



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:32 PM UTC

PDB ID : 8IWH / pdb_00008iwh
EMDB ID : EMD-35766
Title : Structure and characteristics of a photosystem II supercomplex containing monomeric LHCX and dimeric FCP II antennae from the diatom *Thalassiosira pseudonana*
Authors : Feng, Y.; Li, Z.H.; Wang, W.D.; Shen, J.R.
Deposited on : 2023-03-30
Resolution : 2.68 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

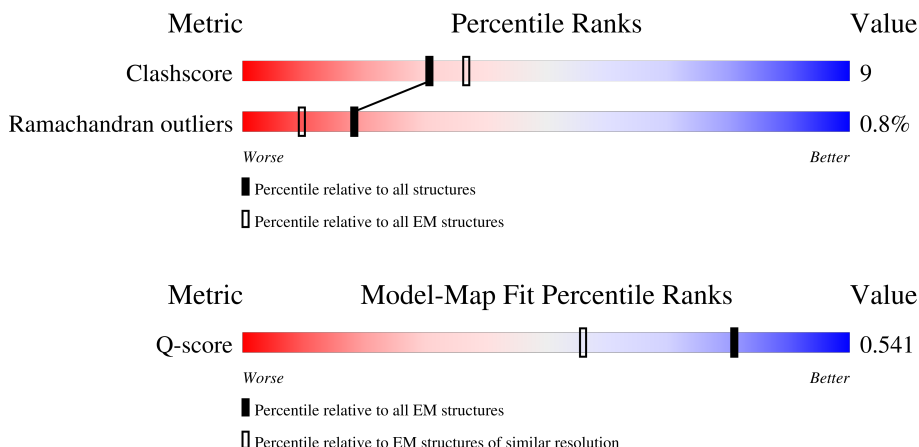
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.68 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.



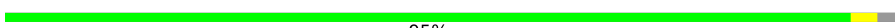
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	9255 (2.18 - 3.18)

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

Mol	Chain	Length	Quality of chain
1	A	333	88% 11% .
1	a	333	93% 7%
2	B	509	86% 7% 6%
2	b	509	83% 11% 6%
3	C	470	85% 11% .

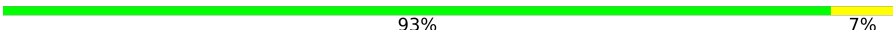
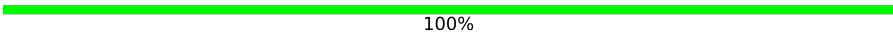
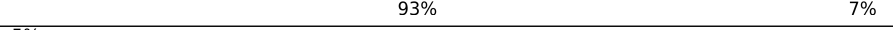
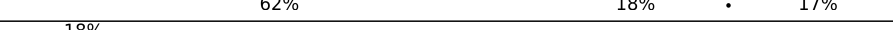
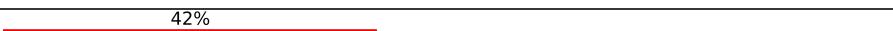
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Mol	Chain	Length	Quality of chain
3	c	470	
4	D	351	
4	d	351	
5	E	84	
5	e	84	
6	F	43	
6	f	43	
7	G	176	
7	g	176	
8	H	66	
8	h	66	
9	I	34	
9	i	34	
10	J	39	
10	j	39	
11	K	44	
11	k	44	
12	L	38	
12	l	38	
13	M	113	
13	m	113	
14	N	30	
14	n	30	
15	O	305	
15	o	305	

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Mol	Chain	Length	Quality of chain
16	T	28	
16	t	28	
17	U	148	
17	u	148	
18	V	162	
18	v	162	
19	W	54	
19	w	54	
20	X	38	
20	x	38	
21	Z	61	
21	z	61	
22	3	220	
23	4	196	
24	5	192	
25	6	199	
26	0	199	
26	7	199	
27	Y	34	
27	y	34	
28	Q	211	
28	q	211	
29	1	193	
29	2	193	
29	8	193	

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Mol	Chain	Length	Quality of chain
29	9	193	

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
33	CLA	0	304	X	-	-	-
33	CLA	0	305	X	-	-	-
33	CLA	0	307	X	-	-	-
33	CLA	0	308	X	-	-	-
33	CLA	0	309	X	-	-	-
33	CLA	0	310	X	-	-	-
33	CLA	0	311	X	-	-	-
33	CLA	0	312	X	-	-	-
33	CLA	0	313	X	-	-	-
33	CLA	1	305	X	-	-	-
33	CLA	1	306	X	-	-	-
33	CLA	1	307	X	-	-	-
33	CLA	1	308	X	-	-	-
33	CLA	1	309	X	-	-	-
33	CLA	1	310	X	-	-	-
33	CLA	1	311	X	-	-	-
33	CLA	1	312	X	-	-	-
33	CLA	1	313	X	-	-	-
33	CLA	1	314	X	-	-	-
33	CLA	1	315	X	-	-	-
33	CLA	1	316	X	-	-	-
33	CLA	2	305	X	-	-	-
33	CLA	2	306	X	-	-	-
33	CLA	2	307	X	-	-	-
33	CLA	2	308	X	-	-	-
33	CLA	2	309	X	-	-	-
33	CLA	2	310	X	-	-	-
33	CLA	2	311	X	-	-	-
33	CLA	2	312	X	-	-	-
33	CLA	2	314	X	-	-	-
33	CLA	2	315	X	-	-	-
33	CLA	2	316	X	-	-	-
33	CLA	2	317	X	-	-	-
33	CLA	3	302	X	-	-	-
33	CLA	3	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	3	304	X	-	-	-
33	CLA	3	305	X	-	-	-
33	CLA	3	306	X	-	-	-
33	CLA	3	307	X	-	-	-
33	CLA	3	308	X	-	-	-
33	CLA	3	309	X	-	-	-
33	CLA	3	311	X	-	-	-
33	CLA	3	312	X	-	-	-
33	CLA	3	313	X	-	-	-
33	CLA	3	319	X	-	-	-
33	CLA	4	305	X	-	-	-
33	CLA	4	306	X	-	-	-
33	CLA	4	308	X	-	-	-
33	CLA	4	309	X	-	-	-
33	CLA	4	310	X	-	-	-
33	CLA	4	311	X	-	-	-
33	CLA	4	312	X	-	-	-
33	CLA	4	313	X	-	-	-
33	CLA	4	314	X	-	-	-
33	CLA	4	315	X	-	-	-
33	CLA	4	316	X	-	-	-
33	CLA	5	308	X	-	-	-
33	CLA	5	309	X	-	-	-
33	CLA	5	311	X	-	-	-
33	CLA	5	312	X	-	-	-
33	CLA	5	313	X	-	-	-
33	CLA	5	314	X	-	-	-
33	CLA	5	316	X	-	-	-
33	CLA	5	317	X	-	-	-
33	CLA	6	307	X	-	-	-
33	CLA	6	308	X	-	-	-
33	CLA	6	310	X	-	-	-
33	CLA	6	311	X	-	-	-
33	CLA	6	312	X	-	-	-
33	CLA	6	313	X	-	-	-
33	CLA	6	315	X	-	-	-
33	CLA	6	316	X	-	-	-
33	CLA	7	304	X	-	-	-
33	CLA	7	305	X	-	-	-
33	CLA	7	307	X	-	-	-
33	CLA	7	308	X	-	-	-
33	CLA	7	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	7	310	X	-	-	-
33	CLA	7	311	X	-	-	-
33	CLA	7	312	X	-	-	-
33	CLA	7	313	X	-	-	-
33	CLA	7	314	X	-	-	-
33	CLA	8	305	X	-	-	-
33	CLA	8	306	X	-	-	-
33	CLA	8	307	X	-	-	-
33	CLA	8	308	X	-	-	-
33	CLA	8	309	X	-	-	-
33	CLA	8	310	X	-	-	-
33	CLA	8	311	X	-	-	-
33	CLA	8	312	X	-	-	-
33	CLA	8	313	X	-	-	-
33	CLA	8	314	X	-	-	-
33	CLA	8	315	X	-	-	-
33	CLA	8	316	X	-	-	-
33	CLA	9	305	X	-	-	-
33	CLA	9	306	X	-	-	-
33	CLA	9	307	X	-	-	-
33	CLA	9	308	X	-	-	-
33	CLA	9	309	X	-	-	-
33	CLA	9	310	X	-	-	-
33	CLA	9	311	X	-	-	-
33	CLA	9	312	X	-	-	-
33	CLA	9	313	X	-	-	-
33	CLA	9	314	X	-	-	-
33	CLA	9	315	X	-	-	-
33	CLA	9	316	X	-	-	-
33	CLA	9	317	X	-	-	-
33	CLA	A	404	X	-	-	-
33	CLA	A	405	X	-	-	-
33	CLA	A	408	X	-	-	-
33	CLA	B	601	X	-	-	-
33	CLA	B	602	X	-	-	-
33	CLA	B	603	X	-	-	-
33	CLA	B	604	X	-	-	-
33	CLA	B	605	X	-	-	-
33	CLA	B	606	X	-	-	-
33	CLA	B	607	X	-	-	-
33	CLA	B	608	X	-	-	-
33	CLA	B	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	B	610	X	-	-	-
33	CLA	B	611	X	-	-	-
33	CLA	B	612	X	-	-	-
33	CLA	B	613	X	-	-	-
33	CLA	B	614	X	-	-	-
33	CLA	B	615	X	-	-	-
33	CLA	B	616	X	-	-	-
33	CLA	C	501	X	-	-	-
33	CLA	C	502	X	-	-	-
33	CLA	C	503	X	-	-	-
33	CLA	C	504	X	-	-	-
33	CLA	C	505	X	-	-	-
33	CLA	C	506	X	-	-	-
33	CLA	C	507	X	-	-	-
33	CLA	C	508	X	-	-	-
33	CLA	C	509	X	-	-	-
33	CLA	C	510	X	-	-	-
33	CLA	C	511	X	-	-	-
33	CLA	C	512	X	-	-	-
33	CLA	C	513	X	-	-	-
33	CLA	D	402	X	-	-	-
33	CLA	D	405	X	-	-	-
33	CLA	D	406	X	-	-	-
33	CLA	H	103	X	-	-	-
33	CLA	W	303	X	-	-	-
33	CLA	Z	101	X	-	-	-
33	CLA	a	407	X	-	-	-
33	CLA	a	408	X	-	-	-
33	CLA	a	411	X	-	-	-
33	CLA	b	602	X	-	-	-
33	CLA	b	603	X	-	-	-
33	CLA	b	604	X	-	-	-
33	CLA	b	605	X	-	-	-
33	CLA	b	606	X	-	-	-
33	CLA	b	607	X	-	-	-
33	CLA	b	608	X	-	-	-
33	CLA	b	609	X	-	-	-
33	CLA	b	610	X	-	-	-
33	CLA	b	611	X	-	-	-
33	CLA	b	612	X	-	-	-
33	CLA	b	613	X	-	-	-
33	CLA	b	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	b	615	X	-	-	-
33	CLA	b	616	X	-	-	-
33	CLA	b	617	X	-	-	-
33	CLA	c	501	X	-	-	-
33	CLA	c	502	X	-	-	-
33	CLA	c	503	X	-	-	-
33	CLA	c	504	X	-	-	-
33	CLA	c	505	X	-	-	-
33	CLA	c	506	X	-	-	-
33	CLA	c	507	X	-	-	-
33	CLA	c	508	X	-	-	-
33	CLA	c	509	X	-	-	-
33	CLA	c	510	X	-	-	-
33	CLA	c	511	X	-	-	-
33	CLA	c	512	X	-	-	-
33	CLA	c	513	X	-	-	-
33	CLA	d	401	X	-	-	-
33	CLA	d	402	X	-	-	-
33	CLA	d	409	X	-	-	-
33	CLA	w	303	X	-	-	-
33	CLA	z	101	X	-	-	-
35	BCT	A	410	-	-	X	-
35	BCT	a	402	-	-	X	-

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 75511 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	333	Total	C	N	O	S	0	0
			2614	1709	427	462	16		
1	a	333	Total	C	N	O	S	0	0
			2614	1709	427	462	16		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	478	Total	C	N	O	S	0	0
			3772	2466	639	654	13		
2	b	478	Total	C	N	O	S	0	0
			3772	2466	639	654	13		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	450	Total	C	N	O	S	0	0
			3489	2277	588	608	16		
3	c	450	Total	C	N	O	S	0	0
			3489	2277	588	608	16		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2699	1784	442	463	10		
4	d	341	Total	C	N	O	S	0	0
			2699	1784	442	463	10		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	76	Total	C	N	O	0	0
			626	407	103	116		
5	e	76	Total	C	N	O	0	0
			626	407	103	116		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	31	Total	C	N	O	S	0	0
			253	173	42	37	1		
6	f	31	Total	C	N	O	S	0	0
			253	173	42	37	1		

- Molecule 7 is a protein called Photosystem II Psb31 protein domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	120	Total	C	N	O	0	0
			890	556	160	174		
7	g	120	Total	C	N	O	0	0
			890	556	160	174		

- Molecule 8 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	65	Total	C	N	O	S	0	0
			512	339	82	89	2		
8	h	65	Total	C	N	O	S	0	0
			512	339	82	89	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total 279	C 188	N 43	O 47	S 1	0	0
9	i	34	Total 279	C 188	N 43	O 47	S 1	0	0

- Molecule 10 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	33	Total	C	N	O	0	0
			243	165	37	41		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	33	Total	C	N	O	0	0
			243	165	37	41		

- Molecule 11 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			303	213	45	45		
11	k	37	Total	C	N	O	0	0
			303	213	45	45		

- Molecule 12 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	37	Total	C	N	O	0	0
			302	203	47	52		
12	l	37	Total	C	N	O	0	0
			302	203	47	52		

- Molecule 13 is a protein called Photosystem II reaction center M protein, plastid.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	41	Total	C	N	O	0	0
			317	208	51	58		
13	m	41	Total	C	N	O	0	0
			317	208	51	58		

- Molecule 14 is a protein called Photosystem II subunit, PsbN..

Mol	Chain	Residues	Atoms				AltConf	Trace
14	n	30	Total	C	N	O	0	0
			150	90	30	30		
14	N	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	248	Total	C	N	O	S	0	0
			1867	1176	309	374	8		
15	o	248	Total	C	N	O	S	0	0
			1867	1176	309	374	8		

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	28	Total	C	N	O	S	0	0
			233	161	34	36	2		
16	t	28	Total	C	N	O	S	0	0
			233	161	34	36	2		

- Molecule 17 is a protein called PS II complex 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	92	Total	C	N	O	S	0	0
			708	451	121	134	2		
17	u	92	Total	C	N	O	S	0	0
			708	451	121	134	2		

- Molecule 18 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	135	Total	C	N	O	S	0	0
			1029	640	179	206	4		
18	v	135	Total	C	N	O	S	0	0
			1029	640	179	206	4		

- Molecule 19 is a protein called Photosystem II subunit, PsbW.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	W	54	Total	C	N	O	0	0
			434	281	64	89		
19	w	54	Total	C	N	O	0	0
			434	281	64	89		

- Molecule 20 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	35	Total	C	N	O	S	0	0
			248	160	41	46	1		
20	x	35	Total	C	N	O	S	0	0
			248	160	41	46	1		

- Molecule 21 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	61	Total	C	N	O	S	0	0
			453	301	68	83	1		
21	z	61	Total	C	N	O	S	0	0
			453	301	68	83	1		

- Molecule 22 is a protein called Fucoxanthin chl a/c protein, lhca clade.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3	220	Total	C	N	O	S	0	0
			1710	1110	281	315	4		

- Molecule 23 is a protein called Fucoxanthin-chlorophyll a-c binding protein, plastid.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	4	163	Total	C	N	O	S	0	0
			1249	809	204	232	4		

- Molecule 24 is a protein called Fucoxanthin chlorophyll a/c protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	5	160	Total	C	N	O	S	0	0
			1229	780	217	227	5		

- Molecule 25 is a protein called Fucoxanthin chlorophyll a/c protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	6	168	Total	C	N	O	S	0	0
			1296	833	219	238	6		

- Molecule 26 is a protein called Fucoxanthin chlorophyll a/c protein-LI818 clade.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	7	165	Total	C	N	O	S	0	0
			1269	819	213	233	4		
26	0	165	Total	C	N	O	S	0	0
			1269	819	213	233	4		

- Molecule 27 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	34	Total	C	N	O	S	0	0
			251	167	41	41	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
27	y	34	Total	C	N	O	S	0	0
			251	167	41	41	2		

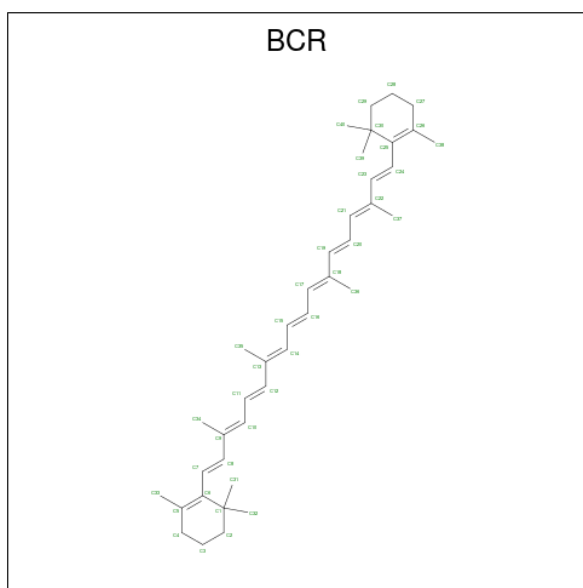
- Molecule 28 is a protein called Photosystem II subunit, PsbQ..

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Q	156	Total	C	N	O	S	0	0
			1198	757	202	237	2		
28	q	156	Total	C	N	O	S	0	0
			1198	757	202	237	2		

- Molecule 29 is a protein called Fucoxanthin chlorophyll a/c light-harvesting protein, major type.

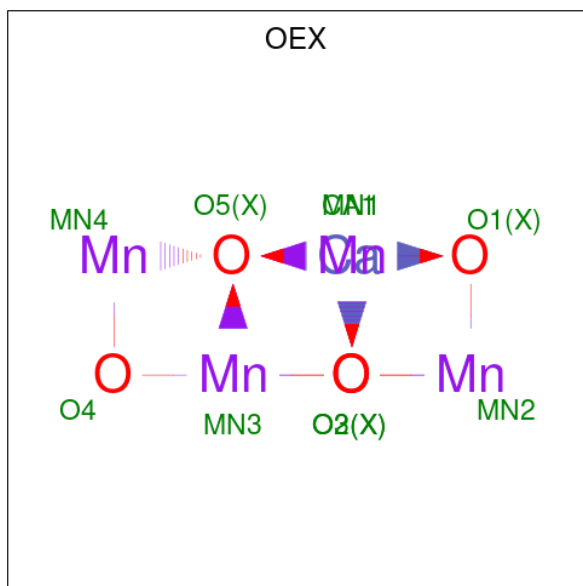
Mol	Chain	Residues	Atoms					AltConf	Trace
29	9	163	Total	C	N	O	S	0	0
			1214	788	206	218	2		
29	2	163	Total	C	N	O	S	0	0
			1214	788	206	218	2		
29	8	163	Total	C	N	O	S	0	0
			1206	783	206	216	1		
29	1	163	Total	C	N	O	S	0	0
			1206	783	206	216	1		

- Molecule 30 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	D	1	Total C 40 40	0
30	d	1	Total C 40 40	0
30	H	1	Total C 40 40	0
30	h	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	k	1	Total C 40 40	0
30	k	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).

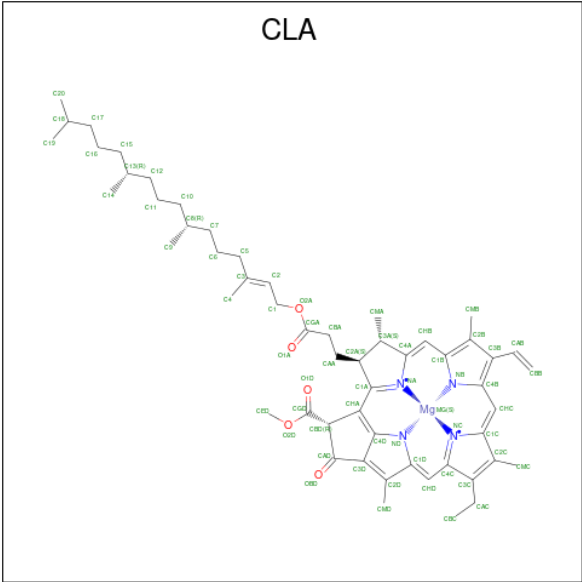


Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
31	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 32 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
32	A	1	Total	Cl	0
			1	1	
32	a	1	Total	Cl	0
			1	1	

- Molecule 33 is CHLOROPHYLL A (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
33	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			61	52	1	4	4	
33	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	C	1	Total 49	C 39	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	c	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	c	1	Total 49	C 39	Mg 1	N 4	O 5	0
33	D	1	Total 59	C 49	Mg 1	N 4	O 5	0
33	D	1	Total 57	C 47	Mg 1	N 4	O 5	0
33	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	d	1	Total 57	C 47	Mg 1	N 4	O 5	0
33	d	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	d	1	Total 59	C 49	Mg 1	N 4	O 5	0
33	H	1	Total 43	C 35	Mg 1	N 4	O 3	0
33	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	Z	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	z	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	3	1	Total 48	C 38	Mg 1	N 4	O 5	0
33	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	3	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
33	3	1	Total 61	C 51	Mg 1	N 4	O 5	0
33	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
33	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	4	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	4	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	4	1	Total 47	C 37	Mg 1	N 4	O 5	0
33	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
33	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
33	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
33	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	5	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	6	1	Total 53	C 43	Mg 1	N 4	O 5	0
33	6	1	Total 54	C 44	Mg 1	N 4	O 5	0
33	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
33	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
33	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
33	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	6	1	Total 39	C 30	Mg 1	N 4	O 4	0
33	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
33	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	7	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	7	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	7	1	Total 34	C 28	Mg 1	N 4	O 1	0
33	7	1	Total 43	C 35	Mg 1	N 4	O 3	0
33	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
33	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
33	b	1	Total 61	C 52	Mg 1	N 4	O 4	0
33	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 64	C 54	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	0	1	Total 47	C 37	Mg 1	N 4	O 5	0
33	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	0	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	0	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	0	1	Total 34	C 28	Mg 1	N 4	O 1	0
33	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	9	1	Total 44	C 34	Mg 1	N 4	O 5	0
33	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	9	1	Total 43	C 33	Mg 1	N 4	O 5	0
33	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	9	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	9	1	Total 36	C 30	Mg 1	N 4	O 1	0
33	9	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	9	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	9	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	2	1	Total 44	C 34	Mg 1	N 4	O 5	0
33	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	2	1	Total 43	C 33	Mg 1	N 4	O 5	0
33	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	2	1	Total 36	C 30	Mg 1	N 4	O 1	0
33	2	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	2	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	2	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	8	1	Total 45	C 35	Mg 1	N 4	O 5	0

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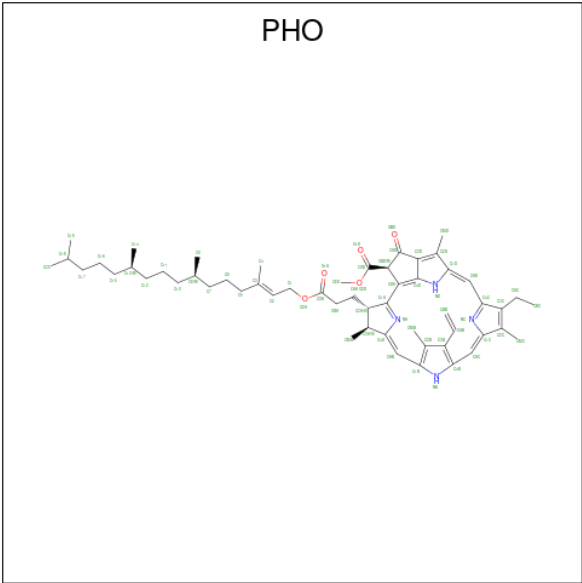
Mol	Chain	Residues	Atoms					AltConf
33	8	1	Total 44	C 34	Mg 1	N 4	O 5	0
33	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	8	1	Total 43	C 33	Mg 1	N 4	O 5	0
33	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	8	1	Total 36	C 30	Mg 1	N 4	O 1	0
33	8	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	8	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	8	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	1	1	Total 44	C 34	Mg 1	N 4	O 5	0
33	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	1	1	Total 43	C 33	Mg 1	N 4	O 5	0
33	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	1	1	Total 36	C 30	Mg 1	N 4	O 1	0
33	1	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	1	1	Total 38	C 32	Mg 1	N 4	O 1	0

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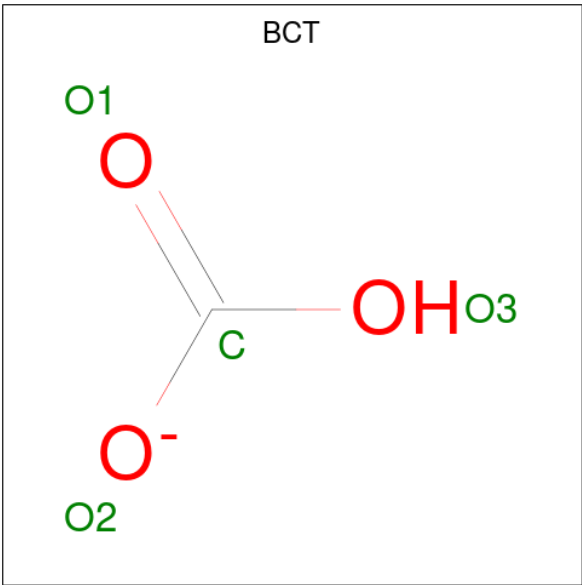
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
33	1	1	38	32	1	4	1	0

- Molecule 34 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



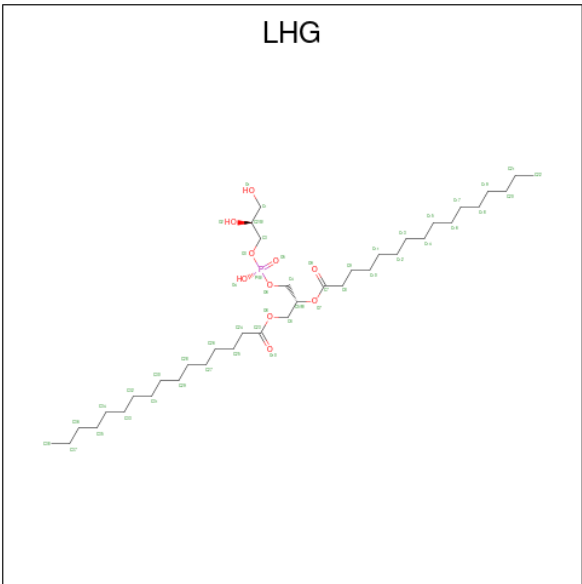
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
34	A	1	64	55	4	5	0
34	A	1	64	55	4	5	0
34	a	1	64	55	4	5	0
34	a	1	64	55	4	5	0

- Molecule 35 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			4	1	3	
35	a	1	Total	C	O	0
			4	1	3	

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



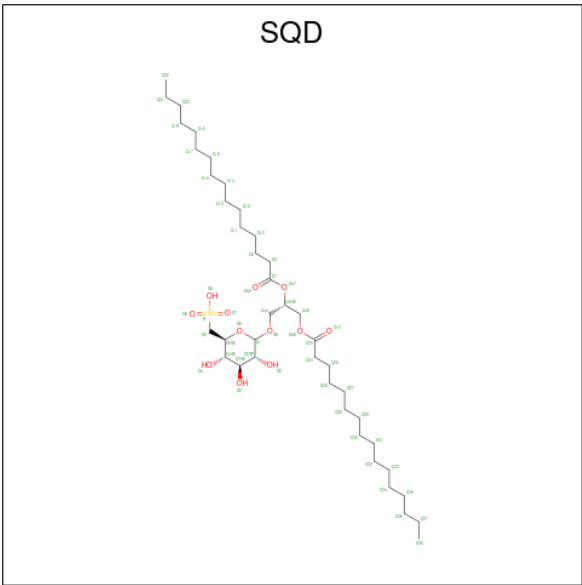
Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	O	P	0
			43	32	10	1	

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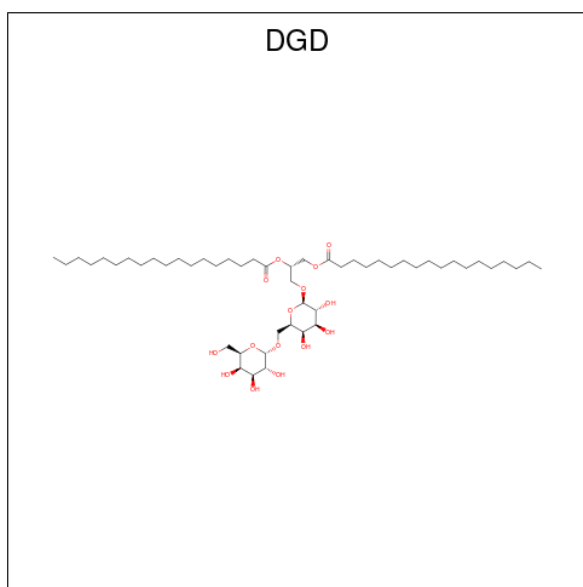
Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	O	P	0
			49	38	10	1	
36	A	1	Total	C	O	P	0
			49	38	10	1	
36	D	1	Total	C	O	P	0
			48	38	9	1	
36	D	1	Total	C	O	P	0
			42	31	10	1	
36	d	1	Total	C	O	P	0
			48	38	9	1	
36	d	1	Total	C	O	P	0
			42	31	10	1	
36	H	1	Total	C	O	P	0
			42	31	10	1	
36	h	1	Total	C	O	P	0
			42	31	10	1	
36	W	1	Total	C	O	P	0
			35	24	10	1	
36	w	1	Total	C	O	P	0
			35	24	10	1	
36	3	1	Total	C	O	P	0
			27	16	10	1	
36	3	1	Total	C	O	P	0
			49	38	10	1	
36	4	1	Total	C	O	P	0
			49	38	10	1	
36	5	1	Total	C	O	P	0
			33	24	8	1	
36	7	1	Total	C	O	P	0
			28	19	8	1	
36	a	1	Total	C	O	P	0
			43	32	10	1	
36	a	1	Total	C	O	P	0
			49	38	10	1	
36	b	1	Total	C	O	P	0
			49	38	10	1	
36	0	1	Total	C	O	P	0
			28	19	8	1	

- Molecule 37 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



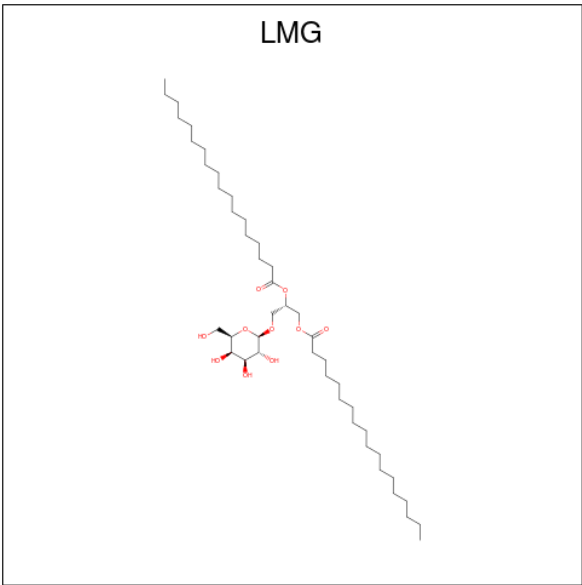
Mol	Chain	Residues	Atoms				AltConf
37	A	1	Total	C	O	S	0
			40	27	12	1	
37	B	1	Total	C	O	S	0
			54	41	12	1	
37	D	1	Total	C	O	S	0
			54	41	12	1	
37	i	1	Total	C	O	S	0
			40	27	12	1	
37	L	1	Total	C	O	S	0
			54	41	12	1	
37	l	1	Total	C	O	S	0
			54	41	12	1	
37	T	1	Total	C	O	S	0
			40	27	12	1	
37	T	1	Total	C	O	S	0
			54	41	12	1	
37	t	1	Total	C	O	S	0
			40	27	12	1	
37	7	1	Total	C	O	S	0
			48	35	12	1	
37	a	1	Total	C	O	S	0
			54	41	12	1	
37	0	1	Total	C	O	S	0
			48	35	12	1	

- Molecule 38 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms			AltConf
38	A	1	Total	C	O	0
			53	39	14	
38	C	1	Total	C	O	0
			55	40	15	
38	C	1	Total	C	O	0
			56	41	15	
38	C	1	Total	C	O	0
			55	40	15	
38	c	1	Total	C	O	0
			55	40	15	
38	c	1	Total	C	O	0
			56	41	15	
38	c	1	Total	C	O	0
			55	40	15	
38	H	1	Total	C	O	0
			62	47	15	
38	h	1	Total	C	O	0
			62	47	15	
38	3	1	Total	C	O	0
			39	34	5	
38	a	1	Total	C	O	0
			53	39	14	

- Molecule 39 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			51	41	10	
39	B	1	Total	C	O	0
			28	18	10	
39	C	1	Total	C	O	0
			46	36	10	
39	C	1	Total	C	O	0
			48	38	10	
39	C	1	Total	C	O	0
			27	17	10	
39	C	1	Total	C	O	0
			23	13	10	
39	c	1	Total	C	O	0
			48	38	10	
39	c	1	Total	C	O	0
			27	17	10	
39	D	1	Total	C	O	0
			40	30	10	
39	D	1	Total	C	O	0
			46	36	10	
39	d	1	Total	C	O	0
			46	36	10	
39	d	1	Total	C	O	0
			37	27	10	
39	M	1	Total	C	O	0
			40	30	10	
39	m	1	Total	C	O	0
			40	30	10	

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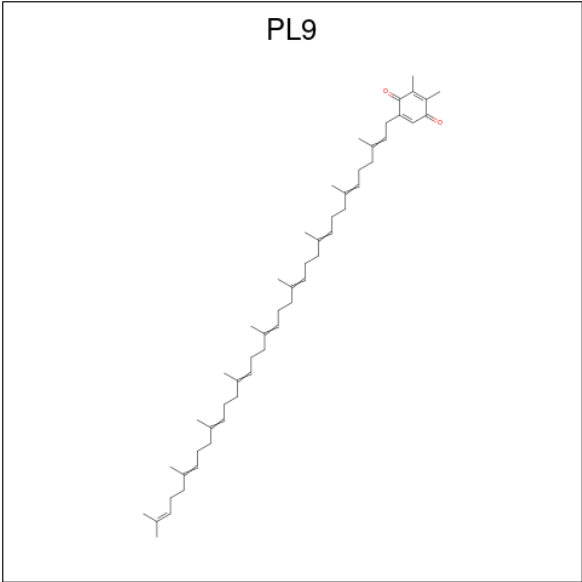
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Mol	Chain	Residues	Atoms			AltConf
39	W	1	Total	C	O	0
			48	38	10	
39	w	1	Total	C	O	0
			48	38	10	
39	3	1	Total	C	O	0
			31	21	10	
39	5	1	Total	C	O	0
			31	21	10	
39	7	1	Total	C	O	0
			55	45	10	
39	b	1	Total	C	O	0
			51	41	10	
39	b	1	Total	C	O	0
			28	18	10	
39	b	1	Total	C	O	0
			40	30	10	
39	Q	1	Total	C	O	0
			37	27	10	
39	q	1	Total	C	O	0
			46	36	10	
39	q	1	Total	C	O	0
			37	27	10	
39	0	1	Total	C	O	0
			42	32	10	

- Molecule 40 is FE (II) ION (CCD ID: FE2) (formula: Fe).

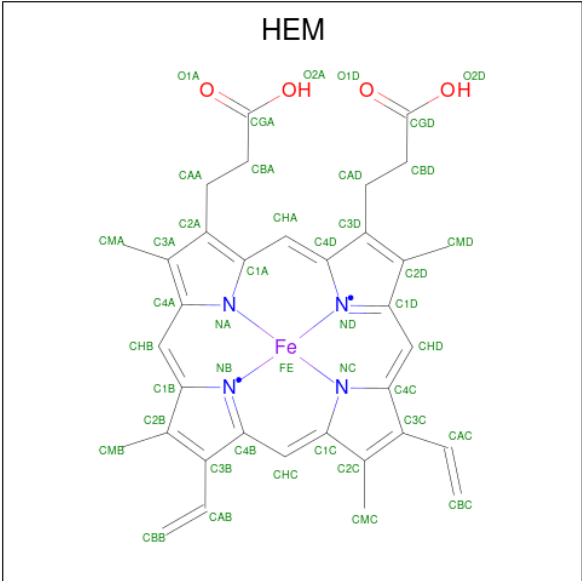
Mol	Chain	Residues	Atoms		AltConf
40	D	1	Total	Fe	0
			1	1	
40	d	1	Total	Fe	0
			1	1	

- Molecule 41 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



Mol	Chain	Residues	Atoms			AltConf
41	D	1	Total	C	O	0
			55	53	2	
41	d	1	Total	C	O	0
			55	53	2	

- Molecule 42 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



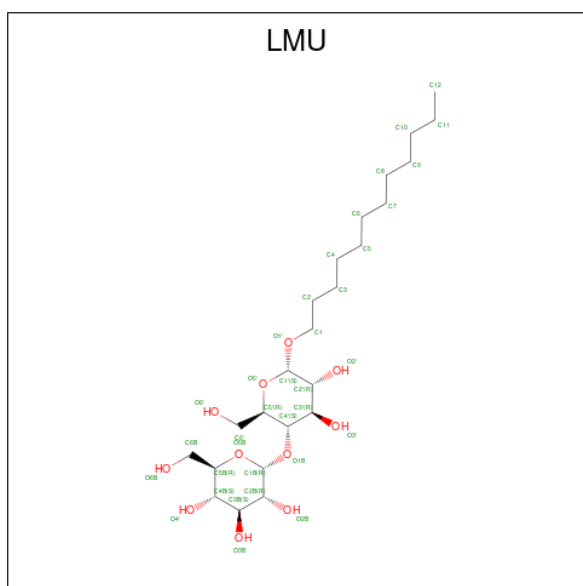
Mol	Chain	Residues	Atoms					AltConf
42	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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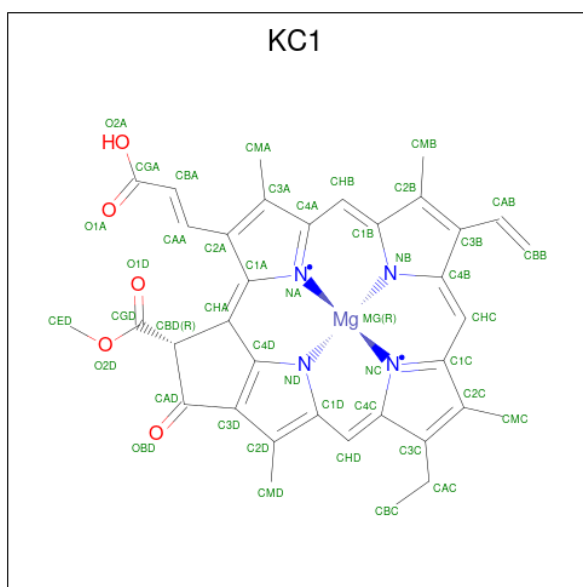
Mol	Chain	Residues	Atoms					AltConf
42	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
42	V	1	Total 43	C 34	Fe 1	N 4	O 4	0
42	v	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 43 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



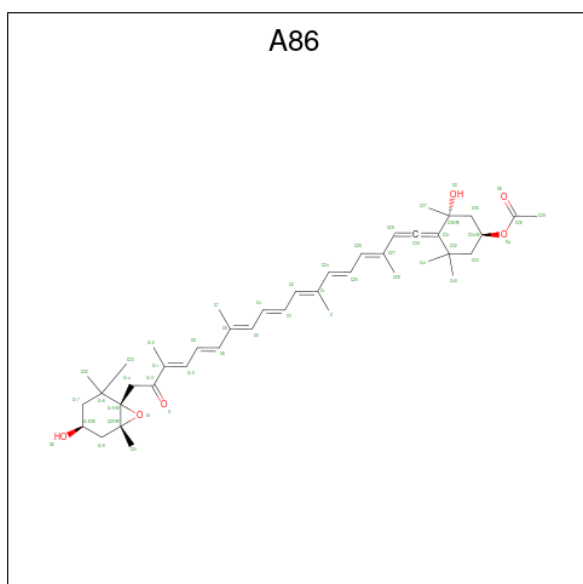
Mol	Chain	Residues	Atoms			AltConf
43	T	1	Total	C	O	0
			31	20	11	
43	t	1	Total	C	O	0
			31	20	11	
43	w	1	Total	C	O	0
			35	24	11	
43	3	1	Total	C	O	0
			35	24	11	
43	4	1	Total	C	O	0
			35	24	11	
43	5	1	Total	C	O	0
			31	20	11	

- Molecule 44 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
44	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 45 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: $C_{42}H_{58}O_6$).



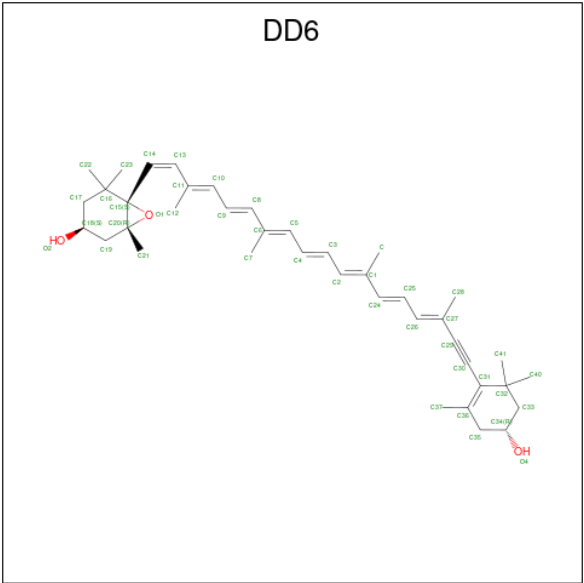
Mol	Chain	Residues	Atoms			AltConf
45	3	1	Total	C	O	0
			48	42	6	
45	4	1	Total	C	O	0
			48	42	6	
45	4	1	Total	C	O	0
			48	42	6	
45	4	1	Total	C	O	0
			48	42	6	
45	5	1	Total	C	O	0
			48	42	6	
45	5	1	Total	C	O	0
			48	42	6	
45	5	1	Total	C	O	0
			48	42	6	
45	5	1	Total	C	O	0
			48	42	6	
45	5	1	Total	C	O	0
			47	41	6	
45	5	1	Total	C	O	0
			48	42	6	
45	5	1	Total	C	O	0
			48	42	6	
45	6	1	Total	C	O	0
			48	42	6	
45	6	1	Total	C	O	0
			48	42	6	
45	6	1	Total	C	O	0
			48	42	6	
45	6	1	Total	C	O	0
			48	42	6	
45	6	1	Total	C	O	0
			48	42	6	
45	6	1	Total	C	O	0
			48	42	6	
45	7	1	Total	C	O	0
			48	42	6	
45	7	1	Total	C	O	0
			48	42	6	
45	0	1	Total	C	O	0
			48	42	6	
45	0	1	Total	C	O	0
			48	42	6	
45	9	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
45	9	1	Total	C	O	0
			48	42	6	
45	2	1	Total	C	O	0
			48	42	6	
45	2	1	Total	C	O	0
			48	42	6	
45	8	1	Total	C	O	0
			48	42	6	
45	8	1	Total	C	O	0
			48	42	6	
45	1	1	Total	C	O	0
			48	42	6	
45	1	1	Total	C	O	0
			48	42	6	

- Molecule 46 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).



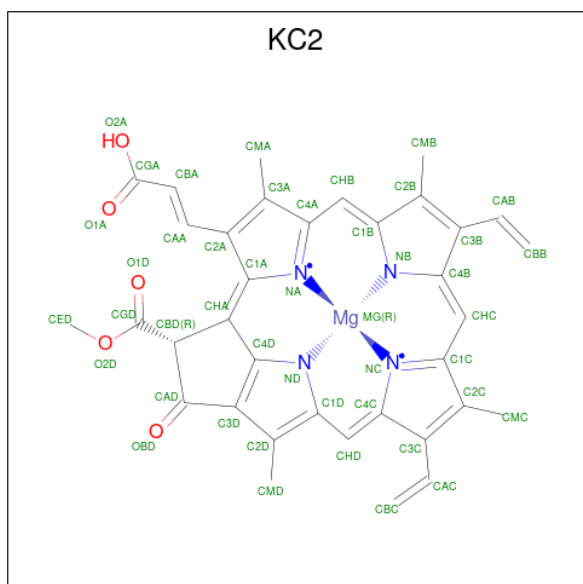
Mol	Chain	Residues	Atoms			AltConf
46	3	1	Total	C	O	0
			43	40	3	
46	4	1	Total	C	O	0
			43	40	3	
46	9	1	Total	C	O	0
			43	40	3	
46	9	1	Total	C	O	0
			43	40	3	

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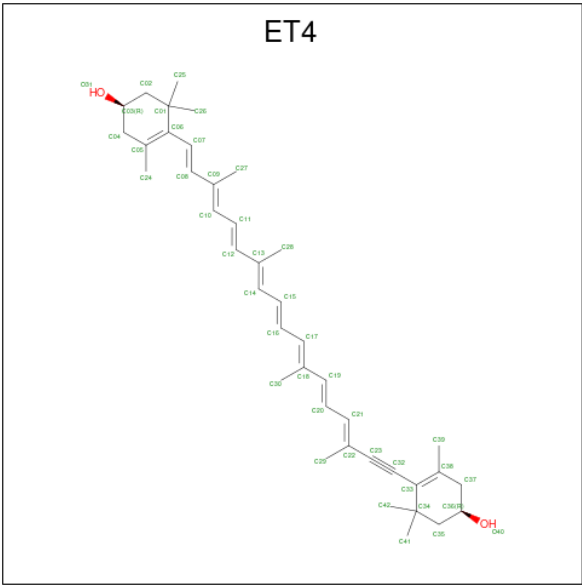
Mol	Chain	Residues	Atoms			AltConf
46	2	1	Total	C	O	0
			43	40	3	
46	2	1	Total	C	O	0
			43	40	3	
46	8	1	Total	C	O	0
			43	40	3	
46	8	1	Total	C	O	0
			43	40	3	
46	1	1	Total	C	O	0
			43	40	3	
46	1	1	Total	C	O	0
			43	40	3	

- Molecule 47 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
47	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 48 is (1 {R})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15-octaen-17-ynyl]cyclohex-3-en-1-ol (CCD ID: ET4) (formula: C₄₀H₅₄O₂).

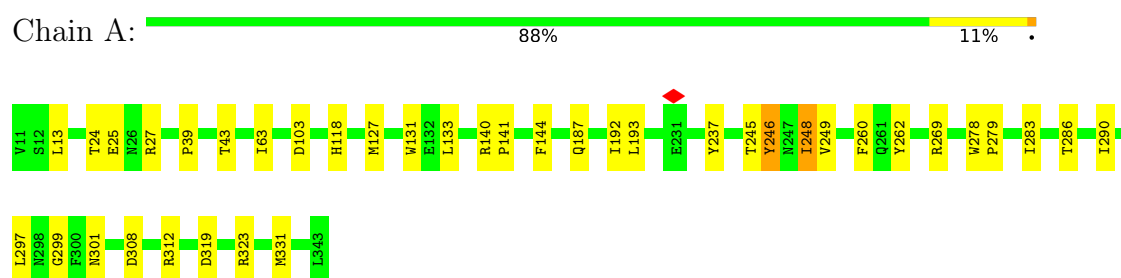


Mol	Chain	Residues	Atoms			AltConf
48	7	1	Total	C	O	0
			42	40	2	
48	0	1	Total	C	O	0
			42	40	2	

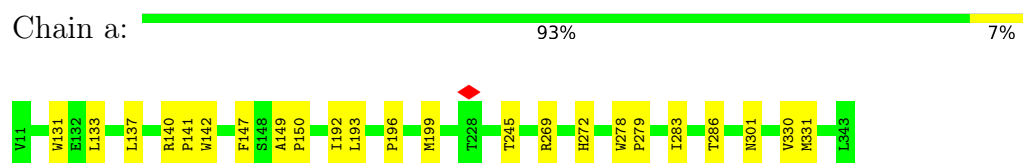
3 Residue-property plots

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

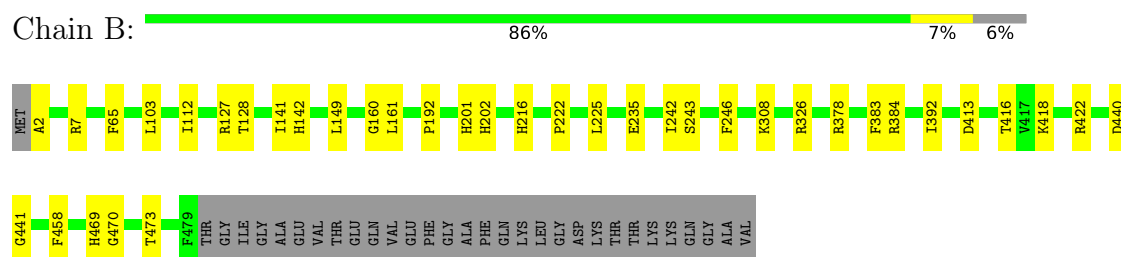
- Molecule 1: Photosystem II protein D1



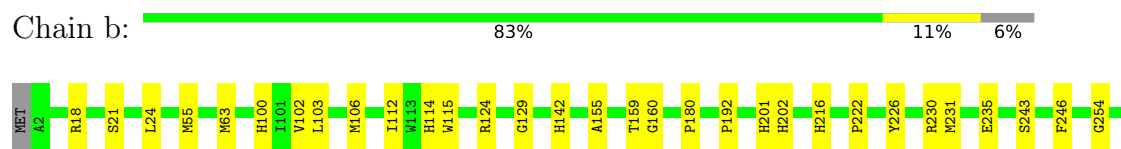
- Molecule 1: Photosystem II protein D1

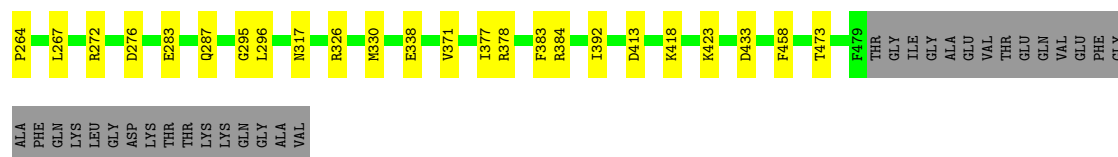


- Molecule 2: Photosystem II CP47 reaction center protein



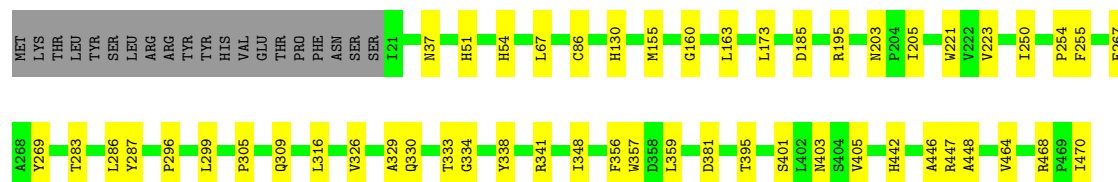
- Molecule 2: Photosystem II CP47 reaction center protein





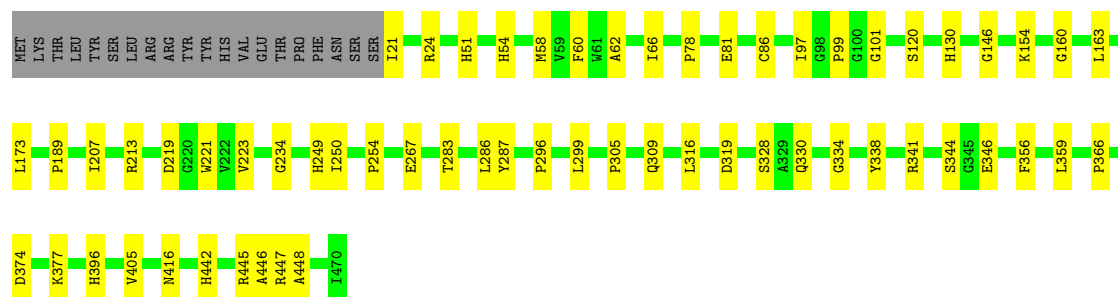
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 85% 11% .



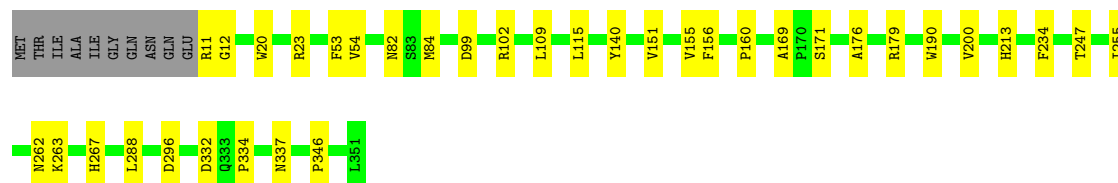
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 83% 13% .



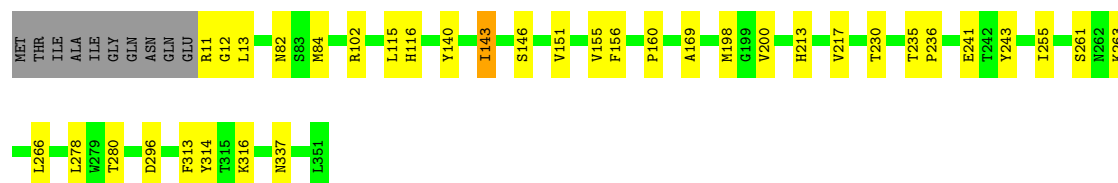
- Molecule 4: Photosystem II D2 protein

Chain D: 87% 10% .



- Molecule 4: Photosystem II D2 protein

Chain d: 87% 10% .



- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 



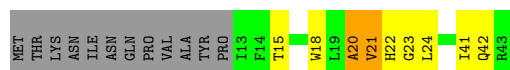
- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 



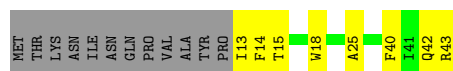
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 



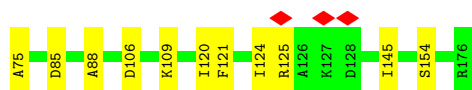
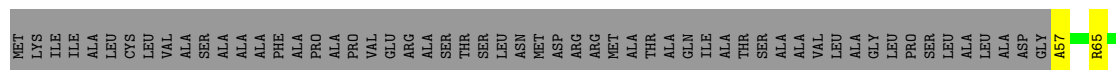
- Molecule 6: Cytochrome b559 subunit beta

Chain f: 



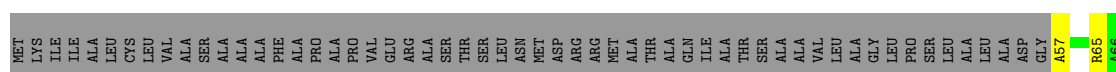
- Molecule 7: Photosystem II Psb31 protein domain-containing protein

Chain G: 



- Molecule 7: Photosystem II Psb31 protein domain-containing protein

Chain g: 





• Molecule 8: Photosystem II reaction center protein H

Chain H: 88% 11% .



• Molecule 8: Photosystem II reaction center protein H

Chain h: 91% 8% .



• Molecule 9: Photosystem II reaction center protein I

Chain I: 91% 9% .



• Molecule 9: Photosystem II reaction center protein I

Chain i: 85% 15% .



• Molecule 10: Photosystem II reaction center protein J

Chain J: 67% 15% 15% .



• Molecule 10: Photosystem II reaction center protein J

Chain j: 77% 8% 15% .



• Molecule 11: Photosystem II reaction center protein K

Chain K: 75% 9% 16% .



- Molecule 11: Photosystem II reaction center protein K

Chain k: 73% 11% 16%



- Molecule 12: Photosystem II reaction center protein L

Chain L: 95% . .



- Molecule 12: Photosystem II reaction center protein L

Chain l: 87% 11% .



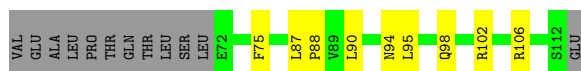
- Molecule 13: Photosystem II reaction center M protein, plastid

Chain M: 27% 9% 64%



- Molecule 13: Photosystem II reaction center M protein, plastid

Chain m: 28% 8% 64%



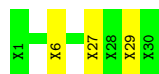
- Molecule 14: Photosystem II subunit, PsbN.

Chain n: 90% 10%



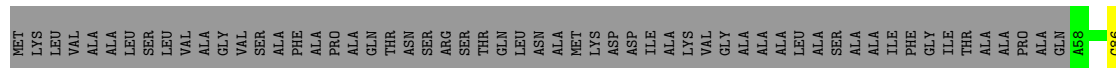
- Molecule 14: Photosystem II subunit, PsbN.

Chain N:  90% 10%



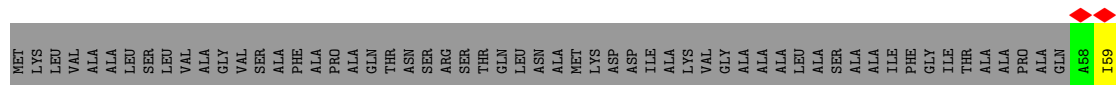
- Molecule 15: Oxygen-evolving enhancer protein 1

Chain O:  72% 10% 19%



- Molecule 15: Oxygen-evolving enhancer protein 1

Chain o:  69% 13% 19%



- Molecule 16: Photosystem II reaction center protein T

Chain T:  93% 7%



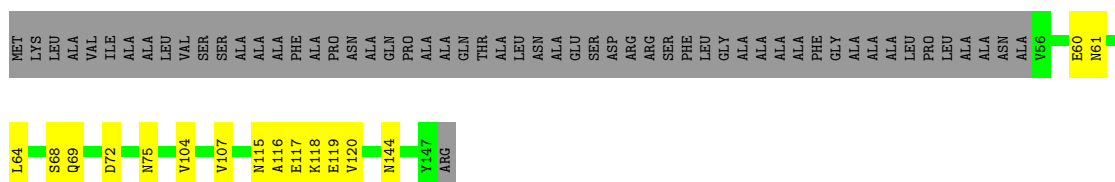
- Molecule 16: Photosystem II reaction center protein T

Chain t:  100%

There are no outlier residues recorded for this chain.

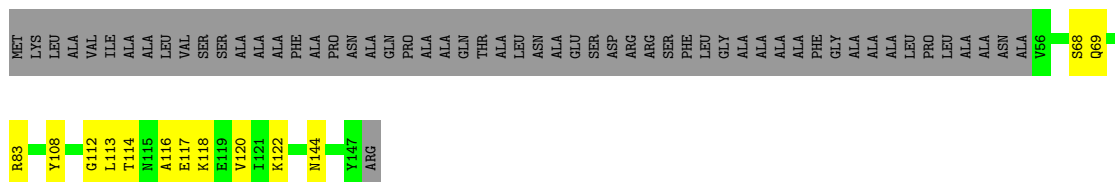
- Molecule 17: PS II complex 12 kDa extrinsic protein

Chain U:  51% 11% 38%



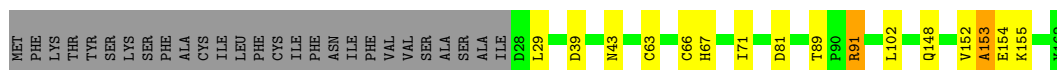
- Molecule 17: PS II complex 12 kDa extrinsic protein

Chain u: 53% 9% 38%



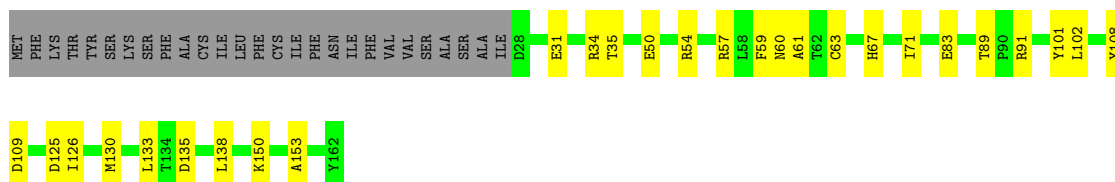
- Molecule 18: Cytochrome c-550

Chain V: 73% 9% 17%



- Molecule 18: Cytochrome c-550

Chain v: 67% 17% 17%



- Molecule 19: Photosystem II subunit, PsbW

Chain W: 91% 9%



- Molecule 19: Photosystem II subunit, PsbW

Chain w: 91% 9%



- Molecule 20: Photosystem II reaction center X protein

Chain X:  74% 18% 8%



- Molecule 20: Photosystem II reaction center X protein

Chain x:  82% 11% 8%



- Molecule 21: Photosystem II reaction center protein Z

Chain Z:  93% 7%



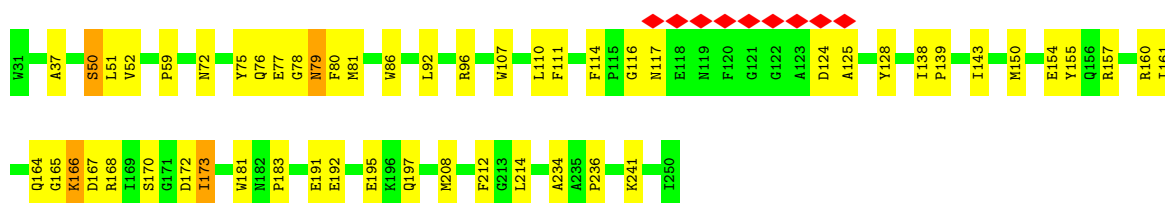
- Molecule 21: Photosystem II reaction center protein Z

Chain z:  5% 89% 11%



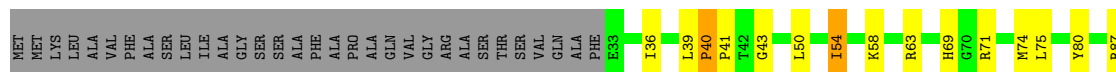
- Molecule 22: Fucoxanthin chl a/c protein, lhca clade

Chain 3:  75% 23% 2%

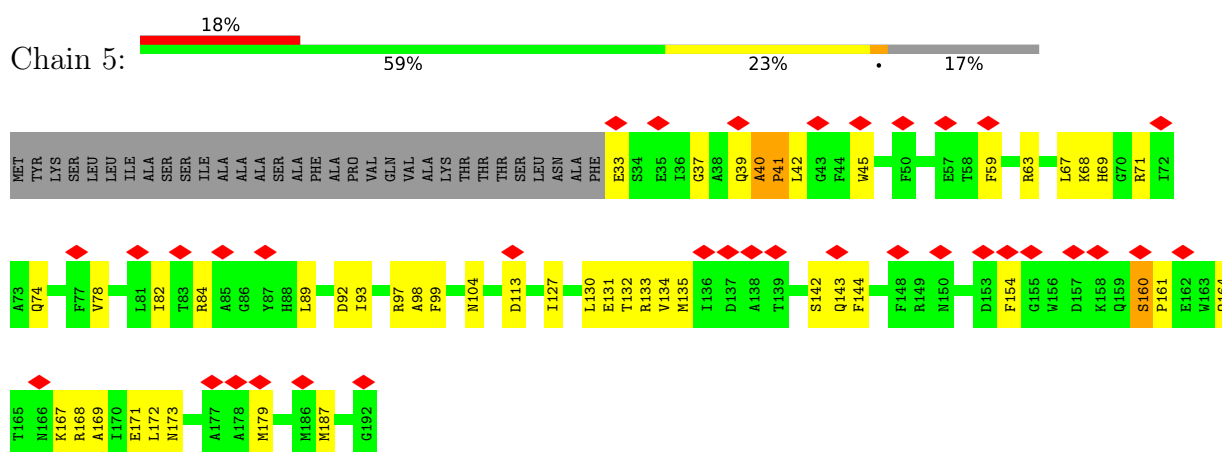


- Molecule 23: Fucoxanthin-chlorophyll a-c binding protein, plastid

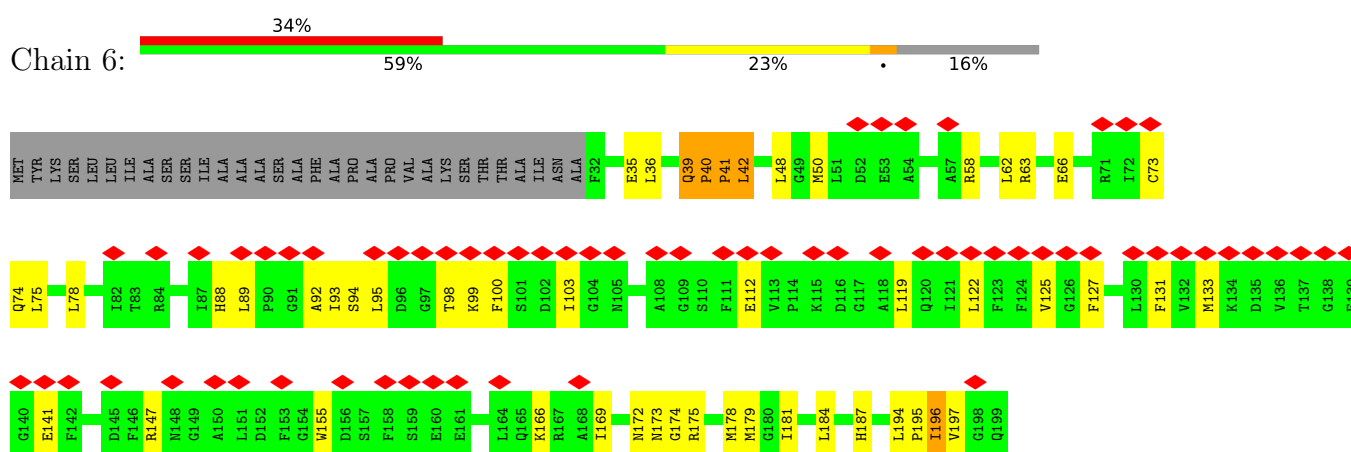
Chain 4:  62% 18% 17%



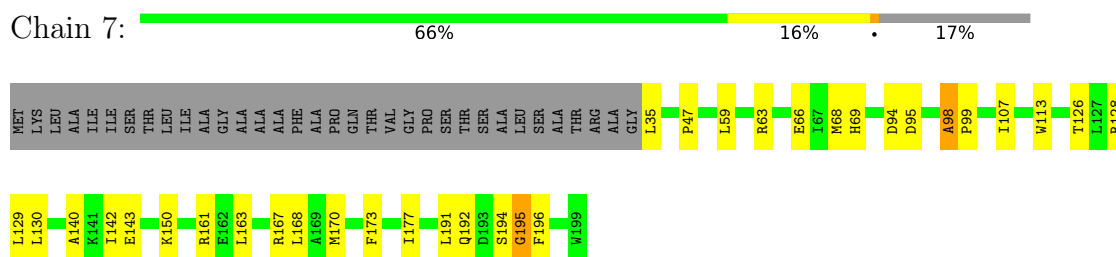
- Molecule 24: Fucoxanthin chlorophyll a/c protein 6



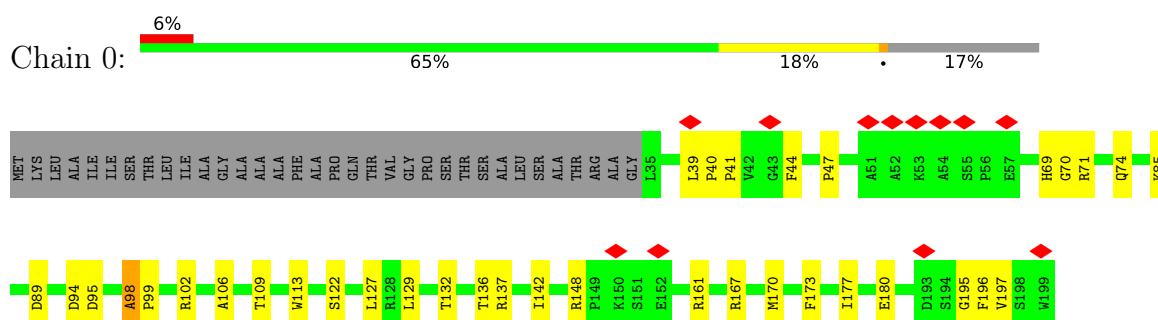
• Molecule 25: Fucoxanthin chlorophyll a/c protein 5



• Molecule 26: Fucoxanthin chlorophyll a/c protein-LI818 clade



• Molecule 26: Fucoxanthin chlorophyll a/c protein-LI818 clade



• Molecule 27: Photosystem II reaction center protein Ycf12

Chain Y:  91% 9%



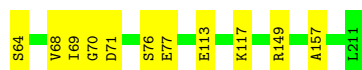
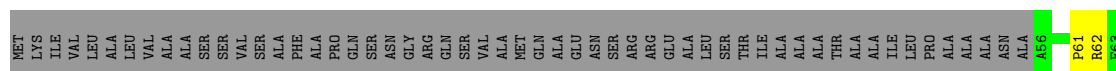
- Molecule 27: Photosystem II reaction center protein Ycf12

Chain y:  88% 12%



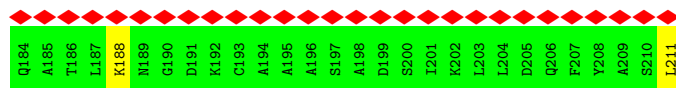
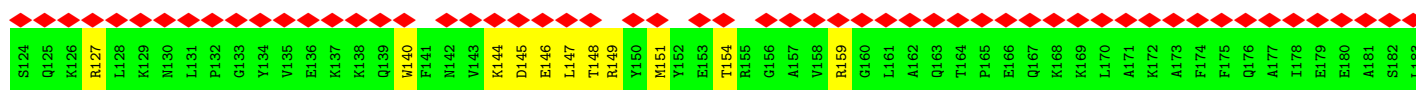
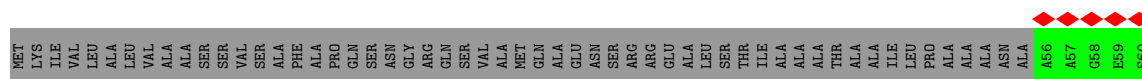
- Molecule 28: Photosystem II subunit, PsbQ.

Chain Q:  68% 6% 26%



- Molecule 28: Photosystem II subunit, PsbQ.

Chain q:  66% 60% 14% 26%



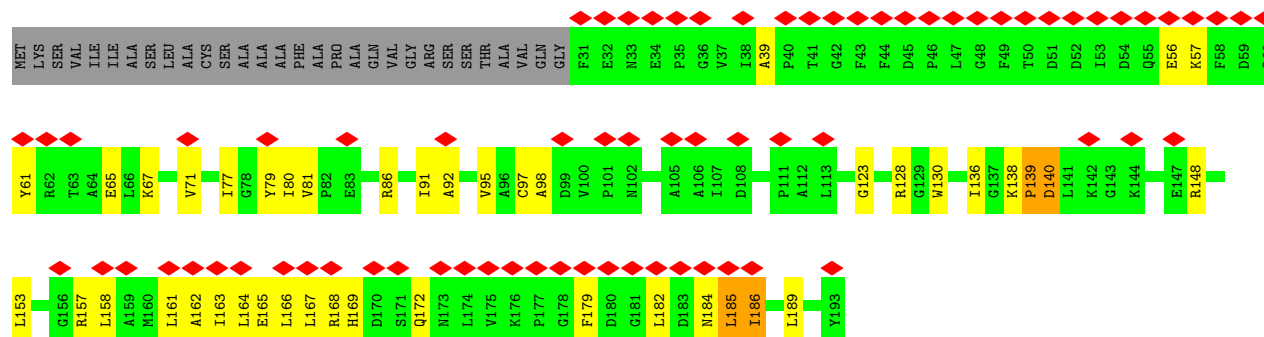
- Molecule 29: Fucoxanthin chlorophyll a/c light-harvesting protein, major type

Chain 9:  60% 23% 16%

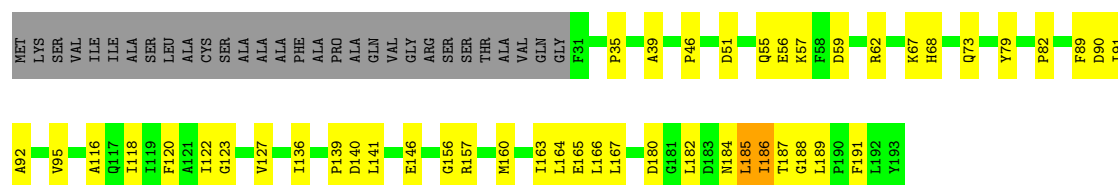




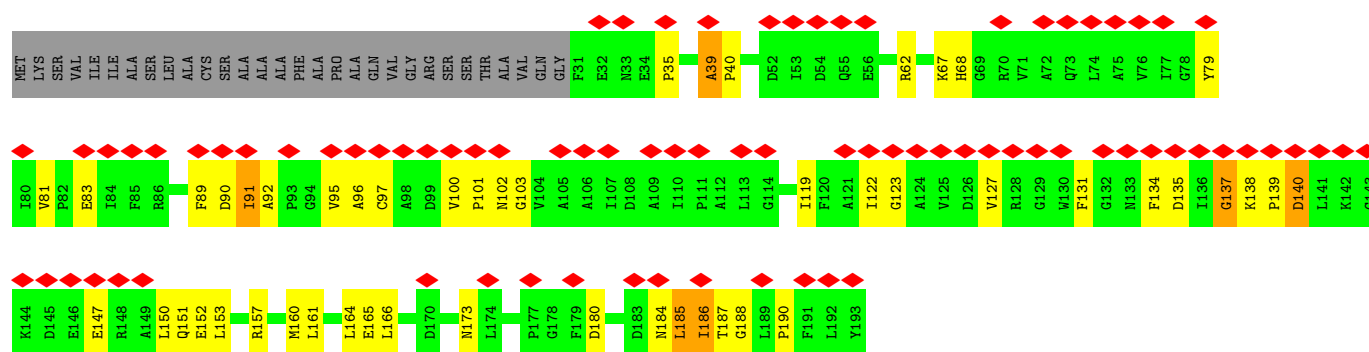
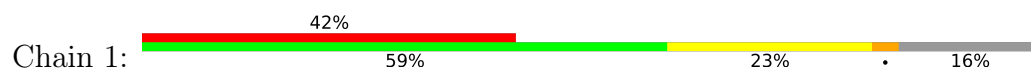
- Molecule 29: Fucoxanthin chlorophyll a/c light-harvesting protein, major type



- Molecule 29: Fucoxanthin chlorophyll a/c light-harvesting protein, major type



- Molecule 29: Fucoxanthin chlorophyll a/c light-harvesting protein, major type



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97098	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	0.719	Depositor
Minimum map value	-0.241	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.088	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, A86, KC1, LMU, HEM, FE2, DGD, DD6, PL9, LMG, BCT, LHG, KC2, PHO, BCR, SQD, OEX, CL, ET4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.23	0/2697	0.39	1/3674 (0.0%)
1	a	0.22	0/2697	0.35	0/3674
2	B	0.25	0/3901	0.33	0/5308
2	b	0.22	0/3901	0.29	0/5308
3	C	0.22	0/3604	0.32	0/4909
3	c	0.20	0/3604	0.31	0/4909
4	D	0.22	0/2791	0.32	0/3804
4	d	0.27	0/2791	0.43	2/3804 (0.1%)
5	E	0.17	0/644	0.29	0/878
5	e	0.16	0/644	0.32	0/878
6	F	0.41	0/261	0.61	0/352
6	f	0.16	0/261	0.29	0/352
7	G	0.11	0/900	0.26	0/1207
7	g	0.11	0/900	0.26	0/1207
8	H	0.19	0/522	0.29	0/712
8	h	0.19	0/522	0.29	0/712
9	I	0.24	0/286	0.32	0/386
9	i	0.19	0/286	0.31	0/386
10	J	0.40	0/249	0.69	1/339 (0.3%)
10	j	0.11	0/249	0.27	0/339
11	K	0.23	0/315	0.44	0/432
11	k	0.22	0/315	0.38	0/432
12	L	0.33	0/311	0.40	0/423
12	l	0.20	0/311	0.23	0/423
13	M	0.19	0/322	0.27	0/435
13	m	0.19	0/322	0.28	0/435
15	O	0.32	0/1896	0.46	0/2549
15	o	0.32	0/1896	0.45	0/2549
16	T	0.19	0/239	0.24	0/323
16	t	0.17	0/239	0.23	0/323
17	U	0.19	0/722	0.34	0/982

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	u	0.28	0/722	0.40	0/982
18	V	0.31	0/1047	0.43	0/1422
18	v	0.34	0/1047	0.46	0/1422
19	W	0.22	0/446	0.32	0/606
19	w	0.18	0/446	0.29	0/606
20	X	0.18	0/248	0.25	0/336
20	x	0.18	0/248	0.26	0/336
21	Z	0.15	0/461	0.26	0/633
21	z	0.12	0/461	0.28	0/633
22	3	0.26	0/1765	0.41	0/2405
23	4	0.35	0/1282	0.56	2/1746 (0.1%)
24	5	0.24	0/1255	0.39	1/1696 (0.1%)
25	6	0.37	1/1324 (0.1%)	0.62	1/1780 (0.1%)
26	0	0.15	0/1298	0.35	0/1764
26	7	0.29	0/1298	0.46	1/1764 (0.1%)
27	Y	0.15	0/253	0.31	0/341
27	y	0.11	0/253	0.23	0/341
28	Q	0.15	0/1220	0.27	0/1638
28	q	0.23	0/1220	0.41	0/1638
29	1	0.29	0/1237	0.47	0/1687
29	2	0.31	0/1246	0.53	1/1700 (0.1%)
29	8	0.29	0/1237	0.50	0/1687
29	9	0.32	0/1246	0.49	1/1700 (0.1%)
All	All	0.25	1/59858 (0.0%)	0.39	11/81307 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	39	GLN	N-CA	5.18	1.49	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	40	PRO	N-CA-C	10.12	123.04	110.70
23	4	40	PRO	N-CA-C	9.97	122.86	110.70
1	A	248	ILE	N-CA-C	9.52	120.13	110.23
29	2	136	ILE	N-CA-C	-7.48	104.20	112.80
24	5	41	PRO	N-CA-CB	6.03	109.58	103.25
4	d	143	ILE	CA-C-N	5.93	128.81	120.28
4	d	143	ILE	C-N-CA	5.93	128.81	120.28
10	J	31	SER	N-CA-C	-5.88	104.95	111.71
29	9	141	LEU	N-CA-C	-5.65	105.96	112.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	196	PHE	N-CA-C	-5.45	106.47	113.23
23	4	88	PHE	CA-CB-CG	5.30	119.10	113.80

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	A	2614	0	2513	35	0
1	a	2614	0	2513	20	0
2	B	3772	0	3654	39	0
2	b	3772	0	3654	40	0
3	C	3489	0	3398	46	0
3	c	3489	0	3398	51	0
4	D	2699	0	2600	30	0
4	d	2699	0	2600	40	0
5	E	626	0	610	12	0
5	e	626	0	610	14	0
6	F	253	0	259	9	0
6	f	253	0	259	8	0
7	G	890	0	896	11	0
7	g	890	0	896	16	0
8	H	512	0	540	8	0
8	h	512	0	540	4	0
9	I	279	0	293	2	0
9	i	279	0	293	4	0
10	J	243	0	253	5	0
10	j	243	0	253	2	0
11	K	303	0	310	4	0
11	k	303	0	310	4	0
12	L	302	0	301	1	0
12	l	302	0	301	4	0
13	M	317	0	323	11	0
13	m	317	0	323	13	0
14	N	150	0	34	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	n	150	0	34	2	0
15	O	1867	0	1862	18	0
15	o	1867	0	1862	27	0
16	T	233	0	244	2	0
16	t	233	0	244	0	0
17	U	708	0	707	11	0
17	u	708	0	707	10	0
18	V	1029	0	1028	15	0
18	v	1029	0	1028	33	0
19	W	434	0	383	6	0
19	w	434	0	383	8	0
20	X	248	0	278	4	0
20	x	248	0	278	3	0
21	Z	453	0	482	3	0
21	z	453	0	482	5	0
22	3	1710	0	1623	59	0
23	4	1249	0	1219	55	0
24	5	1229	0	1184	47	0
25	6	1296	0	1269	64	0
26	0	1269	0	1261	26	0
26	7	1269	0	1262	29	0
27	Y	251	0	289	3	0
27	y	251	0	289	2	0
28	Q	1198	0	1175	9	0
28	q	1198	0	1175	37	0
29	1	1206	0	1119	43	0
29	2	1214	0	1138	40	0
29	8	1206	0	1120	41	0
29	9	1214	0	1137	44	0
30	A	80	0	112	6	0
30	B	120	0	168	6	0
30	C	80	0	112	6	0
30	D	40	0	56	1	0
30	H	40	0	56	1	0
30	K	80	0	112	9	0
30	a	80	0	112	6	0
30	b	120	0	168	7	0
30	c	80	0	112	6	0
30	d	40	0	56	1	0
30	h	40	0	56	5	0
30	k	80	0	112	7	0
31	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	a	10	0	0	0	0
32	A	1	0	0	0	0
32	a	1	0	0	0	0
33	0	478	0	445	16	0
33	1	543	0	422	23	0
33	2	598	0	471	32	0
33	3	702	0	698	35	0
33	4	603	0	556	36	0
33	5	401	0	340	44	0
33	6	396	0	328	11	0
33	7	521	0	475	23	0
33	8	543	0	422	21	0
33	9	598	0	471	19	0
33	A	174	0	170	2	0
33	B	987	0	1039	26	0
33	C	806	0	853	19	0
33	D	176	0	164	3	0
33	H	43	0	30	3	0
33	W	65	0	72	6	0
33	Z	51	0	41	1	0
33	a	174	0	170	0	0
33	b	987	0	1039	29	0
33	c	806	0	853	22	0
33	d	176	0	164	6	0
33	w	65	0	72	5	0
33	z	51	0	41	1	0
34	A	128	0	148	2	0
34	a	128	0	148	2	0
35	A	4	0	1	2	0
35	a	4	0	1	3	0
36	0	28	0	29	0	0
36	3	76	0	98	2	0
36	4	49	0	74	2	0
36	5	33	0	42	1	0
36	7	28	0	29	1	0
36	A	141	0	207	4	0
36	D	90	0	128	1	0
36	H	42	0	54	0	0
36	W	35	0	40	2	0
36	a	92	0	133	2	0
36	b	49	0	74	0	0
36	d	90	0	128	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	h	42	0	54	2	0
36	w	35	0	40	0	0
37	0	48	0	63	1	0
37	7	48	0	62	0	0
37	A	40	0	44	0	0
37	B	54	0	78	3	0
37	D	54	0	77	2	0
37	L	54	0	78	2	0
37	T	94	0	125	2	0
37	a	54	0	78	1	0
37	i	40	0	44	1	0
37	l	54	0	78	2	0
37	t	40	0	47	2	0
38	3	39	0	62	3	0
38	A	53	0	64	3	0
38	C	166	0	206	7	0
38	H	62	0	82	0	0
38	a	53	0	64	2	0
38	c	166	0	206	10	0
38	h	62	0	82	1	0
39	0	42	0	54	2	0
39	3	31	0	32	0	0
39	5	31	0	32	0	0
39	7	55	0	86	1	0
39	B	79	0	98	0	0
39	C	144	0	168	3	0
39	D	86	0	112	2	0
39	M	40	0	50	1	0
39	Q	37	0	44	0	0
39	W	48	0	66	2	0
39	b	119	0	148	6	0
39	c	75	0	90	4	0
39	d	83	0	106	4	0
39	m	40	0	50	2	0
39	q	83	0	106	5	0
39	w	48	0	66	1	0
40	D	1	0	0	0	0
40	d	1	0	0	0	0
41	D	55	0	80	0	0
41	d	55	0	80	1	0
42	F	43	0	30	9	0
42	V	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	e	43	0	30	4	0
42	v	43	0	30	5	0
43	3	35	0	46	5	0
43	4	35	0	46	13	0
43	5	31	0	35	11	0
43	T	31	0	35	1	0
43	t	31	0	35	1	0
43	w	35	0	46	5	0
44	3	45	0	0	0	0
44	5	45	0	0	0	0
44	6	45	0	0	6	0
45	0	96	0	0	1	0
45	1	96	0	0	8	0
45	2	96	0	0	7	0
45	3	48	0	0	2	0
45	4	144	0	0	11	0
45	5	335	0	0	31	0
45	6	288	0	0	18	0
45	7	96	0	0	2	0
45	8	96	0	0	3	0
45	9	96	0	0	1	0
46	1	86	0	0	5	0
46	2	86	0	0	19	0
46	3	43	0	0	1	0
46	4	43	0	0	1	0
46	8	86	0	0	8	0
46	9	86	0	0	5	0
47	0	45	0	0	0	0
47	4	45	0	0	2	0
47	5	45	0	0	16	0
47	6	45	0	0	0	0
47	7	45	0	0	0	0
48	0	42	0	0	2	0
48	7	42	0	0	2	0
All	All	75511	0	72563	1313	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1313) 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)
2:B:243:SER:HA	2:B:246:PHE:CE1	1.47	1.47
25:6:179:MET:SD	45:6:301:A86:C8	2.21	1.28
29:2:158:LEU:HD11	46:2:304:DD6:C	1.72	1.20
18:v:89:THR:OG1	18:v:109:ASP:HA	1.40	1.20
25:6:179:MET:HE1	45:6:301:A86:C10	1.71	1.19
25:6:179:MET:SD	45:6:301:A86:C9	2.34	1.14
45:4:301:A86:C3	33:4:313:CLA:HBC2	1.80	1.12
22:3:150:MET:HE1	33:3:307:CLA:C2C	1.84	1.07
22:3:150:MET:HE1	33:3:307:CLA:CMC	1.85	1.06
23:4:69:HIS:CE1	33:4:310:CLA:HMD2	1.90	1.05
47:5:310:KC2:OBD	33:5:313:CLA:HBD	1.55	1.04
23:4:69:HIS:HD1	33:4:310:CLA:CMD	1.72	1.02
2:B:243:SER:CA	2:B:246:PHE:CE1	2.44	1.00
25:6:179:MET:HE1	45:6:301:A86:C11	1.91	1.00
23:4:69:HIS:HD1	33:4:310:CLA:HMD1	1.27	0.99
25:6:179:MET:HE1	45:6:301:A86:C9	1.93	0.99
24:5:127:ILE:HD11	45:5:302:A86:C8	1.93	0.97
25:6:179:MET:CE	45:6:301:A86:C9	2.41	0.97
23:4:69:HIS:ND1	33:4:310:CLA:CMD	2.27	0.97
45:5:306:A86:C4	47:5:310:KC2:CBB	2.43	0.96
29:1:161:LEU:HB3	33:1:313:CLA:HBB2	1.48	0.95
45:5:302:A86:C37	43:5:320:LMU:H12	1.96	0.94
23:4:69:HIS:CE1	33:4:310:CLA:CMD	2.50	0.94
2:B:243:SER:HA	2:B:246:PHE:HE1	1.15	0.92
23:4:69:HIS:ND1	33:4:310:CLA:HMD1	1.82	0.92
29:9:162:ALA:HB1	46:9:304:DD6:C37	1.99	0.92
22:3:150:MET:HE1	33:3:307:CLA:HMC2	1.51	0.91
23:4:69:HIS:HD2	33:4:306:CLA:CBB	1.84	0.90
46:1:304:DD6:C10	33:1:311:CLA:H71	2.03	0.89
25:6:179:MET:SD	45:6:301:A86:C6	2.61	0.89
11:k:29:PHE:HB3	30:k:101:BCR:H15C	1.54	0.88
47:5:310:KC2:CAD	33:5:313:CLA:HBD	2.03	0.88
18:v:89:THR:OG1	18:v:109:ASP:CA	2.21	0.88
25:6:74:GLN:HE21	25:6:174:GLY:HA2	1.40	0.87
29:1:161:LEU:HB3	33:1:313:CLA:CBB	2.06	0.86
4:d:217:VAL:HG11	1:a:272:HIS:CD2	2.11	0.86
29:2:158:LEU:CD1	46:2:304:DD6:C	2.53	0.85
47:5:310:KC2:CMD	33:5:313:CLA:C4D	2.55	0.85
18:V:66:CYS:SG	42:V:201:HEM:HAC	2.18	0.84
29:1:79:TYR:HD2	29:1:166:LEU:HD13	1.44	0.83
25:6:74:GLN:NE2	25:6:174:GLY:HA2	1.93	0.83
22:3:72:ASN:HB3	22:3:75:TYR:HB2	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:5:127:ILE:CD1	45:5:302:A86:C8	2.57	0.82
23:4:69:HIS:HD2	33:4:306:CLA:HBB2	1.43	0.82
37:0:316:SQD:H352	45:1:301:A86:C3	2.11	0.81
22:3:150:MET:HE1	33:3:307:CLA:C3C	2.10	0.80
3:c:286:LEU:HD12	38:c:516:DGD:HB32	1.64	0.80
43:3:301:LMU:H32	43:3:301:LMU:H112	1.62	0.80
7:G:121:PHE:HB3	7:G:125:ARG:HH21	1.49	0.78
24:5:99:PHE:HE2	43:5:320:LMU:H62	1.48	0.78
45:5:301:A86:C2	33:5:316:CLA:C4C	2.61	0.78
4:d:217:VAL:HG11	1:a:272:HIS:HD2	1.46	0.78
46:2:303:DD6:C22	33:2:306:CLA:C1B	2.62	0.78
23:4:50:LEU:HD23	46:4:303:DD6:O2	1.83	0.78
29:1:161:LEU:CB	33:1:313:CLA:HBB2	2.13	0.78
47:5:310:KC2:C3D	33:5:313:CLA:CAD	2.62	0.77
26:7:167:ARG:HB3	33:7:305:CLA:HBC2	1.66	0.77
29:8:185:LEU:HG	29:8:186:ILE:H	1.50	0.76
26:0:47:PRO:HD2	48:0:302:ET4:O31	1.84	0.76
26:0:69:HIS:HB3	26:0:170:MET:HE2	1.67	0.76
22:3:208:MET:HE1	33:3:303:CLA:HAB	1.68	0.76
45:4:301:A86:C3	33:4:313:CLA:CBC	2.64	0.76
29:9:137:GLY:C	29:9:139:PRO:HD3	2.11	0.75
23:4:69:HIS:CD2	33:4:306:CLA:CBB	2.68	0.75
46:2:303:DD6:C22	33:2:306:CLA:NB	2.50	0.75
4:d:213:HIS:CE1	35:a:402:BCT:O3	2.39	0.75
23:4:93:ILE:HD11	23:4:113:PRO:HG3	1.69	0.74
2:b:114:HIS:HE1	33:b:617:CLA:ND	1.84	0.74
45:6:304:A86:C5	44:6:314:KC1:CAB	2.65	0.74
1:A:331:MET:HE3	4:D:346:PRO:HB2	1.69	0.73
29:2:86:ARG:HD2	29:2:98:ALA:H	1.53	0.73
46:8:304:DD6:C8	33:8:311:CLA:CAB	2.67	0.73
22:3:150:MET:CE	33:3:307:CLA:HMC2	2.18	0.72
11:k:32:LEU:HB3	30:k:101:BCR:H21C	1.72	0.72
23:4:69:HIS:HE1	33:4:310:CLA:HMD2	1.52	0.72
4:d:296:ASP:OD2	2:b:326:ARG:NH2	2.22	0.72
45:4:302:A86:C3	43:4:317:LMU:H123	2.19	0.72
26:7:69:HIS:HB3	26:7:170:MET:HE2	1.71	0.71
26:7:142:ILE:HG13	26:7:143:GLU:H	1.54	0.71
25:6:127:PHE:HB3	25:6:131:PHE:CE2	2.25	0.71
45:4:302:A86:C1	43:4:317:LMU:H122	2.19	0.71
2:B:142:HIS:HE1	33:B:615:CLA:ND	1.88	0.70
33:c:502:CLA:H11	33:c:503:CLA:H2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:2:79:TYR:HD2	29:2:166:LEU:HD23	1.55	0.70
29:2:184:ASN:O	29:2:185:LEU:C	2.35	0.70
36:4:318:LHG:H162	36:4:318:LHG:H302	1.74	0.70
45:4:302:A86:C	43:4:317:LMU:H122	2.22	0.70
2:b:235:GLU:HB3	2:b:473:THR:HG22	1.74	0.70
29:2:138:LYS:CB	33:2:311:CLA:HED2	2.21	0.70
22:3:150:MET:CE	33:3:307:CLA:HAC1	2.21	0.70
25:6:89:LEU:HB2	25:6:92:ALA:HB2	1.74	0.69
23:4:40:PRO:HG2	33:4:305:CLA:HMA1	1.73	0.69
11:K:32:LEU:HB3	30:K:101:BCR:H21C	1.75	0.69
2:B:235:GLU:HB3	2:B:473:THR:HG22	1.73	0.69
42:v:201:HEM:HBC2	42:v:201:HEM:HHD	1.74	0.69
25:6:155:TRP:HZ3	33:6:313:CLA:H2A	1.58	0.68
24:5:135:MET:HE1	45:5:302:A86:C23	2.24	0.68
29:9:86:ARG:HD3	33:9:308:CLA:HED2	1.74	0.68
3:c:316:LEU:HD12	3:c:338:TYR:HB3	1.76	0.68
18:v:57:ARG:CG	28:q:95:VAL:HG13	2.24	0.68
25:6:133:MET:SD	45:6:302:A86:C18	2.81	0.68
3:C:286:LEU:HD12	38:C:516:DGD:HB32	1.76	0.68
46:2:304:DD6:C8	33:2:311:CLA:CAB	2.72	0.68
3:c:366:PRO:HG3	28:q:148:THR:HG23	1.75	0.68
7:g:106:ASP:HB3	7:g:109:LYS:HB2	1.74	0.68
1:A:260:PHE:CE2	1:A:262:TYR:HB3	2.28	0.67
29:8:79:TYR:CD2	29:8:166:LEU:HD12	2.29	0.67
15:o:257:ARG:NH1	15:o:259:GLU:OE2	2.28	0.67
22:3:160:ARG:HG2	22:3:172:ASP:HB3	1.77	0.67
1:a:140:ARG:NH2	36:a:404:LHG:O5	2.26	0.67
21:z:1:MET:HE1	21:z:3:THR:HB	1.76	0.67
29:8:189:LEU:HD22	29:8:191:PHE:HE1	1.59	0.67
23:4:36:ILE:HG13	23:4:63:ARG:HH21	1.58	0.67
3:c:54:HIS:HE1	33:c:510:CLA:NB	1.93	0.67
45:5:301:A86:C24	33:5:316:CLA:C1D	2.72	0.67
26:0:167:ARG:HB3	33:0:305:CLA:HBC3	1.77	0.67
25:6:195:PRO:O	25:6:197:VAL:N	2.27	0.67
4:d:84:MET:HG2	5:e:70:ARG:HG3	1.76	0.66
2:B:242:ILE:O	2:B:246:PHE:HD1	1.79	0.66
6:F:22:HIS:HE1	42:F:101:HEM:ND	1.93	0.66
19:w:183:GLU:HA	43:w:302:LMU:H12	1.75	0.66
22:3:138:ILE:HG23	22:3:143:ILE:HD11	1.77	0.66
22:3:150:MET:HE2	33:3:307:CLA:HAC1	1.75	0.66
47:5:310:KC2:C2D	33:5:313:CLA:C3D	2.74	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:2:304:DD6:C8	33:2:311:CLA:HHC	2.25	0.66
18:v:89:THR:HG1	18:v:109:ASP:HA	1.61	0.66
29:9:123:GLY:HA3	33:9:310:CLA:HAB	1.77	0.66
33:B:606:CLA:H72	30:B:619:BCR:H311	1.78	0.66
26:7:168:LEU:HD21	33:7:310:CLA:HBC3	1.78	0.66
3:c:249:HIS:HE1	33:c:506:CLA:NA	1.92	0.65
25:6:40:PRO:HB2	25:6:41:PRO:HD3	1.76	0.65
18:v:63:CYS:SG	42:v:201:HEM:CAB	2.85	0.65
30:h:101:BCR:H351	33:b:602:CLA:HBB2	1.78	0.65
24:5:42:LEU:HD13	24:5:45:TRP:HB2	1.79	0.65
23:4:39:LEU:HG	23:4:41:PRO:HD2	1.79	0.65
26:7:140:ALA:HA	33:7:312:CLA:HBC2	1.77	0.65
29:9:183:ASP:O	29:9:184:ASN:C	2.40	0.65
10:j:8:PRO:HG2	10:j:11:LEU:HD13	1.77	0.65
3:C:185:ASP:OD2	3:C:195:ARG:NH1	2.29	0.65
13:M:94:ASN:ND2	13:m:94:ASN:HA	2.12	0.65
18:v:57:ARG:HG2	28:q:95:VAL:HG13	1.79	0.65
29:1:122:ILE:HG21	33:1:310:CLA:HMC3	1.77	0.65
2:B:242:ILE:O	2:B:246:PHE:CD1	2.50	0.64
6:F:42:GLN:NE2	28:Q:76:SER:O	2.29	0.64
26:0:136:THR:HG22	26:0:136:THR:O	1.96	0.64
29:8:184:ASN:O	29:8:185:LEU:C	2.40	0.64
26:0:94:ASP:OD1	26:0:95:ASP:N	2.31	0.64
26:7:161:ARG:HH12	29:8:46:PRO:HB3	1.62	0.64
14:N:6:UNK:HA	33:b:617:CLA:HED3	1.79	0.64
33:3:312:CLA:HAC2	33:3:313:CLA:HMA3	1.80	0.64
3:C:54:HIS:HE1	33:C:510:CLA:NB	1.96	0.64
24:5:160:SER:H	24:5:161:PRO:HD2	1.63	0.63
25:6:75:LEU:HD21	45:6:302:A86:O	1.98	0.63
29:8:146:GLU:N	29:8:146:GLU:OE1	2.30	0.63
8:H:30:ILE:HD11	33:H:103:CLA:C2D	2.29	0.63
7:g:121:PHE:HA	7:g:124:ILE:HD12	1.79	0.63
29:1:184:ASN:O	29:1:185:LEU:C	2.41	0.63
29:8:163:ILE:HG23	29:8:164:LEU:HD12	1.81	0.63
2:B:127:ARG:HG3	2:B:128:THR:HG23	1.81	0.62
45:4:302:A86:C	43:4:317:LMU:C12	2.76	0.62
46:8:304:DD6:C10	33:8:311:CLA:H71	2.28	0.62
2:B:103:LEU:HD21	33:B:605:CLA:HMC2	1.81	0.62
13:M:94:ASN:HD21	13:m:94:ASN:HA	1.64	0.62
5:e:14:ILE:HG21	42:e:101:HEM:HAD1	1.82	0.62
46:8:304:DD6:C10	33:8:311:CLA:H52	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:77:LEU:HD11	7:g:92:GLU:HG3	1.81	0.62
33:b:609:CLA:HBC3	33:b:610:CLA:H122	1.79	0.62
45:9:302:A86:C8	33:9:308:CLA:H72	2.29	0.62
29:1:122:ILE:HG23	45:1:302:A86:C22	2.29	0.62
24:5:63:ARG:NH1	33:5:309:CLA:O1D	2.25	0.62
29:9:62:ARG:NH1	29:9:65:GLU:OE1	2.33	0.62
33:B:608:CLA:HBC3	33:B:609:CLA:H122	1.81	0.62
5:E:14:ILE:HG21	42:F:101:HEM:HAD2	1.81	0.62
26:7:94:ASP:OD1	26:7:95:ASP:N	2.30	0.62
7:g:154:SER:O	2:b:378:ARG:NH1	2.33	0.62
39:c:519:LMG:HC92	33:z:101:CLA:H12	1.82	0.61
4:d:213:HIS:CE1	4:d:266:LEU:CD2	2.83	0.61
22:3:76:GLN:HB2	22:3:79:ASN:HB3	1.83	0.61
28:q:127:ARG:HB3	28:q:146:GLU:OE2	2.00	0.61
20:X:24:ILE:HD11	26:0:127:LEU:HB2	1.82	0.61
1:A:140:ARG:NH2	36:A:412:LHG:O5	2.31	0.61
23:4:36:ILE:O	23:4:63:ARG:NH2	2.32	0.61
23:4:89:GLY:O	43:4:317:LMU:H5'	2.00	0.61
45:4:301:A86:C2	33:4:313:CLA:HBC2	2.31	0.61
28:Q:117:LYS:HD2	28:Q:157:ALA:HA	1.83	0.61
22:3:161:ILE:HG12	22:3:168:ARG:NE	2.16	0.61
24:5:167:LYS:HE3	33:5:314:CLA:HMA3	1.80	0.61
26:0:122:SER:HB2	33:0:308:CLA:HAB	1.81	0.61
4:d:255:ILE:HG12	1:a:133:LEU:HD23	1.83	0.61
13:M:94:ASN:ND2	13:m:94:ASN:OD1	2.34	0.61
47:5:310:KC2:CAD	33:5:313:CLA:CBD	2.76	0.61
25:6:179:MET:CE	45:6:301:A86:C10	2.59	0.61
26:0:106:ALA:HA	26:0:109:THR:HG22	1.81	0.61
45:0:301:A86:O	33:0:304:CLA:HAC1	2.01	0.61
29:1:90:ASP:HA	29:1:95:VAL:HA	1.83	0.61
1:A:131:TRP:HZ2	3:C:447:ARG:HD2	1.66	0.61
3:c:305:PRO:HB2	3:c:359:LEU:HD12	1.83	0.61
33:3:307:CLA:HBB2	33:3:312:CLA:C1A	2.30	0.61
23:4:98:SER:O	23:4:99:THR:C	2.44	0.60
45:1:302:A86:C14	33:1:314:CLA:HMB2	2.31	0.60
23:4:40:PRO:O	23:4:41:PRO:C	2.44	0.60
23:4:69:HIS:CD2	33:4:306:CLA:HBB1	2.35	0.60
3:C:267:GLU:HG2	3:C:446:ALA:HB2	1.83	0.60
26:7:161:ARG:HD3	33:7:310:CLA:HBA1	1.83	0.60
17:U:116:ALA:HA	17:U:119:GLU:OE2	2.01	0.60
22:3:214:LEU:HG	45:3:314:A86:C21	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:4:317:LMU:H32	45:6:301:A86:C39	2.31	0.60
39:b:623:LMG:O3	39:b:623:LMG:O1	2.15	0.60
26:0:195:GLY:O	26:0:197:VAL:N	2.35	0.60
45:5:301:A86:C4	33:5:316:CLA:C2C	2.80	0.60
45:6:304:A86:C3	44:6:314:KC1:CAB	2.79	0.60
33:7:312:CLA:H2A	33:7:312:CLA:HED2	1.84	0.60
33:b:607:CLA:H72	30:b:620:BCR:H311	1.84	0.60
30:h:101:BCR:H383	33:b:602:CLA:HAC1	1.83	0.60
22:3:150:MET:CE	33:3:307:CLA:C3C	2.80	0.60
35:A:410:BCT:O3	4:D:213:HIS:NE2	2.33	0.60
3:c:296:PRO:HG2	3:c:299:LEU:HD12	1.83	0.60
33:B:616:CLA:HED3	14:n:6:UNK:HA	1.84	0.60
4:d:198:MET:HE3	4:d:280:THR:CG2	2.30	0.59
18:v:67:HIS:HA	18:v:71:ILE:O	2.02	0.59
22:3:154:GLU:OE2	22:3:157:ARG:NH2	2.35	0.59
33:c:504:CLA:H42	38:c:517:DGD:HB42	1.83	0.59
5:e:63:GLN:HG3	7:g:164:PHE:HA	1.82	0.59
22:3:150:MET:CE	33:3:307:CLA:CAC	2.79	0.59
42:e:101:HEM:HAC	6:f:25:ALA:HB1	1.84	0.59
15:o:86:GLY:C	15:o:87:GLU:HG2	2.28	0.59
23:4:69:HIS:CE1	33:4:310:CLA:HMD1	2.31	0.59
23:4:69:HIS:ND1	33:4:310:CLA:HMD2	2.03	0.59
4:d:278:LEU:HD22	34:a:410:PHO:HBC3	1.83	0.59
11:k:8:ARG:HH21	11:k:14:VAL:HG11	1.67	0.59
1:A:245:THR:O	1:A:246:TYR:HB3	2.03	0.59
45:1:302:A86:C7	33:1:308:CLA:C2	2.81	0.59
4:d:313:PHE:HA	4:d:316:LYS:HD3	1.83	0.59
25:6:179:MET:HE1	45:6:301:A86:C12	2.32	0.59
29:9:184:ASN:O	29:9:185:LEU:C	2.46	0.59
24:5:173:ASN:ND2	33:5:308:CLA:O1D	2.35	0.58
15:O:277:VAL:HG22	15:O:297:LYS:HG2	1.85	0.58
45:1:302:A86:C7	33:1:308:CLA:H2	2.33	0.58
2:B:326:ARG:NH2	4:D:296:ASP:OD2	2.35	0.58
3:c:81:GLU:OE2	3:c:396:HIS:NE2	2.36	0.58
42:F:101:HEM:HBC2	42:F:101:HEM:HMC2	1.84	0.58
29:9:80:ILE:HG13	29:9:186:ILE:HD12	1.84	0.58
29:1:139:PRO:O	29:1:140:ASP:C	2.46	0.58
2:B:440:ASP:OD1	2:B:441:GLY:N	2.37	0.58
26:7:168:LEU:HD21	33:7:310:CLA:CBC	2.33	0.58
22:3:150:MET:HE2	33:3:307:CLA:CAC	2.32	0.58
23:4:91:ASP:O	23:4:92:LEU:C	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:5:132:THR:HG23	24:5:133:ARG:HG2	1.86	0.58
2:b:142:HIS:HE1	33:b:616:CLA:ND	2.00	0.58
4:d:213:HIS:CE1	4:d:266:LEU:HD21	2.39	0.58
18:v:125:ASP:OD1	18:v:126:ILE:N	2.37	0.58
29:1:83:GLU:HG3	29:1:186:ILE:HD13	1.85	0.58
29:1:68:HIS:HE1	33:1:307:CLA:ND	2.00	0.58
36:A:411:LHG:O4	4:D:140:TYR:OH	2.22	0.58
24:5:154:PHE:HB2	33:5:314:CLA:H12	1.86	0.58
28:Q:64:SER:HA	28:Q:70:GLY:HA3	1.84	0.58
15:O:265:VAL:HG22	15:O:272:ILE:HG22	1.86	0.57
3:C:316:LEU:HD12	3:C:338:TYR:HB3	1.85	0.57
4:D:84:MET:HG3	5:E:70:ARG:HG3	1.85	0.57
29:1:81:VAL:HG11	33:1:308:CLA:HAC2	1.85	0.57
29:2:91:ILE:HD13	45:2:302:A86:C29	2.34	0.57
15:o:86:GLY:O	15:o:87:GLU:HG2	2.04	0.57
2:b:103:LEU:HD21	33:b:606:CLA:HMC3	1.87	0.57
18:v:57:ARG:HH11	28:q:95:VAL:HG13	1.68	0.57
25:6:39:GLN:HG3	25:6:41:PRO:HD2	1.86	0.57
46:9:304:DD6:C10	33:9:311:CLA:H72	2.35	0.57
2:B:469:HIS:O	2:B:473:THR:HG23	2.05	0.57
24:5:131:GLU:HA	24:5:135:MET:HE3	1.85	0.56
26:7:113:TRP:NE1	33:7:307:CLA:O1A	2.38	0.56
39:q:301:LMG:H121	39:q:302:LMG:H121	1.87	0.56
1:A:133:LEU:HD23	4:D:255:ILE:HG12	1.86	0.56
9:i:5:LYS:NZ	19:w:188:ASP:OD1	2.35	0.56
3:c:21:ILE:HG21	3:c:24:ARG:HH11	1.70	0.56
6:F:20:ALA:O	6:F:21:VAL:C	2.48	0.56
23:4:153:ALA:O	23:4:157:HIS:CD2	2.58	0.56
24:5:97:ARG:NH2	24:5:113:ASP:OD1	2.38	0.56
45:7:301:A86:C1	33:7:311:CLA:HBC2	2.35	0.56
29:9:120:PHE:HD2	33:8:310:CLA:H122	1.68	0.56
4:D:82:ASN:O	7:G:57:ALA:N	2.38	0.56
7:g:85:ASP:HB3	7:g:88:ALA:HB3	1.87	0.56
8:H:30:ILE:HD11	33:H:103:CLA:C3D	2.35	0.56
19:w:200:HIS:CD2	33:w:303:CLA:ND	2.73	0.56
2:b:243:SER:HA	2:b:246:PHE:CE2	2.41	0.56
22:3:157:ARG:HD3	22:3:173:ILE:HD11	1.87	0.56
29:9:95:VAL:HG22	29:9:97:CYS:H	1.71	0.56
46:8:304:DD6:C8	33:8:311:CLA:CBB	2.83	0.56
3:c:254:PRO:HA	33:c:506:CLA:HED3	1.87	0.56
26:0:41:PRO:HG3	33:0:304:CLA:NB	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:B:601:CLA:HAC1	30:H:101:BCR:H383	1.86	0.56
25:6:78:LEU:HD22	45:6:304:A86:C	2.36	0.56
29:9:87:TRP:HH2	33:9:308:CLA:H43	1.71	0.56
33:2:306:CLA:CGA	33:2:306:CLA:H3A	2.35	0.56
29:1:186:ILE:HD12	29:1:186:ILE:H	1.71	0.56
42:F:101:HEM:HBB2	42:F:101:HEM:HMB2	1.86	0.55
22:3:165:GLY:C	22:3:167:ASP:H	2.14	0.55
14:N:27:UNK:O	14:N:29:UNK:N	2.39	0.55
1:A:246:TYR:HE1	1:A:248:ILE:HD12	1.71	0.55
2:B:7:ARG:HD3	33:B:611:CLA:HED1	1.88	0.55
33:3:307:CLA:HBB2	33:3:312:CLA:NA	2.10	0.55
24:5:69:HIS:HE1	47:5:310:KC2:NA	2.04	0.55
25:6:39:GLN:HE21	25:6:41:PRO:HD3	1.71	0.55
29:2:95:VAL:HG12	29:2:97:CYS:H	1.69	0.55
15:O:101:MET:HB3	15:O:140:ILE:HB	1.87	0.55
25:6:41:PRO:HG3	33:6:307:CLA:C4B	2.36	0.55
28:Q:68:VAL:HG13	28:Q:69:ILE:HG12	1.87	0.55
29:1:147:GLU:OE2	29:1:151:GLN:NE2	2.38	0.55
18:v:63:CYS:SG	42:v:201:HEM:CBB	2.95	0.55
25:6:178:MET:O	25:6:181:ILE:HG22	2.06	0.55
23:4:69:HIS:CD2	33:4:306:CLA:HBB2	2.34	0.55
45:4:302:A86:C3	43:4:317:LMU:C12	2.84	0.55
1:A:248:ILE:O	1:A:249:VAL:C	2.49	0.55
3:c:309:GLN:HG3	3:c:359:LEU:HD13	1.87	0.55
19:W:200:HIS:CD2	33:W:303:CLA:ND	2.73	0.55
29:9:35:PRO:O	29:9:62:ARG:NH2	2.39	0.55
1:A:24:THR:HG22	1:A:24:THR:O	2.05	0.55
47:5:310:KC2:CAD	33:5:313:CLA:CAD	2.85	0.55
47:5:310:KC2:CMD	33:5:313:CLA:C3D	2.85	0.55
2:b:264:PRO:HG2	2:b:267:LEU:HD13	1.89	0.55
29:8:35:PRO:O	29:8:62:ARG:NH2	2.39	0.55
45:6:304:A86:C4	44:6:314:KC1:CAB	2.84	0.55
29:1:137:GLY:O	29:1:138:LYS:C	2.50	0.55
2:B:192:PRO:HG3	8:H:49:TYR:CD1	2.42	0.55
15:o:196:PHE:HE2	15:o:198:MET:HE2	1.71	0.55
39:0:314:LMG:O5	39:0:314:LMG:O4	2.25	0.55
5:e:20:TYR:HE1	42:e:101:HEM:C3D	2.25	0.54
9:i:30:ARG:HA	9:i:34:ARG:HH22	1.72	0.54
25:6:39:GLN:HB2	25:6:40:PRO:HD2	1.89	0.54
28:q:95:VAL:HG12	28:q:95:VAL:O	2.08	0.54
28:q:151:MET:SD	28:q:154:THR:OG1	2.65	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:9:123:GLY:HA3	33:9:310:CLA:CAB	2.38	0.54
4:d:213:HIS:CE1	4:d:266:LEU:HD22	2.42	0.54
15:O:86:GLY:C	15:O:87:GLU:HG2	2.31	0.54
20:x:20:SER:O	20:x:24:ILE:HG12	2.07	0.54
29:1:122:ILE:HG12	45:1:302:A86:C22	2.38	0.54
3:c:223:VAL:HG22	3:c:287:TYR:CD1	2.42	0.54
3:c:330:GLN:HG2	3:c:334:GLY:HA2	1.88	0.54
33:C:507:CLA:H142	30:C:515:BCR:H362	1.90	0.54
17:U:104:VAL:O	17:U:107:VAL:HG12	2.08	0.54
22:3:81:MET:HE3	22:3:86:TRP:HE3	1.73	0.54
25:6:169:ILE:HD11	44:6:314:KC1:CHA	2.38	0.54
2:B:422:ARG:NH2	15:O:225:ASP:OD2	2.37	0.54
45:5:304:A86:C30	33:5:314:CLA:CHB	2.86	0.54
29:8:185:LEU:O	29:8:187:THR:N	2.41	0.54
3:C:341:ARG:NH1	15:O:136:THR:O	2.40	0.54
23:4:90:TYR:CE1	23:4:92:LEU:HG	2.43	0.54
45:5:302:A86:C7	33:5:311:CLA:H2	2.38	0.54
45:5:305:A86:C24	33:5:314:CLA:HAB	2.37	0.54
17:u:144:ASN:O	2:b:384:ARG:NH2	2.40	0.54
23:4:98:SER:O	23:4:100:ASN:N	2.40	0.54
4:d:82:ASN:O	7:g:57:ALA:N	2.41	0.54
29:9:158:LEU:O	29:9:161:LEU:HB2	2.08	0.54
2:B:243:SER:HA	2:B:246:PHE:CD1	2.27	0.54
33:C:502:CLA:H11	33:C:503:CLA:H2	1.90	0.54
4:d:198:MET:HE3	4:d:280:THR:HG21	1.90	0.54
17:u:117:GLU:O	17:u:120:VAL:HG12	2.08	0.54
1:A:278:TRP:HB3	1:A:279:PRO:HD3	1.90	0.53
6:f:42:GLN:OE1	28:q:62:ARG:NH1	2.42	0.53
18:v:59:PHE:C	18:v:61:ALA:H	2.16	0.53
38:C:518:DGD:O2D	10:J:31:SER:O	2.26	0.53
4:d:296:ASP:HA	4:d:314:TYR:OH	2.09	0.53
33:5:308:CLA:H2A	33:5:308:CLA:HED3	1.90	0.53
29:2:139:PRO:O	29:2:140:ASP:C	2.51	0.53
11:K:29:PHE:HB3	30:K:101:BCR:H15C	1.89	0.53
18:V:81:ASP:OD1	18:V:81:ASP:N	2.40	0.53
2:b:295:GLY:C	2:b:296:LEU:HD12	2.34	0.53
39:d:410:LMG:HC62	2:b:230:ARG:HH22	1.73	0.53
25:6:122:LEU:HA	25:6:125:VAL:HG12	1.89	0.53
29:1:122:ILE:HG21	33:1:310:CLA:CMC	2.38	0.53
13:m:102:ARG:NH2	39:m:201:LMG:O4	2.42	0.53
22:3:50:SER:OG	22:3:51:LEU:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:234:ALA:HB2	43:3:301:LMU:H3B	1.89	0.53
33:b:604:CLA:HAB	33:b:606:CLA:H152	1.91	0.53
29:1:35:PRO:O	29:1:62:ARG:NH2	2.42	0.53
28:q:140:TRP:CZ2	28:q:188:LYS:HE2	2.44	0.53
3:C:254:PRO:HA	33:C:506:CLA:HED3	1.91	0.53
9:I:5:LYS:NZ	19:W:188:ASP:OD1	2.41	0.53
25:6:35:GLU:HB3	25:6:63:ARG:HH21	1.73	0.53
22:3:168:ARG:NE	22:3:172:ASP:OD2	2.42	0.53
15:o:68:SER:HB2	15:o:71:GLN:HG2	1.90	0.53
22:3:125:ALA:HA	22:3:128:TYR:HE2	1.74	0.53
25:6:175:ARG:HA	25:6:178:MET:SD	2.49	0.53
29:9:133:ASN:O	29:9:134:PHE:HD1	1.92	0.53
3:C:381:ASP:OD2	28:Q:149:ARG:NH1	2.42	0.52
36:D:409:LHG:H182	16:T:17:ILE:HD11	1.90	0.52
29:2:163:ILE:O	29:2:164:LEU:C	2.52	0.52
1:A:245:THR:HG22	4:D:263:LYS:HD3	1.91	0.52
3:c:267:GLU:HG2	3:c:446:ALA:HB2	1.92	0.52
45:4:302:A86:C1	43:4:317:LMU:C12	2.87	0.52
42:v:201:HEM:HMB2	42:v:201:HEM:HBB2	1.91	0.52
22:3:150:MET:CE	33:3:307:CLA:CMC	2.74	0.52
2:b:272:ARG:NH1	2:b:276:ASP:OD2	2.42	0.52
2:B:243:SER:CA	2:B:246:PHE:HE1	2.03	0.52
23:4:153:ALA:O	23:4:157:HIS:HD2	1.92	0.52
25:6:39:GLN:HE22	33:6:307:CLA:C4A	2.22	0.52
25:6:196:ILE:HG13	25:6:197:VAL:H	1.74	0.52
3:c:51:HIS:CD2	33:c:509:CLA:NA	2.77	0.52
3:c:130:HIS:HE1	33:c:513:CLA:NA	2.05	0.52
10:J:8:PRO:HG2	10:J:11:LEU:HD13	1.92	0.52
22:3:79:ASN:HA	22:3:166:LYS:HG3	1.90	0.52
1:a:272:HIS:CE1	35:a:402:BCT:O2	2.63	0.52
20:X:20:SER:HA	33:0:307:CLA:H18	1.90	0.52
33:4:308:CLA:H101	33:4:314:CLA:H43	1.92	0.52
25:6:95:LEU:HD13	33:6:311:CLA:CGA	2.39	0.52
4:D:151:VAL:O	4:D:155:VAL:HG12	2.10	0.52
29:8:123:GLY:O	29:8:127:VAL:HG12	2.09	0.52
3:c:442:HIS:HE1	33:c:508:CLA:NA	2.05	0.52
4:d:337:ASN:OD1	7:g:65:ARG:NH1	2.43	0.52
1:a:278:TRP:HB3	1:a:279:PRO:HD3	1.92	0.52
26:0:161:ARG:HD3	33:0:310:CLA:HBA1	1.91	0.52
4:D:53:PHE:O	5:E:50:THR:OG1	2.28	0.52
15:o:98:LEU:HD21	15:o:304:ILE:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:5:302:A86:C	33:5:312:CLA:OBD	2.58	0.52
24:5:69:HIS:HE1	47:5:310:KC2:C4A	2.23	0.51
29:2:167:LEU:O	29:2:168:ARG:C	2.53	0.51
2:B:222:PRO:HB3	8:H:25:TRP:O	2.09	0.51
5:e:11:PHE:HA	5:e:14:ILE:HB	1.92	0.51
15:O:110:VAL:HB	15:O:168:LEU:HD21	1.92	0.51
33:3:304:CLA:H18	43:4:317:LMU:H51	1.92	0.51
29:1:135:ASP:N	29:1:135:ASP:OD1	2.44	0.51
15:o:59:ILE:HD12	15:o:83:GLU:OE2	2.10	0.51
18:V:89:THR:C	18:V:91:ARG:H	2.19	0.51
25:6:88:HIS:CD2	25:6:100:PHE:HB2	2.45	0.51
2:b:392:ILE:HD12	2:b:418:LYS:HG2	1.92	0.51
3:C:326:VAL:HG13	3:C:338:TYR:CD2	2.45	0.51
15:O:160:ASP:OD1	15:O:160:ASP:N	2.44	0.51
26:0:39:LEU:HG	26:0:41:PRO:HD2	1.91	0.51
29:8:68:HIS:HE1	33:8:307:CLA:C4D	2.24	0.51
30:c:514:BCR:H352	39:c:519:LMG:H391	1.91	0.51
15:o:266:ASN:ND2	15:o:269:GLU:OE1	2.43	0.51
22:3:212:PHE:HE2	33:3:319:CLA:H43	1.76	0.51
28:q:123:GLU:O	28:q:127:ARG:HG2	2.11	0.51
45:2:302:A86:C3	33:2:308:CLA:H2	2.41	0.51
38:c:518:DGD:O5D	38:c:518:DGD:O4D	2.26	0.51
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.93	0.51
26:0:113:TRP:NE1	33:0:307:CLA:O1A	2.44	0.51
3:C:51:HIS:CD2	33:C:509:CLA:NB	2.79	0.51
3:c:99:PRO:HG3	28:q:159:ARG:HD2	1.91	0.51
29:2:169:HIS:NE2	29:2:182:LEU:HD11	2.26	0.51
3:c:160:GLY:HA3	3:c:250:ILE:HG13	1.93	0.51
15:o:285:ASP:HB2	15:o:289:LYS:HE3	1.93	0.51
24:5:67:LEU:HD21	24:5:71:ARG:HE	1.76	0.51
33:7:312:CLA:H171	39:7:315:LMG:H181	1.91	0.51
29:9:137:GLY:O	29:9:139:PRO:HD3	2.11	0.51
29:1:101:PRO:O	29:1:103:GLY:N	2.39	0.51
37:i:101:SQD:H282	30:a:412:BCR:H363	1.93	0.50
18:v:89:THR:OG1	18:v:109:ASP:C	2.53	0.50
24:5:92:ASP:HA	24:5:98:ALA:HA	1.93	0.50
33:5:313:CLA:H172	36:5:318:LHG:H122	1.93	0.50
46:8:304:DD6:C8	33:8:311:CLA:HAB	2.39	0.50
18:v:35:THR:O	18:v:150:LYS:NZ	2.44	0.50
24:5:45:TRP:HZ2	45:5:303:A86:C39	2.24	0.50
13:m:95:LEU:O	13:m:98:GLN:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:W:210:GLN:O	19:W:210:GLN:NE2	2.43	0.50
1:A:63:ILE:HB	3:C:333:THR:HG21	1.94	0.50
4:D:99:ASP:OD2	4:D:102:ARG:HG2	2.11	0.50
4:d:241:GLU:OE1	4:d:263:LYS:NZ	2.37	0.50
33:0:304:CLA:HBC2	33:0:310:CLA:HBC1	1.93	0.50
17:U:61:ASN:HB3	17:U:64:LEU:HD12	1.92	0.50
45:5:301:A86:C7	33:5:316:CLA:HMC2	2.42	0.50
29:8:55:GLN:NE2	29:8:59:ASP:OD1	2.45	0.50
38:A:415:DGD:HB32	38:A:415:DGD:HA61	1.92	0.50
3:c:54:HIS:HD1	3:c:58:MET:HE2	1.75	0.50
18:V:153:ALA:O	18:V:154:GLU:HG3	2.11	0.50
18:v:31:GLU:HG2	18:v:34:ARG:HH12	1.77	0.50
3:C:296:PRO:HG2	3:C:299:LEU:HD12	1.93	0.50
33:3:313:CLA:HBC2	33:4:314:CLA:HBC3	1.93	0.50
29:8:164:LEU:O	29:8:165:GLU:C	2.55	0.50
4:d:115:LEU:HB3	33:d:402:CLA:HMA1	1.94	0.50
24:5:130:LEU:O	24:5:134:VAL:HB	2.11	0.50
26:7:168:LEU:CD2	33:7:310:CLA:HBC2	2.42	0.50
2:b:458:PHE:HB3	33:b:605:CLA:HBC2	1.92	0.50
29:2:67:LYS:O	29:2:71:VAL:HG23	2.11	0.50
7:G:121:PHE:HA	7:G:124:ILE:HD12	1.93	0.50
29:9:72:ALA:HB2	46:9:303:DD6:C2	2.42	0.50
3:c:249:HIS:HE1	33:c:506:CLA:C1A	2.25	0.49
23:4:130:TYR:HE2	47:5:310:KC2:CED	2.24	0.49
28:q:144:LYS:O	28:q:148:THR:HG22	2.12	0.49
1:A:127:MET:HG2	1:A:144:PHE:HB2	1.93	0.49
1:A:27:ARG:HA	3:C:470:ILE:HD11	1.93	0.49
18:v:89:THR:HG21	18:v:109:ASP:O	2.12	0.49
23:4:74:MET:HE3	33:4:311:CLA:HMC3	1.94	0.49
26:7:129:LEU:HB2	33:7:308:CLA:HMA1	1.93	0.49
29:8:116:ALA:O	29:8:120:PHE:HD2	1.95	0.49
23:4:99:THR:O	23:4:101:ASP:N	2.45	0.49
45:4:302:A86:C2	43:4:317:LMU:C12	2.90	0.49
48:7:302:ET4:C11	33:7:305:CLA:HMC1	2.43	0.49
29:8:67:LYS:HD2	33:8:310:CLA:C3D	2.42	0.49
5:E:22:ILE:HG13	5:E:23:ILE:N	2.26	0.49
6:f:15:THR:HG23	6:f:18:TRP:H	1.76	0.49
21:Z:57:ILE:HG12	33:Z:101:CLA:HBB1	1.95	0.49
29:8:123:GLY:HA3	33:8:310:CLA:CAB	2.43	0.49
3:C:316:LEU:HG	3:C:326:VAL:HG11	1.94	0.49
8:h:25:TRP:O	2:b:222:PRO:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:285:ASP:HB2	15:O:289:LYS:HE3	1.93	0.49
24:5:82:ILE:HG21	33:5:311:CLA:HAC2	1.93	0.49
28:q:145:ASP:O	28:q:149:ARG:HB2	2.13	0.49
33:8:310:CLA:HBD	33:8:310:CLA:HBA1	1.94	0.49
29:1:161:LEU:HD12	45:1:301:A86:C21	2.42	0.49
36:A:412:LHG:H272	37:D:403:SQD:H272	1.95	0.49
38:C:517:DGD:HB22	39:C:519:LMG:H291	1.95	0.49
4:d:263:LYS:HE3	1:a:245:THR:HG22	1.95	0.49
15:O:98:LEU:HD21	15:O:304:ILE:HG13	1.94	0.49
15:o:160:ASP:OD1	15:o:160:ASP:N	2.46	0.49
5:e:19:ARG:HA	5:e:22:ILE:HG12	1.93	0.49
29:9:159:ALA:C	29:9:161:LEU:N	2.69	0.49
1:A:331:MET:CE	4:D:346:PRO:HB2	2.38	0.49
4:D:337:ASN:OD1	7:G:65:ARG:NH1	2.46	0.49
4:d:230:THR:O	1:a:269:ARG:NH1	2.46	0.49
12:l:13:LEU:HD22	13:m:95:LEU:HD23	1.95	0.49
17:U:72:ASP:OD2	17:U:75:ASN:ND2	2.42	0.49
29:1:79:TYR:CD2	29:1:166:LEU:HD13	2.36	0.49
29:1:180:ASP:OD1	29:1:180:ASP:N	2.44	0.49
1:A:301:ASN:HB3	3:C:405:VAL:HG21	1.95	0.49
3:c:223:VAL:HG22	3:c:287:TYR:HD1	1.78	0.49
4:d:102:ARG:HG3	5:e:74:LYS:HD2	1.95	0.48
8:H:30:ILE:CD1	33:H:103:CLA:C2D	2.91	0.48
39:M:201:LMG:H292	39:M:201:LMG:H121	1.95	0.48
15:o:177:LEU:O	15:o:280:GLN:NE2	2.30	0.48
19:W:200:HIS:CD2	33:W:303:CLA:C4D	2.95	0.48
29:8:187:THR:O	46:8:304:DD6:O4	2.31	0.48
3:c:146:GLY:O	3:c:154:LYS:NZ	2.38	0.48
4:d:261:SER:OG	36:d:405:LHG:O4	2.29	0.48
15:o:101:MET:HB3	15:o:140:ILE:HB	1.95	0.48
20:X:5:LEU:O	20:X:9:ILE:HG12	2.12	0.48
25:6:73:CYS:SG	25:6:178:MET:HA	2.52	0.48
29:2:163:ILE:HD11	29:2:167:LEU:HD12	1.94	0.48
2:B:458:PHE:HB3	33:B:604:CLA:HBC2	1.93	0.48
4:d:140:TYR:OH	36:a:403:LHG:O4	2.26	0.48
19:w:204:LEU:HD11	33:w:303:CLA:HBC3	1.94	0.48
22:3:117:ASN:HD21	22:3:124:ASP:H	1.60	0.48
38:a:401:DGD:HB32	38:a:401:DGD:HA61	1.94	0.48
29:1:123:GLY:O	29:1:127:VAL:HG12	2.14	0.48
3:c:213:ARG:HG2	3:c:219:ASP:HB3	1.96	0.48
13:M:94:ASN:HD22	13:m:94:ASN:CG	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:4:167:GLU:HA	23:4:170:ARG:HG2	1.94	0.48
45:5:301:A86:C24	33:5:316:CLA:CHD	2.91	0.48
47:5:310:KC2:C2D	33:5:313:CLA:CAD	2.91	0.48
25:6:88:HIS:HE1	25:6:103:ILE:HB	1.78	0.48
26:7:168:LEU:HD22	33:7:310:CLA:HBC2	1.94	0.48
28:q:64:SER:HA	28:q:70:GLY:HA3	1.94	0.48
29:2:158:LEU:HD12	46:2:304:DD6:C25	2.42	0.48
18:v:57:ARG:NH1	28:q:95:VAL:O	2.46	0.48
20:X:33:ASP:O	20:X:34:ARG:C	2.57	0.48
23:4:187:LEU:O	23:4:195:TYR:OH	2.21	0.48
45:5:302:A86:C37	43:5:320:LMU:C1	2.83	0.48
45:5:302:A86:C37	43:5:320:LMU:O5'	2.62	0.48
27:Y:20:GLY:O	27:Y:23:ILE:HG22	2.13	0.48
36:A:412:LHG:O1	36:A:412:LHG:O3	2.30	0.48
3:C:221:TRP:HE3	38:C:516:DGD:HB21	1.79	0.48
3:c:405:VAL:HG21	1:a:301:ASN:HB3	1.95	0.48
17:U:117:GLU:HA	17:U:120:VAL:HG12	1.96	0.48
24:5:89:LEU:HD23	43:5:320:LMU:H61	1.96	0.48
26:0:132:THR:HG21	26:0:137:ARG:HA	1.94	0.48
2:B:142:HIS:HE1	33:B:615:CLA:C4D	2.27	0.48
4:d:235:THR:OG1	4:d:236:PRO:HD2	2.14	0.48
10:J:33:SER:OG	28:Q:77:GLU:O	2.20	0.48
29:9:162:ALA:CB	46:9:304:DD6:C37	2.81	0.48
29:2:138:LYS:HA	46:2:304:DD6:O2	2.13	0.48
1:A:25:GLU:OE1	3:C:468:ARG:HB2	2.13	0.48
3:C:401:SER:OG	3:C:403:ASN:OD1	2.31	0.48
14:n:27:UNK:O	14:n:29:UNK:N	2.47	0.48
15:o:132:ARG:O	15:o:134:THR:N	2.45	0.48
2:b:124:ARG:NH1	2:b:129:GLY:O	2.43	0.48
46:2:303:DD6:C8	33:2:306:CLA:HBB2	2.44	0.48
29:1:131:PHE:HA	29:1:134:PHE:HE1	1.76	0.48
4:D:171:SER:HB2	4:D:176:ALA:HB1	1.96	0.48
26:0:129:LEU:HB2	33:0:308:CLA:HMA1	1.96	0.48
29:2:86:ARG:HB2	33:2:308:CLA:OBD	2.14	0.48
3:c:447:ARG:HD2	1:a:131:TRP:HZ2	1.79	0.48
4:D:190:TRP:CE3	4:D:288:LEU:HD11	2.47	0.48
4:d:213:HIS:NE2	35:a:402:BCT:O3	2.46	0.48
7:g:65:ARG:O	7:g:69:ILE:HG22	2.14	0.48
9:I:3:THR:O	9:I:7:LEU:HG	2.14	0.48
33:4:315:CLA:HBA1	33:4:315:CLA:H3A	1.71	0.48
29:9:81:VAL:HG21	33:9:308:CLA:HAC2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:2:123:GLY:HA3	33:2:310:CLA:CAB	2.43	0.48
38:c:517:DGD:HA22	38:c:517:DGD:HA52	1.59	0.47
9:i:30:ARG:HA	9:i:34:ARG:NH2	2.28	0.47
17:u:112:GLY:O	17:u:113:LEU:C	2.57	0.47
18:v:57:ARG:NH1	28:q:95:VAL:HA	2.29	0.47
22:3:75:TYR:HE1	22:3:80:PHE:HB2	1.79	0.47
33:3:319:CLA:HED1	23:4:194:LEU:HA	1.95	0.47
27:y:20:GLY:O	27:y:23:ILE:HG22	2.14	0.47
29:9:77:ILE:O	29:9:81:VAL:HG23	2.14	0.47
1:A:290:ILE:HG13	33:A:404:CLA:HED2	1.96	0.47
19:w:183:GLU:CA	43:w:302:LMU:H12	2.44	0.47
20:x:1:MET:HA	20:x:5:LEU:HD12	1.96	0.47
1:a:149:ALA:HB3	1:a:150:PRO:HD3	1.96	0.47
2:b:226:TYR:HA	2:b:231:MET:HG3	1.95	0.47
29:8:118:ILE:O	29:8:122:ILE:HG12	2.15	0.47
29:1:150:LEU:HD23	33:1:305:CLA:HED3	1.96	0.47
34:A:406:PHO:H141	34:A:406:PHO:H161	1.70	0.47
28:q:62:ARG:HH22	28:q:74:SER:HB3	1.79	0.47
29:2:77:ILE:O	29:2:81:VAL:HG22	2.14	0.47
3:C:223:VAL:HG22	3:C:287:TYR:CD1	2.49	0.47
4:d:213:HIS:CD2	4:d:217:VAL:HG23	2.50	0.47
7:G:121:PHE:HB3	7:G:125:ARG:NH2	2.26	0.47
19:w:184:TRP:H	43:w:302:LMU:H12	1.78	0.47
24:5:39:GLN:O	24:5:40:ALA:HB3	2.15	0.47
25:6:40:PRO:C	25:6:42:LEU:H	2.23	0.47
29:2:128:ARG:HB3	29:2:130:TRP:CD1	2.49	0.47
2:B:413:ASP:OD1	2:B:416:THR:OG1	2.30	0.47
5:E:19:ARG:HA	5:E:22:ILE:HG12	1.95	0.47
26:7:150:LYS:NZ	29:8:51:ASP:OD2	2.45	0.47
1:a:192:ILE:HG12	1:a:193:LEU:H	1.79	0.47
25:6:48:LEU:HD23	25:6:50:MET:HE3	1.95	0.47
2:b:100:HIS:HE1	33:b:606:CLA:NA	2.13	0.47
29:9:165:GLU:OE1	29:9:168:ARG:NH1	2.48	0.47
29:2:186:ILE:H	29:2:186:ILE:HG12	1.34	0.47
45:2:302:A86:C40	33:2:309:CLA:HBA2	2.44	0.47
4:d:241:GLU:HG3	4:d:243:TYR:H	1.79	0.47
10:j:33:SER:HB2	28:q:77:GLU:O	2.15	0.47
18:v:57:ARG:HH11	28:q:95:VAL:CG1	2.27	0.47
23:4:39:LEU:HD23	23:4:39:LEU:H	1.79	0.47
24:5:68:LYS:HZ1	45:5:302:A86:C17	2.28	0.47
24:5:187:MET:HE3	33:5:316:CLA:C1D	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:6:307:CLA:HED3	33:6:307:CLA:H2A	1.97	0.47
33:b:610:CLA:H161	33:b:610:CLA:H141	1.70	0.47
33:0:305:CLA:H2A	33:0:305:CLA:O1D	2.14	0.47
29:8:73:GLN:HE21	29:8:156:GLY:N	2.13	0.47
29:1:68:HIS:HB3	29:1:160:MET:HE2	1.96	0.47
3:C:348:ILE:HG21	3:C:357:TRP:HB2	1.97	0.47
3:c:62:ALA:O	3:c:66:ILE:HG12	2.15	0.47
11:k:36:VAL:HG22	30:k:101:BCR:H382	1.96	0.47
24:5:71:ARG:HH12	24:5:171:GLU:CD	2.23	0.47
33:b:604:CLA:H61	33:b:604:CLA:H41	1.72	0.47
29:9:133:ASN:O	29:9:134:PHE:CD1	2.67	0.47
2:B:149:LEU:HD11	33:B:604:CLA:H121	1.97	0.47
33:C:503:CLA:H3A	33:C:503:CLA:HBA2	1.47	0.47
18:v:50:GLU:OE2	28:q:85:GLN:OE1	2.32	0.47
47:5:310:KC2:CMC	33:5:313:CLA:H143	2.45	0.47
9:i:3:THR:O	9:i:7:LEU:HG	2.14	0.47
23:4:93:ILE:O	23:4:94:PRO:C	2.57	0.47
24:5:74:GLN:HG3	33:5:314:CLA:HMC2	1.97	0.47
33:9:308:CLA:CHA	33:9:308:CLA:HBA1	2.45	0.47
29:2:61:TYR:O	29:2:65:GLU:HG3	2.14	0.47
29:8:91:ILE:HG12	45:8:302:A86:C29	2.45	0.47
29:1:161:LEU:CD1	45:1:301:A86:C21	2.93	0.46
22:3:192:GLU:O	22:3:195:GLU:HG3	2.15	0.46
27:y:12:SER:O	27:y:16:ILE:HG12	2.15	0.46
28:q:147:LEU:O	28:q:151:MET:HE3	2.16	0.46
26:0:70:GLY:O	26:0:74:GLN:HG3	2.15	0.46
29:2:153:LEU:O	29:2:157:ARG:HD3	2.15	0.46
45:8:302:A86:C8	33:8:308:CLA:H72	2.45	0.46
3:c:173:LEU:HD22	33:c:501:CLA:C1D	2.45	0.46
7:G:106:ASP:HB3	7:G:109:LYS:HB2	1.97	0.46
30:K:102:BCR:H24C	30:K:102:BCR:H371	1.80	0.46
19:w:200:HIS:CD2	33:w:303:CLA:C4D	2.98	0.46
22:3:150:MET:HE1	33:3:307:CLA:HAC1	1.97	0.46
22:3:208:MET:HE2	46:3:315:DD6:C5	2.44	0.46
29:8:68:HIS:HE1	33:8:307:CLA:ND	2.09	0.46
3:C:37:ASN:HD21	33:C:511:CLA:C1C	2.29	0.46
3:C:442:HIS:HE1	33:C:508:CLA:NA	2.09	0.46
33:3:307:CLA:H72	33:3:313:CLA:HBA2	1.96	0.46
25:6:93:ILE:HG22	25:6:99:LYS:HA	1.97	0.46
1:a:196:PRO:HA	1:a:199:MET:SD	2.55	0.46
33:0:307:CLA:H162	33:0:307:CLA:H141	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:HIS:HE1	33:A:408:CLA:C4D	2.29	0.46
1:A:141:PRO:HG3	3:C:448:ALA:HB2	1.97	0.46
30:C:514:BCR:H15C	30:C:514:BCR:H351	1.84	0.46
3:c:189:PRO:C	28:q:151:MET:HE1	2.41	0.46
6:f:43:ARG:O	28:q:62:ARG:NH2	2.48	0.46
36:3:318:LHG:H151	36:3:318:LHG:H182	1.73	0.46
24:5:68:LYS:NZ	45:5:302:A86:C17	2.79	0.46
45:5:304:A86:C29	33:5:314:CLA:C4A	2.94	0.46
39:b:623:LMG:HC92	39:b:623:LMG:H291	1.65	0.46
29:2:158:LEU:CD1	46:2:304:DD6:C25	2.94	0.46
29:8:163:ILE:HG12	46:8:303:DD6:C24	2.45	0.46
5:E:24:HIS:HE1	42:F:101:HEM:CHD	2.28	0.46
21:Z:22:VAL:HG21	27:Y:26:LEU:HD22	1.98	0.46
24:5:99:PHE:CE2	43:5:320:LMU:H62	2.39	0.46
29:9:134:PHE:HE2	33:9:314:CLA:C2D	2.29	0.46
2:B:392:ILE:HD12	2:B:418:LYS:HG2	1.98	0.46
4:d:116:HIS:HE1	33:d:402:CLA:C4D	2.29	0.46
4:d:155:VAL:HG13	4:d:156:PHE:N	2.31	0.46
5:E:11:PHE:O	5:E:15:ILE:HG12	2.16	0.46
15:o:84:VAL:HG12	15:o:85:ILE:H	1.80	0.46
33:2:311:CLA:H92	33:2:311:CLA:H62	1.72	0.46
29:1:173:ASN:ND2	29:1:180:ASP:OD1	2.48	0.46
33:B:602:CLA:HBB1	33:B:602:CLA:HMB3	1.96	0.46
3:C:155:MET:HE2	3:C:269:TYR:CE2	2.51	0.46
33:C:503:CLA:H62	33:C:503:CLA:H102	1.47	0.46
3:c:207:ILE:HD12	3:c:207:ILE:H	1.81	0.46
4:D:155:VAL:HG13	4:D:156:PHE:N	2.31	0.46
15:O:99:VAL:O	15:O:100:ASP:HB2	2.16	0.46
19:W:204:LEU:HD11	33:W:303:CLA:HBC3	1.97	0.46
25:6:172:ASN:C	25:6:174:GLY:H	2.22	0.46
33:7:307:CLA:H141	33:7:307:CLA:H162	1.73	0.46
33:2:311:CLA:HED2	33:2:311:CLA:HBD	1.86	0.46
46:8:304:DD6:C9	33:8:311:CLA:CBB	2.94	0.46
2:B:112:ILE:HG21	30:B:619:BCR:H393	1.98	0.46
2:B:470:GLY:O	2:B:473:THR:OG1	2.28	0.46
39:c:519:LMG:HC92	39:c:519:LMG:H292	1.59	0.46
37:T:101:SQD:H322	37:T:101:SQD:H351	1.82	0.46
24:5:69:HIS:HB3	24:5:179:MET:SD	2.56	0.46
3:C:395:THR:HG21	18:V:66:CYS:SG	2.56	0.46
38:C:517:DGD:HA22	38:C:517:DGD:HA52	1.58	0.46
3:c:374:ASP:HB3	3:c:377:LYS:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:c:504:CLA:H141	33:c:508:CLA:H143	1.98	0.46
38:h:102:DGD:HB71	2:b:254:GLY:HA3	1.97	0.46
17:U:115:ASN:O	17:U:119:GLU:OE1	2.34	0.46
33:W:303:CLA:H111	33:W:303:CLA:H152	1.59	0.46
23:4:96:GLU:O	23:4:97:LEU:C	2.59	0.46
24:5:164:GLN:O	24:5:168:ARG:HD3	2.16	0.46
25:6:35:GLU:HB3	25:6:63:ARG:NH2	2.31	0.46
25:6:172:ASN:C	25:6:174:GLY:N	2.74	0.46
39:b:623:LMG:H292	39:b:623:LMG:H321	1.65	0.46
4:D:179:ARG:HH21	4:D:332:ASP:CG	2.23	0.45
7:G:120:ILE:O	7:G:124:ILE:HG13	2.16	0.45
18:V:63:CYS:SG	42:V:201:HEM:CAB	3.04	0.45
33:7:307:CLA:H41	33:7:307:CLA:H62	1.56	0.45
29:8:123:GLY:HA3	33:8:310:CLA:HAB	1.98	0.45
29:8:180:ASP:OD1	29:8:180:ASP:N	2.47	0.45
33:B:613:CLA:HBB1	33:B:613:CLA:HMB3	1.96	0.45
38:C:516:DGD:HB81	38:C:516:DGD:HBE2	1.73	0.45
3:c:344:SER:OG	3:c:346:GLU:OE1	2.34	0.45
37:T:103:SQD:H321	37:T:103:SQD:H351	1.80	0.45
18:V:148:GLN:O	18:V:152:VAL:HG22	2.15	0.45
24:5:84:ARG:HD2	24:5:104:ASN:ND2	2.31	0.45
3:c:163:LEU:HD13	33:c:507:CLA:HED1	1.98	0.45
30:h:101:BCR:H20C	30:h:101:BCR:H361	1.83	0.45
15:O:303:LYS:HG2	15:O:305:GLN:H	1.82	0.45
17:u:114:THR:HG23	17:u:117:GLU:OE2	2.17	0.45
18:v:59:PHE:O	18:v:61:ALA:N	2.49	0.45
43:w:302:LMU:H22	43:w:302:LMU:H1'	1.66	0.45
43:w:302:LMU:H32	43:w:302:LMU:H62	1.73	0.45
22:3:92:LEU:O	22:3:96:ARG:HD3	2.16	0.45
24:5:169:ALA:O	24:5:173:ASN:ND2	2.50	0.45
25:6:94:SER:HG	25:6:98:THR:HG1	1.59	0.45
2:b:371:VAL:HG12	2:b:377:ILE:HD13	1.98	0.45
22:3:168:ARG:C	22:3:170:SER:H	2.24	0.45
33:3:304:CLA:H141	33:3:304:CLA:H161	1.73	0.45
33:3:304:CLA:H41	33:4:308:CLA:H193	1.97	0.45
24:5:93:ILE:HB	24:5:99:PHE:HE1	1.82	0.45
2:b:21:SER:OG	2:b:115:TRP:HB2	2.17	0.45
29:8:136:ILE:O	29:8:139:PRO:HD3	2.17	0.45
30:B:617:BCR:H24C	30:B:617:BCR:H371	1.80	0.45
38:c:517:DGD:HA71	39:q:301:LMG:H361	1.99	0.45
33:d:402:CLA:H62	33:d:402:CLA:H41	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:58:THR:O	5:e:62:GLN:NE2	2.50	0.45
13:M:87:LEU:HB2	13:M:88:PRO:HD3	1.98	0.45
17:U:60:GLU:HG2	17:U:61:ASN:N	2.31	0.45
21:z:8:LEU:HD23	21:z:47:LEU:HD21	1.99	0.45
47:5:310:KC2:CMD	33:5:313:CLA:CHA	2.94	0.45
25:6:181:ILE:HD12	25:6:181:ILE:HA	1.84	0.45
25:6:187:HIS:CD2	25:6:194:LEU:HD21	2.52	0.45
2:b:283:GLU:OE2	2:b:287:GLN:NE2	2.42	0.45
29:2:164:LEU:HD13	29:2:164:LEU:H	1.81	0.45
4:d:160:PRO:HG3	4:d:169:ALA:HB2	1.98	0.45
22:3:110:LEU:HD23	22:3:110:LEU:H	1.82	0.45
38:3:320:DGD:HB61	38:3:320:DGD:HB31	1.78	0.45
24:5:59:PHE:O	24:5:63:ARG:HG2	2.17	0.45
24:5:93:ILE:HB	24:5:99:PHE:CE1	2.52	0.45
25:6:42:LEU:HD12	25:6:42:LEU:HA	1.81	0.45
29:9:69:GLY:HA2	29:9:160:MET:HG3	1.98	0.45
3:C:464:VAL:HG21	4:D:247:THR:HG23	1.99	0.45
3:c:416:ASN:ND2	38:c:518:DGD:O6E	2.47	0.45
33:c:503:CLA:H3A	33:c:503:CLA:HBA2	1.44	0.45
24:5:167:LYS:HD3	24:5:168:ARG:HD2	1.99	0.45
25:6:133:MET:SD	45:6:302:A86:O2	2.75	0.45
37:a:413:SQD:H342	37:a:413:SQD:H371	1.73	0.45
39:q:301:LMG:O5	39:q:302:LMG:O5	2.33	0.45
46:2:303:DD6:C22	33:2:306:CLA:C4B	2.94	0.45
39:c:519:LMG:H311	39:c:519:LMG:H341	1.59	0.45
4:D:160:PRO:HG3	4:D:169:ALA:HB2	1.99	0.45
4:d:13:LEU:HD12	36:7:316:LHG:HC92	1.98	0.45
6:F:15:THR:HG23	6:F:18:TRP:H	1.81	0.45
6:F:22:HIS:C	6:F:24:LEU:H	2.25	0.45
30:K:102:BCR:H20C	30:K:102:BCR:H361	1.83	0.45
30:k:102:BCR:H24C	30:k:102:BCR:H371	1.77	0.45
18:V:39:ASP:C	18:V:39:ASP:OD1	2.60	0.45
22:3:75:TYR:HA	22:3:80:PHE:CE2	2.51	0.45
26:7:126:THR:O	26:7:130:LEU:HD23	2.16	0.45
33:b:603:CLA:HBB1	33:b:603:CLA:HMB1	1.99	0.45
29:2:166:LEU:HD12	29:2:166:LEU:HA	1.79	0.45
46:2:304:DD6:C10	33:2:311:CLA:H71	2.47	0.45
1:A:192:ILE:HG12	1:A:193:LEU:H	1.81	0.45
33:B:603:CLA:HAB	33:B:605:CLA:H152	1.99	0.45
3:C:51:HIS:CD2	33:C:509:CLA:C1B	3.00	0.45
13:M:95:LEU:O	13:M:98:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:v:101:TYR:CZ	42:v:201:HEM:HAA2	2.52	0.45
39:w:304:LMG:H161	39:w:304:LMG:H192	1.67	0.45
23:4:80:TYR:CE2	23:4:168:LEU:HD22	2.51	0.45
24:5:78:VAL:HG12	33:5:311:CLA:HAC1	1.99	0.45
45:5:301:A86:C26	33:5:316:CLA:C2D	2.95	0.45
2:b:114:HIS:HE1	33:b:617:CLA:C1D	2.29	0.45
29:1:68:HIS:HE1	33:1:307:CLA:C4D	2.30	0.45
2:B:308:LYS:HB2	15:o:118:GLY:HA2	1.99	0.45
3:c:305:PRO:HB3	3:c:356:PHE:CD1	2.51	0.45
43:5:320:LMU:H1B	43:5:320:LMU:H5'	1.34	0.45
25:6:175:ARG:HB3	33:6:308:CLA:C3C	2.47	0.45
26:7:168:LEU:CD2	33:7:310:CLA:CB	2.95	0.45
1:A:187:GLN:NE2	1:A:192:ILE:O	2.42	0.44
37:B:622:SQD:H321	37:B:622:SQD:H351	1.78	0.44
33:c:508:CLA:H162	33:c:508:CLA:H122	1.58	0.44
17:U:115:ASN:O	17:U:118:LYS:N	2.49	0.44
33:3:309:CLA:H12	33:3:309:CLA:H52	1.80	0.44
23:4:90:TYR:HE1	23:4:92:LEU:HG	1.81	0.44
33:b:607:CLA:OBD	39:b:622:LMG:O5	2.35	0.44
29:9:151:GLN:O	29:9:155:HIS:ND1	2.50	0.44
6:f:40:PHE:CG	28:q:65:VAL:HG12	2.51	0.44
15:O:240:ASP:OD1	15:O:240:ASP:N	2.45	0.44
26:7:35:LEU:HB2	26:7:63:ARG:HH21	1.82	0.44
29:9:87:TRP:CH2	33:9:308:CLA:H43	2.51	0.44
29:8:116:ALA:O	29:8:120:PHE:CD2	2.70	0.44
46:1:304:DD6:C2	33:1:312:CLA:HAB	2.47	0.44
3:C:330:GLN:HG2	3:C:334:GLY:HA2	1.99	0.44
7:g:77:LEU:O	7:g:81:VAL:HG22	2.17	0.44
10:J:29:TYR:O	10:J:32:TYR:N	2.47	0.44
45:5:302:A86:C37	43:5:320:LMU:C6'	2.95	0.44
45:7:301:A86:O1	33:7:305:CLA:HBC1	2.17	0.44
39:0:314:LMG:H131	39:0:314:LMG:H161	1.77	0.44
7:g:148:ILE:HG13	7:g:170:LEU:HD21	1.99	0.44
17:u:68:SER:OG	17:u:69:GLN:N	2.50	0.44
22:3:150:MET:HE1	33:3:307:CLA:CAC	2.41	0.44
22:3:234:ALA:CB	43:3:301:LMU:H3B	2.48	0.44
33:3:313:CLA:H61	33:3:313:CLA:H41	1.68	0.44
26:7:98:ALA:HB1	26:7:99:PRO:HD2	1.99	0.44
29:1:67:LYS:HD2	33:1:310:CLA:C3D	2.47	0.44
29:1:91:ILE:HG12	29:1:96:ALA:HB2	1.99	0.44
29:1:95:VAL:HG13	29:1:97:CYS:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LEU:HD11	30:A:401:BCR:HC21	2.00	0.44
1:A:248:ILE:HG23	1:A:249:VAL:N	2.33	0.44
2:B:141:ILE:HG21	33:B:615:CLA:HBB1	1.99	0.44
30:C:514:BCR:H20C	30:C:514:BCR:H361	1.82	0.44
7:G:75:ALA:HB2	7:G:145:ILE:HG22	1.99	0.44
15:o:223:GLY:HA2	2:b:383:PHE:CZ	2.52	0.44
17:u:108:TYR:HD1	17:u:118:LYS:HG2	1.82	0.44
33:w:303:CLA:H202	33:w:303:CLA:H162	1.76	0.44
22:3:138:ILE:HD12	22:3:139:PRO:HD2	2.00	0.44
43:3:301:LMU:H42	43:3:301:LMU:H11	1.57	0.44
24:5:143:GLN:HB3	24:5:144:PHE:H	1.63	0.44
2:B:383:PHE:CZ	15:O:223:GLY:HA2	2.53	0.44
3:C:163:LEU:HD13	33:C:507:CLA:HED1	2.00	0.44
39:D:404:LMG:HC92	39:D:404:LMG:H291	1.68	0.44
13:m:87:LEU:HB2	13:m:88:PRO:HD3	1.99	0.44
16:T:4:LEU:HG	43:T:102:LMU:H31	1.99	0.44
22:3:52:VAL:HG11	22:3:197:GLN:HB3	2.00	0.44
22:3:79:ASN:CA	22:3:166:LYS:HG3	2.47	0.44
33:4:312:CLA:H11	33:4:312:CLA:H51	1.83	0.44
26:7:163:LEU:O	26:7:167:ARG:HG3	2.17	0.44
3:C:305:PRO:HB3	3:C:356:PHE:CG	2.52	0.44
4:D:54:VAL:HG21	4:D:109:LEU:CD1	2.48	0.44
4:D:334:PRO:HB2	5:E:66:LEU:HD11	2.00	0.44
4:d:198:MET:HB2	4:d:280:THR:HG21	1.98	0.44
30:k:101:BCR:H20C	30:k:101:BCR:H361	1.87	0.44
15:o:59:ILE:HB	15:o:83:GLU:OE1	2.18	0.44
21:z:36:GLN:O	21:z:40:ILE:HG12	2.18	0.44
22:3:75:TYR:CE1	22:3:80:PHE:HB2	2.53	0.44
36:4:318:LHG:H122	36:4:318:LHG:H151	1.59	0.44
30:a:412:BCR:H20C	30:a:412:BCR:H361	1.80	0.44
29:9:167:LEU:HG	33:9:315:CLA:HBC1	2.00	0.44
1:A:319:ASP:O	1:A:323:ARG:HG2	2.17	0.44
2:B:222:PRO:HG2	2:B:225:LEU:HB2	1.99	0.44
3:C:203:ASN:ND2	3:C:205:ILE:HB	2.32	0.44
33:C:512:CLA:H92	33:C:512:CLA:H61	1.82	0.44
17:U:116:ALA:HA	17:U:119:GLU:CD	2.43	0.44
33:3:307:CLA:H62	33:3:307:CLA:H41	1.54	0.44
2:b:202:HIS:HE1	33:b:604:CLA:NA	2.12	0.44
39:b:621:LMG:O4	39:b:621:LMG:O5	2.30	0.44
46:9:304:DD6:C8	33:9:311:CLA:HHC	2.47	0.44
33:9:311:CLA:HED2	33:9:311:CLA:HBD	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:2:77:ILE:HA	29:2:80:ILE:HG12	2.00	0.44
46:2:304:DD6:C22	33:2:311:CLA:C4D	2.96	0.44
46:1:303:DD6:C1	33:1:307:CLA:HMC1	2.48	0.44
33:B:615:CLA:H152	33:B:615:CLA:H112	1.68	0.44
3:C:305:PRO:HB3	3:C:356:PHE:CD1	2.53	0.44
33:c:501:CLA:HBB1	30:c:515:BCR:H21C	2.00	0.44
5:e:20:TYR:HE1	42:e:101:HEM:C4D	2.36	0.44
7:g:107:LYS:HA	7:g:110:LYS:HE2	1.99	0.44
7:g:116:GLN:OE1	7:g:139:TYR:HD1	2.01	0.44
15:o:101:MET:HE2	15:o:101:MET:HB2	1.79	0.44
18:v:89:THR:HG1	18:v:109:ASP:CA	2.23	0.44
21:Z:36:GLN:O	21:Z:40:ILE:HG12	2.18	0.44
33:3:313:CLA:H152	33:3:313:CLA:H112	1.62	0.44
29:2:56:GLU:HG2	29:2:57:LYS:N	2.33	0.44
33:1:306:CLA:H3A	33:1:306:CLA:O1A	2.18	0.44
3:c:66:ILE:HD13	3:c:86:CYS:HB3	1.99	0.43
5:E:24:HIS:CE1	42:F:101:HEM:C1D	3.06	0.43
5:e:19:ARG:HB3	5:e:19:ARG:CZ	2.47	0.43
12:l:5:ASN:HD22	2:b:18:ARG:NH1	2.15	0.43
39:W:301:LMG:H192	39:W:301:LMG:H161	1.54	0.43
22:3:81:MET:H	22:3:81:MET:HG2	1.61	0.43
23:4:87:ARG:HD3	33:4:308:CLA:OBD	2.18	0.43
33:4:308:CLA:H12	43:4:317:LMU:H121	1.99	0.43
45:5:302:A86:C12	33:5:311:CLA:HAB	2.48	0.43
29:9:157:ARG:HA	29:9:160:MET:HE3	2.00	0.43
29:2:162:ALA:HA	46:2:304:DD6:C37	2.48	0.43
46:2:303:DD6:C8	33:2:306:CLA:HAB	2.47	0.43
1:A:39:PRO:O	1:A:43:THR:HG22	2.19	0.43
1:A:299:GLY:O	3:C:401:SER:HB2	2.18	0.43
1:A:308:ASP:C	1:A:308:ASP:OD1	2.60	0.43
33:B:605:CLA:H91	33:B:605:CLA:H111	1.77	0.43
7:g:79:SER:HA	7:g:82:ASN:OD1	2.18	0.43
8:H:5:THR:O	8:H:9:GLU:HG2	2.18	0.43
36:h:103:LHG:H121	36:h:103:LHG:HC91	1.72	0.43
24:5:40:ALA:HA	33:5:308:CLA:CHB	2.48	0.43
28:q:93:TYR:HB3	39:q:301:LMG:HC61	2.00	0.43
29:2:148:ARG:NE	33:2:312:CLA:O2A	2.51	0.43
2:B:201:HIS:HE1	33:B:602:CLA:C1D	2.22	0.43
3:C:309:GLN:HG3	3:C:359:LEU:HD22	1.99	0.43
33:C:513:CLA:H2A	33:C:513:CLA:O1D	2.18	0.43
3:c:283:THR:HG22	3:c:287:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:110:LYS:O	7:g:114:VAL:HG23	2.18	0.43
30:K:101:BCR:H15C	30:K:101:BCR:H351	1.84	0.43
18:V:39:ASP:OD2	18:V:43:ASN:ND2	2.47	0.43
18:V:102:LEU:HA	18:V:102:LEU:HD23	1.65	0.43
33:3:308:CLA:H41	33:3:308:CLA:H61	1.44	0.43
45:5:301:A86:C2	33:5:316:CLA:CHD	2.95	0.43
43:5:320:LMU:H1'	43:5:320:LMU:H6E	1.78	0.43
25:6:174:GLY:O	25:6:175:ARG:C	2.62	0.43
26:7:194:SER:O	26:7:195:GLY:C	2.61	0.43
2:b:112:ILE:HG21	30:b:620:BCR:H393	1.99	0.43
26:0:44:PHE:HD1	33:0:305:CLA:HED3	1.83	0.43
29:8:157:ARG:HA	29:8:160:MET:HE3	1.98	0.43
30:h:101:BCR:H351	30:h:101:BCR:H15C	1.90	0.43
30:K:101:BCR:H24C	30:K:101:BCR:H371	1.85	0.43
15:o:99:VAL:O	15:o:100:ASP:HB2	2.19	0.43
17:u:116:ALA:O	17:u:117:GLU:C	2.62	0.43
18:v:57:ARG:HH12	28:q:95:VAL:C	2.26	0.43
36:W:302:LHG:H262	36:W:302:LHG:H291	1.84	0.43
25:6:187:HIS:CG	25:6:194:LEU:HD21	2.53	0.43
26:0:41:PRO:HG3	33:0:304:CLA:C1B	2.48	0.43
1:A:269:ARG:HH11	4:D:234:PHE:HB2	1.82	0.43
30:B:619:BCR:H11C	30:B:619:BCR:H341	1.90	0.43
3:C:286:LEU:HD23	3:C:286:LEU:HA	1.74	0.43
4:D:54:VAL:HG21	4:D:109:LEU:HD11	1.99	0.43
5:e:65:PRO:HB2	5:e:80:LEU:HD13	2.01	0.43
15:o:59:ILE:HD12	15:o:83:GLU:CD	2.44	0.43
37:t:102:SQD:H322	37:t:102:SQD:H351	1.62	0.43
22:3:155:TYR:HE2	33:3:312:CLA:HED1	1.83	0.43
38:3:320:DGD:HB82	43:4:317:LMU:H2'	2.01	0.43
24:5:164:GLN:HB3	24:5:168:ARG:NH1	2.34	0.43
33:5:312:CLA:H3A	33:5:312:CLA:HBA2	1.25	0.43
26:7:107:ILE:HD12	26:7:107:ILE:H	1.83	0.43
33:7:304:CLA:HBD	33:7:310:CLA:OBD	2.19	0.43
26:0:85:LYS:NZ	26:0:89:ASP:OD1	2.35	0.43
46:2:303:DD6:C10	33:2:306:CLA:CAB	2.97	0.43
29:8:163:ILE:HG13	29:8:167:LEU:HD12	2.00	0.43
29:1:122:ILE:HG22	29:1:123:GLY:N	2.33	0.43
30:B:618:BCR:H24C	30:B:618:BCR:H371	1.85	0.43
37:B:622:SQD:H1	13:m:75:PHE:HE1	1.83	0.43
33:d:402:CLA:H92	33:d:402:CLA:H61	1.68	0.43
6:F:21:VAL:HG13	6:F:22:HIS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:172:ASN:HD22	33:6:307:CLA:C3D	2.32	0.43
26:7:173:PHE:O	26:7:177:ILE:HG12	2.18	0.43
1:a:283:ILE:HG13	34:a:409:PHO:HBC3	2.00	0.43
30:b:619:BCR:H20C	30:b:619:BCR:H361	1.85	0.43
29:9:120:PHE:CD2	33:8:310:CLA:H122	2.52	0.43
29:8:123:GLY:HA3	33:8:310:CLA:C3B	2.48	0.43
29:1:152:GLU:CD	33:1:311:CLA:NB	2.77	0.43
29:1:164:LEU:O	29:1:165:GLU:C	2.61	0.43
2:B:160:GLY:O	2:B:161:LEU:C	2.62	0.43
3:c:445:ARG:HB2	1:a:142:TRP:HZ2	1.84	0.43
4:d:151:VAL:O	4:d:155:VAL:HG12	2.18	0.43
6:f:13:ILE:HG23	6:f:14:PHE:CD2	2.54	0.43
15:O:98:LEU:CD2	15:O:304:ILE:HG13	2.49	0.43
22:3:191:GLU:OE2	22:3:192:GLU:HG2	2.18	0.43
25:6:66:GLU:CD	25:6:175:ARG:HH21	2.27	0.43
2:b:24:LEU:HD21	33:b:617:CLA:HAB	2.01	0.43
29:8:166:LEU:HA	29:8:166:LEU:HD22	1.72	0.43
37:B:622:SQD:H342	37:B:622:SQD:H371	1.76	0.43
7:G:85:ASP:HB3	7:G:88:ALA:HB3	2.01	0.43
11:K:29:PHE:HB3	30:K:101:BCR:C15	2.48	0.43
20:x:1:MET:HG3	20:x:5:LEU:HB2	1.99	0.43
33:3:303:CLA:H162	33:3:303:CLA:H143	1.72	0.43
23:4:41:PRO:HG3	33:4:305:CLA:NB	2.33	0.43
45:5:301:A86:C26	33:5:316:CLA:CMD	2.97	0.43
26:7:47:PRO:HD2	48:7:302:ET4:O31	2.19	0.43
30:A:409:BCR:H24C	30:A:409:BCR:H371	1.78	0.43
3:C:54:HIS:HE1	33:C:510:CLA:C4B	2.32	0.43
3:c:234:GLY:HA3	30:c:515:BCR:H402	2.01	0.43
3:c:305:PRO:HB3	3:c:356:PHE:CG	2.54	0.43
3:c:319:ASP:OD2	3:c:338:TYR:OH	2.27	0.43
30:D:407:BCR:H20C	30:D:407:BCR:H361	1.81	0.43
6:F:22:HIS:CE1	42:F:101:HEM:ND	2.81	0.43
6:f:42:GLN:HB2	28:q:62:ARG:NH1	2.34	0.43
23:4:93:ILE:HD11	23:4:113:PRO:CG	2.44	0.43
28:Q:113:GLU:O	28:Q:117:LYS:HG2	2.18	0.43
29:9:84:ILE:HG13	29:9:85:PHE:N	2.33	0.43
29:2:79:TYR:HD2	29:2:166:LEU:CD2	2.27	0.43
33:1:312:CLA:H2A	33:1:312:CLA:HED2	2.00	0.43
34:A:407:PHO:HBA2	34:A:407:PHO:H3A	1.62	0.43
3:c:78:PRO:HG2	3:c:81:GLU:HG3	2.00	0.43
5:E:24:HIS:CE1	42:F:101:HEM:CHD	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:89:THR:C	18:V:91:ARG:N	2.76	0.43
18:v:59:PHE:C	18:v:61:ALA:N	2.77	0.43
33:W:303:CLA:H143	33:W:303:CLA:H8	2.01	0.43
29:2:67:LYS:HE2	45:2:302:A86:O2	2.18	0.43
45:2:302:A86:C33	33:2:309:CLA:O2A	2.67	0.43
29:8:185:LEU:HG	29:8:186:ILE:N	2.24	0.43
38:A:415:DGD:HA71	33:b:607:CLA:H191	2.00	0.42
5:e:40:SER:O	28:q:61:PRO:HD2	2.19	0.42
13:M:82:LEU:HD23	13:M:82:LEU:HA	1.88	0.42
36:3:318:LHG:H242	36:3:318:LHG:H271	1.57	0.42
23:4:54:ILE:HG22	23:4:58:LYS:HD2	2.01	0.42
24:5:63:ARG:NH1	33:5:309:CLA:HMA3	2.34	0.42
25:6:141:GLU:OE1	25:6:155:TRP:NE1	2.52	0.42
29:2:165:GLU:HG2	33:2:313:CLA:NB	2.34	0.42
29:1:188:GLY:C	29:1:190:PRO:HD3	2.44	0.42
2:B:202:HIS:HE1	33:B:603:CLA:NA	2.16	0.42
2:B:216:HIS:HE1	33:B:609:CLA:C4D	2.24	0.42
33:C:504:CLA:H142	33:C:504:CLA:H111	1.80	0.42
3:c:442:HIS:HE1	33:c:508:CLA:C1A	2.32	0.42
5:E:11:PHE:HE1	42:F:101:HEM:O2D	2.02	0.42
6:F:41:ILE:HG23	28:Q:61:PRO:HB2	2.01	0.42
6:f:40:PHE:CD1	28:q:65:VAL:HG12	2.54	0.42
15:O:132:ARG:O	15:O:134:THR:N	2.50	0.42
18:V:29:LEU:HD12	18:V:29:LEU:HA	1.86	0.42
18:V:89:THR:O	18:V:91:ARG:N	2.52	0.42
18:v:130:MET:CE	18:v:133:LEU:HD12	2.50	0.42
33:4:308:CLA:H3A	33:4:308:CLA:HBA2	1.73	0.42
25:6:40:PRO:O	25:6:42:LEU:N	2.52	0.42
33:7:309:CLA:H61	33:7:309:CLA:H93	1.66	0.42
2:b:216:HIS:HE1	33:b:610:CLA:ND	2.17	0.42
28:q:79:ALA:HB2	39:q:302:LMG:HC71	2.00	0.42
26:0:40:PRO:N	26:0:41:PRO:HD2	2.33	0.42
29:9:134:PHE:CE2	33:9:314:CLA:C2D	3.02	0.42
29:9:153:LEU:O	29:9:157:ARG:HD3	2.18	0.42
29:8:188:GLY:O	29:8:189:LEU:HD23	2.19	0.42
33:1:310:CLA:CHA	33:1:310:CLA:HBA1	2.49	0.42
3:C:130:HIS:HE1	33:C:513:CLA:NA	2.11	0.42
39:C:520:LMG:H361	39:C:520:LMG:H392	1.78	0.42
33:c:508:CLA:H61	33:c:508:CLA:H92	1.75	0.42
4:D:11:ARG:HB3	4:D:12:GLY:H	1.64	0.42
17:u:83:ARG:NH1	18:v:83:GLU:OE2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:5:135:MET:HE1	45:5:302:A86:C22	2.25	0.42
45:5:304:A86:O3	33:5:314:CLA:HMA1	2.19	0.42
33:5:313:CLA:HMB3	33:5:313:CLA:HBB1	2.01	0.42
26:7:191:LEU:O	26:7:192:GLN:C	2.62	0.42
1:a:283:ILE:HA	1:a:286:THR:HG22	2.01	0.42
29:9:159:ALA:O	29:9:160:MET:C	2.61	0.42
29:2:162:ALA:O	29:2:163:ILE:C	2.61	0.42
3:C:173:LEU:HD22	33:C:501:CLA:C1D	2.49	0.42
33:c:503:CLA:H62	33:c:503:CLA:H102	1.68	0.42
8:h:44:ILE:O	8:h:48:ILE:HG13	2.19	0.42
30:K:101:BCR:H16C	27:Y:20:GLY:HA3	2.00	0.42
13:M:90:LEU:HD12	13:m:90:LEU:HD12	2.00	0.42
15:o:88:ASP:OD1	15:o:88:ASP:N	2.50	0.42
18:v:89:THR:OG1	18:v:108:TYR:O	2.29	0.42
18:v:102:LEU:HA	18:v:102:LEU:HD23	1.79	0.42
19:W:181:THR:HG22	22:3:241:LYS:HD2	2.01	0.42
22:3:168:ARG:C	22:3:170:SER:N	2.78	0.42
24:5:33:GLU:OE2	24:5:59:PHE:HD1	2.02	0.42
33:6:308:CLA:H3A	33:6:308:CLA:HBA2	1.63	0.42
26:7:66:GLU:OE2	26:7:167:ARG:NH1	2.52	0.42
26:0:102:ARG:HB3	26:0:180:GLU:OE2	2.19	0.42
29:9:65:GLU:OE2	29:9:157:ARG:NE	2.46	0.42
46:2:304:DD6:C23	33:2:311:CLA:C1D	2.97	0.42
30:A:401:BCR:H15C	30:A:401:BCR:H351	1.90	0.42
38:C:517:DGD:HBW1	38:C:517:DGD:HB91	1.88	0.42
33:c:511:CLA:H202	30:k:102:BCR:H17C	2.02	0.42
39:d:410:LMG:HC3	39:b:623:LMG:HC71	2.01	0.42
8:h:49:TYR:CD1	2:b:192:PRO:HG3	2.54	0.42
15:o:216:LYS:HD2	15:o:216:LYS:HA	1.82	0.42
18:v:54:ARG:HD2	28:q:85:GLN:OE1	2.19	0.42
25:6:169:ILE:O	25:6:173:ASN:HB2	2.19	0.42
2:b:201:HIS:HE1	33:b:603:CLA:ND	2.06	0.42
33:8:308:CLA:H2A	33:8:308:CLA:O2D	2.19	0.42
29:1:119:ILE:O	33:1:310:CLA:HAB	2.19	0.42
38:c:516:DGD:HB72	38:c:516:DGD:HA71	2.01	0.42
4:d:11:ARG:HB3	4:d:12:GLY:H	1.62	0.42
37:l:101:SQD:H271	37:l:101:SQD:H242	1.82	0.42
23:4:188:ILE:HG22	23:4:190:GLY:O	2.20	0.42
29:9:128:ARG:HA	29:9:128:ARG:HD3	1.72	0.42
29:2:161:LEU:HA	29:2:164:LEU:HD22	2.01	0.42
29:8:89:PHE:HB3	45:8:302:A86:C37	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:409:BCR:H20C	30:A:409:BCR:H361	1.80	0.42
30:C:515:BCR:H20C	30:C:515:BCR:H361	1.82	0.42
3:c:60:PHE:HB2	3:c:120:SER:OG	2.19	0.42
18:v:135:ASP:OD1	28:q:105:LEU:HD11	2.19	0.42
33:4:309:CLA:HED3	33:4:309:CLA:H2	2.01	0.42
25:6:58:ARG:O	25:6:62:LEU:HD23	2.19	0.42
2:b:317:ASN:HA	2:b:330:MET:HE1	2.00	0.42
26:0:71:ARG:NH1	33:0:312:CLA:OBD	2.52	0.42
46:2:304:DD6:C8	33:2:311:CLA:CHC	2.96	0.42
29:8:67:LYS:NZ	33:8:310:CLA:O1D	2.38	0.42
29:1:185:LEU:O	29:1:187:THR:N	2.53	0.42
33:B:604:CLA:HMB2	33:B:607:CLA:HAB	2.01	0.42
3:c:189:PRO:O	28:q:151:MET:HE1	2.18	0.42
3:c:341:ARG:NH1	15:o:136:THR:O	2.52	0.42
4:d:200:VAL:HG22	33:d:401:CLA:C1B	2.50	0.42
22:3:59:PRO:HB2	33:4:312:CLA:H42	2.02	0.42
22:3:160:ARG:O	22:3:164:GLN:HG3	2.19	0.42
22:3:165:GLY:HA3	22:3:166:LYS:HZ1	1.84	0.42
23:4:93:ILE:N	23:4:93:ILE:HD12	2.35	0.42
45:5:301:A86:C6	33:5:316:CLA:HMC2	2.49	0.42
43:5:320:LMU:H1'	43:5:320:LMU:H22	1.54	0.42
33:7:312:CLA:H202	33:7:312:CLA:H162	1.92	0.42
30:a:412:BCR:H11C	30:a:412:BCR:H341	1.93	0.42
45:2:301:A86:C37	33:2:315:CLA:HMB2	2.50	0.42
3:C:329:ALA:O	15:O:161:TYR:OH	2.35	0.42
30:c:514:BCR:H20C	30:c:514:BCR:H361	1.82	0.42
8:h:29:PRO:HA	36:h:103:LHG:H112	2.01	0.42
13:M:75:PHE:CE1	13:m:75:PHE:HB3	2.54	0.42
43:t:101:LMU:H71	43:t:101:LMU:H42	1.65	0.42
33:5:313:CLA:H62	33:5:313:CLA:H41	1.79	0.42
33:b:614:CLA:H143	33:b:614:CLA:H161	1.75	0.42
26:0:98:ALA:HB1	26:0:99:PRO:HD2	2.01	0.42
46:1:303:DD6:C22	33:1:306:CLA:NB	2.83	0.42
2:B:192:PRO:HG3	8:H:49:TYR:CE1	2.55	0.42
3:c:51:HIS:CD2	33:c:509:CLA:C4A	3.03	0.42
3:c:97:ILE:HD11	3:c:101:GLY:HA2	2.02	0.42
37:l:101:SQD:H45	37:l:101:SQD:H81	1.83	0.42
17:u:122:LYS:HE2	17:u:122:LYS:HB2	1.88	0.42
33:W:303:CLA:H162	33:W:303:CLA:H202	1.74	0.42
23:4:69:HIS:HE1	47:4:307:KC2:ND	2.02	0.42
45:5:305:A86:C26	33:5:314:CLA:HHC	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:5:320:LMU:H21	43:5:320:LMU:H51	1.18	0.42
28:q:62:ARG:NH1	28:q:74:SER:OG	2.52	0.42
29:9:86:ARG:HD2	29:9:98:ALA:H	1.85	0.42
45:2:302:A86:C26	33:2:309:CLA:HMD1	2.50	0.42
29:1:153:LEU:O	29:1:157:ARG:HD3	2.19	0.42
33:C:501:CLA:H61	33:C:501:CLA:H41	1.81	0.41
3:c:448:ALA:HB2	1:a:141:PRO:HG3	2.02	0.41
17:U:68:SER:OG	17:U:69:GLN:N	2.52	0.41
22:3:114:PHE:C	22:3:116:GLY:H	2.28	0.41
24:5:84:ARG:HA	24:5:104:ASN:HD21	1.84	0.41
33:5:309:CLA:CGA	33:5:309:CLA:H3A	2.49	0.41
25:6:166:LYS:O	25:6:169:ILE:HG22	2.20	0.41
33:b:614:CLA:H143	33:b:614:CLA:H111	1.74	0.41
29:2:185:LEU:HD23	29:2:185:LEU:HA	1.76	0.41
4:D:102:ARG:HD2	5:E:77:LEU:HD13	2.02	0.41
4:d:143:ILE:O	4:d:146:SER:OG	2.37	0.41
7:g:93:LYS:HA	7:g:121:PHE:HZ	1.85	0.41
30:K:102:BCR:H11C	30:K:102:BCR:H341	1.94	0.41
37:L:101:SQD:O47	37:L:101:SQD:O3	2.35	0.41
37:t:102:SQD:H351	37:t:102:SQD:H383	1.88	0.41
33:3:306:CLA:H61	33:3:306:CLA:H41	1.56	0.41
43:4:317:LMU:H31	43:4:317:LMU:H62	1.35	0.41
24:5:37:GLY:HA2	24:5:172:LEU:HD23	2.02	0.41
24:5:142:SER:OG	24:5:143:GLN:N	2.50	0.41
25:6:75:LEU:HB2	33:6:310:CLA:HMC3	2.02	0.41
2:b:338:GLU:OE2	2:b:433:ASP:HB2	2.19	0.41
33:2:308:CLA:CHA	33:2:308:CLA:HBA1	2.51	0.41
33:B:612:CLA:H141	33:B:612:CLA:H161	1.88	0.41
33:c:512:CLA:H202	33:c:512:CLA:H161	1.88	0.41
4:D:20:TRP:CD1	4:D:23:ARG:HH21	2.38	0.41
4:d:116:HIS:HE1	33:d:402:CLA:ND	2.18	0.41
30:h:101:BCR:H371	30:h:101:BCR:H24C	1.77	0.41
25:6:36:LEU:HD11	25:6:63:ARG:HH12	1.85	0.41
25:6:169:ILE:HD11	44:6:314:KC1:CBD	2.50	0.41
45:6:304:A86:C9	44:6:314:KC1:CMC	2.98	0.41
1:a:137:LEU:HD23	1:a:137:LEU:HA	1.89	0.41
33:b:611:CLA:H202	33:b:611:CLA:H161	1.82	0.41
33:b:615:CLA:H52	33:b:615:CLA:H8	1.83	0.41
28:Q:62:ARG:NH2	28:Q:71:ASP:OD2	2.54	0.41
33:9:310:CLA:C2B	33:8:310:CLA:HMB2	2.51	0.41
30:A:401:BCR:H353	33:b:617:CLA:H92	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:213:HIS:HE1	4:d:266:LEU:HD22	1.83	0.41
6:F:22:HIS:O	6:F:24:LEU:N	2.53	0.41
12:l:9:GLN:O	39:m:201:LMG:O3	2.36	0.41
33:3:304:CLA:H71	33:4:308:CLA:H172	2.03	0.41
45:5:306:A86:C2	47:5:310:KC2:CBB	2.98	0.41
25:6:39:GLN:HE21	25:6:41:PRO:CD	2.34	0.41
25:6:103:ILE:HG13	25:6:112:GLU:OE2	2.20	0.41
25:6:147:ARG:HH11	33:6:313:CLA:HED3	1.84	0.41
1:a:330:VAL:HG23	1:a:331:MET:HG2	2.03	0.41
30:a:412:BCR:H371	30:a:412:BCR:H24C	1.81	0.41
29:1:100:VAL:O	29:1:102:ASN:N	2.50	0.41
30:A:401:BCR:H20C	30:A:401:BCR:H361	1.81	0.41
3:c:221:TRP:HE3	38:c:516:DGD:HB21	1.85	0.41
30:c:514:BCR:H24C	30:c:514:BCR:H371	1.81	0.41
15:o:110:VAL:HB	15:o:168:LEU:HD21	2.02	0.41
15:o:225:ASP:OD1	15:o:225:ASP:N	2.53	0.41
18:V:153:ALA:C	18:V:155:LYS:H	2.28	0.41
25:6:119:LEU:O	25:6:122:LEU:HG	2.21	0.41
26:7:68:MET:HE2	26:7:128:ARG:CZ	2.50	0.41
30:a:414:BCR:H24C	30:a:414:BCR:H371	1.83	0.41
26:0:173:PHE:O	26:0:177:ILE:HG12	2.20	0.41
29:9:159:ALA:O	29:9:161:LEU:N	2.53	0.41
29:9:160:MET:O	29:9:163:ILE:HG22	2.21	0.41
1:A:283:ILE:HA	1:A:286:THR:HG22	2.02	0.41
33:B:609:CLA:H161	33:B:609:CLA:H141	1.78	0.41
4:d:13:LEU:HD23	4:d:13:LEU:HA	1.91	0.41
30:d:403:BCR:H20C	30:d:403:BCR:H361	1.84	0.41
5:e:77:LEU:O	5:e:81:THR:HG23	2.20	0.41
37:L:101:SQD:H121	37:L:101:SQD:H302	2.02	0.41
13:M:101:SER:OG	13:m:102:ARG:HB2	2.20	0.41
38:3:320:DGD:HB42	38:3:320:DGD:HB71	1.76	0.41
23:4:36:ILE:HG13	23:4:63:ARG:NH2	2.31	0.41
23:4:71:ARG:O	23:4:75:LEU:HD23	2.20	0.41
23:4:99:THR:C	23:4:101:ASP:H	2.28	0.41
23:4:99:THR:C	23:4:101:ASP:N	2.79	0.41
45:4:301:A86:C23	33:4:306:CLA:HAC2	2.50	0.41
33:4:308:CLA:H162	33:4:308:CLA:H121	1.74	0.41
33:6:307:CLA:H41	33:6:307:CLA:H62	1.89	0.41
33:7:309:CLA:H141	33:7:309:CLA:H161	1.64	0.41
33:b:605:CLA:H61	33:b:605:CLA:H93	1.85	0.41
30:b:618:BCR:H11C	30:b:618:BCR:H341	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:q:118:LYS:NZ	28:q:211:LEU:HB3	2.35	0.41
29:9:171:SER:O	29:9:175:VAL:HG22	2.20	0.41
33:B:605:CLA:H141	33:B:605:CLA:H161	1.76	0.41
33:B:613:CLA:H143	33:B:613:CLA:H111	1.76	0.41
3:c:328:SER:HA	15:o:161:TYR:HE1	1.85	0.41
4:d:213:HIS:CD2	41:d:404:PL9:O2	2.74	0.41
13:M:112:SER:HB3	13:m:106:ARG:HH11	1.85	0.41
18:V:67:HIS:HA	18:V:71:ILE:O	2.20	0.41
25:6:36:LEU:CD1	25:6:63:ARG:HH12	2.34	0.41
33:7:305:CLA:H61	33:7:305:CLA:H93	1.79	0.41
33:b:614:CLA:H72	33:b:614:CLA:H112	1.87	0.41
29:2:163:ILE:O	29:2:166:LEU:N	2.54	0.41
29:8:56:GLU:CD	29:8:57:LYS:N	2.79	0.41
1:A:248:ILE:HG23	1:A:249:VAL:H	1.86	0.41
35:A:410:BCT:C	4:D:267:HIS:HE2	2.34	0.41
2:B:384:ARG:NH2	17:U:144:ASN:O	2.50	0.41
39:C:520:LMG:H322	39:C:520:LMG:H291	1.68	0.41
39:d:410:LMG:HC62	2:b:230:ARG:NH2	2.36	0.41
17:u:117:GLU:O	17:u:118:LYS:C	2.62	0.41
23:4:97:LEU:HD22	23:4:97:LEU:HA	1.70	0.41
23:4:145:ASP:N	23:4:145:ASP:OD1	2.53	0.41
1:a:147:PHE:O	1:a:150:PRO:HD2	2.21	0.41
2:b:102:VAL:O	2:b:106:MET:HG2	2.20	0.41
33:2:310:CLA:H92	33:2:310:CLA:H61	1.86	0.41
1:A:297:LEU:HD12	1:A:297:LEU:HA	1.95	0.41
30:B:618:BCR:H20C	30:B:618:BCR:H361	1.85	0.41
3:C:67:LEU:HD23	3:C:67:LEU:HA	1.92	0.41
3:C:86:CYS:HB3	33:C:503:CLA:HED2	2.02	0.41
30:C:515:BCR:H15C	30:C:515:BCR:H351	1.78	0.41
30:c:514:BCR:H15C	30:c:514:BCR:H351	1.88	0.41
38:c:516:DGD:HBE2	38:c:516:DGD:HB81	1.75	0.41
4:D:200:VAL:HG22	33:D:405:CLA:C1B	2.51	0.41
37:D:403:SQD:H342	37:D:403:SQD:H371	1.80	0.41
8:H:61:ASP:OD1	8:H:62:TRP:N	2.53	0.41
18:v:57:ARG:NH1	28:q:95:VAL:C	2.79	0.41
18:v:102:LEU:HD13	18:v:138:LEU:HD22	2.03	0.41
18:v:133:LEU:HD23	18:v:133:LEU:HA	1.89	0.41
22:3:77:GLU:O	22:3:78:GLY:C	2.64	0.41
26:7:59:LEU:HD23	26:7:59:LEU:HA	1.94	0.41
2:b:55:MET:HE1	2:b:63:MET:HG2	2.02	0.41
33:b:602:CLA:HBA1	33:b:602:CLA:H3A	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:b:618:BCR:H15C	30:b:618:BCR:H351	1.85	0.41
33:9:310:CLA:HED3	33:9:310:CLA:HBD	1.85	0.41
33:2:310:CLA:H62	33:2:310:CLA:H41	1.78	0.41
29:8:140:ASP:HB3	29:8:141:LEU:H	1.70	0.41
29:1:39:ALA:HB3	29:1:40:PRO:HD3	2.02	0.41
46:1:304:DD6:C11	33:1:311:CLA:H71	2.47	0.41
3:C:283:THR:HG22	3:C:287:TYR:CZ	2.56	0.41
33:c:502:CLA:H142	33:c:502:CLA:H111	1.87	0.41
39:D:404:LMG:HC1	39:D:404:LMG:HC8	1.92	0.41
12:l:14:ASN:OD1	12:l:14:ASN:N	2.53	0.41
39:W:301:LMG:H162	39:W:301:LMG:H132	1.88	0.41
22:3:165:GLY:O	22:3:167:ASP:N	2.48	0.41
33:3:302:CLA:HBA1	33:3:302:CLA:H3A	1.63	0.41
33:7:304:CLA:C4D	33:7:310:CLA:HMD3	2.51	0.41
2:b:155:ALA:O	2:b:159:THR:OG1	2.36	0.41
28:q:90:TYR:HA	28:q:98:LYS:CE	2.51	0.41
33:2:310:CLA:HED3	33:2:310:CLA:HBD	1.89	0.41
2:B:378:ARG:NH1	7:G:154:SER:O	2.54	0.40
33:B:604:CLA:H93	33:B:604:CLA:H61	1.75	0.40
3:C:160:GLY:HA3	3:C:250:ILE:HG13	2.02	0.40
15:o:236:GLY:O	2:b:423:LYS:HE2	2.21	0.40
22:3:165:GLY:C	22:3:167:ASP:N	2.78	0.40
23:4:69:HIS:HE1	47:4:307:KC2:C1D	2.34	0.40
38:a:401:DGD:O6D	38:a:401:DGD:O3D	2.25	0.40
26:0:47:PRO:CD	48:0:302:ET4:O31	2.61	0.40
26:0:142:ILE:HB	26:0:148:ARG:HH22	1.86	0.40
33:0:311:CLA:H12	33:0:311:CLA:HBA1	1.90	0.40
29:9:68:HIS:HE1	33:9:307:CLA:ND	2.14	0.40
29:1:89:PHE:O	29:1:95:VAL:HG23	2.21	0.40
1:A:237:TYR:HB3	4:D:262:ASN:ND2	2.36	0.40
2:B:413:ASP:OD1	2:B:413:ASP:N	2.49	0.40
3:C:203:ASN:ND2	22:3:236:PRO:HD3	2.36	0.40
33:D:406:CLA:H92	33:D:406:CLA:H61	1.71	0.40
10:J:26:LEU:HD12	10:J:26:LEU:HA	1.84	0.40
21:z:47:LEU:HD23	21:z:47:LEU:HA	1.91	0.40
22:3:181:TRP:CD1	22:3:183:PRO:HD3	2.56	0.40
22:3:214:LEU:HD21	45:3:314:A86:O1	2.22	0.40
33:4:311:CLA:H61	33:4:311:CLA:H41	1.81	0.40
30:a:414:BCR:H15C	30:a:414:BCR:H351	1.88	0.40
33:0:311:CLA:O1D	33:0:311:CLA:H2A	2.21	0.40
29:9:138:LYS:N	29:9:139:PRO:HD3	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:2:165:GLU:HB2	33:2:313:CLA:CHC	2.51	0.40
33:2:308:CLA:H62	33:2:308:CLA:H92	1.88	0.40
2:B:65:PHE:HE1	33:B:604:CLA:HED2	1.87	0.40
39:d:406:LMG:H112	39:d:406:LMG:H142	1.86	0.40
7:G:85:ASP:O	7:G:88:ALA:N	2.54	0.40
11:K:22:VAL:O	11:K:25:VAL:HG12	2.21	0.40
30:k:102:BCR:H20C	30:k:102:BCR:H361	1.84	0.40
23:4:96:GLU:OE1	23:4:97:LEU:HB2	2.21	0.40
26:7:142:ILE:HG13	26:7:143:GLU:N	2.28	0.40
29:2:189:LEU:HD12	29:2:189:LEU:N	2.36	0.40
29:8:180:ASP:O	29:8:182:LEU:N	2.49	0.40
3:C:255:PHE:CE2	36:W:302:LHG:HC61	2.56	0.40
38:c:516:DGD:HB32	38:c:516:DGD:HB62	1.96	0.40
15:O:101:MET:HG2	15:O:103:ILE:HD11	2.02	0.40
22:3:107:TRP:CD2	22:3:111:PHE:HD2	2.39	0.40
33:3:307:CLA:H51	33:3:313:CLA:H12	2.03	0.40
23:4:119:GLN:HE22	33:4:309:CLA:C1A	2.34	0.40
25:6:181:ILE:HD12	25:6:184:LEU:HD23	2.04	0.40
30:b:618:BCR:H371	30:b:618:BCR:H24C	1.85	0.40
33:9:310:CLA:H152	29:8:120:PHE:CD2	2.56	0.40
29:8:90:ASP:HA	29:8:95:VAL:HA	2.04	0.40
1:A:103:ASP:OD2	38:A:415:DGD:O2D	2.32	0.40
1:A:312:ARG:HE	1:A:312:ARG:HB3	1.72	0.40
2:B:2:ALA:N	12:L:10:ALA:O	2.54	0.40
30:C:514:BCR:H11C	30:C:514:BCR:H341	1.88	0.40
4:D:115:LEU:HB3	33:D:406:CLA:HMA1	2.03	0.40
5:e:17:SER:O	5:e:21:TRP:HD1	2.04	0.40
19:w:204:LEU:CD1	33:w:303:CLA:HBC3	2.52	0.40
21:z:35:ASP:OD1	21:z:35:ASP:N	2.53	0.40
43:3:301:LMU:H41	43:3:301:LMU:H2'	2.03	0.40
33:4:308:CLA:H91	33:4:308:CLA:H112	1.91	0.40
24:5:127:ILE:HD12	45:5:302:A86:C8	2.48	0.40
26:7:68:MET:HE2	26:7:128:ARG:NH2	2.37	0.40
2:b:413:ASP:N	2:b:413:ASP:OD1	2.55	0.40
30:b:619:BCR:H24C	30:b:619:BCR:H371	1.83	0.40
29:9:62:ARG:HA	29:9:62:ARG:HD3	1.96	0.40
29:9:68:HIS:HE1	33:9:307:CLA:C4D	2.34	0.40
29:2:172:GLN:HG3	29:2:179:PHE:HD2	1.87	0.40
46:2:304:DD6:C22	33:2:311:CLA:ND	2.85	0.40
29:8:82:PRO:HG3	33:8:308:CLA:C1D	2.51	0.40
33:8:311:CLA:H92	33:8:311:CLA:H62	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/333 (99%)	311 (94%)	19 (6%)	1 (0%)	36	57
1	a	331/333 (99%)	314 (95%)	17 (5%)	0	100	100
2	B	476/509 (94%)	463 (97%)	13 (3%)	0	100	100
2	b	476/509 (94%)	464 (98%)	12 (2%)	0	100	100
3	C	448/470 (95%)	430 (96%)	18 (4%)	0	100	100
3	c	448/470 (95%)	433 (97%)	15 (3%)	0	100	100
4	D	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
4	d	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
5	E	74/84 (88%)	69 (93%)	5 (7%)	0	100	100
5	e	74/84 (88%)	71 (96%)	3 (4%)	0	100	100
6	F	29/43 (67%)	26 (90%)	0	3 (10%)	0	0
6	f	29/43 (67%)	29 (100%)	0	0	100	100
7	G	118/176 (67%)	108 (92%)	10 (8%)	0	100	100
7	g	118/176 (67%)	108 (92%)	10 (8%)	0	100	100
8	H	63/66 (96%)	58 (92%)	5 (8%)	0	100	100
8	h	63/66 (96%)	56 (89%)	7 (11%)	0	100	100
9	I	32/34 (94%)	32 (100%)	0	0	100	100
9	i	32/34 (94%)	32 (100%)	0	0	100	100
10	J	31/39 (80%)	29 (94%)	2 (6%)	0	100	100
10	j	31/39 (80%)	29 (94%)	2 (6%)	0	100	100
11	K	35/44 (80%)	34 (97%)	1 (3%)	0	100	100
11	k	35/44 (80%)	34 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	35/38 (92%)	35 (100%)	0	0	100	100
12	l	35/38 (92%)	35 (100%)	0	0	100	100
13	M	39/113 (34%)	39 (100%)	0	0	100	100
13	m	39/113 (34%)	38 (97%)	1 (3%)	0	100	100
15	O	246/305 (81%)	230 (94%)	14 (6%)	2 (1%)	16	34
15	o	246/305 (81%)	228 (93%)	16 (6%)	2 (1%)	16	34
16	T	26/28 (93%)	26 (100%)	0	0	100	100
16	t	26/28 (93%)	26 (100%)	0	0	100	100
17	U	90/148 (61%)	88 (98%)	2 (2%)	0	100	100
17	u	90/148 (61%)	82 (91%)	8 (9%)	0	100	100
18	V	133/162 (82%)	125 (94%)	6 (4%)	2 (2%)	8	19
18	v	133/162 (82%)	123 (92%)	7 (5%)	3 (2%)	5	11
19	W	52/54 (96%)	47 (90%)	5 (10%)	0	100	100
19	w	52/54 (96%)	49 (94%)	3 (6%)	0	100	100
20	X	33/38 (87%)	31 (94%)	1 (3%)	1 (3%)	3	7
20	x	33/38 (87%)	31 (94%)	2 (6%)	0	100	100
21	Z	59/61 (97%)	56 (95%)	3 (5%)	0	100	100
21	z	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
22	3	218/220 (99%)	186 (85%)	27 (12%)	5 (2%)	5	11
23	4	161/196 (82%)	139 (86%)	16 (10%)	6 (4%)	2	5
24	5	158/192 (82%)	137 (87%)	18 (11%)	3 (2%)	6	15
25	6	166/199 (83%)	136 (82%)	27 (16%)	3 (2%)	6	15
26	0	163/199 (82%)	148 (91%)	13 (8%)	2 (1%)	10	24
26	7	163/199 (82%)	148 (91%)	13 (8%)	2 (1%)	10	24
27	Y	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
27	y	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
28	Q	154/211 (73%)	145 (94%)	9 (6%)	0	100	100
28	q	154/211 (73%)	144 (94%)	10 (6%)	0	100	100
29	1	161/193 (83%)	128 (80%)	26 (16%)	7 (4%)	2	4
29	2	161/193 (83%)	141 (88%)	14 (9%)	6 (4%)	2	5
29	8	161/193 (83%)	144 (89%)	13 (8%)	4 (2%)	4	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
29	9	161/193 (83%)	138 (86%)	17 (11%)	6 (4%)	2 5
All	All	7423/8659 (86%)	6918 (93%)	447 (6%)	58 (1%)	18 34

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	4	99	THR
24	5	41	PRO
25	6	42	LEU
25	6	196	ILE
29	9	39	ALA
29	2	39	ALA
29	2	92	ALA
29	2	139	PRO
29	2	185	LEU
29	8	39	ALA
29	8	92	ALA
29	8	185	LEU
29	1	39	ALA
29	1	92	ALA
29	1	140	ASP
29	1	185	LEU
1	A	246	TYR
15	o	93	LYS
18	V	91	ARG
18	v	60	ASN
23	4	54	ILE
26	0	196	PHE
29	9	183	ASP
29	9	184	ASN
29	2	140	ASP
6	F	20	ALA
6	F	23	GLY
15	O	93	LYS
18	V	153	ALA
18	v	91	ARG
18	v	153	ALA
22	3	173	ILE
23	4	43	GLY
24	5	160	SER
29	9	92	ALA
29	8	186	ILE

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Mol	Chain	Res	Type
22	3	37	ALA
22	3	79	ASN
22	3	166	LYS
23	4	100	ASN
24	5	40	ALA
29	1	186	ILE
20	X	32	ASN
26	7	98	ALA
26	7	195	GLY
29	9	185	LEU
15	O	91	THR
15	o	91	THR
22	3	50	SER
23	4	188	ILE
26	0	98	ALA
29	2	186	ILE
29	1	137	GLY
23	4	94	PRO
29	9	143	GLY
6	F	21	VAL
25	6	41	PRO
29	1	91	ILE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 347 ligands modelled in this entry, 4 are monoatomic - leaving 343 for Mogul analysis.

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
39	LMG	B	621	-	28,28,55	0.97	0	36,36,63	1.31	4 (11%)
33	CLA	c	506	-	49,53,73	1.36	9 (18%)	58,89,113	1.41	5 (8%)
36	LHG	w	301	-	34,34,48	0.75	2 (5%)	37,40,54	1.26	4 (10%)
33	CLA	9	314	-	40,46,73	1.47	9 (22%)	52,80,113	1.45	5 (9%)
33	CLA	c	508	-	69,73,73	1.15	9 (13%)	82,113,113	1.23	5 (6%)
33	CLA	C	502	-	68,72,73	1.17	10 (14%)	80,111,113	1.24	5 (6%)
33	CLA	4	315	-	51,55,73	1.35	8 (15%)	60,91,113	1.43	6 (10%)
45	A86	4	301	-	47,50,50	1.54	6 (12%)	51,76,76	2.55	16 (31%)
33	CLA	2	312	-	49,53,73	1.40	9 (18%)	58,89,113	1.41	4 (6%)
36	LHG	3	317	33	26,26,48	0.86	1 (3%)	29,32,54	1.35	4 (13%)
33	CLA	6	315	-	45,49,73	1.41	8 (17%)	54,84,113	1.50	5 (9%)
33	CLA	c	507	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	5 (6%)
33	CLA	b	605	-	65,69,73	1.19	9 (13%)	77,108,113	1.35	8 (10%)
33	CLA	B	604	-	65,69,73	1.19	8 (12%)	77,108,113	1.34	7 (9%)
39	LMG	C	520	-	48,48,55	0.81	1 (2%)	56,56,63	1.34	6 (10%)
30	BCR	k	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	5 (8%)
38	DGD	C	518	-	56,56,67	0.99	2 (3%)	70,70,81	1.40	9 (12%)
33	CLA	3	302	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
45	A86	6	306	-	47,50,50	1.43	5 (10%)	51,76,76	7.47	22 (43%)
33	CLA	4	306	23	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
33	CLA	2	305	-	45,49,73	1.43	8 (17%)	54,84,113	1.44	6 (11%)
46	DD6	2	304	-	40,45,45	1.56	2 (5%)	51,67,67	2.18	12 (23%)
33	CLA	B	615	-	69,73,73	1.17	9 (13%)	82,113,113	1.22	5 (6%)
33	CLA	5	317	-	40,46,73	1.47	7 (17%)	52,80,113	1.47	5 (9%)
33	CLA	4	313	23	45,49,73	1.40	8 (17%)	54,84,113	1.48	5 (9%)
33	CLA	2	308	-	59,63,73	1.26	7 (11%)	70,101,113	1.34	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	LMG	B	620	-	51,51,55	0.75	1 (1%)	59,59,63	1.36	6 (10%)
36	LHG	H	104	-	41,41,48	0.68	1 (2%)	44,47,54	1.33	5 (11%)
33	CLA	B	606	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	7 (8%)
33	CLA	C	513	-	53,57,73	1.30	9 (16%)	61,93,113	1.45	8 (13%)
45	A86	4	304	-	47,50,50	1.46	5 (10%)	51,76,76	2.51	18 (35%)
45	A86	1	301	-	47,50,50	1.45	6 (12%)	51,76,76	2.35	15 (29%)
33	CLA	2	309	-	48,51,73	1.47	10 (20%)	56,86,113	1.52	6 (10%)
33	CLA	a	407	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	5 (6%)
39	LMG	q	302	-	37,37,55	0.84	1 (2%)	45,45,63	1.28	5 (11%)
30	BCR	k	102	-	41,41,41	1.18	2 (4%)	56,56,56	1.24	7 (12%)
34	PHO	A	406	-	58,69,69	2.09	10 (17%)	55,99,99	1.48	7 (12%)
33	CLA	B	614	-	68,72,73	1.15	9 (13%)	80,111,113	1.26	6 (7%)
46	DD6	9	304	-	40,45,45	1.56	2 (5%)	51,67,67	2.18	12 (23%)
33	CLA	3	309	36	55,59,73	1.30	9 (16%)	64,96,113	1.37	6 (9%)
33	CLA	3	311	-	45,49,73	1.40	9 (20%)	54,84,113	1.50	5 (9%)
45	A86	6	304	-	47,50,50	1.46	5 (10%)	51,76,76	11.60	22 (43%)
33	CLA	b	606	-	69,73,73	1.15	9 (13%)	82,113,113	1.17	5 (6%)
30	BCR	b	620	-	41,41,41	1.19	4 (9%)	56,56,56	1.22	5 (8%)
39	LMG	q	301	-	46,46,55	0.76	1 (2%)	54,54,63	1.33	6 (11%)
36	LHG	h	103	-	41,41,48	0.70	1 (2%)	44,47,54	1.33	5 (11%)
33	CLA	b	611	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	5 (6%)
33	CLA	C	508	-	69,73,73	1.14	9 (13%)	82,113,113	1.25	7 (8%)
33	CLA	9	309	29	48,51,73	1.48	10 (20%)	56,86,113	1.52	5 (8%)
30	BCR	c	515	-	41,41,41	0.81	1 (2%)	56,56,56	1.98	14 (25%)
45	A86	5	304	-	47,50,50	1.46	5 (10%)	51,76,76	10.37	24 (47%)
37	SQD	L	101	-	52,54,54	0.96	4 (7%)	62,65,65	1.44	9 (14%)
33	CLA	C	507	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	5 (6%)
33	CLA	c	511	3	69,73,73	1.15	9 (13%)	82,113,113	1.30	7 (8%)
33	CLA	1	309	-	48,51,73	1.49	9 (18%)	56,86,113	1.50	6 (10%)
38	DGD	3	320	-	38,38,67	0.65	1 (2%)	40,40,81	1.51	6 (15%)
45	A86	6	303	-	47,50,50	1.49	6 (12%)	51,76,76	8.05	26 (50%)
47	KC2	6	309	-	49,53,53	1.74	9 (18%)	60,89,89	1.99	14 (23%)
33	CLA	C	505	-	69,73,73	1.16	9 (13%)	82,113,113	1.17	6 (7%)
30	BCR	B	617	-	41,41,41	1.23	3 (7%)	56,56,56	1.23	7 (12%)
33	CLA	3	304	-	69,73,73	1.17	9 (13%)	82,113,113	1.25	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	DGD	A	415	-	54,54,67	0.99	3 (5%)	67,67,81	1.46	12 (17%)
31	OEX	A	402	1,3	0,15,15	-	-	-		
30	BCR	A	409	-	41,41,41	1.18	3 (7%)	56,56,56	1.16	4 (7%)
33	CLA	8	311	29	59,63,73	1.26	9 (15%)	70,101,113	1.32	6 (8%)
36	LHG	W	302	-	34,34,48	0.76	2 (5%)	37,40,54	1.25	4 (10%)
41	PL9	D	408	-	55,55,55	1.34	5 (9%)	68,69,69	1.47	12 (17%)
33	CLA	5	309	24	59,63,73	1.26	8 (13%)	70,101,113	1.36	6 (8%)
45	A86	2	302	-	47,50,50	1.55	7 (14%)	51,76,76	2.68	19 (37%)
36	LHG	A	414	-	48,48,48	0.67	1 (2%)	51,54,54	1.29	6 (11%)
39	LMG	C	519	-	46,46,55	0.77	1 (2%)	54,54,63	1.38	7 (12%)
33	CLA	9	307	-	48,52,73	1.48	8 (16%)	59,88,113	1.40	5 (8%)
33	CLA	8	306	29	49,53,73	1.37	9 (18%)	58,89,113	1.44	6 (10%)
37	SQD	l	101	-	52,54,54	0.96	4 (7%)	62,65,65	1.40	9 (14%)
33	CLA	3	308	22	69,73,73	1.16	8 (11%)	82,113,113	1.25	5 (6%)
36	LHG	D	411	-	41,41,48	0.66	1 (2%)	44,47,54	1.31	4 (9%)
39	LMG	b	622	-	28,28,55	0.98	0	36,36,63	1.31	5 (13%)
39	LMG	C	522	-	23,23,55	1.36	3 (13%)	31,31,63	1.51	7 (22%)
48	ET4	0	302	-	41,43,43	2.09	13 (31%)	52,60,60	2.45	18 (34%)
45	A86	9	302	-	47,50,50	1.55	7 (14%)	51,76,76	2.68	19 (37%)
38	DGD	c	517	-	57,57,67	0.96	2 (3%)	71,71,81	1.46	12 (16%)
33	CLA	7	310	26	49,53,73	1.38	8 (16%)	58,89,113	1.43	6 (10%)
38	DGD	c	516	-	56,56,67	0.96	2 (3%)	70,70,81	1.45	11 (15%)
33	CLA	b	602	-	51,55,73	1.31	9 (17%)	60,91,113	1.43	5 (8%)
47	KC2	4	307	-	49,53,53	1.59	10 (20%)	60,89,89	2.28	17 (28%)
33	CLA	8	305	-	45,49,73	1.41	8 (17%)	54,84,113	1.48	5 (9%)
33	CLA	8	308	-	59,63,73	1.25	8 (13%)	70,101,113	1.41	7 (10%)
43	LMU	T	102	-	32,32,36	0.35	0	43,43,47	0.85	0
33	CLA	1	308	-	59,63,73	1.26	6 (10%)	70,101,113	1.36	7 (10%)
33	CLA	b	604	-	68,72,73	1.15	9 (13%)	80,111,113	1.24	6 (7%)
36	LHG	A	411	-	42,42,48	0.70	1 (2%)	45,48,54	1.23	4 (8%)
33	CLA	3	313	-	65,69,73	1.20	8 (12%)	77,108,113	1.27	5 (6%)
36	LHG	D	409	-	44,47,48	0.57	1 (2%)	44,51,54	1.18	5 (11%)
45	A86	6	305	-	47,50,50	1.47	6 (12%)	51,76,76	9.14	23 (45%)
33	CLA	B	602	-	64,69,73	1.17	9 (14%)	73,106,113	1.23	6 (8%)
45	A86	4	302	-	47,50,50	1.46	6 (12%)	51,76,76	12.38	29 (56%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CLA	4	308	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
33	CLA	b	613	-	69,73,73	1.15	9 (13%)	82,113,113	1.33	8 (9%)
37	SQD	A	413	-	38,40,54	1.12	3 (7%)	48,51,65	1.69	11 (22%)
36	LHG	a	403	-	42,42,48	0.69	1 (2%)	45,48,54	1.24	5 (11%)
43	LMU	4	317	-	36,36,36	0.38	0	47,47,47	0.87	2 (4%)
46	DD6	9	303	-	40,45,45	1.59	2 (5%)	51,67,67	2.20	13 (25%)
33	CLA	2	311	29	59,63,73	1.26	8 (13%)	70,101,113	1.31	4 (5%)
33	CLA	4	309	23	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
33	CLA	4	311	23	64,68,73	1.20	9 (14%)	76,107,113	1.27	5 (6%)
45	A86	7	301	-	47,50,50	1.62	8 (17%)	51,76,76	2.60	19 (37%)
39	LMG	m	201	-	40,40,55	0.86	2 (5%)	48,48,63	1.29	5 (10%)
39	LMG	Q	301	-	37,37,55	0.87	1 (2%)	45,45,63	1.27	4 (8%)
30	BCR	C	515	-	41,41,41	0.76	0	56,56,56	1.90	13 (23%)
33	CLA	6	316	-	41,46,73	1.66	6 (14%)	50,79,113	1.60	8 (16%)
45	A86	5	306	-	47,50,50	1.47	6 (12%)	51,76,76	7.76	25 (49%)
33	CLA	3	312	-	60,64,73	1.26	8 (13%)	71,102,113	1.33	5 (7%)
33	CLA	a	408	-	53,57,73	1.30	9 (16%)	61,93,113	1.45	6 (9%)
37	SQD	B	622	-	52,54,54	0.96	4 (7%)	62,65,65	1.71	10 (16%)
36	LHG	4	318	-	48,48,48	0.58	0	51,54,54	1.28	6 (11%)
37	SQD	t	102	-	38,40,54	1.15	3 (7%)	48,51,65	1.96	12 (25%)
33	CLA	d	402	-	64,68,73	1.19	8 (12%)	76,107,113	1.39	7 (9%)
36	LHG	b	601	-	48,48,48	0.66	1 (2%)	51,54,54	1.30	6 (11%)
37	SQD	i	101	-	38,40,54	1.12	3 (7%)	48,51,65	1.66	10 (20%)
33	CLA	1	305	-	45,49,73	1.42	8 (17%)	54,84,113	1.47	5 (9%)
33	CLA	9	316	29	40,46,73	1.48	8 (20%)	52,80,113	1.48	5 (9%)
33	CLA	6	313	25	50,54,73	1.36	7 (14%)	59,90,113	1.36	5 (8%)
38	DGD	h	102	-	63,63,67	0.90	2 (3%)	77,77,81	1.39	9 (11%)
46	DD6	1	304	-	40,45,45	1.62	3 (7%)	51,67,67	2.31	14 (27%)
33	CLA	B	613	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	7 (8%)
38	DGD	H	102	-	63,63,67	0.88	2 (3%)	77,77,81	1.39	10 (12%)
33	CLA	3	305	-	52,56,73	1.33	9 (17%)	61,92,113	1.42	6 (9%)
36	LHG	7	316	-	27,27,48	0.90	2 (7%)	30,32,54	1.75	4 (13%)
33	CLA	7	307	-	69,73,73	1.13	9 (13%)	82,113,113	1.30	7 (8%)
30	BCR	c	514	-	41,41,41	1.16	2 (4%)	56,56,56	1.25	8 (14%)
33	CLA	2	314	-	40,46,73	1.47	8 (20%)	52,80,113	1.47	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CLA	8	315	29	40,46,73	1.45	8 (20%)	52,80,113	1.52	6 (11%)
33	CLA	b	614	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
33	CLA	6	312	-	69,73,73	1.17	7 (10%)	82,113,113	1.22	4 (4%)
37	SQD	0	316	-	46,48,54	1.03	4 (8%)	56,59,65	1.45	8 (14%)
45	A86	5	303	-	47,50,50	1.46	5 (10%)	51,76,76	11.25	23 (45%)
36	LHG	3	318	-	48,48,48	0.63	1 (2%)	51,54,54	1.28	6 (11%)
39	LMG	7	315	-	55,55,55	0.73	1 (1%)	63,63,63	1.35	6 (9%)
33	CLA	1	315	-	40,46,73	1.46	8 (20%)	52,80,113	1.50	5 (9%)
33	CLA	b	612	-	68,72,73	1.15	9 (13%)	80,111,113	1.32	6 (7%)
33	CLA	8	312	-	49,53,73	1.39	9 (18%)	58,89,113	1.46	4 (6%)
45	A86	0	303	-	47,50,50	1.52	6 (12%)	51,76,76	2.45	15 (29%)
33	CLA	3	306	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
43	LMU	w	302	-	36,36,36	0.35	0	47,47,47	1.02	3 (6%)
36	LHG	a	404	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
42	HEM	V	201	18	50,50,50	1.61	9 (18%)	67,82,82	1.67	14 (20%)
33	CLA	c	504	-	68,72,73	1.16	8 (11%)	80,111,113	1.31	6 (7%)
45	A86	5	305	-	46,49,50	1.62	7 (15%)	46,74,76	7.59	22 (47%)
30	BCR	b	619	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	6 (10%)
33	CLA	8	316	29	40,46,73	1.47	8 (20%)	52,80,113	1.50	5 (9%)
33	CLA	A	405	-	53,57,73	1.30	8 (15%)	61,93,113	1.46	6 (9%)
44	KC1	3	310	-	49,53,53	1.33	6 (12%)	61,89,89	1.74	13 (21%)
39	LMG	0	314	-	42,42,55	0.91	2 (4%)	50,50,63	1.27	3 (6%)
33	CLA	9	311	29	59,63,73	1.27	8 (13%)	70,101,113	1.35	6 (8%)
39	LMG	b	623	-	40,40,55	0.85	1 (2%)	48,48,63	1.31	5 (10%)
33	CLA	c	501	-	69,73,73	1.15	9 (13%)	82,113,113	1.20	6 (7%)
33	CLA	B	608	-	69,73,73	1.14	9 (13%)	82,113,113	1.26	5 (6%)
33	CLA	c	510	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	7 (8%)
30	BCR	B	619	-	41,41,41	1.20	3 (7%)	56,56,56	1.21	4 (7%)
33	CLA	w	303	-	69,73,73	1.16	7 (10%)	82,113,113	1.26	6 (7%)
33	CLA	A	408	-	64,68,73	1.19	8 (12%)	76,107,113	1.30	6 (7%)
33	CLA	9	313	-	39,44,73	1.58	10 (25%)	50,77,113	1.60	7 (14%)
33	CLA	5	314	24	59,63,73	1.26	8 (13%)	70,101,113	1.30	6 (8%)
33	CLA	7	304	-	51,55,73	1.34	9 (17%)	60,91,113	1.42	4 (6%)
33	CLA	c	503	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	7 (8%)
42	HEM	F	101	6	50,50,50	1.37	7 (14%)	67,82,82	1.03	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CLA	c	512	-	68,72,73	1.15	9 (13%)	80,111,113	1.28	5 (6%)
33	CLA	1	306	29	49,53,73	1.38	9 (18%)	58,89,113	1.44	5 (8%)
39	LMG	c	520	-	27,27,55	1.02	0	35,35,63	1.18	5 (14%)
33	CLA	1	307	-	48,52,73	1.49	8 (16%)	59,88,113	1.43	5 (8%)
39	LMG	d	406	-	46,46,55	0.80	1 (2%)	54,54,63	1.36	5 (9%)
35	BCT	a	402	40	3,3,3	1.25	0	2,3,3	4.32	2 (100%)
39	LMG	W	301	-	48,48,55	0.79	1 (2%)	56,56,63	1.36	6 (10%)
33	CLA	9	312	-	49,53,73	1.39	8 (16%)	58,89,113	1.40	4 (6%)
30	BCR	h	101	-	41,41,41	1.17	4 (9%)	56,56,56	1.20	3 (5%)
33	CLA	B	601	-	51,55,73	1.33	9 (17%)	60,91,113	1.39	5 (8%)
44	KC1	6	314	25	49,53,53	1.39	7 (14%)	61,89,89	1.71	13 (21%)
46	DD6	2	303	-	40,45,45	1.58	2 (5%)	51,67,67	2.19	13 (25%)
33	CLA	9	306	-	49,53,73	1.38	9 (18%)	58,89,113	1.44	4 (6%)
45	A86	6	301	-	47,50,50	1.46	7 (14%)	51,76,76	12.04	26 (50%)
30	BCR	H	101	-	41,41,41	1.18	4 (9%)	56,56,56	1.19	3 (5%)
33	CLA	C	504	-	68,72,73	1.14	9 (13%)	80,111,113	1.29	6 (7%)
36	LHG	d	407	-	41,41,48	0.68	1 (2%)	44,47,54	1.31	5 (11%)
33	CLA	4	314	23	60,64,73	1.24	8 (13%)	71,102,113	1.28	7 (9%)
33	CLA	8	313	29	39,44,73	1.56	10 (25%)	50,77,113	1.56	7 (14%)
33	CLA	c	509	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	7 (8%)
33	CLA	C	503	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
38	DGD	c	518	-	56,56,67	0.94	2 (3%)	70,70,81	1.38	8 (11%)
30	BCR	d	403	-	41,41,41	1.15	3 (7%)	56,56,56	1.20	5 (8%)
33	CLA	4	305	-	59,63,73	1.25	9 (15%)	70,101,113	1.32	5 (7%)
33	CLA	4	316	-	56,60,73	1.28	9 (16%)	65,97,113	1.39	6 (9%)
46	DD6	3	315	-	40,45,45	1.55	2 (5%)	51,67,67	1.87	14 (27%)
45	A86	5	301	-	47,50,50	1.47	6 (12%)	51,76,76	11.11	26 (50%)
46	DD6	4	303	-	40,45,45	1.61	3 (7%)	51,67,67	2.83	16 (31%)
33	CLA	7	312	-	69,73,73	1.17	9 (13%)	82,113,113	1.24	5 (6%)
33	CLA	B	616	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	6 (7%)
36	LHG	5	318	-	32,32,48	0.84	2 (6%)	35,37,54	1.75	6 (17%)
39	LMG	C	521	-	27,27,55	1.06	1 (3%)	35,35,63	1.16	5 (14%)
30	BCR	D	407	-	41,41,41	1.20	3 (7%)	56,56,56	1.21	7 (12%)
33	CLA	2	307	-	48,52,73	1.49	10 (20%)	59,88,113	1.41	5 (8%)
33	CLA	6	308	25	58,62,73	1.28	8 (13%)	68,99,113	1.35	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CLA	C	506	-	49,53,73	1.37	9 (18%)	58,89,113	1.40	5 (8%)
33	CLA	D	405	-	61,65,73	1.31	10 (16%)	74,103,113	1.35	8 (10%)
33	CLA	a	411	-	64,68,73	1.19	7 (10%)	76,107,113	1.37	7 (9%)
33	CLA	5	313	-	69,73,73	1.17	7 (10%)	82,113,113	1.24	7 (8%)
33	CLA	C	510	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	7 (8%)
33	CLA	B	610	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
33	CLA	9	310	29	69,73,73	1.17	8 (11%)	82,113,113	1.25	7 (8%)
33	CLA	5	316	-	45,49,73	1.42	8 (17%)	54,84,113	1.46	5 (9%)
33	CLA	6	310	-	56,60,73	1.29	8 (14%)	65,97,113	1.37	6 (9%)
45	A86	1	302	-	47,50,50	1.49	5 (10%)	51,76,76	2.55	18 (35%)
46	DD6	1	303	-	40,45,45	1.54	2 (5%)	51,67,67	2.06	13 (25%)
34	PHO	a	409	-	58,69,69	2.09	10 (17%)	55,99,99	1.48	7 (12%)
43	LMU	5	320	-	32,32,36	0.37	0	43,43,47	0.75	1 (2%)
33	CLA	7	309	26	69,73,73	1.16	9 (13%)	82,113,113	1.26	7 (8%)
33	CLA	8	310	29	69,73,73	1.17	9 (13%)	82,113,113	1.28	4 (4%)
36	LHG	A	412	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
45	A86	6	302	-	47,50,50	1.37	5 (10%)	51,76,76	10.82	24 (47%)
33	CLA	5	312	-	50,54,73	1.37	9 (18%)	59,90,113	1.39	4 (6%)
39	LMG	b	621	-	51,51,55	0.75	1 (1%)	59,59,63	1.34	7 (11%)
33	CLA	W	303	-	69,73,73	1.15	8 (11%)	82,113,113	1.30	8 (9%)
33	CLA	7	313	26	36,42,73	1.69	6 (16%)	45,73,113	1.64	7 (15%)
33	CLA	1	314	-	40,46,73	1.48	8 (20%)	52,80,113	1.44	5 (9%)
41	PL9	d	404	-	55,55,55	1.29	5 (9%)	68,69,69	1.46	11 (16%)
33	CLA	d	401	-	61,65,73	1.32	10 (16%)	74,103,113	1.33	8 (10%)
34	PHO	A	407	-	58,69,69	2.11	10 (17%)	55,99,99	1.45	7 (12%)
33	CLA	8	309	-	48,51,73	1.47	10 (20%)	56,86,113	1.53	5 (8%)
33	CLA	C	501	-	69,73,73	1.15	8 (11%)	82,113,113	1.27	6 (7%)
33	CLA	0	309	26	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
33	CLA	0	311	-	55,59,73	1.30	8 (14%)	64,96,113	1.45	6 (9%)
43	LMU	t	101	-	32,32,36	0.35	0	43,43,47	0.81	0
30	BCR	a	412	-	41,41,41	1.19	3 (7%)	56,56,56	1.17	4 (7%)
43	LMU	3	301	-	36,36,36	0.38	0	47,47,47	0.83	1 (2%)
33	CLA	2	310	29	69,73,73	1.17	8 (11%)	82,113,113	1.26	8 (9%)
37	SQD	T	103	-	52,54,54	0.94	2 (3%)	62,65,65	1.52	11 (17%)
33	CLA	1	312	-	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	LMG	3	316	-	31,31,55	0.93	0	39,39,63	1.26	5 (12%)
46	DD6	8	303	-	40,45,45	1.53	2 (5%)	51,67,67	2.06	13 (25%)
39	LMG	c	519	-	48,48,55	0.85	2 (4%)	56,56,63	1.29	6 (10%)
39	LMG	d	410	-	37,37,55	0.86	1 (2%)	45,45,63	1.29	6 (13%)
39	LMG	5	319	-	31,31,55	0.95	0	39,39,63	1.34	5 (12%)
33	CLA	1	316	29	40,46,73	1.48	8 (20%)	52,80,113	1.48	5 (9%)
33	CLA	9	305	-	45,49,73	1.42	8 (17%)	54,84,113	1.45	5 (9%)
45	A86	8	301	-	47,50,50	1.50	5 (10%)	51,76,76	2.56	19 (37%)
33	CLA	4	312	-	55,59,73	1.29	9 (16%)	64,96,113	1.36	5 (7%)
33	CLA	2	306	-	49,53,73	1.38	8 (16%)	58,89,113	1.44	5 (8%)
33	CLA	7	311	-	55,59,73	1.29	8 (14%)	64,96,113	1.44	6 (9%)
36	LHG	d	405	-	44,47,48	0.54	1 (2%)	44,51,54	1.18	5 (11%)
33	CLA	c	513	-	53,57,73	1.31	9 (16%)	61,93,113	1.44	7 (11%)
33	CLA	D	406	-	64,68,73	1.18	9 (14%)	76,107,113	1.38	8 (10%)
33	CLA	0	304	-	51,55,73	1.33	8 (15%)	60,91,113	1.43	5 (8%)
33	CLA	0	312	-	69,73,73	1.17	8 (11%)	82,113,113	1.23	5 (6%)
33	CLA	9	317	-	59,63,73	1.28	9 (15%)	70,101,113	1.35	5 (7%)
33	CLA	A	404	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	6 (7%)
38	DGD	a	401	-	54,54,67	1.00	4 (7%)	67,67,81	1.47	13 (19%)
33	CLA	B	605	-	69,73,73	1.14	9 (13%)	82,113,113	1.18	6 (7%)
38	DGD	C	517	-	57,57,67	0.99	2 (3%)	71,71,81	1.46	10 (14%)
37	SQD	a	413	-	52,54,54	0.94	3 (5%)	62,65,65	1.54	11 (17%)
31	OEX	a	405	1,3	0,15,15	-	-	-	-	-
44	KC1	5	315	-	49,53,53	1.36	5 (10%)	61,89,89	1.71	13 (21%)
30	BCR	K	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.26	6 (10%)
33	CLA	1	313	29	39,44,73	1.57	10 (25%)	50,77,113	1.58	7 (14%)
33	CLA	b	608	-	45,49,73	1.37	9 (20%)	54,84,113	1.53	7 (12%)
33	CLA	8	307	-	48,52,73	1.47	10 (20%)	59,88,113	1.44	6 (10%)
33	CLA	9	308	-	59,63,73	1.26	9 (15%)	70,101,113	1.35	6 (8%)
33	CLA	b	603	-	64,69,73	1.18	7 (10%)	73,106,113	1.07	7 (9%)
33	CLA	c	502	-	68,72,73	1.16	9 (13%)	80,111,113	1.26	5 (6%)
30	BCR	A	401	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	7 (12%)
33	CLA	9	315	-	40,46,73	1.46	8 (20%)	52,80,113	1.48	5 (9%)
39	LMG	D	410	-	46,46,55	0.81	1 (2%)	54,54,63	1.35	4 (7%)
45	A86	9	301	-	47,50,50	1.50	5 (10%)	51,76,76	2.59	18 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PHO	a	410	-	58,69,69	2.10	10 (17%)	55,99,99	1.49	7 (12%)
33	CLA	2	317	-	59,63,73	1.27	8 (13%)	70,101,113	1.32	5 (7%)
33	CLA	C	509	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	8 (9%)
45	A86	7	303	-	47,50,50	1.49	5 (10%)	51,76,76	2.60	15 (29%)
39	LMG	M	201	-	40,40,55	0.85	2 (5%)	48,48,63	1.32	5 (10%)
30	BCR	K	102	-	41,41,41	1.21	2 (4%)	56,56,56	1.22	7 (12%)
33	CLA	b	617	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
33	CLA	Z	101	-	55,59,73	1.30	9 (16%)	64,96,113	1.38	5 (7%)
33	CLA	3	307	-	69,73,73	1.17	9 (13%)	82,113,113	1.25	5 (6%)
33	CLA	7	308	26	45,49,73	1.39	9 (20%)	54,84,113	1.44	5 (9%)
33	CLA	b	609	-	69,73,73	1.14	9 (13%)	82,113,113	1.27	5 (6%)
33	CLA	3	303	-	69,73,73	1.17	9 (13%)	82,113,113	1.23	5 (6%)
45	A86	2	301	-	47,50,50	1.50	5 (10%)	51,76,76	2.58	18 (35%)
33	CLA	5	308	-	50,54,73	1.36	7 (14%)	59,90,113	1.37	4 (6%)
45	A86	8	302	-	47,50,50	1.49	5 (10%)	51,76,76	2.55	18 (35%)
33	CLA	3	319	-	59,63,73	1.26	9 (15%)	70,101,113	1.33	5 (7%)
37	SQD	D	403	-	52,54,54	0.95	3 (5%)	62,65,65	1.42	9 (14%)
33	CLA	b	615	-	68,72,73	1.15	9 (13%)	80,111,113	1.28	6 (7%)
39	LMG	D	404	-	40,40,55	0.82	1 (2%)	48,48,63	1.32	5 (10%)
42	HEM	v	201	18	50,50,50	1.32	7 (14%)	67,82,82	1.21	5 (7%)
33	CLA	1	311	29	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
33	CLA	B	611	-	68,72,73	1.15	9 (13%)	80,111,113	1.26	8 (10%)
33	CLA	4	310	-	50,54,73	1.36	9 (18%)	59,90,113	1.40	6 (10%)
33	CLA	H	103	26	45,51,73	1.40	8 (17%)	57,86,113	1.40	4 (7%)
30	BCR	b	618	-	41,41,41	1.23	3 (7%)	56,56,56	1.24	7 (12%)
33	CLA	D	402	-	63,67,73	1.20	9 (14%)	74,105,113	1.35	7 (9%)
33	CLA	b	607	-	69,73,73	1.14	8 (11%)	82,113,113	1.26	5 (6%)
33	CLA	0	310	-	49,53,73	1.38	7 (14%)	58,89,113	1.45	5 (8%)
33	CLA	B	612	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	6 (7%)
45	A86	3	314	-	47,50,50	1.46	5 (10%)	51,76,76	2.53	18 (35%)
36	LHG	0	315	-	27,27,48	0.93	2 (7%)	30,32,54	1.72	4 (13%)
48	ET4	7	302	-	41,43,43	2.02	11 (26%)	52,60,60	2.38	17 (32%)
30	BCR	a	414	-	41,41,41	1.13	2 (4%)	56,56,56	1.25	7 (12%)
33	CLA	b	616	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	5 (6%)
33	CLA	b	610	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	A86	5	302	-	47,50,50	1.48	7 (14%)	51,76,76	11.77	25 (49%)
33	CLA	6	307	-	57,61,73	1.29	7 (12%)	67,98,113	1.42	7 (10%)
33	CLA	2	316	29	40,46,73	1.48	7 (17%)	52,80,113	1.46	5 (9%)
33	CLA	0	307	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)
30	BCR	B	618	-	41,41,41	1.16	2 (4%)	56,56,56	1.18	4 (7%)
39	LMG	w	304	-	48,48,55	0.77	1 (2%)	56,56,63	1.33	6 (10%)
47	KC2	0	306	-	49,53,53	1.69	9 (18%)	60,89,89	2.09	18 (30%)
45	A86	5	307	-	47,50,50	1.45	6 (12%)	51,76,76	12.72	23 (45%)
33	CLA	C	512	-	68,72,73	1.15	9 (13%)	80,111,113	1.30	5 (6%)
33	CLA	7	305	26	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
33	CLA	0	308	-	45,49,73	1.40	8 (17%)	54,84,113	1.47	6 (11%)
33	CLA	B	609	-	69,73,73	1.13	8 (11%)	82,113,113	1.24	7 (8%)
33	CLA	0	305	26	69,73,73	1.17	8 (11%)	82,113,113	1.31	6 (7%)
33	CLA	c	505	-	69,73,73	1.15	9 (13%)	82,113,113	1.19	5 (6%)
33	CLA	B	607	-	45,49,73	1.38	9 (20%)	54,84,113	1.53	6 (11%)
33	CLA	7	314	-	45,51,73	1.38	9 (20%)	57,86,113	1.41	5 (8%)
33	CLA	B	603	-	68,72,73	1.15	9 (13%)	80,111,113	1.23	6 (7%)
38	DGD	C	516	-	56,56,67	0.98	2 (3%)	70,70,81	1.44	11 (15%)
37	SQD	7	317	-	46,48,54	1.04	5 (10%)	56,59,65	1.48	10 (17%)
33	CLA	1	310	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
47	KC2	5	310	-	49,53,53	1.68	9 (18%)	60,89,89	2.11	18 (30%)
33	CLA	8	314	-	40,46,73	1.47	8 (20%)	52,80,113	1.46	5 (9%)
33	CLA	5	311	-	59,63,73	1.26	6 (10%)	70,101,113	1.33	5 (7%)
47	KC2	7	306	-	49,53,53	1.69	9 (18%)	60,89,89	2.11	16 (26%)
35	BCT	A	410	40	3,3,3	1.18	0	2,3,3	4.08	2 (100%)
33	CLA	C	511	3	69,73,73	1.15	9 (13%)	82,113,113	1.29	5 (6%)
33	CLA	2	313	29	39,44,73	1.70	7 (17%)	50,77,113	1.46	8 (16%)
45	A86	0	301	-	47,50,50	1.62	8 (17%)	51,76,76	2.61	19 (37%)
30	BCR	C	514	-	41,41,41	1.17	2 (4%)	56,56,56	1.26	8 (14%)
37	SQD	T	101	-	38,40,54	1.15	4 (10%)	48,51,65	1.95	12 (25%)
42	HEM	e	101	6	50,50,50	1.60	9 (18%)	67,82,82	1.70	12 (17%)
33	CLA	d	409	-	63,67,73	1.20	9 (14%)	74,105,113	1.37	9 (12%)
33	CLA	2	315	-	40,46,73	1.48	8 (20%)	52,80,113	1.50	5 (9%)
33	CLA	6	311	-	50,54,73	1.37	7 (14%)	59,90,113	1.43	5 (8%)
46	DD6	8	304	-	40,45,45	1.58	2 (5%)	51,67,67	2.46	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CLA	z	101	-	55,59,73	1.32	9 (16%)	64,96,113	1.37	4 (6%)
33	CLA	0	313	-	36,42,73	1.69	6 (16%)	45,73,113	1.62	7 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	LMG	B	621	-	-	6/23/43/70	0/1/1/1
33	CLA	c	506	-	1/1/11/20	4/15/91/115	-
36	LHG	w	301	-	-	20/39/39/53	-
33	CLA	9	314	-	1/1/9/20	2/4/80/115	-
33	CLA	c	508	-	1/1/15/20	8/39/115/115	-
33	CLA	C	502	-	1/1/14/20	16/37/113/115	-
33	CLA	4	315	-	1/1/11/20	4/18/94/115	-
45	A86	4	301	-	-	9/34/90/90	0/3/3/3
33	CLA	2	312	-	1/1/11/20	4/15/91/115	-
36	LHG	3	317	33	-	12/31/31/53	-
33	CLA	6	315	-	1/1/10/20	4/10/86/115	-
33	CLA	c	507	-	1/1/15/20	15/39/115/115	-
33	CLA	b	605	-	1/1/14/20	4/35/111/115	-
33	CLA	B	604	-	1/1/14/20	8/35/111/115	-
39	LMG	C	520	-	-	19/43/63/70	0/1/1/1
30	BCR	k	101	-	-	24/29/63/63	0/2/2/2
38	DGD	C	518	-	-	13/44/84/95	0/2/2/2
33	CLA	3	302	-	1/1/15/20	17/39/115/115	-
45	A86	6	306	-	-	8/34/90/90	0/3/3/3
33	CLA	4	306	23	1/1/15/20	5/39/115/115	-
33	CLA	2	305	-	1/1/10/20	2/10/86/115	-
46	DD6	2	304	-	-	10/26/80/80	0/3/3/3
33	CLA	B	615	-	1/1/15/20	8/39/115/115	-
33	CLA	5	317	-	1/1/9/20	2/4/80/115	-
33	CLA	4	313	23	1/1/10/20	0/10/86/115	-
33	CLA	2	308	-	1/1/13/20	11/27/103/115	-
39	LMG	B	620	-	-	19/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LHG	H	104	-	-	20/46/46/53	-
33	CLA	B	606	-	1/1/15/20	7/39/115/115	-
33	CLA	C	513	-	1/1/11/20	6/20/96/115	-
45	A86	4	304	-	-	3/34/90/90	0/3/3/3
45	A86	1	301	-	-	5/34/90/90	0/3/3/3
33	CLA	2	309	-	1/1/11/20	4/13/89/115	-
33	CLA	a	407	-	1/1/15/20	8/39/115/115	-
39	LMG	q	302	-	-	18/32/52/70	0/1/1/1
30	BCR	k	102	-	-	4/29/63/63	0/2/2/2
34	PHO	A	406	-	-	13/37/103/103	0/5/6/6
33	CLA	B	614	-	1/1/14/20	11/37/113/115	-
46	DD6	9	304	-	-	10/26/80/80	0/3/3/3
33	CLA	3	309	36	1/1/12/20	6/23/99/115	-
33	CLA	3	311	-	1/1/10/20	2/10/86/115	-
45	A86	6	304	-	-	8/34/90/90	0/3/3/3
33	CLA	b	606	-	1/1/15/20	9/39/115/115	-
30	BCR	b	620	-	-	6/29/63/63	0/2/2/2
39	LMG	q	301	-	-	22/41/61/70	0/1/1/1
36	LHG	h	103	-	-	18/46/46/53	-
33	CLA	b	611	-	1/1/15/20	6/39/115/115	-
33	CLA	C	508	-	1/1/15/20	7/39/115/115	-
33	CLA	9	309	29	1/1/11/20	3/13/89/115	-
30	BCR	c	515	-	-	6/29/63/63	0/2/2/2
45	A86	5	304	-	-	8/34/90/90	0/3/3/3
37	SQD	L	101	-	-	23/49/69/69	0/1/1/1
33	CLA	C	507	-	1/1/15/20	15/39/115/115	-
33	CLA	c	511	3	1/1/15/20	7/39/115/115	-
33	CLA	1	309	-	1/1/11/20	5/13/89/115	-
38	DGD	3	320	-	-	20/40/40/95	-
45	A86	6	303	-	-	8/34/90/90	0/3/3/3
47	KC2	6	309	-	-	8/15/71/71	-
33	CLA	C	505	-	1/1/15/20	15/39/115/115	-
30	BCR	B	617	-	-	2/29/63/63	0/2/2/2
33	CLA	3	304	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	DGD	A	415	-	-	24/43/79/95	0/2/2/2
30	BCR	A	409	-	-	2/29/63/63	0/2/2/2
33	CLA	8	311	29	1/1/13/20	4/27/103/115	-
36	LHG	W	302	-	-	23/39/39/53	-
41	PL9	D	408	-	-	5/53/73/73	0/1/1/1
33	CLA	5	309	24	1/1/13/20	5/27/103/115	-
45	A86	2	302	-	-	8/34/90/90	0/3/3/3
36	LHG	A	414	-	-	17/53/53/53	-
39	LMG	C	519	-	-	18/41/61/70	0/1/1/1
33	CLA	9	307	-	1/1/11/20	5/13/89/115	-
33	CLA	8	306	29	1/1/11/20	3/15/91/115	-
37	SQD	l	101	-	-	21/49/69/69	0/1/1/1
33	CLA	3	308	22	1/1/15/20	14/39/115/115	-
36	LHG	D	411	-	-	19/46/46/53	-
39	LMG	b	622	-	-	4/23/43/70	0/1/1/1
39	LMG	C	522	-	-	7/16/36/70	0/1/1/1
48	ET4	0	302	-	-	13/25/67/67	0/2/2/2
45	A86	9	302	-	-	8/34/90/90	0/3/3/3
38	DGD	c	517	-	-	22/45/85/95	0/2/2/2
33	CLA	7	310	26	1/1/11/20	6/15/91/115	-
38	DGD	c	516	-	-	15/44/84/95	0/2/2/2
33	CLA	b	602	-	1/1/11/20	6/18/94/115	-
47	KC2	4	307	-	-	7/15/71/71	-
33	CLA	8	305	-	1/1/10/20	2/10/86/115	-
33	CLA	8	308	-	1/1/13/20	11/27/103/115	-
43	LMU	T	102	-	-	9/17/57/61	0/2/2/2
33	CLA	1	308	-	1/1/13/20	7/27/103/115	-
33	CLA	b	604	-	1/1/14/20	12/37/113/115	-
36	LHG	A	411	-	-	15/47/47/53	-
33	CLA	3	313	-	1/1/14/20	15/35/111/115	-
36	LHG	D	409	-	-	18/47/51/53	-
45	A86	6	305	-	-	8/34/90/90	0/3/3/3
33	CLA	B	602	-	1/1/12/20	11/29/107/115	-
45	A86	4	302	-	-	9/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	4	308	-	1/1/15/20	8/39/115/115	-
33	CLA	b	613	-	1/1/15/20	15/39/115/115	-
37	SQD	A	413	-	-	13/35/55/69	0/1/1/1
36	LHG	a	403	-	-	13/47/47/53	-
43	LMU	4	317	-	-	14/21/61/61	0/2/2/2
46	DD6	9	303	-	-	4/26/80/80	0/3/3/3
33	CLA	2	311	29	1/1/13/20	6/27/103/115	-
33	CLA	4	309	23	1/1/15/20	3/39/115/115	-
33	CLA	4	311	23	1/1/14/20	13/33/109/115	-
45	A86	7	301	-	-	8/34/90/90	0/3/3/3
39	LMG	m	201	-	-	16/35/55/70	0/1/1/1
39	LMG	Q	301	-	-	16/32/52/70	0/1/1/1
30	BCR	C	515	-	-	9/29/63/63	0/2/2/2
33	CLA	6	316	-	1/1/9/20	2/8/80/115	-
45	A86	5	306	-	-	8/34/90/90	0/3/3/3
33	CLA	3	312	-	1/1/13/20	10/29/105/115	-
33	CLA	a	408	-	1/1/11/20	4/20/96/115	-
37	SQD	B	622	-	-	22/49/69/69	0/1/1/1
36	LHG	4	318	-	-	31/53/53/53	-
37	SQD	t	102	-	-	18/34/54/69	0/1/1/1
33	CLA	d	402	-	1/1/14/20	9/33/109/115	-
36	LHG	b	601	-	-	19/53/53/53	-
37	SQD	i	101	-	-	10/35/55/69	0/1/1/1
33	CLA	1	305	-	1/1/10/20	4/10/86/115	-
33	CLA	9	316	29	1/1/9/20	2/4/80/115	-
33	CLA	6	313	25	1/1/11/20	5/17/93/115	-
38	DGD	h	102	-	-	16/51/91/95	0/2/2/2
46	DD6	1	304	-	-	7/26/80/80	0/3/3/3
33	CLA	B	613	-	1/1/15/20	13/39/115/115	-
38	DGD	H	102	-	-	16/51/91/95	0/2/2/2
33	CLA	3	305	-	1/1/11/20	8/19/95/115	-
36	LHG	7	316	-	-	15/29/29/53	-
33	CLA	7	307	-	1/1/15/20	13/39/115/115	-
30	BCR	c	514	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	2	314	-	1/1/9/20	2/4/80/115	-
33	CLA	8	315	29	1/1/9/20	0/4/80/115	-
33	CLA	b	614	-	1/1/15/20	11/39/115/115	-
33	CLA	6	312	-	1/1/15/20	11/39/115/115	-
37	SQD	0	316	-	-	13/43/63/69	0/1/1/1
45	A86	5	303	-	-	8/34/90/90	0/3/3/3
36	LHG	3	318	-	-	21/53/53/53	-
39	LMG	7	315	-	-	26/50/70/70	0/1/1/1
33	CLA	1	315	-	1/1/9/20	0/4/80/115	-
33	CLA	b	612	-	1/1/14/20	6/37/113/115	-
33	CLA	8	312	-	1/1/11/20	4/15/91/115	-
45	A86	0	303	-	-	3/34/90/90	0/3/3/3
33	CLA	3	306	-	1/1/15/20	16/39/115/115	-
43	LMU	w	302	-	-	13/21/61/61	0/2/2/2
36	LHG	a	404	-	-	26/53/53/53	-
42	HEM	V	201	18	-	6/14/54/54	-
33	CLA	c	504	-	1/1/14/20	11/37/113/115	-
45	A86	5	305	-	-	8/33/89/90	0/3/3/3
33	CLA	8	316	29	1/1/9/20	2/4/80/115	-
30	BCR	b	619	-	-	5/29/63/63	0/2/2/2
33	CLA	A	405	-	1/1/11/20	3/20/96/115	-
44	KC1	3	310	-	-	9/15/71/71	-
39	LMG	0	314	-	-	20/37/57/70	0/1/1/1
33	CLA	9	311	29	1/1/13/20	6/27/103/115	-
39	LMG	b	623	-	-	22/35/55/70	0/1/1/1
33	CLA	c	501	-	1/1/15/20	19/39/115/115	-
33	CLA	B	608	-	1/1/15/20	5/39/115/115	-
33	CLA	c	510	-	1/1/15/20	10/39/115/115	-
30	BCR	B	619	-	-	6/29/63/63	0/2/2/2
33	CLA	w	303	-	1/1/15/20	18/39/115/115	-
33	CLA	A	408	-	1/1/14/20	7/33/109/115	-
33	CLA	9	313	-	1/1/9/20	2/2/78/115	-
33	CLA	5	314	24	1/1/13/20	4/27/103/115	-
33	CLA	7	304	-	1/1/11/20	7/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	c	503	-	1/1/15/20	12/39/115/115	-
42	HEM	F	101	6	-	3/14/54/54	-
33	CLA	c	512	-	1/1/14/20	10/37/113/115	-
33	CLA	1	306	29	1/1/11/20	4/15/91/115	-
39	LMG	c	520	-	-	7/21/41/70	0/1/1/1
33	CLA	1	307	-	1/1/11/20	3/13/89/115	-
39	LMG	d	406	-	-	17/41/61/70	0/1/1/1
39	LMG	W	301	-	-	18/43/63/70	0/1/1/1
33	CLA	9	312	-	1/1/11/20	5/15/91/115	-
30	BCR	h	101	-	-	3/29/63/63	0/2/2/2
33	CLA	B	601	-	1/1/11/20	7/18/94/115	-
44	KC1	6	314	25	-	7/15/71/71	-
46	DD6	2	303	-	-	4/26/80/80	0/3/3/3
33	CLA	9	306	-	1/1/11/20	4/15/91/115	-
45	A86	6	301	-	-	7/34/90/90	0/3/3/3
30	BCR	H	101	-	-	2/29/63/63	0/2/2/2
33	CLA	C	504	-	1/1/14/20	12/37/113/115	-
36	LHG	d	407	-	-	18/46/46/53	-
33	CLA	4	314	23	1/1/13/20	4/29/105/115	-
33	CLA	8	313	29	1/1/9/20	0/2/78/115	-
33	CLA	c	509	-	1/1/15/20	5/39/115/115	-
33	CLA	C	503	-	1/1/15/20	13/39/115/115	-
38	DGD	c	518	-	-	15/44/84/95	0/2/2/2
30	BCR	d	403	-	-	4/29/63/63	0/2/2/2
33	CLA	4	305	-	1/1/13/20	5/27/103/115	-
33	CLA	4	316	-	1/1/12/20	4/24/100/115	-
46	DD6	3	315	-	-	5/26/80/80	0/3/3/3
45	A86	5	301	-	-	10/34/90/90	0/3/3/3
46	DD6	4	303	-	-	3/26/80/80	0/3/3/3
33	CLA	7	312	-	1/1/15/20	15/39/115/115	-
33	CLA	B	616	-	1/1/15/20	12/39/115/115	-
36	LHG	5	318	-	-	13/34/34/53	-
39	LMG	C	521	-	-	4/21/41/70	0/1/1/1
30	BCR	D	407	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	2	307	-	1/1/11/20	6/13/89/115	-
33	CLA	6	308	25	1/1/12/20	3/26/102/115	-
33	CLA	C	506	-	1/1/11/20	4/15/91/115	-
33	CLA	D	405	-	1/1/13/20	5/28/104/115	-
33	CLA	a	411	-	1/1/14/20	4/33/109/115	-
33	CLA	5	313	-	1/1/15/20	12/39/115/115	-
33	CLA	C	510	-	1/1/15/20	6/39/115/115	-
33	CLA	B	610	-	1/1/15/20	5/39/115/115	-
33	CLA	9	310	29	1/1/15/20	14/39/115/115	-
33	CLA	5	316	-	1/1/10/20	2/10/86/115	-
33	CLA	6	310	-	1/1/12/20	3/24/100/115	-
45	A86	1	302	-	-	8/34/90/90	0/3/3/3
46	DD6	1	303	-	-	4/26/80/80	0/3/3/3
34	PHO	a	409	-	-	12/37/103/103	0/5/6/6
43	LMU	5	320	-	-	8/17/57/61	0/2/2/2
33	CLA	7	309	26	1/1/15/20	16/39/115/115	-
33	CLA	8	310	29	1/1/15/20	18/39/115/115	-
36	LHG	A	412	-	-	26/53/53/53	-
45	A86	6	302	-	-	8/34/90/90	0/3/3/3
33	CLA	5	312	-	1/1/11/20	9/17/93/115	-
39	LMG	b	621	-	-	21/46/66/70	0/1/1/1
33	CLA	W	303	-	1/1/15/20	17/39/115/115	-
33	CLA	7	313	26	1/1/8/20	0/2/74/115	-
33	CLA	1	314	-	1/1/9/20	2/4/80/115	-
41	PL9	d	404	-	-	7/53/73/73	0/1/1/1
33	CLA	d	401	-	1/1/13/20	5/28/104/115	-
34	PHO	A	407	-	-	8/37/103/103	0/5/6/6
33	CLA	8	309	-	1/1/11/20	3/13/89/115	-
33	CLA	C	501	-	1/1/15/20	19/39/115/115	-
33	CLA	0	309	26	1/1/15/20	13/39/115/115	-
33	CLA	0	311	-	1/1/12/20	7/23/99/115	-
43	LMU	t	101	-	-	12/17/57/61	0/2/2/2
30	BCR	a	412	-	-	3/29/63/63	0/2/2/2
43	LMU	3	301	-	-	17/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	2	310	29	1/1/15/20	12/39/115/115	-
37	SQD	T	103	-	-	22/49/69/69	0/1/1/1
33	CLA	1	312	-	1/1/11/20	6/15/91/115	-
39	LMG	3	316	-	-	6/26/46/70	0/1/1/1
46	DD6	8	303	-	-	4/26/80/80	0/3/3/3
39	LMG	c	519	-	-	21/43/63/70	0/1/1/1
39	LMG	d	410	-	-	18/32/52/70	0/1/1/1
39	LMG	5	319	-	-	13/26/46/70	0/1/1/1
33	CLA	1	316	29	1/1/9/20	2/4/80/115	-
33	CLA	9	305	-	1/1/10/20	2/10/86/115	-
45	A86	8	301	-	-	8/34/90/90	0/3/3/3
33	CLA	4	312	-	1/1/12/20	7/23/99/115	-
33	CLA	2	306	-	1/1/11/20	5/15/91/115	-
33	CLA	7	311	-	1/1/12/20	10/23/99/115	-
36	LHG	d	405	-	-	21/47/51/53	-
33	CLA	c	513	-	1/1/11/20	6/20/96/115	-
33	CLA	D	406	-	1/1/14/20	9/33/109/115	-
33	CLA	0	304	-	1/1/11/20	9/18/94/115	-
33	CLA	0	312	-	1/1/15/20	17/39/115/115	-
33	CLA	9	317	-	1/1/13/20	7/27/103/115	-
33	CLA	A	404	-	1/1/15/20	9/39/115/115	-
38	DGD	a	401	-	-	28/43/79/95	0/2/2/2
33	CLA	B	605	-	1/1/15/20	14/39/115/115	-
38	DGD	C	517	-	-	18/45/85/95	0/2/2/2
37	SQD	a	413	-	-	19/49/69/69	0/1/1/1
44	KC1	5	315	-	-	7/15/71/71	-
30	BCR	K	101	-	-	18/29/63/63	0/2/2/2
33	CLA	1	313	29	1/1/9/20	2/2/78/115	-
33	CLA	b	608	-	1/1/10/20	2/10/86/115	-
33	CLA	8	307	-	1/1/11/20	5/13/89/115	-
33	CLA	9	308	-	1/1/13/20	11/27/103/115	-
33	CLA	b	603	-	1/1/12/20	7/29/107/115	-
33	CLA	c	502	-	1/1/14/20	13/37/113/115	-
30	BCR	A	401	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	9	315	-	1/1/9/20	2/4/80/115	-
39	LMG	D	410	-	-	15/41/61/70	0/1/1/1
45	A86	9	301	-	-	7/34/90/90	0/3/3/3
34	PHO	a	410	-	-	3/37/103/103	0/5/6/6
33	CLA	2	317	-	1/1/13/20	8/27/103/115	-
33	CLA	C	509	-	1/1/15/20	8/39/115/115	-
45	A86	7	303	-	-	6/34/90/90	0/3/3/3
39	LMG	M	201	-	-	15/35/55/70	0/1/1/1
30	BCR	K	102	-	-	4/29/63/63	0/2/2/2
33	CLA	b	617	-	1/1/15/20	18/39/115/115	-
33	CLA	Z	101	-	1/1/12/20	4/23/99/115	-
33	CLA	3	307	-	1/1/15/20	13/39/115/115	-
33	CLA	7	308	26	1/1/10/20	3/10/86/115	-
33	CLA	b	609	-	1/1/15/20	4/39/115/115	-
33	CLA	3	303	-	1/1/15/20	13/39/115/115	-
45	A86	2	301	-	-	7/34/90/90	0/3/3/3
33	CLA	5	308	-	1/1/11/20	6/17/93/115	-
45	A86	8	302	-	-	8/34/90/90	0/3/3/3
33	CLA	3	319	-	1/1/13/20	9/27/103/115	-
37	SQD	D	403	-	-	21/49/69/69	0/1/1/1
33	CLA	b	615	-	1/1/14/20	12/37/113/115	-
39	LMG	D	404	-	-	20/35/55/70	0/1/1/1
42	HEM	v	201	18	-	6/14/54/54	-
33	CLA	1	311	29	1/1/13/20	5/27/103/115	-
33	CLA	B	611	-	1/1/14/20	10/37/113/115	-
33	CLA	4	310	-	1/1/11/20	5/17/93/115	-
33	CLA	H	103	26	1/1/10/20	4/11/87/115	-
30	BCR	b	618	-	-	2/29/63/63	0/2/2/2
33	CLA	D	402	-	1/1/13/20	2/32/108/115	-
33	CLA	b	607	-	1/1/15/20	8/39/115/115	-
33	CLA	0	310	-	1/1/11/20	8/15/91/115	-
33	CLA	B	612	-	1/1/15/20	12/39/115/115	-
45	A86	3	314	-	-	7/34/90/90	0/3/3/3
36	LHG	0	315	-	-	17/29/29/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	ET4	7	302	-	-	11/25/67/67	0/2/2/2
30	BCR	a	414	-	-	4/29/63/63	0/2/2/2
33	CLA	b	616	-	1/1/15/20	7/39/115/115	-
33	CLA	b	610	-	1/1/15/20	9/39/115/115	-
45	A86	5	302	-	-	8/34/90/90	0/3/3/3
33	CLA	6	307	-	1/1/12/20	4/25/101/115	-
33	CLA	2	316	29	1/1/9/20	2/4/80/115	-
33	CLA	0	307	-	1/1/15/20	14/39/115/115	-
30	BCR	B	618	-	-	3/29/63/63	0/2/2/2
39	LMG	w	304	-	-	20/43/63/70	0/1/1/1
47	KC2	0	306	-	-	10/15/71/71	-
45	A86	5	307	-	-	8/34/90/90	0/3/3/3
33	CLA	C	512	-	1/1/14/20	14/37/113/115	-
33	CLA	7	305	26	1/1/15/20	18/39/115/115	-
33	CLA	0	308	-	1/1/10/20	2/10/86/115	-
33	CLA	B	609	-	1/1/15/20	10/39/115/115	-
33	CLA	0	305	26	1/1/15/20	16/39/115/115	-
33	CLA	c	505	-	1/1/15/20	15/39/115/115	-
33	CLA	B	607	-	1/1/10/20	2/10/86/115	-
33	CLA	7	314	-	1/1/10/20	4/11/87/115	-
33	CLA	B	603	-	1/1/14/20	10/37/113/115	-
38	DGD	C	516	-	-	20/44/84/95	0/2/2/2
37	SQD	7	317	-	-	13/43/63/69	0/1/1/1
33	CLA	1	310	-	1/1/15/20	16/39/115/115	-
47	KC2	5	310	-	-	6/15/71/71	-
33	CLA	8	314	-	1/1/9/20	2/4/80/115	-
33	CLA	5	311	-	1/1/13/20	5/27/103/115	-
47	KC2	7	306	-	-	8/15/71/71	-
33	CLA	C	511	3	1/1/15/20	7/39/115/115	-
33	CLA	2	313	29	-	0/2/78/115	-
45	A86	0	301	-	-	8/34/90/90	0/3/3/3
30	BCR	C	514	-	-	0/29/63/63	0/2/2/2
37	SQD	T	101	-	-	17/34/54/69	0/1/1/1
42	HEM	e	101	6	-	9/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	d	409	-	1/1/13/20	4/32/108/115	-
33	CLA	2	315	-	1/1/9/20	2/4/80/115	-
33	CLA	6	311	-	1/1/11/20	11/17/93/115	-
46	DD6	8	304	-	-	10/26/80/80	0/3/3/3
33	CLA	z	101	-	1/1/12/20	6/23/99/115	-
33	CLA	0	313	-	1/1/8/20	0/2/74/115	-

All (2089) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	410	PHO	C1B-C2B	9.44	1.49	1.39
34	A	407	PHO	C1B-C2B	9.43	1.49	1.39
34	a	409	PHO	C1B-C2B	9.33	1.49	1.39
34	A	406	PHO	C1B-C2B	9.33	1.49	1.39
46	1	304	DD6	C30-C31	-8.85	1.25	1.42
46	9	304	DD6	C30-C31	-8.66	1.25	1.42
46	2	304	DD6	C30-C31	-8.66	1.25	1.42
46	8	304	DD6	C30-C31	-8.65	1.25	1.42
46	3	315	DD6	C30-C31	-8.35	1.26	1.42
46	9	303	DD6	C30-C31	-8.33	1.26	1.42
46	2	303	DD6	C30-C31	-8.31	1.26	1.42
34	a	410	PHO	C3B-C4B	8.30	1.49	1.41
46	4	303	DD6	C30-C31	-8.23	1.26	1.42
34	A	407	PHO	C3B-C4B	8.22	1.49	1.41
34	a	409	PHO	C3B-C4B	8.21	1.49	1.41
46	1	303	DD6	C30-C31	-8.20	1.26	1.42
46	8	303	DD6	C30-C31	-8.16	1.26	1.42
34	A	406	PHO	C3B-C4B	8.13	1.49	1.41
45	5	305	A86	O4-C38	5.93	1.45	1.33
44	6	314	KC1	MG-ND	-5.18	1.95	2.05
48	0	302	ET4	C19-C18	5.16	1.57	1.46
47	6	309	KC2	CHD-C4C	5.16	1.48	1.38
44	5	315	KC1	MG-ND	-5.06	1.95	2.05
33	0	313	CLA	C1B-C2B	5.02	1.49	1.41
42	e	101	HEM	FE-NB	5.01	2.10	1.94
33	6	316	CLA	C1B-C2B	4.99	1.49	1.41
47	0	306	KC2	CHD-C4C	4.99	1.48	1.38
33	7	313	CLA	C1B-C2B	4.96	1.49	1.41
47	7	306	KC2	CHD-C4C	4.96	1.48	1.38
45	5	302	A86	O4-C38	4.89	1.46	1.35
45	5	304	A86	O4-C38	4.85	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	6	302	A86	O4-C38	4.84	1.45	1.35
44	6	314	KC1	MG-NB	-4.84	1.96	2.05
45	6	304	A86	O4-C38	4.83	1.45	1.35
45	5	307	A86	O4-C38	4.82	1.45	1.35
45	6	306	A86	O4-C38	4.82	1.45	1.35
42	V	201	HEM	FE-NB	4.81	2.09	1.94
45	4	301	A86	O4-C38	4.81	1.45	1.35
44	3	310	KC1	MG-ND	-4.80	1.96	2.05
45	3	314	A86	O4-C38	4.78	1.45	1.35
45	4	302	A86	O4-C38	4.78	1.45	1.35
44	5	315	KC1	MG-NB	-4.78	1.96	2.05
47	5	310	KC2	CHD-C4C	4.78	1.48	1.38
45	1	301	A86	O4-C38	4.77	1.45	1.35
45	5	306	A86	O4-C38	4.77	1.45	1.35
45	2	301	A86	O4-C38	4.76	1.45	1.35
45	0	303	A86	O4-C38	4.76	1.45	1.35
45	6	301	A86	O4-C38	4.75	1.45	1.35
45	7	301	A86	O4-C38	4.75	1.45	1.35
45	6	305	A86	O4-C38	4.74	1.45	1.35
45	0	301	A86	O4-C38	4.73	1.45	1.35
45	5	303	A86	O4-C38	4.73	1.45	1.35
45	5	301	A86	O4-C38	4.72	1.45	1.35
45	9	301	A86	O4-C38	4.72	1.45	1.35
45	4	304	A86	O4-C38	4.71	1.45	1.35
47	4	307	KC2	CHD-C4C	4.71	1.47	1.38
45	1	302	A86	O4-C38	4.70	1.45	1.35
45	8	302	A86	O4-C38	4.69	1.45	1.35
45	9	302	A86	O4-C38	4.68	1.45	1.35
45	7	303	A86	O4-C38	4.68	1.45	1.35
45	2	302	A86	O4-C38	4.67	1.45	1.35
33	6	316	CLA	C3B-C4B	4.67	1.49	1.39
33	7	313	CLA	C3B-C4B	4.66	1.49	1.39
45	8	301	A86	O4-C38	4.65	1.45	1.35
45	2	302	A86	C30-C31	-4.64	1.25	1.30
45	9	302	A86	C30-C31	-4.62	1.25	1.30
33	0	313	CLA	C3B-C4B	4.60	1.49	1.39
48	7	302	ET4	C08-C07	4.58	1.46	1.33
45	1	302	A86	C30-C31	-4.57	1.25	1.30
45	6	303	A86	O4-C38	4.56	1.45	1.35
48	0	302	ET4	C08-C07	4.56	1.46	1.33
45	8	302	A86	C30-C31	-4.54	1.25	1.30
48	7	302	ET4	C19-C18	4.54	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	0	301	A86	C20-C15	4.49	1.53	1.48
33	2	313	CLA	C4B-NB	4.48	1.43	1.37
45	7	301	A86	C20-C15	4.44	1.53	1.48
45	6	303	A86	C30-C31	-4.44	1.25	1.30
44	3	310	KC1	MG-NB	-4.42	1.97	2.05
45	2	301	A86	C30-C31	-4.41	1.25	1.30
45	9	301	A86	C30-C31	-4.39	1.25	1.30
41	D	408	PL9	C3-C4	-4.35	1.42	1.49
45	0	301	A86	C30-C31	-4.31	1.25	1.30
45	5	301	A86	C30-C31	-4.28	1.25	1.30
45	5	305	A86	C30-C31	-4.28	1.25	1.30
45	0	303	A86	C20-C15	4.26	1.53	1.48
47	6	309	KC2	CHC-C1C	4.26	1.48	1.39
45	7	301	A86	C30-C31	-4.25	1.25	1.30
45	7	303	A86	C20-C15	4.25	1.53	1.48
45	4	301	A86	C30-C31	-4.24	1.25	1.30
45	8	301	A86	C30-C31	-4.22	1.25	1.30
47	6	309	KC2	CHC-C4B	4.21	1.46	1.38
45	6	301	A86	C30-C31	-4.20	1.25	1.30
45	9	301	A86	C20-C15	4.19	1.53	1.48
47	6	309	KC2	MG-NB	-4.18	1.97	2.05
45	6	305	A86	C30-C31	-4.18	1.25	1.30
45	5	306	A86	C30-C31	-4.18	1.25	1.30
48	0	302	ET4	C12-C13	4.17	1.54	1.46
45	5	302	A86	C30-C31	-4.17	1.25	1.30
47	6	309	KC2	MG-ND	-4.17	1.97	2.05
45	4	304	A86	C20-C15	4.16	1.53	1.48
45	2	301	A86	C20-C15	4.16	1.53	1.48
48	0	302	ET4	C04-C03	4.15	1.59	1.52
45	5	307	A86	C30-C31	-4.15	1.25	1.30
48	7	302	ET4	C12-C13	4.12	1.54	1.46
45	4	302	A86	C30-C31	-4.11	1.25	1.30
30	b	618	BCR	C1-C6	-4.10	1.48	1.53
48	0	302	ET4	C08-C09	4.10	1.54	1.46
47	5	310	KC2	CHC-C4B	4.09	1.46	1.38
45	6	304	A86	C30-C31	-4.08	1.25	1.30
30	K	102	BCR	C1-C6	-4.05	1.48	1.53
45	9	302	A86	C30-C29	-4.04	1.25	1.31
47	5	310	KC2	MG-ND	-4.04	1.97	2.05
45	2	302	A86	C30-C29	-4.04	1.25	1.31
47	0	306	KC2	CHC-C1C	4.04	1.48	1.39
30	B	617	BCR	C1-C6	-4.04	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	2	302	A86	C20-C15	4.03	1.53	1.48
45	8	302	A86	C30-C29	-4.03	1.25	1.31
48	7	302	ET4	C08-C09	4.03	1.54	1.46
45	0	303	A86	C30-C31	-4.03	1.25	1.30
47	0	306	KC2	MG-ND	-4.02	1.97	2.05
47	7	306	KC2	MG-ND	-4.02	1.97	2.05
45	5	303	A86	C30-C31	-4.01	1.25	1.30
45	8	301	A86	C20-C15	4.00	1.53	1.48
45	1	302	A86	C30-C29	-3.99	1.25	1.31
33	2	313	CLA	C1D-ND	3.99	1.43	1.37
45	1	301	A86	C30-C31	-3.99	1.25	1.30
42	e	101	HEM	FE-NC	3.99	2.08	1.95
45	9	302	A86	C20-C15	3.99	1.53	1.48
45	5	304	A86	C30-C31	-3.98	1.25	1.30
39	C	522	LMG	C4-C5	3.98	1.61	1.53
47	0	306	KC2	CHC-C4B	3.96	1.46	1.38
47	5	310	KC2	CHC-C1C	3.95	1.48	1.39
47	7	306	KC2	CHC-C1C	3.92	1.48	1.39
45	7	301	A86	C30-C29	-3.91	1.25	1.31
41	D	408	PL9	C6-C1	-3.90	1.42	1.48
45	6	303	A86	C30-C29	-3.90	1.25	1.31
47	7	306	KC2	CHC-C4B	3.88	1.46	1.38
41	d	404	PL9	C3-C4	-3.88	1.43	1.49
47	7	306	KC2	MG-NB	-3.87	1.98	2.05
47	0	306	KC2	MG-NB	-3.86	1.98	2.05
45	5	301	A86	C30-C29	-3.84	1.25	1.31
45	6	306	A86	C30-C31	-3.83	1.26	1.30
45	8	301	A86	C30-C29	-3.82	1.25	1.31
45	4	301	A86	C20-C15	3.82	1.53	1.48
30	B	619	BCR	C1-C6	-3.82	1.48	1.53
45	5	307	A86	C30-C29	-3.82	1.25	1.31
47	5	310	KC2	MG-NB	-3.81	1.98	2.05
45	0	301	A86	C30-C29	-3.80	1.25	1.31
45	6	301	A86	C30-C29	-3.80	1.25	1.31
42	V	201	HEM	FE-NC	3.79	2.07	1.95
45	5	306	A86	C30-C29	-3.79	1.25	1.31
45	6	305	A86	C30-C29	-3.79	1.25	1.31
30	k	102	BCR	C1-C6	-3.78	1.48	1.53
45	5	305	A86	C30-C29	-3.78	1.25	1.31
30	b	620	BCR	C1-C6	-3.78	1.48	1.53
45	7	303	A86	C30-C31	-3.77	1.26	1.30
45	4	301	A86	C30-C29	-3.76	1.25	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	5	302	A86	C30-C29	-3.75	1.25	1.31
47	4	307	KC2	MG-ND	-3.75	1.98	2.05
45	4	302	A86	C30-C29	-3.73	1.25	1.31
30	b	619	BCR	C1-C6	-3.73	1.49	1.53
45	3	314	A86	C20-C15	3.72	1.52	1.48
45	5	303	A86	C30-C29	-3.72	1.25	1.31
30	a	412	BCR	C1-C6	-3.71	1.49	1.53
34	a	409	PHO	C4D-CHA	3.71	1.45	1.39
45	6	304	A86	C30-C29	-3.70	1.25	1.31
30	D	407	BCR	C30-C25	-3.69	1.49	1.53
42	V	201	HEM	C1B-NB	-3.68	1.33	1.40
45	4	304	A86	C30-C31	-3.67	1.26	1.30
45	6	302	A86	C30-C31	-3.67	1.26	1.30
41	d	404	PL9	C6-C1	-3.67	1.42	1.48
34	A	406	PHO	C1D-C2D	3.67	1.43	1.39
45	3	314	A86	C30-C31	-3.66	1.26	1.30
45	5	305	A86	C20-C15	3.66	1.52	1.48
45	6	306	A86	C20-C15	3.65	1.52	1.48
30	A	409	BCR	C1-C6	-3.65	1.49	1.53
45	0	303	A86	C30-C29	-3.64	1.26	1.31
48	7	302	ET4	C04-C03	3.64	1.58	1.52
45	1	301	A86	C30-C29	-3.64	1.26	1.31
34	A	407	PHO	C4D-CHA	3.63	1.45	1.39
33	5	309	CLA	C1D-ND	3.63	1.42	1.37
30	B	617	BCR	C30-C25	-3.63	1.49	1.53
33	2	306	CLA	C1D-ND	3.63	1.42	1.37
33	2	312	CLA	C1D-ND	3.62	1.42	1.37
33	1	309	CLA	C1D-ND	3.62	1.42	1.37
33	1	311	CLA	C1D-ND	3.62	1.42	1.37
30	B	618	BCR	C1-C6	-3.62	1.49	1.53
34	A	406	PHO	C4D-CHA	3.61	1.44	1.39
34	A	407	PHO	C1D-C2D	3.61	1.43	1.39
30	a	414	BCR	C1-C6	-3.60	1.49	1.53
45	5	304	A86	C20-C15	3.60	1.52	1.48
45	5	303	A86	C20-C15	3.60	1.52	1.48
33	6	307	CLA	C1D-ND	3.59	1.42	1.37
33	2	305	CLA	C1D-ND	3.59	1.42	1.37
34	a	409	PHO	C1D-C2D	3.59	1.43	1.39
33	6	313	CLA	C1D-ND	3.58	1.42	1.37
30	K	101	BCR	C1-C6	-3.57	1.49	1.53
33	5	314	CLA	C1D-ND	3.56	1.42	1.37
30	C	514	BCR	C30-C25	-3.56	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	6	308	CLA	C1D-ND	3.56	1.42	1.37
30	D	407	BCR	C1-C6	-3.56	1.49	1.53
45	5	304	A86	C30-C29	-3.55	1.26	1.31
30	A	401	BCR	C1-C6	-3.55	1.49	1.53
33	9	316	CLA	C1D-ND	3.55	1.42	1.37
45	5	301	A86	C20-C15	3.55	1.52	1.48
33	1	312	CLA	C1D-ND	3.54	1.42	1.37
33	1	306	CLA	C1D-ND	3.54	1.42	1.37
33	z	101	CLA	C1D-ND	3.54	1.42	1.37
42	V	201	HEM	C4D-ND	-3.54	1.34	1.40
33	9	311	CLA	C1D-ND	3.54	1.42	1.37
33	1	305	CLA	C1D-ND	3.54	1.42	1.37
45	5	306	A86	C20-C15	3.54	1.52	1.48
30	b	618	BCR	C30-C25	-3.54	1.49	1.53
33	8	312	CLA	C1D-ND	3.53	1.42	1.37
34	a	410	PHO	C1D-C2D	3.53	1.43	1.39
30	k	101	BCR	C1-C6	-3.53	1.49	1.53
30	c	514	BCR	C30-C25	-3.53	1.49	1.53
33	2	307	CLA	C1D-ND	3.52	1.42	1.37
33	8	314	CLA	C1D-ND	3.52	1.42	1.37
33	9	309	CLA	C1D-ND	3.52	1.42	1.37
33	1	314	CLA	C1D-ND	3.52	1.42	1.37
45	6	302	A86	C30-C29	-3.52	1.26	1.31
33	3	312	CLA	C1D-ND	3.52	1.42	1.37
33	1	316	CLA	C1D-ND	3.52	1.42	1.37
33	5	317	CLA	C1D-ND	3.51	1.42	1.37
33	1	308	CLA	C1D-ND	3.51	1.42	1.37
33	2	310	CLA	C1D-ND	3.51	1.42	1.37
45	5	302	A86	C20-C15	3.50	1.52	1.48
33	9	307	CLA	C1D-ND	3.50	1.42	1.37
33	1	315	CLA	C1D-ND	3.50	1.42	1.37
45	3	314	A86	C30-C29	-3.50	1.26	1.31
45	6	306	A86	C30-C29	-3.50	1.26	1.31
33	5	316	CLA	C1D-ND	3.50	1.42	1.37
33	0	310	CLA	C1D-ND	3.50	1.42	1.37
33	4	315	CLA	C1D-ND	3.50	1.42	1.37
47	6	309	KC2	CHD-C1D	3.49	1.47	1.39
33	1	310	CLA	C1D-ND	3.49	1.42	1.37
33	2	308	CLA	C1D-ND	3.49	1.42	1.37
33	9	308	CLA	C1D-ND	3.49	1.42	1.37
30	B	619	BCR	C30-C25	-3.49	1.49	1.53
33	9	305	CLA	C1D-ND	3.49	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	0	313	CLA	C2D-C1D	3.48	1.48	1.42
45	1	301	A86	C20-C15	3.48	1.52	1.48
34	a	410	PHO	C4D-CHA	3.48	1.44	1.39
33	1	307	CLA	C1D-ND	3.48	1.42	1.37
33	3	307	CLA	C1D-ND	3.48	1.42	1.37
33	6	311	CLA	C1D-ND	3.48	1.42	1.37
33	9	312	CLA	C1D-ND	3.48	1.42	1.37
33	5	312	CLA	C1D-ND	3.48	1.42	1.37
33	w	303	CLA	C1D-ND	3.48	1.42	1.37
33	0	305	CLA	C1D-ND	3.47	1.42	1.37
33	8	306	CLA	C1D-ND	3.47	1.42	1.37
33	3	306	CLA	C1D-ND	3.47	1.42	1.37
45	6	304	A86	C20-C15	3.47	1.52	1.48
33	0	312	CLA	C1D-ND	3.47	1.42	1.37
33	2	309	CLA	C1D-ND	3.47	1.42	1.37
42	e	101	HEM	C1B-NB	-3.47	1.34	1.40
33	4	309	CLA	C1D-ND	3.47	1.42	1.37
33	8	308	CLA	C1D-ND	3.47	1.42	1.37
33	8	305	CLA	C1D-ND	3.47	1.42	1.37
33	9	317	CLA	C1D-ND	3.46	1.42	1.37
33	2	314	CLA	C1D-ND	3.46	1.42	1.37
45	6	303	A86	C20-C15	3.46	1.52	1.48
33	0	308	CLA	C1D-ND	3.46	1.42	1.37
33	B	615	CLA	C1D-ND	3.45	1.42	1.37
33	8	311	CLA	C1D-ND	3.45	1.42	1.37
33	7	310	CLA	C1D-ND	3.45	1.42	1.37
33	5	308	CLA	C1D-ND	3.45	1.42	1.37
30	H	101	BCR	C30-C25	-3.45	1.49	1.53
33	B	602	CLA	C1D-ND	3.45	1.42	1.37
33	9	310	CLA	C1D-ND	3.45	1.42	1.37
33	2	311	CLA	C1D-ND	3.45	1.42	1.37
45	7	303	A86	C30-C29	-3.45	1.26	1.31
33	8	310	CLA	C1D-ND	3.44	1.42	1.37
33	8	313	CLA	C1D-ND	3.44	1.42	1.37
42	e	101	HEM	C4D-ND	-3.44	1.34	1.40
33	9	313	CLA	C1D-ND	3.44	1.42	1.37
33	9	314	CLA	C1D-ND	3.44	1.42	1.37
33	0	309	CLA	C1D-ND	3.44	1.42	1.37
33	6	315	CLA	C1D-ND	3.44	1.42	1.37
30	d	403	BCR	C30-C25	-3.44	1.49	1.53
33	2	315	CLA	C1D-ND	3.43	1.42	1.37
30	H	101	BCR	C1-C6	-3.43	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	4	304	A86	C30-C29	-3.43	1.26	1.31
33	2	316	CLA	C1D-ND	3.43	1.42	1.37
33	1	313	CLA	C1D-ND	3.43	1.42	1.37
45	6	305	A86	C20-C15	3.43	1.52	1.48
47	0	306	KC2	CHD-C1D	3.43	1.47	1.39
33	8	316	CLA	C1D-ND	3.43	1.42	1.37
30	c	514	BCR	C1-C6	-3.43	1.49	1.53
33	2	317	CLA	C1D-ND	3.43	1.42	1.37
33	8	309	CLA	C1D-ND	3.43	1.42	1.37
30	a	412	BCR	C30-C25	-3.42	1.49	1.53
33	7	304	CLA	C1D-ND	3.42	1.42	1.37
33	0	311	CLA	C1D-ND	3.42	1.42	1.37
33	6	312	CLA	C1D-ND	3.42	1.42	1.37
33	5	311	CLA	C1D-ND	3.42	1.42	1.37
33	9	306	CLA	C1D-ND	3.42	1.42	1.37
30	k	101	BCR	C30-C25	-3.42	1.49	1.53
33	4	308	CLA	C1D-ND	3.42	1.42	1.37
33	c	503	CLA	C1D-ND	3.41	1.42	1.37
33	5	313	CLA	C1D-ND	3.41	1.42	1.37
33	7	313	CLA	C2D-C1D	3.41	1.48	1.42
33	4	306	CLA	C1D-ND	3.41	1.42	1.37
33	6	310	CLA	C1D-ND	3.41	1.42	1.37
33	3	308	CLA	C1D-ND	3.40	1.42	1.37
33	9	315	CLA	C1D-ND	3.39	1.42	1.37
33	Z	101	CLA	C1D-ND	3.39	1.42	1.37
33	7	312	CLA	C1D-ND	3.39	1.42	1.37
33	3	311	CLA	C1D-ND	3.38	1.42	1.37
33	3	303	CLA	C1D-ND	3.38	1.42	1.37
33	c	509	CLA	C1D-ND	3.38	1.42	1.37
33	B	616	CLA	C1D-ND	3.38	1.42	1.37
33	3	319	CLA	C1D-ND	3.38	1.42	1.37
33	A	408	CLA	C1D-ND	3.38	1.42	1.37
33	8	315	CLA	C1D-ND	3.38	1.42	1.37
33	4	314	CLA	C1D-ND	3.38	1.42	1.37
33	3	305	CLA	C1D-ND	3.37	1.42	1.37
33	3	309	CLA	C1D-ND	3.37	1.42	1.37
33	4	312	CLA	C1D-ND	3.37	1.42	1.37
33	a	411	CLA	C1D-ND	3.37	1.42	1.37
33	4	305	CLA	C1D-ND	3.36	1.42	1.37
33	B	604	CLA	C1D-ND	3.36	1.42	1.37
33	c	513	CLA	C1D-ND	3.36	1.42	1.37
33	7	311	CLA	C1D-ND	3.36	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	6	316	CLA	C1D-ND	3.36	1.42	1.37
45	5	307	A86	C20-C15	3.36	1.52	1.48
33	C	509	CLA	C1D-ND	3.36	1.42	1.37
33	H	103	CLA	C1D-ND	3.36	1.42	1.37
33	b	616	CLA	C1D-ND	3.35	1.42	1.37
33	B	612	CLA	C1D-ND	3.35	1.42	1.37
33	4	313	CLA	C1D-ND	3.35	1.42	1.37
33	4	310	CLA	C1D-ND	3.35	1.42	1.37
30	C	514	BCR	C1-C6	-3.35	1.49	1.53
30	A	409	BCR	C30-C25	-3.35	1.49	1.53
33	a	407	CLA	C1D-ND	3.34	1.42	1.37
33	b	613	CLA	C1D-ND	3.34	1.42	1.37
33	B	603	CLA	C1D-ND	3.34	1.42	1.37
33	0	304	CLA	C1D-ND	3.34	1.42	1.37
30	h	101	BCR	C1-C6	-3.34	1.49	1.53
33	A	405	CLA	C1D-ND	3.34	1.42	1.37
47	5	310	KC2	CHD-C1D	3.33	1.46	1.39
33	3	313	CLA	C1D-ND	3.33	1.42	1.37
47	7	306	KC2	CHD-C1D	3.33	1.46	1.39
37	t	102	SQD	O47-C7	3.33	1.42	1.35
33	C	503	CLA	C1D-ND	3.33	1.42	1.37
33	c	512	CLA	C1D-ND	3.32	1.42	1.37
33	8	307	CLA	C1D-ND	3.32	1.42	1.37
47	4	307	KC2	MG-NB	-3.32	1.99	2.05
33	C	506	CLA	C1D-ND	3.32	1.42	1.37
37	T	101	SQD	O47-C7	3.32	1.42	1.35
33	3	302	CLA	C1D-ND	3.32	1.42	1.37
33	C	513	CLA	C1D-ND	3.31	1.42	1.37
45	4	302	A86	C20-C15	3.31	1.52	1.48
30	d	403	BCR	C1-C6	-3.31	1.49	1.53
33	4	311	CLA	C1D-ND	3.31	1.42	1.37
33	3	304	CLA	C1D-ND	3.31	1.42	1.37
33	d	402	CLA	C1D-ND	3.31	1.42	1.37
33	d	409	CLA	C1D-ND	3.31	1.42	1.37
33	c	504	CLA	C1D-ND	3.30	1.42	1.37
33	4	316	CLA	C1D-ND	3.30	1.42	1.37
33	7	308	CLA	C1D-ND	3.30	1.42	1.37
30	h	101	BCR	C30-C25	-3.30	1.49	1.53
30	b	620	BCR	C30-C25	-3.30	1.49	1.53
33	c	511	CLA	C1D-ND	3.30	1.42	1.37
33	B	606	CLA	C1D-ND	3.29	1.42	1.37
33	b	617	CLA	C1D-ND	3.29	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	0	307	CLA	C1D-ND	3.29	1.42	1.37
33	C	501	CLA	C1D-ND	3.29	1.42	1.37
33	B	601	CLA	C1D-ND	3.29	1.42	1.37
33	b	608	CLA	C1D-ND	3.29	1.42	1.37
33	b	615	CLA	C1D-ND	3.28	1.42	1.37
33	C	510	CLA	C1D-ND	3.28	1.42	1.37
33	7	305	CLA	C1D-ND	3.28	1.42	1.37
33	b	604	CLA	C1D-ND	3.28	1.42	1.37
33	B	610	CLA	C1D-ND	3.28	1.42	1.37
33	b	603	CLA	C1D-ND	3.27	1.42	1.37
30	B	618	BCR	C30-C25	-3.27	1.49	1.53
33	b	602	CLA	C1D-ND	3.27	1.42	1.37
48	0	302	ET4	C20-C21	3.27	1.53	1.43
33	a	408	CLA	C1D-ND	3.27	1.42	1.37
33	c	505	CLA	C1D-ND	3.26	1.42	1.37
33	7	307	CLA	C1D-ND	3.26	1.42	1.37
33	B	614	CLA	C1D-ND	3.26	1.42	1.37
33	d	401	CLA	CAB-C3B	-3.26	1.44	1.50
33	b	605	CLA	C1D-ND	3.26	1.42	1.37
30	b	619	BCR	C30-C25	-3.26	1.49	1.53
33	D	406	CLA	C1D-ND	3.25	1.42	1.37
33	7	309	CLA	C1D-ND	3.25	1.42	1.37
33	b	610	CLA	C1D-ND	3.25	1.42	1.37
33	c	506	CLA	C1D-ND	3.25	1.42	1.37
30	K	102	BCR	C30-C25	-3.25	1.49	1.53
33	D	405	CLA	CAB-C3B	-3.25	1.44	1.50
33	d	401	CLA	C1D-ND	3.24	1.42	1.37
33	C	511	CLA	C1D-ND	3.24	1.42	1.37
33	C	504	CLA	C1D-ND	3.24	1.42	1.37
33	b	606	CLA	C1D-ND	3.24	1.42	1.37
30	k	102	BCR	C30-C25	-3.24	1.49	1.53
33	c	507	CLA	C1D-ND	3.23	1.42	1.37
33	1	307	CLA	CAB-C3B	-3.23	1.44	1.50
33	c	502	CLA	C1D-ND	3.23	1.42	1.37
45	6	301	A86	C20-C15	3.22	1.52	1.48
33	b	612	CLA	C1D-ND	3.22	1.42	1.37
33	C	502	CLA	C1D-ND	3.22	1.42	1.37
33	b	611	CLA	C1D-ND	3.22	1.42	1.37
33	9	313	CLA	C4B-NB	3.22	1.42	1.37
33	C	508	CLA	C1D-ND	3.21	1.42	1.37
33	B	607	CLA	C1D-ND	3.21	1.42	1.37
33	c	501	CLA	C1D-ND	3.21	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	8	307	CLA	CAB-C3B	-3.21	1.44	1.50
33	C	505	CLA	C1D-ND	3.20	1.42	1.37
33	D	402	CLA	C1D-ND	3.20	1.42	1.37
33	7	314	CLA	C1D-ND	3.19	1.42	1.37
33	b	607	CLA	C1D-ND	3.19	1.42	1.37
33	c	508	CLA	C1D-ND	3.19	1.42	1.37
33	b	609	CLA	C1D-ND	3.19	1.42	1.37
33	A	404	CLA	C1D-ND	3.19	1.42	1.37
33	2	305	CLA	C4B-NB	3.18	1.42	1.37
33	2	307	CLA	C4B-NB	3.18	1.42	1.37
33	C	512	CLA	C1D-ND	3.18	1.42	1.37
33	1	314	CLA	C4B-NB	3.17	1.42	1.37
33	2	315	CLA	C4B-NB	3.16	1.42	1.37
30	K	101	BCR	C30-C25	-3.16	1.49	1.53
33	9	307	CLA	CAB-C3B	-3.16	1.44	1.50
33	3	306	CLA	C4B-NB	3.16	1.42	1.37
33	c	510	CLA	C1D-ND	3.16	1.42	1.37
45	9	301	A86	C30-C29	-3.15	1.26	1.31
33	3	312	CLA	C4B-NB	3.15	1.42	1.37
33	B	605	CLA	C1D-ND	3.15	1.42	1.37
33	B	611	CLA	C1D-ND	3.14	1.42	1.37
47	4	307	KC2	CHC-C1C	3.14	1.46	1.39
33	B	608	CLA	C1D-ND	3.14	1.42	1.37
33	C	507	CLA	C1D-ND	3.14	1.42	1.37
33	W	303	CLA	C1D-ND	3.14	1.42	1.37
33	9	305	CLA	C4B-NB	3.14	1.42	1.37
33	6	311	CLA	C4B-NB	3.13	1.42	1.37
33	2	316	CLA	C4B-NB	3.13	1.42	1.37
33	1	305	CLA	C4B-NB	3.13	1.42	1.37
37	T	103	SQD	O48-C23	3.13	1.42	1.33
45	2	301	A86	C30-C29	-3.13	1.26	1.31
37	i	101	SQD	O48-C23	3.13	1.42	1.33
33	B	613	CLA	C1D-ND	3.12	1.42	1.37
33	1	309	CLA	C4B-NB	3.12	1.42	1.37
33	5	312	CLA	C4B-NB	3.12	1.42	1.37
33	2	307	CLA	CAB-C3B	-3.12	1.44	1.50
30	A	401	BCR	C30-C25	-3.12	1.49	1.53
37	B	622	SQD	O48-C23	3.12	1.42	1.33
33	1	316	CLA	C4B-NB	3.11	1.41	1.37
45	8	302	A86	C20-C15	3.11	1.52	1.48
37	0	316	SQD	O48-C23	3.11	1.42	1.33
33	D	405	CLA	C1D-ND	3.11	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	5	311	CLA	C4B-NB	3.11	1.41	1.37
37	7	317	SQD	O48-C23	3.10	1.42	1.33
33	1	307	CLA	C4B-NB	3.10	1.41	1.37
45	1	302	A86	C20-C15	3.09	1.52	1.48
33	6	312	CLA	C4B-NB	3.09	1.41	1.37
33	9	307	CLA	C4B-NB	3.09	1.41	1.37
37	l	101	SQD	O48-C23	3.09	1.42	1.33
37	A	413	SQD	O48-C23	3.08	1.42	1.33
33	B	609	CLA	C1D-ND	3.08	1.41	1.37
37	a	413	SQD	O48-C23	3.08	1.42	1.33
42	v	201	HEM	CAB-C3B	3.07	1.55	1.47
33	8	310	CLA	C4B-NB	3.07	1.41	1.37
37	t	102	SQD	O48-C23	3.07	1.42	1.33
33	9	317	CLA	C4B-NB	3.07	1.41	1.37
33	1	312	CLA	C4B-NB	3.07	1.41	1.37
37	L	101	SQD	O48-C23	3.06	1.42	1.33
33	b	614	CLA	C1D-ND	3.06	1.41	1.37
33	B	616	CLA	C4B-NB	3.06	1.41	1.37
33	8	314	CLA	C4B-NB	3.06	1.41	1.37
33	1	313	CLA	C4B-NB	3.05	1.41	1.37
30	a	414	BCR	C30-C25	-3.05	1.49	1.53
33	5	317	CLA	C4B-NB	3.05	1.41	1.37
33	w	303	CLA	C4B-NB	3.05	1.41	1.37
33	z	101	CLA	C4B-NB	3.05	1.41	1.37
33	8	305	CLA	C4B-NB	3.05	1.41	1.37
33	6	313	CLA	C4B-NB	3.05	1.41	1.37
42	F	101	HEM	CAC-C3C	3.05	1.55	1.47
37	T	101	SQD	O48-C23	3.04	1.42	1.33
33	3	304	CLA	C4B-NB	3.04	1.41	1.37
42	F	101	HEM	CAB-C3B	3.03	1.55	1.47
42	F	101	HEM	FE-NB	3.03	2.04	1.94
33	2	312	CLA	C4B-NB	3.03	1.41	1.37
33	2	317	CLA	C4B-NB	3.02	1.41	1.37
33	5	308	CLA	C4B-NB	3.02	1.41	1.37
33	2	311	CLA	C4B-NB	3.01	1.41	1.37
33	9	306	CLA	C4B-NB	3.01	1.41	1.37
33	9	312	CLA	C4B-NB	3.01	1.41	1.37
33	2	314	CLA	C4B-NB	3.01	1.41	1.37
37	D	403	SQD	O48-C23	3.01	1.42	1.33
33	1	306	CLA	C4B-NB	3.01	1.41	1.37
33	5	313	CLA	C4B-NB	3.00	1.41	1.37
33	8	316	CLA	C4B-NB	3.00	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	9	316	CLA	C4B-NB	3.00	1.41	1.37
33	6	310	CLA	C4B-NB	3.00	1.41	1.37
33	6	308	CLA	C4B-NB	2.99	1.41	1.37
48	0	302	ET4	C16-C17	2.99	1.52	1.43
33	9	315	CLA	C4B-NB	2.99	1.41	1.37
33	9	309	CLA	C4B-NB	2.98	1.41	1.37
33	1	311	CLA	C4B-NB	2.98	1.41	1.37
33	4	309	CLA	C4B-NB	2.98	1.41	1.37
33	W	303	CLA	C4B-NB	2.97	1.41	1.37
33	0	312	CLA	C4B-NB	2.97	1.41	1.37
33	2	313	CLA	C3C-C4C	2.96	1.46	1.40
33	1	309	CLA	C3C-C4C	2.96	1.46	1.40
33	2	306	CLA	C4B-NB	2.96	1.41	1.37
33	5	316	CLA	C4B-NB	2.96	1.41	1.37
33	1	310	CLA	C1B-C2B	2.95	1.50	1.43
33	9	308	CLA	C4B-NB	2.95	1.41	1.37
33	9	314	CLA	C4B-NB	2.95	1.41	1.37
48	7	302	ET4	C20-C21	2.95	1.52	1.43
33	b	616	CLA	C4B-NB	2.95	1.41	1.37
33	6	315	CLA	C4B-NB	2.95	1.41	1.37
33	5	314	CLA	C4B-NB	2.95	1.41	1.37
33	8	307	CLA	C4B-NB	2.94	1.41	1.37
33	0	305	CLA	C4B-NB	2.94	1.41	1.37
33	4	305	CLA	C4B-NB	2.94	1.41	1.37
33	4	310	CLA	C4B-NB	2.94	1.41	1.37
33	3	307	CLA	C4B-NB	2.94	1.41	1.37
33	d	401	CLA	C4B-NB	2.94	1.41	1.37
42	v	201	HEM	CAC-C3C	2.94	1.55	1.47
33	B	615	CLA	C4B-NB	2.93	1.41	1.37
33	4	315	CLA	C4B-NB	2.93	1.41	1.37
33	8	312	CLA	C4B-NB	2.93	1.41	1.37
33	3	319	CLA	C4B-NB	2.93	1.41	1.37
33	H	103	CLA	C4B-NB	2.93	1.41	1.37
33	2	308	CLA	C4B-NB	2.93	1.41	1.37
33	0	309	CLA	C4B-NB	2.93	1.41	1.37
33	0	308	CLA	C4B-NB	2.92	1.41	1.37
33	8	309	CLA	C4B-NB	2.92	1.41	1.37
33	6	307	CLA	C4B-NB	2.92	1.41	1.37
33	0	311	CLA	C4B-NB	2.92	1.41	1.37
33	9	313	CLA	C3C-C4C	2.92	1.46	1.40
33	3	303	CLA	C4B-NB	2.92	1.41	1.37
33	8	313	CLA	C3C-C4C	2.92	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	505	CLA	C4B-NB	2.92	1.41	1.37
33	1	315	CLA	C4B-NB	2.92	1.41	1.37
33	b	611	CLA	C4B-NB	2.92	1.41	1.37
33	1	308	CLA	C4B-NB	2.92	1.41	1.37
33	9	311	CLA	C4B-NB	2.91	1.41	1.37
37	A	413	SQD	O47-C7	2.91	1.42	1.34
33	7	308	CLA	C4B-NB	2.91	1.41	1.37
33	2	310	CLA	C4B-NB	2.91	1.41	1.37
37	i	101	SQD	O47-C7	2.91	1.42	1.34
33	4	314	CLA	C4B-NB	2.91	1.41	1.37
33	4	308	CLA	C4B-NB	2.90	1.41	1.37
33	4	313	CLA	C4B-NB	2.90	1.41	1.37
37	L	101	SQD	O47-C7	2.90	1.42	1.34
33	D	405	CLA	C4B-NB	2.90	1.41	1.37
33	8	313	CLA	C4B-NB	2.90	1.41	1.37
45	7	303	A86	O1-C20	-2.90	1.42	1.46
33	4	312	CLA	C4B-NB	2.89	1.41	1.37
33	2	309	CLA	C3C-C4C	2.89	1.46	1.40
33	7	309	CLA	C4B-NB	2.89	1.41	1.37
33	3	313	CLA	C4B-NB	2.89	1.41	1.37
33	0	304	CLA	C4B-NB	2.89	1.41	1.37
33	2	309	CLA	C4B-NB	2.89	1.41	1.37
34	a	410	PHO	CMC-C2C	-2.88	1.46	1.50
33	4	316	CLA	C4B-NB	2.88	1.41	1.37
33	9	310	CLA	C4B-NB	2.88	1.41	1.37
46	4	303	DD6	O1-C20	-2.88	1.42	1.46
42	F	101	HEM	FE-ND	2.88	2.03	1.94
33	0	310	CLA	C4B-NB	2.88	1.41	1.37
33	1	313	CLA	C3C-C4C	2.87	1.46	1.40
33	3	305	CLA	C4B-NB	2.87	1.41	1.37
33	7	312	CLA	C4B-NB	2.87	1.41	1.37
33	8	309	CLA	C3C-C4C	2.87	1.46	1.40
48	7	302	ET4	C02-C03	2.87	1.56	1.52
33	7	304	CLA	C4B-NB	2.87	1.41	1.37
33	a	411	CLA	C4B-NB	2.87	1.41	1.37
47	4	307	KC2	CHD-C1D	2.87	1.45	1.39
33	c	513	CLA	C4B-NB	2.87	1.41	1.37
33	1	310	CLA	C4B-NB	2.87	1.41	1.37
37	a	413	SQD	O47-C7	2.86	1.42	1.34
33	B	610	CLA	C4B-NB	2.86	1.41	1.37
37	0	316	SQD	O47-C7	2.86	1.42	1.34
33	C	508	CLA	C4B-NB	2.86	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	510	CLA	C4B-NB	2.86	1.41	1.37
33	C	506	CLA	C4B-NB	2.85	1.41	1.37
33	9	309	CLA	C3C-C4C	2.85	1.46	1.40
33	8	306	CLA	C4B-NB	2.85	1.41	1.37
33	Z	101	CLA	C4B-NB	2.85	1.41	1.37
33	c	501	CLA	C4B-NB	2.84	1.41	1.37
37	D	403	SQD	O47-C7	2.84	1.42	1.34
33	B	609	CLA	C4B-NB	2.84	1.41	1.37
33	4	311	CLA	C4B-NB	2.84	1.41	1.37
45	3	314	A86	O1-C20	-2.84	1.42	1.46
37	B	622	SQD	O47-C7	2.84	1.42	1.34
33	3	309	CLA	C4B-NB	2.84	1.41	1.37
33	7	310	CLA	C4B-NB	2.84	1.41	1.37
33	b	617	CLA	C4B-NB	2.84	1.41	1.37
33	7	305	CLA	C4B-NB	2.83	1.41	1.37
38	C	517	DGD	O2G-C2G	-2.83	1.39	1.46
37	T	103	SQD	O47-C7	2.83	1.42	1.34
33	0	307	CLA	C4B-NB	2.83	1.41	1.37
37	1	101	SQD	O47-C7	2.83	1.42	1.34
37	7	317	SQD	O47-C7	2.83	1.42	1.34
33	8	311	CLA	C4B-NB	2.83	1.41	1.37
33	8	315	CLA	C4B-NB	2.83	1.41	1.37
42	V	201	HEM	FE-ND	-2.83	1.86	1.94
33	A	408	CLA	C4B-NB	2.82	1.41	1.37
33	b	612	CLA	C4B-NB	2.82	1.41	1.37
33	c	508	CLA	C4B-NB	2.82	1.41	1.37
33	C	511	CLA	C4B-NB	2.82	1.41	1.37
33	3	302	CLA	C4B-NB	2.81	1.41	1.37
33	3	311	CLA	C4B-NB	2.81	1.41	1.37
33	c	512	CLA	C4B-NB	2.81	1.41	1.37
33	c	503	CLA	C4B-NB	2.81	1.41	1.37
33	B	608	CLA	C4B-NB	2.81	1.41	1.37
33	8	308	CLA	C4B-NB	2.81	1.41	1.37
33	c	505	CLA	C4B-NB	2.80	1.41	1.37
33	c	506	CLA	C4B-NB	2.80	1.41	1.37
33	c	510	CLA	C4B-NB	2.80	1.41	1.37
33	7	314	CLA	C4B-NB	2.80	1.41	1.37
42	v	201	HEM	FE-NC	2.80	2.04	1.95
33	6	307	CLA	C1B-C2B	2.80	1.49	1.43
33	b	609	CLA	C4B-NB	2.79	1.41	1.37
33	1	314	CLA	C1B-C2B	2.79	1.49	1.43
38	c	517	DGD	O2G-C2G	-2.79	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	b	614	CLA	C4B-NB	2.79	1.41	1.37
33	B	613	CLA	C4B-NB	2.79	1.41	1.37
41	d	404	PL9	C7-C3	-2.79	1.47	1.51
33	c	502	CLA	C4B-NB	2.79	1.41	1.37
48	7	302	ET4	C16-C17	2.79	1.51	1.43
34	A	406	PHO	CMC-C2C	-2.79	1.46	1.50
33	4	306	CLA	C4B-NB	2.79	1.41	1.37
47	4	307	KC2	CHC-C4B	2.79	1.43	1.38
46	9	303	DD6	C19-C20	-2.78	1.48	1.52
46	2	303	DD6	C19-C20	-2.78	1.48	1.52
33	5	309	CLA	C4B-NB	2.78	1.41	1.37
33	5	311	CLA	C1B-C2B	2.78	1.49	1.43
33	8	310	CLA	C1B-C2B	2.78	1.49	1.43
45	7	301	A86	C13-C11	-2.78	1.44	1.49
33	5	308	CLA	C1B-C2B	2.78	1.49	1.43
33	d	402	CLA	C4B-NB	2.77	1.41	1.37
33	c	507	CLA	C4B-NB	2.77	1.41	1.37
45	0	301	A86	C13-C11	-2.77	1.44	1.49
33	C	513	CLA	C4B-NB	2.77	1.41	1.37
34	A	407	PHO	CMC-C2C	-2.77	1.46	1.50
34	a	409	PHO	CMC-C2C	-2.77	1.46	1.50
33	5	309	CLA	C1B-C2B	2.77	1.49	1.43
33	2	317	CLA	C1B-C2B	2.77	1.49	1.43
33	4	315	CLA	C1B-C2B	2.77	1.49	1.43
33	B	606	CLA	C4B-NB	2.77	1.41	1.37
39	b	623	LMG	C4-C5	2.76	1.58	1.53
33	c	509	CLA	C4B-NB	2.76	1.41	1.37
33	0	304	CLA	C1B-C2B	2.76	1.49	1.43
33	1	312	CLA	C1B-C2B	2.76	1.49	1.43
33	B	605	CLA	C4B-NB	2.76	1.41	1.37
33	3	308	CLA	C4B-NB	2.76	1.41	1.37
33	4	310	CLA	C1B-C2B	2.76	1.49	1.43
33	9	306	CLA	C1B-C2B	2.76	1.49	1.43
33	3	304	CLA	C1B-C2B	2.76	1.49	1.43
33	b	606	CLA	C4B-NB	2.75	1.41	1.37
33	2	315	CLA	C1B-C2B	2.75	1.49	1.43
33	2	306	CLA	C1B-C2B	2.75	1.49	1.43
33	1	308	CLA	C1B-C2B	2.75	1.49	1.43
41	d	404	PL9	C53-C6	-2.75	1.45	1.50
33	6	312	CLA	C1B-C2B	2.75	1.49	1.43
45	6	301	A86	O1-C20	-2.75	1.42	1.46
33	c	511	CLA	C4B-NB	2.75	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	9	315	CLA	C1B-C2B	2.74	1.49	1.43
33	B	601	CLA	C4B-NB	2.74	1.41	1.37
33	B	611	CLA	C4B-NB	2.74	1.41	1.37
33	b	613	CLA	C4B-NB	2.74	1.41	1.37
33	2	308	CLA	C1B-C2B	2.74	1.49	1.43
41	D	408	PL9	C7-C3	-2.74	1.47	1.51
33	0	307	CLA	C1B-C2B	2.74	1.49	1.43
45	5	305	A86	O4-C34	-2.74	1.43	1.46
45	6	302	A86	C20-C15	2.74	1.51	1.48
33	2	316	CLA	C1B-C2B	2.74	1.49	1.43
41	D	408	PL9	C53-C6	-2.74	1.45	1.50
33	B	604	CLA	C1B-C2B	2.73	1.49	1.43
47	4	307	KC2	C4A-C3A	-2.73	1.39	1.44
33	1	315	CLA	C1B-C2B	2.73	1.49	1.43
33	6	313	CLA	C1B-C2B	2.73	1.49	1.43
33	3	302	CLA	C1B-C2B	2.73	1.49	1.43
33	2	311	CLA	C1B-C2B	2.73	1.49	1.43
33	8	309	CLA	C1B-C2B	2.73	1.49	1.43
33	2	309	CLA	C1B-C2B	2.73	1.49	1.43
46	4	303	DD6	C28-C27	-2.73	1.49	1.50
33	1	311	CLA	C1B-C2B	2.73	1.49	1.43
33	4	305	CLA	C1B-C2B	2.73	1.49	1.43
33	5	317	CLA	C1B-C2B	2.73	1.49	1.43
33	0	305	CLA	C1B-C2B	2.72	1.49	1.43
33	C	502	CLA	C4B-NB	2.72	1.41	1.37
33	6	315	CLA	C1B-C2B	2.72	1.49	1.43
33	9	312	CLA	C1B-C2B	2.72	1.49	1.43
33	1	307	CLA	C4B-C3B	2.72	1.49	1.43
45	5	305	A86	O1-C20	-2.72	1.42	1.46
42	F	101	HEM	FE-NA	2.72	2.04	1.95
33	1	316	CLA	C1B-C2B	2.72	1.49	1.43
33	b	615	CLA	C4B-NB	2.72	1.41	1.37
48	0	302	ET4	C15-C14	2.72	1.51	1.43
33	C	507	CLA	C4B-NB	2.72	1.41	1.37
33	0	311	CLA	C1B-C2B	2.72	1.49	1.43
33	8	305	CLA	C1B-C2B	2.72	1.49	1.43
33	H	103	CLA	C1B-C2B	2.71	1.49	1.43
33	C	503	CLA	C4B-NB	2.71	1.41	1.37
42	F	101	HEM	FE-NC	2.71	2.04	1.95
45	6	305	A86	O1-C20	-2.71	1.42	1.46
33	B	603	CLA	C4B-NB	2.71	1.41	1.37
33	C	512	CLA	C4B-NB	2.71	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	407	CLA	C4B-NB	2.71	1.41	1.37
33	b	604	CLA	C4B-NB	2.71	1.41	1.37
33	8	312	CLA	C1B-C2B	2.71	1.49	1.43
33	9	317	CLA	C1B-C2B	2.71	1.49	1.43
33	0	308	CLA	C1B-C2B	2.71	1.49	1.43
33	B	612	CLA	C4B-NB	2.71	1.41	1.37
33	3	307	CLA	C1B-C2B	2.71	1.49	1.43
33	6	311	CLA	C1B-C2B	2.71	1.49	1.43
33	2	313	CLA	C1B-C2B	2.71	1.49	1.43
33	c	504	CLA	C4B-NB	2.71	1.41	1.37
33	9	305	CLA	C1B-C2B	2.71	1.49	1.43
42	V	201	HEM	C1C-C2C	-2.70	1.40	1.45
44	6	314	KC1	C4B-NB	-2.70	1.34	1.37
33	4	309	CLA	C1B-C2B	2.70	1.49	1.43
33	3	306	CLA	C1B-C2B	2.70	1.49	1.43
33	1	309	CLA	C1B-C2B	2.70	1.49	1.43
48	7	302	ET4	C01-C06	2.70	1.57	1.53
33	8	316	CLA	C1B-C2B	2.70	1.49	1.43
33	z	101	CLA	C1B-C2B	2.70	1.49	1.43
33	2	312	CLA	C1B-C2B	2.70	1.49	1.43
33	9	314	CLA	C1B-C2B	2.70	1.49	1.43
33	0	310	CLA	C1B-C2B	2.69	1.49	1.43
33	9	311	CLA	C1B-C2B	2.69	1.49	1.43
33	2	305	CLA	C1B-C2B	2.69	1.49	1.43
33	B	614	CLA	C4B-NB	2.69	1.41	1.37
33	8	315	CLA	C1B-C2B	2.69	1.49	1.43
33	1	305	CLA	C1B-C2B	2.69	1.49	1.43
33	B	607	CLA	C4B-NB	2.69	1.41	1.37
33	8	314	CLA	C1B-C2B	2.69	1.49	1.43
33	w	303	CLA	C1B-C2B	2.68	1.49	1.43
33	5	313	CLA	C1B-C2B	2.68	1.49	1.43
33	9	307	CLA	C4B-C3B	2.68	1.49	1.43
33	8	313	CLA	C1B-C2B	2.68	1.49	1.43
33	5	314	CLA	C1B-C2B	2.68	1.49	1.43
42	e	101	HEM	FE-ND	-2.68	1.86	1.94
33	b	603	CLA	MG-NB	-2.68	2.00	2.05
33	b	607	CLA	C4B-NB	2.68	1.41	1.37
33	9	309	CLA	C1B-C2B	2.68	1.49	1.43
33	1	307	CLA	C1B-C2B	2.68	1.49	1.43
33	5	316	CLA	C1B-C2B	2.68	1.49	1.43
33	7	311	CLA	C4B-NB	2.68	1.41	1.37
33	7	311	CLA	C1B-C2B	2.67	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c	509	CLA	C1B-C2B	2.67	1.49	1.43
33	4	312	CLA	C1B-C2B	2.67	1.49	1.43
33	b	610	CLA	C4B-NB	2.67	1.41	1.37
33	3	313	CLA	C1B-C2B	2.67	1.49	1.43
33	7	314	CLA	C1B-C2B	2.67	1.49	1.43
33	6	308	CLA	C1B-C2B	2.67	1.49	1.43
33	4	308	CLA	C1B-C2B	2.66	1.49	1.43
33	2	314	CLA	C1B-C2B	2.66	1.49	1.43
38	C	516	DGD	O2G-C2G	-2.66	1.40	1.46
33	3	312	CLA	C1B-C2B	2.66	1.49	1.43
33	7	309	CLA	C1B-C2B	2.66	1.49	1.43
44	5	315	KC1	C4B-NB	-2.66	1.34	1.37
33	8	307	CLA	C4B-C3B	2.66	1.49	1.43
33	B	604	CLA	C4B-NB	2.66	1.41	1.37
33	8	308	CLA	C1B-C2B	2.65	1.49	1.43
33	7	307	CLA	C4B-NB	2.65	1.41	1.37
45	6	304	A86	O1-C20	-2.65	1.42	1.46
33	6	310	CLA	C1B-C2B	2.65	1.49	1.43
33	b	608	CLA	C4B-NB	2.65	1.41	1.37
33	0	309	CLA	C1B-C2B	2.65	1.49	1.43
39	0	314	LMG	C4-C5	2.64	1.58	1.53
33	1	306	CLA	C1B-C2B	2.64	1.49	1.43
33	1	313	CLA	C1B-C2B	2.64	1.49	1.43
33	B	602	CLA	C4B-NB	2.64	1.41	1.37
39	c	519	LMG	C4-C5	2.64	1.58	1.53
33	9	308	CLA	C1B-C2B	2.64	1.49	1.43
33	2	307	CLA	C4B-C3B	2.64	1.49	1.43
33	3	308	CLA	C1B-C2B	2.64	1.49	1.43
42	v	201	HEM	FE-NA	2.64	2.03	1.95
48	7	302	ET4	C15-C14	2.64	1.51	1.43
34	A	407	PHO	CMD-C2D	-2.64	1.46	1.51
36	A	411	LHG	O7-C5	-2.64	1.40	1.46
33	a	408	CLA	C4B-NB	2.64	1.41	1.37
33	C	504	CLA	C4B-NB	2.64	1.41	1.37
33	0	312	CLA	C1B-C2B	2.64	1.49	1.43
33	C	509	CLA	C4B-NB	2.64	1.41	1.37
33	D	406	CLA	C1B-C2B	2.63	1.49	1.43
33	4	313	CLA	C1B-C2B	2.63	1.49	1.43
48	0	302	ET4	C11-C10	2.63	1.51	1.43
33	8	307	CLA	C1B-C2B	2.63	1.49	1.43
33	b	607	CLA	C1B-C2B	2.63	1.49	1.43
33	9	313	CLA	C1B-C2B	2.63	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	7	308	CLA	C1B-C2B	2.63	1.49	1.43
33	C	503	CLA	C1B-C2B	2.63	1.49	1.43
33	D	402	CLA	C4B-NB	2.63	1.41	1.37
33	b	605	CLA	C4B-NB	2.63	1.41	1.37
34	a	410	PHO	CMD-C2D	-2.63	1.46	1.51
33	8	311	CLA	C1B-C2B	2.63	1.49	1.43
33	4	311	CLA	C1B-C2B	2.63	1.49	1.43
33	3	319	CLA	C1B-C2B	2.63	1.49	1.43
33	3	311	CLA	C1B-C2B	2.62	1.49	1.43
33	7	304	CLA	C1B-C2B	2.62	1.49	1.43
33	b	603	CLA	C4B-NB	2.62	1.41	1.37
44	3	310	KC1	C4B-NB	-2.62	1.34	1.37
33	7	310	CLA	C1B-C2B	2.62	1.49	1.43
38	a	401	DGD	O2G-C2G	-2.62	1.40	1.46
34	a	409	PHO	CMD-C2D	-2.62	1.46	1.51
33	B	612	CLA	C1B-C2B	2.62	1.49	1.43
44	6	314	KC1	CBA-CGA	-2.62	1.41	1.48
36	b	601	LHG	O7-C5	-2.62	1.40	1.46
33	C	511	CLA	C1B-C2B	2.62	1.49	1.43
33	b	613	CLA	C1B-C2B	2.62	1.49	1.43
45	0	303	A86	O1-C20	-2.62	1.42	1.46
33	B	607	CLA	C1B-C2B	2.62	1.49	1.43
33	A	405	CLA	C4B-NB	2.62	1.41	1.37
33	3	303	CLA	C1B-C2B	2.62	1.49	1.43
38	C	517	DGD	O1G-C1G	-2.62	1.39	1.45
33	c	507	CLA	C1B-C2B	2.62	1.49	1.43
33	9	307	CLA	C1B-C2B	2.61	1.49	1.43
33	5	312	CLA	C1B-C2B	2.61	1.49	1.43
36	D	409	LHG	O7-C5	-2.61	1.40	1.46
42	e	101	HEM	C1C-C2C	-2.61	1.40	1.45
33	4	314	CLA	C1B-C2B	2.61	1.49	1.43
33	7	312	CLA	C1B-C2B	2.61	1.49	1.43
33	2	307	CLA	C1B-C2B	2.61	1.49	1.43
33	A	404	CLA	C4B-NB	2.60	1.41	1.37
33	2	313	CLA	MG-NB	-2.60	2.00	2.05
33	c	505	CLA	C1B-C2B	2.60	1.49	1.43
33	c	503	CLA	C1B-C2B	2.60	1.49	1.43
33	d	402	CLA	C1B-C2B	2.60	1.49	1.43
47	7	306	KC2	CBA-CGA	-2.60	1.41	1.48
33	9	316	CLA	C1B-C2B	2.60	1.49	1.43
45	9	302	A86	O1-C20	-2.60	1.42	1.46
33	A	404	CLA	C1B-C2B	2.60	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	4	306	CLA	C1B-C2B	2.60	1.49	1.43
33	c	513	CLA	C1B-C2B	2.59	1.49	1.43
33	c	511	CLA	C1B-C2B	2.59	1.49	1.43
45	6	303	A86	O1-C20	-2.59	1.42	1.46
33	c	508	CLA	C1B-C2B	2.58	1.49	1.43
33	C	513	CLA	C1B-C2B	2.58	1.49	1.43
33	c	502	CLA	C1B-C2B	2.58	1.49	1.43
33	a	411	CLA	C1B-C2B	2.58	1.49	1.43
33	Z	101	CLA	C1B-C2B	2.58	1.49	1.43
33	d	409	CLA	C4B-NB	2.58	1.41	1.37
34	A	406	PHO	CMD-C2D	-2.58	1.46	1.51
33	3	305	CLA	C1B-C2B	2.58	1.49	1.43
48	7	302	ET4	C11-C10	2.58	1.51	1.43
33	4	316	CLA	C1B-C2B	2.57	1.49	1.43
33	b	602	CLA	C4B-NB	2.57	1.41	1.37
33	7	305	CLA	C1B-C2B	2.57	1.49	1.43
45	5	306	A86	O1-C20	-2.57	1.42	1.46
33	d	401	CLA	C4B-C3B	2.57	1.49	1.43
33	C	504	CLA	C1B-C2B	2.57	1.49	1.43
33	C	501	CLA	C4B-NB	2.57	1.41	1.37
45	4	304	A86	O1-C20	-2.56	1.42	1.46
33	b	615	CLA	C1B-C2B	2.56	1.49	1.43
39	d	406	LMG	O7-C8	-2.56	1.40	1.46
33	c	510	CLA	C1B-C2B	2.56	1.49	1.43
44	3	310	KC1	CBA-CGA	-2.56	1.42	1.48
33	D	406	CLA	C4B-NB	2.56	1.41	1.37
47	5	310	KC2	CBA-CGA	-2.55	1.42	1.48
47	6	309	KC2	CBA-CGA	-2.55	1.42	1.48
47	0	306	KC2	CBA-CGA	-2.55	1.42	1.48
33	C	507	CLA	C1B-C2B	2.55	1.49	1.43
33	c	501	CLA	C1B-C2B	2.55	1.49	1.43
45	8	302	A86	O1-C20	-2.55	1.42	1.46
33	b	612	CLA	C1B-C2B	2.55	1.49	1.43
33	b	608	CLA	C1B-C2B	2.55	1.49	1.43
45	2	302	A86	O1-C20	-2.55	1.42	1.46
38	c	516	DGD	O1G-C1G	-2.55	1.39	1.45
33	C	505	CLA	C1B-C2B	2.55	1.49	1.43
33	a	408	CLA	C1B-C2B	2.55	1.49	1.43
45	1	302	A86	O1-C20	-2.55	1.42	1.46
33	8	306	CLA	C1B-C2B	2.54	1.49	1.43
33	C	512	CLA	C1B-C2B	2.54	1.49	1.43
36	3	317	LHG	O7-C5	-2.54	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	v	201	HEM	FE-NB	2.54	2.02	1.94
36	a	403	LHG	O7-C5	-2.54	1.40	1.46
33	b	605	CLA	C1B-C2B	2.54	1.49	1.43
33	C	508	CLA	C1B-C2B	2.54	1.49	1.43
33	c	504	CLA	C1B-C2B	2.54	1.49	1.43
33	D	405	CLA	C4B-C3B	2.54	1.49	1.43
34	A	407	PHO	CMB-C2B	-2.53	1.46	1.51
34	a	409	PHO	CMB-C2B	-2.53	1.46	1.51
33	C	502	CLA	C1B-C2B	2.53	1.49	1.43
33	c	512	CLA	C1B-C2B	2.53	1.49	1.43
33	3	309	CLA	C1B-C2B	2.53	1.49	1.43
33	B	613	CLA	C1B-C2B	2.53	1.49	1.43
33	C	506	CLA	C1B-C2B	2.53	1.49	1.43
33	D	402	CLA	C1B-C2B	2.53	1.49	1.43
33	a	407	CLA	C1B-C2B	2.53	1.49	1.43
36	h	103	LHG	O7-C5	-2.52	1.40	1.46
33	B	601	CLA	C1B-C2B	2.52	1.49	1.43
34	A	406	PHO	CAC-C3C	-2.52	1.47	1.51
33	B	605	CLA	C1B-C2B	2.52	1.49	1.43
33	C	510	CLA	C1B-C2B	2.52	1.49	1.43
33	2	310	CLA	C1B-C2B	2.52	1.49	1.43
33	b	602	CLA	C1B-C2B	2.52	1.49	1.43
33	d	409	CLA	C1B-C2B	2.52	1.49	1.43
45	4	302	A86	O1-C20	-2.51	1.43	1.46
33	W	303	CLA	C1B-C2B	2.51	1.49	1.43
34	a	409	PHO	CAC-C3C	-2.51	1.47	1.51
39	D	410	LMG	O7-C8	-2.51	1.40	1.46
33	B	610	CLA	C1B-C2B	2.51	1.49	1.43
33	C	509	CLA	C1B-C2B	2.51	1.49	1.43
45	4	301	A86	O1-C20	-2.51	1.43	1.46
45	5	303	A86	O1-C20	-2.51	1.43	1.46
34	A	406	PHO	CMB-C2B	-2.51	1.46	1.51
45	5	307	A86	O1-C20	-2.50	1.43	1.46
33	B	614	CLA	C1B-C2B	2.50	1.49	1.43
45	5	304	A86	O1-C20	-2.50	1.43	1.46
33	A	408	CLA	C1B-C2B	2.50	1.49	1.43
38	c	516	DGD	O2G-C2G	-2.50	1.40	1.46
44	5	315	KC1	CBA-CGA	-2.50	1.42	1.48
34	a	410	PHO	CMB-C2B	-2.50	1.46	1.51
38	A	415	DGD	O2G-C2G	-2.49	1.40	1.46
47	4	307	KC2	CBA-CGA	-2.49	1.42	1.48
45	5	302	A86	O1-C20	-2.49	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	501	CLA	C1B-C2B	2.49	1.49	1.43
33	b	604	CLA	C1B-C2B	2.48	1.49	1.43
33	b	616	CLA	C1B-C2B	2.48	1.49	1.43
33	b	611	CLA	C1B-C2B	2.48	1.49	1.43
38	h	102	DGD	O2G-C2G	-2.48	1.40	1.46
33	9	310	CLA	C1B-C2B	2.48	1.48	1.43
33	B	608	CLA	C1B-C2B	2.48	1.48	1.43
33	b	617	CLA	C1B-C2B	2.47	1.48	1.43
33	7	307	CLA	C1B-C2B	2.47	1.48	1.43
33	A	405	CLA	C1B-C2B	2.47	1.48	1.43
33	B	602	CLA	C1B-C2B	2.47	1.48	1.43
33	B	611	CLA	C1B-C2B	2.47	1.48	1.43
33	B	615	CLA	C1B-C2B	2.46	1.48	1.43
36	d	405	LHG	O7-C5	-2.46	1.40	1.46
33	B	603	CLA	C1B-C2B	2.46	1.48	1.43
33	D	405	CLA	C1B-C2B	2.46	1.48	1.43
33	B	606	CLA	C1B-C2B	2.46	1.48	1.43
30	c	515	BCR	C1-C6	-2.46	1.50	1.53
42	V	201	HEM	C4B-NB	-2.46	1.34	1.38
33	b	610	CLA	CMC-C2C	-2.45	1.45	1.50
33	c	510	CLA	CMD-C2D	-2.45	1.45	1.50
42	V	201	HEM	C1D-ND	-2.45	1.34	1.38
36	A	414	LHG	O7-C5	-2.45	1.40	1.46
39	C	520	LMG	O7-C8	-2.44	1.40	1.46
33	c	506	CLA	C1B-C2B	2.44	1.48	1.43
33	b	614	CLA	C1B-C2B	2.44	1.48	1.43
33	B	616	CLA	C1B-C2B	2.43	1.48	1.43
33	b	609	CLA	C1B-C2B	2.43	1.48	1.43
33	b	606	CLA	C1B-C2B	2.43	1.48	1.43
46	1	304	DD6	O1-C20	-2.43	1.43	1.46
33	d	401	CLA	C1B-C2B	2.42	1.48	1.43
45	6	302	A86	O1-C20	-2.42	1.43	1.46
38	c	518	DGD	O2G-C2G	-2.42	1.40	1.46
34	a	410	PHO	CAC-C3C	-2.42	1.47	1.51
42	V	201	HEM	C3C-C4C	-2.41	1.41	1.46
33	b	610	CLA	C1B-C2B	2.41	1.48	1.43
44	3	310	KC1	C1B-NB	-2.41	1.34	1.37
33	9	316	CLA	C3B-C4B	2.41	1.49	1.42
33	1	311	CLA	C3B-C4B	2.40	1.49	1.42
38	a	401	DGD	O1G-C1G	-2.40	1.39	1.45
33	d	402	CLA	MG-NB	-2.40	2.01	2.05
33	A	408	CLA	MG-NB	-2.40	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	1	313	CLA	C3B-C4B	2.40	1.49	1.42
45	4	301	A86	C32-C31	-2.40	1.50	1.54
38	C	518	DGD	O2G-C2G	-2.39	1.41	1.46
34	A	407	PHO	CAC-C3C	-2.39	1.47	1.51
33	6	316	CLA	CHC-C1C	2.39	1.43	1.38
33	4	312	CLA	MG-ND	-2.38	2.01	2.05
33	9	313	CLA	C3B-C4B	2.38	1.49	1.42
38	C	516	DGD	O1G-C1G	-2.38	1.39	1.45
38	h	102	DGD	O1G-C1G	-2.38	1.39	1.45
33	5	312	CLA	C3B-C4B	2.38	1.49	1.42
33	5	316	CLA	C3B-C4B	2.38	1.49	1.42
33	3	312	CLA	C3B-C4B	2.38	1.49	1.42
38	A	415	DGD	O1G-C1G	-2.38	1.39	1.45
33	6	313	CLA	C3B-C4B	2.38	1.49	1.42
45	8	301	A86	O1-C20	-2.38	1.43	1.46
39	7	315	LMG	O7-C8	-2.38	1.41	1.46
33	3	306	CLA	C3B-C4B	2.37	1.49	1.42
36	0	315	LHG	O7-C5	-2.37	1.41	1.46
33	b	603	CLA	C1B-C2B	2.37	1.48	1.43
33	2	316	CLA	C3B-C4B	2.37	1.49	1.42
46	1	303	DD6	O1-C20	-2.37	1.43	1.46
41	d	404	PL9	C52-C5	-2.37	1.45	1.50
33	6	311	CLA	C3B-C4B	2.37	1.49	1.42
33	2	310	CLA	C3B-C4B	2.36	1.49	1.42
46	8	303	DD6	O1-C20	-2.36	1.43	1.46
33	1	316	CLA	C3B-C4B	2.36	1.49	1.42
38	H	102	DGD	O2G-C2G	-2.36	1.41	1.46
33	9	305	CLA	C3B-C4B	2.36	1.49	1.42
33	B	609	CLA	C1B-C2B	2.36	1.48	1.43
33	2	311	CLA	C3B-C4B	2.36	1.49	1.42
47	4	307	KC2	C4B-NB	-2.36	1.34	1.37
33	9	311	CLA	C3B-C4B	2.35	1.49	1.42
33	a	407	CLA	CMD-C2D	-2.35	1.45	1.50
33	1	305	CLA	C3B-C4B	2.35	1.49	1.42
33	A	404	CLA	CMD-C2D	-2.35	1.46	1.50
33	b	611	CLA	C3B-C4B	2.35	1.49	1.42
33	B	610	CLA	C3B-C4B	2.35	1.49	1.42
33	6	310	CLA	C3B-C4B	2.35	1.49	1.42
33	6	310	CLA	CHC-C1C	2.34	1.43	1.38
33	3	309	CLA	C3B-C4B	2.34	1.49	1.42
33	1	309	CLA	C3B-C4B	2.34	1.49	1.42
33	z	101	CLA	C3B-C4B	2.34	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2	315	CLA	C3B-C4B	2.34	1.49	1.42
38	c	517	DGD	O1G-C1G	-2.34	1.39	1.45
33	1	308	CLA	C3B-C4B	2.34	1.49	1.42
45	2	301	A86	O1-C20	-2.34	1.43	1.46
33	8	311	CLA	C3B-C4B	2.34	1.49	1.42
33	5	313	CLA	C3B-C4B	2.34	1.49	1.42
33	6	311	CLA	CHC-C1C	2.34	1.43	1.38
38	H	102	DGD	O1G-C1G	-2.33	1.40	1.45
39	m	201	LMG	O7-C8	-2.33	1.41	1.46
45	5	301	A86	O1-C20	-2.33	1.43	1.46
33	9	314	CLA	C3B-C4B	2.33	1.49	1.42
33	8	305	CLA	C3B-C4B	2.33	1.49	1.42
33	C	512	CLA	MG-NB	-2.33	2.01	2.05
36	H	104	LHG	O7-C5	-2.33	1.41	1.46
33	5	308	CLA	C3B-C4B	2.33	1.49	1.42
33	4	306	CLA	CHC-C1C	2.33	1.43	1.38
33	D	402	CLA	CMD-C2D	-2.33	1.46	1.50
45	0	301	A86	O1-C20	-2.33	1.43	1.46
33	9	316	CLA	CHC-C1C	2.32	1.43	1.38
33	9	310	CLA	C3B-C4B	2.32	1.49	1.42
36	7	316	LHG	O7-C5	-2.32	1.41	1.46
33	2	305	CLA	C3B-C4B	2.32	1.49	1.42
33	2	312	CLA	C3B-C4B	2.32	1.49	1.42
33	4	310	CLA	C3B-C4B	2.32	1.49	1.42
33	8	314	CLA	C3B-C4B	2.32	1.49	1.42
33	C	505	CLA	MG-NB	-2.32	2.01	2.05
33	4	309	CLA	C3B-C4B	2.32	1.49	1.42
33	0	310	CLA	C3B-C4B	2.32	1.49	1.42
33	6	313	CLA	CHC-C1C	2.32	1.43	1.38
42	e	101	HEM	C1D-ND	-2.32	1.34	1.38
33	6	308	CLA	C3B-C4B	2.31	1.49	1.42
33	8	316	CLA	C3B-C4B	2.31	1.49	1.42
46	2	304	DD6	O1-C20	-2.31	1.43	1.46
33	B	606	CLA	MG-NB	-2.31	2.01	2.05
33	9	309	CLA	C3B-C4B	2.31	1.49	1.42
44	6	314	KC1	C1B-NB	-2.31	1.34	1.37
33	2	309	CLA	C3B-C4B	2.31	1.49	1.42
33	1	313	CLA	CHC-C1C	2.31	1.43	1.38
45	6	306	A86	O1-C20	-2.31	1.43	1.46
33	8	313	CLA	C3B-C4B	2.31	1.49	1.42
33	b	606	CLA	MG-NB	-2.31	2.01	2.05
33	6	312	CLA	C3B-C4B	2.31	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	B	615	CLA	MG-NB	-2.31	2.01	2.05
33	B	612	CLA	CMD-C2D	-2.30	1.46	1.50
41	D	408	PL9	C52-C5	-2.30	1.46	1.50
33	B	605	CLA	MG-NB	-2.30	2.01	2.05
33	c	512	CLA	MG-NB	-2.30	2.01	2.05
33	8	312	CLA	C3B-C4B	2.30	1.49	1.42
45	7	301	A86	O1-C20	-2.30	1.43	1.46
33	A	405	CLA	MG-NB	-2.30	2.01	2.05
33	7	309	CLA	C3B-C4B	2.30	1.49	1.42
33	2	308	CLA	C3B-C4B	2.30	1.49	1.42
33	2	310	CLA	CHC-C1C	2.30	1.43	1.38
33	b	616	CLA	C3B-C4B	2.30	1.49	1.42
33	2	305	CLA	CHC-C1C	2.30	1.43	1.38
33	2	309	CLA	CHC-C1C	2.30	1.43	1.38
33	9	313	CLA	CHC-C1C	2.30	1.43	1.38
33	4	308	CLA	C3B-C4B	2.29	1.49	1.42
33	9	317	CLA	CHC-C1C	2.29	1.43	1.38
33	c	505	CLA	MG-NB	-2.29	2.01	2.05
33	0	305	CLA	C3B-C4B	2.29	1.49	1.42
33	3	303	CLA	CHC-C1C	2.29	1.43	1.38
33	b	610	CLA	MG-NB	-2.29	2.01	2.05
33	b	605	CLA	CMD-C2D	-2.29	1.46	1.50
47	7	306	KC2	C4A-C3A	-2.29	1.39	1.44
33	5	313	CLA	CHC-C1C	2.29	1.43	1.38
47	5	310	KC2	C4B-NB	-2.29	1.34	1.37
33	c	513	CLA	C3B-C4B	2.29	1.49	1.42
33	3	313	CLA	C3B-C4B	2.29	1.49	1.42
33	7	305	CLA	C3B-C4B	2.29	1.49	1.42
33	b	602	CLA	MG-NB	-2.29	2.01	2.05
33	3	304	CLA	C3B-C4B	2.29	1.49	1.42
33	8	315	CLA	C3B-C4B	2.29	1.49	1.42
36	w	301	LHG	O7-C5	-2.29	1.41	1.46
33	b	617	CLA	MG-NB	-2.29	2.01	2.05
45	9	301	A86	O1-C20	-2.29	1.43	1.46
38	C	518	DGD	O1G-C1G	-2.29	1.40	1.45
33	1	306	CLA	C3B-C4B	2.29	1.49	1.42
33	5	316	CLA	CHC-C1C	2.29	1.43	1.38
33	d	409	CLA	MG-NB	-2.29	2.01	2.05
46	8	304	DD6	O1-C20	-2.29	1.43	1.46
45	4	302	A86	C32-C31	-2.29	1.50	1.54
33	2	315	CLA	CHC-C1C	2.28	1.43	1.38
33	C	506	CLA	MG-NB	-2.28	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	B	601	CLA	C3B-C4B	2.28	1.49	1.42
33	3	305	CLA	C3B-C4B	2.28	1.49	1.42
33	9	314	CLA	CHC-C1C	2.28	1.43	1.38
38	c	518	DGD	O1G-C1G	-2.28	1.40	1.45
46	3	315	DD6	O1-C20	-2.28	1.43	1.46
33	7	309	CLA	CHC-C1C	2.28	1.43	1.38
33	1	314	CLA	C3B-C4B	2.28	1.49	1.42
33	Z	101	CLA	MG-NB	-2.28	2.01	2.05
33	0	311	CLA	C3B-C4B	2.28	1.49	1.42
33	9	306	CLA	C3B-C4B	2.28	1.49	1.42
33	C	507	CLA	CMD-C2D	-2.28	1.46	1.50
33	b	614	CLA	CHC-C1C	2.28	1.43	1.38
33	5	314	CLA	C3B-C4B	2.28	1.49	1.42
33	5	313	CLA	CMD-C2D	-2.28	1.46	1.50
46	9	304	DD6	O1-C20	-2.28	1.43	1.46
33	B	611	CLA	MG-NB	-2.28	2.01	2.05
33	3	303	CLA	C3B-C4B	2.28	1.49	1.42
34	a	409	PHO	C3D-C4D	2.27	1.44	1.41
33	0	307	CLA	C3B-C4B	2.27	1.49	1.42
33	C	501	CLA	CMD-C2D	-2.27	1.46	1.50
39	w	304	LMG	O7-C8	-2.27	1.41	1.46
33	4	309	CLA	CHC-C1C	2.27	1.43	1.38
33	2	313	CLA	CMD-C2D	-2.27	1.46	1.50
33	0	309	CLA	C3B-C4B	2.27	1.49	1.42
33	8	309	CLA	C3B-C4B	2.27	1.49	1.42
33	5	317	CLA	C3B-C4B	2.27	1.49	1.42
33	1	306	CLA	CHC-C1C	2.27	1.43	1.38
33	B	615	CLA	C3B-C4B	2.27	1.49	1.42
33	4	314	CLA	C3B-C4B	2.27	1.49	1.42
33	a	408	CLA	CMD-C2D	-2.27	1.46	1.50
33	8	314	CLA	CHC-C1C	2.27	1.43	1.38
44	3	310	KC1	C4A-C3A	-2.27	1.39	1.44
39	C	519	LMG	O7-C8	-2.27	1.41	1.46
33	a	407	CLA	MG-NB	-2.27	2.01	2.05
33	9	308	CLA	C3B-C4B	2.27	1.49	1.42
33	z	101	CLA	CHC-C1C	2.27	1.43	1.38
33	2	317	CLA	CHC-C1C	2.27	1.43	1.38
33	c	501	CLA	CMD-C2D	-2.27	1.46	1.50
33	4	306	CLA	C3B-C4B	2.27	1.49	1.42
33	9	306	CLA	CHC-C1C	2.27	1.43	1.38
33	2	307	CLA	CHC-C1C	2.27	1.43	1.38
33	2	312	CLA	CHC-C1C	2.27	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	4	308	CLA	CHC-C1C	2.27	1.43	1.38
33	2	316	CLA	CHC-C1C	2.26	1.43	1.38
33	3	307	CLA	C3B-C4B	2.26	1.49	1.42
33	5	317	CLA	CHC-C1C	2.26	1.43	1.38
33	0	313	CLA	CHC-C1C	2.26	1.43	1.38
39	q	301	LMG	O7-C8	-2.26	1.41	1.46
33	9	309	CLA	CHC-C1C	2.26	1.43	1.38
33	C	507	CLA	MG-NB	-2.26	2.01	2.05
33	B	603	CLA	CMD-C2D	-2.26	1.46	1.50
33	B	606	CLA	CMC-C2C	-2.26	1.46	1.50
33	B	606	CLA	CMD-C2D	-2.26	1.46	1.50
33	b	610	CLA	CMD-C2D	-2.26	1.46	1.50
33	b	614	CLA	C3B-C4B	2.26	1.49	1.42
33	c	506	CLA	CMB-C2B	-2.26	1.46	1.50
33	8	306	CLA	C3B-C4B	2.26	1.49	1.42
33	8	310	CLA	C3B-C4B	2.26	1.49	1.42
33	1	312	CLA	C3B-C4B	2.26	1.49	1.42
33	b	607	CLA	MG-NB	-2.26	2.01	2.05
33	8	311	CLA	CHC-C1C	2.26	1.43	1.38
33	2	314	CLA	C3B-C4B	2.26	1.49	1.42
33	c	505	CLA	CMD-C2D	-2.26	1.46	1.50
33	B	604	CLA	CMD-C2D	-2.26	1.46	1.50
33	B	607	CLA	CMD-C2D	-2.26	1.46	1.50
33	B	610	CLA	CMB-C2B	-2.26	1.46	1.50
33	C	505	CLA	CMD-C2D	-2.26	1.46	1.50
33	7	314	CLA	CMD-C2D	-2.26	1.46	1.50
33	3	304	CLA	CHC-C1C	2.26	1.43	1.38
33	a	408	CLA	MG-NB	-2.26	2.01	2.05
34	a	410	PHO	C4D-ND	-2.26	1.35	1.38
33	B	605	CLA	CMD-C2D	-2.26	1.46	1.50
33	b	613	CLA	MG-NB	-2.26	2.01	2.05
33	4	311	CLA	C3B-C4B	2.26	1.49	1.42
33	b	603	CLA	CMD-C2D	-2.26	1.46	1.50
33	6	312	CLA	CHC-C1C	2.26	1.43	1.38
33	8	308	CLA	C3B-C4B	2.26	1.49	1.42
33	B	610	CLA	CMD-C2D	-2.25	1.46	1.50
33	4	313	CLA	C3B-C4B	2.25	1.49	1.42
33	C	501	CLA	MG-NB	-2.25	2.01	2.05
33	b	602	CLA	CMD-C2D	-2.25	1.46	1.50
33	B	602	CLA	MG-NB	-2.25	2.01	2.05
33	8	309	CLA	CHC-C1C	2.25	1.43	1.38
33	5	311	CLA	C3B-C4B	2.25	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	3	319	CLA	MG-NB	-2.25	2.01	2.05
33	2	311	CLA	CHC-C1C	2.25	1.43	1.38
33	b	611	CLA	CMD-C2D	-2.25	1.46	1.50
33	2	317	CLA	C3B-C4B	2.25	1.49	1.42
33	b	616	CLA	MG-NB	-2.25	2.01	2.05
33	B	609	CLA	CMD-C2D	-2.25	1.46	1.50
33	6	315	CLA	C3B-C4B	2.25	1.49	1.42
33	1	309	CLA	CHC-C1C	2.25	1.43	1.38
33	C	503	CLA	MG-NB	-2.25	2.01	2.05
33	d	409	CLA	CMD-C2D	-2.25	1.46	1.50
33	d	401	CLA	CMD-C2D	-2.25	1.46	1.50
33	3	306	CLA	CHC-C1C	2.25	1.43	1.38
33	b	604	CLA	MG-NB	-2.25	2.01	2.05
33	B	602	CLA	CMD-C2D	-2.25	1.46	1.50
33	C	502	CLA	CMD-C2D	-2.25	1.46	1.50
33	W	303	CLA	CMB-C2B	-2.25	1.46	1.50
36	a	404	LHG	O7-C5	-2.25	1.41	1.46
33	5	308	CLA	CHC-C1C	2.25	1.43	1.38
33	4	310	CLA	CHC-C1C	2.25	1.43	1.38
33	7	312	CLA	MG-NB	-2.25	2.01	2.05
33	9	312	CLA	C3B-C4B	2.25	1.49	1.42
33	C	503	CLA	CMD-C2D	-2.25	1.46	1.50
33	H	103	CLA	C3B-C4B	2.25	1.49	1.42
33	7	304	CLA	C3B-C4B	2.25	1.49	1.42
39	M	201	LMG	O8-C9	-2.25	1.40	1.45
33	0	308	CLA	C3B-C4B	2.25	1.49	1.42
33	B	616	CLA	C3B-C4B	2.24	1.49	1.42
33	C	513	CLA	C3B-C4B	2.24	1.49	1.42
33	9	317	CLA	C3B-C4B	2.24	1.49	1.42
44	5	315	KC1	C1B-NB	-2.24	1.34	1.37
33	1	311	CLA	CHC-C1C	2.24	1.43	1.38
33	C	506	CLA	CMB-C2B	-2.24	1.46	1.50
33	b	603	CLA	CMB-C2B	-2.24	1.46	1.50
36	d	407	LHG	O7-C5	-2.24	1.41	1.46
48	0	302	ET4	C02-C03	2.24	1.55	1.52
33	4	315	CLA	C3B-C4B	2.24	1.49	1.42
33	7	310	CLA	C3B-C4B	2.24	1.49	1.42
33	8	308	CLA	CHC-C1C	2.24	1.43	1.38
33	9	310	CLA	CHC-C1C	2.24	1.43	1.38
33	c	507	CLA	MG-NB	-2.24	2.01	2.05
47	4	307	KC2	C1C-C2C	-2.24	1.40	1.44
33	2	306	CLA	C3B-C4B	2.24	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	4	316	CLA	CHC-C1C	2.24	1.43	1.38
33	4	305	CLA	C3B-C4B	2.24	1.49	1.42
33	1	315	CLA	C3B-C4B	2.24	1.49	1.42
33	B	614	CLA	C3B-C4B	2.24	1.49	1.42
33	9	315	CLA	C3B-C4B	2.24	1.49	1.42
33	D	406	CLA	CMD-C2D	-2.24	1.46	1.50
33	0	309	CLA	CHC-C1C	2.24	1.43	1.38
33	H	103	CLA	CHC-C1C	2.24	1.43	1.38
33	b	611	CLA	MG-NB	-2.24	2.01	2.05
33	3	308	CLA	C3B-C4B	2.24	1.49	1.42
33	3	313	CLA	CHC-C1C	2.24	1.43	1.38
33	9	305	CLA	CHC-C1C	2.24	1.43	1.38
33	d	401	CLA	CHC-C1C	2.24	1.43	1.38
33	7	312	CLA	C3B-C4B	2.24	1.49	1.42
33	3	302	CLA	MG-NB	-2.24	2.01	2.05
33	8	313	CLA	CHC-C1C	2.24	1.43	1.38
33	B	607	CLA	MG-NB	-2.23	2.01	2.05
33	C	502	CLA	MG-NB	-2.23	2.01	2.05
33	7	307	CLA	MG-NB	-2.23	2.01	2.05
33	0	312	CLA	C3B-C4B	2.23	1.49	1.42
33	1	316	CLA	CHC-C1C	2.23	1.43	1.38
33	b	613	CLA	CMD-C2D	-2.23	1.46	1.50
33	B	608	CLA	CMD-C2D	-2.23	1.46	1.50
33	b	611	CLA	CMB-C2B	-2.23	1.46	1.50
33	b	609	CLA	CMD-C2D	-2.23	1.46	1.50
33	b	614	CLA	CMD-C2D	-2.23	1.46	1.50
33	2	308	CLA	CHC-C1C	2.23	1.43	1.38
33	8	315	CLA	CHC-C1C	2.23	1.43	1.38
33	1	308	CLA	CHC-C1C	2.23	1.43	1.38
33	3	319	CLA	C3B-C4B	2.23	1.49	1.42
33	c	504	CLA	MG-NB	-2.23	2.01	2.05
33	C	510	CLA	CMD-C2D	-2.23	1.46	1.50
33	4	316	CLA	MG-NB	-2.23	2.01	2.05
33	b	607	CLA	CMD-C2D	-2.23	1.46	1.50
33	0	308	CLA	CHC-C1C	2.23	1.43	1.38
33	b	604	CLA	CMD-C2D	-2.23	1.46	1.50
39	Q	301	LMG	O7-C8	-2.23	1.41	1.46
42	e	101	HEM	C4B-NB	-2.23	1.34	1.38
33	B	611	CLA	CMB-C2B	-2.23	1.46	1.50
36	A	412	LHG	O7-C5	-2.23	1.41	1.46
33	Z	101	CLA	C3B-C4B	2.23	1.49	1.42
33	A	405	CLA	CMD-C2D	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	w	303	CLA	C3B-C4B	2.23	1.49	1.42
33	7	313	CLA	CHC-C1C	2.23	1.42	1.38
33	a	408	CLA	CMB-C2B	-2.23	1.46	1.50
33	1	310	CLA	C3B-C4B	2.23	1.49	1.42
33	4	314	CLA	CHC-C1C	2.23	1.42	1.38
33	3	308	CLA	MG-NB	-2.23	2.01	2.05
33	c	503	CLA	MG-NB	-2.22	2.01	2.05
33	3	313	CLA	CMD-C2D	-2.22	1.46	1.50
33	B	610	CLA	MG-NB	-2.22	2.01	2.05
33	B	614	CLA	CMD-C2D	-2.22	1.46	1.50
33	B	603	CLA	MG-NB	-2.22	2.01	2.05
33	8	305	CLA	CHC-C1C	2.22	1.42	1.38
33	D	405	CLA	CMB-C2B	-2.22	1.46	1.50
33	4	305	CLA	CHC-C1C	2.22	1.42	1.38
33	5	314	CLA	CHC-C1C	2.22	1.42	1.38
33	A	404	CLA	MG-NB	-2.22	2.01	2.05
33	B	603	CLA	CMB-C2B	-2.22	1.46	1.50
33	1	305	CLA	CHC-C1C	2.22	1.42	1.38
33	5	312	CLA	CHC-C1C	2.22	1.42	1.38
33	1	314	CLA	CHC-C1C	2.22	1.42	1.38
45	1	301	A86	O1-C20	-2.22	1.43	1.46
33	b	609	CLA	MG-NB	-2.22	2.01	2.05
33	B	616	CLA	CMD-C2D	-2.22	1.46	1.50
33	3	304	CLA	CMD-C2D	-2.22	1.46	1.50
33	b	608	CLA	CMD-C2D	-2.22	1.46	1.50
33	8	306	CLA	CHC-C1C	2.22	1.42	1.38
33	D	406	CLA	MG-NB	-2.21	2.01	2.05
33	B	615	CLA	CMB-C2B	-2.21	1.46	1.50
33	3	311	CLA	C3B-C4B	2.21	1.49	1.42
36	W	302	LHG	O7-C5	-2.21	1.41	1.46
33	4	310	CLA	MG-NB	-2.21	2.01	2.05
33	4	311	CLA	MG-NB	-2.21	2.01	2.05
33	c	502	CLA	CMB-C2B	-2.21	1.46	1.50
33	b	604	CLA	CMB-C2B	-2.21	1.46	1.50
33	b	612	CLA	CMB-C2B	-2.21	1.46	1.50
33	7	305	CLA	CHC-C1C	2.21	1.42	1.38
33	3	302	CLA	CMD-C2D	-2.21	1.46	1.50
33	C	509	CLA	CMB-C2B	-2.21	1.46	1.50
33	b	606	CLA	CMD-C2D	-2.21	1.46	1.50
33	4	316	CLA	C3B-C4B	2.21	1.49	1.42
33	D	402	CLA	CMB-C2B	-2.21	1.46	1.50
33	c	513	CLA	CHC-C1C	2.21	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	7	307	CLA	CMD-C2D	-2.21	1.46	1.50
33	b	608	CLA	MG-NB	-2.21	2.01	2.05
33	a	407	CLA	CHC-C1C	2.21	1.42	1.38
33	c	501	CLA	MG-NB	-2.21	2.01	2.05
33	B	616	CLA	CMB-C2B	-2.21	1.46	1.50
33	C	508	CLA	CMC-C2C	-2.21	1.46	1.50
33	4	312	CLA	C3B-C4B	2.21	1.49	1.42
33	3	308	CLA	CHC-C1C	2.21	1.42	1.38
33	0	312	CLA	CHC-C1C	2.21	1.42	1.38
33	A	408	CLA	CMD-C2D	-2.21	1.46	1.50
33	B	601	CLA	CMD-C2D	-2.21	1.46	1.50
33	C	511	CLA	MG-NB	-2.21	2.01	2.05
33	b	616	CLA	CMD-C2D	-2.21	1.46	1.50
33	7	311	CLA	MG-NB	-2.21	2.01	2.05
33	a	407	CLA	C3B-C4B	2.21	1.49	1.42
33	9	310	CLA	MG-NB	-2.21	2.01	2.05
36	5	318	LHG	O7-C5	-2.20	1.41	1.46
33	7	309	CLA	CMD-C2D	-2.20	1.46	1.50
33	c	506	CLA	MG-NB	-2.20	2.01	2.05
33	B	611	CLA	CMD-C2D	-2.20	1.46	1.50
33	C	508	CLA	CMD-C2D	-2.20	1.46	1.50
33	A	405	CLA	CMB-C2B	-2.20	1.46	1.50
33	C	504	CLA	CMD-C2D	-2.20	1.46	1.50
33	d	402	CLA	CMD-C2D	-2.20	1.46	1.50
33	B	613	CLA	CMD-C2D	-2.20	1.46	1.50
33	C	511	CLA	CMD-C2D	-2.20	1.46	1.50
36	3	318	LHG	O7-C5	-2.20	1.41	1.46
33	5	309	CLA	C3B-C4B	2.20	1.49	1.42
33	c	511	CLA	MG-NB	-2.20	2.01	2.05
45	2	302	A86	C32-C31	-2.20	1.50	1.54
33	Z	101	CLA	CHC-C1C	2.20	1.42	1.38
33	C	509	CLA	MG-NB	-2.20	2.01	2.05
33	C	508	CLA	CMB-C2B	-2.20	1.46	1.50
33	b	617	CLA	CMD-C2D	-2.20	1.46	1.50
33	b	616	CLA	CMB-C2B	-2.20	1.46	1.50
33	D	405	CLA	MG-NB	-2.20	2.01	2.05
33	B	601	CLA	CMB-C2B	-2.20	1.46	1.50
33	C	508	CLA	C3B-C4B	2.20	1.49	1.42
33	C	510	CLA	C3B-C4B	2.20	1.49	1.42
33	1	307	CLA	CHC-C1C	2.20	1.42	1.38
33	c	511	CLA	CMD-C2D	-2.20	1.46	1.50
33	b	609	CLA	CMB-C2B	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	B	601	CLA	MG-NB	-2.20	2.01	2.05
33	c	502	CLA	MG-NB	-2.20	2.01	2.05
33	0	304	CLA	C3B-C4B	2.20	1.49	1.42
33	c	506	CLA	C3B-C4B	2.19	1.49	1.42
33	2	314	CLA	CHC-C1C	2.19	1.42	1.38
39	W	301	LMG	O7-C8	-2.19	1.41	1.46
33	b	617	CLA	CMB-C2B	-2.19	1.46	1.50
33	3	302	CLA	C3B-C4B	2.19	1.49	1.42
36	5	318	LHG	P-O6	2.19	1.67	1.60
33	c	510	CLA	C3B-C4B	2.19	1.49	1.42
47	0	306	KC2	C4A-C3A	-2.19	1.40	1.44
33	B	602	CLA	C3B-C4B	2.19	1.49	1.42
33	7	307	CLA	C3B-C4B	2.19	1.49	1.42
33	c	510	CLA	MG-NB	-2.19	2.01	2.05
33	7	311	CLA	C3B-C4B	2.19	1.49	1.42
45	7	301	A86	C17-C16	-2.19	1.51	1.54
36	0	315	LHG	P-O6	2.19	1.67	1.60
33	c	509	CLA	CMB-C2B	-2.19	1.46	1.50
33	b	612	CLA	CMD-C2D	-2.19	1.46	1.50
39	C	522	LMG	C4-C3	2.19	1.58	1.52
45	9	302	A86	C32-C31	-2.19	1.50	1.54
33	D	402	CLA	MG-NB	-2.19	2.01	2.05
33	A	408	CLA	CMB-C2B	-2.19	1.46	1.50
33	6	307	CLA	C3B-C4B	2.19	1.49	1.42
33	c	508	CLA	C3B-C4B	2.19	1.49	1.42
33	3	309	CLA	MG-NB	-2.19	2.01	2.05
33	b	614	CLA	CMC-C2C	-2.19	1.46	1.50
33	0	311	CLA	CHC-C1C	2.19	1.42	1.38
33	7	314	CLA	MG-NB	-2.19	2.01	2.05
33	1	312	CLA	CHC-C1C	2.19	1.42	1.38
33	C	502	CLA	CMB-C2B	-2.19	1.46	1.50
33	d	401	CLA	CMB-C2B	-2.19	1.46	1.50
46	1	304	DD6	C36-C31	-2.19	1.32	1.35
33	0	305	CLA	CHC-C1C	2.19	1.42	1.38
33	9	312	CLA	CHC-C1C	2.19	1.42	1.38
33	C	512	CLA	CMD-C2D	-2.19	1.46	1.50
33	0	310	CLA	CHC-C1C	2.19	1.42	1.38
33	b	612	CLA	MG-NB	-2.19	2.01	2.05
33	d	409	CLA	CMB-C2B	-2.19	1.46	1.50
33	a	411	CLA	CMB-C2B	-2.19	1.46	1.50
33	D	405	CLA	CHC-C1C	2.19	1.42	1.38
33	b	617	CLA	CMC-C2C	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	509	CLA	CMD-C2D	-2.18	1.46	1.50
33	d	401	CLA	CMC-C2C	-2.18	1.46	1.50
33	3	311	CLA	MG-NB	-2.18	2.01	2.05
33	4	311	CLA	CHC-C1C	2.18	1.42	1.38
33	B	613	CLA	C3B-C4B	2.18	1.49	1.42
36	D	411	LHG	O7-C5	-2.18	1.41	1.46
33	c	507	CLA	CMD-C2D	-2.18	1.46	1.50
33	B	614	CLA	MG-NB	-2.18	2.01	2.05
33	b	614	CLA	CMB-C2B	-2.18	1.46	1.50
33	3	305	CLA	CHC-C1C	2.18	1.42	1.38
33	4	313	CLA	MG-NB	-2.18	2.01	2.05
33	9	308	CLA	MG-NB	-2.18	2.01	2.05
47	7	306	KC2	C4B-NB	-2.18	1.35	1.37
33	D	405	CLA	CMD-C2D	-2.18	1.46	1.50
33	3	303	CLA	MG-NB	-2.18	2.01	2.05
33	C	509	CLA	CHC-C1C	2.18	1.42	1.38
33	B	611	CLA	CMC-C2C	-2.18	1.46	1.50
33	C	506	CLA	CMD-C2D	-2.18	1.46	1.50
33	c	508	CLA	CMD-C2D	-2.18	1.46	1.50
33	C	505	CLA	CMB-C2B	-2.18	1.46	1.50
33	c	508	CLA	CMB-C2B	-2.18	1.46	1.50
33	8	307	CLA	MG-NB	-2.18	2.01	2.05
33	8	310	CLA	CMC-C2C	-2.18	1.46	1.50
33	b	615	CLA	C3B-C4B	2.18	1.49	1.42
33	c	504	CLA	CMD-C2D	-2.18	1.46	1.50
33	c	506	CLA	CHC-C1C	2.18	1.42	1.38
33	B	615	CLA	CMD-C2D	-2.18	1.46	1.50
33	C	501	CLA	CMB-C2B	-2.18	1.46	1.50
33	4	310	CLA	CMD-C2D	-2.18	1.46	1.50
45	6	305	A86	C32-C31	-2.18	1.50	1.54
33	B	614	CLA	CHC-C1C	2.18	1.42	1.38
33	B	616	CLA	CMC-C2C	-2.18	1.46	1.50
33	c	508	CLA	MG-NB	-2.18	2.01	2.05
33	3	311	CLA	CMD-C2D	-2.18	1.46	1.50
33	6	308	CLA	CHC-C1C	2.18	1.42	1.38
33	9	308	CLA	CHC-C1C	2.18	1.42	1.38
33	c	509	CLA	MG-NB	-2.18	2.01	2.05
33	7	309	CLA	MG-NB	-2.18	2.01	2.05
33	c	507	CLA	CMB-C2B	-2.17	1.46	1.50
33	6	316	CLA	CMD-C2D	-2.17	1.46	1.50
33	c	503	CLA	CHC-C1C	2.17	1.42	1.38
33	7	305	CLA	MG-NB	-2.17	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	h	101	BCR	C33-C5	-2.17	1.47	1.50
34	A	406	PHO	C3D-C4D	2.17	1.44	1.41
33	9	309	CLA	C1C-C2C	2.17	1.46	1.42
39	M	201	LMG	O7-C8	-2.17	1.41	1.46
38	A	415	DGD	C2E-C1E	2.17	1.56	1.50
33	B	608	CLA	MG-NB	-2.17	2.01	2.05
33	C	504	CLA	MG-NB	-2.17	2.01	2.05
33	C	512	CLA	CMB-C2B	-2.17	1.46	1.50
33	b	606	CLA	CMB-C2B	-2.17	1.46	1.50
33	c	503	CLA	CMD-C2D	-2.17	1.46	1.50
33	Z	101	CLA	CMD-C2D	-2.17	1.46	1.50
33	9	315	CLA	CHC-C1C	2.17	1.42	1.38
33	b	612	CLA	CMC-C2C	-2.17	1.46	1.50
33	7	310	CLA	CHC-C1C	2.17	1.42	1.38
33	9	306	CLA	MG-NB	-2.17	2.01	2.05
33	a	407	CLA	CMB-C2B	-2.17	1.46	1.50
33	B	604	CLA	CMB-C2B	-2.17	1.46	1.50
33	3	304	CLA	MG-NB	-2.17	2.01	2.05
39	0	314	LMG	O7-C8	-2.17	1.41	1.46
33	7	314	CLA	CHC-C1C	2.17	1.42	1.38
47	0	306	KC2	C4B-NB	-2.17	1.35	1.37
33	7	308	CLA	MG-NB	-2.17	2.01	2.05
33	c	512	CLA	C3B-C4B	2.17	1.49	1.42
33	C	513	CLA	CMD-C2D	-2.17	1.46	1.50
33	3	307	CLA	CHC-C1C	2.17	1.42	1.38
33	C	503	CLA	CMB-C2B	-2.17	1.46	1.50
33	H	103	CLA	MG-NB	-2.17	2.01	2.05
33	0	304	CLA	CHC-C1C	2.17	1.42	1.38
45	5	302	A86	C32-C31	-2.17	1.50	1.54
33	b	605	CLA	CMB-C2B	-2.17	1.46	1.50
33	7	310	CLA	MG-NB	-2.17	2.01	2.05
33	7	312	CLA	CHC-C1C	2.17	1.42	1.38
33	7	308	CLA	C3B-C4B	2.17	1.49	1.42
33	B	612	CLA	CMB-C2B	-2.17	1.46	1.50
33	9	310	CLA	CMB-C2B	-2.17	1.46	1.50
33	W	303	CLA	CMD-C2D	-2.17	1.46	1.50
34	A	406	PHO	C4D-ND	-2.17	1.35	1.38
33	B	605	CLA	CMB-C2B	-2.16	1.46	1.50
33	4	315	CLA	CHC-C1C	2.16	1.42	1.38
45	2	302	A86	C13-C11	-2.16	1.45	1.49
33	2	313	CLA	C1C-C2C	2.16	1.46	1.42
33	A	404	CLA	C3B-C4B	2.16	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2	306	CLA	CHC-C1C	2.16	1.42	1.38
33	C	511	CLA	CMB-C2B	-2.16	1.46	1.50
33	c	507	CLA	C3B-C4B	2.16	1.49	1.42
33	4	315	CLA	MG-NB	-2.16	2.01	2.05
33	C	507	CLA	CMB-C2B	-2.16	1.46	1.50
33	c	506	CLA	CMD-C2D	-2.16	1.46	1.50
33	8	309	CLA	CMD-C2D	-2.16	1.46	1.50
33	B	603	CLA	C3B-C4B	2.16	1.49	1.42
33	B	609	CLA	C3B-C4B	2.16	1.49	1.42
33	0	307	CLA	CHC-C1C	2.16	1.42	1.38
33	B	612	CLA	CMC-C2C	-2.16	1.46	1.50
33	b	602	CLA	CMB-C2B	-2.16	1.46	1.50
33	A	404	CLA	CHC-C1C	2.16	1.42	1.38
33	C	510	CLA	CHC-C1C	2.16	1.42	1.38
33	7	308	CLA	CMB-C2B	-2.16	1.46	1.50
33	b	615	CLA	MG-NB	-2.16	2.01	2.05
33	c	502	CLA	CMD-C2D	-2.16	1.46	1.50
34	A	407	PHO	C3D-C4D	2.16	1.44	1.41
42	e	101	HEM	C3C-C4C	-2.16	1.42	1.46
33	8	309	CLA	MG-NB	-2.16	2.01	2.05
33	C	505	CLA	C3B-C4B	2.16	1.49	1.42
33	8	316	CLA	CHC-C1C	2.16	1.42	1.38
33	2	310	CLA	CMB-C2B	-2.16	1.46	1.50
33	4	314	CLA	MG-NB	-2.16	2.01	2.05
33	C	513	CLA	CHC-C1C	2.16	1.42	1.38
33	D	402	CLA	CHC-C1C	2.16	1.42	1.38
33	3	319	CLA	CHC-C1C	2.16	1.42	1.38
33	4	305	CLA	MG-NB	-2.16	2.01	2.05
33	b	616	CLA	CMC-C2C	-2.16	1.46	1.50
34	a	410	PHO	C3D-C4D	2.16	1.44	1.41
33	c	508	CLA	CMC-C2C	-2.16	1.46	1.50
33	B	601	CLA	CHC-C1C	2.16	1.42	1.38
33	B	612	CLA	MG-NB	-2.16	2.01	2.05
33	8	312	CLA	CHC-C1C	2.16	1.42	1.38
33	D	405	CLA	CMC-C2C	-2.15	1.46	1.50
33	7	310	CLA	CMD-C2D	-2.15	1.46	1.50
33	c	511	CLA	C3B-C4B	2.15	1.49	1.42
45	0	301	A86	C17-C16	-2.15	1.51	1.54
33	b	617	CLA	C3B-C4B	2.15	1.49	1.42
33	3	309	CLA	CHC-C1C	2.15	1.42	1.38
33	C	504	CLA	CMB-C2B	-2.15	1.46	1.50
33	c	503	CLA	CMB-C2B	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	7	314	CLA	C3B-C4B	2.15	1.49	1.42
45	5	306	A86	C32-C31	-2.15	1.50	1.54
39	C	521	LMG	O7-C8	-2.15	1.41	1.46
33	c	504	CLA	C3B-C4B	2.15	1.49	1.42
33	0	309	CLA	MG-NB	-2.15	2.01	2.05
33	7	304	CLA	MG-NB	-2.15	2.01	2.05
33	c	513	CLA	CMD-C2D	-2.15	1.46	1.50
33	b	615	CLA	CMC-C2C	-2.15	1.46	1.50
33	d	401	CLA	MG-NB	-2.15	2.01	2.05
47	6	309	KC2	C4B-NB	-2.15	1.35	1.37
33	b	615	CLA	CMD-C2D	-2.15	1.46	1.50
33	c	510	CLA	CHC-C1C	2.15	1.42	1.38
33	4	306	CLA	MG-NB	-2.15	2.01	2.05
33	6	308	CLA	MG-NB	-2.15	2.01	2.05
33	b	608	CLA	C3B-C4B	2.15	1.49	1.42
33	1	310	CLA	CHC-C1C	2.15	1.42	1.38
33	c	512	CLA	CMD-C2D	-2.15	1.46	1.50
33	b	607	CLA	CMC-C2C	-2.15	1.46	1.50
33	8	307	CLA	CHC-C1C	2.15	1.42	1.38
33	3	305	CLA	MG-NB	-2.15	2.01	2.05
33	8	315	CLA	MG-NB	-2.15	2.01	2.05
33	2	309	CLA	C1C-C2C	2.15	1.46	1.42
33	C	507	CLA	CMC-C2C	-2.15	1.46	1.50
33	0	308	CLA	MG-NB	-2.15	2.01	2.05
33	C	512	CLA	C3B-C4B	2.15	1.49	1.42
33	9	311	CLA	CHC-C1C	2.15	1.42	1.38
33	c	501	CLA	C3B-C4B	2.15	1.49	1.42
33	7	312	CLA	CMD-C2D	-2.15	1.46	1.50
33	B	608	CLA	C3B-C4B	2.15	1.49	1.42
33	C	512	CLA	CMC-C2C	-2.15	1.46	1.50
33	a	411	CLA	CMD-C2D	-2.15	1.46	1.50
33	b	607	CLA	CMB-C2B	-2.15	1.46	1.50
33	8	310	CLA	CMB-C2B	-2.15	1.46	1.50
33	d	409	CLA	C3B-C4B	2.15	1.49	1.42
33	B	613	CLA	CMB-C2B	-2.15	1.46	1.50
33	b	604	CLA	C3B-C4B	2.15	1.49	1.42
33	3	319	CLA	CMD-C2D	-2.15	1.46	1.50
33	8	307	CLA	CMD-C2D	-2.15	1.46	1.50
33	b	606	CLA	CHC-C1C	2.15	1.42	1.38
33	3	309	CLA	CMD-C2D	-2.15	1.46	1.50
33	2	316	CLA	CMD-C2D	-2.15	1.46	1.50
33	C	506	CLA	C3B-C4B	2.15	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	511	CLA	C3B-C4B	2.15	1.49	1.42
33	d	402	CLA	CMB-C2B	-2.14	1.46	1.50
33	8	316	CLA	MG-NB	-2.14	2.01	2.05
33	c	504	CLA	CMB-C2B	-2.14	1.46	1.50
33	b	613	CLA	CMB-C2B	-2.14	1.46	1.50
33	C	504	CLA	C3B-C4B	2.14	1.49	1.42
45	0	303	A86	C32-C31	-2.14	1.51	1.54
33	c	501	CLA	CMB-C2B	-2.14	1.46	1.50
33	3	311	CLA	CMB-C2B	-2.14	1.46	1.50
33	B	606	CLA	CMB-C2B	-2.14	1.46	1.50
33	4	313	CLA	CHC-C1C	2.14	1.42	1.38
33	b	614	CLA	MG-NB	-2.14	2.01	2.05
39	b	621	LMG	O7-C8	-2.14	1.41	1.46
33	7	304	CLA	CHC-C1C	2.14	1.42	1.38
33	8	308	CLA	MG-NB	-2.14	2.01	2.05
33	4	305	CLA	CMD-C2D	-2.14	1.46	1.50
33	b	605	CLA	C3B-C4B	2.14	1.49	1.42
33	D	402	CLA	C3B-C4B	2.14	1.49	1.42
33	B	614	CLA	CMB-C2B	-2.14	1.46	1.50
33	8	310	CLA	MG-NB	-2.14	2.01	2.05
33	3	313	CLA	MG-NB	-2.14	2.01	2.05
33	1	309	CLA	C1C-C2C	2.14	1.46	1.42
33	B	614	CLA	CMC-C2C	-2.14	1.46	1.50
33	9	313	CLA	C1C-C2C	2.14	1.46	1.42
33	a	408	CLA	C3B-C4B	2.14	1.49	1.42
33	b	610	CLA	CMB-C2B	-2.14	1.46	1.50
33	B	605	CLA	C3B-C4B	2.14	1.49	1.42
33	b	610	CLA	CHC-C1C	2.14	1.42	1.38
33	4	308	CLA	MG-NB	-2.14	2.01	2.05
33	6	310	CLA	MG-NB	-2.14	2.01	2.05
33	B	611	CLA	C3B-C4B	2.14	1.49	1.42
33	B	602	CLA	CMB-C2B	-2.14	1.46	1.50
33	B	607	CLA	CMB-C2B	-2.14	1.46	1.50
33	7	311	CLA	CMD-C2D	-2.14	1.46	1.50
33	9	317	CLA	MG-NB	-2.14	2.01	2.05
33	1	310	CLA	CMD-C2D	-2.14	1.46	1.50
34	A	407	PHO	C4D-ND	-2.14	1.35	1.38
37	7	317	SQD	O2-C2	-2.14	1.37	1.43
33	6	315	CLA	CHC-C1C	2.14	1.42	1.38
33	c	509	CLA	CMD-C2D	-2.14	1.46	1.50
33	c	510	CLA	CMC-C2C	-2.14	1.46	1.50
33	5	309	CLA	CHC-C1C	2.14	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	7	308	CLA	CHC-C1C	2.14	1.42	1.38
33	b	609	CLA	C3B-C4B	2.14	1.49	1.42
33	C	502	CLA	C3B-C4B	2.14	1.49	1.42
33	C	513	CLA	MG-NB	-2.13	2.01	2.05
33	b	613	CLA	CMC-C2C	-2.13	1.46	1.50
33	b	615	CLA	CMB-C2B	-2.13	1.46	1.50
33	c	501	CLA	CMC-C2C	-2.13	1.46	1.50
33	a	407	CLA	CMC-C2C	-2.13	1.46	1.50
33	9	307	CLA	CHC-C1C	2.13	1.42	1.38
33	7	305	CLA	CMC-C2C	-2.13	1.46	1.50
33	B	603	CLA	CHC-C1C	2.13	1.42	1.38
33	C	508	CLA	CHC-C1C	2.13	1.42	1.38
33	H	103	CLA	CMD-C2D	-2.13	1.46	1.50
33	1	313	CLA	CMB-C2B	-2.13	1.46	1.50
44	6	314	KC1	C1D-ND	-2.13	1.35	1.37
33	2	305	CLA	CMD-C2D	-2.13	1.46	1.50
48	0	302	ET4	C01-C06	2.13	1.56	1.53
33	b	602	CLA	C3B-C4B	2.13	1.48	1.42
33	C	510	CLA	CMB-C2B	-2.13	1.46	1.50
33	9	311	CLA	CMD-C2D	-2.13	1.46	1.50
33	5	311	CLA	CHC-C1C	2.13	1.42	1.38
33	3	312	CLA	MG-NB	-2.13	2.01	2.05
33	8	306	CLA	MG-NB	-2.13	2.01	2.05
33	B	608	CLA	CMB-C2B	-2.13	1.46	1.50
39	C	522	LMG	O7-C8	-2.13	1.41	1.46
33	B	610	CLA	CMC-C2C	-2.13	1.46	1.50
33	8	310	CLA	CMD-C2D	-2.13	1.46	1.50
33	B	610	CLA	CHC-C1C	2.13	1.42	1.38
33	3	311	CLA	CHC-C1C	2.13	1.42	1.38
33	c	511	CLA	CMB-C2B	-2.13	1.46	1.50
33	0	307	CLA	MG-NB	-2.13	2.01	2.05
33	5	311	CLA	MG-NB	-2.13	2.01	2.05
33	6	316	CLA	MG-NB	-2.13	2.01	2.05
33	B	603	CLA	CMC-C2C	-2.13	1.46	1.50
33	3	307	CLA	CMB-C2B	-2.13	1.46	1.50
33	0	308	CLA	CMD-C2D	-2.13	1.46	1.50
33	9	309	CLA	MG-NB	-2.13	2.01	2.05
33	B	602	CLA	CHC-C1C	2.12	1.42	1.38
33	C	513	CLA	CMC-C2C	-2.12	1.46	1.50
33	5	312	CLA	MG-NB	-2.12	2.01	2.05
38	a	401	DGD	C3E-C4E	2.12	1.55	1.52
33	c	505	CLA	CMB-C2B	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	411	CLA	MG-NB	-2.12	2.01	2.05
33	2	310	CLA	MG-NB	-2.12	2.01	2.05
33	3	312	CLA	CHC-C1C	2.12	1.42	1.38
33	9	307	CLA	CMD-C2D	-2.12	1.46	1.50
33	C	509	CLA	CMC-C2C	-2.12	1.46	1.50
33	Z	101	CLA	CMB-C2B	-2.12	1.46	1.50
33	b	606	CLA	C3B-C4B	2.12	1.48	1.42
33	D	406	CLA	C3B-C4B	2.12	1.48	1.42
33	W	303	CLA	C3B-C4B	2.12	1.48	1.42
33	D	406	CLA	CMC-C2C	-2.12	1.46	1.50
33	4	310	CLA	CMC-C2C	-2.12	1.46	1.50
33	b	610	CLA	C3B-C4B	2.12	1.48	1.42
33	A	404	CLA	CMC-C2C	-2.12	1.46	1.50
33	0	304	CLA	CMD-C2D	-2.12	1.46	1.50
33	C	503	CLA	CMC-C2C	-2.12	1.46	1.50
33	c	510	CLA	CMB-C2B	-2.12	1.46	1.50
33	B	616	CLA	MG-NB	-2.12	2.01	2.05
33	b	608	CLA	CMB-C2B	-2.12	1.46	1.50
33	b	605	CLA	MG-NB	-2.12	2.01	2.05
33	6	307	CLA	MG-NB	-2.12	2.01	2.05
45	9	302	A86	C13-C11	-2.12	1.45	1.49
33	b	608	CLA	CHC-C1C	2.12	1.42	1.38
33	B	607	CLA	C3B-C4B	2.12	1.48	1.42
33	0	307	CLA	CMB-C2B	-2.12	1.46	1.50
33	3	303	CLA	CMD-C2D	-2.11	1.46	1.50
33	1	315	CLA	CHC-C1C	2.11	1.42	1.38
33	8	315	CLA	CMD-C2D	-2.11	1.46	1.50
33	C	509	CLA	C3B-C4B	2.11	1.48	1.42
33	c	511	CLA	CMC-C2C	-2.11	1.46	1.50
33	c	512	CLA	CMB-C2B	-2.11	1.46	1.50
33	6	308	CLA	CMB-C2B	-2.11	1.46	1.50
33	b	608	CLA	CMC-C2C	-2.11	1.46	1.50
33	9	315	CLA	CMD-C2D	-2.11	1.46	1.50
33	B	608	CLA	CHC-C1C	2.11	1.42	1.38
33	2	309	CLA	MG-NB	-2.11	2.01	2.05
33	c	513	CLA	MG-NB	-2.11	2.01	2.05
33	C	506	CLA	CMC-C2C	-2.11	1.46	1.50
33	4	306	CLA	CMD-C2D	-2.11	1.46	1.50
33	b	606	CLA	CMC-C2C	-2.11	1.46	1.50
33	C	511	CLA	CHC-C1C	2.11	1.42	1.38
47	5	310	KC2	C4A-C3A	-2.11	1.40	1.44
33	9	309	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	4	312	CLA	CMB-C2B	-2.11	1.46	1.50
33	0	311	CLA	MG-NB	-2.11	2.01	2.05
33	2	314	CLA	MG-NB	-2.11	2.01	2.05
33	B	612	CLA	CHC-C1C	2.11	1.42	1.38
33	w	303	CLA	CMB-C2B	-2.11	1.46	1.50
33	C	507	CLA	C3B-C4B	2.11	1.48	1.42
33	4	309	CLA	MG-NB	-2.11	2.01	2.05
33	C	501	CLA	CMC-C2C	-2.11	1.46	1.50
33	8	310	CLA	CHC-C1C	2.11	1.42	1.38
33	9	312	CLA	CMB-C2B	-2.11	1.46	1.50
33	0	312	CLA	CMD-C2D	-2.11	1.46	1.50
33	2	314	CLA	CMB-C2B	-2.11	1.46	1.50
33	2	308	CLA	MG-NB	-2.11	2.01	2.05
33	A	404	CLA	CMB-C2B	-2.11	1.46	1.50
33	9	317	CLA	CMB-C2B	-2.11	1.46	1.50
33	7	304	CLA	CMD-C2D	-2.11	1.46	1.50
33	4	311	CLA	CMC-C2C	-2.11	1.46	1.50
33	6	315	CLA	CMD-C2D	-2.11	1.46	1.50
37	B	622	SQD	O2-C2	-2.11	1.37	1.43
33	c	505	CLA	CMC-C2C	-2.11	1.46	1.50
33	3	302	CLA	CHC-C1C	2.11	1.42	1.38
33	A	405	CLA	C3B-C4B	2.11	1.48	1.42
33	b	609	CLA	CHC-C1C	2.10	1.42	1.38
33	c	503	CLA	C3B-C4B	2.10	1.48	1.42
33	C	503	CLA	CHC-C1C	2.10	1.42	1.38
33	5	313	CLA	MG-NB	-2.10	2.01	2.05
33	1	308	CLA	MG-NB	-2.10	2.01	2.05
33	1	315	CLA	MG-NB	-2.10	2.01	2.05
33	c	509	CLA	CHC-C1C	2.10	1.42	1.38
33	b	604	CLA	CMC-C2C	-2.10	1.46	1.50
33	B	608	CLA	CMC-C2C	-2.10	1.46	1.50
33	0	310	CLA	CMD-C2D	-2.10	1.46	1.50
33	9	312	CLA	MG-NB	-2.10	2.01	2.05
33	b	615	CLA	CHC-C1C	2.10	1.42	1.38
33	B	612	CLA	C3B-C4B	2.10	1.48	1.42
33	2	306	CLA	MG-NB	-2.10	2.01	2.05
33	9	317	CLA	CMD-C2D	-2.10	1.46	1.50
33	4	316	CLA	CMD-C2D	-2.10	1.46	1.50
33	7	311	CLA	CHC-C1C	2.10	1.42	1.38
33	8	306	CLA	CMD-C2D	-2.10	1.46	1.50
33	4	314	CLA	CMD-C2D	-2.10	1.46	1.50
33	B	611	CLA	CHC-C1C	2.10	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	B	613	CLA	CMC-C2C	-2.10	1.46	1.50
33	6	312	CLA	CMD-C2D	-2.10	1.46	1.50
33	9	308	CLA	CMD-C2D	-2.10	1.46	1.50
37	i	101	SQD	O2-C2	-2.10	1.37	1.43
33	8	312	CLA	MG-NB	-2.10	2.01	2.05
33	3	309	CLA	CMB-C2B	-2.10	1.46	1.50
33	C	503	CLA	C3B-C4B	2.10	1.48	1.42
33	4	315	CLA	CMD-C2D	-2.10	1.46	1.50
33	8	313	CLA	CMD-C2D	-2.10	1.46	1.50
33	0	305	CLA	MG-NB	-2.10	2.01	2.05
33	5	309	CLA	MG-NB	-2.10	2.01	2.05
33	b	612	CLA	C3B-C4B	2.10	1.48	1.42
48	0	302	ET4	C37-C38	-2.10	1.47	1.51
33	5	316	CLA	MG-NB	-2.10	2.01	2.05
33	9	305	CLA	MG-NB	-2.10	2.01	2.05
33	C	504	CLA	CMC-C2C	-2.09	1.46	1.50
33	9	316	CLA	MG-NB	-2.09	2.01	2.05
33	1	312	CLA	MG-NB	-2.09	2.01	2.05
33	B	605	CLA	CHC-C1C	2.09	1.42	1.38
33	7	305	CLA	CMB-C2B	-2.09	1.46	1.50
33	4	311	CLA	CMD-C2D	-2.09	1.46	1.50
33	C	510	CLA	MG-NB	-2.09	2.01	2.05
33	B	616	CLA	CHC-C1C	2.09	1.42	1.38
33	c	501	CLA	CHC-C1C	2.09	1.42	1.38
33	D	402	CLA	CMC-C2C	-2.09	1.46	1.50
33	1	314	CLA	CMB-C2B	-2.09	1.46	1.50
33	2	317	CLA	CMD-C2D	-2.09	1.46	1.50
37	T	101	SQD	O2-C2	-2.09	1.37	1.43
33	7	308	CLA	CMD-C2D	-2.09	1.46	1.50
33	b	605	CLA	CMC-C2C	-2.09	1.46	1.50
30	B	617	BCR	C33-C5	-2.09	1.47	1.50
33	6	310	CLA	CMC-C2C	-2.09	1.46	1.50
33	3	303	CLA	CMB-C2B	-2.09	1.46	1.50
33	9	306	CLA	CMD-C2D	-2.09	1.46	1.50
33	C	505	CLA	CHC-C1C	2.09	1.42	1.38
33	8	311	CLA	MG-NB	-2.09	2.01	2.05
33	B	609	CLA	CMB-C2B	-2.09	1.46	1.50
33	1	313	CLA	C1C-C2C	2.09	1.46	1.42
33	8	308	CLA	CMD-C2D	-2.09	1.46	1.50
37	0	316	SQD	O2-C2	-2.09	1.37	1.43
33	9	314	CLA	CMD-C2D	-2.09	1.46	1.50
33	1	307	CLA	CMB-C2B	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	B	615	CLA	CMC-C2C	-2.09	1.46	1.50
33	7	309	CLA	CMC-C2C	-2.09	1.46	1.50
33	c	504	CLA	CMC-C2C	-2.09	1.46	1.50
33	3	307	CLA	CMD-C2D	-2.09	1.46	1.50
33	C	506	CLA	CHC-C1C	2.09	1.42	1.38
33	6	315	CLA	MG-NB	-2.09	2.01	2.05
33	B	605	CLA	CMC-C2C	-2.09	1.46	1.50
33	C	511	CLA	CMC-C2C	-2.09	1.46	1.50
33	3	303	CLA	CMC-C2C	-2.09	1.46	1.50
33	b	609	CLA	CMC-C2C	-2.09	1.46	1.50
33	6	307	CLA	CHC-C1C	2.09	1.42	1.38
36	7	316	LHG	P-O6	2.09	1.66	1.60
33	a	411	CLA	CMC-C2C	-2.09	1.46	1.50
33	0	311	CLA	CMD-C2D	-2.09	1.46	1.50
33	w	303	CLA	CHC-C1C	2.08	1.42	1.38
33	d	409	CLA	CMC-C2C	-2.08	1.46	1.50
33	9	316	CLA	CMB-C2B	-2.08	1.46	1.50
39	B	620	LMG	O7-C8	-2.08	1.41	1.46
33	0	313	CLA	CBD-CAD	2.08	1.56	1.51
33	0	312	CLA	MG-NB	-2.08	2.01	2.05
33	C	502	CLA	CMC-C2C	-2.08	1.46	1.50
33	8	305	CLA	CMB-C2B	-2.08	1.46	1.50
33	3	307	CLA	MG-NB	-2.08	2.01	2.05
33	8	305	CLA	MG-NB	-2.08	2.01	2.05
33	c	512	CLA	CMC-C2C	-2.08	1.46	1.50
33	3	305	CLA	CMC-C2C	-2.08	1.46	1.50
33	8	312	CLA	CMD-C2D	-2.08	1.46	1.50
33	3	305	CLA	CMD-C2D	-2.08	1.46	1.50
33	4	315	CLA	CMB-C2B	-2.08	1.46	1.50
33	c	502	CLA	CHC-C1C	2.08	1.42	1.38
33	9	314	CLA	CMB-C2B	-2.08	1.46	1.50
33	B	606	CLA	C3B-C4B	2.08	1.48	1.42
33	7	313	CLA	MG-NB	-2.08	2.01	2.05
33	B	602	CLA	CMC-C2C	-2.08	1.46	1.50
33	8	316	CLA	CMD-C2D	-2.08	1.46	1.50
33	0	307	CLA	CMD-C2D	-2.08	1.46	1.50
33	b	604	CLA	CHC-C1C	2.08	1.42	1.38
33	c	513	CLA	CMC-C2C	-2.08	1.46	1.50
33	3	319	CLA	CMB-C2B	-2.08	1.46	1.50
33	0	309	CLA	CMD-C2D	-2.08	1.46	1.50
33	C	513	CLA	CMB-C2B	-2.08	1.46	1.50
33	8	311	CLA	CMB-C2B	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	z	101	CLA	MG-NB	-2.08	2.01	2.05
33	c	509	CLA	C3B-C4B	2.08	1.48	1.42
33	a	408	CLA	CHC-C1C	2.08	1.42	1.38
33	6	312	CLA	MG-NB	-2.08	2.01	2.05
33	A	408	CLA	CMC-C2C	-2.08	1.46	1.50
33	7	304	CLA	CMB-C2B	-2.08	1.46	1.50
30	D	407	BCR	C33-C5	-2.08	1.47	1.50
45	0	301	A86	O1-C15	-2.08	1.42	1.45
33	3	312	CLA	CMD-C2D	-2.08	1.46	1.50
33	a	408	CLA	CMC-C2C	-2.08	1.46	1.50
33	8	314	CLA	MG-NB	-2.08	2.01	2.05
30	b	618	BCR	C33-C5	-2.08	1.47	1.50
34	a	409	PHO	C4D-ND	-2.08	1.35	1.38
33	c	508	CLA	CHC-C1C	2.08	1.42	1.38
33	8	306	CLA	CMB-C2B	-2.08	1.46	1.50
33	2	317	CLA	MG-NB	-2.08	2.01	2.05
33	d	402	CLA	CMC-C2C	-2.08	1.46	1.50
33	0	309	CLA	CMB-C2B	-2.08	1.46	1.50
33	c	505	CLA	C3B-C4B	2.08	1.48	1.42
33	B	607	CLA	CMC-C2C	-2.08	1.46	1.50
33	9	315	CLA	MG-NB	-2.08	2.01	2.05
33	8	313	CLA	MG-NB	-2.08	2.01	2.05
33	b	611	CLA	CMC-C2C	-2.07	1.46	1.50
33	D	406	CLA	CMB-C2B	-2.07	1.46	1.50
33	4	306	CLA	CMC-C2C	-2.07	1.46	1.50
33	7	305	CLA	CMD-C2D	-2.07	1.46	1.50
33	6	307	CLA	CMD-C2D	-2.07	1.46	1.50
33	5	314	CLA	MG-NB	-2.07	2.01	2.05
33	c	512	CLA	CHC-C1C	2.07	1.42	1.38
33	7	307	CLA	CHC-C1C	2.07	1.42	1.38
33	2	315	CLA	CMB-C2B	-2.07	1.46	1.50
33	6	313	CLA	MG-NB	-2.07	2.01	2.05
30	H	101	BCR	C33-C5	-2.07	1.47	1.50
33	0	305	CLA	CMB-C2B	-2.07	1.46	1.50
33	8	307	CLA	CMB-C2B	-2.07	1.46	1.50
45	6	303	A86	C32-C31	-2.07	1.51	1.54
33	C	508	CLA	MG-NB	-2.07	2.01	2.05
33	0	304	CLA	MG-NB	-2.07	2.01	2.05
33	4	308	CLA	CMD-C2D	-2.07	1.46	1.50
33	1	313	CLA	MG-NB	-2.07	2.01	2.05
33	c	513	CLA	CMB-C2B	-2.07	1.46	1.50
33	w	303	CLA	CMD-C2D	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	5	312	CLA	CMB-C2B	-2.07	1.46	1.50
33	2	307	CLA	CMD-C2D	-2.07	1.46	1.50
33	2	312	CLA	CMD-C2D	-2.07	1.46	1.50
37	D	403	SQD	O2-C2	-2.07	1.37	1.43
33	A	405	CLA	CMC-C2C	-2.07	1.46	1.50
33	4	316	CLA	CMB-C2B	-2.07	1.46	1.50
33	0	312	CLA	CMB-C2B	-2.07	1.46	1.50
33	B	613	CLA	CHC-C1C	2.06	1.42	1.38
37	A	413	SQD	O2-C2	-2.06	1.37	1.43
33	9	317	CLA	CMC-C2C	-2.06	1.46	1.50
33	2	310	CLA	CMD-C2D	-2.06	1.46	1.50
45	5	301	A86	C32-C31	-2.06	1.51	1.54
33	c	502	CLA	CMC-C2C	-2.06	1.46	1.50
33	8	314	CLA	CMD-C2D	-2.06	1.46	1.50
33	A	408	CLA	C3B-C4B	2.06	1.48	1.42
33	b	602	CLA	CHC-C1C	2.06	1.42	1.38
37	a	413	SQD	O2-C2	-2.06	1.37	1.43
33	1	309	CLA	CMD-C2D	-2.06	1.46	1.50
33	1	305	CLA	MG-NB	-2.06	2.01	2.05
33	1	313	CLA	CMD-C2D	-2.06	1.46	1.50
33	7	313	CLA	CBD-CAD	2.06	1.56	1.51
33	2	311	CLA	MG-NB	-2.06	2.01	2.05
33	3	312	CLA	CMB-C2B	-2.06	1.46	1.50
33	4	312	CLA	CMD-C2D	-2.06	1.46	1.50
33	0	305	CLA	CMD-C2D	-2.06	1.46	1.50
33	9	315	CLA	CMB-C2B	-2.06	1.46	1.50
33	9	316	CLA	CMD-C2D	-2.06	1.46	1.50
33	1	311	CLA	MG-NB	-2.06	2.01	2.05
33	c	507	CLA	CMC-C2C	-2.06	1.46	1.50
33	1	306	CLA	MG-NB	-2.06	2.01	2.05
42	v	201	HEM	C2A-C3A	-2.06	1.33	1.38
45	5	305	A86	C32-C31	-2.06	1.51	1.54
33	9	305	CLA	CMB-C2B	-2.06	1.46	1.50
33	1	316	CLA	CMB-C2B	-2.06	1.46	1.50
33	9	314	CLA	MG-NB	-2.06	2.01	2.05
33	4	313	CLA	CMD-C2D	-2.06	1.46	1.50
33	2	315	CLA	CMD-C2D	-2.06	1.46	1.50
33	8	311	CLA	CMD-C2D	-2.06	1.46	1.50
33	4	312	CLA	CHC-C1C	2.06	1.42	1.38
33	4	311	CLA	CMB-C2B	-2.06	1.46	1.50
33	4	316	CLA	CMC-C2C	-2.06	1.46	1.50
33	9	310	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	8	315	CLA	CMB-C2B	-2.06	1.46	1.50
39	d	410	LMG	O7-C8	-2.06	1.41	1.46
33	3	304	CLA	CMB-C2B	-2.06	1.46	1.50
33	5	317	CLA	MG-NB	-2.06	2.01	2.05
33	c	503	CLA	CMC-C2C	-2.06	1.46	1.50
33	6	315	CLA	CMB-C2B	-2.06	1.46	1.50
33	2	315	CLA	MG-NB	-2.06	2.01	2.05
33	B	604	CLA	C3B-C4B	2.06	1.48	1.42
33	C	505	CLA	CMC-C2C	-2.05	1.46	1.50
33	0	310	CLA	MG-NB	-2.05	2.01	2.05
45	6	301	A86	C13-C11	-2.05	1.45	1.49
33	c	502	CLA	C3B-C4B	2.05	1.48	1.42
33	9	311	CLA	MG-NB	-2.05	2.01	2.05
33	1	314	CLA	CMD-C2D	-2.05	1.46	1.50
33	b	613	CLA	C3B-C4B	2.05	1.48	1.42
33	7	312	CLA	CMC-C2C	-2.05	1.46	1.50
33	9	313	CLA	CMB-C2B	-2.05	1.46	1.50
33	2	316	CLA	MG-NB	-2.05	2.01	2.05
33	3	313	CLA	CMB-C2B	-2.05	1.46	1.50
33	4	313	CLA	CMB-C2B	-2.05	1.46	1.50
33	8	314	CLA	CMB-C2B	-2.05	1.46	1.50
33	c	509	CLA	CMC-C2C	-2.05	1.46	1.50
33	4	308	CLA	CMB-C2B	-2.05	1.46	1.50
33	2	317	CLA	CMB-C2B	-2.05	1.46	1.50
33	1	307	CLA	CMD-C2D	-2.05	1.46	1.50
45	7	301	A86	O1-C15	-2.05	1.42	1.45
33	8	313	CLA	C1C-C2C	2.05	1.46	1.42
33	4	309	CLA	CMB-C2B	-2.05	1.46	1.50
33	c	506	CLA	CMC-C2C	-2.05	1.46	1.50
33	5	308	CLA	CMD-C2D	-2.05	1.46	1.50
33	9	312	CLA	CMD-C2D	-2.05	1.46	1.50
33	b	612	CLA	CHC-C1C	2.05	1.42	1.38
37	L	101	SQD	O2-C2	-2.05	1.37	1.43
33	8	309	CLA	C1C-C2C	2.05	1.46	1.42
33	B	609	CLA	CMC-C2C	-2.05	1.46	1.50
33	z	101	CLA	CMD-C2D	-2.05	1.46	1.50
33	3	311	CLA	CMC-C2C	-2.05	1.46	1.50
33	7	309	CLA	CMB-C2B	-2.05	1.46	1.50
38	a	401	DGD	C2E-C1E	2.05	1.56	1.50
33	3	308	CLA	CMD-C2D	-2.05	1.46	1.50
45	6	301	A86	C32-C31	-2.05	1.51	1.54
33	6	308	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	1	315	CLA	CMD-C2D	-2.05	1.46	1.50
42	F	101	HEM	CMB-C2B	2.05	1.55	1.50
33	1	316	CLA	MG-NB	-2.05	2.01	2.05
33	W	303	CLA	CHC-C1C	2.05	1.42	1.38
47	6	309	KC2	C4A-C3A	-2.05	1.40	1.44
33	C	510	CLA	CMC-C2C	-2.05	1.46	1.50
33	3	304	CLA	CMC-C2C	-2.05	1.46	1.50
37	t	102	SQD	O3-C3	-2.05	1.37	1.43
33	3	306	CLA	MG-NB	-2.04	2.01	2.05
33	8	311	CLA	CMC-C2C	-2.04	1.46	1.50
33	b	611	CLA	CHC-C1C	2.04	1.42	1.38
33	b	616	CLA	CHC-C1C	2.04	1.42	1.38
33	5	314	CLA	CMC-C2C	-2.04	1.46	1.50
33	9	306	CLA	CMC-C2C	-2.04	1.46	1.50
33	6	310	CLA	CMD-C2D	-2.04	1.46	1.50
33	B	607	CLA	CHC-C1C	2.04	1.42	1.38
33	7	310	CLA	CMB-C2B	-2.04	1.46	1.50
33	1	310	CLA	CMB-C2B	-2.04	1.46	1.50
33	3	306	CLA	CMB-C2B	-2.04	1.46	1.50
33	7	307	CLA	CMB-C2B	-2.04	1.46	1.50
33	9	307	CLA	CMB-C2B	-2.04	1.46	1.50
33	9	308	CLA	CMB-C2B	-2.04	1.46	1.50
33	8	316	CLA	CMB-C2B	-2.04	1.46	1.50
33	3	308	CLA	CMB-C2B	-2.04	1.46	1.50
33	9	309	CLA	CMB-C2B	-2.04	1.46	1.50
33	H	103	CLA	CMB-C2B	-2.04	1.46	1.50
33	7	308	CLA	CMC-C2C	-2.04	1.46	1.50
33	2	307	CLA	CMB-C2B	-2.04	1.46	1.50
33	1	306	CLA	CMD-C2D	-2.04	1.46	1.50
33	1	312	CLA	CMB-C2B	-2.04	1.46	1.50
33	7	314	CLA	CMB-C2B	-2.04	1.46	1.50
33	1	315	CLA	CMB-C2B	-2.04	1.46	1.50
33	4	305	CLA	CMB-C2B	-2.04	1.46	1.50
33	1	305	CLA	CMD-C2D	-2.04	1.46	1.50
33	2	305	CLA	MG-NB	-2.04	2.01	2.05
33	4	306	CLA	CMB-C2B	-2.04	1.46	1.50
33	4	314	CLA	CMC-C2C	-2.04	1.46	1.50
33	2	306	CLA	CMD-C2D	-2.04	1.46	1.50
33	1	312	CLA	CMD-C2D	-2.04	1.46	1.50
30	b	620	BCR	C33-C5	-2.04	1.47	1.50
33	8	313	CLA	CMB-C2B	-2.04	1.46	1.50
33	1	316	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	B	604	CLA	CMC-C2C	-2.04	1.46	1.50
33	5	309	CLA	CMD-C2D	-2.04	1.46	1.50
33	7	307	CLA	CMC-C2C	-2.04	1.46	1.50
33	8	307	CLA	CMC-C2C	-2.04	1.46	1.50
42	v	201	HEM	FE-ND	2.04	2.01	1.94
33	3	307	CLA	CMC-C2C	-2.04	1.46	1.50
33	5	312	CLA	CMD-C2D	-2.04	1.46	1.50
33	b	607	CLA	C3B-C4B	2.04	1.48	1.42
30	K	101	BCR	C33-C5	-2.04	1.47	1.50
33	C	512	CLA	CHC-C1C	2.04	1.42	1.38
33	B	615	CLA	CHC-C1C	2.04	1.42	1.38
38	3	320	DGD	O1G-C1G	-2.04	1.40	1.45
33	b	602	CLA	CMC-C2C	-2.03	1.46	1.50
33	1	311	CLA	CMD-C2D	-2.03	1.46	1.50
33	5	309	CLA	CMB-C2B	-2.03	1.46	1.50
33	B	609	CLA	MG-NB	-2.03	2.01	2.05
33	0	308	CLA	CMB-C2B	-2.03	1.46	1.50
33	8	312	CLA	CMB-C2B	-2.03	1.46	1.50
37	7	317	SQD	O3-C3	-2.03	1.37	1.43
33	5	314	CLA	CMD-C2D	-2.03	1.46	1.50
33	c	505	CLA	CHC-C1C	2.03	1.42	1.38
33	6	311	CLA	MG-NB	-2.03	2.01	2.05
33	0	304	CLA	CMB-C2B	-2.03	1.46	1.50
33	1	306	CLA	CMC-C2C	-2.03	1.46	1.50
33	C	501	CLA	C3B-C4B	2.03	1.48	1.42
33	C	502	CLA	CHC-C1C	2.03	1.42	1.38
45	1	301	A86	C32-C31	-2.03	1.51	1.54
33	5	316	CLA	CMD-C2D	-2.03	1.46	1.50
33	0	307	CLA	CMC-C2C	-2.03	1.46	1.50
45	5	302	A86	C13-C11	-2.03	1.45	1.49
33	9	313	CLA	CMD-C2D	-2.03	1.46	1.50
33	D	406	CLA	CHC-C1C	2.03	1.42	1.38
33	W	303	CLA	MG-NB	-2.03	2.01	2.05
33	2	312	CLA	MG-NB	-2.03	2.01	2.05
33	B	604	CLA	MG-NB	-2.03	2.01	2.05
33	4	305	CLA	CMC-C2C	-2.03	1.46	1.50
33	9	313	CLA	MG-NB	-2.03	2.01	2.05
33	3	302	CLA	CMB-C2B	-2.03	1.46	1.50
33	3	309	CLA	CMC-C2C	-2.03	1.46	1.50
39	m	201	LMG	O8-C9	-2.03	1.40	1.45
33	z	101	CLA	CMB-C2B	-2.03	1.46	1.50
33	0	313	CLA	MG-NB	-2.03	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	504	CLA	CHC-C1C	2.03	1.42	1.38
33	c	507	CLA	CHC-C1C	2.03	1.42	1.38
33	2	307	CLA	MG-NB	-2.03	2.01	2.05
33	b	605	CLA	CHC-C1C	2.03	1.42	1.38
33	5	308	CLA	MG-NB	-2.03	2.01	2.05
33	5	316	CLA	CMB-C2B	-2.03	1.46	1.50
33	2	309	CLA	CMD-C2D	-2.03	1.46	1.50
33	8	312	CLA	CMC-C2C	-2.03	1.46	1.50
33	0	311	CLA	CMC-C2C	-2.03	1.46	1.50
33	1	305	CLA	CMB-C2B	-2.03	1.46	1.50
30	d	403	BCR	C33-C5	-2.03	1.47	1.50
33	z	101	CLA	CMC-C2C	-2.02	1.46	1.50
33	2	312	CLA	CMC-C2C	-2.02	1.46	1.50
37	l	101	SQD	O2-C2	-2.02	1.37	1.43
33	8	308	CLA	CMB-C2B	-2.02	1.46	1.50
33	3	302	CLA	CMC-C2C	-2.02	1.46	1.50
33	2	311	CLA	CMB-C2B	-2.02	1.46	1.50
48	0	302	ET4	C04-C05	2.02	1.54	1.51
30	H	101	BCR	C38-C26	-2.02	1.47	1.50
39	q	302	LMG	O7-C8	-2.02	1.41	1.46
33	4	310	CLA	CMB-C2B	-2.02	1.46	1.50
45	5	307	A86	C32-C31	-2.02	1.51	1.54
33	3	305	CLA	CMB-C2B	-2.02	1.46	1.50
33	6	311	CLA	CMD-C2D	-2.02	1.46	1.50
33	9	305	CLA	CMD-C2D	-2.02	1.46	1.50
33	1	314	CLA	MG-NB	-2.02	2.01	2.05
33	2	314	CLA	CMD-C2D	-2.02	1.46	1.50
33	9	314	CLA	CMC-C2C	-2.02	1.46	1.50
30	a	412	BCR	C38-C26	-2.02	1.47	1.50
33	8	306	CLA	CMC-C2C	-2.02	1.46	1.50
33	8	309	CLA	CMB-C2B	-2.02	1.46	1.50
44	6	314	KC1	C4A-C3A	-2.02	1.40	1.44
33	9	308	CLA	CMC-C2C	-2.02	1.46	1.50
33	8	305	CLA	CMD-C2D	-2.02	1.46	1.50
30	h	101	BCR	C38-C26	-2.02	1.47	1.50
33	1	310	CLA	MG-NB	-2.02	2.01	2.05
33	5	317	CLA	CMD-C2D	-2.01	1.46	1.50
39	D	404	LMG	O8-C9	-2.01	1.40	1.45
33	b	617	CLA	CHC-C1C	2.01	1.42	1.38
36	W	302	LHG	P-O6	2.01	1.67	1.59
33	4	309	CLA	CMD-C2D	-2.01	1.46	1.50
33	4	312	CLA	CMC-C2C	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	9	306	CLA	CMB-C2B	-2.01	1.46	1.50
37	0	316	SQD	O3-C3	-2.01	1.38	1.43
33	C	507	CLA	CHC-C1C	2.01	1.42	1.38
33	b	613	CLA	CHC-C1C	2.01	1.42	1.38
33	3	306	CLA	CMD-C2D	-2.01	1.46	1.50
33	1	309	CLA	MG-NB	-2.01	2.01	2.05
33	7	311	CLA	CMC-C2C	-2.01	1.46	1.50
33	2	307	CLA	CMC-C2C	-2.01	1.46	1.50
39	c	519	LMG	C4-C3	2.01	1.57	1.52
33	7	312	CLA	CMB-C2B	-2.01	1.46	1.50
33	b	603	CLA	CMC-C2C	-2.01	1.46	1.50
33	2	306	CLA	CMB-C2B	-2.01	1.46	1.50
33	d	402	CLA	C3B-C4B	2.01	1.48	1.42
33	7	304	CLA	CMC-C2C	-2.01	1.46	1.50
33	d	409	CLA	CHC-C1C	2.01	1.42	1.38
33	1	311	CLA	CMC-C2C	-2.01	1.46	1.50
33	Z	101	CLA	CMC-C2C	-2.01	1.46	1.50
33	6	313	CLA	CMD-C2D	-2.01	1.46	1.50
33	1	306	CLA	CMB-C2B	-2.01	1.46	1.50
33	C	502	CLA	MG-ND	-2.01	2.01	2.05
37	T	101	SQD	O3-C3	-2.01	1.38	1.43
33	B	601	CLA	CMC-C2C	-2.01	1.46	1.50
33	3	319	CLA	CMC-C2C	-2.01	1.46	1.50
33	7	314	CLA	CMC-C2C	-2.01	1.46	1.50
30	b	620	BCR	C38-C26	-2.01	1.47	1.50
33	5	312	CLA	CMC-C2C	-2.01	1.46	1.50
33	4	308	CLA	CMC-C2C	-2.01	1.46	1.50
33	2	311	CLA	CMD-C2D	-2.01	1.46	1.50
33	B	613	CLA	MG-ND	-2.01	2.01	2.05
37	1	101	SQD	O4-C4	-2.01	1.38	1.43
33	2	308	CLA	CMD-C2D	-2.01	1.46	1.50
33	2	309	CLA	CMB-C2B	-2.01	1.46	1.50
36	w	301	LHG	P-O6	2.00	1.67	1.59
37	L	101	SQD	O4-C4	-2.00	1.38	1.43
33	9	311	CLA	CMB-C2B	-2.00	1.46	1.50
30	A	409	BCR	C33-C5	-2.00	1.47	1.50
30	B	619	BCR	C38-C26	-2.00	1.47	1.50
33	c	511	CLA	CHC-C1C	2.00	1.42	1.38
33	2	312	CLA	CMB-C2B	-2.00	1.46	1.50
33	2	305	CLA	CMB-C2B	-2.00	1.46	1.50
37	7	317	SQD	O4-C4	-2.00	1.38	1.43
37	B	622	SQD	O4-C4	-2.00	1.38	1.43

All (2660) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	5	302	A86	C23-C16-C22	-72.53	2.00	107.37
45	6	304	A86	C23-C16-C22	-72.36	2.25	107.37
45	5	303	A86	C23-C16-C22	-71.86	2.97	107.37
45	4	302	A86	C23-C16-C22	-71.36	3.70	107.37
45	5	307	A86	C23-C16-C22	-69.94	5.76	107.37
45	6	302	A86	C23-C16-C22	-68.85	7.35	107.37
45	5	304	A86	C23-C16-C22	-67.20	9.74	107.37
45	5	301	A86	C23-C16-C22	-65.86	11.69	107.37
45	6	301	A86	C23-C16-C22	-64.73	13.33	107.37
45	6	305	A86	C23-C16-C22	-45.58	41.16	107.37
45	5	307	A86	C29-C30-C31	-44.45	125.21	177.66
45	6	306	A86	C23-C16-C22	-37.05	53.55	107.37
45	5	306	A86	C23-C16-C17	-31.92	52.87	108.97
45	6	301	A86	C29-C30-C31	-30.78	141.35	177.66
45	6	301	A86	O1-C20-C19	30.57	142.14	113.49
45	5	305	A86	C29-C30-C31	-30.49	141.69	177.66
45	6	303	A86	C23-C16-C17	-30.32	55.69	108.97
45	4	302	A86	O1-C20-C19	28.97	140.64	113.49
45	6	303	A86	C34-O4-C38	28.95	168.98	117.85
45	6	303	A86	O1-C20-C19	28.49	140.19	113.49
45	5	306	A86	O1-C20-C19	28.35	140.06	113.49
45	6	305	A86	O1-C20-C19	28.18	139.91	113.49
45	6	304	A86	O1-C20-C19	26.20	138.05	113.49
45	5	305	A86	O1-C20-C19	26.17	138.02	113.49
45	5	302	A86	C34-O4-C38	25.34	162.59	117.85
45	6	306	A86	O1-C20-C19	25.30	137.21	113.49
45	5	303	A86	C34-O4-C38	24.80	161.65	117.85
45	5	307	A86	C34-O4-C38	23.17	158.76	117.85
45	6	302	A86	O1-C20-C19	-22.86	92.07	113.49
45	5	302	A86	O1-C20-C19	22.44	134.52	113.49
45	6	305	A86	C29-C30-C31	-22.21	151.45	177.66
45	5	306	A86	C29-C30-C31	-21.55	152.23	177.66
45	5	301	A86	O1-C20-C19	20.89	133.07	113.49
45	5	305	A86	C23-C16-C22	20.41	137.03	107.37
45	4	302	A86	O4-C34-C35	-19.78	57.00	107.64
45	5	301	A86	C29-C30-C31	-19.43	154.73	177.66
45	5	307	A86	O1-C20-C19	18.87	131.17	113.49
45	5	301	A86	C34-O4-C38	18.39	150.33	117.85
45	6	305	A86	C23-C16-C17	-18.31	76.78	108.97
45	6	301	A86	C35-C34-C33	-17.88	77.77	109.89
45	4	302	A86	O4-C34-C33	17.68	152.88	107.64
45	6	304	A86	C34-O4-C38	16.75	147.44	117.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	5	304	A86	O1-C20-C19	16.47	128.93	113.49
45	5	304	A86	C29-C30-C31	-15.30	159.61	177.66
45	5	302	A86	C29-C30-C31	-15.17	159.76	177.66
45	5	301	A86	C35-C34-C33	-14.65	83.56	109.89
45	5	303	A86	O1-C20-C19	14.36	126.95	113.49
45	6	304	A86	C29-C30-C31	-14.28	160.82	177.66
45	6	301	A86	C21-C20-C15	-14.18	77.57	123.35
45	4	302	A86	C34-O4-C38	-13.36	94.25	117.85
45	6	306	A86	C34-O4-C38	13.30	141.33	117.85
45	4	302	A86	C21-C20-C15	-12.74	82.22	123.35
45	6	302	A86	C29-C30-C31	-12.58	162.82	177.66
45	6	306	A86	C23-C16-C17	-12.21	87.51	108.97
45	6	301	A86	O4-C34-C33	11.57	137.25	107.64
45	6	301	A86	O4-C34-C35	11.49	137.06	107.64
45	5	306	A86	C21-C20-C15	-11.39	86.60	123.35
45	5	307	A86	C35-C34-C33	-11.38	89.45	109.89
45	4	302	A86	C29-C30-C31	-11.37	164.25	177.66
45	6	301	A86	C23-C16-C17	-10.93	89.75	108.97
45	6	303	A86	C29-C30-C31	-10.79	164.93	177.66
45	5	306	A86	C23-C16-C22	10.76	123.00	107.37
45	5	305	A86	C35-C34-C33	-10.70	90.67	109.89
45	5	306	A86	C35-C34-C33	-10.37	91.26	109.89
45	6	303	A86	C23-C16-C22	-10.36	92.33	107.37
45	4	302	A86	C33-C32-C31	10.22	119.14	109.21
45	6	302	A86	C35-C34-C33	-10.16	91.64	109.89
46	4	303	DD6	C10-C9-C8	9.92	151.95	123.20
45	5	301	A86	O4-C34-C33	9.89	132.95	107.64
45	0	301	A86	C20-O1-C15	9.84	65.26	61.03
45	5	301	A86	O4-C34-C35	9.81	132.74	107.64
45	7	303	A86	C20-O1-C15	9.80	65.24	61.03
45	6	305	A86	C21-C20-C15	-9.75	91.87	123.35
45	7	301	A86	C20-O1-C15	9.72	65.21	61.03
45	6	303	A86	C21-C20-C15	-9.67	92.12	123.35
45	4	302	A86	C23-C16-C17	-9.65	92.01	108.97
45	0	303	A86	C20-O1-C15	9.42	65.08	61.03
45	4	304	A86	C20-O1-C15	9.23	65.00	61.03
45	5	305	A86	C19-C18-C17	-9.21	93.56	110.79
45	5	304	A86	C35-C34-C33	-9.19	93.38	109.89
45	4	302	A86	C22-C16-C17	-9.14	92.90	108.97
45	6	306	A86	C35-C34-C33	-9.13	93.48	109.89
45	9	302	A86	C20-O1-C15	8.97	64.88	61.03
45	2	302	A86	C20-O1-C15	8.97	64.88	61.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	9	301	A86	C20-O1-C15	8.96	64.88	61.03
45	2	301	A86	C20-O1-C15	8.95	64.87	61.03
45	4	301	A86	C20-O1-C15	8.84	64.83	61.03
45	6	305	A86	C35-C34-C33	-8.80	94.07	109.89
45	4	302	A86	C41-C32-C40	-8.80	83.44	108.63
45	8	301	A86	C20-O1-C15	8.77	64.80	61.03
45	3	314	A86	C20-O1-C15	8.70	64.77	61.03
45	5	303	A86	C29-C30-C31	-8.66	167.44	177.66
46	4	303	DD6	C9-C10-C11	8.56	139.28	127.28
45	6	302	A86	C21-C20-C15	8.55	150.94	123.35
45	5	305	A86	C20-O1-C15	8.45	64.66	61.03
45	5	306	A86	C22-C16-C17	-8.40	94.21	108.97
45	5	303	A86	C20-O1-C15	8.35	64.61	61.03
45	6	306	A86	C20-O1-C15	8.30	64.59	61.03
45	5	304	A86	C20-O1-C15	8.23	64.57	61.03
45	6	301	A86	C22-C16-C17	-8.21	94.54	108.97
45	6	303	A86	C20-O1-C15	8.19	64.55	61.03
45	6	304	A86	C20-O1-C15	8.18	64.54	61.03
46	8	304	DD6	C4-C5-C6	-8.14	115.86	127.28
45	5	301	A86	C20-O1-C15	8.13	64.52	61.03
45	6	305	A86	C20-O1-C15	8.12	64.52	61.03
45	5	306	A86	C20-O1-C15	8.09	64.50	61.03
45	5	302	A86	C20-O1-C15	8.03	64.48	61.03
45	1	301	A86	C20-O1-C15	7.91	64.43	61.03
46	4	303	DD6	C9-C8-C6	7.85	147.88	126.36
45	6	301	A86	C20-O1-C15	7.81	64.39	61.03
45	5	302	A86	C35-C34-C33	-7.76	95.94	109.89
45	5	307	A86	C20-O1-C15	7.75	64.36	61.03
45	6	305	A86	C22-C16-C17	-7.74	95.36	108.97
45	4	302	A86	C20-O1-C15	7.70	64.34	61.03
45	8	302	A86	C20-O1-C15	7.66	64.32	61.03
45	5	301	A86	C23-C16-C17	-7.65	95.52	108.97
45	1	302	A86	C20-O1-C15	7.63	64.31	61.03
45	5	303	A86	C35-C34-C33	-7.58	96.28	109.89
46	8	304	DD6	C14-C13-C11	-7.54	113.83	125.53
45	5	306	A86	C34-O4-C38	7.45	131.01	117.85
45	5	305	A86	C22-C16-C17	-7.35	96.06	108.97
33	b	613	CLA	C4A-NA-C1A	7.28	110.00	106.68
33	d	402	CLA	C4A-NA-C1A	7.26	109.99	106.68
45	6	303	A86	C35-C34-C33	-7.25	96.86	109.89
45	6	306	A86	C19-C18-C17	-7.22	97.28	110.79
33	B	612	CLA	C4A-NA-C1A	7.22	109.97	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	1	304	DD6	C4-C5-C6	-7.18	117.21	127.28
33	1	310	CLA	C4A-NA-C1A	7.13	109.93	106.68
33	8	310	CLA	C4A-NA-C1A	7.08	109.91	106.68
45	6	302	A86	C34-O4-C38	7.07	130.33	117.85
33	c	509	CLA	C4A-NA-C1A	7.06	109.90	106.68
33	8	308	CLA	C4A-NA-C1A	7.05	109.89	106.68
33	C	507	CLA	C4A-NA-C1A	7.04	109.89	106.68
46	1	303	DD6	C9-C10-C11	-7.02	117.44	127.28
45	6	306	A86	C22-C16-C17	-7.01	96.66	108.97
46	8	303	DD6	C9-C10-C11	-7.00	117.46	127.28
33	a	411	CLA	C4A-NA-C1A	6.93	109.84	106.68
46	8	304	DD6	C9-C10-C11	-6.90	117.60	127.28
33	0	311	CLA	C4A-NA-C1A	6.87	109.81	106.68
33	c	507	CLA	C4A-NA-C1A	6.85	109.81	106.68
33	5	309	CLA	C4A-NA-C1A	6.84	109.80	106.68
33	b	617	CLA	C4A-NA-C1A	6.83	109.79	106.68
33	6	311	CLA	C4A-NA-C1A	6.81	109.79	106.68
33	3	302	CLA	C4A-NA-C1A	6.81	109.79	106.68
33	C	509	CLA	C4A-NA-C1A	6.81	109.78	106.68
45	6	304	A86	C21-C20-C15	-6.80	101.38	123.35
46	2	303	DD6	O1-C20-C21	6.79	122.64	115.05
33	6	307	CLA	C4A-NA-C1A	6.79	109.78	106.68
48	7	302	ET4	C29-C22-C21	-6.79	111.00	124.18
33	2	306	CLA	C4A-NA-C1A	6.78	109.77	106.68
33	0	305	CLA	C4A-NA-C1A	6.78	109.77	106.68
33	6	308	CLA	C4A-NA-C1A	6.78	109.77	106.68
46	9	303	DD6	O1-C20-C21	6.78	122.62	115.05
48	0	302	ET4	C29-C22-C21	-6.75	111.06	124.18
33	C	511	CLA	C4A-NA-C1A	6.75	109.76	106.68
33	C	503	CLA	C4A-NA-C1A	6.74	109.75	106.68
33	5	311	CLA	C4A-NA-C1A	6.73	109.75	106.68
33	B	607	CLA	C4A-NA-C1A	6.72	109.75	106.68
33	4	308	CLA	C4A-NA-C1A	6.71	109.74	106.68
33	7	311	CLA	C4A-NA-C1A	6.71	109.74	106.68
33	2	315	CLA	C4A-NA-C1A	6.71	109.74	106.68
33	D	406	CLA	C4A-NA-C1A	6.71	109.74	106.68
33	C	504	CLA	C4A-NA-C1A	6.70	109.73	106.68
33	9	317	CLA	C4A-NA-C1A	6.66	109.72	106.68
33	4	315	CLA	C4A-NA-C1A	6.66	109.72	106.68
33	1	312	CLA	C4A-NA-C1A	6.66	109.72	106.68
33	0	304	CLA	C4A-NA-C1A	6.65	109.72	106.68
33	c	504	CLA	C4A-NA-C1A	6.65	109.71	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	8	312	CLA	C4A-NA-C1A	6.64	109.71	106.68
33	1	308	CLA	C4A-NA-C1A	6.64	109.71	106.68
33	7	313	CLA	C4A-NA-C1A	6.64	109.71	106.68
33	b	610	CLA	C4A-NA-C1A	6.63	109.71	106.68
33	9	306	CLA	C4A-NA-C1A	6.63	109.71	106.68
33	6	315	CLA	C4A-NA-C1A	6.63	109.70	106.68
45	9	302	A86	O1-C20-C19	-6.62	107.28	113.49
45	2	302	A86	O1-C20-C19	-6.62	107.29	113.49
33	c	513	CLA	C4A-NA-C1A	6.62	109.70	106.68
33	8	309	CLA	C4A-NA-C1A	6.62	109.70	106.68
45	6	302	A86	C20-O1-C15	6.60	63.87	61.03
33	A	408	CLA	C4A-NA-C1A	6.60	109.69	106.68
33	3	319	CLA	C4A-NA-C1A	6.60	109.69	106.68
33	c	503	CLA	C4A-NA-C1A	6.60	109.69	106.68
33	3	307	CLA	C4A-NA-C1A	6.60	109.69	106.68
33	0	310	CLA	C4A-NA-C1A	6.59	109.69	106.68
33	0	313	CLA	C4A-NA-C1A	6.59	109.69	106.68
33	4	310	CLA	C4A-NA-C1A	6.58	109.68	106.68
33	c	511	CLA	C4A-NA-C1A	6.57	109.68	106.68
33	b	608	CLA	C4A-NA-C1A	6.55	109.67	106.68
33	8	315	CLA	C4A-NA-C1A	6.55	109.67	106.68
33	C	513	CLA	C4A-NA-C1A	6.55	109.67	106.68
33	9	315	CLA	C4A-NA-C1A	6.53	109.66	106.68
33	3	312	CLA	C4A-NA-C1A	6.53	109.66	106.68
45	6	306	A86	C21-C20-C15	-6.53	102.28	123.35
33	C	512	CLA	C4A-NA-C1A	6.53	109.66	106.68
33	9	308	CLA	C4A-NA-C1A	6.52	109.66	106.68
33	2	309	CLA	C4A-NA-C1A	6.52	109.66	106.68
33	0	307	CLA	C4A-NA-C1A	6.52	109.65	106.68
33	1	305	CLA	C4A-NA-C1A	6.52	109.65	106.68
33	9	311	CLA	C4A-NA-C1A	6.51	109.65	106.68
45	6	303	A86	C4-C3-C2	-6.51	110.21	123.52
33	3	305	CLA	C4A-NA-C1A	6.51	109.65	106.68
33	3	306	CLA	C4A-NA-C1A	6.50	109.64	106.68
33	1	315	CLA	C4A-NA-C1A	6.50	109.64	106.68
33	9	312	CLA	C4A-NA-C1A	6.49	109.64	106.68
33	2	308	CLA	C4A-NA-C1A	6.49	109.64	106.68
33	4	309	CLA	C4A-NA-C1A	6.49	109.64	106.68
33	1	306	CLA	C4A-NA-C1A	6.49	109.64	106.68
33	B	610	CLA	C4A-NA-C1A	6.48	109.64	106.68
46	9	304	DD6	C4-C5-C6	-6.47	118.20	127.28
33	B	601	CLA	C4A-NA-C1A	6.47	109.63	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	6	310	CLA	C4A-NA-C1A	6.47	109.63	106.68
33	7	310	CLA	C4A-NA-C1A	6.47	109.63	106.68
33	b	611	CLA	C4A-NA-C1A	6.47	109.63	106.68
33	A	405	CLA	C4A-NA-C1A	6.47	109.63	106.68
33	8	314	CLA	C4A-NA-C1A	6.47	109.63	106.68
33	A	404	CLA	C4A-NA-C1A	6.47	109.63	106.68
45	5	305	A86	O1-C20-C21	-6.46	107.82	115.05
33	7	304	CLA	C4A-NA-C1A	6.46	109.63	106.68
33	9	309	CLA	C4A-NA-C1A	6.46	109.63	106.68
46	2	304	DD6	C4-C5-C6	-6.46	118.22	127.28
33	4	305	CLA	C4A-NA-C1A	6.46	109.62	106.68
33	0	309	CLA	C4A-NA-C1A	6.46	109.62	106.68
33	2	317	CLA	C4A-NA-C1A	6.45	109.62	106.68
33	4	311	CLA	C4A-NA-C1A	6.45	109.62	106.68
33	8	305	CLA	C4A-NA-C1A	6.44	109.62	106.68
33	b	602	CLA	C4A-NA-C1A	6.44	109.62	106.68
33	8	306	CLA	C4A-NA-C1A	6.44	109.62	106.68
33	H	103	CLA	C4A-NA-C1A	6.43	109.61	106.68
33	5	314	CLA	C4A-NA-C1A	6.43	109.61	106.68
45	6	301	A86	C34-O4-C38	6.42	129.19	117.85
33	2	311	CLA	C4A-NA-C1A	6.42	109.61	106.68
33	1	314	CLA	C4A-NA-C1A	6.42	109.61	106.68
33	5	317	CLA	C4A-NA-C1A	6.41	109.60	106.68
33	d	409	CLA	C4A-NA-C1A	6.41	109.60	106.68
33	5	312	CLA	C4A-NA-C1A	6.41	109.60	106.68
33	5	308	CLA	C4A-NA-C1A	6.40	109.60	106.68
33	B	604	CLA	C4A-NA-C1A	6.40	109.60	106.68
33	2	314	CLA	C4A-NA-C1A	6.40	109.60	106.68
46	2	304	DD6	C9-C10-C11	-6.39	118.31	127.28
33	b	612	CLA	C4A-NA-C1A	6.39	109.59	106.68
33	8	311	CLA	C4A-NA-C1A	6.39	109.59	106.68
33	1	309	CLA	C4A-NA-C1A	6.39	109.59	106.68
45	6	303	A86	C22-C16-C17	-6.38	97.75	108.97
33	3	311	CLA	C4A-NA-C1A	6.37	109.59	106.68
33	8	316	CLA	C4A-NA-C1A	6.36	109.58	106.68
33	9	313	CLA	C4A-NA-C1A	6.36	109.58	106.68
46	9	304	DD6	C9-C10-C11	-6.36	118.36	127.28
33	6	312	CLA	C4A-NA-C1A	6.36	109.58	106.68
33	7	305	CLA	C4A-NA-C1A	6.36	109.58	106.68
33	a	407	CLA	C4A-NA-C1A	6.35	109.58	106.68
33	2	305	CLA	C4A-NA-C1A	6.35	109.58	106.68
33	7	309	CLA	C4A-NA-C1A	6.35	109.58	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	1	316	CLA	C4A-NA-C1A	6.35	109.58	106.68
33	B	616	CLA	C4A-NA-C1A	6.34	109.57	106.68
33	3	313	CLA	C4A-NA-C1A	6.34	109.57	106.68
33	D	402	CLA	C4A-NA-C1A	6.33	109.57	106.68
33	7	314	CLA	C4A-NA-C1A	6.33	109.57	106.68
33	C	501	CLA	C4A-NA-C1A	6.32	109.56	106.68
33	1	311	CLA	C4A-NA-C1A	6.32	109.56	106.68
45	6	301	A86	O1-C20-C21	-6.32	107.99	115.05
33	6	313	CLA	C4A-NA-C1A	6.31	109.56	106.68
33	9	310	CLA	C4A-NA-C1A	6.31	109.56	106.68
33	c	512	CLA	C4A-NA-C1A	6.30	109.56	106.68
33	2	316	CLA	C4A-NA-C1A	6.30	109.56	106.68
33	0	308	CLA	C4A-NA-C1A	6.30	109.55	106.68
33	b	607	CLA	C4A-NA-C1A	6.29	109.55	106.68
33	5	313	CLA	C4A-NA-C1A	6.29	109.55	106.68
33	9	305	CLA	C4A-NA-C1A	6.28	109.55	106.68
33	a	408	CLA	C4A-NA-C1A	6.28	109.54	106.68
33	9	316	CLA	C4A-NA-C1A	6.28	109.54	106.68
33	4	313	CLA	C4A-NA-C1A	6.27	109.54	106.68
33	z	101	CLA	C4A-NA-C1A	6.26	109.54	106.68
33	3	308	CLA	C4A-NA-C1A	6.26	109.54	106.68
33	b	616	CLA	C4A-NA-C1A	6.26	109.54	106.68
33	2	312	CLA	C4A-NA-C1A	6.26	109.54	106.68
33	C	510	CLA	C4A-NA-C1A	6.26	109.53	106.68
33	4	312	CLA	C4A-NA-C1A	6.26	109.53	106.68
33	1	313	CLA	C4A-NA-C1A	6.25	109.53	106.68
33	7	307	CLA	C4A-NA-C1A	6.25	109.53	106.68
33	9	314	CLA	C4A-NA-C1A	6.24	109.53	106.68
33	4	316	CLA	C4A-NA-C1A	6.22	109.52	106.68
33	3	304	CLA	C4A-NA-C1A	6.22	109.52	106.68
33	4	306	CLA	C4A-NA-C1A	6.22	109.52	106.68
33	6	316	CLA	C4A-NA-C1A	6.22	109.52	106.68
33	5	316	CLA	C4A-NA-C1A	6.21	109.51	106.68
33	7	312	CLA	C4A-NA-C1A	6.21	109.51	106.68
33	2	310	CLA	C4A-NA-C1A	6.21	109.51	106.68
33	8	307	CLA	C4A-NA-C1A	6.21	109.51	106.68
33	c	502	CLA	C4A-NA-C1A	6.20	109.51	106.68
33	c	510	CLA	C4A-NA-C1A	6.19	109.50	106.68
33	0	312	CLA	C4A-NA-C1A	6.19	109.50	106.68
33	7	308	CLA	C4A-NA-C1A	6.18	109.50	106.68
33	8	313	CLA	C4A-NA-C1A	6.18	109.50	106.68
33	C	506	CLA	C4A-NA-C1A	6.17	109.49	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	1	307	CLA	C4A-NA-C1A	6.16	109.49	106.68
45	4	302	A86	C35-C34-C33	6.16	120.95	109.89
45	6	305	A86	O1-C20-C21	-6.16	108.17	115.05
34	A	406	PHO	C4D-CHA-CBD	-6.15	105.51	108.45
33	B	614	CLA	C4A-NA-C1A	6.14	109.48	106.68
45	7	303	A86	O1-C20-C19	-6.14	107.74	113.49
33	B	613	CLA	C4A-NA-C1A	6.11	109.47	106.68
33	Z	101	CLA	C4A-NA-C1A	6.11	109.47	106.68
33	3	309	CLA	C4A-NA-C1A	6.10	109.46	106.68
47	4	307	KC2	C1D-CHD-C4C	-6.10	111.91	126.25
33	c	508	CLA	C4A-NA-C1A	6.10	109.46	106.68
33	b	615	CLA	C4A-NA-C1A	6.09	109.46	106.68
46	8	303	DD6	C4-C5-C6	-6.09	118.74	127.28
46	1	303	DD6	C4-C5-C6	-6.07	118.76	127.28
33	b	609	CLA	C4A-NA-C1A	6.05	109.44	106.68
33	b	605	CLA	C4A-NA-C1A	6.04	109.43	106.68
45	7	301	A86	C4-C5-C6	-6.03	118.83	127.28
33	3	303	CLA	C4A-NA-C1A	6.01	109.42	106.68
33	c	506	CLA	C4A-NA-C1A	6.01	109.42	106.68
46	2	304	DD6	C21-C20-C19	6.00	120.98	114.24
34	a	410	PHO	C4D-CHA-CBD	-6.00	105.58	108.45
46	2	303	DD6	C4-C5-C6	-6.00	118.86	127.28
46	9	303	DD6	C4-C5-C6	-6.00	118.86	127.28
46	9	304	DD6	C21-C20-C19	6.00	120.98	114.24
33	4	314	CLA	C4A-NA-C1A	5.99	109.41	106.68
33	W	303	CLA	C4A-NA-C1A	5.99	109.41	106.68
45	0	301	A86	C4-C5-C6	-5.99	118.88	127.28
33	B	608	CLA	C4A-NA-C1A	5.97	109.40	106.68
45	5	307	A86	O1-C20-C21	-5.96	108.38	115.05
45	6	302	A86	C4-C3-C2	-5.96	111.33	123.52
45	6	304	A86	O1-C20-C21	-5.94	108.41	115.05
33	B	602	CLA	C4A-NA-C1A	5.94	109.39	106.68
45	6	304	A86	C35-C34-C33	-5.94	99.22	109.89
33	2	307	CLA	C4A-NA-C1A	5.93	109.39	106.68
45	5	305	A86	C25-C26-C27	-5.91	118.99	127.28
34	a	409	PHO	C4D-CHA-CBD	-5.91	105.62	108.45
45	5	306	A86	O1-C20-C21	-5.86	108.50	115.05
33	D	405	CLA	C4A-NA-C1A	5.86	109.35	106.68
45	4	304	A86	O1-C20-C19	-5.84	108.02	113.49
34	A	407	PHO	C4D-CHA-CBD	-5.80	105.67	108.45
33	B	615	CLA	C4A-NA-C1A	5.79	109.32	106.68
46	1	304	DD6	C21-C20-C19	5.78	120.73	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	9	307	CLA	C4A-NA-C1A	5.77	109.31	106.68
33	C	508	CLA	C4A-NA-C1A	5.77	109.31	106.68
33	b	614	CLA	C4A-NA-C1A	5.74	109.30	106.68
45	5	302	A86	O1-C20-C21	-5.74	108.64	115.05
33	d	401	CLA	C4A-NA-C1A	5.74	109.30	106.68
33	w	303	CLA	C4A-NA-C1A	5.73	109.29	106.68
33	B	606	CLA	C4A-NA-C1A	5.72	109.29	106.68
45	4	301	A86	O1-C20-C19	-5.72	108.13	113.49
30	c	515	BCR	C20-C21-C22	-5.72	119.26	127.28
45	8	301	A86	O1-C20-C21	-5.70	108.67	115.05
36	7	316	LHG	O4-P-O5	5.69	133.00	110.83
30	C	515	BCR	C20-C21-C22	-5.68	119.31	127.28
36	5	318	LHG	O4-P-O5	5.67	132.92	110.83
45	0	303	A86	O1-C20-C19	-5.67	108.18	113.49
45	7	303	A86	O1-C20-C21	-5.65	108.73	115.05
33	b	604	CLA	C4A-NA-C1A	5.64	109.25	106.68
36	0	315	LHG	O4-P-O5	5.63	132.78	110.83
45	6	304	A86	C22-C16-C17	-5.60	99.13	108.97
45	6	304	A86	C23-C16-C17	-5.58	99.16	108.97
33	B	609	CLA	C4A-NA-C1A	5.58	109.23	106.68
45	1	302	A86	C33-C32-C31	5.58	114.63	109.21
33	C	502	CLA	C4A-NA-C1A	5.57	109.22	106.68
45	8	302	A86	C33-C32-C31	5.56	114.62	109.21
45	4	302	A86	O1-C20-C21	-5.55	108.84	115.05
45	7	301	A86	O1-C20-C21	-5.52	108.88	115.05
33	B	603	CLA	C4A-NA-C1A	5.51	109.19	106.68
45	0	301	A86	O1-C20-C21	-5.51	108.89	115.05
45	5	307	A86	C19-C18-C17	5.49	121.06	110.79
33	c	501	CLA	C4A-NA-C1A	5.47	109.17	106.68
45	6	305	A86	C3-C2-C1	-5.45	119.63	127.28
45	5	302	A86	C3-C2-C1	-5.45	119.64	127.28
45	6	303	A86	O1-C20-C21	-5.45	108.96	115.05
45	5	305	A86	C3-C2-C1	-5.43	119.66	127.28
44	5	315	KC1	C1D-ND-C4D	5.43	110.12	106.31
45	4	301	A86	C4-C5-C6	-5.43	119.67	127.28
45	2	302	A86	C4-C5-C6	-5.38	119.73	127.28
45	9	302	A86	C4-C5-C6	-5.38	119.74	127.28
45	5	307	A86	C25-C26-C27	-5.37	119.75	127.28
45	5	304	A86	C25-C26-C27	-5.37	119.75	127.28
45	6	305	A86	C25-C26-C27	-5.35	119.78	127.28
45	2	301	A86	C4-C5-C6	-5.35	119.78	127.28
45	3	314	A86	C3-C2-C1	-5.34	119.79	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	e	101	HEM	CHC-C4B-NB	5.32	130.15	124.42
33	c	505	CLA	C4A-NA-C1A	5.31	109.10	106.68
45	0	301	A86	O1-C20-C15	-5.30	57.10	59.23
47	4	307	KC2	C4B-CHC-C1C	-5.30	114.75	126.02
35	A	410	BCT	O2-C-O1	5.30	133.22	119.68
45	5	302	A86	C4-C5-C6	-5.28	119.88	127.28
45	9	301	A86	C4-C5-C6	-5.27	119.89	127.28
33	B	605	CLA	C4A-NA-C1A	5.26	109.08	106.68
42	V	201	HEM	CHC-C4B-NB	5.25	130.08	124.42
45	8	302	A86	C25-C26-C27	-5.24	119.93	127.28
45	1	302	A86	C25-C26-C27	-5.24	119.93	127.28
45	5	305	A86	O4-C38-O5	-5.24	118.98	125.70
47	5	310	KC2	C1D-CHD-C4C	-5.23	113.95	126.25
45	7	301	A86	O1-C20-C15	-5.23	57.13	59.23
33	b	606	CLA	C4A-NA-C1A	5.23	109.06	106.68
45	5	303	A86	C22-C16-C17	-5.21	99.81	108.97
45	5	304	A86	C22-C16-C17	-5.20	99.82	108.97
47	7	306	KC2	C1D-CHD-C4C	-5.20	114.02	126.25
45	8	301	A86	C3-C2-C1	-5.18	120.01	127.28
45	3	314	A86	C41-C32-C31	-5.16	105.86	110.47
45	5	307	A86	C3-C2-C1	-5.16	120.04	127.28
45	5	305	A86	C4-C5-C6	-5.16	120.05	127.28
46	3	315	DD6	C4-C5-C6	-5.13	120.08	127.28
46	1	304	DD6	C9-C10-C11	-5.12	120.09	127.28
45	6	303	A86	C3-C2-C1	-5.11	120.11	127.28
45	5	302	A86	C21-C20-C19	-5.11	108.50	114.24
45	5	303	A86	O1-C20-C21	-5.11	109.33	115.05
45	7	303	A86	C3-C2-C1	-5.11	120.12	127.28
33	B	611	CLA	C4A-NA-C1A	5.10	109.01	106.68
47	4	307	KC2	C1A-NA-C4A	-5.10	104.35	106.68
45	5	303	A86	C23-C16-C17	-5.10	100.01	108.97
37	T	101	SQD	C1-O5-C5	5.10	123.67	113.72
45	4	302	A86	C3-C2-C1	-5.09	120.14	127.28
35	a	402	BCT	O2-C-O1	5.09	132.69	119.68
45	6	302	A86	C3-C2-C1	-5.08	120.16	127.28
45	0	303	A86	O4-C38-C39	5.07	120.13	111.09
41	d	404	PL9	C7-C3-C4	5.06	121.08	116.91
45	6	302	A86	C22-C16-C17	5.06	117.86	108.97
37	B	622	SQD	C1-O5-C5	5.05	123.59	113.72
45	6	302	A86	C25-C26-C27	-5.05	120.19	127.28
45	5	302	A86	C25-C26-C27	-5.05	120.20	127.28
45	3	314	A86	C4-C5-C6	-5.02	120.24	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	5	301	A86	C25-C26-C27	-5.01	120.25	127.28
37	t	102	SQD	C1-O5-C5	5.01	123.50	113.72
45	6	302	A86	C4-C5-C6	-5.00	120.26	127.28
45	5	305	A86	C23-C16-C17	-5.00	100.18	108.97
41	D	408	PL9	C7-C3-C4	5.00	121.03	116.91
45	4	301	A86	O1-C20-C21	-4.99	109.47	115.05
45	6	302	A86	O1-C20-C21	-4.99	109.47	115.05
46	9	303	DD6	C3-C2-C1	-4.99	120.28	127.28
45	6	306	A86	C25-C26-C27	-4.98	120.29	127.28
47	0	306	KC2	C1D-CHD-C4C	-4.98	114.54	126.25
45	2	301	A86	O1-C20-C21	-4.97	109.50	115.05
46	2	303	DD6	C3-C2-C1	-4.97	120.31	127.28
46	1	304	DD6	C14-C13-C11	-4.97	117.82	125.53
45	9	301	A86	O1-C20-C21	-4.96	109.50	115.05
45	5	301	A86	C3-C2-C1	-4.95	120.34	127.28
45	6	301	A86	C19-C18-C17	4.94	120.03	110.79
46	9	303	DD6	C21-C20-C19	-4.93	108.70	114.24
48	7	302	ET4	C16-C15-C14	4.93	133.60	123.52
46	3	315	DD6	C21-C20-C19	4.93	119.78	114.24
45	4	302	A86	C21-C20-C19	-4.92	108.71	114.24
46	4	303	DD6	C4-C5-C6	-4.92	120.38	127.28
45	4	301	A86	O4-C38-C39	4.92	119.86	111.09
45	5	304	A86	C19-C18-C17	-4.92	101.59	110.79
46	2	303	DD6	C21-C20-C19	-4.91	108.73	114.24
45	4	302	A86	C4-C3-C2	-4.90	113.50	123.52
45	4	304	A86	C3-C2-C1	-4.86	120.46	127.28
45	6	301	A86	C21-C20-C19	-4.86	108.78	114.24
45	5	306	A86	C25-C26-C27	-4.86	120.46	127.28
47	5	310	KC2	C4B-CHC-C1C	-4.84	115.73	126.02
45	4	302	A86	C25-C26-C27	-4.84	120.49	127.28
46	1	303	DD6	C3-C2-C1	-4.83	120.51	127.28
47	6	309	KC2	C1D-CHD-C4C	-4.82	114.91	126.25
47	4	307	KC2	CHD-C4C-NC	4.82	131.57	124.31
33	C	505	CLA	C4A-NA-C1A	4.81	108.87	106.68
44	3	310	KC1	O2D-CGD-CBD	4.81	119.63	111.23
45	5	304	A86	C3-C2-C1	-4.80	120.54	127.28
45	6	304	A86	C3-C2-C1	-4.80	120.54	127.28
45	2	302	A86	O1-C20-C21	-4.80	109.68	115.05
48	0	302	ET4	C16-C15-C14	4.80	133.34	123.52
45	9	302	A86	O1-C20-C21	-4.79	109.69	115.05
45	5	305	A86	C21-C20-C19	-4.79	108.86	114.24
46	8	303	DD6	C3-C2-C1	-4.79	120.56	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	3	314	A86	O4-C38-C39	4.78	119.62	111.09
45	5	306	A86	C3-C2-C1	-4.78	120.57	127.28
45	5	301	A86	C4-C5-C6	-4.78	120.58	127.28
45	9	302	A86	C3-C2-C1	-4.77	120.58	127.28
45	5	307	A86	C4-C5-C6	-4.76	120.60	127.28
45	6	301	A86	C25-C26-C27	-4.76	120.60	127.28
45	2	302	A86	C3-C2-C1	-4.75	120.62	127.28
45	6	304	A86	C21-C20-C19	-4.74	108.91	114.24
45	6	303	A86	C25-C26-C27	-4.74	120.63	127.28
45	6	301	A86	C3-C2-C1	-4.74	120.64	127.28
45	0	303	A86	O1-C20-C21	-4.73	109.76	115.05
47	0	306	KC2	C4B-CHC-C1C	-4.73	115.96	126.02
47	7	306	KC2	O2D-CGD-CBD	4.73	119.50	111.23
46	4	303	DD6	C21-C20-C19	4.73	119.55	114.24
45	6	306	A86	C3-C2-C1	-4.72	120.66	127.28
45	5	301	A86	C21-C20-C19	-4.72	108.94	114.24
45	8	301	A86	O4-C38-C39	4.71	119.50	111.09
45	6	301	A86	O4-C38-C39	4.71	119.48	111.09
45	4	304	A86	O4-C38-C39	4.70	119.48	111.09
45	5	302	A86	O4-C38-C39	4.70	119.47	111.09
45	5	307	A86	C21-C20-C19	-4.70	108.96	114.24
45	7	303	A86	C4-C5-C6	-4.70	120.69	127.28
47	5	310	KC2	O2D-CGD-CBD	4.69	119.43	111.23
37	T	101	SQD	O47-C7-C8	4.69	119.45	111.09
47	6	309	KC2	O2D-CGD-CBD	4.68	119.41	111.23
45	8	302	A86	O4-C38-C39	4.67	119.42	111.09
45	1	302	A86	O4-C38-C39	4.66	119.40	111.09
47	5	310	KC2	CHD-C4C-NC	4.66	131.33	124.31
46	3	315	DD6	C3-C2-C1	-4.65	120.75	127.28
30	c	515	BCR	C7-C8-C9	-4.65	119.35	126.23
45	6	304	A86	O4-C38-C39	4.65	119.38	111.09
45	5	304	A86	C4-C3-C2	4.65	133.03	123.52
45	6	306	A86	O4-C38-C39	4.64	119.36	111.09
45	5	304	A86	O4-C38-C39	4.64	119.36	111.09
45	4	302	A86	O4-C38-C39	4.64	119.36	111.09
45	4	304	A86	O1-C20-C21	-4.63	109.87	115.05
45	6	305	A86	C4-C3-C2	-4.62	114.06	123.52
45	5	303	A86	C3-C2-C1	-4.62	120.79	127.28
45	0	301	A86	O4-C38-C39	4.62	119.33	111.09
45	2	302	A86	O4-C38-C39	4.62	119.33	111.09
45	3	314	A86	C33-C32-C31	4.62	113.70	109.21
47	7	306	KC2	C4B-CHC-C1C	-4.61	116.21	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	9	302	A86	O4-C38-C39	4.61	119.31	111.09
45	1	301	A86	C26-C25-C24	-4.60	109.88	123.20
48	0	302	ET4	C27-C09-C10	-4.60	115.37	122.82
45	6	305	A86	O4-C38-C39	4.60	119.28	111.09
45	5	301	A86	O4-C38-C39	4.59	119.28	111.09
45	6	302	A86	O4-C38-C39	4.59	119.27	111.09
37	B	622	SQD	O5-C5-C4	4.59	117.96	109.70
45	7	301	A86	O4-C38-C39	4.58	119.26	111.09
45	5	301	A86	O1-C20-C21	-4.58	109.93	115.05
47	6	309	KC2	CHD-C4C-NC	4.57	131.20	124.31
47	7	306	KC2	CHD-C4C-NC	4.57	131.19	124.31
44	6	314	KC1	C1D-ND-C4D	4.56	109.51	106.31
45	2	301	A86	C36-C31-C32	4.55	124.21	119.70
45	5	303	A86	O4-C38-C39	4.54	119.19	111.09
45	5	307	A86	O4-C38-C39	4.54	119.19	111.09
38	c	517	DGD	O3G-C3G-C2G	-4.53	99.79	110.82
48	0	302	ET4	C19-C18-C17	4.53	126.14	119.01
45	9	301	A86	C36-C31-C32	4.53	124.19	119.70
36	5	318	LHG	O3-P-O6	-4.52	94.87	106.67
48	7	302	ET4	C27-C09-C10	-4.52	115.50	122.82
45	4	301	A86	C3-C2-C1	-4.51	120.95	127.28
45	9	301	A86	O4-C38-C39	4.51	119.14	111.09
45	1	301	A86	O4-C38-C39	4.51	119.14	111.09
45	1	302	A86	C3-C2-C1	-4.51	120.95	127.28
47	0	306	KC2	CHD-C4C-NC	4.51	131.10	124.31
45	7	303	A86	O1-C20-C15	-4.51	57.42	59.23
48	0	302	ET4	C30-C18-C17	-4.50	115.52	122.82
45	7	303	A86	O4-C38-C39	4.50	119.12	111.09
45	8	302	A86	C3-C2-C1	-4.50	120.97	127.28
45	5	304	A86	C4-C5-C6	-4.50	120.97	127.28
46	9	304	DD6	C14-C13-C11	-4.50	118.55	125.53
36	7	316	LHG	O3-P-O6	-4.49	94.96	106.67
46	2	304	DD6	C14-C13-C11	-4.49	118.56	125.53
36	b	601	LHG	O4-P-O5	4.49	133.33	112.44
45	1	301	A86	C41-C32-C31	-4.49	106.46	110.47
33	2	313	CLA	C4A-NA-C1A	4.49	108.73	106.68
38	3	320	DGD	O3G-C3G-C2G	-4.48	100.26	111.77
48	0	302	ET4	C24-C05-C06	-4.48	119.60	124.48
45	6	306	A86	C4-C5-C6	-4.47	121.00	127.28
45	2	301	A86	O4-C38-C39	4.47	119.06	111.09
44	6	314	KC1	O2D-CGD-CBD	4.47	119.04	111.23
36	A	414	LHG	O4-P-O5	4.45	133.16	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	d	407	LHG	O4-P-O5	4.44	133.09	112.44
36	H	104	LHG	O4-P-O5	4.43	133.07	112.44
45	8	301	A86	C36-C31-C32	4.43	124.09	119.70
36	3	318	LHG	O4-P-O5	4.43	133.05	112.44
36	h	103	LHG	O4-P-O5	4.43	133.04	112.44
37	t	102	SQD	O47-C7-C8	4.43	118.98	111.09
36	a	404	LHG	O4-P-O5	4.43	133.03	112.44
36	A	412	LHG	O4-P-O5	4.42	133.01	112.44
45	5	306	A86	O4-C38-C39	4.42	118.97	111.09
36	3	317	LHG	O4-P-O5	4.42	133.01	112.44
42	e	101	HEM	CHD-C1D-ND	4.42	129.18	124.42
45	5	303	A86	C4-C5-C6	-4.42	121.08	127.28
36	A	411	LHG	O4-P-O5	4.41	132.98	112.44
36	D	411	LHG	O4-P-O5	4.41	132.97	112.44
36	W	302	LHG	O4-P-O5	4.41	132.97	112.44
36	a	403	LHG	O4-P-O5	4.41	132.95	112.44
45	6	304	A86	C25-C26-C27	-4.41	121.10	127.28
45	5	304	A86	O1-C20-C21	-4.41	110.12	115.05
36	w	301	LHG	O4-P-O5	4.40	132.93	112.44
44	5	315	KC1	O2D-CGD-CBD	4.40	118.93	111.23
36	4	318	LHG	O4-P-O5	4.40	132.92	112.44
48	7	302	ET4	C19-C18-C17	4.40	125.93	119.01
45	5	303	A86	C25-C26-C27	-4.40	121.11	127.28
47	0	306	KC2	CHB-C1B-NB	4.39	130.98	124.80
37	T	103	SQD	O7-S-C6	4.38	113.30	106.76
47	4	307	KC2	CHB-C1B-NB	4.38	130.97	124.80
47	6	309	KC2	CHB-C1B-NB	4.37	130.96	124.80
37	T	101	SQD	O5-C5-C4	4.37	117.58	109.70
45	5	301	A86	C21-C20-C15	-4.37	109.25	123.35
45	0	303	A86	O1-C20-C15	-4.36	57.48	59.23
45	6	304	A86	C4-C5-C6	-4.35	121.17	127.28
36	0	315	LHG	O3-P-O6	-4.35	95.33	106.67
47	7	306	KC2	CHB-C1B-NB	4.35	130.92	124.80
45	4	301	A86	O1-C20-C15	-4.34	57.48	59.23
47	5	310	KC2	CHB-C1B-NB	4.33	130.89	124.80
45	9	301	A86	O1-C20-C15	-4.32	57.49	59.23
45	4	304	A86	O1-C20-C15	-4.32	57.49	59.23
45	5	303	A86	C21-C20-C19	-4.31	109.40	114.24
45	7	303	A86	C26-C25-C24	-4.30	110.73	123.20
45	0	303	A86	C3-C2-C1	-4.28	121.28	127.28
45	8	301	A86	C4-C5-C6	-4.27	121.29	127.28
45	2	301	A86	O1-C20-C15	-4.25	57.52	59.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	C	517	DGD	O3G-C3G-C2G	-4.24	100.50	110.82
45	5	301	A86	C22-C16-C17	-4.21	101.57	108.97
45	4	302	A86	C4-C5-C6	-4.19	121.40	127.28
47	6	309	KC2	CHC-C4B-NB	4.17	130.67	124.80
30	c	515	BCR	C15-C14-C13	-4.16	121.44	127.28
45	6	303	A86	O4-C38-C39	4.16	118.51	111.09
47	0	306	KC2	O2D-CGD-CBD	4.16	118.50	111.23
48	0	302	ET4	C35-C34-C33	4.15	117.67	109.49
48	7	302	ET4	C30-C18-C17	-4.15	116.10	122.82
45	8	301	A86	O1-C20-C15	-4.14	57.56	59.23
38	c	518	DGD	O3G-C3G-C2G	-4.14	100.75	110.82
37	t	102	SQD	O5-C5-C4	4.12	117.13	109.70
45	6	304	A86	C19-C18-C17	4.12	118.50	110.79
45	6	305	A86	C21-C20-C19	-4.12	109.61	114.24
46	1	304	DD6	O1-C20-C19	-4.12	109.63	113.49
38	c	516	DGD	O3G-C3G-C2G	-4.12	100.81	110.82
45	1	302	A86	C34-O4-C38	-4.11	110.59	117.85
45	8	302	A86	C34-O4-C38	-4.11	110.59	117.85
45	2	302	A86	O1-C20-C15	-4.09	57.58	59.23
45	9	302	A86	O1-C20-C15	-4.09	57.58	59.23
47	6	309	KC2	C4B-CHC-C1C	-4.09	117.33	126.02
46	8	304	DD6	C21-C20-C15	-4.08	115.59	122.30
38	C	518	DGD	O3G-C3G-C2G	-4.08	100.90	110.82
45	9	301	A86	C3-C2-C1	-4.08	121.56	127.28
48	0	302	ET4	C01-C06-C07	4.08	126.71	115.65
45	8	302	A86	O1-C20-C21	-4.07	110.50	115.05
45	6	306	A86	O1-C20-C15	-4.07	57.59	59.23
47	4	307	KC2	CHC-C4B-NB	4.07	130.53	124.80
45	6	305	A86	C4-C5-C6	-4.07	121.57	127.28
47	5	310	KC2	CHC-C4B-NB	4.06	130.51	124.80
45	6	306	A86	O1-C20-C21	-4.06	110.51	115.05
45	2	301	A86	C3-C2-C1	-4.06	121.59	127.28
47	7	306	KC2	CHC-C4B-NB	4.05	130.50	124.80
47	4	307	KC2	CHD-C1D-ND	4.05	130.12	124.05
45	1	302	A86	O1-C20-C21	-4.04	110.53	115.05
37	t	102	SQD	O7-S-C6	4.03	112.77	106.76
42	V	201	HEM	CHD-C1D-ND	4.03	128.76	124.42
37	a	413	SQD	O9-S-O7	-4.02	100.74	113.82
48	0	302	ET4	C08-C09-C10	4.01	125.32	119.01
30	C	515	BCR	C7-C8-C9	-4.01	120.30	126.23
45	4	304	A86	C4-C5-C6	-4.00	121.67	127.28
45	1	302	A86	C4-C5-C6	-3.98	121.69	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	3	310	KC1	CHB-C1B-NB	3.98	130.41	124.80
44	3	310	KC1	C1D-ND-C4D	3.98	109.10	106.31
47	4	307	KC2	CHC-C4B-C3B	-3.98	118.50	125.21
37	7	317	SQD	O47-C7-C8	3.97	120.08	111.48
37	T	103	SQD	O9-S-O7	-3.97	100.92	113.82
38	C	516	DGD	O3G-C3G-C2G	-3.97	101.17	110.82
30	C	515	BCR	C15-C14-C13	-3.96	121.72	127.28
44	6	314	KC1	CHB-C1B-NB	3.96	130.38	124.80
48	7	302	ET4	C08-C09-C10	3.96	125.23	119.01
37	B	622	SQD	O9-S-O7	-3.95	100.97	113.82
30	c	515	BCR	C33-C5-C6	-3.95	120.18	124.48
37	L	101	SQD	O9-S-O7	-3.95	100.99	113.82
37	l	101	SQD	O9-S-O7	-3.94	101.02	113.82
45	7	301	A86	C34-O4-C38	-3.94	110.90	117.85
37	T	101	SQD	O7-S-C6	3.93	112.63	106.76
45	1	302	A86	C40-C32-C31	-3.93	106.95	110.47
45	8	302	A86	C4-C5-C6	-3.93	121.76	127.28
45	0	301	A86	C34-O4-C38	-3.93	110.90	117.85
37	t	102	SQD	O9-S-O7	-3.93	101.04	113.82
45	6	303	A86	C21-C20-C19	-3.93	109.83	114.24
39	C	522	LMG	O6-C5-C4	3.93	116.77	109.70
45	2	302	A86	C34-O4-C38	-3.92	110.92	117.85
45	5	306	A86	C21-C20-C19	-3.92	109.84	114.24
45	9	302	A86	C34-O4-C38	-3.91	110.94	117.85
45	8	302	A86	C40-C32-C31	-3.91	106.97	110.47
44	6	314	KC1	CHC-C4B-NB	3.90	130.29	124.80
45	2	302	A86	C25-C26-C27	-3.90	121.81	127.28
42	V	201	HEM	C1B-NB-C4B	3.89	109.82	105.21
45	5	301	A86	O1-C20-C15	-3.89	57.66	59.23
45	5	304	A86	C34-O4-C38	3.89	124.72	117.85
45	9	302	A86	C25-C26-C27	-3.89	121.83	127.28
37	D	403	SQD	O9-S-O7	-3.89	101.18	113.82
47	0	306	KC2	CHC-C4B-NB	3.89	130.27	124.80
46	1	304	DD6	C4-C3-C2	-3.89	115.57	123.52
45	5	306	A86	C4-C5-C6	-3.88	121.83	127.28
30	C	515	BCR	C33-C5-C6	-3.88	120.25	124.48
37	i	101	SQD	O9-S-O7	-3.88	101.19	113.82
37	0	316	SQD	O9-S-O7	-3.88	101.20	113.82
47	5	310	KC2	CHD-C1D-ND	3.88	129.87	124.05
46	4	303	DD6	C14-C13-C11	-3.86	119.53	125.53
45	5	303	A86	O1-C20-C15	-3.86	57.68	59.23
45	1	301	A86	O1-C20-C15	-3.85	57.68	59.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	T	101	SQD	O9-S-O7	-3.85	101.29	113.82
48	7	302	ET4	C01-C06-C05	-3.85	117.37	122.64
37	A	413	SQD	O9-S-O7	-3.85	101.30	113.82
45	1	301	A86	O1-C20-C21	-3.84	110.75	115.05
45	6	301	A86	C4-C5-C6	-3.84	121.89	127.28
46	9	304	DD6	C3-C2-C1	-3.83	121.90	127.28
45	4	304	A86	C25-C26-C27	-3.83	121.91	127.28
46	2	303	DD6	C9-C10-C11	-3.82	121.92	127.28
46	2	304	DD6	C3-C2-C1	-3.81	121.93	127.28
45	5	304	A86	C21-C20-C19	-3.81	109.97	114.24
45	5	305	A86	C33-C32-C31	-3.80	105.51	109.21
46	9	303	DD6	C9-C10-C11	-3.80	121.95	127.28
33	b	603	CLA	C4A-NA-C1A	3.80	108.41	106.68
47	4	307	KC2	O2D-CGD-CBD	3.79	117.86	111.23
39	D	404	LMG	O6-C1-O1	-3.79	101.08	110.04
37	7	317	SQD	O9-S-O7	-3.79	101.50	113.82
45	5	304	A86	C23-C16-C17	-3.79	102.31	108.97
46	3	315	DD6	C9-C10-C11	-3.76	122.01	127.28
38	a	401	DGD	O3G-C3G-C2G	-3.75	101.69	110.82
44	3	310	KC1	CHD-C1D-ND	3.74	129.66	124.05
34	A	406	PHO	C2B-C1B-NB	-3.73	106.73	109.43
45	5	301	A86	C4-C3-C2	3.73	131.15	123.52
45	5	307	A86	O4-C34-C35	-3.73	98.09	107.64
37	B	622	SQD	C44-O6-C1	3.73	121.79	113.80
38	H	102	DGD	O3G-C3G-C2G	-3.72	101.77	110.82
41	d	404	PL9	C7-C3-C2	-3.72	119.01	123.39
42	e	101	HEM	CHA-C4D-ND	3.72	128.97	124.37
46	8	304	DD6	O1-C20-C19	3.71	116.97	113.49
38	h	102	DGD	O3G-C3G-C2G	-3.71	101.79	110.82
33	a	408	CLA	O2D-CGD-O1D	-3.71	116.63	123.85
30	C	515	BCR	C16-C17-C18	-3.71	122.08	127.28
47	7	306	KC2	CHD-C1D-ND	3.70	129.59	124.05
33	a	411	CLA	O2D-CGD-O1D	-3.69	116.66	123.85
37	a	413	SQD	O5-C5-C4	3.69	116.35	109.70
37	T	101	SQD	C44-O6-C1	3.69	121.70	113.80
44	5	315	KC1	CHC-C4B-NB	3.68	129.98	124.80
37	a	413	SQD	O47-C7-C8	3.68	119.43	111.48
48	7	302	ET4	C24-C05-C06	-3.67	120.48	124.48
46	1	303	DD6	C15-C14-C13	-3.67	118.24	125.99
30	c	515	BCR	C16-C17-C18	-3.66	122.14	127.28
45	6	303	A86	O1-C20-C15	-3.66	57.76	59.23
45	3	314	A86	C34-O4-C38	-3.66	111.38	117.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	4	303	DD6	C37-C36-C35	3.66	121.15	114.42
45	3	314	A86	C9-C8-C6	-3.66	116.32	126.36
45	5	304	A86	O1-C20-C15	-3.65	57.76	59.23
48	7	302	ET4	C35-C34-C33	3.65	116.69	109.49
37	B	622	SQD	O9-S-C6	3.65	112.21	106.76
45	2	301	A86	C41-C32-C31	-3.65	107.20	110.47
46	8	304	DD6	C21-C20-C19	3.65	118.34	114.24
34	a	409	PHO	C2B-C1B-NB	-3.64	106.80	109.43
41	D	408	PL9	C7-C3-C2	-3.64	119.09	123.39
46	8	303	DD6	C15-C14-C13	-3.64	118.30	125.99
45	1	301	A86	C4-C5-C6	-3.63	122.18	127.28
33	b	604	CLA	O2D-CGD-O1D	-3.62	116.80	123.85
33	A	405	CLA	O2D-CGD-O1D	-3.62	116.81	123.85
47	5	310	KC2	CHC-C4B-C3B	-3.61	119.11	125.21
47	5	310	KC2	C1A-NA-C4A	-3.61	105.03	106.68
48	0	302	ET4	C01-C06-C05	-3.61	117.71	122.64
42	e	101	HEM	CHB-C1B-NB	3.60	128.82	124.37
47	0	306	KC2	CHD-C1D-ND	3.60	129.45	124.05
34	A	407	PHO	C2B-C1B-NB	-3.60	106.83	109.43
48	0	302	ET4	O40-C36-C35	3.60	117.10	109.75
45	9	301	A86	C41-C32-C31	-3.59	107.26	110.47
45	3	314	A86	O1-C20-C15	-3.59	57.79	59.23
45	1	301	A86	C36-C31-C32	3.59	123.26	119.70
37	0	316	SQD	O47-C7-C8	3.58	119.24	111.48
38	A	415	DGD	O3G-C3G-C2G	-3.58	102.11	110.82
33	0	305	CLA	O2D-CGD-O1D	-3.58	116.89	123.85
47	7	306	KC2	CHC-C4B-C3B	-3.57	119.19	125.21
33	C	513	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
46	4	303	DD6	C37-C36-C31	-3.57	117.49	124.16
47	4	307	KC2	CHB-C1B-C2B	-3.56	118.08	125.49
47	7	306	KC2	CHB-C1B-C2B	-3.56	118.08	125.49
37	B	622	SQD	O47-C7-C8	3.56	119.18	111.48
37	A	413	SQD	O47-C7-C8	3.56	119.18	111.48
37	A	413	SQD	O7-S-C6	3.56	112.07	106.76
37	7	317	SQD	O7-S-C6	3.56	112.07	106.76
37	t	102	SQD	C44-O6-C1	3.55	121.40	113.80
45	0	303	A86	C4-C5-C6	-3.55	122.31	127.28
37	L	101	SQD	O7-S-C6	3.54	112.04	106.76
33	B	603	CLA	O2D-CGD-O1D	-3.54	116.96	123.85
45	9	302	A86	C40-C32-C31	-3.54	107.31	110.47
45	5	306	A86	O4-C34-C35	-3.53	98.59	107.64
44	3	310	KC1	CHC-C4B-NB	3.53	129.78	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	6	304	A86	C4-C3-C2	-3.53	116.29	123.52
47	0	306	KC2	CHB-C1B-C2B	-3.53	118.15	125.49
47	5	310	KC2	CHB-C1B-C2B	-3.52	118.16	125.49
37	L	101	SQD	O47-C7-C8	3.52	119.10	111.48
45	6	303	A86	C4-C5-C6	-3.52	122.35	127.28
48	7	302	ET4	O40-C36-C35	3.51	116.93	109.75
43	w	302	LMU	C1B-O1B-C4'	-3.51	109.65	117.98
45	2	302	A86	C40-C32-C31	-3.51	107.33	110.47
46	1	304	DD6	C37-C36-C35	3.50	120.86	114.42
37	T	103	SQD	O47-C7-C8	3.50	119.05	111.48
43	3	301	LMU	C1B-O1B-C4'	-3.50	109.69	117.98
33	D	406	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
44	5	315	KC1	CHB-C1B-NB	3.49	129.71	124.80
37	i	101	SQD	O47-C7-C8	3.48	119.02	111.48
45	8	301	A86	C34-O4-C38	-3.48	111.69	117.85
33	W	303	CLA	O2D-CGD-O1D	-3.48	117.07	123.85
46	1	304	DD6	C3-C2-C1	-3.48	122.40	127.28
45	5	305	A86	O1-C20-C15	-3.48	57.83	59.23
45	6	304	A86	O1-C20-C15	-3.48	57.83	59.23
33	C	508	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
33	B	604	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
42	e	101	HEM	C1B-NB-C4B	3.47	109.32	105.21
45	5	302	A86	O1-C20-C15	-3.47	57.83	59.23
37	A	413	SQD	O5-C5-C4	3.47	115.94	109.70
45	5	302	A86	C23-C16-C17	-3.46	102.88	108.97
33	A	408	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
37	l	101	SQD	O47-C7-C8	3.46	118.97	111.48
37	i	101	SQD	O9-S-C6	3.45	111.91	106.76
45	7	301	A86	C25-C26-C27	-3.45	122.44	127.28
45	0	301	A86	C25-C26-C27	-3.45	122.44	127.28
47	0	306	KC2	CHC-C4B-C3B	-3.45	119.39	125.21
45	0	301	A86	C36-C31-C32	3.45	123.12	119.70
45	9	301	A86	C34-O4-C38	-3.45	111.76	117.85
45	9	301	A86	C25-C26-C27	-3.45	122.44	127.28
47	7	306	KC2	C1A-NA-C4A	-3.44	105.11	106.68
33	b	605	CLA	O2D-CGD-O1D	-3.44	117.15	123.85
38	C	517	DGD	O6D-C1D-O3G	-3.44	101.92	110.04
45	7	301	A86	C36-C31-C32	3.44	123.11	119.70
45	2	301	A86	C34-O4-C38	-3.43	111.78	117.85
37	B	622	SQD	O7-S-C6	3.43	111.88	106.76
38	C	518	DGD	O6D-C1D-O3G	-3.43	101.93	110.04
37	l	101	SQD	O7-S-C6	3.42	111.87	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	4	303	DD6	O1-C15-C14	-3.42	107.08	116.88
45	1	301	A86	C3-C2-C1	-3.42	122.48	127.28
48	7	302	ET4	C01-C06-C07	3.42	124.92	115.65
37	0	316	SQD	O9-S-C6	3.42	111.86	106.76
45	2	301	A86	C25-C26-C27	-3.41	122.50	127.28
37	A	413	SQD	O9-S-C6	3.41	111.84	106.76
34	a	410	PHO	C2B-C1B-NB	-3.40	106.97	109.43
45	8	302	A86	O1-C20-C15	-3.40	57.86	59.23
47	6	309	KC2	CHD-C1D-ND	3.40	129.15	124.05
33	8	308	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
45	5	307	A86	O4-C34-C33	-3.40	98.93	107.64
33	C	509	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
30	c	515	BCR	C38-C26-C25	-3.40	120.78	124.48
45	1	302	A86	O1-C20-C15	-3.40	57.86	59.23
37	t	102	SQD	O9-S-C6	3.39	111.82	106.76
35	a	402	BCT	O3-C-O1	-3.39	111.01	119.68
33	D	405	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
39	b	623	LMG	O6-C5-C4	3.38	115.80	109.70
33	b	609	CLA	O2D-CGD-O1D	-3.38	117.28	123.85
33	b	611	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
38	c	518	DGD	O6D-C1D-O3G	-3.35	102.12	110.04
43	w	302	LMU	C1-O1'-C1'	-3.35	107.96	113.68
45	1	301	A86	O1-C20-C19	-3.35	110.36	113.49
45	5	306	A86	O1-C20-C15	-3.35	57.88	59.23
45	5	306	A86	O4-C34-C33	-3.34	99.09	107.64
33	d	402	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
33	7	305	CLA	O2D-CGD-O1D	-3.34	117.36	123.85
45	6	306	A86	C21-C20-C19	-3.33	110.50	114.24
37	0	316	SQD	O7-S-C6	3.33	111.73	106.76
33	B	611	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
47	6	309	KC2	CHC-C4B-C3B	-3.33	119.60	125.21
45	5	306	A86	C4-C3-C2	-3.33	116.71	123.52
37	i	101	SQD	O7-S-C6	3.32	111.72	106.76
45	8	301	A86	C33-C32-C31	3.32	112.44	109.21
45	6	305	A86	O1-C20-C15	-3.32	57.89	59.23
46	9	303	DD6	O1-C15-C14	-3.31	107.39	116.88
33	b	614	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
46	2	303	DD6	O1-C15-C14	-3.30	107.42	116.88
33	C	505	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
42	V	201	HEM	CHA-C4D-ND	3.30	128.45	124.37
33	3	312	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
45	1	302	A86	C36-C31-C32	3.30	122.97	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	B	608	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
33	C	512	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
45	8	302	A86	C36-C31-C32	3.30	122.97	119.70
33	B	606	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
44	3	310	KC1	C4B-CHC-C1C	-3.29	119.03	126.02
37	D	403	SQD	O47-C7-C8	3.28	118.58	111.48
38	c	517	DGD	O6D-C1D-O3G	-3.28	102.29	110.04
43	4	317	LMU	C1B-O1B-C4'	-3.28	110.21	117.98
39	0	314	LMG	O6-C1-O1	-3.27	102.31	110.04
45	1	301	A86	C34-O4-C38	-3.27	112.07	117.85
46	1	303	DD6	C13-C11-C10	3.27	124.15	119.01
46	8	303	DD6	C13-C11-C10	3.27	124.15	119.01
30	C	515	BCR	C38-C26-C25	-3.26	120.92	124.48
37	t	102	SQD	O5-C1-C2	3.26	117.07	110.37
33	c	505	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
44	5	315	KC1	CHD-C1D-ND	3.26	128.93	124.05
45	4	302	A86	C40-C32-C31	3.26	113.39	110.47
45	2	301	A86	C9-C8-C6	-3.25	117.44	126.36
33	d	401	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
33	b	615	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
47	6	309	KC2	CHB-C1B-C2B	-3.25	118.73	125.49
33	0	311	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
45	3	314	A86	C36-C31-C32	3.24	122.91	119.70
37	T	101	SQD	O9-S-C6	3.24	111.59	106.76
30	K	101	BCR	C15-C14-C13	-3.24	122.73	127.28
45	9	301	A86	C9-C8-C6	-3.24	117.48	126.36
33	7	311	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
45	6	302	A86	C21-C20-C19	-3.23	110.61	114.24
33	b	612	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
33	C	501	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
47	4	307	KC2	C1B-CHB-C4A	-3.22	119.18	126.02
33	C	511	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
45	6	303	A86	C33-C32-C31	-3.21	106.09	109.21
33	C	510	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
33	C	507	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
33	6	316	CLA	C1B-NB-C4B	3.21	108.56	106.31
45	8	301	A86	C41-C32-C31	-3.20	107.60	110.47
45	4	301	A86	C25-C26-C27	-3.20	122.78	127.28
45	5	307	A86	O1-C20-C15	-3.19	57.94	59.23
33	b	607	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
33	b	602	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
33	B	610	CLA	O2D-CGD-O1D	-3.18	117.66	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	a	413	SQD	O7-S-C6	3.18	111.50	106.76
45	4	302	A86	O1-C20-C15	-3.17	57.95	59.23
33	B	612	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
38	C	516	DGD	O6D-C1D-O3G	-3.17	102.56	110.04
33	c	509	CLA	O2D-CGD-O1D	-3.17	117.69	123.85
33	c	513	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
33	c	508	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
33	w	303	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
33	4	315	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
33	8	315	CLA	CBD-CHA-C1A	3.16	132.14	127.38
33	4	306	CLA	C3B-C4B-NB	-3.15	107.72	110.53
48	0	302	ET4	C28-C13-C14	-3.15	117.71	122.82
44	6	314	KC1	CHD-C1D-ND	3.15	128.77	124.05
38	c	516	DGD	O6D-C1D-O3G	-3.15	102.61	110.04
37	i	101	SQD	C44-O6-C1	3.15	120.54	113.80
33	0	304	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
33	9	315	CLA	CBD-CHA-C1A	3.14	132.12	127.38
34	a	409	PHO	O2D-CGD-O1D	-3.14	117.74	123.85
33	B	605	CLA	O2D-CGD-O1D	-3.14	117.75	123.85
33	c	507	CLA	O2D-CGD-O1D	-3.14	117.75	123.85
33	d	409	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
34	A	406	PHO	O1D-CGD-CBD	3.13	129.47	124.72
34	a	409	PHO	O1D-CGD-CBD	3.13	129.46	124.72
45	5	302	A86	C4-C3-C2	-3.12	117.12	123.52
33	2	315	CLA	CBD-CHA-C1A	3.12	132.09	127.38
33	c	503	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
45	9	301	A86	O1-C20-C19	-3.12	110.57	113.49
33	B	615	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
33	7	314	CLA	CBD-CHA-C1A	3.12	132.08	127.38
33	8	314	CLA	CBD-CHA-C1A	3.12	132.08	127.38
33	3	304	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
33	B	614	CLA	O2D-CGD-O1D	-3.11	117.78	123.85
34	A	407	PHO	O1D-CGD-CBD	3.11	129.44	124.72
48	7	302	ET4	C28-C13-C14	-3.11	117.77	122.82
33	H	103	CLA	CBD-CHA-C1A	3.11	132.08	127.38
33	c	504	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
37	D	403	SQD	O7-S-C6	3.11	111.39	106.76
37	a	413	SQD	O9-S-C6	3.11	111.39	106.76
45	5	302	A86	C21-C20-C15	-3.11	113.32	123.35
46	1	304	DD6	O1-C15-C14	-3.10	107.99	116.88
34	a	410	PHO	O1D-CGD-CBD	3.10	129.42	124.72
33	C	506	CLA	O2D-CGD-O1D	-3.10	117.82	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	b	616	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
33	c	512	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
33	c	511	CLA	O2D-CGD-O1D	-3.09	117.82	123.85
33	8	316	CLA	CBD-CHA-C1A	3.09	132.05	127.38
33	C	502	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
33	B	607	CLA	CAA-C2A-C3A	-3.09	109.14	116.23
33	z	101	CLA	C3B-C4B-NB	-3.09	107.78	110.53
46	9	303	DD6	C19-C18-C17	-3.09	105.02	110.79
47	4	307	KC2	CHB-C4A-C3A	-3.08	120.16	125.03
33	1	313	CLA	CBD-CHA-C1A	3.08	132.03	127.38
37	D	403	SQD	O9-S-C6	3.08	111.36	106.76
33	7	313	CLA	CHB-C1B-C2B	-3.08	123.99	130.51
33	1	314	CLA	CBD-CHA-C1A	3.08	132.03	127.38
44	5	315	KC1	C2D-C1D-ND	-3.08	107.13	110.33
33	c	510	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
33	9	314	CLA	CBD-CHA-C1A	3.07	132.02	127.38
46	2	303	DD6	C19-C18-C17	-3.07	105.04	110.79
33	0	313	CLA	CHB-C1B-C2B	-3.07	124.01	130.51
45	1	301	A86	C33-C32-C31	3.07	112.19	109.21
45	6	301	A86	O1-C20-C15	-3.06	58.00	59.23
33	2	314	CLA	CBD-CHA-C1A	3.06	132.00	127.38
33	2	316	CLA	CBD-CHA-C1A	3.06	132.00	127.38
33	9	313	CLA	CBD-CHA-C1A	3.06	131.99	127.38
33	9	308	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
33	1	315	CLA	CBD-CHA-C1A	3.06	131.99	127.38
33	6	316	CLA	CHB-C1B-C2B	-3.06	124.04	130.51
33	5	312	CLA	C3B-C4B-NB	-3.06	107.80	110.53
34	a	410	PHO	O2D-CGD-O1D	-3.06	117.90	123.85
33	C	503	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
38	A	415	DGD	C3G-C2G-C1G	-3.05	104.67	111.78
48	0	302	ET4	C12-C13-C14	3.05	123.81	119.01
33	4	312	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
33	1	316	CLA	CBD-CHA-C1A	3.05	131.98	127.38
33	0	307	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
46	4	303	DD6	C4-C3-C2	-3.05	117.28	123.52
45	2	301	A86	O1-C20-C19	-3.05	110.64	113.49
33	6	315	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
33	b	613	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
30	C	515	BCR	C11-C10-C9	-3.04	123.02	127.28
33	Z	101	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
37	i	101	SQD	O6-C1-C2	3.04	112.89	108.27
33	B	601	CLA	C3B-C4B-NB	-3.04	107.82	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	3	306	CLA	C3B-C4B-NB	-3.03	107.82	110.53
37	7	317	SQD	O9-S-C6	3.03	111.28	106.76
33	4	314	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
33	3	309	CLA	C3B-C4B-NB	-3.03	107.83	110.53
33	9	313	CLA	C3B-C4B-NB	-3.02	107.83	110.53
45	5	302	A86	C19-C18-C17	3.02	116.44	110.79
44	3	310	KC1	CHB-C1B-C2B	-3.02	119.20	125.49
33	6	310	CLA	C3B-C4B-NB	-3.02	107.83	110.53
33	1	313	CLA	C3B-C4B-NB	-3.02	107.83	110.53
46	3	315	DD6	C21-C20-C15	-3.02	117.33	122.30
33	9	316	CLA	C3B-C4B-NB	-3.02	107.84	110.53
33	8	316	CLA	C3B-C4B-NB	-3.02	107.84	110.53
33	z	101	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
47	7	306	KC2	C4C-C3C-C2C	-3.01	104.51	107.28
33	C	504	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
33	9	307	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
33	C	509	CLA	C3B-C4B-NB	-3.01	107.84	110.53
33	3	311	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
45	6	302	A86	O4-C34-C33	-3.01	99.94	107.64
33	c	502	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
33	9	316	CLA	CBD-CHA-C1A	3.01	131.92	127.38
33	4	308	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
45	2	302	A86	C12-C11-C13	3.01	120.87	116.00
48	7	302	ET4	C12-C13-C14	3.00	123.73	119.01
33	Z	101	CLA	C3B-C4B-NB	-3.00	107.85	110.53
33	3	319	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
47	6	309	KC2	C1D-ND-C4D	3.00	108.42	106.31
33	5	317	CLA	CBD-CHA-C1A	3.00	131.90	127.38
33	8	313	CLA	CBD-CHA-C1A	3.00	131.90	127.38
45	8	301	A86	C25-C26-C27	-3.00	123.08	127.28
34	a	410	PHO	CMB-C2B-C3B	2.99	130.66	124.68
33	7	304	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
36	3	317	LHG	O8-C23-C24	2.99	120.23	111.15
45	6	301	A86	C33-C32-C31	-2.99	106.31	109.21
33	1	312	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
33	b	608	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
47	5	310	KC2	C4C-C3C-C2C	-2.99	104.53	107.28
33	b	610	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
33	b	611	CLA	C3B-C4B-NB	-2.98	107.87	110.53
33	7	307	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
30	c	515	BCR	C11-C10-C9	-2.98	123.09	127.28
45	9	302	A86	C12-C11-C13	2.98	120.84	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2	315	CLA	C3B-C4B-NB	-2.98	107.87	110.53
45	9	301	A86	C33-C32-C31	2.98	112.11	109.21
37	B	622	SQD	O5-C1-C2	2.98	116.49	110.37
33	B	610	CLA	C3B-C4B-NB	-2.98	107.87	110.53
33	c	506	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
33	D	402	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
45	6	303	A86	O4-C34-C33	-2.97	100.02	107.64
33	B	607	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
33	6	311	CLA	C3B-C4B-NB	-2.97	107.88	110.53
33	4	311	CLA	C3B-C4B-NB	-2.97	107.88	110.53
33	8	305	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
33	b	617	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
33	B	613	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
33	2	312	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
33	1	316	CLA	C3B-C4B-NB	-2.96	107.89	110.53
33	B	601	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
33	9	314	CLA	C3B-C4B-NB	-2.96	107.89	110.53
33	8	305	CLA	C3B-C4B-NB	-2.96	107.89	110.53
46	8	304	DD6	C37-C36-C35	2.95	119.85	114.42
33	7	310	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
33	4	316	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
33	0	309	CLA	C3B-C4B-NB	-2.95	107.89	110.53
36	A	412	LHG	O8-C23-C24	2.95	120.83	111.83
47	0	306	KC2	C1A-NA-C4A	-2.95	105.33	106.68
45	4	304	A86	C34-O4-C38	-2.94	112.64	117.85
33	8	306	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
45	2	301	A86	C33-C32-C31	2.93	112.06	109.21
38	H	102	DGD	O6D-C1D-O3G	-2.93	103.11	110.04
33	9	309	CLA	C3B-C4B-NB	-2.93	107.91	110.53
33	B	616	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
33	b	606	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
33	5	308	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
34	A	406	PHO	CMB-C2B-C3B	2.92	130.53	124.68
45	5	307	A86	C22-C16-C17	-2.92	103.83	108.97
33	9	305	CLA	C3B-C4B-NB	-2.92	107.92	110.53
45	5	305	A86	C25-C24-C1	-2.92	118.35	126.36
33	c	501	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
45	6	302	A86	O4-C34-C35	-2.92	100.16	107.64
34	A	407	PHO	O2D-CGD-O1D	-2.92	118.17	123.85
38	a	401	DGD	C3G-C2G-C1G	-2.92	104.99	111.78
33	1	305	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
33	0	310	CLA	O2D-CGD-O1D	-2.91	118.18	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	7	301	A86	C12-C11-C13	2.91	120.72	116.00
30	c	515	BCR	C1-C6-C5	-2.91	118.66	122.64
33	6	311	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
33	9	317	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
33	9	306	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
33	1	309	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
45	2	302	A86	C4-C3-C2	-2.90	117.58	123.52
33	2	317	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
45	0	301	A86	C12-C11-C13	2.90	120.70	116.00
38	h	102	DGD	O6D-C1D-O3G	-2.90	103.19	110.04
33	6	312	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
33	a	407	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
33	2	308	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
42	V	201	HEM	CHB-C1B-NB	2.90	127.95	124.37
45	1	302	A86	O1-C20-C19	-2.90	110.78	113.49
33	8	314	CLA	C3B-C4B-NB	-2.90	107.94	110.53
33	2	309	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
39	C	519	LMG	O6-C1-O1	-2.89	103.21	110.04
33	5	312	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
34	A	406	PHO	O2D-CGD-O1D	-2.89	118.22	123.85
37	T	101	SQD	O5-C1-C2	2.89	116.31	110.37
33	6	316	CLA	C3A-C2A-C1A	-2.89	103.34	106.30
33	b	608	CLA	CAA-C2A-C3A	-2.89	109.60	116.23
44	3	310	KC1	CHC-C4B-C3B	-2.89	120.34	125.21
45	8	302	A86	O1-C20-C19	-2.89	110.78	113.49
33	b	614	CLA	O1D-CGD-CBD	2.89	130.22	124.52
34	A	407	PHO	CMB-C2B-C3B	2.89	130.45	124.68
33	b	614	CLA	C3B-C4B-NB	-2.88	107.96	110.53
33	3	305	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
45	9	302	A86	C4-C3-C2	-2.88	117.62	123.52
33	3	319	CLA	C3B-C4B-NB	-2.88	107.96	110.53
39	W	301	LMG	O6-C1-O1	-2.88	103.25	110.04
33	8	316	CLA	CAA-C2A-C3A	-2.88	109.64	116.23
36	4	318	LHG	O8-C23-C24	2.87	120.59	111.83
30	C	515	BCR	C28-C27-C26	-2.87	108.93	114.06
30	B	617	BCR	C27-C26-C25	2.87	126.58	122.70
33	5	314	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
37	a	413	SQD	C3-C4-C5	2.86	115.42	110.23
33	8	311	CLA	C3B-C4B-NB	-2.86	107.97	110.53
38	A	415	DGD	CDB-CCB-CBB	-2.86	99.90	114.37
33	2	307	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
38	a	401	DGD	O6D-C1D-O3G	-2.86	103.28	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	C	520	LMG	O6-C1-O1	-2.86	103.28	110.04
33	1	311	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
33	1	308	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
33	9	305	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
33	1	306	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
33	3	307	CLA	C3B-C4B-NB	-2.86	107.98	110.53
33	9	311	CLA	C3B-C4B-NB	-2.86	107.98	110.53
33	7	308	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
33	9	311	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
33	4	311	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
33	4	306	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
33	5	309	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
33	8	305	CLA	CAA-C2A-C3A	-2.85	109.69	116.23
33	8	309	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
33	3	312	CLA	C3B-C4B-NB	-2.85	107.98	110.53
33	6	316	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
36	d	407	LHG	O8-C23-C24	2.85	120.53	111.83
38	c	516	DGD	CDB-CCB-CBB	-2.85	99.96	114.37
47	0	306	KC2	C4C-C3C-C2C	-2.85	104.66	107.28
33	c	510	CLA	C3B-C4B-NB	-2.85	107.99	110.53
39	q	302	LMG	O6-C1-O1	-2.85	103.31	110.04
33	c	512	CLA	C3B-C4B-NB	-2.85	107.99	110.53
33	1	305	CLA	C3B-C4B-NB	-2.85	107.99	110.53
33	3	302	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
30	c	515	BCR	C28-C27-C26	-2.84	108.98	114.06
38	C	517	DGD	CDB-CCB-CBB	-2.84	100.00	114.37
44	6	314	KC1	C1D-CHD-C4C	-2.84	119.57	126.25
33	7	305	CLA	C3B-C4B-NB	-2.84	108.00	110.53
33	7	312	CLA	C3B-C4B-NB	-2.84	108.00	110.53
44	5	315	KC1	C1D-CHD-C4C	-2.84	119.58	126.25
33	1	311	CLA	C3B-C4B-NB	-2.84	108.00	110.53
30	K	101	BCR	C15-C16-C17	-2.84	117.72	123.52
33	2	314	CLA	C3B-C4B-NB	-2.84	108.00	110.53
33	3	313	CLA	C3B-C4B-NB	-2.83	108.00	110.53
30	b	618	BCR	C27-C26-C25	2.83	126.53	122.70
37	A	413	SQD	O6-C1-C2	2.83	112.57	108.27
30	b	618	BCR	C33-C5-C6	-2.83	121.39	124.48
33	8	307	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
37	D	403	SQD	O5-C5-C4	2.83	114.80	109.70
33	b	617	CLA	C3B-C4B-NB	-2.83	108.00	110.53
44	5	315	KC1	O1D-CGD-CBD	-2.83	118.94	124.52
33	C	503	CLA	C3B-C4B-NB	-2.83	108.01	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	5	316	CLA	C3B-C4B-NB	-2.83	108.01	110.53
33	9	312	CLA	C3B-C4B-NB	-2.83	108.01	110.53
33	3	306	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
39	D	404	LMG	O1-C1-C2	-2.82	103.98	108.27
45	5	302	A86	C9-C10-C11	-2.82	118.66	126.64
30	D	407	BCR	C27-C26-C25	2.82	126.52	122.70
37	L	101	SQD	O9-S-C6	2.82	110.97	106.76
33	a	408	CLA	C3B-C4B-NB	-2.82	108.01	110.53
33	9	317	CLA	C3B-C4B-NB	-2.82	108.01	110.53
34	a	409	PHO	CMB-C2B-C3B	2.82	130.32	124.68
33	c	503	CLA	C3B-C4B-NB	-2.82	108.01	110.53
34	a	410	PHO	C1-C2-C3	-2.82	121.57	126.20
33	2	310	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
33	9	309	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
33	4	305	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
33	3	308	CLA	C3B-C4B-NB	-2.82	108.02	110.53
33	7	309	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
44	3	310	KC1	C1D-CHD-C4C	-2.81	119.63	126.25
30	B	618	BCR	C27-C26-C25	2.81	126.51	122.70
33	8	306	CLA	C3B-C4B-NB	-2.81	108.02	110.53
30	C	515	BCR	C3-C4-C5	-2.81	109.04	114.06
33	6	308	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
33	8	315	CLA	CAA-C2A-C3A	-2.81	109.78	116.23
33	1	310	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
30	h	101	BCR	C27-C26-C25	2.81	126.50	122.70
33	2	311	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
33	0	307	CLA	C3B-C4B-NB	-2.81	108.02	110.53
33	2	316	CLA	C3B-C4B-NB	-2.81	108.02	110.53
33	B	609	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
33	5	311	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
45	9	301	A86	C25-C24-C1	-2.81	118.66	126.36
33	5	316	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
33	0	312	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
33	2	306	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
45	5	302	A86	C33-C32-C31	-2.81	106.48	109.21
33	A	404	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
36	D	409	LHG	O8-C23-C24	2.80	120.38	111.83
39	B	620	LMG	O6-C1-O1	-2.80	103.42	110.04
33	7	313	CLA	CAA-C2A-C3A	-2.80	109.80	116.23
30	B	617	BCR	C33-C5-C6	-2.80	121.43	124.48
45	4	301	A86	C9-C10-C11	-2.80	118.72	126.64
33	3	313	CLA	O2D-CGD-O1D	-2.80	118.39	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	2	301	A86	C25-C24-C1	-2.80	118.68	126.36
33	8	309	CLA	CHC-C1C-C2C	-2.80	123.82	129.94
33	H	103	CLA	C3B-C4B-NB	-2.80	108.03	110.53
33	b	609	CLA	C3B-C4B-NB	-2.80	108.03	110.53
33	8	311	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
30	a	414	BCR	C24-C23-C22	-2.80	122.10	126.23
33	b	602	CLA	C3B-C4B-NB	-2.80	108.03	110.53
38	C	516	DGD	CDB-CCB-CBB	-2.79	100.24	114.37
33	b	607	CLA	C3B-C4B-NB	-2.79	108.04	110.53
33	9	310	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
33	9	306	CLA	C3B-C4B-NB	-2.79	108.04	110.53
33	2	305	CLA	C3B-C4B-NB	-2.79	108.04	110.53
33	5	313	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
36	5	318	LHG	O8-C23-C24	2.79	120.34	111.83
37	A	413	SQD	O48-C23-C24	2.79	120.34	111.83
33	0	309	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
46	1	303	DD6	C12-C11-C10	-2.79	118.30	122.82
33	6	313	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
33	1	307	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
33	9	313	CLA	CHC-C1C-C2C	-2.79	123.84	129.94
39	w	304	LMG	O6-C1-O1	-2.79	103.46	110.04
33	1	315	CLA	CAA-C2A-C3A	-2.79	109.84	116.23
45	8	301	A86	O1-C20-C19	-2.78	110.88	113.49
36	D	411	LHG	O8-C23-C24	2.78	120.33	111.83
33	4	310	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
33	2	309	CLA	CHC-C1C-C2C	-2.78	123.85	129.94
39	d	410	LMG	O6-C1-O1	-2.78	103.47	110.04
33	0	313	CLA	C1B-NB-C4B	2.78	108.26	106.31
38	a	401	DGD	CDB-CCB-CBB	-2.78	100.32	114.37
42	e	101	HEM	CHD-C4C-NC	2.78	127.48	124.45
33	9	312	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
33	3	303	CLA	C3B-C4B-NB	-2.78	108.05	110.53
30	k	102	BCR	C24-C23-C22	-2.78	122.13	126.23
33	B	614	CLA	C3B-C4B-NB	-2.78	108.05	110.53
33	b	613	CLA	C3B-C4B-NB	-2.78	108.05	110.53
33	8	310	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
33	4	305	CLA	C3B-C4B-NB	-2.77	108.05	110.53
30	H	101	BCR	C27-C26-C25	2.77	126.45	122.70
30	k	101	BCR	C15-C14-C13	-2.77	123.39	127.28
33	4	309	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
33	6	312	CLA	C3B-C4B-NB	-2.77	108.05	110.53
33	2	311	CLA	C3B-C4B-NB	-2.77	108.05	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	9	316	CLA	CAA-C2A-C3A	-2.77	109.87	116.23
37	A	413	SQD	C44-O6-C1	2.77	119.74	113.80
46	8	303	DD6	C12-C11-C10	-2.77	118.33	122.82
33	8	309	CLA	C3B-C4B-NB	-2.77	108.06	110.53
33	8	312	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
37	i	101	SQD	O48-C23-C24	2.77	120.28	111.83
39	C	522	LMG	C1-C2-C3	-2.77	104.19	110.01
33	1	313	CLA	CHC-C1C-C2C	-2.77	123.89	129.94
33	6	307	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
30	k	101	BCR	C15-C16-C17	-2.76	117.86	123.52
33	4	313	CLA	C3B-C4B-NB	-2.76	108.06	110.53
33	b	615	CLA	C3B-C4B-NB	-2.76	108.06	110.53
33	9	308	CLA	C3B-C4B-NB	-2.76	108.06	110.53
33	3	309	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
33	2	313	CLA	CHC-C4B-NB	2.76	128.19	124.05
45	5	304	A86	O4-C34-C35	-2.76	100.57	107.64
45	5	305	A86	C12-C11-C13	2.76	120.48	116.00
33	0	305	CLA	C3B-C4B-NB	-2.76	108.07	110.53
39	q	301	LMG	O6-C1-O1	-2.76	103.53	110.04
47	6	309	KC2	C4C-C3C-C2C	-2.76	104.75	107.28
38	A	415	DGD	O6D-C1D-O3G	-2.76	103.53	110.04
46	8	304	DD6	C19-C18-C17	2.75	115.94	110.79
33	C	511	CLA	C3B-C4B-NB	-2.75	108.07	110.53
36	A	414	LHG	O8-C23-C24	2.75	120.23	111.83
45	5	303	A86	C12-C11-C13	2.75	120.46	116.00
33	9	313	CLA	CAA-C2A-C3A	-2.75	109.92	116.23
33	2	317	CLA	C3B-C4B-NB	-2.75	108.07	110.53
45	2	302	A86	C35-C34-C33	2.75	114.83	109.89
33	D	402	CLA	C3B-C4B-NB	-2.75	108.07	110.53
33	d	402	CLA	C1-C2-C3	-2.75	121.69	126.20
33	3	311	CLA	C3B-C4B-NB	-2.75	108.08	110.53
33	8	313	CLA	CHC-C1C-C2C	-2.75	123.92	129.94
33	5	317	CLA	C3B-C4B-NB	-2.75	108.08	110.53
30	b	618	BCR	C11-C10-C9	-2.75	123.42	127.28
33	7	313	CLA	C1B-NB-C4B	2.75	108.24	106.31
36	w	301	LHG	O8-C23-C24	2.75	120.21	111.83
30	a	412	BCR	C27-C26-C25	2.75	126.42	122.70
30	c	514	BCR	C24-C23-C22	-2.75	122.17	126.23
38	3	320	DGD	CDB-CCB-CBB	-2.74	100.50	114.37
33	0	308	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
45	6	305	A86	O4-C34-C33	-2.74	100.62	107.64
38	H	102	DGD	CDB-CCB-CBB	-2.74	100.51	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	3	315	DD6	C15-C14-C13	-2.74	120.20	125.99
44	6	314	KC1	CHC-C4B-C3B	-2.74	120.59	125.21
33	4	315	CLA	C3B-C4B-NB	-2.74	108.08	110.53
48	7	302	ET4	C07-C06-C05	-2.74	115.25	121.56
33	b	614	CLA	CHB-C4A-NA	2.74	128.35	124.40
45	0	303	A86	O4-C38-O5	-2.74	117.70	122.99
33	D	406	CLA	CHB-C4A-NA	2.74	128.35	124.40
44	6	314	KC1	C2D-C1D-ND	-2.74	107.49	110.33
45	5	302	A86	C9-C8-C6	-2.74	118.86	126.36
33	c	501	CLA	C3B-C4B-NB	-2.74	108.09	110.53
33	9	309	CLA	CHC-C1C-C2C	-2.73	123.96	129.94
33	5	309	CLA	CHB-C4A-NA	2.73	128.34	124.40
33	2	309	CLA	C3B-C4B-NB	-2.73	108.09	110.53
33	C	510	CLA	C3B-C4B-NB	-2.73	108.09	110.53
38	c	517	DGD	CDB-CCB-CBB	-2.73	100.56	114.37
36	h	103	LHG	O8-C23-C24	2.73	120.16	111.83
44	6	314	KC1	O1D-CGD-CBD	-2.73	119.13	124.52
37	l	101	SQD	O9-S-C6	2.73	110.83	106.76
45	7	301	A86	O1-C20-C19	-2.73	110.93	113.49
33	3	308	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
33	2	305	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
45	0	303	A86	C25-C26-C27	-2.73	123.45	127.28
33	3	305	CLA	C3B-C4B-NB	-2.73	108.10	110.53
33	B	604	CLA	O2D-CGD-CBD	2.73	116.00	111.23
39	7	315	LMG	O6-C1-O1	-2.73	103.60	110.04
45	9	302	A86	C35-C34-C33	2.73	114.78	109.89
39	m	201	LMG	O6-C1-O1	-2.72	103.61	110.04
33	C	507	CLA	C3B-C4B-NB	-2.72	108.10	110.53
33	8	312	CLA	CHB-C4A-NA	2.72	128.33	124.40
44	6	314	KC1	CHB-C1B-C2B	-2.72	119.83	125.49
33	7	304	CLA	C3B-C4B-NB	-2.72	108.10	110.53
33	3	303	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
33	b	610	CLA	C3B-C4B-NB	-2.72	108.10	110.53
33	1	313	CLA	CAA-C2A-C3A	-2.72	110.00	116.23
33	7	309	CLA	C1-C2-C3	-2.72	121.75	126.20
33	9	315	CLA	C3B-C4B-NB	-2.71	108.11	110.53
33	1	315	CLA	C3B-C4B-NB	-2.71	108.11	110.53
39	b	621	LMG	O6-C1-O1	-2.71	103.64	110.04
36	W	302	LHG	O8-C23-C24	2.71	120.09	111.83
33	b	605	CLA	O2D-CGD-CBD	2.71	115.96	111.23
33	4	308	CLA	C3B-C4B-NB	-2.71	108.11	110.53
45	0	301	A86	O1-C20-C19	-2.71	110.95	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2	310	CLA	CMB-C2B-C1B	-2.71	121.30	125.42
30	A	401	BCR	C27-C26-C25	2.71	126.36	122.70
33	A	405	CLA	C3B-C4B-NB	-2.71	108.11	110.53
33	3	304	CLA	C3B-C4B-NB	-2.71	108.11	110.53
30	C	514	BCR	C27-C26-C25	2.70	126.36	122.70
36	A	411	LHG	O8-C23-C24	2.70	120.08	111.83
33	b	616	CLA	C3B-C4B-NB	-2.70	108.12	110.53
30	B	617	BCR	C24-C23-C22	-2.70	122.23	126.23
47	4	307	KC2	C4C-C3C-C2C	-2.70	104.80	107.28
30	k	101	BCR	C27-C26-C25	2.70	126.36	122.70
30	c	515	BCR	C24-C23-C22	-2.70	122.24	126.23
33	B	615	CLA	C3B-C4B-NB	-2.70	108.12	110.53
36	a	403	LHG	O8-C23-C24	2.70	120.07	111.83
33	B	609	CLA	C3B-C4B-NB	-2.70	108.12	110.53
33	5	309	CLA	C3B-C4B-NB	-2.70	108.12	110.53
30	c	514	BCR	C27-C26-C25	2.70	126.35	122.70
33	2	308	CLA	C3B-C4B-NB	-2.70	108.12	110.53
36	7	316	LHG	O8-C23-C24	2.70	120.06	111.83
33	1	309	CLA	CHC-C1C-C2C	-2.70	124.04	129.94
45	5	307	A86	C12-C11-C13	2.70	120.37	116.00
36	3	318	LHG	O8-C23-C24	2.69	120.05	111.83
41	d	404	PL9	C27-C28-C29	-2.69	121.46	127.62
30	A	409	BCR	C27-C26-C25	2.69	126.34	122.70
33	B	611	CLA	C3B-C4B-NB	-2.69	108.13	110.53
33	6	315	CLA	C3B-C4B-NB	-2.69	108.13	110.53
33	b	615	CLA	C1-C2-C3	-2.69	121.79	126.20
33	8	312	CLA	C3B-C4B-NB	-2.69	108.13	110.53
45	6	305	A86	C12-C11-C13	2.69	120.36	116.00
36	H	104	LHG	O8-C23-C24	2.69	120.04	111.83
33	1	316	CLA	CAA-C2A-C3A	-2.69	110.06	116.23
33	C	502	CLA	C3B-C4B-NB	-2.69	108.13	110.53
33	8	313	CLA	C3B-C4B-NB	-2.69	108.13	110.53
33	4	313	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
33	c	507	CLA	CHB-C4A-NA	2.68	128.27	124.40
33	B	612	CLA	C3B-C4B-NB	-2.68	108.14	110.53
45	5	301	A86	C12-C11-C13	2.68	120.35	116.00
45	7	303	A86	C9-C8-C6	-2.68	119.01	126.36
45	6	303	A86	O4-C34-C35	-2.68	100.78	107.64
30	a	414	BCR	C27-C26-C25	2.68	126.33	122.70
33	a	407	CLA	C3B-C4B-NB	-2.68	108.14	110.53
33	b	606	CLA	C3B-C4B-NB	-2.68	108.14	110.53
39	d	410	LMG	O1-C1-C2	-2.68	104.21	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	C	517	DGD	C3G-C2G-C1G	-2.68	105.54	111.78
33	9	310	CLA	C3B-C4B-NB	-2.68	108.14	110.53
37	T	101	SQD	O48-C23-C24	2.68	119.99	111.83
33	0	308	CLA	C3B-C4B-NB	-2.68	108.14	110.53
42	e	101	HEM	CHD-C1D-C2D	-2.67	120.81	125.03
33	6	315	CLA	CAA-C2A-C3A	-2.67	110.11	116.23
37	a	413	SQD	O48-C23-C24	2.67	119.98	111.83
33	A	404	CLA	C3B-C4B-NB	-2.67	108.15	110.53
33	7	314	CLA	C3B-C4B-NB	-2.67	108.15	110.53
33	0	304	CLA	C3B-C4B-NB	-2.67	108.15	110.53
33	1	314	CLA	C3B-C4B-NB	-2.67	108.15	110.53
33	7	310	CLA	C3B-C4B-NB	-2.67	108.15	110.53
41	D	408	PL9	C7-C8-C9	-2.67	122.23	126.83
33	4	312	CLA	CHB-C4A-NA	2.67	128.25	124.40
36	a	404	LHG	O8-C23-C24	2.67	119.96	111.83
33	6	313	CLA	C3B-C4B-NB	-2.66	108.15	110.53
45	9	301	A86	C9-C10-C11	-2.66	119.11	126.64
33	4	316	CLA	C3B-C4B-NB	-2.66	108.15	110.53
39	C	522	LMG	O6-C1-O1	-2.66	103.75	110.04
33	C	507	CLA	CHB-C4A-NA	2.66	128.24	124.40
33	3	302	CLA	C3B-C4B-NB	-2.66	108.16	110.53
41	D	408	PL9	C40-C39-C41	2.66	119.84	115.23
47	0	306	KC2	O1D-CGD-CBD	-2.66	119.27	124.52
45	6	306	A86	C29-C30-C31	-2.66	174.52	177.66
33	8	310	CLA	CHB-C4A-NA	2.66	128.24	124.40
33	7	313	CLA	CMB-C2B-C1B	-2.66	123.29	125.94
45	0	301	A86	C21-C20-C15	2.66	131.93	123.35
33	8	308	CLA	CHB-C4A-NA	2.66	128.23	124.40
33	B	613	CLA	CHB-C4A-NA	2.65	128.23	124.40
30	c	515	BCR	C33-C5-C4	2.65	119.25	113.60
41	d	404	PL9	C22-C23-C24	-2.65	121.55	127.62
36	b	601	LHG	O8-C23-C24	2.65	119.92	111.83
45	1	302	A86	C9-C8-C6	-2.65	119.09	126.36
37	L	101	SQD	C1-O5-C5	2.65	118.89	113.72
45	6	306	A86	O4-C34-C35	-2.65	100.86	107.64
45	2	301	A86	C9-C10-C11	-2.65	119.16	126.64
45	8	302	A86	C9-C8-C6	-2.65	119.11	126.36
45	8	302	A86	C12-C11-C13	2.64	120.29	116.00
45	7	301	A86	C21-C20-C15	2.64	131.89	123.35
38	h	102	DGD	CDB-CCB-CBB	-2.64	101.00	114.37
42	e	101	HEM	C3B-C4B-NB	-2.64	107.57	109.47
45	5	302	A86	C25-C24-C1	-2.64	119.12	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	Q	301	LMG	O6-C1-O1	-2.64	103.81	110.04
45	6	304	A86	C12-C11-C13	2.64	120.28	116.00
39	d	406	LMG	O6-C1-O1	-2.64	103.81	110.04
33	4	316	CLA	C1-C2-C3	-2.64	121.87	126.20
30	b	619	BCR	C27-C26-C25	2.64	126.27	122.70
33	b	605	CLA	C1-C2-C3	-2.64	121.87	126.20
45	1	302	A86	C12-C11-C13	2.64	120.28	116.00
33	7	312	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
33	7	307	CLA	C3B-C4B-NB	-2.64	108.18	110.53
39	3	316	LMG	O6-C1-O1	-2.64	103.81	110.04
33	2	316	CLA	CAA-C2A-C3A	-2.63	110.19	116.23
45	1	302	A86	C4-C3-C2	-2.63	118.13	123.52
44	6	314	KC1	C4B-CHC-C1C	-2.63	120.42	126.02
33	B	616	CLA	C3B-C4B-NB	-2.63	108.18	110.53
33	7	308	CLA	C3B-C4B-NB	-2.63	108.18	110.53
33	c	509	CLA	C3B-C4B-NB	-2.63	108.18	110.53
44	5	315	KC1	C4B-CHC-C1C	-2.63	120.42	126.02
33	c	507	CLA	C3B-C4B-NB	-2.63	108.18	110.53
33	1	308	CLA	C3B-C4B-NB	-2.63	108.18	110.53
45	6	302	A86	C9-C10-C11	-2.63	119.21	126.64
33	1	306	CLA	C3B-C4B-NB	-2.62	108.19	110.53
30	d	403	BCR	C27-C26-C25	2.62	126.25	122.70
33	0	311	CLA	C3B-C4B-NB	-2.62	108.19	110.53
45	6	302	A86	C9-C8-C6	-2.62	119.18	126.36
33	7	313	CLA	CHB-C4A-NA	2.62	128.18	124.40
33	1	312	CLA	C3B-C4B-NB	-2.62	108.19	110.53
33	4	313	CLA	CAA-C2A-C3A	-2.62	110.23	116.23
45	4	301	A86	C19-C18-C17	-2.62	105.89	110.79
30	h	101	BCR	C2-C1-C6	2.62	114.24	110.44
45	5	307	A86	C23-C16-C17	-2.62	104.37	108.97
36	0	315	LHG	O8-C23-C24	2.62	119.81	111.83
33	6	310	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
33	0	310	CLA	CHB-C4A-NA	2.61	128.17	124.40
33	8	308	CLA	C3B-C4B-NB	-2.61	108.20	110.53
33	2	307	CLA	CMB-C2B-C3B	2.61	130.47	123.53
37	B	622	SQD	O48-C23-C24	2.61	119.80	111.83
33	9	314	CLA	CAA-C2A-C3A	-2.61	110.24	116.23
33	B	604	CLA	CHB-C4A-NA	2.61	128.17	124.40
33	7	309	CLA	C3B-C4B-NB	-2.61	108.20	110.53
39	M	201	LMG	O6-C1-O1	-2.61	103.88	110.04
39	B	621	LMG	O6-C1-O1	-2.61	103.88	110.04
33	6	308	CLA	C3B-C4B-NB	-2.61	108.20	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	3	315	DD6	C37-C36-C35	2.61	119.22	114.42
33	C	509	CLA	CHB-C4A-NA	2.61	128.16	124.40
33	0	311	CLA	CHB-C4A-NA	2.61	128.16	124.40
30	b	619	BCR	C15-C14-C13	-2.61	123.62	127.28
45	6	303	A86	C12-C11-C13	2.60	120.22	116.00
33	B	612	CLA	CHB-C4A-NA	2.60	128.16	124.40
33	b	613	CLA	CHB-C4A-NA	2.60	128.16	124.40
30	C	515	BCR	C24-C23-C22	-2.60	122.39	126.23
45	8	302	A86	C4-C3-C2	-2.60	118.20	123.52
30	c	514	BCR	C15-C14-C13	-2.60	123.63	127.28
33	B	609	CLA	O2A-CGA-O1A	-2.60	117.13	123.63
39	D	410	LMG	O6-C1-O1	-2.59	103.91	110.04
47	7	306	KC2	C1B-CHB-C4A	-2.59	120.50	126.02
33	c	506	CLA	C3B-C4B-NB	-2.59	108.22	110.53
48	0	302	ET4	C07-C06-C05	-2.59	115.58	121.56
30	H	101	BCR	C2-C1-C6	2.59	114.20	110.44
42	V	201	HEM	C4D-ND-C1D	2.59	108.27	105.21
37	t	102	SQD	C45-O47-C7	2.59	122.42	117.85
48	0	302	ET4	C42-C34-C33	-2.59	105.88	110.52
30	K	101	BCR	C27-C26-C25	2.59	126.20	122.70
33	C	513	CLA	CHB-C4A-NA	2.59	128.13	124.40
45	4	304	A86	C19-C18-C17	-2.59	105.95	110.79
33	9	311	CLA	CHB-C4A-NA	2.59	128.13	124.40
39	5	319	LMG	O6-C5-C4	2.58	114.36	109.70
33	2	312	CLA	C3B-C4B-NB	-2.58	108.22	110.53
33	b	612	CLA	C1-C2-C3	-2.58	121.96	126.20
33	b	617	CLA	CHB-C4A-NA	2.58	128.13	124.40
33	d	409	CLA	C3B-C4B-NB	-2.58	108.23	110.53
30	A	401	BCR	C33-C5-C6	-2.58	121.67	124.48
33	C	512	CLA	C3B-C4B-NB	-2.58	108.23	110.53
38	C	518	DGD	C3G-C2G-C1G	-2.58	105.77	111.78
33	8	315	CLA	C3B-C4B-NB	-2.58	108.23	110.53
44	5	315	KC1	CHC-C4B-C3B	-2.58	120.86	125.21
30	a	414	BCR	C33-C5-C6	-2.58	121.67	124.48
33	A	408	CLA	C3B-C4B-NB	-2.58	108.23	110.53
33	b	603	CLA	C3B-C4B-NB	-2.58	108.23	110.53
33	C	513	CLA	C3B-C4B-NB	-2.57	108.23	110.53
45	5	306	A86	C19-C18-C17	2.57	115.60	110.79
45	7	303	A86	C34-O4-C38	-2.57	113.30	117.85
33	2	315	CLA	CHB-C4A-NA	2.57	128.11	124.40
46	4	303	DD6	C26-C25-C24	-2.57	115.75	123.20
45	5	302	A86	C22-C16-C17	-2.57	104.45	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	0	305	CLA	CHB-C4A-NA	2.57	128.11	124.40
33	6	316	CLA	CMB-C2B-C1B	-2.57	123.38	125.94
33	9	315	CLA	CAA-C2A-C3A	-2.57	110.34	116.23
46	9	304	DD6	C4-C3-C2	-2.57	118.26	123.52
45	4	301	A86	O4-C38-O5	-2.57	118.03	122.99
43	w	302	LMU	C1'-O5'-C5'	-2.57	108.70	113.72
33	1	305	CLA	CAA-C2A-C3A	-2.57	110.34	116.23
33	B	603	CLA	C3B-C4B-NB	-2.57	108.24	110.53
33	b	612	CLA	C3B-C4B-NB	-2.57	108.24	110.53
30	A	401	BCR	C24-C23-C22	-2.57	122.44	126.23
38	H	102	DGD	C3G-C2G-C1G	-2.57	105.80	111.78
45	7	301	A86	C3-C2-C1	-2.57	123.68	127.28
34	a	409	PHO	C1-C2-C3	-2.57	121.99	126.20
37	T	103	SQD	O9-S-C6	2.57	110.59	106.76
33	b	604	CLA	C3B-C4B-NB	-2.57	108.24	110.53
46	2	304	DD6	C4-C3-C2	-2.56	118.27	123.52
33	3	313	CLA	CHB-C4A-NA	2.56	128.10	124.40
46	4	303	DD6	O1-C20-C21	-2.56	112.18	115.05
41	D	408	PL9	C22-C23-C24	-2.56	121.76	127.62
33	B	608	CLA	C3B-C4B-NB	-2.56	108.24	110.53
37	L	101	SQD	C44-O6-C1	2.56	119.29	113.80
42	v	201	HEM	C4D-ND-C1D	2.56	108.24	105.21
45	9	302	A86	C19-C18-C17	-2.56	106.00	110.79
33	c	511	CLA	CHB-C4A-NA	2.56	128.10	124.40
33	7	304	CLA	CHB-C4A-NA	2.56	128.09	124.40
46	9	303	DD6	C9-C8-C6	-2.56	119.34	126.36
33	7	311	CLA	C3B-C4B-NB	-2.56	108.25	110.53
33	7	311	CLA	CHB-C4A-NA	2.55	128.09	124.40
45	1	301	A86	C12-C11-C13	2.55	120.14	116.00
33	8	308	CLA	O2D-CGD-CBD	2.55	115.69	111.23
33	2	314	CLA	CAA-C2A-C3A	-2.55	110.38	116.23
33	4	306	CLA	CHB-C4A-NA	2.55	128.08	124.40
33	7	307	CLA	CMB-C2B-C1B	-2.55	121.53	125.42
33	2	313	CLA	CHC-C1C-C2C	-2.55	124.36	129.94
38	C	516	DGD	C3G-C2G-C1G	-2.55	105.84	111.78
33	c	504	CLA	C3B-C4B-NB	-2.55	108.26	110.53
33	2	307	CLA	CAB-C3B-C2B	2.55	130.30	123.53
45	5	306	A86	C12-C11-C13	2.55	120.13	116.00
33	3	311	CLA	CAA-C2A-C3A	-2.55	110.39	116.23
39	b	622	LMG	O6-C1-O1	-2.55	104.03	110.04
33	3	307	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
47	0	306	KC2	C1D-ND-C4D	2.55	108.10	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2	312	CLA	CHB-C4A-NA	2.55	128.07	124.40
33	2	313	CLA	CHB-C1B-NB	2.55	127.87	124.05
45	2	302	A86	C19-C18-C17	-2.55	106.03	110.79
37	i	101	SQD	O5-C5-C4	2.54	114.28	109.70
36	d	405	LHG	O8-C23-C24	2.54	119.59	111.83
33	0	313	CLA	CAA-C2A-C3A	-2.54	110.40	116.23
33	c	513	CLA	C3B-C4B-NB	-2.54	108.26	110.53
33	5	316	CLA	CAA-C2A-C3A	-2.54	110.40	116.23
46	1	303	DD6	C28-C27-C26	-2.54	119.25	124.18
46	2	303	DD6	C9-C8-C6	-2.54	119.39	126.36
46	8	303	DD6	C28-C27-C26	-2.54	119.25	124.18
33	4	315	CLA	CHB-C4A-NA	2.54	128.07	124.40
38	c	516	DGD	C3G-C2G-C1G	-2.54	105.86	111.78
33	B	601	CLA	CHB-C4A-NA	2.54	128.06	124.40
33	5	314	CLA	C3B-C4B-NB	-2.54	108.26	110.53
47	5	310	KC2	C1D-ND-C4D	2.54	108.09	106.31
47	4	307	KC2	CBA-CAA-C2A	-2.54	115.27	125.45
33	C	508	CLA	C3B-C4B-NB	-2.54	108.27	110.53
33	C	511	CLA	CHB-C4A-NA	2.53	128.06	124.40
33	1	312	CLA	CHB-C4A-NA	2.53	128.06	124.40
30	C	514	BCR	C15-C14-C13	-2.53	123.72	127.28
34	A	406	PHO	C1-C2-C3	-2.53	122.05	126.20
37	L	101	SQD	O5-C5-C4	2.53	114.26	109.70
45	1	302	A86	O4-C38-O5	-2.53	118.10	122.99
33	4	310	CLA	C3B-C4B-NB	-2.53	108.27	110.53
33	9	305	CLA	CAA-C2A-C3A	-2.53	110.43	116.23
42	V	201	HEM	CHD-C4C-NC	2.53	127.21	124.45
33	B	607	CLA	C3B-C4B-NB	-2.53	108.27	110.53
33	c	511	CLA	C3B-C4B-NB	-2.53	108.27	110.53
38	A	415	DGD	O5D-C6D-C5D	-2.53	103.72	109.42
46	4	303	DD6	C3-C2-C1	-2.53	123.73	127.28
36	b	601	LHG	C11-C10-C9	-2.53	101.59	114.37
37	T	103	SQD	C44-O6-C1	2.53	119.21	113.80
33	B	604	CLA	C1-C2-C3	-2.53	122.06	126.20
33	0	304	CLA	CHB-C4A-NA	2.53	128.04	124.40
45	5	303	A86	O4-C34-C35	-2.53	101.17	107.64
48	0	302	ET4	C11-C10-C09	-2.52	123.74	127.28
33	a	408	CLA	O2D-CGD-CBD	2.52	115.64	111.23
33	5	313	CLA	C3B-C4B-NB	-2.52	108.28	110.53
45	8	302	A86	O4-C38-O5	-2.52	118.12	122.99
33	3	305	CLA	CHB-C4A-NA	2.52	128.04	124.40
33	6	315	CLA	CHB-C4A-NA	2.52	128.04	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	0	313	CLA	CMB-C2B-C1B	-2.52	123.43	125.94
33	c	512	CLA	CHB-C4A-NA	2.52	128.04	124.40
33	4	308	CLA	CHB-C4A-NA	2.52	128.04	124.40
33	1	306	CLA	CHB-C4A-NA	2.52	128.04	124.40
38	c	518	DGD	C3G-C2G-C1G	-2.52	105.90	111.78
45	5	301	A86	C33-C32-C31	-2.52	106.76	109.21
37	7	317	SQD	O5-C5-C4	2.52	114.24	109.70
33	C	504	CLA	CHB-C4A-NA	2.52	128.04	124.40
33	6	307	CLA	CHB-C4A-NA	2.52	128.04	124.40
33	b	608	CLA	C3B-C4B-NB	-2.52	108.28	110.53
38	C	517	DGD	O5D-C6D-C5D	-2.52	103.74	109.42
33	4	309	CLA	C3B-C4B-NB	-2.52	108.28	110.53
33	2	315	CLA	CAA-C2A-C3A	-2.52	110.46	116.23
33	c	513	CLA	CHB-C4A-NA	2.52	128.03	124.40
45	8	301	A86	O4-C38-O5	-2.52	118.13	122.99
33	1	308	CLA	CHB-C4A-NA	2.52	128.03	124.40
30	b	618	BCR	C24-C23-C22	-2.52	122.51	126.23
47	0	306	KC2	C1B-CHB-C4A	-2.51	120.68	126.02
37	T	103	SQD	O5-C5-C4	2.51	114.23	109.70
33	8	309	CLA	CHB-C4A-NA	2.51	128.02	124.40
37	T	103	SQD	O48-C23-C24	2.51	119.49	111.83
30	b	619	BCR	C15-C16-C17	-2.51	118.39	123.52
33	B	602	CLA	C3B-C4B-NB	-2.51	108.29	110.53
30	C	514	BCR	C24-C23-C22	-2.51	122.53	126.23
37	T	103	SQD	C1-O5-C5	2.51	118.61	113.72
47	5	310	KC2	CHD-C4C-C3C	-2.51	117.48	125.91
33	c	504	CLA	CHB-C4A-NA	2.50	128.01	124.40
30	h	101	BCR	C24-C23-C22	-2.50	122.53	126.23
47	0	306	KC2	O2D-CGD-O1D	-2.50	118.97	123.85
45	4	304	A86	O4-C38-O5	-2.50	118.16	122.99
38	a	401	DGD	O5D-C6D-C5D	-2.50	103.78	109.42
33	6	308	CLA	CHB-C4A-NA	2.50	128.01	124.40
42	V	201	HEM	C1A-CHA-C4D	-2.50	120.36	126.25
33	C	510	CLA	CHB-C4A-NA	2.50	128.01	124.40
47	0	306	KC2	CHB-C4A-C3A	-2.50	121.08	125.03
33	6	311	CLA	CHB-C4A-NA	2.50	128.01	124.40
33	9	306	CLA	CHB-C4A-NA	2.50	128.01	124.40
37	1	101	SQD	C44-O6-C1	2.50	119.16	113.80
46	3	315	DD6	C25-C24-C1	-2.50	119.51	126.36
33	B	605	CLA	C3B-C4B-NB	-2.50	108.30	110.53
41	D	408	PL9	C27-C28-C29	-2.50	121.90	127.62
33	9	308	CLA	CHB-C4A-NA	2.50	128.01	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2	309	CLA	CHB-C4A-NA	2.50	128.01	124.40
30	K	102	BCR	C27-C26-C25	2.50	126.08	122.70
33	C	512	CLA	CHB-C4A-NA	2.50	128.00	124.40
33	4	311	CLA	CHB-C4A-NA	2.50	128.00	124.40
36	d	405	LHG	C11-C10-C9	-2.50	101.74	114.37
33	3	319	CLA	CHB-C4A-NA	2.50	128.00	124.40
48	7	302	ET4	C42-C34-C33	-2.50	106.05	110.52
46	8	304	DD6	C37-C36-C31	-2.50	119.49	124.16
33	8	313	CLA	CAA-C2A-C3A	-2.49	110.51	116.23
36	A	412	LHG	C20-C19-C18	-2.49	101.76	114.37
33	b	602	CLA	CHB-C4A-NA	2.49	128.00	124.40
33	2	311	CLA	CHB-C4A-NA	2.49	128.00	124.40
46	9	304	DD6	C26-C25-C24	-2.49	115.97	123.20
45	0	301	A86	C3-C2-C1	-2.49	123.78	127.28
30	k	102	BCR	C33-C5-C6	-2.49	121.77	124.48
33	b	611	CLA	CHB-C4A-NA	2.49	127.99	124.40
33	0	310	CLA	C3B-C4B-NB	-2.49	108.31	110.53
46	2	304	DD6	C26-C25-C24	-2.49	115.99	123.20
33	1	311	CLA	CHB-C4A-NA	2.49	127.99	124.40
33	2	313	CLA	CBD-CHA-C1A	2.49	131.13	127.38
39	B	620	LMG	C40-C39-C38	-2.49	101.79	114.37
33	c	508	CLA	C3B-C4B-NB	-2.49	108.31	110.53
33	c	510	CLA	CHB-C4A-NA	2.49	127.99	124.40
39	c	519	LMG	O6-C1-O1	-2.49	104.17	110.04
33	8	310	CLA	C3B-C4B-NB	-2.49	108.31	110.53
33	1	310	CLA	CHB-C4A-NA	2.48	127.99	124.40
45	7	303	A86	O1-C15-C20	-2.48	57.34	59.45
33	c	508	CLA	CHB-C4A-NA	2.48	127.98	124.40
36	A	414	LHG	C11-C10-C9	-2.48	101.81	114.37
30	B	618	BCR	C15-C16-C17	-2.48	118.44	123.52
33	5	317	CLA	CAA-C2A-C3A	-2.48	110.53	116.23
30	A	401	BCR	C15-C16-C17	-2.48	118.45	123.52
30	a	414	BCR	C15-C16-C17	-2.48	118.45	123.52
47	5	310	KC2	CHB-C4A-C3A	-2.48	121.11	125.03
33	C	501	CLA	C3B-C4B-NB	-2.48	108.32	110.53
33	9	309	CLA	CHB-C4A-NA	2.48	127.98	124.40
37	A	413	SQD	C1-O5-C5	2.48	118.56	113.72
30	B	619	BCR	C27-C26-C25	2.48	126.05	122.70
33	8	305	CLA	CHB-C4A-NA	2.48	127.97	124.40
36	4	318	LHG	C11-C10-C9	-2.48	101.85	114.37
33	2	310	CLA	C1-C2-C3	-2.48	122.14	126.20
33	1	316	CLA	CHB-C4A-NA	2.48	127.97	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	8	306	CLA	CHB-C4A-NA	2.47	127.97	124.40
33	a	411	CLA	CHB-C4A-NA	2.47	127.97	124.40
33	2	316	CLA	CHB-C4A-NA	2.47	127.97	124.40
45	4	302	A86	C12-C11-C13	2.47	120.01	116.00
33	8	315	CLA	CHB-C4A-NA	2.47	127.97	124.40
42	v	201	HEM	C2A-C1A-NA	-2.47	107.41	110.15
33	B	607	CLA	CHB-C4A-NA	2.47	127.97	124.40
45	3	314	A86	C12-C11-C13	2.47	120.01	116.00
30	K	101	BCR	C35-C13-C14	-2.47	118.81	122.82
33	1	315	CLA	CHB-C4A-NA	2.47	127.97	124.40
48	0	302	ET4	C10-C11-C12	2.47	130.36	123.20
30	b	618	BCR	C7-C8-C9	-2.47	122.58	126.23
33	3	308	CLA	CHB-C4A-NA	2.47	127.97	124.40
33	C	501	CLA	CHB-C4A-NA	2.47	127.96	124.40
33	4	305	CLA	CHB-C4A-NA	2.47	127.96	124.40
39	d	410	LMG	O1-C7-C8	-2.47	104.81	110.82
36	D	409	LHG	C11-C10-C9	-2.47	101.89	114.37
33	2	306	CLA	CHB-C4A-NA	2.47	127.96	124.40
33	4	312	CLA	C3B-C4B-NB	-2.47	108.33	110.53
37	i	101	SQD	C4-C3-C2	2.47	115.16	110.83
33	9	316	CLA	CHB-C4A-NA	2.47	127.96	124.40
39	M	201	LMG	O2-C2-C1	-2.47	104.19	110.08
33	0	312	CLA	C3B-C4B-NB	-2.47	108.33	110.53
39	W	301	LMG	O3-C3-C2	-2.47	104.56	110.38
33	8	311	CLA	CHB-C4A-NA	2.47	127.96	124.40
37	T	103	SQD	C4-C3-C2	2.47	115.16	110.83
36	a	403	LHG	C11-C10-C9	-2.47	101.90	114.37
33	d	402	CLA	CHB-C4A-NA	2.47	127.96	124.40
33	4	313	CLA	CHB-C4A-NA	2.47	127.96	124.40
33	7	305	CLA	CHB-C4A-NA	2.47	127.96	124.40
45	3	314	A86	O4-C38-O5	-2.47	118.23	122.99
36	d	407	LHG	C11-C10-C9	-2.46	101.91	114.37
33	3	302	CLA	CHB-C4A-NA	2.46	127.96	124.40
36	3	318	LHG	C11-C10-C9	-2.46	101.91	114.37
33	b	605	CLA	CHB-C4A-NA	2.46	127.96	124.40
33	0	308	CLA	CHB-C4A-NA	2.46	127.95	124.40
33	C	503	CLA	CHB-C4A-NA	2.46	127.95	124.40
30	D	407	BCR	C24-C23-C22	-2.46	122.59	126.23
33	3	306	CLA	CHB-C4A-NA	2.46	127.95	124.40
33	1	305	CLA	CHB-C4A-NA	2.46	127.95	124.40
36	3	317	LHG	C11-C10-C9	-2.46	101.92	114.37
42	V	201	HEM	C3B-C4B-NB	-2.46	107.70	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	7	306	KC2	CHB-C4A-C3A	-2.46	121.14	125.03
36	A	414	LHG	C20-C19-C18	-2.46	101.93	114.37
38	c	517	DGD	C3G-C2G-C1G	-2.46	106.05	111.78
30	K	102	BCR	C24-C23-C22	-2.46	122.59	126.23
33	a	411	CLA	O2D-CGD-CBD	2.46	115.53	111.23
39	b	621	LMG	C38-C37-C36	-2.46	101.93	114.37
45	4	301	A86	C40-C32-C31	-2.46	108.27	110.47
33	b	608	CLA	CHB-C4A-NA	2.46	127.95	124.40
33	2	308	CLA	CHB-C4A-NA	2.46	127.95	124.40
45	5	307	A86	C25-C24-C1	-2.46	119.62	126.36
33	3	307	CLA	CHB-C4A-NA	2.46	127.95	124.40
33	4	314	CLA	C3B-C4B-NB	-2.46	108.34	110.53
45	0	301	A86	O4-C38-O5	-2.46	118.25	122.99
33	3	304	CLA	CHB-C4A-NA	2.46	127.94	124.40
39	q	301	LMG	C40-C39-C38	-2.45	101.96	114.37
33	A	408	CLA	CHB-C4A-NA	2.45	127.94	124.40
30	c	514	BCR	C11-C10-C9	-2.45	123.84	127.28
33	B	611	CLA	O2A-CGA-O1A	-2.45	117.49	123.63
33	3	311	CLA	CHB-C4A-NA	2.45	127.94	124.40
30	c	515	BCR	C37-C22-C21	-2.45	118.84	122.82
33	H	103	CLA	CHB-C4A-NA	2.45	127.94	124.40
45	8	302	A86	C19-C18-C17	2.45	115.38	110.79
33	a	411	CLA	C1-C2-C3	-2.45	122.18	126.20
39	W	301	LMG	C38-C37-C36	-2.45	101.98	114.37
33	d	409	CLA	CHB-C4A-NA	2.45	127.94	124.40
30	B	619	BCR	C11-C10-C9	-2.45	123.84	127.28
33	b	612	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
39	d	406	LMG	C1-C2-C3	-2.45	104.86	110.01
39	0	314	LMG	O6-C5-C4	2.45	114.11	109.70
33	D	402	CLA	CHB-C4A-NA	2.45	127.93	124.40
33	1	313	CLA	CHB-C4A-NA	2.45	127.93	124.40
45	2	302	A86	O4-C38-O5	-2.45	118.26	122.99
33	C	505	CLA	C3B-C4B-NB	-2.45	108.35	110.53
36	A	412	LHG	C11-C10-C9	-2.45	102.00	114.37
37	a	413	SQD	O6-C1-C2	2.45	111.99	108.27
33	9	314	CLA	CHB-C4A-NA	2.45	127.93	124.40
33	B	606	CLA	C3B-C4B-NB	-2.45	108.35	110.53
36	D	411	LHG	C11-C10-C9	-2.44	102.01	114.37
39	W	301	LMG	C40-C39-C38	-2.44	102.01	114.37
45	6	301	A86	C12-C11-C13	2.44	119.96	116.00
33	d	401	CLA	CMB-C2B-C3B	2.44	130.03	123.53
36	A	411	LHG	C11-C10-C9	-2.44	102.02	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	414	BCR	C11-C10-C9	-2.44	123.85	127.28
45	9	302	A86	O4-C38-O5	-2.44	118.28	122.99
33	1	307	CLA	CMB-C2B-C3B	2.44	130.02	123.53
33	0	313	CLA	CHB-C4A-NA	2.44	127.92	124.40
36	a	404	LHG	C20-C19-C18	-2.44	102.03	114.37
39	b	621	LMG	C40-C39-C38	-2.44	102.03	114.37
33	7	307	CLA	CHB-C4A-NA	2.44	127.92	124.40
45	0	303	A86	C19-C18-C17	-2.44	106.23	110.79
36	a	404	LHG	C11-C10-C9	-2.44	102.04	114.37
46	8	304	DD6	C26-C25-C24	-2.44	116.14	123.20
33	0	309	CLA	C1-C2-C3	-2.44	122.20	126.20
33	B	610	CLA	CHB-C4A-NA	2.44	127.92	124.40
47	5	310	KC2	C1B-CHB-C4A	-2.44	120.84	126.02
33	5	312	CLA	CHB-C4A-NA	2.44	127.92	124.40
46	2	304	DD6	C37-C36-C31	-2.44	119.61	124.16
33	b	612	CLA	CHB-C4A-NA	2.44	127.92	124.40
36	4	318	LHG	C20-C19-C18	-2.44	102.06	114.37
41	d	404	PL9	C7-C8-C9	-2.43	122.64	126.83
45	6	306	A86	C12-C11-C13	2.43	119.95	116.00
39	w	304	LMG	C38-C37-C36	-2.43	102.07	114.37
36	5	318	LHG	C20-C19-C18	-2.43	102.07	114.37
33	0	308	CLA	CAA-C2A-C3A	-2.43	110.65	116.23
37	D	403	SQD	O8-S-C6	2.43	110.67	105.97
45	5	302	A86	O4-C34-C35	-2.43	101.41	107.64
33	B	616	CLA	CHB-C4A-NA	2.43	127.91	124.40
45	6	306	A86	O4-C38-O5	-2.43	118.30	122.99
33	8	316	CLA	CHB-C4A-NA	2.43	127.91	124.40
33	a	408	CLA	CHB-C4A-NA	2.43	127.91	124.40
33	D	405	CLA	CMB-C2B-C3B	2.43	129.99	123.53
42	V	201	HEM	C4C-CHD-C1D	-2.43	120.86	126.02
36	H	104	LHG	C11-C10-C9	-2.43	102.09	114.37
37	l	101	SQD	O48-C23-C24	2.43	119.24	111.83
33	9	307	CLA	CAB-C3B-C2B	2.43	129.98	123.53
33	8	307	CLA	CAB-C3B-C2B	2.43	129.98	123.53
33	3	309	CLA	CHB-C4A-NA	2.43	127.90	124.40
33	c	509	CLA	CHB-C4A-NA	2.43	127.90	124.40
30	d	403	BCR	C15-C16-C17	-2.43	118.56	123.52
33	B	611	CLA	C1-C2-C3	-2.43	122.22	126.20
33	B	613	CLA	C3B-C4B-NB	-2.43	108.36	110.53
33	C	510	CLA	C1-C2-C3	-2.42	122.22	126.20
30	C	514	BCR	C11-C10-C9	-2.42	123.88	127.28
33	B	615	CLA	CHB-C4A-NA	2.42	127.90	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	503	CLA	CHB-C4A-NA	2.42	127.90	124.40
45	1	302	A86	C19-C18-C17	2.42	115.32	110.79
33	9	315	CLA	CHB-C4A-NA	2.42	127.90	124.40
36	b	601	LHG	C20-C19-C18	-2.42	102.12	114.37
45	7	301	A86	O4-C38-O5	-2.42	118.31	122.99
47	7	306	KC2	CHD-C4C-C3C	-2.42	117.76	125.91
39	m	201	LMG	O2-C2-C1	-2.42	104.30	110.08
33	d	409	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
33	A	405	CLA	O2D-CGD-CBD	2.42	115.46	111.23
33	5	317	CLA	CHB-C4A-NA	2.42	127.89	124.40
41	D	408	PL9	C37-C38-C39	-2.42	122.08	127.62
30	k	102	BCR	C15-C16-C17	-2.42	118.57	123.52
37	0	316	SQD	O5-C5-C4	2.42	114.06	109.70
33	z	101	CLA	CHB-C4A-NA	2.42	127.89	124.40
33	9	317	CLA	CHB-C4A-NA	2.42	127.89	124.40
45	8	302	A86	C41-C32-C31	-2.42	108.31	110.47
33	0	309	CLA	CHB-C4A-NA	2.42	127.89	124.40
36	h	103	LHG	C11-C10-C9	-2.42	102.15	114.37
33	9	307	CLA	CMB-C2B-C3B	2.42	129.96	123.53
30	C	515	BCR	C37-C22-C21	-2.42	118.90	122.82
39	C	520	LMG	O1-C7-C8	-2.42	104.94	110.82
30	a	412	BCR	C33-C5-C6	-2.42	121.85	124.48
33	5	316	CLA	CHB-C4A-NA	2.41	127.88	124.40
33	b	607	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
33	Z	101	CLA	CHB-C4A-NA	2.41	127.88	124.40
42	e	101	HEM	C1A-CHA-C4D	-2.41	120.57	126.25
33	b	604	CLA	O2D-CGD-CBD	2.41	115.45	111.23
33	2	313	CLA	CAA-C2A-C3A	-2.41	110.70	116.23
39	c	520	LMG	O6-C1-O1	-2.41	104.35	110.04
33	b	616	CLA	CHB-C4A-NA	2.41	127.88	124.40
33	9	312	CLA	CHB-C4A-NA	2.41	127.88	124.40
33	c	502	CLA	C3B-C4B-NB	-2.41	108.38	110.53
39	c	519	LMG	C38-C37-C36	-2.41	102.19	114.37
33	9	313	CLA	CHB-C4A-NA	2.41	127.88	124.40
30	C	515	BCR	C23-C22-C21	2.41	122.80	119.01
33	7	309	CLA	CHB-C4A-NA	2.41	127.88	124.40
33	7	310	CLA	CHB-C4A-NA	2.41	127.88	124.40
33	b	610	CLA	C1-C2-C3	-2.41	122.25	126.20
33	7	314	CLA	CHB-C4A-NA	2.41	127.88	124.40
33	8	307	CLA	CHB-C4A-NA	2.41	127.88	124.40
38	c	517	DGD	O5D-C6D-C5D	-2.41	103.99	109.42
33	D	405	CLA	CAB-C3B-C2B	2.41	129.93	123.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	1	307	CLA	CHB-C4A-NA	2.41	127.88	124.40
33	6	307	CLA	C3B-C4B-NB	-2.41	108.38	110.53
45	1	302	A86	C41-C32-C31	-2.41	108.32	110.47
33	5	313	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
33	5	313	CLA	CHB-C4A-NA	2.40	127.87	124.40
33	b	610	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
33	8	307	CLA	CMB-C2B-C3B	2.40	129.92	123.53
45	5	304	A86	O4-C38-O5	-2.40	118.35	122.99
37	T	101	SQD	C45-O47-C7	2.40	122.09	117.85
33	8	314	CLA	CHB-C4A-NA	2.40	127.87	124.40
39	C	521	LMG	O6-C1-O1	-2.40	104.37	110.04
30	b	619	BCR	C33-C5-C6	-2.40	121.87	124.48
33	C	508	CLA	CHB-C4A-NA	2.40	127.86	124.40
47	4	307	KC2	CHD-C4C-C3C	-2.40	117.84	125.91
46	9	304	DD6	C37-C36-C31	-2.40	119.68	124.16
33	A	405	CLA	CHB-C4A-NA	2.40	127.86	124.40
33	B	608	CLA	CHB-C4A-NA	2.40	127.86	124.40
45	6	303	A86	C3-C4-C5	-2.40	118.62	123.52
33	b	605	CLA	C3B-C4B-NB	-2.39	108.39	110.53
30	K	102	BCR	C15-C16-C17	-2.39	118.62	123.52
45	0	303	A86	C41-C32-C31	-2.39	108.33	110.47
30	k	101	BCR	C33-C5-C6	-2.39	121.87	124.48
45	8	301	A86	C3-C4-C5	-2.39	118.62	123.52
33	2	317	CLA	CHB-C4A-NA	2.39	127.85	124.40
33	1	307	CLA	CAB-C3B-C2B	2.39	129.89	123.53
45	3	314	A86	C-C1-C2	-2.39	118.94	122.82
45	5	301	A86	O4-C38-O5	-2.39	118.38	122.99
39	7	315	LMG	C40-C39-C38	-2.39	102.28	114.37
38	h	102	DGD	C3G-C2G-C1G	-2.39	106.21	111.78
45	4	301	A86	C34-O4-C38	-2.39	113.62	117.85
33	A	404	CLA	CHB-C4A-NA	2.39	127.85	124.40
33	a	407	CLA	CHB-C4A-NA	2.39	127.85	124.40
47	4	307	KC2	CHD-C1D-C2D	-2.39	120.49	127.43
45	6	302	A86	O4-C38-O5	-2.39	118.38	122.99
39	C	519	LMG	C40-C39-C38	-2.39	102.30	114.37
30	K	102	BCR	C33-C5-C6	-2.39	121.88	124.48
33	4	309	CLA	CHB-C4A-NA	2.39	127.84	124.40
33	4	316	CLA	CHB-C4A-NA	2.39	127.84	124.40
33	7	308	CLA	CAA-C2A-C3A	-2.39	110.76	116.23
45	5	302	A86	O4-C38-O5	-2.39	118.38	122.99
46	8	304	DD6	C-C1-C24	2.39	121.73	118.09
33	B	606	CLA	O2A-CGA-O1A	-2.39	117.66	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	w	304	LMG	C40-C39-C38	-2.39	102.31	114.37
39	D	410	LMG	C1-C2-C3	-2.39	104.99	110.01
46	2	304	DD6	C37-C36-C35	2.38	118.81	114.42
33	b	610	CLA	CHB-C4A-NA	2.38	127.84	124.40
45	6	305	A86	O4-C38-O5	-2.38	118.39	122.99
37	L	101	SQD	O48-C23-C24	2.38	119.10	111.83
46	2	303	DD6	C-C1-C2	-2.38	118.96	122.82
33	4	310	CLA	CHB-C4A-NA	2.38	127.84	124.40
30	B	619	BCR	C33-C5-C6	-2.38	121.89	124.48
37	0	316	SQD	O6-C1-C2	2.38	111.89	108.27
30	a	414	BCR	C15-C14-C13	-2.38	123.94	127.28
33	b	603	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
30	b	620	BCR	C27-C26-C25	2.38	125.92	122.70
33	8	314	CLA	CAA-C2A-C3A	-2.38	110.77	116.23
45	6	302	A86	O1-C20-C15	-2.38	58.27	59.23
33	3	303	CLA	CHB-C4A-NA	2.38	127.83	124.40
46	9	303	DD6	C23-C16-C22	2.38	110.83	107.37
33	2	305	CLA	CAA-C2A-C3A	-2.38	110.78	116.23
33	d	401	CLA	CAB-C3B-C2B	2.38	129.85	123.53
45	6	304	A86	O4-C38-O5	-2.38	118.40	122.99
33	b	609	CLA	CHB-C4A-NA	2.38	127.83	124.40
33	2	314	CLA	CHB-C4A-NA	2.38	127.83	124.40
45	6	305	A86	C25-C24-C1	-2.38	119.84	126.36
44	5	315	KC1	C2A-C3A-C4A	2.38	108.20	106.41
45	4	302	A86	C36-C31-C32	-2.38	117.34	119.70
45	4	302	A86	O4-C38-O5	-2.38	118.40	122.99
33	1	309	CLA	CHB-C4A-NA	2.38	127.83	124.40
45	4	302	A86	C9-C10-C11	-2.38	119.92	126.64
38	C	516	DGD	C1D-C2D-C3D	-2.38	105.01	110.01
39	B	620	LMG	C38-C37-C36	-2.38	102.36	114.37
36	3	318	LHG	C20-C19-C18	-2.37	102.36	114.37
33	C	504	CLA	C3B-C4B-NB	-2.37	108.41	110.53
33	2	306	CLA	C3B-C4B-NB	-2.37	108.41	110.53
33	6	310	CLA	CHB-C4A-NA	2.37	127.82	124.40
45	5	303	A86	O4-C38-O5	-2.37	118.42	122.99
33	8	313	CLA	CHB-C4A-NA	2.37	127.82	124.40
33	B	616	CLA	C1-C2-C3	-2.37	122.32	126.20
46	9	303	DD6	C-C1-C2	-2.37	118.98	122.82
33	6	312	CLA	CHB-C4A-NA	2.37	127.81	124.40
45	5	307	A86	O4-C38-O5	-2.37	118.42	122.99
33	C	504	CLA	CMB-C2B-C1B	-2.37	121.82	125.42
47	7	306	KC2	C1D-ND-C4D	2.36	107.97	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	5	308	CLA	CHB-C4A-NA	2.36	127.81	124.40
45	0	303	A86	O1-C15-C20	-2.36	57.45	59.45
44	5	315	KC1	O2D-CGD-O1D	-2.36	119.25	123.85
33	b	608	CLA	CMB-C2B-C1B	-2.36	121.82	125.42
45	7	301	A86	C40-C32-C31	-2.36	108.36	110.47
45	3	314	A86	O1-C15-C20	-2.36	57.45	59.45
33	a	407	CLA	CMB-C2B-C1B	-2.36	121.82	125.42
33	7	308	CLA	CHB-C4A-NA	2.36	127.81	124.40
33	b	615	CLA	CHB-C4A-NA	2.36	127.81	124.40
33	1	309	CLA	C3B-C4B-NB	-2.36	108.42	110.53
45	7	303	A86	C12-C11-C13	2.36	119.82	116.00
39	D	410	LMG	O3-C3-C2	-2.36	104.82	110.38
46	9	304	DD6	C37-C36-C35	2.36	118.75	114.42
33	6	310	CLA	C1-C2-C3	-2.35	122.34	126.20
37	D	403	SQD	O6-C1-C2	2.35	111.85	108.27
37	l	101	SQD	O5-C5-C4	2.35	113.94	109.70
45	5	306	A86	O4-C38-O5	-2.35	118.45	122.99
46	8	303	DD6	C-C1-C2	-2.35	119.00	122.82
46	2	303	DD6	C23-C16-C22	2.35	110.79	107.37
36	5	318	LHG	C11-C10-C9	-2.35	102.47	114.37
39	d	406	LMG	O2-C2-C1	-2.35	104.47	110.08
37	t	102	SQD	O48-C23-C24	2.35	119.01	111.83
33	C	503	CLA	C1-C2-C3	-2.35	122.35	126.20
30	a	414	BCR	C7-C8-C9	-2.35	122.76	126.23
45	6	305	A86	O4-C34-C35	-2.35	101.62	107.64
30	b	620	BCR	C11-C10-C9	-2.35	123.98	127.28
37	t	102	SQD	O6-C1-C2	2.35	111.84	108.27
30	c	514	BCR	C15-C16-C17	-2.34	118.72	123.52
33	3	312	CLA	CHB-C4A-NA	2.34	127.78	124.40
39	C	519	LMG	C38-C37-C36	-2.34	102.53	114.37
33	9	305	CLA	CHB-C4A-NA	2.34	127.78	124.40
45	5	301	A86	C9-C8-C6	-2.34	119.94	126.36
39	3	316	LMG	C1-C2-C3	-2.34	105.09	110.01
33	C	506	CLA	C3B-C4B-NB	-2.34	108.44	110.53
30	k	102	BCR	C27-C26-C25	2.34	125.86	122.70
33	B	614	CLA	CHB-C4A-NA	2.34	127.78	124.40
42	e	101	HEM	CHA-C4D-C3D	-2.34	120.92	125.23
39	C	519	LMG	O1-C7-C8	-2.34	105.13	110.82
39	b	622	LMG	O3-C3-C2	-2.34	104.86	110.38
33	d	401	CLA	C3B-C4B-NB	-2.34	107.90	110.33
33	C	508	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
38	A	415	DGD	O2D-C2D-C1D	-2.34	104.51	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	1	303	DD6	C7-C6-C5	-2.34	119.03	122.82
45	4	304	A86	C12-C11-C13	2.34	119.79	116.00
45	6	301	A86	O4-C38-O5	-2.34	118.48	122.99
39	B	620	LMG	O2-C2-C1	-2.33	104.51	110.08
39	D	404	LMG	O3-C3-C2	-2.33	104.88	110.38
45	5	301	A86	C25-C24-C1	-2.33	119.97	126.36
46	1	303	DD6	C-C1-C2	-2.33	119.04	122.82
45	7	301	A86	C21-C20-C19	-2.33	111.62	114.24
33	2	305	CLA	CHB-C4A-NA	2.33	127.77	124.40
33	c	502	CLA	CHB-C4A-NA	2.33	127.77	124.40
33	B	602	CLA	CHB-C4A-NA	2.33	127.76	124.40
46	8	303	DD6	C7-C6-C5	-2.33	119.04	122.82
45	0	301	A86	C21-C20-C19	-2.33	111.62	114.24
33	7	312	CLA	CHB-C4A-NA	2.33	127.76	124.40
39	7	315	LMG	C38-C37-C36	-2.33	102.59	114.37
30	C	514	BCR	C15-C16-C17	-2.33	118.76	123.52
39	b	623	LMG	O7-C10-O9	-2.33	118.26	123.70
33	B	602	CLA	CMB-C2B-C1B	-2.33	121.88	125.42
33	2	313	CLA	C3B-C4B-NB	-2.33	108.45	110.53
37	l	101	SQD	O8-S-C6	2.33	110.46	105.97
45	5	304	A86	C25-C24-C1	-2.33	119.99	126.36
33	4	314	CLA	CMB-C2B-C1B	-2.33	121.88	125.42
30	B	618	BCR	C33-C5-C6	-2.33	121.95	124.48
37	D	403	SQD	O48-C23-C24	2.32	118.92	111.83
48	7	302	ET4	C34-C35-C36	-2.32	108.50	113.59
33	5	311	CLA	CHB-C4A-NA	2.32	127.75	124.40
45	9	301	A86	O4-C38-O5	-2.32	118.51	122.99
33	4	310	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
45	5	303	A86	C33-C32-C31	-2.32	106.96	109.21
33	c	501	CLA	CHB-C4A-NA	2.32	127.75	124.40
30	H	101	BCR	C24-C23-C22	-2.32	122.81	126.23
39	B	621	LMG	O3-C3-C2	-2.32	104.91	110.38
39	M	201	LMG	O3-C3-C2	-2.32	104.92	110.38
33	b	607	CLA	CHB-C4A-NA	2.32	127.74	124.40
46	1	303	DD6	C37-C36-C31	-2.32	119.83	124.16
33	c	513	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
34	A	407	PHO	C1-C2-C3	-2.32	122.40	126.20
30	A	401	BCR	C15-C14-C13	-2.32	124.03	127.28
39	C	519	LMG	O3-C3-C2	-2.31	104.92	110.38
33	D	406	CLA	C3B-C4B-NB	-2.31	108.47	110.53
39	C	522	LMG	O1-C7-C8	-2.31	105.19	110.82
33	6	313	CLA	CHB-C4A-NA	2.31	127.74	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	2	302	A86	C9-C8-C6	-2.31	120.02	126.36
37	a	413	SQD	C44-O6-C1	2.31	118.75	113.80
33	d	409	CLA	C1-C2-C3	-2.31	122.41	126.20
37	7	317	SQD	O48-C23-C24	2.31	118.88	111.83
47	0	306	KC2	CHD-C4C-C3C	-2.31	118.13	125.91
39	3	316	LMG	O3-C3-C2	-2.31	104.93	110.38
33	8	313	CLA	C1C-NC-C4C	2.31	107.73	106.68
45	9	302	A86	C9-C8-C6	-2.31	120.03	126.36
41	D	408	PL9	O1-C4-C3	-2.31	118.30	120.73
47	5	310	KC2	C4D-CHA-C1A	-2.31	115.41	122.45
39	C	520	LMG	C40-C39-C38	-2.31	102.70	114.37
30	b	620	BCR	C24-C23-C22	-2.31	122.82	126.23
33	B	614	CLA	C1-C2-C3	-2.31	122.42	126.20
36	D	409	LHG	C20-C19-C18	-2.31	102.70	114.37
30	B	618	BCR	C15-C14-C13	-2.31	124.04	127.28
37	D	403	SQD	C44-O6-C1	2.31	118.74	113.80
33	d	401	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
37	7	317	SQD	O6-C1-C2	2.31	111.78	108.27
47	6	309	KC2	O1D-CGD-CBD	-2.31	119.97	124.52
33	C	508	CLA	O2D-CGD-CBD	2.30	115.26	111.23
45	0	301	A86	C40-C32-C31	-2.30	108.41	110.47
33	0	312	CLA	CHB-C4A-NA	2.30	127.72	124.40
30	b	619	BCR	C24-C23-C22	-2.30	122.83	126.23
46	8	303	DD6	C37-C36-C31	-2.30	119.86	124.16
33	c	506	CLA	CHB-C4A-NA	2.30	127.72	124.40
35	A	410	BCT	O3-C-O1	-2.30	113.79	119.68
33	W	303	CLA	CHB-C4A-NA	2.30	127.72	124.40
36	d	405	LHG	C20-C19-C18	-2.30	102.74	114.37
33	1	314	CLA	CHB-C4A-NA	2.30	127.72	124.40
37	L	101	SQD	O8-S-C6	2.30	110.41	105.97
33	3	312	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
33	7	312	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
39	5	319	LMG	C4-C3-C2	-2.30	106.80	110.83
33	1	310	CLA	C3B-C4B-NB	-2.30	108.48	110.53
44	5	315	KC1	CHB-C1B-C2B	-2.30	120.71	125.49
34	A	406	PHO	O2A-CGA-O1A	-2.30	117.89	123.63
33	0	307	CLA	CHB-C4A-NA	2.30	127.71	124.40
33	B	613	CLA	CMB-C2B-C1B	-2.29	121.92	125.42
33	C	513	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
33	0	309	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
45	4	304	A86	C26-C25-C24	-2.29	116.56	123.20
33	1	314	CLA	CAA-C2A-C3A	-2.29	110.97	116.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	7	305	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
33	C	510	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
39	c	519	LMG	C40-C39-C38	-2.29	102.79	114.37
39	C	520	LMG	O1-C1-C2	-2.29	104.79	108.27
39	5	319	LMG	O1-C7-C8	-2.29	105.25	110.82
45	4	304	A86	O1-C15-C20	-2.29	57.51	59.45
30	b	620	BCR	C33-C5-C6	-2.29	121.99	124.48
39	d	410	LMG	O7-C10-O9	-2.29	118.36	123.70
45	5	305	A86	O1-C15-C20	-2.29	57.51	59.45
46	9	303	DD6	C28-C27-C26	-2.29	119.74	124.18
33	9	310	CLA	CHB-C4A-NA	2.29	127.70	124.40
30	K	102	BCR	C15-C14-C13	-2.29	124.07	127.28
39	C	519	LMG	O2-C2-C1	-2.29	104.63	110.08
39	d	410	LMG	O2-C2-C1	-2.29	104.63	110.08
39	q	301	LMG	C38-C37-C36	-2.29	102.81	114.37
46	2	303	DD6	C28-C27-C26	-2.29	119.74	124.18
33	5	308	CLA	C3B-C4B-NB	-2.29	108.49	110.53
46	2	304	DD6	C21-C20-C15	-2.29	118.54	122.30
30	c	515	BCR	C23-C22-C21	2.28	122.60	119.01
33	C	506	CLA	CHB-C4A-NA	2.28	127.69	124.40
39	b	621	LMG	O3-C3-C2	-2.28	104.99	110.38
41	d	404	PL9	C20-C19-C21	2.28	119.19	115.23
34	a	409	PHO	O2A-CGA-O1A	-2.28	117.92	123.63
38	a	401	DGD	O2D-C2D-C1D	-2.28	104.64	110.08
46	8	303	DD6	C9-C8-C6	-2.28	120.11	126.36
33	C	502	CLA	CHB-C4A-NA	2.28	127.68	124.40
46	1	304	DD6	O1-C20-C21	-2.27	112.51	115.05
33	d	402	CLA	C3B-C4B-NB	-2.27	108.50	110.53
33	W	303	CLA	C3B-C4B-NB	-2.27	108.50	110.53
33	b	604	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
46	9	304	DD6	C21-C20-C15	-2.27	118.56	122.30
39	B	620	LMG	O3-C3-C2	-2.27	105.02	110.38
33	C	513	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
46	3	315	DD6	C28-C27-C26	-2.27	119.77	124.18
46	1	303	DD6	C9-C8-C6	-2.27	120.13	126.36
45	6	301	A86	C3-C4-C5	-2.27	118.87	123.52
45	6	306	A86	O4-C34-C33	-2.27	101.82	107.64
45	5	306	A86	C33-C32-C31	-2.27	107.00	109.21
46	9	304	DD6	C15-C14-C13	-2.27	121.19	125.99
30	D	407	BCR	C15-C16-C17	-2.27	118.88	123.52
45	2	301	A86	O4-C38-O5	-2.27	118.61	122.99
33	C	505	CLA	C1-C2-C3	-2.27	122.48	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	Q	301	LMG	O3-C3-C2	-2.27	105.03	110.38
33	A	404	CLA	C1-C2-C3	-2.27	122.48	126.20
47	6	309	KC2	CHD-C4C-C3C	-2.27	118.28	125.91
33	D	402	CLA	C1-C2-C3	-2.27	122.49	126.20
39	5	319	LMG	O3-C3-C2	-2.26	105.04	110.38
46	2	304	DD6	C15-C14-C13	-2.26	121.21	125.99
47	0	306	KC2	C4D-CHA-C1A	-2.26	115.56	122.45
47	4	307	KC2	C4D-CHA-C1A	-2.26	115.56	122.45
45	9	302	A86	O1-C15-C20	-2.26	57.53	59.45
38	3	320	DGD	CFB-CEB-CDB	-2.26	102.93	114.37
39	7	315	LMG	O2-C2-C1	-2.26	104.69	110.08
45	2	302	A86	O1-C15-C20	-2.26	57.54	59.45
37	a	413	SQD	C4-C3-C2	2.26	114.80	110.83
33	1	310	CLA	C1-C2-C3	-2.26	122.50	126.20
33	b	611	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
45	0	303	A86	C33-C32-C31	2.26	111.41	109.21
45	7	303	A86	C19-C18-C17	-2.26	106.57	110.79
33	D	405	CLA	CHB-C4A-NA	2.26	127.66	124.40
30	B	617	BCR	C15-C16-C17	-2.25	118.91	123.52
30	k	102	BCR	C11-C10-C9	-2.25	124.12	127.28
45	6	301	A86	C25-C24-C1	-2.25	120.19	126.36
33	A	408	CLA	O2D-CGD-CBD	2.25	115.17	111.23
36	D	409	LHG	C27-C26-C25	-2.25	102.99	114.37
30	k	102	BCR	C15-C14-C13	-2.25	124.12	127.28
46	1	304	DD6	C25-C26-C27	-2.25	120.32	126.61
45	6	303	A86	C25-C24-C1	-2.25	120.20	126.36
30	C	514	BCR	C33-C5-C6	-2.25	122.03	124.48
39	q	301	LMG	O2-C2-C1	-2.25	104.72	110.08
38	A	415	DGD	CBB-CAB-C9B	-2.25	103.02	114.37
39	C	520	LMG	C38-C37-C36	-2.25	103.02	114.37
30	b	618	BCR	C15-C14-C13	-2.25	124.13	127.28
33	7	311	CLA	CMB-C2B-C1B	-2.24	122.00	125.42
33	4	308	CLA	C1-C2-C3	-2.24	122.52	126.20
46	9	304	DD6	C9-C8-C6	-2.24	120.21	126.36
36	3	318	LHG	C18-C17-C16	-2.24	103.04	114.37
33	5	311	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
30	c	514	BCR	C33-C5-C6	-2.24	122.04	124.48
46	2	304	DD6	C9-C8-C6	-2.24	120.22	126.36
33	B	610	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
47	7	306	KC2	O1D-CGD-CBD	-2.24	120.10	124.52
39	5	319	LMG	O2-C2-C1	-2.24	104.74	110.08
39	q	301	LMG	O1-C7-C8	-2.24	105.38	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	3	314	A86	C40-C32-C31	-2.24	108.47	110.47
46	8	304	DD6	C3-C4-C5	-2.23	118.95	123.52
30	A	409	BCR	C24-C23-C22	-2.23	122.93	126.23
37	a	413	SQD	O8-S-C6	2.23	110.28	105.97
39	Q	301	LMG	O2-C2-C1	-2.23	104.75	110.08
33	C	502	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
33	b	609	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
36	d	405	LHG	C27-C26-C25	-2.23	103.09	114.37
33	c	510	CLA	C1-C2-C3	-2.23	122.54	126.20
44	3	310	KC1	C2D-C1D-ND	-2.23	108.01	110.33
38	a	401	DGD	C1D-C2D-C3D	-2.23	105.32	110.01
39	b	621	LMG	C1-C2-C3	-2.23	105.32	110.01
36	h	103	LHG	C18-C17-C16	-2.23	103.09	114.37
33	7	307	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
39	d	406	LMG	O3-C3-C2	-2.23	105.12	110.38
45	4	304	A86	C-C1-C24	2.23	121.50	118.09
45	4	302	A86	C3-C4-C5	-2.23	118.96	123.52
39	C	522	LMG	O3-C3-C2	-2.23	105.12	110.38
36	h	103	LHG	C27-C26-C25	-2.23	103.11	114.37
45	6	306	A86	C25-C24-C1	-2.23	120.26	126.36
39	b	621	LMG	O2-C2-C1	-2.23	104.77	110.08
41	d	404	PL9	O1-C4-C3	-2.23	118.38	120.73
38	c	517	DGD	CBB-CAB-C9B	-2.23	103.12	114.37
30	A	409	BCR	C33-C5-C6	-2.23	122.06	124.48
46	4	303	DD6	C21-C20-C15	-2.22	118.64	122.30
38	A	415	DGD	C1D-C2D-C3D	-2.22	105.33	110.01
33	7	314	CLA	CMB-C2B-C1B	-2.22	122.03	125.42
33	3	313	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
30	K	101	BCR	C33-C5-C6	-2.22	122.06	124.48
45	4	304	A86	C-C1-C2	-2.22	119.22	122.82
30	B	617	BCR	C11-C10-C9	-2.22	124.16	127.28
33	0	305	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
39	d	406	LMG	O1-C7-C8	-2.22	105.42	110.82
45	1	301	A86	O4-C38-O5	-2.22	118.70	122.99
39	C	521	LMG	O3-C3-C2	-2.22	105.14	110.38
33	9	310	CLA	C1-C2-C3	-2.22	122.56	126.20
45	5	301	A86	C9-C10-C11	-2.22	120.37	126.64
45	0	303	A86	C9-C10-C11	-2.22	120.37	126.64
39	W	301	LMG	O2-C2-C1	-2.22	104.80	110.08
45	4	301	A86	C25-C24-C1	-2.21	120.29	126.36
46	9	303	DD6	C37-C36-C31	-2.21	120.02	124.16
33	B	606	CLA	CMB-C2B-C1B	-2.21	122.05	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	7	307	CLA	CMB-C2B-C3B	2.21	131.76	126.55
33	c	505	CLA	C3B-C4B-NB	-2.21	108.55	110.53
45	0	301	A86	C7-C6-C5	-2.21	119.23	122.82
33	c	502	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
33	2	310	CLA	CMB-C2B-C3B	2.21	131.75	126.55
33	0	310	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
39	c	520	LMG	O2-C2-C1	-2.21	104.81	110.08
39	q	302	LMG	O3-C3-C2	-2.21	105.17	110.38
39	q	302	LMG	O2-C2-C1	-2.21	104.81	110.08
33	w	303	CLA	CHB-C4A-NA	2.21	127.59	124.40
33	B	603	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
33	D	406	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
33	5	309	CLA	C1-C2-C3	-2.21	122.58	126.20
41	d	404	PL9	C37-C38-C39	-2.20	122.58	127.62
39	B	621	LMG	O2-C2-C1	-2.20	104.82	110.08
46	1	304	DD6	C10-C9-C8	-2.20	116.81	123.20
36	4	318	LHG	C27-C26-C25	-2.20	103.23	114.37
39	D	410	LMG	O2-C2-C1	-2.20	104.83	110.08
33	B	605	CLA	CHB-C4A-NA	2.20	127.58	124.40
42	v	201	HEM	C3D-C4D-ND	-2.20	107.76	110.17
39	b	622	LMG	O2-C2-C1	-2.20	104.83	110.08
33	d	401	CLA	CHB-C4A-NA	2.20	127.58	124.40
33	4	314	CLA	CHB-C4A-NA	2.20	127.58	124.40
36	b	601	LHG	C18-C17-C16	-2.20	103.24	114.37
33	D	405	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
39	m	201	LMG	O3-C3-C2	-2.20	105.19	110.38
39	q	302	LMG	O1-C1-C2	-2.20	104.93	108.27
33	B	603	CLA	CHB-C4A-NA	2.20	127.57	124.40
36	4	318	LHG	C18-C17-C16	-2.20	103.25	114.37
42	F	101	HEM	C4D-ND-C1D	2.20	107.81	105.21
30	A	409	BCR	C7-C8-C9	-2.20	122.98	126.23
33	3	308	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
46	2	303	DD6	C37-C36-C31	-2.20	120.05	124.16
45	6	305	A86	O1-C15-C20	-2.20	57.59	59.45
36	a	403	LHG	C27-C26-C25	-2.20	103.26	114.37
45	5	303	A86	C19-C18-C17	-2.20	106.68	110.79
37	A	413	SQD	C4-C3-C2	2.20	114.69	110.83
45	8	301	A86	C9-C10-C11	-2.20	120.43	126.64
39	q	302	LMG	O1-C7-C8	-2.20	105.48	110.82
41	D	408	PL9	C20-C19-C21	2.20	119.04	115.23
38	3	320	DGD	CBB-CAB-C9B	-2.20	103.27	114.37
33	1	306	CLA	CMB-C2B-C1B	-2.20	122.08	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	d	410	LMG	O3-C3-C2	-2.20	105.20	110.38
42	V	201	HEM	C1C-CHC-C4B	-2.20	121.35	126.02
33	5	311	CLA	C3B-C4B-NB	-2.19	108.57	110.53
39	7	315	LMG	O3-C3-C2	-2.19	105.20	110.38
30	c	514	BCR	C7-C8-C9	-2.19	122.99	126.23
36	w	301	LHG	C27-C26-C25	-2.19	103.28	114.37
38	H	102	DGD	C1D-C2D-C3D	-2.19	105.40	110.01
33	8	308	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
30	d	403	BCR	C33-C5-C6	-2.19	122.09	124.48
33	4	311	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
45	7	301	A86	C7-C6-C5	-2.19	119.26	122.82
45	8	301	A86	C12-C11-C13	2.19	119.55	116.00
30	K	101	BCR	C11-C10-C9	-2.19	124.20	127.28
45	0	303	A86	C26-C25-C24	-2.19	116.85	123.20
33	4	306	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
39	w	304	LMG	O3-C3-C2	-2.19	105.21	110.38
38	C	516	DGD	O5D-C6D-C5D	-2.19	104.48	109.42
37	A	413	SQD	C3-C4-C5	2.19	114.20	110.23
38	c	516	DGD	C1D-C2D-C3D	-2.19	105.40	110.01
33	0	311	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
33	C	509	CLA	C1-C2-C3	-2.19	122.61	126.20
33	C	507	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
36	D	411	LHG	C27-C26-C25	-2.19	103.30	114.37
37	7	317	SQD	C44-O6-C1	2.19	118.49	113.80
39	D	404	LMG	O7-C10-O9	-2.19	118.59	123.70
45	9	301	A86	C7-C6-C5	-2.19	119.27	122.82
30	B	617	BCR	C15-C14-C13	-2.19	124.21	127.28
33	B	604	CLA	C3B-C4B-NB	-2.19	108.58	110.53
33	9	310	CLA	CMB-C2B-C1B	-2.19	122.09	125.42
33	B	608	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
36	b	601	LHG	C27-C26-C25	-2.19	103.32	114.37
38	a	401	DGD	CBB-CAB-C9B	-2.19	103.32	114.37
39	c	520	LMG	O3-C3-C2	-2.18	105.23	110.38
43	4	317	LMU	O5'-C5'-C6'	2.18	111.85	106.44
39	7	315	LMG	C42-C41-C40	-2.18	103.33	114.37
39	M	201	LMG	O1-C7-C8	-2.18	105.51	110.82
33	w	303	CLA	C1-C2-C3	-2.18	122.62	126.20
33	b	606	CLA	CHB-C4A-NA	2.18	127.55	124.40
33	1	311	CLA	C1-C2-C3	-2.18	122.62	126.20
46	4	303	DD6	C28-C27-C26	-2.18	119.94	124.18
41	D	408	PL9	O2-C1-C6	2.18	123.95	120.48
39	C	522	LMG	O1-C1-C2	-2.18	104.96	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	1	308	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
33	9	313	CLA	C1C-NC-C4C	2.18	107.67	106.68
38	c	516	DGD	O5D-C6D-C5D	-2.18	104.50	109.42
33	b	604	CLA	CHB-C4A-NA	2.18	127.55	124.40
36	d	405	LHG	C18-C17-C16	-2.18	103.35	114.37
37	7	317	SQD	C4-C3-C2	2.18	114.66	110.83
33	c	509	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
38	h	102	DGD	CBB-CAB-C9B	-2.18	103.36	114.37
33	2	317	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
33	4	315	CLA	O2D-CGD-CBD	2.18	115.03	111.23
38	c	517	DGD	O3E-C3E-C2E	-2.18	105.25	110.38
45	2	301	A86	O1-C15-C20	-2.18	57.61	59.45
33	7	313	CLA	CMB-C2B-C3B	2.18	129.84	124.63
47	6	309	KC2	C1B-CHB-C4A	-2.17	121.40	126.02
38	C	516	DGD	O2D-C2D-C1D	-2.17	104.89	110.08
37	B	622	SQD	O8-S-C6	2.17	110.17	105.97
33	5	314	CLA	CHB-C4A-NA	2.17	127.54	124.40
45	5	305	A86	C9-C8-C6	-2.17	120.40	126.36
37	0	316	SQD	O48-C23-C24	2.17	118.46	111.83
38	H	102	DGD	CBB-CAB-C9B	-2.17	103.38	114.37
33	0	308	CLA	CMA-C3A-C2A	-2.17	111.25	116.23
33	c	511	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
36	5	318	LHG	C18-C17-C16	-2.17	103.38	114.37
38	h	102	DGD	O3E-C3E-C2E	-2.17	105.25	110.38
39	C	520	LMG	O3-C3-C2	-2.17	105.25	110.38
33	7	309	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
33	b	613	CLA	C1-C2-C3	-2.17	122.64	126.20
33	C	509	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
45	6	302	A86	C23-C16-C17	2.17	112.78	108.97
33	w	303	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
33	c	508	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
39	m	201	LMG	O1-C7-C8	-2.17	105.54	110.82
33	a	411	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
33	B	609	CLA	CHB-C4A-NA	2.17	127.53	124.40
39	b	623	LMG	O1-C7-C8	-2.17	105.54	110.82
33	9	311	CLA	C1-C2-C3	-2.17	122.64	126.20
33	A	405	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
45	5	306	A86	O1-C15-C20	-2.17	57.61	59.45
33	3	305	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
36	H	104	LHG	C27-C26-C25	-2.17	103.41	114.37
30	b	618	BCR	C15-C16-C17	-2.17	119.09	123.52
46	1	304	DD6	C37-C36-C31	-2.17	120.11	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	C	517	DGD	O3E-C3E-C2E	-2.17	105.27	110.38
33	c	506	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
33	b	603	CLA	CHC-C4B-NB	2.17	127.30	124.05
33	1	308	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
33	B	614	CLA	CMB-C2B-C1B	-2.16	122.12	125.42
46	3	315	DD6	C37-C36-C31	-2.16	120.11	124.16
45	5	303	A86	O4-C34-C33	-2.16	102.10	107.64
42	v	201	HEM	CAA-C2A-C1A	2.16	129.16	124.94
45	6	303	A86	C10-C9-C8	-2.16	116.94	123.20
45	5	306	A86	C3-C4-C5	-2.16	119.09	123.52
45	6	301	A86	O1-C15-C20	-2.16	57.62	59.45
33	B	615	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
36	W	302	LHG	C27-C26-C25	-2.16	103.45	114.37
36	7	316	LHG	C27-C26-C25	-2.16	103.45	114.37
33	c	513	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
33	2	310	CLA	CHB-C4A-NA	2.16	127.52	124.40
33	B	605	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
33	B	612	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
38	C	518	DGD	CAB-C9B-C8B	-2.16	103.45	114.37
33	2	308	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
38	a	401	DGD	C3D-C4D-C5D	-2.16	106.32	110.23
45	5	304	A86	O4-C34-C33	-2.16	102.11	107.64
38	c	517	DGD	CAB-C9B-C8B	-2.16	103.46	114.37
33	6	307	CLA	CAC-C3C-C4C	2.16	127.60	124.79
42	V	201	HEM	CHD-C1D-C2D	-2.16	121.62	125.03
39	c	519	LMG	O3-C3-C2	-2.16	105.29	110.38
44	3	310	KC1	C2A-C3A-C4A	2.16	108.03	106.41
38	h	102	DGD	C7B-C6B-C5B	-2.16	103.47	114.37
45	3	314	A86	C-C1-C24	2.15	121.38	118.09
38	c	516	DGD	O2D-C2D-C1D	-2.15	104.94	110.08
33	B	605	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
42	V	201	HEM	C4A-CHB-C1B	-2.15	121.18	126.25
39	C	522	LMG	O2-C2-C1	-2.15	104.94	110.08
33	4	308	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
45	3	314	A86	O1-C20-C19	-2.15	111.47	113.49
33	2	310	CLA	C3B-C4B-NB	-2.15	108.61	110.53
36	A	414	LHG	C27-C26-C25	-2.15	103.48	114.37
30	B	617	BCR	C7-C8-C9	-2.15	123.05	126.23
33	4	305	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
36	A	414	LHG	C18-C17-C16	-2.15	103.49	114.37
33	W	303	CLA	CAA-C2A-C1A	-2.15	104.92	111.97
45	6	304	A86	O1-C15-C20	-2.15	57.63	59.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	d	407	LHG	C27-C26-C25	-2.15	103.49	114.37
36	0	315	LHG	C27-C26-C25	-2.15	103.50	114.37
38	A	415	DGD	C3D-C4D-C5D	-2.15	106.33	110.23
38	c	517	DGD	C3D-C4D-C5D	-2.15	106.33	110.23
36	A	411	LHG	C27-C26-C25	-2.15	103.50	114.37
30	C	514	BCR	C2-C1-C6	2.15	113.56	110.44
33	B	611	CLA	CHB-C4A-NA	2.15	127.50	124.40
45	9	301	A86	O1-C15-C20	-2.15	57.63	59.45
38	a	401	DGD	C1E-O6E-C5E	2.15	116.36	113.05
33	9	307	CLA	C2A-C1A-CHA	2.15	127.59	123.87
33	D	405	CLA	C3B-C4B-NB	-2.15	108.10	110.33
42	V	201	HEM	C4C-NC-C1C	2.15	109.32	105.82
36	H	104	LHG	C18-C17-C16	-2.15	103.52	114.37
39	3	316	LMG	O2-C2-C1	-2.15	104.96	110.08
38	C	518	DGD	O3D-C3D-C4D	-2.15	105.32	110.38
39	D	404	LMG	O8-C28-O10	-2.15	118.26	123.63
38	C	517	DGD	C5B-C4B-C3B	-2.15	103.53	114.37
36	A	412	LHG	C27-C26-C25	-2.14	103.53	114.37
33	a	408	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
33	c	509	CLA	C1-C2-C3	-2.14	122.68	126.20
42	e	101	HEM	CHA-C1A-NA	2.14	127.75	123.86
38	h	102	DGD	C1D-C2D-C3D	-2.14	105.50	110.01
33	0	311	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
33	A	408	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
34	A	407	PHO	O2A-CGA-O1A	-2.14	118.27	123.63
39	w	304	LMG	O2-C2-C1	-2.14	104.97	110.08
33	3	307	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
41	D	408	PL9	C12-C13-C14	-2.14	122.72	127.62
33	4	314	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
39	c	520	LMG	O1-C1-C2	-2.14	105.02	108.27
33	1	311	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
33	2	313	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
33	2	306	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
41	d	404	PL9	O2-C1-C6	2.14	123.88	120.48
44	6	314	KC1	C2A-C3A-C4A	2.14	108.02	106.41
34	a	410	PHO	O2A-CGA-O1A	-2.14	118.28	123.63
39	c	520	LMG	O1-C7-C8	-2.14	105.62	110.82
45	2	301	A86	C7-C6-C5	-2.14	119.35	122.82
45	8	301	A86	O1-C15-C20	-2.14	57.64	59.45
45	2	302	A86	C26-C25-C24	-2.14	117.01	123.20
33	b	605	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
30	D	407	BCR	C7-C8-C9	-2.14	123.08	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	0	312	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
38	C	517	DGD	CBB-CAB-C9B	-2.13	103.58	114.37
39	C	521	LMG	O2-C2-C1	-2.13	104.99	110.08
33	B	603	CLA	O2D-CGD-CBD	2.13	114.96	111.23
36	a	404	LHG	C27-C26-C25	-2.13	103.59	114.37
46	4	303	DD6	C12-C11-C10	-2.13	119.36	122.82
33	C	508	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
38	C	516	DGD	C5B-C4B-C3B	-2.13	103.60	114.37
38	c	518	DGD	CAB-C9B-C8B	-2.13	103.60	114.37
45	9	302	A86	C26-C25-C24	-2.13	117.03	123.20
33	8	311	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
33	b	610	CLA	CMB-C2B-C3B	2.13	131.56	126.55
38	H	102	DGD	O2D-C2D-C1D	-2.13	105.00	110.08
45	0	301	A86	O1-C15-C20	-2.13	57.65	59.45
33	7	305	CLA	CAC-C3C-C4C	2.13	127.56	124.79
33	B	609	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
33	6	316	CLA	CMB-C2B-C3B	2.13	129.73	124.63
33	A	404	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
38	c	516	DGD	C4E-C3E-C2E	-2.13	107.10	110.83
45	8	301	A86	C25-C24-C1	-2.13	120.53	126.36
38	C	518	DGD	O2D-C2D-C1D	-2.13	105.01	110.08
46	8	304	DD6	C8-C6-C5	2.13	122.35	119.01
33	0	313	CLA	CMB-C2B-C3B	2.12	129.72	124.63
38	c	518	DGD	O2D-C2D-C1D	-2.12	105.02	110.08
45	7	303	A86	O4-C38-O5	-2.12	118.89	122.99
38	C	518	DGD	O3E-C3E-C2E	-2.12	105.37	110.38
39	b	622	LMG	O1-C1-C2	-2.12	105.05	108.27
33	w	303	CLA	C3B-C4B-NB	-2.12	108.64	110.53
43	5	320	LMU	C1B-O1B-C4'	-2.12	112.95	117.98
36	D	409	LHG	C18-C17-C16	-2.12	103.64	114.37
46	1	304	DD6	C26-C25-C24	-2.12	117.05	123.20
33	2	309	CLA	C1C-NC-C4C	2.12	107.65	106.68
37	l	101	SQD	C1-O5-C5	2.12	117.86	113.72
39	M	201	LMG	O7-C10-O9	-2.12	118.75	123.70
33	C	510	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
39	3	316	LMG	O1-C7-C8	-2.12	105.67	110.82
33	3	303	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
38	C	518	DGD	CBB-CAB-C9B	-2.12	103.67	114.37
36	d	407	LHG	C18-C17-C16	-2.12	103.67	114.37
45	6	303	A86	O4-C38-O5	-2.12	118.91	122.99
33	3	306	CLA	C1-C2-C3	-2.11	122.73	126.20
33	C	501	CLA	O2A-CGA-O1A	-2.11	118.34	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	9	303	DD6	C4-C3-C2	-2.11	119.19	123.52
33	b	610	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
33	2	307	CLA	CHB-C4A-NA	2.11	127.45	124.40
33	3	309	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
33	6	307	CLA	C1-C2-C3	-2.11	122.74	126.20
33	4	309	CLA	C1-C2-C3	-2.11	122.74	126.20
30	b	620	BCR	C28-C27-C26	-2.11	110.29	114.06
33	6	316	CLA	CHB-C4A-NA	2.11	127.44	124.40
36	a	404	LHG	C18-C17-C16	-2.11	103.70	114.37
46	3	315	DD6	C7-C6-C5	-2.11	119.40	122.82
33	c	503	CLA	O1D-CGD-CBD	2.11	128.68	124.52
30	D	407	BCR	C2-C1-C6	2.11	113.50	110.44
33	8	315	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
39	B	620	LMG	O7-C10-O9	-2.11	118.78	123.70
30	k	101	BCR	C35-C13-C14	-2.11	119.40	122.82
33	3	302	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
33	3	305	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
30	K	102	BCR	C7-C8-C9	-2.11	123.12	126.23
33	a	411	CLA	C3B-C4B-NB	-2.11	108.65	110.53
33	c	505	CLA	O2D-CGD-CBD	2.11	114.92	111.23
38	C	516	DGD	O3E-C3E-C2E	-2.11	105.41	110.38
33	Z	101	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
39	q	301	LMG	O3-C3-C2	-2.11	105.41	110.38
45	7	301	A86	O1-C15-C20	-2.10	57.67	59.45
33	9	317	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
33	6	307	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
45	4	302	A86	C25-C24-C1	-2.10	120.59	126.36
38	C	518	DGD	O6E-C1E-O5D	-2.10	105.07	110.04
33	b	605	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
33	3	302	CLA	C1-C2-C3	-2.10	122.75	126.20
39	C	519	LMG	O1-C1-C2	-2.10	105.08	108.27
41	d	404	PL9	C12-C13-C14	-2.10	122.81	127.62
38	c	516	DGD	O3E-C3E-C2E	-2.10	105.42	110.38
33	C	513	CLA	O2D-CGD-CBD	2.10	114.90	111.23
33	d	402	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
47	5	310	KC2	CHD-C1D-C2D	-2.10	121.33	127.43
30	B	619	BCR	C15-C14-C13	-2.10	124.33	127.28
37	T	103	SQD	O47-C7-O49	-2.10	118.79	123.70
44	3	310	KC1	O2D-CGD-O1D	-2.10	119.76	123.85
39	Q	301	LMG	O1-C7-C8	-2.10	105.71	110.82
45	5	303	A86	C3-C4-C5	-2.10	119.22	123.52
44	6	314	KC1	O2D-CGD-O1D	-2.10	119.76	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	1	301	A86	C3-C4-C5	-2.10	119.22	123.52
33	6	313	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
45	6	302	A86	C25-C24-C1	-2.10	120.61	126.36
39	b	623	LMG	O3-C3-C2	-2.10	105.43	110.38
45	5	305	A86	C9-C10-C11	-2.10	120.71	126.64
33	c	512	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
33	7	310	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
33	B	602	CLA	CMB-C2B-C3B	2.10	131.48	126.55
45	5	304	A86	O1-C15-C20	-2.10	57.67	59.45
39	b	623	LMG	O2-C2-C1	-2.10	105.08	110.08
33	C	503	CLA	O1D-CGD-CBD	2.10	128.65	124.52
33	d	401	CLA	O2D-CGD-CBD	2.09	114.89	111.23
33	b	613	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
38	A	415	DGD	O3D-C3D-C4D	-2.09	105.44	110.38
37	7	317	SQD	O8-S-C6	2.09	110.01	105.97
38	c	518	DGD	CBB-CAB-C9B	-2.09	103.79	114.37
33	W	303	CLA	C1-C2-C3	-2.09	122.77	126.20
46	1	303	DD6	O1-C20-C19	-2.09	111.53	113.49
39	w	304	LMG	O1-C7-C8	-2.09	105.74	110.82
33	d	409	CLA	CMB-C2B-C3B	2.09	131.46	126.55
36	w	301	LHG	C5-O7-C7	-2.09	112.80	117.80
45	4	301	A86	C35-C34-C33	2.09	113.64	109.89
33	B	611	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
33	1	308	CLA	C1-C2-C3	-2.09	122.78	126.20
36	A	412	LHG	C18-C17-C16	-2.09	103.82	114.37
33	B	612	CLA	O1D-CGD-CBD	2.09	128.63	124.52
38	3	320	DGD	CAB-C9B-C8B	-2.09	103.82	114.37
38	3	320	DGD	C1G-C2G-C3G	-2.09	106.98	111.80
46	3	315	DD6	C-C1-C2	-2.09	119.44	122.82
33	5	314	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
47	5	310	KC2	O1D-CGD-CBD	-2.09	120.41	124.52
33	b	606	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
38	c	517	DGD	O2D-C2D-C1D	-2.08	105.11	110.08
38	h	102	DGD	O2D-C2D-C1D	-2.08	105.11	110.08
33	4	316	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
33	W	303	CLA	O2D-CGD-CBD	2.08	114.87	111.23
38	C	517	DGD	C3D-C4D-C5D	-2.08	106.46	110.23
38	a	401	DGD	O3D-C3D-C4D	-2.08	105.47	110.38
33	C	505	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
33	4	314	CLA	CMB-C2B-C3B	2.08	131.44	126.55
45	5	302	A86	O1-C15-C20	-2.08	57.69	59.45
46	3	315	DD6	C32-C33-C34	-2.08	109.03	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	8	307	CLA	C3B-C4B-NB	-2.08	108.17	110.33
33	5	313	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
39	0	314	LMG	O1-C7-C8	-2.08	105.76	110.82
33	b	603	CLA	CMB-C2B-C3B	2.08	131.44	126.55
45	4	301	A86	O1-C15-C20	-2.08	57.69	59.45
33	6	308	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
30	a	412	BCR	C24-C23-C22	-2.08	123.16	126.23
38	H	102	DGD	CAB-C9B-C8B	-2.08	103.88	114.37
33	C	513	CLA	CMB-C2B-C3B	2.08	131.43	126.55
48	0	302	ET4	C20-C21-C22	2.07	132.42	126.61
33	B	606	CLA	CHB-C1B-NB	2.07	127.16	124.05
33	4	312	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
37	0	316	SQD	C44-O6-C1	2.07	118.24	113.80
33	8	308	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
46	2	303	DD6	C4-C3-C2	-2.07	119.28	123.52
38	C	517	DGD	CAB-C9B-C8B	-2.07	103.89	114.37
45	6	303	A86	O1-C15-C20	-2.07	57.69	59.45
33	b	603	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
33	1	309	CLA	C1C-NC-C4C	2.07	107.62	106.68
45	5	307	A86	O1-C15-C20	-2.07	57.70	59.45
45	3	314	A86	C7-C6-C5	-2.07	119.46	122.82
33	B	604	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
33	8	306	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
33	5	313	CLA	CMB-C2B-C3B	2.07	131.42	126.55
30	C	514	BCR	C7-C8-C9	-2.07	123.17	126.23
39	W	301	LMG	C1-C2-C3	-2.07	105.66	110.01
33	c	511	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
39	C	521	LMG	O1-C1-C2	-2.07	105.13	108.27
33	0	304	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
33	8	311	CLA	C1-C2-C3	-2.07	122.81	126.20
37	t	102	SQD	O47-C7-O49	-2.07	119.00	122.99
33	c	510	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
33	3	306	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
33	0	307	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
45	5	304	A86	C12-C11-C13	2.07	119.35	116.00
38	c	518	DGD	O6E-C1E-O5D	-2.07	105.16	110.04
38	c	516	DGD	C5B-C4B-C3B	-2.06	103.93	114.37
33	D	405	CLA	O2D-CGD-CBD	2.06	114.84	111.23
33	c	511	CLA	C1-C2-C3	-2.06	122.82	126.20
30	A	401	BCR	C11-C10-C9	-2.06	124.39	127.28
38	H	102	DGD	C3D-C4D-C5D	-2.06	106.49	110.23
33	B	611	CLA	O2D-CGD-CBD	2.06	114.83	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	4	304	A86	C3-C4-C5	-2.06	119.30	123.52
33	b	617	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
48	7	302	ET4	C11-C10-C09	-2.06	124.39	127.28
33	D	402	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
45	7	301	A86	C10-C9-C8	-2.06	117.23	123.20
37	T	101	SQD	O47-C7-O49	-2.06	119.02	122.99
30	C	515	BCR	C33-C5-C4	2.06	117.98	113.60
33	B	613	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
33	0	305	CLA	O2D-CGD-CBD	2.06	114.83	111.23
45	5	303	A86	O1-C15-C20	-2.06	57.71	59.45
39	m	201	LMG	O7-C10-O9	-2.06	118.90	123.70
38	H	102	DGD	O3E-C3E-C2E	-2.06	105.53	110.38
45	0	301	A86	C41-C32-C31	-2.06	108.63	110.47
38	c	517	DGD	O3G-C1D-C2D	-2.06	105.15	108.27
38	A	415	DGD	C5B-C4B-C3B	-2.06	103.98	114.37
38	c	516	DGD	CBB-CAB-C9B	-2.05	103.98	114.37
45	4	302	A86	O1-C15-C20	-2.05	57.71	59.45
33	C	511	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
33	3	309	CLA	C1-C2-C3	-2.05	122.83	126.20
33	C	505	CLA	O2D-CGD-CBD	2.05	114.82	111.23
45	6	304	A86	C3-C4-C5	-2.05	119.32	123.52
46	8	303	DD6	O1-C15-C14	-2.05	110.99	116.88
46	1	303	DD6	O1-C15-C14	-2.05	110.99	116.88
45	5	301	A86	C3-C4-C5	-2.05	119.32	123.52
30	d	403	BCR	C7-C8-C9	-2.05	123.20	126.23
33	b	615	CLA	O2D-CGD-CBD	2.05	114.82	111.23
33	b	602	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
38	a	401	DGD	C5B-C4B-C3B	-2.05	104.00	114.37
46	3	315	DD6	C9-C8-C6	-2.05	120.74	126.36
30	K	102	BCR	C11-C10-C9	-2.05	124.40	127.28
33	c	513	CLA	CMB-C2B-C3B	2.05	131.37	126.55
38	a	401	DGD	CAB-C9B-C8B	-2.05	104.02	114.37
39	b	621	LMG	O7-C10-O9	-2.05	118.92	123.70
33	b	616	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
30	D	407	BCR	C33-C5-C6	-2.05	122.25	124.48
42	F	101	HEM	C3D-C4D-ND	-2.05	107.93	110.17
33	C	509	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
33	B	602	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
33	9	308	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
30	D	407	BCR	C11-C10-C9	-2.05	124.41	127.28
33	C	501	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
33	d	402	CLA	O2A-CGA-O1A	-2.05	118.51	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	5	309	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
45	5	307	A86	C21-C20-C15	-2.04	116.75	123.35
36	3	317	LHG	C5-O7-C7	-2.04	112.90	117.80
30	A	401	BCR	C7-C8-C9	-2.04	123.21	126.23
37	T	103	SQD	O5-C1-C2	2.04	114.57	110.37
33	7	309	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
45	0	301	A86	C10-C9-C8	-2.04	117.28	123.20
33	9	311	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
33	4	310	CLA	CMB-C2B-C3B	2.04	131.35	126.55
41	D	408	PL9	O2-C1-C2	-2.04	117.19	121.83
36	3	318	LHG	C27-C26-C25	-2.04	104.05	114.37
42	e	101	HEM	C4C-CHD-C1D	-2.04	121.68	126.02
33	c	510	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
33	7	311	CLA	CMB-C2B-C3B	2.04	131.35	126.55
33	B	616	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
33	6	308	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
44	3	310	KC1	O1D-CGD-CBD	-2.04	120.50	124.52
39	c	519	LMG	O1-C7-C8	-2.04	105.86	110.82
39	C	521	LMG	O1-C7-C8	-2.04	105.86	110.82
33	B	613	CLA	CMB-C2B-C3B	2.04	131.34	126.55
33	4	315	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
33	W	303	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
33	C	509	CLA	O2D-CGD-CBD	2.04	114.79	111.23
33	c	505	CLA	CHB-C4A-NA	2.04	127.34	124.40
45	5	304	A86	C9-C10-C11	-2.03	120.89	126.64
45	7	303	A86	C3-C4-C5	-2.03	119.36	123.52
36	W	302	LHG	C5-O7-C7	-2.03	112.93	117.80
33	c	509	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
33	4	309	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
45	7	301	A86	C41-C32-C31	-2.03	108.65	110.47
33	D	406	CLA	C1-C2-C3	-2.03	122.87	126.20
46	8	304	DD6	C3-C2-C1	-2.03	124.43	127.28
33	B	609	CLA	C1-C2-C3	-2.03	122.87	126.20
33	c	503	CLA	C1-C2-C3	-2.03	122.87	126.20
45	6	305	A86	C3-C4-C5	-2.03	119.37	123.52
33	c	503	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
38	c	517	DGD	C8B-C7B-C6B	-2.03	104.11	114.37
33	c	504	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
30	k	102	BCR	C7-C8-C9	-2.03	123.23	126.23
33	2	310	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
38	C	516	DGD	CBB-CAB-C9B	-2.03	104.12	114.37
33	D	406	CLA	O2D-CGD-CBD	2.03	114.77	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	0	307	CLA	CAA-C2A-C3A	-2.03	107.53	113.00
33	C	512	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
37	i	101	SQD	C1-O5-C5	2.03	117.67	113.72
45	8	301	A86	C9-C8-C6	-2.03	120.81	126.36
33	D	406	CLA	CMB-C2B-C3B	2.02	131.31	126.55
37	T	101	SQD	O8-S-C6	2.02	109.88	105.97
33	C	504	CLA	CMB-C2B-C3B	2.02	131.31	126.55
33	d	409	CLA	O2D-CGD-CBD	2.02	114.76	111.23
33	D	402	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
33	6	310	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
46	8	303	DD6	O1-C20-C19	-2.02	111.60	113.49
33	c	501	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
33	B	601	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
30	b	619	BCR	C11-C10-C9	-2.02	124.44	127.28
33	2	308	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
39	c	519	LMG	O2-C2-C1	-2.02	105.26	110.08
33	c	501	CLA	O1D-CGD-CBD	2.02	128.50	124.52
30	c	515	BCR	C20-C19-C18	-2.02	120.83	126.36
33	b	617	CLA	C1-C2-C3	-2.02	122.89	126.20
33	B	606	CLA	O1D-CGD-CBD	2.02	128.50	124.52
33	7	310	CLA	O2A-CGA-O1A	-2.02	118.14	123.33
39	B	621	LMG	O1-C1-C2	-2.02	105.21	108.27
33	b	613	CLA	O1D-CGD-CBD	2.02	128.50	124.52
33	3	304	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
45	5	305	A86	C28-C27-C26	-2.02	119.55	122.82
33	b	613	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
42	v	201	HEM	C1B-NB-C4B	2.01	107.59	105.21
45	4	304	A86	C9-C10-C11	-2.01	120.94	126.64
33	d	409	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
45	6	301	A86	C10-C9-C8	-2.01	117.37	123.20
33	5	314	CLA	C1-C2-C3	-2.01	122.90	126.20
30	d	403	BCR	C2-C1-C6	2.01	113.36	110.44
33	B	607	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
38	C	516	DGD	CAB-C9B-C8B	-2.01	104.20	114.37
30	c	514	BCR	C2-C1-C6	2.01	113.36	110.44
45	2	302	A86	C25-C24-C1	-2.01	120.85	126.36
38	c	518	DGD	O3E-C3E-C2E	-2.01	105.64	110.38
33	C	506	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
38	A	415	DGD	CAB-C9B-C8B	-2.01	104.21	114.37
36	a	403	LHG	C5-O7-C7	-2.01	112.99	117.80
33	b	608	CLA	CMB-C2B-C3B	2.01	131.28	126.55
41	d	404	PL9	O2-C1-C2	-2.01	117.26	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	412	BCR	C7-C8-C9	-2.01	123.27	126.23
33	2	305	CLA	O2D-CGD-CBD	2.01	114.74	111.23
45	6	302	A86	C12-C11-C13	2.01	119.25	116.00
33	c	504	CLA	C1-C2-C3	-2.01	122.91	126.20
39	b	622	LMG	C6-C5-C4	-2.01	108.10	113.02
33	9	310	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
33	8	306	CLA	O2A-CGA-O1A	-2.00	118.18	123.33
33	9	308	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
33	6	311	CLA	C3A-C2A-C1A	2.00	104.34	101.34
33	1	313	CLA	C1C-NC-C4C	2.00	107.59	106.68
45	9	302	A86	C25-C24-C1	-2.00	120.87	126.36
33	b	603	CLA	CHB-C1B-NB	2.00	127.05	124.05
33	c	507	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
33	3	319	CLA	O2A-CGA-O1A	-2.00	118.62	123.63

All (182) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	A	404	CLA	ND
33	A	405	CLA	ND
33	A	408	CLA	ND
33	B	601	CLA	ND
33	B	602	CLA	ND
33	B	603	CLA	ND
33	B	604	CLA	ND
33	B	605	CLA	ND
33	B	606	CLA	ND
33	B	607	CLA	ND
33	B	608	CLA	ND
33	B	609	CLA	ND
33	B	610	CLA	ND
33	B	611	CLA	ND
33	B	612	CLA	ND
33	B	613	CLA	ND
33	B	614	CLA	ND
33	B	615	CLA	ND
33	B	616	CLA	ND
33	C	501	CLA	ND
33	C	502	CLA	ND
33	C	503	CLA	ND
33	C	504	CLA	ND
33	C	505	CLA	ND

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Mol	Chain	Res	Type	Atom
33	C	506	CLA	ND
33	C	507	CLA	ND
33	C	508	CLA	ND
33	C	509	CLA	ND
33	C	510	CLA	ND
33	C	511	CLA	ND
33	C	512	CLA	ND
33	C	513	CLA	ND
33	c	501	CLA	ND
33	c	502	CLA	ND
33	c	503	CLA	ND
33	c	504	CLA	ND
33	c	505	CLA	ND
33	c	506	CLA	ND
33	c	507	CLA	ND
33	c	508	CLA	ND
33	c	509	CLA	ND
33	c	510	CLA	ND
33	c	511	CLA	ND
33	c	512	CLA	ND
33	c	513	CLA	ND
33	D	402	CLA	ND
33	D	405	CLA	ND
33	D	406	CLA	ND
33	d	401	CLA	ND
33	d	402	CLA	ND
33	d	409	CLA	ND
33	H	103	CLA	ND
33	W	303	CLA	ND
33	w	303	CLA	ND
33	Z	101	CLA	ND
33	z	101	CLA	ND
33	3	302	CLA	ND
33	3	303	CLA	ND
33	3	304	CLA	ND
33	3	305	CLA	ND
33	3	306	CLA	ND
33	3	307	CLA	ND
33	3	308	CLA	ND
33	3	309	CLA	ND
33	3	311	CLA	ND
33	3	312	CLA	ND

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Mol	Chain	Res	Type	Atom
33	3	313	CLA	ND
33	3	319	CLA	ND
33	4	305	CLA	ND
33	4	306	CLA	ND
33	4	308	CLA	ND
33	4	309	CLA	ND
33	4	310	CLA	ND
33	4	311	CLA	ND
33	4	312	CLA	ND
33	4	313	CLA	ND
33	4	314	CLA	ND
33	4	315	CLA	ND
33	4	316	CLA	ND
33	5	308	CLA	ND
33	5	309	CLA	ND
33	5	311	CLA	ND
33	5	312	CLA	ND
33	5	313	CLA	ND
33	5	314	CLA	ND
33	5	316	CLA	ND
33	5	317	CLA	ND
33	6	307	CLA	ND
33	6	308	CLA	ND
33	6	310	CLA	ND
33	6	311	CLA	ND
33	6	312	CLA	ND
33	6	313	CLA	ND
33	6	315	CLA	ND
33	6	316	CLA	ND
33	7	304	CLA	ND
33	7	305	CLA	ND
33	7	307	CLA	ND
33	7	308	CLA	ND
33	7	309	CLA	ND
33	7	310	CLA	ND
33	7	311	CLA	ND
33	7	312	CLA	ND
33	7	313	CLA	ND
33	7	314	CLA	ND
33	a	407	CLA	ND
33	a	408	CLA	ND
33	a	411	CLA	ND

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Mol	Chain	Res	Type	Atom
33	b	602	CLA	ND
33	b	603	CLA	ND
33	b	604	CLA	ND
33	b	605	CLA	ND
33	b	606	CLA	ND
33	b	607	CLA	ND
33	b	608	CLA	ND
33	b	609	CLA	ND
33	b	610	CLA	ND
33	b	611	CLA	ND
33	b	612	CLA	ND
33	b	613	CLA	ND
33	b	614	CLA	ND
33	b	615	CLA	ND
33	b	616	CLA	ND
33	b	617	CLA	ND
33	0	304	CLA	ND
33	0	305	CLA	ND
33	0	307	CLA	ND
33	0	308	CLA	ND
33	0	309	CLA	ND
33	0	310	CLA	ND
33	0	311	CLA	ND
33	0	312	CLA	ND
33	0	313	CLA	ND
33	9	305	CLA	ND
33	9	306	CLA	ND
33	9	307	CLA	ND
33	9	308	CLA	ND
33	9	309	CLA	ND
33	9	310	CLA	ND
33	9	311	CLA	ND
33	9	312	CLA	ND
33	9	313	CLA	ND
33	9	314	CLA	ND
33	9	315	CLA	ND
33	9	316	CLA	ND
33	9	317	CLA	ND
33	2	305	CLA	ND
33	2	306	CLA	ND
33	2	307	CLA	ND
33	2	308	CLA	ND

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Mol	Chain	Res	Type	Atom
33	2	309	CLA	ND
33	2	310	CLA	ND
33	2	311	CLA	ND
33	2	312	CLA	ND
33	2	314	CLA	ND
33	2	315	CLA	ND
33	2	316	CLA	ND
33	2	317	CLA	ND
33	8	305	CLA	ND
33	8	306	CLA	ND
33	8	307	CLA	ND
33	8	308	CLA	ND
33	8	309	CLA	ND
33	8	310	CLA	ND
33	8	311	CLA	ND
33	8	312	CLA	ND
33	8	313	CLA	ND
33	8	314	CLA	ND
33	8	315	CLA	ND
33	8	316	CLA	ND
33	1	305	CLA	ND
33	1	306	CLA	ND
33	1	307	CLA	ND
33	1	308	CLA	ND
33	1	309	CLA	ND
33	1	310	CLA	ND
33	1	311	CLA	ND
33	1	312	CLA	ND
33	1	313	CLA	ND
33	1	314	CLA	ND
33	1	315	CLA	ND
33	1	316	CLA	ND

All (3206) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	B	619	BCR	C7-C8-C9-C10
30	B	619	BCR	C21-C22-C23-C24
30	B	619	BCR	C37-C22-C23-C24
30	B	619	BCR	C22-C23-C24-C25
30	C	515	BCR	C7-C8-C9-C10
30	C	515	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
30	D	407	BCR	C21-C22-C23-C24
30	K	101	BCR	C7-C8-C9-C10
30	K	101	BCR	C11-C10-C9-C8
30	K	101	BCR	C11-C10-C9-C34
30	K	101	BCR	C10-C11-C12-C13
30	K	101	BCR	C14-C15-C16-C17
30	K	101	BCR	C16-C17-C18-C19
30	K	101	BCR	C16-C17-C18-C36
30	K	101	BCR	C20-C21-C22-C37
30	k	101	BCR	C6-C7-C8-C9
30	k	101	BCR	C7-C8-C9-C10
30	k	101	BCR	C7-C8-C9-C34
30	k	101	BCR	C11-C10-C9-C8
30	k	101	BCR	C11-C10-C9-C34
30	k	101	BCR	C10-C11-C12-C13
30	k	101	BCR	C12-C13-C14-C15
30	k	101	BCR	C16-C17-C18-C36
30	k	101	BCR	C20-C21-C22-C37
30	b	620	BCR	C7-C8-C9-C10
30	b	620	BCR	C7-C8-C9-C34
30	b	620	BCR	C21-C22-C23-C24
30	b	620	BCR	C22-C23-C24-C25
33	B	601	CLA	C1A-C2A-CAA-CBA
33	B	601	CLA	C3A-C2A-CAA-CBA
33	B	601	CLA	CAD-CBD-CGD-O1D
33	B	601	CLA	CAD-CBD-CGD-O2D
33	B	605	CLA	CAD-CBD-CGD-O2D
33	B	605	CLA	CBD-CGD-O2D-CED
33	B	605	CLA	C2-C3-C5-C6
33	B	605	CLA	C4-C3-C5-C6
33	B	614	CLA	CAD-CBD-CGD-O1D
33	B	614	CLA	CAD-CBD-CGD-O2D
33	B	614	CLA	C11-C10-C8-C9
33	C	501	CLA	CAD-CBD-CGD-O1D
33	C	501	CLA	CAD-CBD-CGD-O2D
33	C	503	CLA	C1A-C2A-CAA-CBA
33	C	503	CLA	C3A-C2A-CAA-CBA
33	C	507	CLA	CHA-CBD-CGD-O1D
33	C	507	CLA	CHA-CBD-CGD-O2D
33	C	507	CLA	C11-C12-C13-C14
33	c	501	CLA	CAD-CBD-CGD-O1D
33	c	501	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
33	c	503	CLA	C1A-C2A-CAA-CBA
33	c	503	CLA	C3A-C2A-CAA-CBA
33	c	503	CLA	CBD-CGD-O2D-CED
33	c	506	CLA	CAD-CBD-CGD-O2D
33	c	507	CLA	CHA-CBD-CGD-O2D
33	c	512	CLA	CHA-CBD-CGD-O1D
33	c	512	CLA	CHA-CBD-CGD-O2D
33	D	405	CLA	C1A-C2A-CAA-CBA
33	d	401	CLA	C1A-C2A-CAA-CBA
33	d	401	CLA	C3A-C2A-CAA-CBA
33	w	303	CLA	C2B-C3B-CAB-CBB
33	w	303	CLA	C4B-C3B-CAB-CBB
33	Z	101	CLA	C2B-C3B-CAB-CBB
33	Z	101	CLA	C4B-C3B-CAB-CBB
33	3	302	CLA	C1A-C2A-CAA-CBA
33	3	302	CLA	C3A-C2A-CAA-CBA
33	3	302	CLA	CBD-CGD-O2D-CED
33	3	305	CLA	CAD-CBD-CGD-O1D
33	3	305	CLA	CAD-CBD-CGD-O2D
33	3	305	CLA	CBD-CGD-O2D-CED
33	3	306	CLA	CHA-CBD-CGD-O2D
33	3	307	CLA	C2B-C3B-CAB-CBB
33	3	307	CLA	C4B-C3B-CAB-CBB
33	3	312	CLA	C1A-C2A-CAA-CBA
33	3	313	CLA	CHA-CBD-CGD-O1D
33	3	313	CLA	CHA-CBD-CGD-O2D
33	3	313	CLA	CBD-CGD-O2D-CED
33	3	313	CLA	C11-C10-C8-C9
33	3	319	CLA	CAD-CBD-CGD-O1D
33	3	319	CLA	CAD-CBD-CGD-O2D
33	3	319	CLA	CBD-CGD-O2D-CED
33	4	308	CLA	CHA-CBD-CGD-O1D
33	4	308	CLA	CHA-CBD-CGD-O2D
33	4	310	CLA	CBA-CGA-O2A-C1
33	4	310	CLA	CBD-CGD-O2D-CED
33	4	312	CLA	CHA-CBD-CGD-O1D
33	4	312	CLA	CHA-CBD-CGD-O2D
33	4	315	CLA	C1A-C2A-CAA-CBA
33	4	315	CLA	C3A-C2A-CAA-CBA
33	4	315	CLA	CHA-CBD-CGD-O1D
33	4	315	CLA	CHA-CBD-CGD-O2D
33	5	308	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	5	312	CLA	C3A-C2A-CAA-CBA
33	5	316	CLA	CBD-CGD-O2D-CED
33	5	316	CLA	O1D-CGD-O2D-CED
33	6	308	CLA	C1A-C2A-CAA-CBA
33	6	310	CLA	CBD-CGD-O2D-CED
33	6	311	CLA	CBD-CGD-O2D-CED
33	6	313	CLA	CBD-CGD-O2D-CED
33	6	315	CLA	CBD-CGD-O2D-CED
33	7	305	CLA	CBA-CGA-O2A-C1
33	7	305	CLA	CAD-CBD-CGD-O1D
33	7	305	CLA	CAD-CBD-CGD-O2D
33	7	307	CLA	CHA-CBD-CGD-O1D
33	7	307	CLA	CHA-CBD-CGD-O2D
33	7	307	CLA	C11-C12-C13-C14
33	7	310	CLA	CHA-CBD-CGD-O1D
33	7	310	CLA	CHA-CBD-CGD-O2D
33	7	311	CLA	CAD-CBD-CGD-O1D
33	7	311	CLA	CAD-CBD-CGD-O2D
33	7	311	CLA	CBD-CGD-O2D-CED
33	7	312	CLA	CHA-CBD-CGD-O1D
33	7	312	CLA	CHA-CBD-CGD-O2D
33	a	407	CLA	C1A-C2A-CAA-CBA
33	a	407	CLA	C3A-C2A-CAA-CBA
33	b	602	CLA	C1A-C2A-CAA-CBA
33	b	602	CLA	C3A-C2A-CAA-CBA
33	b	602	CLA	CAD-CBD-CGD-O1D
33	b	602	CLA	CAD-CBD-CGD-O2D
33	b	604	CLA	CAD-CBD-CGD-O1D
33	b	604	CLA	CAD-CBD-CGD-O2D
33	b	606	CLA	C2-C3-C5-C6
33	b	606	CLA	C4-C3-C5-C6
33	b	613	CLA	C1A-C2A-CAA-CBA
33	b	613	CLA	C3A-C2A-CAA-CBA
33	b	615	CLA	CAD-CBD-CGD-O1D
33	b	615	CLA	CAD-CBD-CGD-O2D
33	0	304	CLA	C3A-C2A-CAA-CBA
33	0	304	CLA	CBD-CGD-O2D-CED
33	0	305	CLA	CBA-CGA-O2A-C1
33	0	305	CLA	CAD-CBD-CGD-O1D
33	0	305	CLA	CAD-CBD-CGD-O2D
33	0	305	CLA	CBD-CGD-O2D-CED
33	0	307	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
33	0	307	CLA	CHA-CBD-CGD-O2D
33	0	310	CLA	CHA-CBD-CGD-O1D
33	0	310	CLA	CHA-CBD-CGD-O2D
33	0	311	CLA	CAD-CBD-CGD-O1D
33	0	311	CLA	CAD-CBD-CGD-O2D
33	9	308	CLA	C1A-C2A-CAA-CBA
33	9	310	CLA	C1A-C2A-CAA-CBA
33	9	310	CLA	CBD-CGD-O2D-CED
33	9	311	CLA	CBD-CGD-O2D-CED
33	9	312	CLA	CHA-CBD-CGD-O1D
33	9	312	CLA	CHA-CBD-CGD-O2D
33	9	317	CLA	CBD-CGD-O2D-CED
33	2	305	CLA	C4B-C3B-CAB-CBB
33	2	307	CLA	C1A-C2A-CAA-CBA
33	2	308	CLA	CAD-CBD-CGD-O1D
33	2	308	CLA	CAD-CBD-CGD-O2D
33	2	310	CLA	C1A-C2A-CAA-CBA
33	2	310	CLA	CBD-CGD-O2D-CED
33	2	311	CLA	CBD-CGD-O2D-CED
33	2	317	CLA	CBD-CGD-O2D-CED
33	8	308	CLA	CHA-CBD-CGD-O1D
33	8	308	CLA	CHA-CBD-CGD-O2D
33	8	310	CLA	C1A-C2A-CAA-CBA
33	8	310	CLA	CBD-CGD-O2D-CED
33	8	310	CLA	O1D-CGD-O2D-CED
33	8	312	CLA	CHA-CBD-CGD-O1D
33	8	312	CLA	CHA-CBD-CGD-O2D
33	1	310	CLA	C1A-C2A-CAA-CBA
33	1	310	CLA	CBD-CGD-O2D-CED
33	1	311	CLA	CBD-CGD-O2D-CED
33	1	312	CLA	CHA-CBD-CGD-O1D
33	1	312	CLA	CHA-CBD-CGD-O2D
33	1	314	CLA	C4B-C3B-CAB-CBB
34	A	407	PHO	C3A-C2A-CAA-CBA
36	A	411	LHG	O1-C1-C2-C3
36	A	412	LHG	C3-O3-P-O4
36	A	412	LHG	C8-C7-O7-C5
36	A	414	LHG	C3-O3-P-O5
36	A	414	LHG	C3-O3-P-O6
36	D	409	LHG	O1-C1-C2-C3
36	D	411	LHG	C2-C3-O3-P
36	D	411	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
36	D	411	LHG	C3-O3-P-O6
36	d	405	LHG	O1-C1-C2-C3
36	d	407	LHG	C2-C3-O3-P
36	d	407	LHG	C3-O3-P-O4
36	d	407	LHG	C3-O3-P-O6
36	H	104	LHG	C3-O3-P-O4
36	H	104	LHG	C3-O3-P-O5
36	H	104	LHG	C3-O3-P-O6
36	H	104	LHG	C4-O6-P-O5
36	H	104	LHG	C8-C7-O7-C5
36	h	103	LHG	O1-C1-C2-C3
36	h	103	LHG	C3-O3-P-O5
36	h	103	LHG	C3-O3-P-O6
36	h	103	LHG	O9-C7-O7-C5
36	h	103	LHG	C8-C7-O7-C5
36	W	302	LHG	C3-O3-P-O6
36	W	302	LHG	C4-O6-P-O4
36	w	301	LHG	C3-O3-P-O5
36	w	301	LHG	C3-O3-P-O6
36	w	301	LHG	C4-O6-P-O4
36	w	301	LHG	C4-O6-P-O5
36	3	317	LHG	C4-O6-P-O3
36	3	317	LHG	C4-O6-P-O5
36	3	318	LHG	O2-C2-C3-O3
36	3	318	LHG	C3-O3-P-O5
36	3	318	LHG	C4-O6-P-O4
36	4	318	LHG	C3-O3-P-O4
36	4	318	LHG	C3-O3-P-O5
36	4	318	LHG	C3-O3-P-O6
36	4	318	LHG	C4-O6-P-O3
36	4	318	LHG	C4-O6-P-O4
36	4	318	LHG	C4-O6-P-O5
36	5	318	LHG	C8-C7-O7-C5
36	7	316	LHG	C4-O6-P-O3
36	7	316	LHG	C4-O6-P-O4
36	7	316	LHG	C4-O6-P-O5
36	7	316	LHG	O9-C7-O7-C5
36	7	316	LHG	C8-C7-O7-C5
36	a	403	LHG	O1-C1-C2-C3
36	a	403	LHG	C4-O6-P-O5
36	a	404	LHG	O1-C1-C2-C3
36	a	404	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
36	b	601	LHG	C3-O3-P-O6
36	0	315	LHG	C4-O6-P-O3
36	0	315	LHG	C4-O6-P-O5
36	0	315	LHG	C8-C7-O7-C5
37	A	413	SQD	C2-C1-O6-C44
37	A	413	SQD	O5-C1-O6-C44
37	A	413	SQD	O49-C7-O47-C45
37	A	413	SQD	O5-C5-C6-S
37	B	622	SQD	C2-C1-O6-C44
37	B	622	SQD	O49-C7-O47-C45
37	B	622	SQD	C8-C7-O47-C45
37	B	622	SQD	C5-C6-S-O9
37	i	101	SQD	O5-C1-O6-C44
37	i	101	SQD	O49-C7-O47-C45
37	i	101	SQD	C8-C7-O47-C45
37	L	101	SQD	O5-C1-O6-C44
37	L	101	SQD	O49-C7-O47-C45
37	L	101	SQD	C8-C7-O47-C45
37	L	101	SQD	O5-C5-C6-S
37	l	101	SQD	C2-C1-O6-C44
37	l	101	SQD	O5-C1-O6-C44
37	l	101	SQD	O49-C7-O47-C45
37	l	101	SQD	C8-C7-O47-C45
37	l	101	SQD	O5-C5-C6-S
37	T	101	SQD	C2-C1-O6-C44
37	T	101	SQD	O5-C1-O6-C44
37	T	101	SQD	O49-C7-O47-C45
37	T	101	SQD	C8-C7-O47-C45
37	T	101	SQD	C5-C6-S-O7
37	T	103	SQD	C8-C7-O47-C45
37	T	103	SQD	C5-C6-S-O7
37	T	103	SQD	C5-C6-S-O8
37	T	103	SQD	C5-C6-S-O9
37	t	102	SQD	C8-C7-O47-C45
37	t	102	SQD	C5-C6-S-O7
37	7	317	SQD	O47-C45-C46-O48
37	7	317	SQD	O5-C5-C6-S
37	0	316	SQD	O5-C5-C6-S
38	A	415	DGD	O1G-C1G-C2G-O2G
38	A	415	DGD	C2E-C1E-O5D-C6D
38	A	415	DGD	O6E-C1E-O5D-C6D
38	3	320	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
38	3	320	DGD	O2G-C2G-C3G-O3G
38	a	401	DGD	C2B-C1B-O2G-C2G
38	a	401	DGD	O1G-C1G-C2G-O2G
38	a	401	DGD	C2E-C1E-O5D-C6D
38	a	401	DGD	O6E-C1E-O5D-C6D
39	C	520	LMG	O7-C8-C9-O8
39	C	521	LMG	C2-C1-O1-C7
39	C	521	LMG	O6-C1-O1-C7
39	c	520	LMG	O6-C1-O1-C7
39	D	404	LMG	C29-C28-O8-C9
39	d	410	LMG	C11-C10-O7-C8
39	5	319	LMG	O6-C1-O1-C7
39	5	319	LMG	O7-C8-C9-O8
39	7	315	LMG	O6-C1-O1-C7
39	7	315	LMG	O7-C8-C9-O8
39	b	623	LMG	C2-C1-O1-C7
39	b	623	LMG	C9-C8-O7-C10
39	Q	301	LMG	C11-C10-O7-C8
39	q	301	LMG	O7-C8-C9-O8
39	q	302	LMG	O9-C10-O7-C8
39	q	302	LMG	C11-C10-O7-C8
39	0	314	LMG	O6-C1-O1-C7
41	d	404	PL9	C37-C38-C39-C41
42	e	101	HEM	C2C-C3C-CAC-CBC
42	e	101	HEM	C4C-C3C-CAC-CBC
42	V	201	HEM	C2C-C3C-CAC-CBC
42	V	201	HEM	C4C-C3C-CAC-CBC
42	v	201	HEM	C1A-C2A-CAA-CBA
43	T	102	LMU	O5'-C1'-O1'-C1
43	t	101	LMU	O5'-C1'-O1'-C1
43	w	302	LMU	O5'-C1'-O1'-C1
43	3	301	LMU	O5'-C1'-O1'-C1
43	5	320	LMU	C2-C1-O1'-C1'
44	3	310	KC1	C1A-C2A-CAA-CBA
44	3	310	KC1	C2B-C3B-CAB-CBB
44	3	310	KC1	C2A-CAA-CBA-CGA
44	3	310	KC1	CBD-CGD-O2D-CED
44	5	315	KC1	C1A-C2A-CAA-CBA
44	5	315	KC1	C3A-C2A-CAA-CBA
44	5	315	KC1	C2B-C3B-CAB-CBB
44	6	314	KC1	C3A-C2A-CAA-CBA
44	6	314	KC1	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
44	6	314	KC1	C4B-C3B-CAB-CBB
44	6	314	KC1	C2A-CAA-CBA-CGA
44	6	314	KC1	CBD-CGD-O2D-CED
45	3	314	A86	C24-C25-C26-C27
45	4	301	A86	C39-C38-O4-C34
45	4	301	A86	O5-C38-O4-C34
45	4	301	A86	C5-C6-C8-C9
45	4	301	A86	C7-C6-C8-C9
45	4	302	A86	C10-C11-C13-O
45	4	302	A86	C12-C11-C13-O
45	4	302	A86	C39-C38-O4-C34
45	4	304	A86	O5-C38-O4-C34
45	5	301	A86	C10-C11-C13-C14
45	5	301	A86	C12-C11-C13-C14
45	5	301	A86	C13-C14-C15-C16
45	5	302	A86	C10-C11-C13-O
45	5	302	A86	C10-C11-C13-C14
45	5	302	A86	C12-C11-C13-O
45	5	302	A86	C13-C14-C15-C16
45	5	302	A86	C35-C34-O4-C38
45	5	302	A86	O5-C38-O4-C34
45	5	303	A86	C10-C11-C13-C14
45	5	303	A86	C12-C11-C13-O
45	5	303	A86	C13-C14-C15-C16
45	5	304	A86	C10-C11-C13-C14
45	5	304	A86	C12-C11-C13-C14
45	5	304	A86	C13-C14-C15-C16
45	5	305	A86	C10-C11-C13-C14
45	5	305	A86	C12-C11-C13-C14
45	5	305	A86	C13-C14-C15-C20
45	5	305	A86	C13-C14-C15-O1
45	5	305	A86	C35-C34-O4-C38
45	5	305	A86	O5-C38-O4-C34
45	5	306	A86	C10-C11-C13-C14
45	5	306	A86	C12-C11-C13-O
45	5	306	A86	C12-C11-C13-C14
45	5	306	A86	C13-C14-C15-C16
45	5	307	A86	C10-C11-C13-C14
45	5	307	A86	C12-C11-C13-C14
45	5	307	A86	C13-C14-C15-C16
45	6	301	A86	C10-C11-C13-O
45	6	302	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
45	6	303	A86	C10-C11-C13-O
45	6	303	A86	C12-C11-C13-O
45	6	303	A86	C13-C14-C15-C16
45	6	304	A86	C10-C11-C13-O
45	6	304	A86	C12-C11-C13-O
45	6	304	A86	C13-C14-C15-C16
45	6	305	A86	C10-C11-C13-O
45	6	305	A86	C12-C11-C13-O
45	6	305	A86	C13-C14-C15-C16
45	6	306	A86	C10-C11-C13-C14
45	6	306	A86	C12-C11-C13-C14
45	6	306	A86	C13-C14-C15-C16
45	7	301	A86	C13-C14-C15-O1
45	7	301	A86	C39-C38-O4-C34
45	7	301	A86	O5-C38-O4-C34
45	7	301	A86	C5-C6-C8-C9
45	7	301	A86	C7-C6-C8-C9
45	7	303	A86	C39-C38-O4-C34
45	7	303	A86	O5-C38-O4-C34
45	0	301	A86	C13-C14-C15-O1
45	0	301	A86	C39-C38-O4-C34
45	0	301	A86	O5-C38-O4-C34
45	0	301	A86	C5-C6-C8-C9
45	0	301	A86	C7-C6-C8-C9
45	9	301	A86	C39-C38-O4-C34
45	9	302	A86	O-C13-C14-C15
45	9	302	A86	C5-C6-C8-C9
45	9	302	A86	C7-C6-C8-C9
45	2	301	A86	C39-C38-O4-C34
45	2	302	A86	O-C13-C14-C15
45	2	302	A86	C5-C6-C8-C9
45	2	302	A86	C7-C6-C8-C9
45	8	301	A86	C12-C11-C13-O
45	8	301	A86	C39-C38-O4-C34
45	8	301	A86	O5-C38-O4-C34
45	8	302	A86	C39-C38-O4-C34
45	8	302	A86	O5-C38-O4-C34
45	8	302	A86	C3-C4-C5-C6
45	8	302	A86	C5-C6-C8-C9
45	8	302	A86	C7-C6-C8-C9
45	1	301	A86	O-C13-C14-C15
45	1	301	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
45	1	302	A86	C39-C38-O4-C34
45	1	302	A86	O5-C38-O4-C34
45	1	302	A86	C3-C4-C5-C6
45	1	302	A86	C5-C6-C8-C9
45	1	302	A86	C7-C6-C8-C9
46	3	315	DD6	C10-C11-C13-C14
46	3	315	DD6	C12-C11-C13-C14
46	9	303	DD6	C10-C11-C13-C14
46	9	303	DD6	C12-C11-C13-C14
46	9	304	DD6	C2-C1-C24-C25
46	9	304	DD6	C11-C10-C9-C8
46	9	304	DD6	C10-C11-C13-C14
46	9	304	DD6	C5-C6-C8-C9
46	2	303	DD6	C10-C11-C13-C14
46	2	303	DD6	C12-C11-C13-C14
46	2	304	DD6	C2-C1-C24-C25
46	2	304	DD6	C11-C10-C9-C8
46	2	304	DD6	C10-C11-C13-C14
46	2	304	DD6	C5-C6-C8-C9
46	8	304	DD6	C-C1-C24-C25
46	8	304	DD6	C2-C1-C24-C25
46	8	304	DD6	C13-C14-C15-C16
46	8	304	DD6	C13-C14-C15-C20
46	1	304	DD6	C10-C11-C13-C14
46	1	304	DD6	C5-C6-C8-C9
46	1	304	DD6	C7-C6-C8-C9
47	4	307	KC2	C3A-C2A-CAA-CBA
47	4	307	KC2	C2B-C3B-CAB-CBB
47	4	307	KC2	C4B-C3B-CAB-CBB
47	4	307	KC2	C2C-C3C-CAC-CBC
47	4	307	KC2	C4C-C3C-CAC-CBC
47	4	307	KC2	C2A-CAA-CBA-CGA
47	5	310	KC2	C2C-C3C-CAC-CBC
47	5	310	KC2	C4C-C3C-CAC-CBC
47	6	309	KC2	C2B-C3B-CAB-CBB
47	6	309	KC2	C4B-C3B-CAB-CBB
47	6	309	KC2	C2C-C3C-CAC-CBC
47	7	306	KC2	C1A-C2A-CAA-CBA
47	7	306	KC2	C2B-C3B-CAB-CBB
47	0	306	KC2	C1A-C2A-CAA-CBA
47	0	306	KC2	C3A-C2A-CAA-CBA
47	0	306	KC2	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
47	0	306	KC2	C4B-C3B-CAB-CBB
47	0	306	KC2	CBD-CGD-O2D-CED
48	7	302	ET4	C11-C12-C13-C14
48	7	302	ET4	C11-C12-C13-C28
48	7	302	ET4	C13-C14-C15-C16
48	7	302	ET4	C05-C06-C07-C08
48	0	302	ET4	C13-C14-C15-C16
48	0	302	ET4	C15-C16-C17-C18
43	5	320	LMU	C5'-C4'-O1B-C1B
33	4	306	CLA	O1D-CGD-O2D-CED
33	6	313	CLA	O1D-CGD-O2D-CED
33	7	304	CLA	O1D-CGD-O2D-CED
33	0	307	CLA	O1D-CGD-O2D-CED
33	0	311	CLA	O1D-CGD-O2D-CED
33	9	310	CLA	O1D-CGD-O2D-CED
33	9	311	CLA	O1D-CGD-O2D-CED
33	9	317	CLA	O1D-CGD-O2D-CED
33	2	310	CLA	O1D-CGD-O2D-CED
33	2	311	CLA	O1D-CGD-O2D-CED
33	1	309	CLA	O1D-CGD-O2D-CED
33	1	310	CLA	O1D-CGD-O2D-CED
33	1	311	CLA	O1D-CGD-O2D-CED
47	0	306	KC2	O1D-CGD-O2D-CED
37	t	102	SQD	O49-C7-O47-C45
39	C	522	LMG	C11-C10-O7-C8
45	4	302	A86	O5-C38-O4-C34
45	5	301	A86	C39-C38-O4-C34
45	5	302	A86	C39-C38-O4-C34
45	5	306	A86	C39-C38-O4-C34
45	5	307	A86	C39-C38-O4-C34
45	6	302	A86	C39-C38-O4-C34
45	6	306	A86	C39-C38-O4-C34
45	0	303	A86	O5-C38-O4-C34
45	1	301	A86	O5-C38-O4-C34
43	T	102	LMU	O5B-C1B-O1B-C4'
33	3	306	CLA	O1D-CGD-O2D-CED
33	4	310	CLA	O1D-CGD-O2D-CED
33	6	311	CLA	O1D-CGD-O2D-CED
33	7	308	CLA	O1D-CGD-O2D-CED
33	0	304	CLA	O1D-CGD-O2D-CED
33	8	309	CLA	O1D-CGD-O2D-CED
33	8	311	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	C	522	LMG	O9-C10-O7-C8
45	4	304	A86	C39-C38-O4-C34
45	5	304	A86	C39-C38-O4-C34
45	6	305	A86	C39-C38-O4-C34
45	0	303	A86	C39-C38-O4-C34
45	9	301	A86	O5-C38-O4-C34
45	9	302	A86	C39-C38-O4-C34
45	2	301	A86	O5-C38-O4-C34
45	2	302	A86	C39-C38-O4-C34
33	B	609	CLA	CBD-CGD-O2D-CED
33	B	613	CLA	CBD-CGD-O2D-CED
33	c	506	CLA	CBD-CGD-O2D-CED
33	z	101	CLA	CBD-CGD-O2D-CED
33	3	306	CLA	CBD-CGD-O2D-CED
33	3	309	CLA	CBD-CGD-O2D-CED
33	4	306	CLA	CBD-CGD-O2D-CED
33	5	311	CLA	CBD-CGD-O2D-CED
33	6	312	CLA	CBD-CGD-O2D-CED
33	7	304	CLA	CBD-CGD-O2D-CED
33	7	305	CLA	CBD-CGD-O2D-CED
33	7	307	CLA	CBD-CGD-O2D-CED
33	7	308	CLA	CBD-CGD-O2D-CED
33	7	312	CLA	CBD-CGD-O2D-CED
33	a	407	CLA	CBD-CGD-O2D-CED
33	b	610	CLA	CBD-CGD-O2D-CED
33	0	307	CLA	CBD-CGD-O2D-CED
33	0	308	CLA	CBD-CGD-O2D-CED
33	0	311	CLA	CBD-CGD-O2D-CED
33	0	312	CLA	CBD-CGD-O2D-CED
33	9	309	CLA	CBD-CGD-O2D-CED
33	9	312	CLA	CBD-CGD-O2D-CED
33	2	306	CLA	CBD-CGD-O2D-CED
33	8	309	CLA	CBD-CGD-O2D-CED
33	8	311	CLA	CBD-CGD-O2D-CED
33	1	309	CLA	CBD-CGD-O2D-CED
33	A	404	CLA	O1A-CGA-O2A-C1
33	3	302	CLA	O1A-CGA-O2A-C1
33	5	311	CLA	O1A-CGA-O2A-C1
33	7	305	CLA	O1A-CGA-O2A-C1
33	7	311	CLA	O1A-CGA-O2A-C1
33	0	305	CLA	O1A-CGA-O2A-C1
33	0	311	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	8	308	CLA	O1A-CGA-O2A-C1
33	1	308	CLA	O1A-CGA-O2A-C1
33	1	310	CLA	O1A-CGA-O2A-C1
34	a	409	PHO	O1A-CGA-O2A-C1
36	D	411	LHG	O10-C23-O8-C6
36	d	407	LHG	O10-C23-O8-C6
36	h	103	LHG	O10-C23-O8-C6
37	L	101	SQD	O10-C23-O48-C46
38	C	517	DGD	O1A-C1A-O1G-C1G
39	c	519	LMG	O10-C28-O8-C9
39	0	314	LMG	O10-C28-O8-C9
33	4	310	CLA	O1A-CGA-O2A-C1
33	5	308	CLA	O1A-CGA-O2A-C1
33	c	503	CLA	O1D-CGD-O2D-CED
44	3	310	KC1	O1D-CGD-O2D-CED
45	5	303	A86	C39-C38-O4-C34
43	t	101	LMU	O5B-C1B-O1B-C4'
45	4	301	A86	C33-C34-O4-C38
45	5	301	A86	C35-C34-O4-C38
45	5	303	A86	C35-C34-O4-C38
33	3	309	CLA	O1D-CGD-O2D-CED
33	6	312	CLA	O1D-CGD-O2D-CED
33	2	306	CLA	O1D-CGD-O2D-CED
33	3	302	CLA	CBA-CGA-O2A-C1
33	5	311	CLA	CBA-CGA-O2A-C1
33	7	311	CLA	CBA-CGA-O2A-C1
33	0	311	CLA	CBA-CGA-O2A-C1
33	8	308	CLA	CBA-CGA-O2A-C1
33	1	308	CLA	CBA-CGA-O2A-C1
34	A	406	PHO	CBA-CGA-O2A-C1
34	a	409	PHO	CBA-CGA-O2A-C1
36	3	317	LHG	C24-C23-O8-C6
39	c	519	LMG	C29-C28-O8-C9
39	b	623	LMG	C29-C28-O8-C9
39	q	302	LMG	C29-C28-O8-C9
45	5	303	A86	O5-C38-O4-C34
33	A	404	CLA	CBD-CGD-O2D-CED
33	2	309	CLA	CBD-CGD-O2D-CED
33	4	305	CLA	O1A-CGA-O2A-C1
33	4	314	CLA	O1A-CGA-O2A-C1
33	9	308	CLA	O1A-CGA-O2A-C1
33	9	310	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	9	317	CLA	O1A-CGA-O2A-C1
33	2	308	CLA	O1A-CGA-O2A-C1
33	2	310	CLA	O1A-CGA-O2A-C1
33	2	317	CLA	O1A-CGA-O2A-C1
34	A	406	PHO	O1A-CGA-O2A-C1
36	w	301	LHG	O10-C23-O8-C6
36	3	317	LHG	O10-C23-O8-C6
36	3	318	LHG	O10-C23-O8-C6
36	4	318	LHG	O10-C23-O8-C6
37	B	622	SQD	O10-C23-O48-C46
37	l	101	SQD	O10-C23-O48-C46
39	D	404	LMG	O10-C28-O8-C9
39	d	410	LMG	O10-C28-O8-C9
39	m	201	LMG	O10-C28-O8-C9
39	7	315	LMG	O10-C28-O8-C9
39	b	623	LMG	O10-C28-O8-C9
39	Q	301	LMG	O10-C28-O8-C9
39	q	301	LMG	O10-C28-O8-C9
39	q	302	LMG	O10-C28-O8-C9
39	w	304	LMG	C4-C5-C6-O5
33	3	319	CLA	O1D-CGD-O2D-CED
33	6	310	CLA	O1D-CGD-O2D-CED
33	7	311	CLA	O1D-CGD-O2D-CED
33	0	312	CLA	O1D-CGD-O2D-CED
33	9	309	CLA	O1D-CGD-O2D-CED
33	2	317	CLA	O1D-CGD-O2D-CED
47	0	306	KC2	CAA-CBA-CGA-O2A
33	B	605	CLA	O1D-CGD-O2D-CED
33	3	302	CLA	O1D-CGD-O2D-CED
33	3	313	CLA	O1D-CGD-O2D-CED
33	0	305	CLA	O1D-CGD-O2D-CED
45	5	301	A86	O5-C38-O4-C34
45	6	302	A86	O5-C38-O4-C34
45	6	306	A86	O5-C38-O4-C34
33	5	308	CLA	CBD-CGD-O2D-CED
33	3	304	CLA	O1A-CGA-O2A-C1
36	H	104	LHG	O10-C23-O8-C6
36	A	412	LHG	O9-C7-O7-C5
36	H	104	LHG	O9-C7-O7-C5
36	5	318	LHG	O9-C7-O7-C5
36	a	404	LHG	O9-C7-O7-C5
36	0	315	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
39	c	519	LMG	O9-C10-O7-C8
39	D	404	LMG	O9-C10-O7-C8
39	d	410	LMG	O9-C10-O7-C8
39	m	201	LMG	O9-C10-O7-C8
39	Q	301	LMG	O9-C10-O7-C8
39	b	621	LMG	C4-C5-C6-O5
33	C	502	CLA	C3-C5-C6-C7
33	c	503	CLA	C3-C5-C6-C7
33	w	303	CLA	C3-C5-C6-C7
33	3	308	CLA	C3-C5-C6-C7
33	5	309	CLA	C3-C5-C6-C7
33	b	605	CLA	C3-C5-C6-C7
33	0	312	CLA	C3-C5-C6-C7
33	1	308	CLA	C3-C5-C6-C7
34	A	406	PHO	C3-C5-C6-C7
34	A	407	PHO	C3-C5-C6-C7
33	b	610	CLA	O1D-CGD-O2D-CED
33	A	404	CLA	CBA-CGA-O2A-C1
33	4	305	CLA	CBA-CGA-O2A-C1
33	0	304	CLA	CBA-CGA-O2A-C1
33	9	308	CLA	CBA-CGA-O2A-C1
33	9	310	CLA	CBA-CGA-O2A-C1
33	9	317	CLA	CBA-CGA-O2A-C1
33	2	308	CLA	CBA-CGA-O2A-C1
33	2	317	CLA	CBA-CGA-O2A-C1
33	1	310	CLA	CBA-CGA-O2A-C1
36	D	411	LHG	C24-C23-O8-C6
36	d	407	LHG	C24-C23-O8-C6
36	4	318	LHG	C24-C23-O8-C6
37	B	622	SQD	C24-C23-O48-C46
37	l	101	SQD	C24-C23-O48-C46
38	C	517	DGD	C2A-C1A-O1G-C1G
39	d	410	LMG	C29-C28-O8-C9
39	m	201	LMG	C29-C28-O8-C9
39	7	315	LMG	C29-C28-O8-C9
39	Q	301	LMG	C29-C28-O8-C9
33	C	504	CLA	CBD-CGD-O2D-CED
33	C	506	CLA	CBD-CGD-O2D-CED
33	c	501	CLA	CBD-CGD-O2D-CED
33	6	307	CLA	CBD-CGD-O2D-CED
33	7	309	CLA	CBD-CGD-O2D-CED
33	9	306	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
33	9	308	CLA	CBD-CGD-O2D-CED
33	8	308	CLA	CBD-CGD-O2D-CED
33	1	305	CLA	CBD-CGD-O2D-CED
33	1	306	CLA	CBD-CGD-O2D-CED
33	1	312	CLA	CBD-CGD-O2D-CED
37	A	413	SQD	C8-C7-O47-C45
38	A	415	DGD	C2B-C1B-O2G-C2G
38	3	320	DGD	C2B-C1B-O2G-C2G
33	3	305	CLA	O1D-CGD-O2D-CED
33	7	305	CLA	O1D-CGD-O2D-CED
33	7	307	CLA	O1D-CGD-O2D-CED
33	5	313	CLA	O1A-CGA-O2A-C1
33	w	303	CLA	C2C-C3C-CAC-CBC
33	6	315	CLA	O1D-CGD-O2D-CED
45	5	307	A86	O5-C38-O4-C34
47	0	306	KC2	CAA-CBA-CGA-O1A
33	d	402	CLA	C4-C3-C5-C6
33	3	306	CLA	C4-C3-C5-C6
33	3	307	CLA	C4-C3-C5-C6
33	3	312	CLA	C4-C3-C5-C6
33	5	314	CLA	C4-C3-C5-C6
33	7	307	CLA	C4-C3-C5-C6
33	b	604	CLA	C4-C3-C5-C6
33	d	402	CLA	C2-C3-C5-C6
33	3	306	CLA	C2-C3-C5-C6
33	3	307	CLA	C2-C3-C5-C6
33	3	312	CLA	C2-C3-C5-C6
33	5	314	CLA	C2-C3-C5-C6
33	7	307	CLA	C2-C3-C5-C6
33	z	101	CLA	O1D-CGD-O2D-CED
33	5	311	CLA	O1D-CGD-O2D-CED
45	5	306	A86	O5-C38-O4-C34
33	4	316	CLA	C3-C5-C6-C7
33	B	604	CLA	C3-C5-C6-C7
33	3	302	CLA	C3-C5-C6-C7
33	4	305	CLA	C3-C5-C6-C7
33	7	312	CLA	C3-C5-C6-C7
33	a	411	CLA	C3-C5-C6-C7
33	b	617	CLA	C3-C5-C6-C7
33	3	304	CLA	CBA-CGA-O2A-C1
33	3	308	CLA	CBA-CGA-O2A-C1
33	4	314	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	6	307	CLA	CBA-CGA-O2A-C1
33	a	407	CLA	CBA-CGA-O2A-C1
33	2	310	CLA	CBA-CGA-O2A-C1
36	H	104	LHG	C24-C23-O8-C6
36	w	301	LHG	C24-C23-O8-C6
36	3	318	LHG	C24-C23-O8-C6
37	L	101	SQD	C24-C23-O48-C46
38	c	517	DGD	C2A-C1A-O1G-C1G
39	M	201	LMG	C29-C28-O8-C9
39	0	314	LMG	C29-C28-O8-C9
45	5	304	A86	O5-C38-O4-C34
45	9	302	A86	O5-C38-O4-C34
36	d	405	LHG	C23-C24-C25-C26
39	c	520	LMG	O10-C28-O8-C9
39	c	520	LMG	C29-C28-O8-C9
45	6	305	A86	O5-C38-O4-C34
45	2	302	A86	O5-C38-O4-C34
39	b	621	LMG	O6-C5-C6-O5
30	K	101	BCR	C9-C10-C11-C12
30	k	101	BCR	C9-C10-C11-C12
45	4	301	A86	C1-C2-C3-C4
45	4	301	A86	C3-C4-C5-C6
45	4	304	A86	C24-C25-C26-C27
45	7	301	A86	C3-C4-C5-C6
45	0	301	A86	C3-C4-C5-C6
45	9	302	A86	C3-C4-C5-C6
45	2	302	A86	C3-C4-C5-C6
46	9	304	DD6	C24-C25-C26-C27
46	2	304	DD6	C24-C25-C26-C27
46	8	304	DD6	C24-C25-C26-C27
33	3	308	CLA	O1A-CGA-O2A-C1
33	6	312	CLA	O1A-CGA-O2A-C1
33	a	407	CLA	O1A-CGA-O2A-C1
38	c	517	DGD	O1A-C1A-O1G-C1G
39	M	201	LMG	O10-C28-O8-C9
33	W	303	CLA	C2C-C3C-CAC-CBC
36	4	318	LHG	O9-C7-O7-C5
39	b	623	LMG	O9-C10-O7-C8
33	9	312	CLA	O1D-CGD-O2D-CED
39	w	304	LMG	O6-C5-C6-O5
38	C	516	DGD	C4E-C5E-C6E-O5E
38	c	516	DGD	C4E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
45	6	301	A86	C39-C38-O4-C34
44	3	310	KC1	CAA-CBA-CGA-O1A
33	C	503	CLA	C3-C5-C6-C7
33	d	402	CLA	C3-C5-C6-C7
33	2	311	CLA	C3-C5-C6-C7
33	8	311	CLA	C3-C5-C6-C7
34	a	409	PHO	C3-C5-C6-C7
33	5	312	CLA	CBD-CGD-O2D-CED
43	t	101	LMU	C2-C3-C4-C5
43	5	320	LMU	C2-C3-C4-C5
36	A	412	LHG	O2-C2-C3-O3
36	a	404	LHG	O2-C2-C3-O3
33	B	613	CLA	O1D-CGD-O2D-CED
33	3	313	CLA	CBA-CGA-O2A-C1
33	5	313	CLA	CBA-CGA-O2A-C1
36	h	103	LHG	C24-C23-O8-C6
39	q	301	LMG	C29-C28-O8-C9
38	C	517	DGD	O6E-C5E-C6E-O5E
38	c	517	DGD	O6E-C5E-C6E-O5E
38	a	401	DGD	O6E-C5E-C6E-O5E
33	6	307	CLA	O1A-CGA-O2A-C1
33	0	304	CLA	O1A-CGA-O2A-C1
37	t	102	SQD	O10-C23-O48-C46
33	B	609	CLA	O1D-CGD-O2D-CED
45	6	301	A86	O5-C38-O4-C34
45	6	303	A86	C39-C38-O4-C34
45	6	303	A86	O5-C38-O4-C34
45	6	304	A86	C39-C38-O4-C34
45	6	304	A86	O5-C38-O4-C34
43	T	102	LMU	O5B-C5B-C6B-O6B
39	q	301	LMG	C4-C5-C6-O5
33	c	502	CLA	CBD-CGD-O2D-CED
36	4	318	LHG	C8-C7-O7-C5
36	a	404	LHG	C8-C7-O7-C5
37	D	403	SQD	C8-C7-O47-C45
39	D	404	LMG	C11-C10-O7-C8
39	b	623	LMG	C11-C10-O7-C8
33	H	103	CLA	CBA-CGA-O2A-C1
33	a	407	CLA	O1D-CGD-O2D-CED
33	0	308	CLA	O1D-CGD-O2D-CED
39	7	315	LMG	O6-C5-C6-O5
39	b	623	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
33	D	406	CLA	C3-C5-C6-C7
33	4	314	CLA	CBD-CGD-O2D-CED
44	5	315	KC1	CBD-CGD-O2D-CED
39	d	406	LMG	O6-C5-C6-O5
39	q	301	LMG	O6-C5-C6-O5
43	5	320	LMU	O5'-C5'-C6'-O6'
38	C	517	DGD	C4E-C5E-C6E-O5E
33	c	506	CLA	O1D-CGD-O2D-CED
33	7	312	CLA	O1D-CGD-O2D-CED
33	6	312	CLA	CBA-CGA-O2A-C1
33	B	603	CLA	C4-C3-C5-C6
33	D	406	CLA	C4-C3-C5-C6
33	B	603	CLA	C2-C3-C5-C6
33	D	406	CLA	C2-C3-C5-C6
33	b	604	CLA	C2-C3-C5-C6
39	m	201	LMG	O6-C5-C6-O5
41	d	404	PL9	C39-C41-C42-C43
43	3	301	LMU	C6-C7-C8-C9
43	4	317	LMU	O5'-C5'-C6'-O6'
42	F	101	HEM	C2A-CAA-CBA-CGA
33	B	610	CLA	C2A-CAA-CBA-CGA
33	w	303	CLA	C4C-C3C-CAC-CBC
33	2	317	CLA	C3-C5-C6-C7
37	T	103	SQD	O5-C1-O6-C44
38	A	415	DGD	O6D-C1D-O3G-C3G
38	C	518	DGD	O6D-C1D-O3G-C3G
38	c	517	DGD	O6E-C1E-O5D-C6D
39	C	519	LMG	O6-C1-O1-C7
39	C	520	LMG	O6-C1-O1-C7
39	c	519	LMG	O6-C1-O1-C7
39	b	623	LMG	O6-C1-O1-C7
39	Q	301	LMG	O6-C1-O1-C7
39	q	301	LMG	O6-C1-O1-C7
39	q	302	LMG	O6-C1-O1-C7
33	c	504	CLA	CBA-CGA-O2A-C1
33	Z	101	CLA	CBA-CGA-O2A-C1
33	3	307	CLA	CBA-CGA-O2A-C1
33	B	603	CLA	CBD-CGD-O2D-CED
33	6	316	CLA	CBD-CGD-O2D-CED
33	b	615	CLA	CBD-CGD-O2D-CED
38	c	516	DGD	O6E-C5E-C6E-O5E
39	D	410	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
39	M	201	LMG	O6-C5-C6-O5
43	3	301	LMU	C1-C2-C3-C4
33	3	313	CLA	O1A-CGA-O2A-C1
38	C	516	DGD	O6E-C5E-C6E-O5E
33	A	404	CLA	O1D-CGD-O2D-CED
43	t	101	LMU	C4'-C5'-C6'-O6'
36	d	405	LHG	C32-C33-C34-C35
33	3	311	CLA	CBD-CGD-O2D-CED
33	0	309	CLA	CBD-CGD-O2D-CED
36	a	403	LHG	C32-C33-C34-C35
38	a	401	DGD	C4E-C5E-C6E-O5E
45	3	314	A86	C11-C10-C9-C8
45	7	303	A86	C11-C10-C9-C8
45	9	302	A86	C11-C10-C9-C8
45	2	302	A86	C11-C10-C9-C8
45	8	302	A86	C11-C10-C9-C8
45	1	302	A86	C11-C10-C9-C8
46	9	304	DD6	C1-C2-C3-C4
46	2	304	DD6	C1-C2-C3-C4
46	1	304	DD6	C24-C25-C26-C27
33	c	504	CLA	O1A-CGA-O2A-C1
33	Z	101	CLA	O1A-CGA-O2A-C1
36	A	412	LHG	C1-C2-C3-O3
36	a	403	LHG	C1-C2-C3-O3
36	a	404	LHG	C1-C2-C3-O3
33	2	309	CLA	O1D-CGD-O2D-CED
33	c	503	CLA	CBA-CGA-O2A-C1
33	c	512	CLA	CBA-CGA-O2A-C1
33	3	306	CLA	CBA-CGA-O2A-C1
33	3	309	CLA	CBA-CGA-O2A-C1
33	5	314	CLA	CBA-CGA-O2A-C1
33	7	307	CLA	CBA-CGA-O2A-C1
36	a	404	LHG	C24-C23-O8-C6
37	t	102	SQD	C24-C23-O48-C46
37	0	316	SQD	C24-C23-O48-C46
39	C	519	LMG	C29-C28-O8-C9
36	A	414	LHG	C32-C33-C34-C35
45	6	305	A86	C33-C34-O4-C38
38	h	102	DGD	O6E-C5E-C6E-O5E
38	c	517	DGD	C4E-C5E-C6E-O5E
36	A	412	LHG	C29-C30-C31-C32
38	a	401	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
33	5	308	CLA	O1D-CGD-O2D-CED
33	8	308	CLA	O1D-CGD-O2D-CED
33	3	308	CLA	C4-C3-C5-C6
33	3	308	CLA	C2-C3-C5-C6
33	3	303	CLA	C3-C5-C6-C7
33	3	313	CLA	C3-C5-C6-C7
33	b	604	CLA	CBD-CGD-O2D-CED
33	A	408	CLA	C11-C10-C8-C9
33	B	602	CLA	C11-C12-C13-C14
33	B	604	CLA	C6-C7-C8-C9
33	B	605	CLA	C11-C10-C8-C9
33	B	605	CLA	C14-C13-C15-C16
33	B	610	CLA	C11-C12-C13-C14
33	B	613	CLA	C14-C13-C15-C16
33	B	616	CLA	C6-C7-C8-C9
33	C	501	CLA	C14-C13-C15-C16
33	C	509	CLA	C6-C7-C8-C9
33	c	501	CLA	C14-C13-C15-C16
33	c	504	CLA	C11-C12-C13-C14
33	c	507	CLA	C11-C12-C13-C14
33	3	307	CLA	C11-C12-C13-C14
33	7	305	CLA	C14-C13-C15-C16
33	7	309	CLA	C11-C10-C8-C9
33	b	614	CLA	C11-C12-C13-C14
33	b	615	CLA	C11-C10-C8-C9
33	0	305	CLA	C14-C13-C15-C16
33	0	307	CLA	C11-C12-C13-C14
33	0	309	CLA	C11-C10-C8-C9
33	0	309	CLA	C14-C13-C15-C16
33	0	312	CLA	C6-C7-C8-C9
34	A	406	PHO	C14-C13-C15-C16
39	b	622	LMG	O6-C5-C6-O5
33	1	305	CLA	O1D-CGD-O2D-CED
33	1	312	CLA	O1D-CGD-O2D-CED
37	T	103	SQD	C2-C1-O6-C44
37	t	102	SQD	C2-C1-O6-C44
38	c	517	DGD	C2E-C1E-O5D-C6D
39	C	519	LMG	C2-C1-O1-C7
39	c	519	LMG	C2-C1-O1-C7
39	5	319	LMG	C2-C1-O1-C7
39	Q	301	LMG	C2-C1-O1-C7
39	q	301	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
39	q	302	LMG	C2-C1-O1-C7
39	0	314	LMG	C2-C1-O1-C7
43	3	301	LMU	C2'-C1'-O1'-C1
43	4	317	LMU	C3-C4-C5-C6
38	a	401	DGD	O6D-C5D-C6D-O5D
36	a	403	LHG	O2-C2-C3-O3
43	3	301	LMU	O5'-C5'-C6'-O6'
33	3	307	CLA	O1A-CGA-O2A-C1
33	5	314	CLA	O1A-CGA-O2A-C1
30	B	618	BCR	C7-C8-C9-C34
30	B	619	BCR	C7-C8-C9-C34
30	C	515	BCR	C37-C22-C23-C24
30	c	515	BCR	C37-C22-C23-C24
30	D	407	BCR	C37-C22-C23-C24
30	k	101	BCR	C11-C12-C13-C35
30	b	620	BCR	C37-C22-C23-C24
45	3	314	A86	C7-C6-C8-C9
45	7	303	A86	C7-C6-C8-C9
46	4	303	DD6	C12-C11-C13-C14
46	9	304	DD6	C-C1-C24-C25
46	9	304	DD6	C12-C11-C13-C14
46	9	304	DD6	C7-C6-C8-C9
46	2	304	DD6	C-C1-C24-C25
46	2	304	DD6	C12-C11-C13-C14
46	2	304	DD6	C7-C6-C8-C9
46	1	304	DD6	C12-C11-C13-C14
48	7	302	ET4	C07-C08-C09-C27
48	0	302	ET4	C11-C12-C13-C28
48	0	302	ET4	C30-C18-C19-C20
43	4	317	LMU	O5B-C5B-C6B-O6B
30	C	515	BCR	C21-C22-C23-C24
30	c	515	BCR	C21-C22-C23-C24
30	K	101	BCR	C11-C12-C13-C14
45	3	314	A86	C5-C6-C8-C9
45	7	303	A86	C5-C6-C8-C9
43	5	320	LMU	C4'-C5'-C6'-O6'
33	C	501	CLA	C2A-CAA-CBA-CGA
33	9	307	CLA	C2A-CAA-CBA-CGA
33	1	307	CLA	C2A-CAA-CBA-CGA
36	H	104	LHG	C23-C24-C25-C26
33	3	306	CLA	O1A-CGA-O2A-C1
43	w	302	LMU	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
38	a	401	DGD	O1B-C1B-O2G-C2G
39	m	201	LMG	C11-C10-O7-C8
44	5	315	KC1	CAA-CBA-CGA-O2A
47	6	309	KC2	CAA-CBA-CGA-O2A
33	7	314	CLA	CBA-CGA-O2A-C1
33	W	303	CLA	C4C-C3C-CAC-CBC
36	7	316	LHG	O7-C5-C6-O8
33	7	309	CLA	O1D-CGD-O2D-CED
33	C	504	CLA	CBA-CGA-O2A-C1
36	4	318	LHG	C7-C8-C9-C10
36	b	601	LHG	C23-C24-C25-C26
33	c	501	CLA	O1D-CGD-O2D-CED
44	6	314	KC1	O1D-CGD-O2D-CED
33	3	304	CLA	CBD-CGD-O2D-CED
36	b	601	LHG	C32-C33-C34-C35
43	w	302	LMU	C3-C4-C5-C6
43	w	302	LMU	C6-C7-C8-C9
33	B	606	CLA	C10-C11-C12-C13
33	B	612	CLA	C15-C16-C17-C18
33	c	502	CLA	C10-C11-C12-C13
33	c	505	CLA	C5-C6-C7-C8
33	7	305	CLA	C5-C6-C7-C8
36	a	404	LHG	O1-C1-C2-O2
38	A	415	DGD	C4D-C5D-C6D-O5D
45	5	306	A86	C35-C34-O4-C38
33	C	503	CLA	C6-C7-C8-C10
33	3	313	CLA	C11-C12-C13-C15
33	7	309	CLA	C11-C12-C13-C15
33	7	309	CLA	CBA-CGA-O2A-C1
33	8	310	CLA	CBA-CGA-O2A-C1
33	B	611	CLA	C12-C13-C15-C16
44	5	315	KC1	CAA-CBA-CGA-O1A
39	B	621	LMG	O6-C5-C6-O5
43	4	317	LMU	C4B-C5B-C6B-O6B
36	A	412	LHG	C23-C24-C25-C26
36	3	318	LHG	C7-C8-C9-C10
38	A	415	DGD	C1B-C2B-C3B-C4B
39	b	623	LMG	C10-C11-C12-C13
39	0	314	LMG	C10-C11-C12-C13
30	K	101	BCR	C15-C16-C17-C18
45	4	301	A86	C11-C10-C9-C8
45	7	303	A86	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
46	9	303	DD6	C1-C2-C3-C4
46	2	303	DD6	C1-C2-C3-C4
46	8	304	DD6	C1-C2-C3-C4
33	C	506	CLA	O1D-CGD-O2D-CED
33	9	306	CLA	O1D-CGD-O2D-CED
33	c	503	CLA	C10-C11-C12-C13
33	0	305	CLA	C5-C6-C7-C8
43	w	302	LMU	C4B-C5B-C6B-O6B
36	A	411	LHG	C7-C8-C9-C10
36	h	103	LHG	C23-C24-C25-C26
36	a	404	LHG	C23-C24-C25-C26
37	D	403	SQD	C7-C8-C9-C10
37	0	316	SQD	C7-C8-C9-C10
33	c	512	CLA	O1A-CGA-O2A-C1
33	7	307	CLA	O1A-CGA-O2A-C1
33	7	304	CLA	CBA-CGA-O2A-C1
33	B	604	CLA	C8-C10-C11-C12
33	B	611	CLA	C8-C10-C11-C12
33	B	613	CLA	C8-C10-C11-C12
33	B	614	CLA	C8-C10-C11-C12
33	C	507	CLA	C10-C11-C12-C13
33	D	406	CLA	C5-C6-C7-C8
33	W	303	CLA	C10-C11-C12-C13
33	9	310	CLA	C5-C6-C7-C8
38	C	518	DGD	O6E-C5E-C6E-O5E
38	A	415	DGD	O6D-C5D-C6D-O5D
33	5	312	CLA	C2A-CAA-CBA-CGA
33	7	305	CLA	C2A-CAA-CBA-CGA
33	b	607	CLA	C2A-CAA-CBA-CGA
33	b	611	CLA	C2A-CAA-CBA-CGA
33	0	305	CLA	C2A-CAA-CBA-CGA
33	B	608	CLA	C15-C16-C17-C18
33	B	613	CLA	C10-C11-C12-C13
33	c	503	CLA	C8-C10-C11-C12
33	c	507	CLA	C13-C15-C16-C17
33	3	313	CLA	C8-C10-C11-C12
33	7	309	CLA	C10-C11-C12-C13
33	b	614	CLA	C10-C11-C12-C13
33	9	317	CLA	C5-C6-C7-C8
36	A	414	LHG	C23-C24-C25-C26
36	D	409	LHG	C7-C8-C9-C10
36	d	405	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
36	w	301	LHG	C7-C8-C9-C10
36	3	318	LHG	C23-C24-C25-C26
36	5	318	LHG	C23-C24-C25-C26
38	3	320	DGD	C1A-C2A-C3A-C4A
39	w	304	LMG	C10-C11-C12-C13
39	7	315	LMG	C28-C29-C30-C31
39	q	302	LMG	C28-C29-C30-C31
33	6	307	CLA	O1D-CGD-O2D-CED
33	9	308	CLA	O1D-CGD-O2D-CED
33	c	503	CLA	O1A-CGA-O2A-C1
38	c	518	DGD	O1A-C1A-O1G-C1G
37	B	622	SQD	O5-C1-O6-C44
38	C	517	DGD	O6E-C1E-O5D-C6D
38	a	401	DGD	O6D-C1D-O3G-C3G
39	D	404	LMG	O6-C1-O1-C7
38	H	102	DGD	O6E-C5E-C6E-O5E
33	C	504	CLA	O1D-CGD-O2D-CED
33	B	605	CLA	C5-C6-C7-C8
33	C	503	CLA	C10-C11-C12-C13
33	C	508	CLA	C5-C6-C7-C8
33	c	502	CLA	C15-C16-C17-C18
33	w	303	CLA	C10-C11-C12-C13
33	3	303	CLA	C13-C15-C16-C17
33	b	614	CLA	C8-C10-C11-C12
33	b	615	CLA	C11-C12-C13-C15
36	A	411	LHG	O2-C2-C3-O3
36	D	409	LHG	O2-C2-C3-O3
36	d	405	LHG	O2-C2-C3-O3
36	4	318	LHG	O2-C2-C3-O3
43	3	301	LMU	O1'-C1-C2-C3
33	c	505	CLA	CBA-CGA-O2A-C1
33	c	513	CLA	CBA-CGA-O2A-C1
33	3	309	CLA	O1A-CGA-O2A-C1
36	H	104	LHG	C7-C8-C9-C10
37	a	413	SQD	C7-C8-C9-C10
38	a	401	DGD	C1B-C2B-C3B-C4B
39	C	521	LMG	C10-C11-C12-C13
39	b	621	LMG	C28-C29-C30-C31
33	C	502	CLA	C10-C11-C12-C13
33	8	308	CLA	C5-C6-C7-C8
43	T	102	LMU	C4B-C5B-C6B-O6B
43	t	101	LMU	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
33	A	408	CLA	C3-C5-C6-C7
33	5	312	CLA	O1D-CGD-O2D-CED
33	1	306	CLA	O1D-CGD-O2D-CED
33	b	610	CLA	C13-C15-C16-C17
36	A	411	LHG	C23-C24-C25-C26
39	D	410	LMG	C10-C11-C12-C13
33	H	103	CLA	O1A-CGA-O2A-C1
33	A	404	CLA	C15-C16-C17-C18
33	C	510	CLA	C8-C10-C11-C12
33	3	304	CLA	C8-C10-C11-C12
33	3	313	CLA	C10-C11-C12-C13
33	4	311	CLA	C8-C10-C11-C12
33	b	607	CLA	C10-C11-C12-C13
33	b	615	CLA	C15-C16-C17-C18
33	8	310	CLA	C5-C6-C7-C8
33	C	503	CLA	CBA-CGA-O2A-C1
33	4	311	CLA	CBA-CGA-O2A-C1
33	B	612	CLA	CBD-CGD-O2D-CED
39	c	519	LMG	C11-C10-O7-C8
47	7	306	KC2	C2A-CAA-CBA-CGA
33	C	504	CLA	O1A-CGA-O2A-C1
33	c	508	CLA	C5-C6-C7-C8
46	9	304	DD6	C3-C4-C5-C6
46	2	304	DD6	C3-C4-C5-C6
46	8	304	DD6	C11-C10-C9-C8
46	8	304	DD6	C3-C4-C5-C6
48	0	302	ET4	C19-C20-C21-C22
33	7	307	CLA	C10-C11-C12-C13
39	w	304	LMG	C28-C29-C30-C31
36	A	411	LHG	C1-C2-C3-O3
36	D	409	LHG	C1-C2-C3-O3
36	d	405	LHG	C1-C2-C3-O3
36	4	318	LHG	C1-C2-C3-O3
33	c	501	CLA	C2A-CAA-CBA-CGA
33	B	616	CLA	CBA-CGA-O2A-C1
36	W	302	LHG	C24-C23-O8-C6
37	D	403	SQD	C24-C23-O48-C46
33	B	609	CLA	C15-C16-C17-C18
33	B	613	CLA	C15-C16-C17-C18
33	C	503	CLA	C5-C6-C7-C8
33	C	504	CLA	C13-C15-C16-C17
33	C	505	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	b	609	CLA	C15-C16-C17-C18
33	b	610	CLA	C15-C16-C17-C18
33	c	502	CLA	O1D-CGD-O2D-CED
42	v	201	HEM	C3A-C2A-CAA-CBA
33	B	615	CLA	C15-C16-C17-C18
33	C	501	CLA	C10-C11-C12-C13
33	C	505	CLA	C15-C16-C17-C18
33	d	402	CLA	C5-C6-C7-C8
33	b	606	CLA	C15-C16-C17-C18
33	b	615	CLA	C8-C10-C11-C12
39	C	522	LMG	C4-C5-C6-O5
39	7	315	LMG	C4-C5-C6-O5
33	C	503	CLA	C8-C10-C11-C12
33	C	512	CLA	C15-C16-C17-C18
33	c	512	CLA	C8-C10-C11-C12
33	3	302	CLA	C10-C11-C12-C13
33	4	308	CLA	C15-C16-C17-C18
33	7	305	CLA	C8-C10-C11-C12
33	3	312	CLA	CBA-CGA-O2A-C1
33	3	319	CLA	CBA-CGA-O2A-C1
33	0	309	CLA	CBA-CGA-O2A-C1
36	h	103	LHG	C7-C8-C9-C10
33	3	313	CLA	C4-C3-C5-C6
33	b	605	CLA	C4-C3-C5-C6
36	3	318	LHG	C8-C7-O7-C5
34	a	409	PHO	C14-C13-C15-C16
39	b	622	LMG	C4-C5-C6-O5
33	8	310	CLA	O1A-CGA-O2A-C1
37	T	103	SQD	O49-C7-O47-C45
37	i	101	SQD	C2-C1-O6-C44
37	L	101	SQD	C2-C1-O6-C44
38	A	415	DGD	C2D-C1D-O3G-C3G
38	C	517	DGD	C2E-C1E-O5D-C6D
38	C	518	DGD	C2D-C1D-O3G-C3G
38	a	401	DGD	C2D-C1D-O3G-C3G
39	c	520	LMG	C2-C1-O1-C7
39	D	404	LMG	C2-C1-O1-C7
43	w	302	LMU	C2'-C1'-O1'-C1
38	H	102	DGD	C1A-C2A-C3A-C4A
43	4	317	LMU	C4'-C5'-C6'-O6'
36	b	601	LHG	O2-C2-C3-O3
43	4	317	LMU	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
33	C	505	CLA	CBA-CGA-O2A-C1
33	c	501	CLA	CBA-CGA-O2A-C1
33	3	305	CLA	CBA-CGA-O2A-C1
33	0	312	CLA	C16-C17-C18-C19
43	3	301	LMU	C3-C4-C5-C6
33	b	613	CLA	C15-C16-C17-C18
33	1	308	CLA	C5-C6-C7-C8
30	d	403	BCR	C20-C21-C22-C37
30	b	620	BCR	C20-C21-C22-C37
43	t	101	LMU	O5'-C5'-C6'-O6'
33	b	606	CLA	C5-C6-C7-C8
33	b	607	CLA	C8-C10-C11-C12
30	c	515	BCR	C7-C8-C9-C34
30	h	101	BCR	C7-C8-C9-C34
30	K	101	BCR	C11-C12-C13-C35
46	8	303	DD6	C12-C11-C13-C14
46	8	304	DD6	C7-C6-C8-C9
46	1	303	DD6	C12-C11-C13-C14
46	1	304	DD6	C-C1-C24-C25
48	7	302	ET4	C30-C18-C19-C20
48	0	302	ET4	C07-C08-C09-C27
30	k	101	BCR	C11-C12-C13-C14
46	8	303	DD6	C10-C11-C13-C14
46	8	304	DD6	C5-C6-C8-C9
46	1	303	DD6	C10-C11-C13-C14
46	1	304	DD6	C2-C1-C24-C25
48	7	302	ET4	C07-C08-C09-C10
48	0	302	ET4	C11-C12-C13-C14
48	0	302	ET4	C17-C18-C19-C20
48	0	302	ET4	C07-C08-C09-C10
42	v	201	HEM	C2A-CAA-CBA-CGA
33	C	503	CLA	O1A-CGA-O2A-C1
33	4	311	CLA	O1A-CGA-O2A-C1
33	7	309	CLA	O1A-CGA-O2A-C1
45	6	306	A86	C35-C34-O4-C38
33	B	602	CLA	C2A-CAA-CBA-CGA
33	B	616	CLA	C2A-CAA-CBA-CGA
33	c	503	CLA	C2A-CAA-CBA-CGA
33	c	507	CLA	C2A-CAA-CBA-CGA
33	b	604	CLA	C2A-CAA-CBA-CGA
33	B	615	CLA	C10-C11-C12-C13
36	D	411	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
36	d	407	LHG	O1-C1-C2-C3
36	H	104	LHG	O1-C1-C2-C3
36	W	302	LHG	O1-C1-C2-C3
36	w	301	LHG	O1-C1-C2-C3
39	W	301	LMG	C10-C11-C12-C13
36	4	318	LHG	C6-C5-O7-C7
37	T	101	SQD	C46-C45-O47-C7
37	t	102	SQD	C46-C45-O47-C7
33	3	302	CLA	C16-C17-C18-C20
33	b	613	CLA	C16-C17-C18-C19
33	c	505	CLA	O1A-CGA-O2A-C1
33	7	304	CLA	O1A-CGA-O2A-C1
33	c	509	CLA	C3-C5-C6-C7
33	B	609	CLA	C13-C15-C16-C17
33	c	504	CLA	C13-C15-C16-C17
33	a	407	CLA	C15-C16-C17-C18
30	K	101	BCR	C20-C21-C22-C23
30	k	101	BCR	C16-C17-C18-C19
30	k	101	BCR	C20-C21-C22-C23
37	a	413	SQD	C12-C13-C14-C15
43	5	320	LMU	C1-C2-C3-C4
38	C	516	DGD	O6D-C1D-O3G-C3G
38	c	518	DGD	O6D-C1D-O3G-C3G
39	q	301	LMG	C11-C10-O7-C8
33	4	314	CLA	O1D-CGD-O2D-CED
33	B	606	CLA	C8-C10-C11-C12
33	b	617	CLA	C5-C6-C7-C8
33	c	505	CLA	C16-C17-C18-C20
33	D	406	CLA	C11-C12-C13-C15
33	7	309	CLA	C16-C17-C18-C20
33	C	507	CLA	C13-C15-C16-C17
33	3	306	CLA	C15-C16-C17-C18
39	D	404	LMG	O6-C5-C6-O5
36	H	104	LHG	C12-C13-C14-C15
36	0	315	LHG	C28-C29-C30-C31
37	7	317	SQD	C31-C32-C33-C34
39	q	301	LMG	C14-C15-C16-C17
39	q	301	LMG	C38-C39-C40-C41
36	A	412	LHG	C26-C27-C28-C29
36	W	302	LHG	C11-C10-C9-C8
37	L	101	SQD	C30-C31-C32-C33
37	T	103	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
38	H	102	DGD	C9A-CAA-CBA-CCA
36	h	103	LHG	C15-C16-C17-C18
37	L	101	SQD	C9-C10-C11-C12
37	l	101	SQD	C9-C10-C11-C12
37	T	103	SQD	C11-C12-C13-C14
39	M	201	LMG	C30-C31-C32-C33
33	c	513	CLA	O1A-CGA-O2A-C1
36	D	409	LHG	C14-C15-C16-C17
36	7	316	LHG	C24-C25-C26-C27
36	b	601	LHG	C12-C13-C14-C15
36	0	315	LHG	C29-C30-C31-C32
37	a	413	SQD	C10-C11-C12-C13
38	c	518	DGD	C6B-C7B-C8B-C9B
39	B	620	LMG	C31-C32-C33-C34
39	B	620	LMG	C33-C34-C35-C36
39	B	620	LMG	C37-C38-C39-C40
39	C	520	LMG	C19-C20-C21-C22
39	d	406	LMG	C32-C33-C34-C35
39	W	301	LMG	C12-C13-C14-C15
39	w	304	LMG	C18-C19-C20-C21
39	b	621	LMG	C13-C14-C15-C16
39	b	621	LMG	C36-C37-C38-C39
36	3	318	LHG	O9-C7-O7-C5
38	A	415	DGD	O1B-C1B-O2G-C2G
36	A	411	LHG	O1-C1-C2-O2
36	D	409	LHG	O1-C1-C2-O2
36	D	411	LHG	O1-C1-C2-O2
36	h	103	LHG	O1-C1-C2-O2
36	W	302	LHG	O1-C1-C2-O2
43	w	302	LMU	C2-C1-O1'-C1'
33	c	504	CLA	C11-C10-C8-C7
38	C	518	DGD	C6A-C7A-C8A-C9A
39	d	410	LMG	C32-C33-C34-C35
39	m	201	LMG	C30-C31-C32-C33
43	w	302	LMU	C7-C8-C9-C10
33	W	303	CLA	C4B-C3B-CAB-CBB
33	8	305	CLA	C4B-C3B-CAB-CBB
33	8	314	CLA	C4B-C3B-CAB-CBB
33	8	316	CLA	C4B-C3B-CAB-CBB
36	D	409	LHG	C23-C24-C25-C26
33	b	604	CLA	C13-C15-C16-C17
36	a	404	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
38	C	518	DGD	C2B-C3B-C4B-C5B
38	c	518	DGD	C6A-C7A-C8A-C9A
39	w	304	LMG	C33-C34-C35-C36
43	3	301	LMU	C4-C5-C6-C7
33	6	313	CLA	CBA-CGA-O2A-C1
33	B	615	CLA	C16-C17-C18-C19
33	B	615	CLA	C16-C17-C18-C20
33	c	504	CLA	C16-C17-C18-C20
33	5	309	CLA	C6-C7-C8-C9
33	7	309	CLA	C16-C17-C18-C19
33	b	613	CLA	C16-C17-C18-C20
33	0	312	CLA	C16-C17-C18-C20
33	6	316	CLA	O1D-CGD-O2D-CED
33	C	503	CLA	C2A-CAA-CBA-CGA
39	b	621	LMG	C15-C16-C17-C18
33	5	313	CLA	C10-C11-C12-C13
36	D	411	LHG	C8-C7-O7-C5
36	a	404	LHG	C14-C15-C16-C17
39	0	314	LMG	C32-C33-C34-C35
43	3	301	LMU	C4B-C5B-C6B-O6B
43	3	301	LMU	C4'-C5'-C6'-O6'
33	c	503	CLA	C6-C7-C8-C10
33	c	508	CLA	C12-C13-C15-C16
33	W	303	CLA	C11-C12-C13-C15
33	W	303	CLA	C12-C13-C15-C16
33	4	311	CLA	C6-C7-C8-C10
43	w	302	LMU	O1'-C1-C2-C3
36	D	411	LHG	C27-C28-C29-C30
38	C	517	DGD	C5B-C6B-C7B-C8B
39	b	623	LMG	C31-C32-C33-C34
37	B	622	SQD	C7-C8-C9-C10
39	c	520	LMG	C10-C11-C12-C13
33	3	319	CLA	O1A-CGA-O2A-C1
33	C	511	CLA	C3-C5-C6-C7
33	A	404	CLA	C3A-C2A-CAA-CBA
33	B	616	CLA	C3A-C2A-CAA-CBA
33	D	405	CLA	C3A-C2A-CAA-CBA
33	3	304	CLA	C3A-C2A-CAA-CBA
33	4	309	CLA	C3A-C2A-CAA-CBA
33	6	308	CLA	C3A-C2A-CAA-CBA
33	6	311	CLA	C3A-C2A-CAA-CBA
33	7	310	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
33	b	617	CLA	C3A-C2A-CAA-CBA
33	0	310	CLA	C3A-C2A-CAA-CBA
33	9	307	CLA	C3A-C2A-CAA-CBA
33	2	307	CLA	C3A-C2A-CAA-CBA
33	2	312	CLA	C3A-C2A-CAA-CBA
33	8	310	CLA	C3A-C2A-CAA-CBA
33	1	312	CLA	C3A-C2A-CAA-CBA
36	d	405	LHG	C30-C31-C32-C33
38	C	518	DGD	C4B-C5B-C6B-C7B
39	C	520	LMG	C34-C35-C36-C37
39	W	301	LMG	C18-C19-C20-C21
43	5	320	LMU	C3-C4-C5-C6
33	6	311	CLA	CBA-CGA-O2A-C1
36	D	411	LHG	C11-C10-C9-C8
36	H	104	LHG	C15-C16-C17-C18
38	c	517	DGD	C5B-C6B-C7B-C8B
39	M	201	LMG	C32-C33-C34-C35
39	w	304	LMG	C29-C30-C31-C32
33	C	508	CLA	C10-C11-C12-C13
33	c	505	CLA	C15-C16-C17-C18
39	0	314	LMG	C28-C29-C30-C31
36	b	601	LHG	C30-C31-C32-C33
30	k	101	BCR	C13-C14-C15-C16
45	7	301	A86	C1-C2-C3-C4
45	0	301	A86	C1-C2-C3-C4
45	8	302	A86	C24-C25-C26-C27
45	1	302	A86	C24-C25-C26-C27
48	7	302	ET4	C15-C16-C17-C18
33	5	309	CLA	C6-C7-C8-C10
33	B	616	CLA	O1A-CGA-O2A-C1
33	3	312	CLA	O1A-CGA-O2A-C1
37	T	101	SQD	C27-C28-C29-C30
38	c	518	DGD	C5B-C6B-C7B-C8B
38	3	320	DGD	C6A-C7A-C8A-C9A
39	D	410	LMG	C12-C13-C14-C15
39	7	315	LMG	C21-C22-C23-C24
33	B	607	CLA	CBD-CGD-O2D-CED
36	4	318	LHG	C32-C33-C34-C35
36	0	315	LHG	C24-C25-C26-C27
38	A	415	DGD	C4B-C5B-C6B-C7B
38	C	518	DGD	C5B-C6B-C7B-C8B
39	D	404	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
39	M	201	LMG	C14-C15-C16-C17
36	b	601	LHG	C1-C2-C3-O3
33	d	402	CLA	CBA-CGA-O2A-C1
33	b	613	CLA	CBA-CGA-O2A-C1
33	b	617	CLA	CBA-CGA-O2A-C1
39	C	520	LMG	C29-C28-O8-C9
39	b	622	LMG	O1-C7-C8-C9
33	B	602	CLA	C8-C10-C11-C12
36	A	414	LHG	C24-C25-C26-C27
36	0	315	LHG	C27-C28-C29-C30
37	D	403	SQD	C9-C10-C11-C12
37	L	101	SQD	C16-C17-C18-C19
37	0	316	SQD	C31-C32-C33-C34
38	c	518	DGD	C2B-C3B-C4B-C5B
38	3	320	DGD	C5A-C6A-C7A-C8A
36	d	407	LHG	C23-C24-C25-C26
36	0	315	LHG	C23-C24-C25-C26
39	c	519	LMG	C10-C11-C12-C13
37	0	316	SQD	C10-C11-C12-C13
38	C	516	DGD	C5B-C6B-C7B-C8B
39	m	201	LMG	C32-C33-C34-C35
33	C	505	CLA	O1A-CGA-O2A-C1
33	c	501	CLA	O1A-CGA-O2A-C1
33	3	305	CLA	O1A-CGA-O2A-C1
33	0	309	CLA	O1A-CGA-O2A-C1
36	b	601	LHG	C24-C25-C26-C27
38	c	517	DGD	C6A-C7A-C8A-C9A
39	c	519	LMG	C13-C14-C15-C16
39	c	519	LMG	C30-C31-C32-C33
39	7	315	LMG	C30-C31-C32-C33
36	W	302	LHG	C28-C29-C30-C31
36	4	318	LHG	C24-C25-C26-C27
33	2	310	CLA	C5-C6-C7-C8
36	3	318	LHG	C27-C28-C29-C30
36	4	318	LHG	C27-C28-C29-C30
39	w	304	LMG	C34-C35-C36-C37
39	b	623	LMG	C11-C12-C13-C14
39	0	314	LMG	C33-C34-C35-C36
43	3	301	LMU	C11-C10-C9-C8
30	B	617	BCR	C1-C6-C7-C8
30	b	618	BCR	C1-C6-C7-C8
30	b	618	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	B	601	CLA	C2B-C3B-CAB-CBB
33	W	303	CLA	C2B-C3B-CAB-CBB
33	2	305	CLA	C2B-C3B-CAB-CBB
33	8	305	CLA	C2B-C3B-CAB-CBB
33	8	314	CLA	C2B-C3B-CAB-CBB
33	8	316	CLA	C2B-C3B-CAB-CBB
33	1	314	CLA	C2B-C3B-CAB-CBB
48	7	302	ET4	C01-C06-C07-C08
48	0	302	ET4	C01-C06-C07-C08
48	0	302	ET4	C05-C06-C07-C08
36	D	409	LHG	C32-C33-C34-C35
36	h	103	LHG	C11-C10-C9-C8
37	t	102	SQD	C26-C27-C28-C29
37	7	317	SQD	C24-C25-C26-C27
38	c	517	DGD	C4B-C5B-C6B-C7B
39	C	520	LMG	C30-C31-C32-C33
39	7	315	LMG	C12-C13-C14-C15
39	Q	301	LMG	C30-C31-C32-C33
33	C	502	CLA	CBD-CGD-O2D-CED
33	5	313	CLA	CBD-CGD-O2D-CED
33	0	310	CLA	CBD-CGD-O2D-CED
36	d	407	LHG	C8-C7-O7-C5
33	C	501	CLA	CBA-CGA-O2A-C1
33	3	307	CLA	C5-C6-C7-C8
33	0	307	CLA	C15-C16-C17-C18
33	3	307	CLA	C3-C5-C6-C7
33	3	319	CLA	C3-C5-C6-C7
37	7	317	SQD	C10-C11-C12-C13
39	B	620	LMG	C13-C14-C15-C16
43	4	317	LMU	C11-C10-C9-C8
33	b	617	CLA	C2A-CAA-CBA-CGA
33	8	307	CLA	C2A-CAA-CBA-CGA
36	4	318	LHG	C23-C24-C25-C26
36	a	403	LHG	C7-C8-C9-C10
33	0	307	CLA	C10-C11-C12-C13
39	B	620	LMG	C17-C18-C19-C20
39	b	621	LMG	C31-C32-C33-C34
37	0	316	SQD	C12-C13-C14-C15
39	b	621	LMG	C17-C18-C19-C20
39	C	520	LMG	O9-C10-O7-C8
33	c	502	CLA	C4-C3-C5-C6
39	B	620	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
39	q	301	LMG	C13-C14-C15-C16
33	3	302	CLA	C15-C16-C17-C18
33	3	313	CLA	C2-C3-C5-C6
33	b	605	CLA	C2-C3-C5-C6
36	d	405	LHG	C13-C14-C15-C16
36	a	404	LHG	C27-C28-C29-C30
37	T	103	SQD	C10-C11-C12-C13
38	C	517	DGD	C6A-C7A-C8A-C9A
39	B	620	LMG	C15-C16-C17-C18
39	c	519	LMG	C33-C34-C35-C36
33	C	512	CLA	CBA-CGA-O2A-C1
33	c	511	CLA	CBA-CGA-O2A-C1
36	0	315	LHG	C24-C23-O8-C6
33	C	504	CLA	C11-C12-C13-C14
33	6	312	CLA	C6-C7-C8-C9
33	b	612	CLA	C12-C13-C15-C16
38	A	415	DGD	C3B-C4B-C5B-C6B
38	H	102	DGD	C4A-C5A-C6A-C7A
33	2	308	CLA	C5-C6-C7-C8
36	A	412	LHG	C14-C15-C16-C17
38	a	401	DGD	C5B-C6B-C7B-C8B
39	w	304	LMG	C31-C32-C33-C34
43	T	102	LMU	C4-C5-C6-C7
39	0	314	LMG	C17-C18-C19-C20
43	T	102	LMU	O5'-C5'-C6'-O6'
43	t	101	LMU	C2'-C1'-O1'-C1
33	B	614	CLA	CBD-CGD-O2D-CED
33	2	311	CLA	C5-C6-C7-C8
36	D	409	LHG	C13-C14-C15-C16
36	D	409	LHG	C28-C29-C30-C31
36	d	405	LHG	C14-C15-C16-C17
39	Q	301	LMG	C28-C29-C30-C31
36	D	409	LHG	C11-C12-C13-C14
37	l	101	SQD	C29-C30-C31-C32
37	0	316	SQD	C11-C12-C13-C14
38	c	516	DGD	C5B-C6B-C7B-C8B
39	q	302	LMG	C30-C31-C32-C33
37	l	101	SQD	C16-C17-C18-C19
39	C	520	LMG	C32-C33-C34-C35
33	C	511	CLA	CBA-CGA-O2A-C1
45	9	302	A86	C1-C2-C3-C4
45	2	302	A86	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
48	7	302	ET4	C09-C10-C11-C12
48	0	302	ET4	C09-C10-C11-C12
33	A	408	CLA	C11-C12-C13-C14
33	c	505	CLA	C16-C17-C18-C19
33	d	402	CLA	C11-C12-C13-C15
33	9	311	CLA	C6-C7-C8-C10
39	C	520	LMG	C11-C10-O7-C8
36	3	317	LHG	C7-C8-C9-C10
36	A	412	LHG	C24-C25-C26-C27
39	w	304	LMG	C12-C13-C14-C15
39	7	315	LMG	C31-C32-C33-C34
33	3	302	CLA	C8-C10-C11-C12
34	a	409	PHO	C5-C6-C7-C8
33	7	314	CLA	O1A-CGA-O2A-C1
36	h	103	LHG	C16-C17-C18-C19
38	h	102	DGD	C4A-C5A-C6A-C7A
38	C	516	DGD	C5A-C6A-C7A-C8A
45	4	302	A86	C35-C34-O4-C38
39	D	410	LMG	C32-C33-C34-C35
41	d	404	PL9	C37-C38-C39-C40
36	A	414	LHG	C11-C10-C9-C8
36	d	407	LHG	C11-C10-C9-C8
38	h	102	DGD	CAB-CBB-CCB-CDB
33	9	317	CLA	C3-C5-C6-C7
48	7	302	ET4	C17-C18-C19-C20
37	a	413	SQD	C45-C44-O6-C1
39	b	623	LMG	C8-C7-O1-C1
36	D	409	LHG	C24-C25-C26-C27
38	C	516	DGD	C4B-C5B-C6B-C7B
39	D	404	LMG	C33-C34-C35-C36
39	m	201	LMG	C11-C12-C13-C14
33	6	311	CLA	C2A-CAA-CBA-CGA
33	A	408	CLA	C11-C12-C13-C15
33	C	508	CLA	C16-C17-C18-C20
33	D	406	CLA	C11-C12-C13-C14
36	h	103	LHG	C12-C13-C14-C15
36	7	316	LHG	C27-C28-C29-C30
39	C	519	LMG	C14-C15-C16-C17
39	0	314	LMG	C30-C31-C32-C33
33	B	609	CLA	C4-C3-C5-C6
33	C	502	CLA	C4-C3-C5-C6
33	d	402	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
42	e	101	HEM	C2B-C3B-CAB-CBB
47	7	306	KC2	C2C-C3C-CAC-CBC
33	b	612	CLA	C13-C15-C16-C17
38	H	102	DGD	CBA-CCA-CDA-CEA
39	D	404	LMG	C32-C33-C34-C35
43	4	317	LMU	C4-C5-C6-C7
33	B	603	CLA	O1D-CGD-O2D-CED
33	C	507	CLA	C15-C16-C17-C18
33	b	612	CLA	C8-C10-C11-C12
33	0	309	CLA	C5-C6-C7-C8
33	0	312	CLA	C13-C15-C16-C17
38	a	401	DGD	C3B-C4B-C5B-C6B
33	0	309	CLA	O1D-CGD-O2D-CED
33	b	613	CLA	O1A-CGA-O2A-C1
33	b	617	CLA	O1A-CGA-O2A-C1
33	B	612	CLA	C8-C10-C11-C12
34	A	406	PHO	C13-C15-C16-C17
36	A	414	LHG	C12-C13-C14-C15
39	W	301	LMG	C37-C38-C39-C40
39	0	314	LMG	O6-C5-C6-O5
36	7	316	LHG	C28-C29-C30-C31
39	d	410	LMG	C31-C32-C33-C34
43	4	317	LMU	C1-C2-C3-C4
39	5	319	LMG	C11-C10-O7-C8
33	7	309	CLA	C5-C6-C7-C8
33	b	612	CLA	C15-C16-C17-C18
33	b	617	CLA	C13-C15-C16-C17
33	0	307	CLA	C8-C10-C11-C12
42	v	201	HEM	C4C-C3C-CAC-CBC
47	5	310	KC2	C2A-CAA-CBA-CGA
47	6	309	KC2	C4C-C3C-CAC-CBC
47	7	306	KC2	C4B-C3B-CAB-CBB
33	C	508	CLA	C16-C17-C18-C19
33	3	302	CLA	C16-C17-C18-C19
37	L	101	SQD	C29-C30-C31-C32
39	d	406	LMG	C18-C19-C20-C21
39	C	519	LMG	O10-C28-O8-C9
33	b	615	CLA	O1D-CGD-O2D-CED
38	c	517	DGD	C3A-C4A-C5A-C6A
39	W	301	LMG	C34-C35-C36-C37
37	T	103	SQD	C7-C8-C9-C10
33	0	305	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
36	A	411	LHG	C27-C28-C29-C30
36	w	301	LHG	C11-C10-C9-C8
36	w	301	LHG	C27-C28-C29-C30
39	q	301	LMG	C39-C40-C41-C42
36	0	315	LHG	O7-C5-C6-O8
37	T	101	SQD	O6-C44-C45-O47
39	C	522	LMG	O7-C8-C9-O8
39	M	201	LMG	O7-C8-C9-O8
36	D	409	LHG	C30-C31-C32-C33
37	l	101	SQD	C30-C31-C32-C33
39	q	302	LMG	C32-C33-C34-C35
33	0	312	CLA	CBA-CGA-O2A-C1
36	a	404	LHG	C10-C11-C12-C13
39	7	315	LMG	C16-C17-C18-C19
39	7	315	LMG	C33-C34-C35-C36
33	C	512	CLA	C5-C6-C7-C8
39	W	301	LMG	O6-C5-C6-O5
36	A	414	LHG	C27-C28-C29-C30
37	i	101	SQD	C9-C10-C11-C12
39	C	519	LMG	C33-C34-C35-C36
43	w	302	LMU	C11-C10-C9-C8
36	b	601	LHG	C27-C28-C29-C30
37	T	103	SQD	C24-C25-C26-C27
38	C	517	DGD	C3A-C4A-C5A-C6A
38	c	518	DGD	C4B-C5B-C6B-C7B
33	3	311	CLA	O1D-CGD-O2D-CED
36	w	301	LHG	C5-C4-O6-P
36	3	317	LHG	C11-C10-C9-C8
39	B	620	LMG	C19-C20-C21-C22
33	C	502	CLA	C6-C7-C8-C10
33	3	303	CLA	C4-C3-C5-C6
42	F	101	HEM	C3D-CAD-CBD-CGD
33	B	609	CLA	C2-C3-C5-C6
41	D	408	PL9	C13-C14-C16-C17
37	D	403	SQD	O49-C7-O47-C45
36	3	318	LHG	C1-C2-C3-O3
36	A	414	LHG	C26-C27-C28-C29
39	B	620	LMG	C36-C37-C38-C39
39	0	314	LMG	C34-C35-C36-C37
33	B	603	CLA	C2A-CAA-CBA-CGA
33	c	505	CLA	C2A-CAA-CBA-CGA
33	3	308	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
33	4	311	CLA	C2A-CAA-CBA-CGA
33	9	312	CLA	C2A-CAA-CBA-CGA
33	2	308	CLA	CBD-CGD-O2D-CED
36	A	411	LHG	C29-C30-C31-C32
39	Q	301	LMG	C31-C32-C33-C34
43	t	101	LMU	C3-C4-C5-C6
37	B	622	SQD	C9-C10-C11-C12
38	H	102	DGD	C1B-C2B-C3B-C4B
39	C	520	LMG	C18-C19-C20-C21
39	W	301	LMG	C32-C33-C34-C35
37	a	413	SQD	C9-C10-C11-C12
39	M	201	LMG	C11-C12-C13-C14
33	9	311	CLA	C6-C7-C8-C9
36	d	405	LHG	O1-C1-C2-O2
36	w	301	LHG	O1-C1-C2-O2
36	a	403	LHG	O1-C1-C2-O2
33	C	501	CLA	O1A-CGA-O2A-C1
33	3	306	CLA	C3-C5-C6-C7
33	9	311	CLA	C3-C5-C6-C7
39	D	404	LMG	C11-C12-C13-C14
37	0	316	SQD	C9-C10-C11-C12
38	H	102	DGD	CAB-CBB-CCB-CDB
39	d	410	LMG	C12-C13-C14-C15
33	A	404	CLA	C1A-C2A-CAA-CBA
33	B	612	CLA	C1A-C2A-CAA-CBA
33	B	614	CLA	C1A-C2A-CAA-CBA
33	B	616	CLA	C1A-C2A-CAA-CBA
33	C	501	CLA	C1A-C2A-CAA-CBA
33	c	501	CLA	C1A-C2A-CAA-CBA
33	D	402	CLA	C1A-C2A-CAA-CBA
33	d	409	CLA	C1A-C2A-CAA-CBA
33	3	304	CLA	C1A-C2A-CAA-CBA
33	4	309	CLA	C1A-C2A-CAA-CBA
33	4	311	CLA	C1A-C2A-CAA-CBA
33	5	311	CLA	C1A-C2A-CAA-CBA
33	5	312	CLA	C1A-C2A-CAA-CBA
33	6	311	CLA	C1A-C2A-CAA-CBA
33	7	307	CLA	C1A-C2A-CAA-CBA
33	7	310	CLA	C1A-C2A-CAA-CBA
33	7	311	CLA	C1A-C2A-CAA-CBA
33	b	615	CLA	C1A-C2A-CAA-CBA
33	b	617	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
33	0	304	CLA	C1A-C2A-CAA-CBA
33	0	307	CLA	C1A-C2A-CAA-CBA
33	0	310	CLA	C1A-C2A-CAA-CBA
33	0	311	CLA	C1A-C2A-CAA-CBA
33	9	307	CLA	C1A-C2A-CAA-CBA
33	2	308	CLA	C1A-C2A-CAA-CBA
33	2	312	CLA	C1A-C2A-CAA-CBA
33	8	308	CLA	C1A-C2A-CAA-CBA
33	8	309	CLA	C1A-C2A-CAA-CBA
33	1	308	CLA	C1A-C2A-CAA-CBA
33	1	309	CLA	C1A-C2A-CAA-CBA
33	1	312	CLA	C1A-C2A-CAA-CBA
33	0	312	CLA	C15-C16-C17-C18
43	4	317	LMU	C6-C7-C8-C9
38	c	518	DGD	C5A-C6A-C7A-C8A
33	c	511	CLA	O1A-CGA-O2A-C1
36	3	318	LHG	C32-C33-C34-C35
38	h	102	DGD	CBA-CCA-CDA-CEA
39	d	410	LMG	C29-C30-C31-C32
39	M	201	LMG	C31-C32-C33-C34
43	3	301	LMU	C7-C8-C9-C10
33	c	504	CLA	C10-C11-C12-C13
36	4	318	LHG	O6-C4-C5-C6
38	c	518	DGD	O6E-C5E-C6E-O5E
38	c	517	DGD	CBB-CCB-CDB-CEB
38	h	102	DGD	C9B-CAB-CBB-CCB
33	7	305	CLA	C3-C5-C6-C7
33	A	408	CLA	C6-C7-C8-C10
33	A	408	CLA	C11-C10-C8-C7
33	C	502	CLA	C12-C13-C15-C16
33	C	509	CLA	C6-C7-C8-C10
33	C	512	CLA	C11-C12-C13-C15
33	c	507	CLA	C11-C12-C13-C15
33	c	507	CLA	C12-C13-C15-C16
33	c	508	CLA	C11-C10-C8-C7
33	c	511	CLA	C12-C13-C15-C16
33	w	303	CLA	C12-C13-C15-C16
33	3	303	CLA	C11-C12-C13-C15
33	3	308	CLA	C12-C13-C15-C16
33	3	313	CLA	C11-C10-C8-C7
33	b	614	CLA	C11-C10-C8-C7
33	b	614	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
33	8	310	CLA	C6-C7-C8-C10
33	1	310	CLA	C11-C12-C13-C15
33	1	310	CLA	C12-C13-C15-C16
37	L	101	SQD	C17-C18-C19-C20
33	d	402	CLA	C11-C12-C13-C14
33	C	512	CLA	O1A-CGA-O2A-C1
38	c	517	DGD	C2A-C3A-C4A-C5A
39	C	519	LMG	C39-C40-C41-C42
36	D	411	LHG	C23-C24-C25-C26
33	9	308	CLA	C4-C3-C5-C6
36	a	404	LHG	C32-C33-C34-C35
39	0	314	LMG	C14-C15-C16-C17
38	3	320	DGD	C4A-C5A-C6A-C7A
33	7	309	CLA	C8-C10-C11-C12
33	C	505	CLA	C2A-CAA-CBA-CGA
33	3	303	CLA	C2A-CAA-CBA-CGA
33	3	305	CLA	C2A-CAA-CBA-CGA
33	7	309	CLA	C2A-CAA-CBA-CGA
33	B	616	CLA	C11-C10-C8-C9
33	C	507	CLA	C6-C7-C8-C9
33	C	507	CLA	C14-C13-C15-C16
33	C	511	CLA	C14-C13-C15-C16
33	C	512	CLA	C11-C12-C13-C14
33	c	505	CLA	C11-C12-C13-C14
33	3	308	CLA	C14-C13-C15-C16
33	4	309	CLA	C6-C7-C8-C9
33	4	311	CLA	C6-C7-C8-C9
33	b	603	CLA	C11-C12-C13-C14
33	0	305	CLA	C6-C7-C8-C9
33	8	310	CLA	C6-C7-C8-C9
33	8	310	CLA	C14-C13-C15-C16
36	5	318	LHG	C11-C12-C13-C14
39	c	519	LMG	C17-C18-C19-C20
43	4	317	LMU	C2-C3-C4-C5
39	D	410	LMG	C18-C19-C20-C21
39	d	406	LMG	C12-C13-C14-C15
33	C	510	CLA	CBA-CGA-O2A-C1
33	C	513	CLA	CBA-CGA-O2A-C1
36	d	405	LHG	C24-C23-O8-C6
37	A	413	SQD	C24-C23-O48-C46
39	w	304	LMG	C37-C38-C39-C40
38	c	516	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
39	d	410	LMG	C4-C5-C6-O5
43	T	102	LMU	C2'-C1'-O1'-C1
37	A	413	SQD	C7-C8-C9-C10
39	D	404	LMG	C10-C11-C12-C13
36	A	414	LHG	C4-C5-C6-O8
36	W	302	LHG	C4-C5-C6-O8
36	b	601	LHG	C4-C5-C6-O8
36	0	315	LHG	C4-C5-C6-O8
37	D	403	SQD	O6-C44-C45-C46
38	A	415	DGD	O1G-C1G-C2G-C3G
38	A	415	DGD	C1G-C2G-C3G-O3G
38	C	518	DGD	O1G-C1G-C2G-C3G
38	a	401	DGD	O1G-C1G-C2G-C3G
39	C	519	LMG	O1-C7-C8-C9
39	c	520	LMG	C7-C8-C9-O8
39	d	410	LMG	O1-C7-C8-C9
39	w	304	LMG	O1-C7-C8-C9
39	3	316	LMG	O1-C7-C8-C9
39	Q	301	LMG	O1-C7-C8-C9
39	q	301	LMG	O1-C7-C8-C9
39	q	302	LMG	O1-C7-C8-C9
36	w	301	LHG	C28-C29-C30-C31
36	a	403	LHG	C11-C12-C13-C14
39	b	621	LMG	C19-C20-C21-C22
33	B	604	CLA	C10-C11-C12-C13
33	W	303	CLA	C5-C6-C7-C8
34	a	410	PHO	C5-C6-C7-C8
38	A	415	DGD	C4A-C5A-C6A-C7A
39	B	620	LMG	C16-C17-C18-C19
39	b	621	LMG	C33-C34-C35-C36
38	c	518	DGD	C2A-C1A-O1G-C1G
36	W	302	LHG	C7-C8-C9-C10
38	c	517	DGD	C1B-C2B-C3B-C4B
39	3	316	LMG	O6-C5-C6-O5
43	t	101	LMU	O5B-C5B-C6B-O6B
33	a	411	CLA	C11-C12-C13-C14
36	D	411	LHG	C16-C17-C18-C19
38	c	517	DGD	C7B-C8B-C9B-CAB
36	d	407	LHG	C27-C28-C29-C30
30	B	619	BCR	C20-C21-C22-C37
34	a	410	PHO	CHA-CBD-CGD-O1D
34	a	410	PHO	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
34	A	406	PHO	C5-C6-C7-C8
33	b	603	CLA	C5-C6-C7-C8
36	A	411	LHG	C11-C12-C13-C14
37	L	101	SQD	C18-C19-C20-C21
37	t	102	SQD	C24-C25-C26-C27
39	b	623	LMG	C13-C14-C15-C16
36	A	414	LHG	C7-C8-C9-C10
36	W	302	LHG	C23-C24-C25-C26
33	C	511	CLA	O1A-CGA-O2A-C1
33	0	312	CLA	O1A-CGA-O2A-C1
39	q	301	LMG	C33-C34-C35-C36
30	H	101	BCR	C7-C8-C9-C34
30	K	101	BCR	C7-C8-C9-C34
37	l	101	SQD	C25-C26-C27-C28
39	d	406	LMG	C21-C22-C23-C24
46	4	303	DD6	C10-C11-C13-C14
36	a	404	LHG	O10-C23-O8-C6
33	1	310	CLA	C5-C6-C7-C8
36	5	318	LHG	C4-O6-P-O5
39	W	301	LMG	C30-C31-C32-C33
38	3	320	DGD	CEB-CFB-CGB-CHB
38	a	401	DGD	C6B-C7B-C8B-C9B
39	B	620	LMG	C38-C39-C40-C41
38	H	102	DGD	C4B-C5B-C6B-C7B
39	D	410	LMG	C16-C17-C18-C19
36	A	414	LHG	C28-C29-C30-C31
36	a	404	LHG	C16-C17-C18-C19
39	b	621	LMG	C38-C39-C40-C41
33	3	304	CLA	O1D-CGD-O2D-CED
33	7	312	CLA	CBA-CGA-O2A-C1
38	3	320	DGD	C1G-C2G-O2G-C1B
39	c	519	LMG	C7-C8-O7-C10
39	D	404	LMG	C9-C8-O7-C10
39	d	406	LMG	C16-C17-C18-C19
39	b	623	LMG	C32-C33-C34-C35
30	k	101	BCR	C18-C19-C20-C21
33	B	614	CLA	C12-C13-C15-C16
37	T	103	SQD	C12-C13-C14-C15
38	h	102	DGD	C4B-C5B-C6B-C7B
39	C	519	LMG	C38-C39-C40-C41
39	Q	301	LMG	C32-C33-C34-C35
39	q	301	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
46	9	303	DD6	C3-C4-C5-C6
46	2	303	DD6	C3-C4-C5-C6
33	C	510	CLA	O1A-CGA-O2A-C1
33	w	303	CLA	CBD-CGD-O2D-CED
36	D	411	LHG	C9-C10-C11-C12
36	d	405	LHG	C28-C29-C30-C31
33	b	604	CLA	O1D-CGD-O2D-CED
38	a	401	DGD	C4A-C5A-C6A-C7A
33	B	605	CLA	C15-C16-C17-C18
37	7	317	SQD	C12-C13-C14-C15
38	C	517	DGD	C4A-C5A-C6A-C7A
43	w	302	LMU	C2-C3-C4-C5
43	w	302	LMU	C5-C6-C7-C8
36	3	318	LHG	C24-C25-C26-C27
39	b	621	LMG	C34-C35-C36-C37
44	3	310	KC1	CAA-CBA-CGA-O2A
36	A	411	LHG	C28-C29-C30-C31
39	d	406	LMG	C19-C20-C21-C22
38	C	517	DGD	C2A-C3A-C4A-C5A
39	w	304	LMG	C30-C31-C32-C33
36	d	405	LHG	C27-C28-C29-C30
36	a	403	LHG	O7-C5-C6-O8
37	0	316	SQD	O47-C45-C46-O48
36	A	411	LHG	C32-C33-C34-C35
36	4	318	LHG	C26-C27-C28-C29
37	t	102	SQD	C27-C28-C29-C30
33	D	406	CLA	CBA-CGA-O2A-C1
37	A	413	SQD	C10-C11-C12-C13
39	5	319	LMG	C30-C31-C32-C33
39	7	315	LMG	C42-C43-C44-C45
36	A	412	LHG	C33-C34-C35-C36
39	d	406	LMG	C35-C36-C37-C38
38	C	516	DGD	CAB-CBB-CCB-CDB
37	T	101	SQD	C34-C35-C36-C37
39	d	410	LMG	C33-C34-C35-C36
33	0	312	CLA	C5-C6-C7-C8
39	B	621	LMG	C4-C5-C6-O5
39	m	201	LMG	C31-C32-C33-C34
36	a	404	LHG	C28-C29-C30-C31
39	7	315	LMG	C13-C14-C15-C16
33	C	513	CLA	O1A-CGA-O2A-C1
39	5	319	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
33	a	407	CLA	C13-C15-C16-C17
36	A	412	LHG	C16-C17-C18-C19
33	4	316	CLA	CBA-CGA-O2A-C1
37	i	101	SQD	C10-C11-C12-C13
38	3	320	DGD	C6B-C7B-C8B-C9B
36	H	104	LHG	C11-C10-C9-C8
37	B	622	SQD	C14-C15-C16-C17
33	3	303	CLA	C15-C16-C17-C18
39	d	410	LMG	C11-C12-C13-C14
33	0	309	CLA	C13-C15-C16-C17
33	B	612	CLA	O1D-CGD-O2D-CED
41	d	404	PL9	C15-C14-C16-C17
41	d	404	PL9	C40-C39-C41-C42
33	B	608	CLA	CBA-CGA-O2A-C1
36	7	316	LHG	C24-C23-O8-C6
37	D	403	SQD	C27-C28-C29-C30
37	a	413	SQD	C32-C33-C34-C35
38	c	517	DGD	C2B-C3B-C4B-C5B
36	H	104	LHG	O1-C1-C2-O2
43	t	101	LMU	C2-C1-O1'-C1'
43	4	317	LMU	C2-C1-O1'-C1'
46	4	303	DD6	C27-C29-C30-C31
48	0	302	ET4	C22-C23-C32-C33
33	7	307	CLA	C3-C5-C6-C7
33	B	606	CLA	C11-C12-C13-C14
33	C	502	CLA	C14-C13-C15-C16
33	C	512	CLA	C6-C7-C8-C9
33	c	507	CLA	C14-C13-C15-C16
33	c	508	CLA	C11-C10-C8-C9
33	c	511	CLA	C14-C13-C15-C16
33	W	303	CLA	C14-C13-C15-C16
33	w	303	CLA	C14-C13-C15-C16
33	3	303	CLA	C11-C12-C13-C14
33	3	306	CLA	C14-C13-C15-C16
33	3	308	CLA	C6-C7-C8-C9
33	7	305	CLA	C6-C7-C8-C9
33	a	411	CLA	C11-C10-C8-C9
33	b	604	CLA	C6-C7-C8-C9
33	b	606	CLA	C14-C13-C15-C16
33	b	607	CLA	C14-C13-C15-C16
33	b	611	CLA	C11-C12-C13-C14
33	1	310	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
33	1	310	CLA	C14-C13-C15-C16
33	C	505	CLA	C10-C11-C12-C13
33	C	511	CLA	C13-C15-C16-C17
33	c	502	CLA	C13-C15-C16-C17
36	W	302	LHG	C5-C4-O6-P
36	7	316	LHG	C5-C4-O6-P
33	B	601	CLA	C4B-C3B-CAB-CBB
33	z	101	CLA	C4B-C3B-CAB-CBB
33	3	306	CLA	C4B-C3B-CAB-CBB
33	4	311	CLA	C4B-C3B-CAB-CBB
33	5	309	CLA	C4B-C3B-CAB-CBB
33	6	311	CLA	C4B-C3B-CAB-CBB
33	6	312	CLA	C4B-C3B-CAB-CBB
33	9	314	CLA	C4B-C3B-CAB-CBB
33	2	314	CLA	C4B-C3B-CAB-CBB
33	2	316	CLA	C4B-C3B-CAB-CBB
36	A	414	LHG	C30-C31-C32-C33
36	W	302	LHG	C24-C25-C26-C27
37	l	101	SQD	C17-C18-C19-C20
39	q	301	LMG	C32-C33-C34-C35
39	q	302	LMG	C4-C5-C6-O5
38	A	415	DGD	C5B-C6B-C7B-C8B
39	7	315	LMG	C34-C35-C36-C37
33	c	501	CLA	C10-C11-C12-C13
43	3	301	LMU	C9-C10-C11-C12
33	0	309	CLA	C2A-CAA-CBA-CGA
37	B	622	SQD	C26-C27-C28-C29
38	c	518	DGD	C2D-C1D-O3G-C3G
39	7	315	LMG	C2-C1-O1-C7
36	A	412	LHG	C28-C29-C30-C31
36	b	601	LHG	C15-C16-C17-C18
39	w	304	LMG	C32-C33-C34-C35
36	D	409	LHG	O6-C4-C5-C6
36	d	405	LHG	O6-C4-C5-C6
36	3	317	LHG	O6-C4-C5-C6
36	D	409	LHG	C12-C13-C14-C15
36	d	407	LHG	C9-C10-C11-C12
39	d	406	LMG	C30-C31-C32-C33
39	W	301	LMG	C11-C12-C13-C14
38	h	102	DGD	CDA-CEA-CFA-CGA
38	H	102	DGD	O2G-C1B-C2B-C3B
39	m	201	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
33	B	603	CLA	C6-C7-C8-C10
33	B	606	CLA	C11-C12-C13-C15
33	B	606	CLA	C12-C13-C15-C16
33	B	614	CLA	C11-C10-C8-C7
33	B	616	CLA	C11-C10-C8-C7
33	C	505	CLA	C11-C12-C13-C15
33	C	507	CLA	C6-C7-C8-C10
33	C	507	CLA	C11-C12-C13-C15
33	C	507	CLA	C12-C13-C15-C16
33	C	511	CLA	C12-C13-C15-C16
33	C	512	CLA	C11-C10-C8-C7
33	C	512	CLA	C12-C13-C15-C16
33	c	501	CLA	C11-C12-C13-C15
33	c	505	CLA	C11-C12-C13-C15
33	c	512	CLA	C11-C10-C8-C7
33	3	302	CLA	C6-C7-C8-C10
33	3	306	CLA	C12-C13-C15-C16
33	3	308	CLA	C11-C10-C8-C7
33	7	305	CLA	C11-C10-C8-C7
33	7	307	CLA	C11-C12-C13-C15
33	b	604	CLA	C6-C7-C8-C10
33	b	607	CLA	C11-C12-C13-C15
33	b	607	CLA	C12-C13-C15-C16
33	b	616	CLA	C12-C13-C15-C16
33	0	305	CLA	C11-C10-C8-C7
33	8	310	CLA	C12-C13-C15-C16
33	1	310	CLA	C6-C7-C8-C10
39	3	316	LMG	C28-C29-C30-C31
33	a	411	CLA	C11-C12-C13-C15
33	b	617	CLA	C16-C17-C18-C20
36	w	301	LHG	C30-C31-C32-C33
37	0	316	SQD	O10-C23-O48-C46
43	3	301	LMU	C2-C3-C4-C5
33	B	612	CLA	C3A-C2A-CAA-CBA
33	3	312	CLA	C3A-C2A-CAA-CBA
33	9	308	CLA	C3A-C2A-CAA-CBA
33	2	310	CLA	C3A-C2A-CAA-CBA
41	D	408	PL9	C40-C39-C41-C42
39	C	520	LMG	C20-C21-C22-C23
33	c	502	CLA	C11-C10-C8-C7
36	5	318	LHG	C10-C11-C12-C13
33	C	504	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
33	1	311	CLA	CBA-CGA-O2A-C1
37	T	101	SQD	C24-C23-O48-C46
39	d	406	LMG	C33-C34-C35-C36
39	w	304	LMG	C15-C16-C17-C18
39	q	302	LMG	C31-C32-C33-C34
45	1	301	A86	C24-C25-C26-C27
37	A	413	SQD	C9-C10-C11-C12
36	3	318	LHG	C17-C18-C19-C20
39	3	316	LMG	C30-C31-C32-C33
37	l	101	SQD	C28-C29-C30-C31
33	3	305	CLA	O2A-C1-C2-C3
36	A	412	LHG	C30-C31-C32-C33
33	c	503	CLA	C5-C6-C7-C8
33	7	309	CLA	C13-C15-C16-C17
36	A	411	LHG	C4-C5-C6-O8
36	w	301	LHG	C4-C5-C6-O8
36	7	316	LHG	C4-C5-C6-O8
36	a	403	LHG	C4-C5-C6-O8
37	i	101	SQD	C44-C45-C46-O48
37	T	101	SQD	O6-C44-C45-C46
37	T	103	SQD	C44-C45-C46-O48
38	c	518	DGD	O1G-C1G-C2G-C3G
38	a	401	DGD	C1G-C2G-C3G-O3G
39	B	621	LMG	O1-C7-C8-C9
39	C	520	LMG	O1-C7-C8-C9
39	C	522	LMG	C7-C8-C9-O8
39	Q	301	LMG	C7-C8-C9-O8
45	5	301	A86	C12-C11-C13-O
45	5	304	A86	C12-C11-C13-O
45	5	305	A86	C12-C11-C13-O
45	5	307	A86	C12-C11-C13-O
45	6	301	A86	C12-C11-C13-O
45	6	306	A86	C12-C11-C13-O
45	9	301	A86	C12-C11-C13-O
45	2	301	A86	C12-C11-C13-O
39	d	406	LMG	C4-C5-C6-O5
33	C	502	CLA	C8-C10-C11-C12
33	3	312	CLA	C3-C5-C6-C7
33	b	605	CLA	C8-C10-C11-C12
33	7	312	CLA	O1A-CGA-O2A-C1
37	T	103	SQD	C28-C29-C30-C31
38	A	415	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
38	C	516	DGD	C2A-C3A-C4A-C5A
39	c	519	LMG	C32-C33-C34-C35
34	A	407	PHO	C1A-C2A-CAA-CBA
38	3	320	DGD	C1G-C2G-C3G-O3G
36	d	405	LHG	C31-C32-C33-C34
37	D	403	SQD	C12-C13-C14-C15
37	L	101	SQD	C12-C13-C14-C15
33	B	611	CLA	C4-C3-C5-C6
41	D	408	PL9	C15-C14-C16-C17
39	W	301	LMG	C28-C29-C30-C31
33	B	611	CLA	C10-C11-C12-C13
33	c	502	CLA	C8-C10-C11-C12
45	5	301	A86	C10-C11-C13-O
45	5	303	A86	C10-C11-C13-O
45	5	304	A86	C10-C11-C13-O
45	5	305	A86	C10-C11-C13-O
45	5	306	A86	C10-C11-C13-O
45	5	307	A86	C10-C11-C13-O
45	6	302	A86	C10-C11-C13-O
45	6	306	A86	C10-C11-C13-O
45	9	301	A86	C10-C11-C13-O
45	2	301	A86	C10-C11-C13-O
45	8	301	A86	C10-C11-C13-O
36	a	404	LHG	C11-C10-C9-C8
36	3	317	LHG	O6-C4-C5-O7
36	a	404	LHG	O6-C4-C5-O7
39	q	302	LMG	C29-C30-C31-C32
30	A	401	BCR	C1-C6-C7-C8
30	B	617	BCR	C5-C6-C7-C8
30	C	515	BCR	C1-C6-C7-C8
30	c	515	BCR	C23-C24-C25-C30
30	K	102	BCR	C1-C6-C7-C8
30	k	101	BCR	C23-C24-C25-C30
30	k	102	BCR	C1-C6-C7-C8
30	a	414	BCR	C1-C6-C7-C8
33	z	101	CLA	C2B-C3B-CAB-CBB
33	9	314	CLA	C2B-C3B-CAB-CBB
45	5	301	A86	C33-C34-O4-C38
36	w	301	LHG	C24-C25-C26-C27
39	c	519	LMG	C36-C37-C38-C39
33	W	303	CLA	C15-C16-C17-C18
33	b	614	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	W	301	LMG	C15-C16-C17-C18
43	3	301	LMU	C5-C6-C7-C8
37	a	413	SQD	C11-C10-C9-C8
33	6	310	CLA	C2A-CAA-CBA-CGA
33	9	317	CLA	C2A-CAA-CBA-CGA
36	7	316	LHG	C23-C24-C25-C26
36	A	411	LHG	O7-C5-C6-O8
36	3	317	LHG	O7-C5-C6-O8
37	T	103	SQD	O6-C44-C45-O47
37	t	102	SQD	O6-C44-C45-O47
37	7	317	SQD	O6-C44-C45-O47
38	C	516	DGD	O2G-C2G-C3G-O3G
38	C	518	DGD	O1G-C1G-C2G-O2G
38	c	518	DGD	O1G-C1G-C2G-O2G
39	C	522	LMG	O1-C7-C8-O7
39	D	404	LMG	O7-C8-C9-O8
39	Q	301	LMG	O1-C7-C8-O7
39	q	302	LMG	O1-C7-C8-O7
37	T	101	SQD	C23-C24-C25-C26
33	C	505	CLA	C4-C3-C5-C6
33	b	604	CLA	C11-C12-C13-C15
38	H	102	DGD	CCA-CDA-CEA-CFA
38	a	401	DGD	C4B-C5B-C6B-C7B
39	d	406	LMG	C34-C35-C36-C37
33	A	404	CLA	C13-C15-C16-C17
33	B	611	CLA	C2-C3-C5-C6
33	C	505	CLA	C2-C3-C5-C6
39	0	314	LMG	C18-C19-C20-C21
36	A	412	LHG	C15-C16-C17-C18
37	L	101	SQD	C14-C15-C16-C17
37	l	101	SQD	C12-C13-C14-C15
37	a	413	SQD	C16-C17-C18-C19
33	c	504	CLA	C16-C17-C18-C19
39	C	519	LMG	C32-C33-C34-C35
39	7	315	LMG	C38-C39-C40-C41
39	b	621	LMG	C16-C17-C18-C19
33	B	611	CLA	C13-C15-C16-C17
36	a	404	LHG	C24-C25-C26-C27
33	B	606	CLA	C14-C13-C15-C16
33	C	503	CLA	C6-C7-C8-C9
33	C	505	CLA	C11-C12-C13-C14
33	c	501	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
33	c	507	CLA	C11-C10-C8-C9
33	c	510	CLA	C6-C7-C8-C9
33	7	305	CLA	C11-C10-C8-C9
33	b	607	CLA	C11-C12-C13-C14
33	0	305	CLA	C11-C10-C8-C9
33	1	310	CLA	C6-C7-C8-C9
37	a	413	SQD	C25-C26-C27-C28
39	m	201	LMG	C29-C30-C31-C32
37	D	403	SQD	C35-C36-C37-C38
43	w	302	LMU	C9-C10-C11-C12
33	7	309	CLA	C3-C5-C6-C7
38	C	516	DGD	C3A-C4A-C5A-C6A
33	C	512	CLA	O2A-C1-C2-C3
33	b	613	CLA	CBD-CGD-O2D-CED
36	0	315	LHG	C11-C10-C9-C8
37	L	101	SQD	C10-C11-C12-C13
39	b	621	LMG	C37-C38-C39-C40
33	w	303	CLA	C5-C6-C7-C8
33	0	305	CLA	C3-C5-C6-C7
36	H	104	LHG	C29-C30-C31-C32
41	d	404	PL9	C13-C14-C16-C17
33	8	310	CLA	C16-C17-C18-C20
33	B	611	CLA	C11-C12-C13-C15
36	4	318	LHG	C33-C34-C35-C36
39	0	314	LMG	C35-C36-C37-C38
33	5	313	CLA	O1D-CGD-O2D-CED
33	0	310	CLA	O1D-CGD-O2D-CED
33	C	504	CLA	C10-C11-C12-C13
33	7	312	CLA	C15-C16-C17-C18
37	7	317	SQD	C11-C12-C13-C14
30	c	514	BCR	C16-C17-C18-C36
30	d	403	BCR	C16-C17-C18-C36
38	c	517	DGD	CCB-CDB-CEB-CFB
39	7	315	LMG	C37-C38-C39-C40
36	A	412	LHG	O6-C4-C5-C6
33	b	617	CLA	C16-C17-C18-C19
38	H	102	DGD	C5B-C6B-C7B-C8B
33	b	617	CLA	C15-C16-C17-C18
30	b	619	BCR	C7-C8-C9-C34
46	3	315	DD6	C-C1-C24-C25
38	c	517	DGD	C8B-C9B-CAB-CBB
33	B	602	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
33	C	501	CLA	C11-C12-C13-C15
33	C	509	CLA	C11-C10-C8-C7
33	c	508	CLA	C11-C12-C13-C15
33	c	510	CLA	C6-C7-C8-C10
33	c	510	CLA	C11-C10-C8-C7
33	3	307	CLA	C11-C10-C8-C7
33	b	617	CLA	C11-C10-C8-C7
33	0	307	CLA	C11-C12-C13-C15
33	9	310	CLA	C12-C13-C15-C16
33	8	310	CLA	C11-C12-C13-C15
34	a	409	PHO	C6-C7-C8-C10
39	q	301	LMG	C28-C29-C30-C31
43	3	301	LMU	O5B-C5B-C6B-O6B
36	A	412	LHG	C32-C33-C34-C35
36	h	103	LHG	C28-C29-C30-C31
33	c	511	CLA	C3-C5-C6-C7
30	c	515	BCR	C7-C8-C9-C10
33	6	313	CLA	O1A-CGA-O2A-C1
37	L	101	SQD	C24-C25-C26-C27
37	a	413	SQD	C14-C15-C16-C17
39	m	201	LMG	C13-C14-C15-C16
33	B	608	CLA	O1A-CGA-O2A-C1
33	D	406	CLA	O1A-CGA-O2A-C1
36	0	315	LHG	C4-O6-P-O4
37	B	622	SQD	C5-C6-S-O8
37	a	413	SQD	C5-C6-S-O8
37	0	316	SQD	C45-C44-O6-C1
39	3	316	LMG	C8-C7-O1-C1
39	5	319	LMG	C8-C7-O1-C1
39	0	314	LMG	C8-C7-O1-C1
33	C	502	CLA	O1D-CGD-O2D-CED
33	B	606	CLA	C2A-CAA-CBA-CGA
33	b	609	CLA	C2A-CAA-CBA-CGA
33	2	307	CLA	C2A-CAA-CBA-CGA
33	8	306	CLA	C2A-CAA-CBA-CGA
33	1	311	CLA	O1A-CGA-O2A-C1
42	V	201	HEM	C2B-C3B-CAB-CBB
47	0	306	KC2	C2C-C3C-CAC-CBC
43	t	101	LMU	C2B-C1B-O1B-C4'
33	B	602	CLA	C6-C7-C8-C10
33	4	316	CLA	O1A-CGA-O2A-C1
36	W	302	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
36	D	411	LHG	C28-C29-C30-C31
33	b	609	CLA	CBA-CGA-O2A-C1
39	b	623	LMG	C4-C5-C6-O5
30	d	403	BCR	C20-C21-C22-C23
39	b	623	LMG	C33-C34-C35-C36
33	B	607	CLA	O1D-CGD-O2D-CED
39	q	301	LMG	O9-C10-O7-C8
36	A	412	LHG	O6-C4-C5-O7
33	b	612	CLA	C11-C12-C13-C15
37	7	317	SQD	C29-C30-C31-C32
38	C	517	DGD	C7B-C8B-C9B-CAB
38	3	320	DGD	C9A-CAA-CBA-CCA
39	q	301	LMG	C29-C30-C31-C32
37	A	413	SQD	C44-C45-C46-O48
37	D	403	SQD	C44-C45-C46-O48
37	t	102	SQD	O6-C44-C45-C46
37	7	317	SQD	C44-C45-C46-O48
37	a	413	SQD	O6-C44-C45-C46
37	0	316	SQD	C44-C45-C46-O48
38	C	516	DGD	C1G-C2G-C3G-O3G
38	3	320	DGD	O1G-C1G-C2G-C3G
39	C	520	LMG	C7-C8-C9-O8
39	C	522	LMG	O1-C7-C8-C9
39	D	404	LMG	C7-C8-C9-O8
39	d	410	LMG	C7-C8-C9-O8
39	5	319	LMG	C7-C8-C9-O8
39	7	315	LMG	C7-C8-C9-O8
39	b	623	LMG	C7-C8-C9-O8
39	q	301	LMG	C7-C8-C9-O8
38	a	401	DGD	C6A-C7A-C8A-C9A
44	3	310	KC1	C4B-C3B-CAB-CBB
44	5	315	KC1	C4B-C3B-CAB-CBB
47	7	306	KC2	C4C-C3C-CAC-CBC
33	8	310	CLA	C16-C17-C18-C19
33	W	303	CLA	C3-C5-C6-C7
37	L	101	SQD	C25-C26-C27-C28
38	a	401	DGD	O1G-C1A-C2A-C3A
33	C	502	CLA	C2-C3-C5-C6
33	c	502	CLA	C2-C3-C5-C6
37	T	103	SQD	C23-C24-C25-C26
33	8	308	CLA	C3-C5-C6-C7
39	c	519	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
33	2	308	CLA	O1D-CGD-O2D-CED
36	b	601	LHG	O7-C5-C6-O8
38	3	320	DGD	O1G-C1G-C2G-O2G
38	a	401	DGD	O2G-C2G-C3G-O3G
39	C	520	LMG	O1-C7-C8-O7
39	d	410	LMG	O7-C8-C9-O8
39	b	622	LMG	O1-C7-C8-O7
39	b	623	LMG	O7-C8-C9-O8
33	4	311	CLA	C10-C11-C12-C13
33	c	508	CLA	C11-C12-C13-C14
33	c	510	CLA	C11-C10-C8-C9
33	d	402	CLA	C6-C7-C8-C9
33	3	308	CLA	C11-C10-C8-C9
33	b	606	CLA	C11-C10-C8-C9
34	a	409	PHO	C6-C7-C8-C9
34	a	409	PHO	C11-C10-C8-C9
33	B	616	CLA	C16-C17-C18-C20
38	3	320	DGD	C8A-C9A-CAA-CBA
39	D	410	LMG	C13-C14-C15-C16
39	b	621	LMG	C30-C31-C32-C33
33	b	612	CLA	C10-C11-C12-C13
36	3	318	LHG	C11-C12-C13-C14
36	H	104	LHG	C27-C28-C29-C30
37	l	101	SQD	C10-C11-C12-C13
33	0	309	CLA	C8-C10-C11-C12
45	3	314	A86	C13-C14-C15-O1
37	a	413	SQD	C27-C28-C29-C30
36	d	405	LHG	C11-C12-C13-C14
45	6	302	A86	C35-C34-O4-C38
33	B	604	CLA	C5-C6-C7-C8
36	D	409	LHG	C27-C28-C29-C30
39	D	410	LMG	C15-C16-C17-C18
38	c	518	DGD	C8A-C9A-CAA-CBA
33	6	311	CLA	O1A-CGA-O2A-C1
37	L	101	SQD	C26-C27-C28-C29
33	B	614	CLA	C11-C12-C13-C15
33	b	615	CLA	C13-C15-C16-C17
36	4	318	LHG	C35-C36-C37-C38
33	B	613	CLA	C13-C15-C16-C17
37	T	103	SQD	C16-C17-C18-C19
30	k	101	BCR	C14-C15-C16-C17
33	7	305	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
33	b	609	CLA	O1A-CGA-O2A-C1
33	b	611	CLA	C13-C15-C16-C17
45	3	314	A86	C39-C38-O4-C34
37	L	101	SQD	C4-C5-C6-S
36	A	412	LHG	C10-C11-C12-C13
43	t	101	LMU	C4-C5-C6-C7
43	3	301	LMU	C2-C1-O1'-C1'
46	8	303	DD6	C27-C29-C30-C31
37	l	101	SQD	C11-C12-C13-C14
33	B	609	CLA	C1A-C2A-CAA-CBA
33	B	611	CLA	C1A-C2A-CAA-CBA
33	B	615	CLA	C4B-C3B-CAB-CBB
33	3	309	CLA	C4B-C3B-CAB-CBB
33	5	308	CLA	C1A-C2A-CAA-CBA
33	b	604	CLA	C1A-C2A-CAA-CBA
33	b	617	CLA	C4B-C3B-CAB-CBB
33	9	305	CLA	C4B-C3B-CAB-CBB
33	9	313	CLA	C4B-C3B-CAB-CBB
33	9	316	CLA	C4B-C3B-CAB-CBB
33	1	305	CLA	C4B-C3B-CAB-CBB
33	1	313	CLA	C4B-C3B-CAB-CBB
33	1	316	CLA	C4B-C3B-CAB-CBB
45	7	301	A86	O-C13-C14-C15
45	0	301	A86	O-C13-C14-C15
45	8	302	A86	O-C13-C14-C15
45	1	302	A86	O-C13-C14-C15
39	d	410	LMG	O6-C5-C6-O5
33	B	614	CLA	O1D-CGD-O2D-CED
33	z	101	CLA	CBA-CGA-O2A-C1
38	C	517	DGD	C7A-C8A-C9A-CAA
33	C	501	CLA	C4-C3-C5-C6
30	k	101	BCR	C22-C23-C24-C25
36	7	316	LHG	C29-C30-C31-C32
46	3	315	DD6	C2-C1-C24-C25
36	W	302	LHG	C27-C28-C29-C30
39	B	620	LMG	C4-C5-C6-O5
38	C	516	DGD	C4D-C5D-C6D-O5D
33	2	306	CLA	C2A-CAA-CBA-CGA
39	m	201	LMG	C35-C36-C37-C38
39	D	410	LMG	C4-C5-C6-O5
33	c	505	CLA	C13-C15-C16-C17
36	5	318	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
36	a	404	LHG	O6-C4-C5-C6
38	A	415	DGD	C6A-C7A-C8A-C9A
36	D	411	LHG	O9-C7-O7-C5
38	h	102	DGD	C6A-C7A-C8A-C9A
33	4	312	CLA	C2-C3-C5-C6
39	c	519	LMG	C38-C39-C40-C41
39	M	201	LMG	C33-C34-C35-C36
33	C	501	CLA	C6-C7-C8-C10
33	c	501	CLA	C6-C7-C8-C10
33	c	505	CLA	C6-C7-C8-C10
33	c	509	CLA	C11-C10-C8-C7
33	3	312	CLA	C6-C7-C8-C10
33	7	309	CLA	C11-C10-C8-C7
33	0	309	CLA	C11-C10-C8-C7
33	0	309	CLA	C12-C13-C15-C16
34	A	407	PHO	C6-C7-C8-C10
36	w	301	LHG	C29-C30-C31-C32
36	5	318	LHG	C15-C16-C17-C18
38	C	517	DGD	C6B-C7B-C8B-C9B
39	w	304	LMG	C39-C40-C41-C42
38	c	518	DGD	C4A-C5A-C6A-C7A
33	B	612	CLA	CBA-CGA-O2A-C1
33	C	502	CLA	CBA-CGA-O2A-C1
33	B	605	CLA	C10-C11-C12-C13
37	B	622	SQD	C23-C24-C25-C26
36	4	318	LHG	C2-C3-O3-P
39	b	623	LMG	C12-C13-C14-C15
33	B	609	CLA	C3A-C2A-CAA-CBA
45	6	301	A86	C33-C34-O4-C38
36	b	601	LHG	C28-C29-C30-C31
33	9	307	CLA	CBD-CGD-O2D-CED
36	D	409	LHG	O6-C4-C5-O7
36	D	411	LHG	O6-C4-C5-O7
36	d	405	LHG	O6-C4-C5-O7
33	C	502	CLA	C11-C10-C8-C7
39	d	406	LMG	C11-C10-O7-C8
33	A	405	CLA	C2A-CAA-CBA-CGA
33	B	608	CLA	C2A-CAA-CBA-CGA
33	C	501	CLA	C11-C12-C13-C14
33	C	512	CLA	C14-C13-C15-C16
33	3	307	CLA	C11-C10-C8-C9
33	b	617	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
33	9	310	CLA	C14-C13-C15-C16
33	8	310	CLA	C11-C12-C13-C14
38	H	102	DGD	C9B-CAB-CBB-CCB
39	d	406	LMG	C17-C18-C19-C20
36	4	318	LHG	C29-C30-C31-C32
30	C	515	BCR	C9-C10-C11-C12
45	0	303	A86	C24-C25-C26-C27
39	C	519	LMG	C36-C37-C38-C39
33	B	605	CLA	C13-C15-C16-C17
39	C	519	LMG	C30-C31-C32-C33
39	7	315	LMG	C41-C42-C43-C44
33	A	405	CLA	C1-C2-C3-C4
33	C	513	CLA	C1-C2-C3-C4
33	c	513	CLA	C1-C2-C3-C4
33	a	408	CLA	C1-C2-C3-C4
37	i	101	SQD	O5-C5-C6-S
44	3	310	KC1	C3A-C2A-CAA-CBA
47	6	309	KC2	C1A-C2A-CAA-CBA
47	7	306	KC2	C3A-C2A-CAA-CBA
33	d	409	CLA	C11-C12-C13-C14
39	7	315	LMG	C17-C18-C19-C20
33	C	509	CLA	C8-C10-C11-C12
39	M	201	LMG	C4-C5-C6-O5
33	z	101	CLA	O1A-CGA-O2A-C1
39	C	520	LMG	O10-C28-O8-C9
36	A	414	LHG	O7-C5-C6-O8
36	W	302	LHG	O7-C5-C6-O8
36	w	301	LHG	O7-C5-C6-O8
37	D	403	SQD	O6-C44-C45-O47
37	D	403	SQD	O47-C45-C46-O48
37	T	103	SQD	O47-C45-C46-O48
37	a	413	SQD	O6-C44-C45-O47
38	A	415	DGD	O2G-C2G-C3G-O3G
38	c	516	DGD	O2G-C2G-C3G-O3G
39	B	621	LMG	O1-C7-C8-O7
39	c	520	LMG	O7-C8-C9-O8
39	d	410	LMG	O1-C7-C8-O7
39	W	301	LMG	O1-C7-C8-O7
39	w	304	LMG	O1-C7-C8-O7
39	3	316	LMG	O1-C7-C8-O7
39	Q	301	LMG	O7-C8-C9-O8
39	q	301	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
36	A	412	LHG	C12-C13-C14-C15
38	C	516	DGD	CDB-CEB-CFB-CGB
33	c	512	CLA	O2A-C1-C2-C3
38	C	516	DGD	C2D-C1D-O3G-C3G
33	C	509	CLA	C13-C15-C16-C17
38	c	516	DGD	C1G-C2G-C3G-O3G
39	B	620	LMG	C7-C8-C9-O8
39	M	201	LMG	C7-C8-C9-O8
39	W	301	LMG	O1-C7-C8-C9
36	3	318	LHG	C11-C10-C9-C8
33	7	312	CLA	C5-C6-C7-C8
33	3	303	CLA	C2-C3-C5-C6
33	8	307	CLA	CBD-CGD-O2D-CED
33	B	603	CLA	CAD-CBD-CGD-O2D
33	B	609	CLA	CAD-CBD-CGD-O2D
33	C	502	CLA	CAD-CBD-CGD-O2D
33	C	505	CLA	CAD-CBD-CGD-O2D
33	C	506	CLA	CAD-CBD-CGD-O2D
33	C	513	CLA	CAD-CBD-CGD-O2D
33	c	502	CLA	CAD-CBD-CGD-O2D
33	c	504	CLA	CAD-CBD-CGD-O2D
33	c	505	CLA	CAD-CBD-CGD-O2D
33	c	513	CLA	CAD-CBD-CGD-O2D
33	6	311	CLA	CAD-CBD-CGD-O2D
33	b	610	CLA	CAD-CBD-CGD-O2D
45	4	302	A86	C13-C14-C15-C20
33	b	613	CLA	C8-C10-C11-C12
33	w	303	CLA	O1D-CGD-O2D-CED
33	b	613	CLA	O1D-CGD-O2D-CED
38	c	516	DGD	C2A-C3A-C4A-C5A
33	B	612	CLA	O1A-CGA-O2A-C1
33	3	304	CLA	C13-C15-C16-C17
33	C	504	CLA	C16-C17-C18-C19
33	b	603	CLA	C6-C7-C8-C10
38	c	516	DGD	C6B-C7B-C8B-C9B
33	C	502	CLA	O1A-CGA-O2A-C1
38	C	518	DGD	O1A-C1A-O1G-C1G
37	l	101	SQD	C11-C10-C9-C8
39	D	404	LMG	C12-C13-C14-C15
33	B	603	CLA	CAD-CBD-CGD-O1D
33	B	605	CLA	CAD-CBD-CGD-O1D
33	B	609	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
33	C	502	CLA	CAD-CBD-CGD-O1D
33	C	505	CLA	CAD-CBD-CGD-O1D
33	C	506	CLA	CAD-CBD-CGD-O1D
33	C	512	CLA	CHA-CBD-CGD-O1D
33	C	512	CLA	CHA-CBD-CGD-O2D
33	C	513	CLA	CAD-CBD-CGD-O1D
33	c	502	CLA	CAD-CBD-CGD-O1D
33	c	504	CLA	CAD-CBD-CGD-O1D
33	c	505	CLA	CAD-CBD-CGD-O1D
33	c	506	CLA	CAD-CBD-CGD-O1D
33	c	507	CLA	CHA-CBD-CGD-O1D
33	c	513	CLA	CAD-CBD-CGD-O1D
33	3	306	CLA	CHA-CBD-CGD-O1D
33	6	311	CLA	CAD-CBD-CGD-O1D
33	6	315	CLA	CAD-CBD-CGD-O1D
33	b	610	CLA	CAD-CBD-CGD-O1D
33	b	617	CLA	CHA-CBD-CGD-O1D
33	b	617	CLA	CHA-CBD-CGD-O2D
33	2	312	CLA	CHA-CBD-CGD-O1D
33	2	312	CLA	CHA-CBD-CGD-O2D
33	8	310	CLA	CHA-CBD-CGD-O1D
33	1	308	CLA	CHA-CBD-CGD-O1D
33	1	308	CLA	CHA-CBD-CGD-O2D
34	A	407	PHO	CHA-CBD-CGD-O2D
36	W	302	LHG	C3-O3-P-O5
36	W	302	LHG	C4-O6-P-O3
36	W	302	LHG	C4-O6-P-O5
36	w	301	LHG	C4-O6-P-O3
36	3	317	LHG	C3-O3-P-O5
36	3	317	LHG	C4-O6-P-O4
36	3	318	LHG	C3-O3-P-O6
36	b	601	LHG	C3-O3-P-O5
45	4	302	A86	C10-C11-C13-C14
45	6	301	A86	C10-C11-C13-C14
45	6	302	A86	C10-C11-C13-C14
45	6	303	A86	C10-C11-C13-C14
45	6	304	A86	C10-C11-C13-C14
45	6	305	A86	C10-C11-C13-C14
45	8	301	A86	C10-C11-C13-C14
36	d	407	LHG	C30-C31-C32-C33
33	B	604	CLA	C4-C3-C5-C6
33	B	612	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
33	b	613	CLA	C4-C3-C5-C6
33	2	310	CLA	C4-C3-C5-C6
34	A	406	PHO	C4-C3-C5-C6
30	A	401	BCR	C23-C24-C25-C30
33	B	615	CLA	C2B-C3B-CAB-CBB
33	3	306	CLA	C2B-C3B-CAB-CBB
33	3	309	CLA	C2B-C3B-CAB-CBB
33	6	311	CLA	C2B-C3B-CAB-CBB
33	b	617	CLA	C2B-C3B-CAB-CBB
33	9	316	CLA	C2B-C3B-CAB-CBB
33	2	314	CLA	C2B-C3B-CAB-CBB
33	2	316	CLA	C2B-C3B-CAB-CBB
33	1	305	CLA	C2B-C3B-CAB-CBB
33	1	313	CLA	C2B-C3B-CAB-CBB
33	1	316	CLA	C2B-C3B-CAB-CBB
33	9	308	CLA	C2-C3-C5-C6
39	D	410	LMG	C20-C21-C22-C23
36	W	302	LHG	C2-C3-O3-P
36	w	301	LHG	C2-C3-O3-P
36	0	315	LHG	C5-C4-O6-P
45	9	301	A86	C-C1-C24-C25
45	2	301	A86	C-C1-C24-C25
36	a	404	LHG	C31-C32-C33-C34
39	M	201	LMG	O9-C10-O7-C8
33	2	310	CLA	C4C-C3C-CAC-CBC
33	b	614	CLA	O1D-CGD-O2D-CED
39	C	521	LMG	C29-C28-O8-C9
36	d	407	LHG	C28-C29-C30-C31
33	b	616	CLA	C15-C16-C17-C18
33	C	507	CLA	C16-C17-C18-C20
33	b	611	CLA	C15-C16-C17-C18
45	4	302	A86	C12-C11-C13-C14
45	5	302	A86	C12-C11-C13-C14
45	5	303	A86	C12-C11-C13-C14
45	6	301	A86	C12-C11-C13-C14
45	6	302	A86	C12-C11-C13-C14
45	6	303	A86	C12-C11-C13-C14
45	6	304	A86	C12-C11-C13-C14
45	6	305	A86	C12-C11-C13-C14
45	8	301	A86	C12-C11-C13-C14
39	7	315	LMG	C29-C30-C31-C32
36	H	104	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
36	W	302	LHG	C30-C31-C32-C33
39	d	410	LMG	C10-C11-C12-C13
39	5	319	LMG	C28-C29-C30-C31
36	a	403	LHG	C30-C31-C32-C33
33	c	505	CLA	C10-C11-C12-C13
37	T	103	SQD	C13-C14-C15-C16
39	C	520	LMG	C7-C8-O7-C10
33	B	610	CLA	C15-C16-C17-C18
33	W	303	CLA	C8-C10-C11-C12
33	w	303	CLA	C15-C16-C17-C18
33	9	308	CLA	C5-C6-C7-C8
41	D	408	PL9	C38-C39-C41-C42
37	t	102	SQD	C23-C24-C25-C26
38	h	102	DGD	C2B-C3B-C4B-C5B
39	c	519	LMG	C31-C32-C33-C34
38	h	102	DGD	CAA-CBA-CCA-CDA
33	B	616	CLA	C16-C17-C18-C19
33	c	512	CLA	C5-C6-C7-C8
37	7	317	SQD	C30-C31-C32-C33
33	C	508	CLA	O1A-CGA-O2A-C1
33	B	603	CLA	C6-C7-C8-C9
33	C	509	CLA	C11-C10-C8-C9
33	C	512	CLA	C11-C10-C8-C9
33	c	512	CLA	C11-C10-C8-C9
33	3	302	CLA	C6-C7-C8-C9
33	7	309	CLA	C11-C12-C13-C14
33	b	603	CLA	C14-C13-C15-C16
33	b	616	CLA	C14-C13-C15-C16
36	d	407	LHG	C16-C17-C18-C19
39	w	304	LMG	C17-C18-C19-C20
33	4	306	CLA	C11-C12-C13-C15
33	7	305	CLA	C12-C13-C15-C16
36	a	403	LHG	C23-C24-C25-C26
37	B	622	SQD	C13-C14-C15-C16
36	4	318	LHG	O6-C4-C5-O7
36	5	318	LHG	O6-C4-C5-O7
39	7	315	LMG	C39-C40-C41-C42
38	C	517	DGD	C8B-C9B-CAB-CBB
36	A	412	LHG	O10-C23-O8-C6
33	b	616	CLA	C5-C6-C7-C8
33	B	613	CLA	C16-C17-C18-C20
39	W	301	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
36	7	316	LHG	C7-C8-C9-C10
33	B	605	CLA	C8-C10-C11-C12
33	B	611	CLA	C15-C16-C17-C18
36	4	318	LHG	O7-C5-C6-O8
39	C	519	LMG	O1-C7-C8-O7
38	h	102	DGD	O2G-C1B-C2B-C3B
39	c	519	LMG	C11-C12-C13-C14
39	b	623	LMG	C34-C35-C36-C37
39	B	620	LMG	C34-C35-C36-C37
39	b	621	LMG	O8-C28-C29-C30
37	B	622	SQD	C12-C13-C14-C15
39	c	519	LMG	C34-C35-C36-C37
33	C	508	CLA	CBA-CGA-O2A-C1
33	3	304	CLA	C2-C1-O2A-CGA
38	H	102	DGD	C6A-C7A-C8A-C9A
33	c	513	CLA	O2A-C1-C2-C3
36	4	318	LHG	C4-C5-C6-O8
39	5	319	LMG	O1-C7-C8-C9
39	q	302	LMG	O6-C5-C6-O5
36	A	412	LHG	C11-C10-C9-C8
38	a	401	DGD	C2B-C3B-C4B-C5B
39	0	314	LMG	C31-C32-C33-C34
33	B	611	CLA	C16-C17-C18-C20
38	C	517	DGD	C2B-C1B-O2G-C2G
38	C	516	DGD	O6D-C5D-C6D-O5D
37	L	101	SQD	C11-C12-C13-C14
37	l	101	SQD	C26-C27-C28-C29
38	3	320	DGD	C7B-C8B-C9B-CAB
45	9	301	A86	C2-C1-C24-C25
45	2	301	A86	C2-C1-C24-C25
38	3	320	DGD	CFB-CGB-CHB-CIB
37	A	413	SQD	C45-C44-O6-C1
37	L	101	SQD	C45-C44-O6-C1
39	D	410	LMG	C8-C7-O1-C1
36	d	405	LHG	C12-C13-C14-C15
39	b	621	LMG	C35-C36-C37-C38
36	A	414	LHG	C15-C16-C17-C18
39	w	304	LMG	C38-C39-C40-C41
36	0	315	LHG	C7-C8-C9-C10
33	4	311	CLA	C4-C3-C5-C6
33	7	312	CLA	C13-C15-C16-C17
45	5	307	A86	C35-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
45	4	302	A86	C13-C14-C15-C16
45	6	302	A86	C13-C14-C15-C16
46	1	303	DD6	C27-C29-C30-C31
33	B	602	CLA	C16-C17-C18-C20
33	c	505	CLA	C6-C7-C8-C9
33	w	303	CLA	C6-C7-C8-C9
33	9	307	CLA	O1D-CGD-O2D-CED
33	8	307	CLA	O1D-CGD-O2D-CED
33	b	603	CLA	CBA-CGA-O2A-C1
33	5	312	CLA	C4B-C3B-CAB-CBB
33	5	317	CLA	C4B-C3B-CAB-CBB
33	b	616	CLA	C4B-C3B-CAB-CBB
33	0	304	CLA	C4B-C3B-CAB-CBB
33	2	315	CLA	C4B-C3B-CAB-CBB
37	a	413	SQD	C24-C25-C26-C27
33	C	505	CLA	C13-C15-C16-C17
37	B	622	SQD	C30-C31-C32-C33
39	D	410	LMG	C30-C31-C32-C33
33	C	504	CLA	C16-C17-C18-C20
33	3	307	CLA	C16-C17-C18-C20
33	b	611	CLA	C16-C17-C18-C20
37	i	101	SQD	C24-C23-O48-C46
36	b	601	LHG	C19-C20-C21-C22
33	d	409	CLA	C2A-CAA-CBA-CGA
39	C	519	LMG	C29-C30-C31-C32
33	B	612	CLA	C2-C3-C5-C6
34	A	406	PHO	C2-C3-C5-C6
36	4	318	LHG	C10-C11-C12-C13
36	5	318	LHG	C14-C15-C16-C17
36	a	404	LHG	C15-C16-C17-C18
37	D	403	SQD	C10-C11-C12-C13
33	b	603	CLA	O1A-CGA-O2A-C1
33	3	302	CLA	C5-C6-C7-C8
38	c	517	DGD	C6B-C7B-C8B-C9B
42	e	101	HEM	C4B-C3B-CAB-CBB
47	0	306	KC2	C4C-C3C-CAC-CBC
39	b	621	LMG	C18-C19-C20-C21
37	l	101	SQD	C14-C15-C16-C17
33	B	613	CLA	C12-C13-C15-C16
33	B	615	CLA	C11-C12-C13-C15
33	c	504	CLA	C11-C12-C13-C15
33	4	308	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
37	D	403	SQD	O10-C23-O48-C46
36	D	411	LHG	C24-C25-C26-C27
33	B	602	CLA	C16-C17-C18-C19
36	4	318	LHG	C30-C31-C32-C33
39	Q	301	LMG	C11-C12-C13-C14
33	b	606	CLA	C13-C15-C16-C17
37	D	403	SQD	C24-C25-C26-C27
37	B	622	SQD	O47-C45-C46-O48
39	B	620	LMG	O7-C8-C9-O8
39	b	623	LMG	C14-C15-C16-C17
33	w	303	CLA	C3A-C2A-CAA-CBA
33	7	314	CLA	C3A-C2A-CAA-CBA
33	C	504	CLA	C6-C7-C8-C10
36	b	601	LHG	C11-C10-C9-C8
33	1	310	CLA	C13-C15-C16-C17
36	d	405	LHG	C25-C26-C27-C28
36	W	302	LHG	C29-C30-C31-C32
30	k	101	BCR	C19-C20-C21-C22
33	B	613	CLA	C2-C1-O2A-CGA
30	A	401	BCR	C7-C8-C9-C34
45	6	304	A86	C35-C34-O4-C38
33	4	312	CLA	C4-C3-C5-C6
37	D	403	SQD	C25-C26-C27-C28
33	b	614	CLA	C13-C15-C16-C17
36	D	409	LHG	C33-C34-C35-C36
33	B	614	CLA	C13-C15-C16-C17
37	L	101	SQD	C11-C10-C9-C8
39	d	406	LMG	C31-C32-C33-C34
33	b	613	CLA	C2-C3-C5-C6
33	B	610	CLA	C16-C17-C18-C20
33	C	505	CLA	C16-C17-C18-C19
34	a	409	PHO	C16-C17-C18-C19
33	3	313	CLA	C5-C6-C7-C8
45	6	303	A86	C35-C34-O4-C38
37	T	101	SQD	C25-C26-C27-C28
38	h	102	DGD	C4E-C5E-C6E-O5E
33	C	507	CLA	C11-C10-C8-C9
33	c	501	CLA	C6-C7-C8-C9
33	D	406	CLA	C6-C7-C8-C9
33	3	304	CLA	C6-C7-C8-C9
33	3	306	CLA	C11-C10-C8-C9
33	7	312	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
33	7	312	CLA	C11-C10-C8-C9
38	c	516	DGD	C7B-C8B-C9B-CAB
33	2	311	CLA	C6-C7-C8-C9
45	3	314	A86	O5-C38-O4-C34
39	m	201	LMG	C9-C8-O7-C10
36	A	414	LHG	C19-C20-C21-C22
36	H	104	LHG	C10-C11-C12-C13
38	3	320	DGD	C2B-C3B-C4B-C5B
39	c	519	LMG	C14-C15-C16-C17
33	2	310	CLA	C2C-C3C-CAC-CBC
38	A	415	DGD	O1G-C1A-C2A-C3A
36	d	407	LHG	O1-C1-C2-O2
33	C	501	CLA	CBD-CGD-O2D-CED
33	A	404	CLA	C2A-CAA-CBA-CGA
38	c	516	DGD	C4B-C5B-C6B-C7B
33	A	405	CLA	C1A-C2A-CAA-CBA
33	B	602	CLA	C1A-C2A-CAA-CBA
33	C	508	CLA	C1A-C2A-CAA-CBA
33	H	103	CLA	C1A-C2A-CAA-CBA
33	w	303	CLA	C1A-C2A-CAA-CBA
33	3	303	CLA	C1A-C2A-CAA-CBA
33	4	310	CLA	C1A-C2A-CAA-CBA
33	4	312	CLA	C1A-C2A-CAA-CBA
33	5	313	CLA	C1A-C2A-CAA-CBA
33	6	312	CLA	C1A-C2A-CAA-CBA
33	7	314	CLA	C1A-C2A-CAA-CBA
33	9	309	CLA	C1A-C2A-CAA-CBA
33	1	306	CLA	C1A-C2A-CAA-CBA
30	A	401	BCR	C5-C6-C7-C8
30	C	515	BCR	C5-C6-C7-C8
30	C	515	BCR	C23-C24-C25-C30
30	c	515	BCR	C23-C24-C25-C26
30	H	101	BCR	C23-C24-C25-C30
30	h	101	BCR	C23-C24-C25-C30
30	K	102	BCR	C5-C6-C7-C8
30	K	102	BCR	C23-C24-C25-C30
30	k	102	BCR	C5-C6-C7-C8
30	k	102	BCR	C23-C24-C25-C30
30	a	412	BCR	C1-C6-C7-C8
30	a	414	BCR	C5-C6-C7-C8
30	a	414	BCR	C23-C24-C25-C30
30	b	619	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
33	5	312	CLA	C2B-C3B-CAB-CBB
33	5	317	CLA	C2B-C3B-CAB-CBB
33	7	304	CLA	C2B-C3B-CAB-CBB
33	0	304	CLA	C2B-C3B-CAB-CBB
33	9	305	CLA	C2B-C3B-CAB-CBB
33	9	313	CLA	C2B-C3B-CAB-CBB
33	2	315	CLA	C2B-C3B-CAB-CBB
33	8	310	CLA	C2B-C3B-CAB-CBB
37	t	102	SQD	C29-C30-C31-C32
33	8	312	CLA	CAA-CBA-CGA-O1A
42	e	101	HEM	CAD-CBD-CGD-O2D
38	h	102	DGD	O1A-C1A-O1G-C1G
36	3	318	LHG	C5-C4-O6-P
38	C	516	DGD	C6B-C7B-C8B-C9B
33	c	511	CLA	C4-C3-C5-C6
33	0	307	CLA	C4-C3-C5-C6
41	d	404	PL9	C38-C39-C41-C42
45	5	304	A86	C35-C34-O4-C38
42	e	101	HEM	C3D-CAD-CBD-CGD
38	c	517	DGD	CAB-CBB-CCB-CDB
30	k	101	BCR	C15-C16-C17-C18
33	C	503	CLA	C11-C10-C8-C7
33	c	501	CLA	C12-C13-C15-C16
33	w	303	CLA	C6-C7-C8-C10
33	b	615	CLA	C11-C10-C8-C7
33	0	305	CLA	C12-C13-C15-C16
38	H	102	DGD	CCB-CDB-CEB-CFB
33	4	308	CLA	C16-C17-C18-C20
33	6	312	CLA	C13-C15-C16-C17
39	B	621	LMG	O7-C8-C9-O8
33	8	312	CLA	CAA-CBA-CGA-O2A
33	1	307	CLA	CAA-CBA-CGA-O1A
38	A	415	DGD	C8B-C9B-CAB-CBB
38	C	518	DGD	C4A-C5A-C6A-C7A
33	9	310	CLA	C4C-C3C-CAC-CBC
36	5	318	LHG	C11-C10-C9-C8
33	B	613	CLA	C16-C17-C18-C19
33	7	305	CLA	C16-C17-C18-C20
33	c	508	CLA	C4-C3-C5-C6
33	4	305	CLA	C4-C3-C5-C6
33	5	313	CLA	C4-C3-C5-C6
39	D	404	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
33	8	308	CLA	C2-C1-O2A-CGA
36	3	318	LHG	C13-C14-C15-C16
37	A	413	SQD	O10-C23-O48-C46
39	M	201	LMG	C35-C36-C37-C38
42	e	101	HEM	CAD-CBD-CGD-O1D
33	9	310	CLA	C11-C12-C13-C14
36	d	407	LHG	C24-C25-C26-C27
45	8	301	A86	C11-C10-C9-C8
33	c	507	CLA	C15-C16-C17-C18
33	C	505	CLA	C16-C17-C18-C20
33	b	617	CLA	C10-C11-C12-C13
30	K	101	BCR	C6-C7-C8-C9
33	3	306	CLA	C13-C15-C16-C17
33	1	307	CLA	CAA-CBA-CGA-O2A
39	D	410	LMG	C33-C34-C35-C36
33	C	501	CLA	C2-C3-C5-C6
33	B	602	CLA	O2A-C1-C2-C3
33	b	603	CLA	O2A-C1-C2-C3
37	A	413	SQD	C23-C24-C25-C26
39	B	621	LMG	C7-C8-C9-O8
36	0	315	LHG	O10-C23-O8-C6
41	D	408	PL9	C47-C48-C49-C51
33	1	306	CLA	C2A-CAA-CBA-CGA
33	c	509	CLA	C13-C15-C16-C17
33	b	616	CLA	C16-C17-C18-C19
39	C	519	LMG	O7-C10-C11-C12
39	W	301	LMG	C31-C32-C33-C34
38	c	516	DGD	C6A-C7A-C8A-C9A
33	2	309	CLA	CAA-CBA-CGA-O2A
42	V	201	HEM	CAD-CBD-CGD-O2D
42	v	201	HEM	CAA-CBA-CGA-O1A
38	h	102	DGD	C4D-C5D-C6D-O5D
36	5	318	LHG	C24-C25-C26-C27
34	a	409	PHO	C4-C3-C5-C6
34	a	409	PHO	C2-C3-C5-C6
33	7	304	CLA	C4B-C3B-CAB-CBB
33	7	308	CLA	C4B-C3B-CAB-CBB
33	a	408	CLA	C4B-C3B-CAB-CBB
33	b	607	CLA	C4B-C3B-CAB-CBB
33	0	312	CLA	C4B-C3B-CAB-CBB
33	2	317	CLA	C4B-C3B-CAB-CBB
33	8	310	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
37	T	101	SQD	C28-C29-C30-C31
33	8	306	CLA	CAA-CBA-CGA-O2A
38	C	517	DGD	C4B-C5B-C6B-C7B
47	6	309	KC2	CAA-CBA-CGA-O1A
33	2	306	CLA	CAA-CBA-CGA-O2A
36	h	103	LHG	C27-C28-C29-C30
38	h	102	DGD	C6B-C7B-C8B-C9B
33	c	501	CLA	C16-C17-C18-C20
33	c	507	CLA	C16-C17-C18-C20
33	3	307	CLA	C16-C17-C18-C19
33	b	616	CLA	C16-C17-C18-C20
33	1	310	CLA	C16-C17-C18-C19
39	C	519	LMG	C28-C29-C30-C31
36	W	302	LHG	C1-C2-C3-O3
34	A	406	PHO	CHA-CBD-CGD-O1D
34	A	407	PHO	CHA-CBD-CGD-O1D
33	7	310	CLA	CAA-CBA-CGA-O1A
33	7	310	CLA	CAA-CBA-CGA-O2A
33	1	309	CLA	CAA-CBA-CGA-O2A
36	b	601	LHG	C7-C8-C9-C10
33	5	313	CLA	C16-C17-C18-C20
33	c	501	CLA	C4-C3-C5-C6
39	5	319	LMG	O1-C7-C8-O7
43	T	102	LMU	C5-C6-C7-C8
39	q	301	LMG	O7-C10-C11-C12
36	a	404	LHG	C25-C26-C27-C28
43	5	320	LMU	O5'-C1'-O1'-C1
39	C	519	LMG	C17-C18-C19-C20
36	h	103	LHG	C24-C25-C26-C27
38	3	320	DGD	CAB-CBB-CCB-CDB
39	0	314	LMG	C15-C16-C17-C18
33	B	605	CLA	C11-C10-C8-C7
33	b	613	CLA	C6-C7-C8-C10
33	9	310	CLA	C6-C7-C8-C10
34	A	406	PHO	C6-C7-C8-C10
38	h	102	DGD	C8B-C9B-CAB-CBB
36	5	318	LHG	C9-C10-C11-C12
39	C	520	LMG	C17-C18-C19-C20
33	b	606	CLA	C10-C11-C12-C13
36	A	411	LHG	C10-C11-C12-C13
43	4	317	LMU	C3'-C4'-O1B-C1B
33	B	603	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
38	a	401	DGD	O1A-C1A-C2A-C3A
33	c	507	CLA	C6-C7-C8-C9
33	c	509	CLA	C6-C7-C8-C9
33	c	510	CLA	C14-C13-C15-C16
33	3	312	CLA	C6-C7-C8-C9
33	5	313	CLA	C11-C10-C8-C9
33	7	312	CLA	C14-C13-C15-C16
33	0	312	CLA	C11-C12-C13-C14
37	T	101	SQD	C5-C6-S-O8
37	t	102	SQD	C5-C6-S-O8
38	A	415	DGD	C5D-C6D-O5D-C1E
39	D	404	LMG	C8-C7-O1-C1
39	d	406	LMG	C8-C7-O1-C1
39	d	410	LMG	C8-C7-O1-C1
39	M	201	LMG	C8-C7-O1-C1
33	B	601	CLA	C2A-CAA-CBA-CGA
33	c	510	CLA	C2-C1-O2A-CGA
33	4	316	CLA	C2-C1-O2A-CGA
33	2	308	CLA	C2-C1-O2A-CGA
43	4	317	LMU	C5'-C4'-O1B-C1B
33	B	602	CLA	C5-C6-C7-C8
39	w	304	LMG	C14-C15-C16-C17
33	H	103	CLA	C3A-C2A-CAA-CBA
33	4	308	CLA	C3A-C2A-CAA-CBA
33	4	312	CLA	C3A-C2A-CAA-CBA
33	7	311	CLA	C3A-C2A-CAA-CBA
33	1	310	CLA	C3A-C2A-CAA-CBA
39	W	301	LMG	C40-C41-C42-C43
33	B	604	CLA	C2-C3-C5-C6
47	5	310	KC2	C2B-C3B-CAB-CBB
39	C	520	LMG	O7-C10-C11-C12
39	B	620	LMG	C18-C19-C20-C21
30	c	514	BCR	C10-C11-C12-C13
33	C	509	CLA	C10-C11-C12-C13
39	b	621	LMG	O10-C28-C29-C30
39	m	201	LMG	C12-C13-C14-C15
33	2	309	CLA	CAA-CBA-CGA-O1A
33	0	307	CLA	C13-C15-C16-C17
46	3	315	DD6	C13-C14-C15-O1
36	A	412	LHG	C24-C23-O8-C6
33	1	309	CLA	CAA-CBA-CGA-O1A
42	e	101	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
42	V	201	HEM	CAD-CBD-CGD-O1D
36	A	412	LHG	C4-C5-C6-O8
37	B	622	SQD	C44-C45-C46-O48
38	C	518	DGD	C1G-C2G-C3G-O3G
36	a	404	LHG	C26-C27-C28-C29
33	b	602	CLA	O1A-CGA-O2A-C1
42	V	201	HEM	C4B-C3B-CAB-CBB
47	5	310	KC2	C4B-C3B-CAB-CBB
36	4	318	LHG	C12-C13-C14-C15
33	0	309	CLA	C3-C5-C6-C7
39	W	301	LMG	C35-C36-C37-C38
33	8	306	CLA	CAA-CBA-CGA-O1A
42	e	101	HEM	CAA-CBA-CGA-O1A
47	7	306	KC2	CAA-CBA-CGA-O1A
47	5	310	KC2	CBD-CGD-O2D-CED
33	0	312	CLA	C4-C3-C5-C6
33	D	402	CLA	C2A-CAA-CBA-CGA
33	b	613	CLA	C2A-CAA-CBA-CGA
33	2	310	CLA	C2-C3-C5-C6
45	8	301	A86	C3-C4-C5-C6
37	0	316	SQD	C29-C30-C31-C32
45	5	301	A86	C28-C27-C29-C30
36	D	411	LHG	C11-C12-C13-C14
38	C	517	DGD	CBB-CCB-CDB-CEB
37	D	403	SQD	C17-C18-C19-C20
33	C	501	CLA	C6-C7-C8-C9
33	c	508	CLA	C14-C13-C15-C16
33	c	509	CLA	C11-C10-C8-C9
33	W	303	CLA	C11-C12-C13-C14
33	b	606	CLA	C11-C12-C13-C14
33	9	310	CLA	C2C-C3C-CAC-CBC
39	q	302	LMG	C35-C36-C37-C38
39	0	314	LMG	O8-C28-C29-C30
33	b	602	CLA	CBA-CGA-O2A-C1
39	D	410	LMG	C29-C28-O8-C9
38	H	102	DGD	C3B-C4B-C5B-C6B
33	b	610	CLA	C4-C3-C5-C6
45	4	301	A86	C13-C14-C15-O1
45	1	301	A86	C13-C14-C15-O1
33	C	501	CLA	O1D-CGD-O2D-CED
39	5	319	LMG	O7-C10-C11-C12
33	2	306	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
33	C	507	CLA	C2A-CAA-CBA-CGA
33	2	311	CLA	C2A-CAA-CBA-CGA
36	D	411	LHG	C30-C31-C32-C33
33	B	604	CLA	C6-C7-C8-C10
33	c	507	CLA	C6-C7-C8-C10
33	c	510	CLA	C12-C13-C15-C16
33	3	308	CLA	C11-C12-C13-C15
33	5	313	CLA	C11-C10-C8-C7
33	0	312	CLA	C11-C12-C13-C15
33	9	310	CLA	C11-C12-C13-C15
30	A	401	BCR	C23-C24-C25-C26
30	A	409	BCR	C1-C6-C7-C8
30	A	409	BCR	C5-C6-C7-C8
30	B	618	BCR	C1-C6-C7-C8
30	B	618	BCR	C23-C24-C25-C30
30	C	515	BCR	C23-C24-C25-C26
30	h	101	BCR	C23-C24-C25-C26
30	K	101	BCR	C1-C6-C7-C8
30	K	101	BCR	C23-C24-C25-C26
30	K	101	BCR	C23-C24-C25-C30
30	K	102	BCR	C23-C24-C25-C26
30	k	101	BCR	C1-C6-C7-C8
30	k	101	BCR	C5-C6-C7-C8
30	k	101	BCR	C23-C24-C25-C26
30	k	102	BCR	C23-C24-C25-C26
30	a	412	BCR	C5-C6-C7-C8
30	a	412	BCR	C23-C24-C25-C30
30	a	414	BCR	C23-C24-C25-C26
30	b	619	BCR	C1-C6-C7-C8
30	b	619	BCR	C5-C6-C7-C8
30	b	619	BCR	C23-C24-C25-C26
33	3	319	CLA	C2B-C3B-CAB-CBB
33	4	311	CLA	C2B-C3B-CAB-CBB
33	5	309	CLA	C2B-C3B-CAB-CBB
33	5	313	CLA	C2B-C3B-CAB-CBB
33	6	312	CLA	C2B-C3B-CAB-CBB
33	a	408	CLA	C2B-C3B-CAB-CBB
33	9	315	CLA	C2B-C3B-CAB-CBB
33	2	317	CLA	C2B-C3B-CAB-CBB
33	B	613	CLA	CAA-CBA-CGA-O2A
33	D	405	CLA	CAA-CBA-CGA-O2A
33	3	302	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
38	c	517	DGD	C9B-CAB-CBB-CCB
33	b	611	CLA	C2-C1-O2A-CGA
33	b	614	CLA	C2-C1-O2A-CGA
33	0	307	CLA	C2-C1-O2A-CGA
37	T	103	SQD	C19-C20-C21-C22
33	C	513	CLA	O2A-C1-C2-C3
38	a	401	DGD	O2G-C1B-C2B-C3B
34	a	409	PHO	C8-C10-C11-C12
33	6	312	CLA	C3-C5-C6-C7
33	b	608	CLA	CBD-CGD-O2D-CED
33	c	511	CLA	C2-C3-C5-C6
33	b	610	CLA	C2-C3-C5-C6
39	5	319	LMG	C11-C12-C13-C14
36	W	302	LHG	O2-C2-C3-O3
33	C	510	CLA	CAA-CBA-CGA-O2A
33	c	510	CLA	CAA-CBA-CGA-O2A
33	b	614	CLA	CAA-CBA-CGA-O2A
39	D	404	LMG	C29-C30-C31-C32
33	3	308	CLA	CAA-CBA-CGA-O2A
38	c	516	DGD	O2G-C1B-C2B-C3B
36	A	412	LHG	C27-C28-C29-C30
39	C	519	LMG	C10-C11-C12-C13
37	B	622	SQD	C4-C5-C6-S
37	l	101	SQD	C4-C5-C6-S
37	T	101	SQD	C4-C5-C6-S
37	t	102	SQD	C4-C5-C6-S
42	v	201	HEM	CAA-CBA-CGA-O2A
38	3	320	DGD	C1B-C2B-C3B-C4B
33	C	501	CLA	CAA-CBA-CGA-O2A
33	W	303	CLA	CAA-CBA-CGA-O2A
33	4	311	CLA	C2-C3-C5-C6
38	a	401	DGD	O1A-C1A-O1G-C1G
33	C	510	CLA	C2A-CAA-CBA-CGA
33	a	408	CLA	C2A-CAA-CBA-CGA
33	w	303	CLA	CAA-CBA-CGA-O2A
43	T	102	LMU	C2-C1-O1'-C1'
33	3	303	CLA	C5-C6-C7-C8
33	0	310	CLA	CAA-CBA-CGA-O2A
33	3	303	CLA	C6-C7-C8-C9
33	5	313	CLA	C11-C12-C13-C14
33	b	610	CLA	C14-C13-C15-C16
33	b	613	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
34	A	407	PHO	C6-C7-C8-C9
33	2	307	CLA	O1D-CGD-O2D-CED
33	C	503	CLA	C15-C16-C17-C18
33	6	312	CLA	C15-C16-C17-C18
33	5	312	CLA	CAA-CBA-CGA-O2A
33	7	312	CLA	CAA-CBA-CGA-O2A
33	0	312	CLA	CAA-CBA-CGA-O2A
37	a	413	SQD	O48-C23-C24-C25
39	b	623	LMG	O8-C28-C29-C30
36	H	104	LHG	C4-C5-C6-O8
39	B	620	LMG	O1-C7-C8-C9
36	d	407	LHG	C15-C16-C17-C18
33	B	610	CLA	C4B-C3B-CAB-CBB
33	B	616	CLA	C4B-C3B-CAB-CBB
33	C	504	CLA	C1A-C2A-CAA-CBA
33	C	511	CLA	C1A-C2A-CAA-CBA
33	3	312	CLA	C4B-C3B-CAB-CBB
33	3	319	CLA	C4B-C3B-CAB-CBB
33	4	305	CLA	C1A-C2A-CAA-CBA
33	9	306	CLA	C1A-C2A-CAA-CBA
33	9	315	CLA	C4B-C3B-CAB-CBB
33	8	307	CLA	C1A-C2A-CAA-CBA
38	a	401	DGD	C8B-C9B-CAB-CBB
39	C	520	LMG	C14-C15-C16-C17
33	7	311	CLA	C2C-C3C-CAC-CBC
33	W	303	CLA	C4-C3-C5-C6
39	W	301	LMG	C16-C17-C18-C19
38	C	518	DGD	O6E-C1E-O5D-C6D
33	3	303	CLA	CAA-CBA-CGA-O2A
30	d	403	BCR	C7-C8-C9-C10
45	9	301	A86	C11-C10-C9-C8
45	2	301	A86	C11-C10-C9-C8
36	d	405	LHG	C15-C16-C17-C18
37	D	403	SQD	C26-C27-C28-C29
33	c	501	CLA	CAA-CBA-CGA-O2A
33	d	401	CLA	CAA-CBA-CGA-O2A
33	2	308	CLA	CAA-CBA-CGA-O2A
37	D	403	SQD	O47-C7-C8-C9
33	9	311	CLA	C2A-CAA-CBA-CGA
33	8	311	CLA	C2A-CAA-CBA-CGA
33	1	311	CLA	C2A-CAA-CBA-CGA
39	d	406	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
36	h	103	LHG	O6-C4-C5-C6
33	9	308	CLA	CAA-CBA-CGA-O2A
39	q	302	LMG	O8-C28-C29-C30
37	B	622	SQD	C5-C6-S-O7
37	a	413	SQD	C5-C6-S-O9
33	c	510	CLA	C8-C10-C11-C12
33	2	317	CLA	C5-C6-C7-C8
33	6	308	CLA	C2-C1-O2A-CGA
33	C	509	CLA	C11-C12-C13-C15
33	c	512	CLA	C12-C13-C15-C16
34	A	406	PHO	C12-C13-C15-C16
37	7	317	SQD	C24-C23-O48-C46
38	H	102	DGD	C2B-C3B-C4B-C5B
39	c	519	LMG	C16-C17-C18-C19
36	A	414	LHG	C29-C30-C31-C32
33	C	507	CLA	C8-C10-C11-C12
46	8	303	DD6	C24-C25-C26-C27
46	1	303	DD6	C24-C25-C26-C27
33	4	306	CLA	C2A-CAA-CBA-CGA
33	6	313	CLA	C2A-CAA-CBA-CGA
33	9	306	CLA	C2A-CAA-CBA-CGA
33	2	310	CLA	C2A-CAA-CBA-CGA
33	1	310	CLA	C2A-CAA-CBA-CGA
33	C	502	CLA	C16-C17-C18-C20
36	b	601	LHG	C26-C27-C28-C29
39	B	620	LMG	C39-C40-C41-C42
36	4	318	LHG	C5-C4-O6-P
33	2	307	CLA	CAA-CBA-CGA-O1A
33	B	602	CLA	C3A-C2A-CAA-CBA
33	7	305	CLA	C4-C3-C5-C6
33	9	310	CLA	C3A-C2A-CAA-CBA
33	8	307	CLA	C3A-C2A-CAA-CBA
33	D	405	CLA	CAA-CBA-CGA-O1A
38	c	516	DGD	O6D-C5D-C6D-O5D
33	b	615	CLA	C12-C13-C15-C16
33	0	307	CLA	C2-C3-C5-C6
42	F	101	HEM	C4D-C3D-CAD-CBD
33	B	613	CLA	CAA-CBA-CGA-O1A
33	c	510	CLA	CAA-CBA-CGA-O1A
36	d	405	LHG	O10-C23-C24-C25
33	c	507	CLA	O1A-CGA-O2A-C1
33	c	507	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	7	311	CLA	C4C-C3C-CAC-CBC
38	c	516	DGD	O6D-C1D-O3G-C3G
39	D	410	LMG	C21-C22-C23-C24
39	7	315	LMG	O9-C10-C11-C12
39	0	314	LMG	O10-C28-C29-C30
37	B	622	SQD	C19-C20-C21-C22
34	A	406	PHO	CBD-CGD-O2D-CED
33	5	308	CLA	C2A-CAA-CBA-CGA
36	b	601	LHG	C24-C23-O8-C6
33	0	310	CLA	CAA-CBA-CGA-O1A
33	4	306	CLA	C11-C12-C13-C14
33	4	308	CLA	C6-C7-C8-C9
33	C	501	CLA	CAA-CBA-CGA-O1A
38	A	415	DGD	O1B-C1B-C2B-C3B
36	d	407	LHG	C11-C12-C13-C14
33	d	409	CLA	O1D-CGD-O2D-CED
33	C	510	CLA	CAA-CBA-CGA-O1A
37	t	102	SQD	C32-C33-C34-C35
33	B	612	CLA	C10-C11-C12-C13
44	6	314	KC1	C1A-C2A-CAA-CBA
47	4	307	KC2	C1A-C2A-CAA-CBA
47	6	309	KC2	C3A-C2A-CAA-CBA
38	C	516	DGD	C6A-C7A-C8A-C9A
33	w	303	CLA	CAA-CBA-CGA-O1A
33	3	302	CLA	CAA-CBA-CGA-O1A
33	5	312	CLA	CAA-CBA-CGA-O1A
33	0	312	CLA	CAA-CBA-CGA-O1A
37	D	403	SQD	O10-C23-C24-C25
33	b	608	CLA	O1D-CGD-O2D-CED
33	B	615	CLA	C5-C6-C7-C8
33	4	312	CLA	O1A-CGA-O2A-C1
39	7	315	LMG	O7-C10-C11-C12
39	B	620	LMG	O6-C5-C6-O5
33	2	307	CLA	CBD-CGD-O2D-CED
34	A	406	PHO	O1D-CGD-O2D-CED
33	b	614	CLA	CAA-CBA-CGA-O1A
34	A	407	PHO	C8-C10-C11-C12
38	A	415	DGD	C3A-C4A-C5A-C6A
37	T	101	SQD	C45-C44-O6-C1
37	7	317	SQD	C45-C44-O6-C1
38	C	516	DGD	C5D-C6D-O5D-C1E
38	c	517	DGD	C2G-C3G-O3G-C1D

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Mol	Chain	Res	Type	Atoms
38	a	401	DGD	C5D-C6D-O5D-C1E
37	i	101	SQD	O47-C45-C46-O48
33	3	303	CLA	CAA-CBA-CGA-O1A
33	7	312	CLA	CAA-CBA-CGA-O1A
37	a	413	SQD	O10-C23-C24-C25
39	b	621	LMG	O7-C10-C11-C12
33	B	608	CLA	C13-C15-C16-C17
39	m	201	LMG	C36-C37-C38-C39
36	3	318	LHG	C29-C30-C31-C32
38	c	517	DGD	C3B-C4B-C5B-C6B
36	3	317	LHG	C4-C5-C6-O8
36	a	404	LHG	C4-C5-C6-O8
39	b	621	LMG	O1-C7-C8-C9
33	3	308	CLA	CAA-CBA-CGA-O1A
33	B	612	CLA	CAA-CBA-CGA-O2A
33	7	304	CLA	CAA-CBA-CGA-O2A
38	C	516	DGD	O2G-C1B-C2B-C3B
39	D	404	LMG	O8-C28-C29-C30
36	A	412	LHG	C35-C36-C37-C38
37	B	622	SQD	C25-C26-C27-C28
33	c	501	CLA	CAA-CBA-CGA-O1A
33	d	401	CLA	CAA-CBA-CGA-O1A
33	9	308	CLA	CAA-CBA-CGA-O1A
33	2	308	CLA	CAA-CBA-CGA-O1A
39	q	302	LMG	O10-C28-C29-C30
33	c	502	CLA	O1A-CGA-O2A-C1
33	A	408	CLA	CAD-CBD-CGD-O2D
33	B	616	CLA	CAD-CBD-CGD-O2D
33	D	405	CLA	CAD-CBD-CGD-O2D
33	d	401	CLA	CAD-CBD-CGD-O2D
33	W	303	CLA	CAD-CBD-CGD-O2D
33	6	315	CLA	CAD-CBD-CGD-O2D
33	0	305	CLA	CAA-CBA-CGA-O2A
38	C	516	DGD	CCB-CDB-CEB-CFB
33	W	303	CLA	CAA-CBA-CGA-O1A
33	0	304	CLA	CAA-CBA-CGA-O2A
36	a	403	LHG	C29-C30-C31-C32
38	c	516	DGD	C4D-C5D-C6D-O5D
37	T	103	SQD	C27-C28-C29-C30
37	t	102	SQD	C33-C34-C35-C36
33	4	308	CLA	CAA-CBA-CGA-O2A
33	C	501	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
36	A	411	LHG	C12-C13-C14-C15
33	4	311	CLA	CAA-CBA-CGA-O2A
33	8	308	CLA	CAA-CBA-CGA-O2A
37	a	413	SQD	O47-C7-C8-C9
39	Q	301	LMG	O8-C28-C29-C30
33	c	502	CLA	CBA-CGA-O2A-C1
37	D	403	SQD	O49-C7-C8-C9
36	3	318	LHG	C28-C29-C30-C31

There are no ring outliers.

259 monomers are involved in 635 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	c	506	CLA	3	0
33	9	314	CLA	2	0
33	c	508	CLA	5	0
33	C	502	CLA	1	0
33	4	315	CLA	1	0
45	4	301	A86	4	0
33	2	312	CLA	1	0
33	c	507	CLA	1	0
33	b	605	CLA	2	0
33	B	604	CLA	5	0
39	C	520	LMG	2	0
30	k	101	BCR	4	0
38	C	518	DGD	1	0
33	3	302	CLA	1	0
33	4	306	CLA	6	0
46	2	304	DD6	13	0
33	B	615	CLA	4	0
33	4	313	CLA	3	0
33	2	308	CLA	4	0
33	B	606	CLA	1	0
33	C	513	CLA	2	0
45	1	301	A86	3	0
33	2	309	CLA	3	0
39	q	302	LMG	3	0
30	k	102	BCR	3	0
34	A	406	PHO	1	0
46	9	304	DD6	4	0
33	3	309	CLA	1	0
45	6	304	A86	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	b	606	CLA	3	0
30	b	620	BCR	2	0
39	q	301	LMG	4	0
36	h	103	LHG	2	0
33	b	611	CLA	1	0
33	C	508	CLA	1	0
30	c	515	BCR	2	0
45	5	304	A86	3	0
37	L	101	SQD	2	0
33	C	507	CLA	2	0
33	c	511	CLA	1	0
38	3	320	DGD	3	0
30	B	617	BCR	1	0
33	3	304	CLA	4	0
38	A	415	DGD	3	0
30	A	409	BCR	2	0
33	8	311	CLA	7	0
36	W	302	LHG	2	0
33	5	309	CLA	3	0
45	2	302	A86	6	0
39	C	519	LMG	1	0
33	9	307	CLA	2	0
37	l	101	SQD	2	0
33	3	308	CLA	1	0
39	b	622	LMG	1	0
48	0	302	ET4	2	0
45	9	302	A86	1	0
38	c	517	DGD	3	0
33	7	310	CLA	8	0
38	c	516	DGD	5	0
33	b	602	CLA	3	0
47	4	307	KC2	2	0
33	8	308	CLA	3	0
43	T	102	LMU	1	0
33	1	308	CLA	3	0
33	b	604	CLA	3	0
36	A	411	LHG	1	0
33	3	313	CLA	6	0
36	D	409	LHG	1	0
33	B	602	CLA	2	0
45	4	302	A86	7	0
33	4	308	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	a	403	LHG	1	0
43	4	317	LMU	13	0
46	9	303	DD6	1	0
33	2	311	CLA	10	0
33	4	309	CLA	2	0
33	4	311	CLA	2	0
45	7	301	A86	2	0
39	m	201	LMG	2	0
30	C	515	BCR	3	0
45	5	306	A86	2	0
33	3	312	CLA	4	0
37	B	622	SQD	3	0
36	4	318	LHG	2	0
37	t	102	SQD	2	0
33	d	402	CLA	5	0
37	i	101	SQD	1	0
33	1	305	CLA	1	0
33	6	313	CLA	2	0
38	h	102	DGD	1	0
46	1	304	DD6	3	0
33	B	613	CLA	2	0
36	7	316	LHG	1	0
33	7	307	CLA	3	0
30	c	514	BCR	4	0
33	b	614	CLA	3	0
37	0	316	SQD	1	0
45	5	303	A86	1	0
36	3	318	LHG	2	0
39	7	315	LMG	1	0
33	3	306	CLA	1	0
43	w	302	LMU	5	0
36	a	404	LHG	1	0
42	V	201	HEM	2	0
33	c	504	CLA	2	0
45	5	305	A86	2	0
30	b	619	BCR	2	0
39	0	314	LMG	2	0
33	9	311	CLA	3	0
39	b	623	LMG	4	0
33	c	501	CLA	2	0
33	B	608	CLA	1	0
33	c	510	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	B	619	BCR	3	0
33	w	303	CLA	5	0
33	A	408	CLA	1	0
33	5	314	CLA	8	0
33	7	304	CLA	2	0
33	c	503	CLA	3	0
42	F	101	HEM	9	0
33	c	512	CLA	1	0
33	1	306	CLA	2	0
33	1	307	CLA	3	0
39	d	406	LMG	1	0
35	a	402	BCT	3	0
39	W	301	LMG	2	0
30	h	101	BCR	5	0
33	B	601	CLA	1	0
44	6	314	KC1	6	0
46	2	303	DD6	6	0
45	6	301	A86	10	0
30	H	101	BCR	1	0
33	C	504	CLA	1	0
33	4	314	CLA	2	0
33	c	509	CLA	2	0
33	C	503	CLA	4	0
38	c	518	DGD	2	0
30	d	403	BCR	1	0
33	4	305	CLA	2	0
46	3	315	DD6	1	0
45	5	301	A86	9	0
46	4	303	DD6	1	0
33	7	312	CLA	4	0
33	B	616	CLA	1	0
36	5	318	LHG	1	0
30	D	407	BCR	1	0
33	6	308	CLA	2	0
33	C	506	CLA	1	0
33	D	405	CLA	1	0
33	5	313	CLA	14	0
33	C	510	CLA	2	0
33	9	310	CLA	5	0
33	5	316	CLA	10	0
33	6	310	CLA	1	0
45	1	302	A86	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	1	303	DD6	2	0
34	a	409	PHO	1	0
43	5	320	LMU	11	0
33	7	309	CLA	2	0
33	8	310	CLA	9	0
36	A	412	LHG	3	0
45	6	302	A86	3	0
33	5	312	CLA	2	0
39	b	621	LMG	1	0
33	W	303	CLA	6	0
33	1	314	CLA	1	0
41	d	404	PL9	1	0
33	d	401	CLA	1	0
34	A	407	PHO	1	0
33	C	501	CLA	2	0
33	0	311	CLA	2	0
43	t	101	LMU	1	0
30	a	412	BCR	4	0
43	3	301	LMU	5	0
33	2	310	CLA	4	0
37	T	103	SQD	1	0
33	1	312	CLA	2	0
46	8	303	DD6	1	0
39	c	519	LMG	4	0
39	d	410	LMG	3	0
33	4	312	CLA	2	0
33	2	306	CLA	7	0
33	7	311	CLA	1	0
36	d	405	LHG	1	0
33	c	513	CLA	1	0
33	D	406	CLA	2	0
33	0	304	CLA	4	0
33	0	312	CLA	1	0
33	A	404	CLA	1	0
38	a	401	DGD	2	0
33	B	605	CLA	4	0
38	C	517	DGD	3	0
37	a	413	SQD	1	0
30	K	101	BCR	6	0
33	1	313	CLA	3	0
33	8	307	CLA	2	0
33	9	308	CLA	6	0

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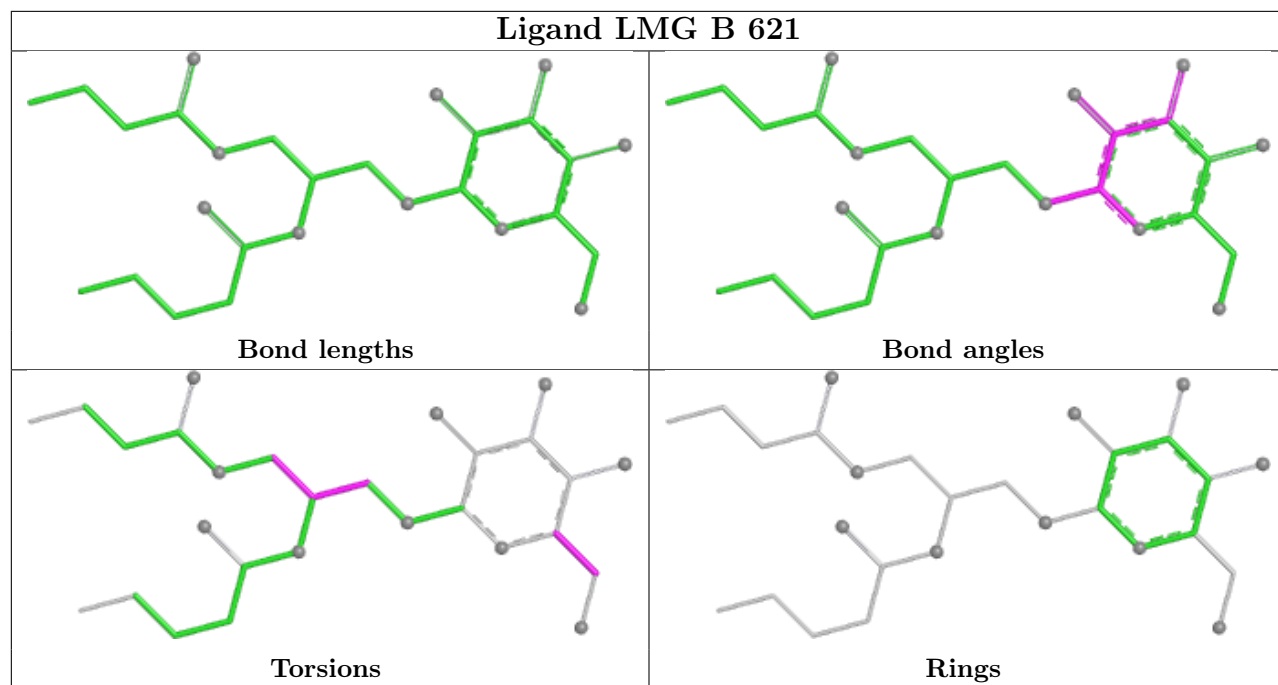
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33	c	502	CLA	2	0
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33	9	315	CLA	1	0
34	a	410	PHO	1	0
33	C	509	CLA	2	0
39	M	201	LMG	1	0
30	K	102	BCR	3	0
33	b	617	CLA	5	0
33	Z	101	CLA	1	0
33	3	307	CLA	18	0
33	7	308	CLA	1	0
33	b	609	CLA	1	0
33	3	303	CLA	2	0
45	2	301	A86	1	0
33	5	308	CLA	3	0
45	8	302	A86	3	0
33	3	319	CLA	2	0
37	D	403	SQD	2	0
33	b	615	CLA	1	0
39	D	404	LMG	2	0
42	v	201	HEM	5	0
33	1	311	CLA	3	0
33	B	611	CLA	1	0
33	4	310	CLA	9	0
33	H	103	CLA	3	0
30	b	618	BCR	3	0
33	b	607	CLA	3	0
33	0	310	CLA	2	0
33	B	612	CLA	1	0
45	3	314	A86	2	0
48	7	302	ET4	2	0
30	a	414	BCR	2	0
33	b	616	CLA	1	0
33	b	610	CLA	3	0
45	5	302	A86	14	0
33	6	307	CLA	5	0
33	0	307	CLA	3	0
30	B	618	BCR	2	0
39	w	304	LMG	1	0
33	C	512	CLA	1	0
33	7	305	CLA	4	0

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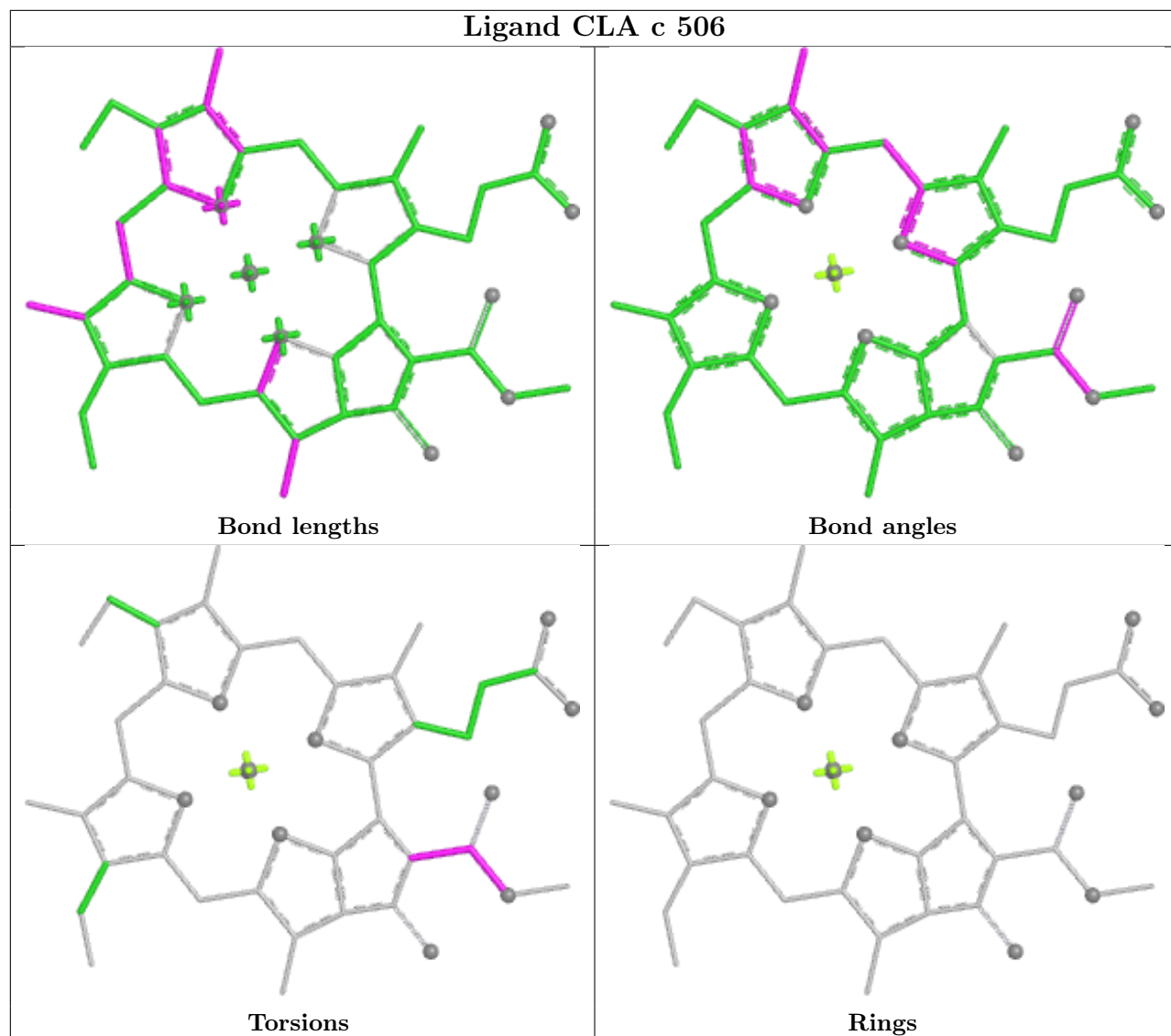
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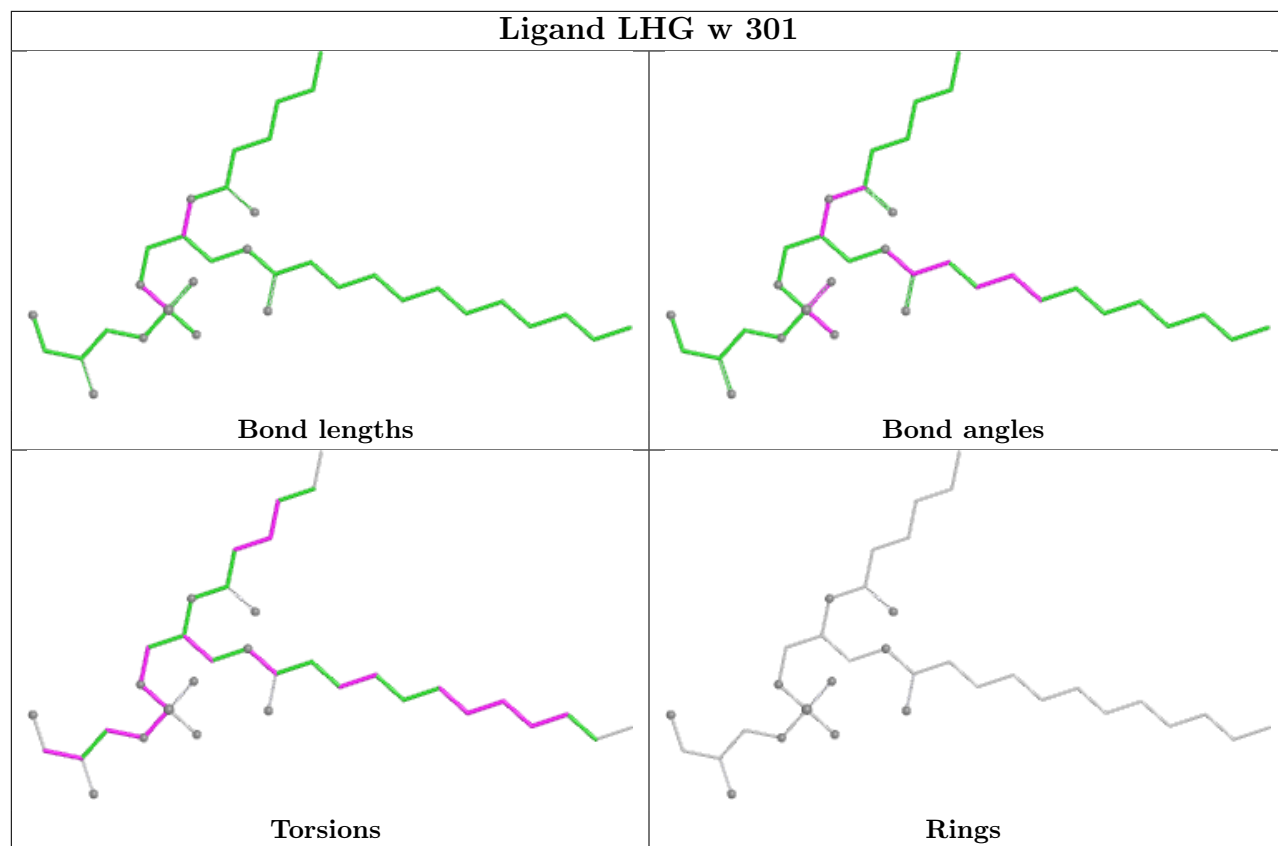
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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33	B	609	CLA	3	0
33	0	305	CLA	3	0
33	B	607	CLA	1	0
33	B	603	CLA	2	0
38	C	516	DGD	3	0
33	1	310	CLA	5	0
47	5	310	KC2	16	0
33	5	311	CLA	4	0
35	A	410	BCT	2	0
33	C	511	CLA	1	0
33	2	313	CLA	2	0
45	0	301	A86	1	0
30	C	514	BCR	3	0
37	T	101	SQD	1	0
42	e	101	HEM	4	0
33	2	315	CLA	1	0
33	6	311	CLA	1	0
46	8	304	DD6	7	0
33	z	101	CLA	1	0

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

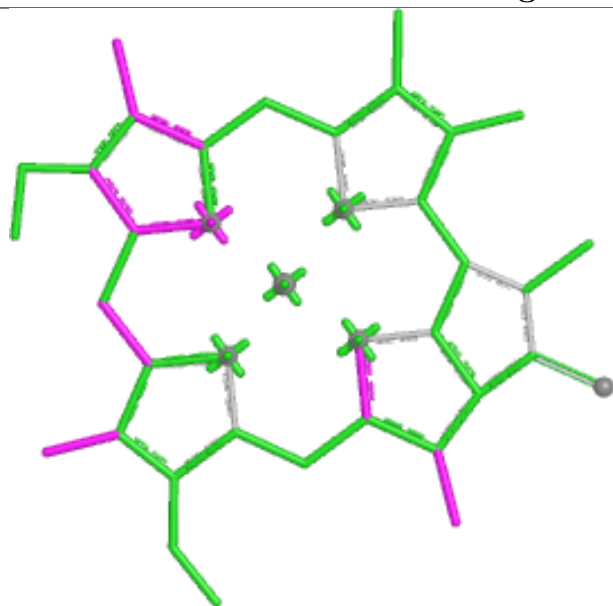


Ligand CLA c 506

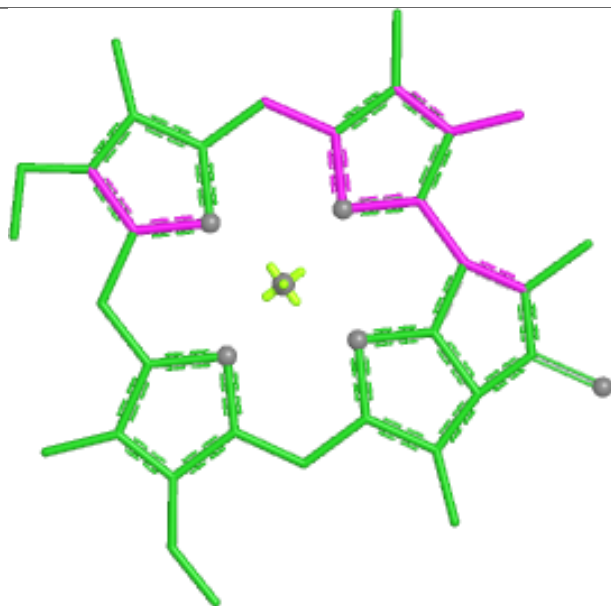




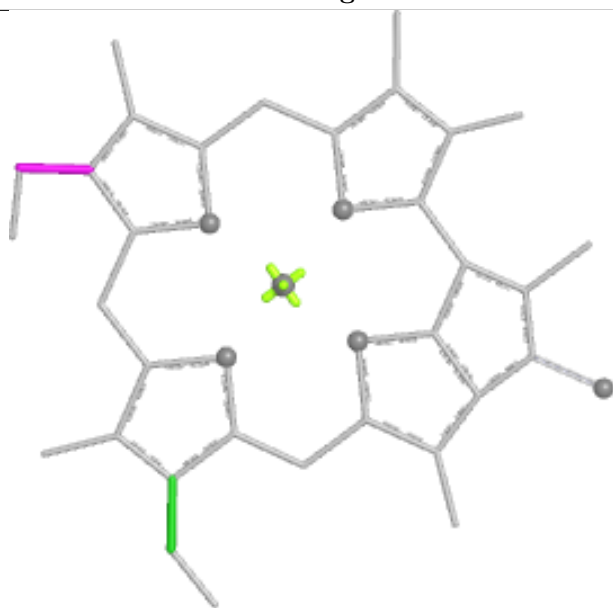
Ligand CLA 9 314



Bond lengths



Bond angles

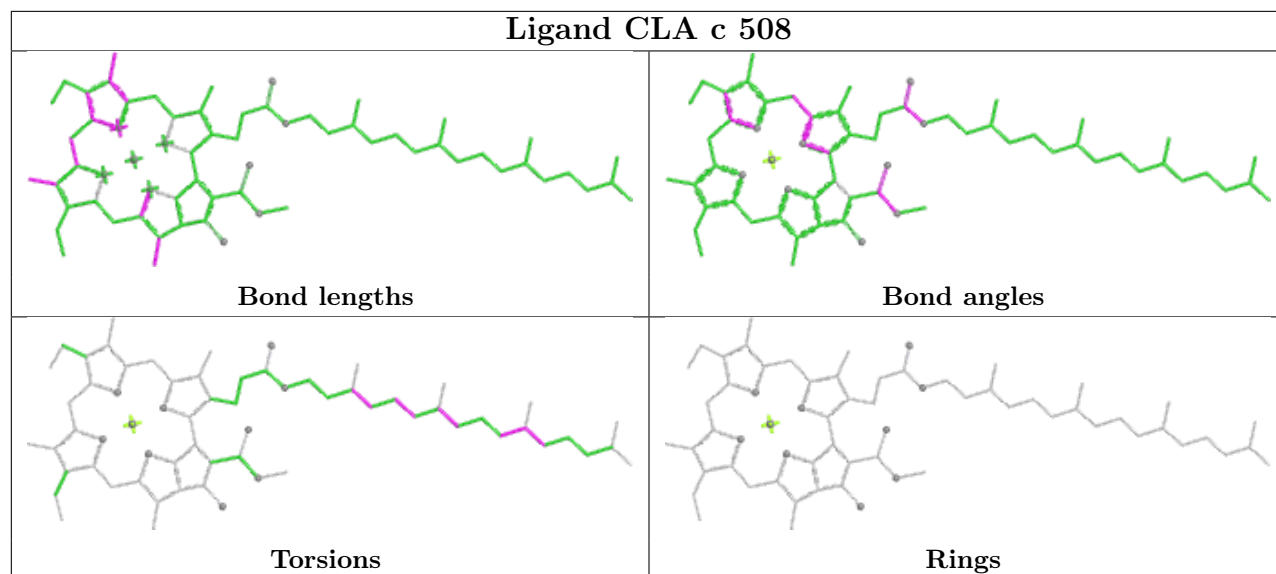


Torsions

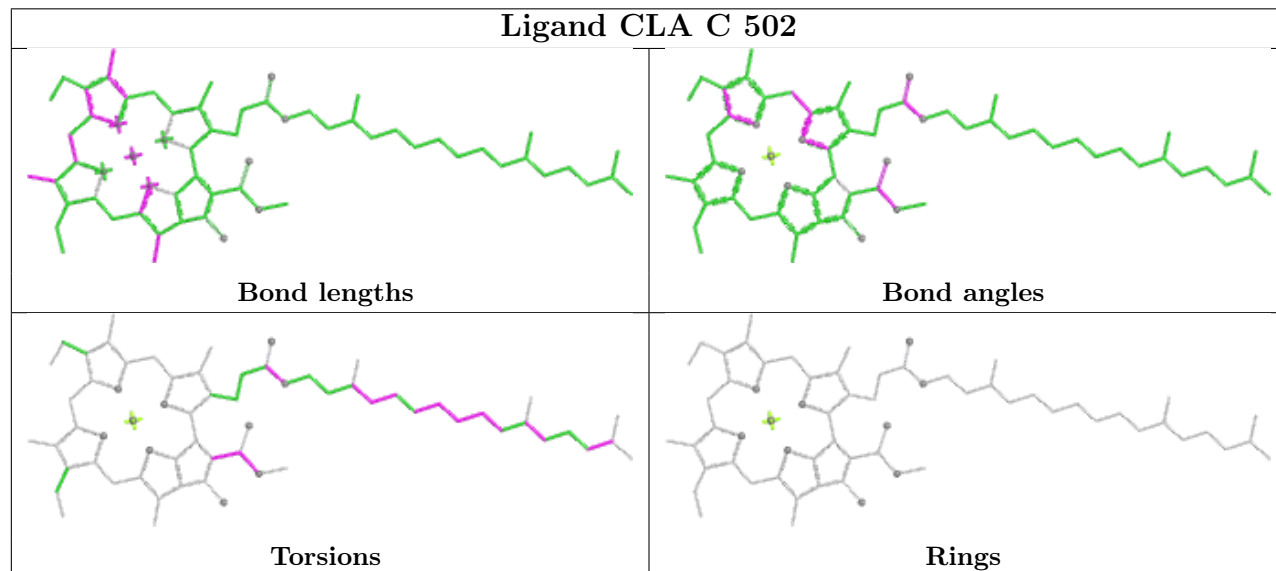


Rings

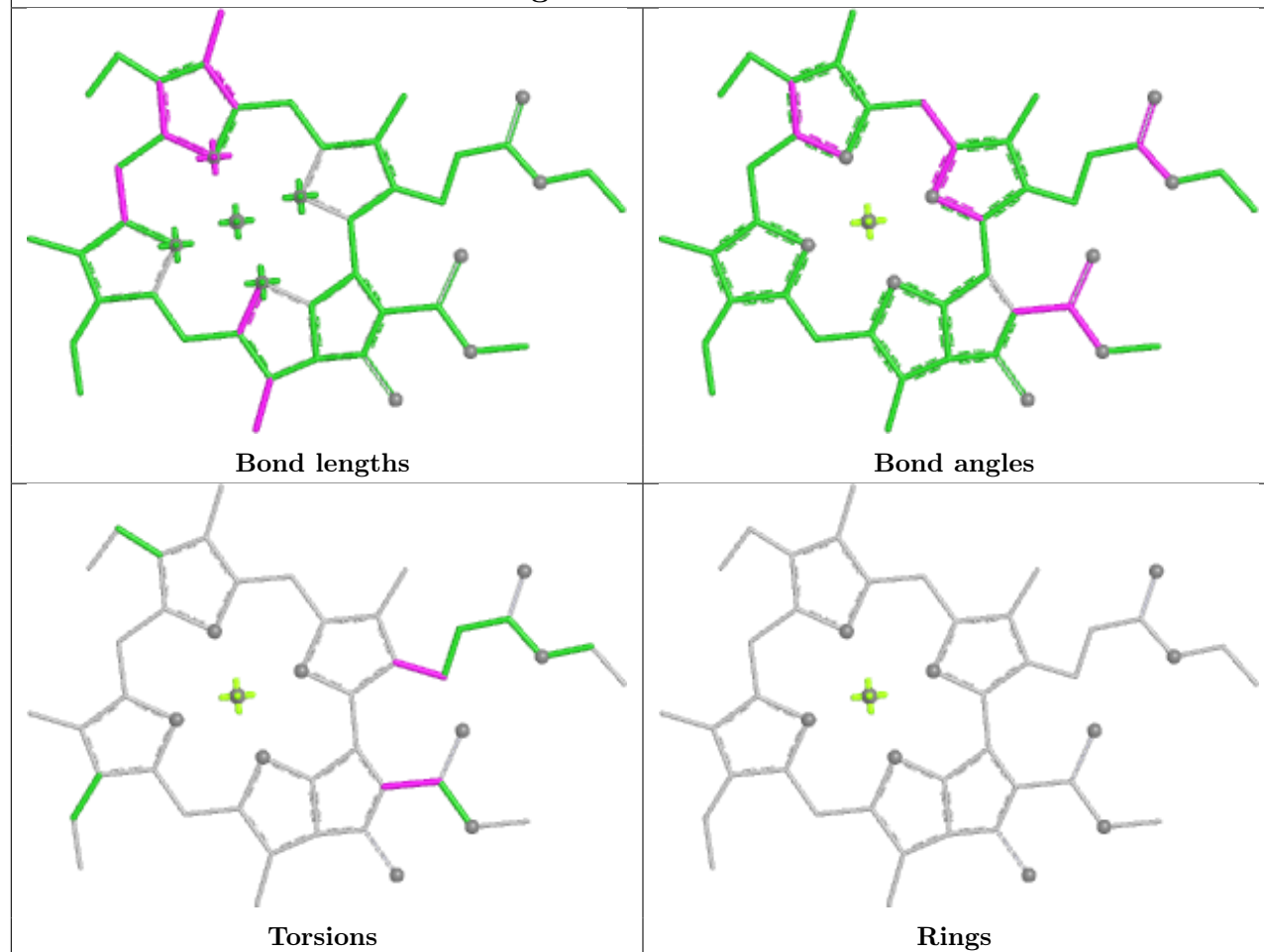
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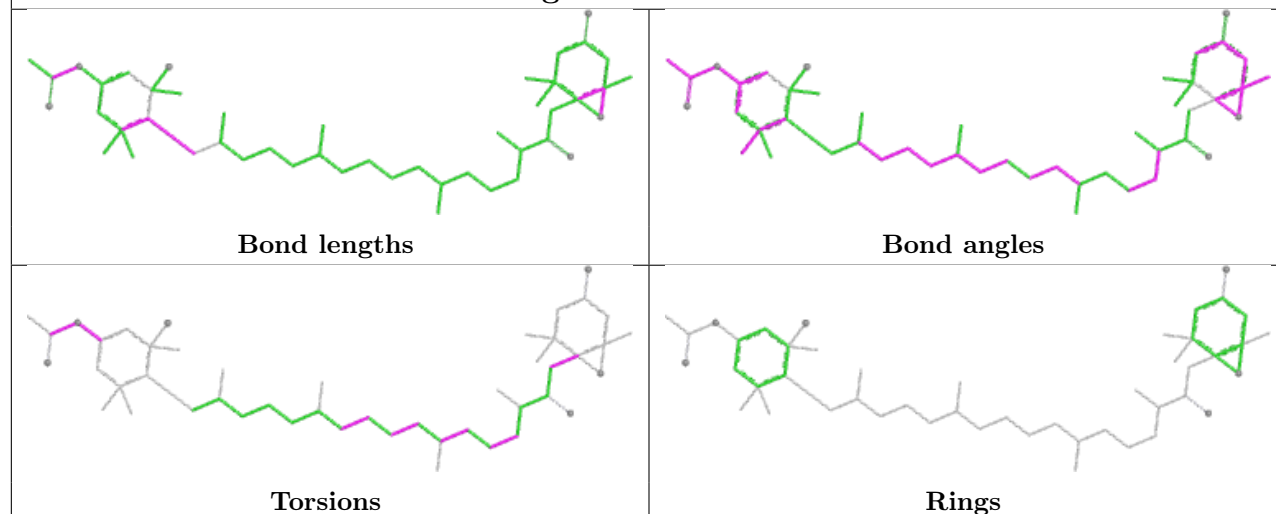
Ligand CLA C 502



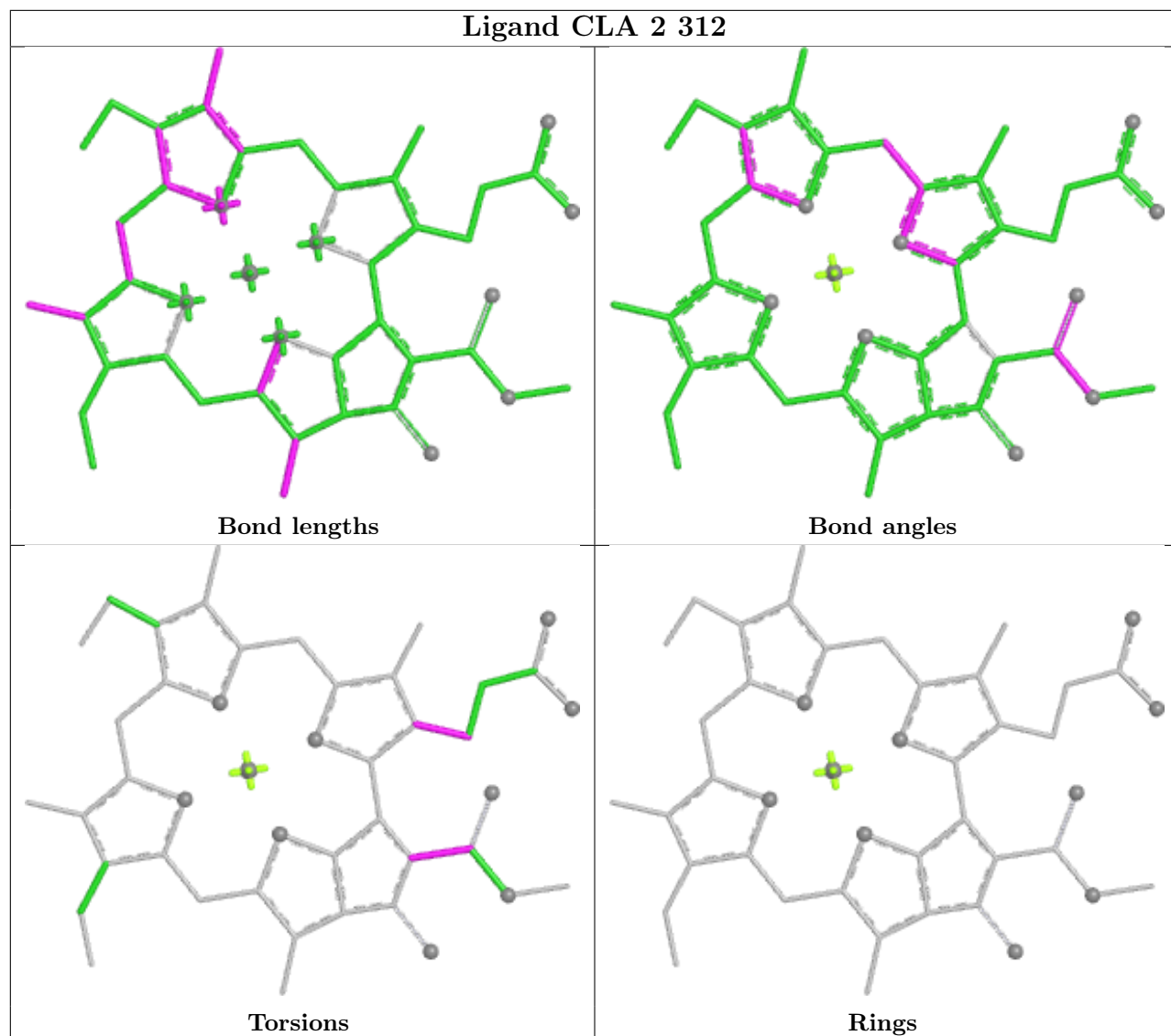
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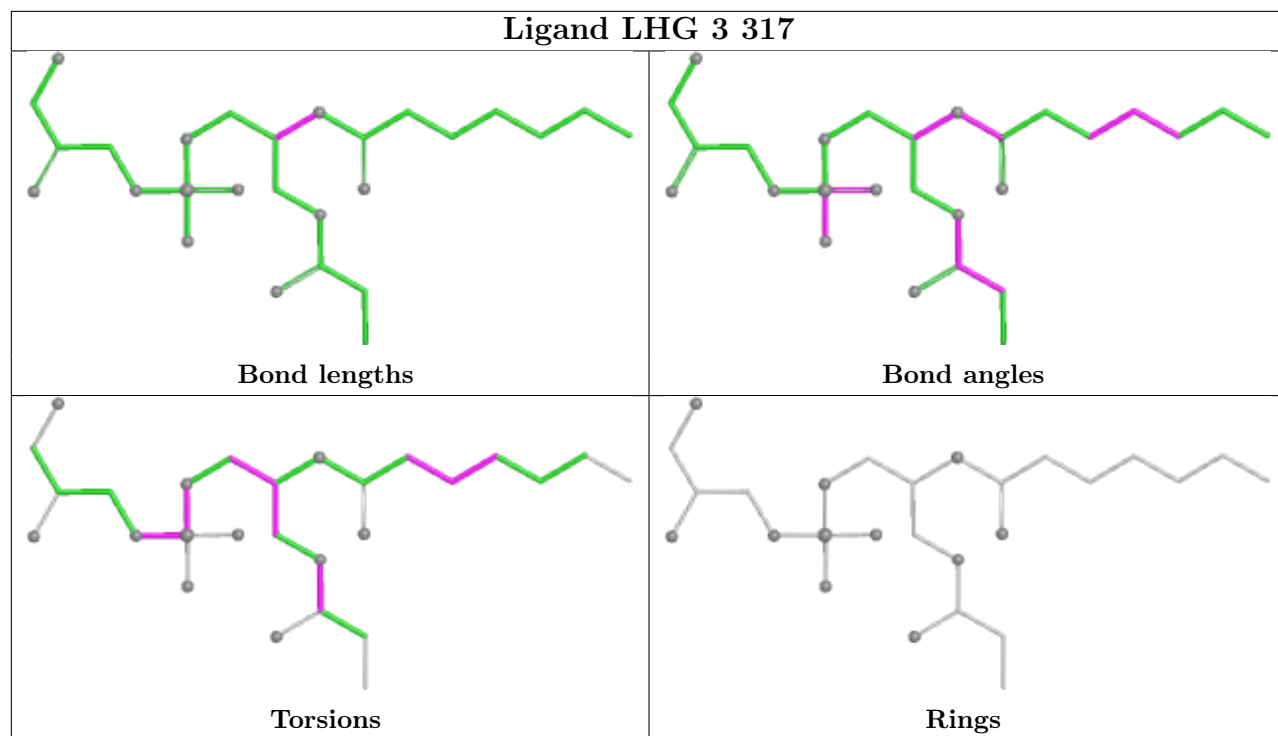


Ligand A86 4 301

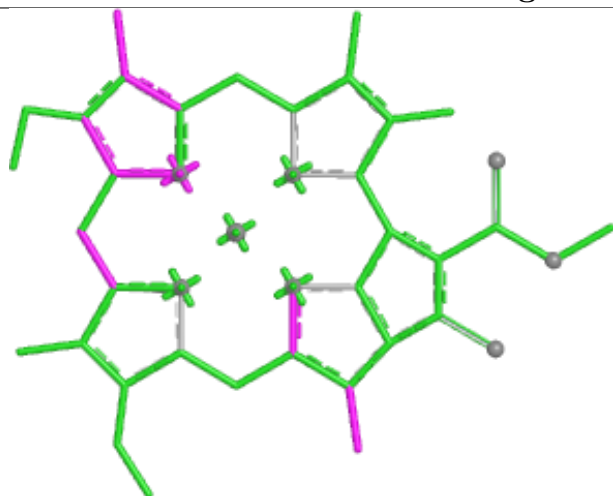


Ligand CLA 2 312

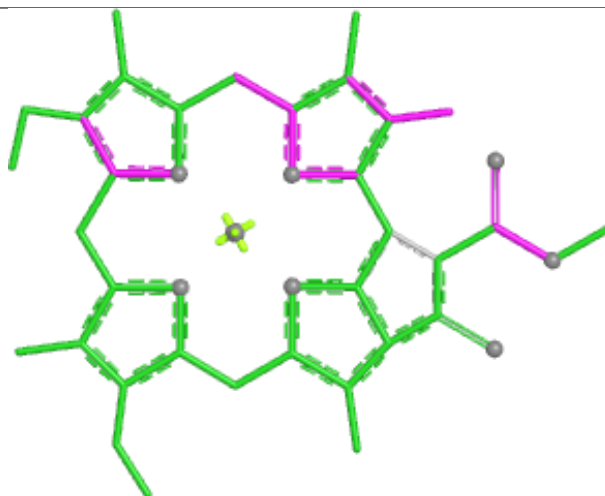




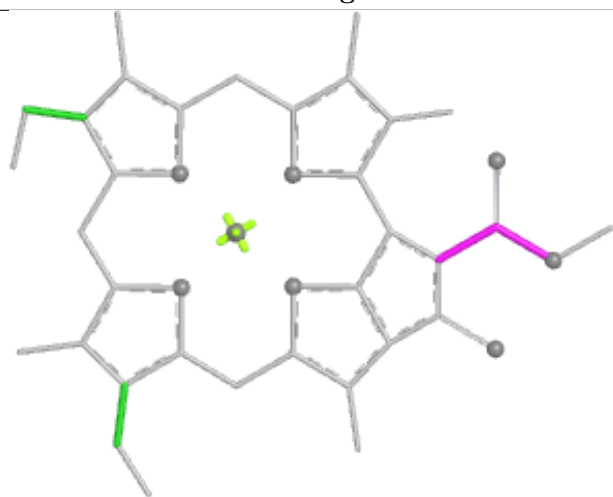
Ligand CLA 6 315



Bond lengths



Bond angles

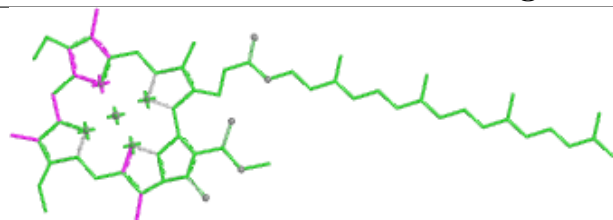


Torsions

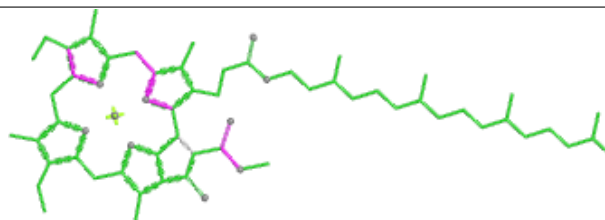


Rings

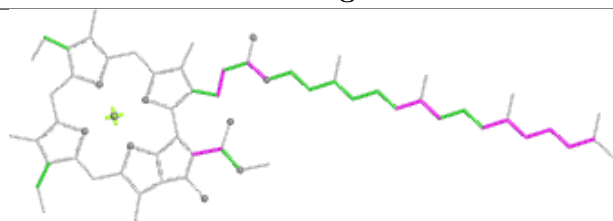
Ligand CLA c 507



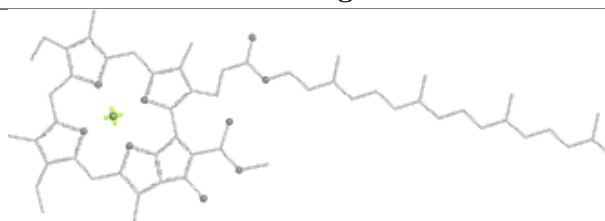
Bond lengths



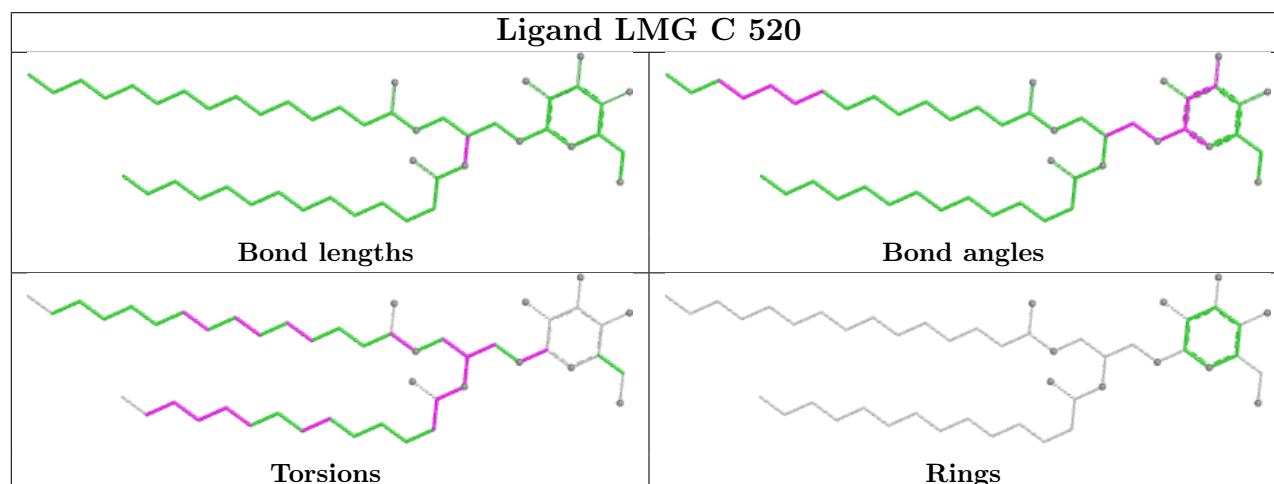
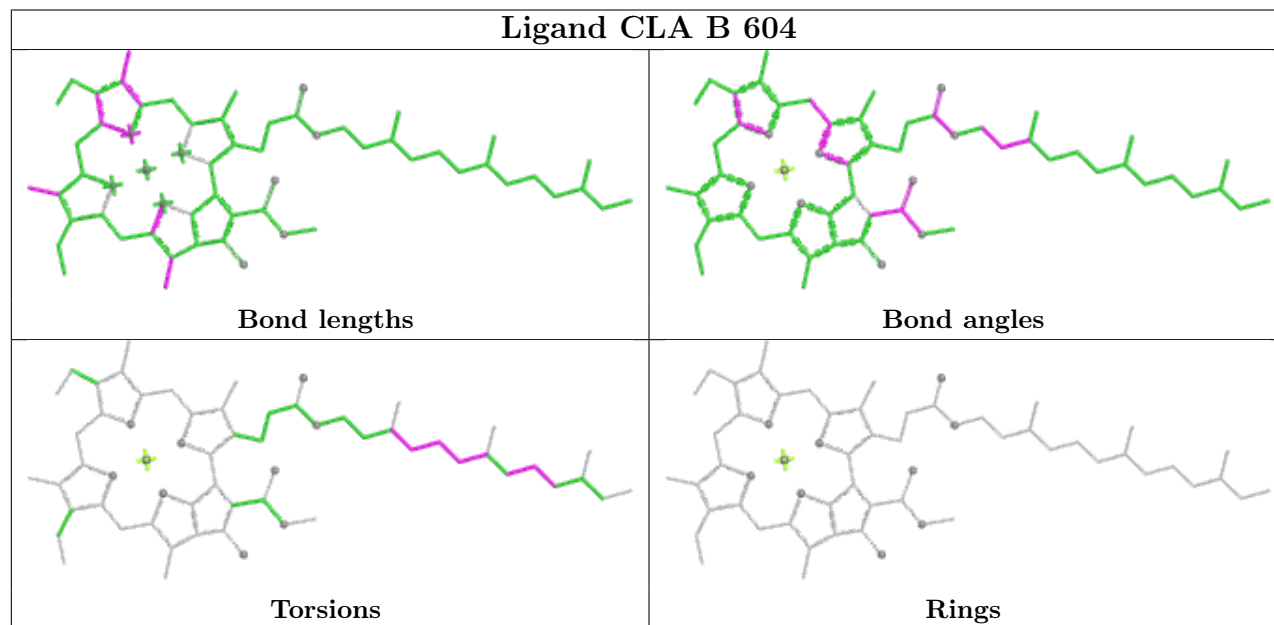
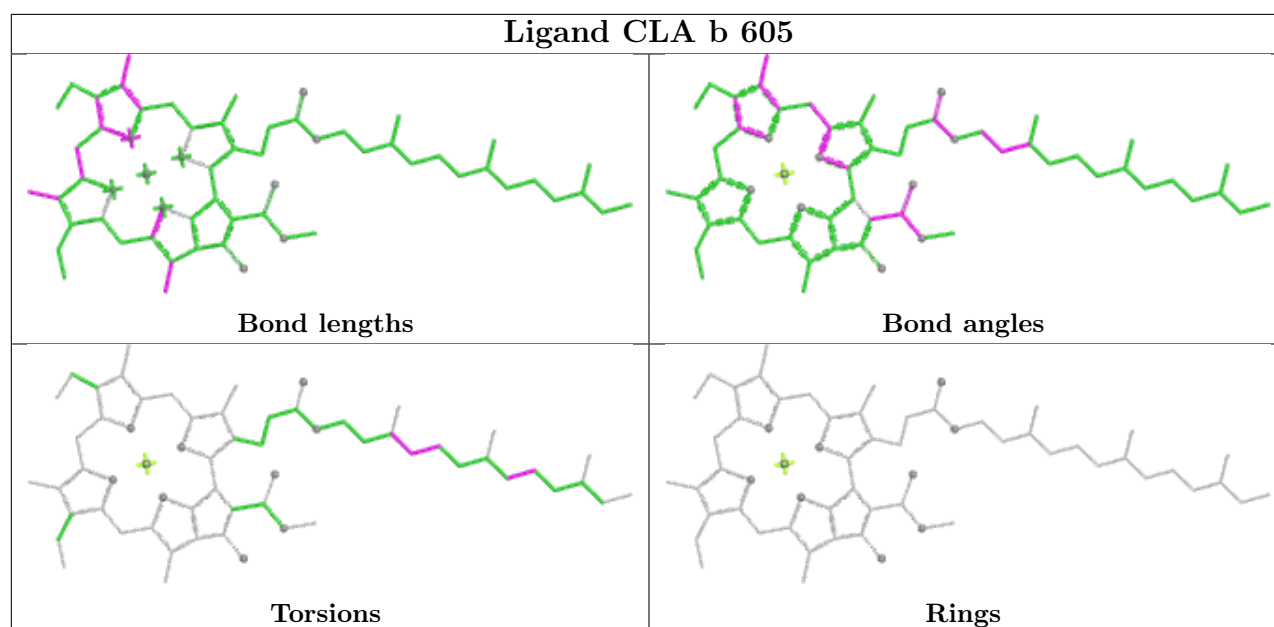
Bond angles

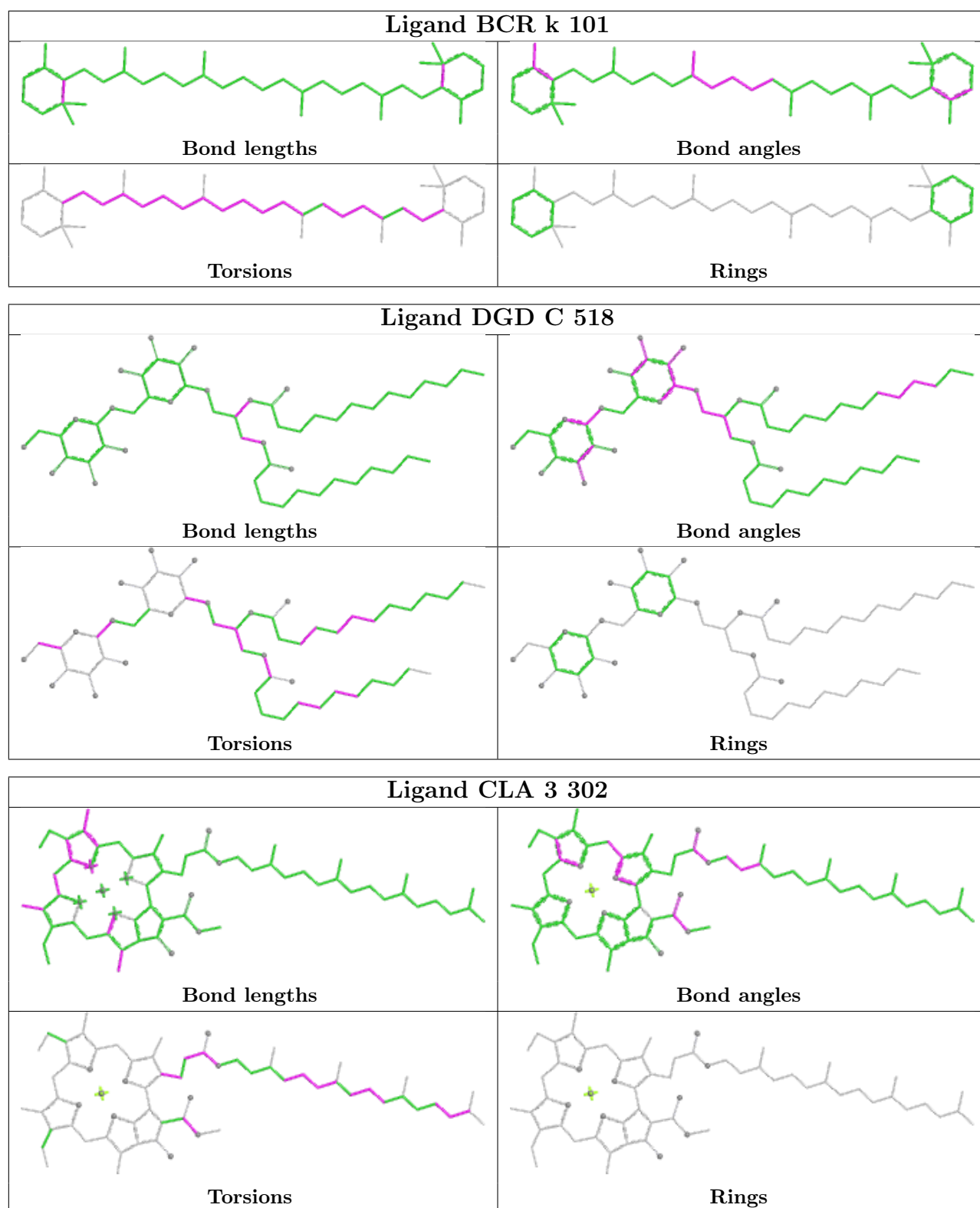


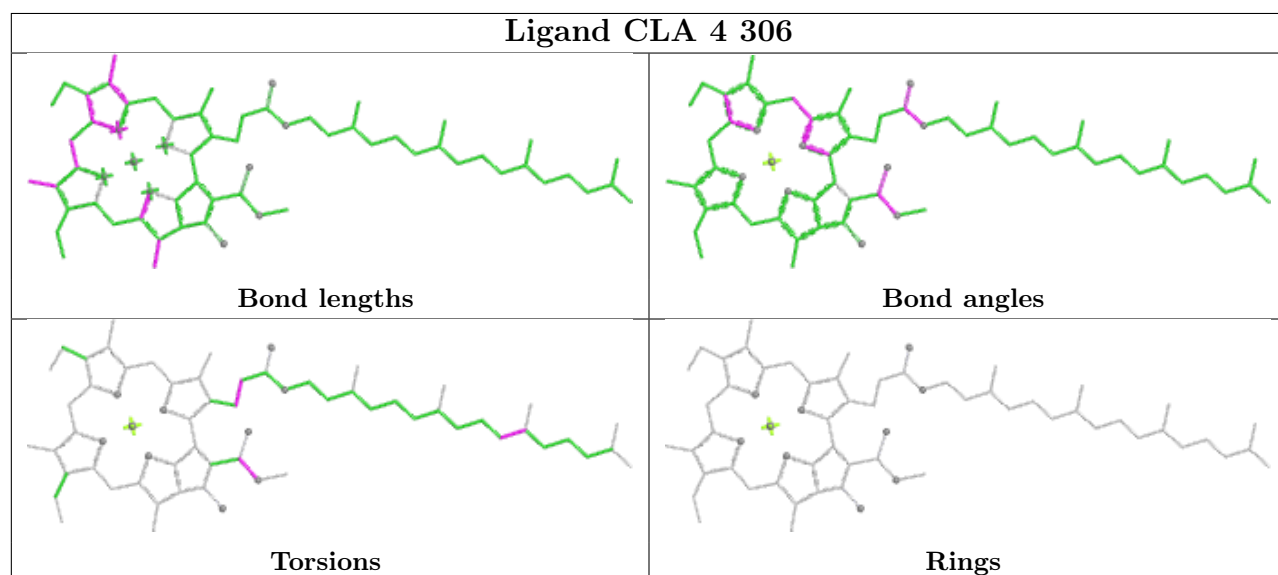
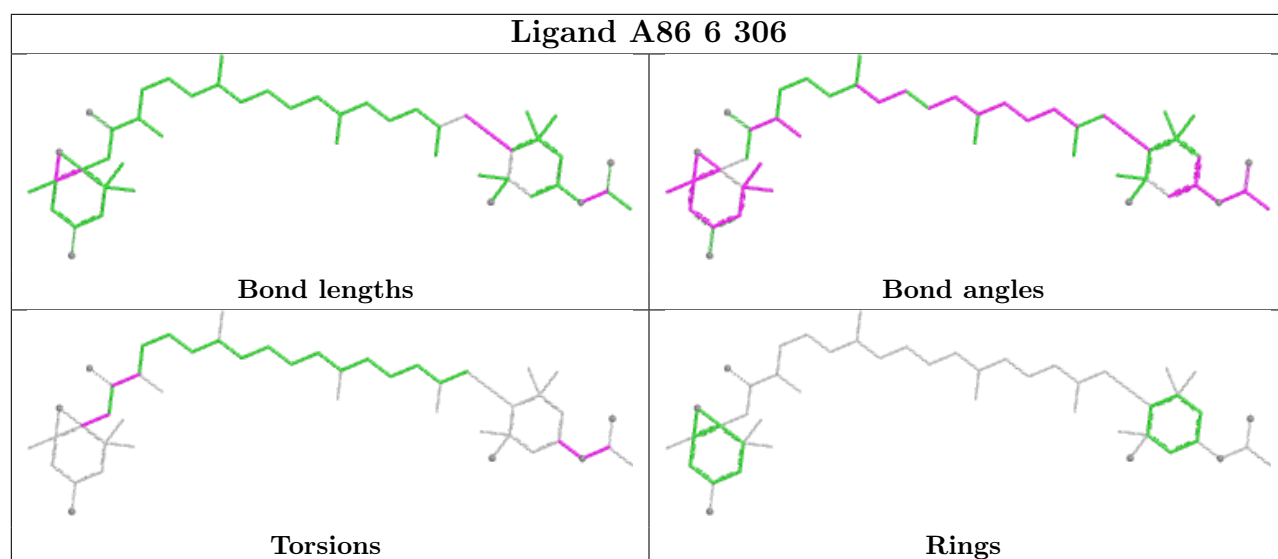
Torsions



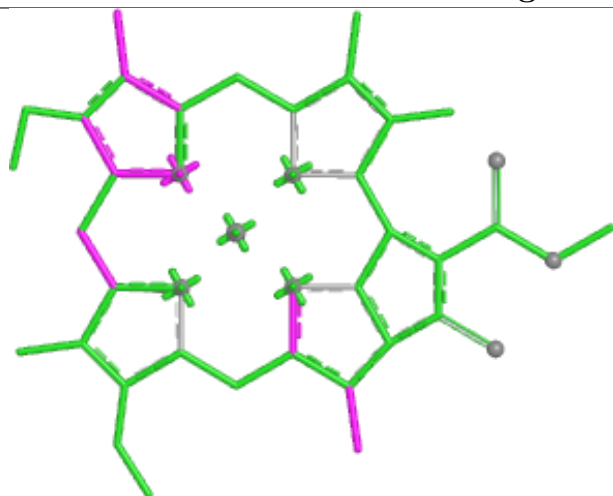
Rings



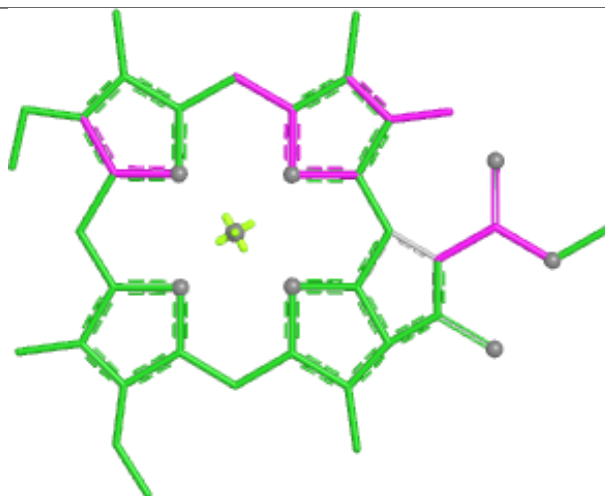




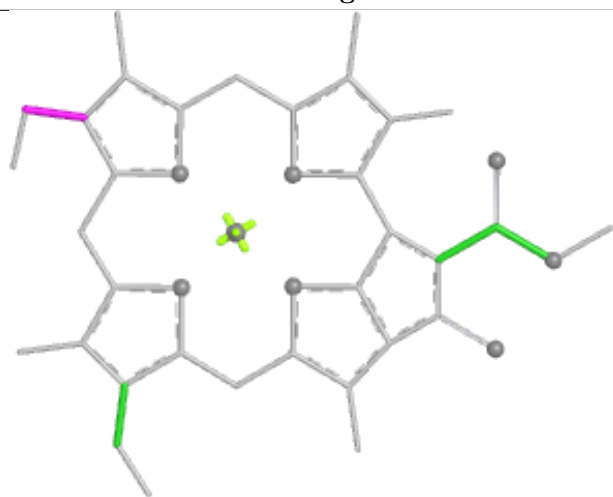
Ligand CLA 2 305



Bond lengths



Bond angles

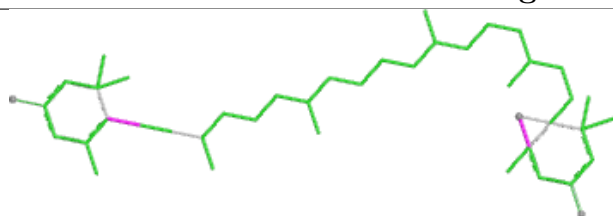


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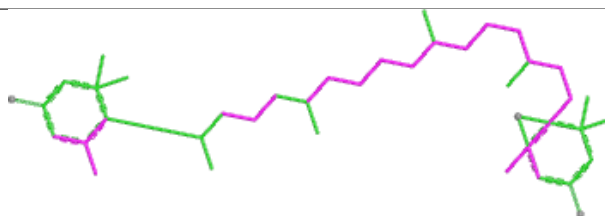


Rings

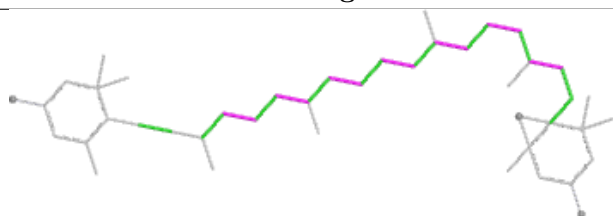
Ligand DD6 2 304



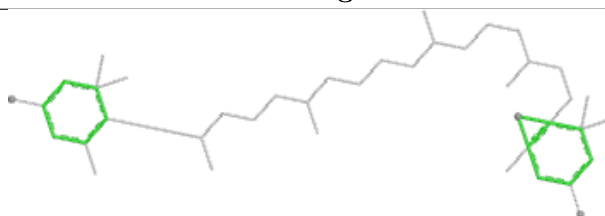
Bond lengths



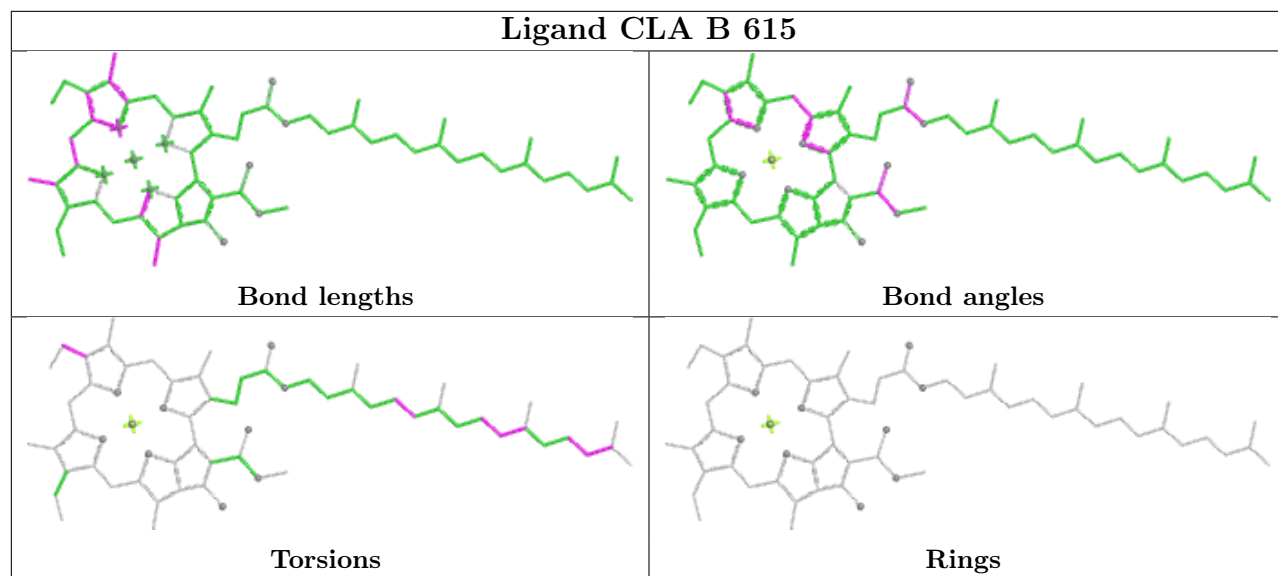
Bond angles



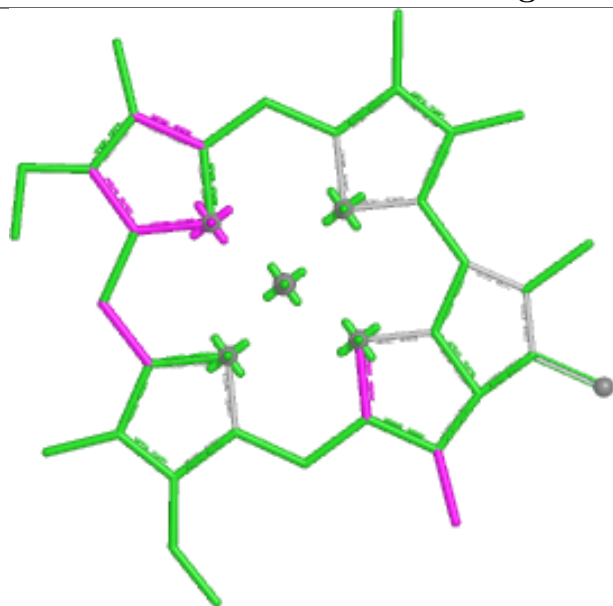
Torsions



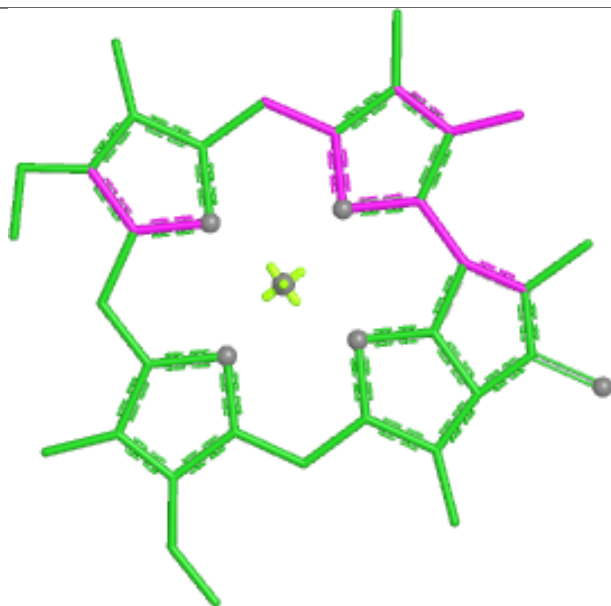
Rings



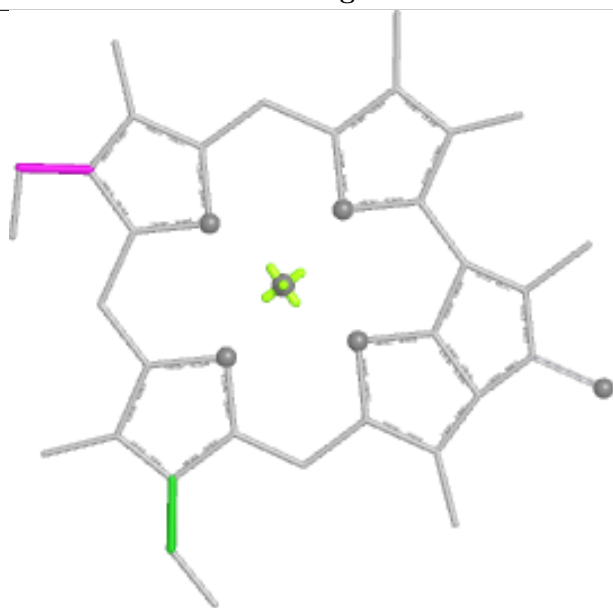
Ligand CLA 5 317



Bond lengths



Bond angles

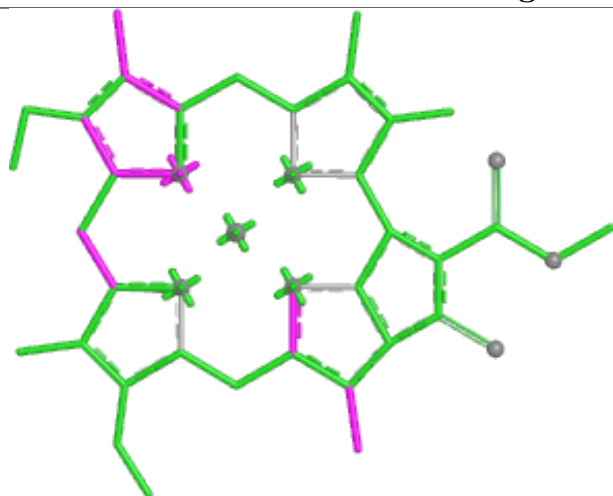


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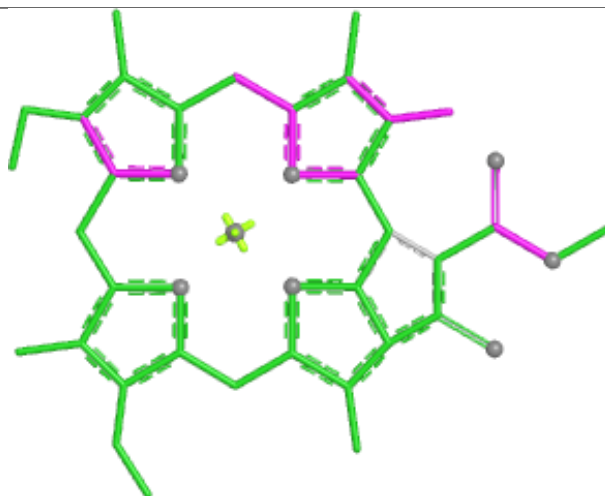


Rings

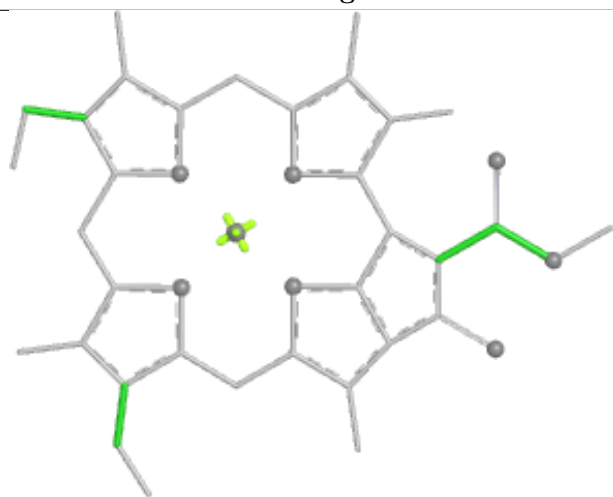
Ligand CLA 4 313



Bond lengths



Bond angles

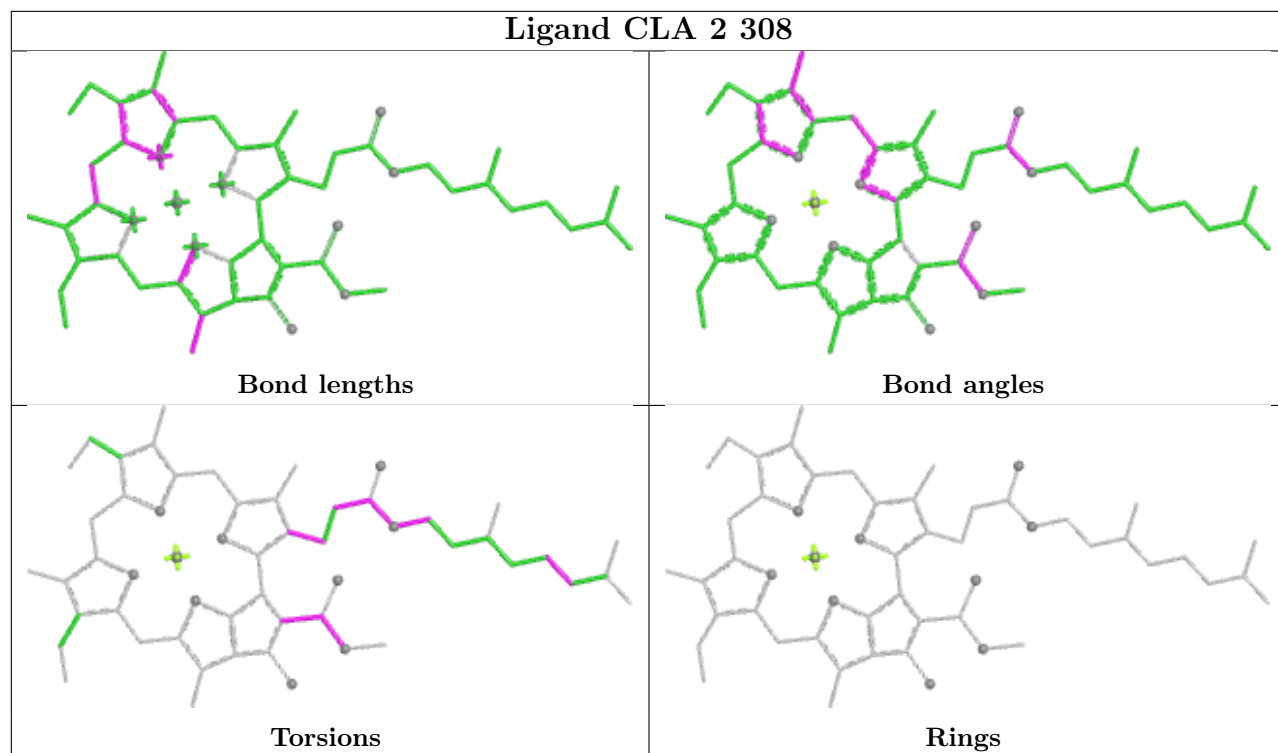


Torsions

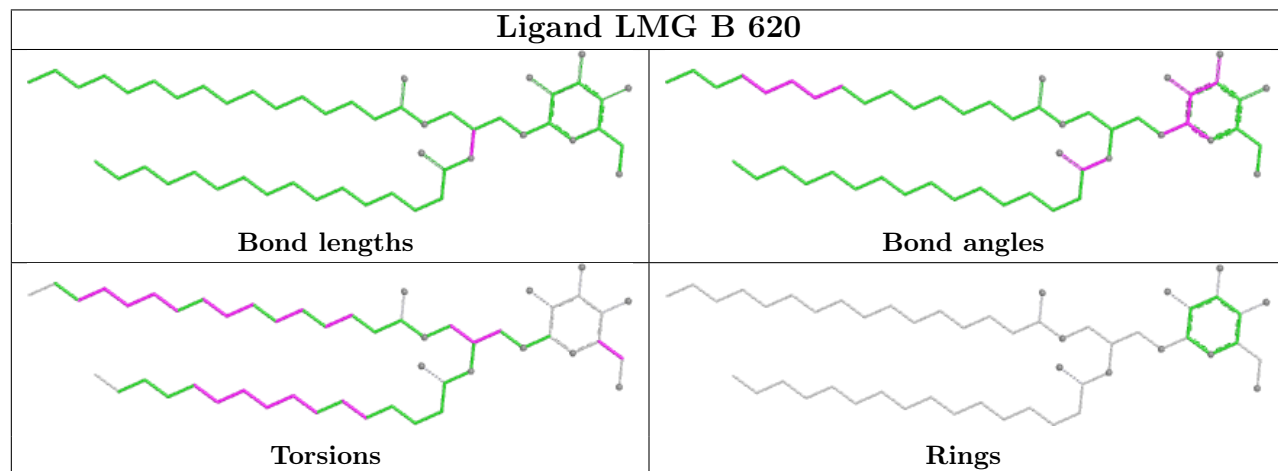


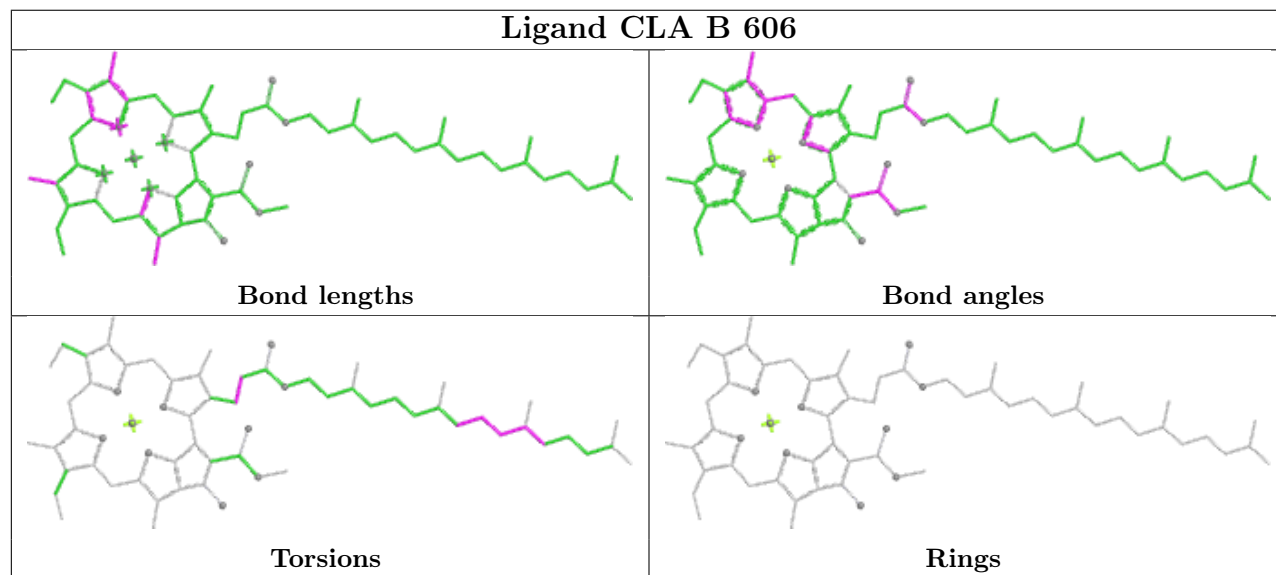
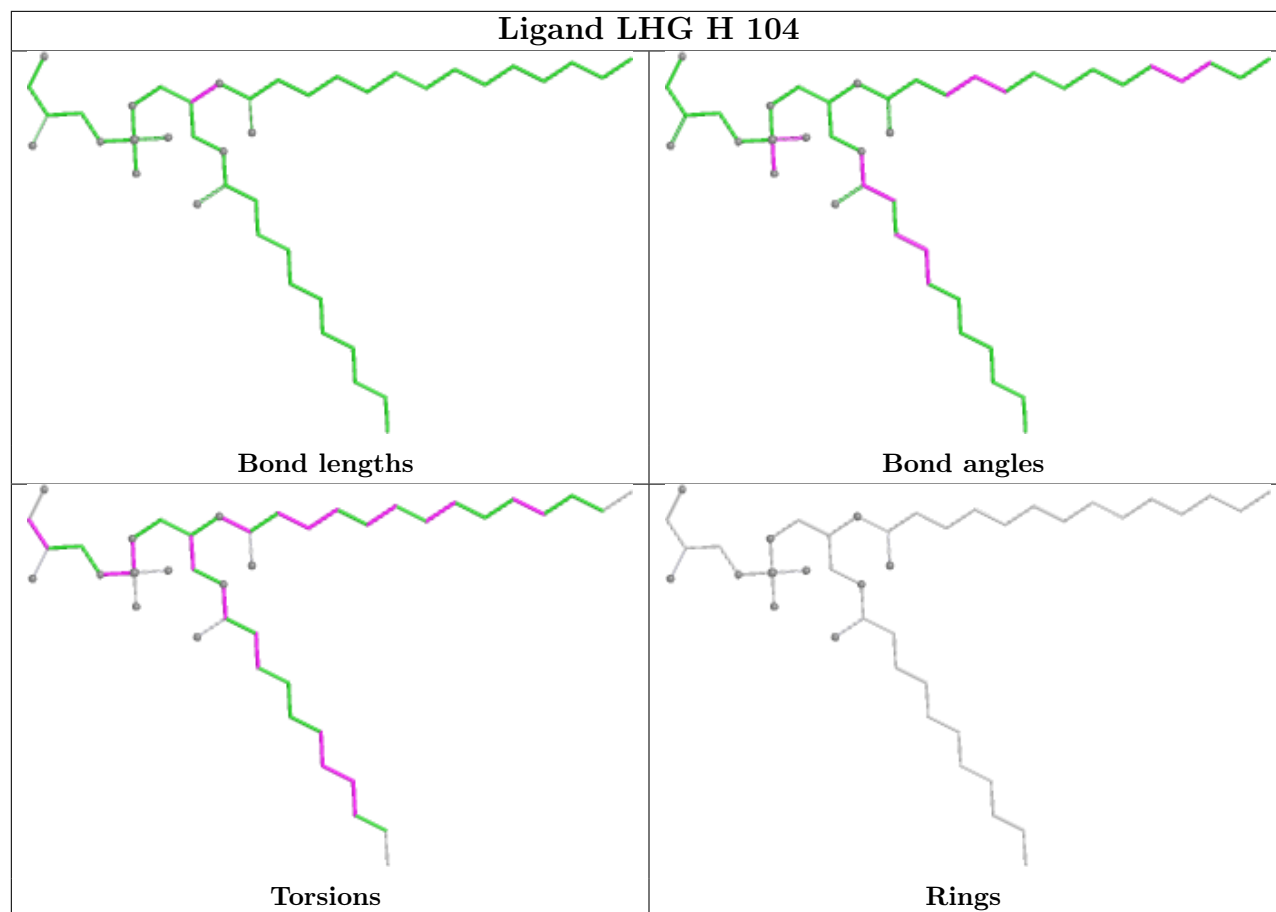
Rings

Ligand CLA 2 308

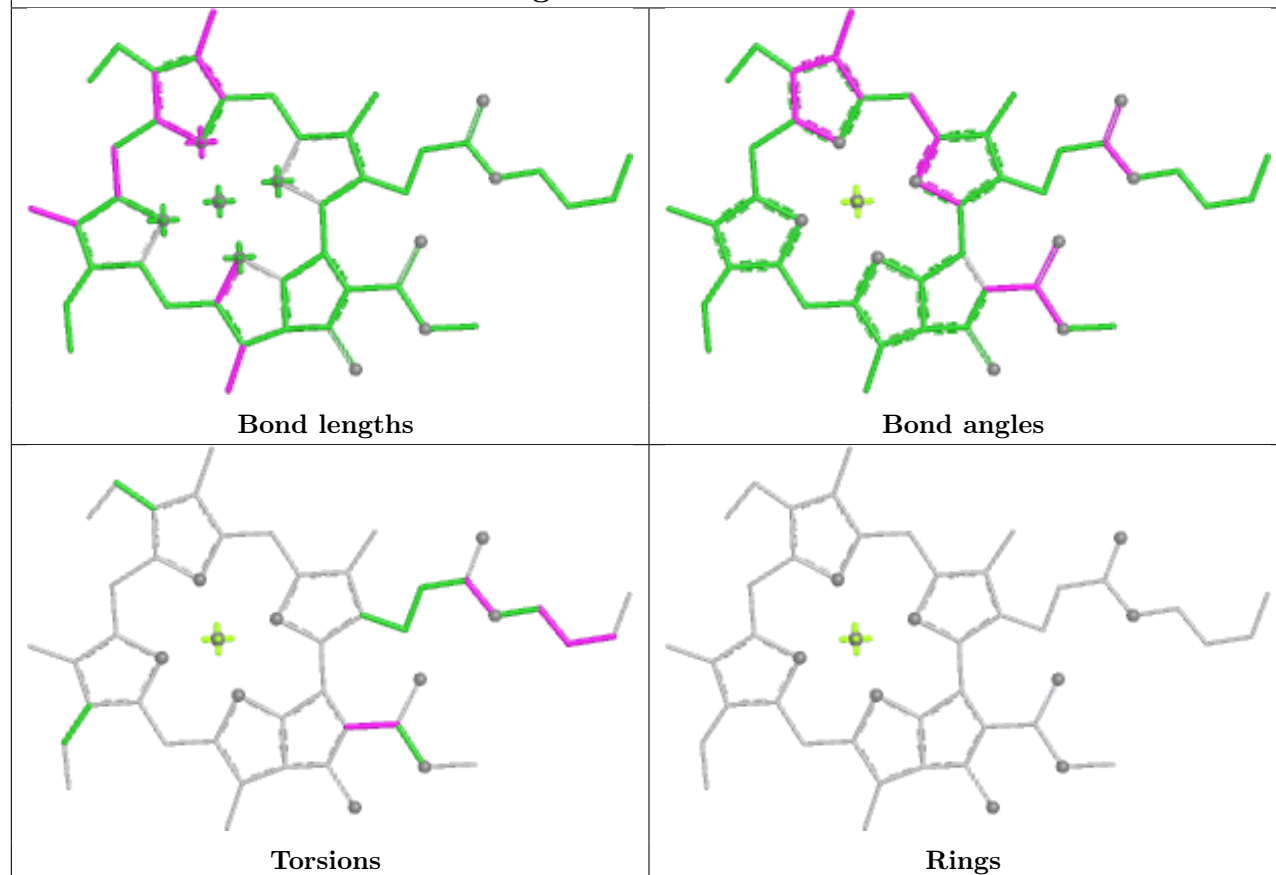


Ligand LMG B 620

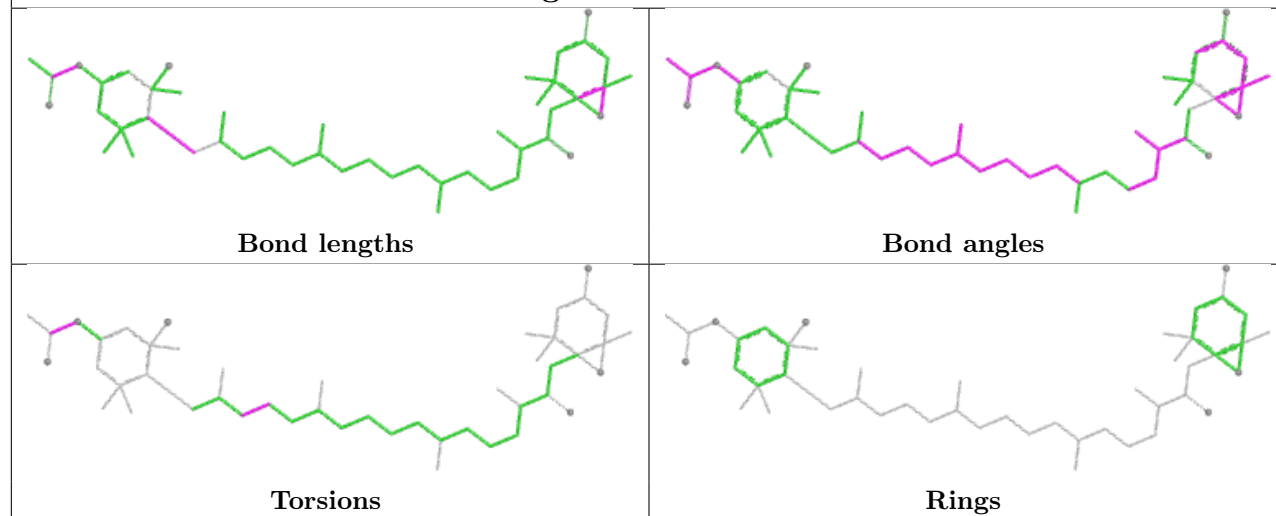


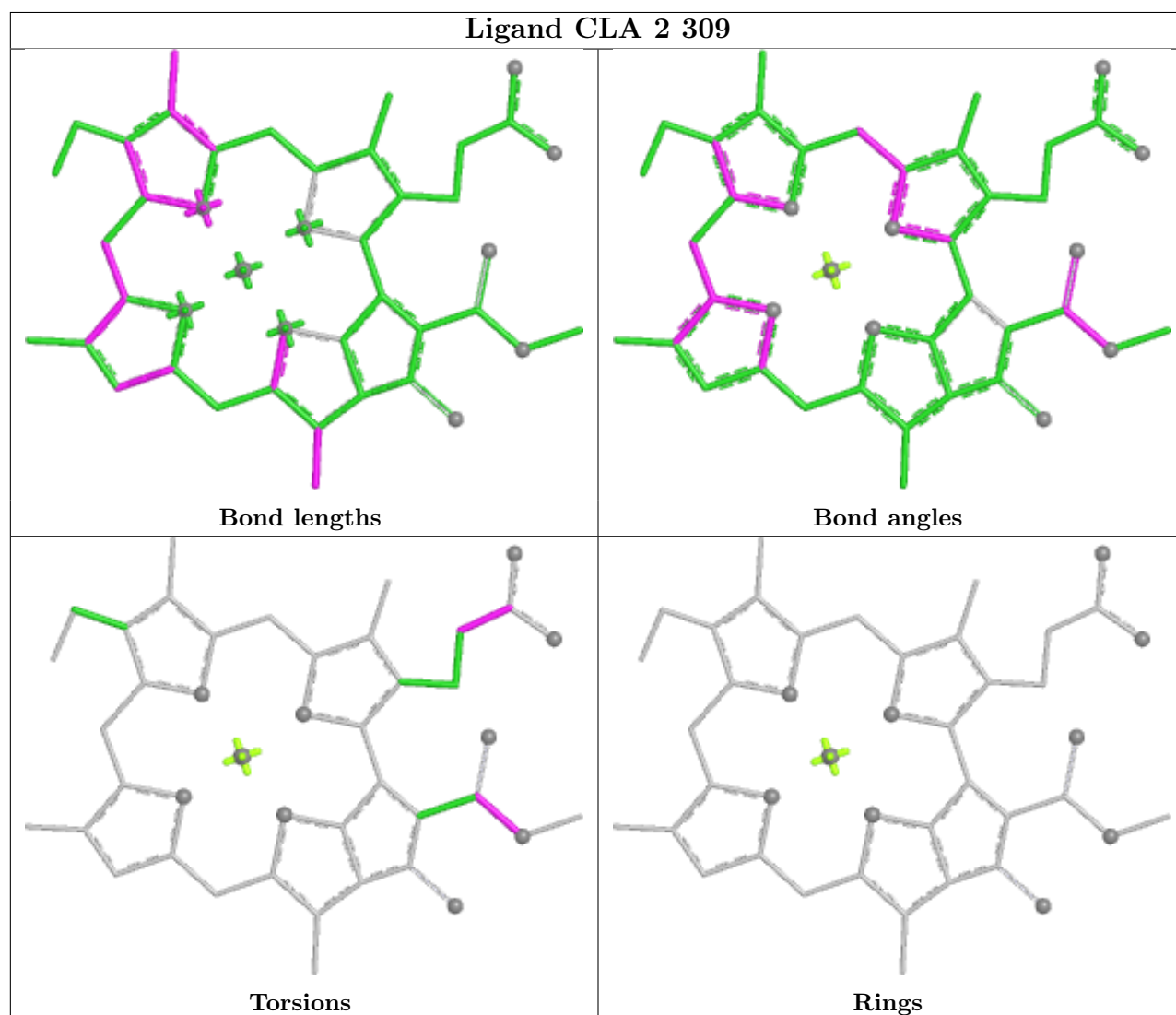
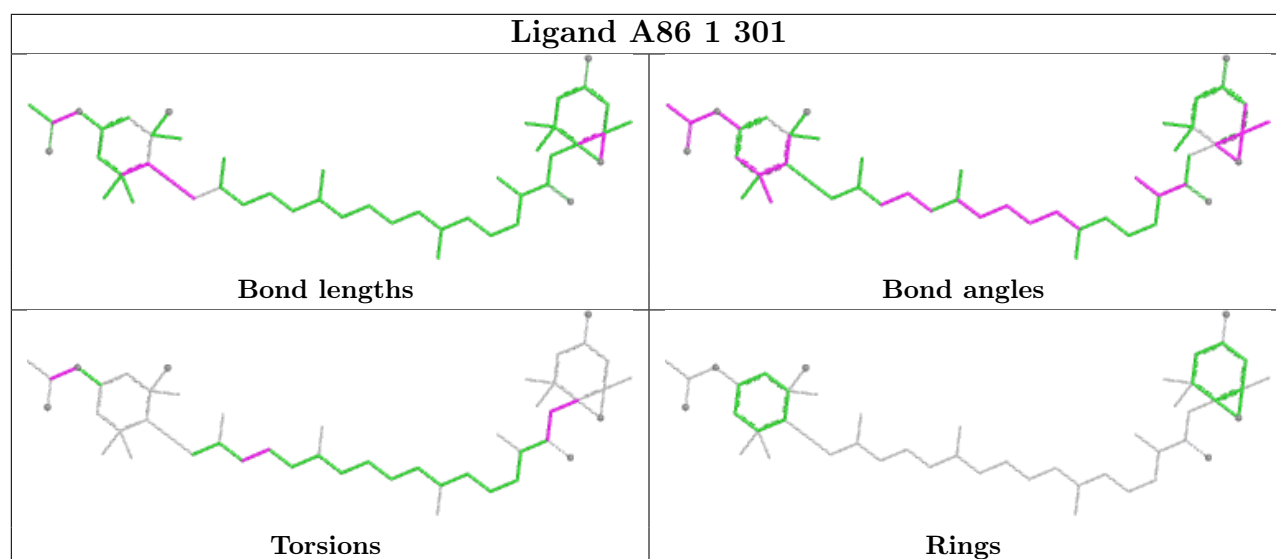


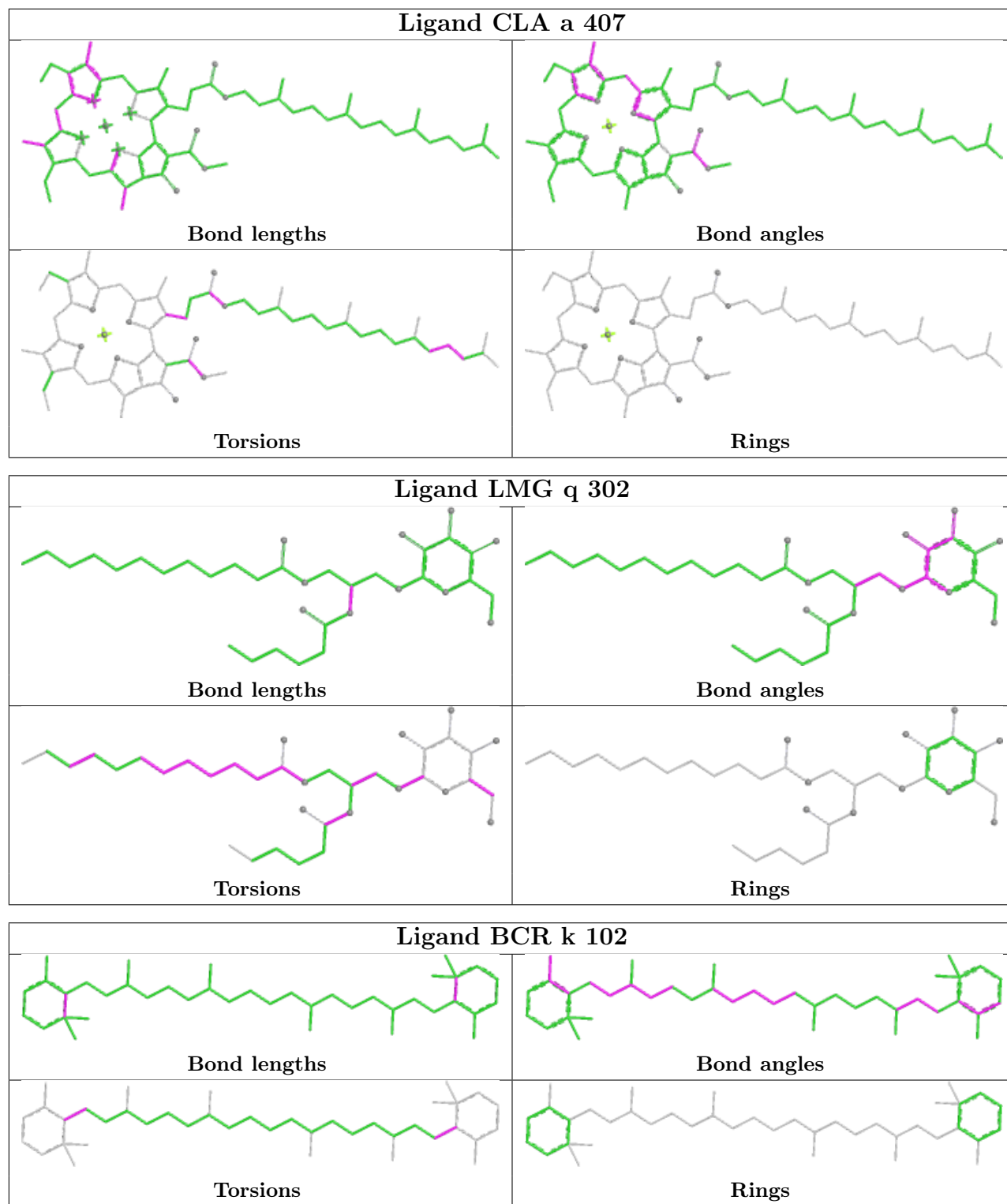
Ligand CLA C 513

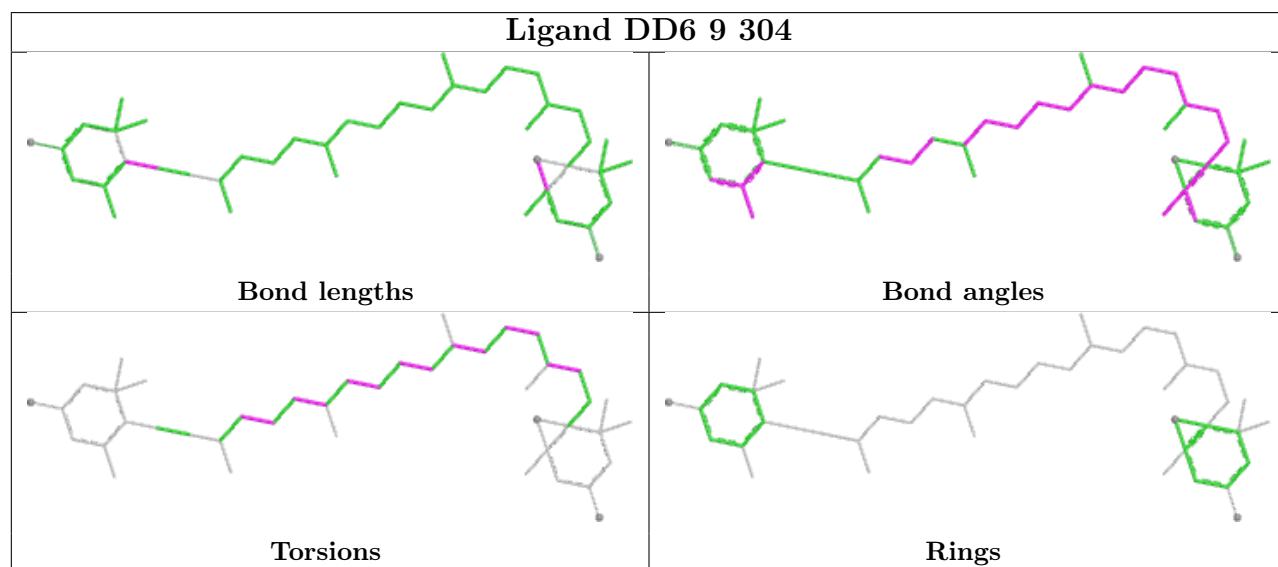
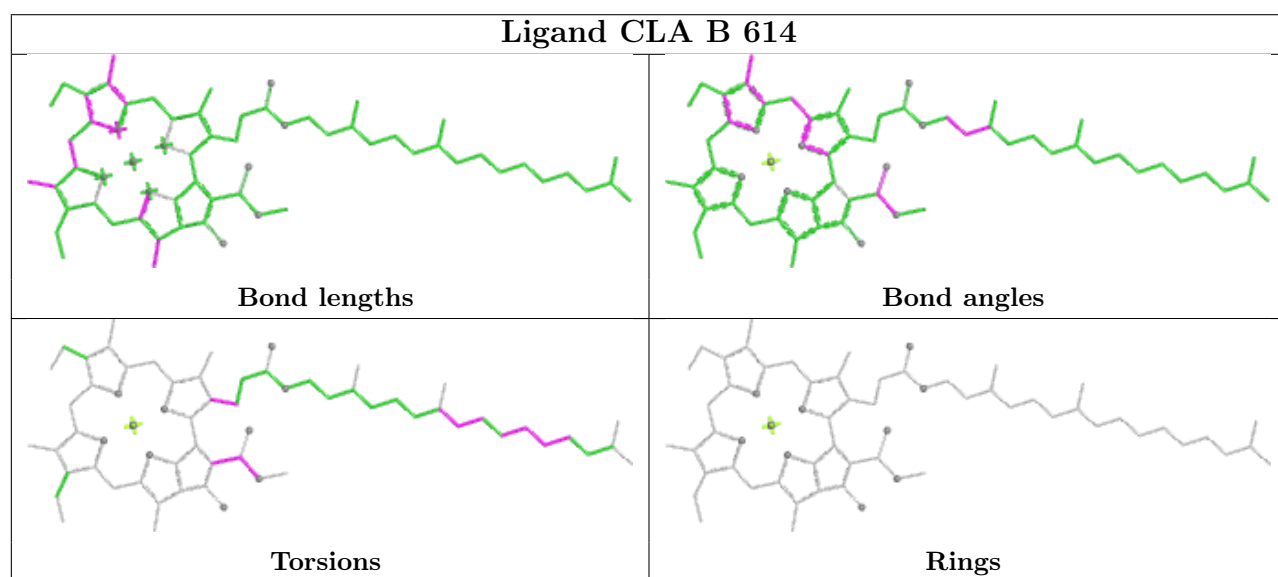
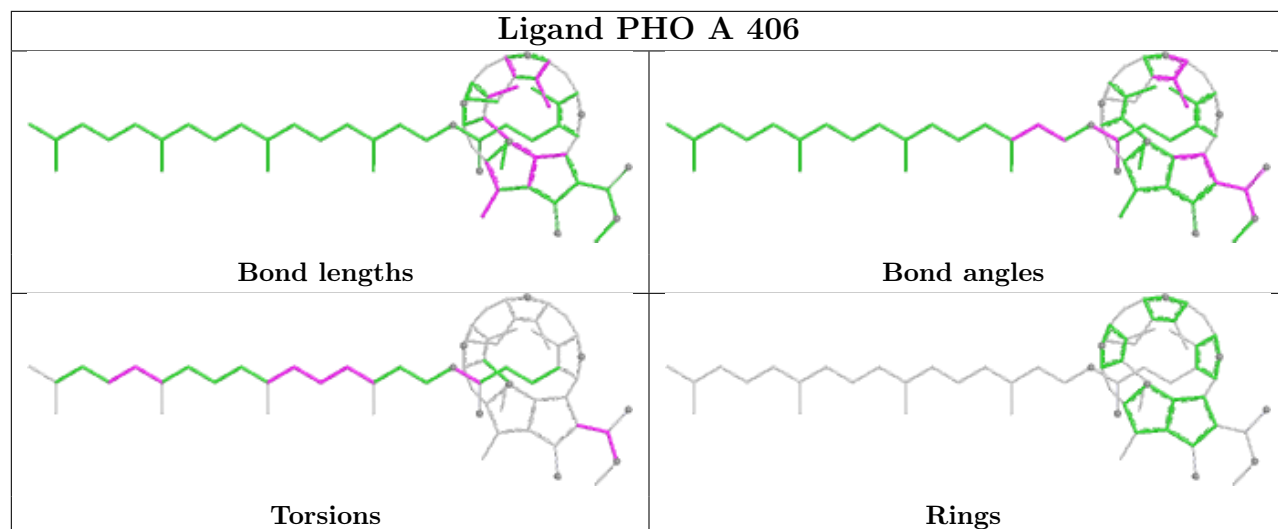


Ligand A86 4 304

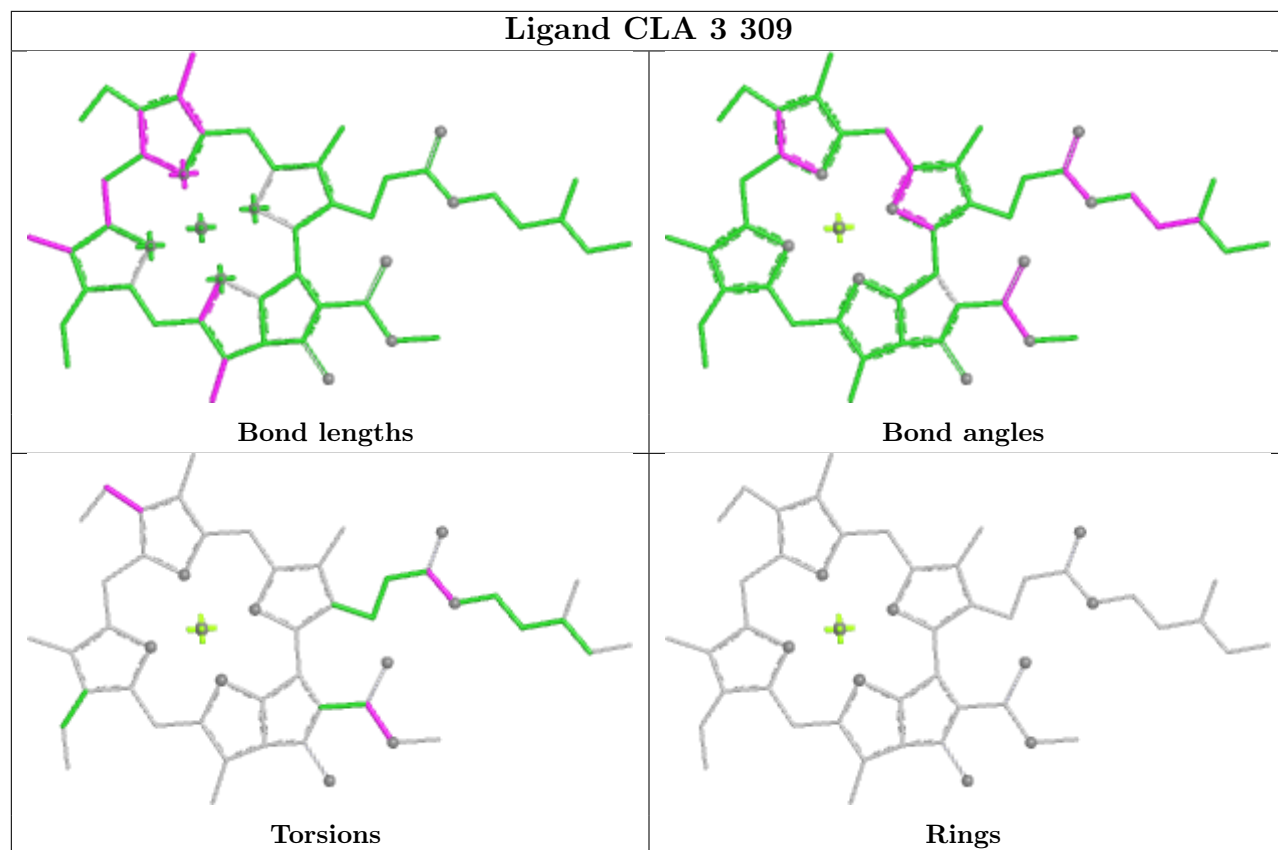




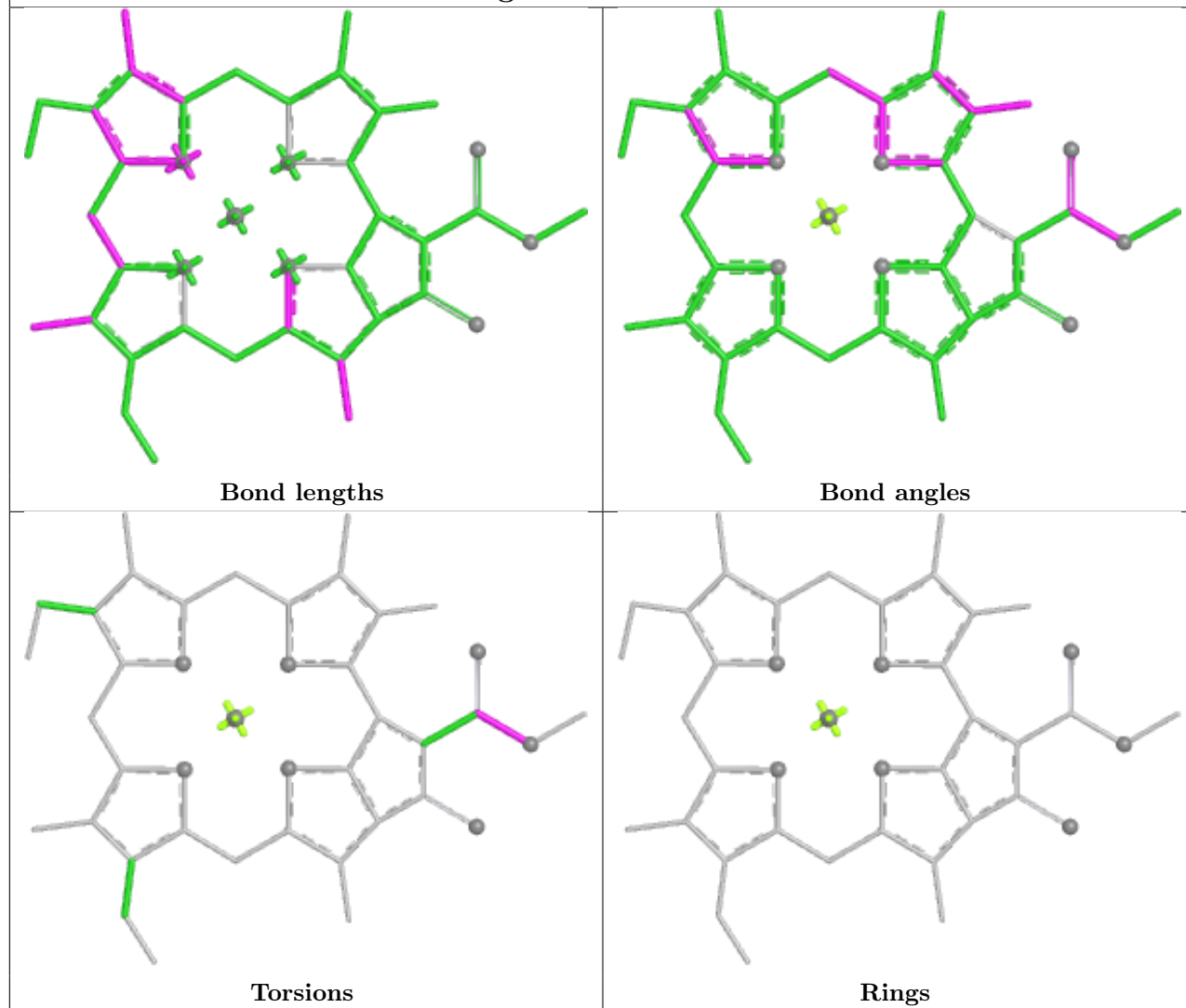




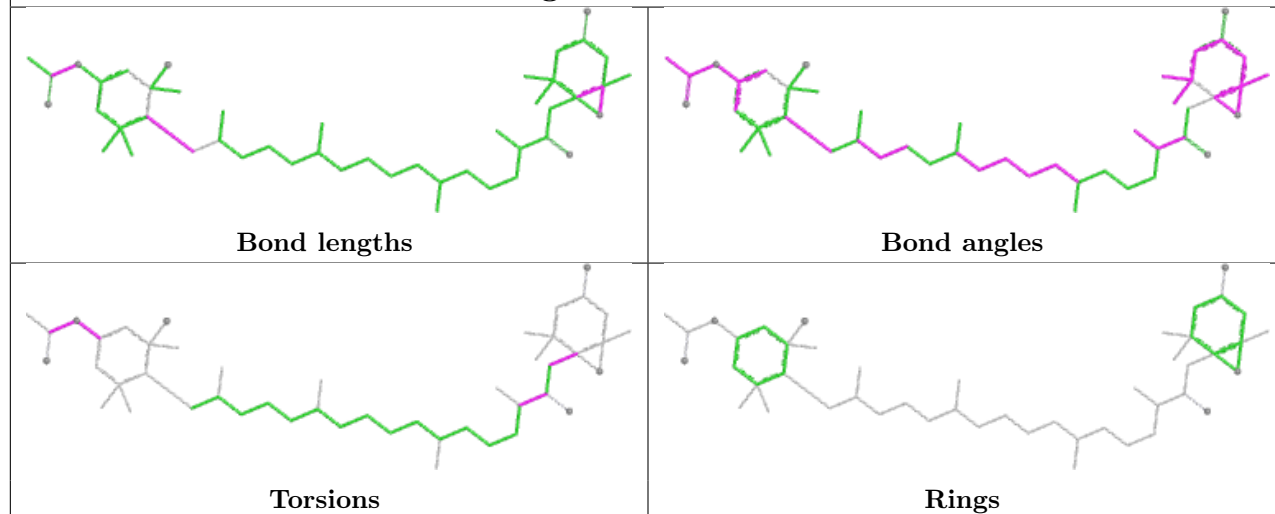
Ligand CLA 3 309

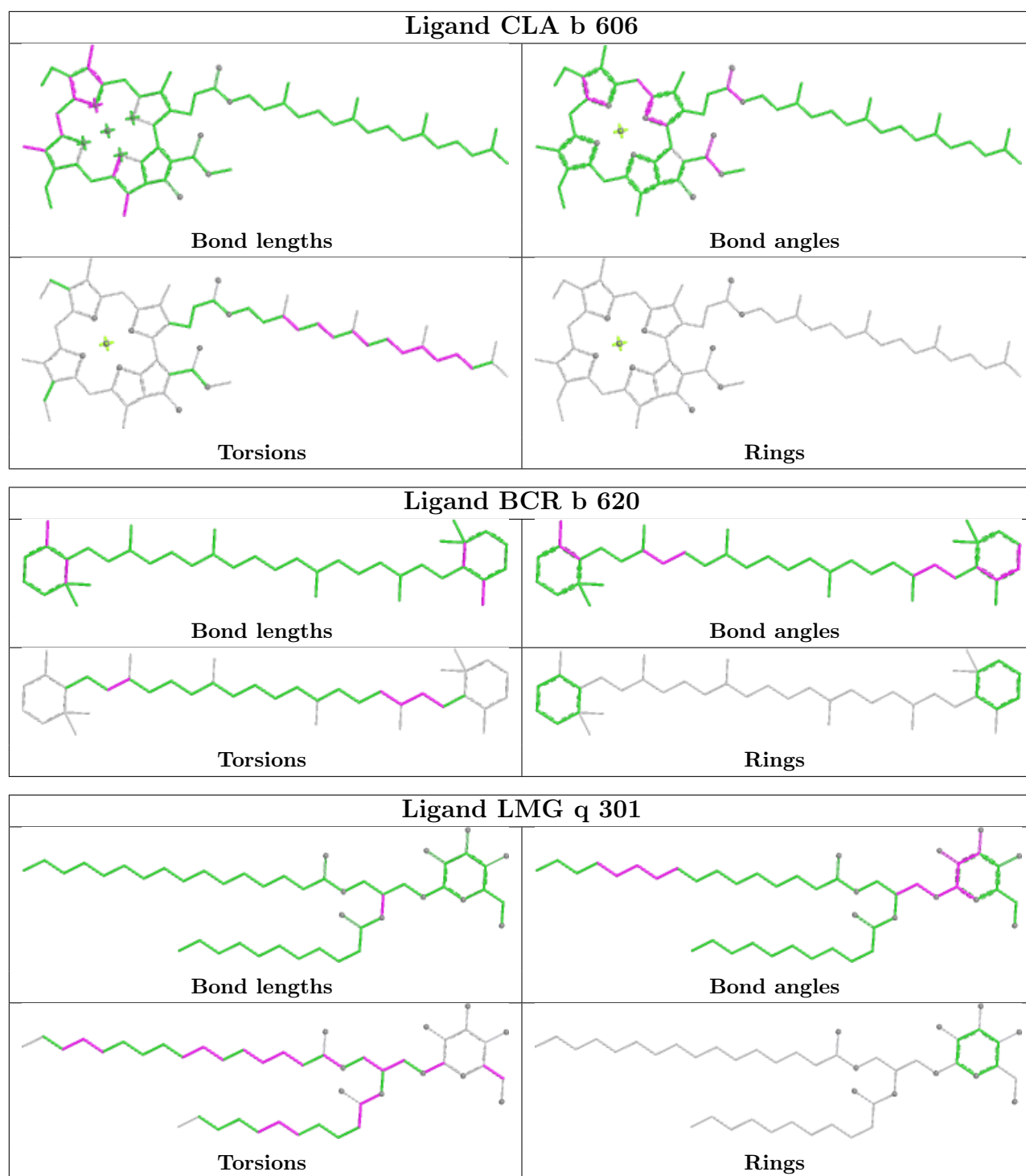


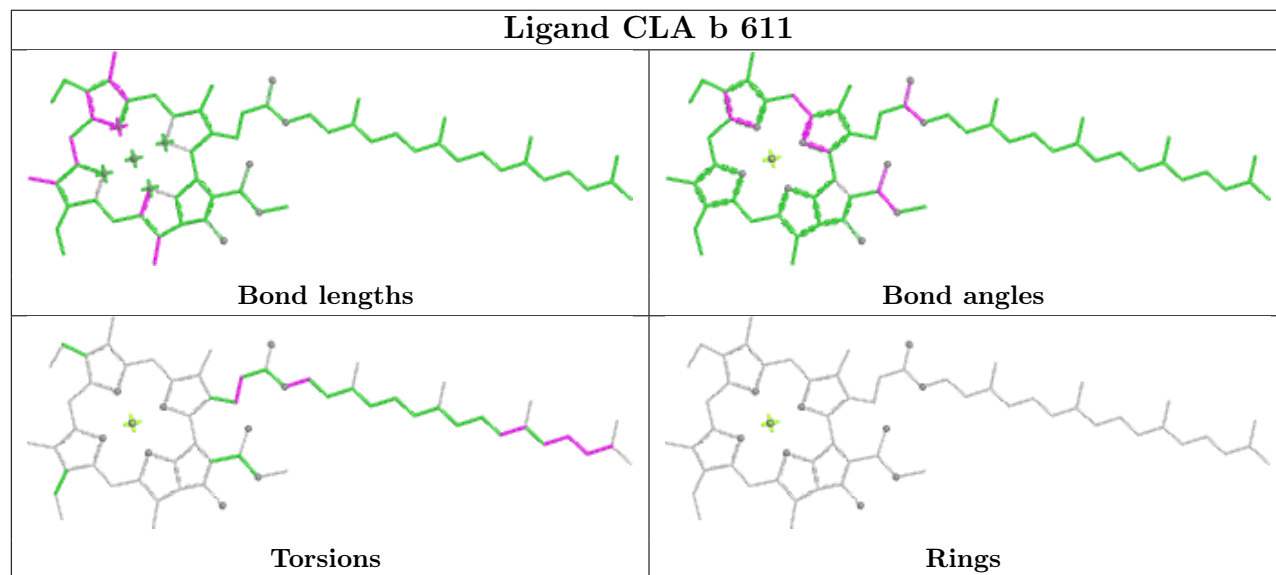
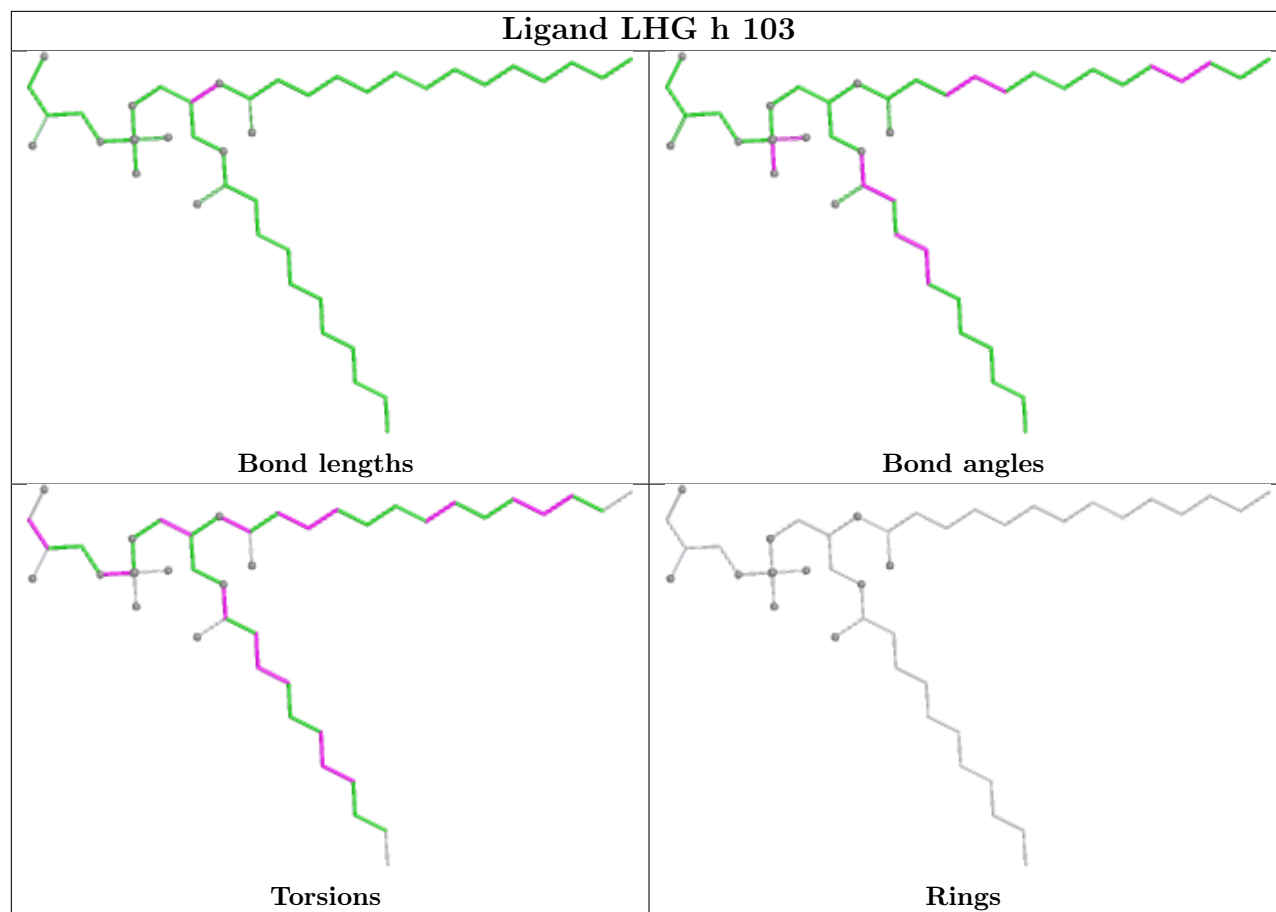
Ligand CLA 3 311

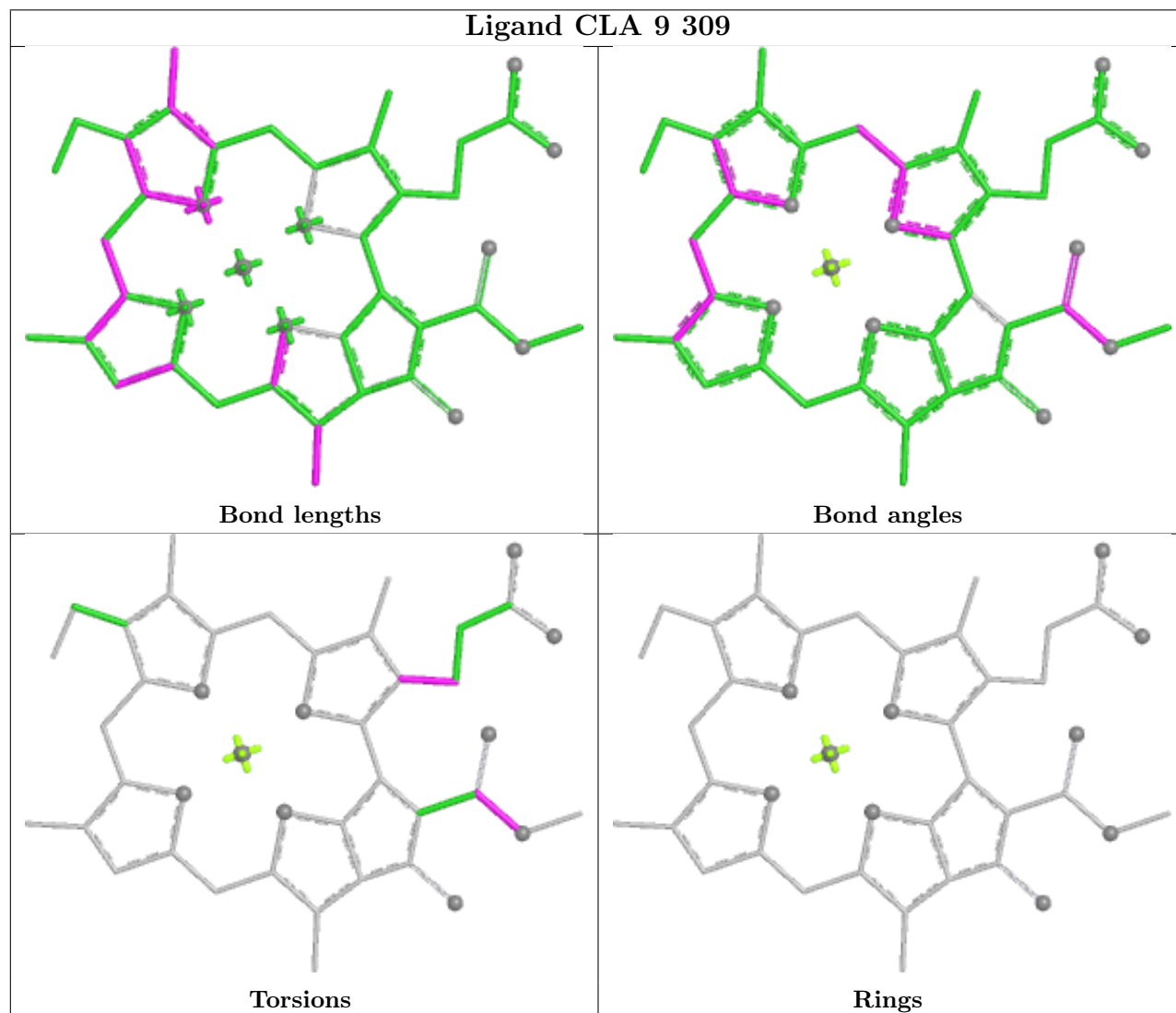
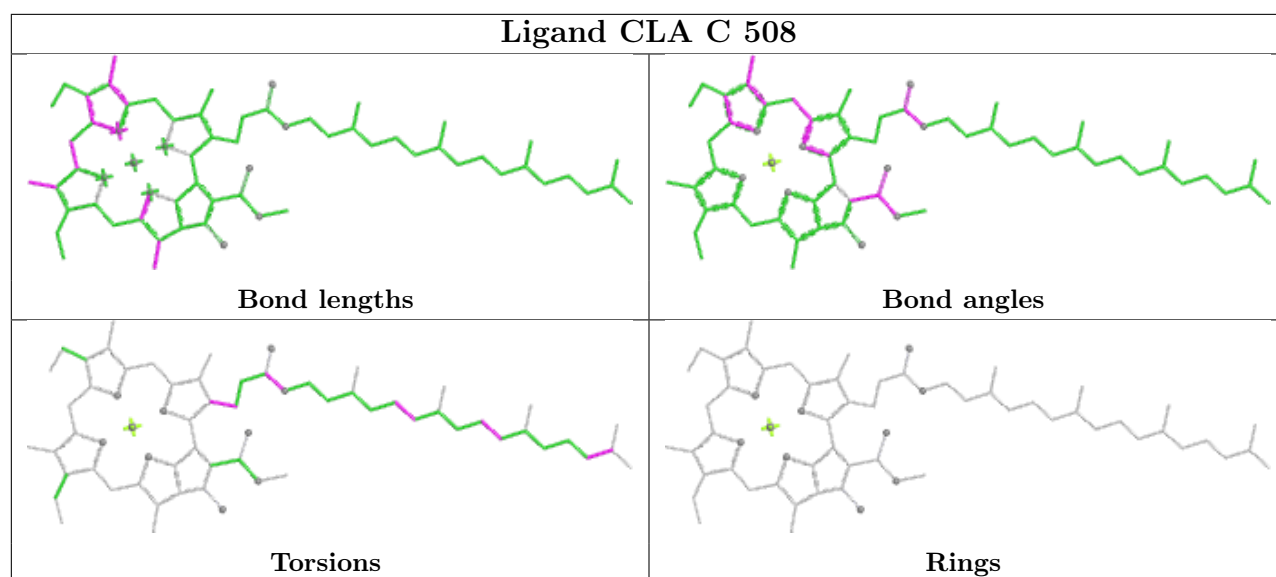


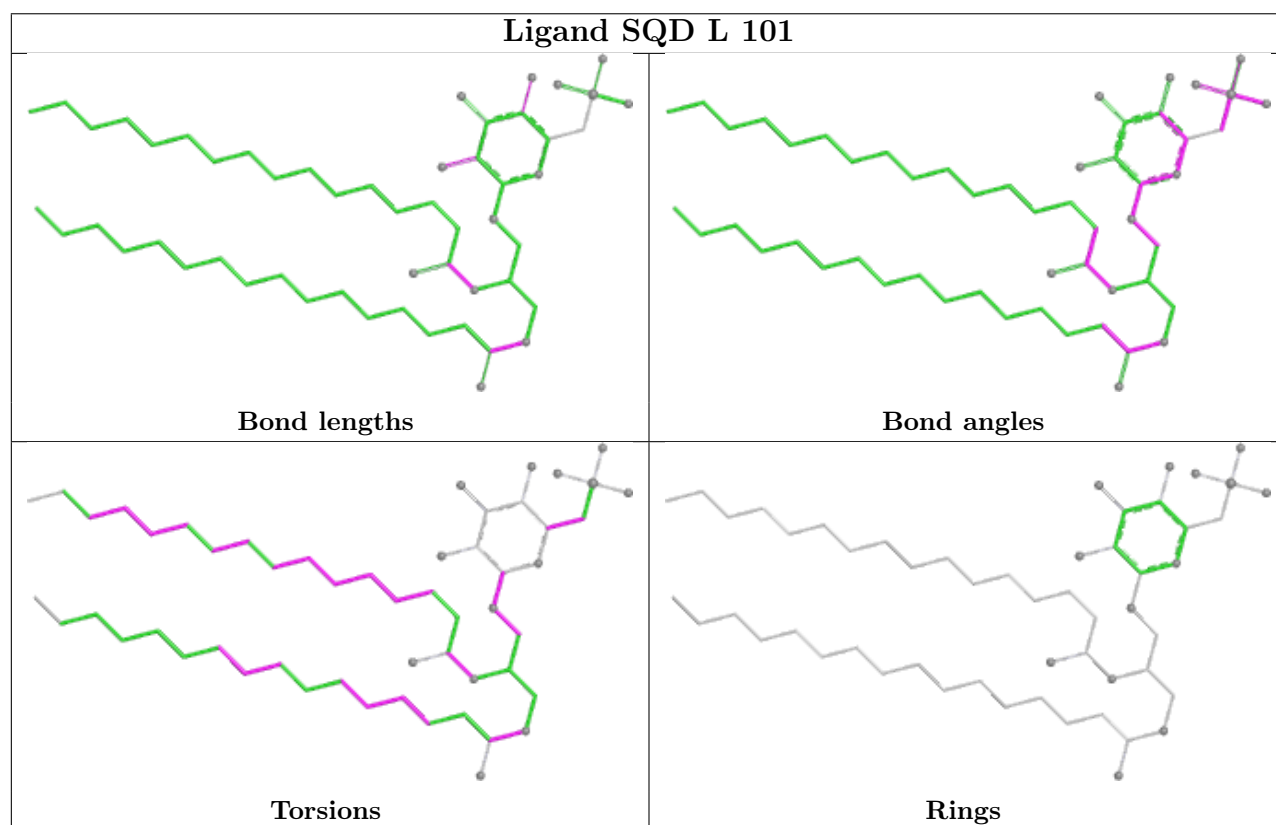
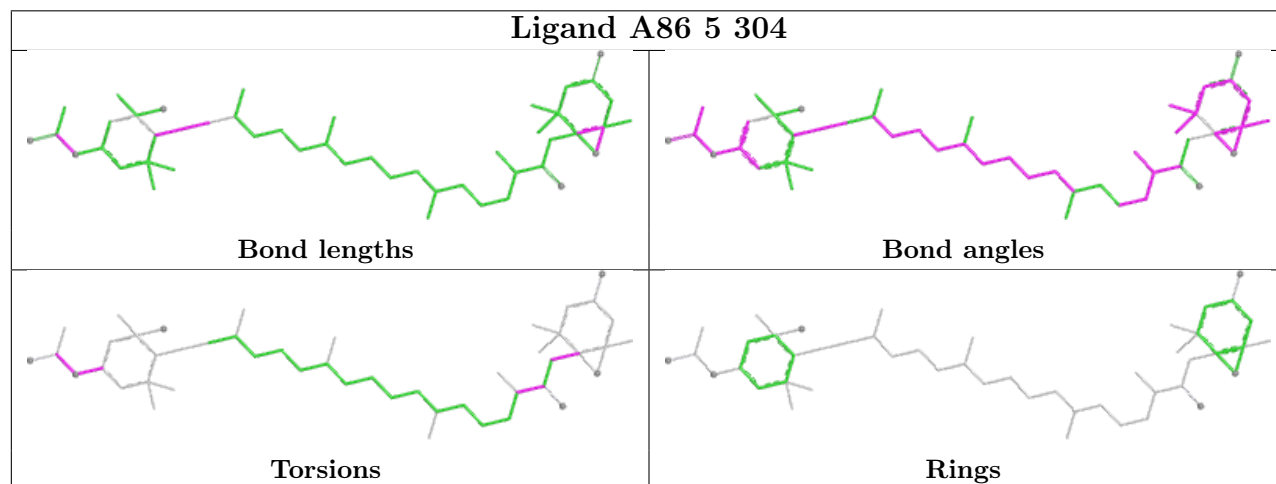
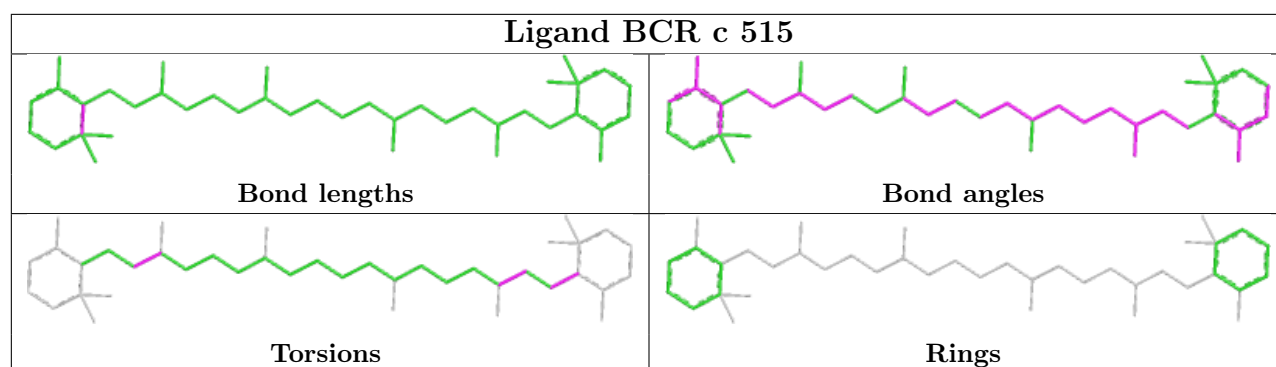
Ligand A86 6 304

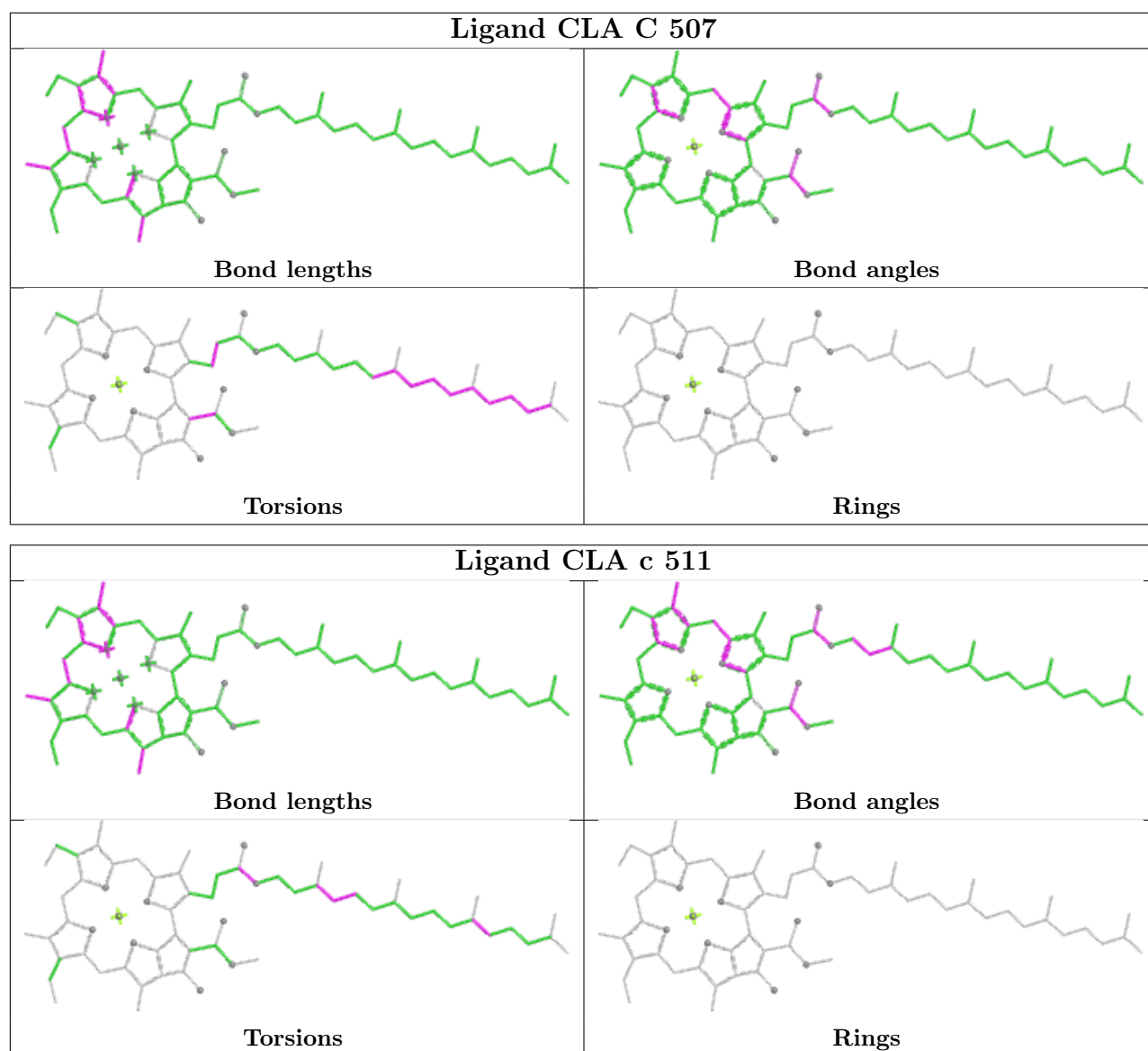




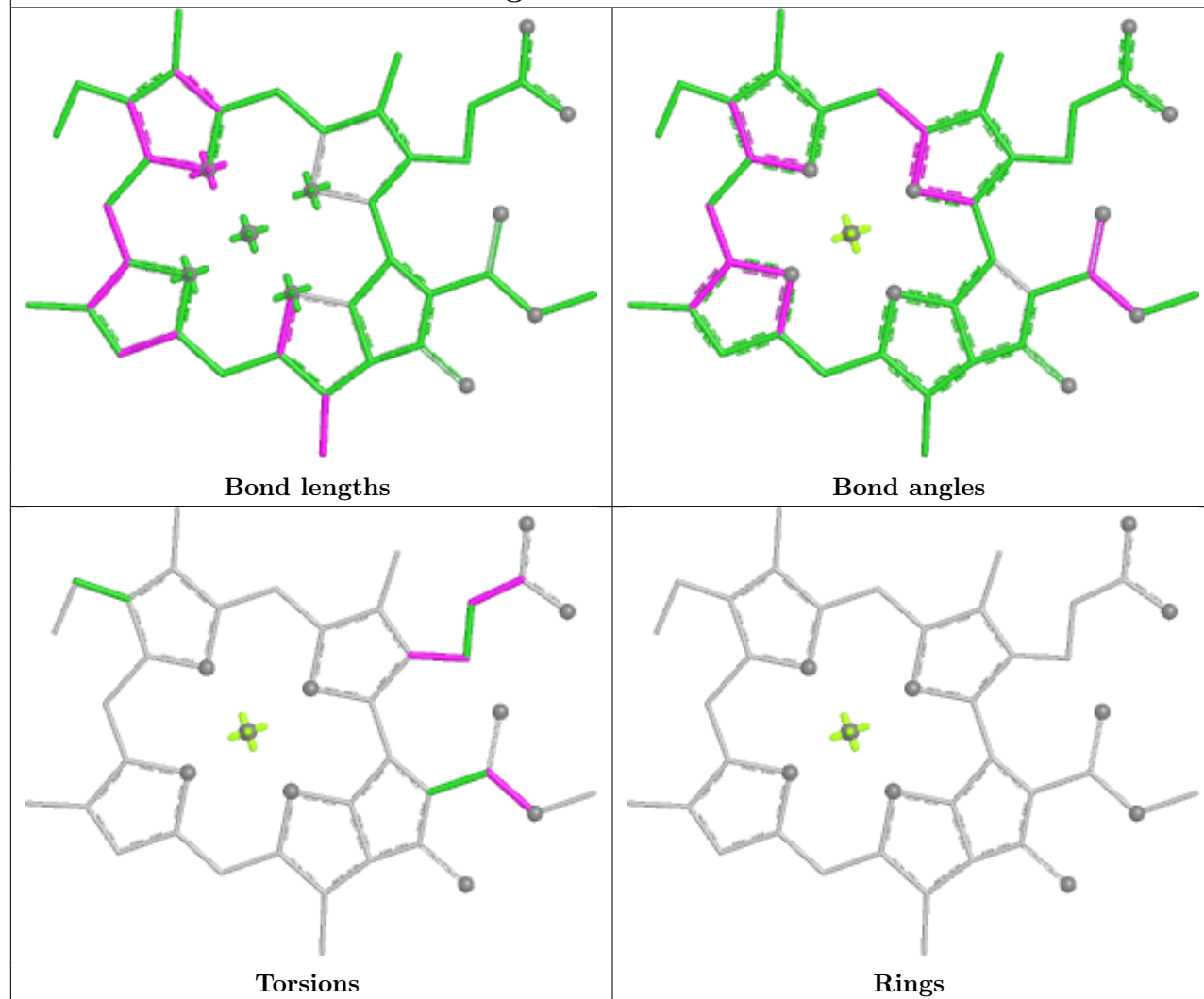




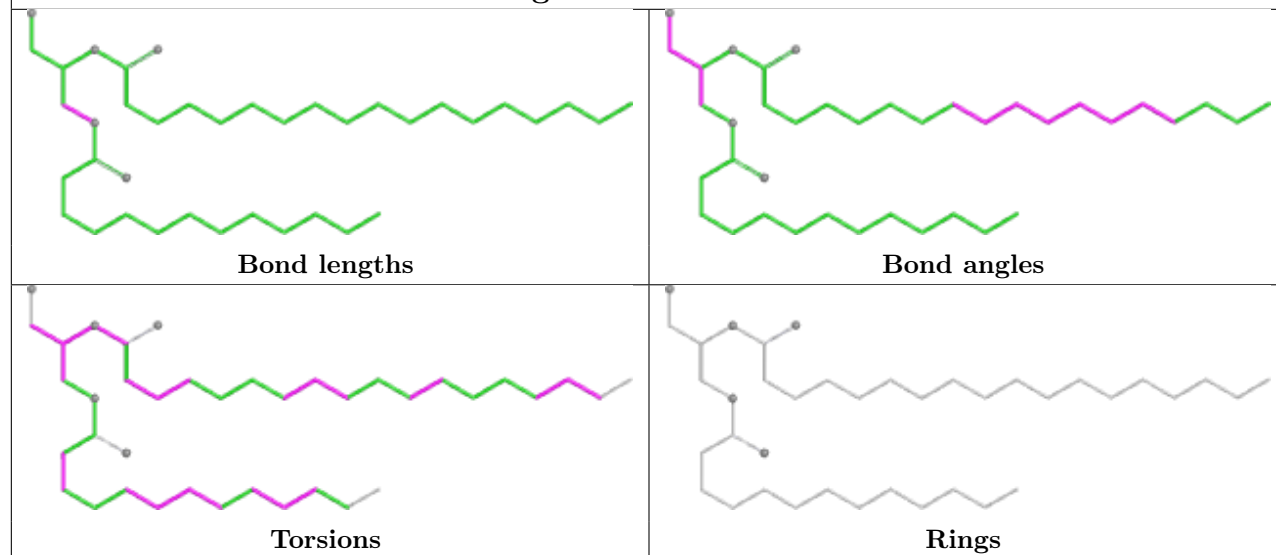


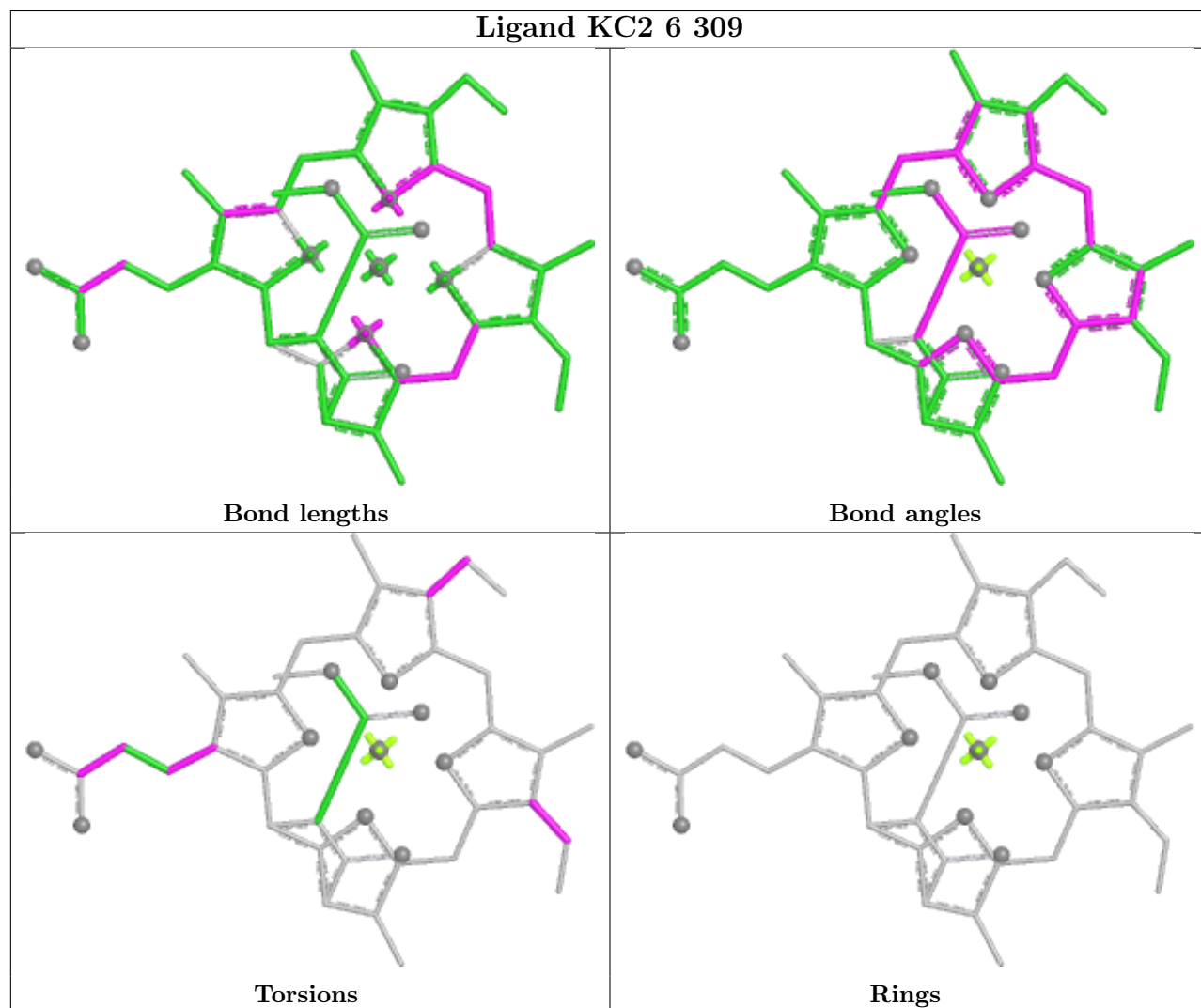
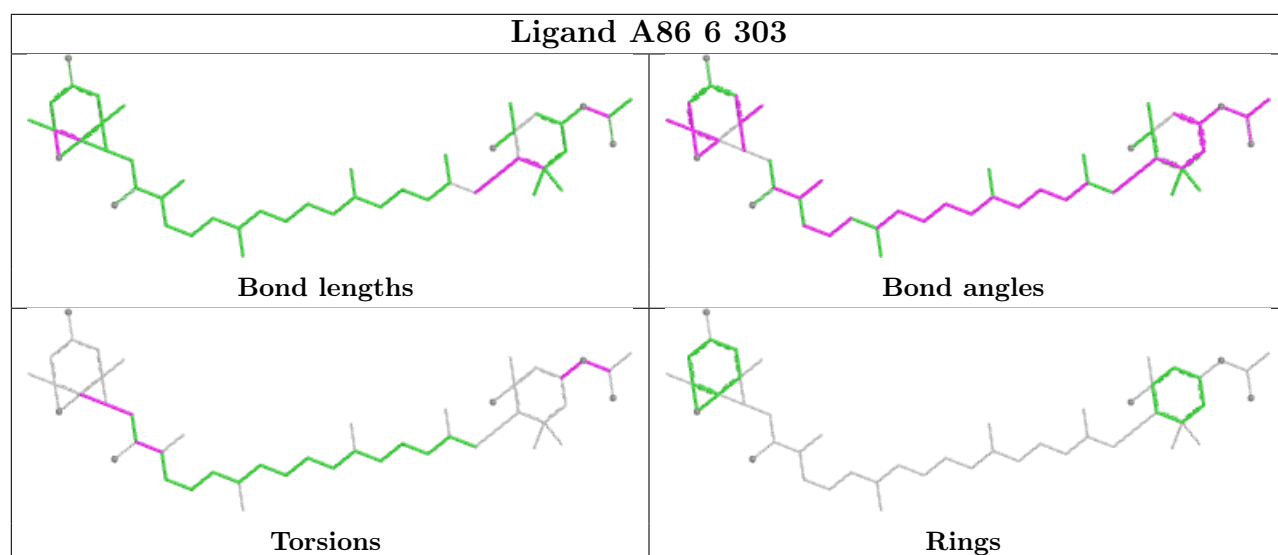


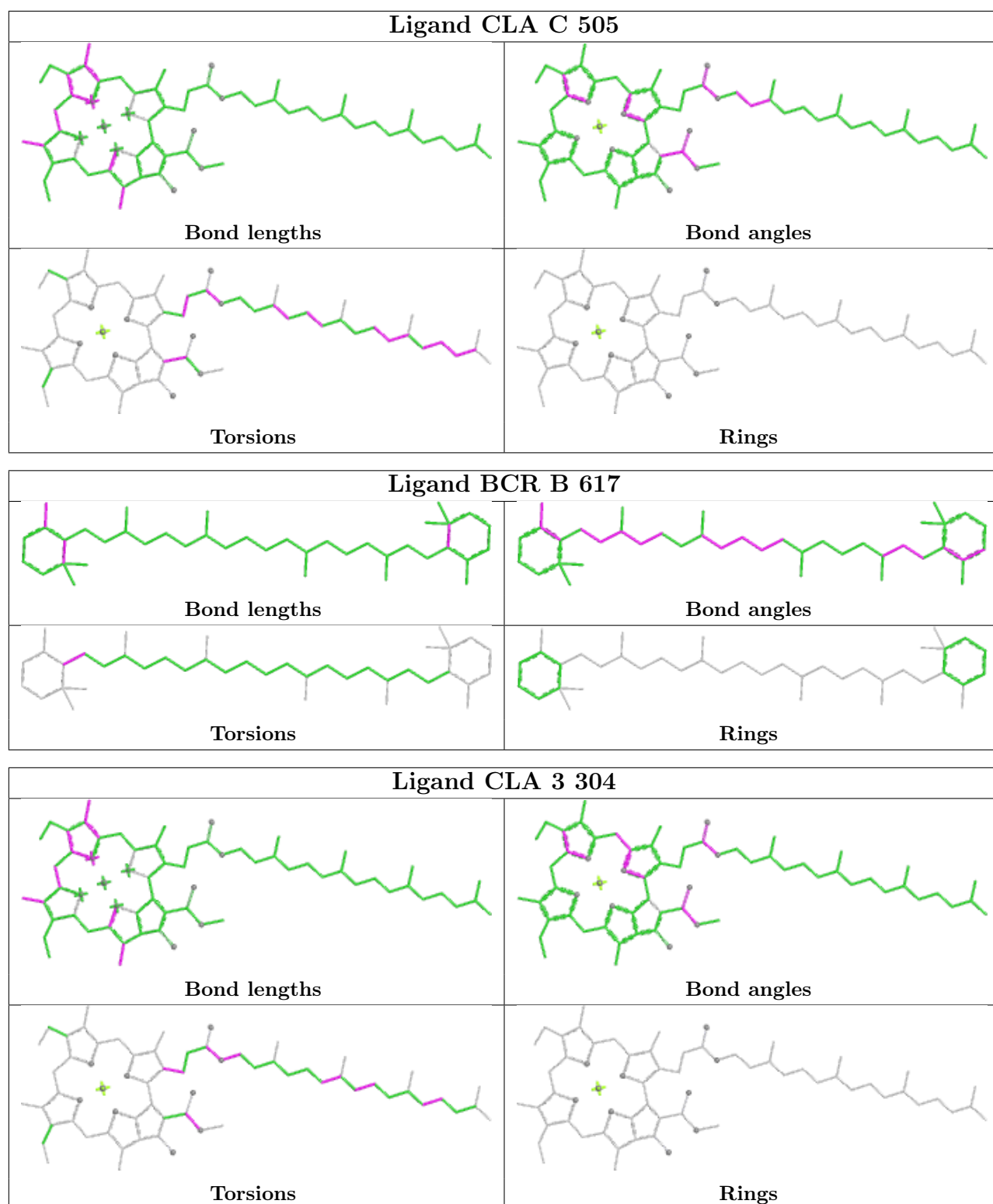
Ligand CLA 1 309

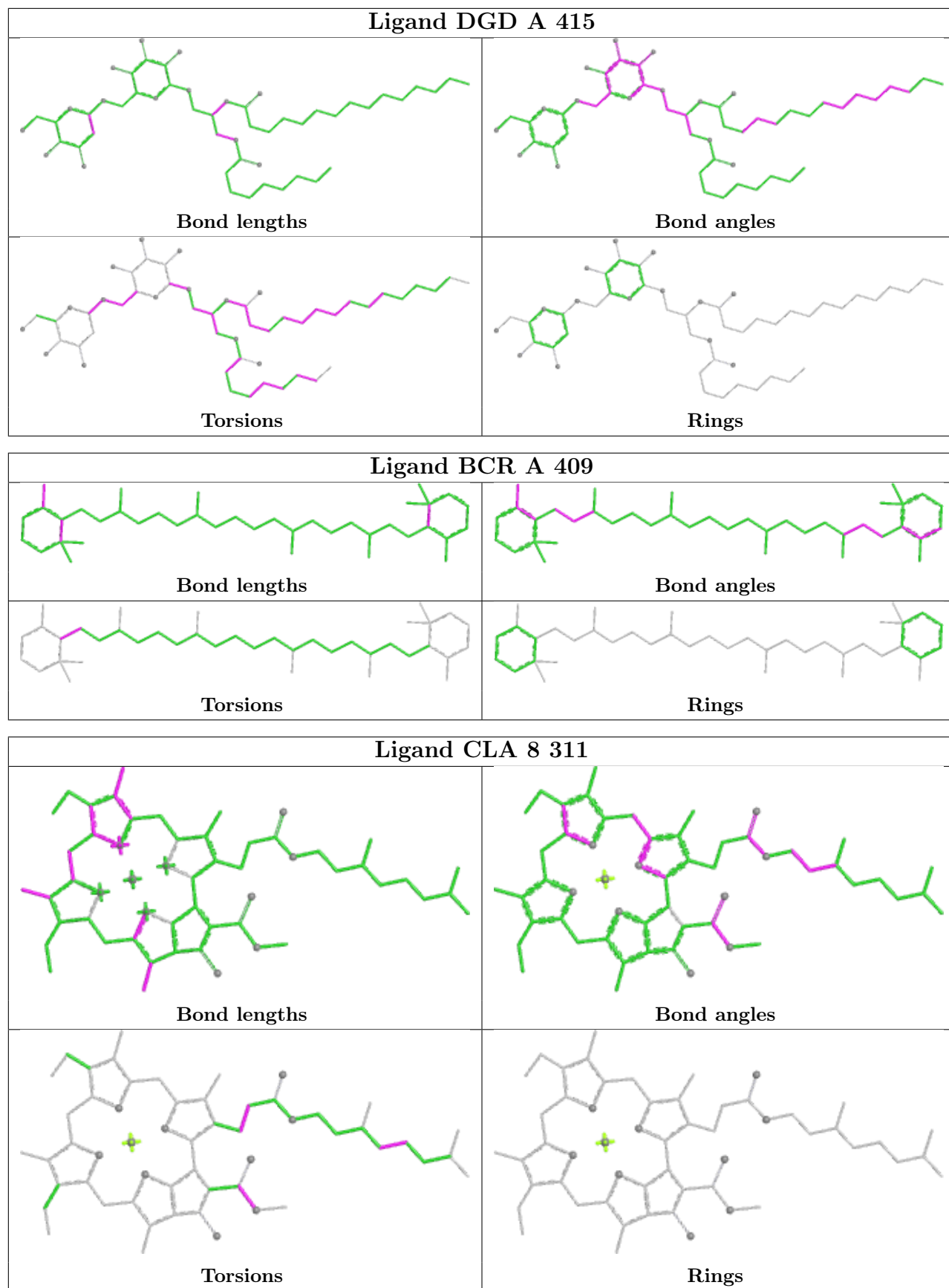


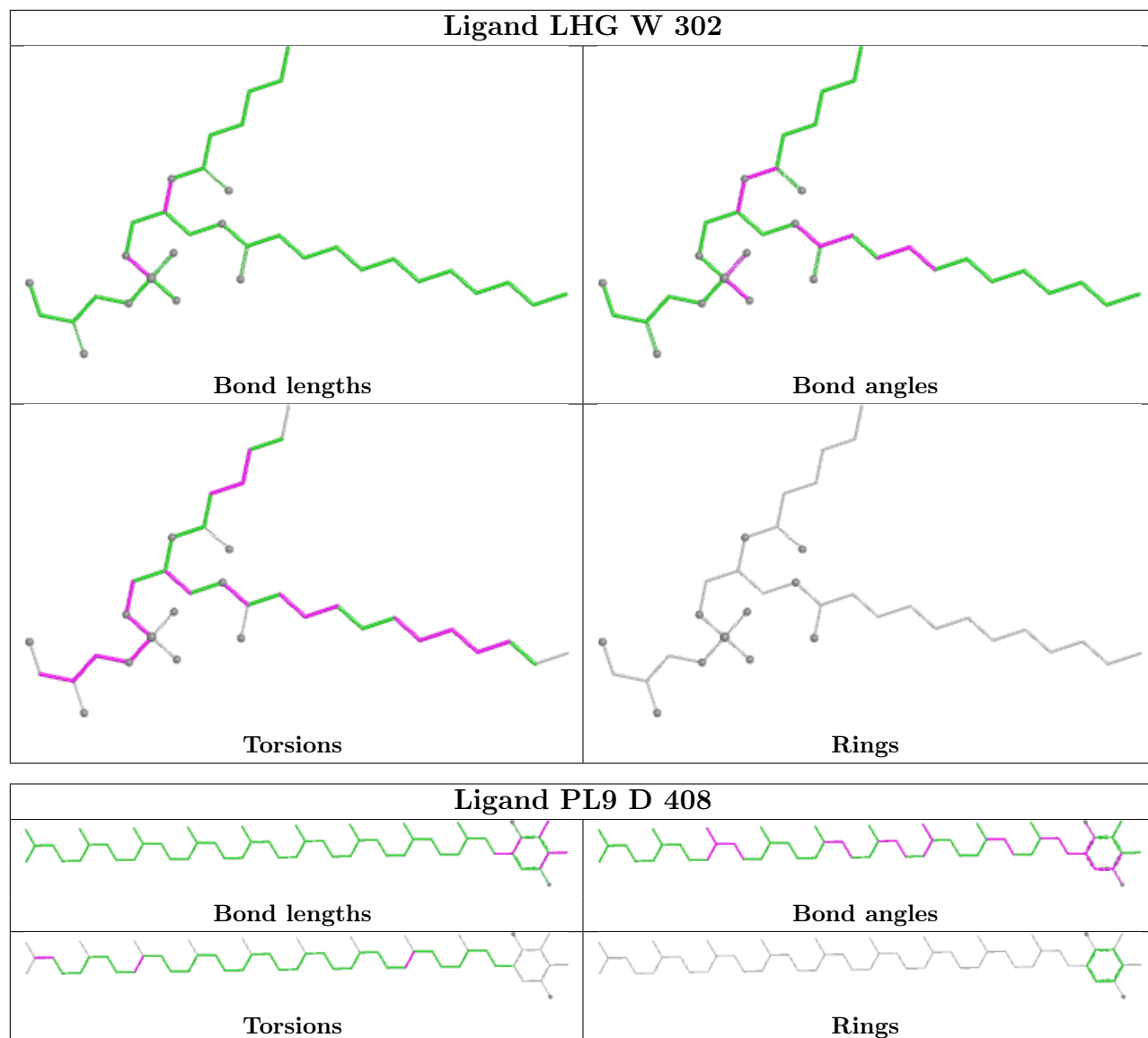
Ligand DGD 3 320



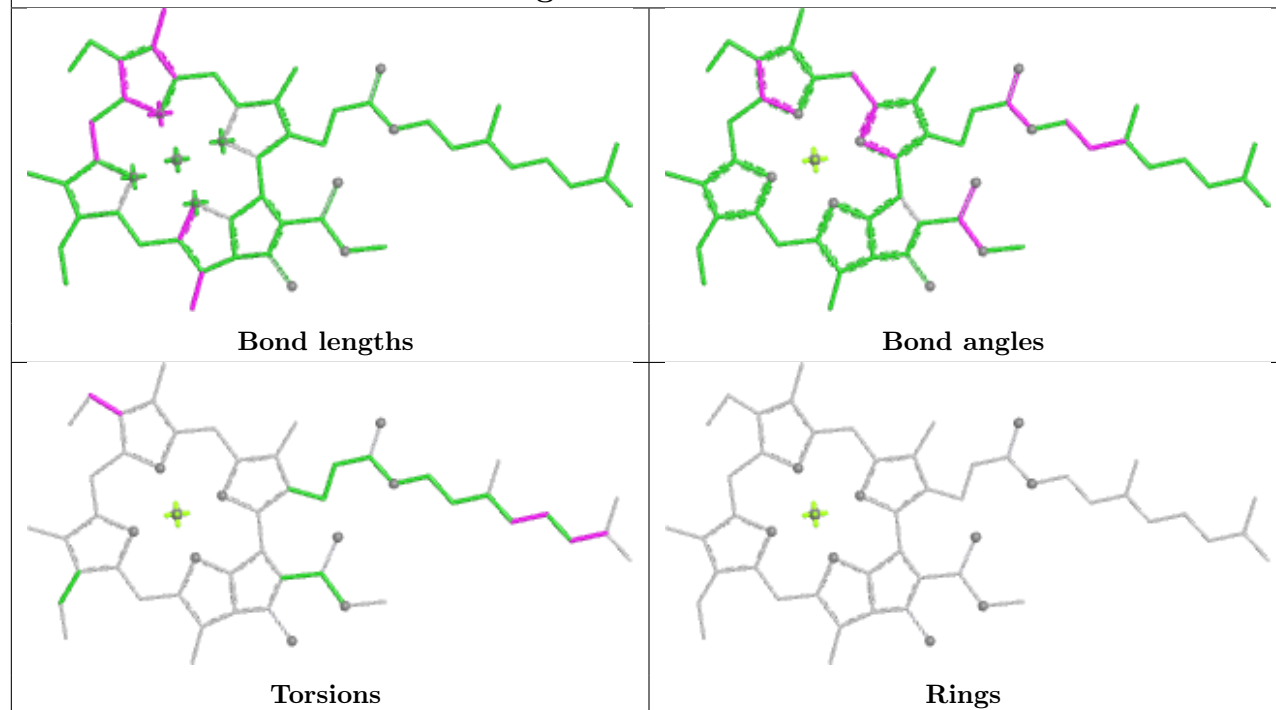




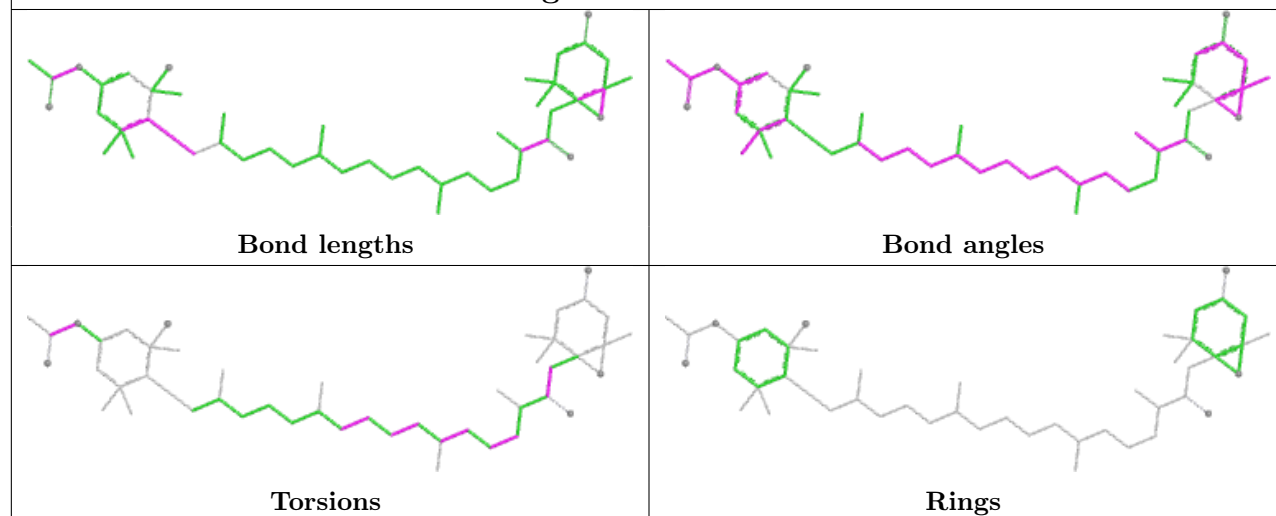


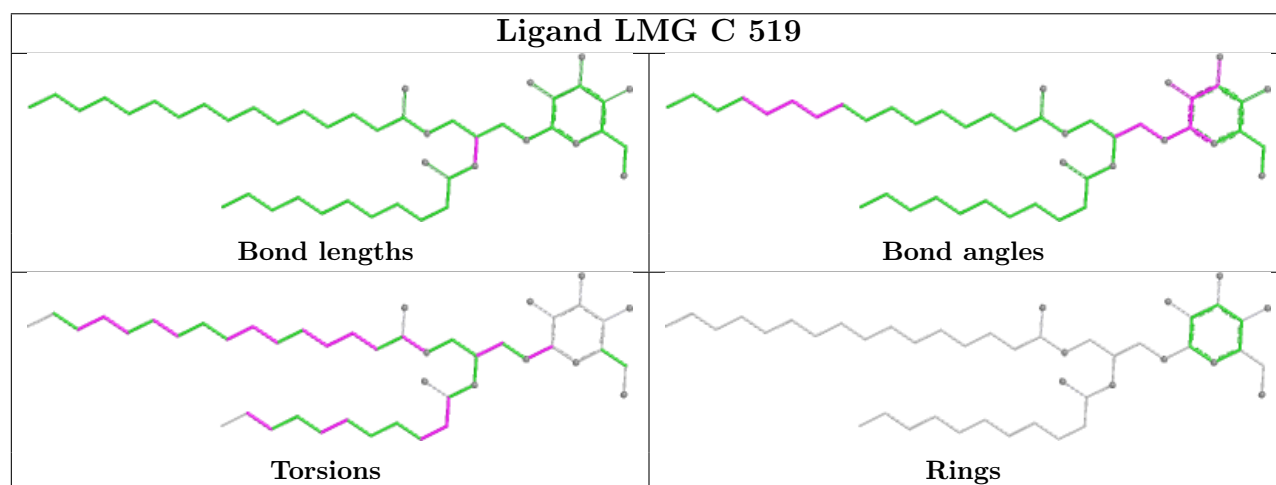
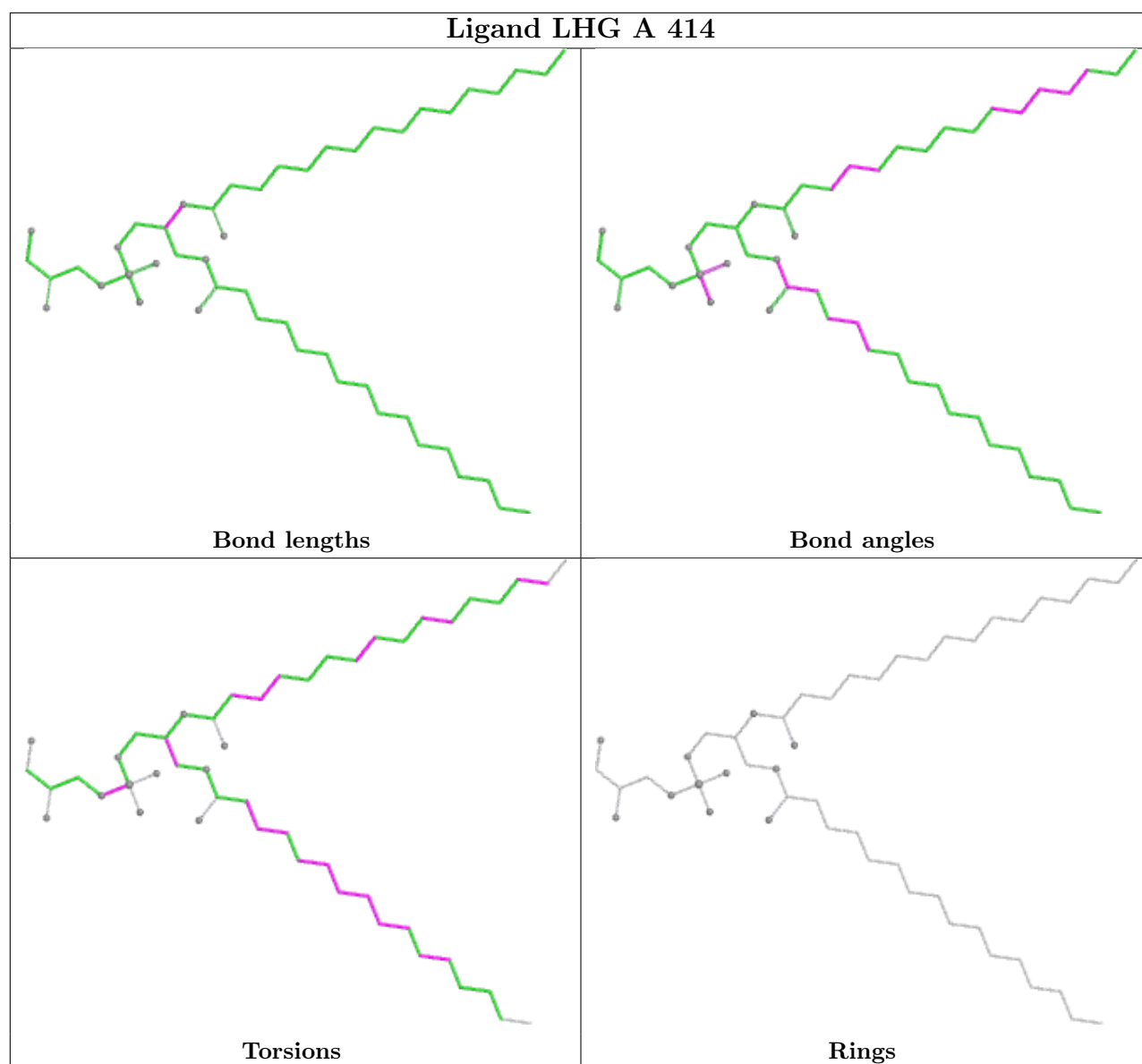


Ligand CLA 5 309

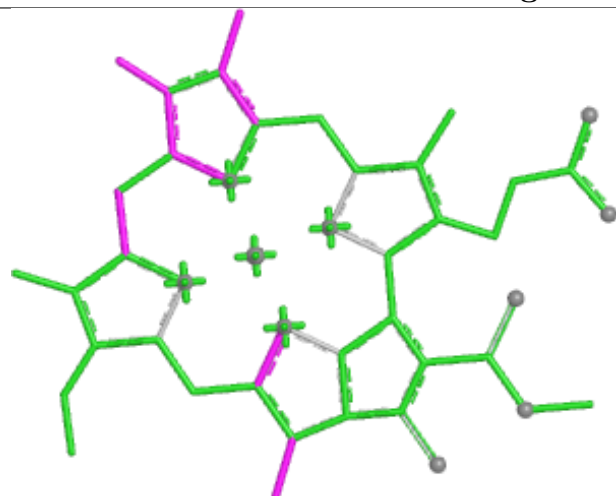


Ligand A86 2 302

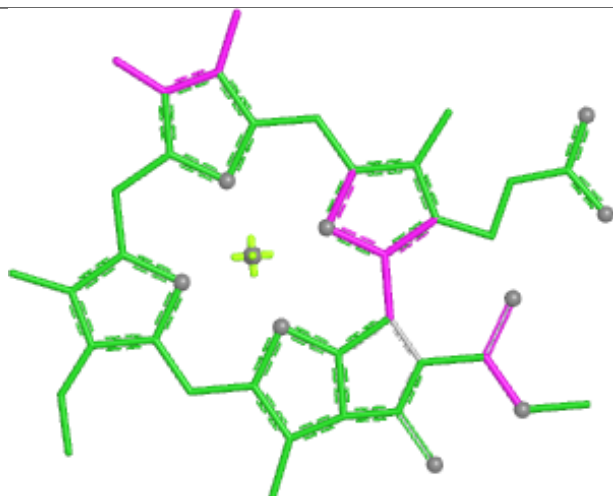




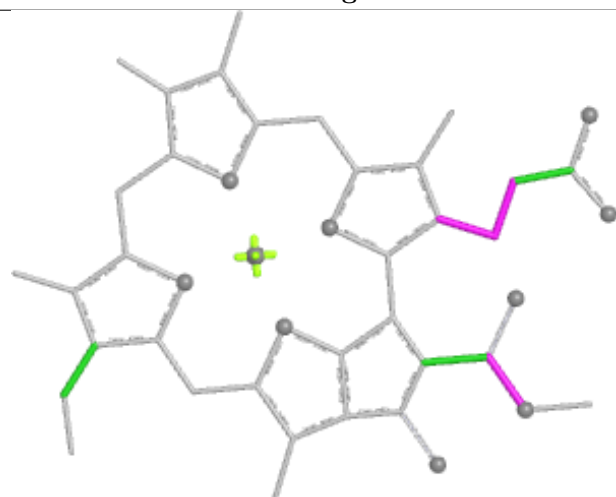
Ligand CLA 9 307



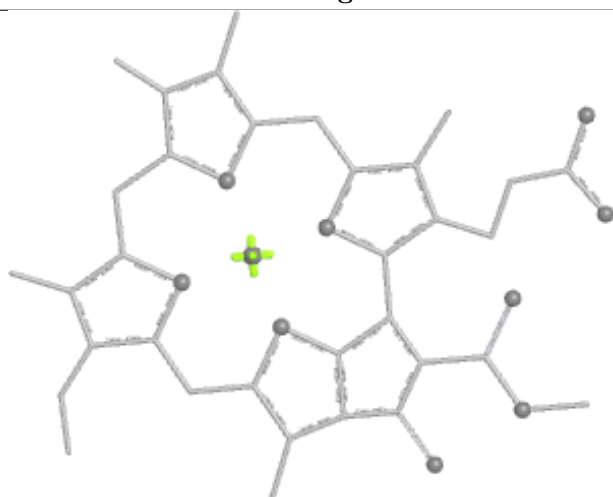
Bond lengths



Bond angles

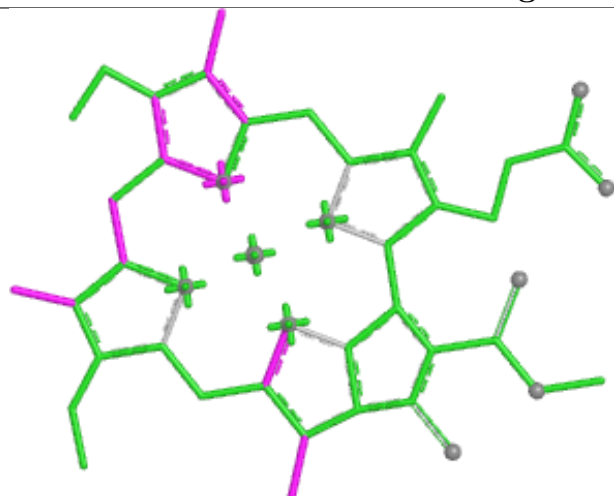


Torsions

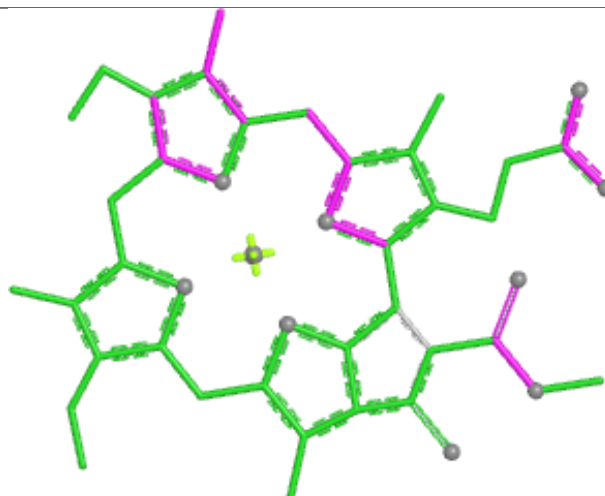


Rings

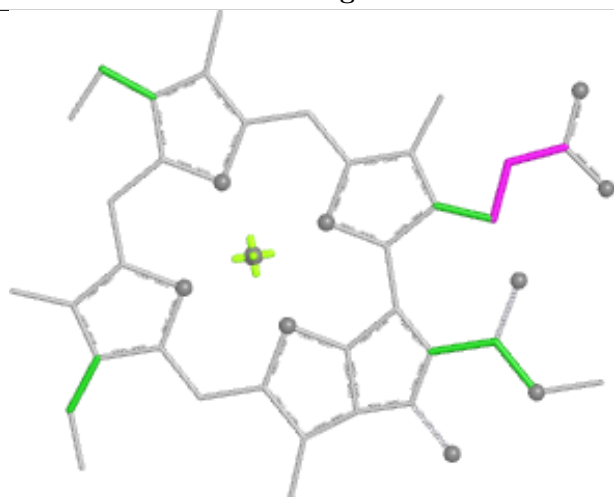
Ligand CLA 8 306



Bond lengths



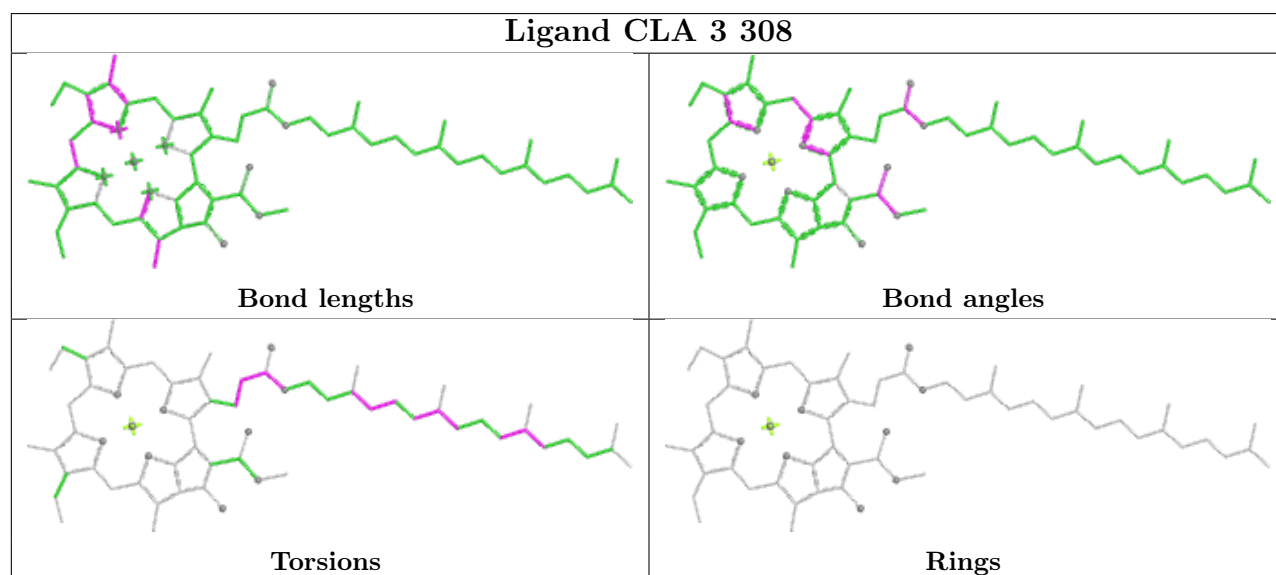
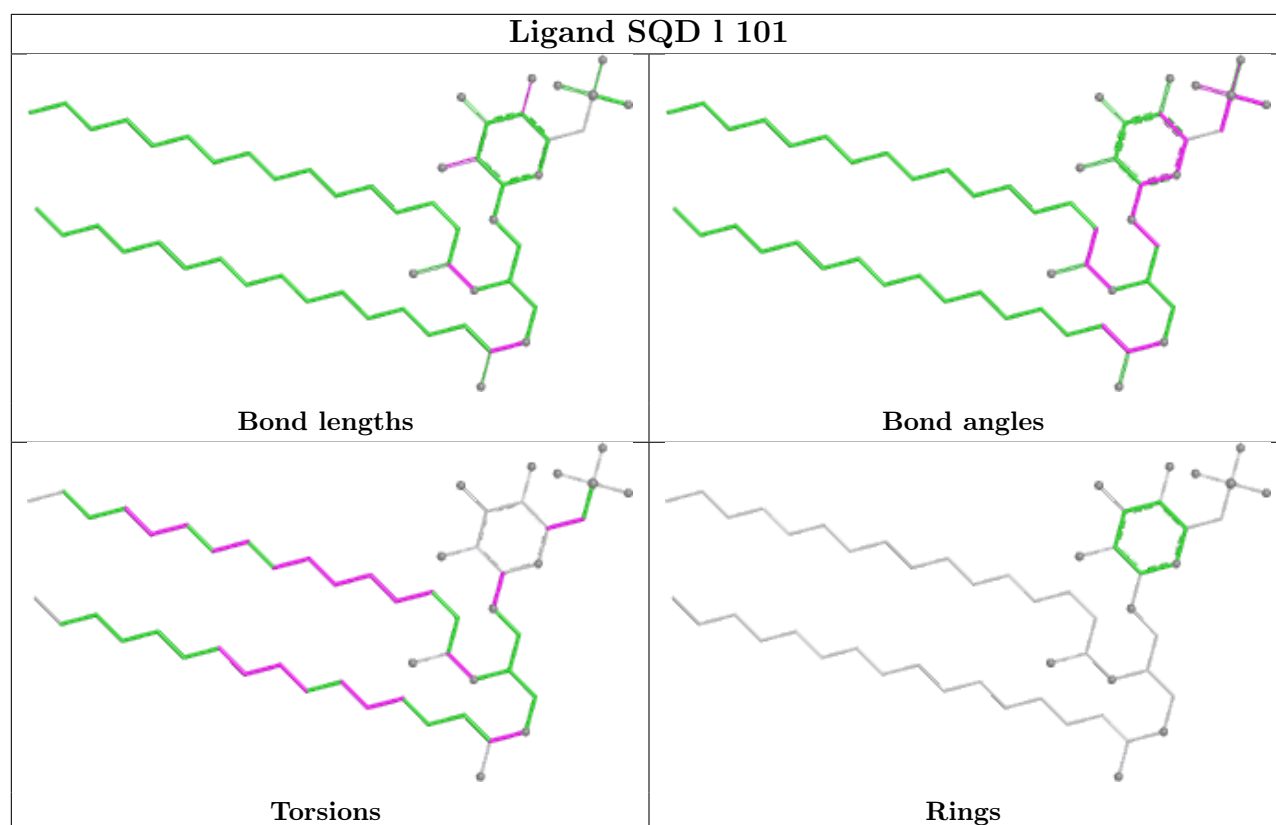
Bond angles

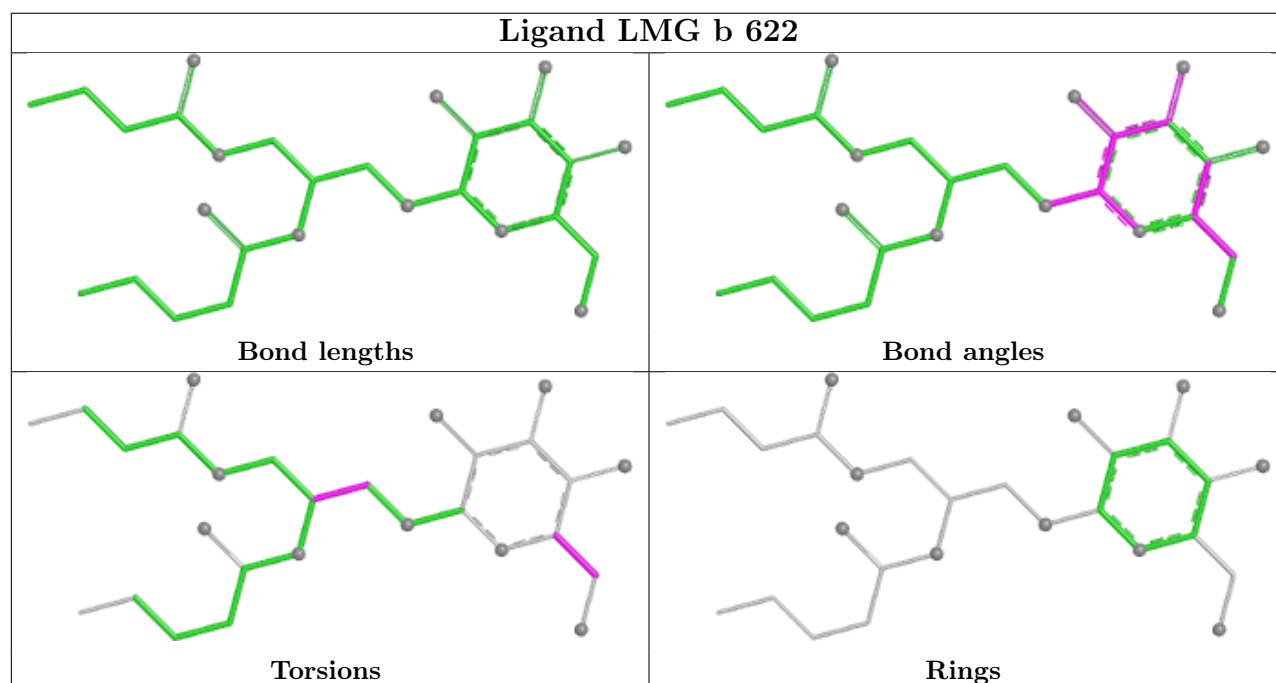
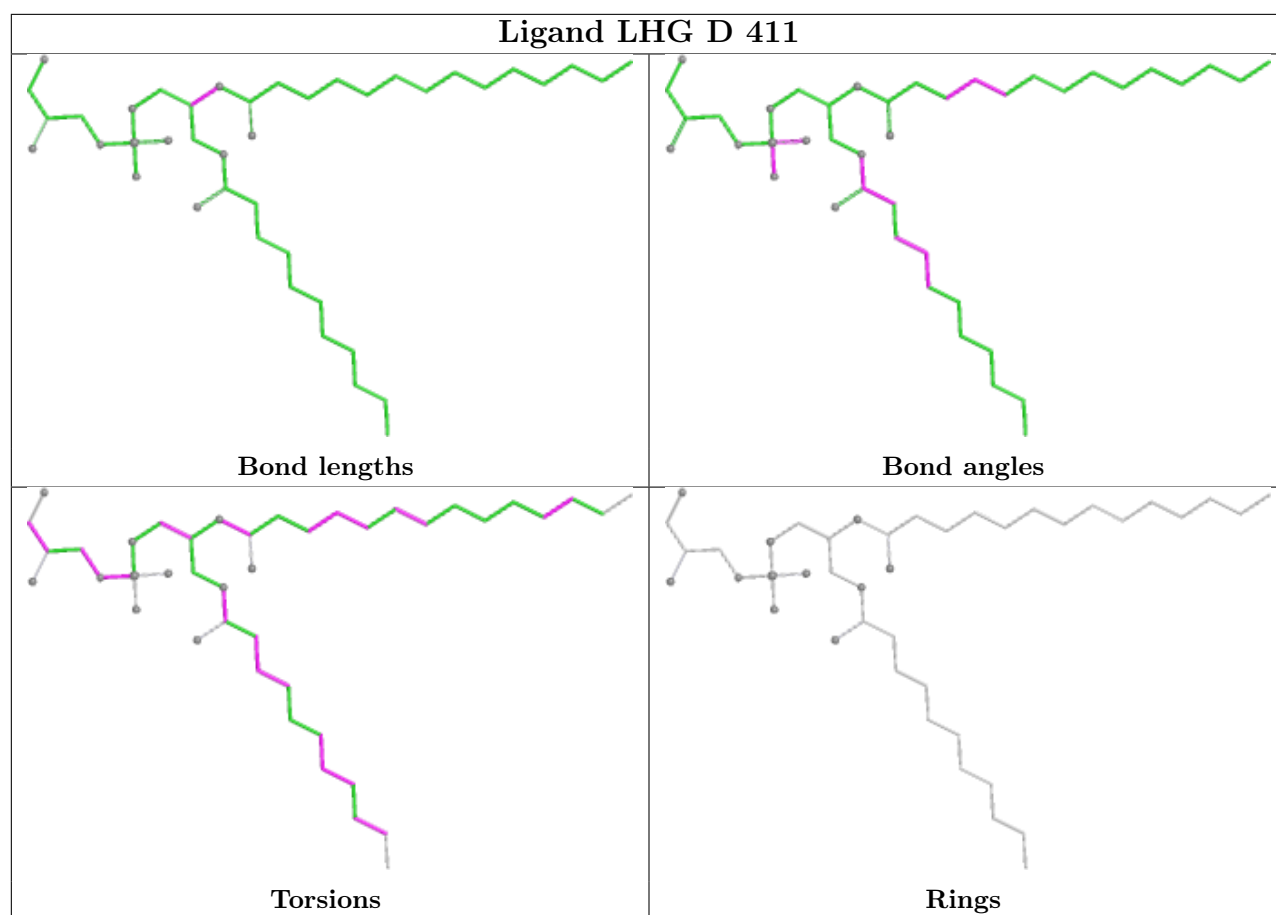


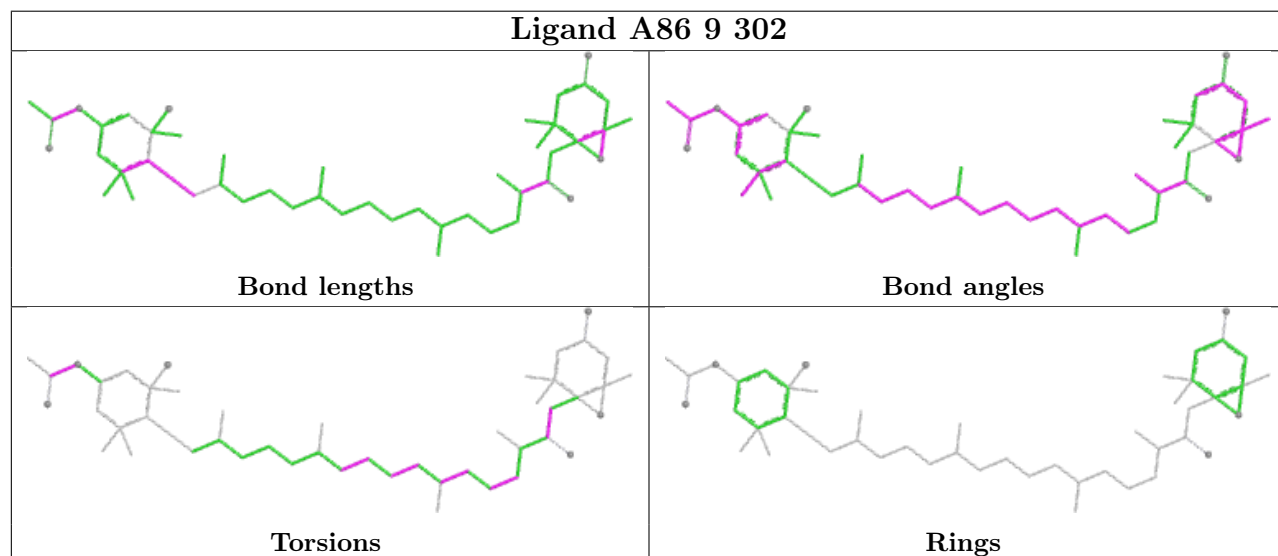
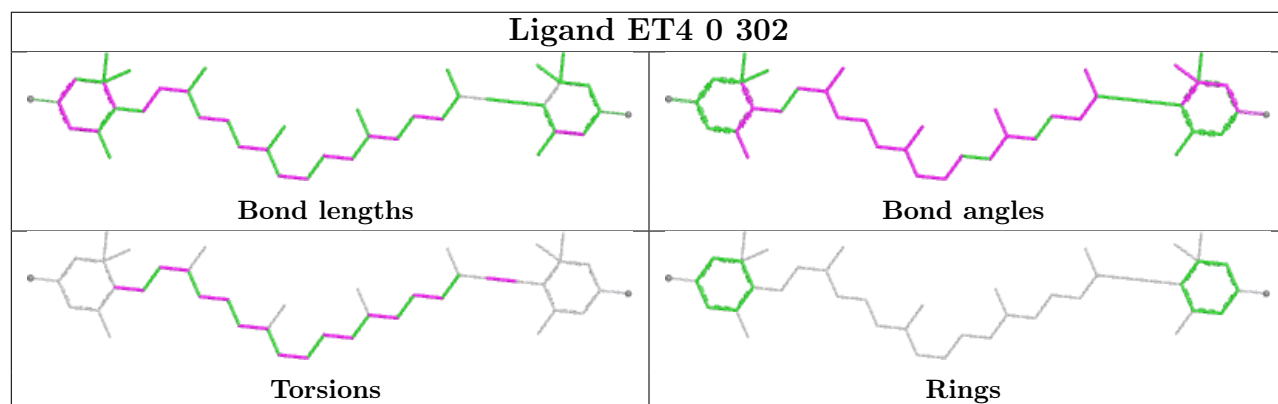
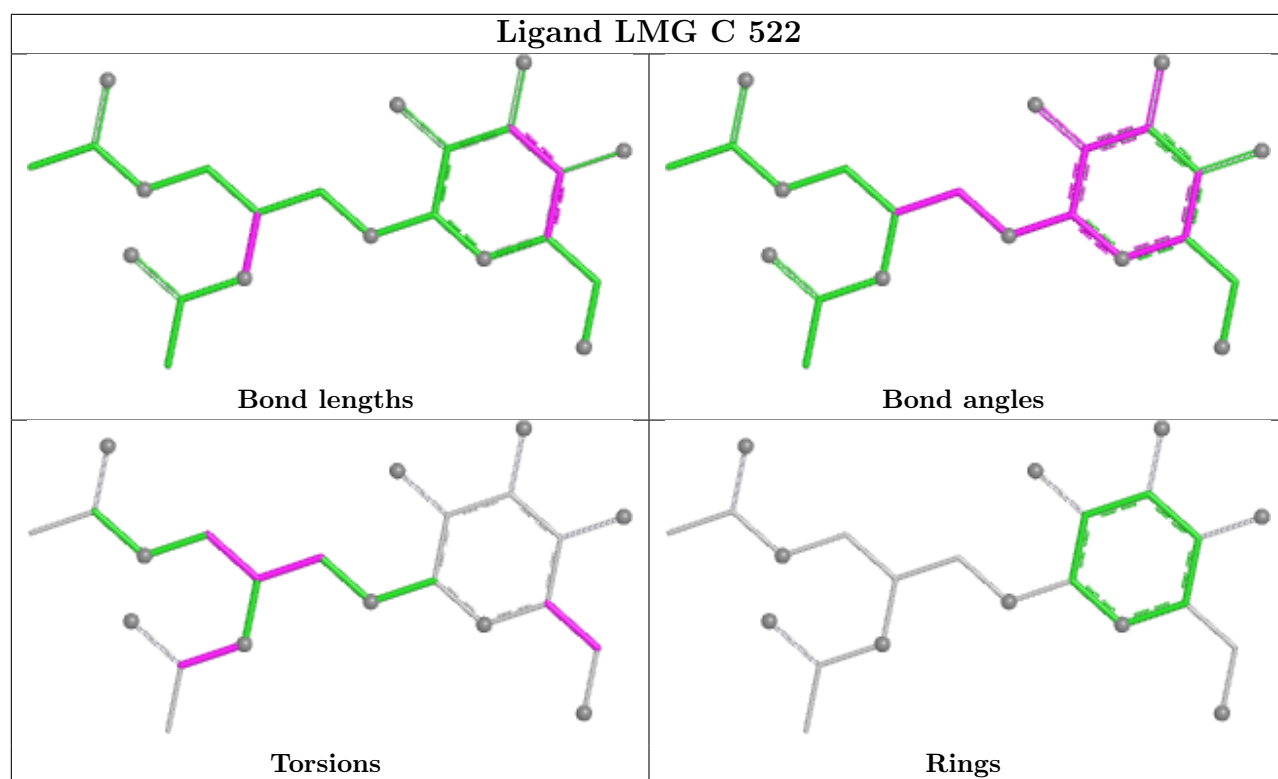
Torsions

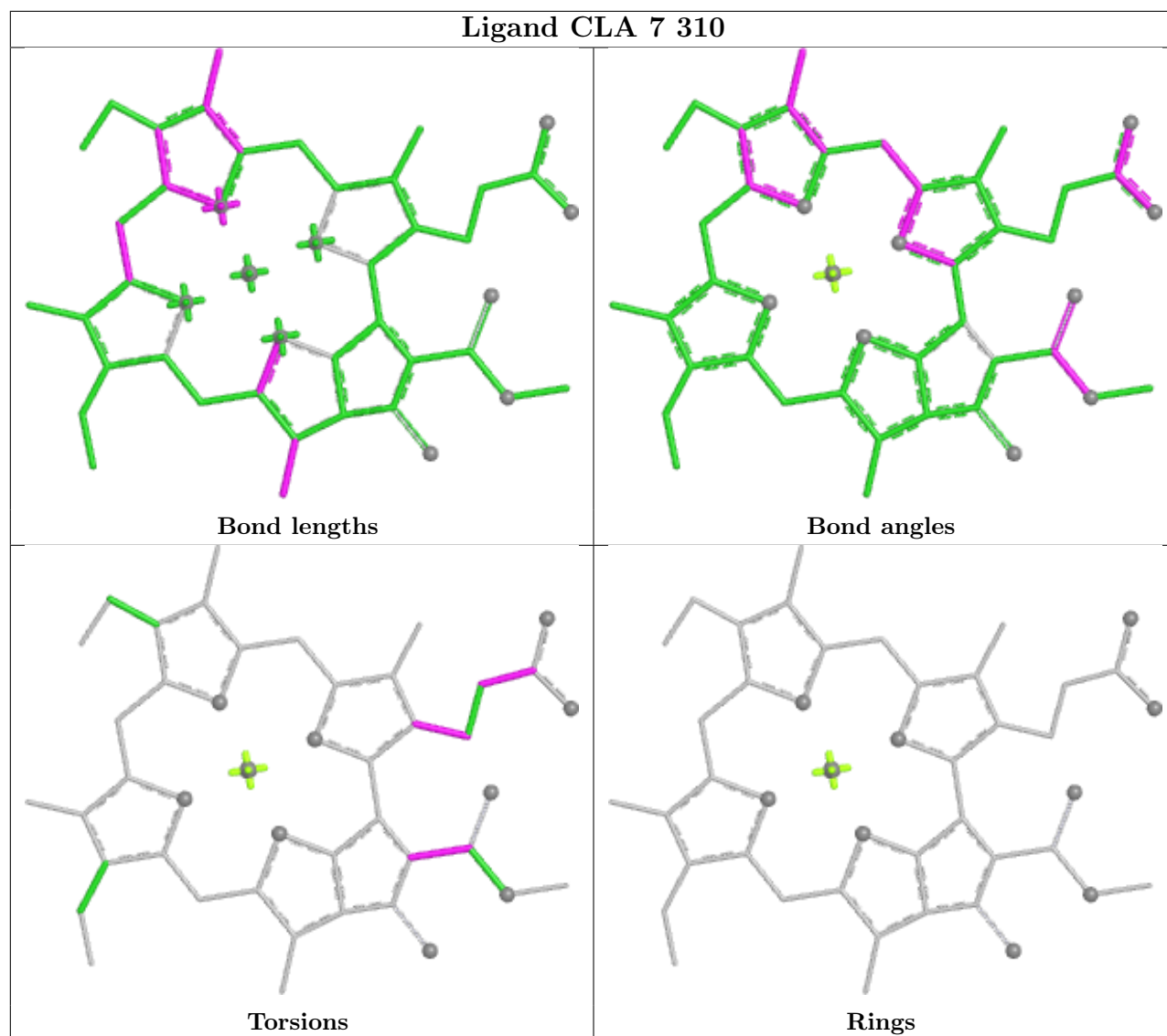
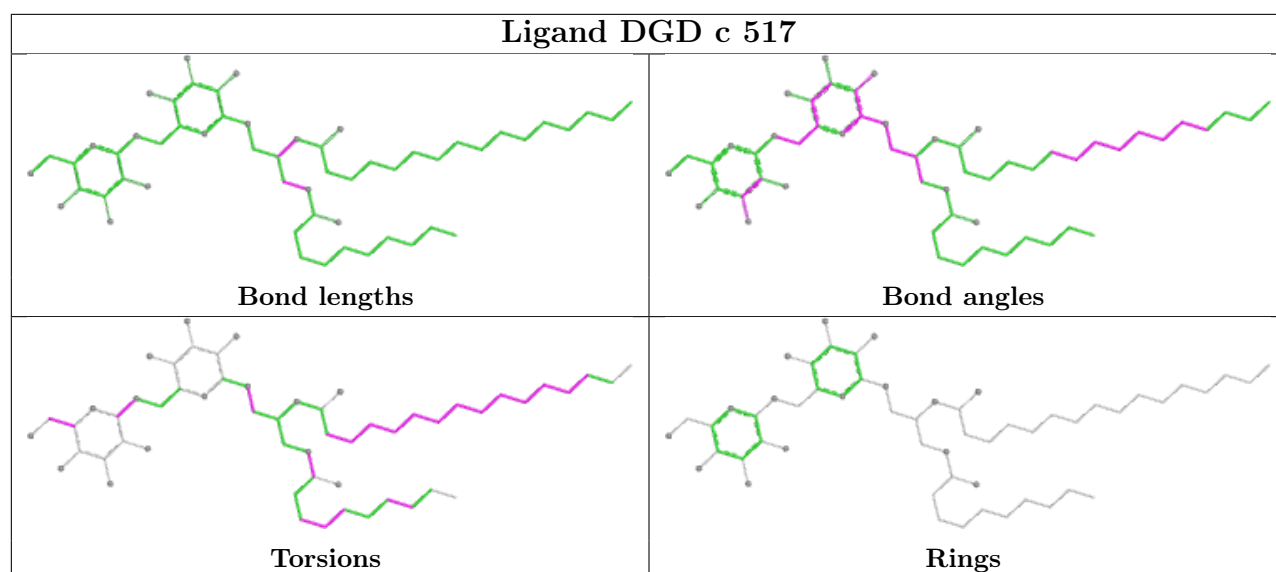


Rings

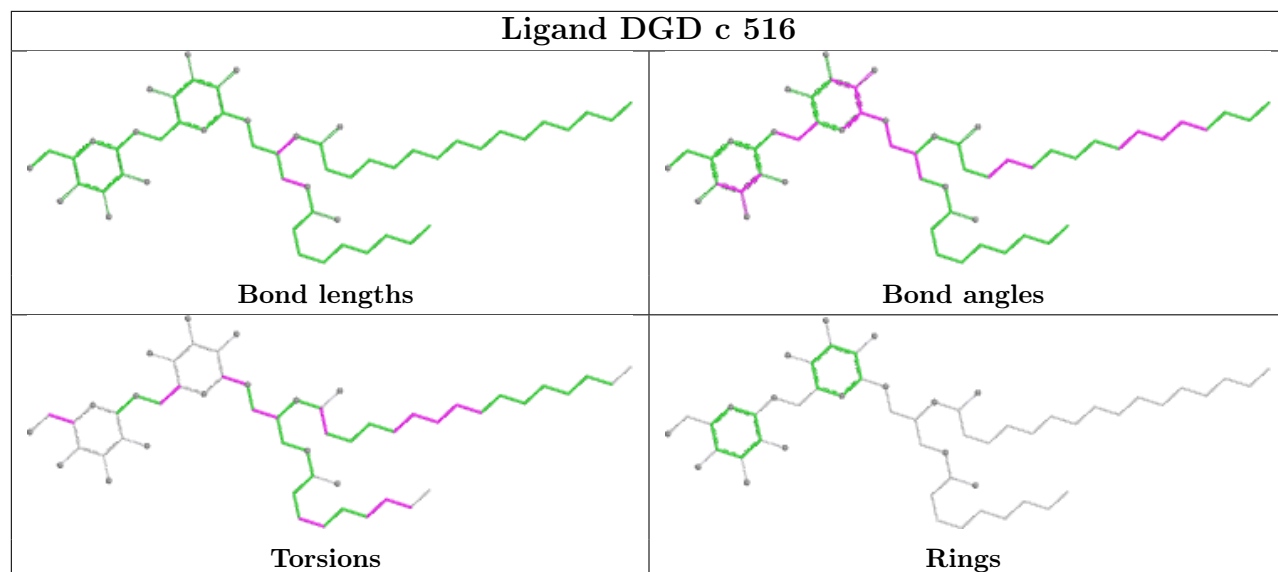




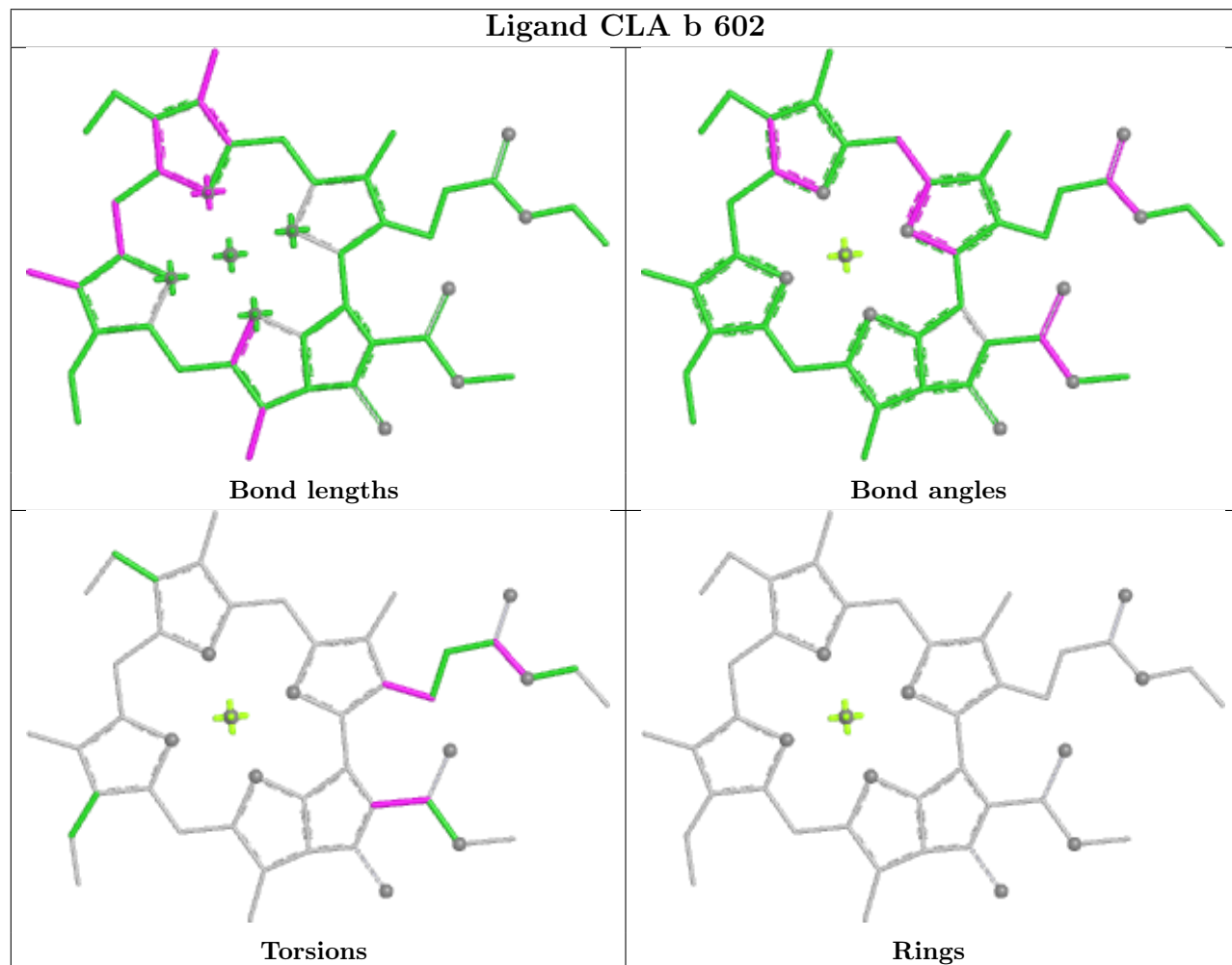




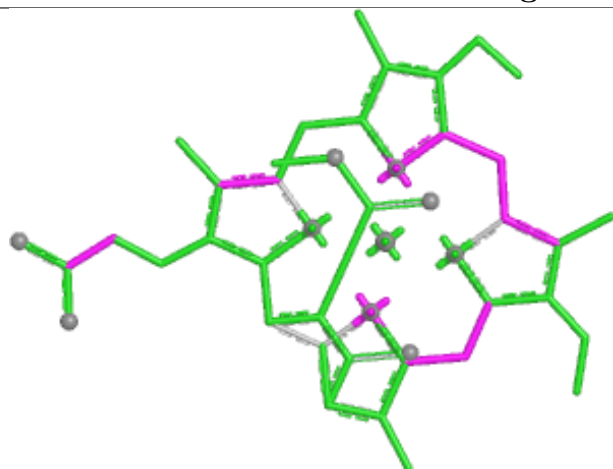
Ligand DGD c 516



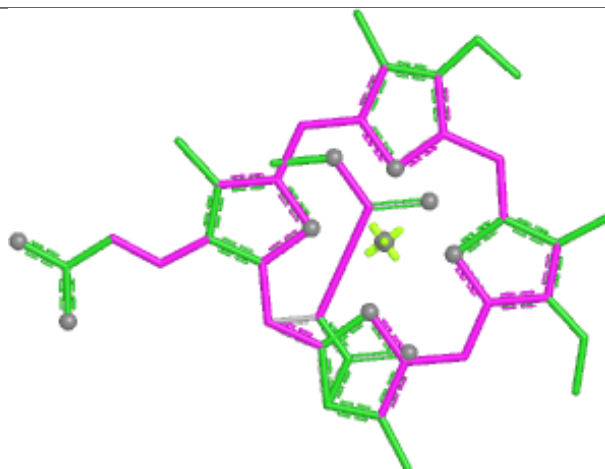
Ligand CLA b 602



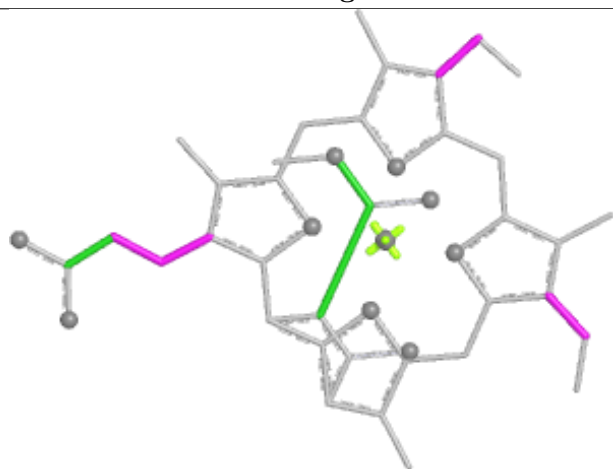
Ligand KC2 4 307



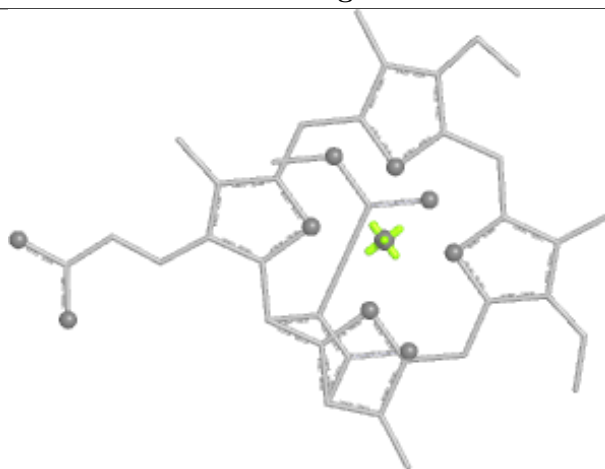
Bond lengths



Bond angles

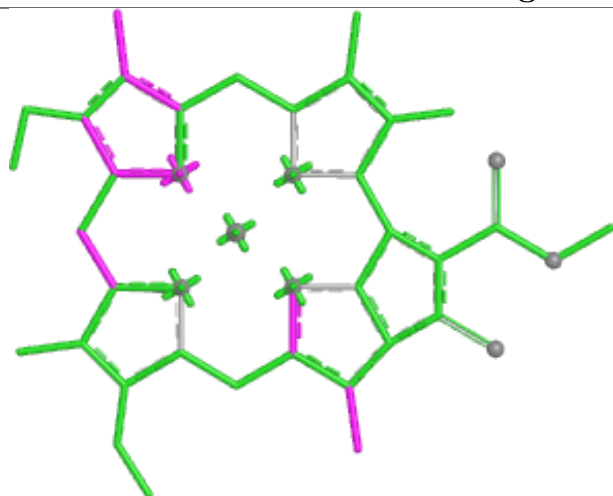


Torsions

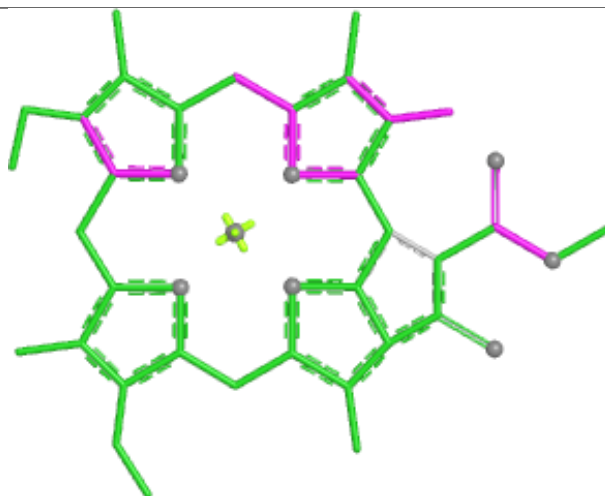


Rings

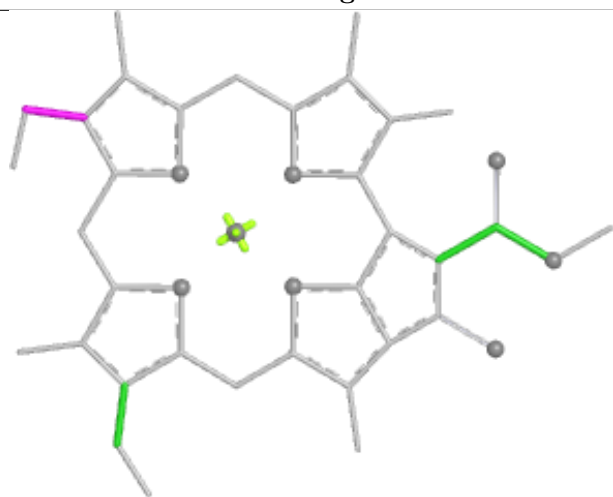
Ligand CLA 8 305



Bond lengths



Bond angles

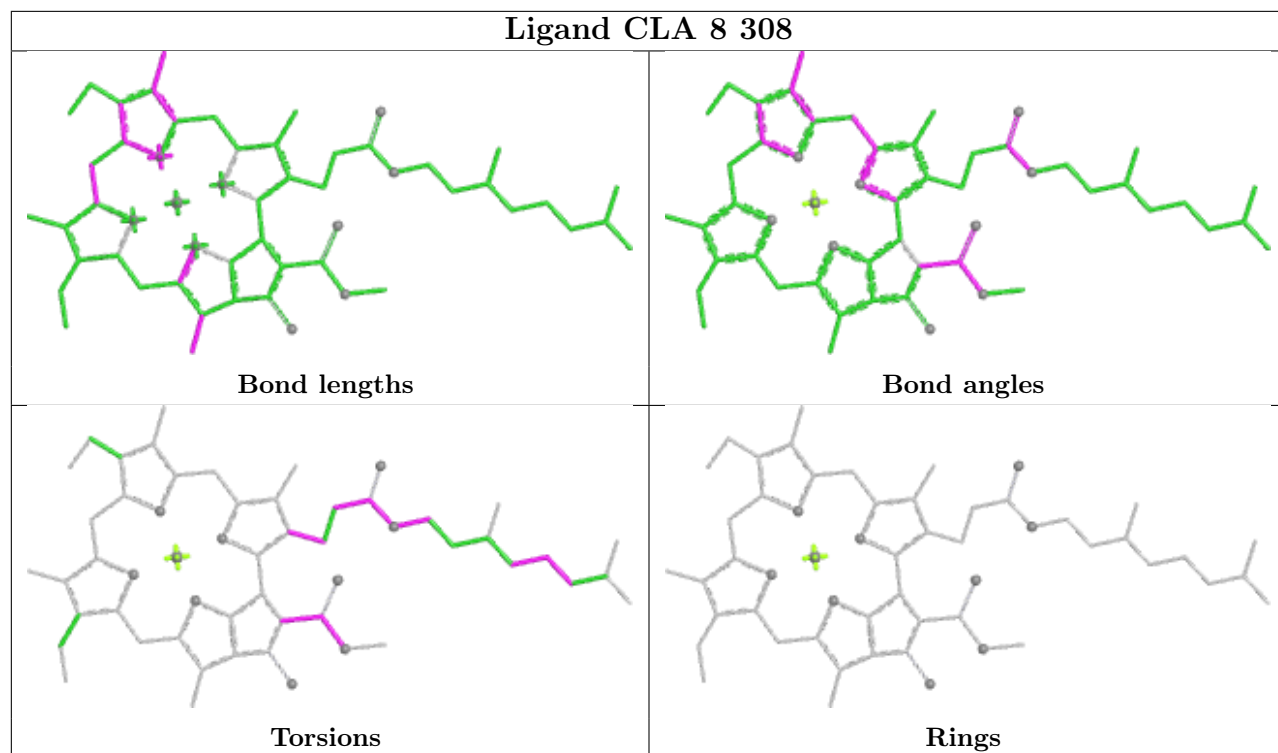


Torsions

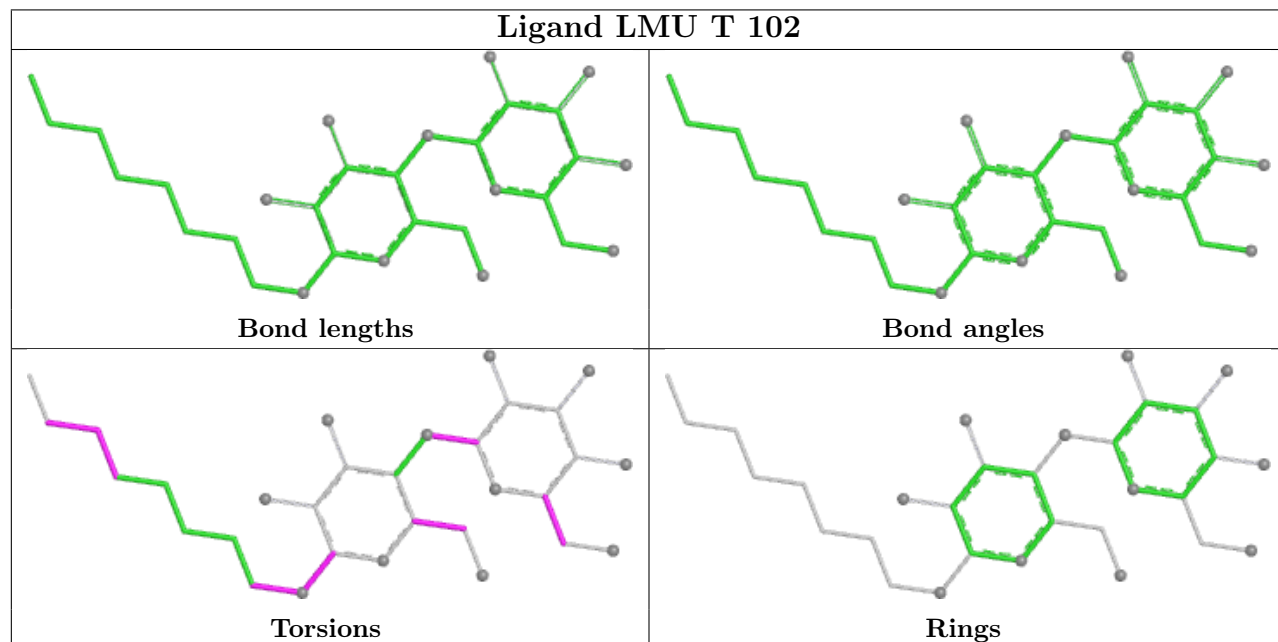


Rings

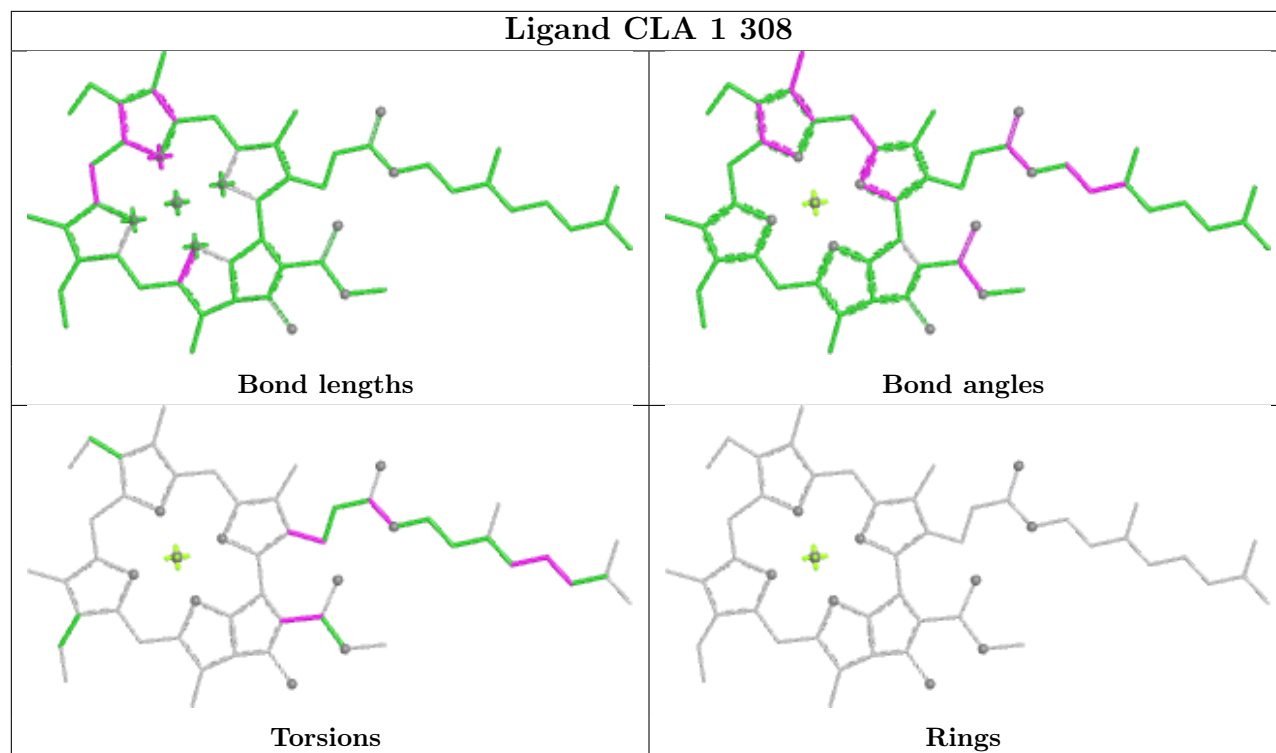
Ligand CLA 8 308



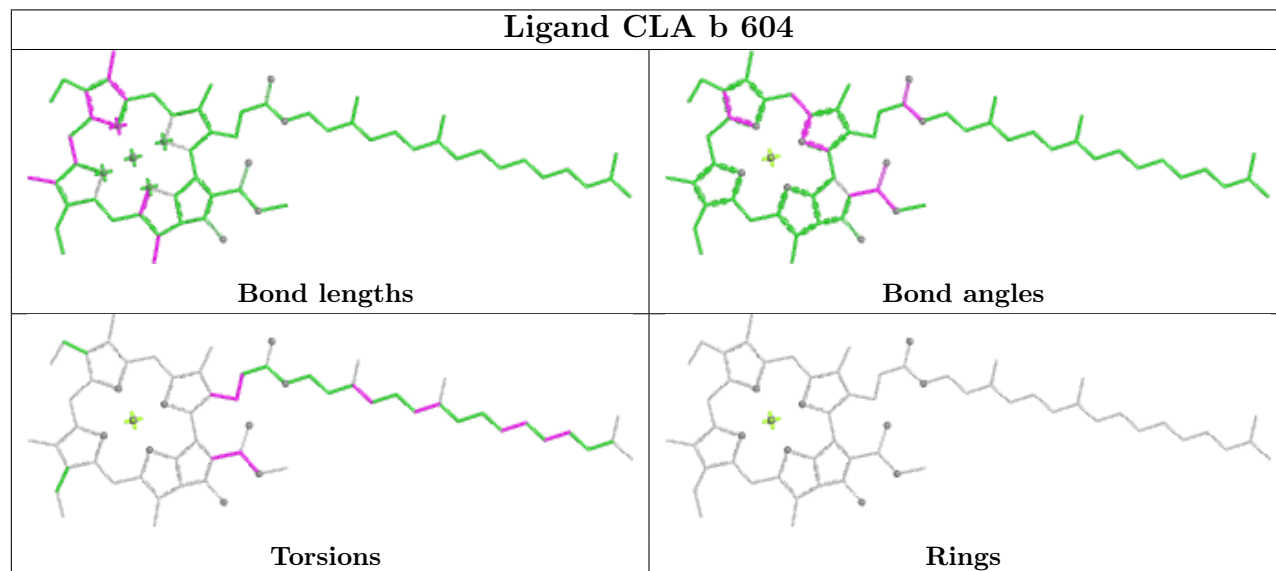
Ligand LMU T 102

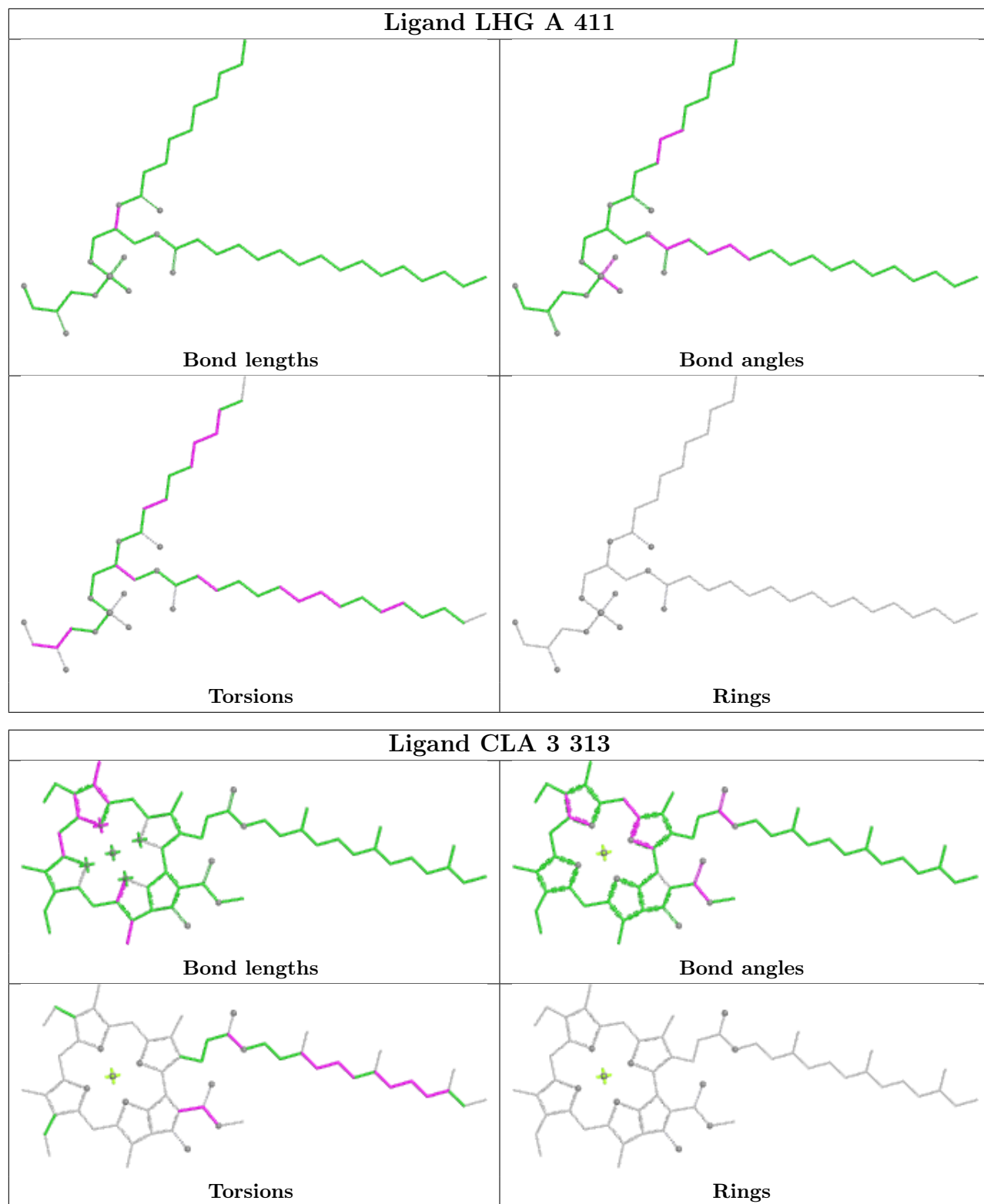


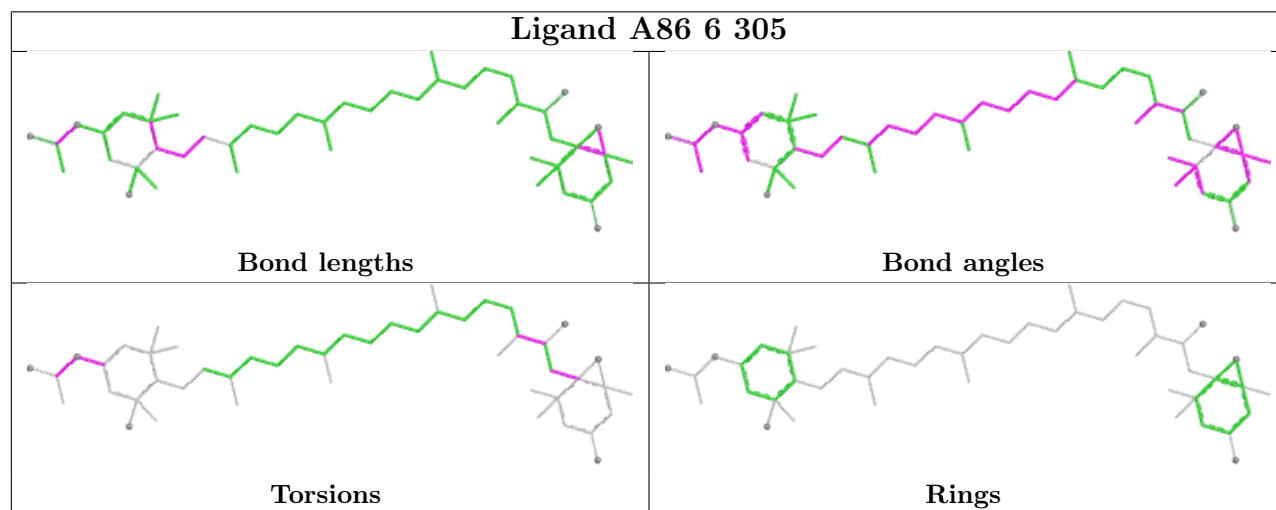
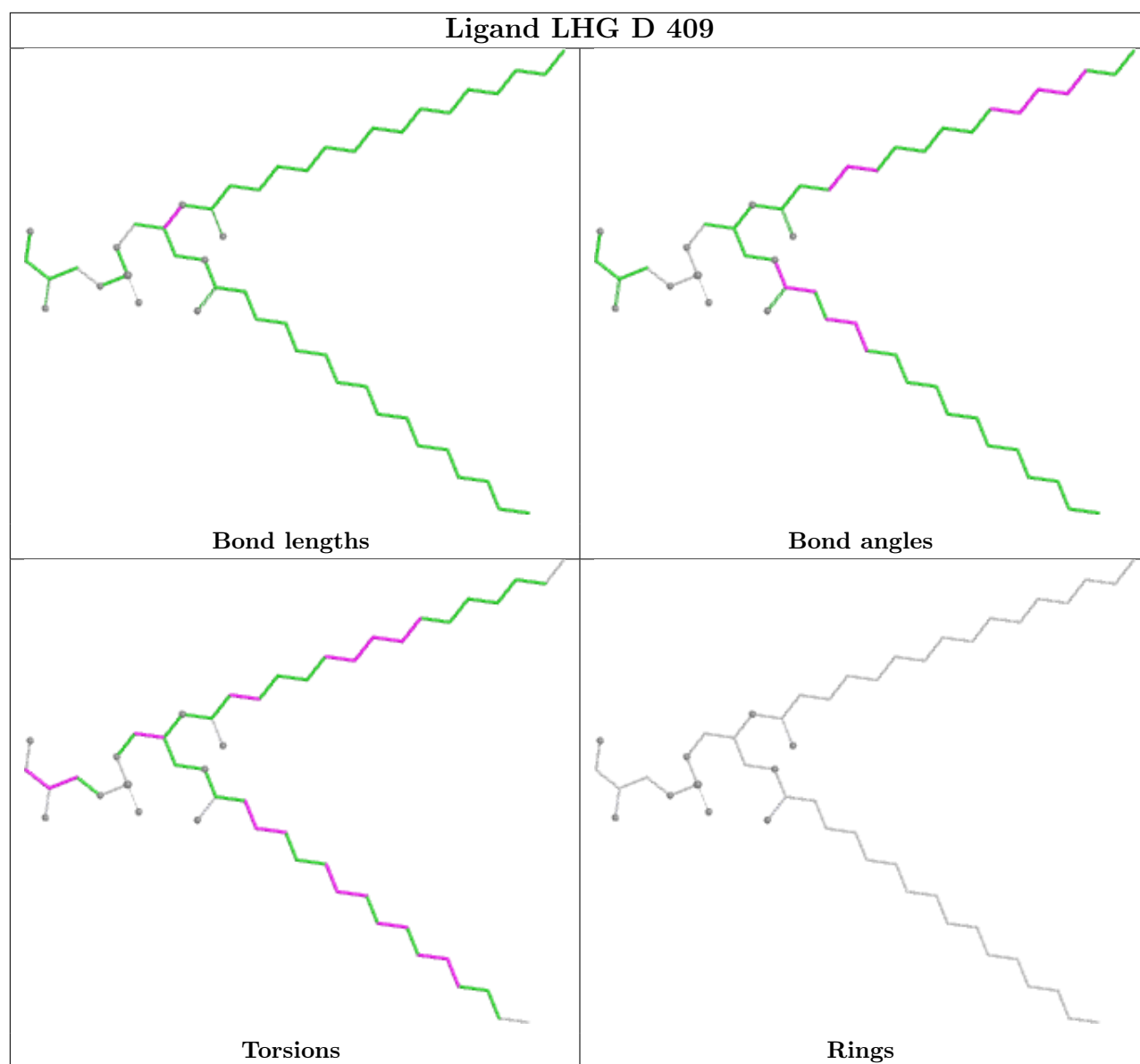
Ligand CLA 1 308

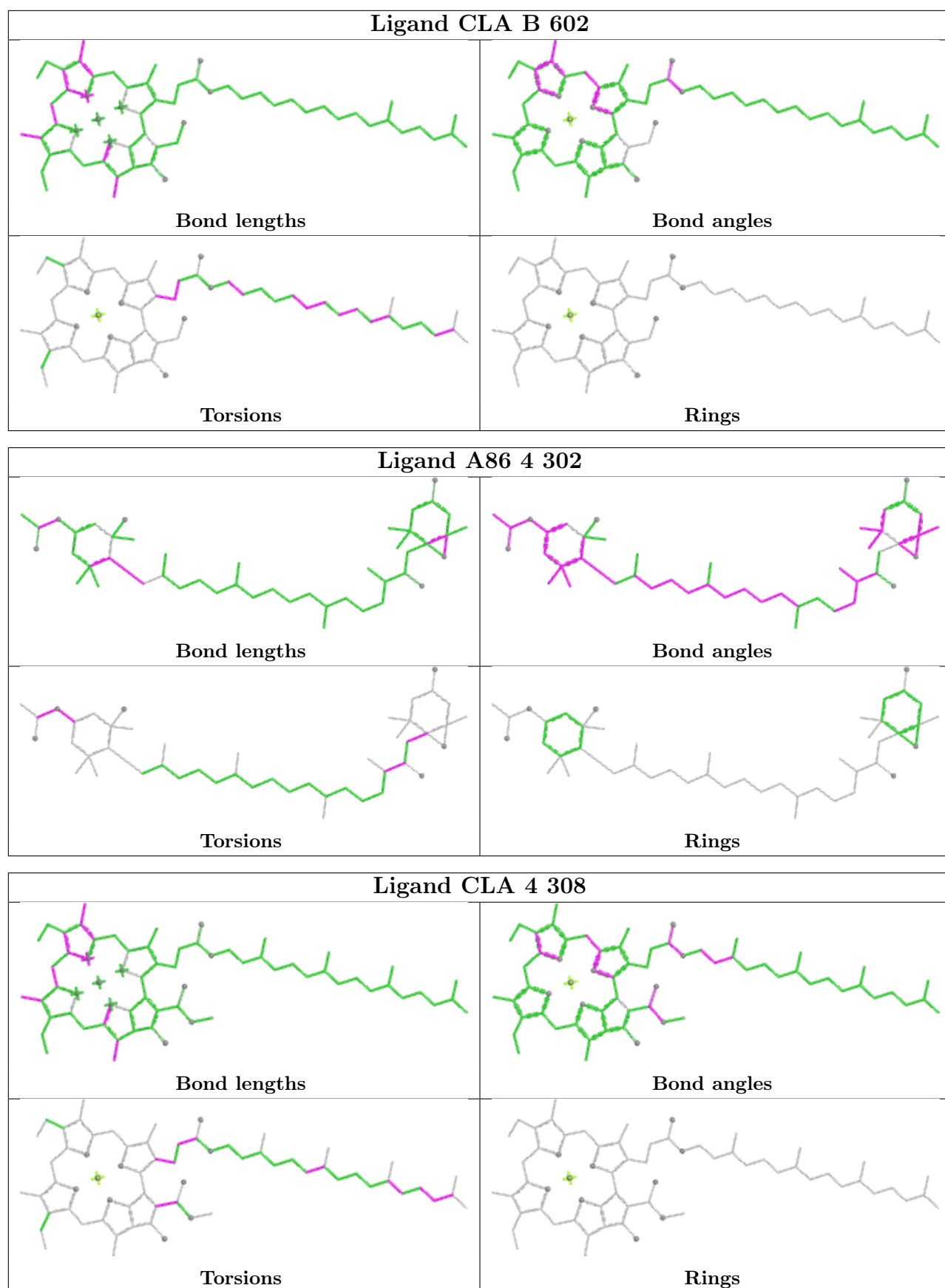


Ligand CLA b 604

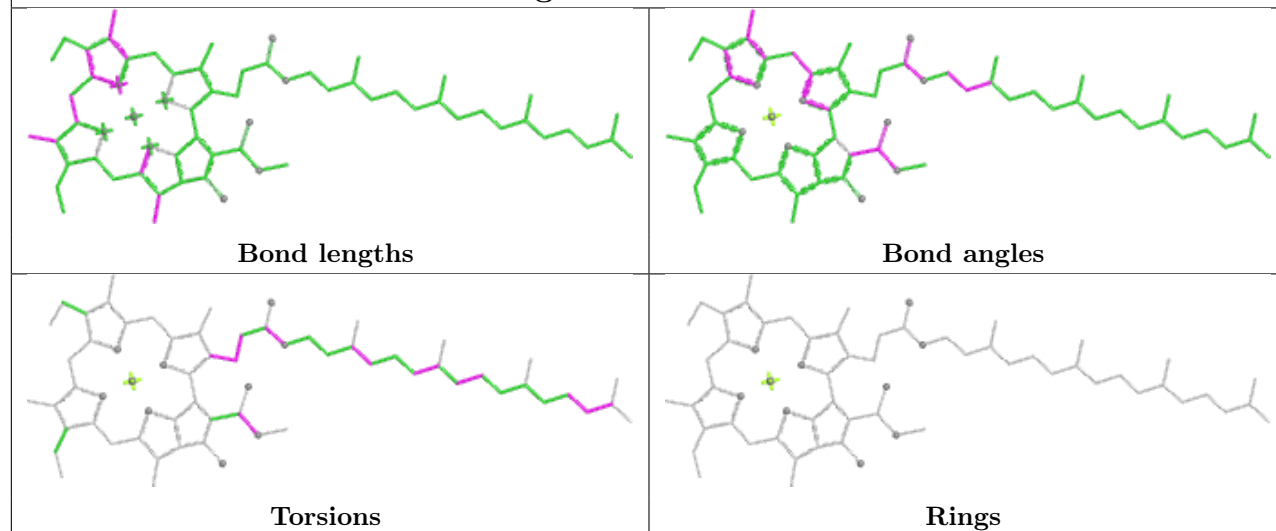




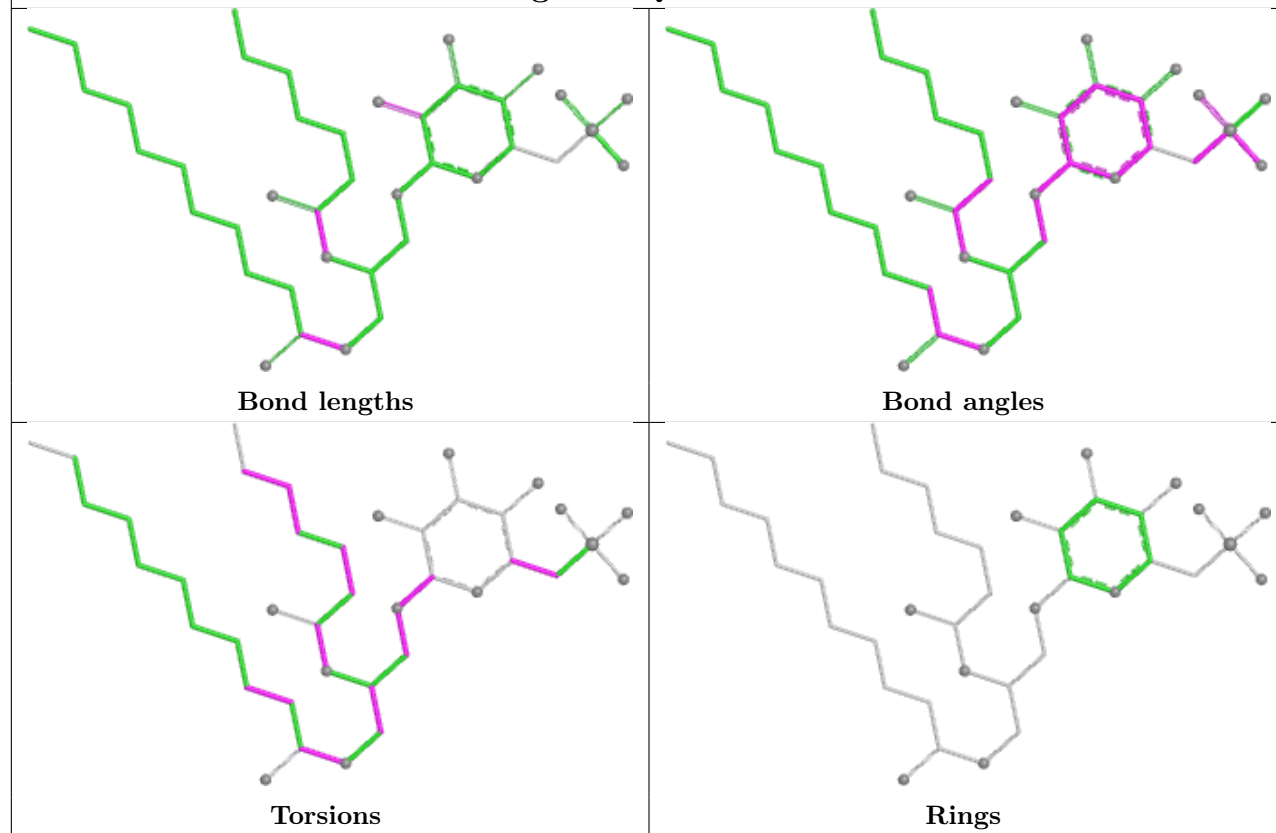




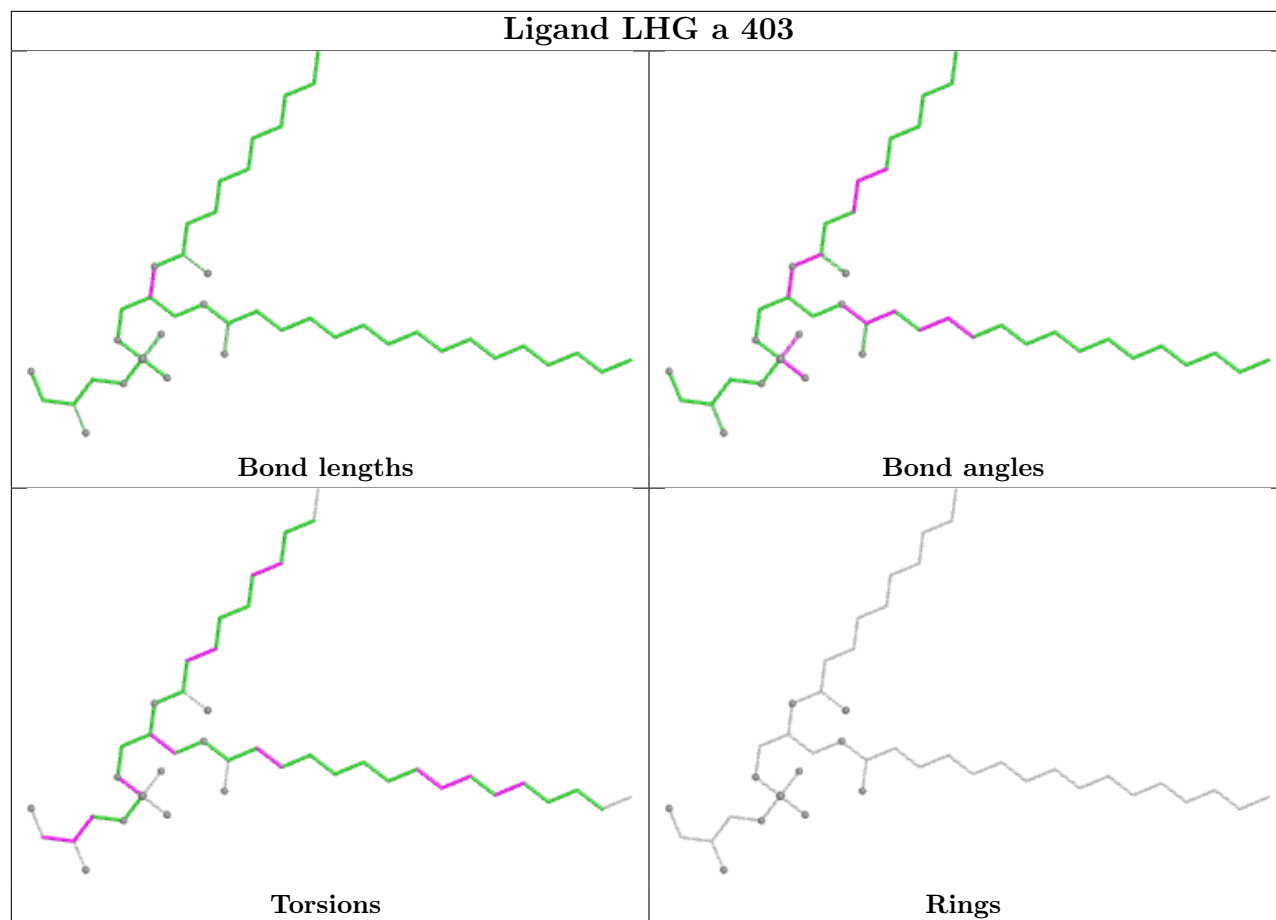
Ligand CLA b 613



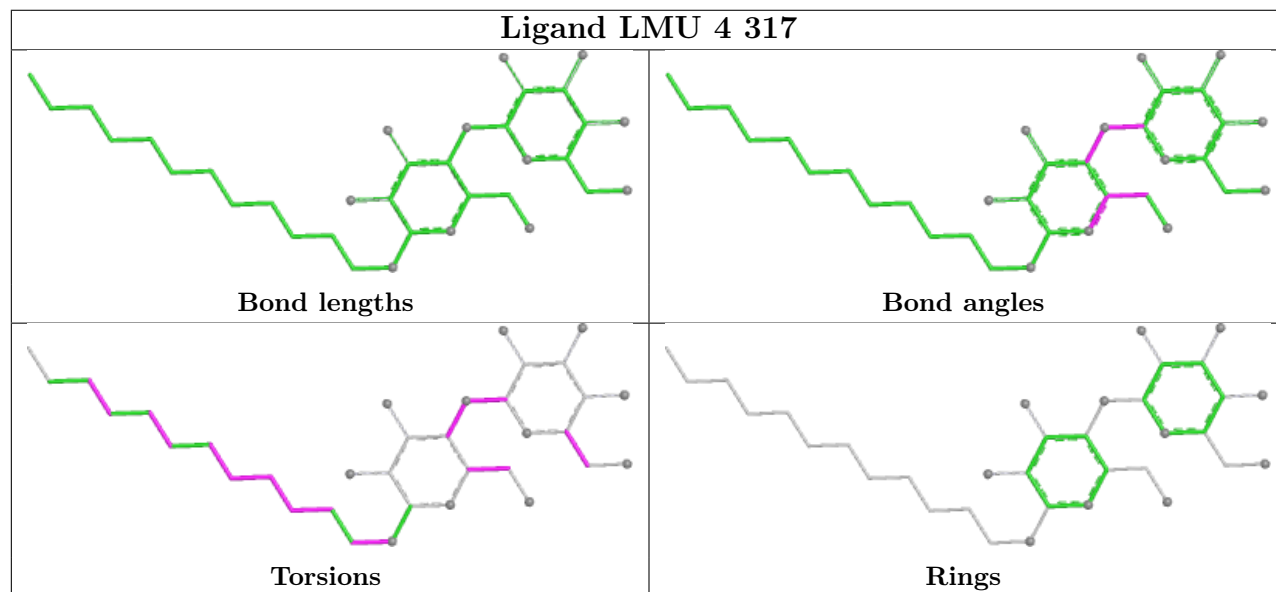
Ligand SQD A 413

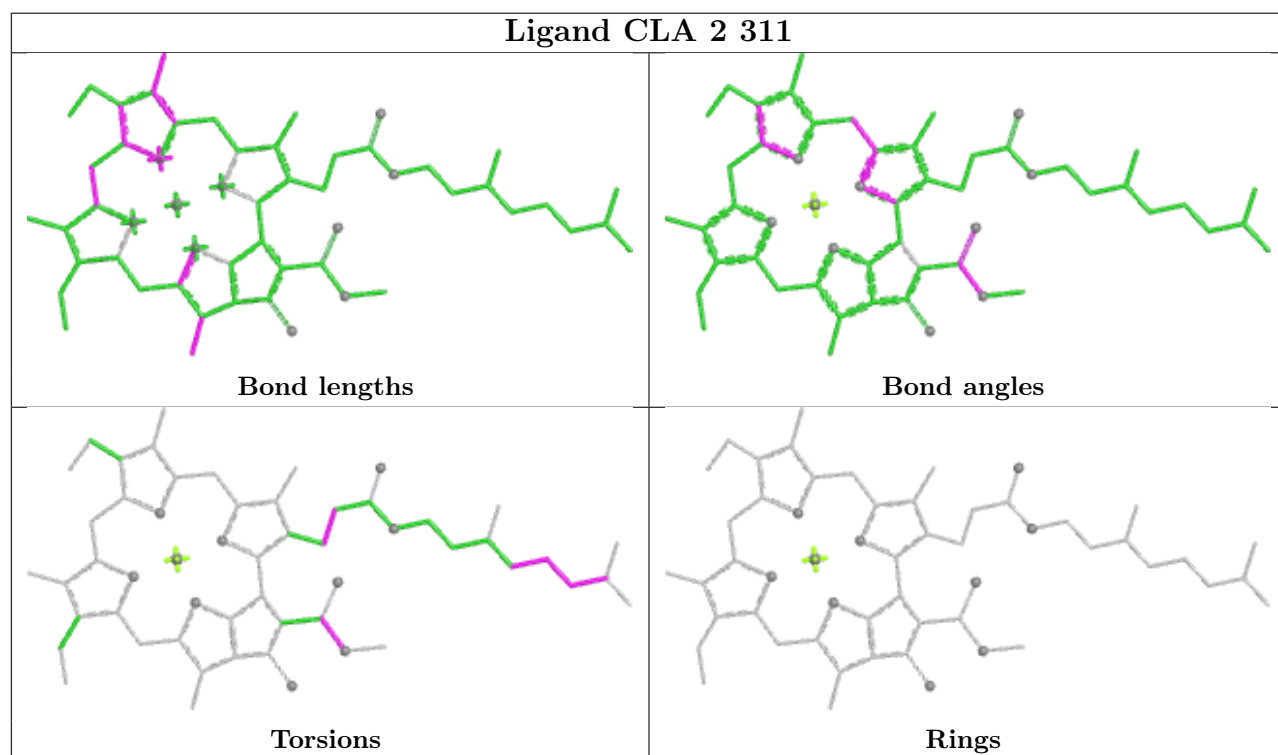
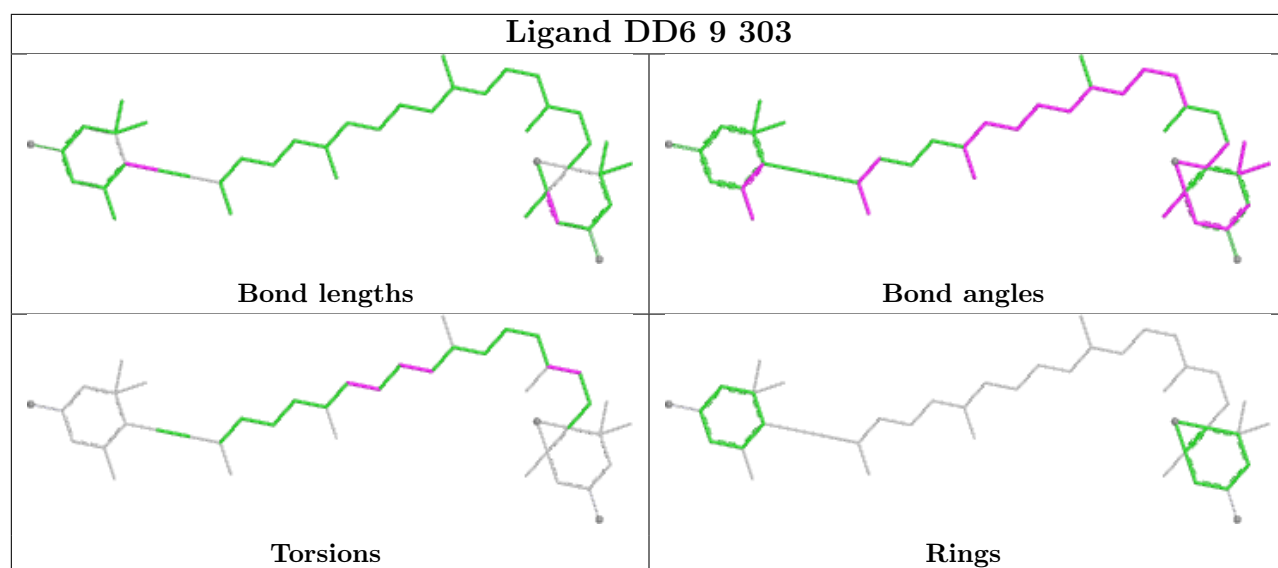


Ligand LHG a 403

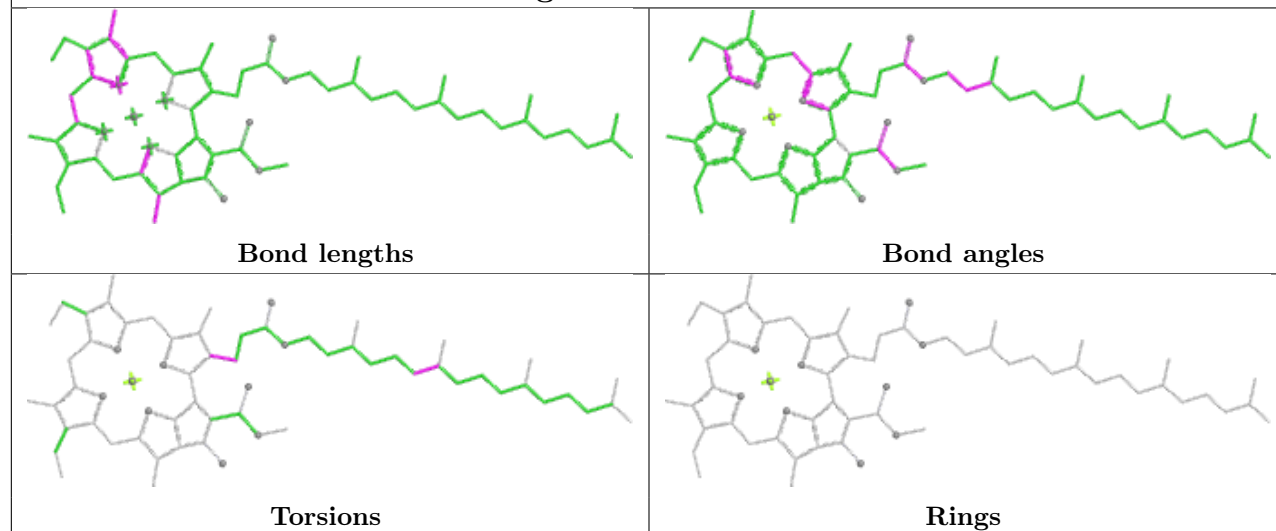


Ligand LMU 4 317

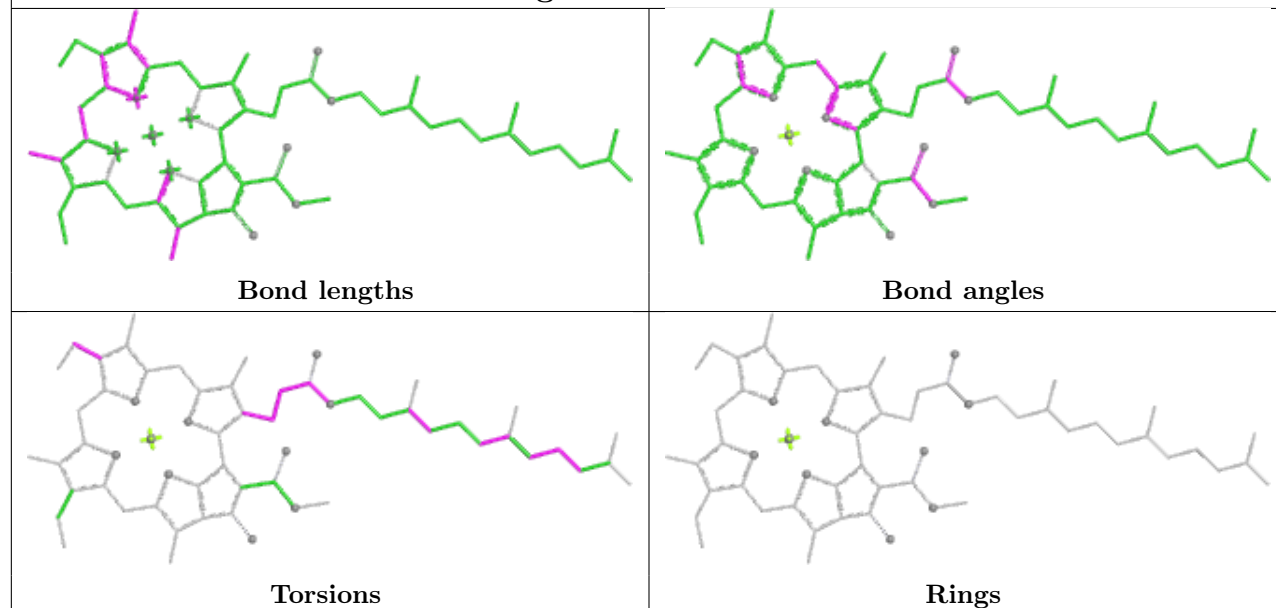




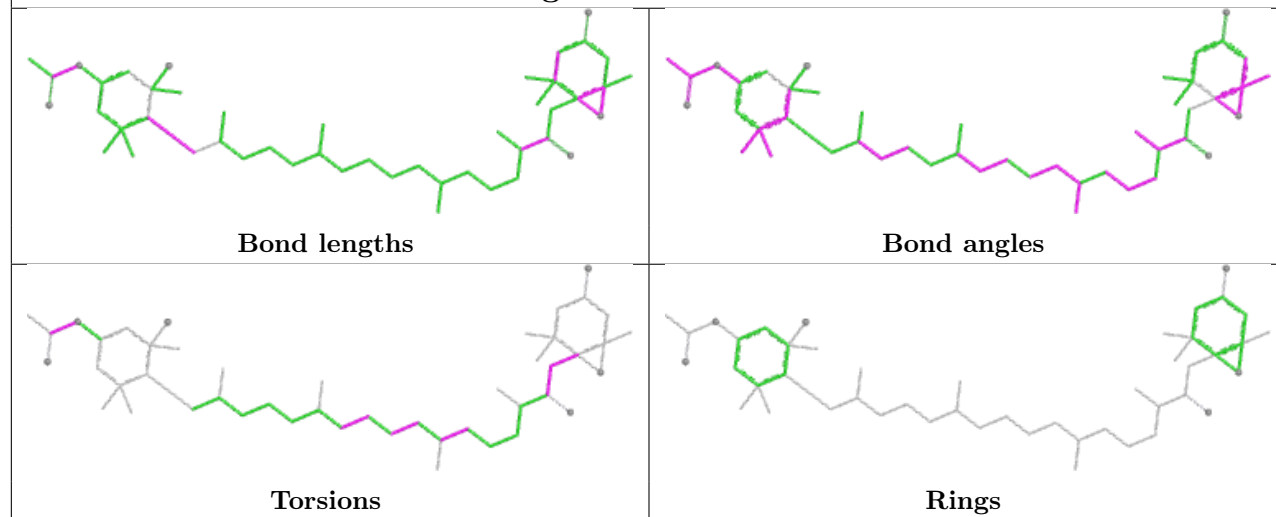
Ligand CLA 4 309

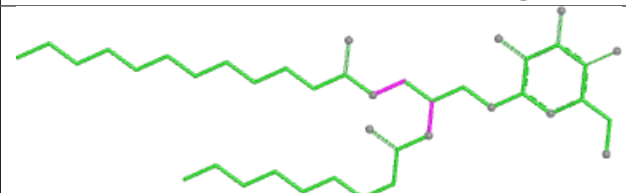
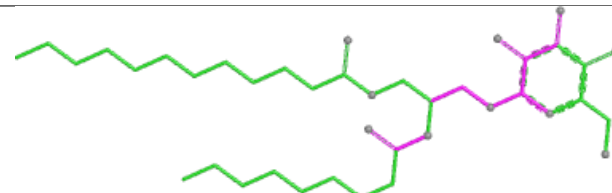
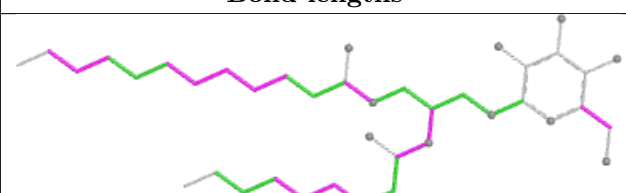
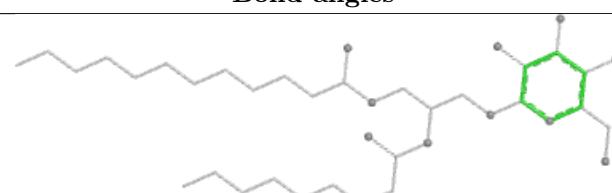
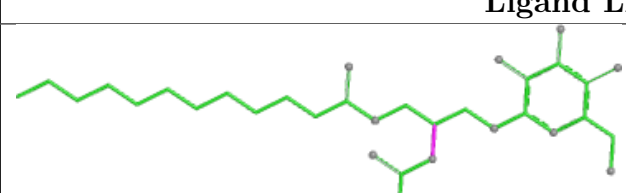
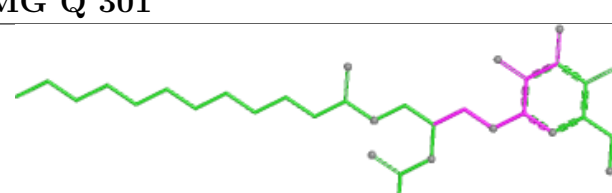
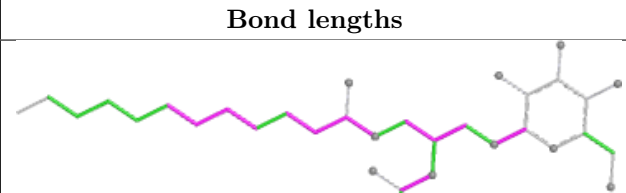
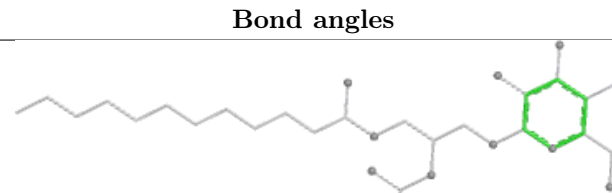
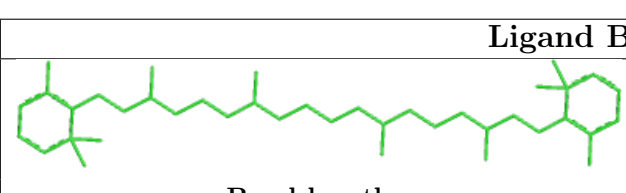
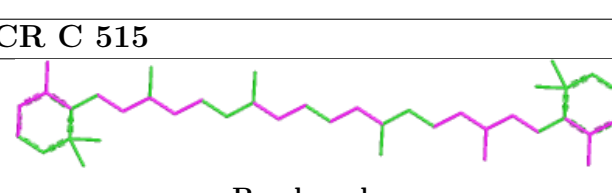
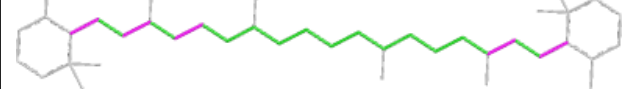
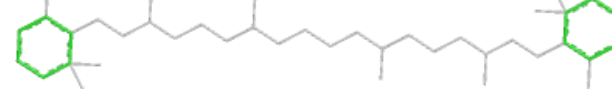


Ligand CLA 4 311

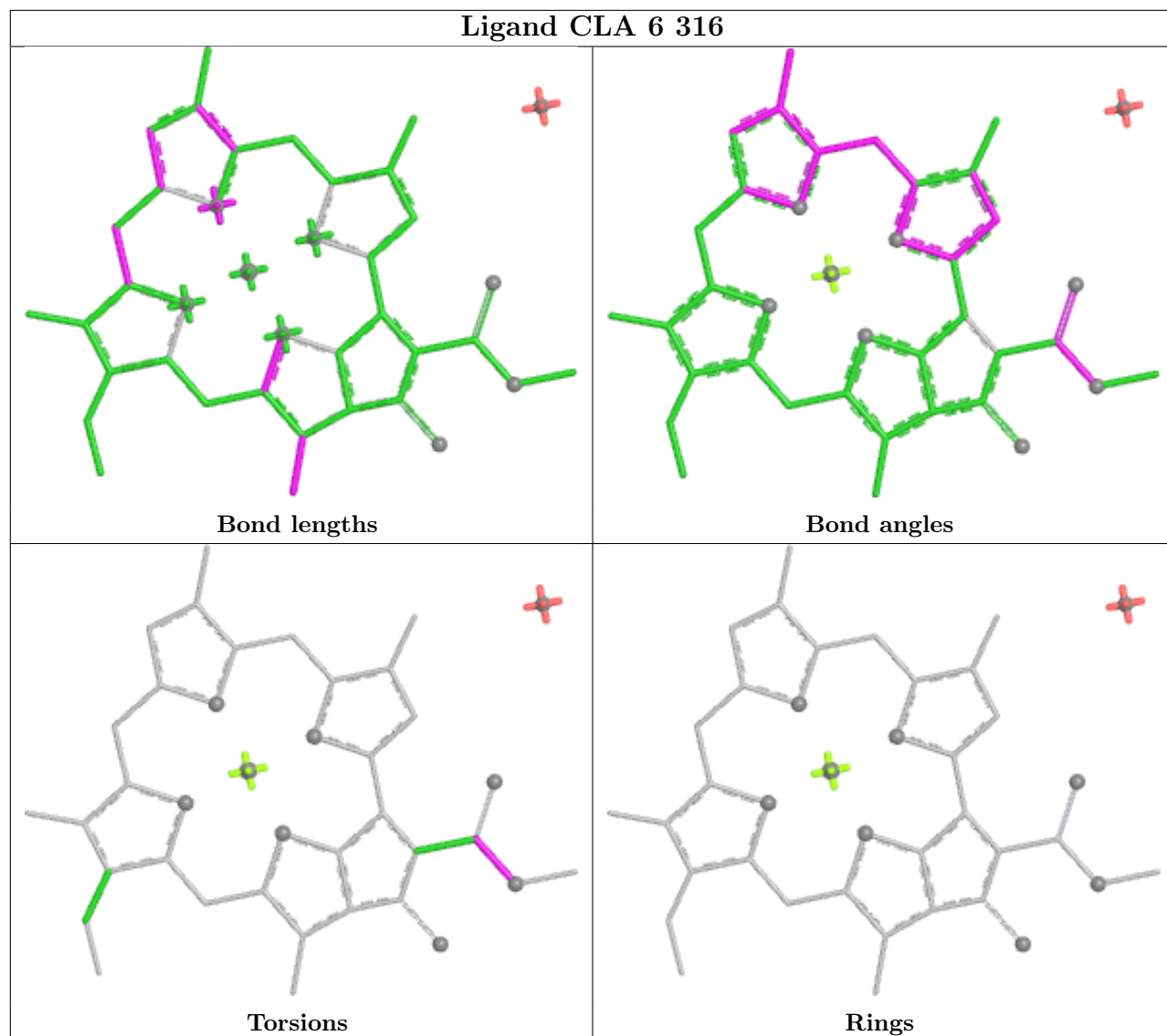


Ligand A86 7 301

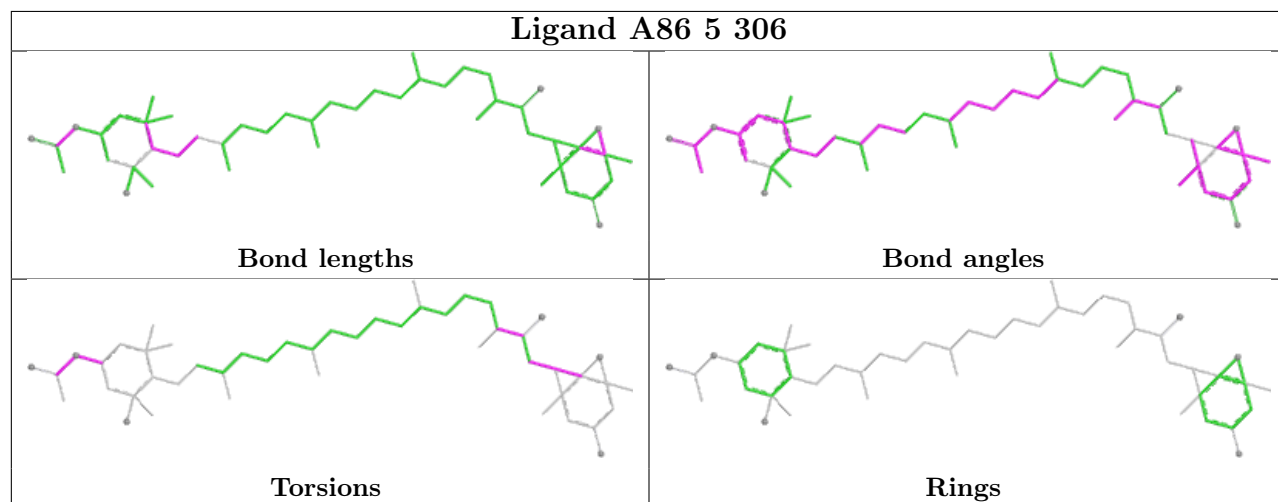


Ligand LMG m 201	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG Q 301	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

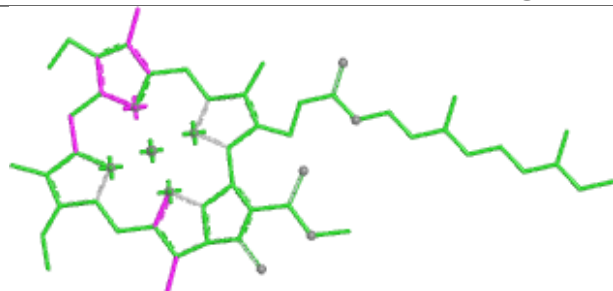
Ligand CLA 6 316



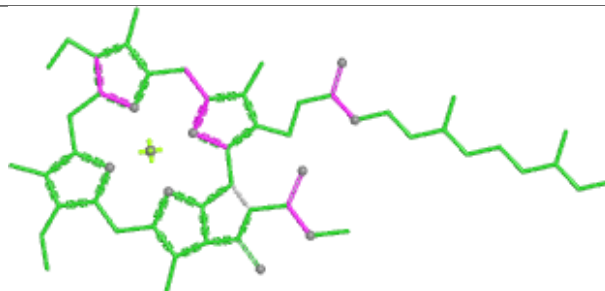
Ligand A86 5 306



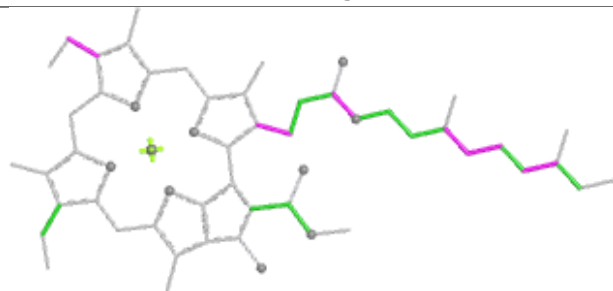
Ligand CLA 3 312



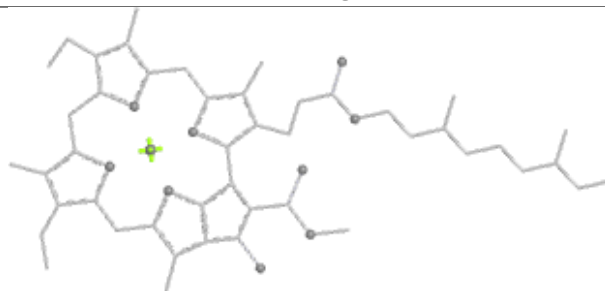
Bond lengths



Bond angles

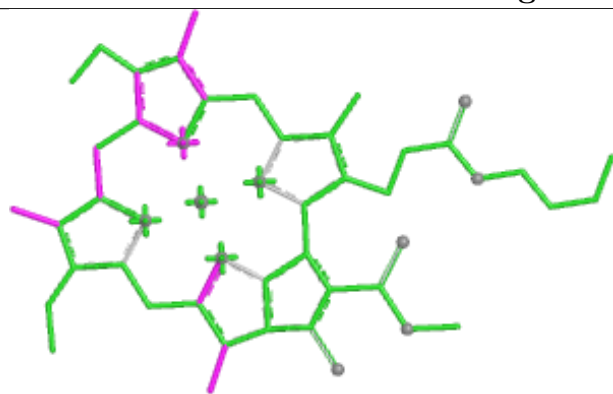


Torsions

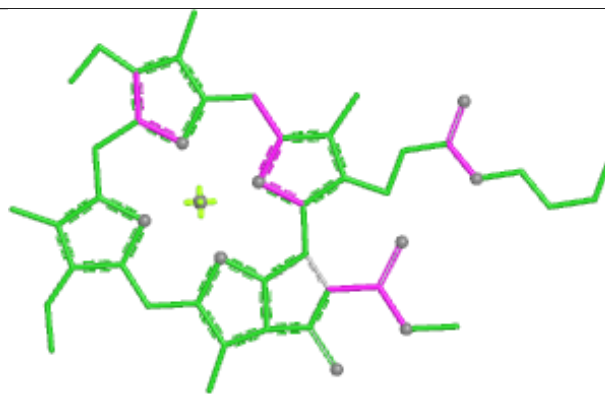


Rings

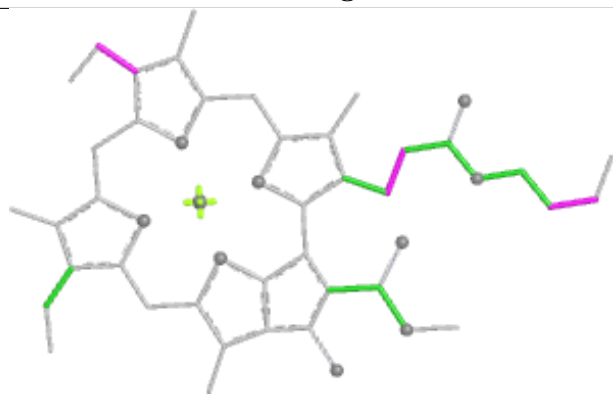
Ligand CLA a 408



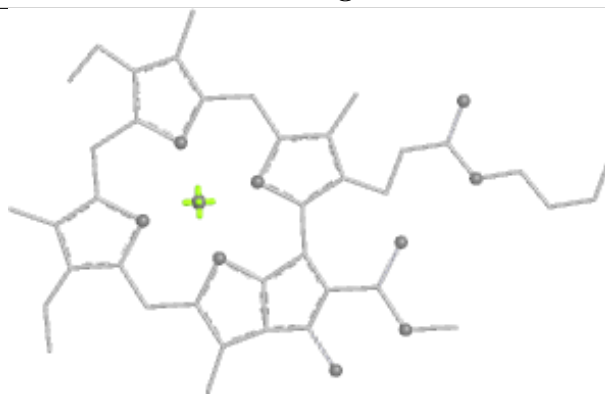
Bond lengths



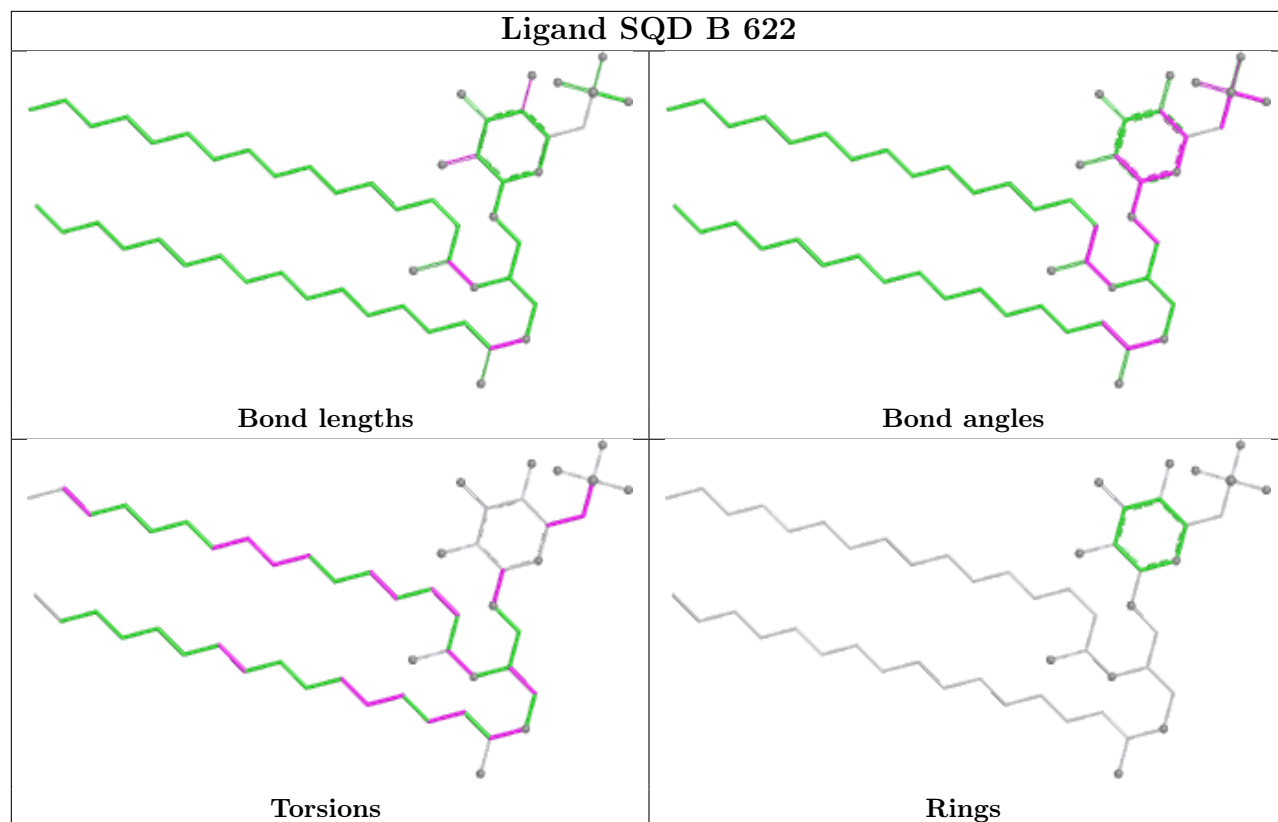
Bond angles

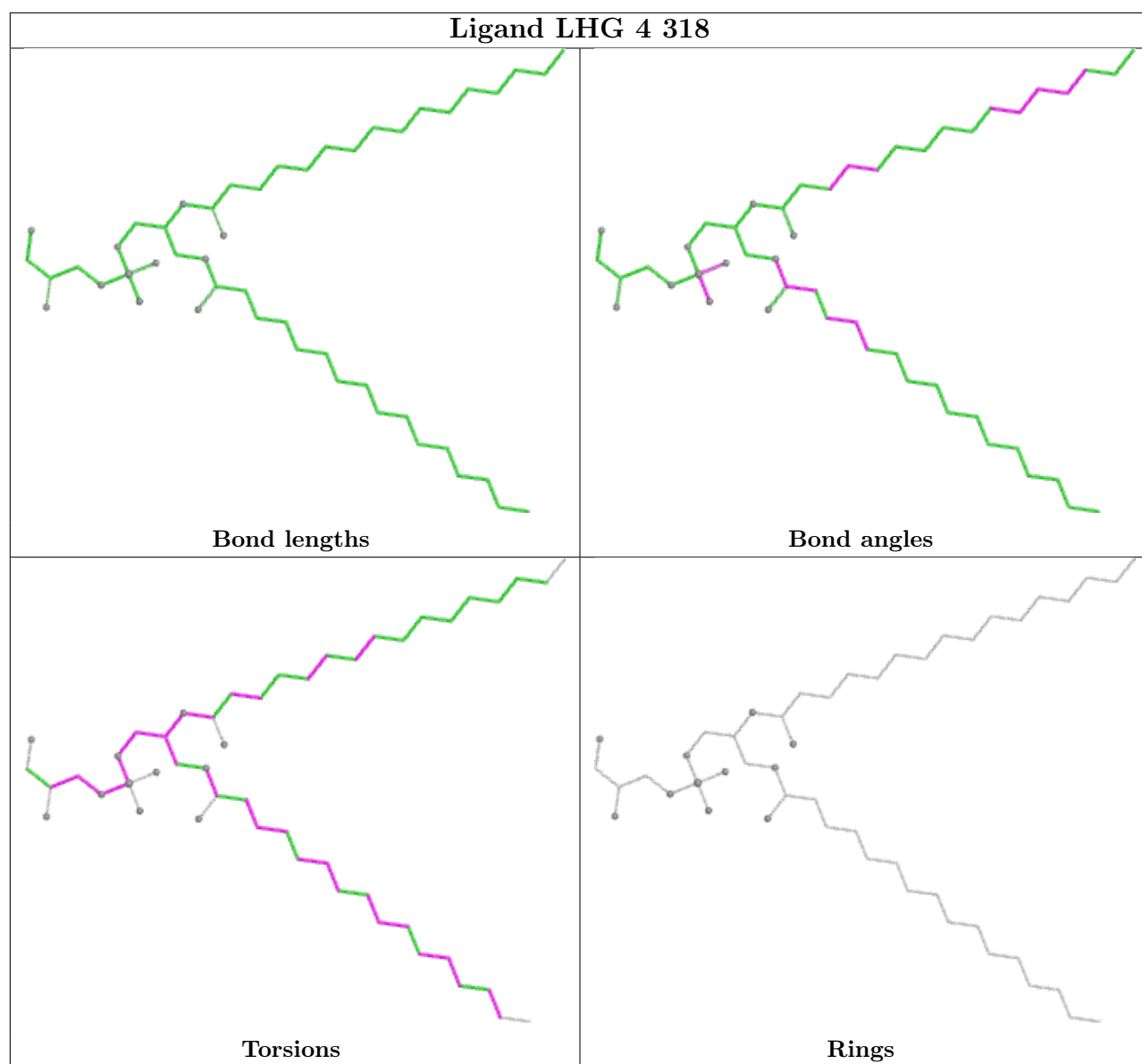


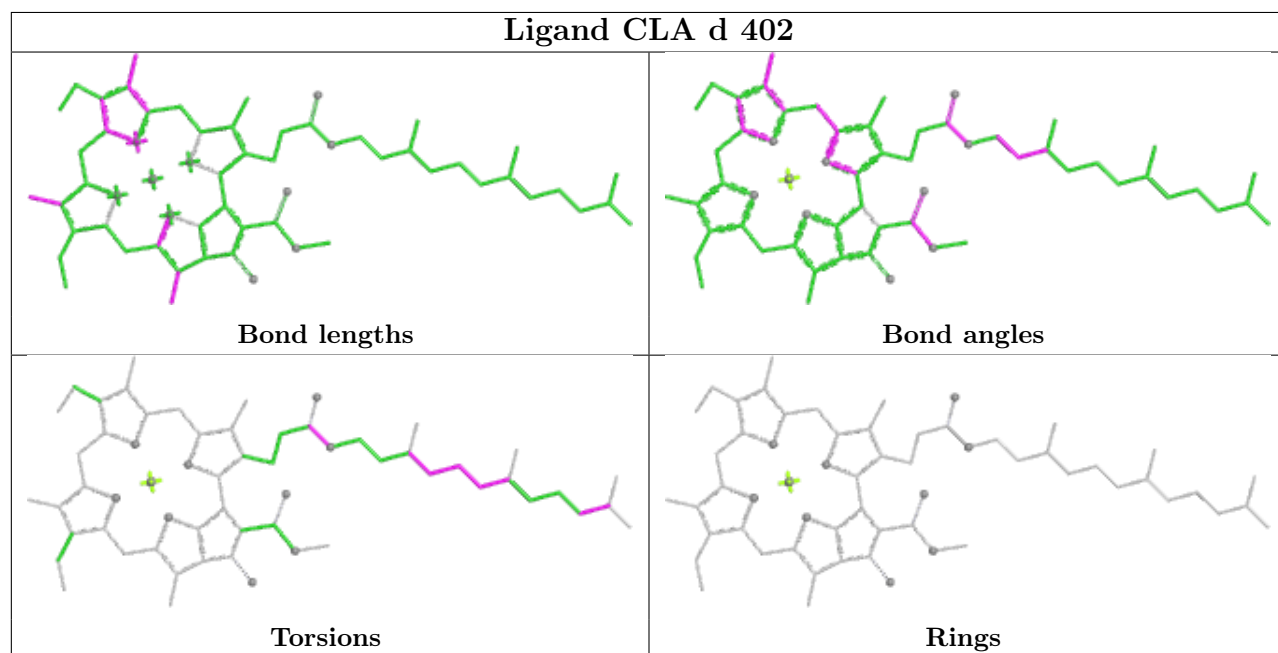
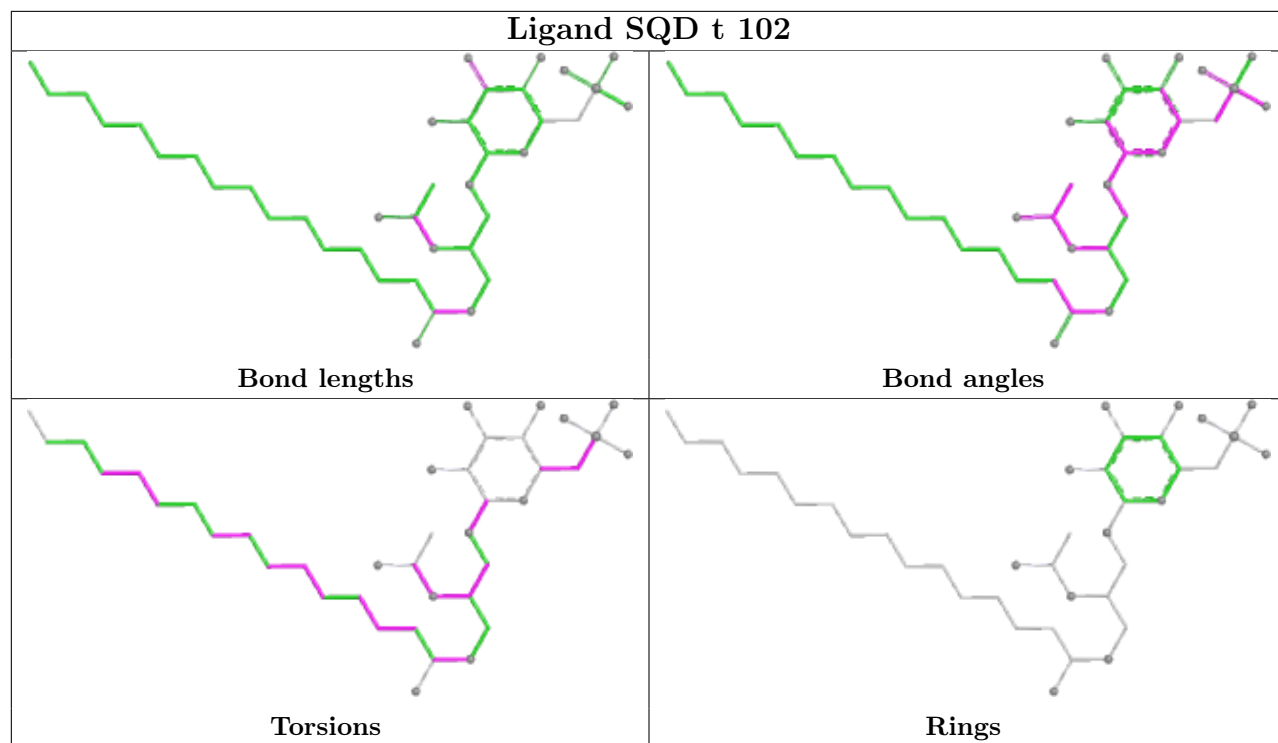
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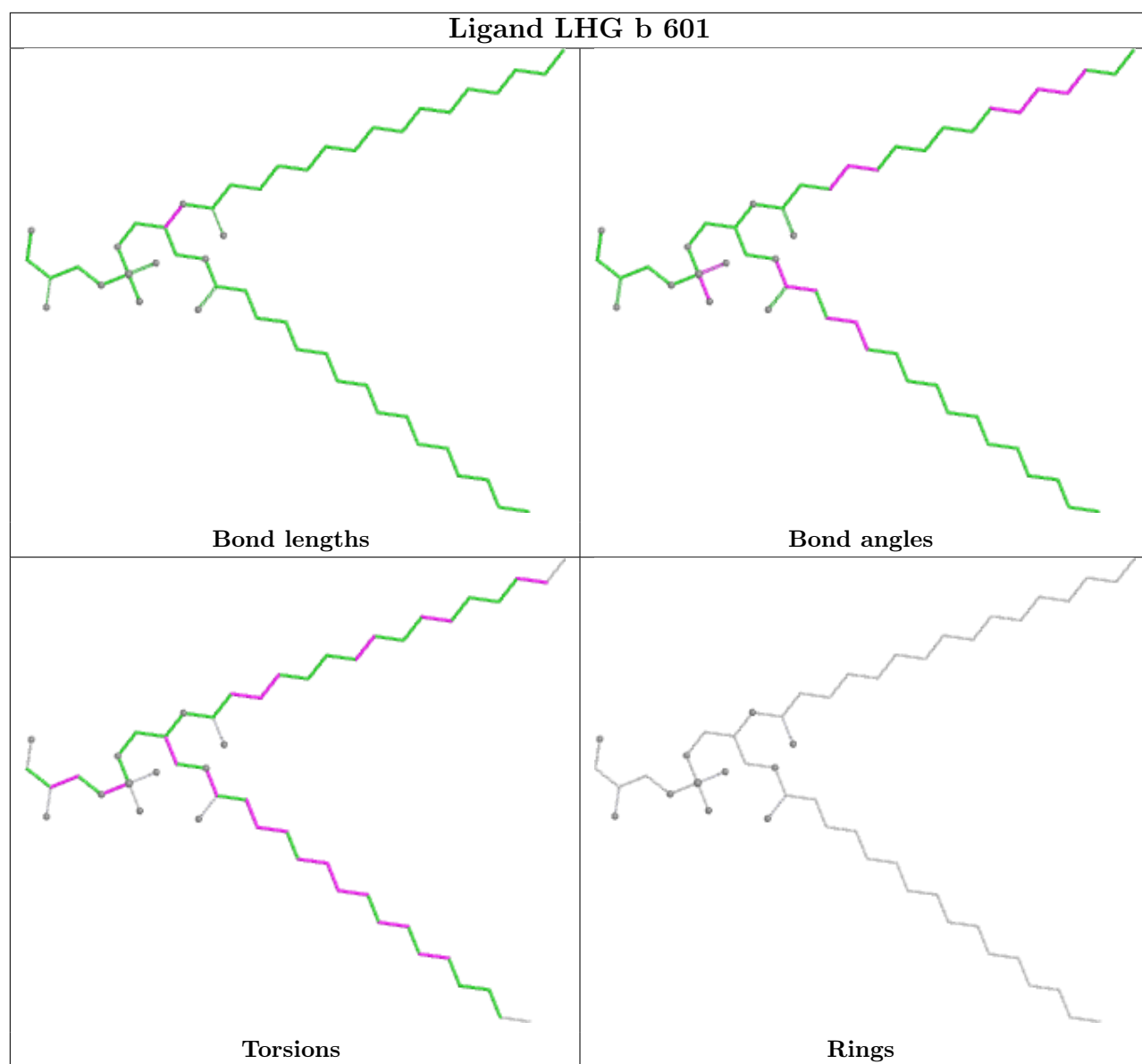


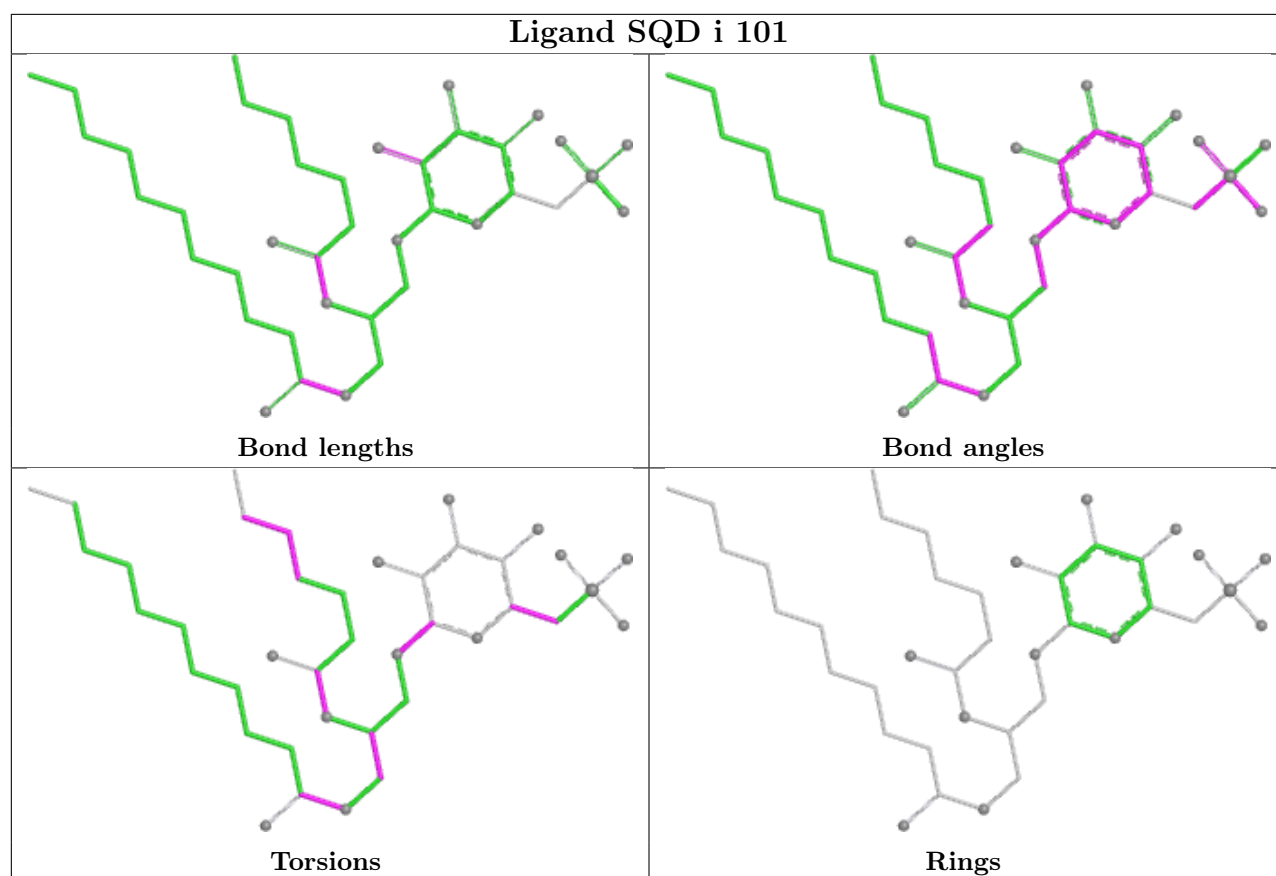
Rings



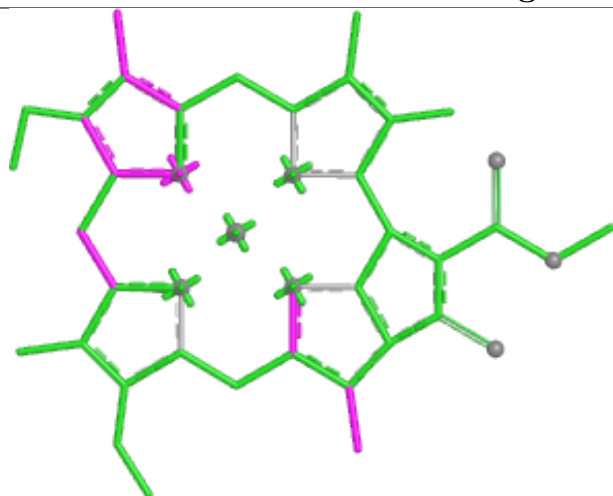




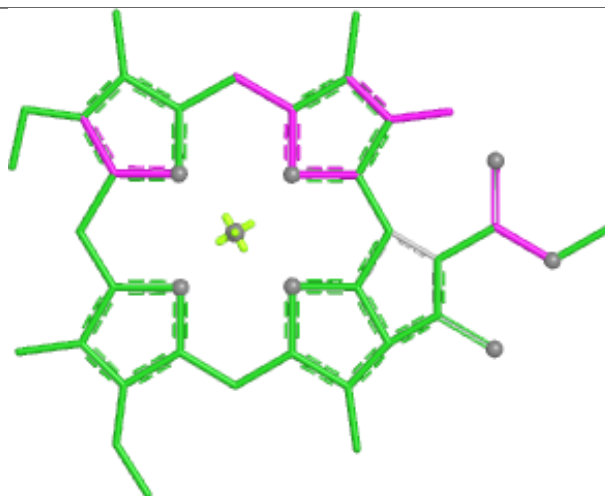




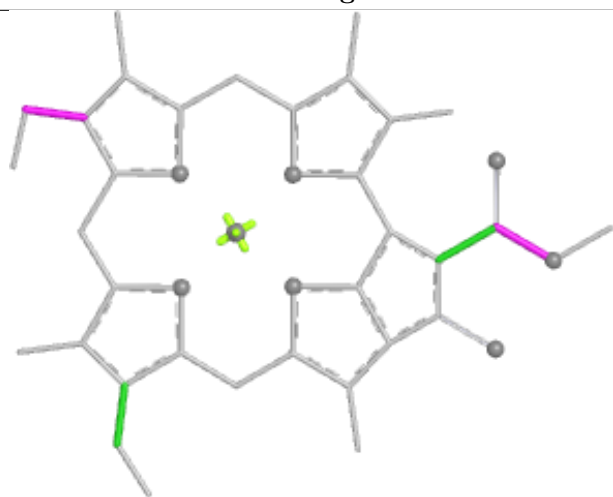
Ligand CLA 1 305



Bond lengths



Bond angles

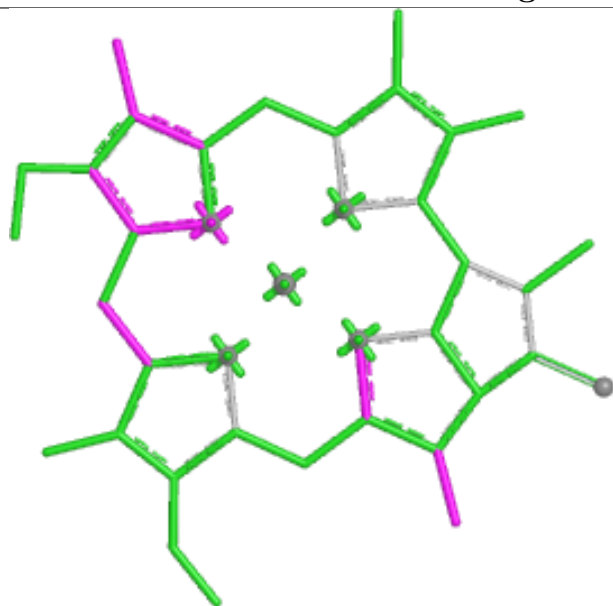


Torsions

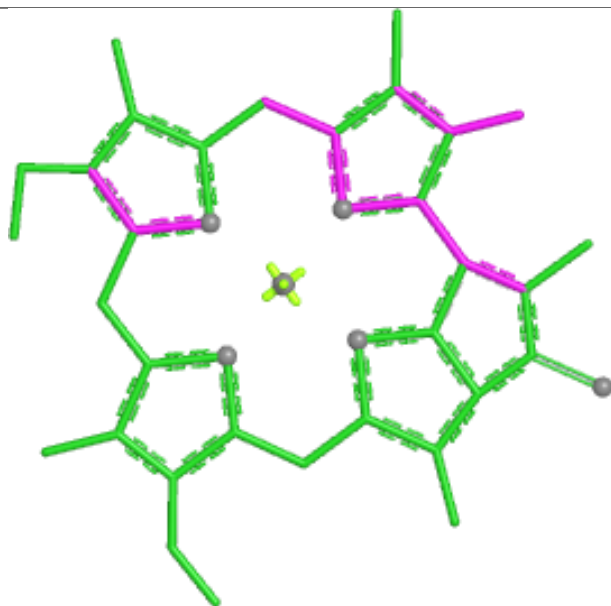


Rings

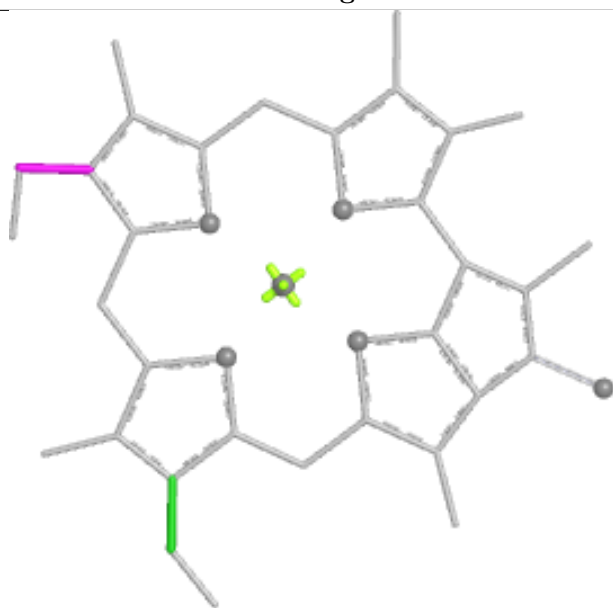
Ligand CLA 9 316



Bond lengths



Bond angles

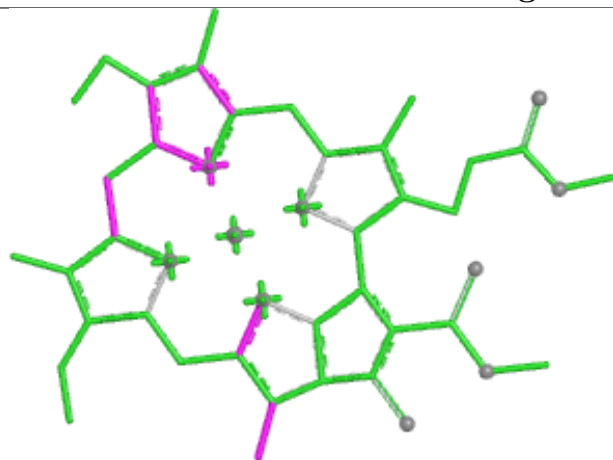


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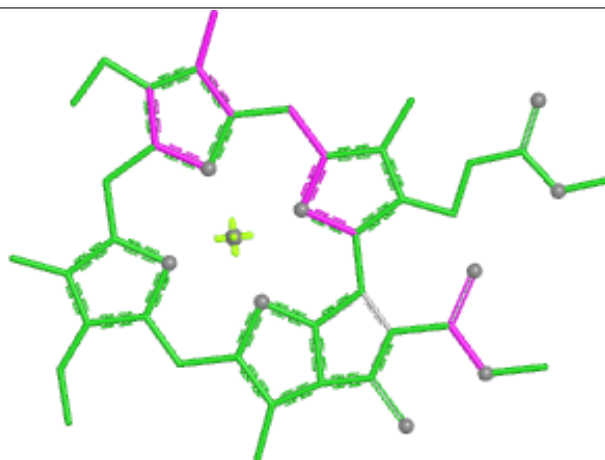


Rings

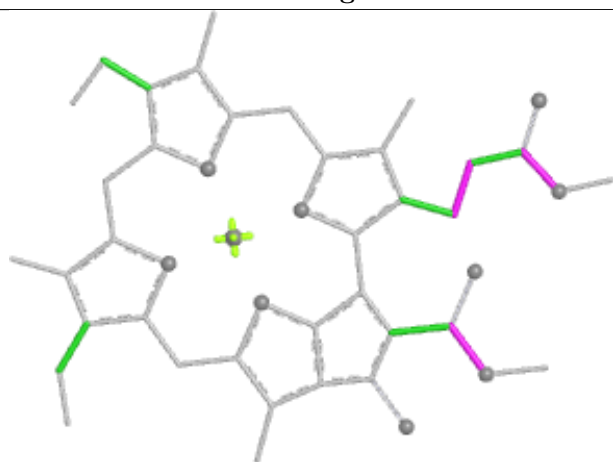
Ligand CLA 6 313



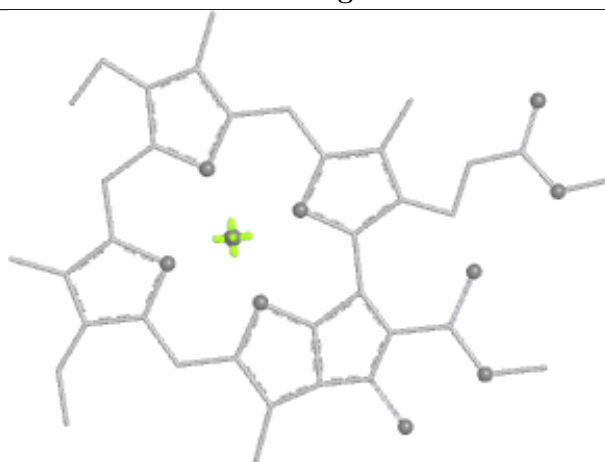
Bond lengths



Bond angles

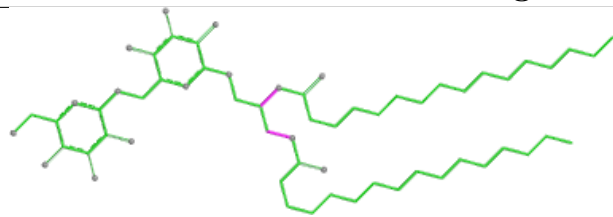


Torsions

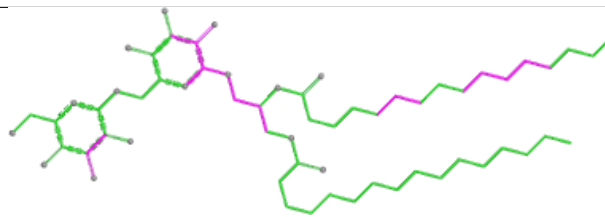


Rings

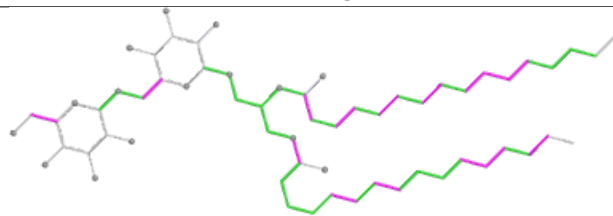
Ligand DGD h 102



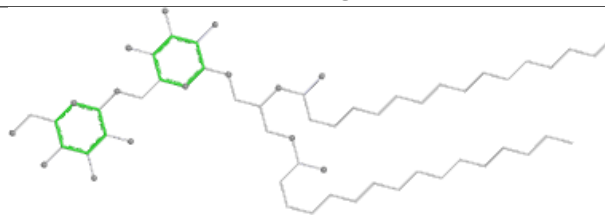
Bond lengths



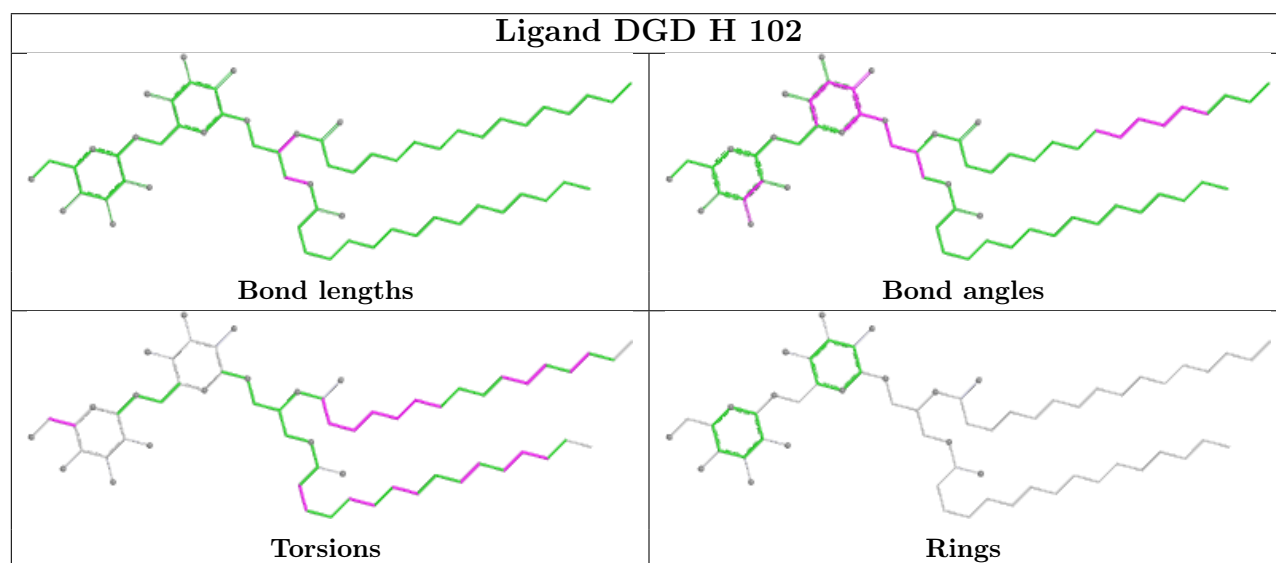
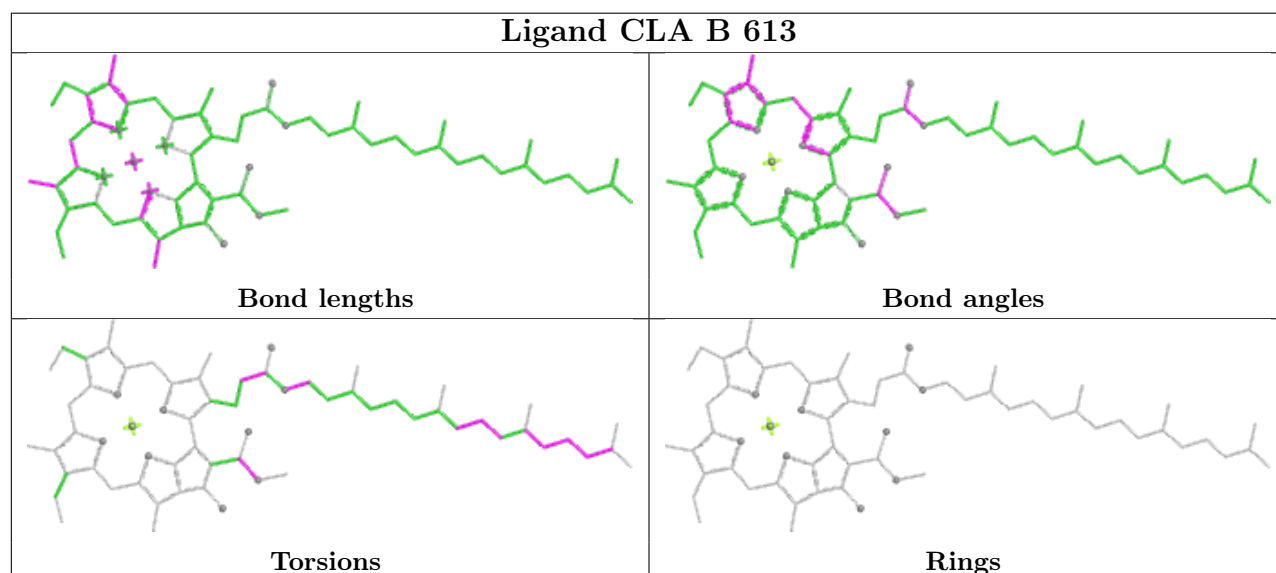
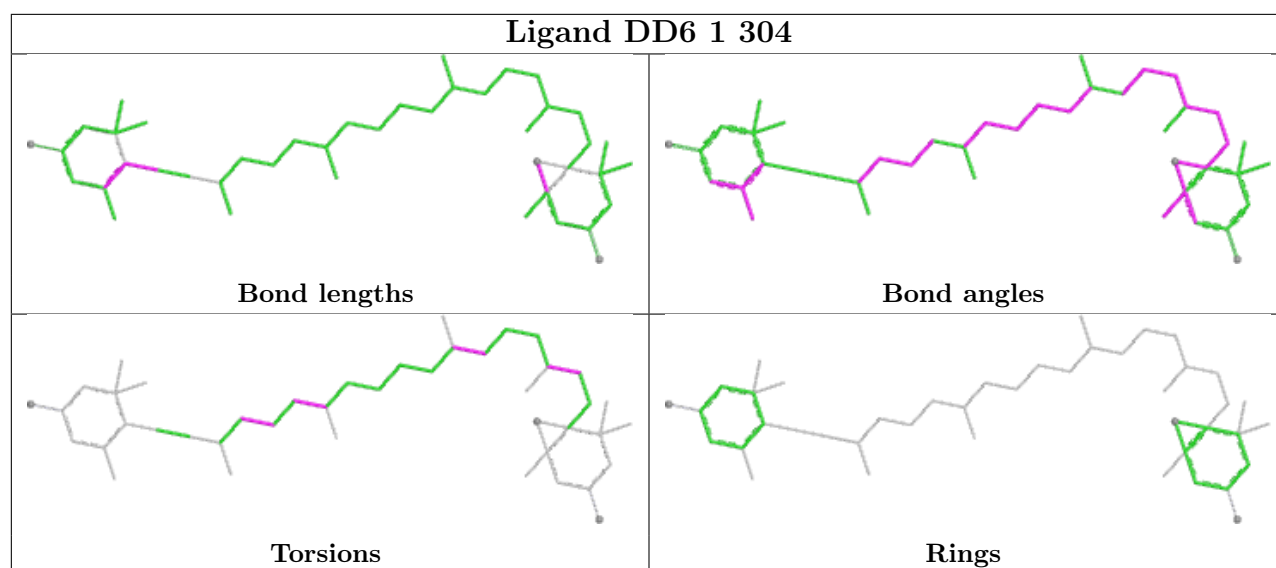
Bond angles



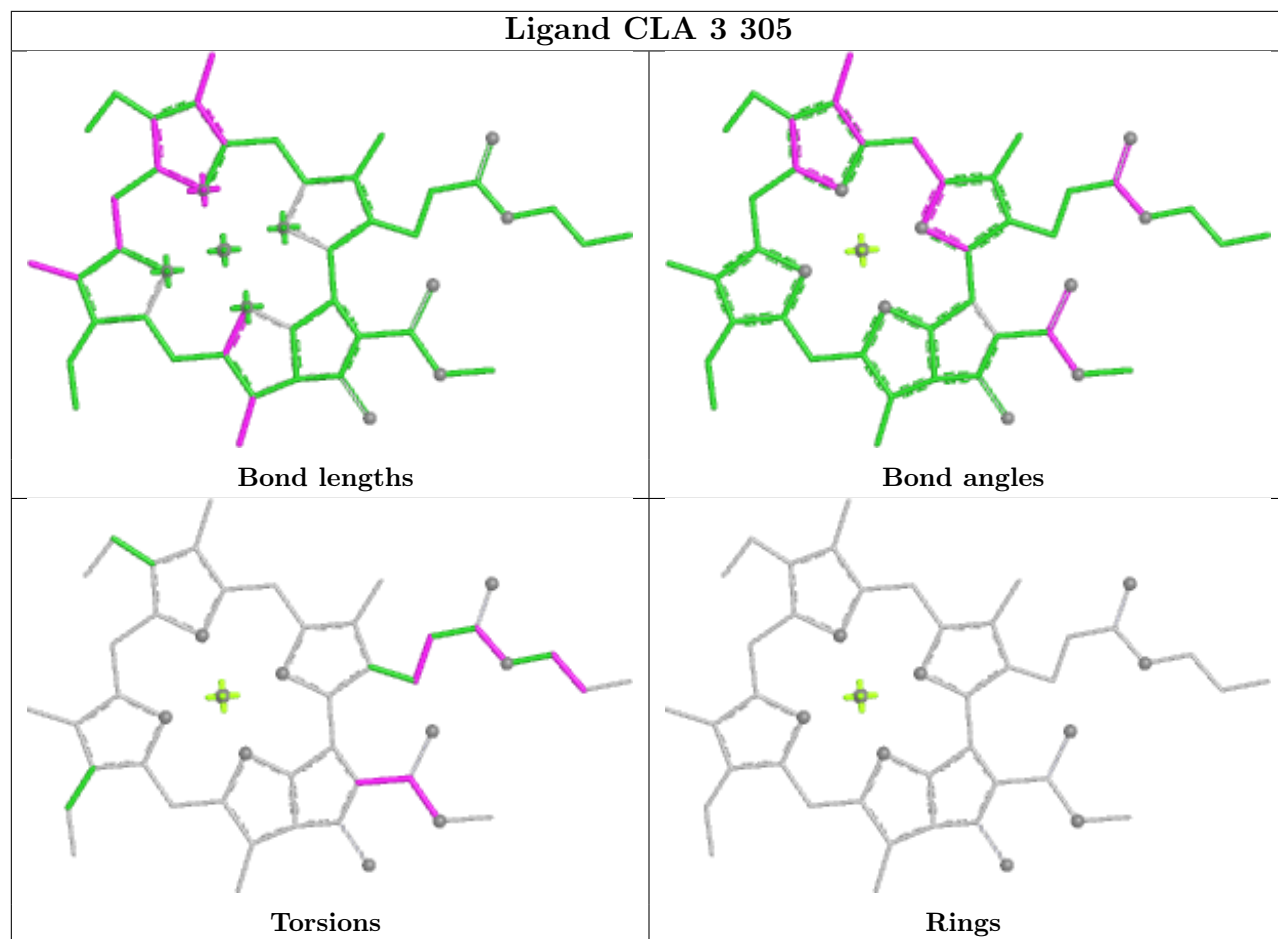
Torsions



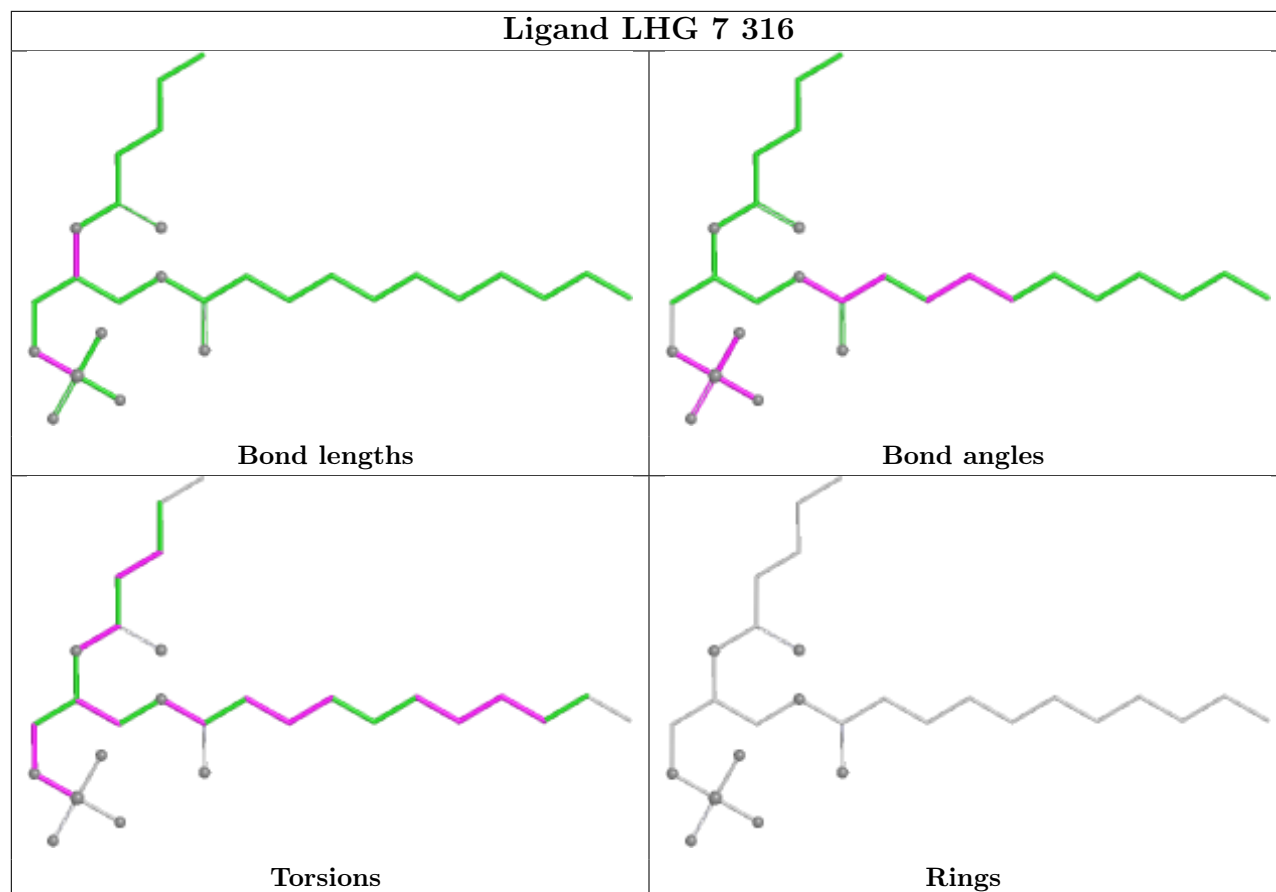
Rings



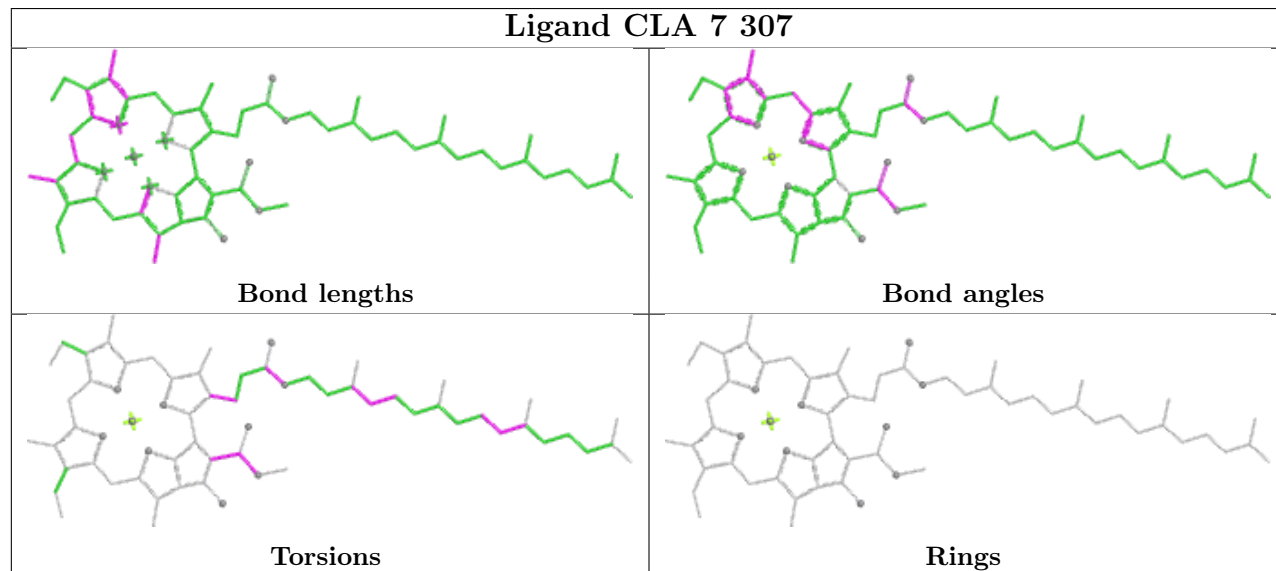
Ligand CLA 3 305

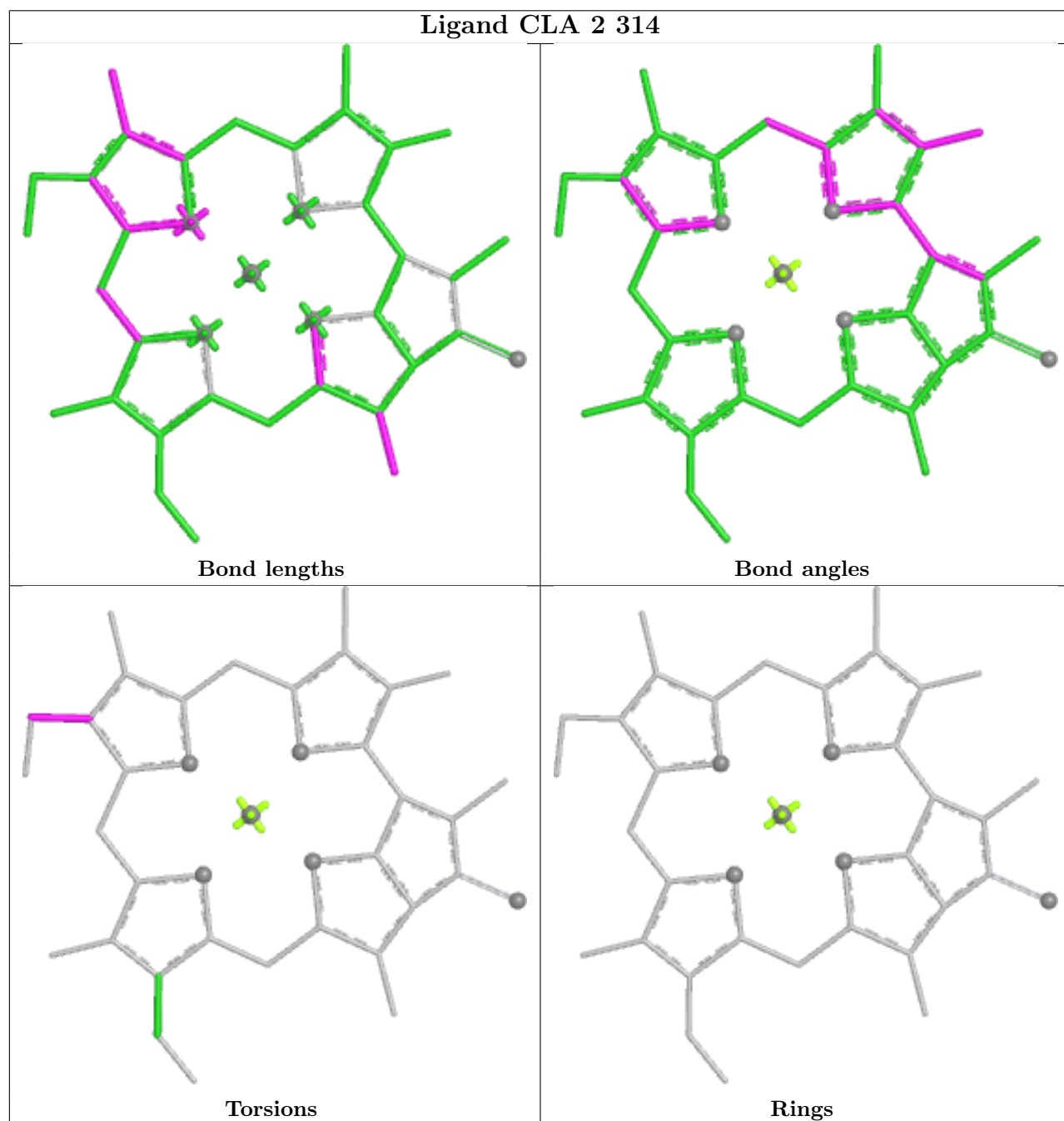
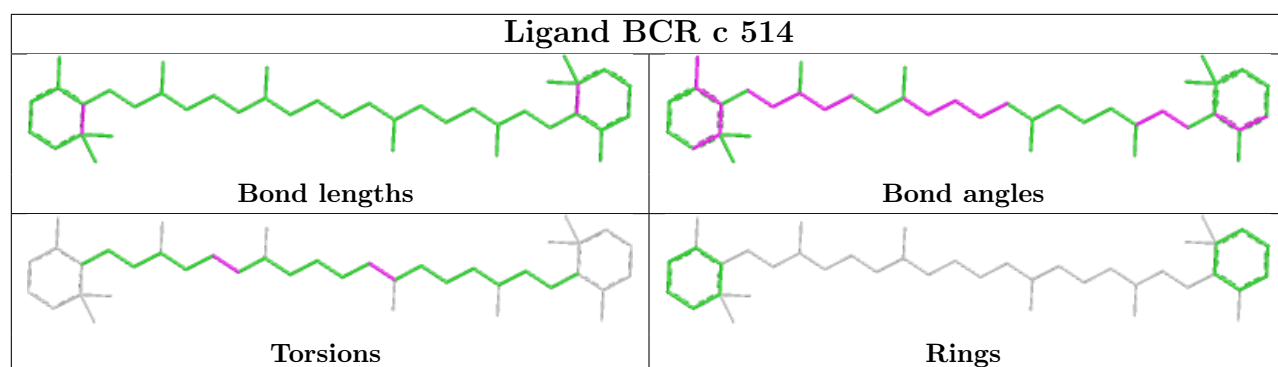


Ligand LHG 7 316

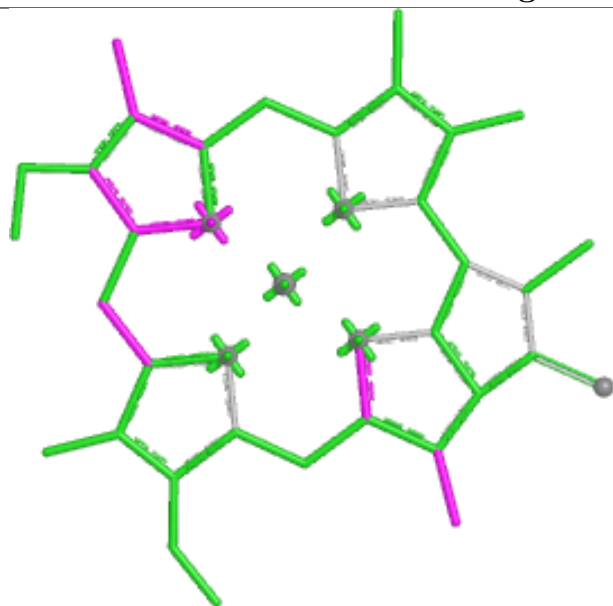


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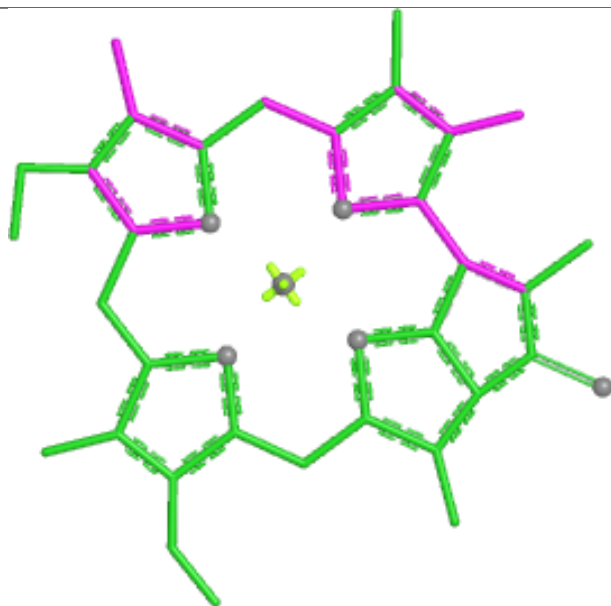




Ligand CLA 8 315



Bond lengths



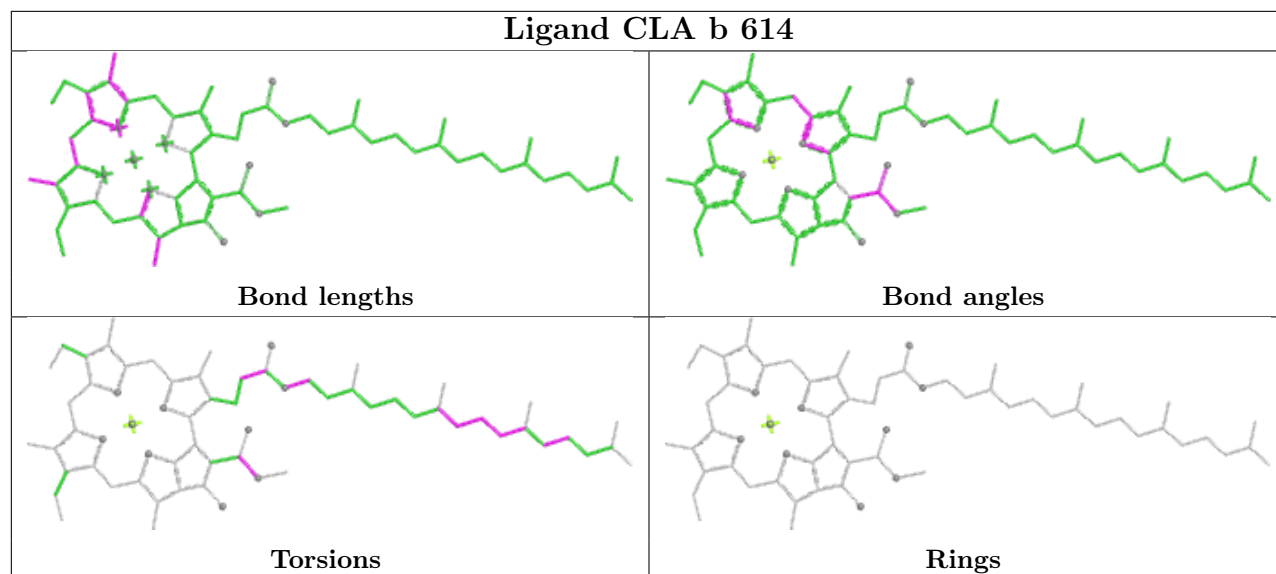
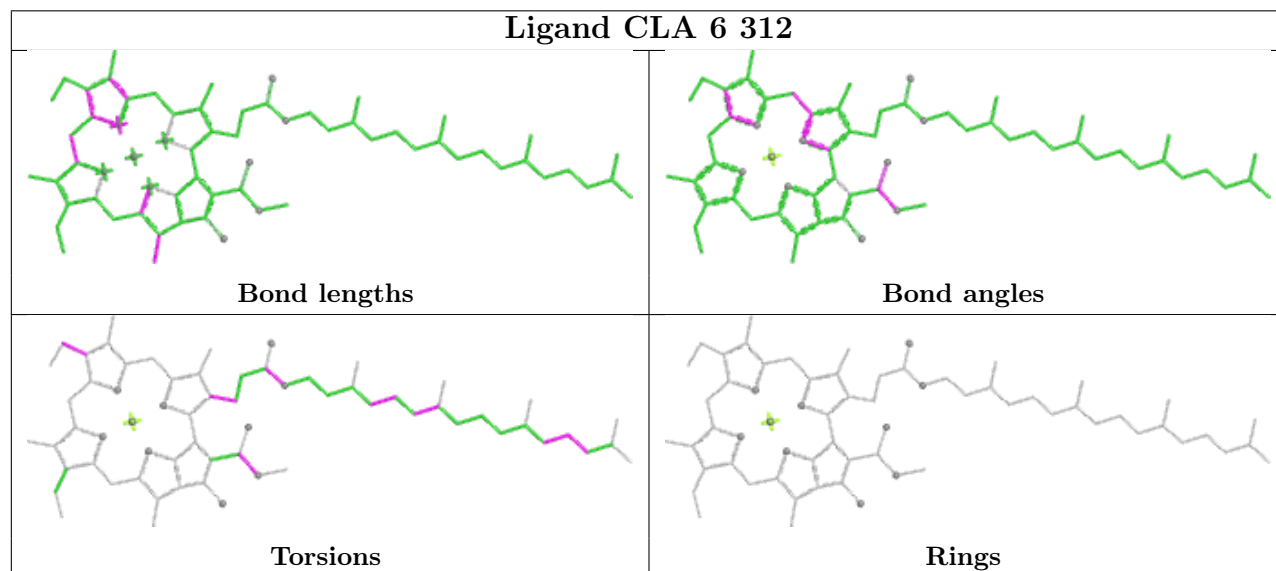
Bond angles

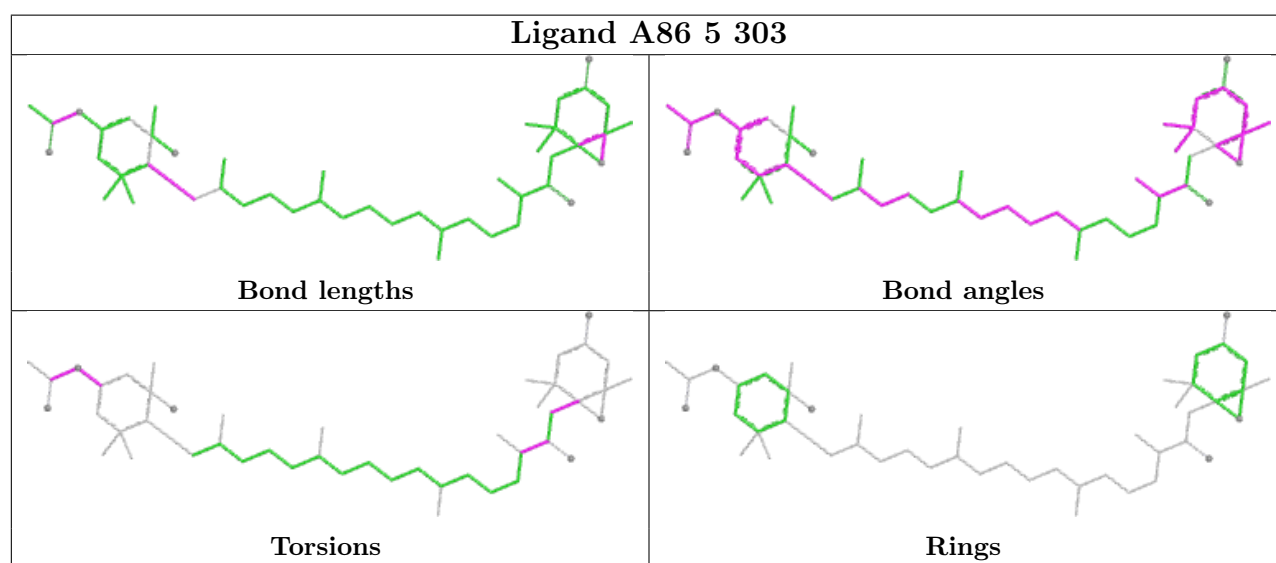
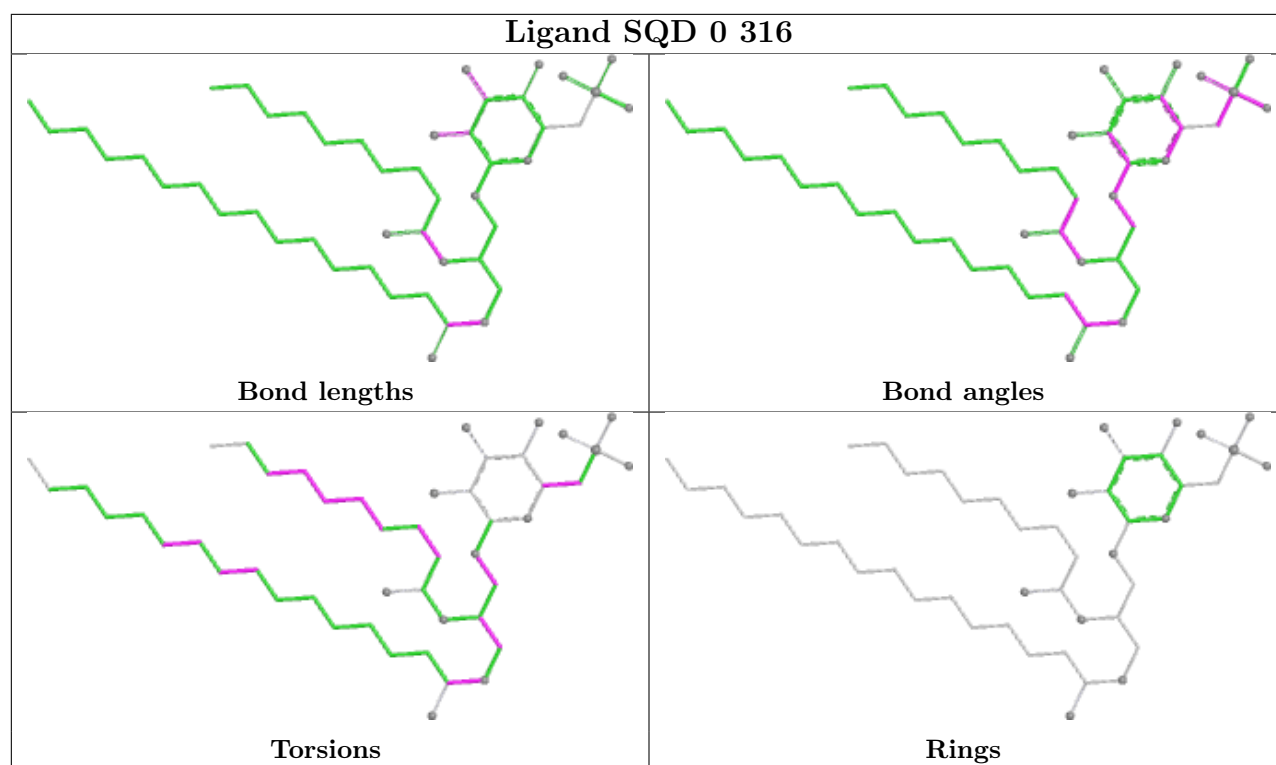


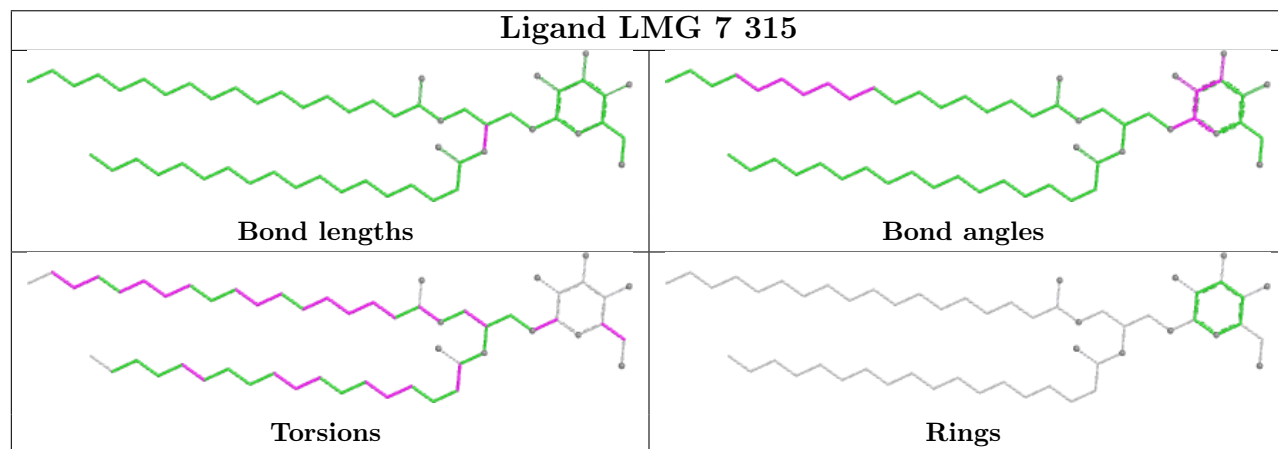
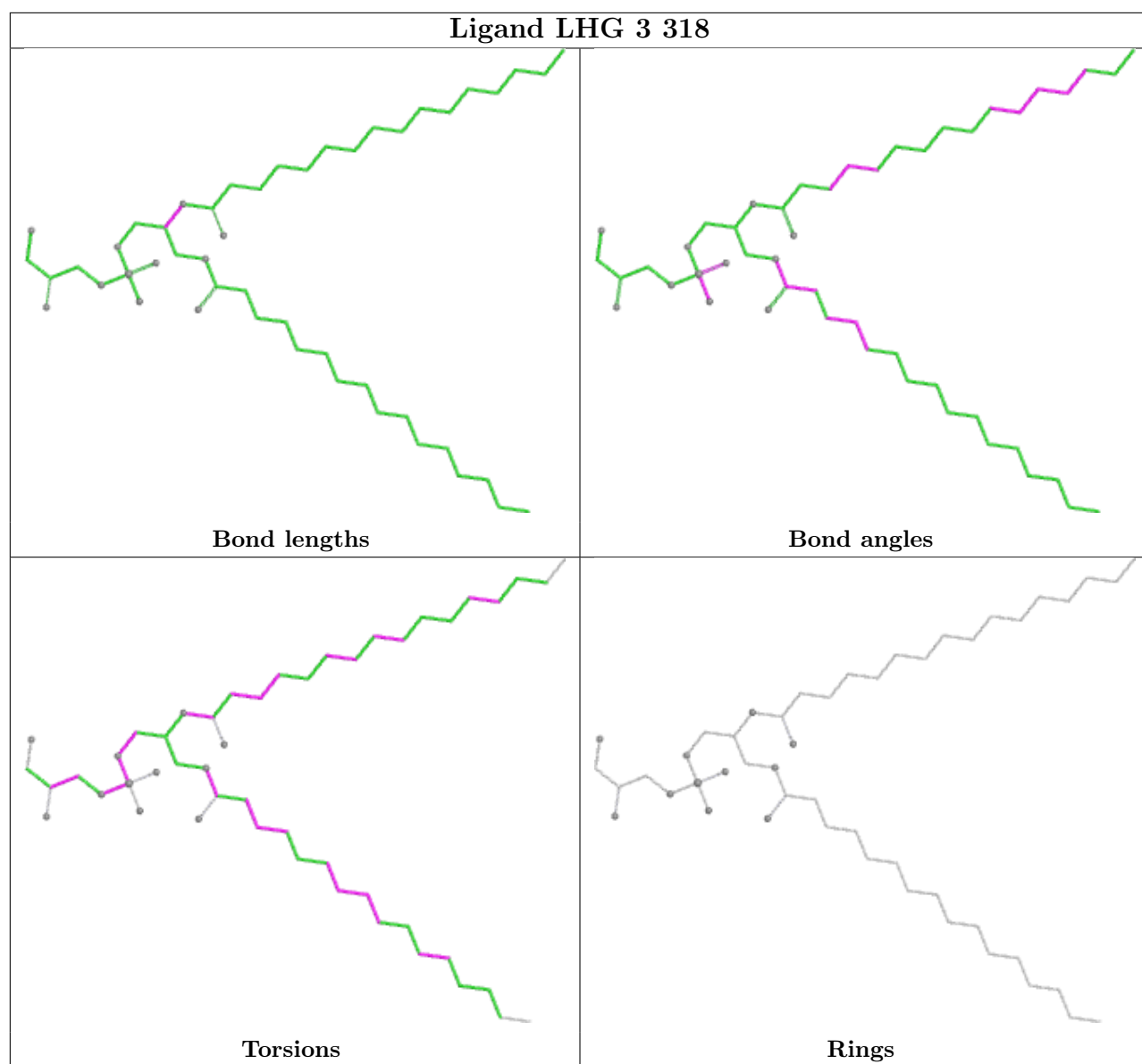
Torsions



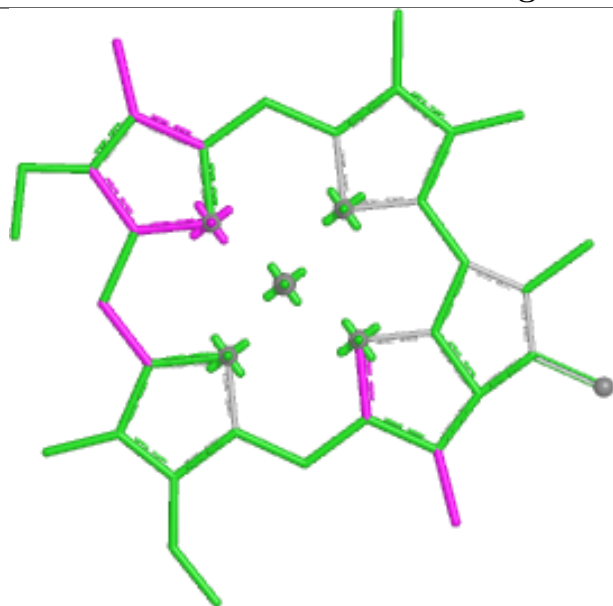
Rings

Ligand CLA b 614**Ligand CLA 6 312**

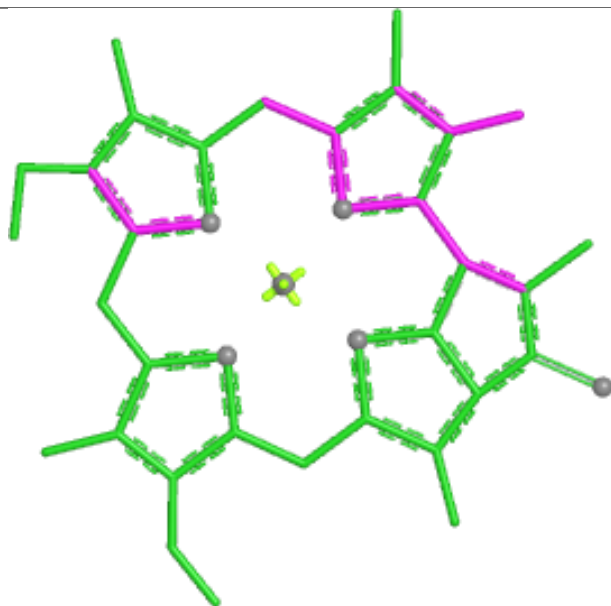




Ligand CLA 1 315



Bond lengths



Bond angles

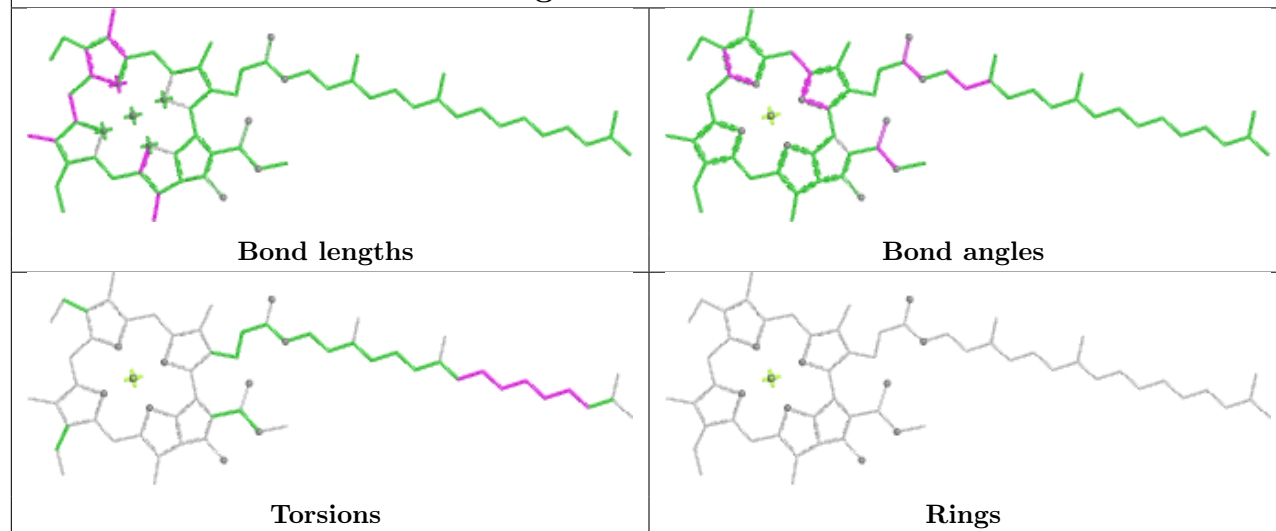


Torsions

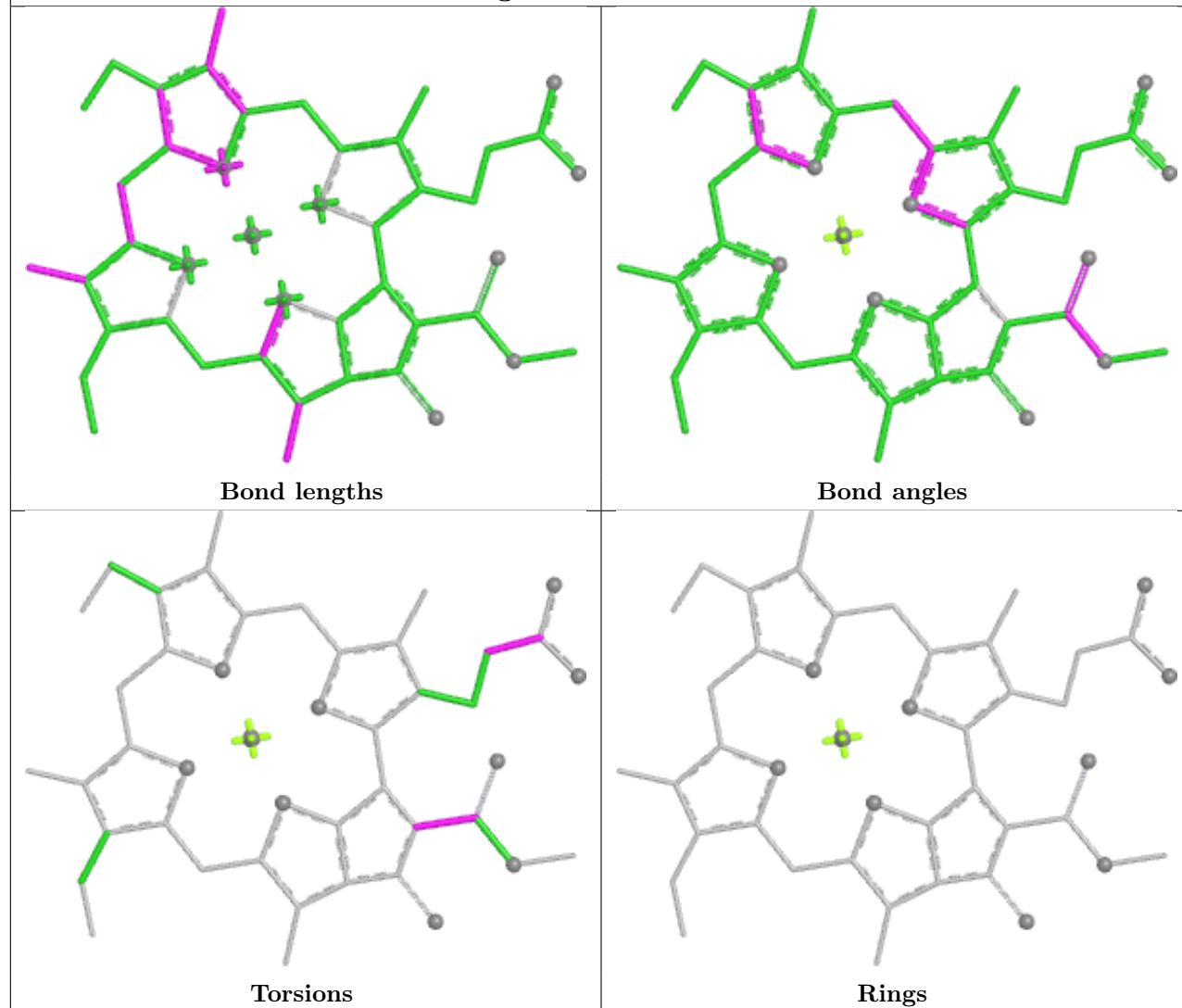


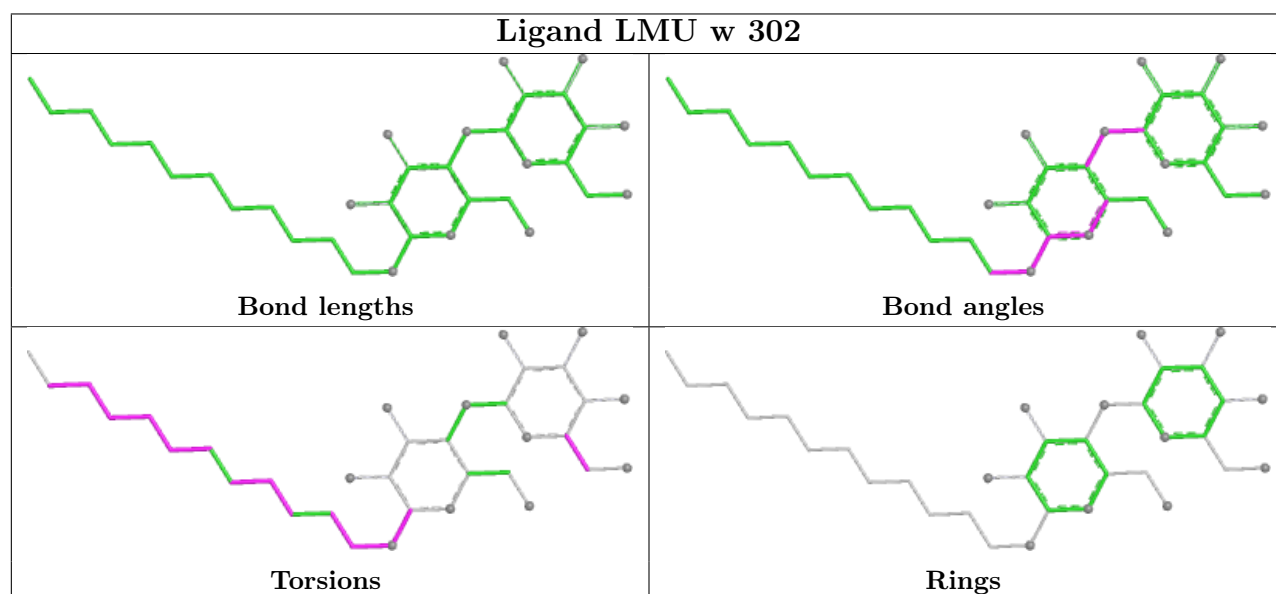
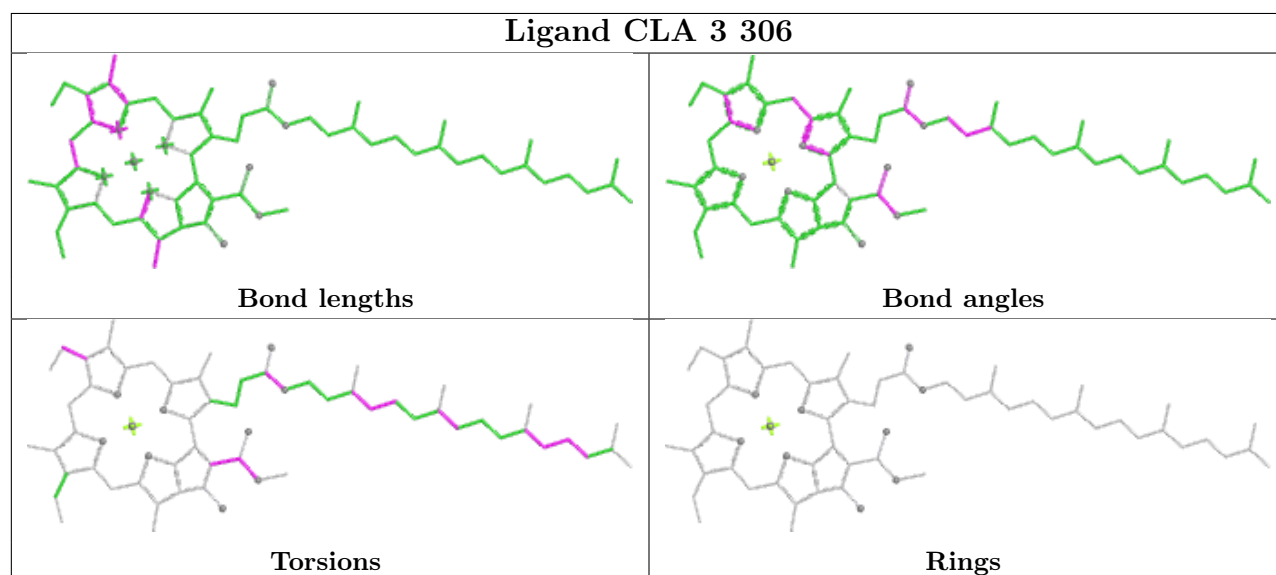
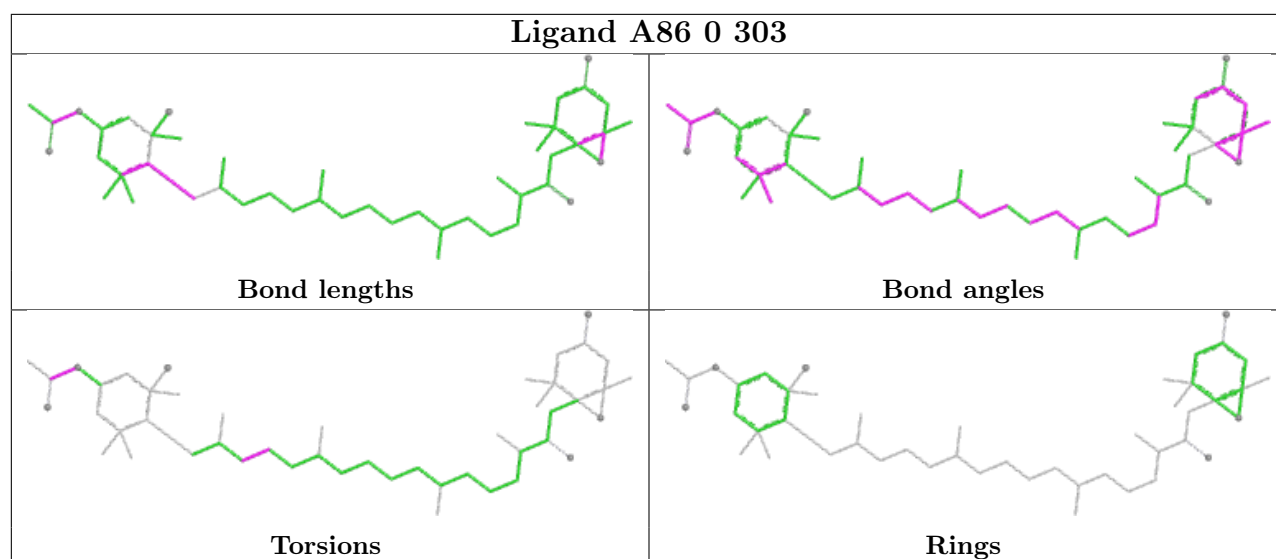
Rings

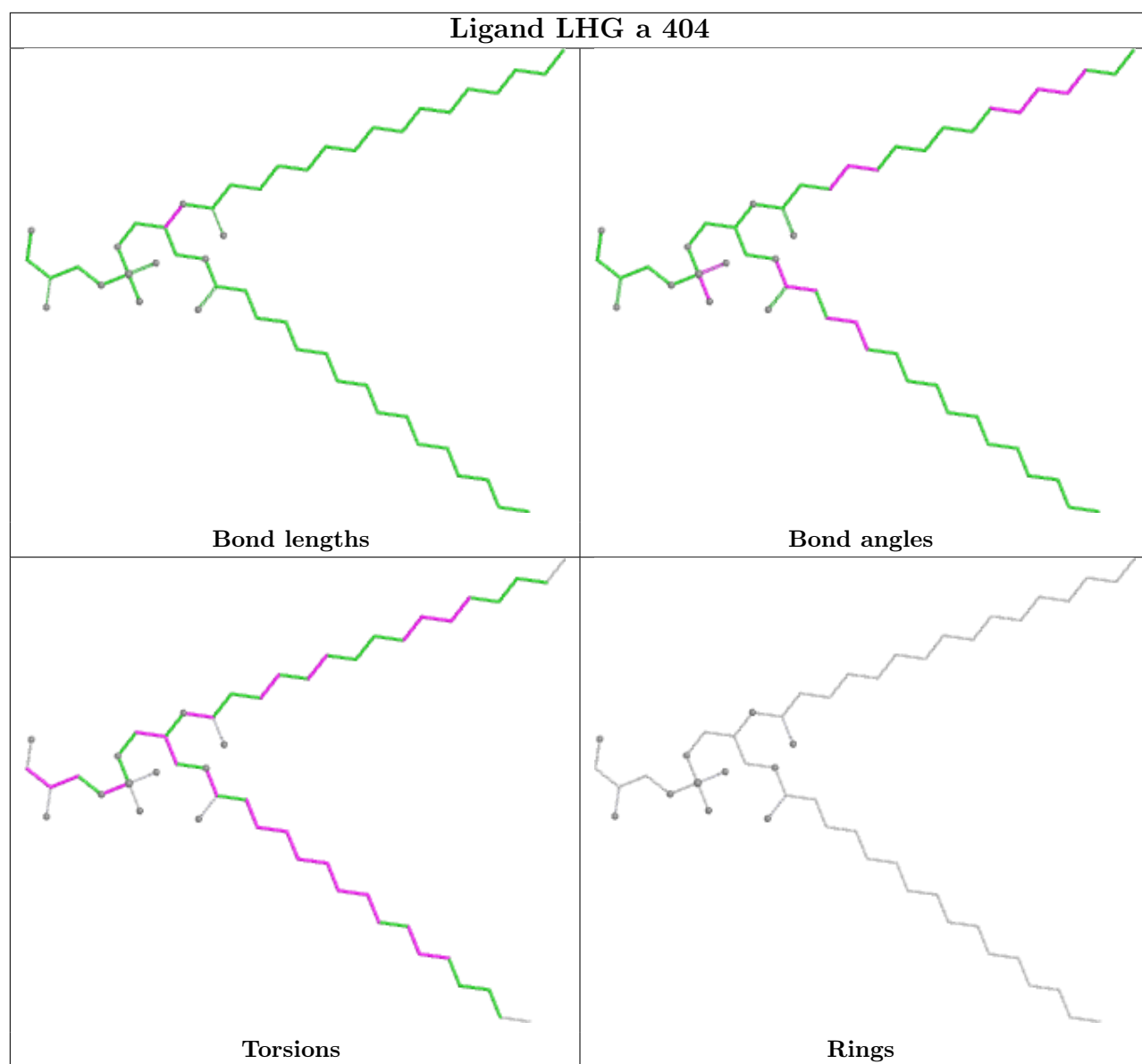
Ligand CLA b 612

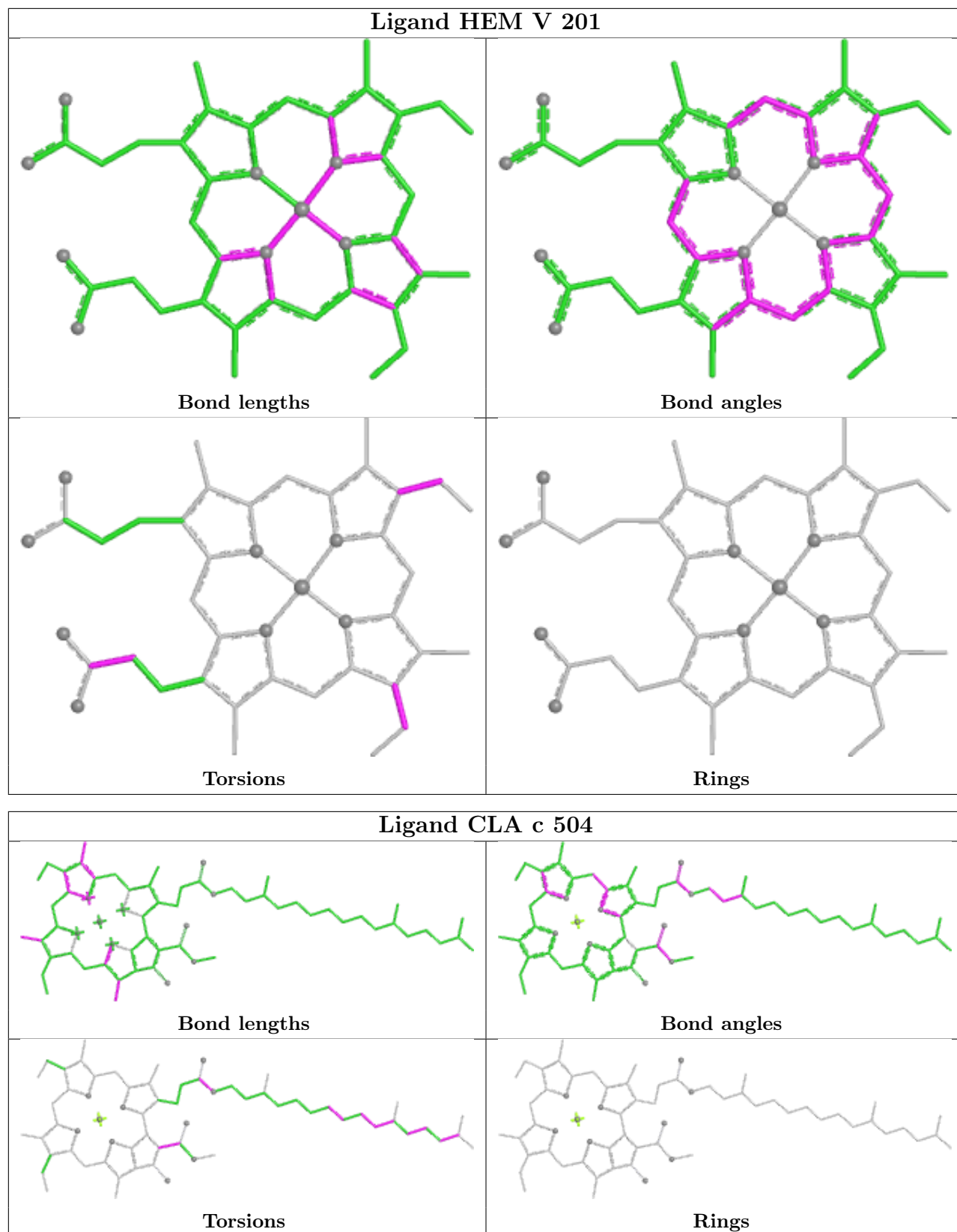


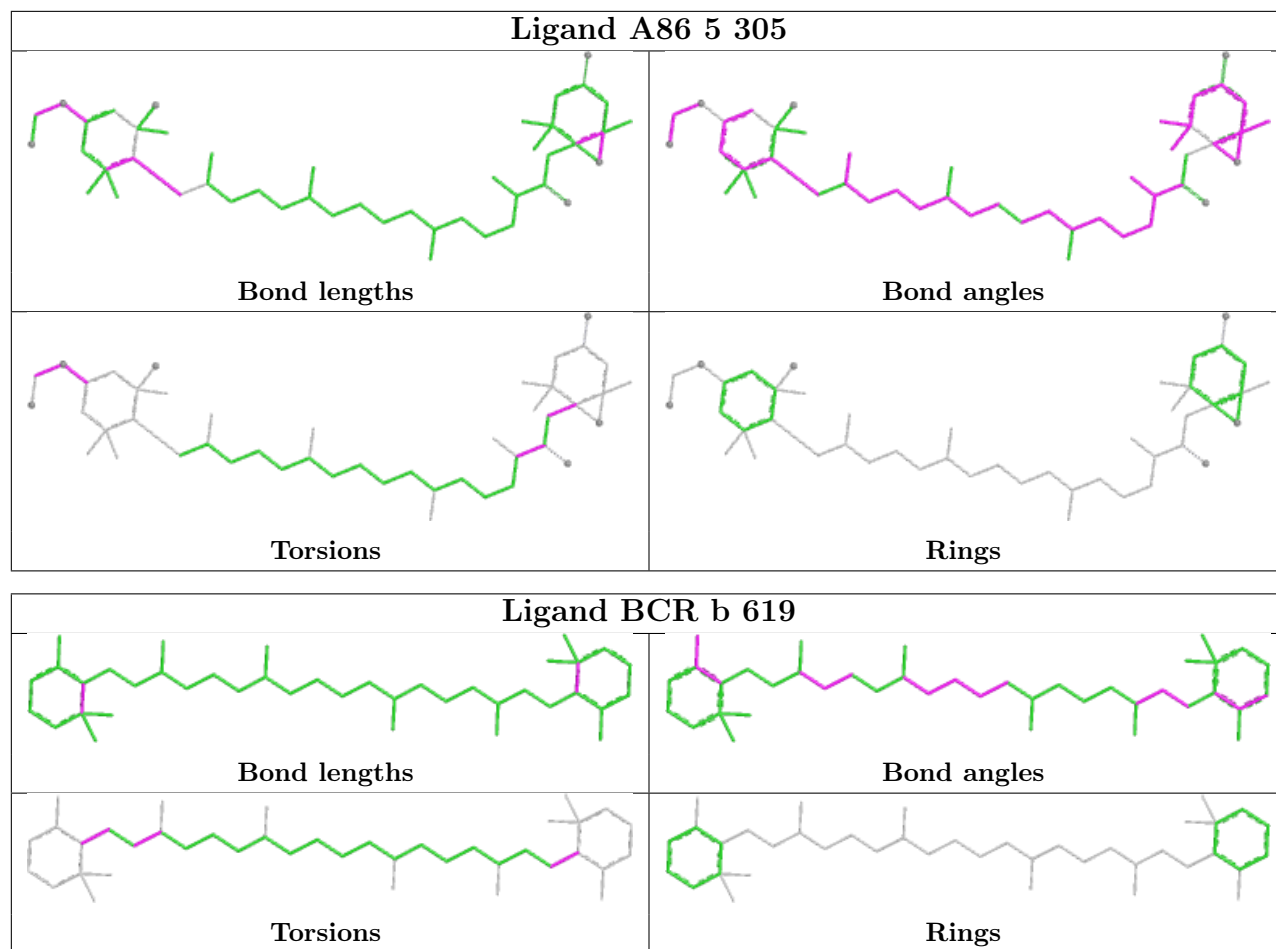
Ligand CLA 8 312



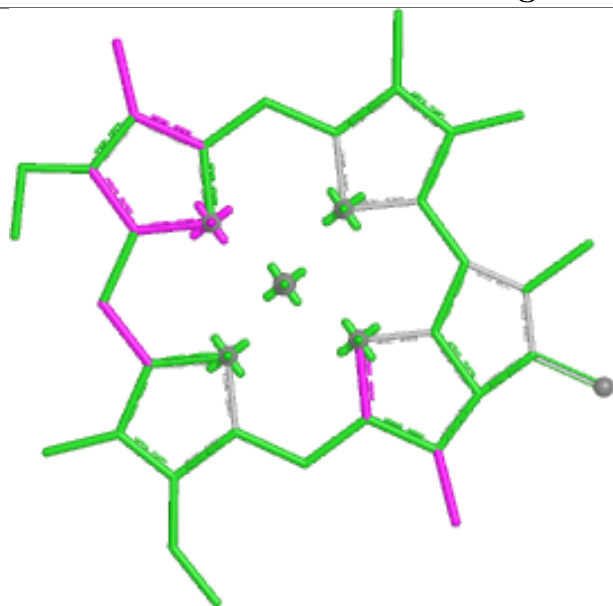




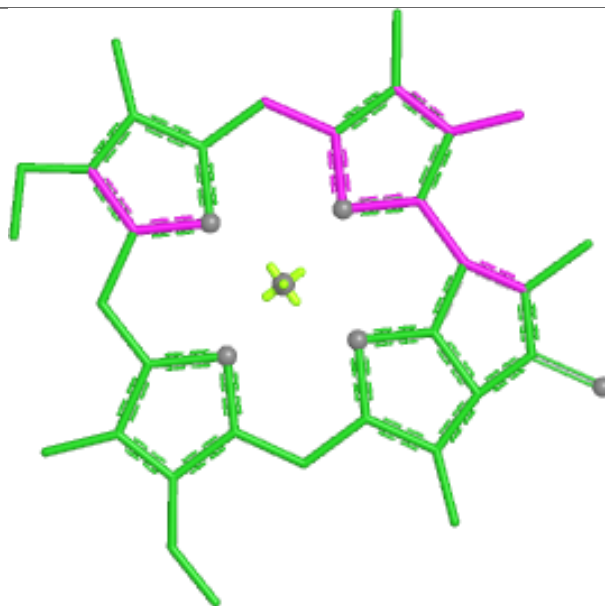




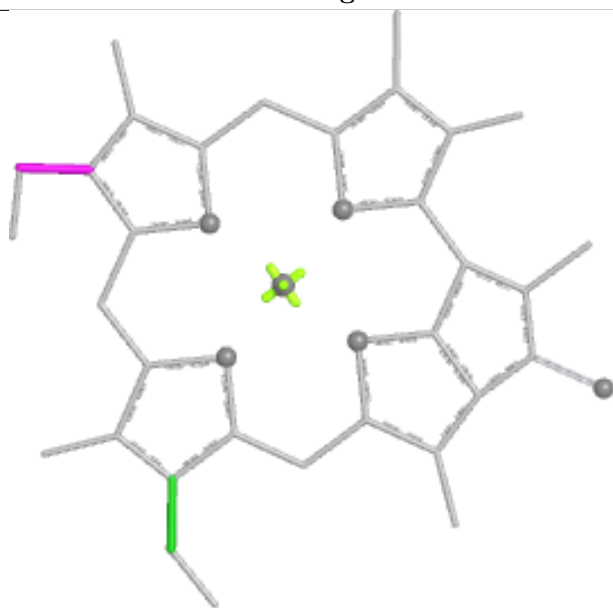
Ligand CLA 8 316



Bond lengths



Bond angles

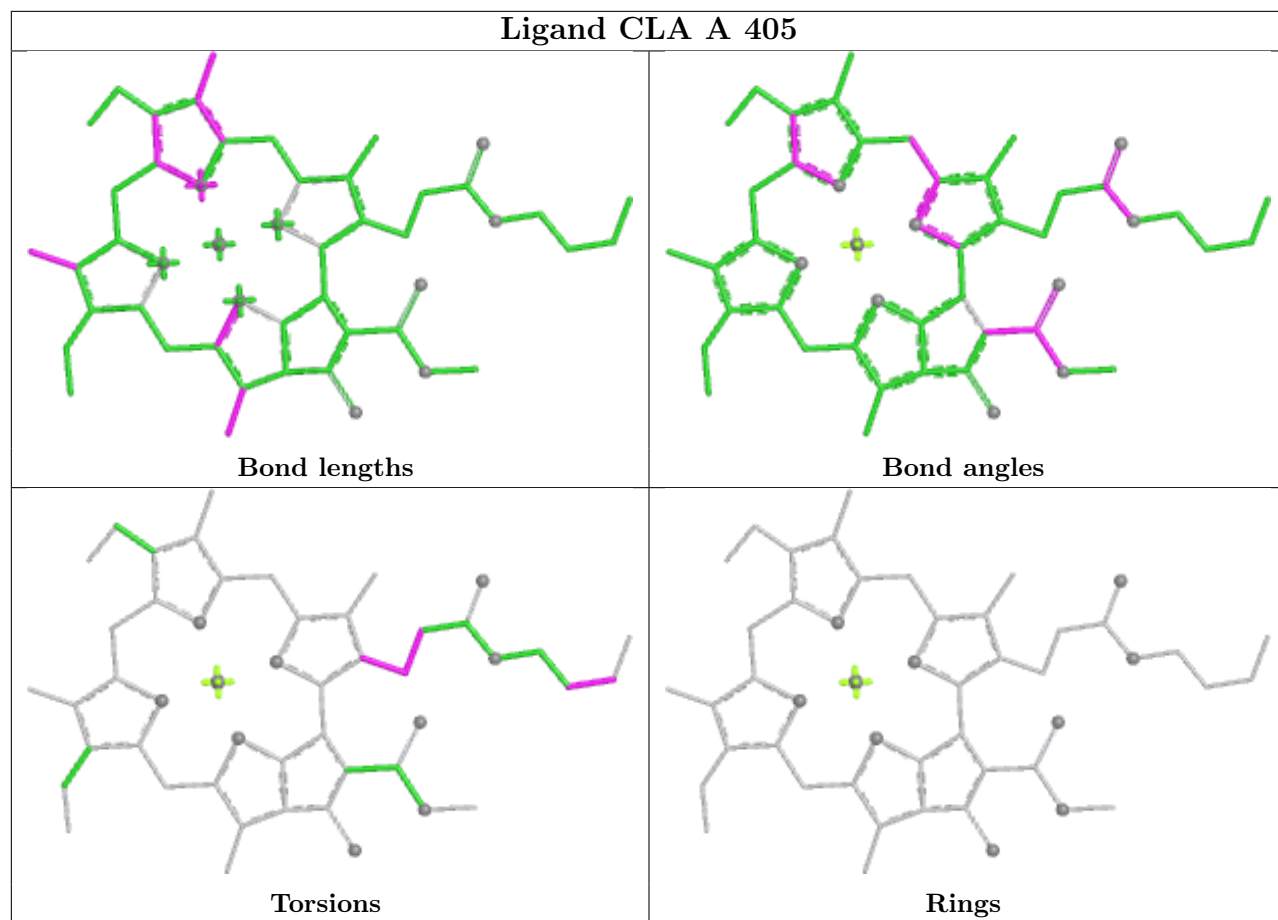


Torsions

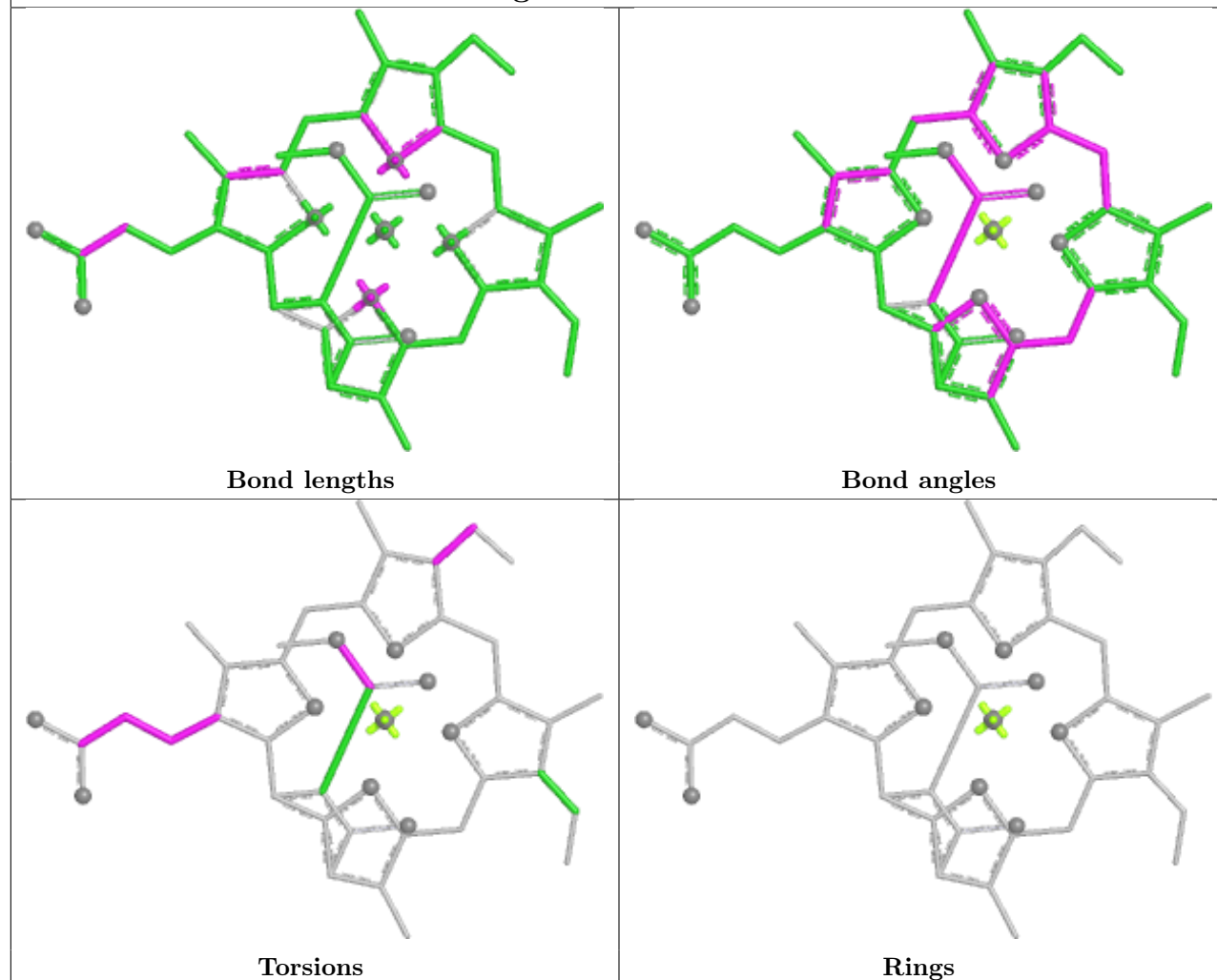


Rings

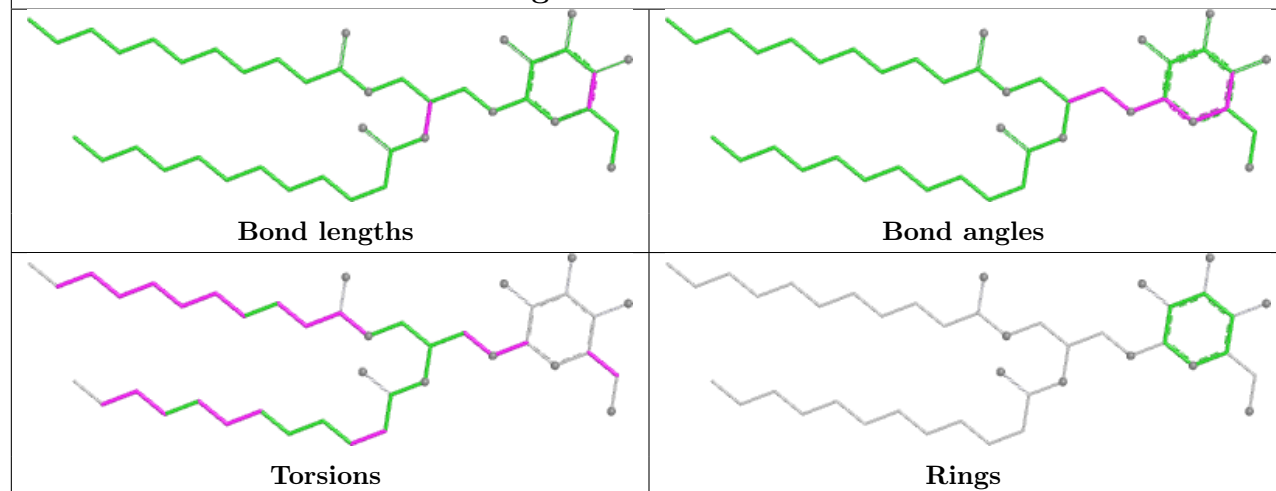
Ligand CLA A 405

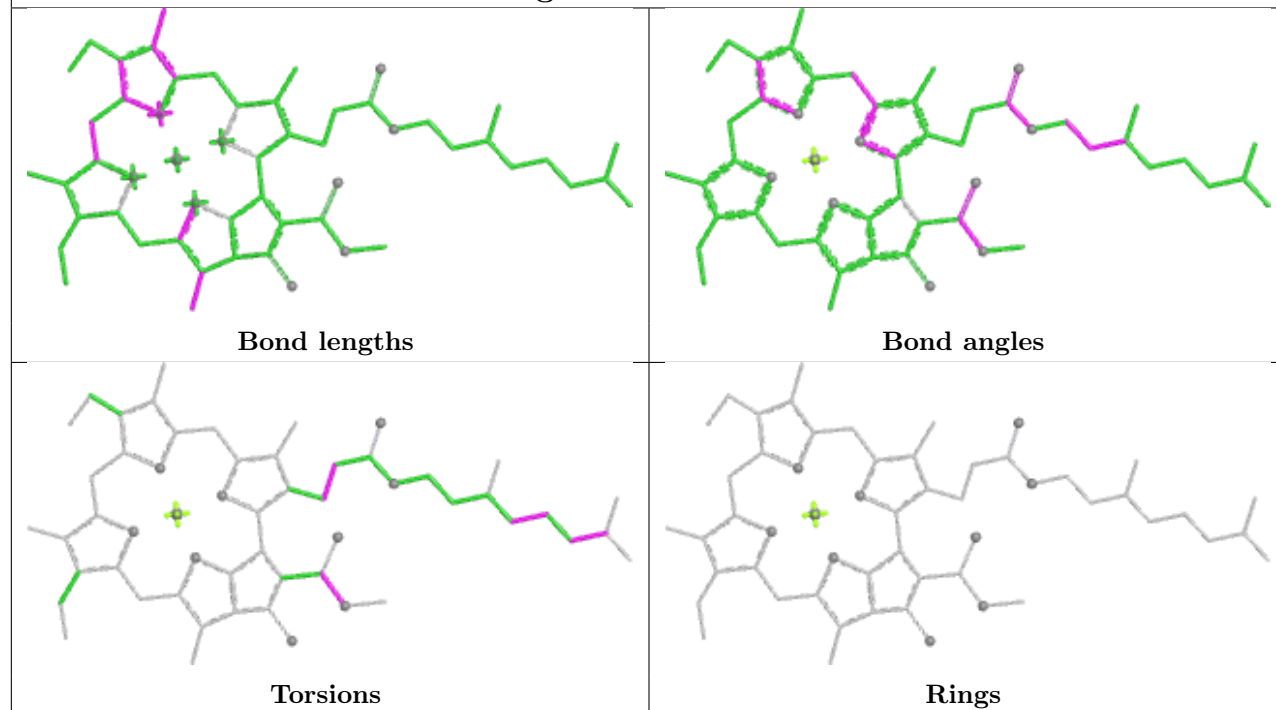
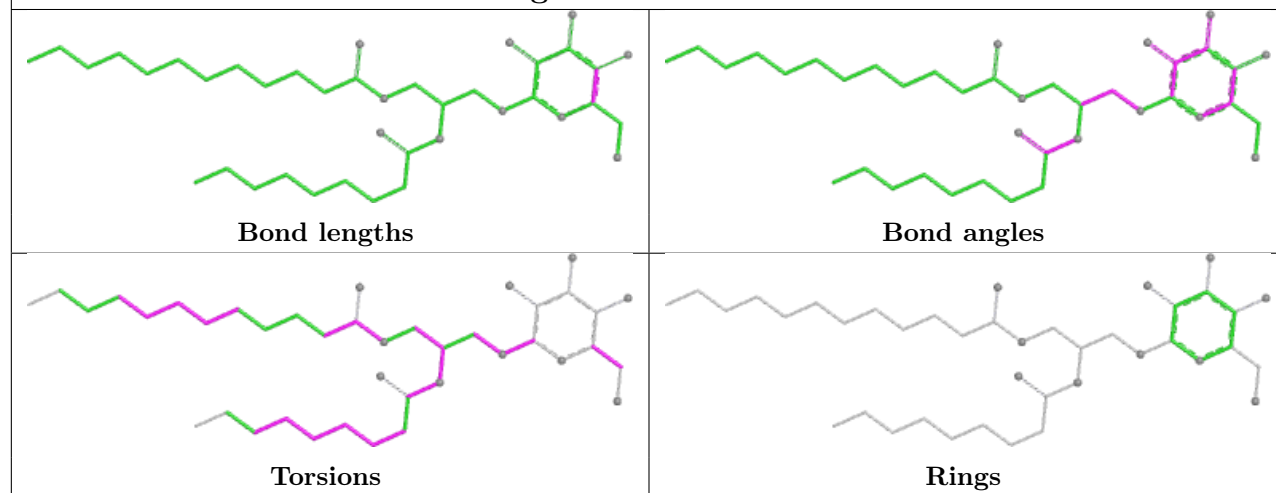


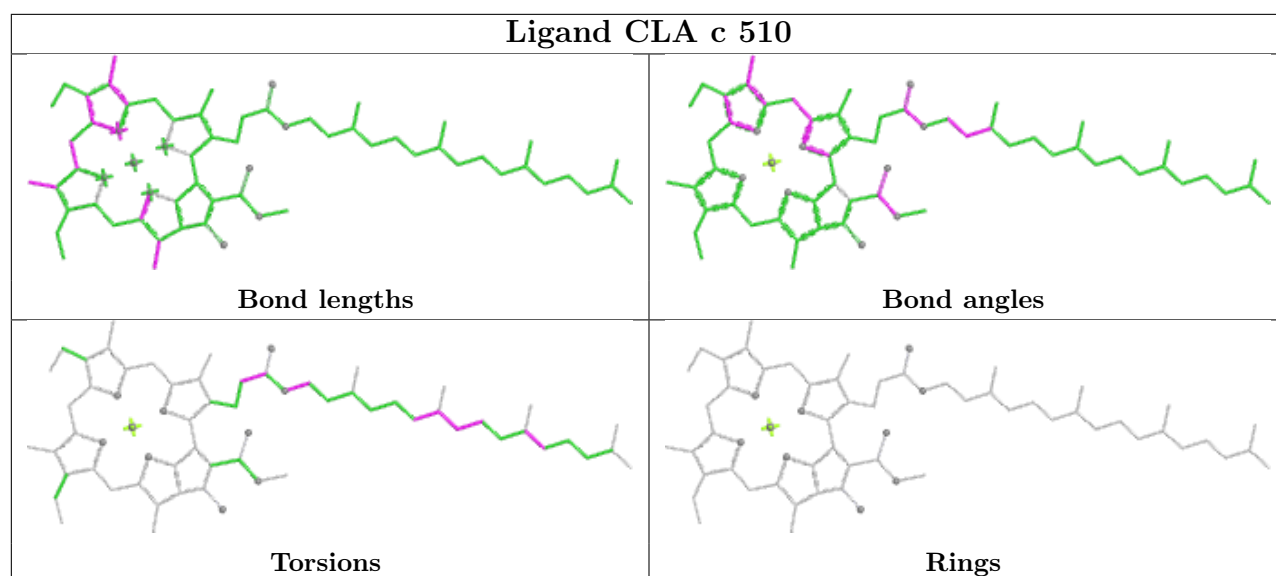
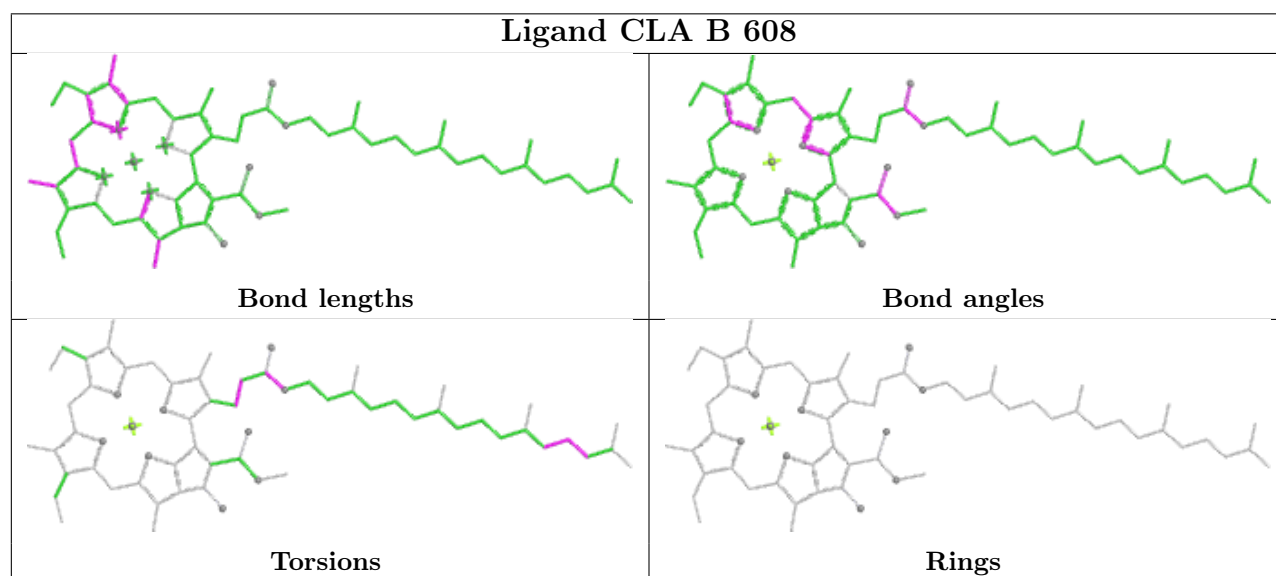
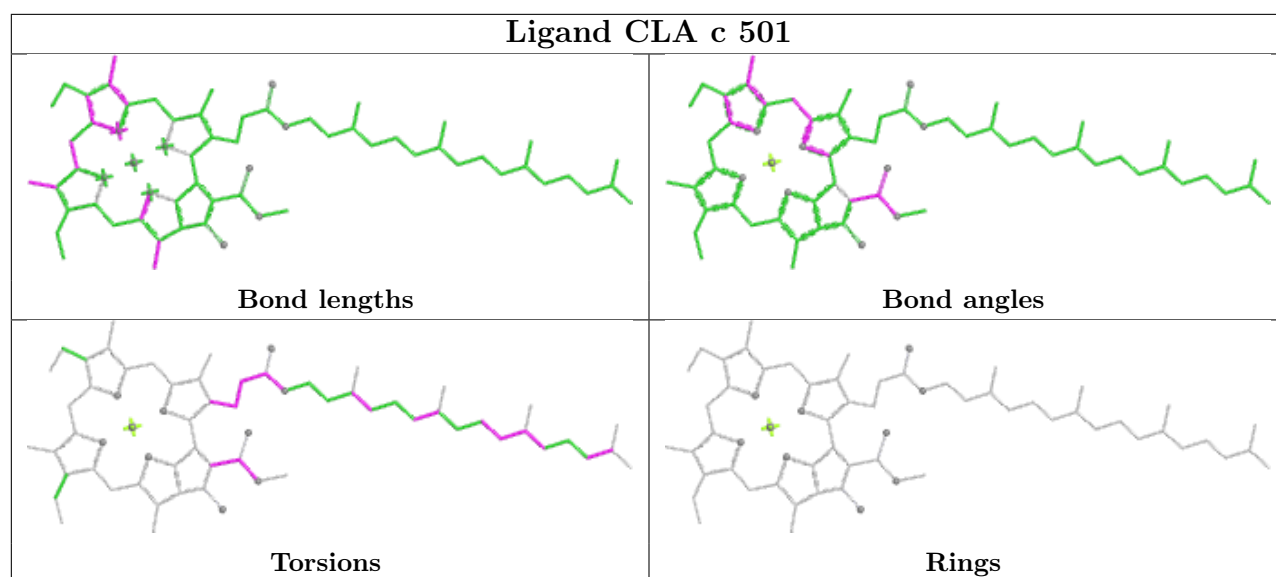
Ligand KC1 3 310

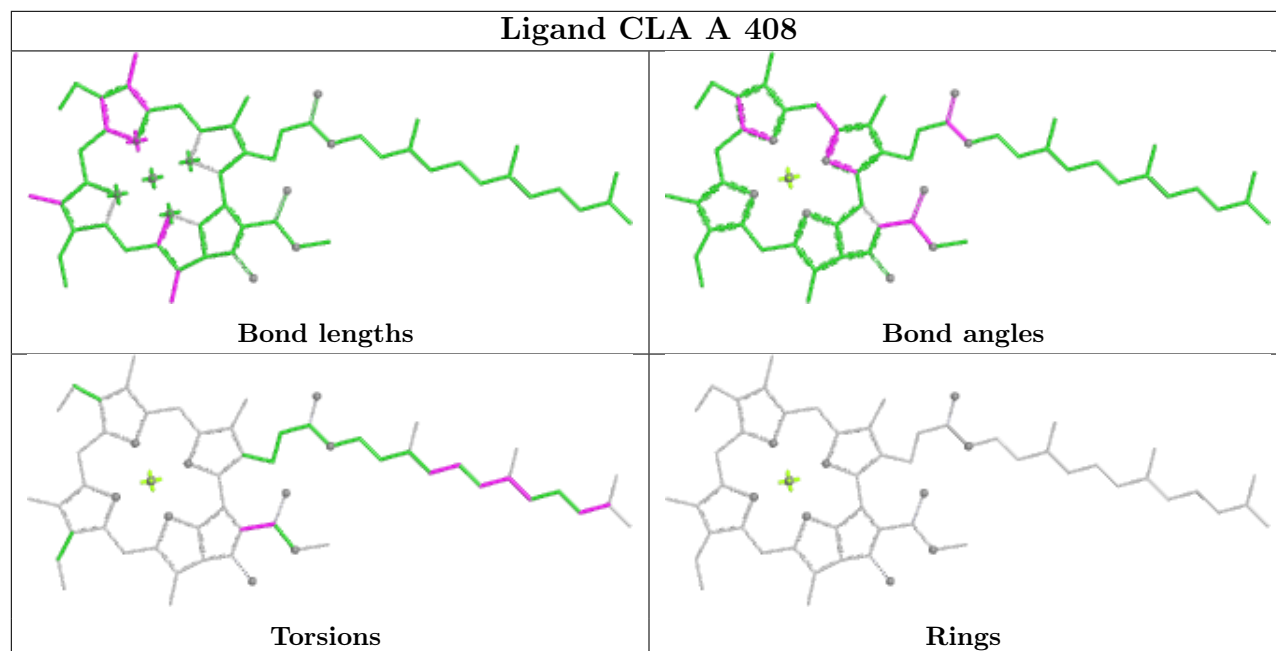
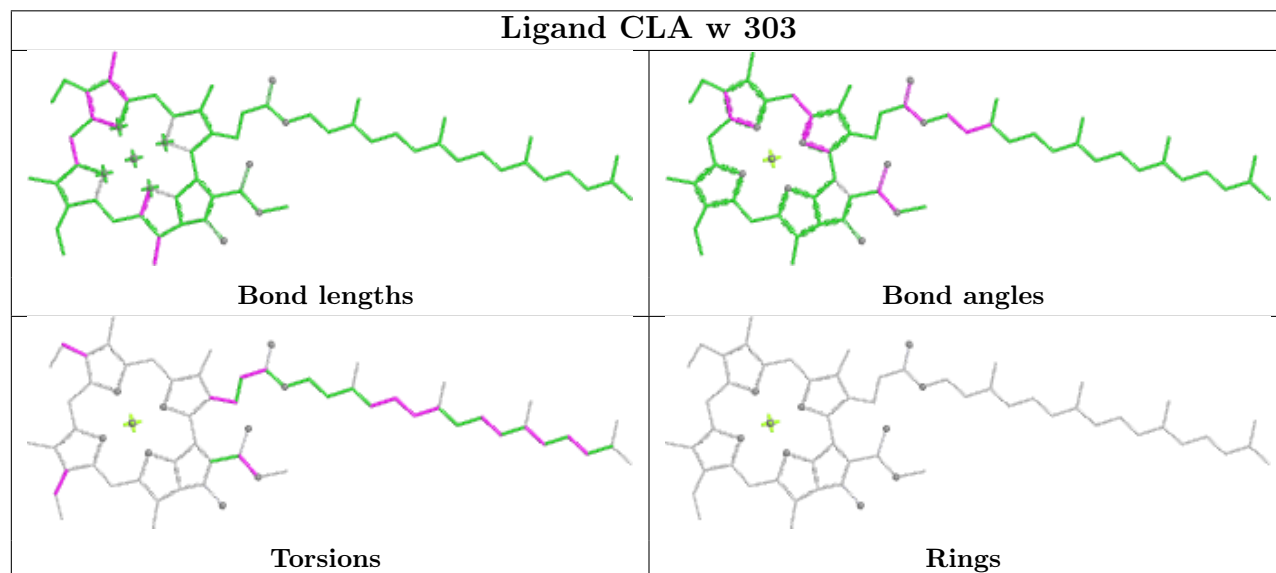
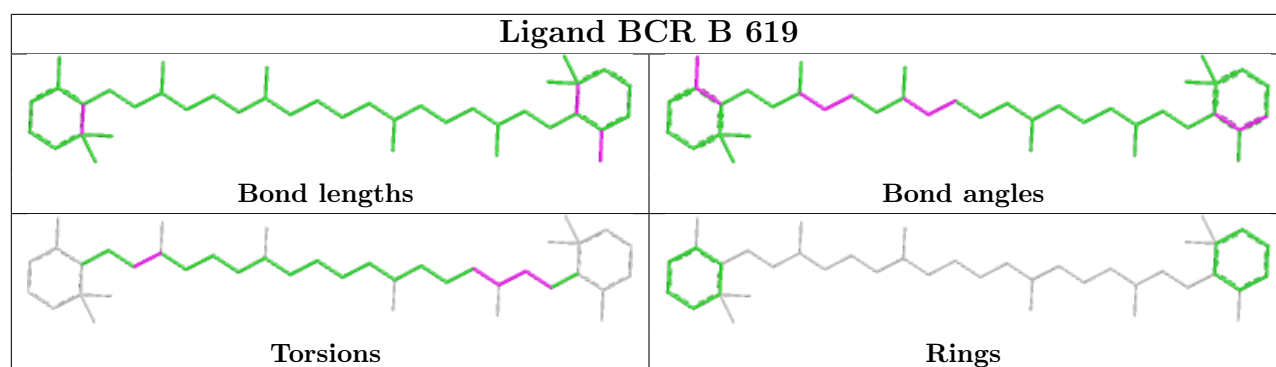


Ligand LMG 0 314

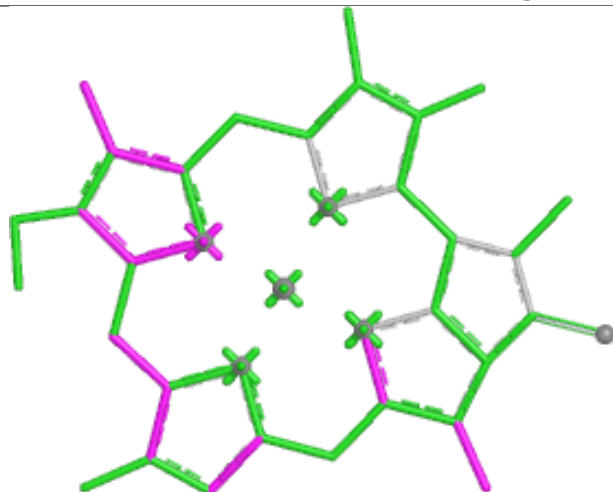


Ligand CLA 9 311**Ligand LMG b 623**

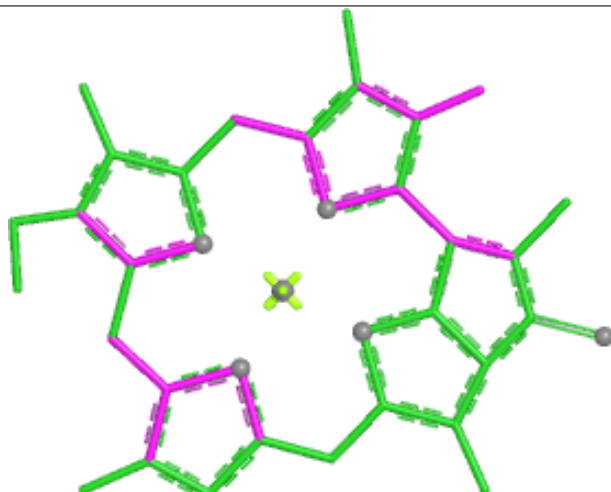




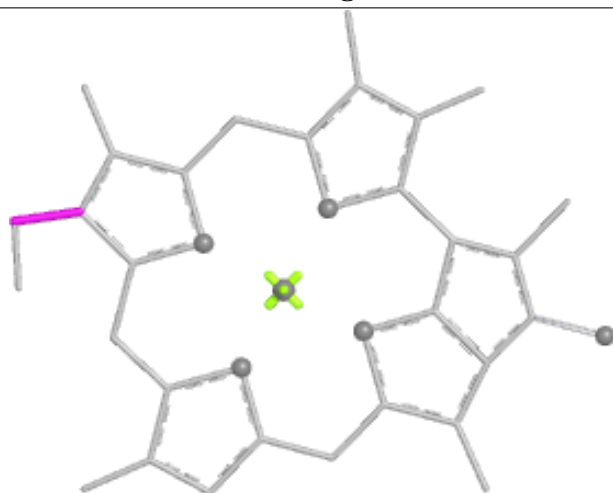
Ligand CLA 9 313



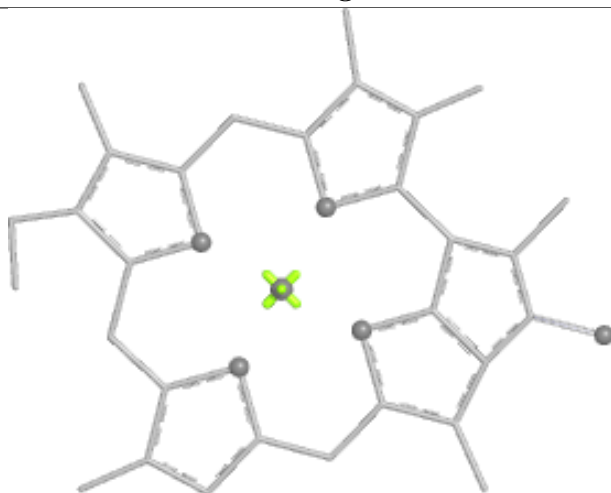
Bond lengths



Bond angles

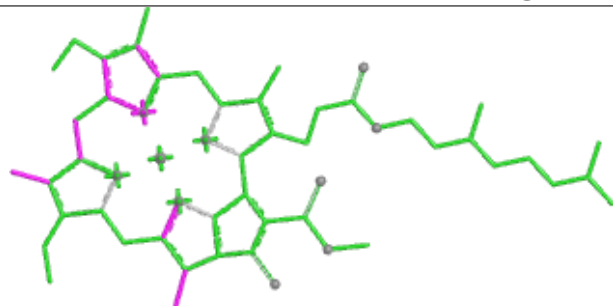


Torsions

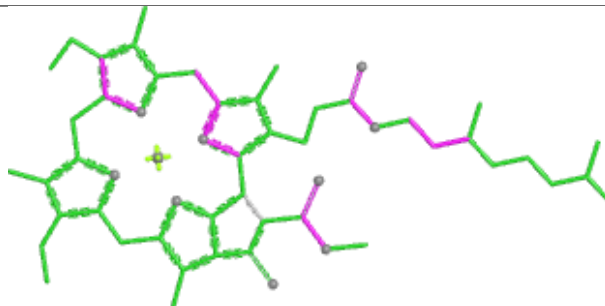


Rings

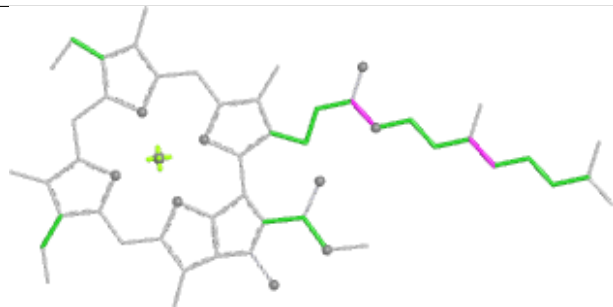
Ligand CLA 5 314



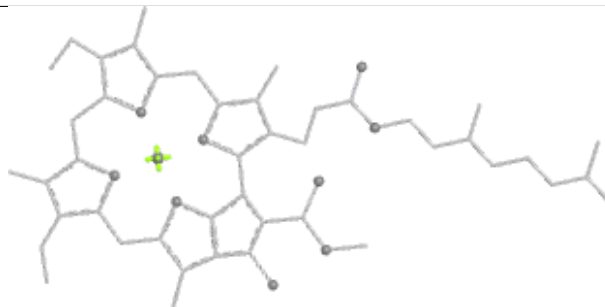
Bond lengths



Bond angles

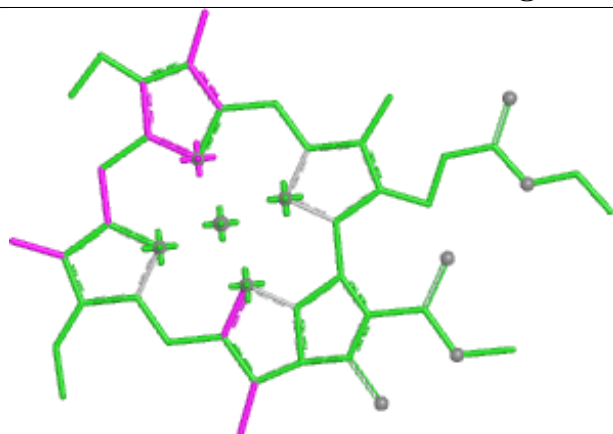


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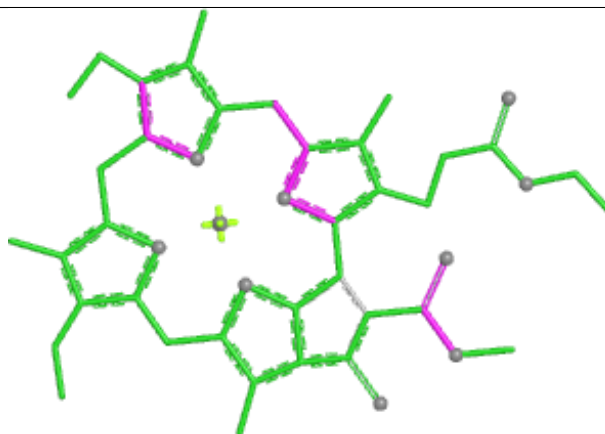


Rings

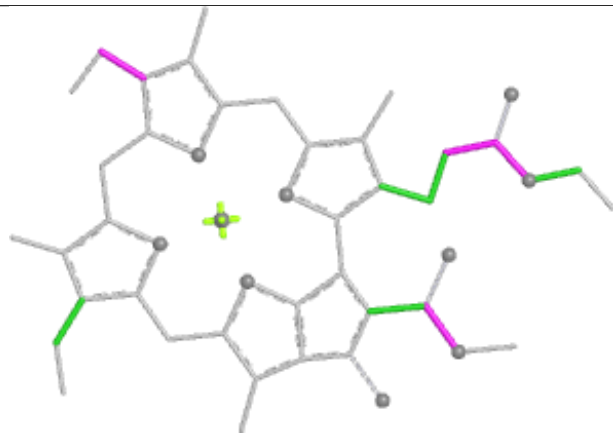
Ligand CLA 7 304



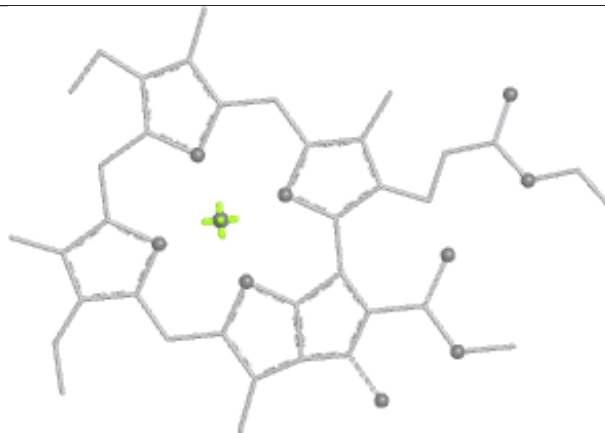
Bond lengths



Bond angles

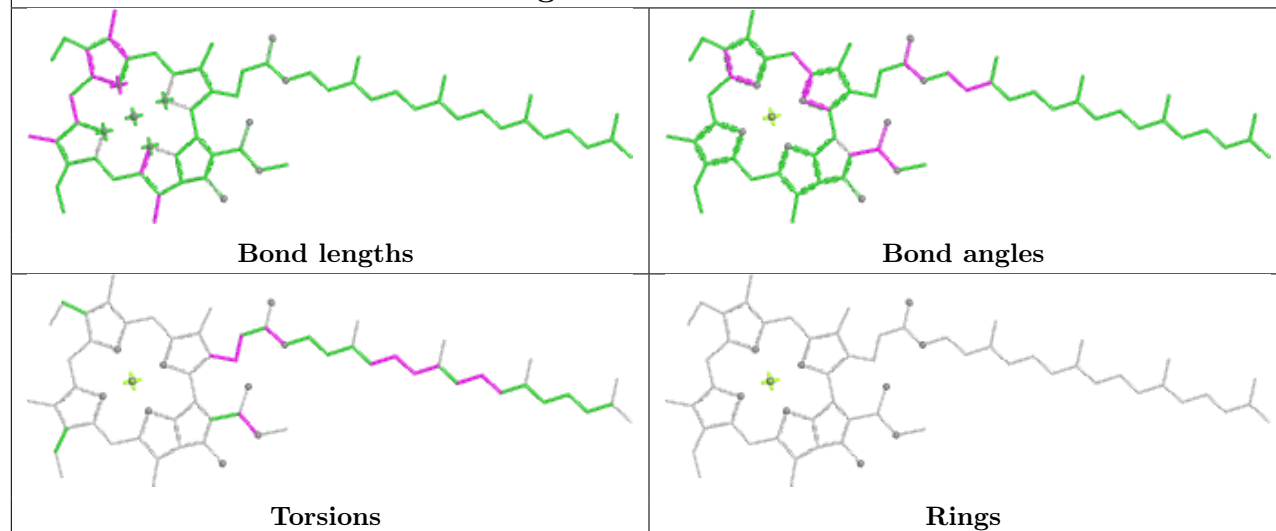


Torsions

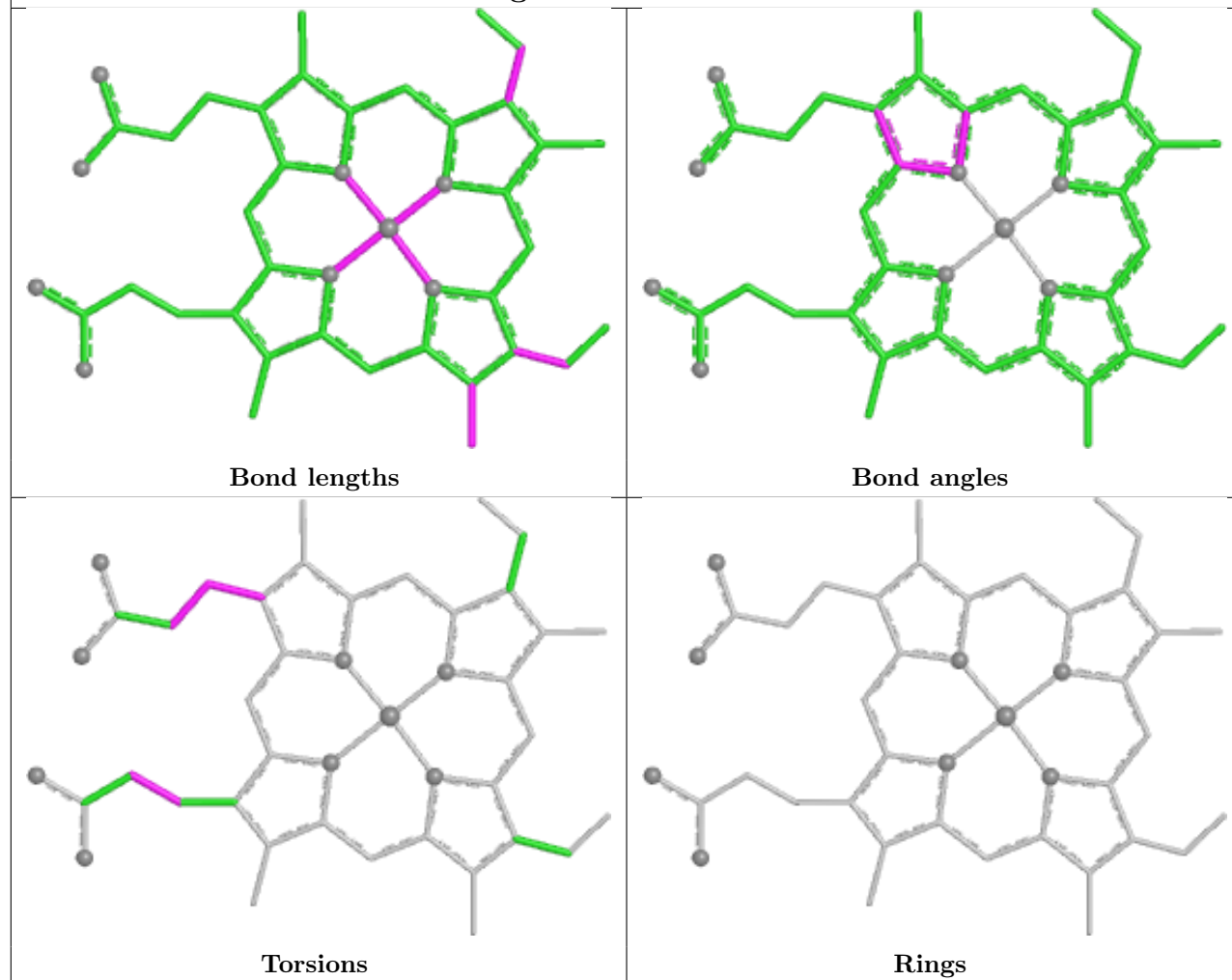


Rings

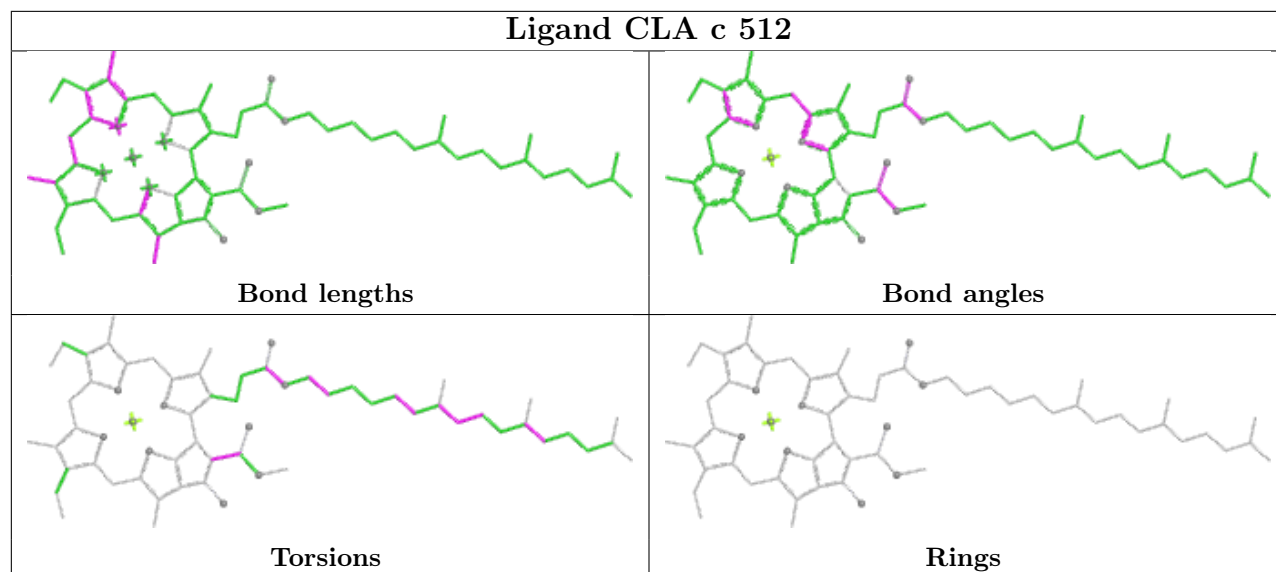
Ligand CLA c 503



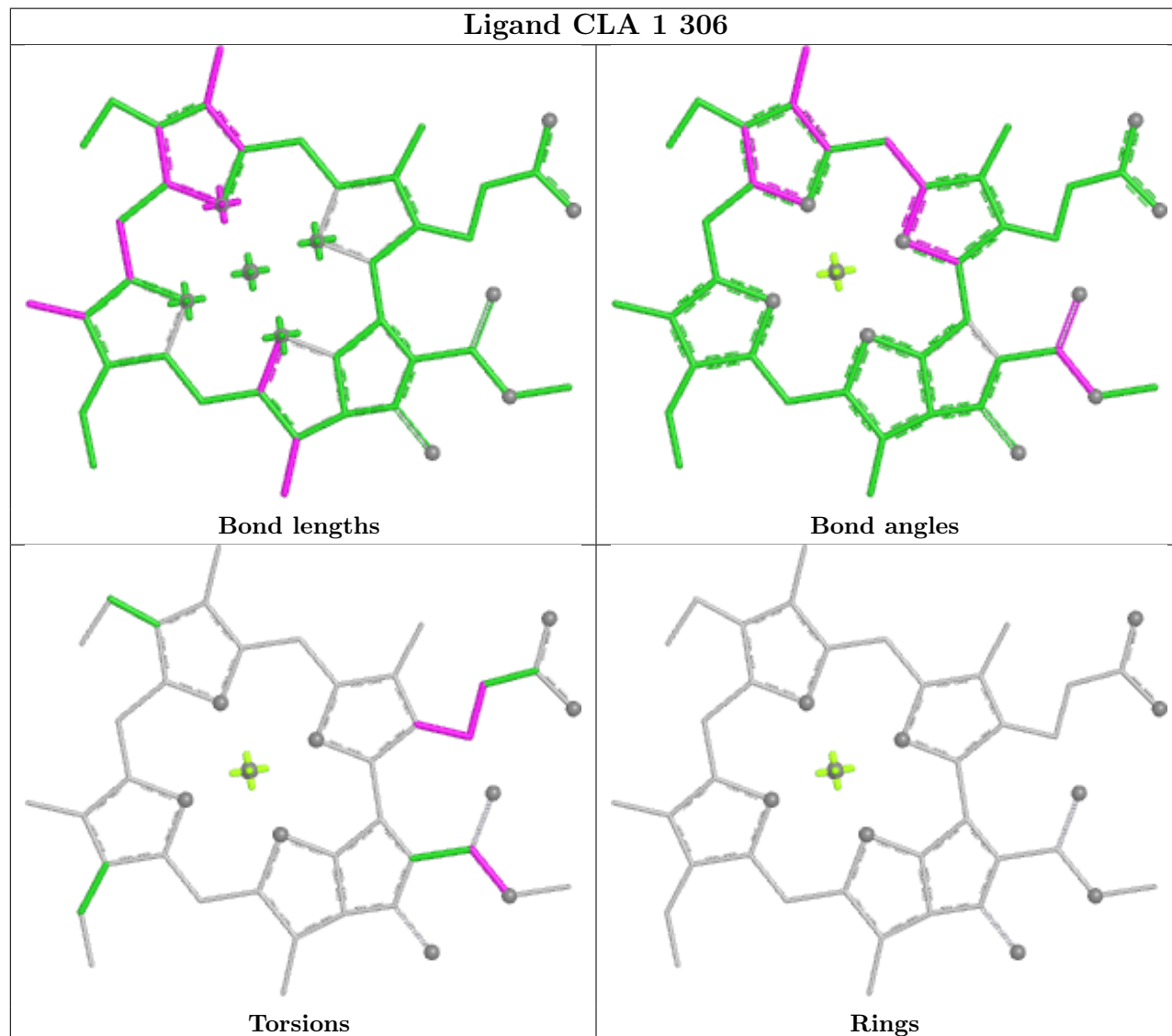
Ligand HEM F 101

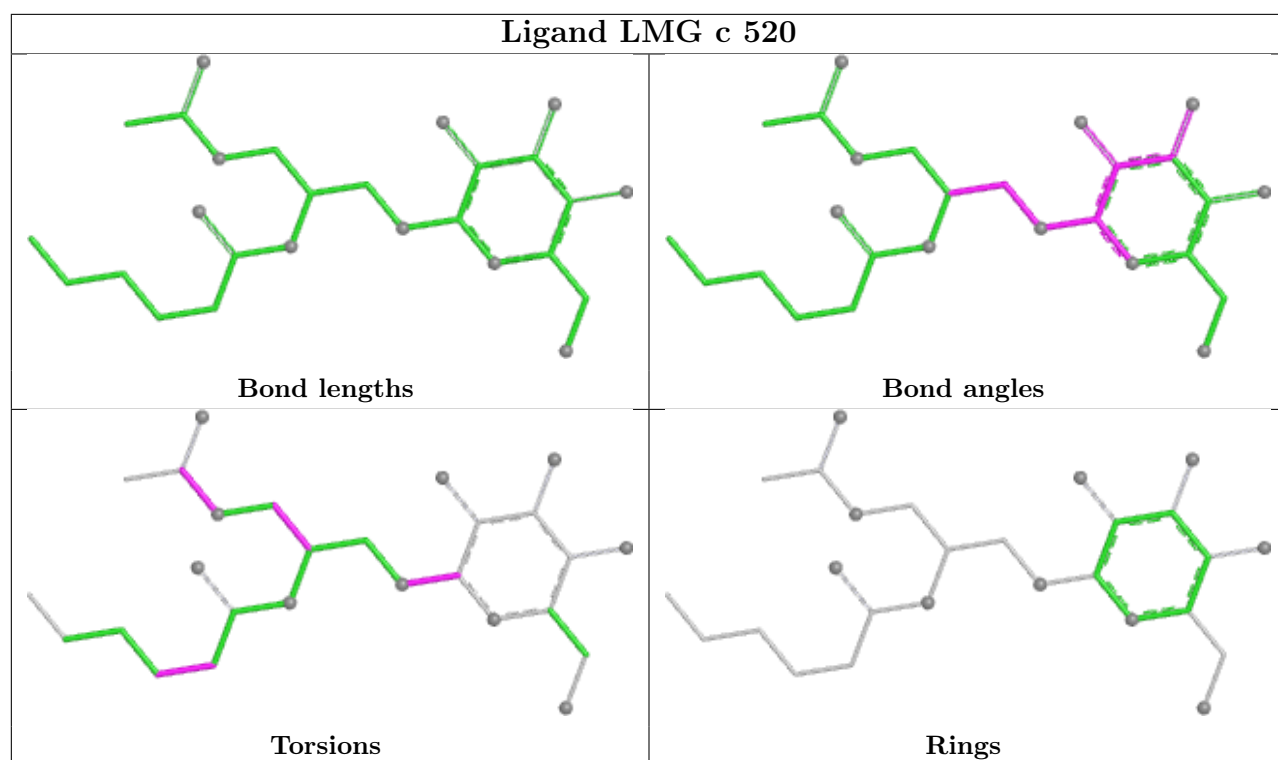


Ligand CLA c 512

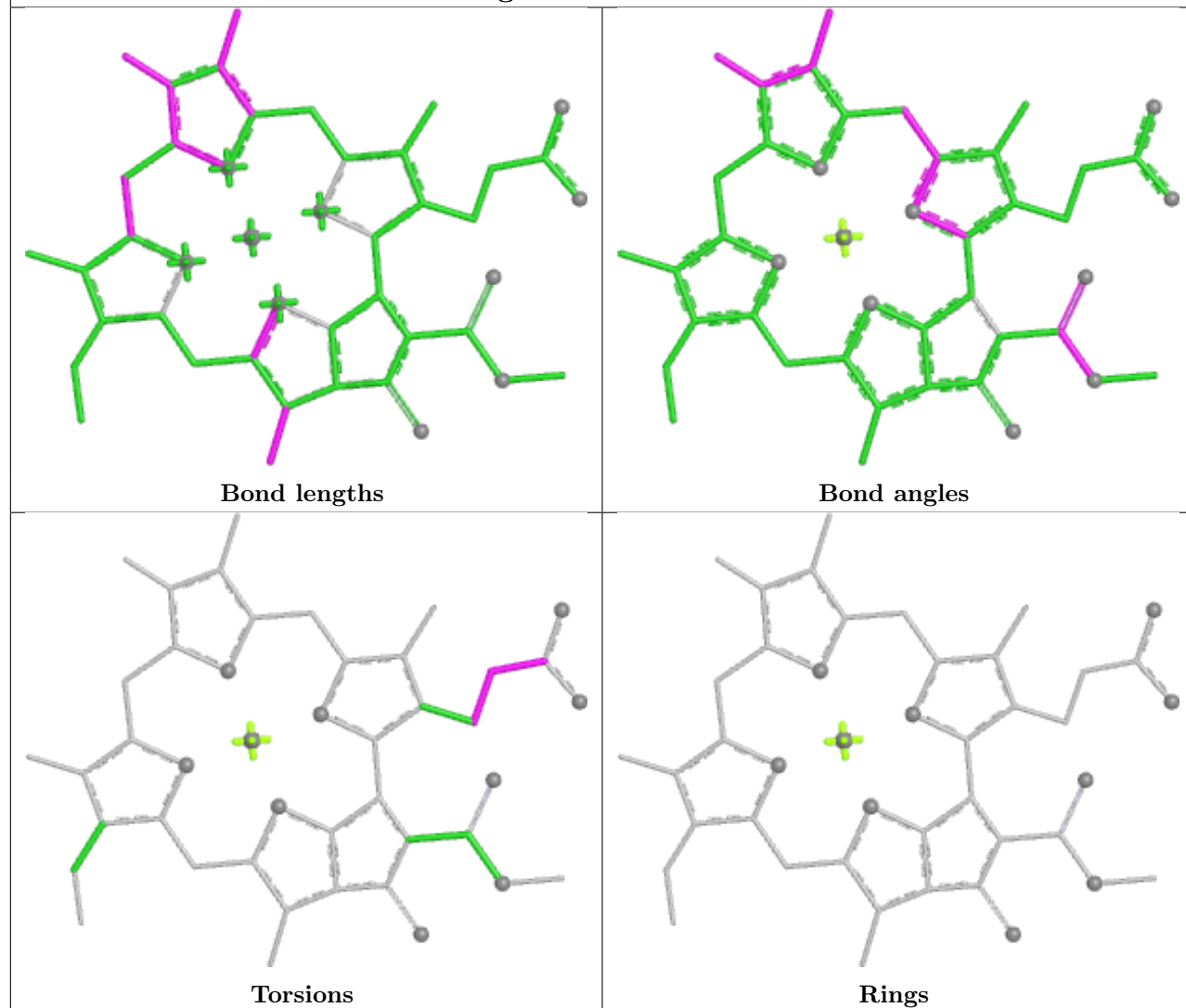


Ligand CLA 1 306

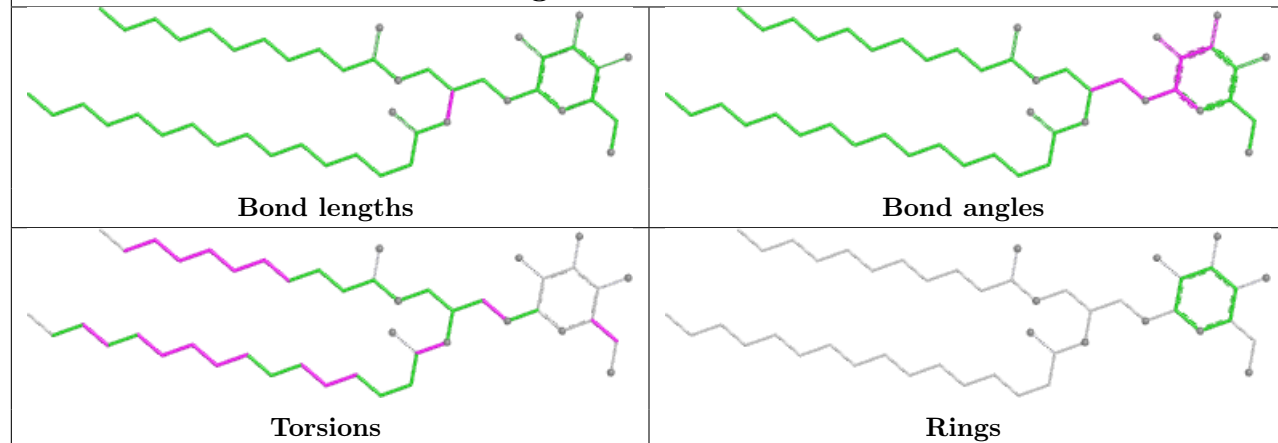


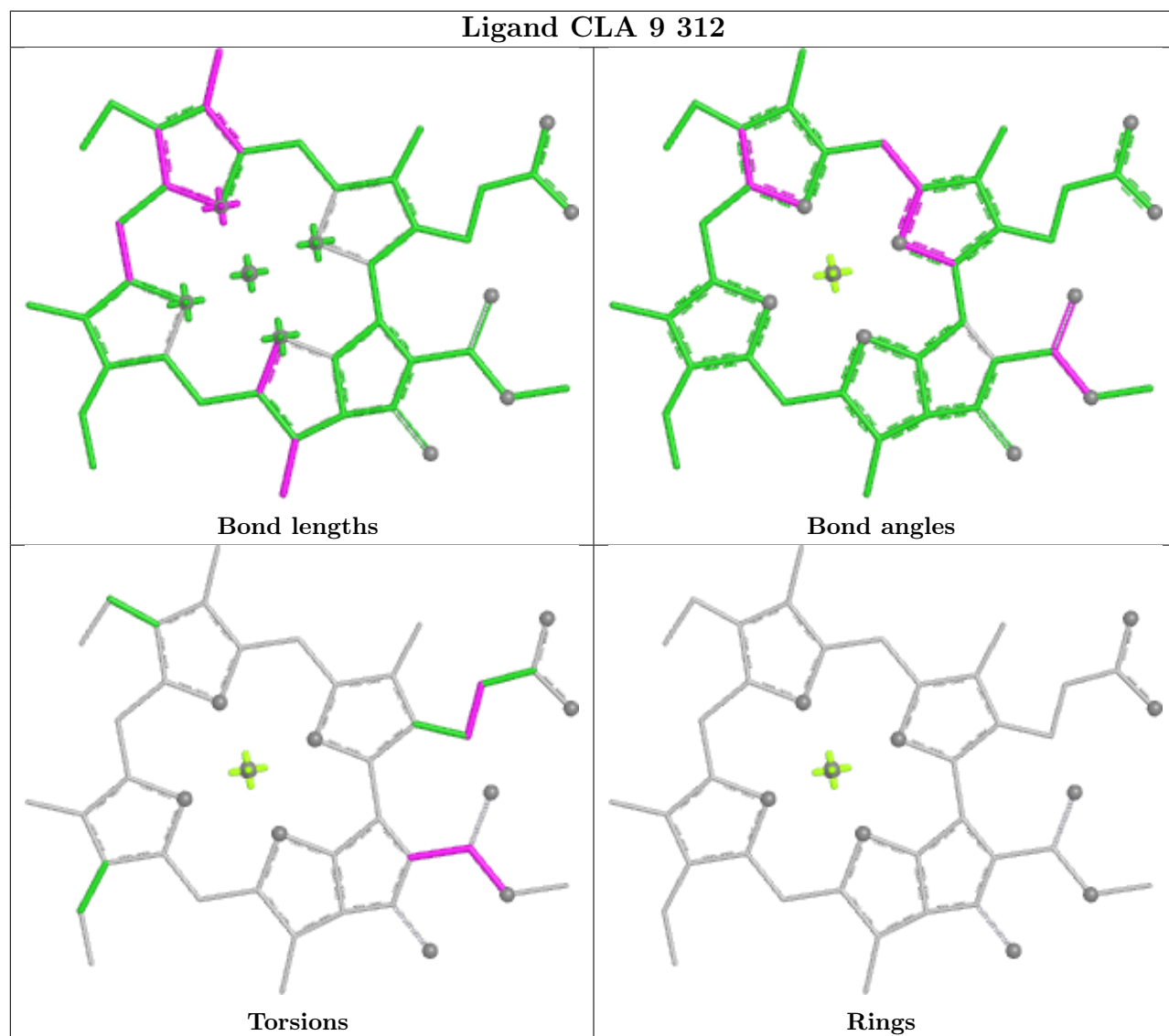
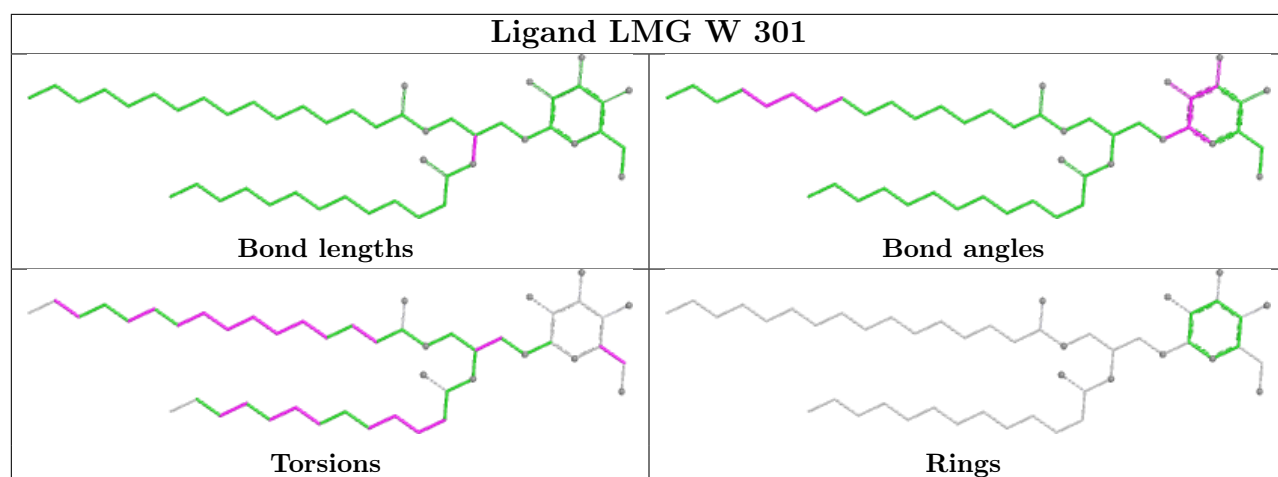


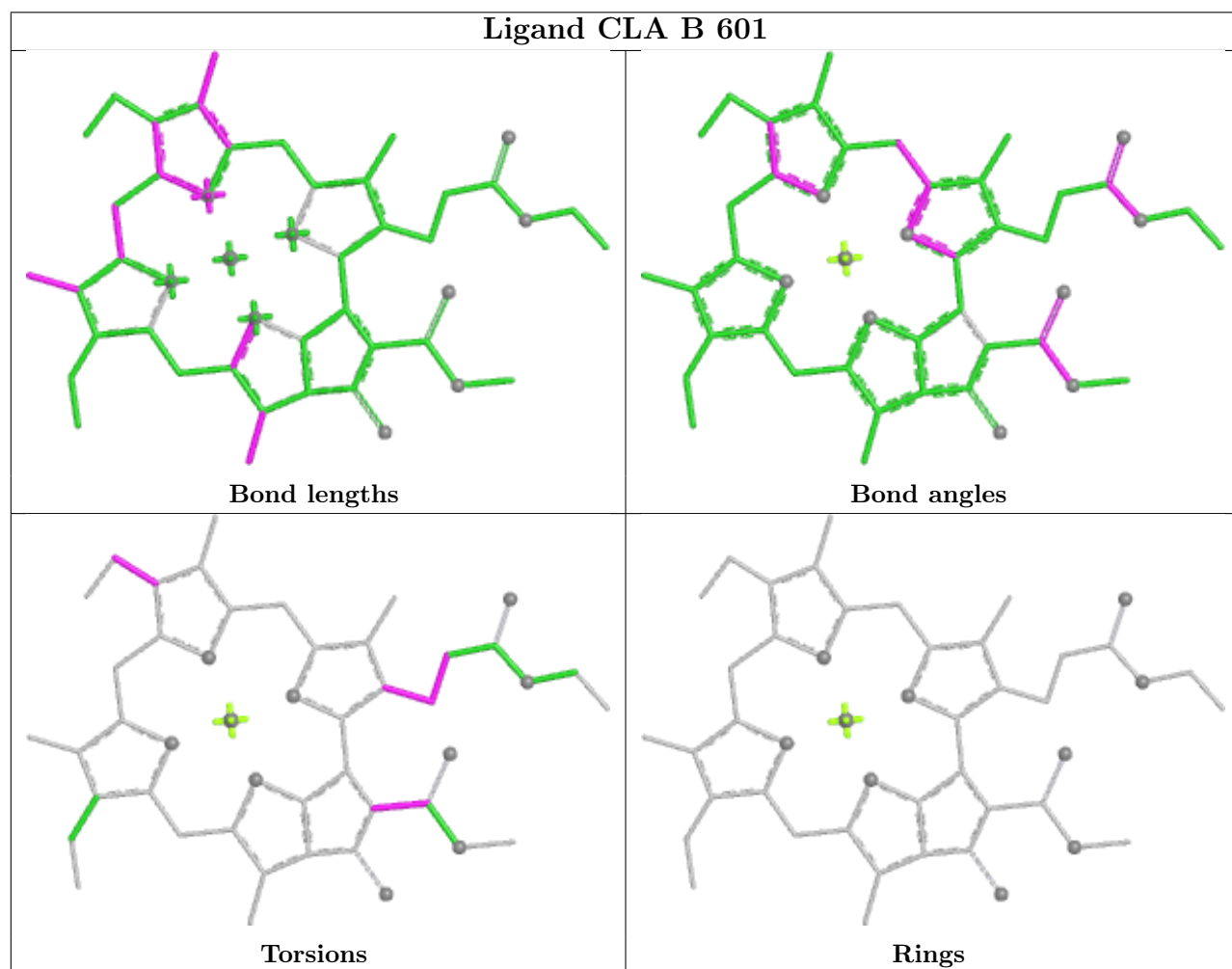
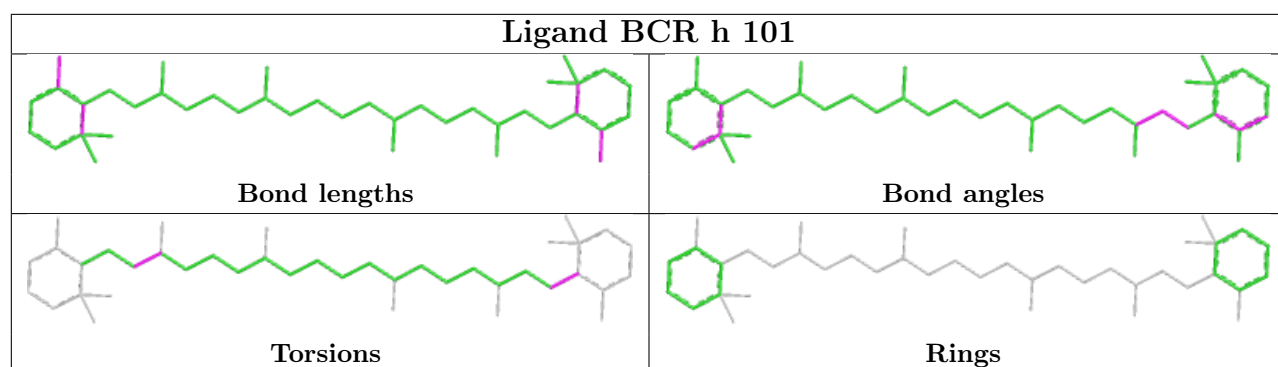
Ligand CLA 1 307



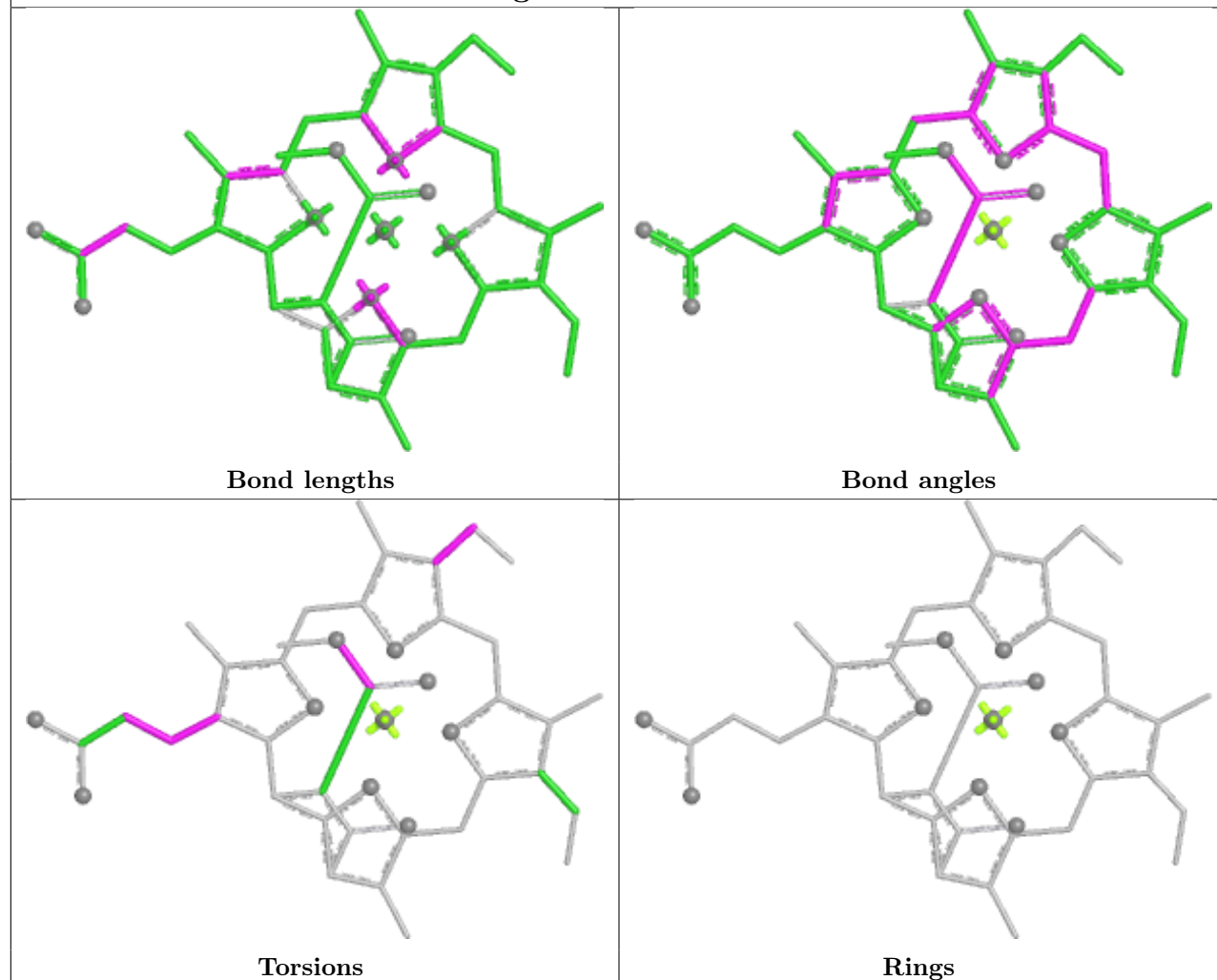
Ligand LMG d 406



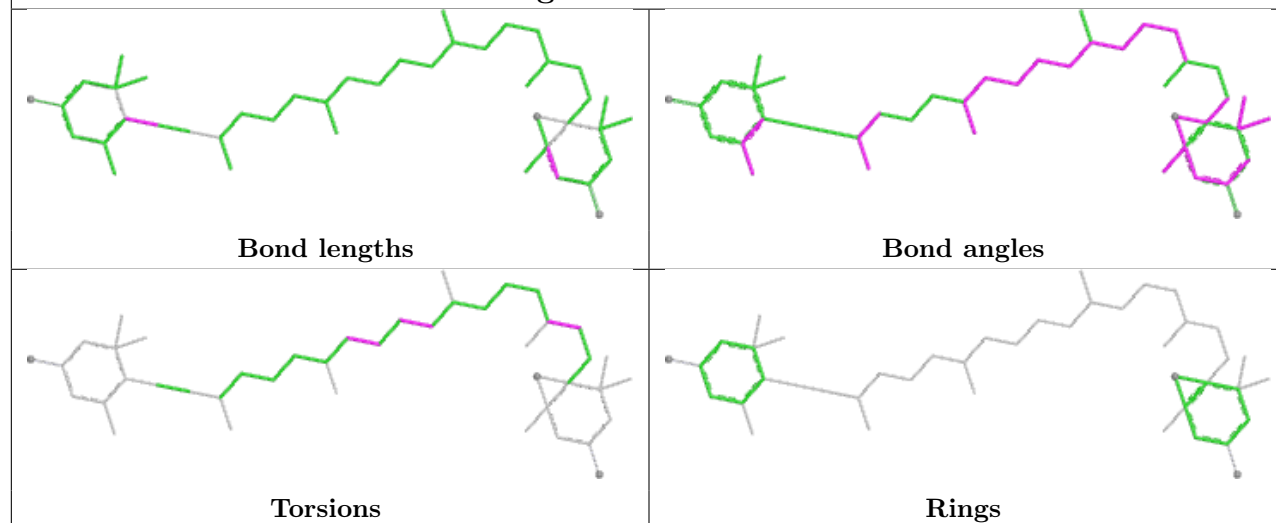




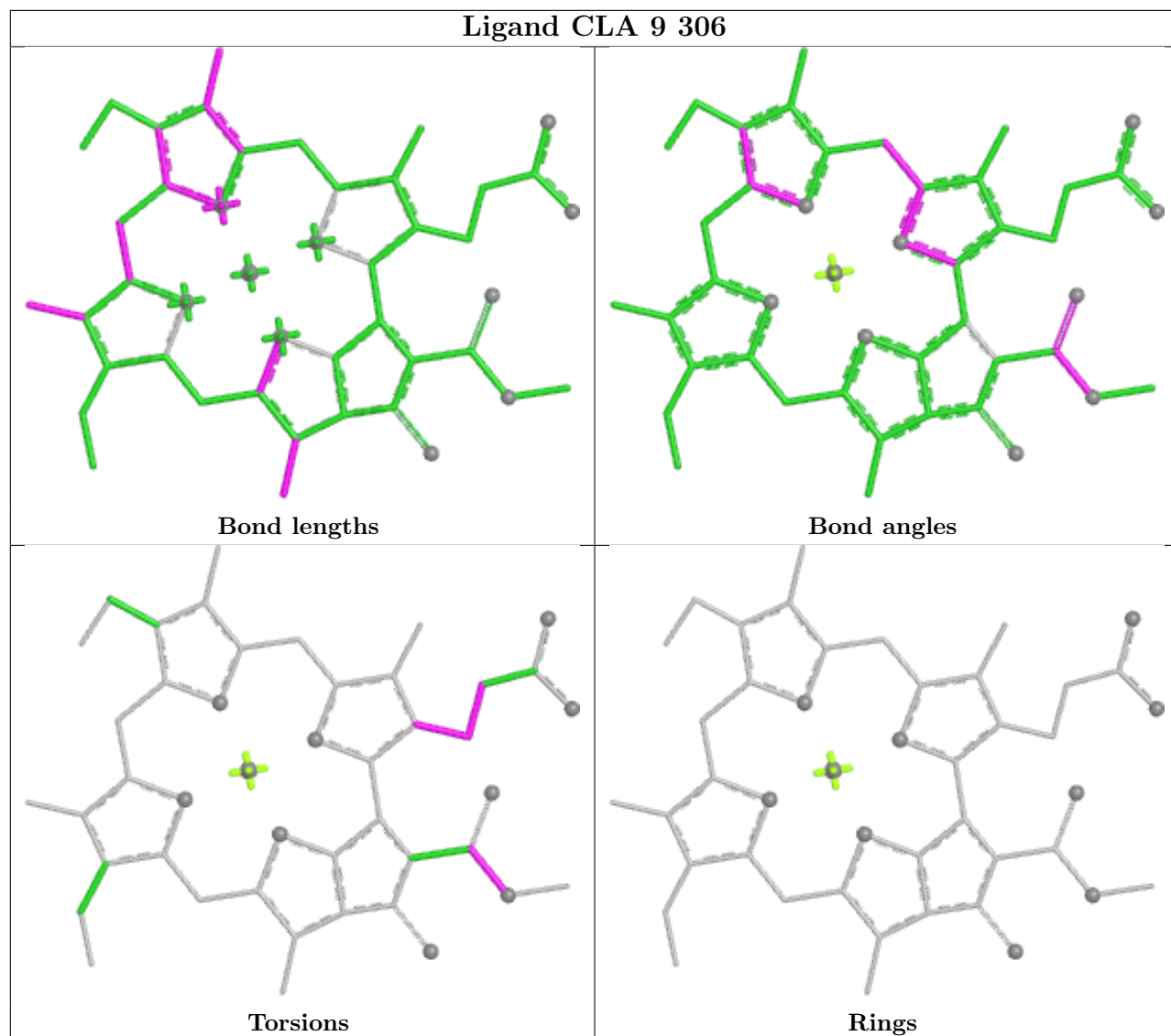
Ligand KC1 6 314



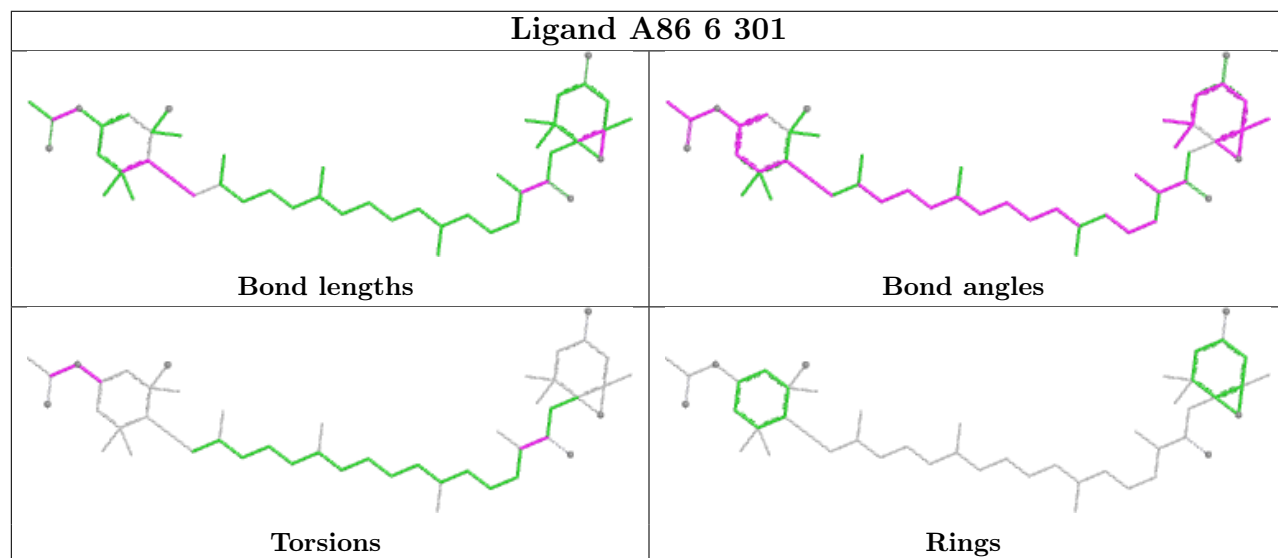
Ligand DD6 2 303

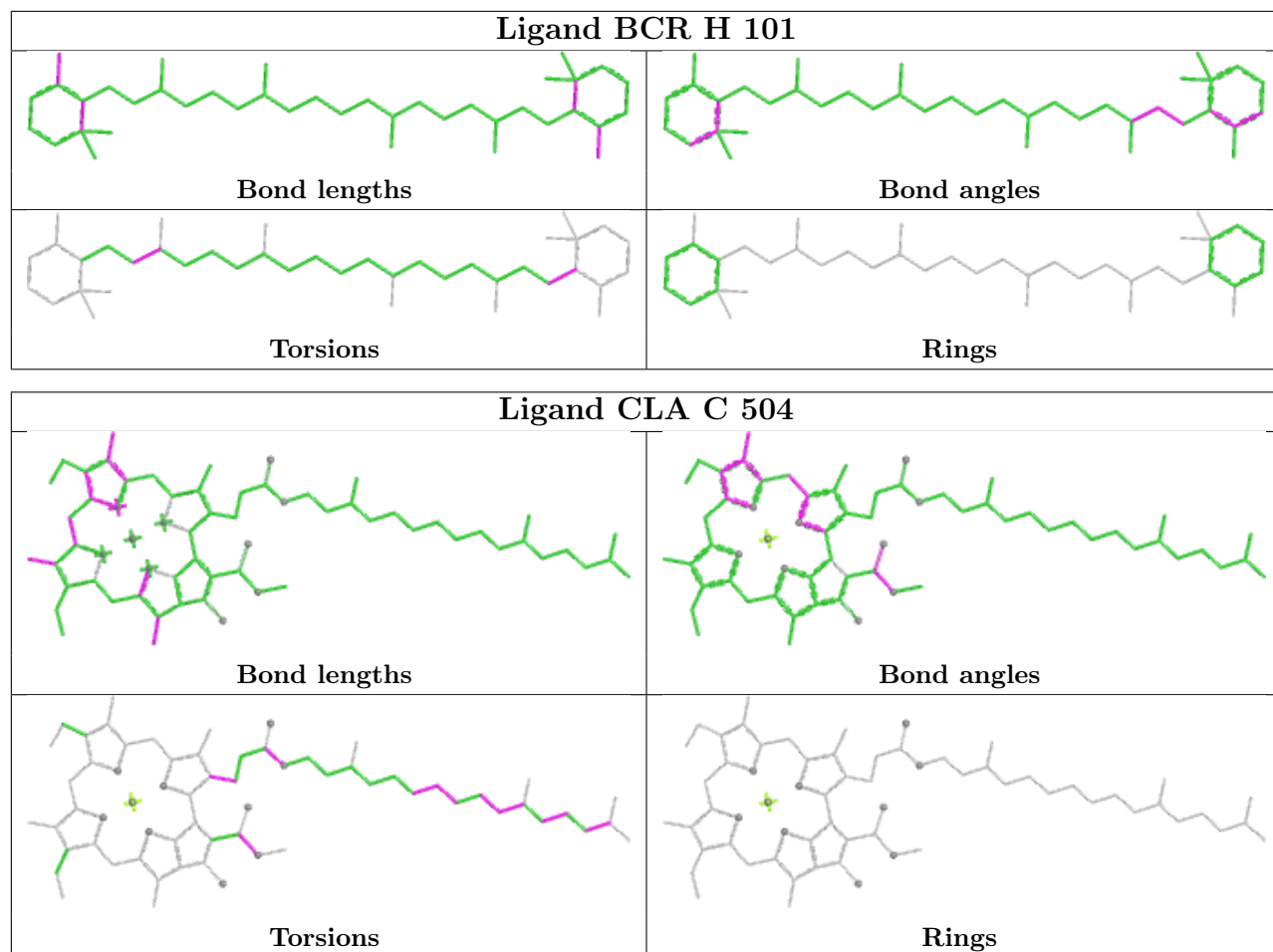


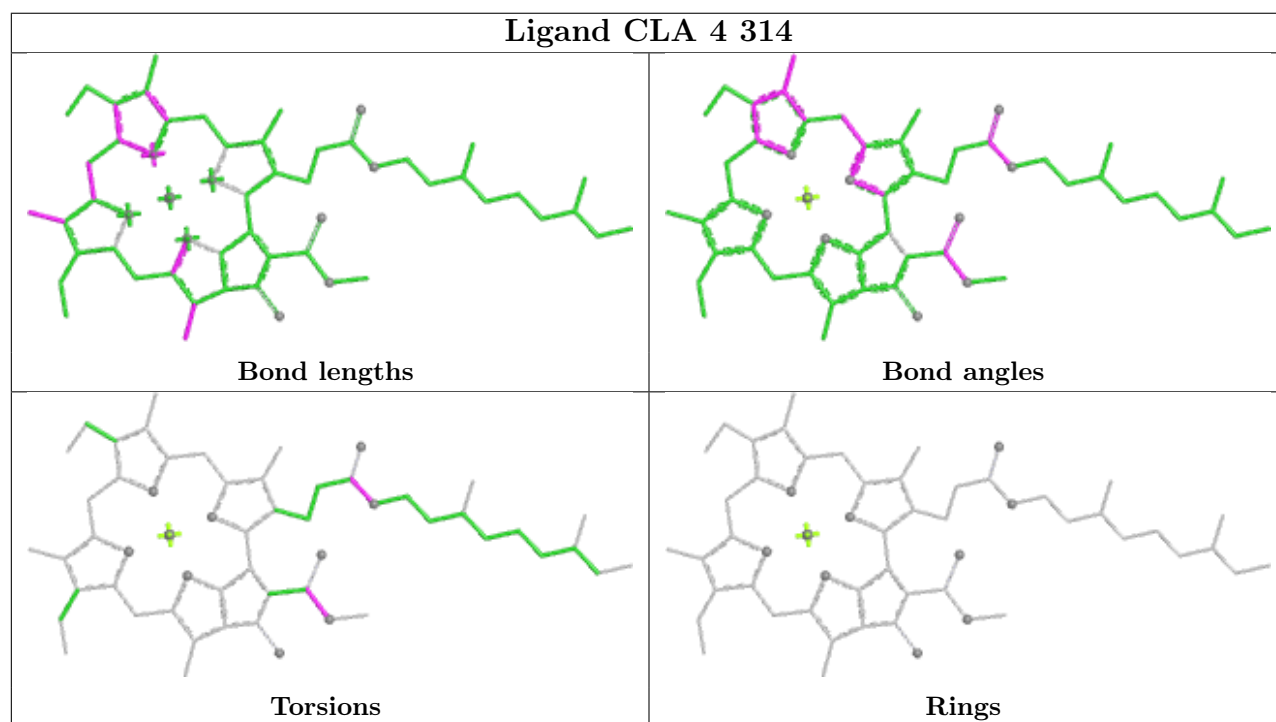
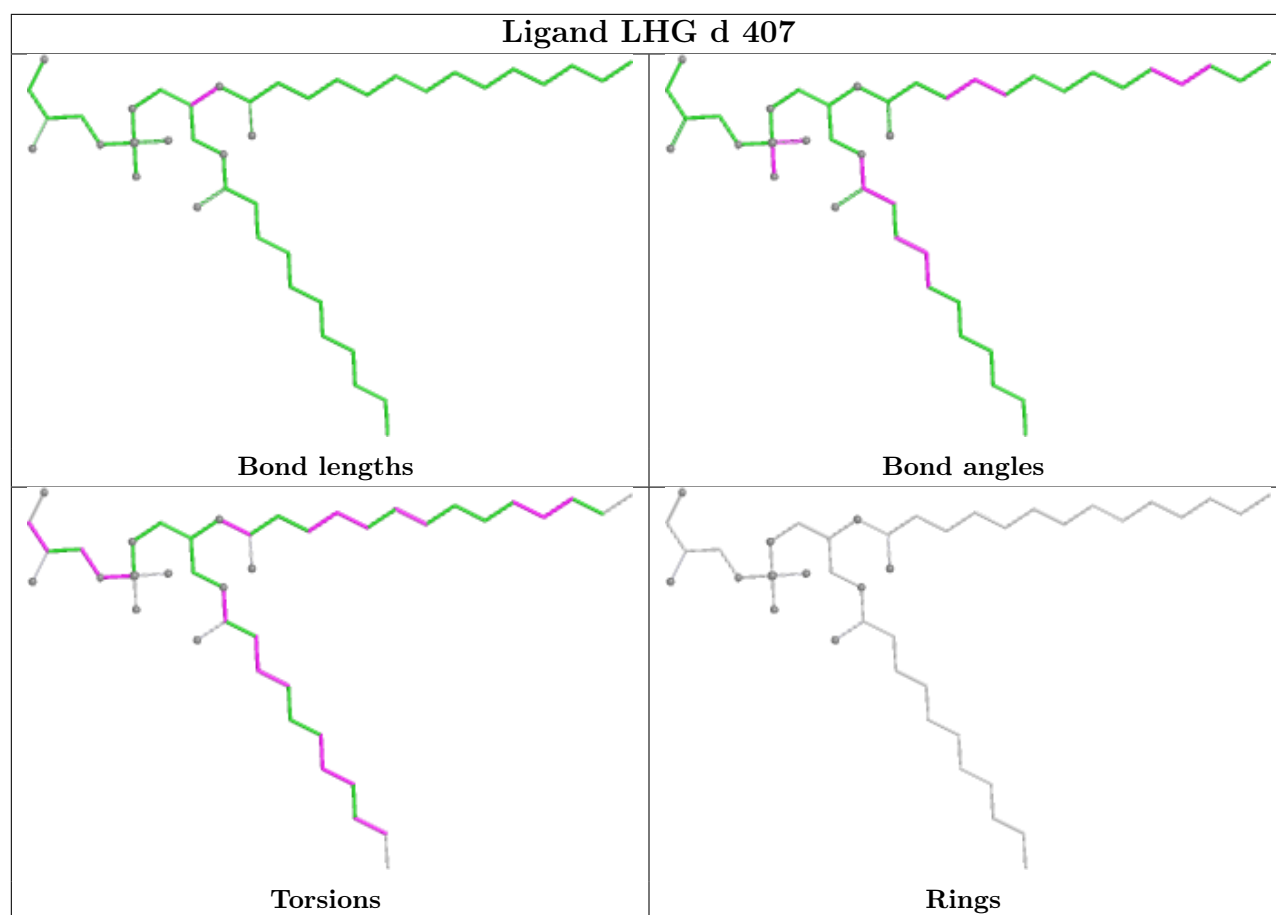
Ligand CLA 9 306



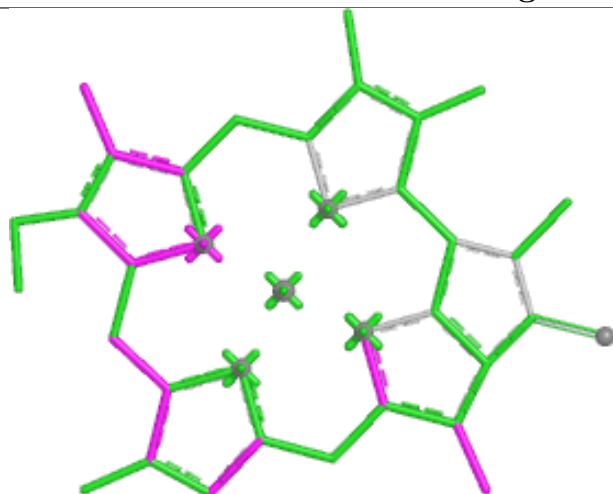
Ligand A86 6 301



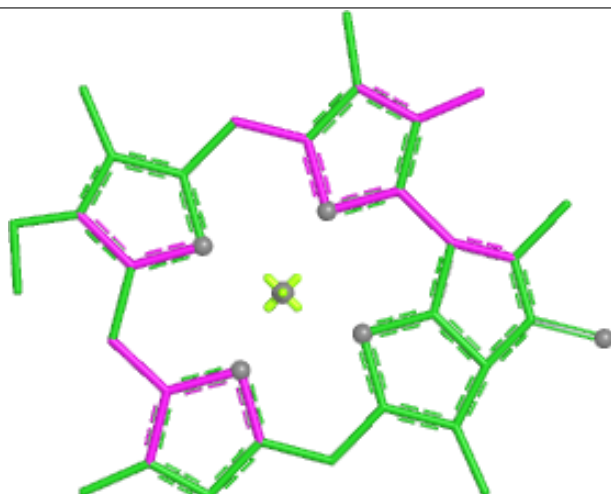




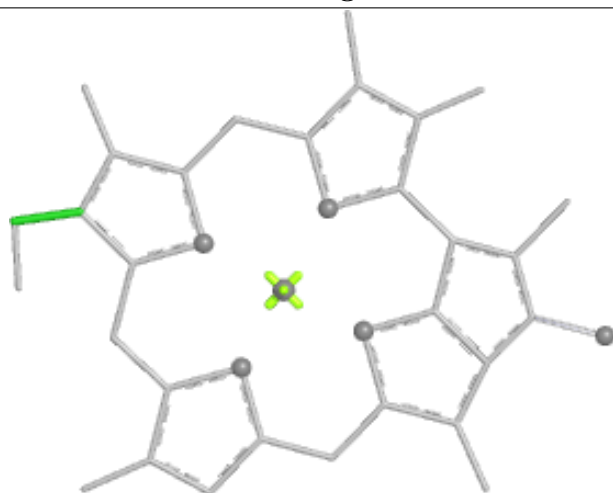
Ligand CLA 8 313



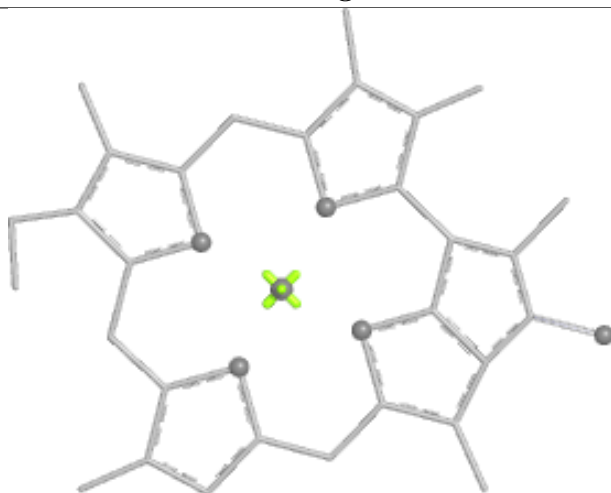
Bond lengths



Bond angles

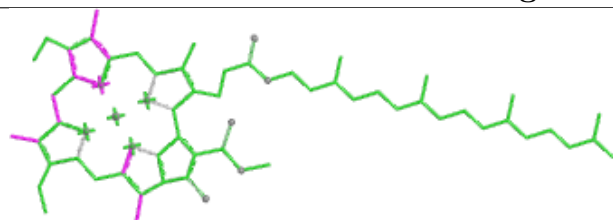


Torsions

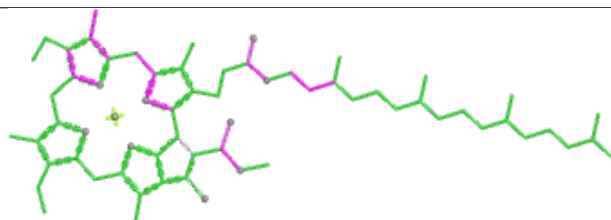


Rings

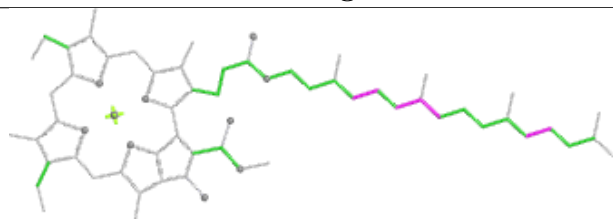
Ligand CLA c 509



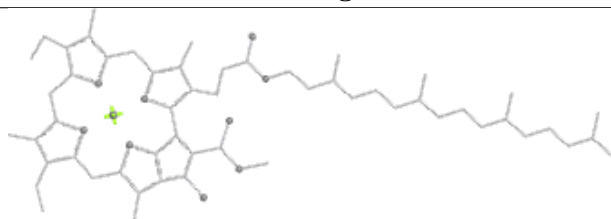
Bond lengths



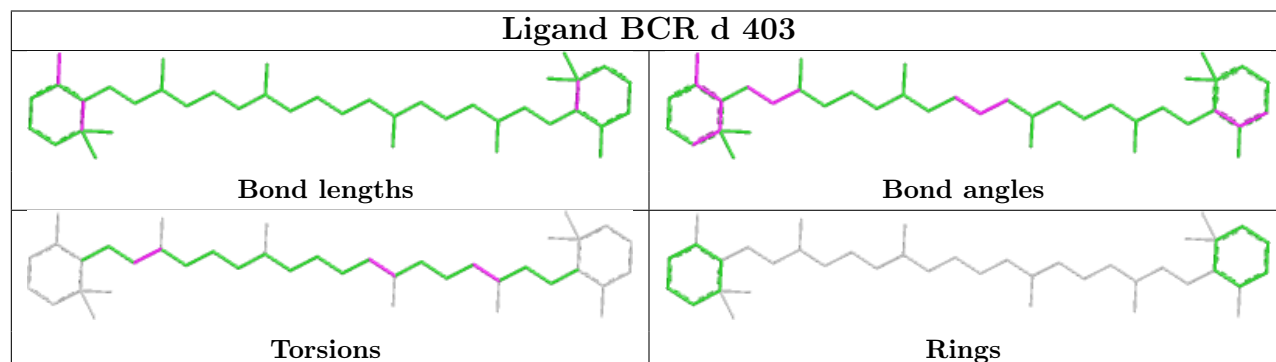
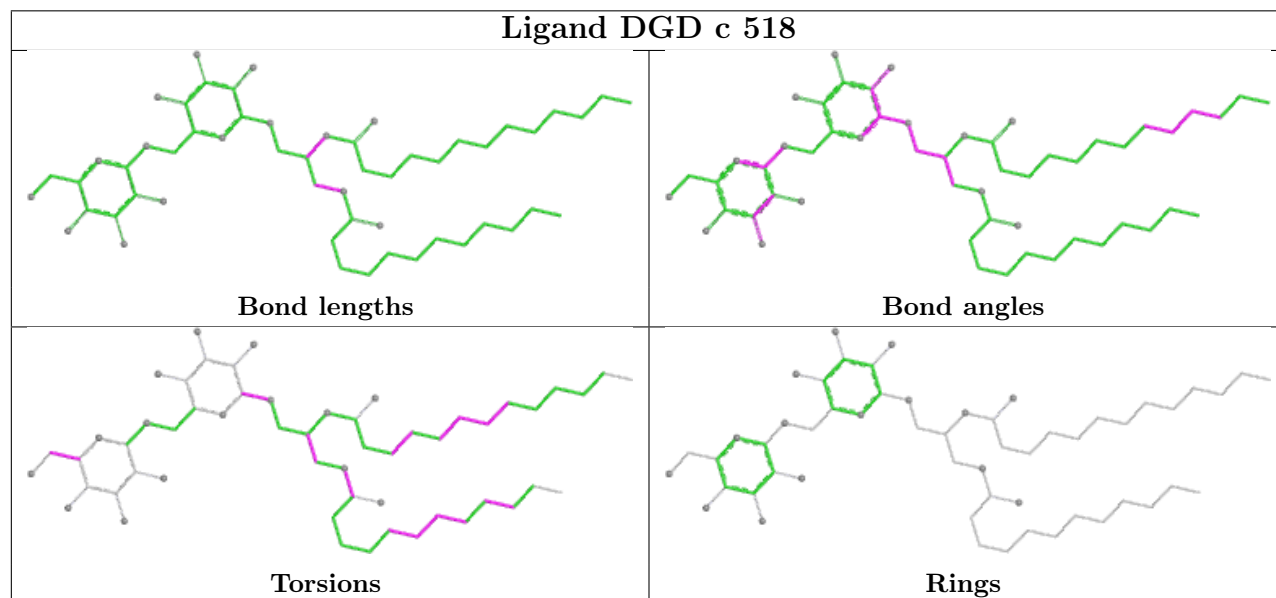
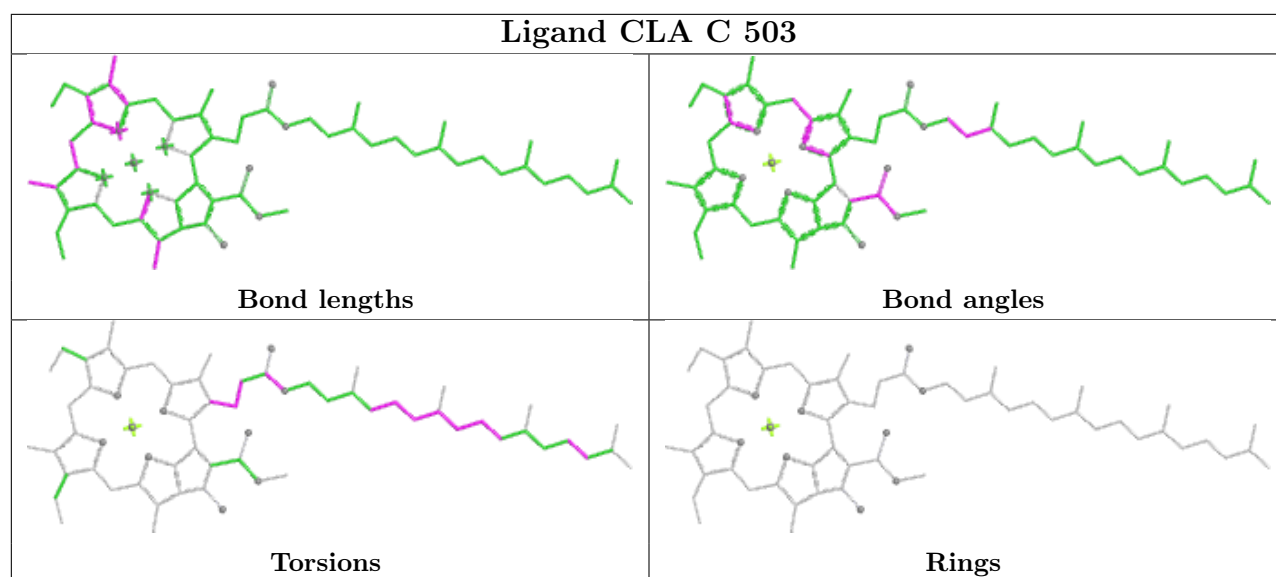
Bond angles



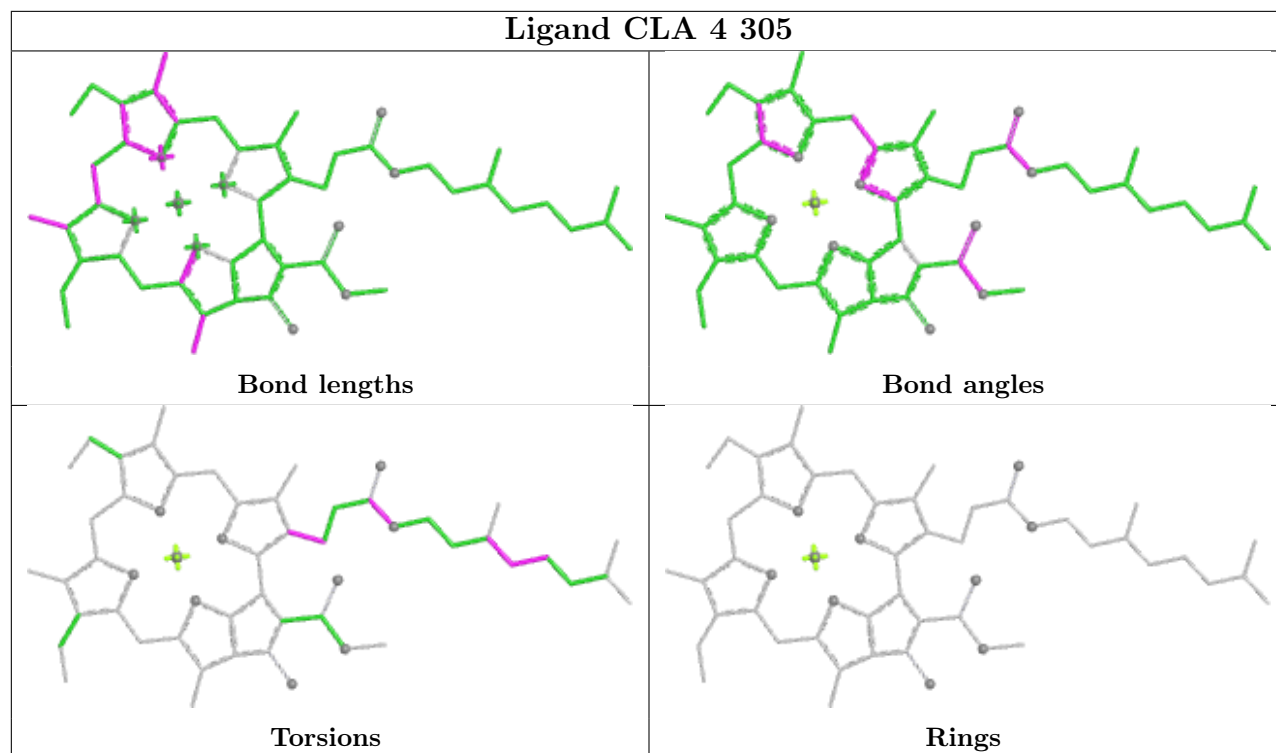
Torsions



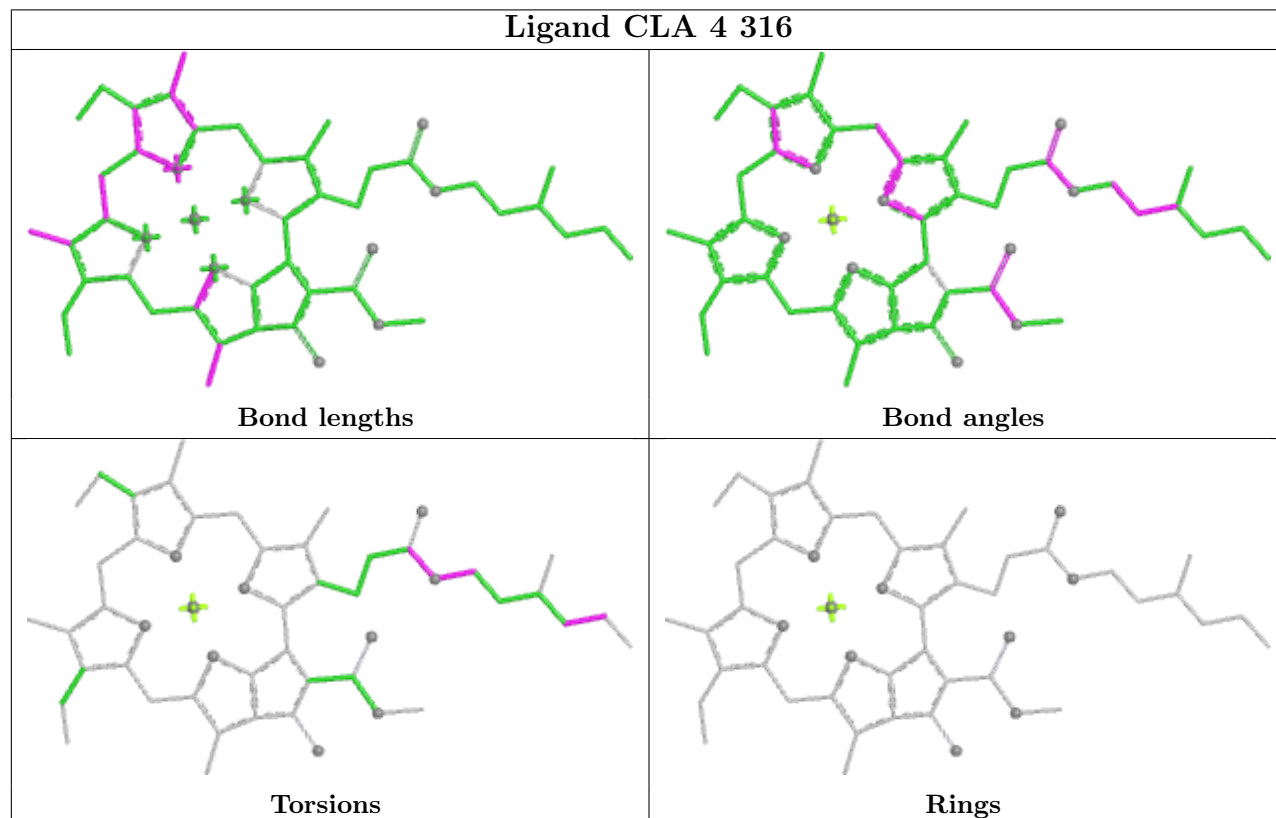
Rings



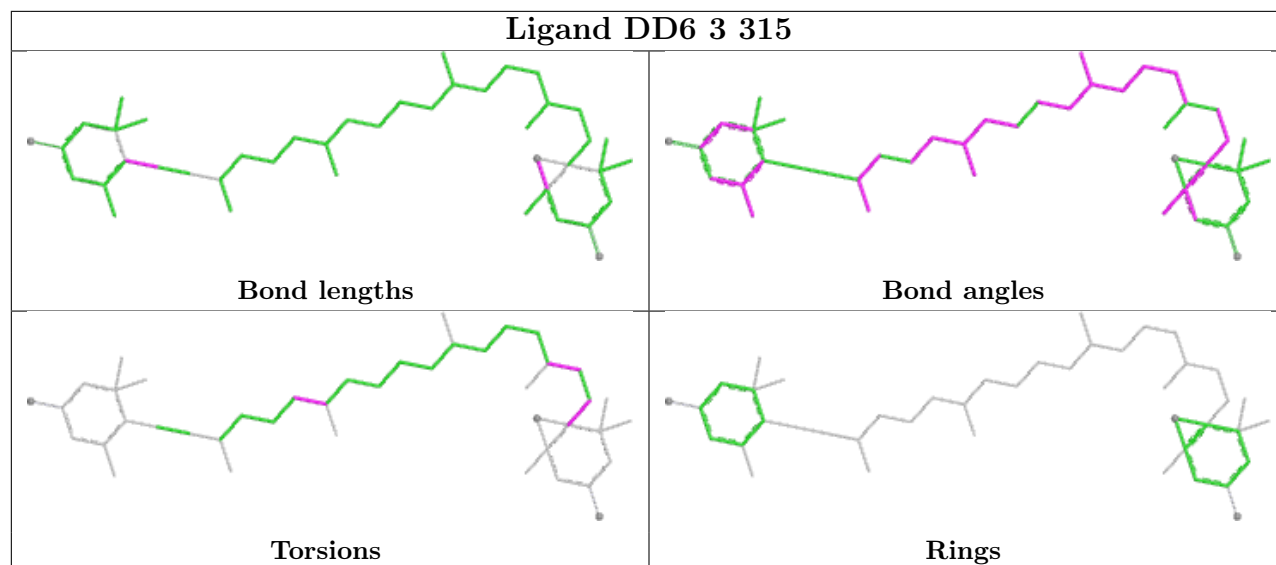
Ligand CLA 4 305



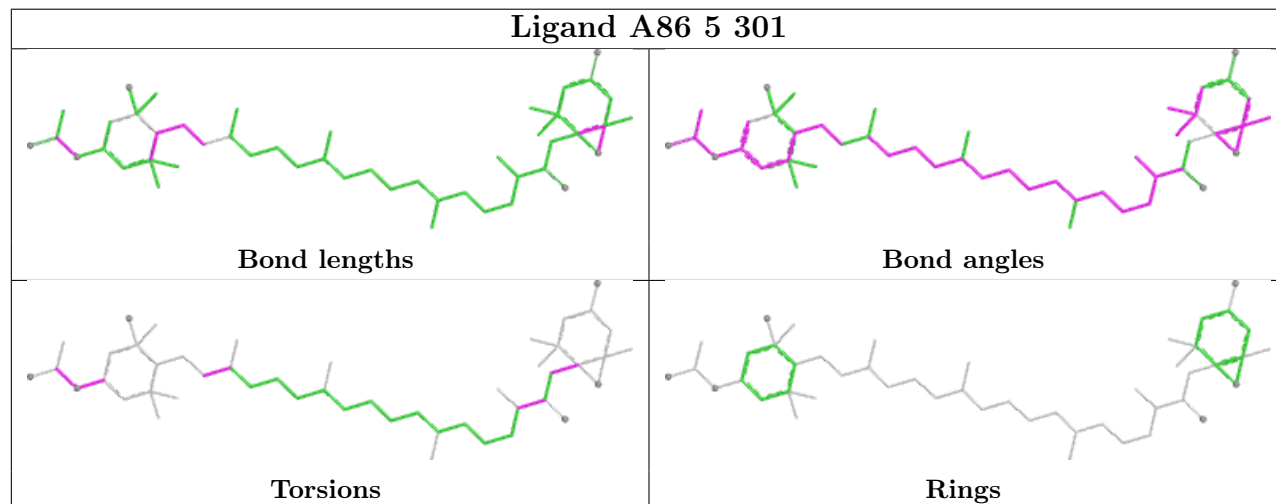
Ligand CLA 4 316



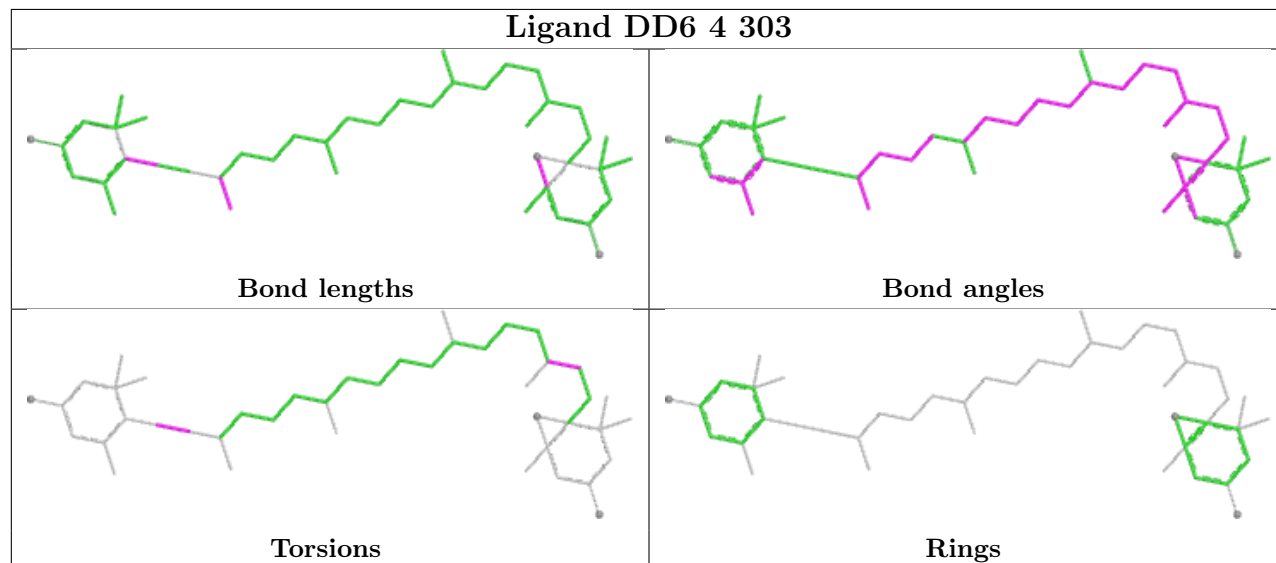
Ligand DD6 3 315



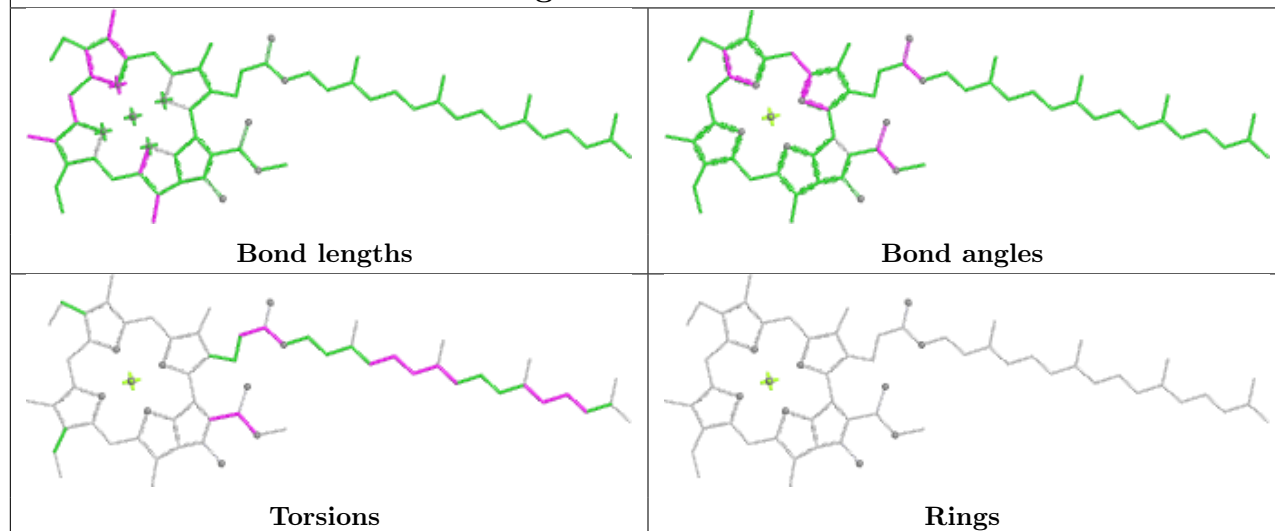
Ligand A86 5 301



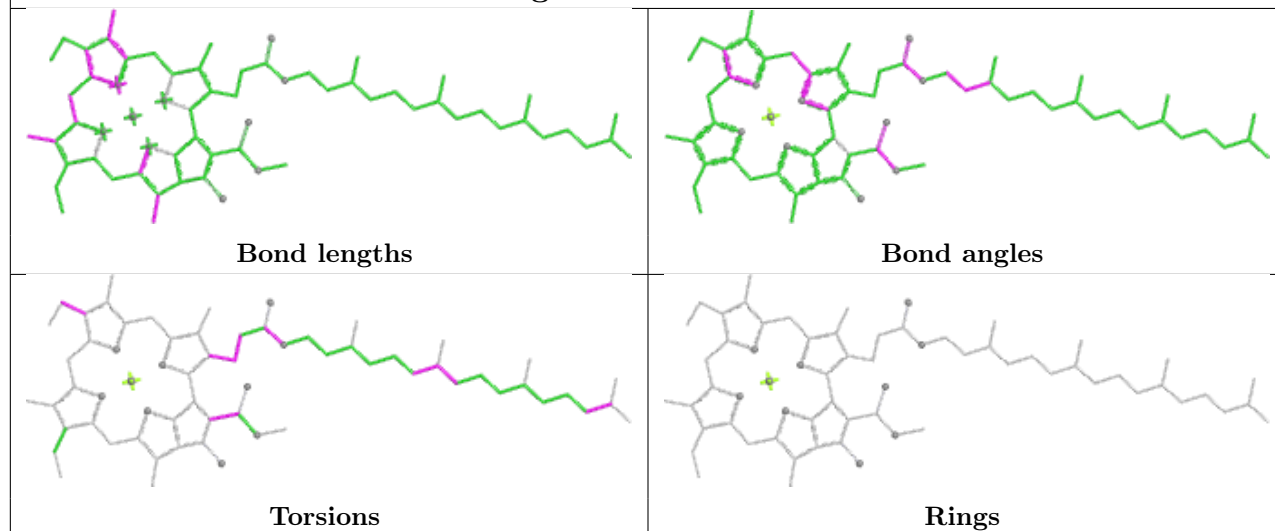
Ligand DD6 4 303



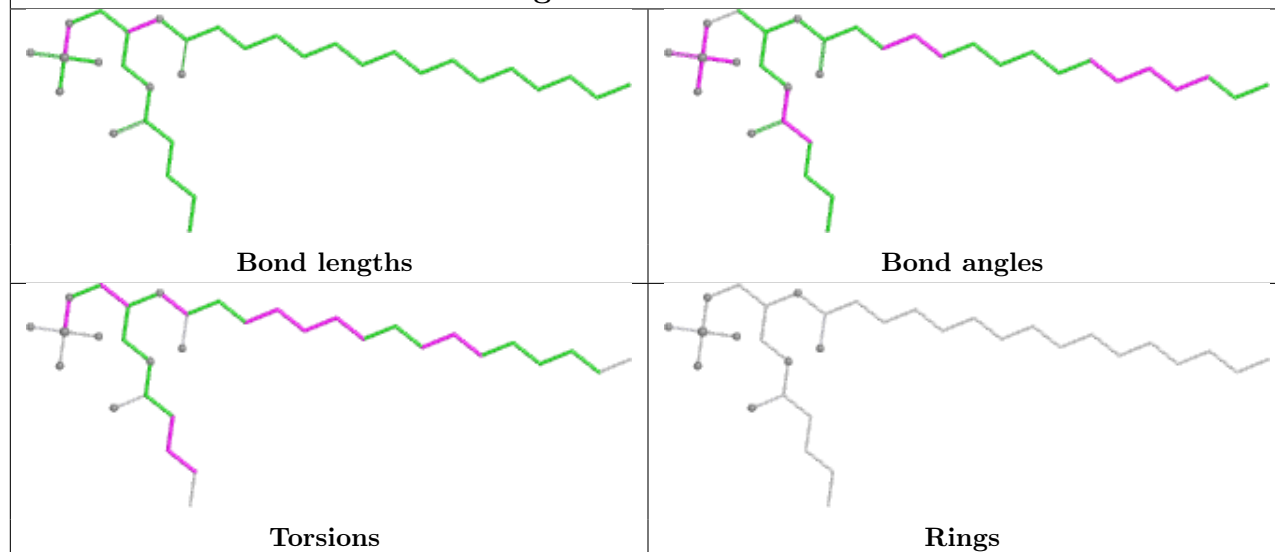
Ligand CLA 7 312

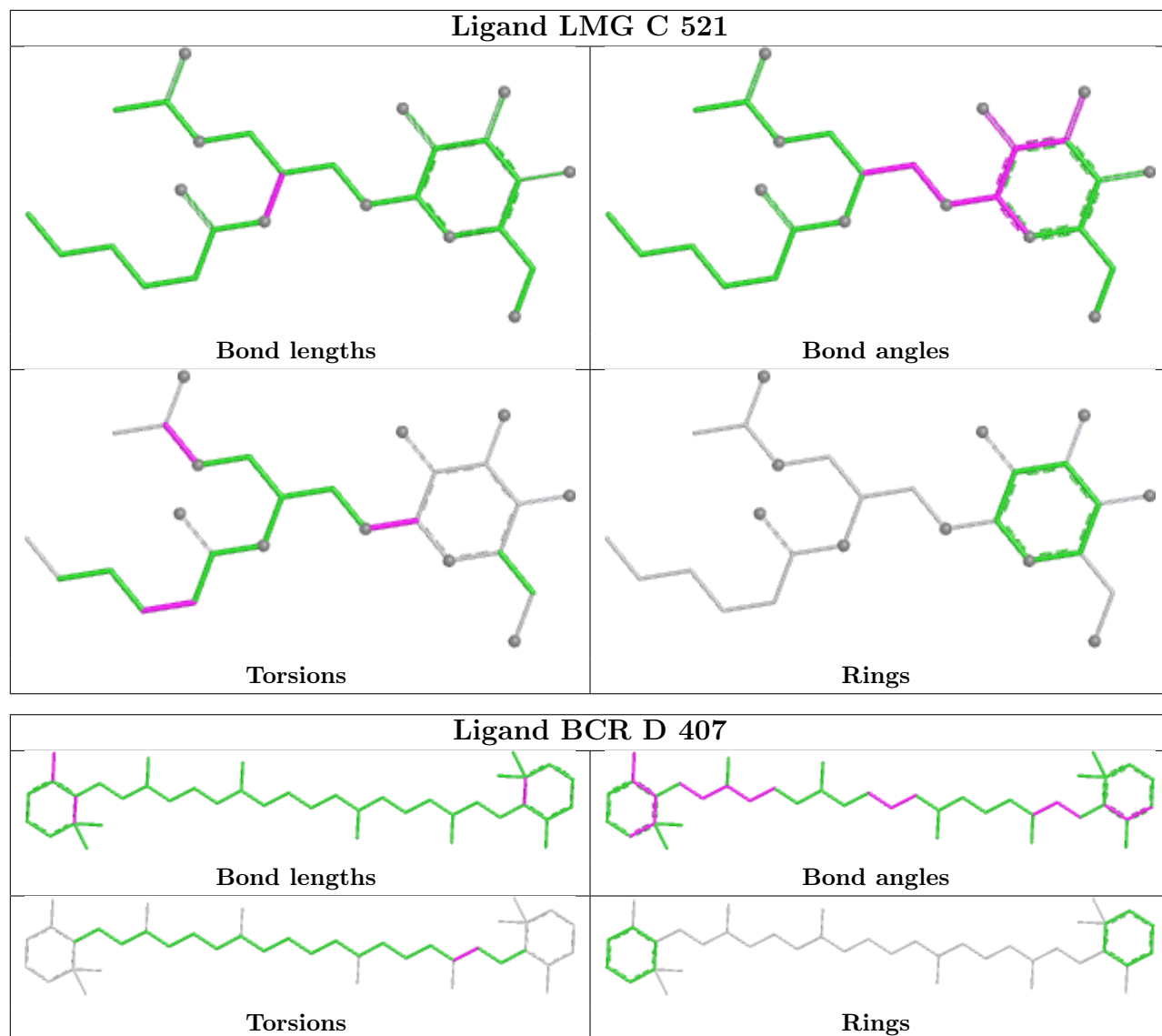


Ligand CLA B 616

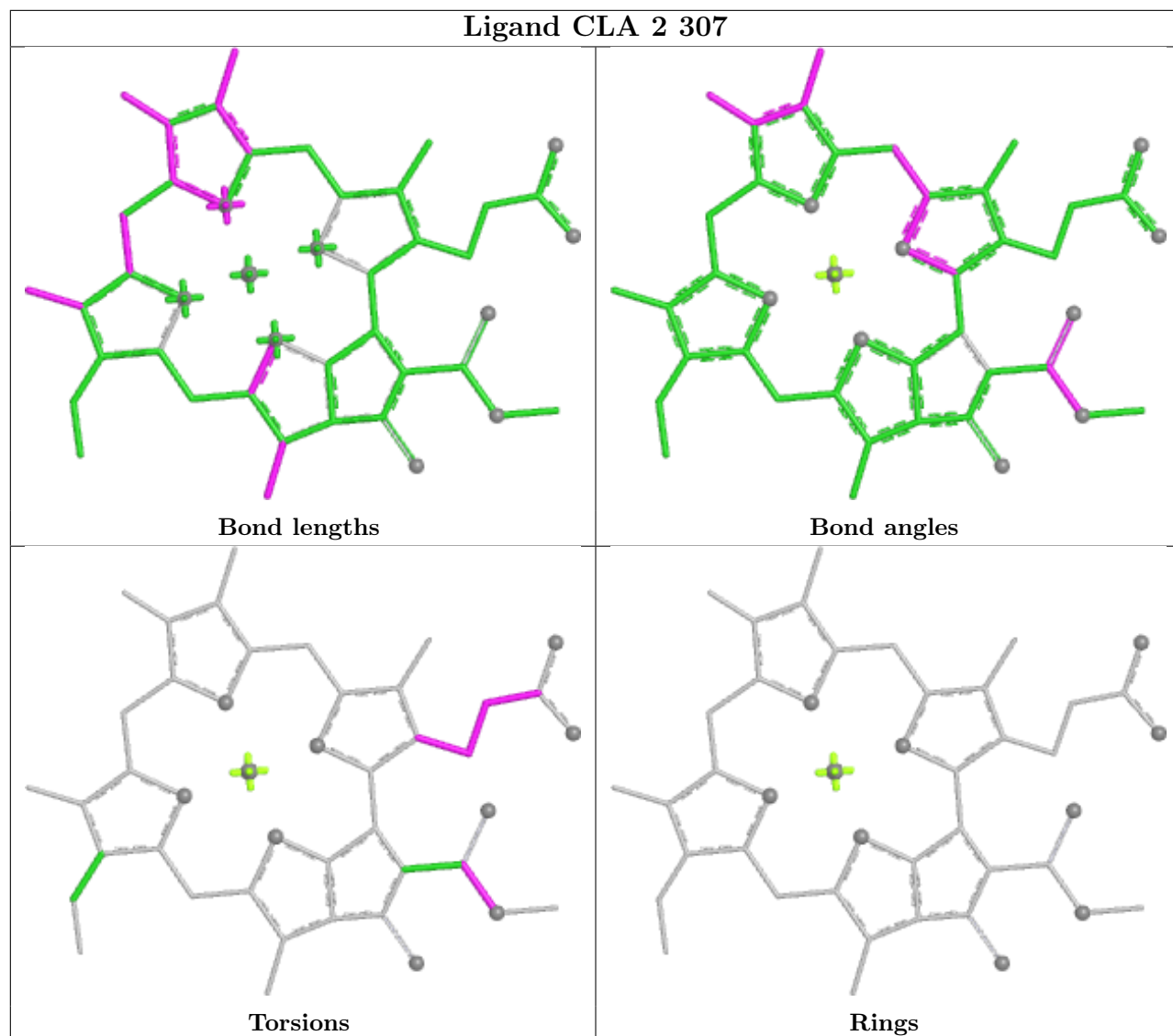


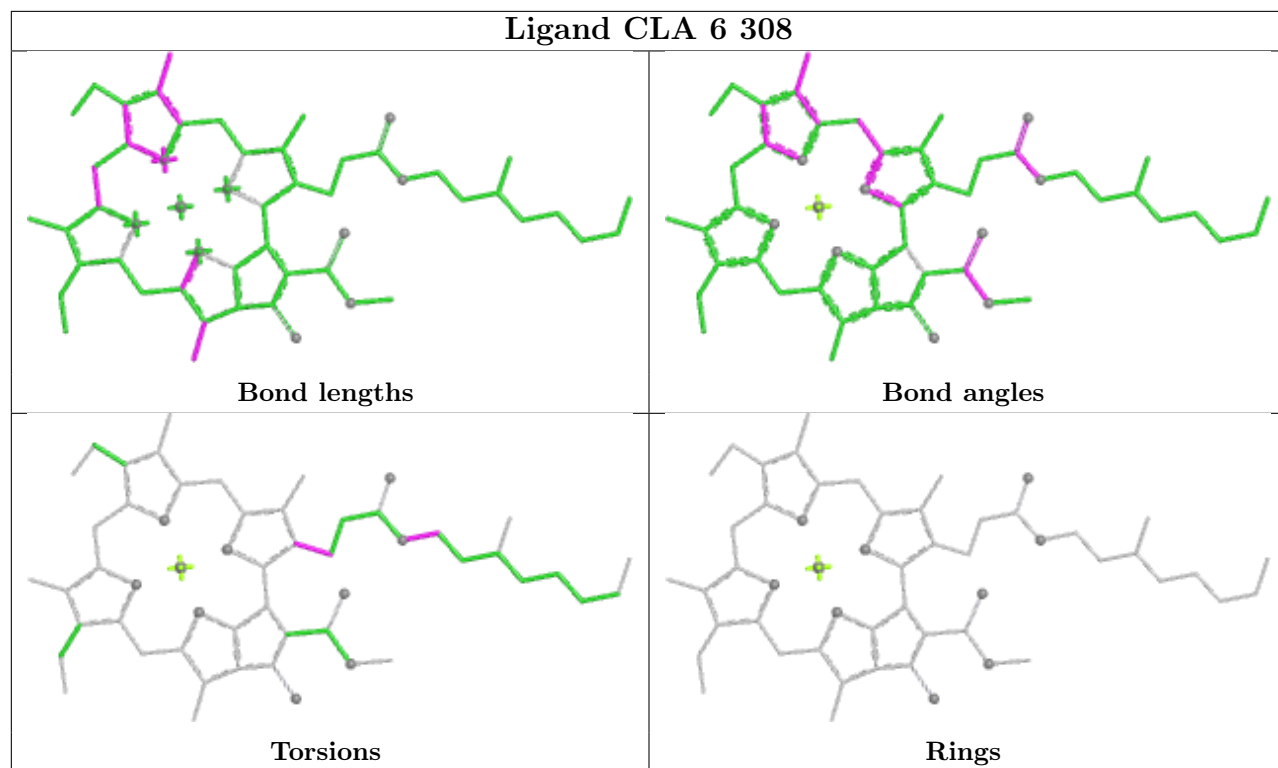
Ligand LHG 5 318



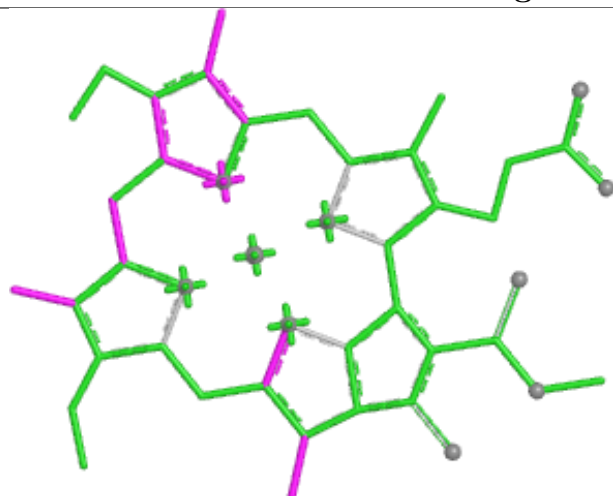


Ligand CLA 2 307

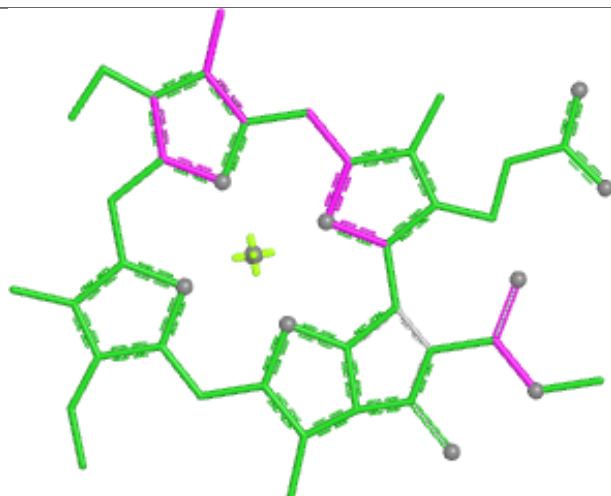




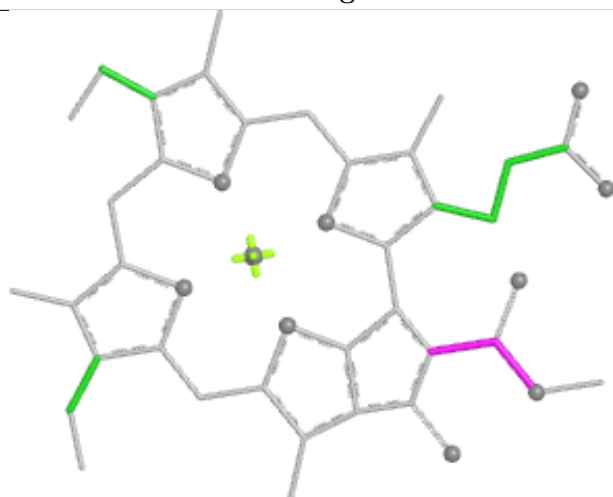
Ligand CLA C 506



Bond lengths



Bond angles

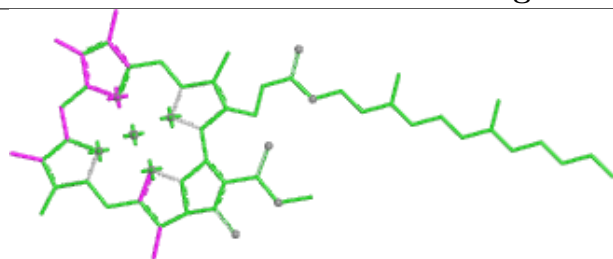


Torsions

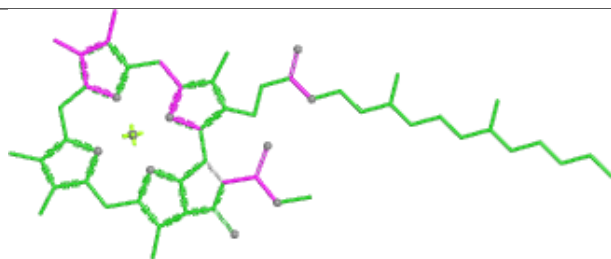


Rings

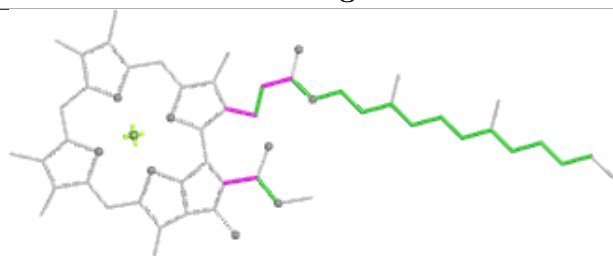
Ligand CLA D 405



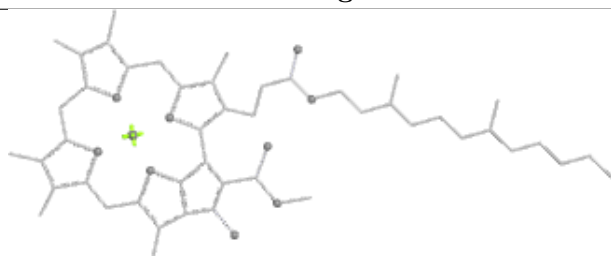
Bond lengths



Bond angles

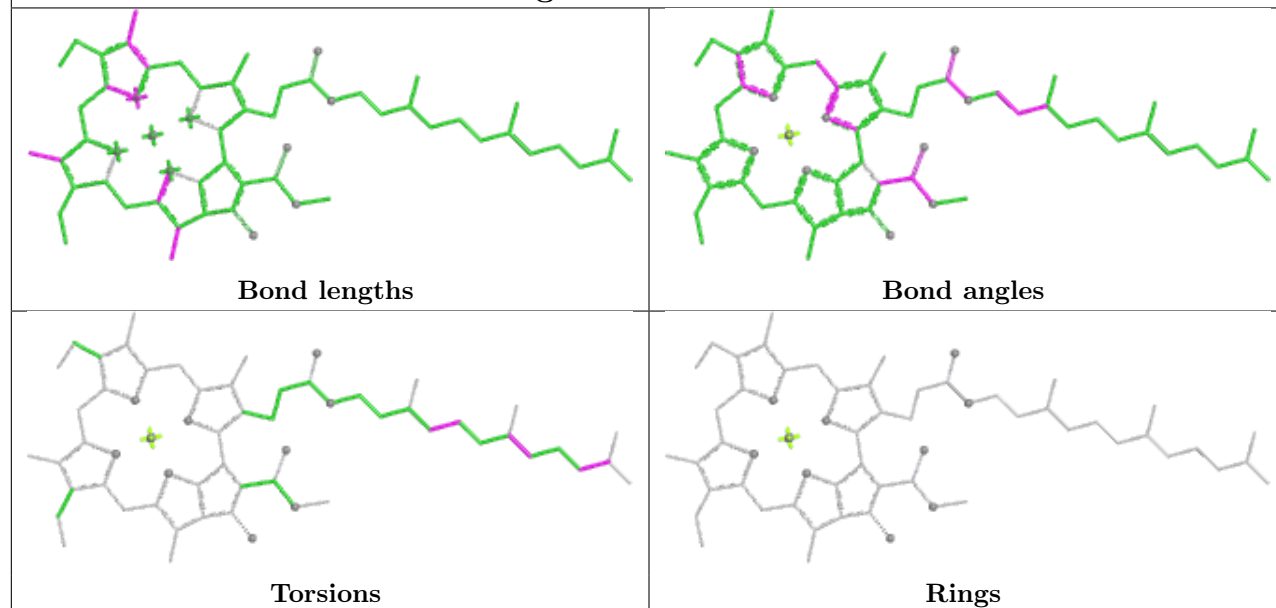


Torsions

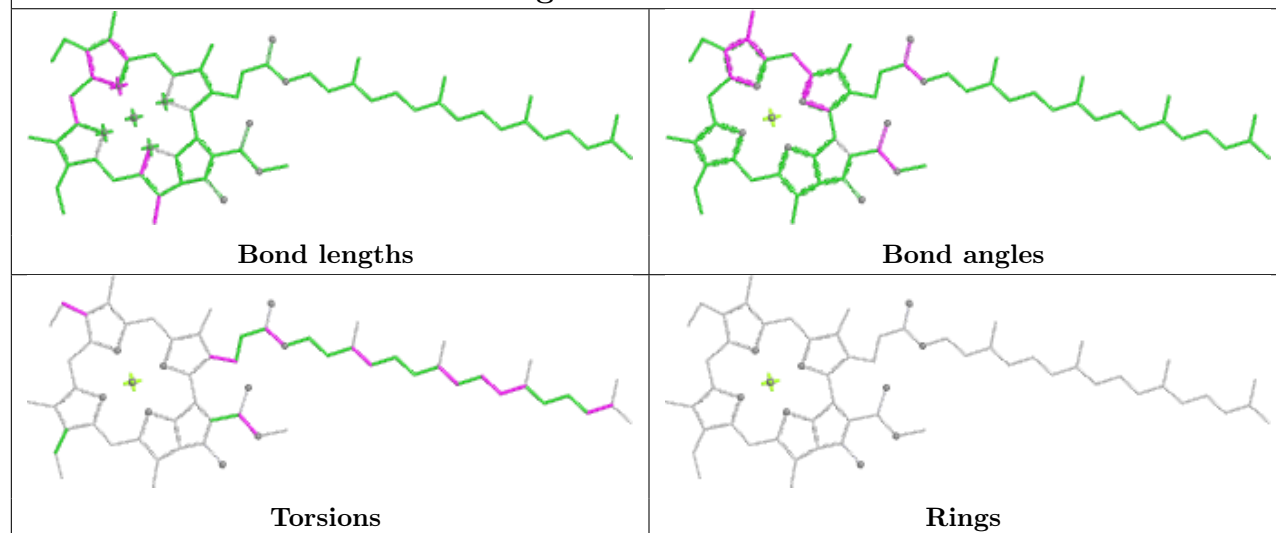


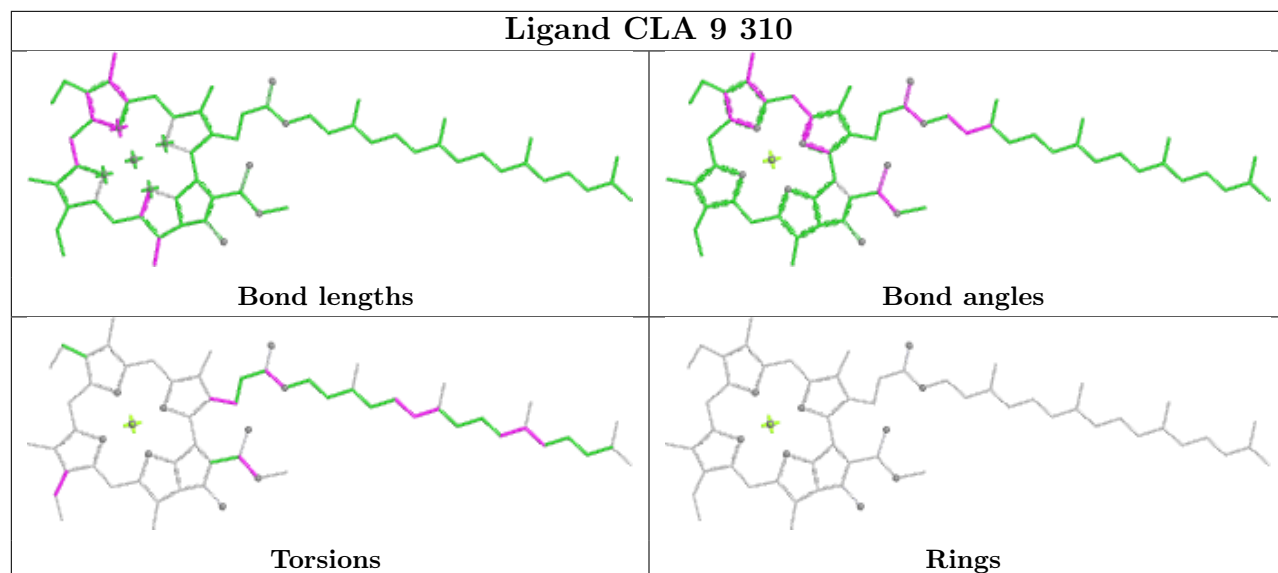
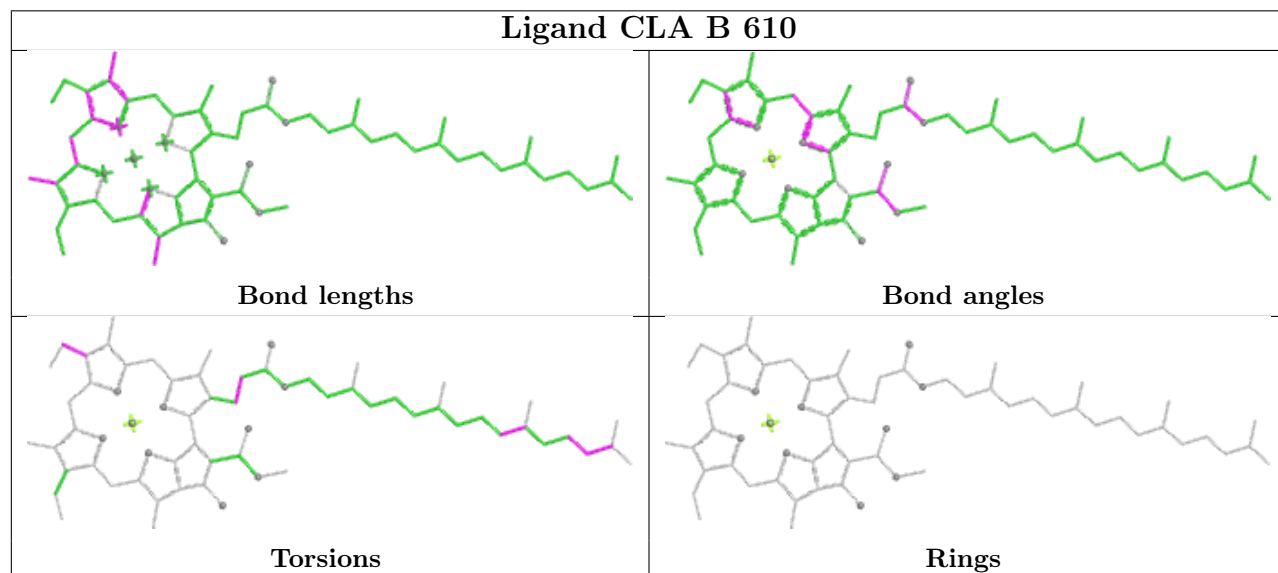
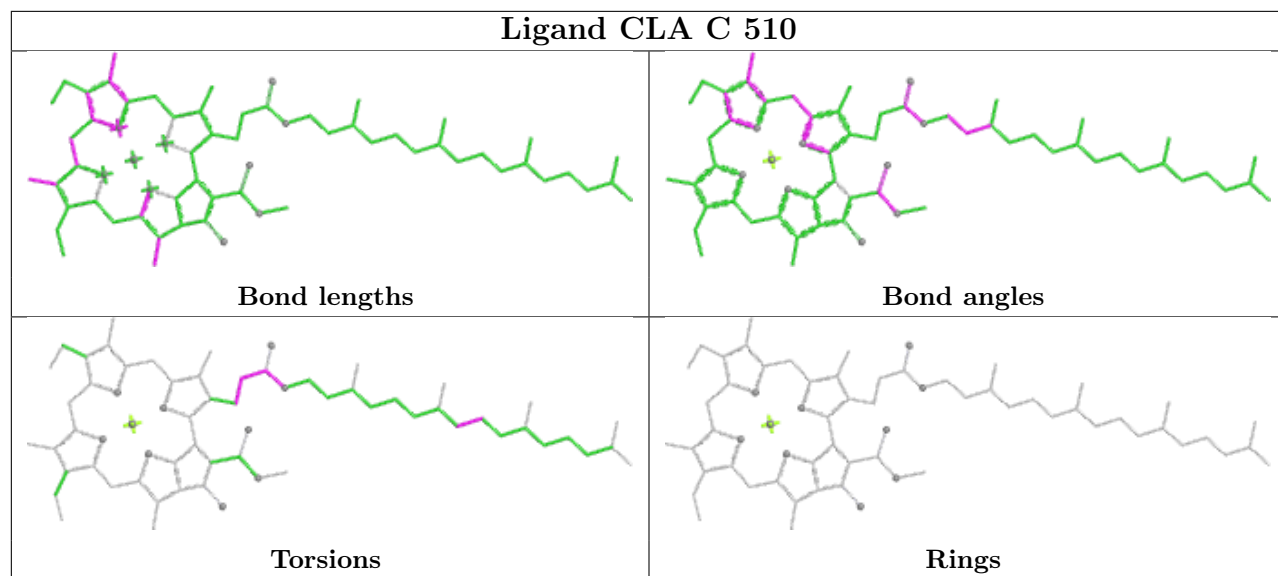
Rings

Ligand CLA a 411

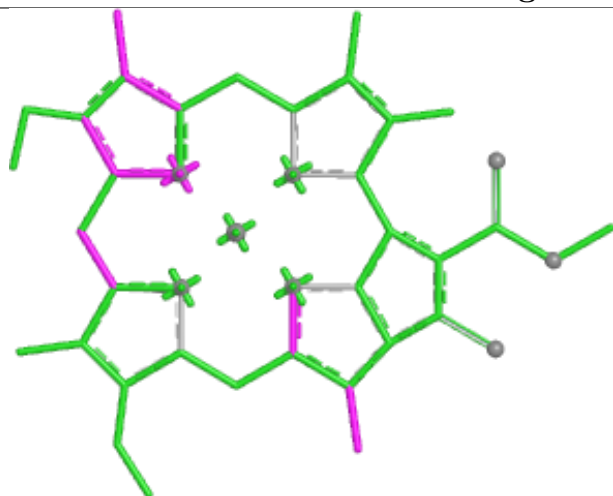


Ligand CLA 5 313

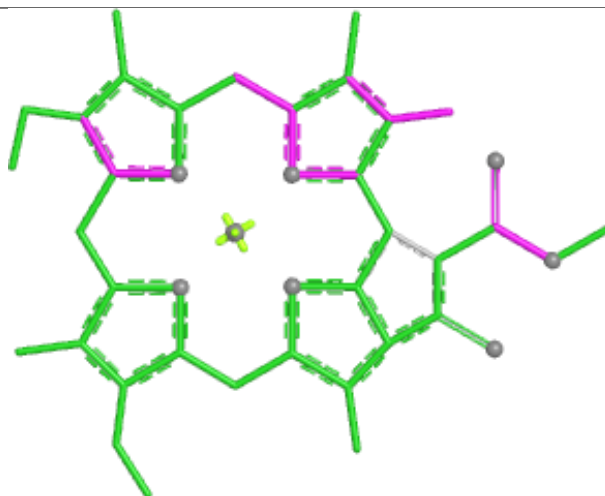




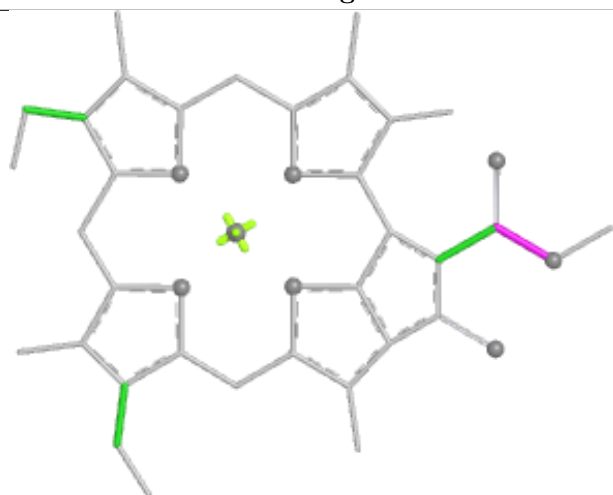
Ligand CLA 5 316



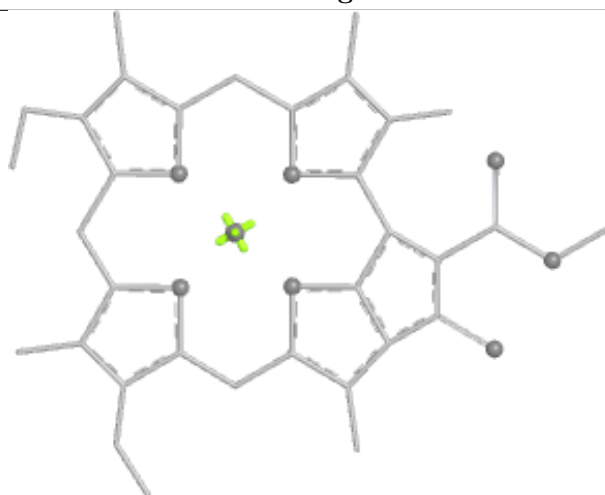
Bond lengths



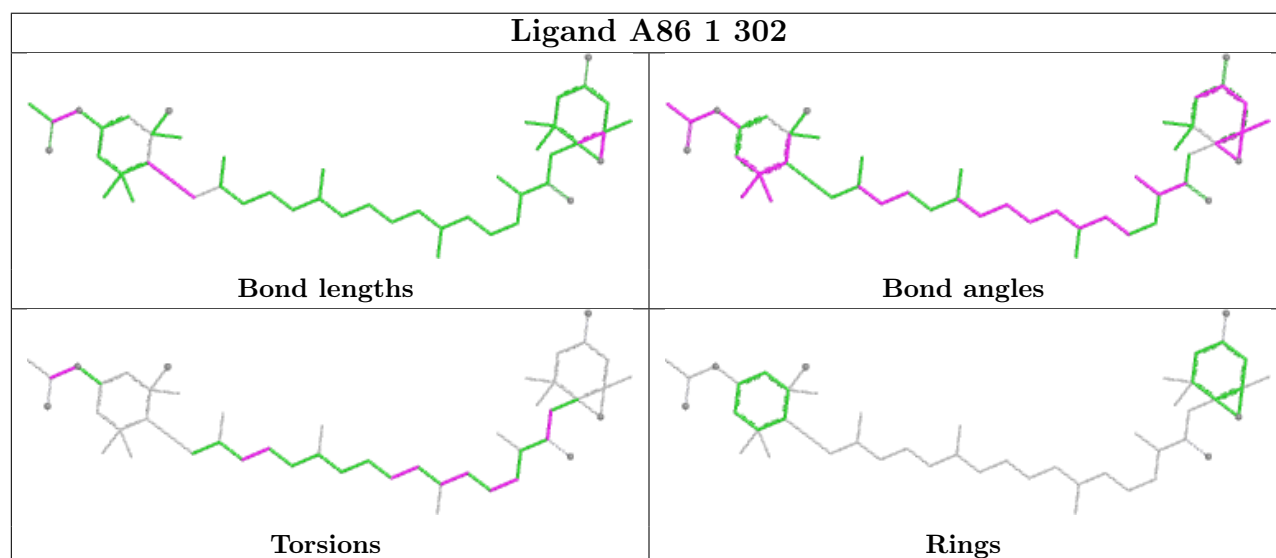
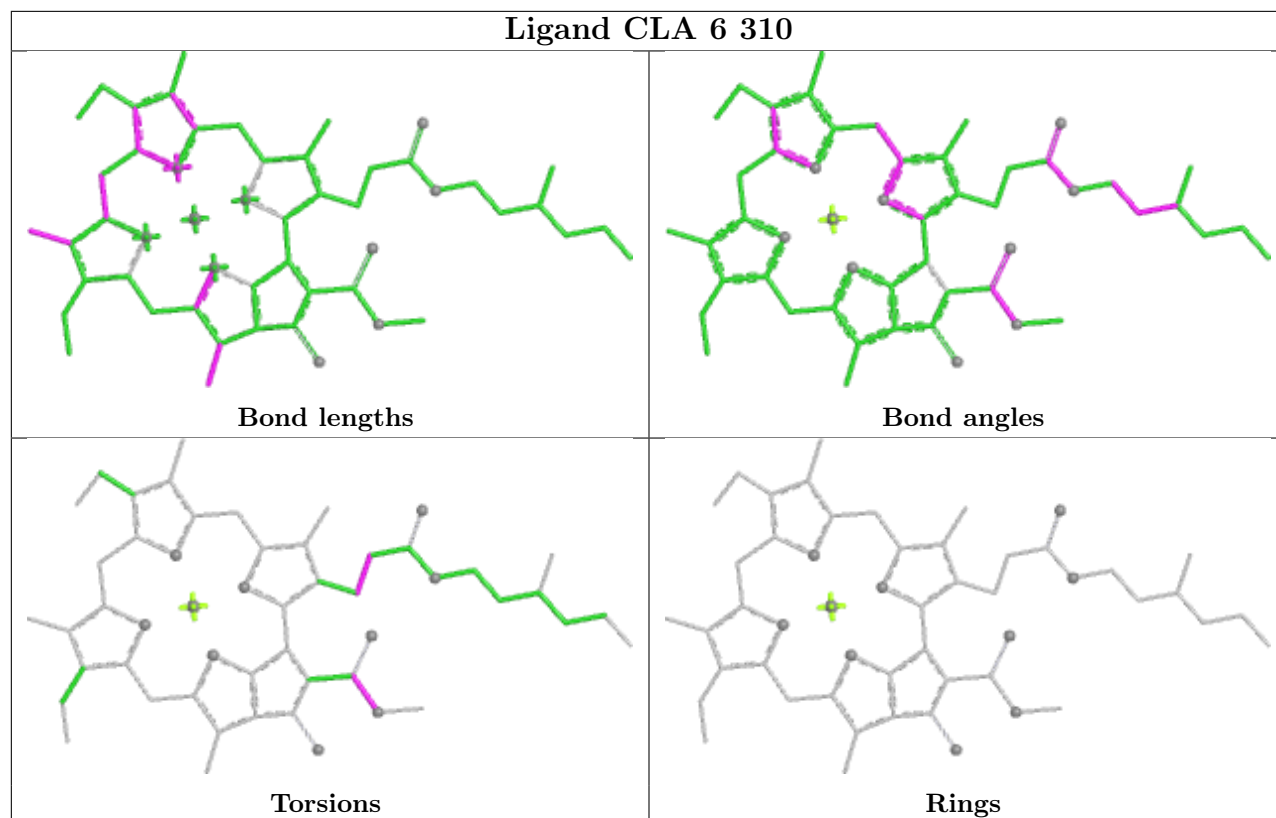
Bond angles

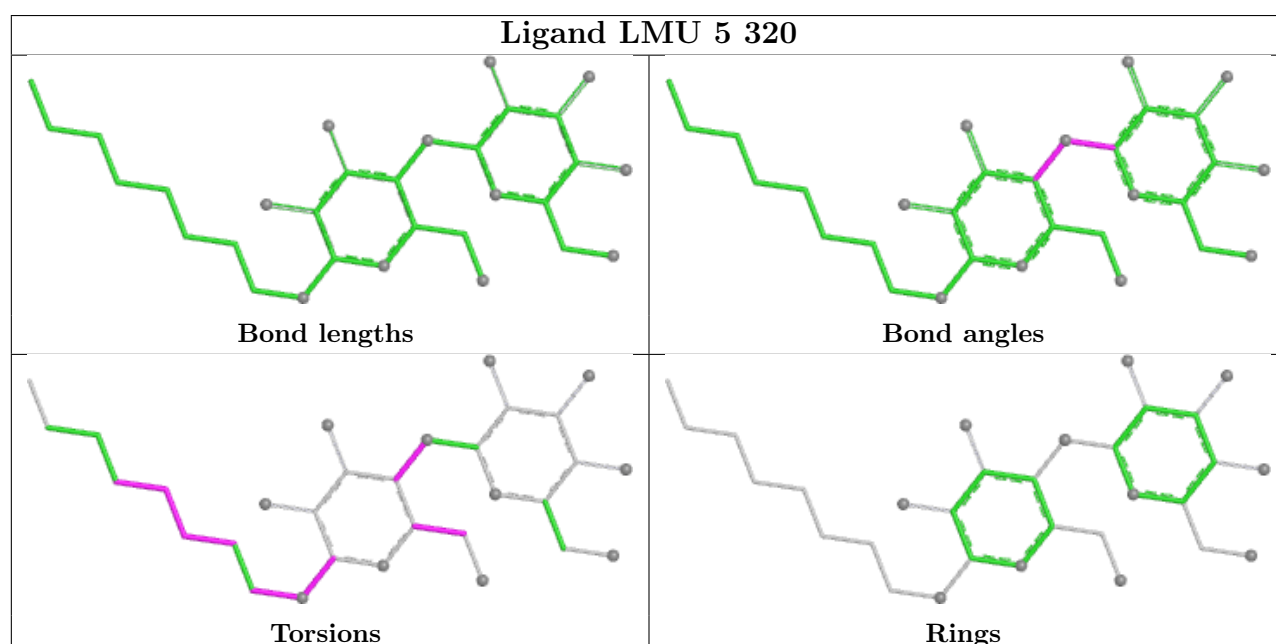
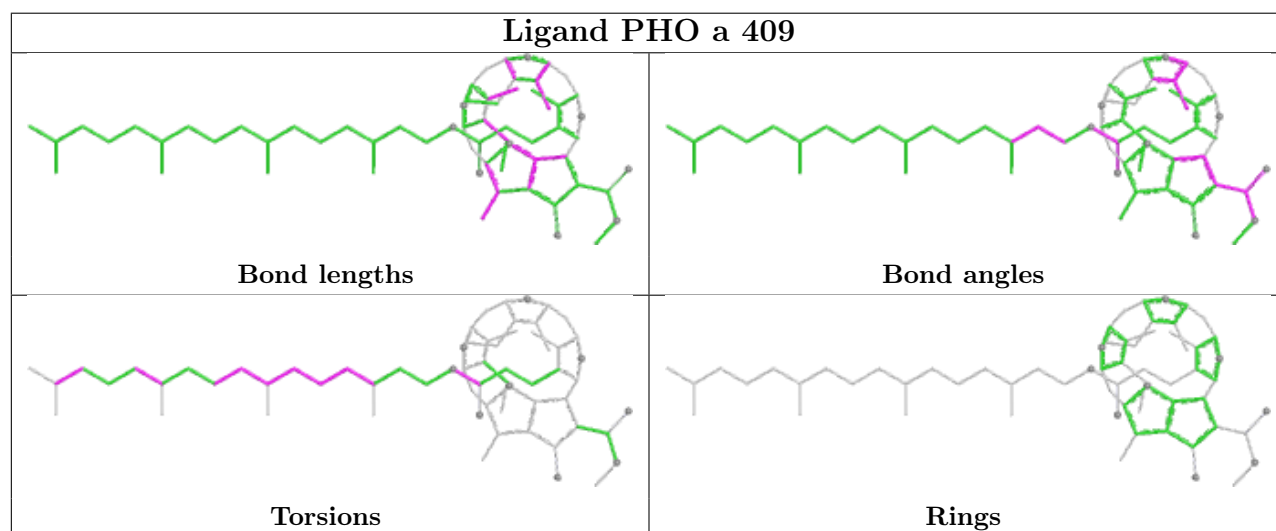
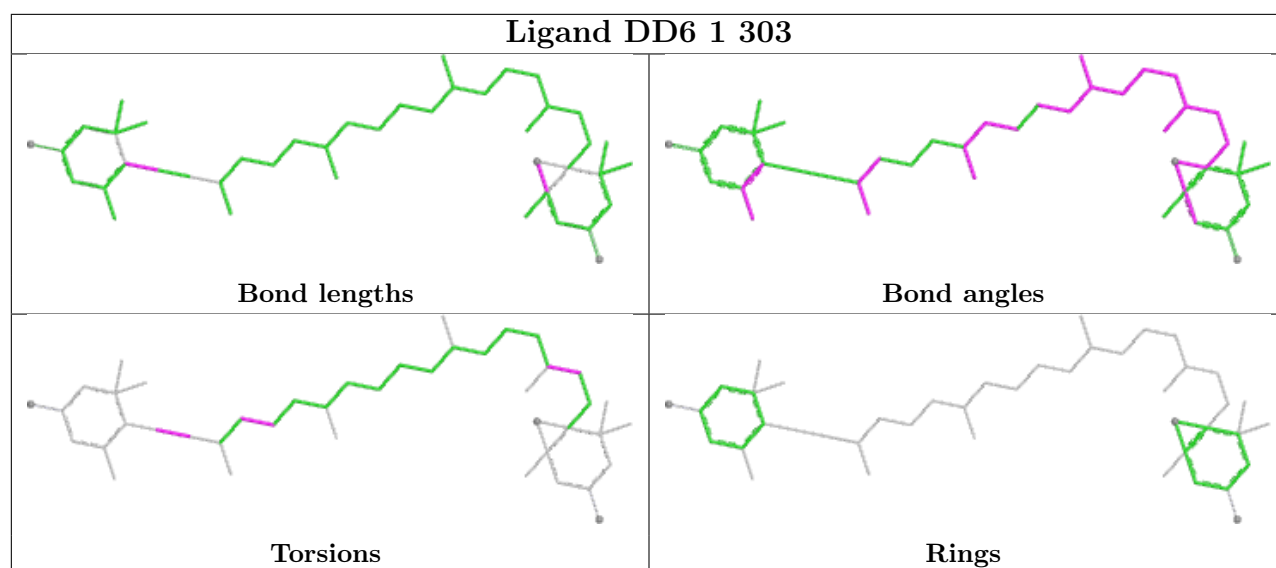


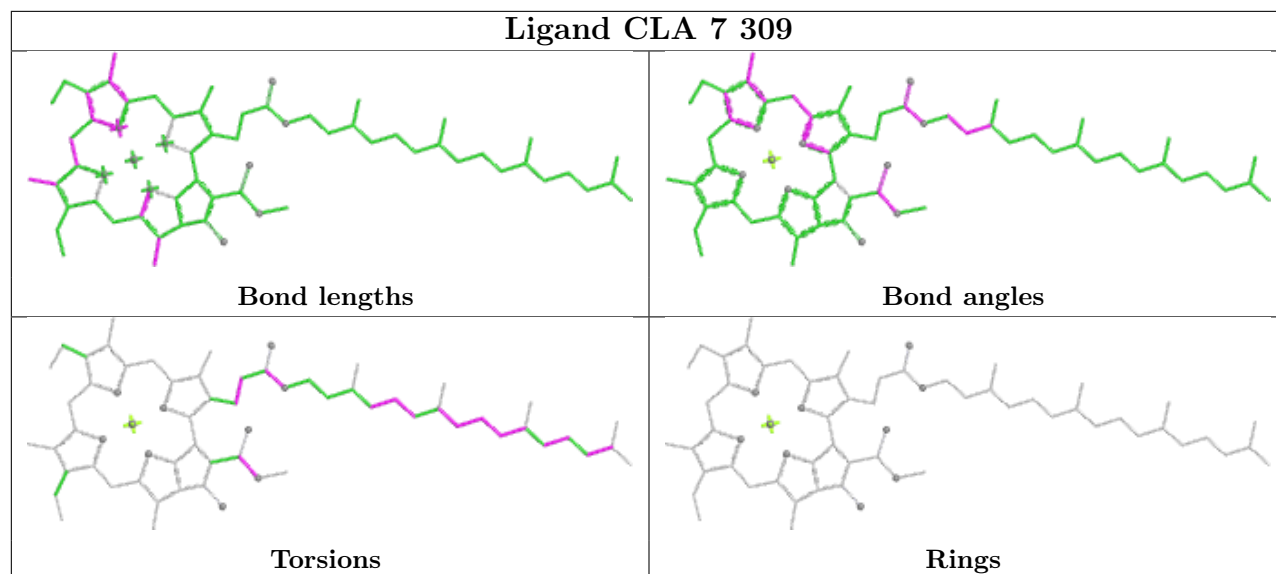
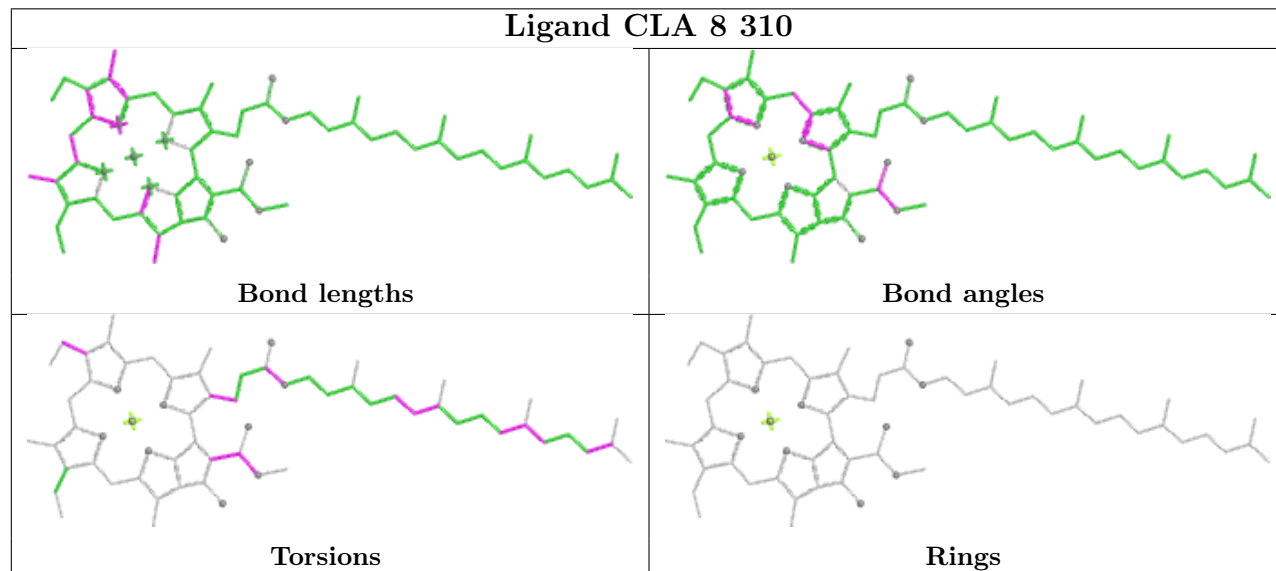
Torsions

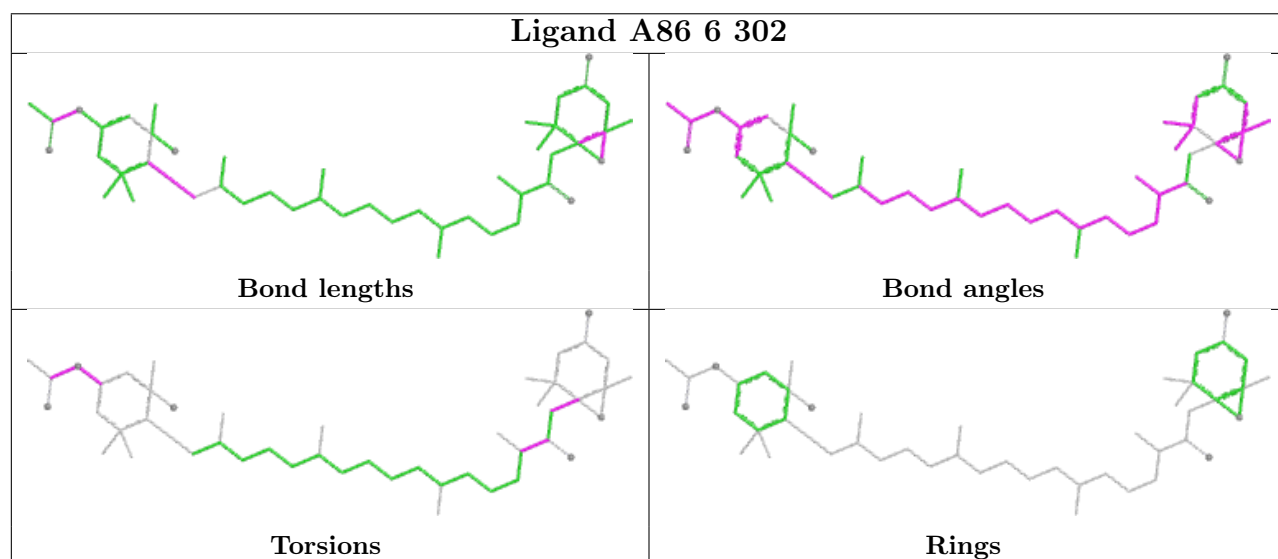
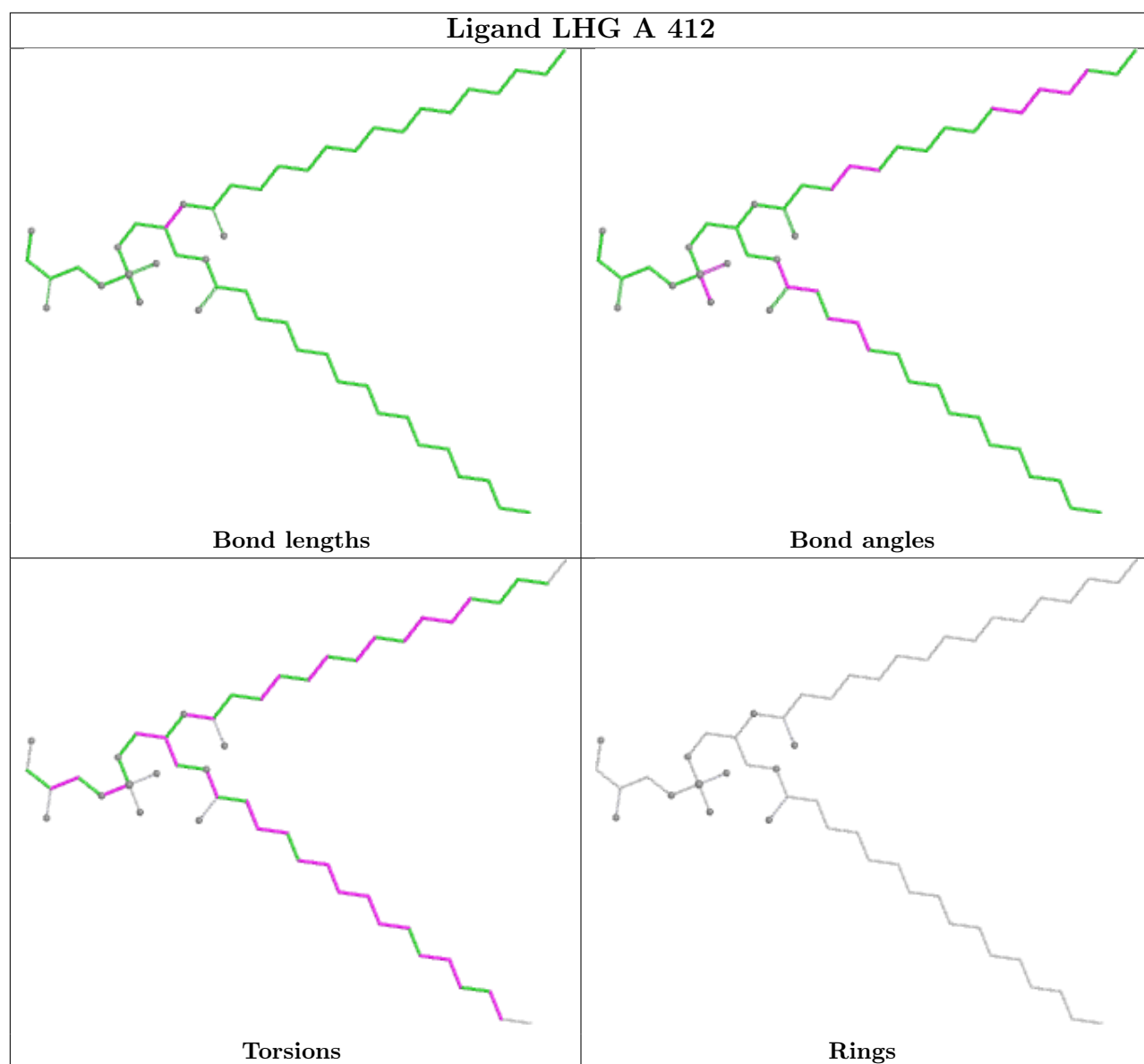


Rings

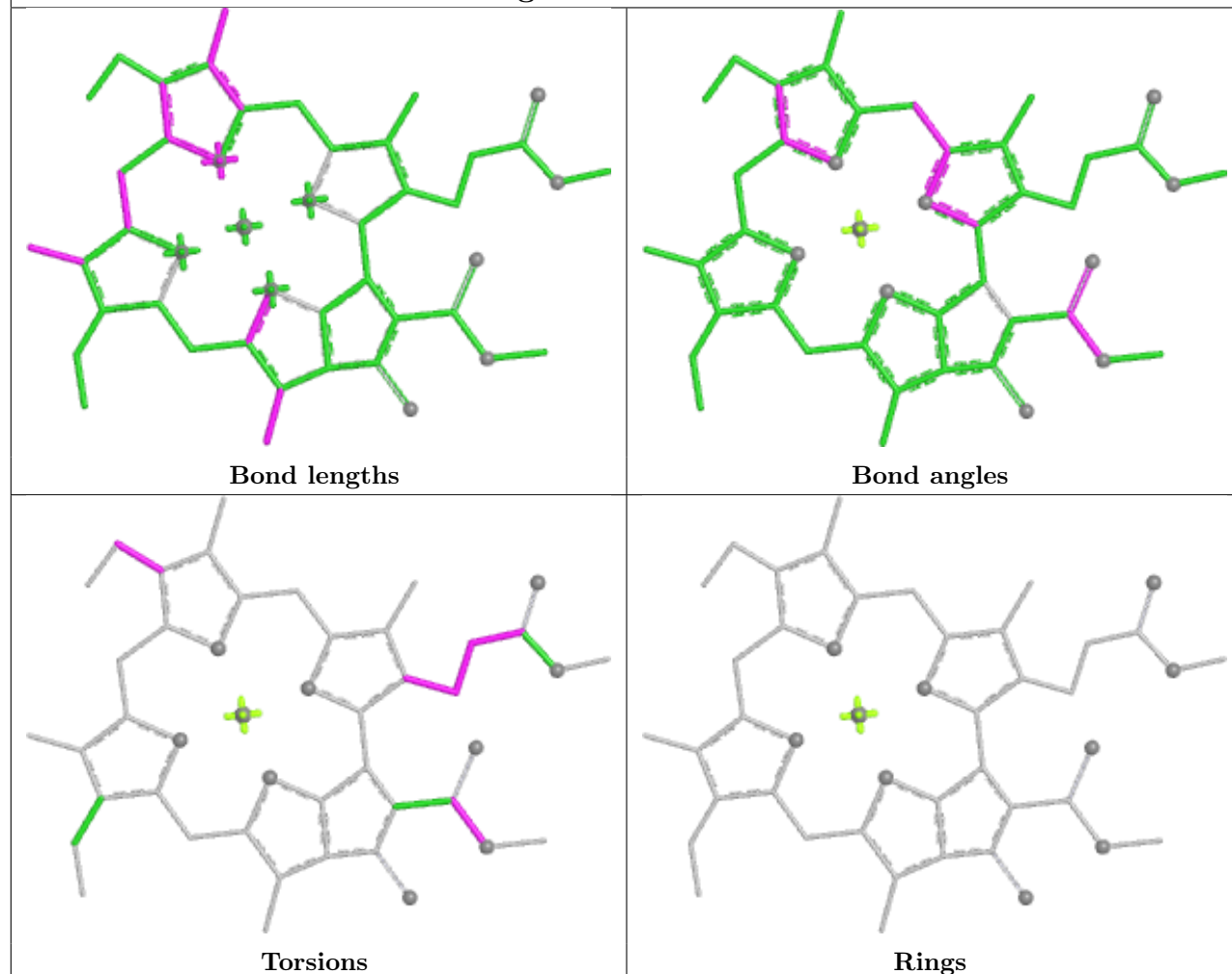




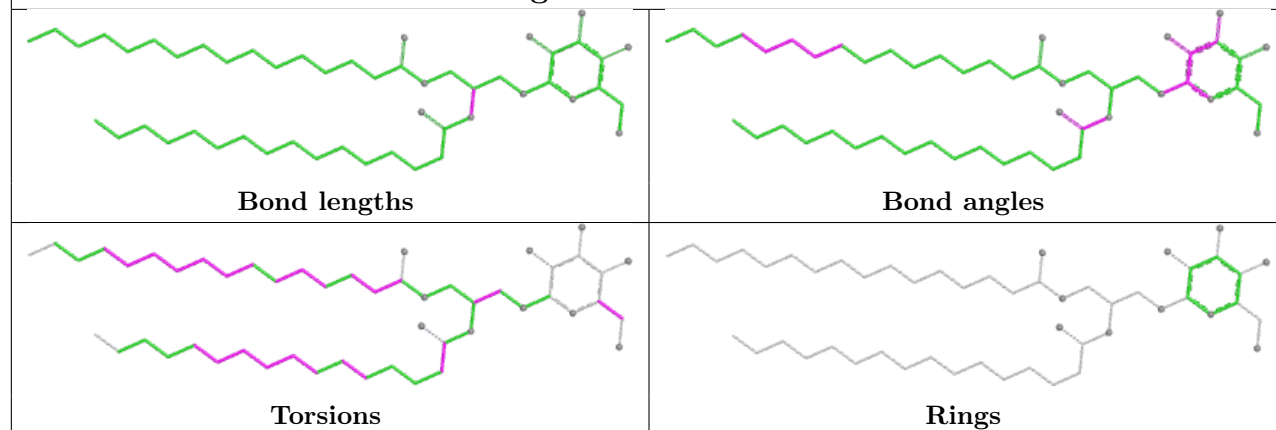
Ligand CLA 7 309**Ligand CLA 8 310**

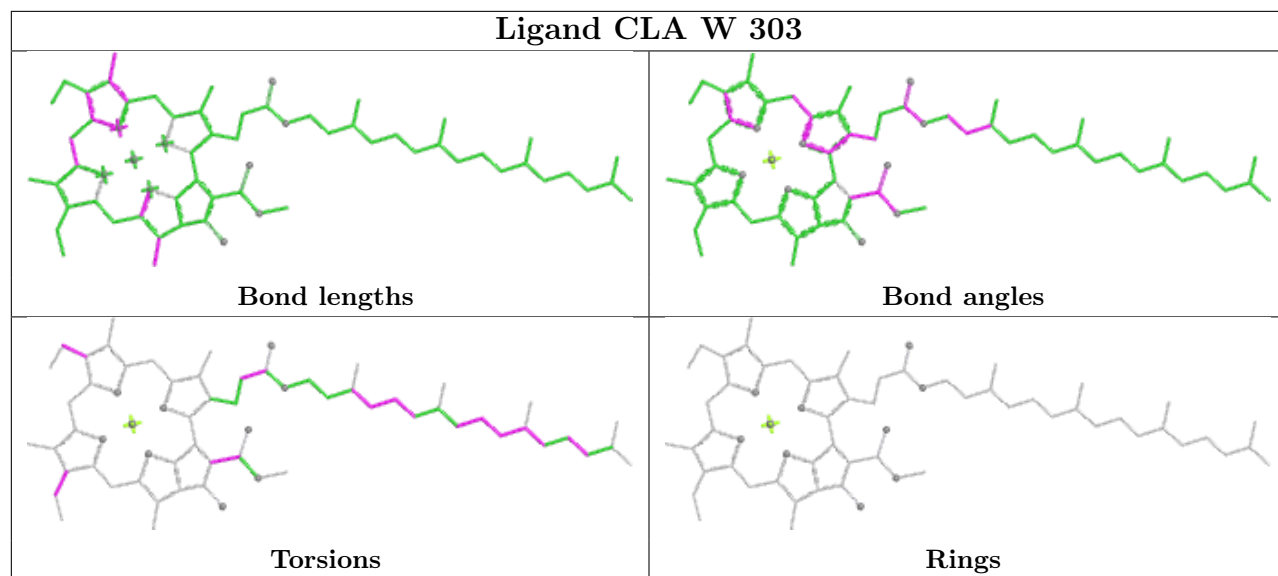


Ligand CLA 5 312

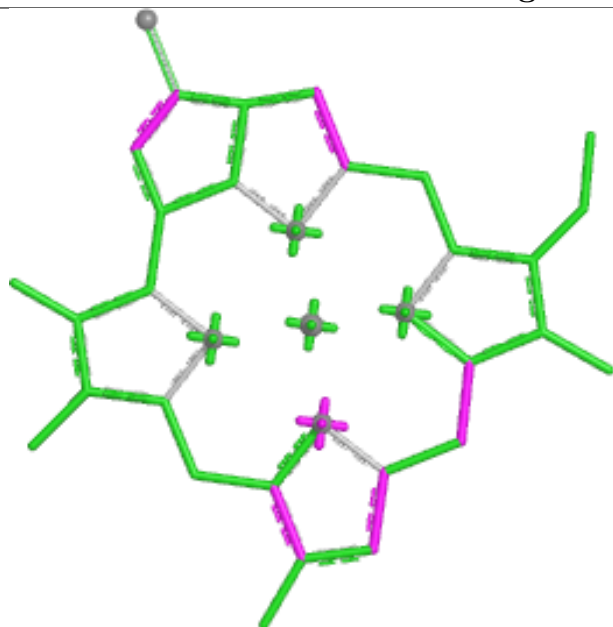


Ligand LMG b 621

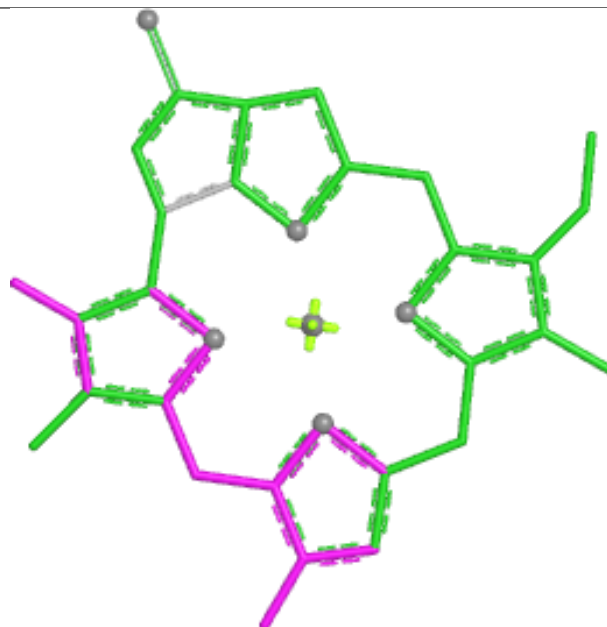




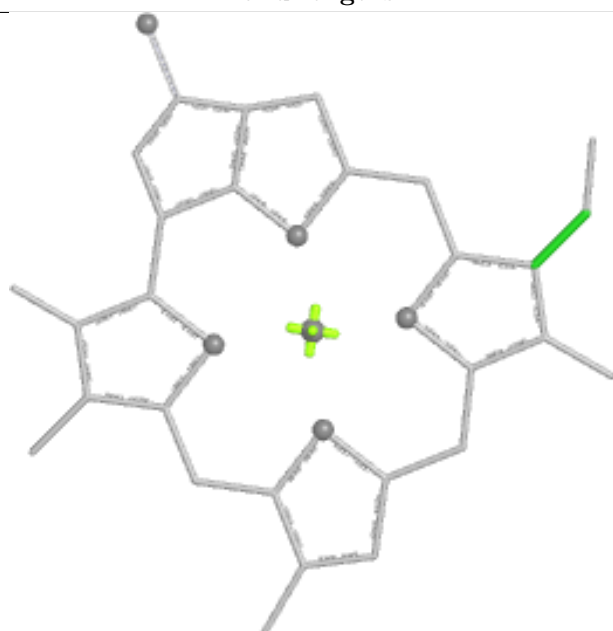
Ligand CLA 7 313



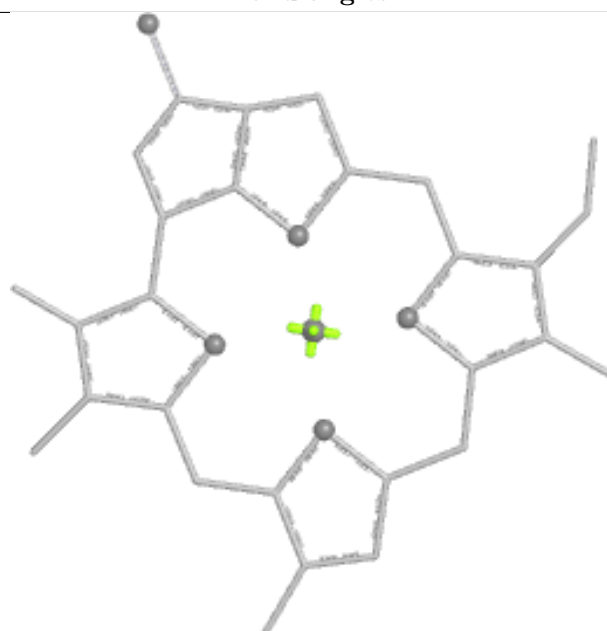
Bond lengths



Bond angles

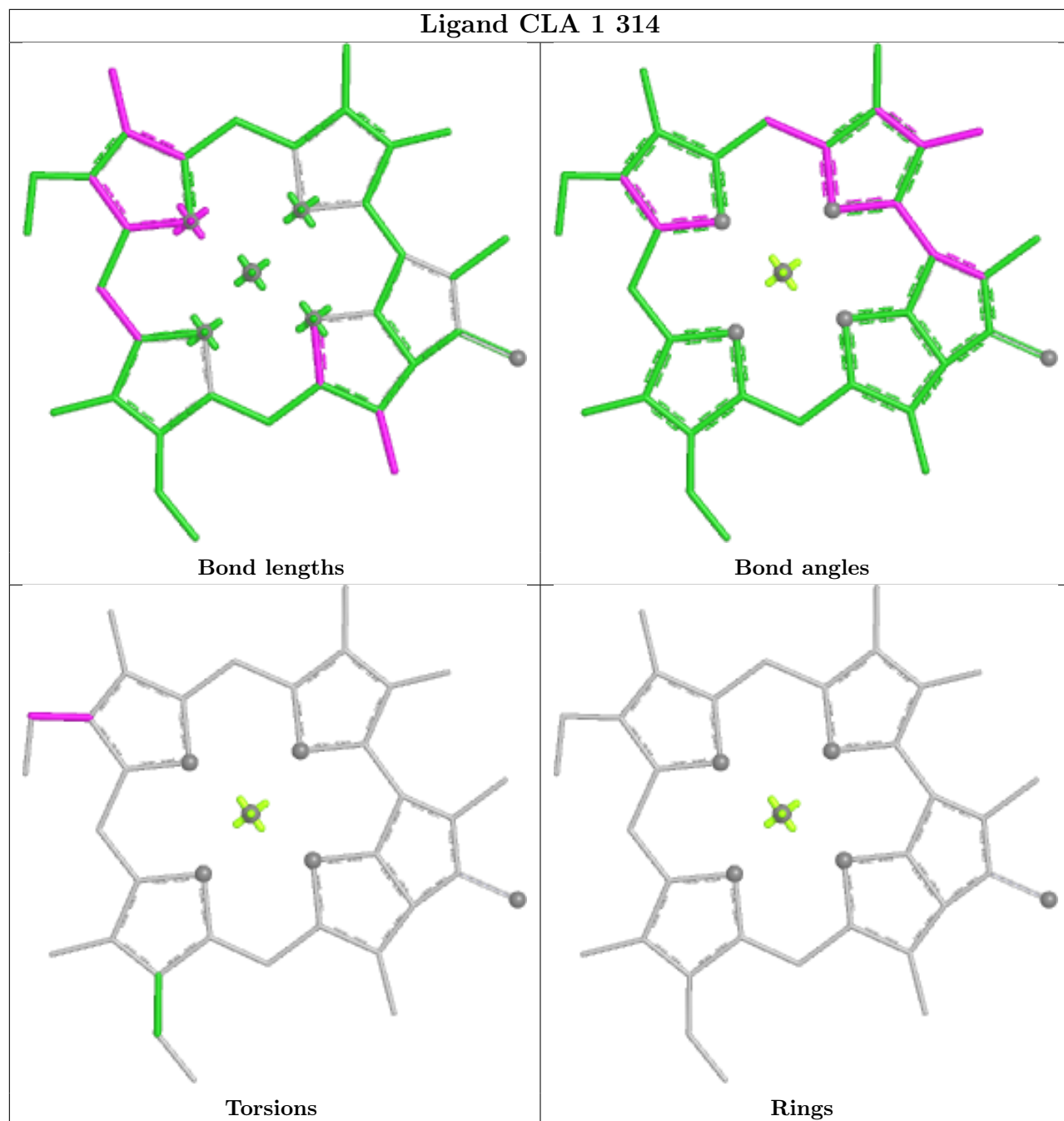


Torsions

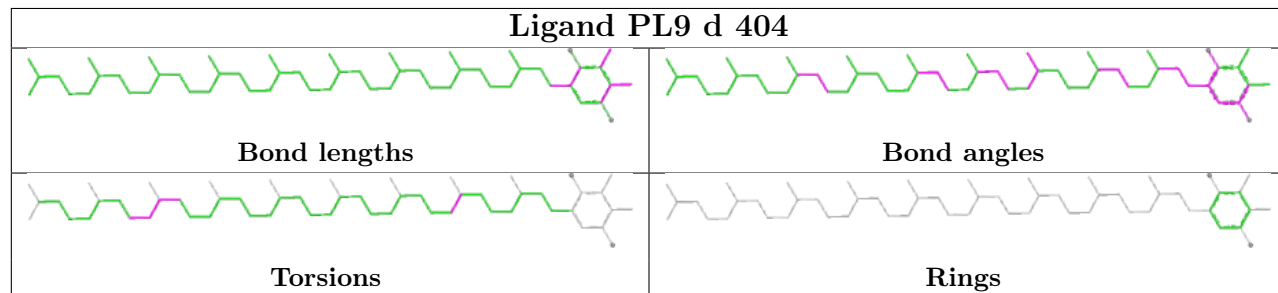


Rings

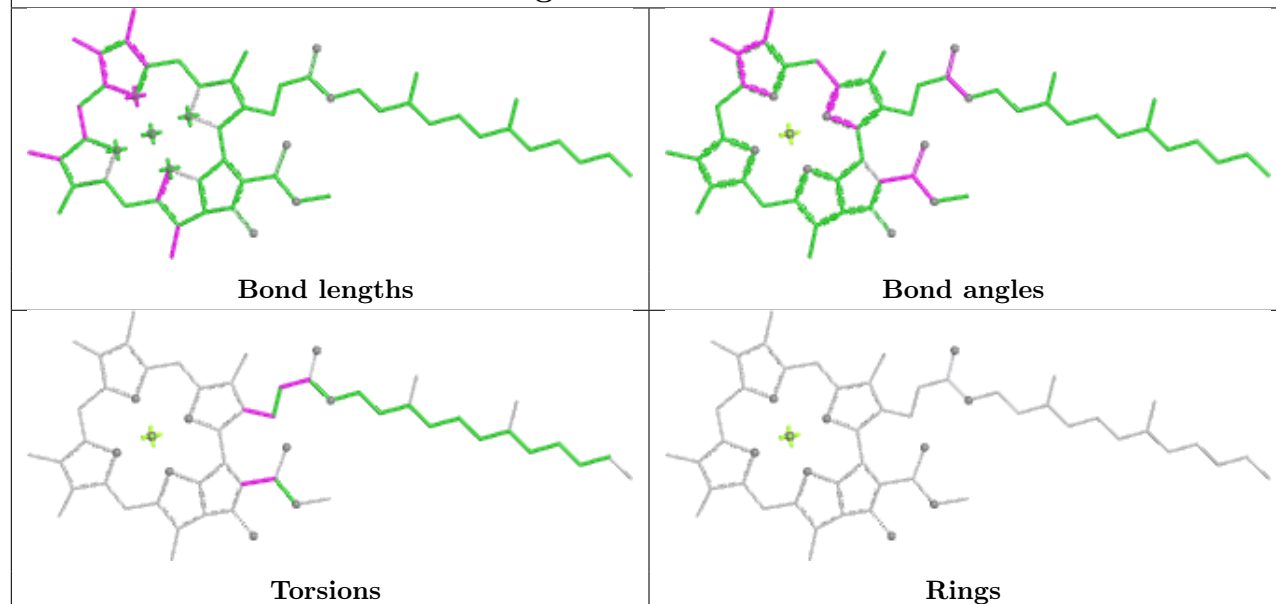
Ligand CLA 1 314



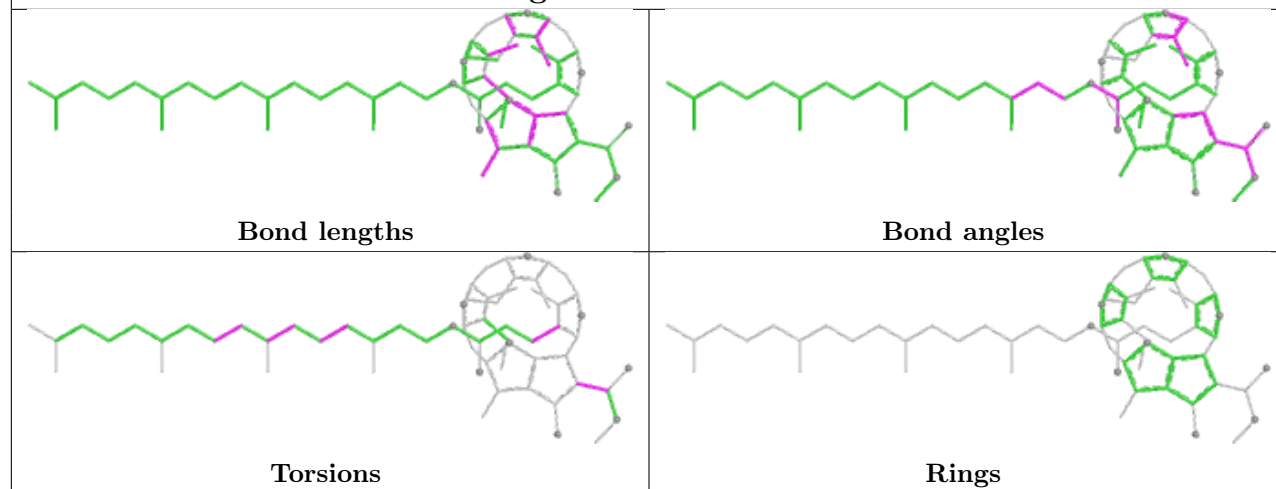
Ligand PL9 d 404



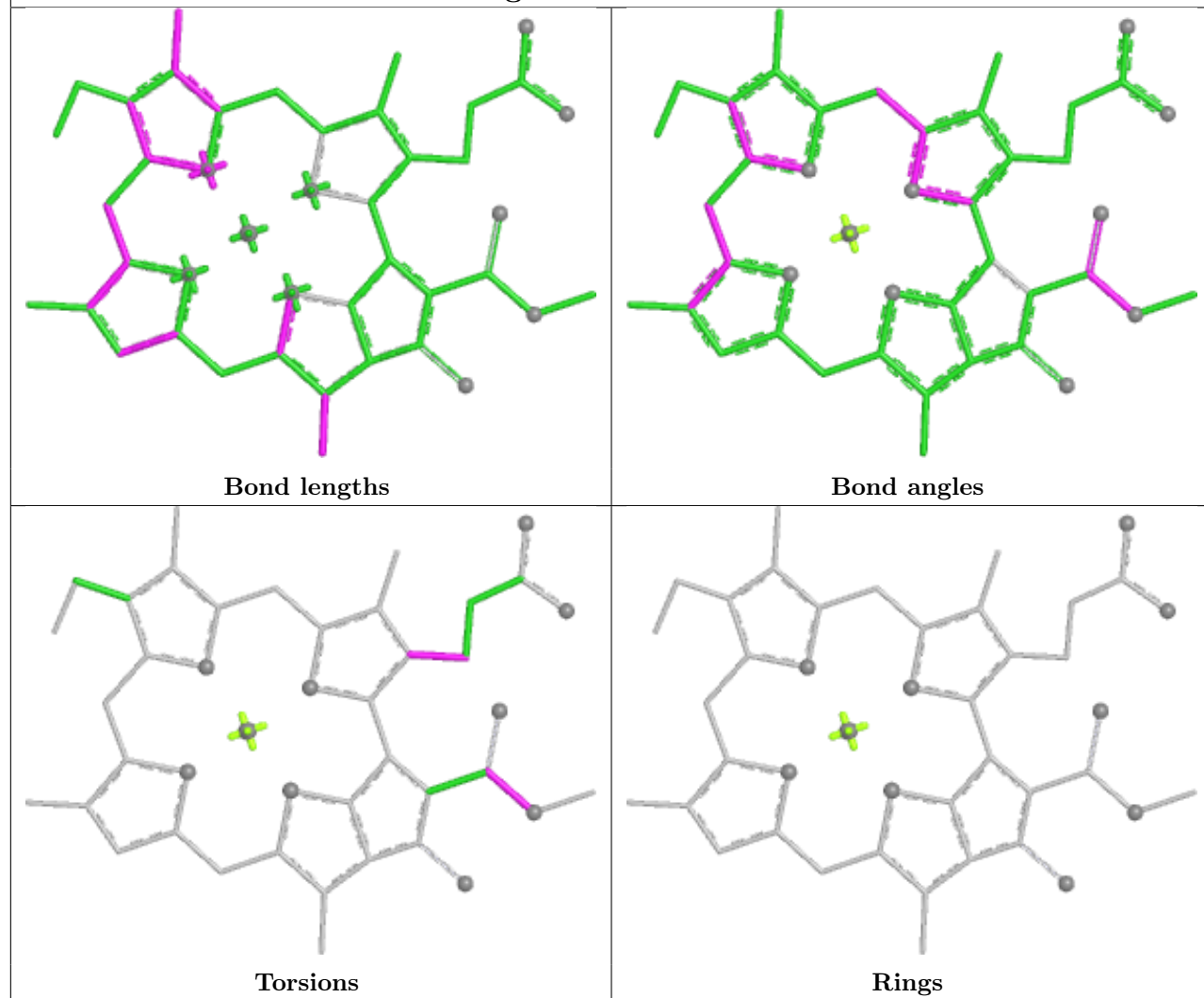
Ligand CLA d 401



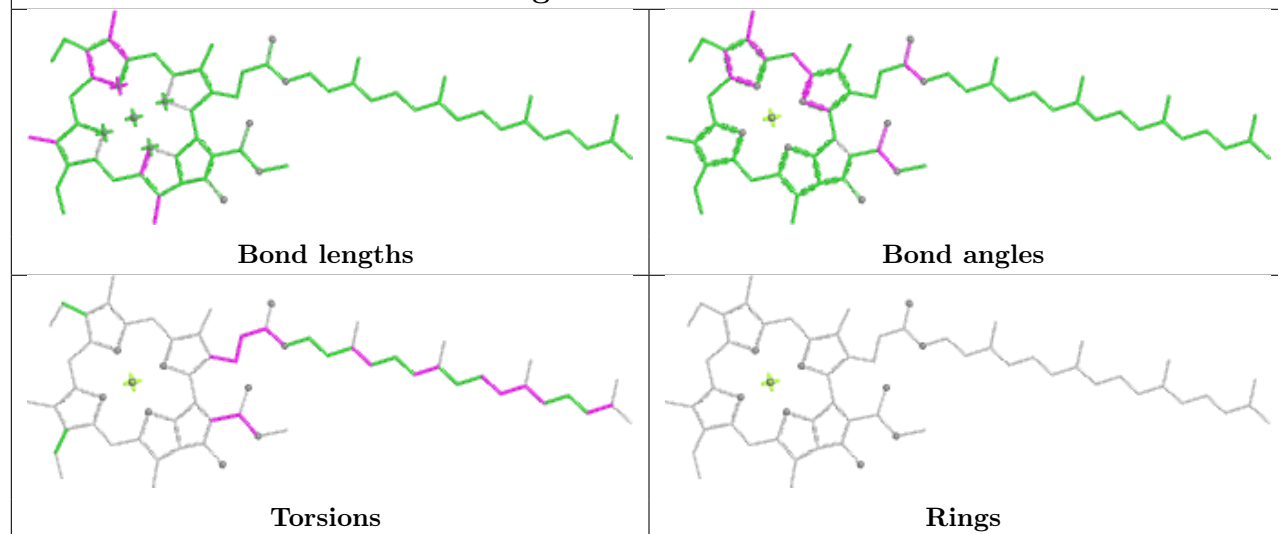
Ligand PHO A 407



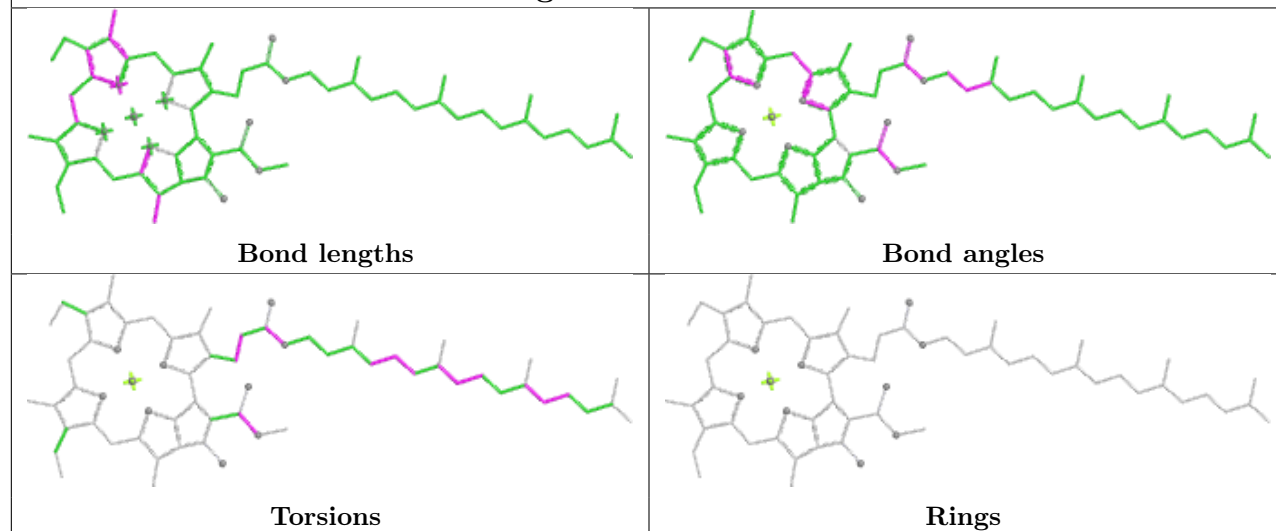
Ligand CLA 8 309



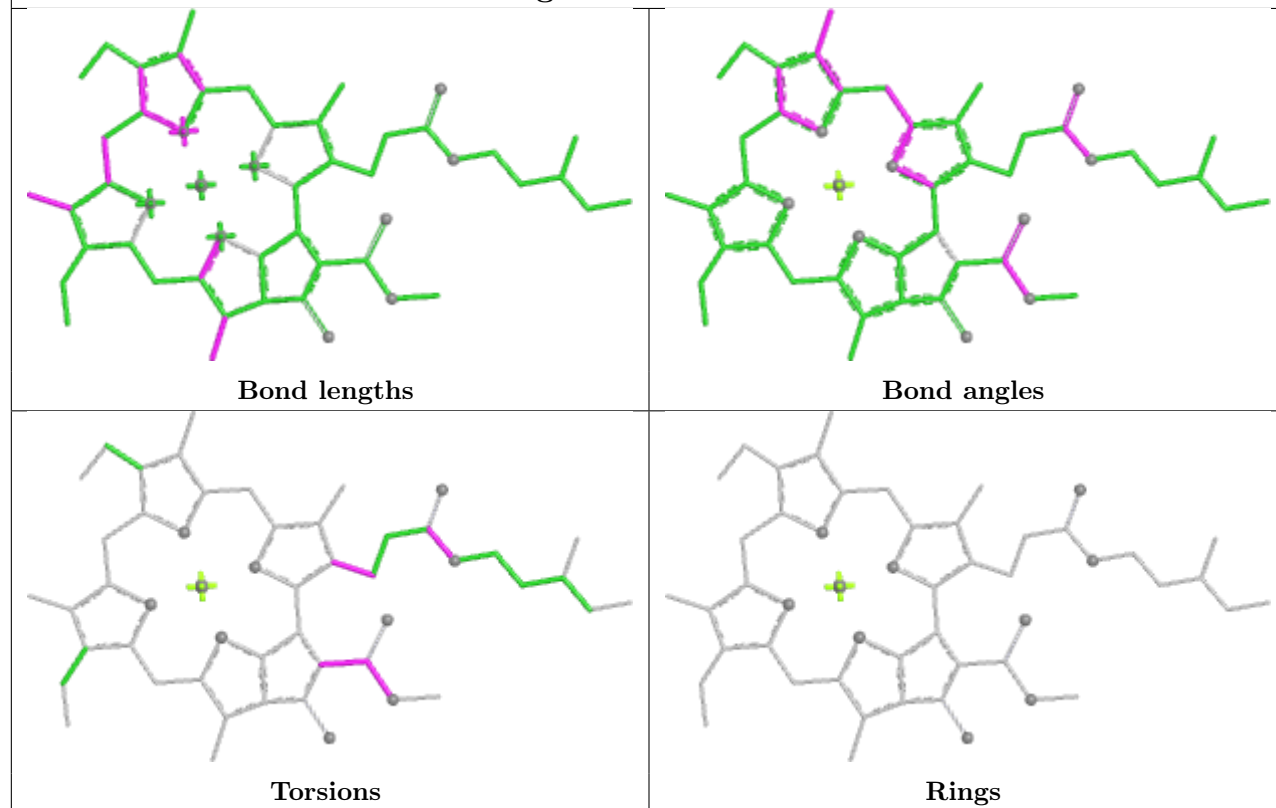
Ligand CLA C 501

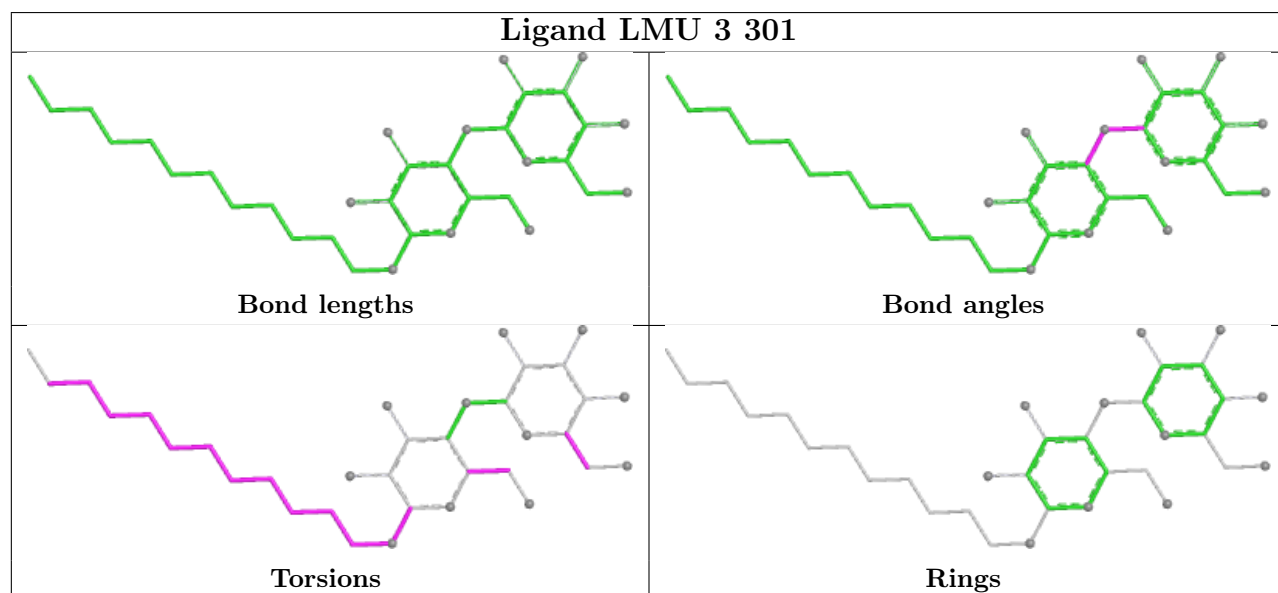
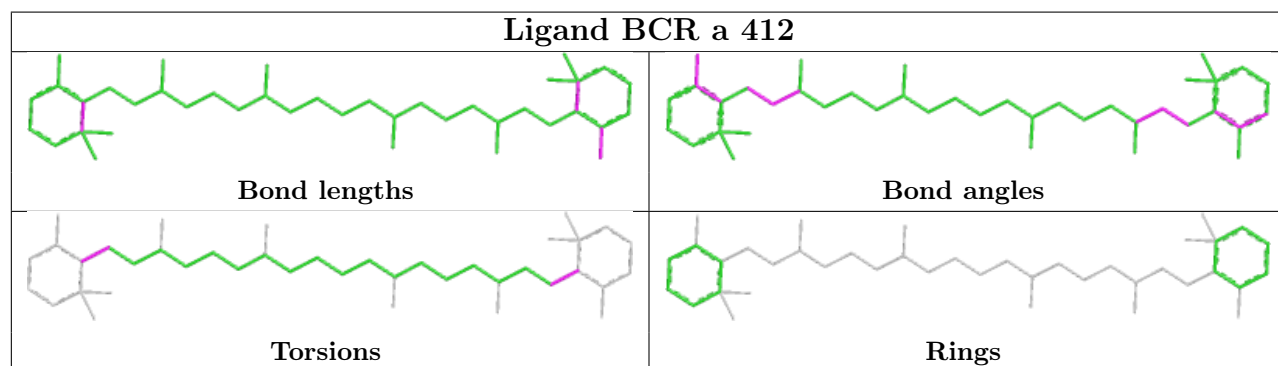
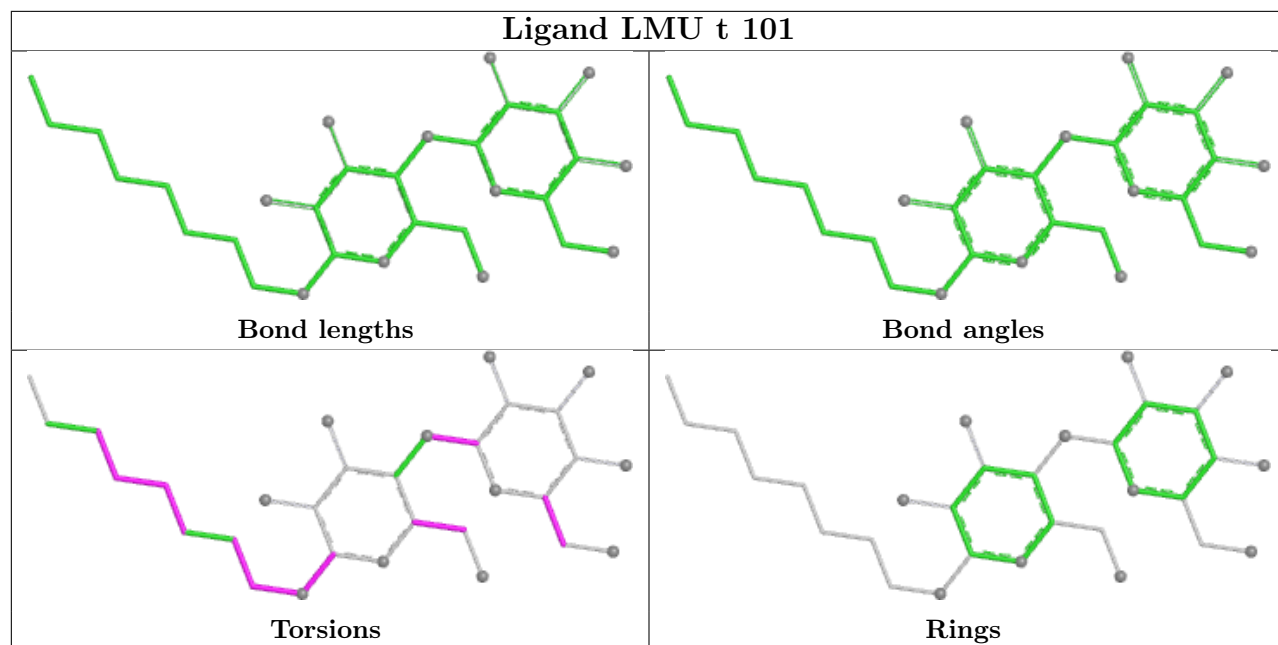


Ligand CLA 0 309

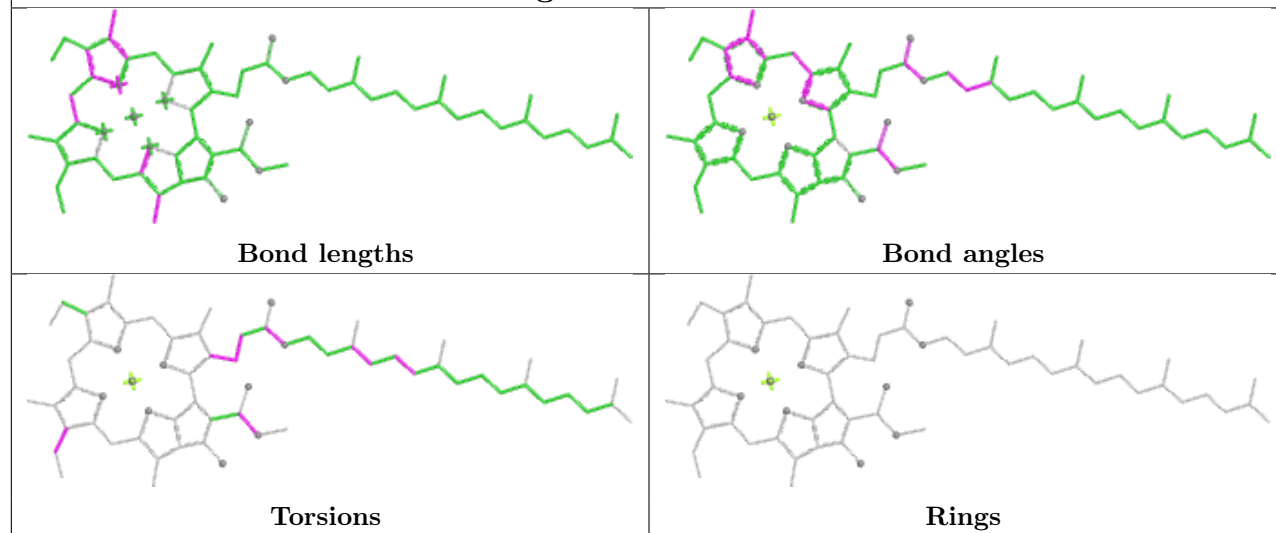


Ligand CLA 0 311

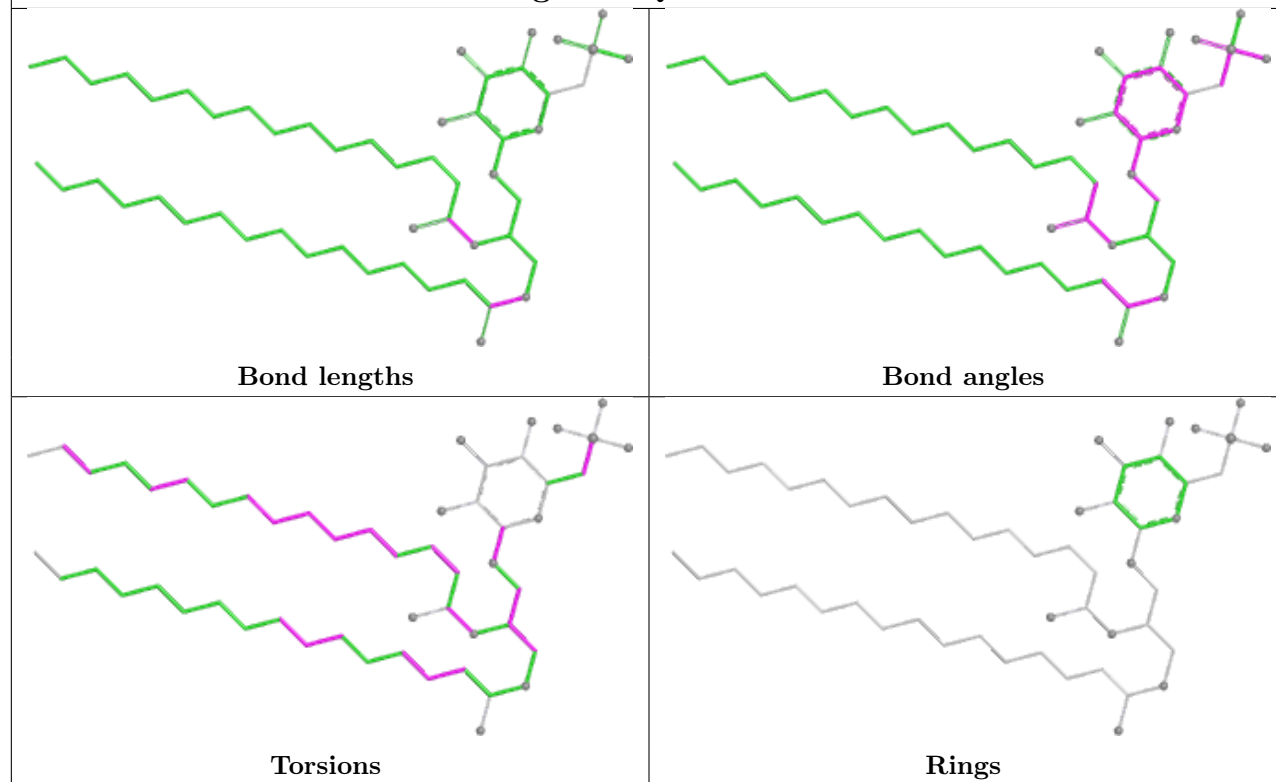




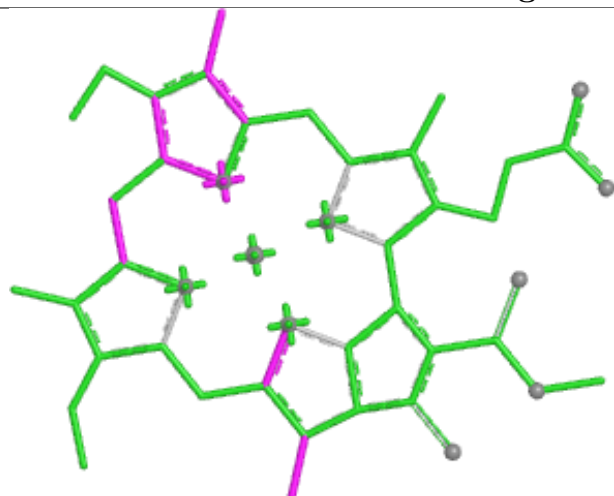
Ligand CLA 2 310



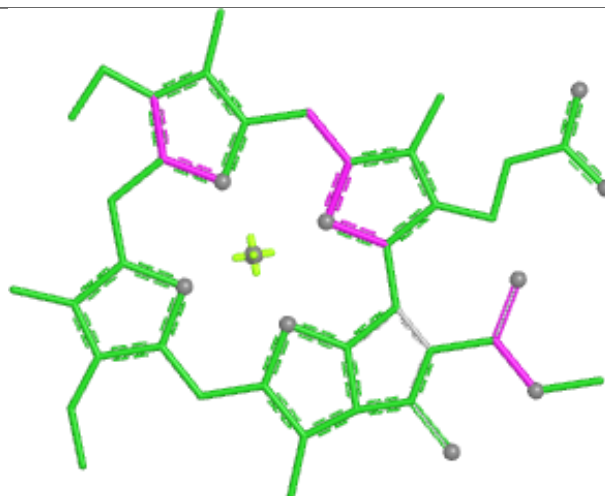
Ligand SQD T 103



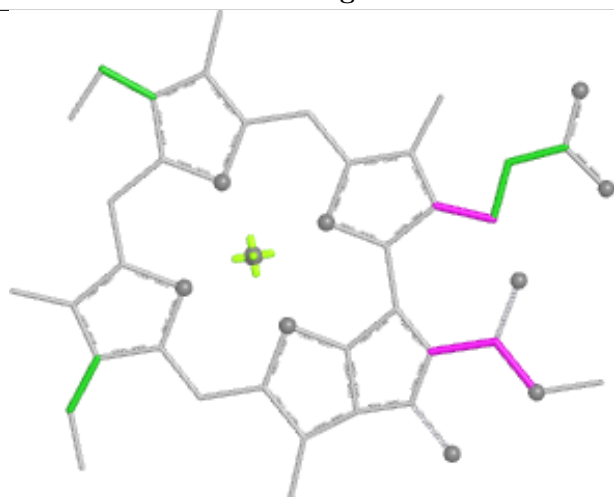
Ligand CLA 1 312



Bond lengths



Bond angles

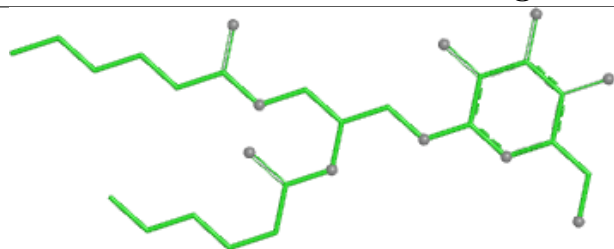


Torsions

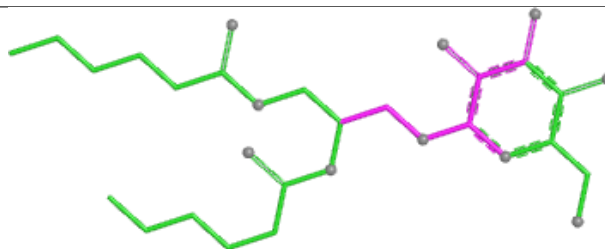


Rings

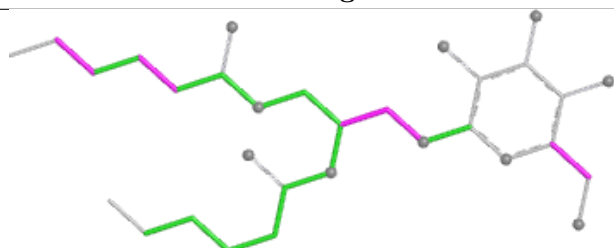
Ligand LMG 3 316



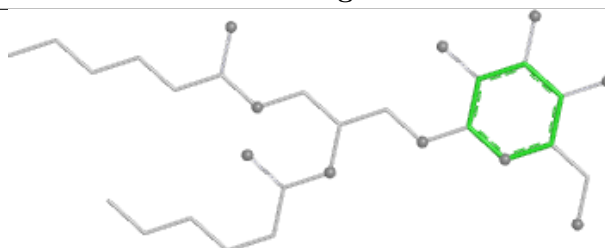
Bond lengths



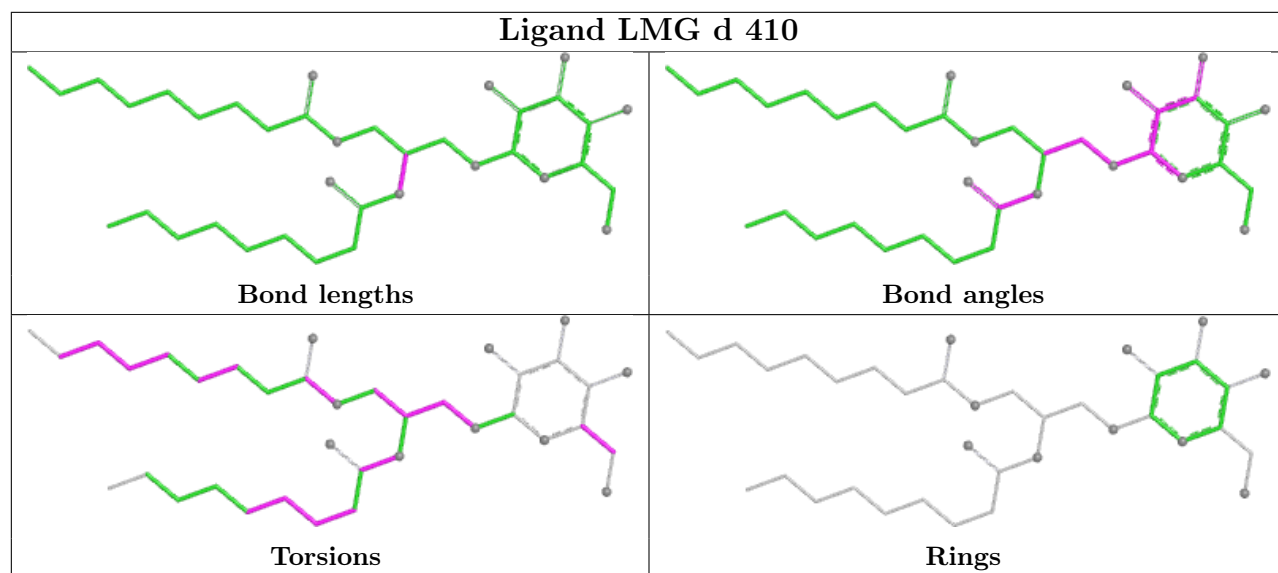
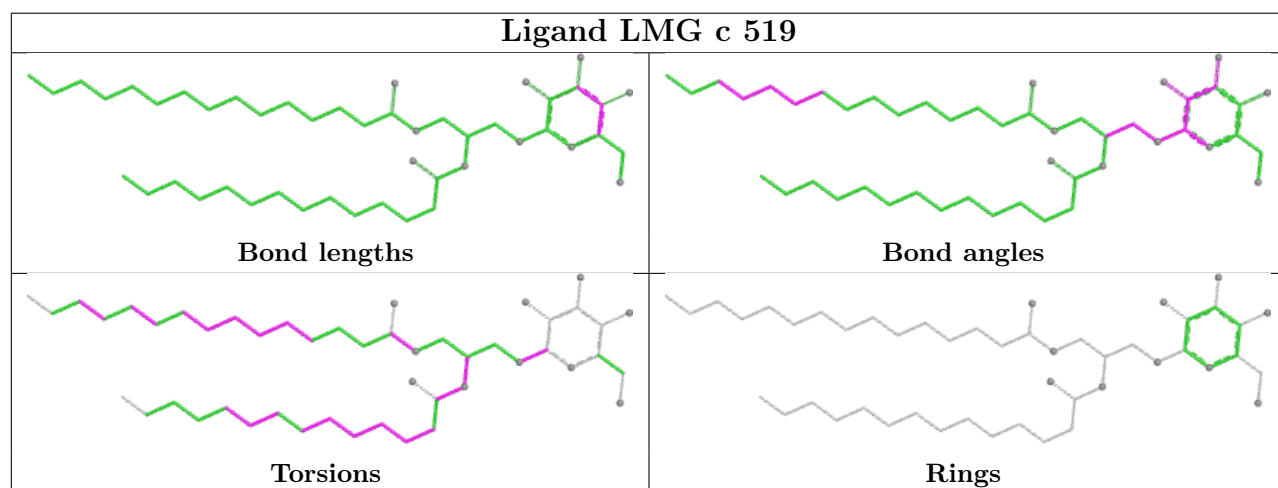
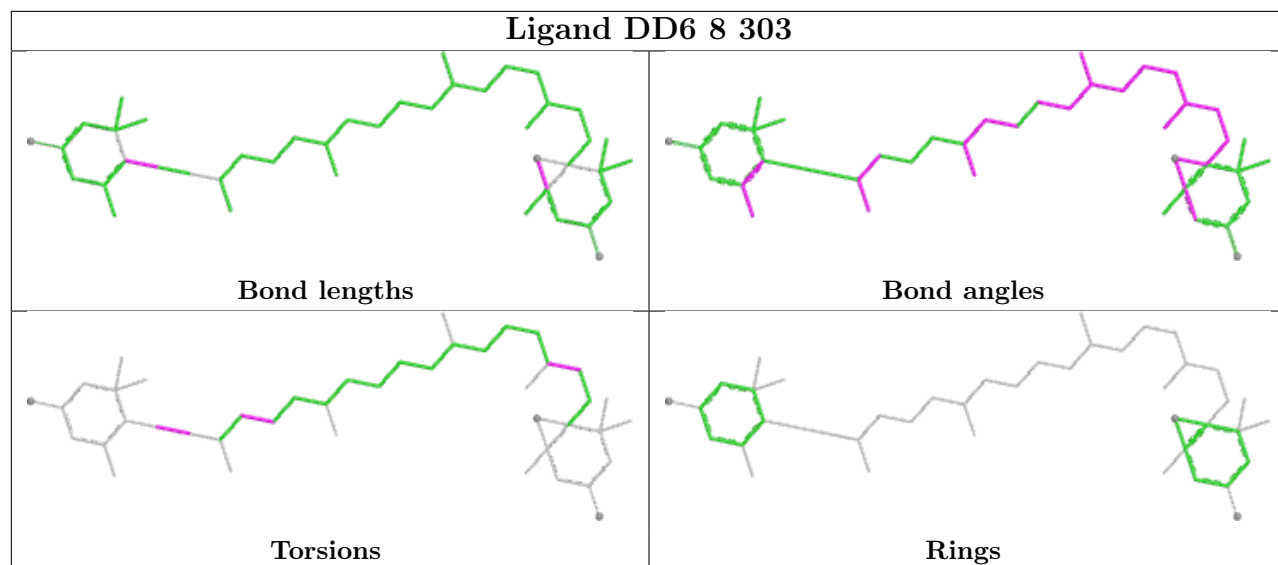
Bond angles

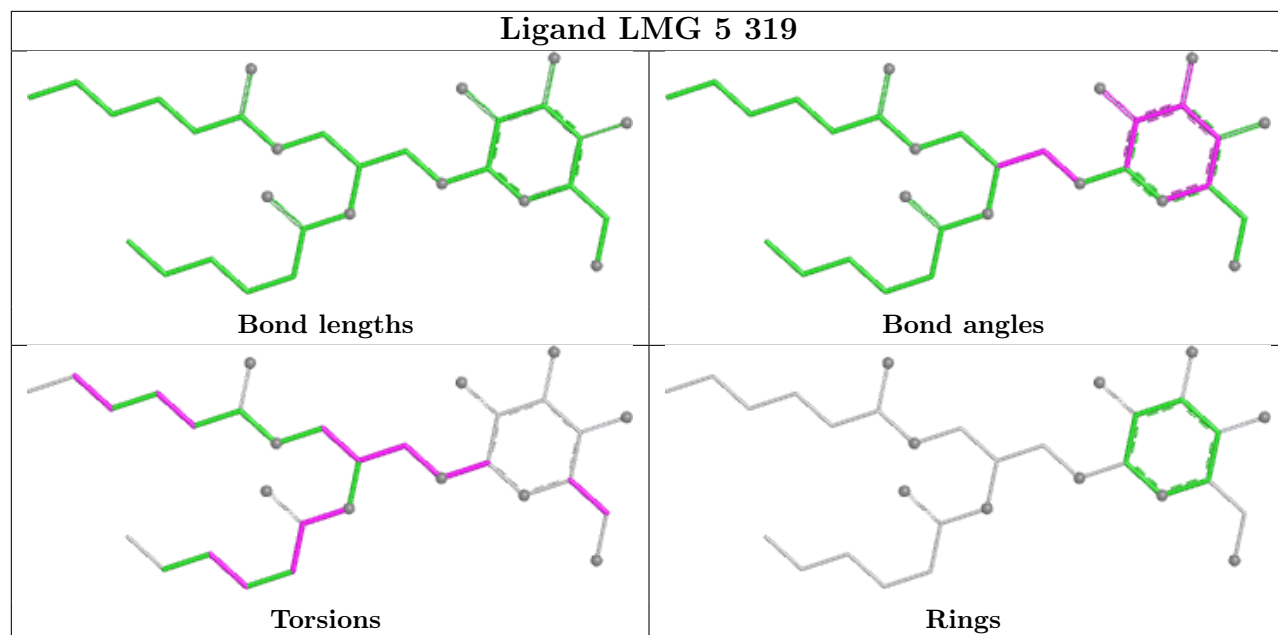


Torsions

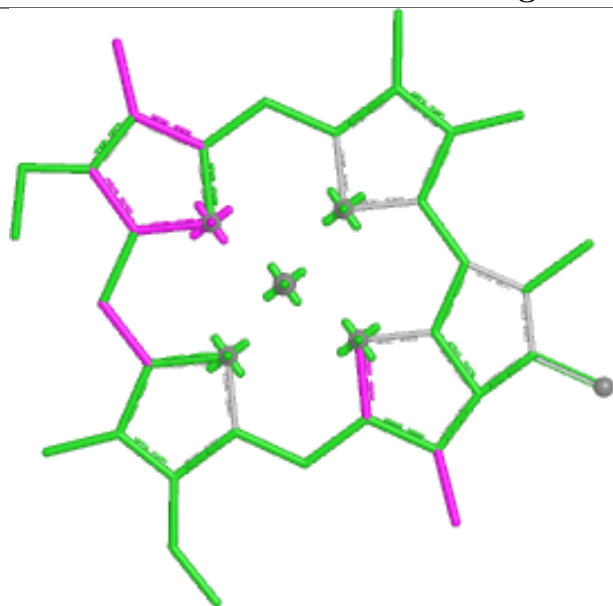


Rings

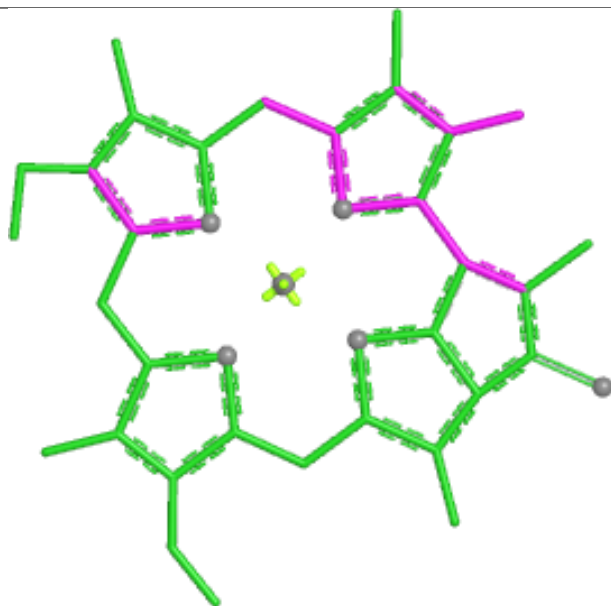




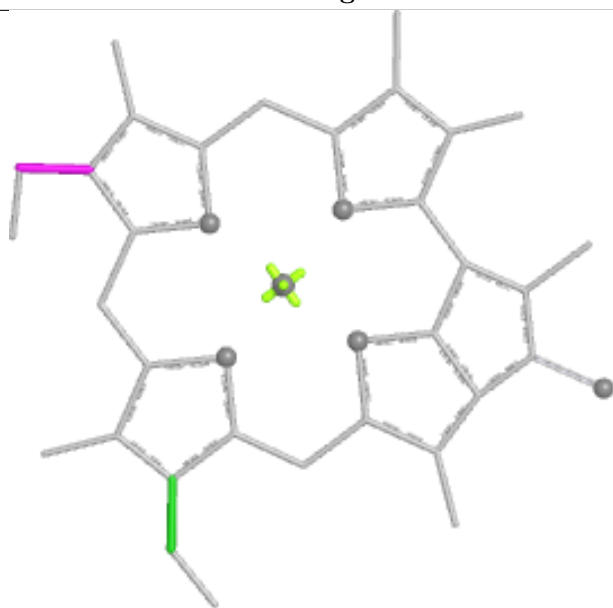
Ligand CLA 1 316



Bond lengths



Bond angles

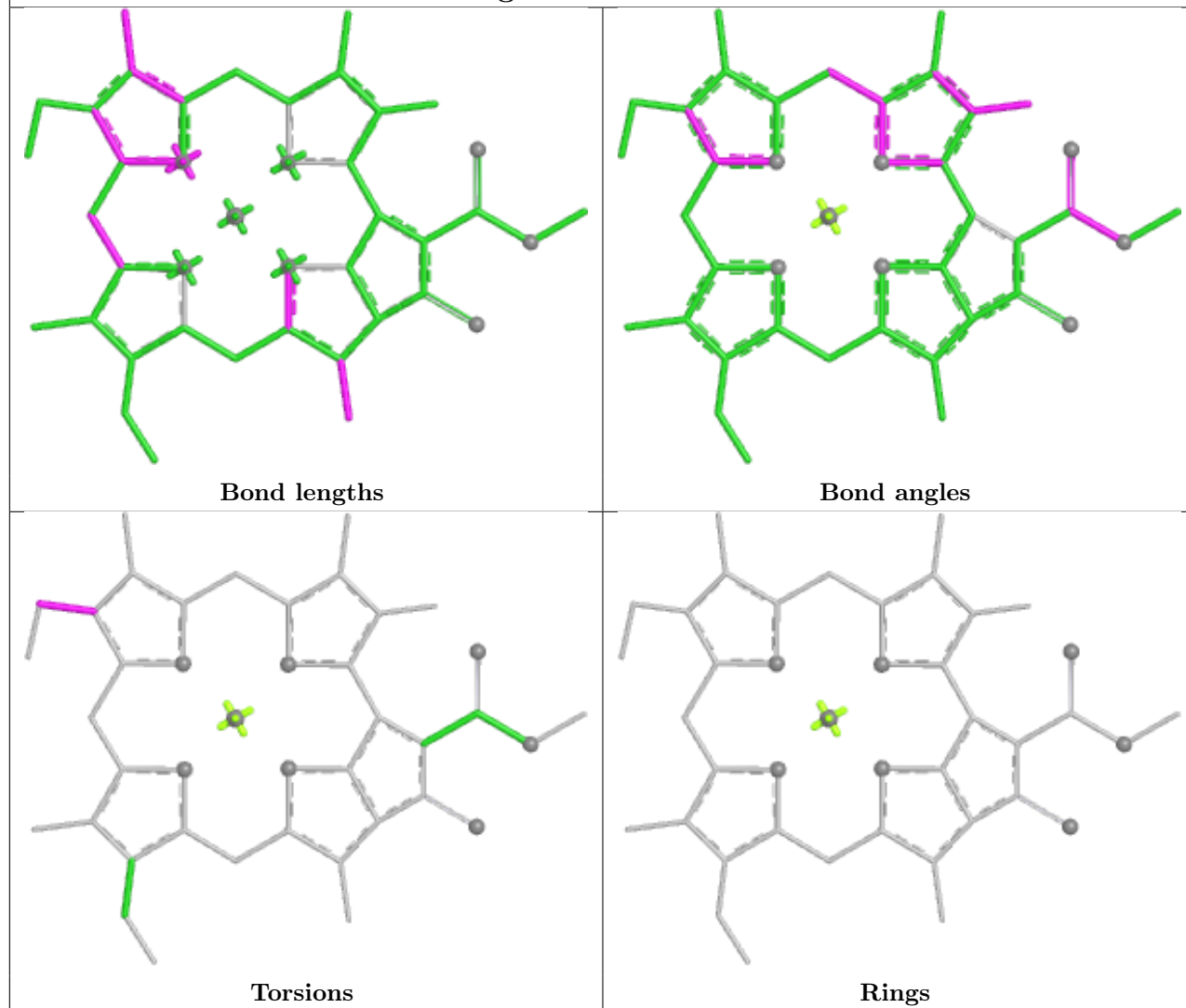


Torsions

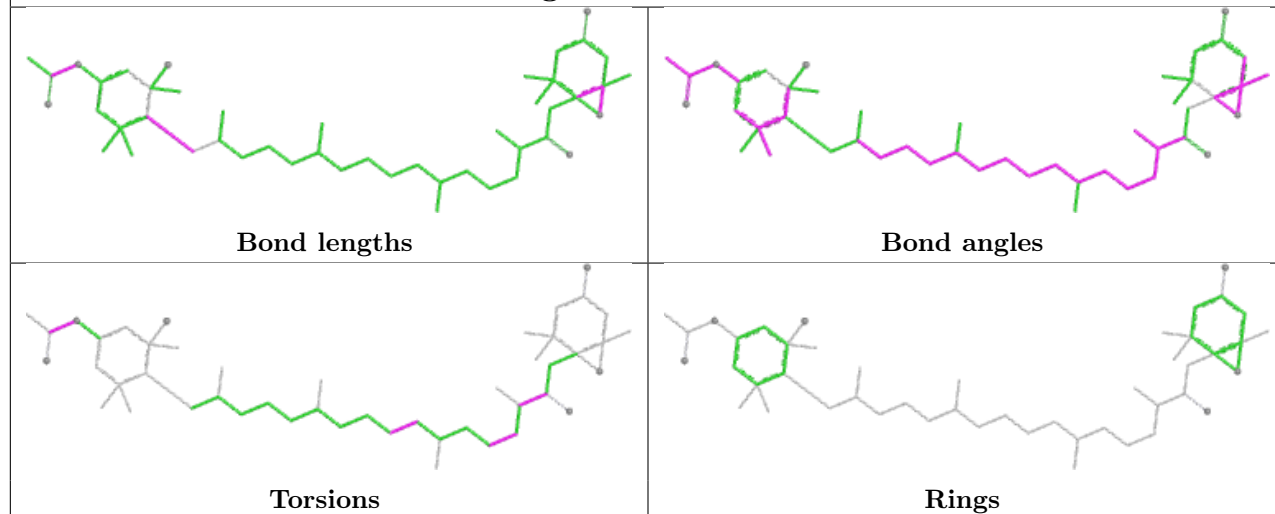


Rings

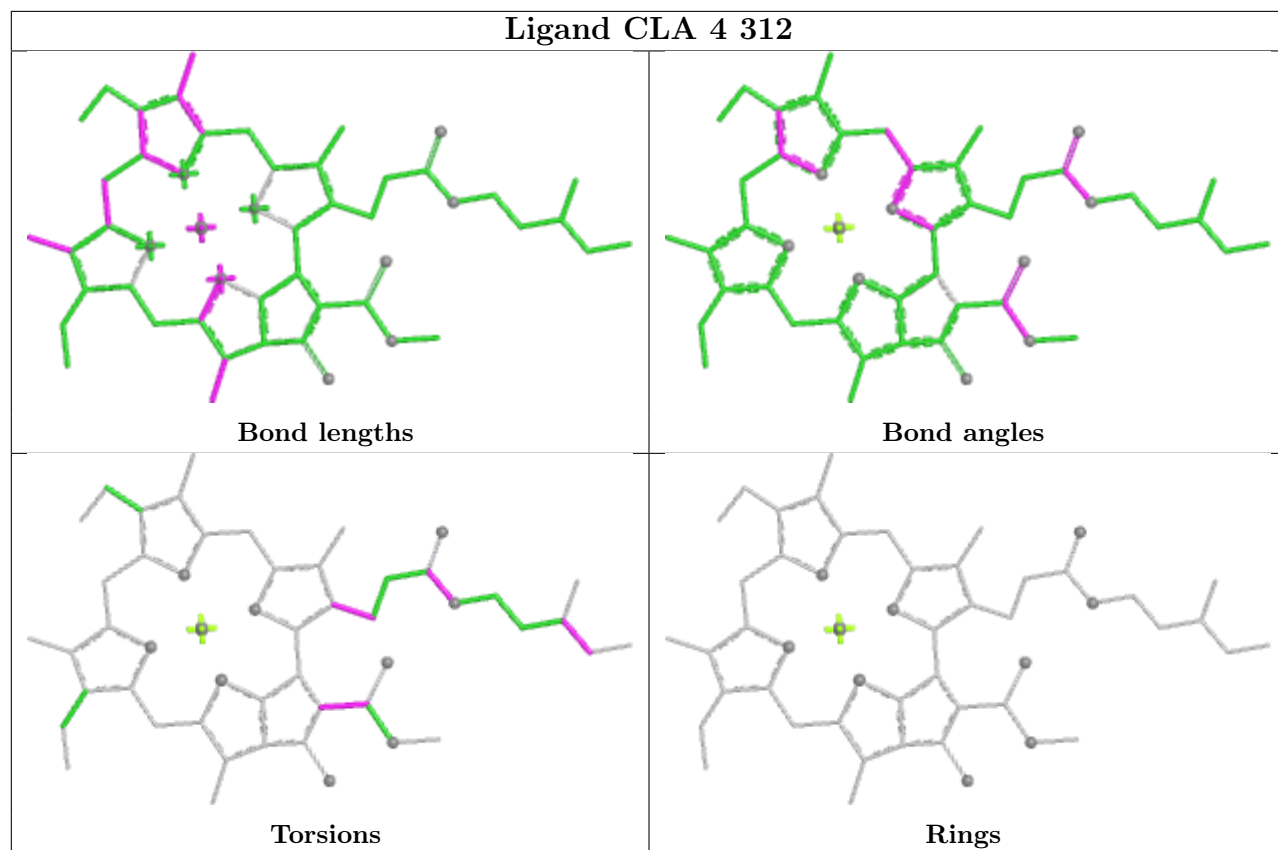
Ligand CLA 9 305



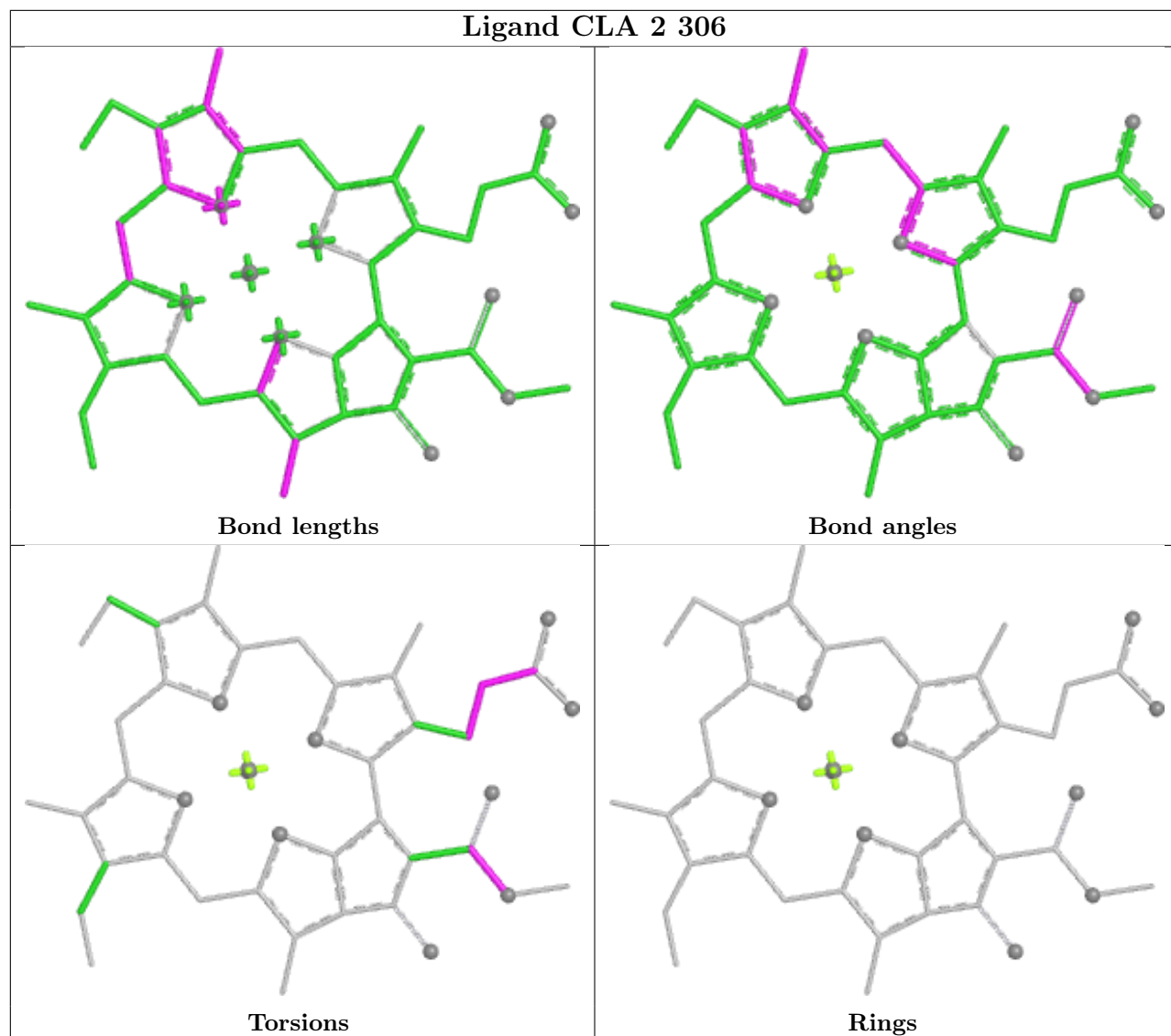
Ligand A86 8 301



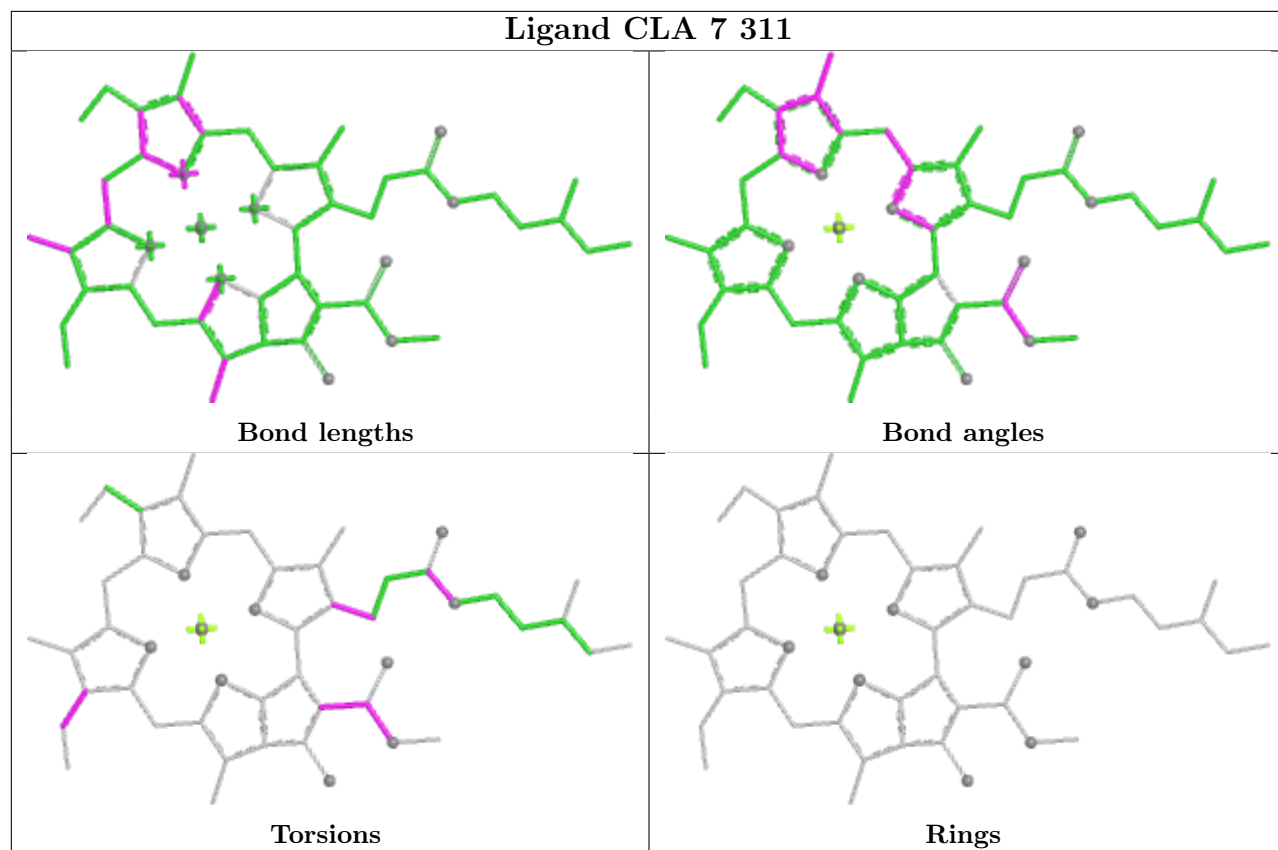
Ligand CLA 4 312

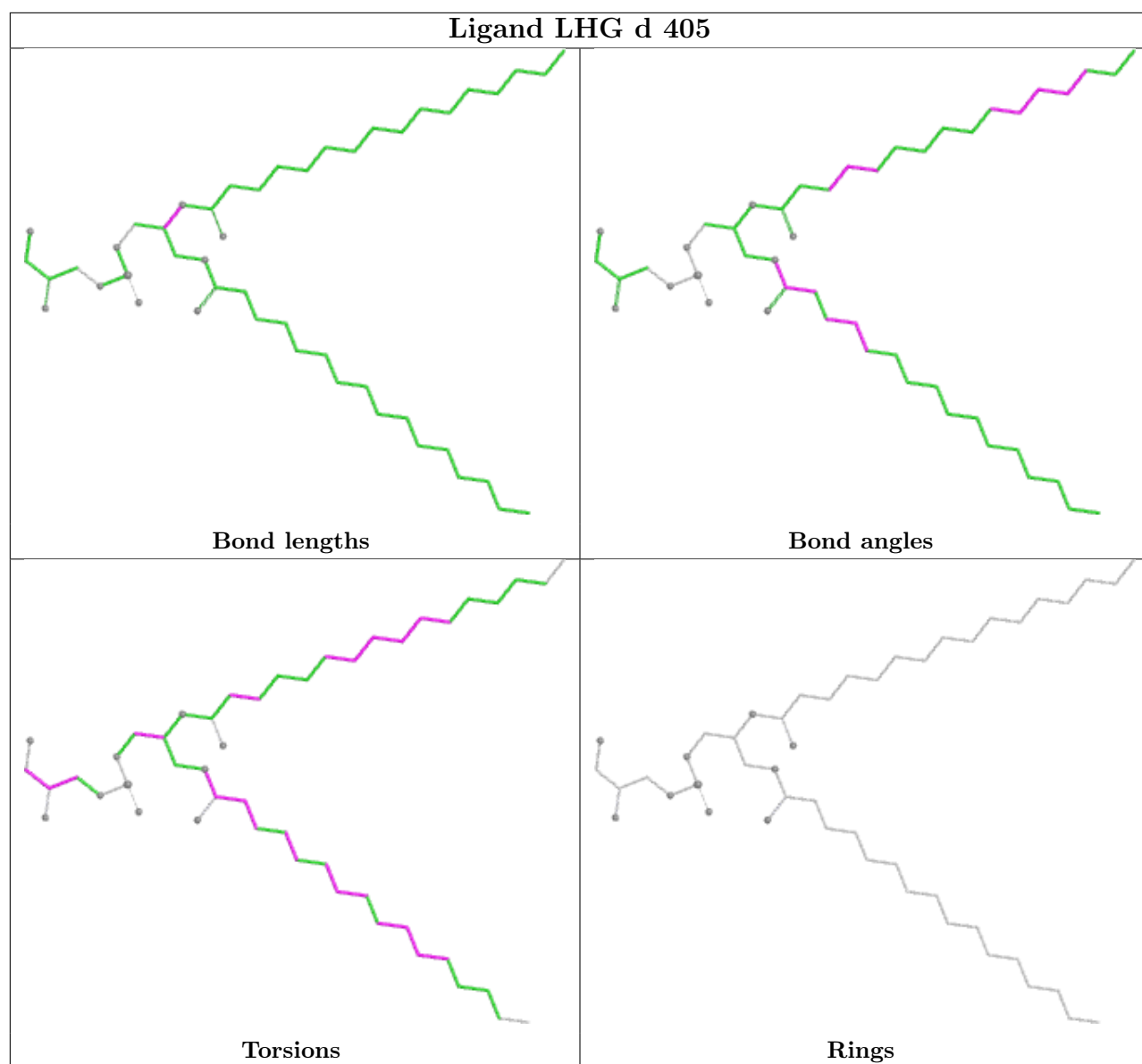


Ligand CLA 2 306

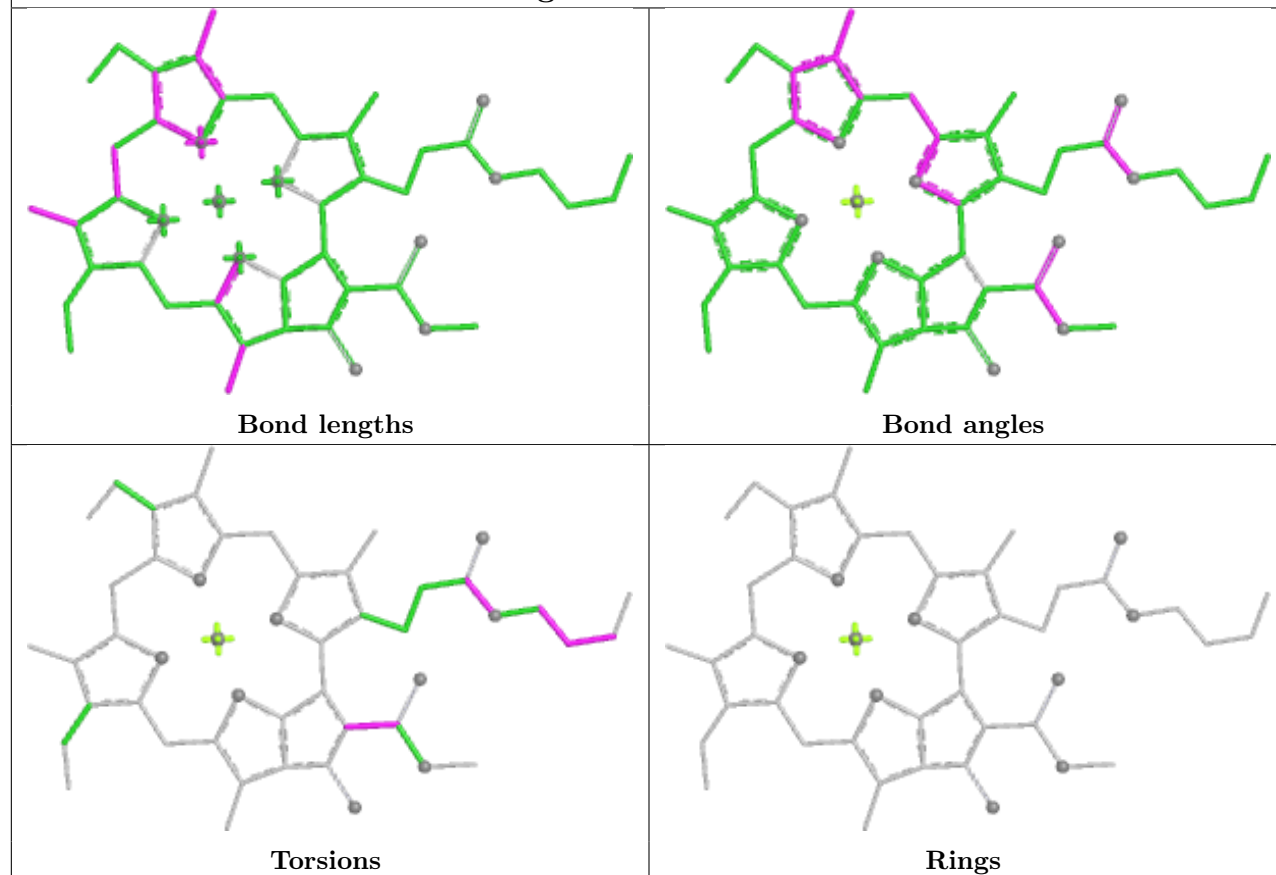


Ligand CLA 7 311

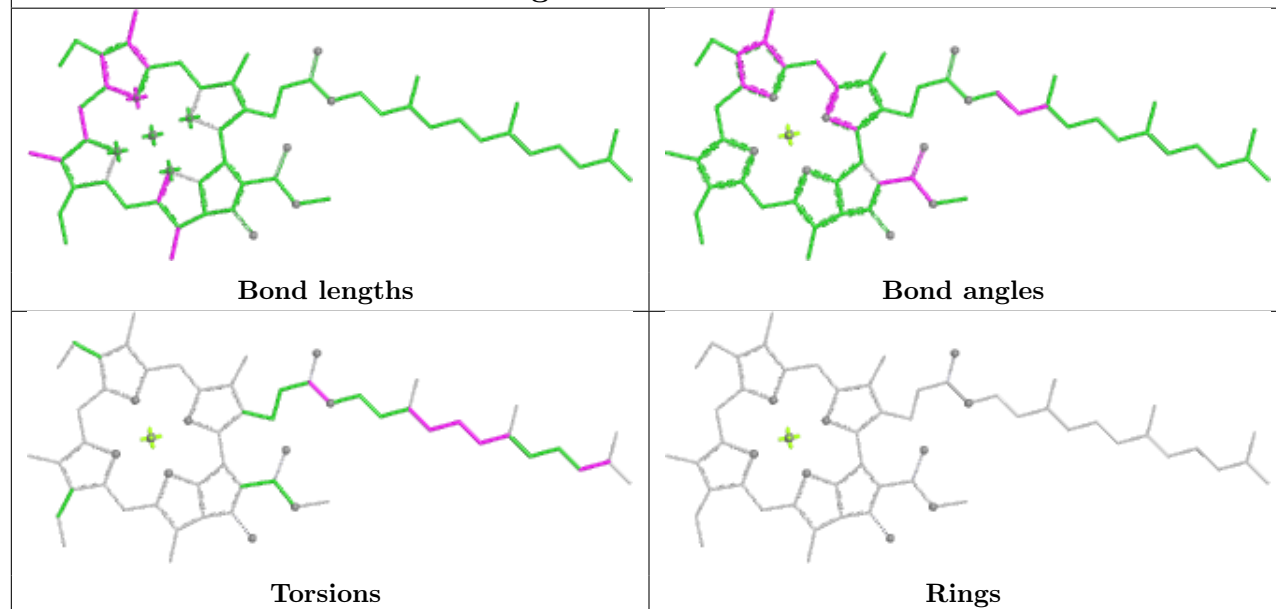




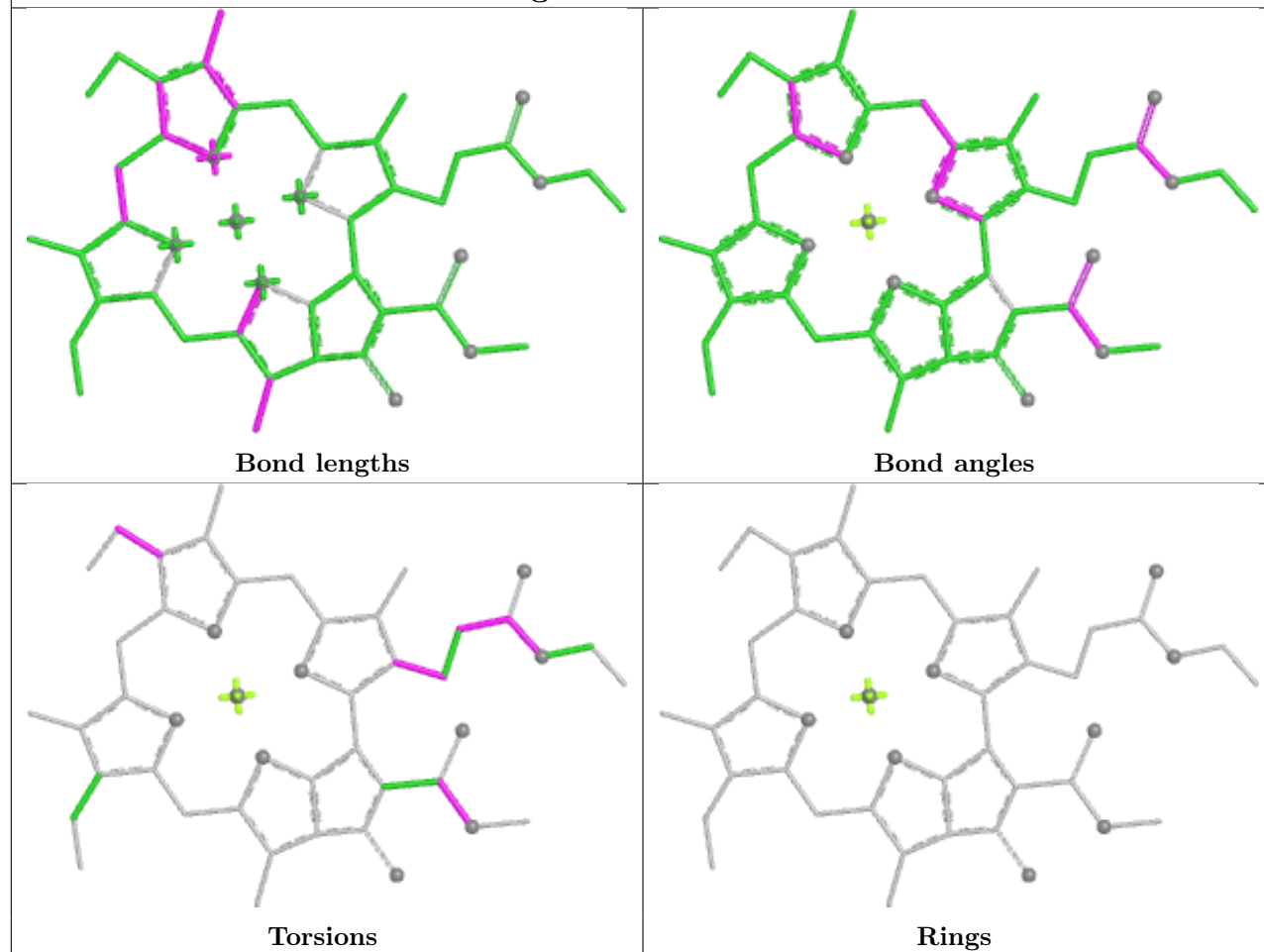
Ligand CLA c 513



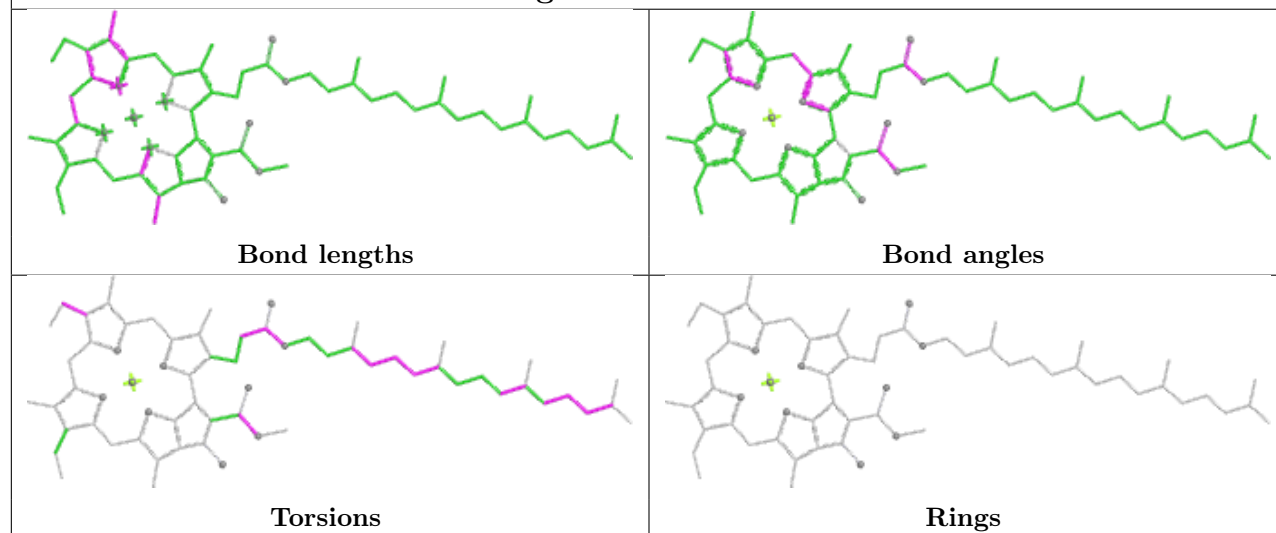
Ligand CLA D 406



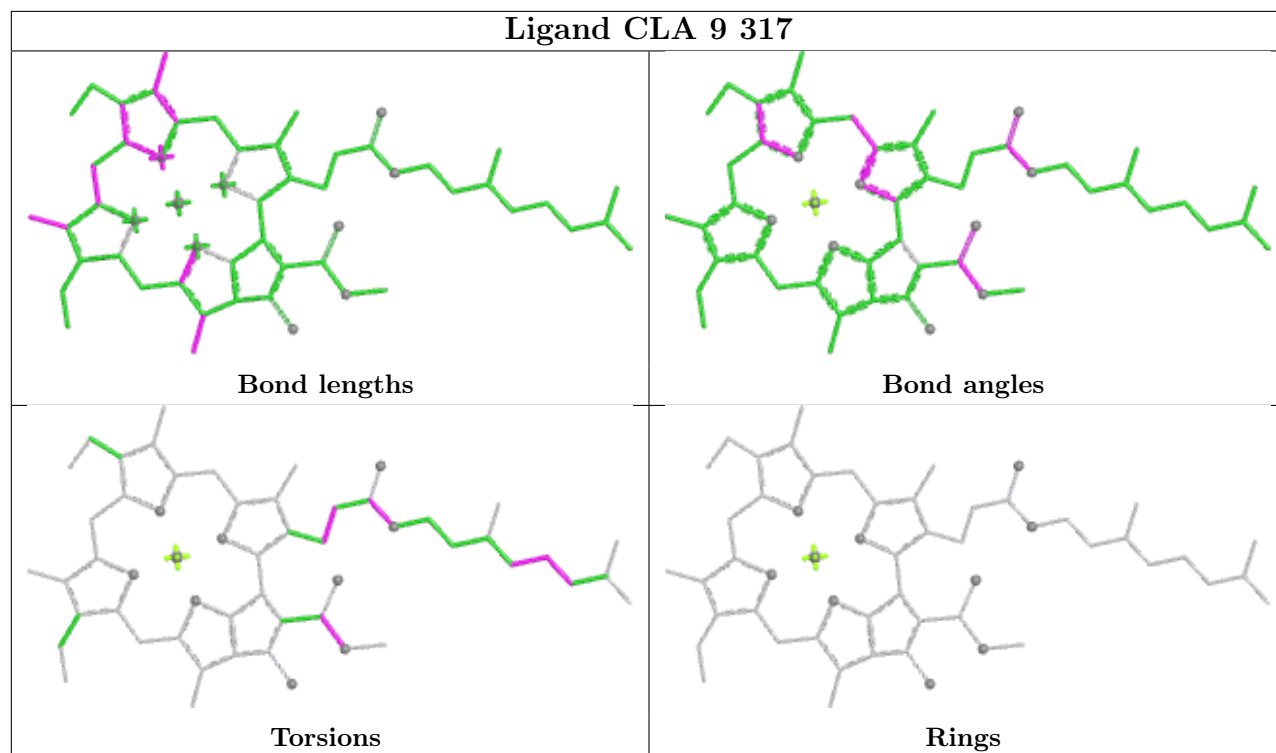
Ligand CLA 0 304



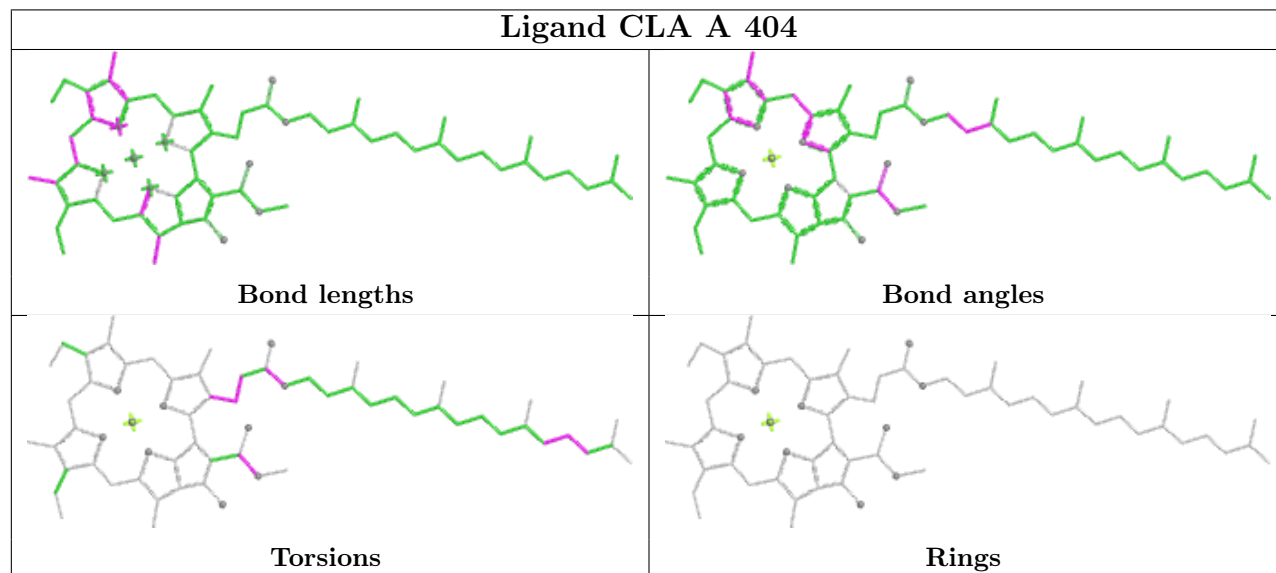
Ligand CLA 0 312

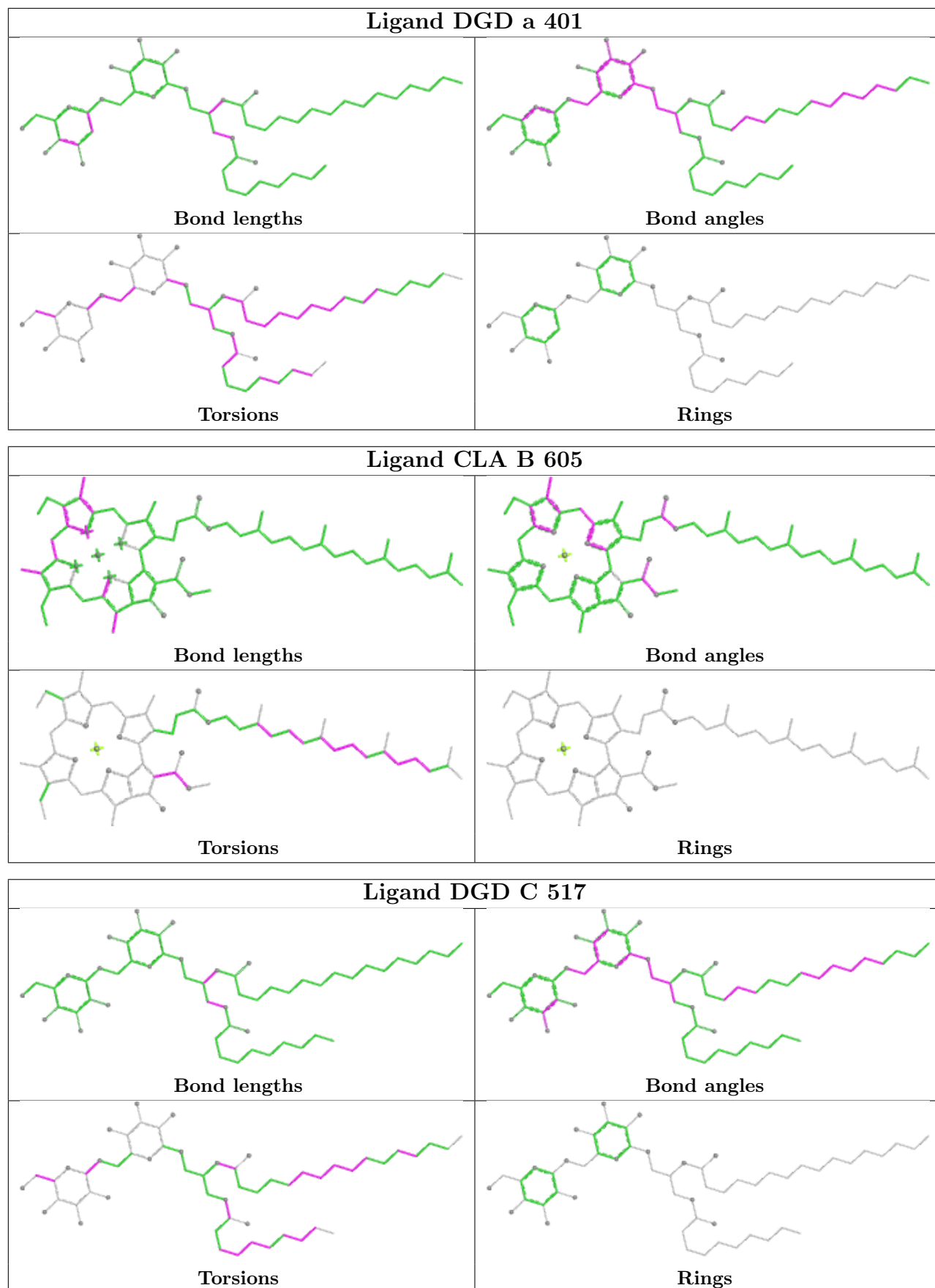


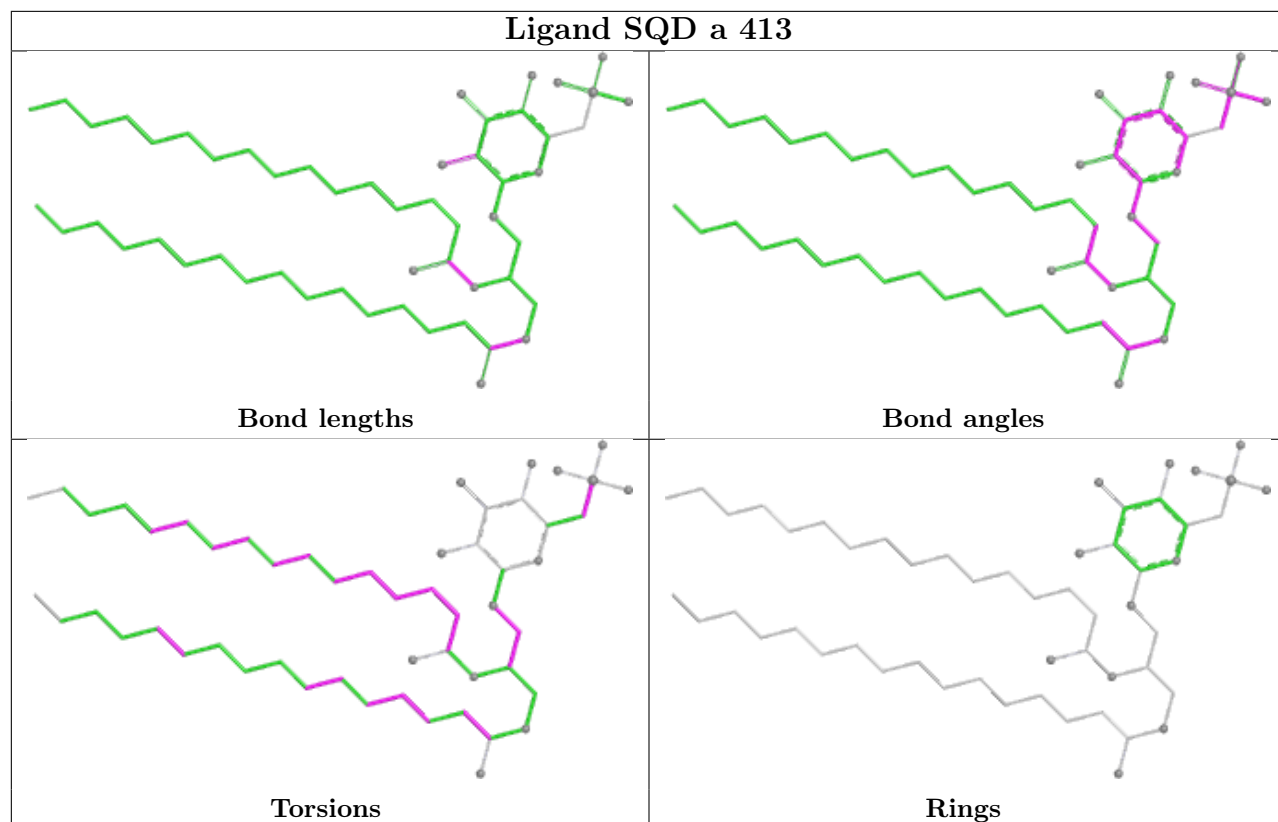
Ligand CLA 9 317



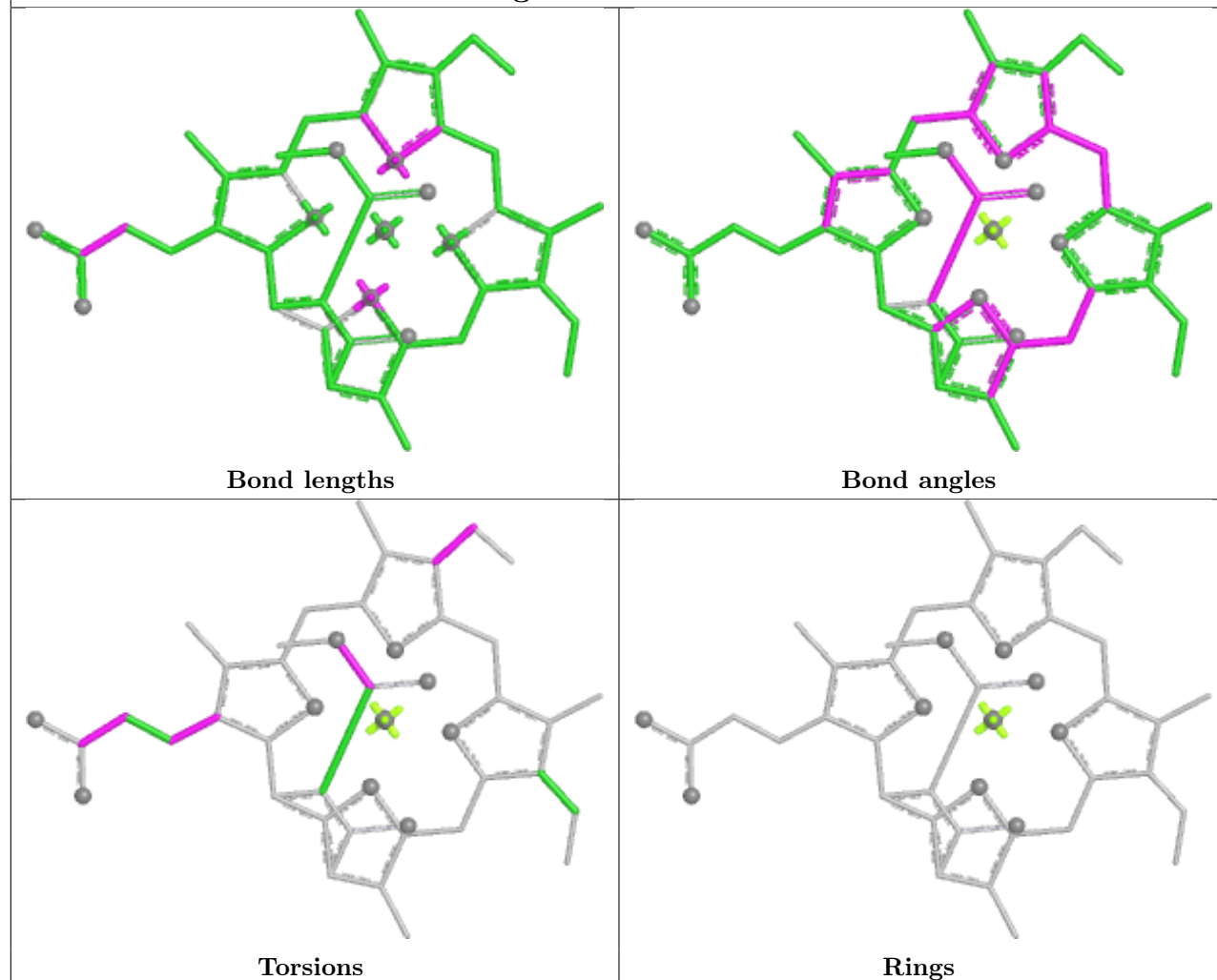
Ligand CLA A 404



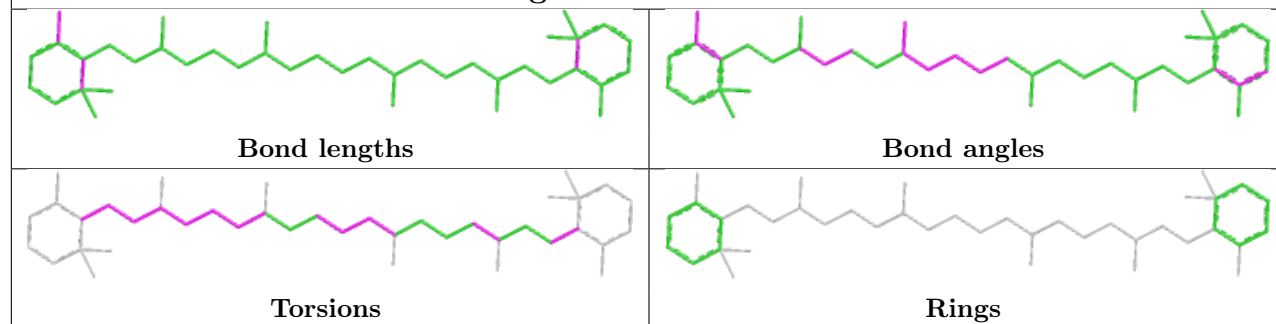




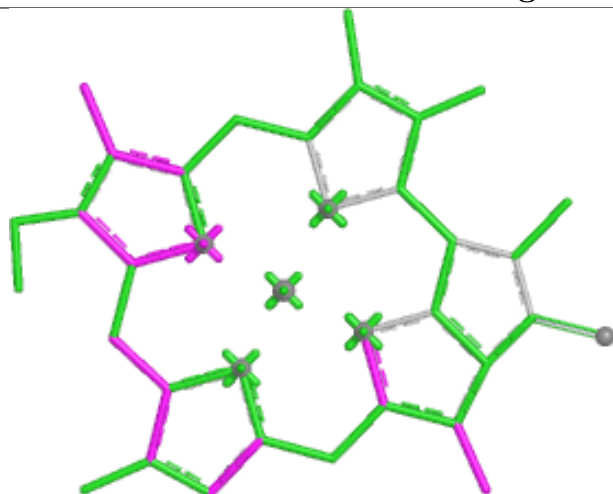
Ligand KC1 5 315



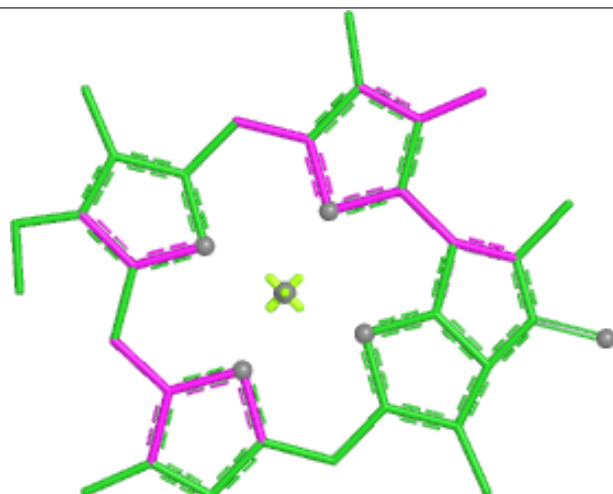
Ligand BCR K 101



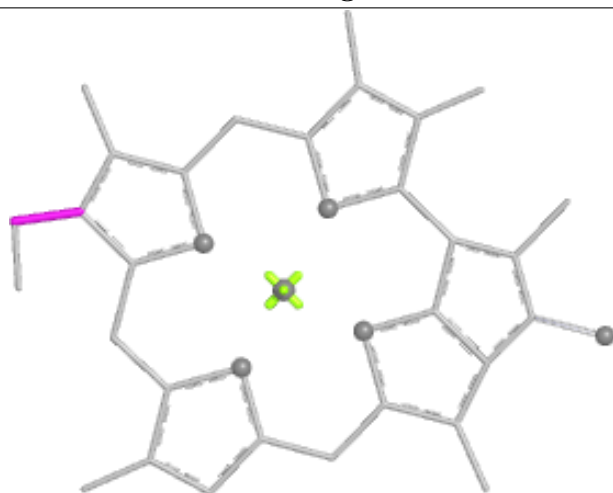
Ligand CLA 1 313



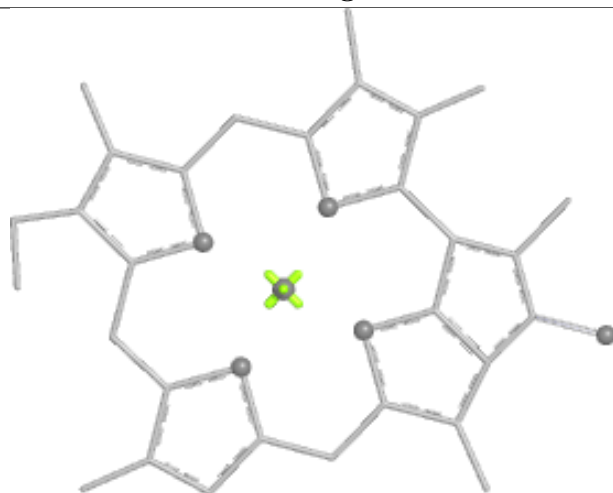
Bond lengths



Bond angles

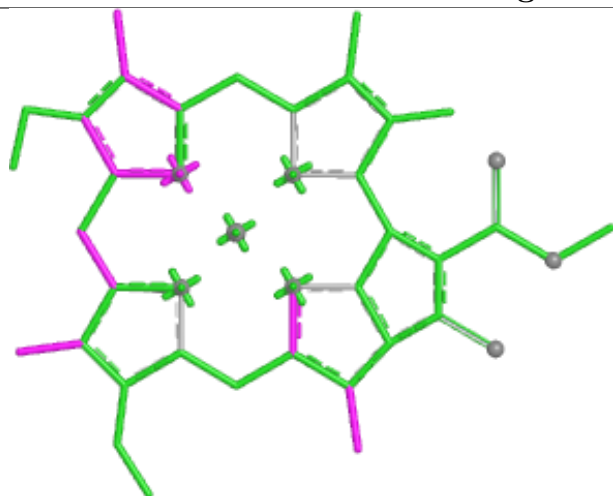


Torsions

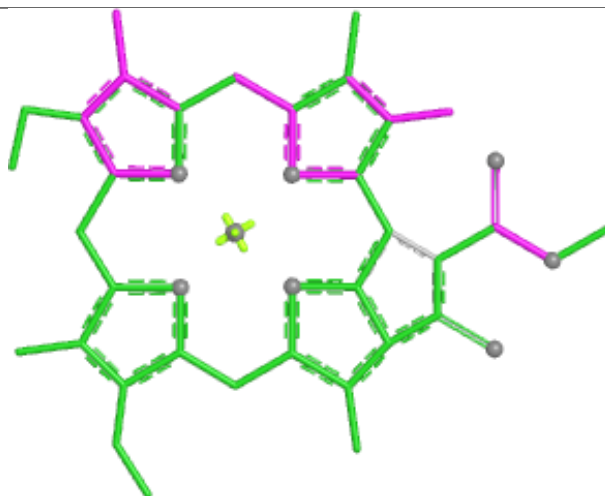


Rings

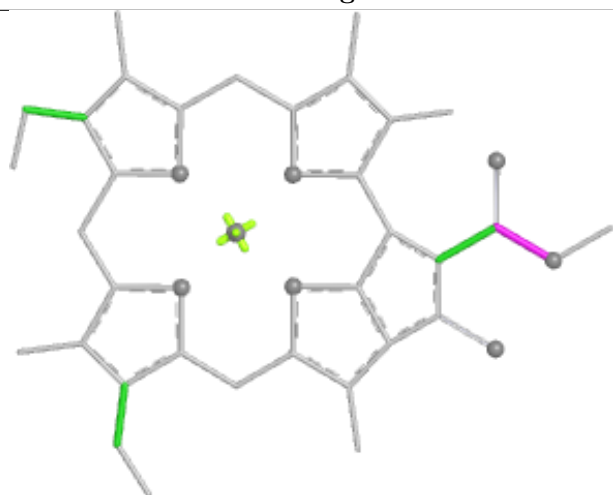
Ligand CLA b 608



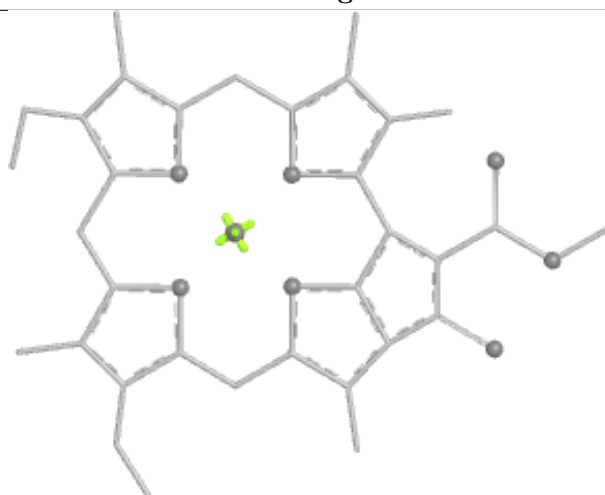
Bond lengths



Bond angles

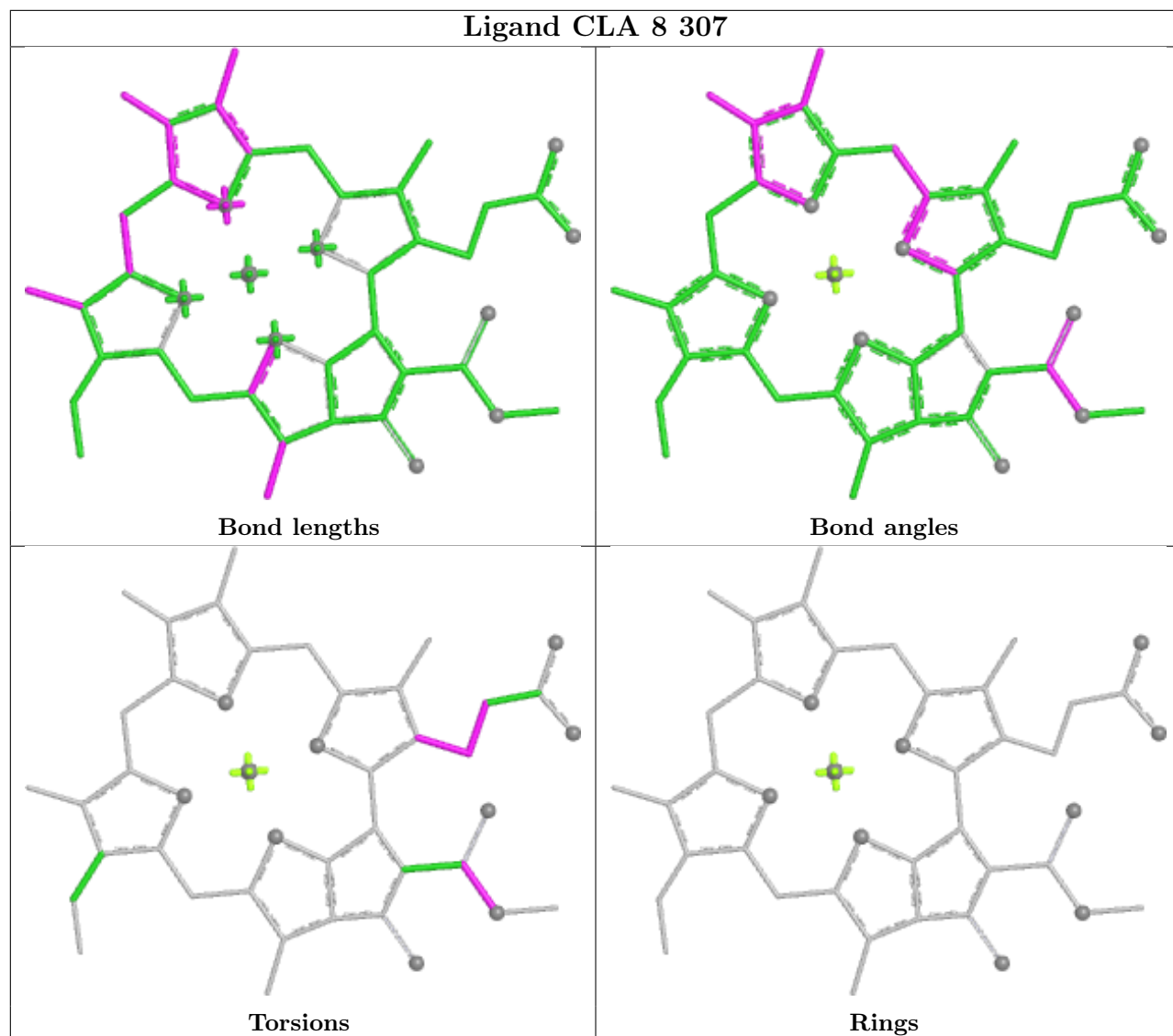


Torsions

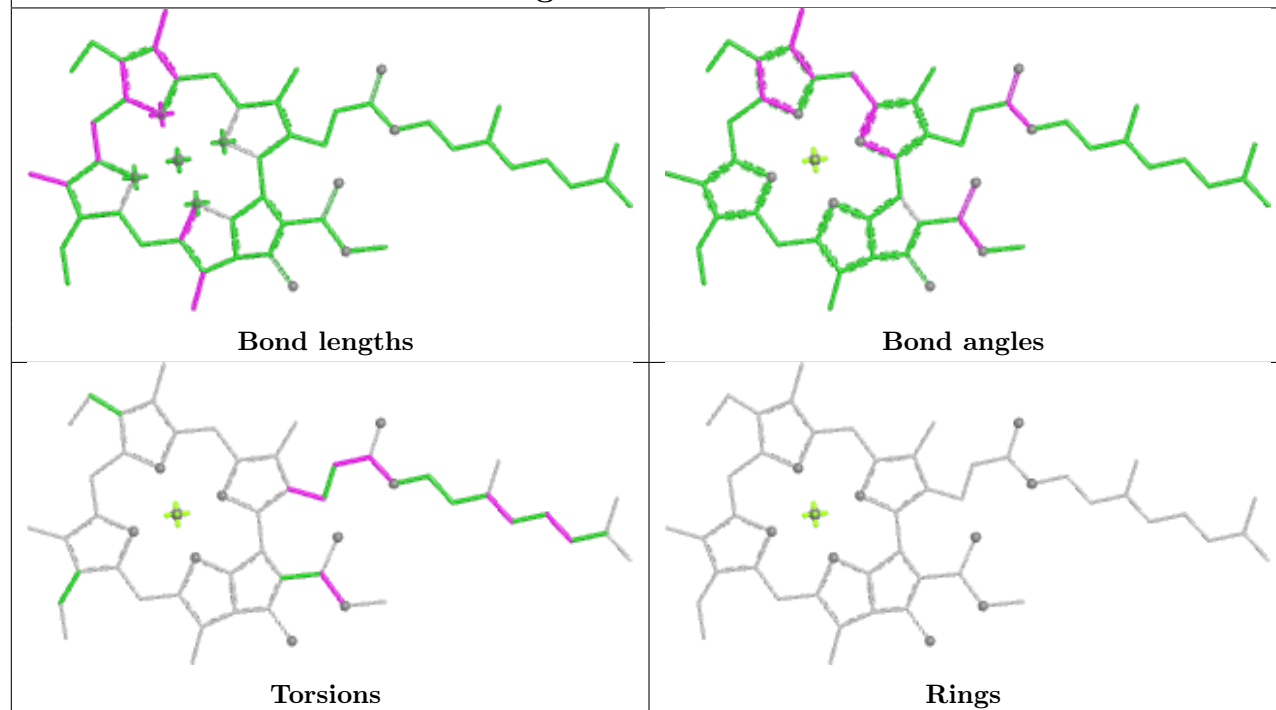


Rings

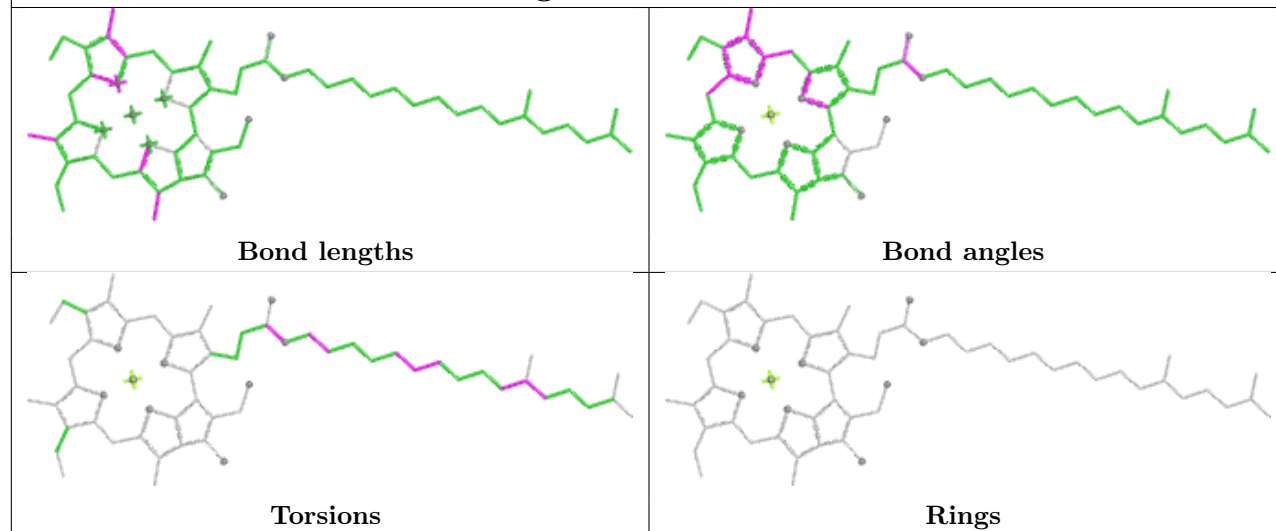
Ligand CLA 8 307

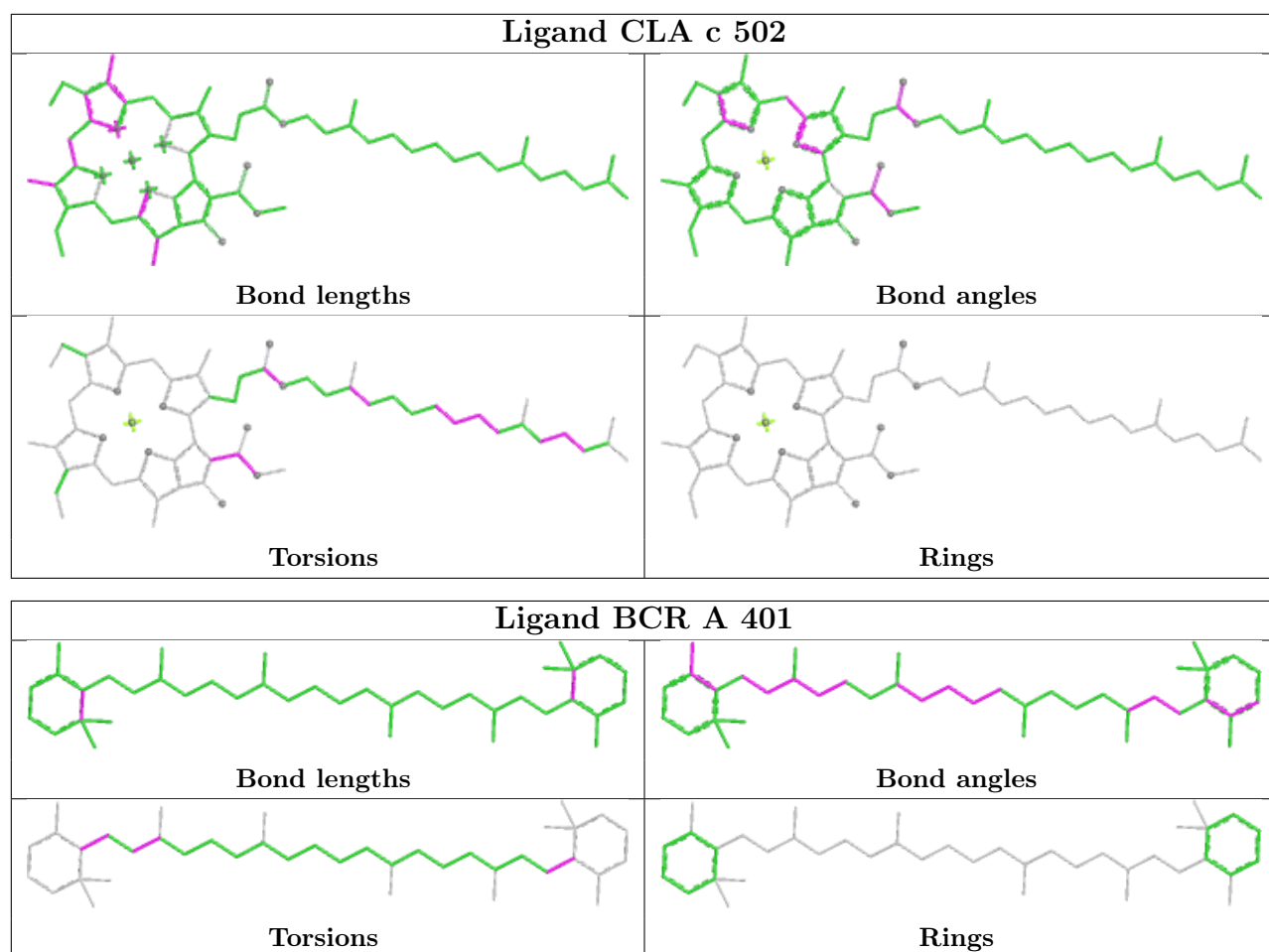


Ligand CLA 9 308

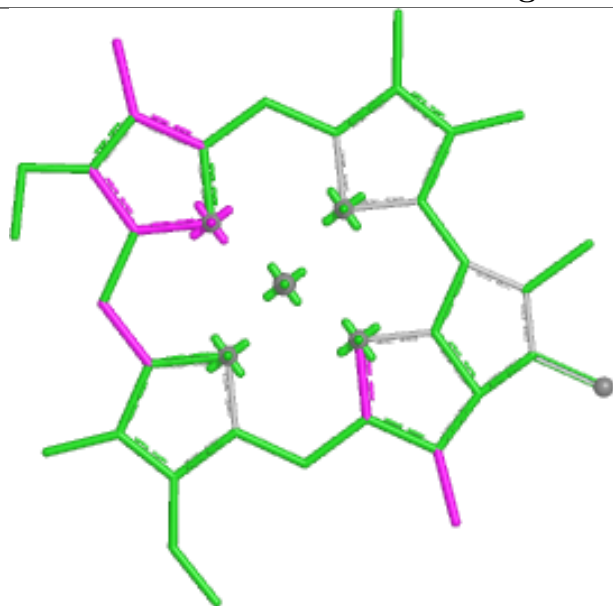


Ligand CLA b 603

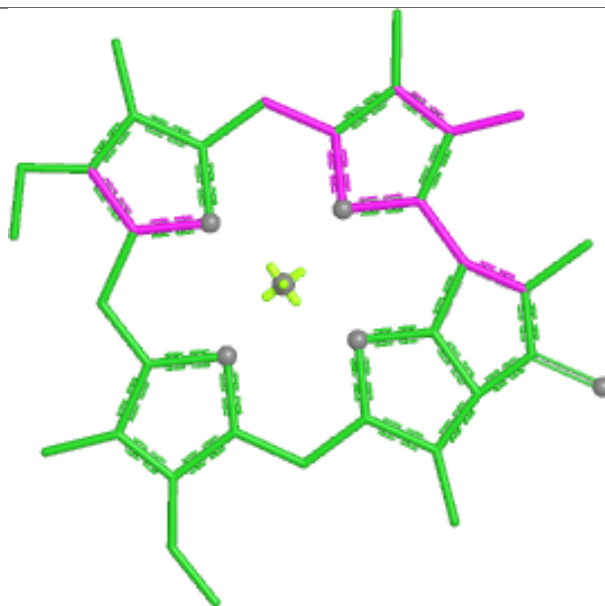




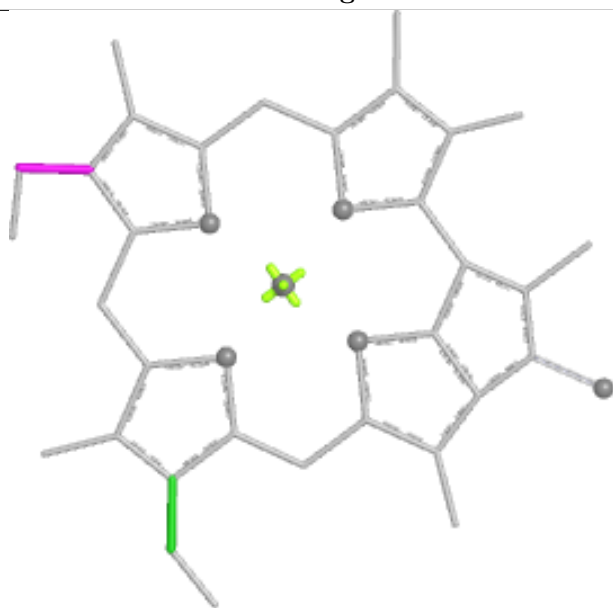
Ligand CLA 9 315



Bond lengths



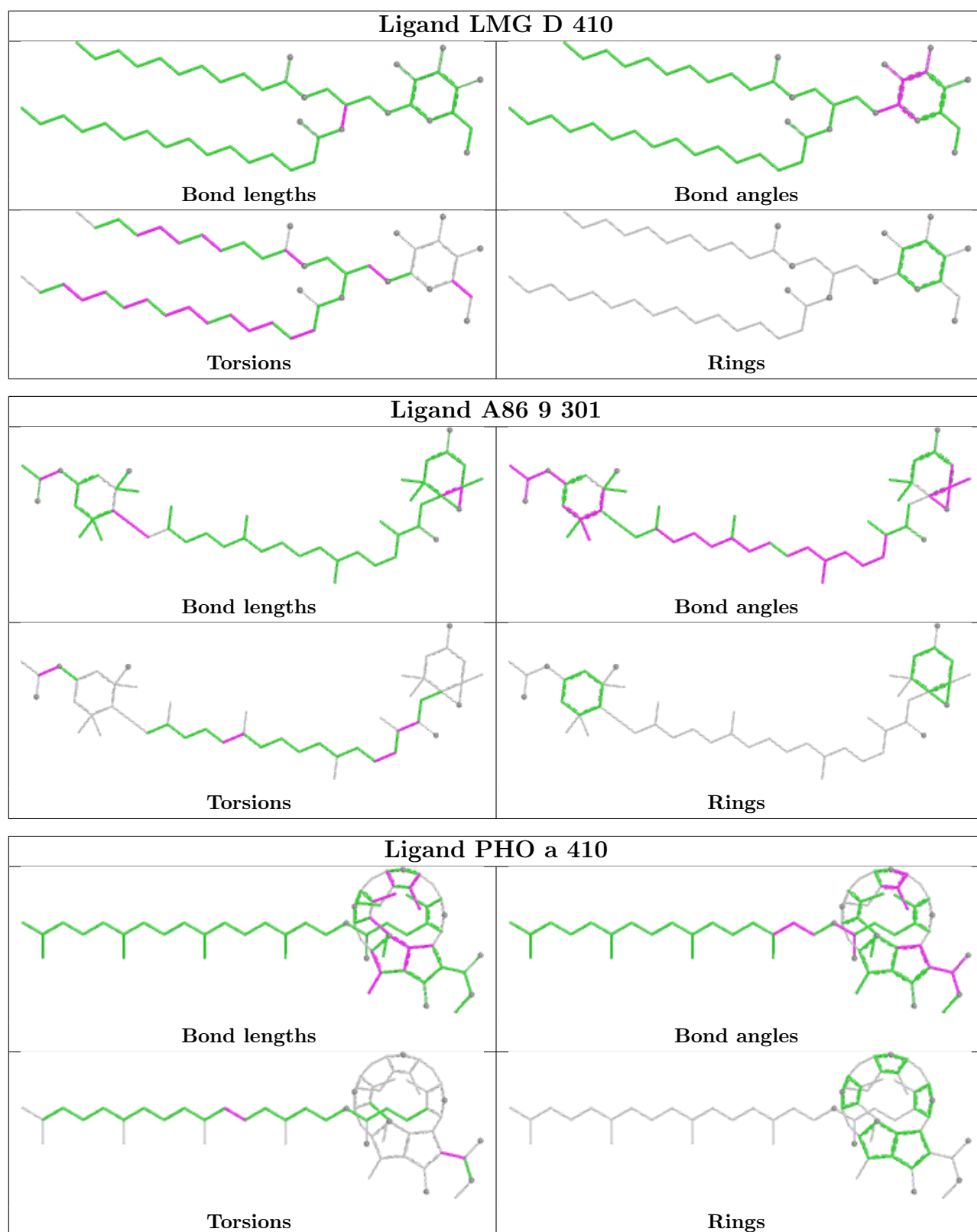
Bond angles



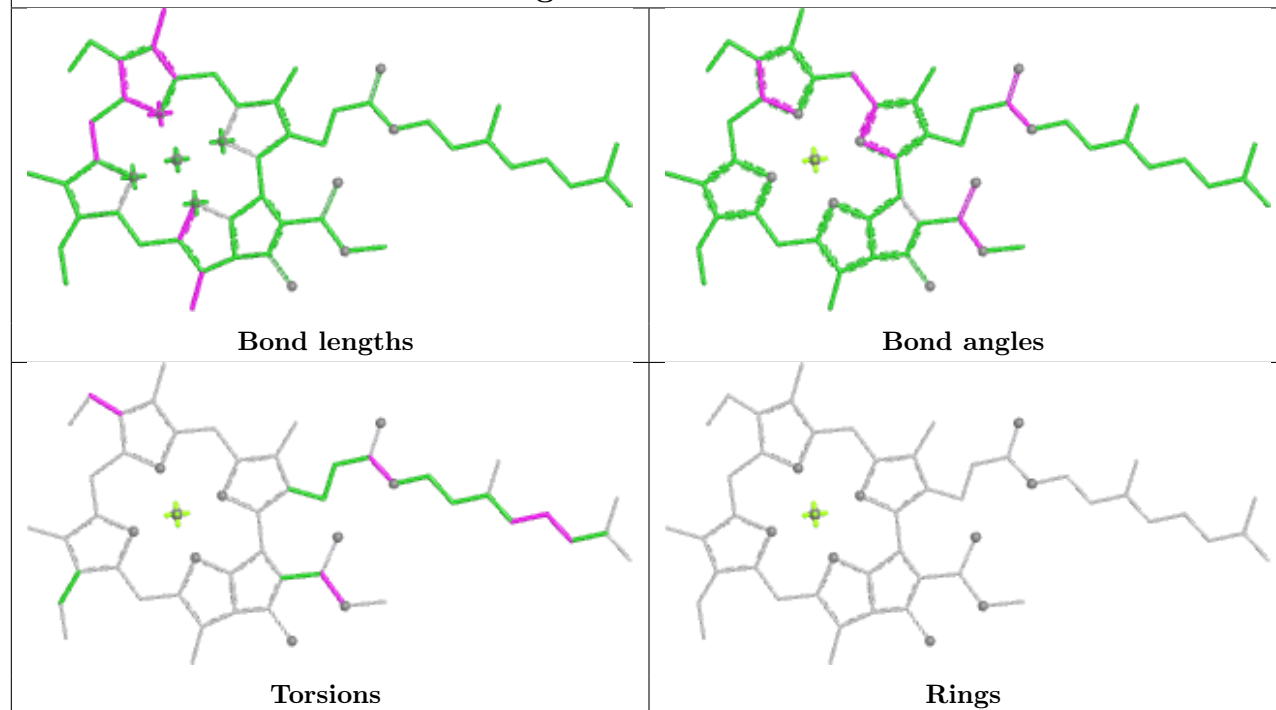
Torsions



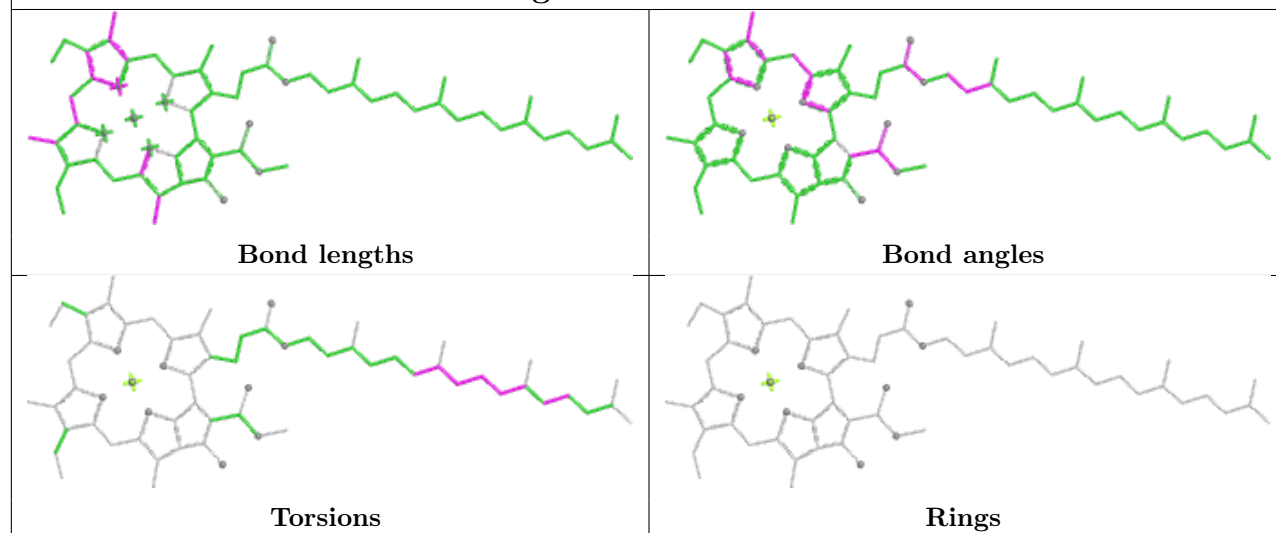
Rings

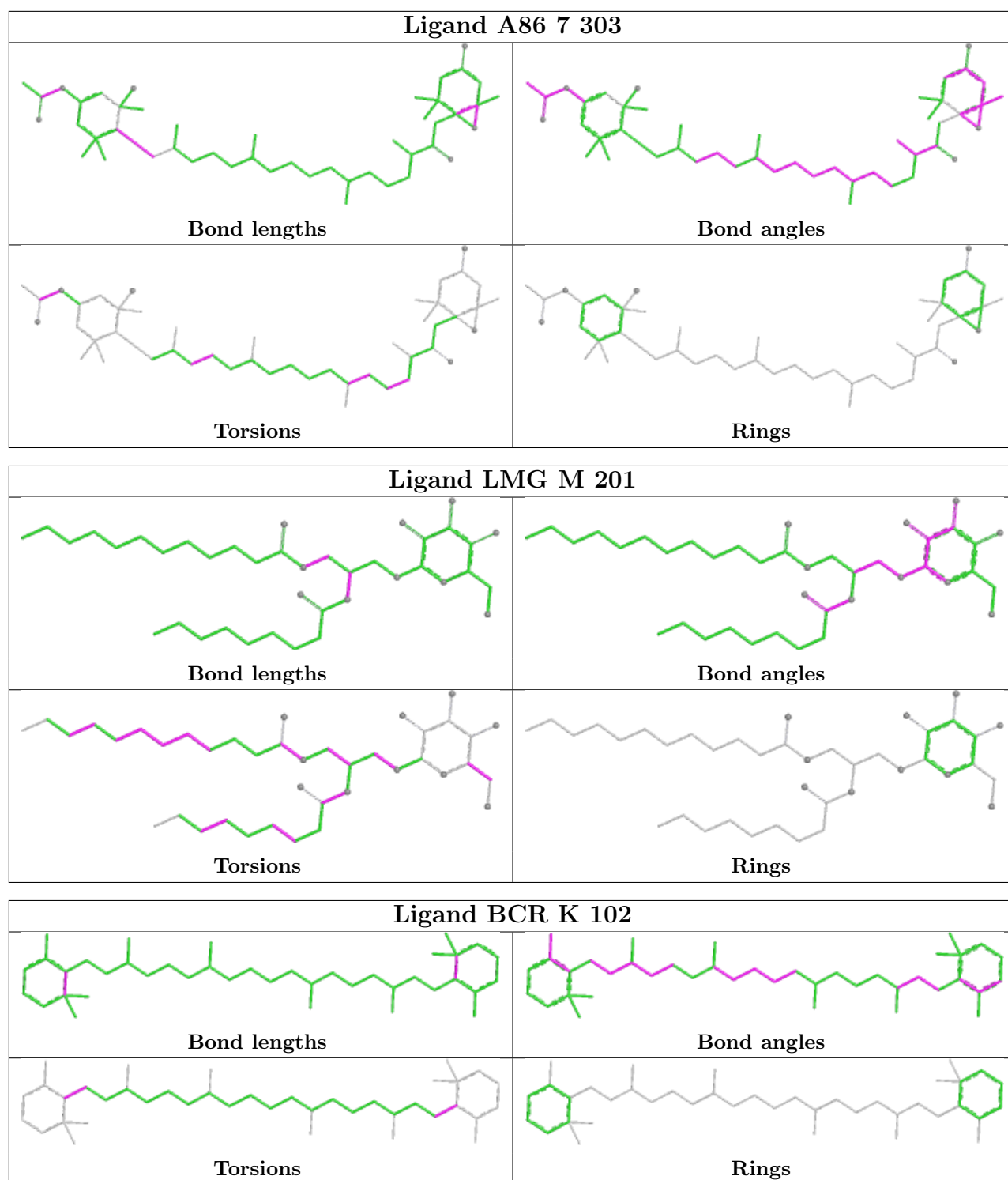


Ligand CLA 2 317

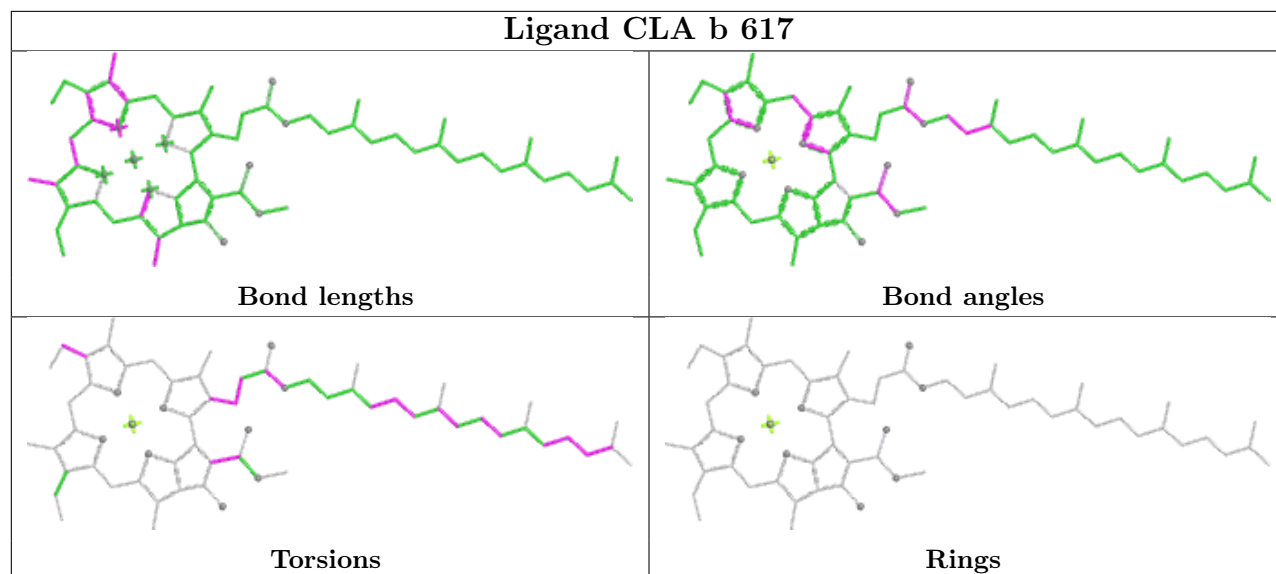


Ligand CLA C 509

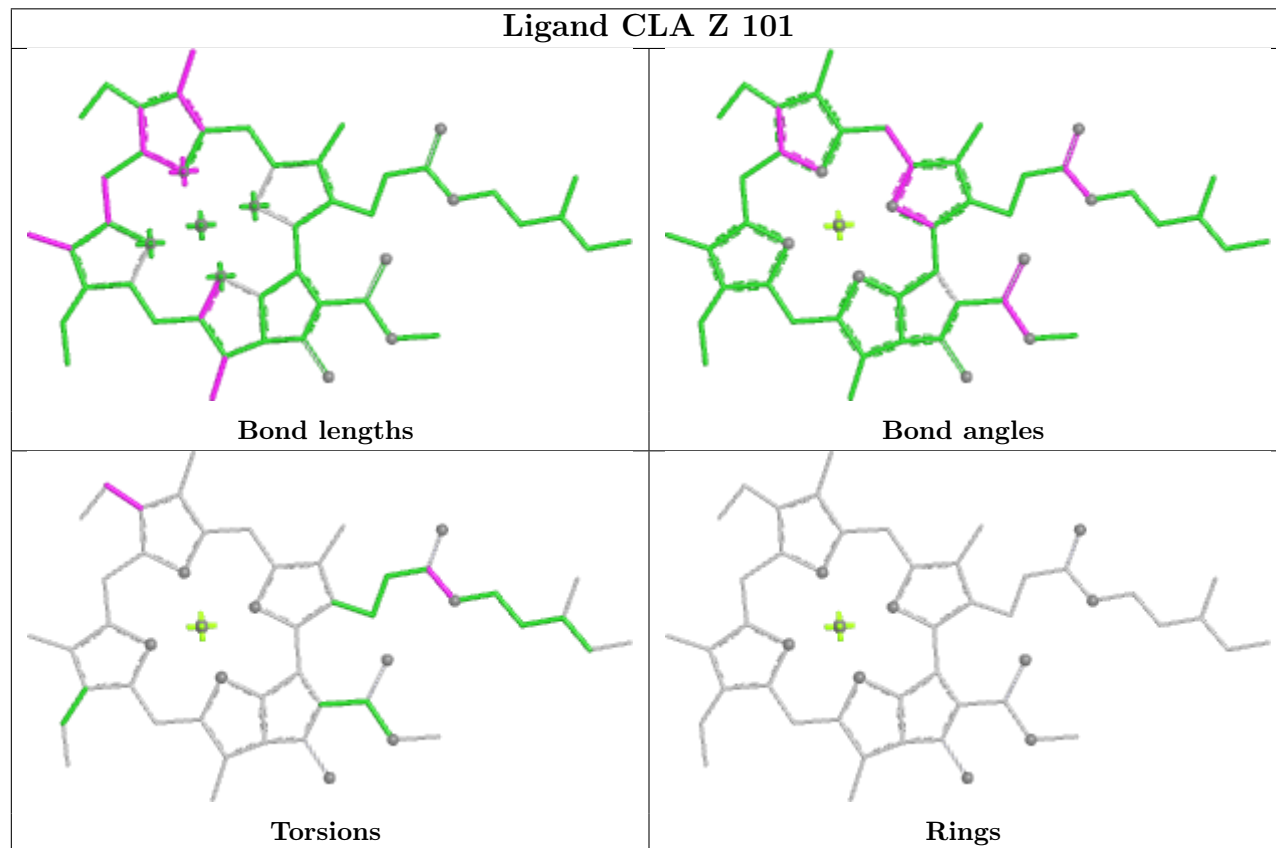




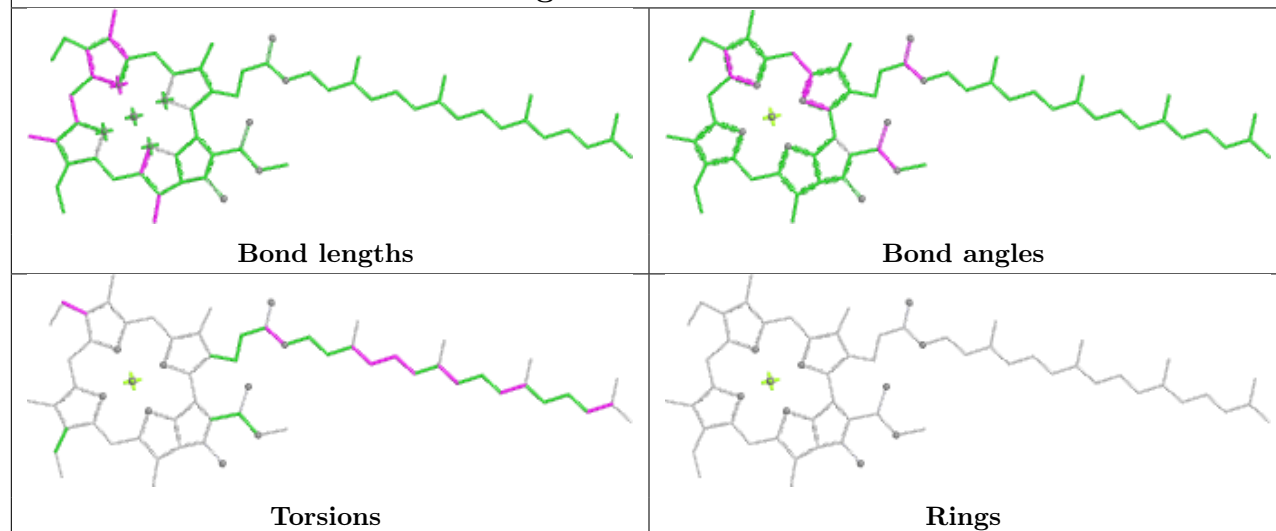
Ligand CLA b 617



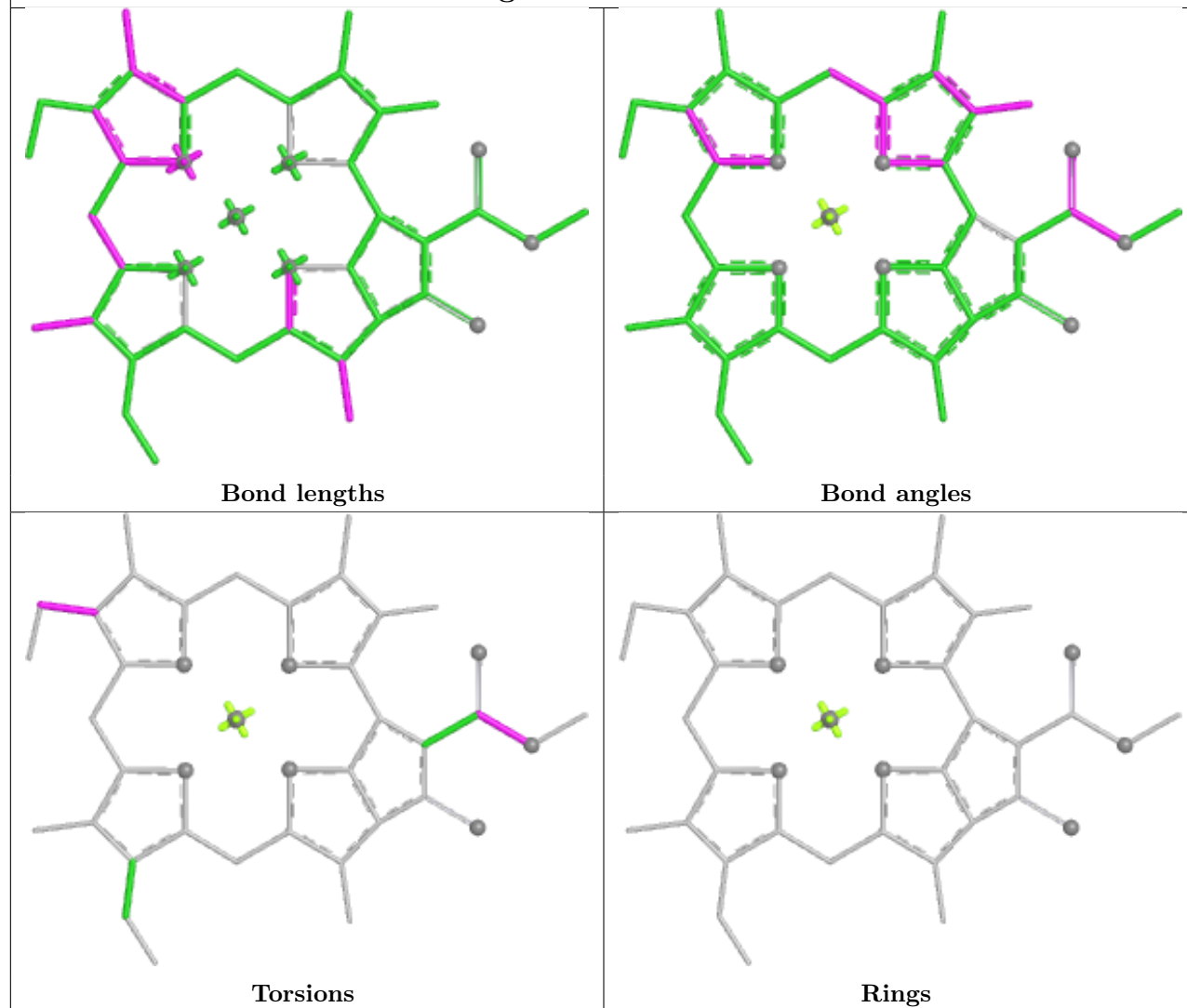
Ligand CLA Z 101

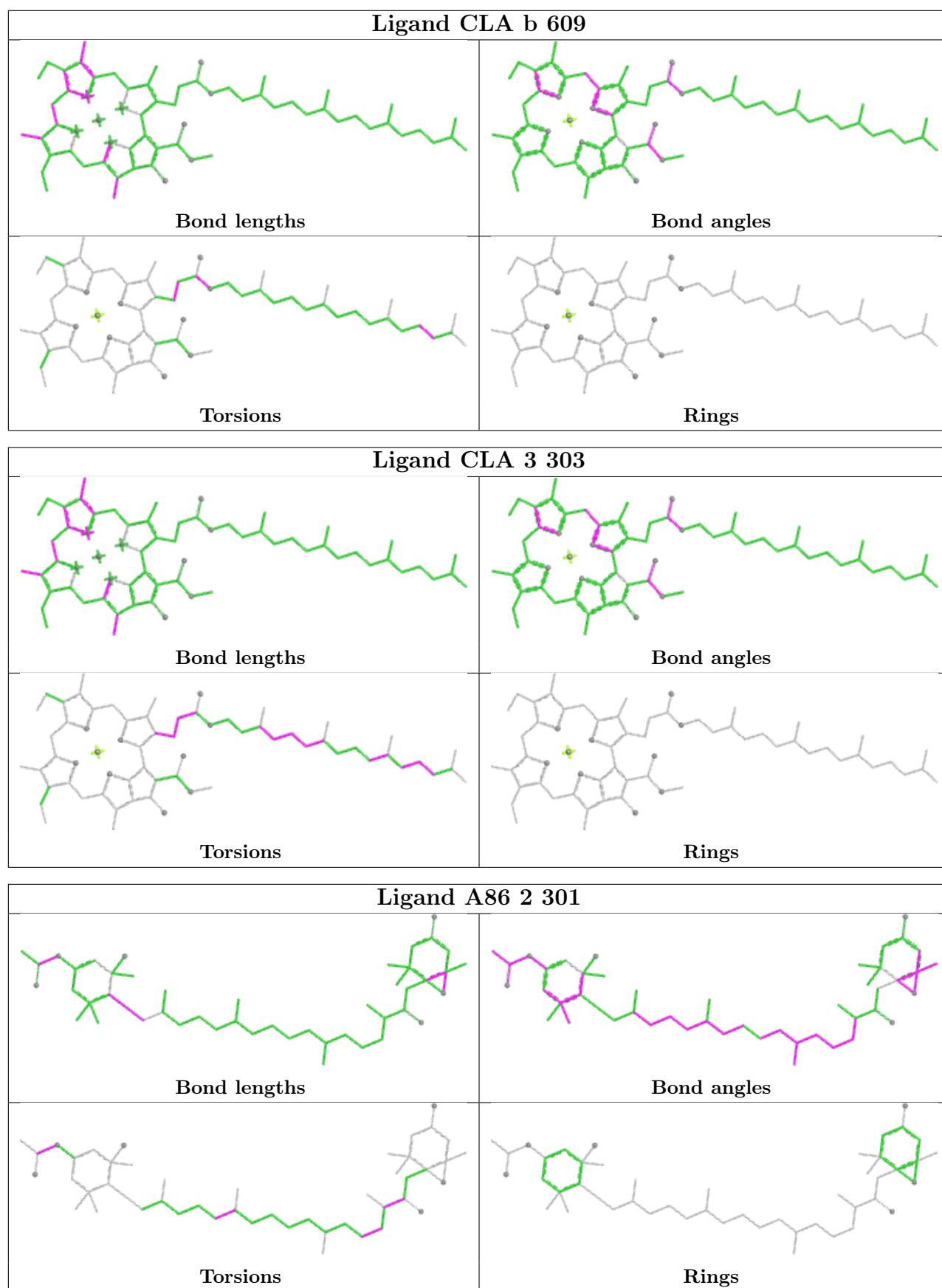


Ligand CLA 3 307

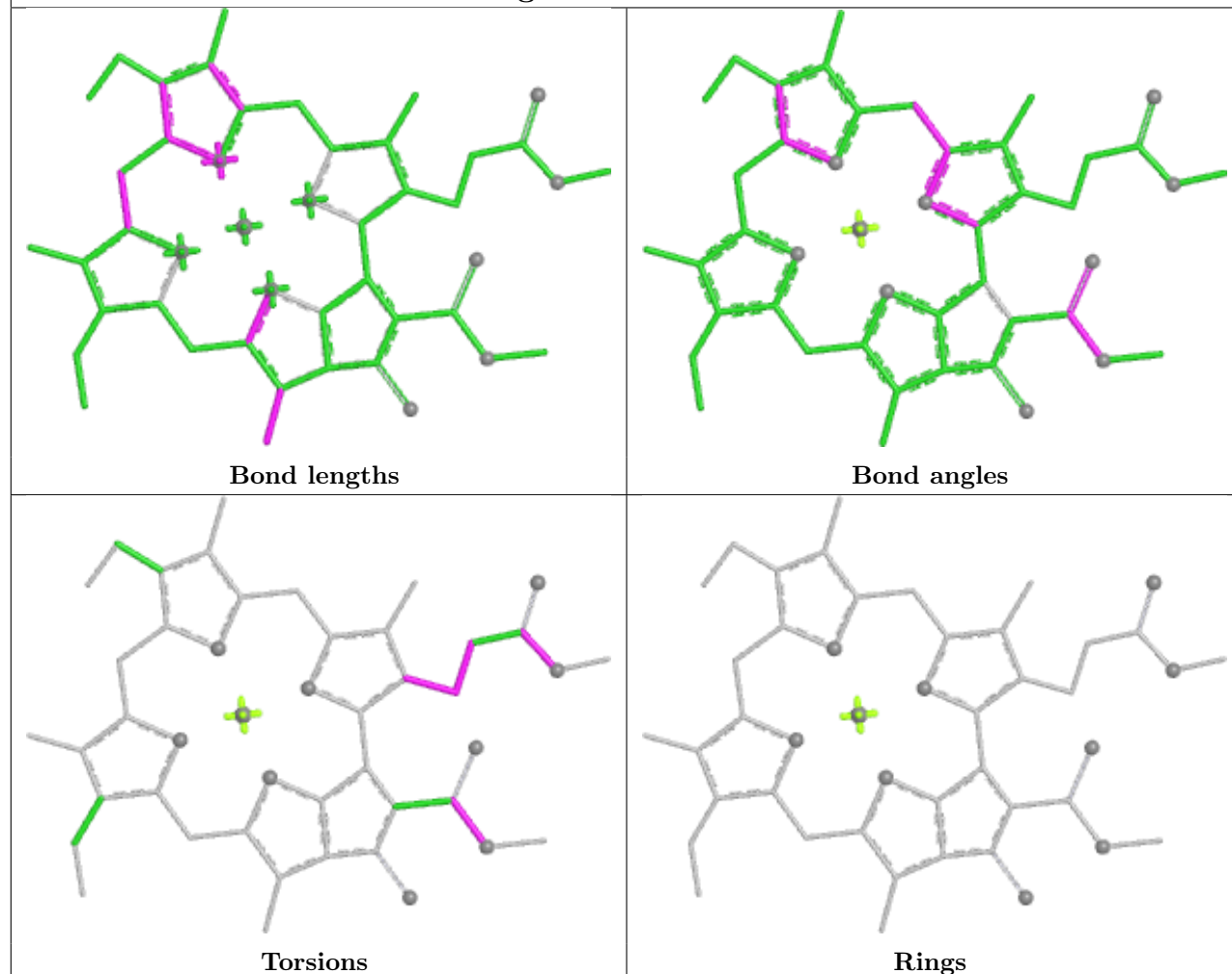


Ligand CLA 7 308

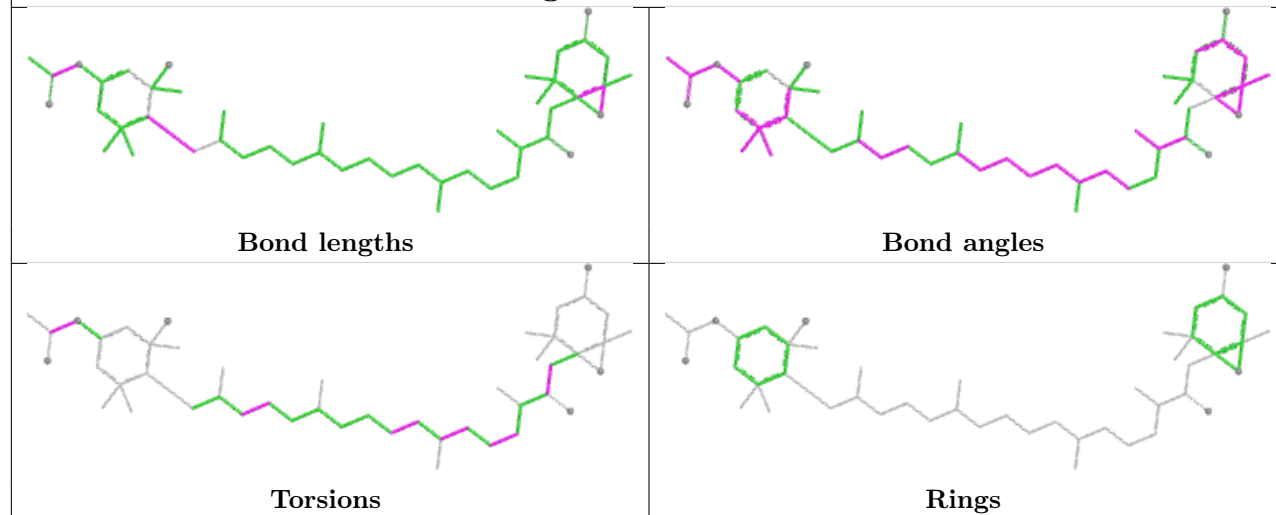




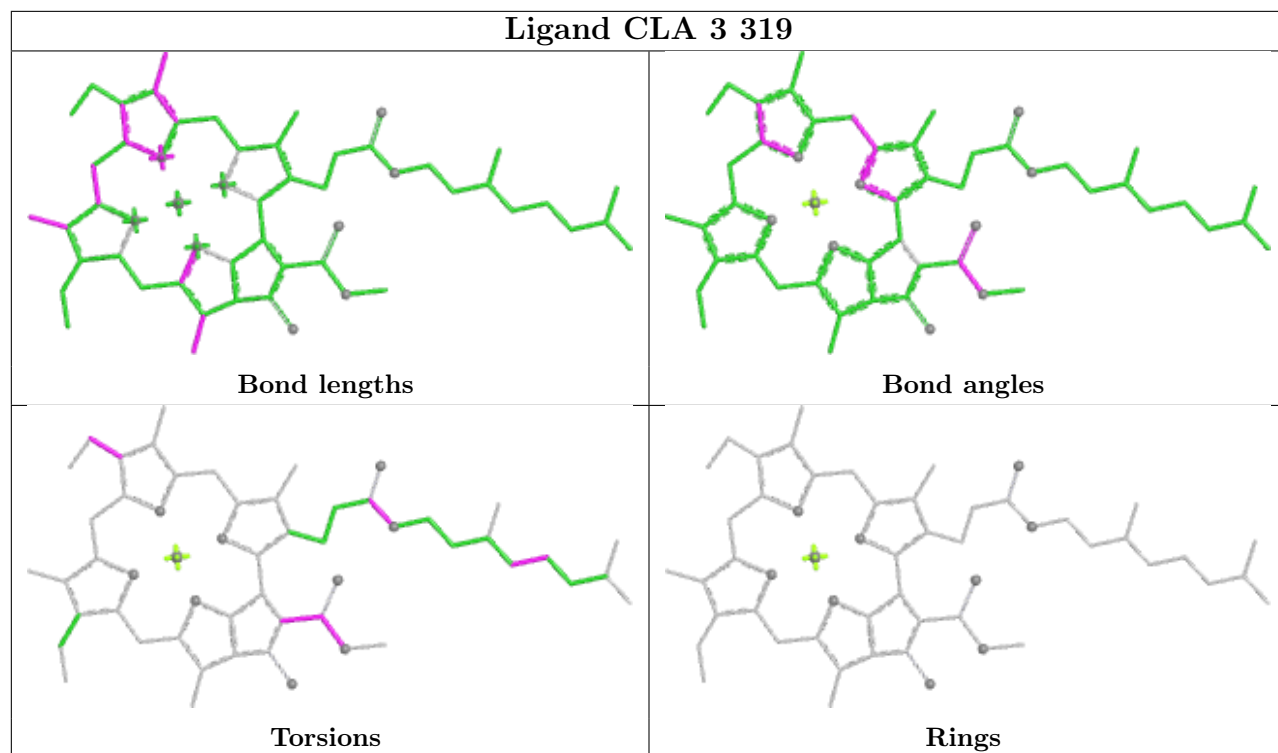
Ligand CLA 5 308



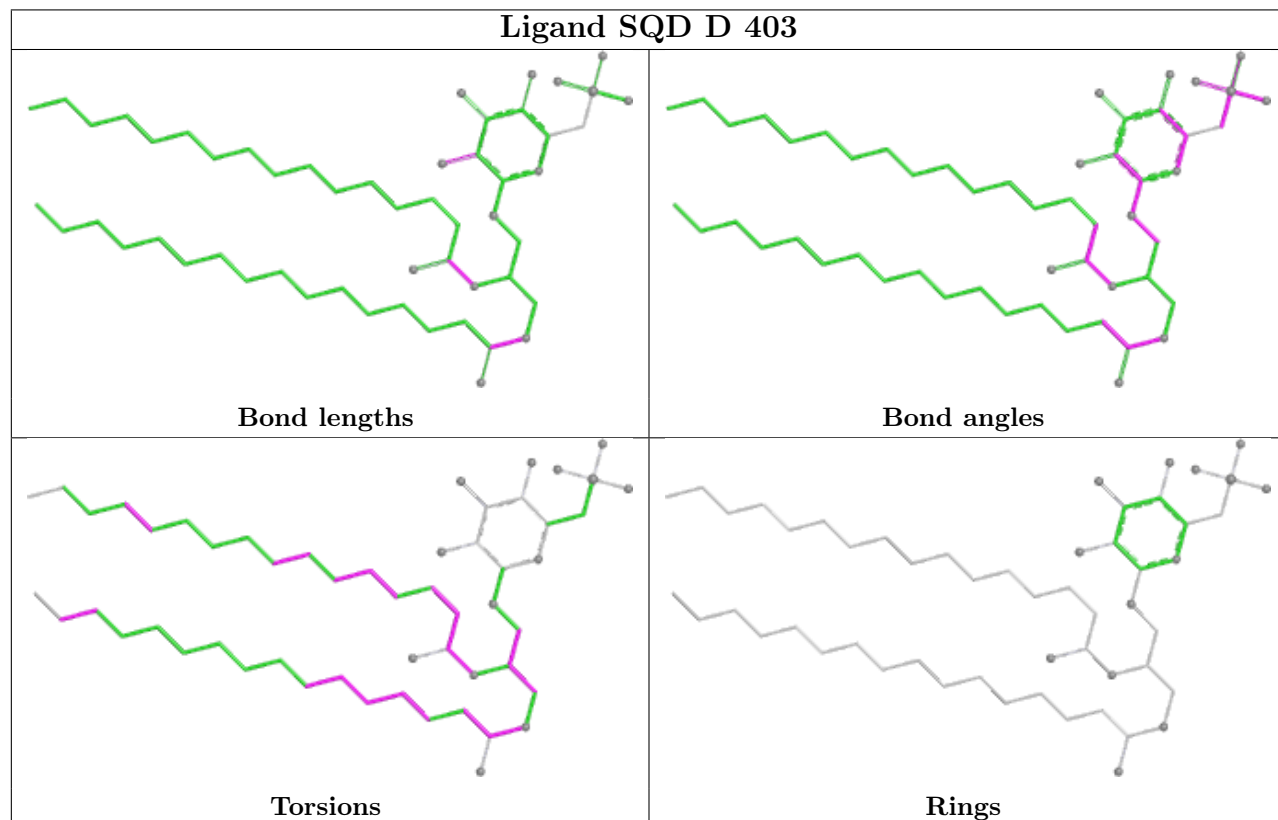
Ligand A86 8 302

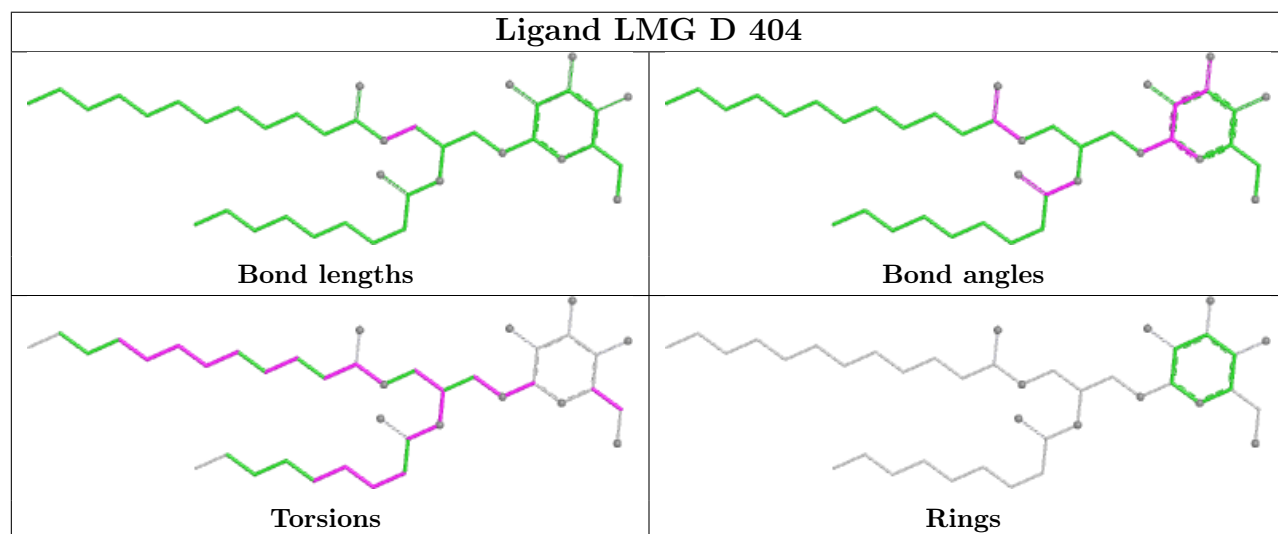
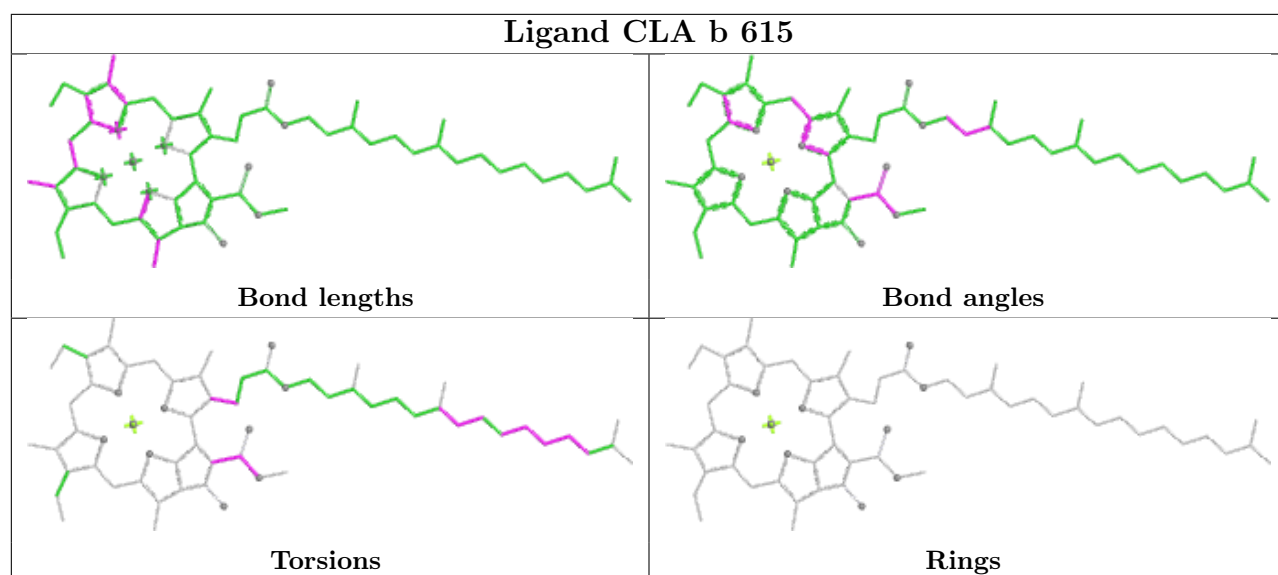


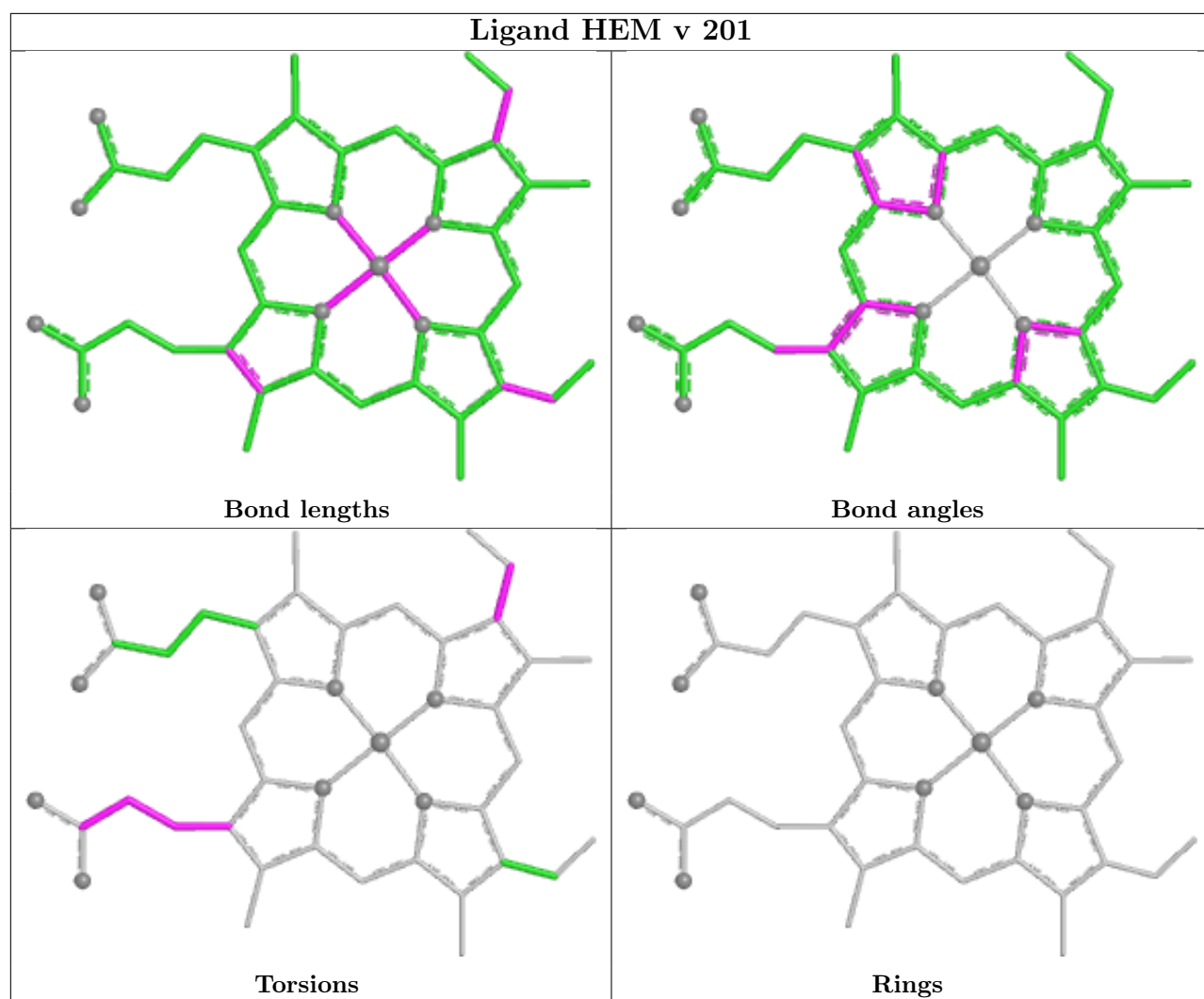
Ligand CLA 3 319

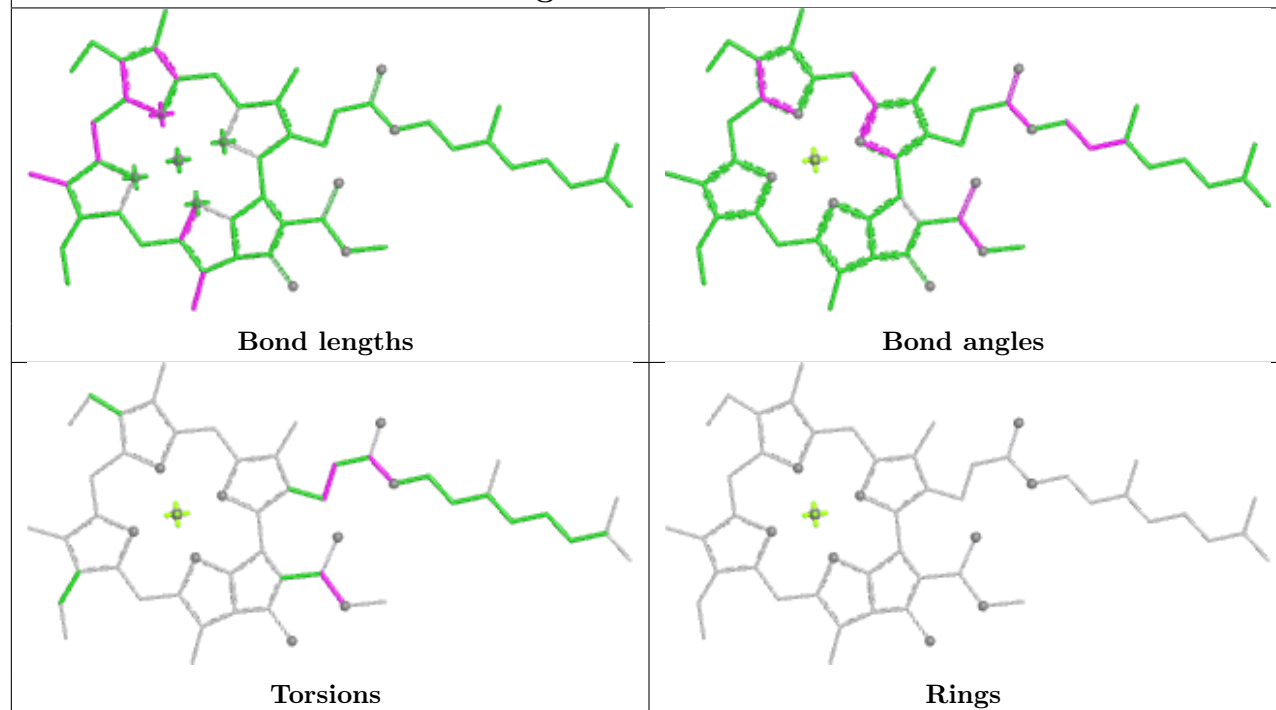
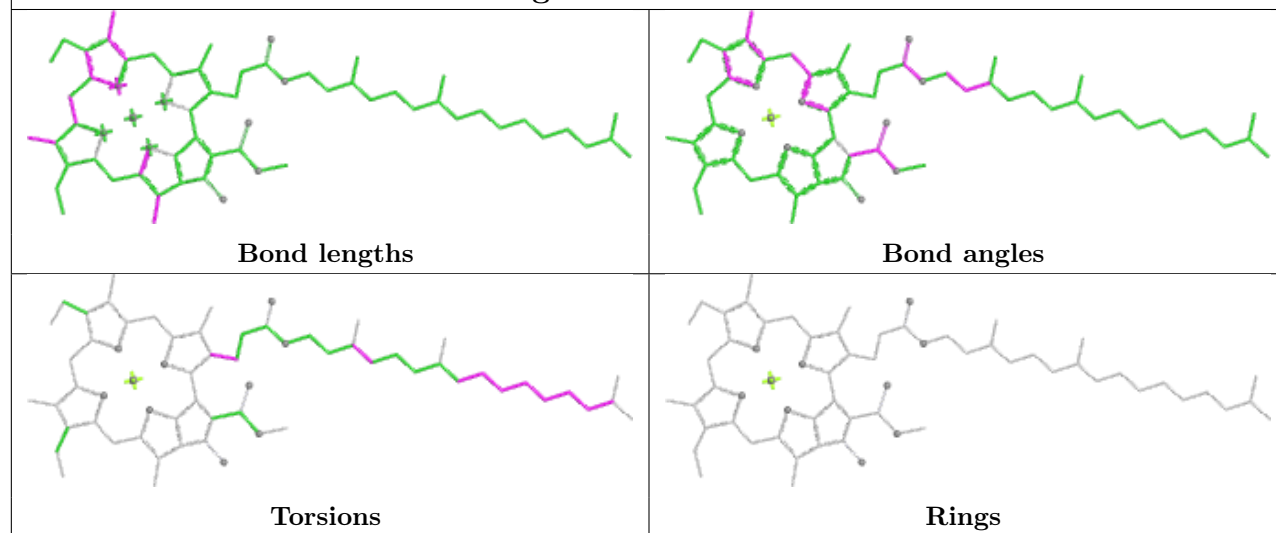


Ligand SQD D 403

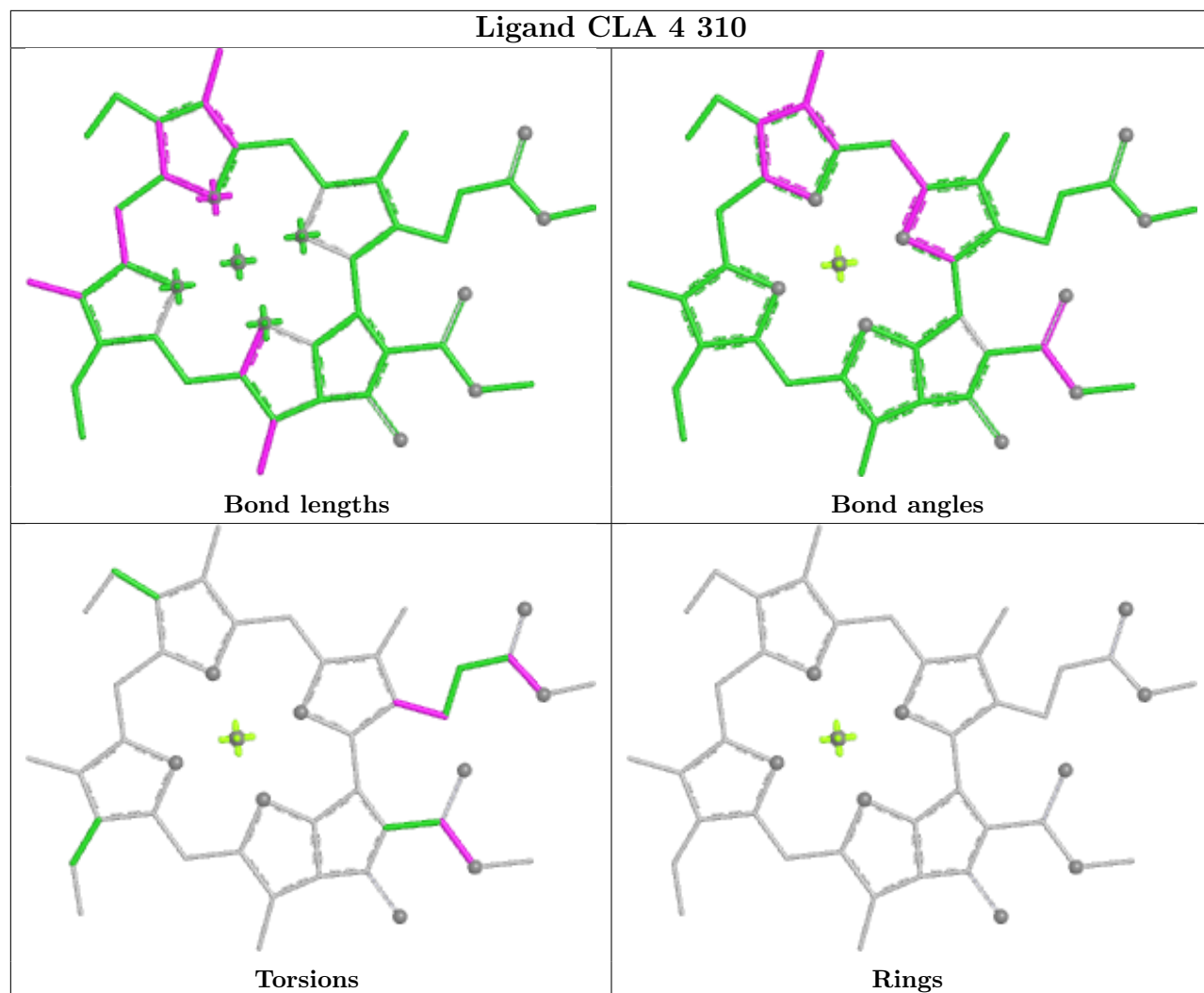


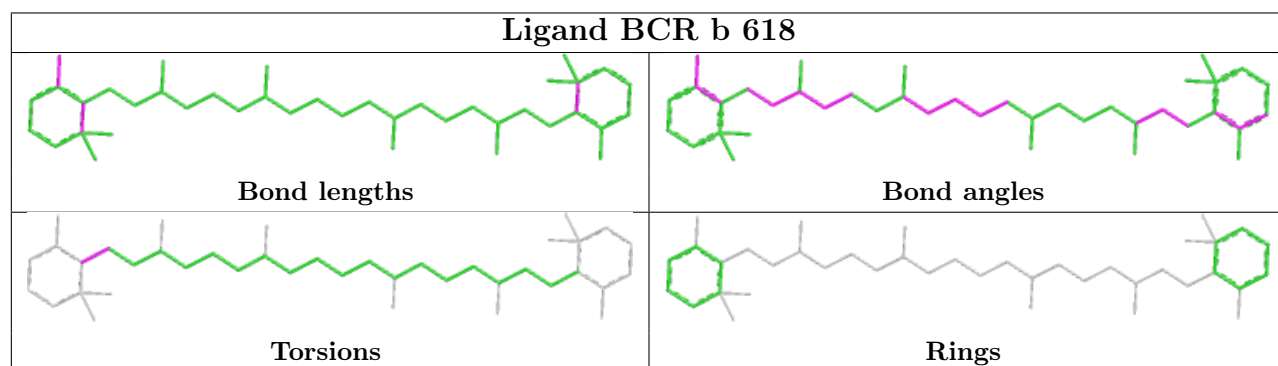
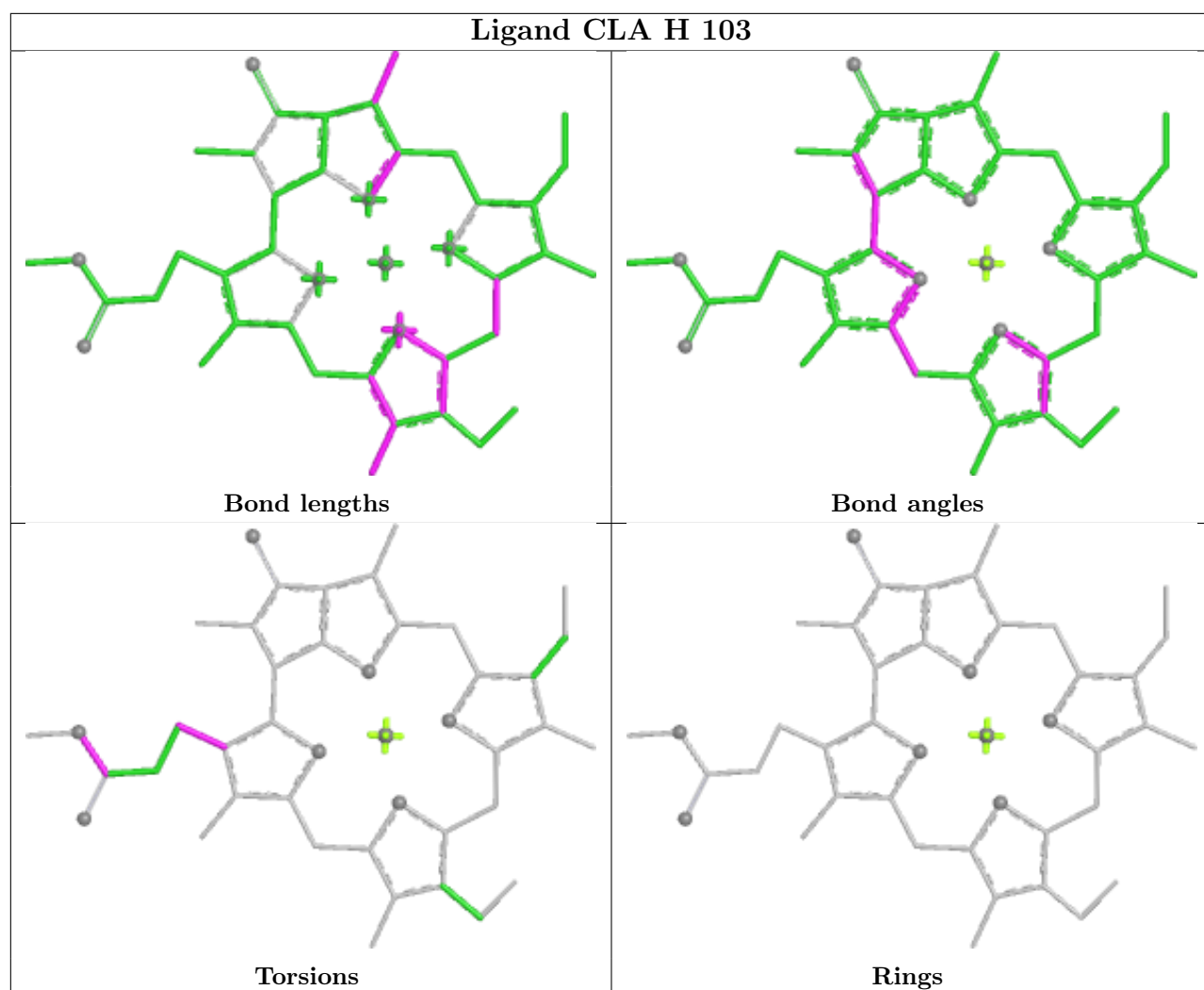


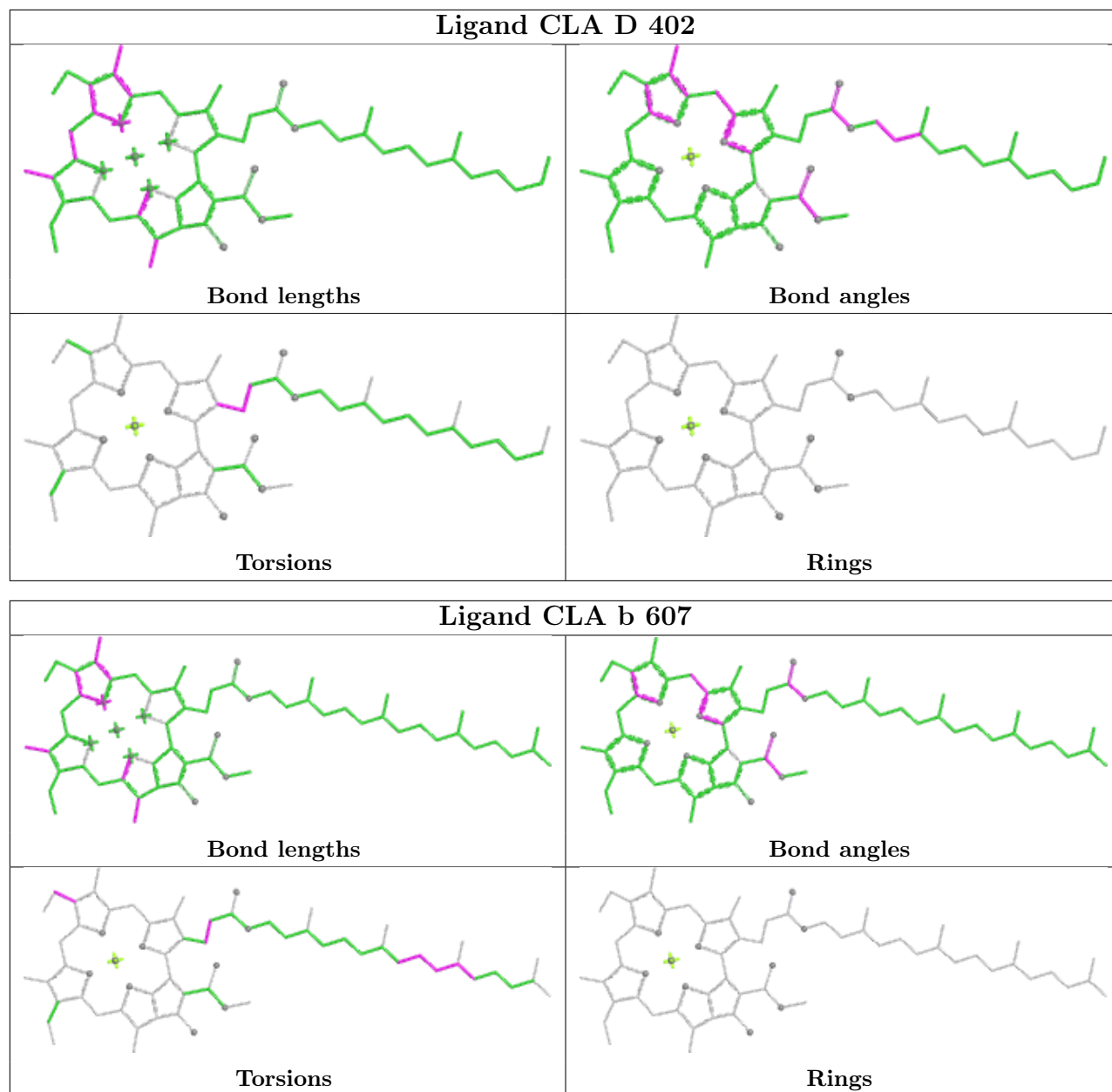


Ligand CLA 1 311**Ligand CLA B 611**

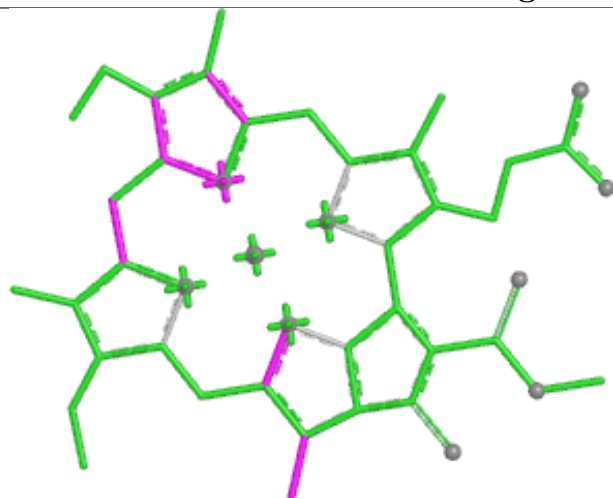
Ligand CLA 4 310



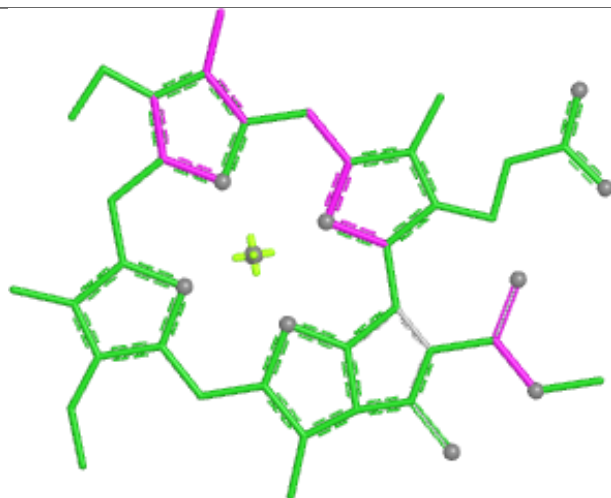




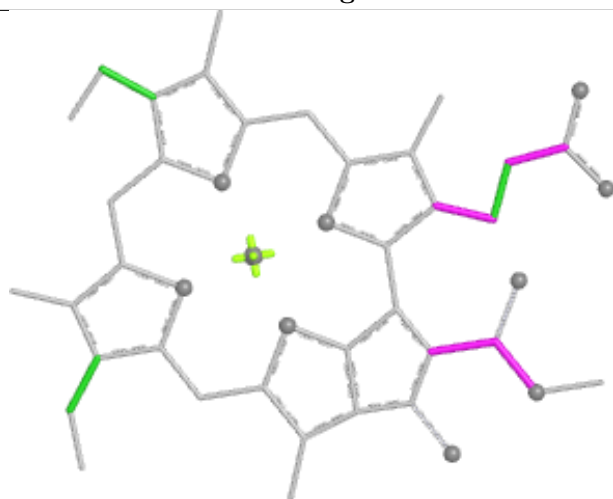
Ligand CLA 0 310



Bond lengths



Bond angles

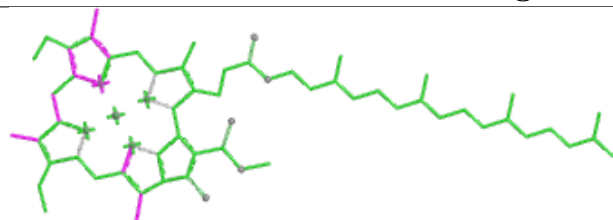


Torsions

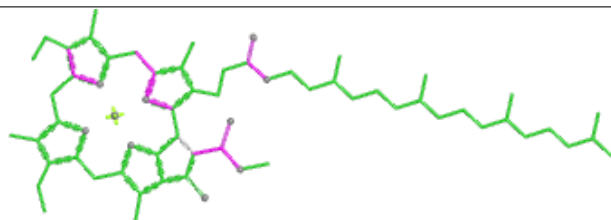


Rings

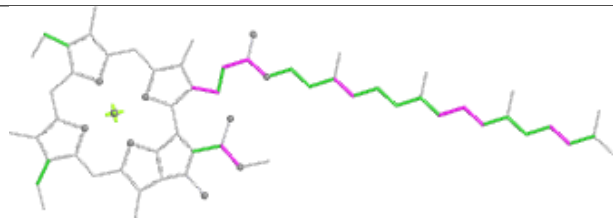
Ligand CLA B 612



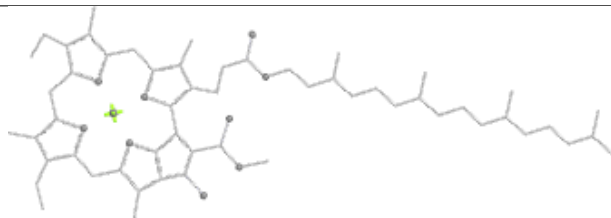
Bond lengths



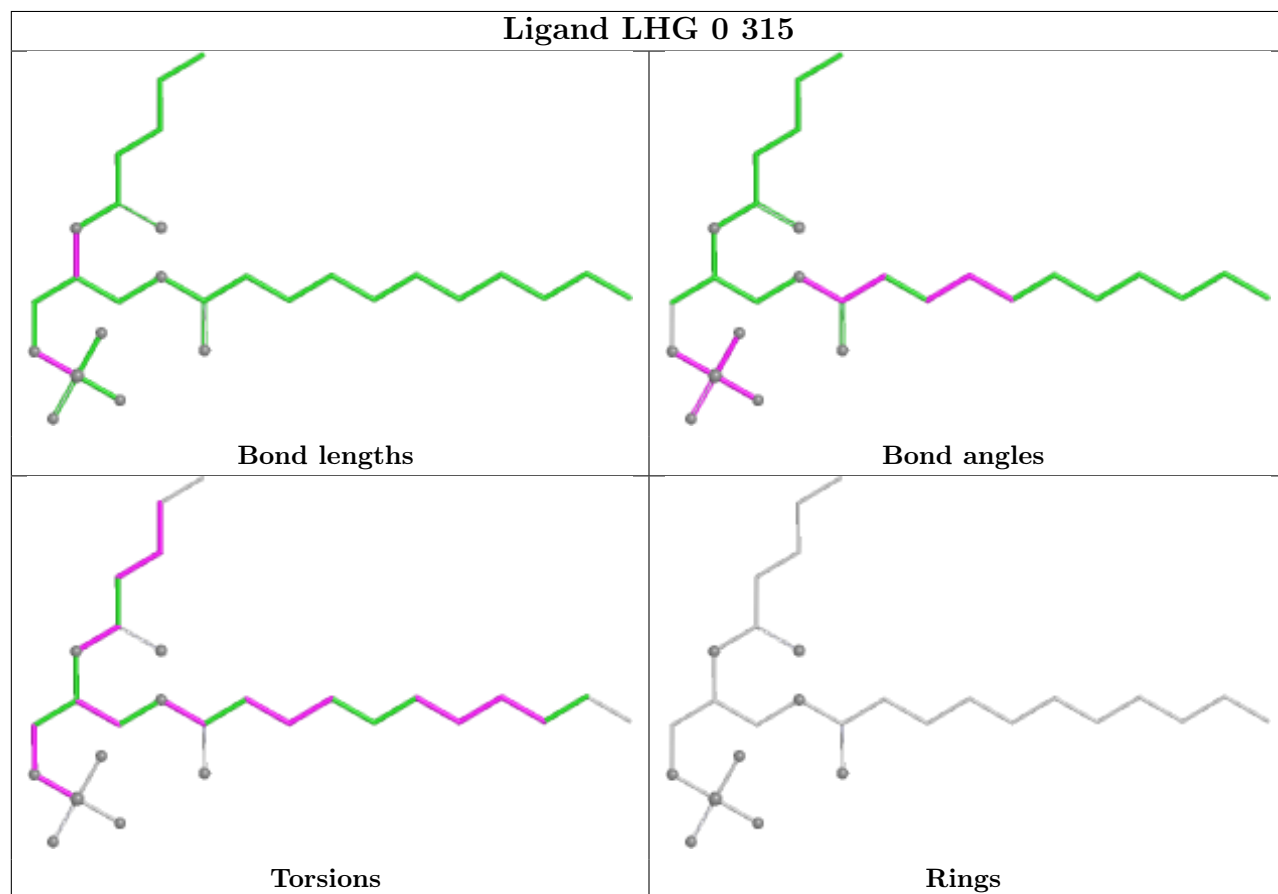
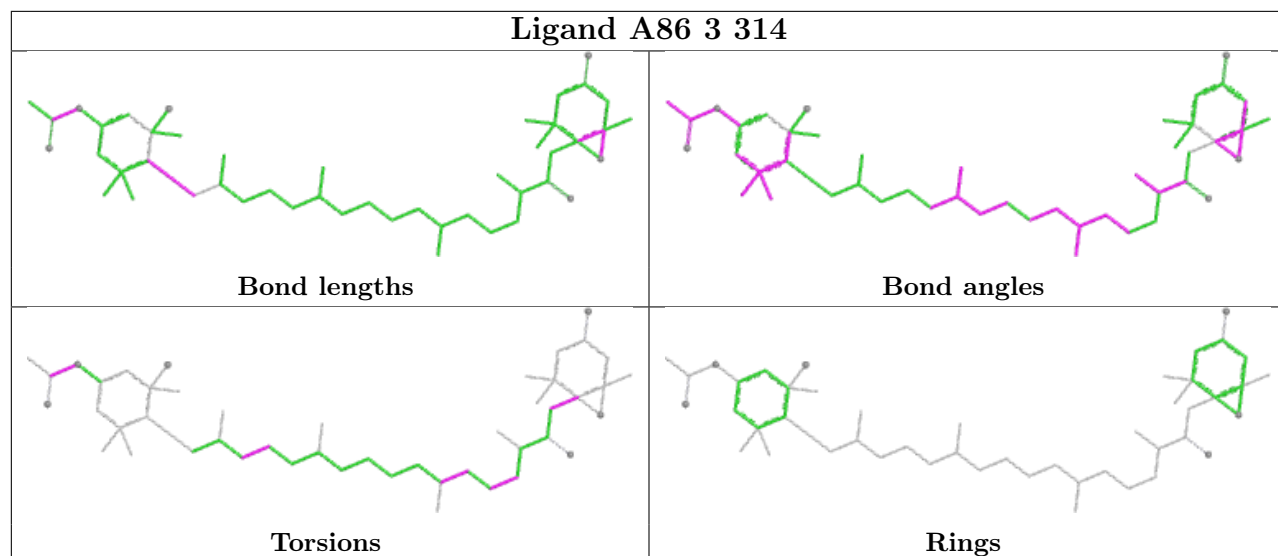
Bond angles

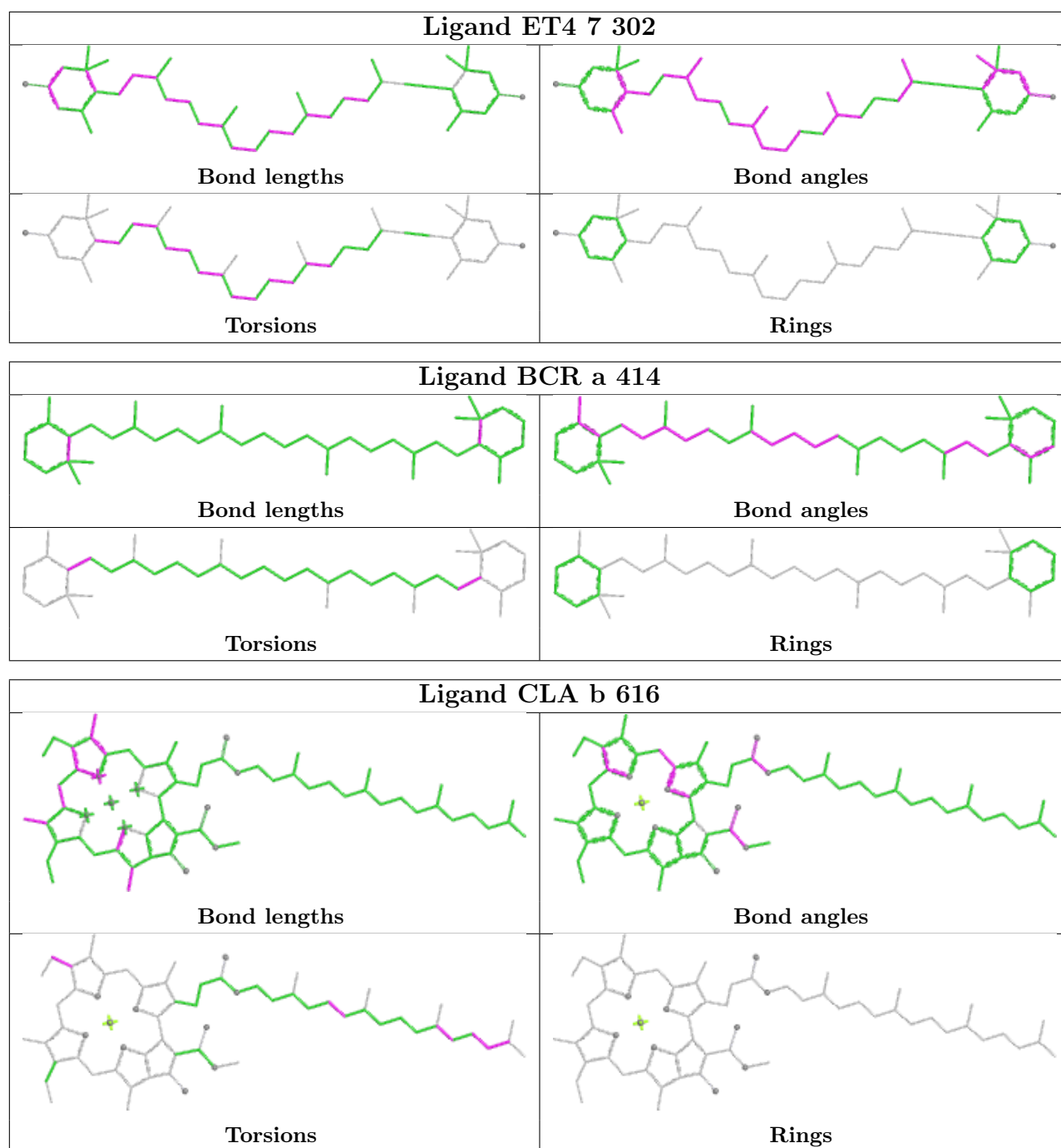


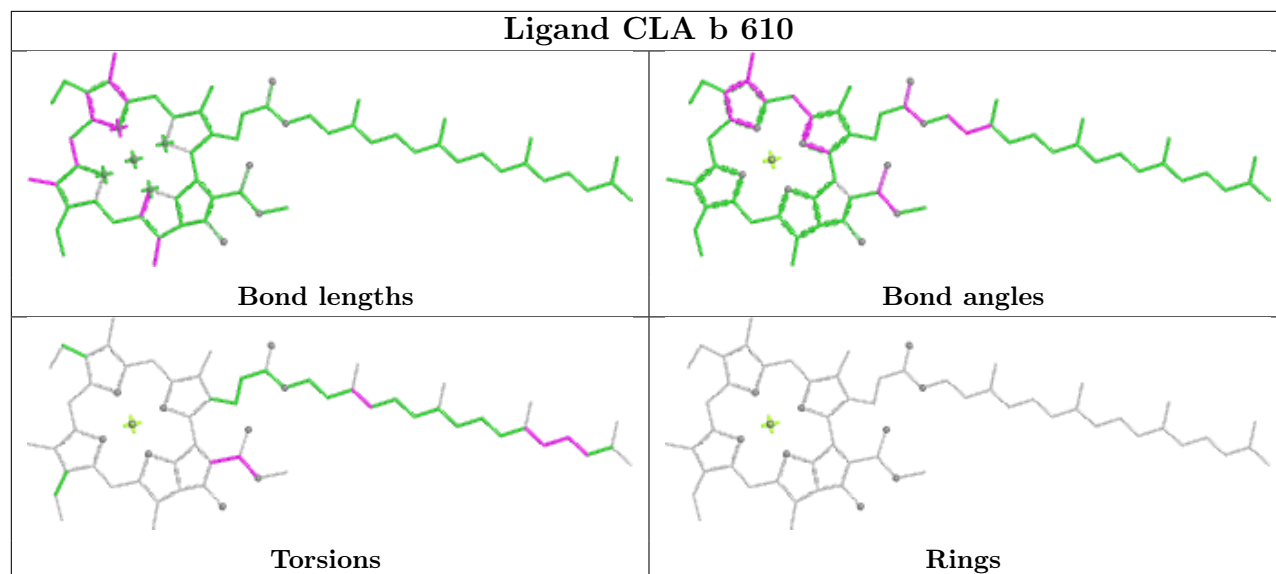
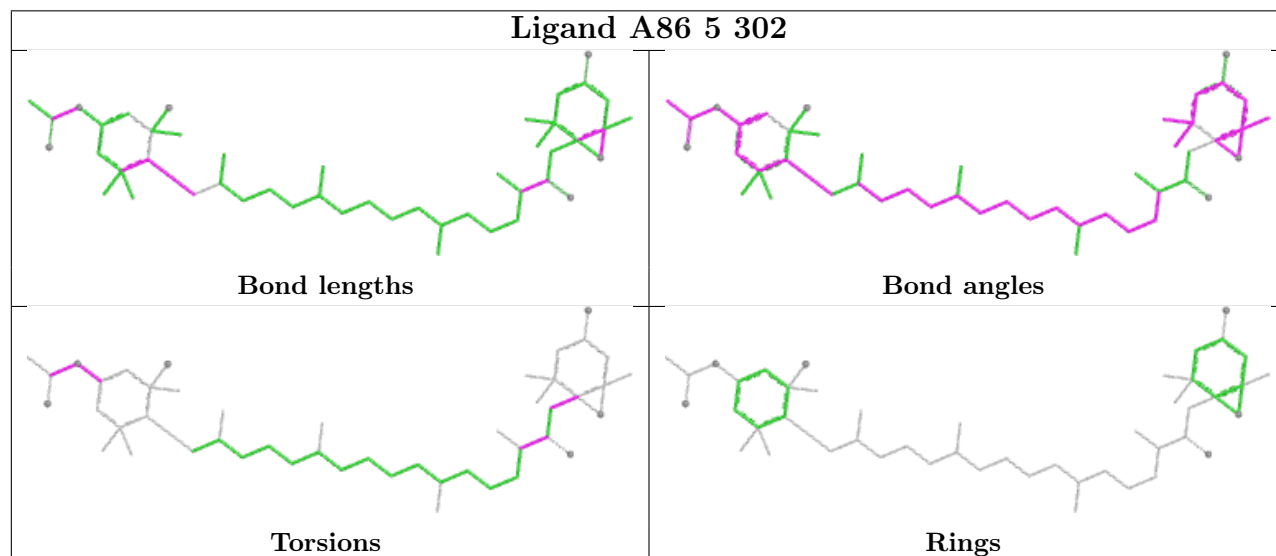
Torsions

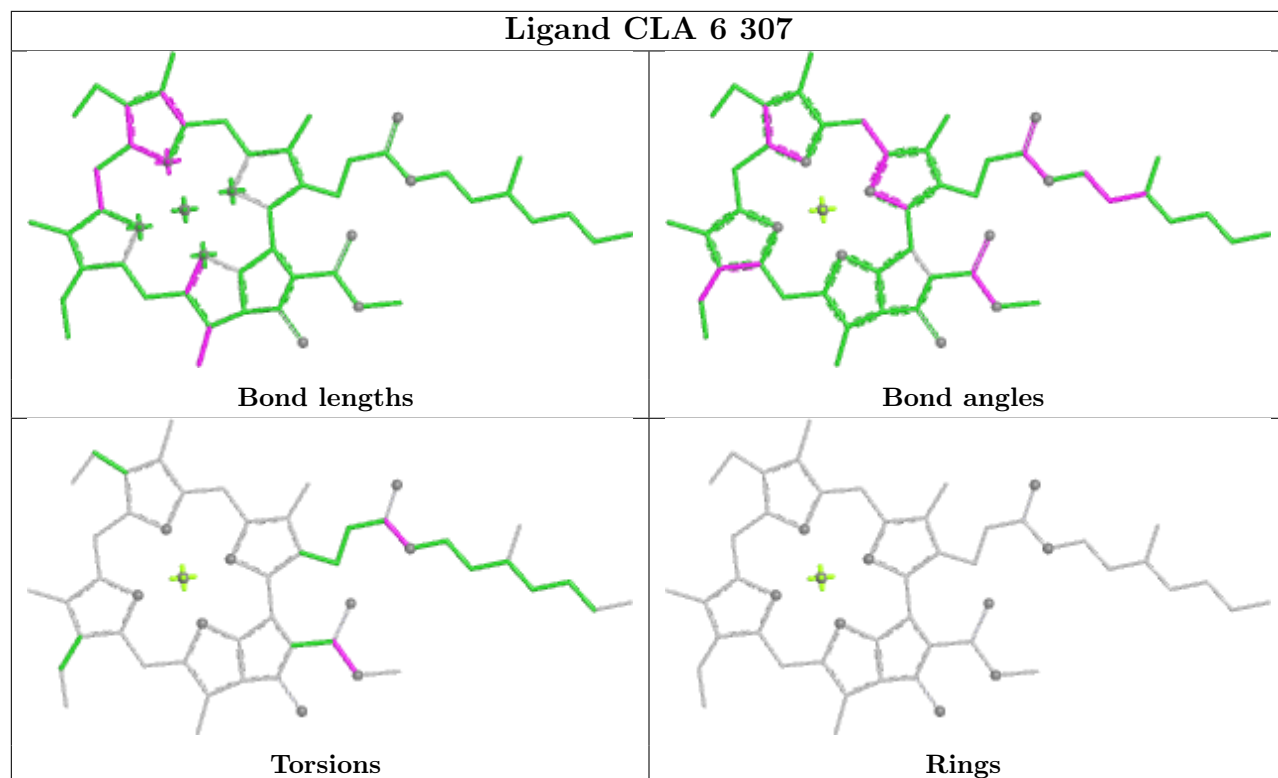


Rings

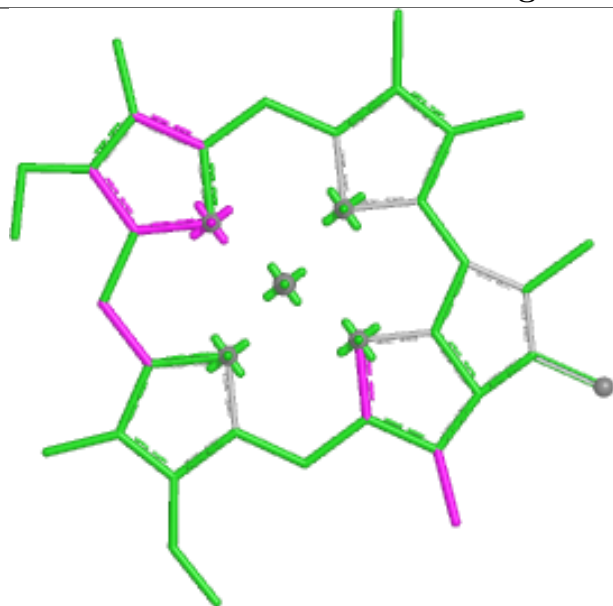




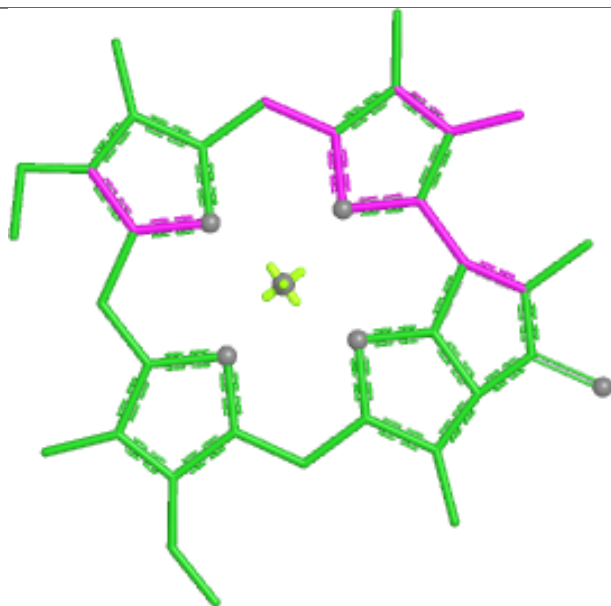
Ligand CLA b 610**Ligand A86 5 302**



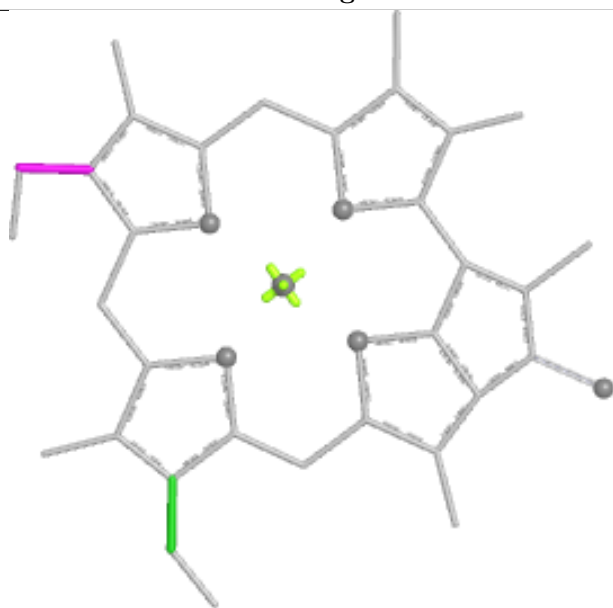
Ligand CLA 2 316



Bond lengths



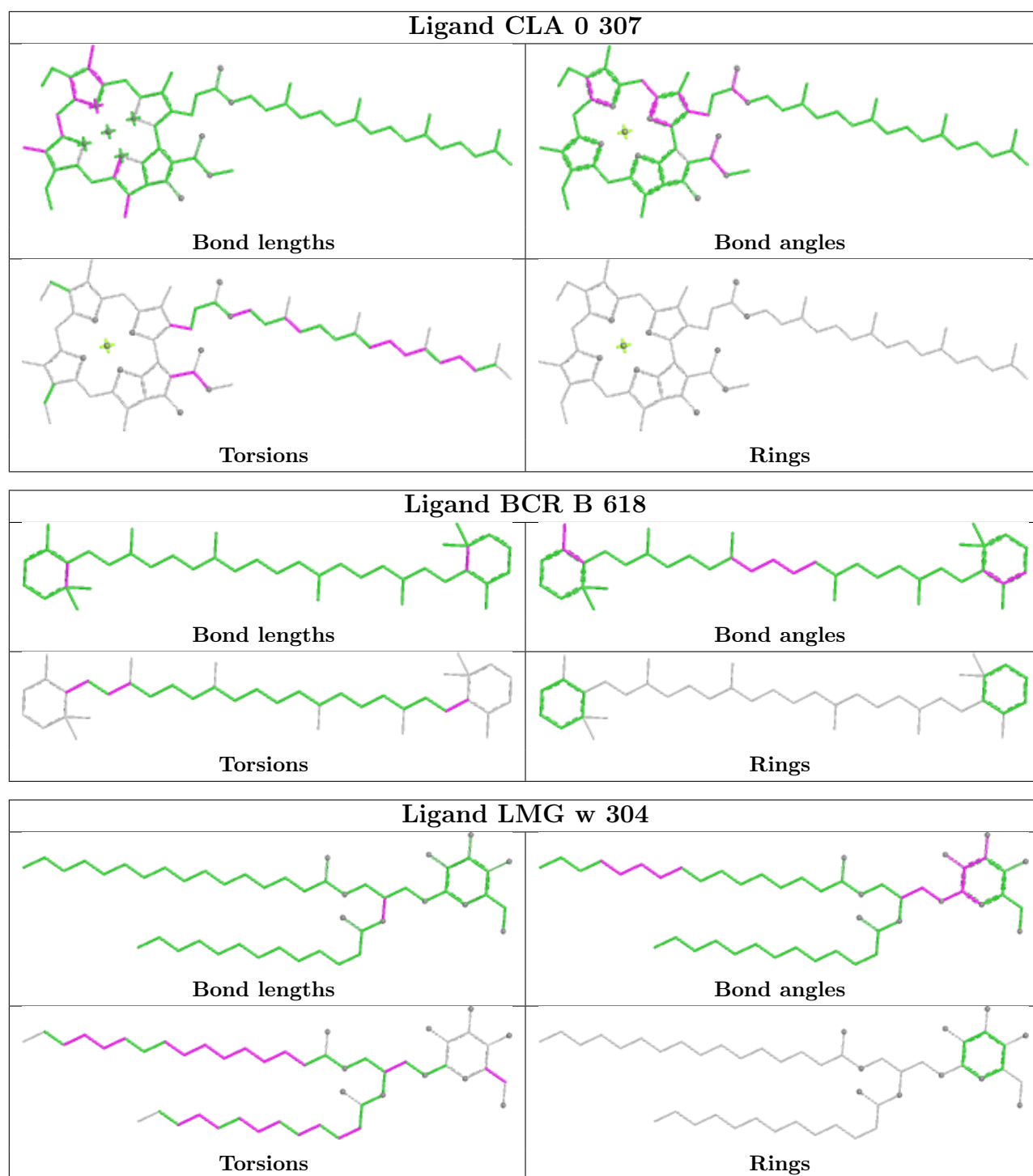
Bond angles



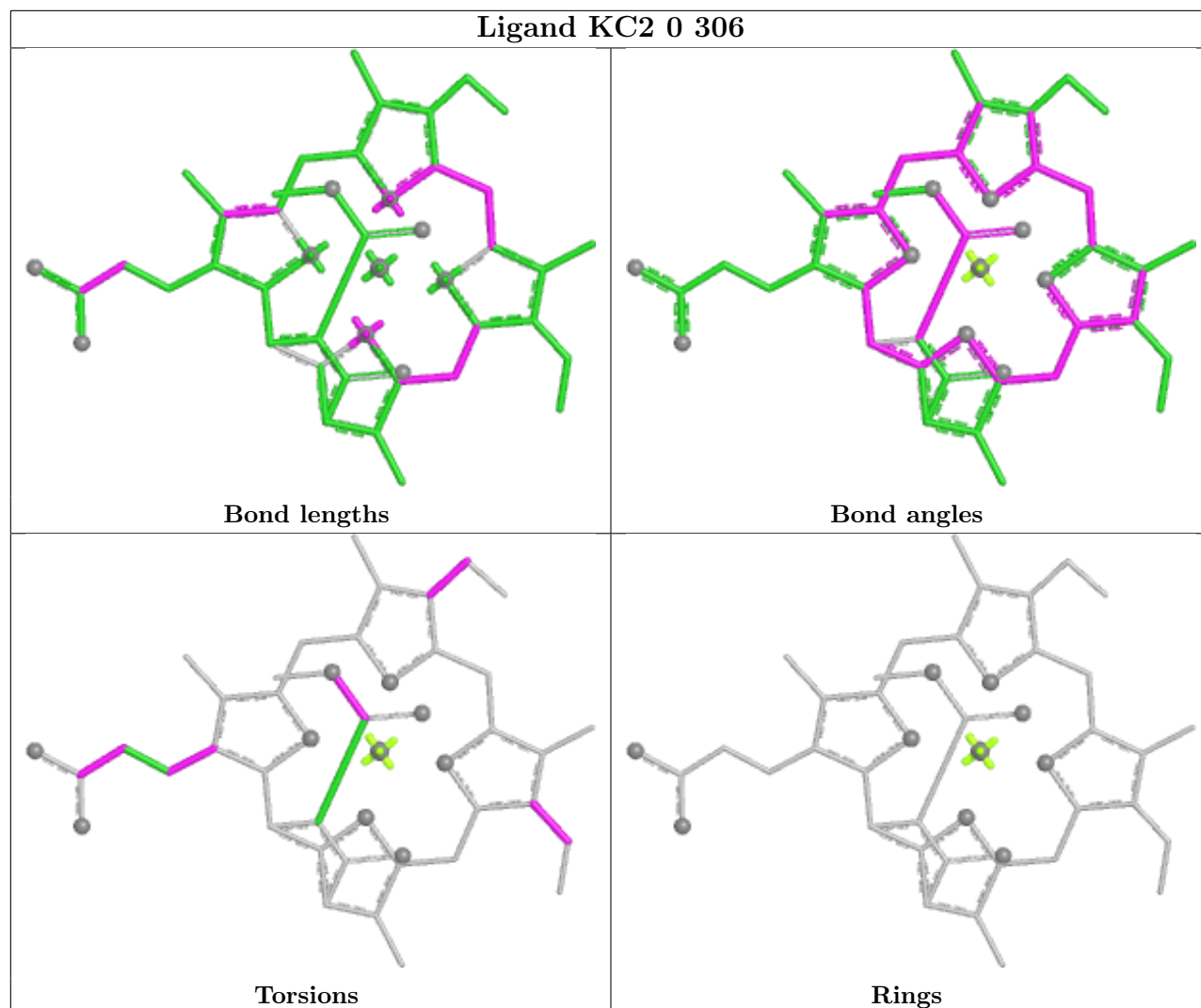
Torsions



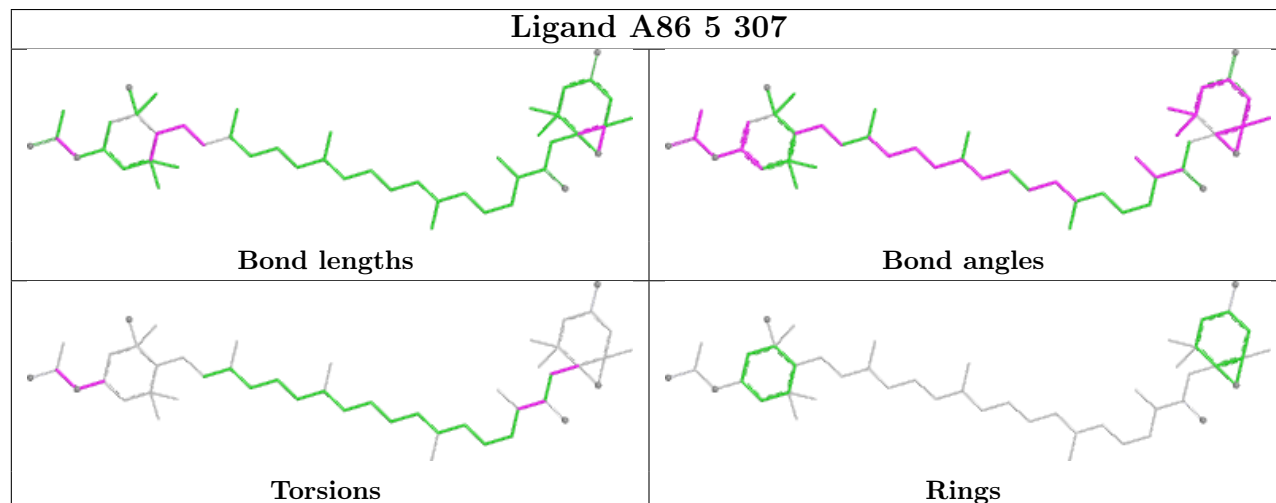
Rings

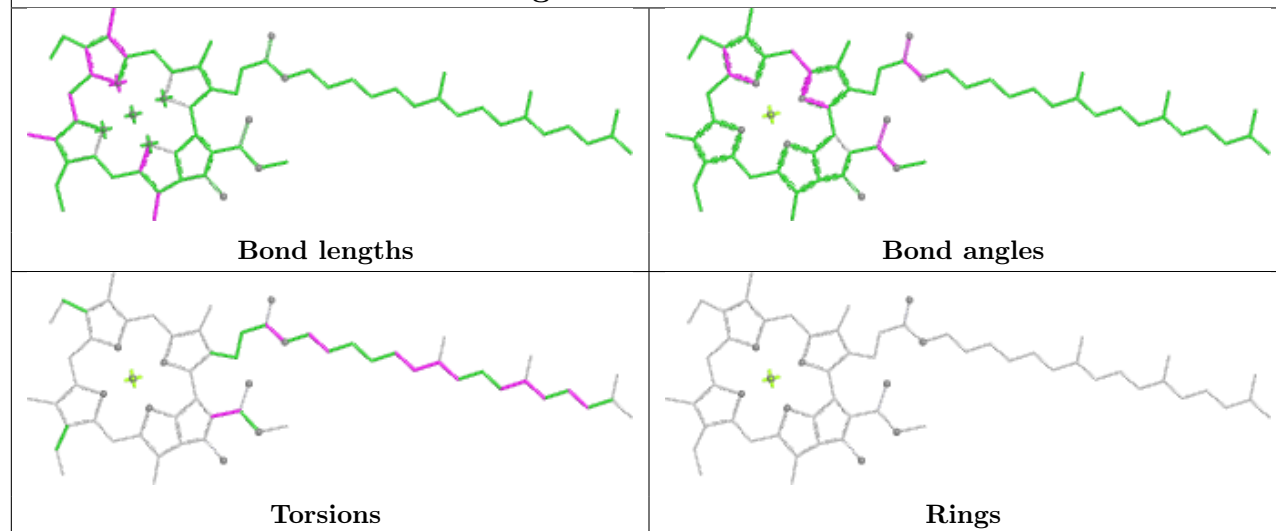
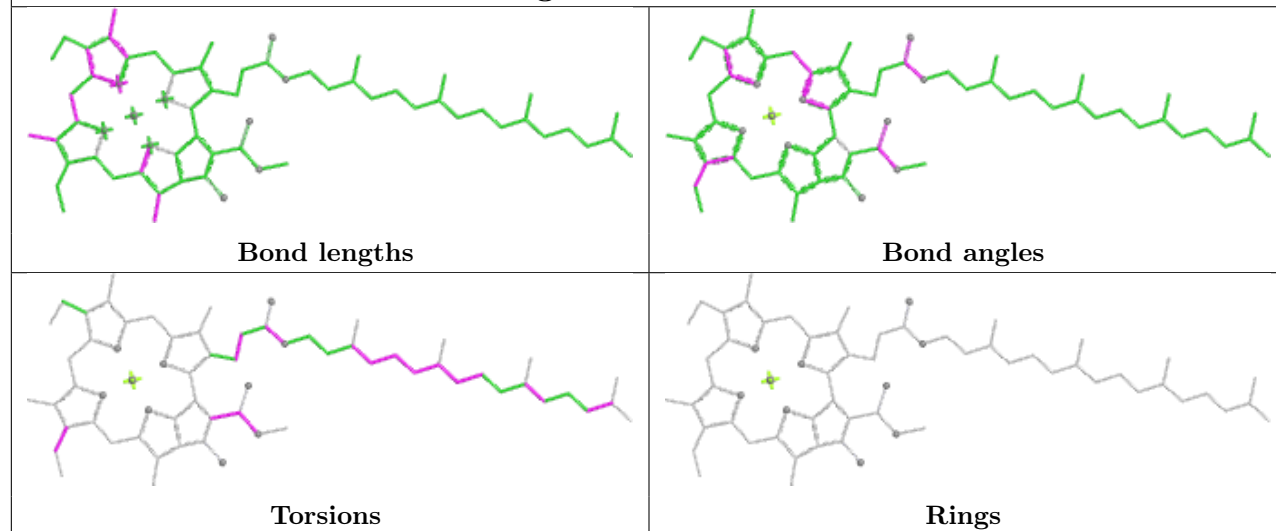


Ligand KC2 0 306

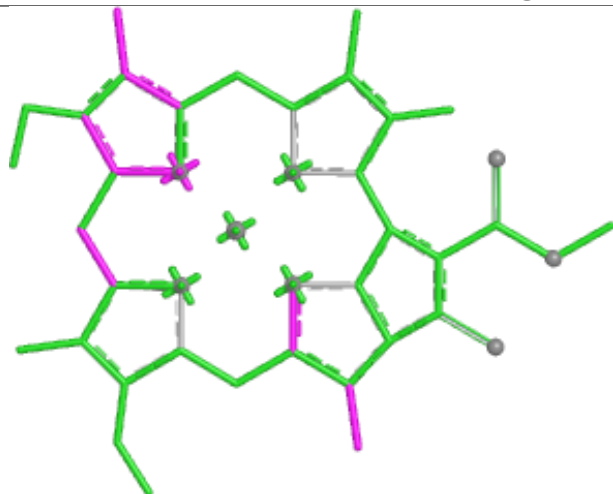


Ligand A86 5 307

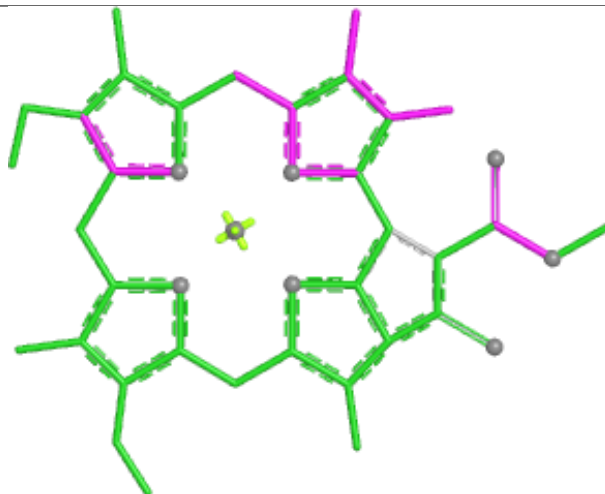


Ligand CLA C 512**Ligand CLA 7 305**

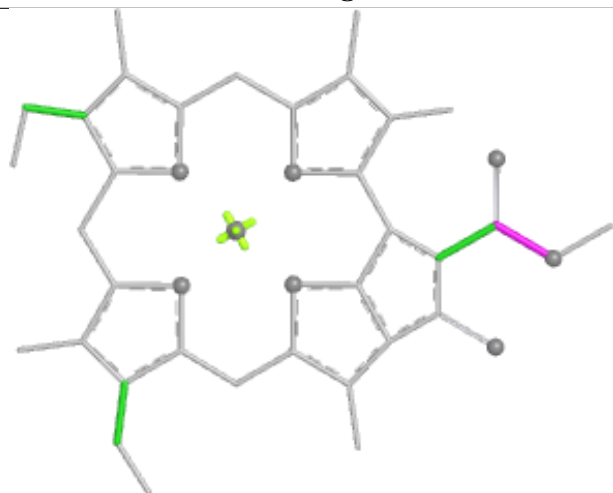
Ligand CLA 0 308



Bond lengths



Bond angles

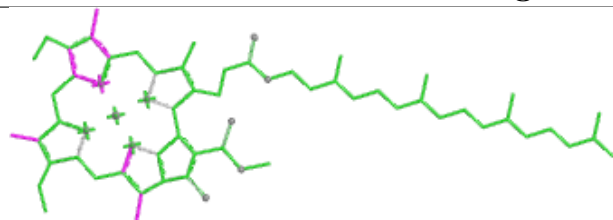


Torsions

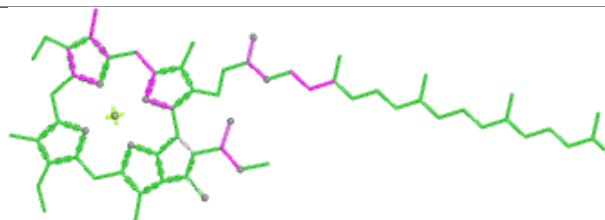


Rings

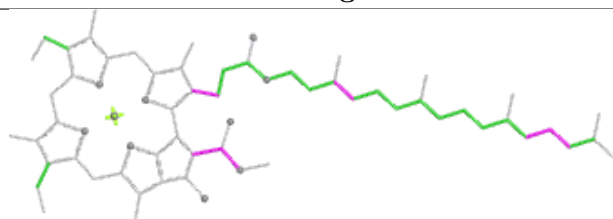
Ligand CLA B 609



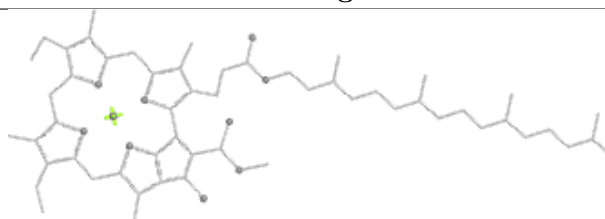
Bond lengths



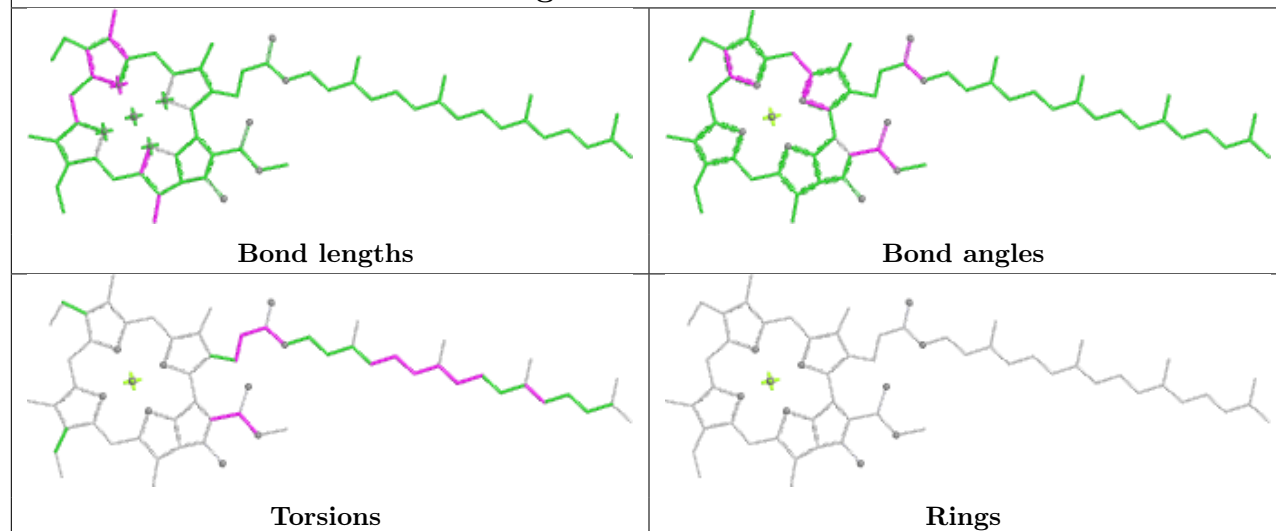
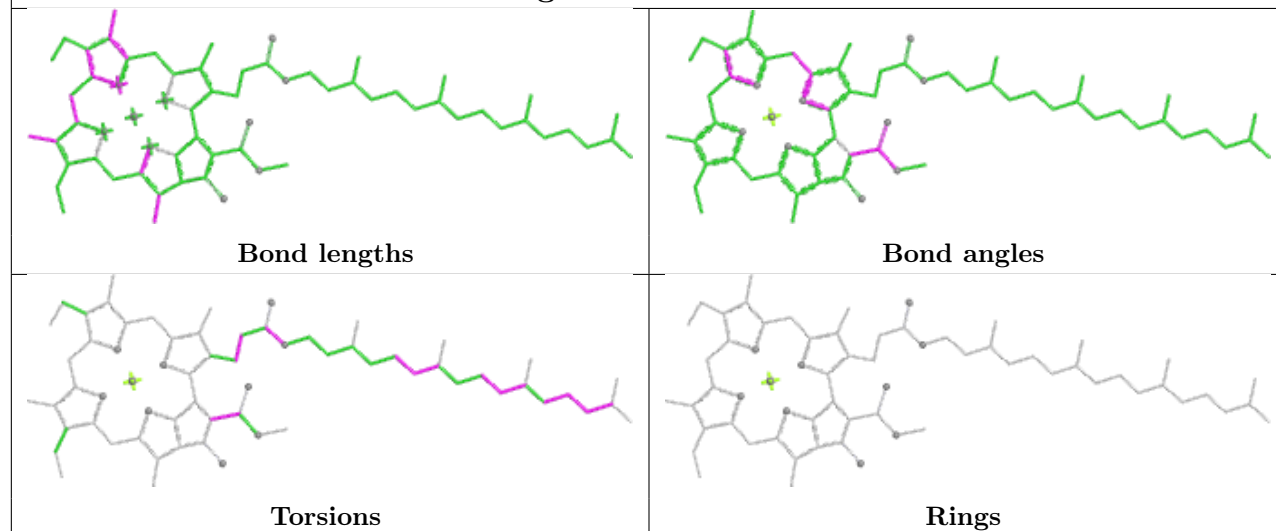
Bond angles



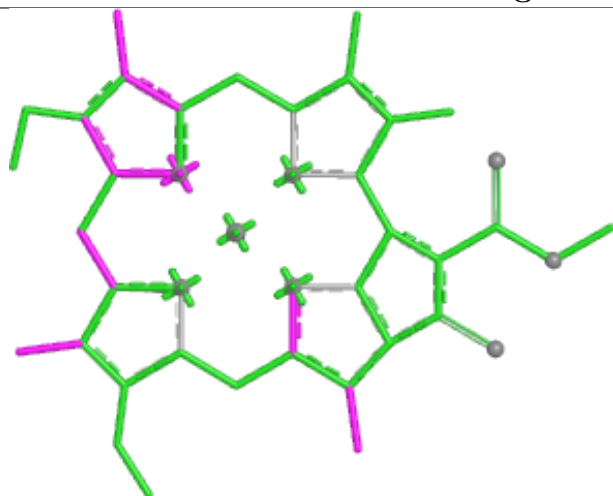
Torsions



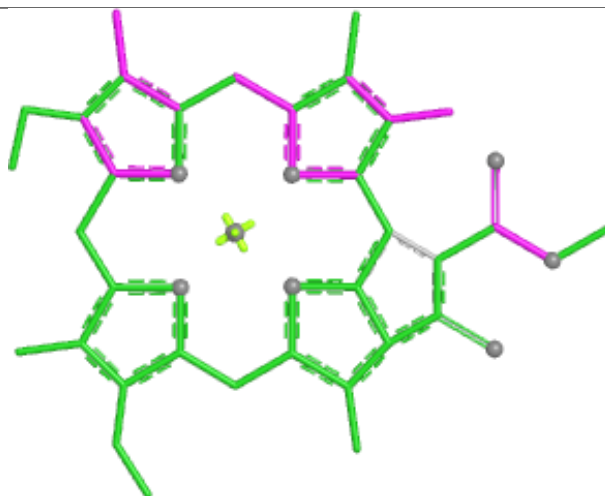
Rings

Ligand CLA 0 305**Ligand CLA c 505**

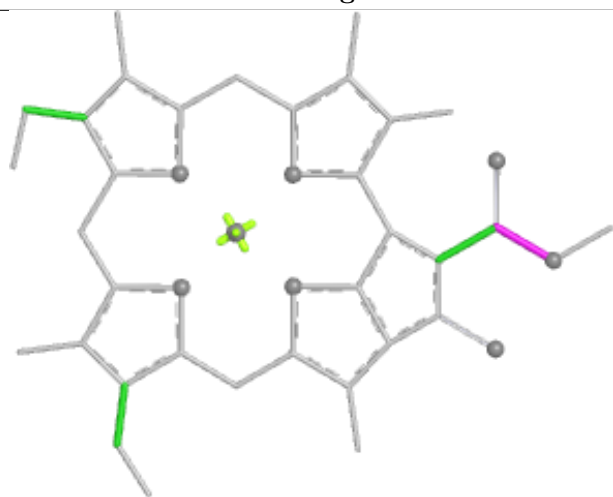
Ligand CLA B 607



Bond lengths



Bond angles

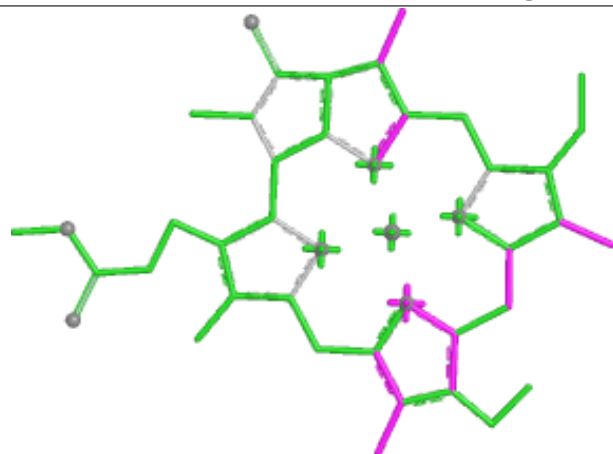


Torsions

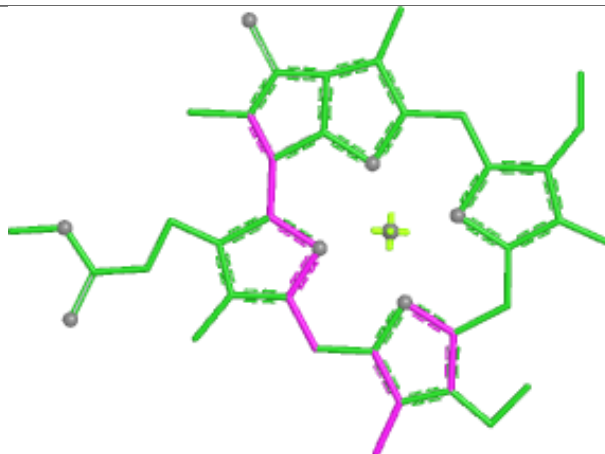


Rings

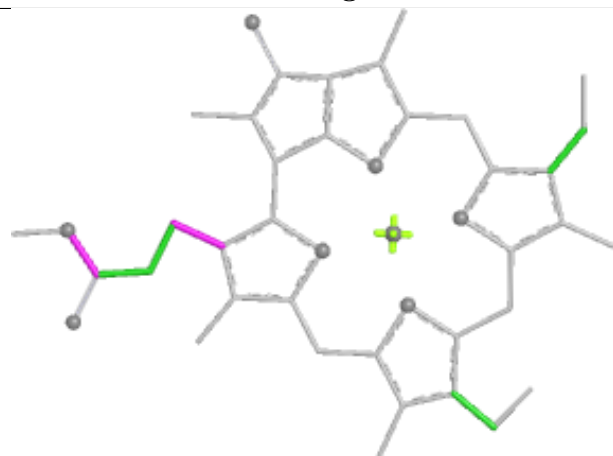
Ligand CLA 7 314



Bond lengths



Bond angles

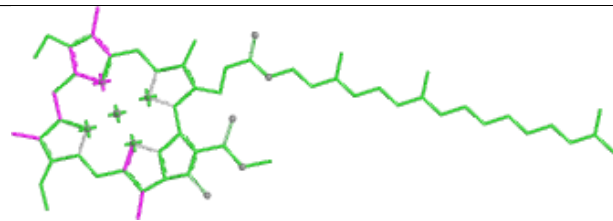


Torsions

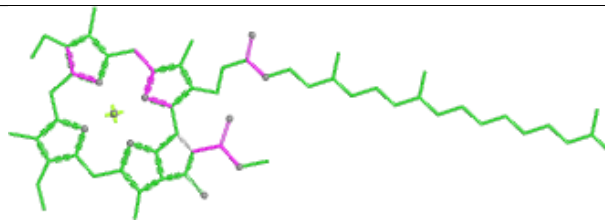


Rings

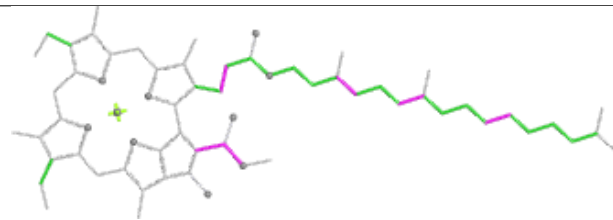
Ligand CLA B 603



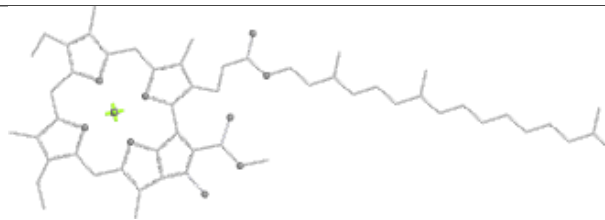
Bond lengths



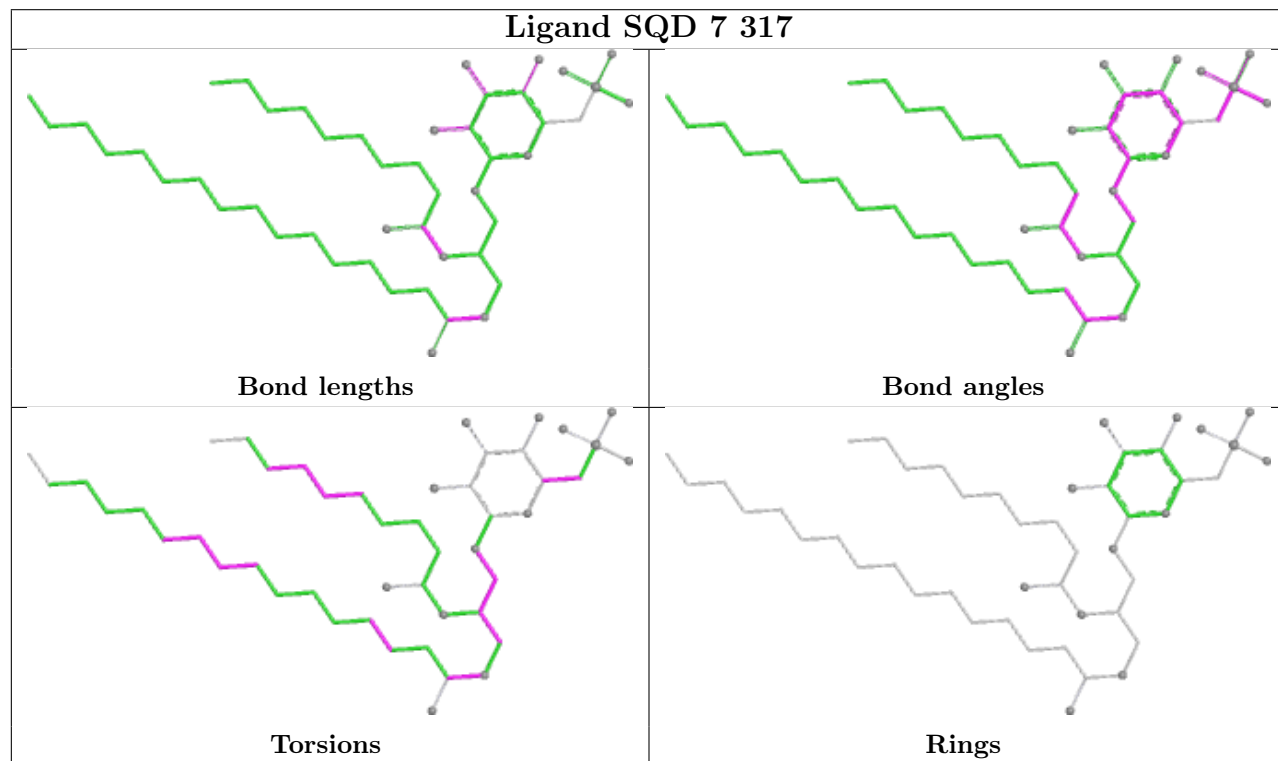
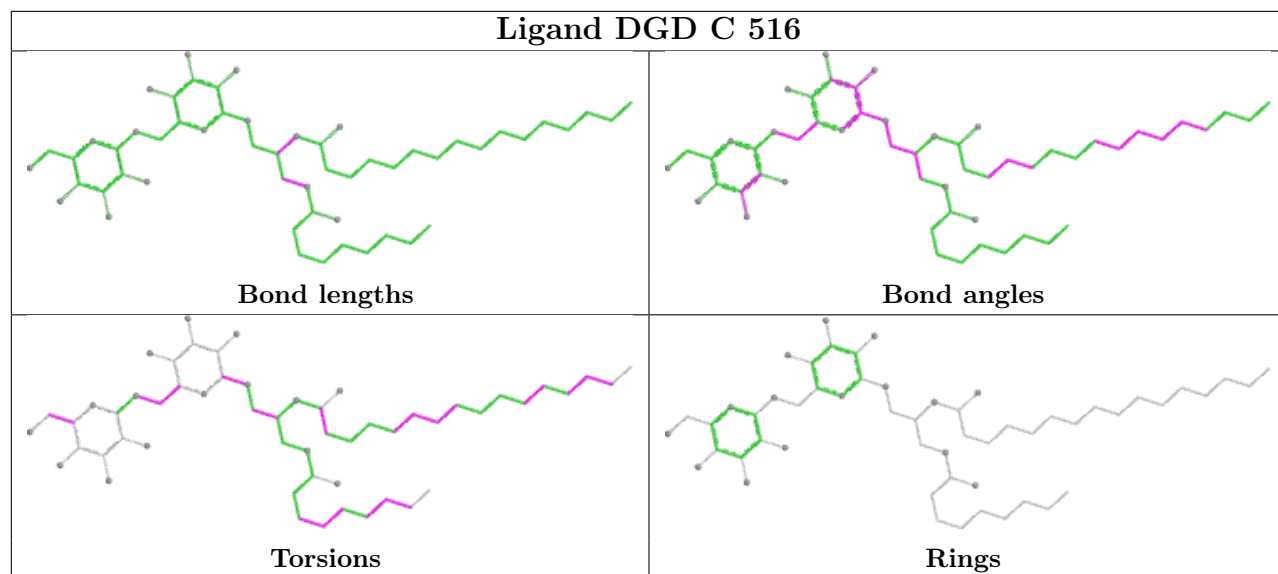
Bond angles



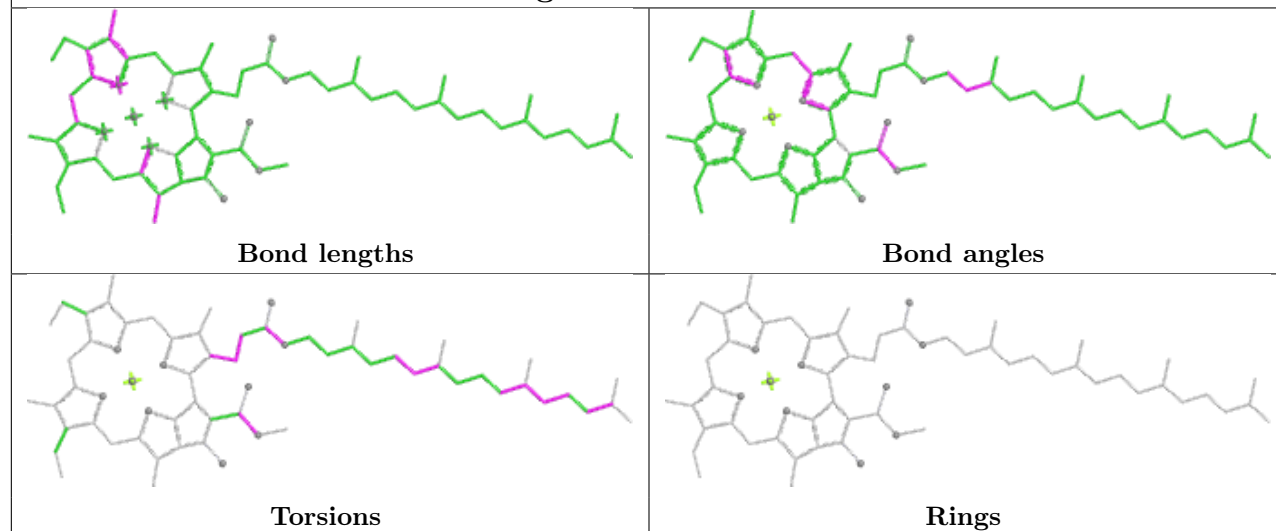
Torsions



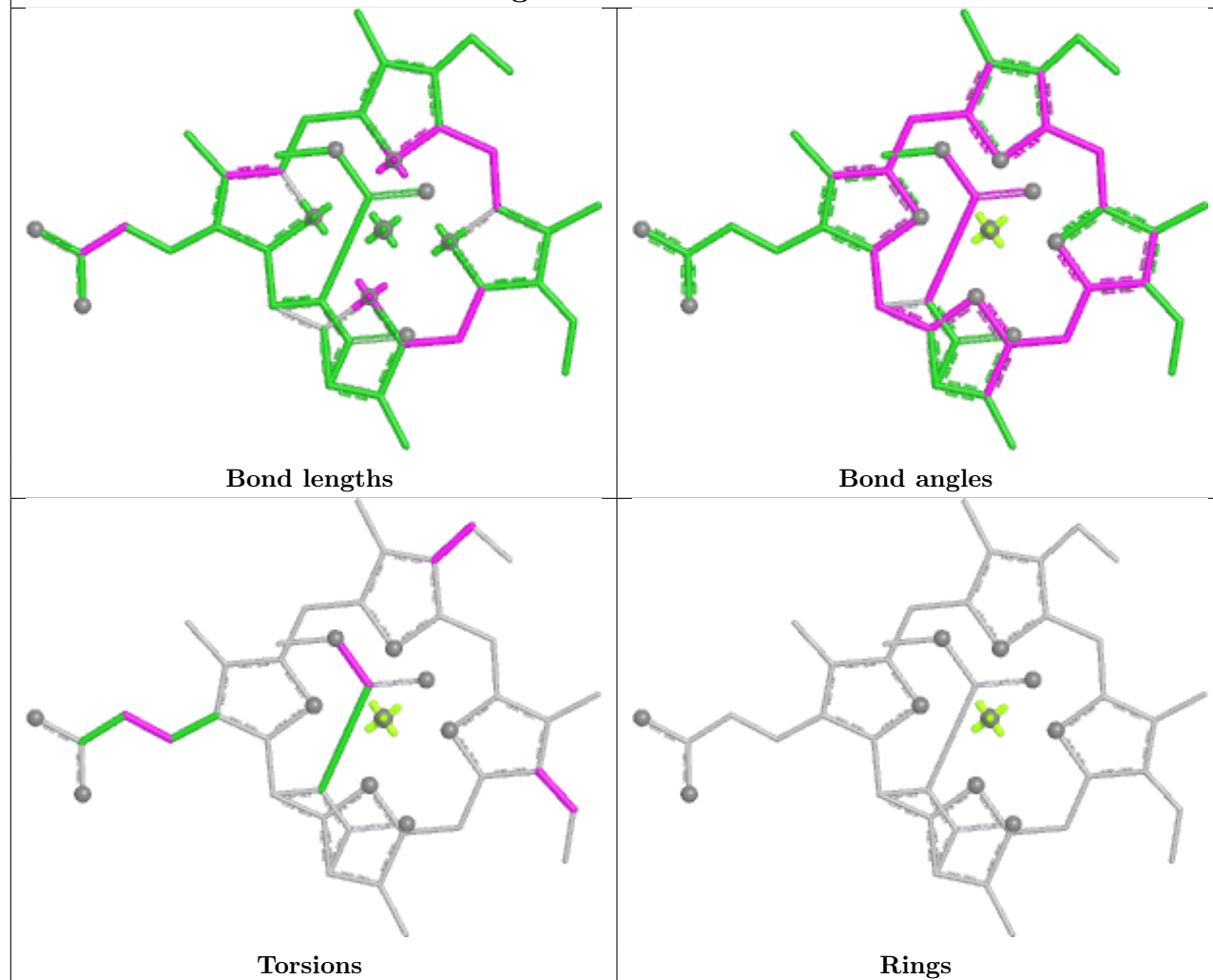
Rings



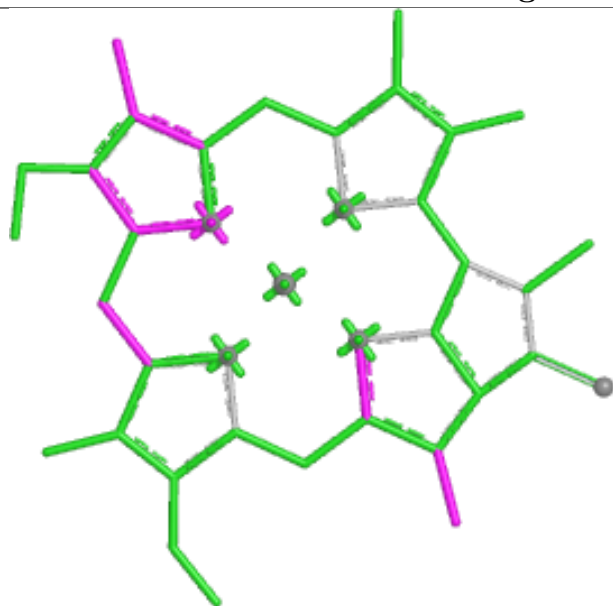
Ligand CLA 1 310



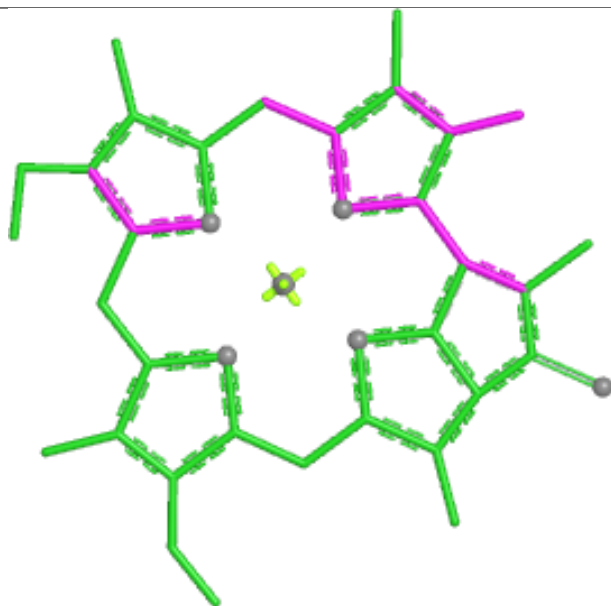
Ligand KC2 5 310



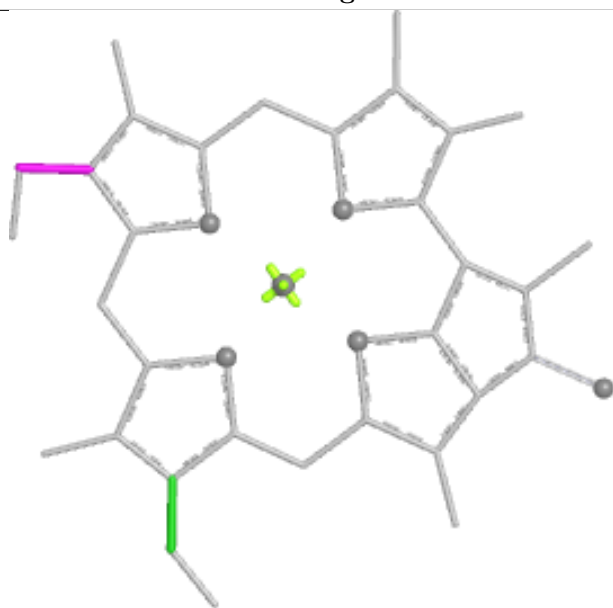
Ligand CLA 8 314



Bond lengths



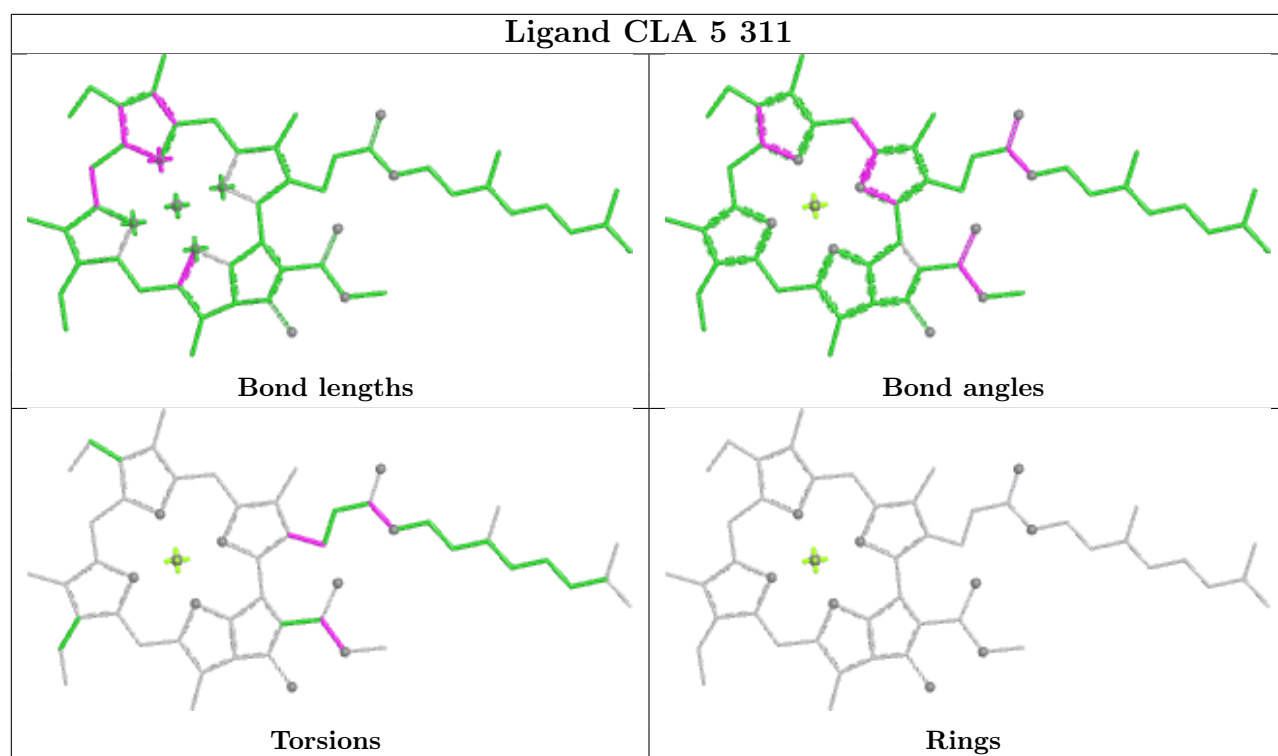
Bond angles



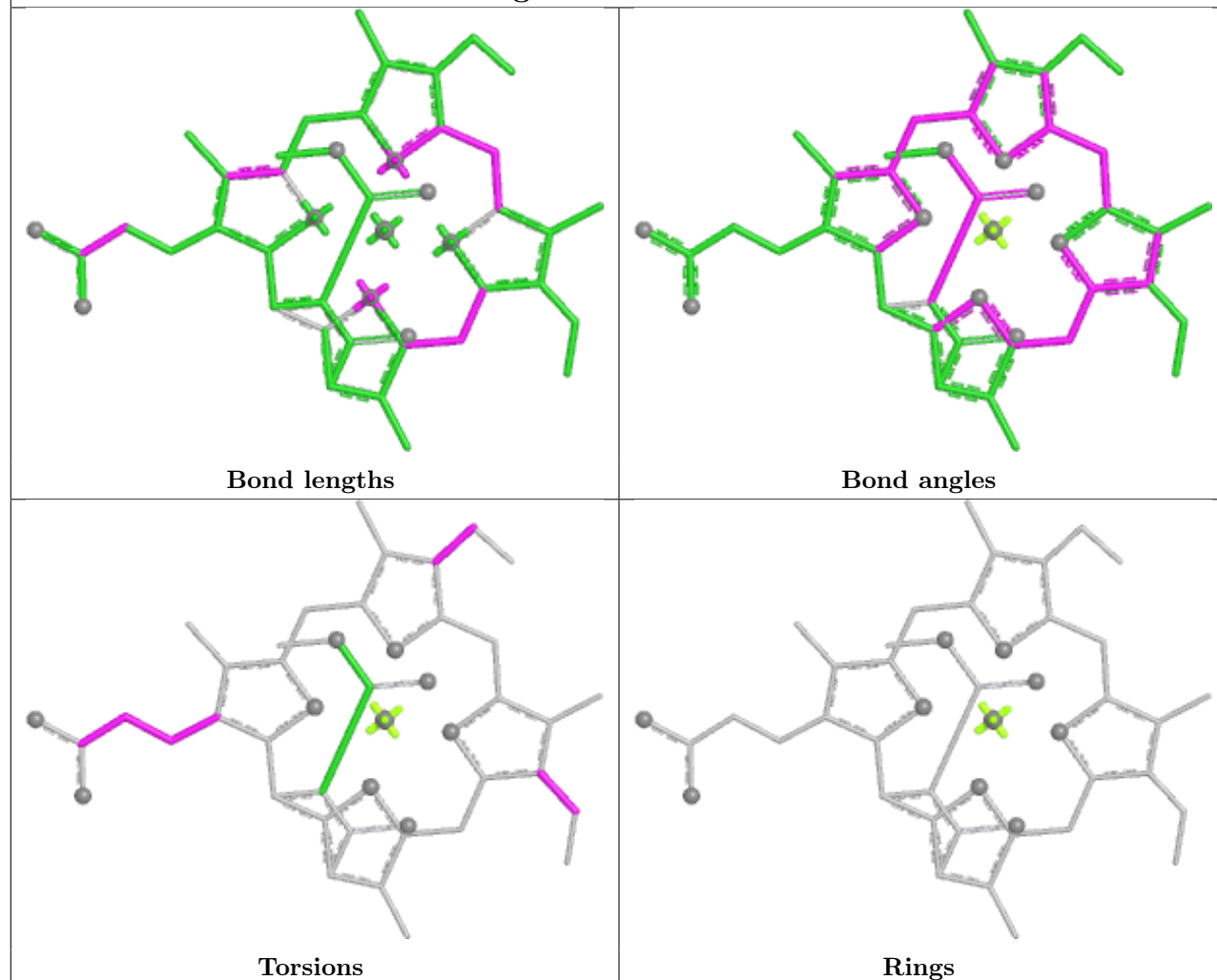
Torsions



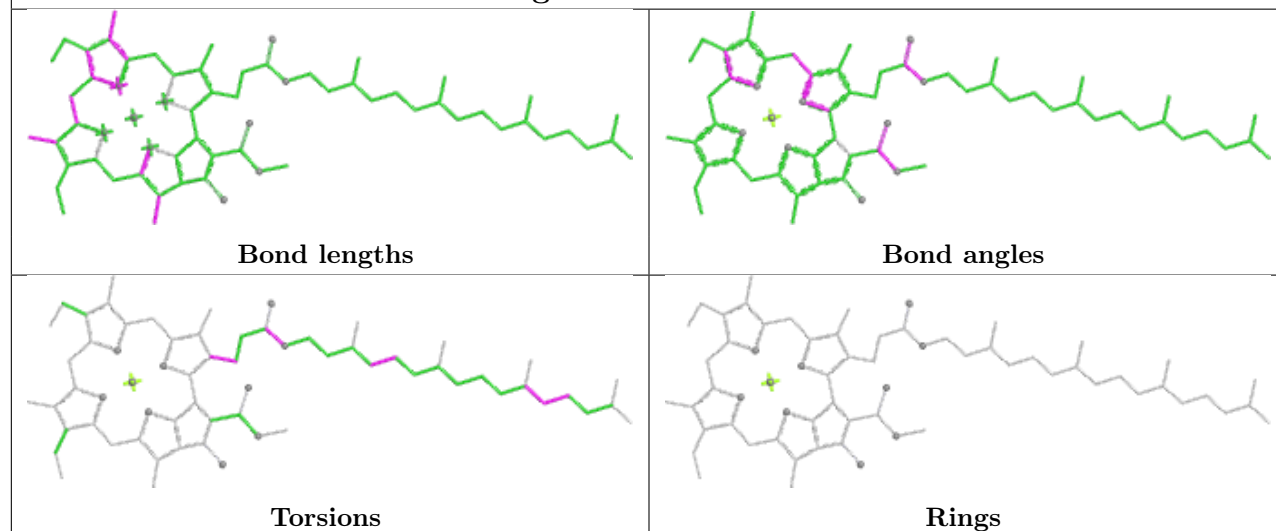
Rings



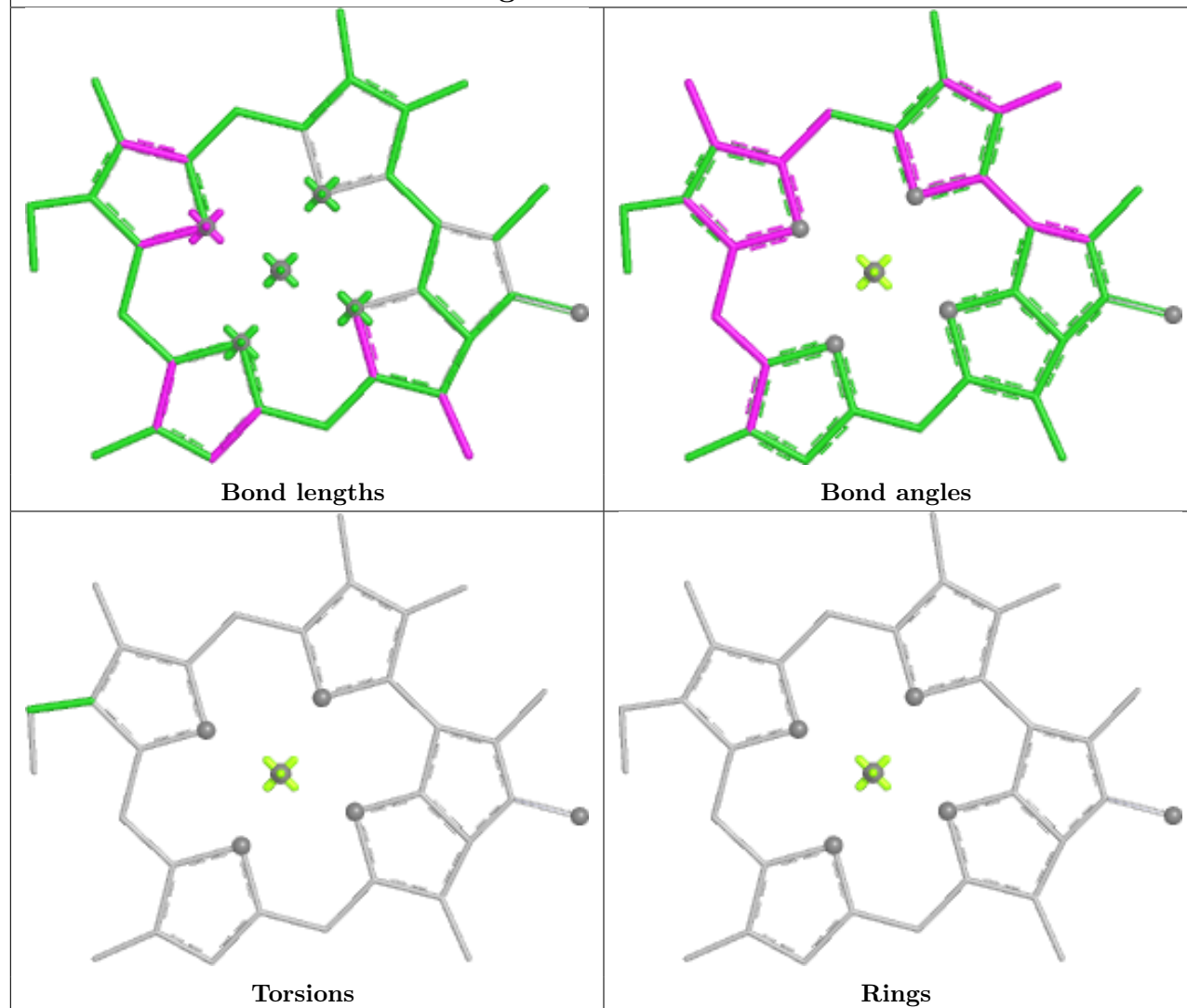
Ligand KC2 7 306



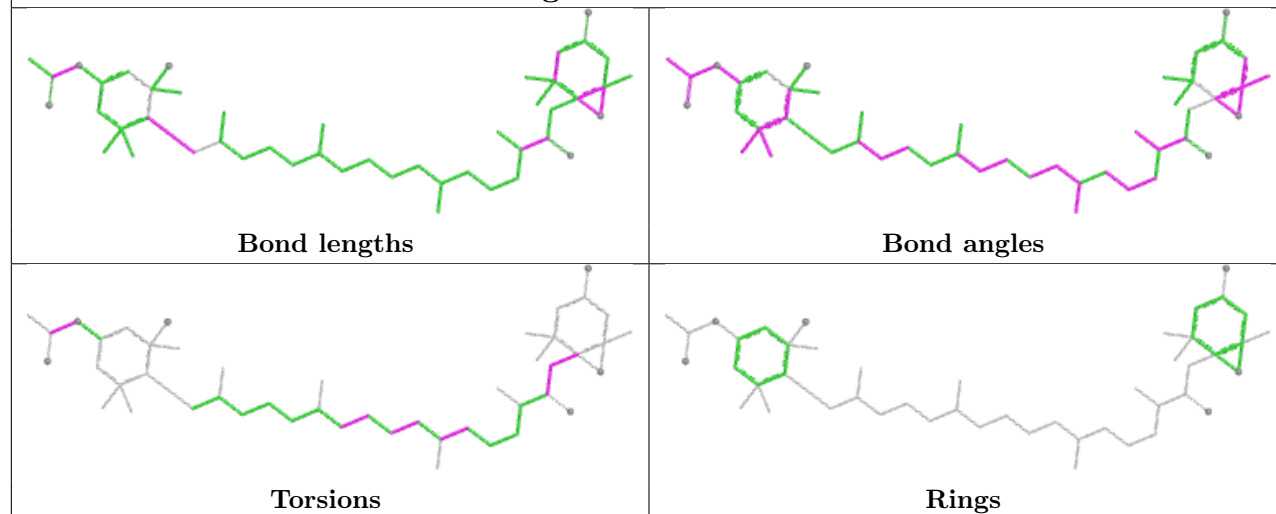
Ligand CLA C 511

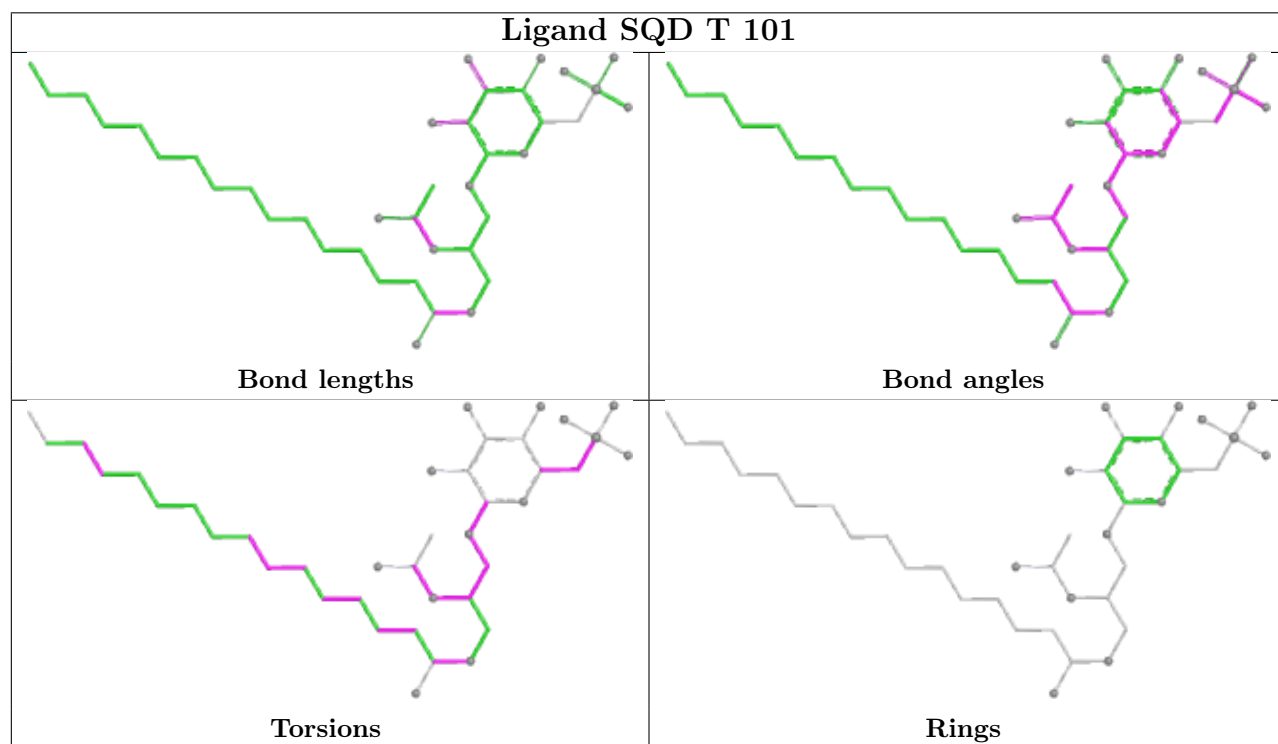
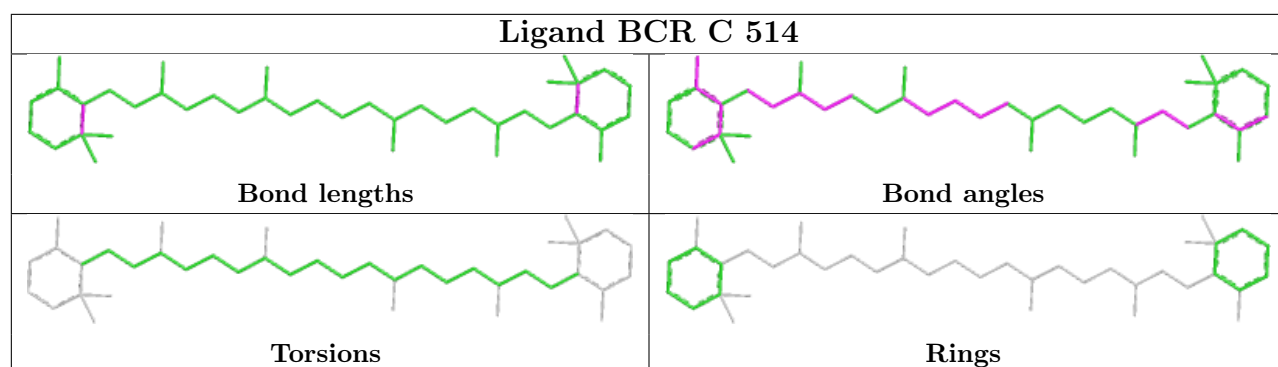


Ligand CLA 2 313

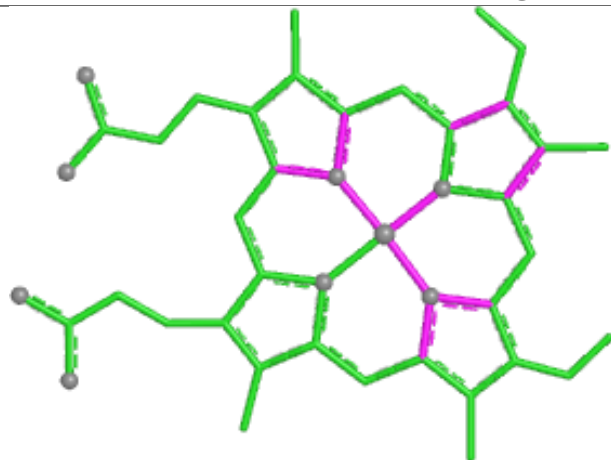


Ligand A86 0 301

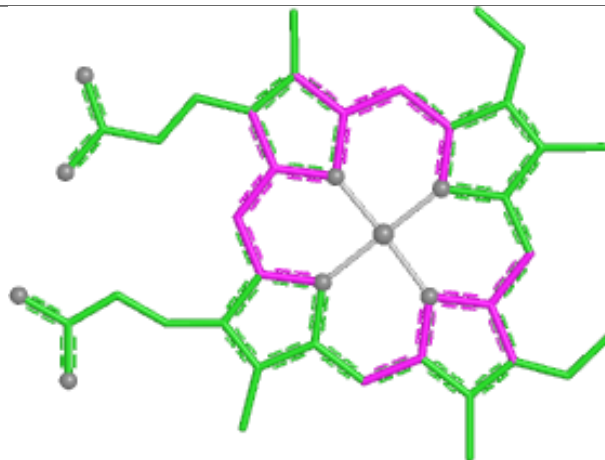




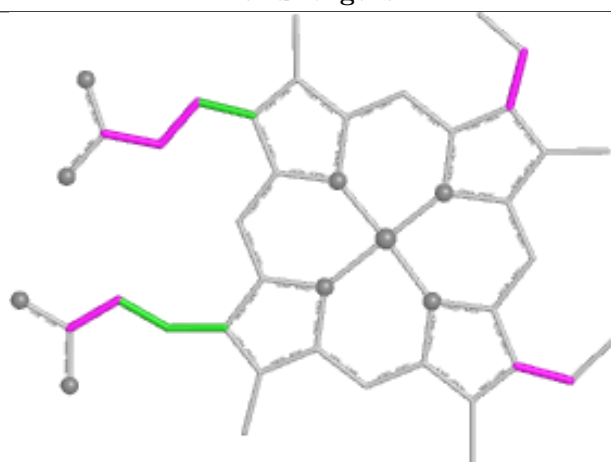
Ligand HEM e 101



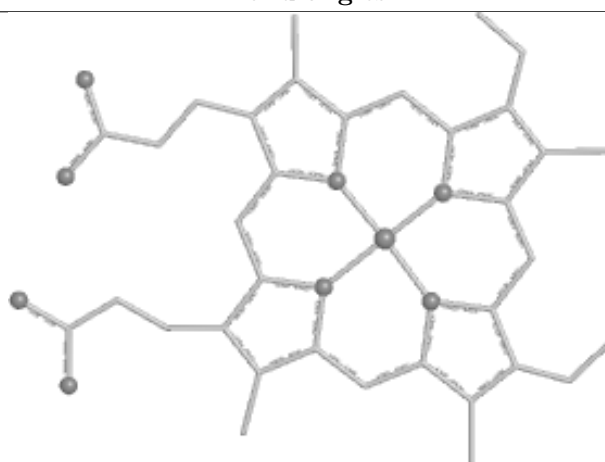
Bond lengths



Bond angles

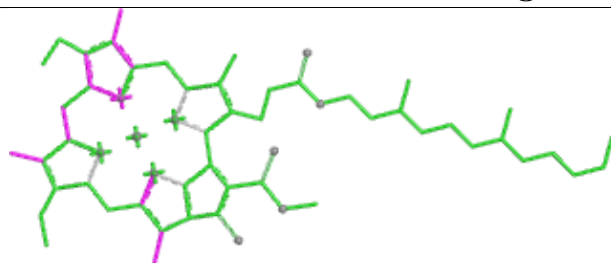


Torsions

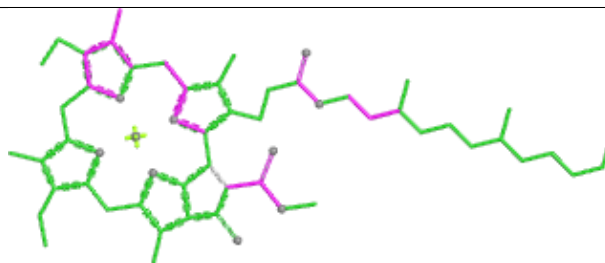


Rings

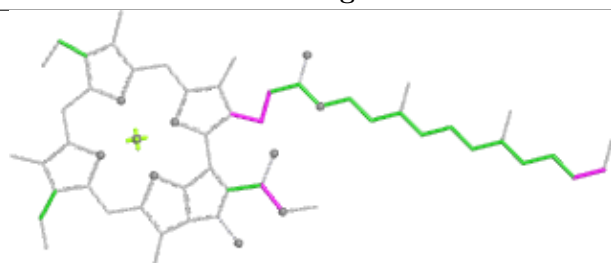
Ligand CLA d 409



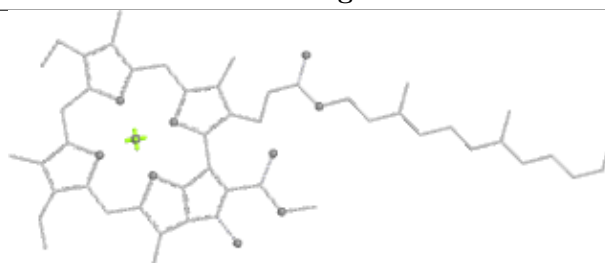
Bond lengths



Bond angles

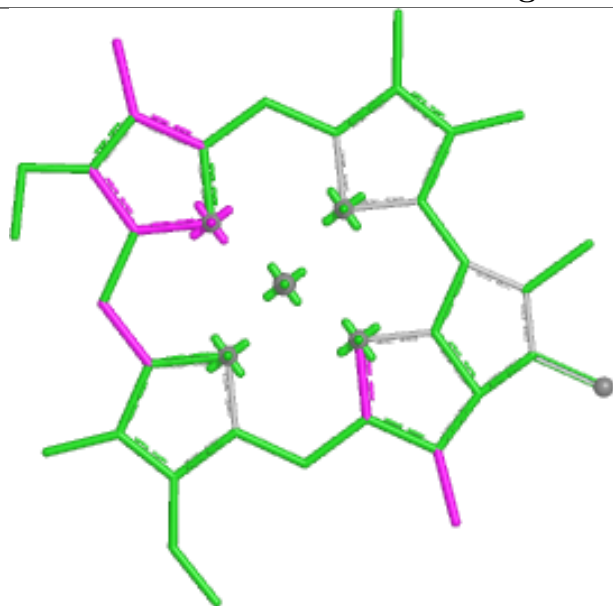


Torsions

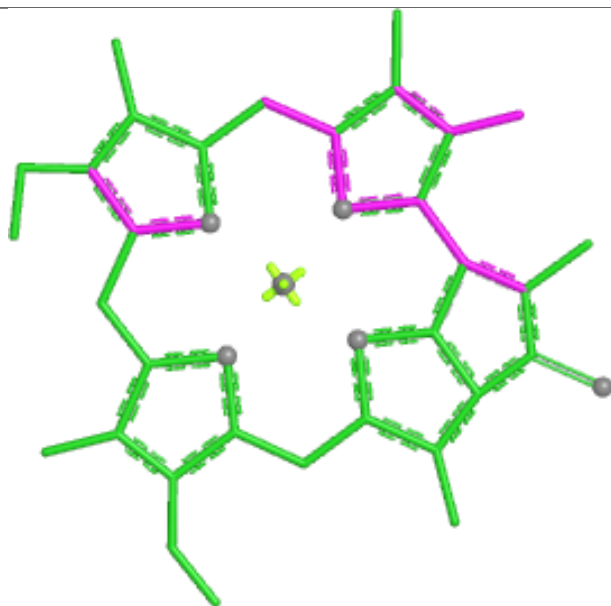


Rings

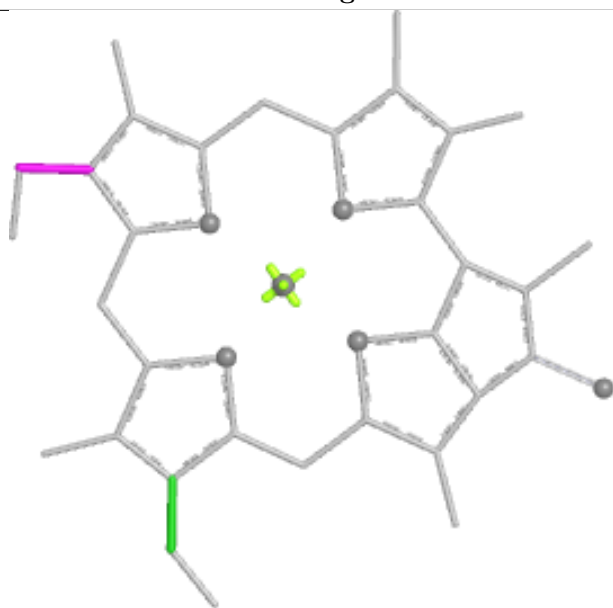
Ligand CLA 2 315



Bond lengths



Bond angles

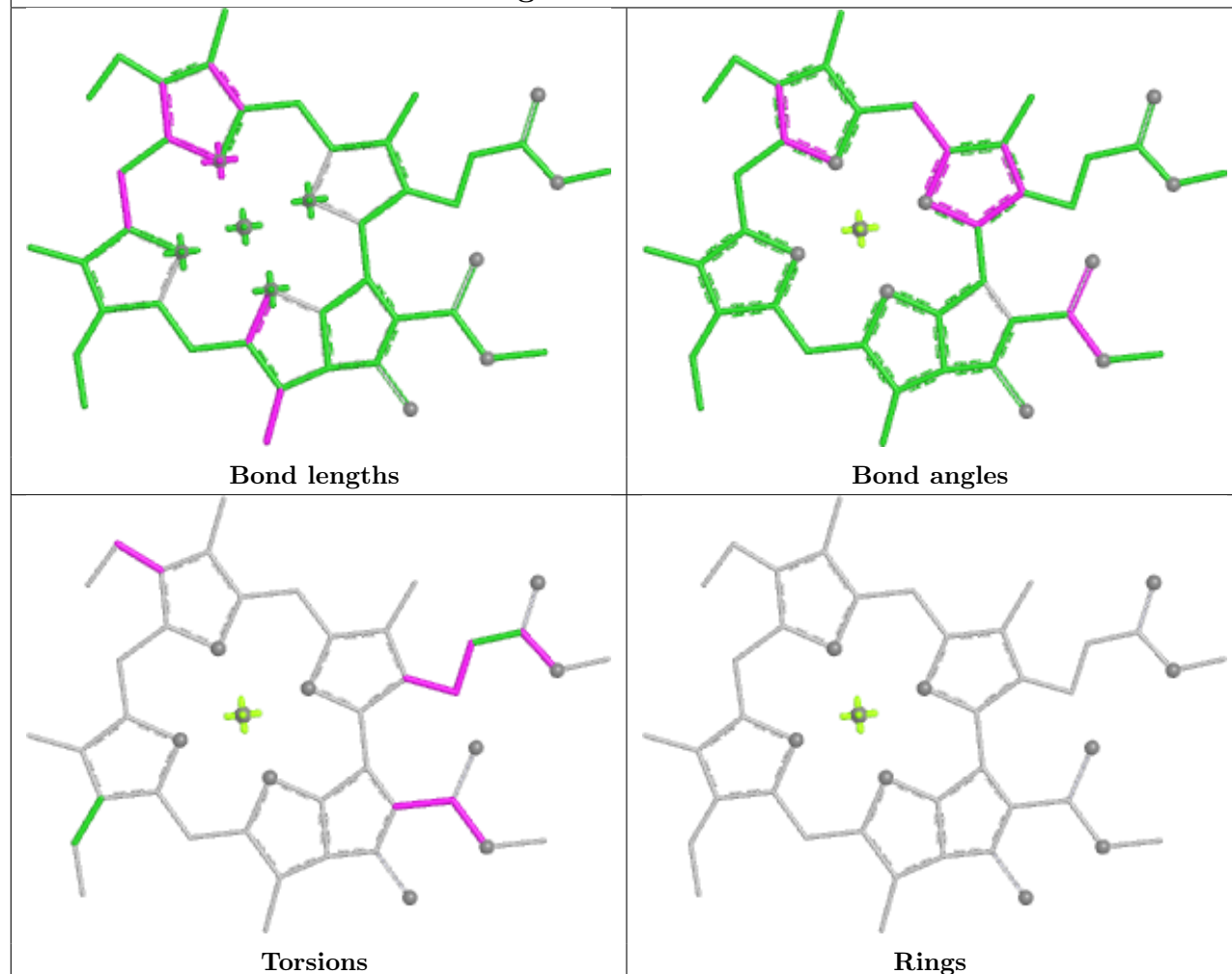


Torsions

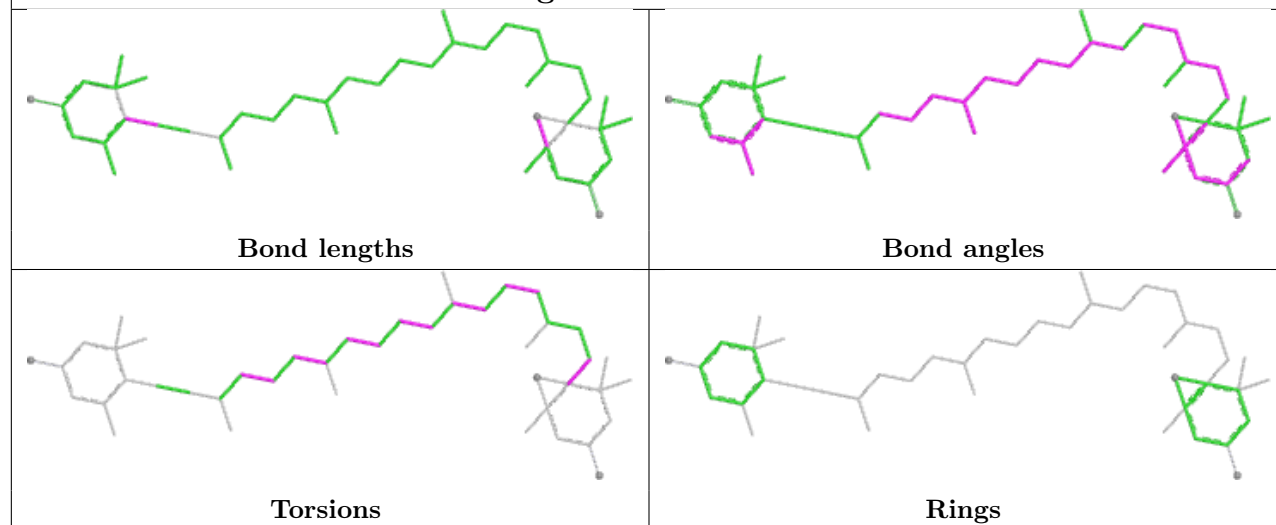


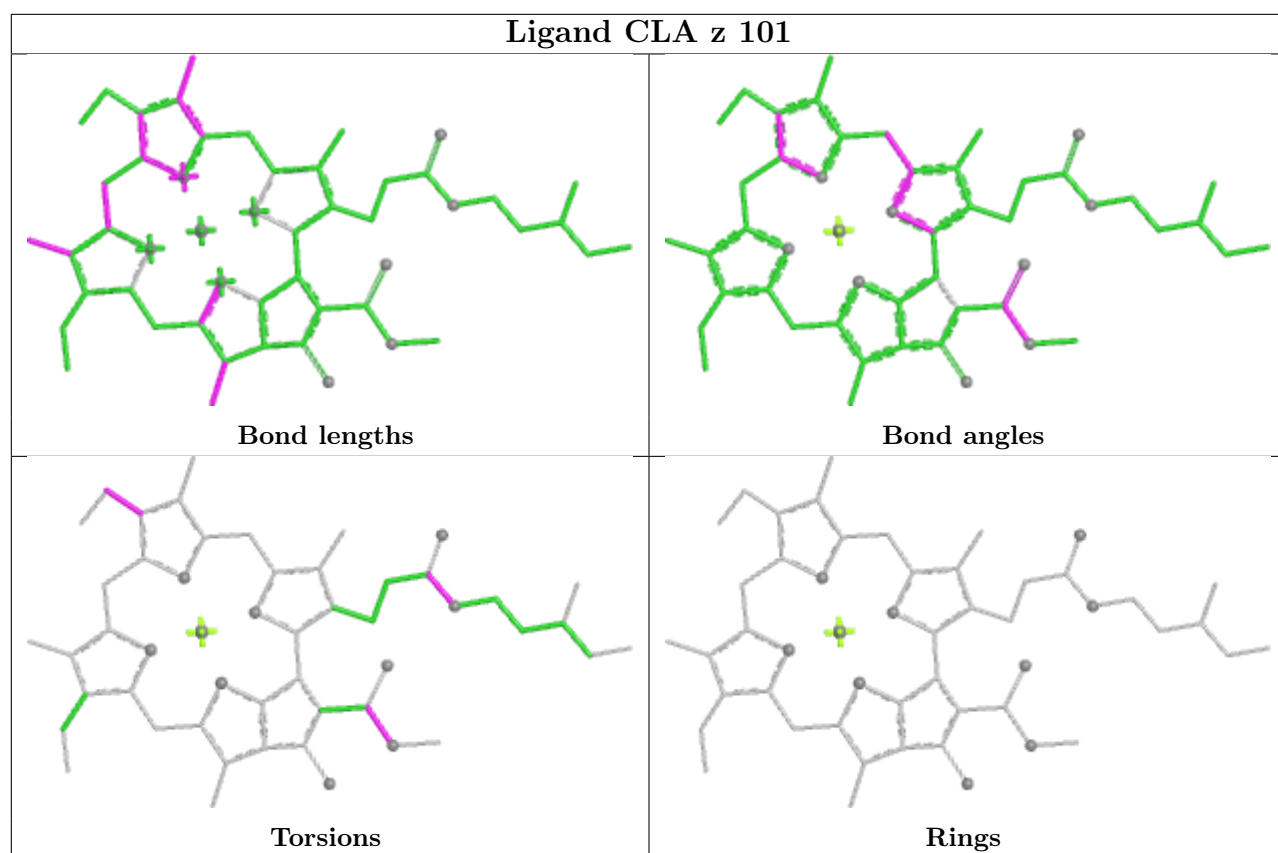
Rings

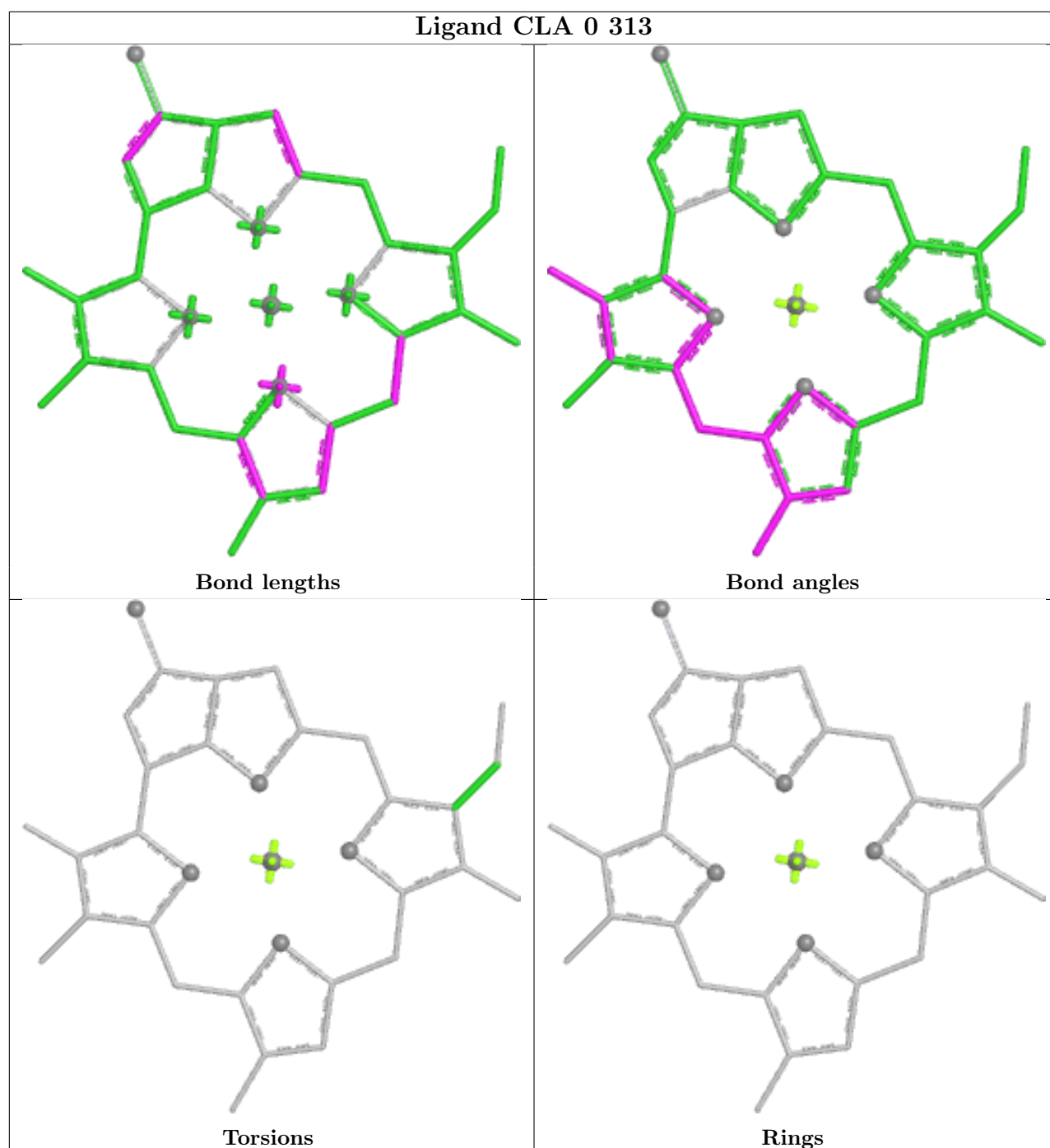
Ligand CLA 6 311



Ligand DD6 8 304







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

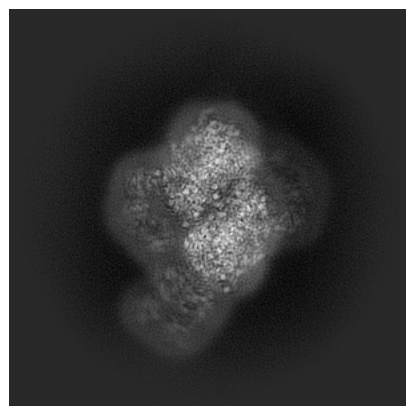
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35766. These allow visual inspection of the internal detail of the map and identification of artifacts.

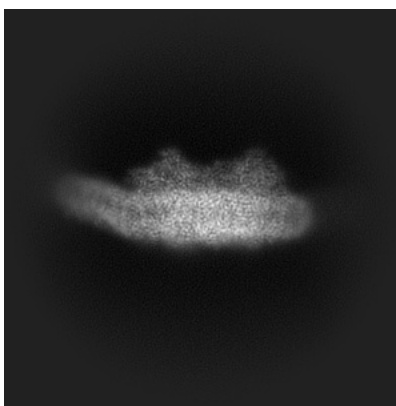
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

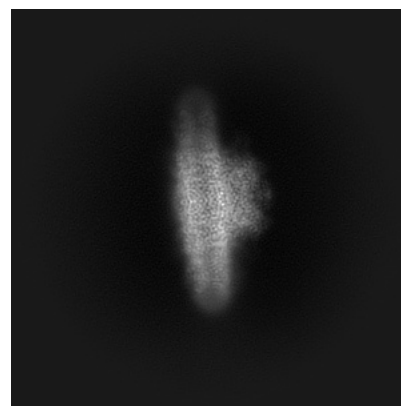
6.1.1 Primary map



X

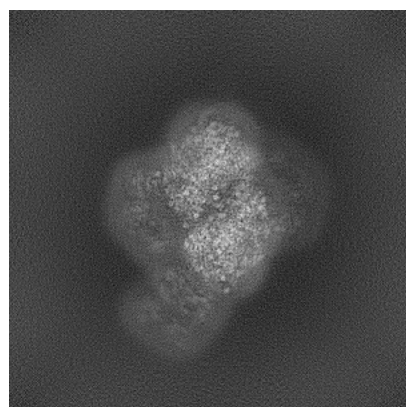


Y

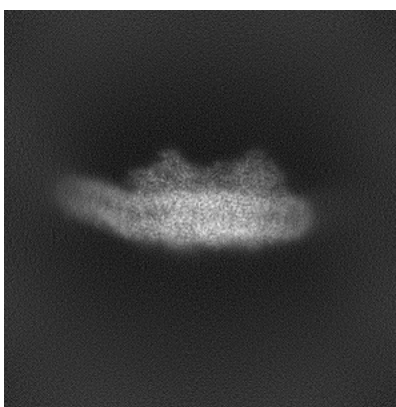


Z

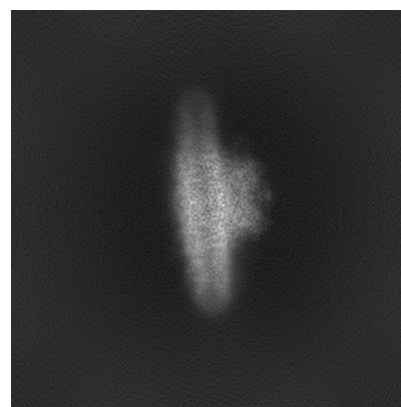
6.1.2 Raw map



X



Y

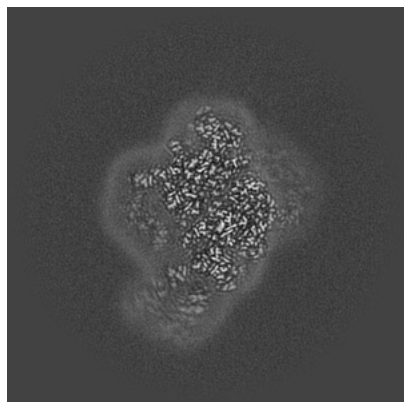


Z

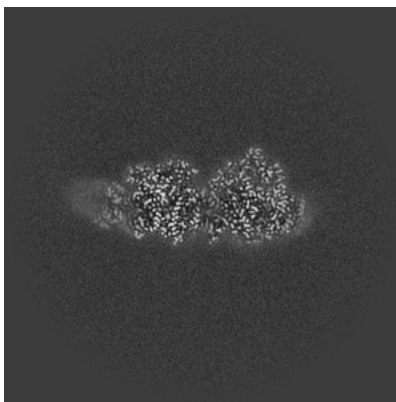
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

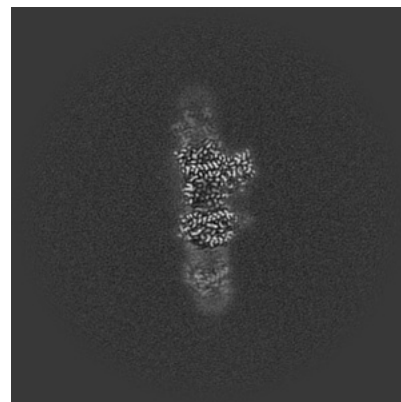
6.2.1 Primary map



X Index: 250

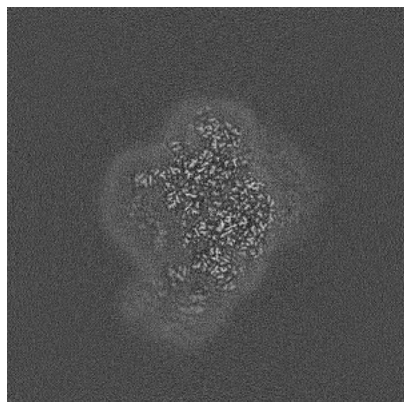


Y Index: 250

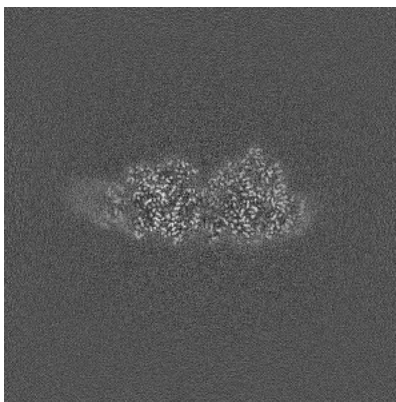


Z Index: 250

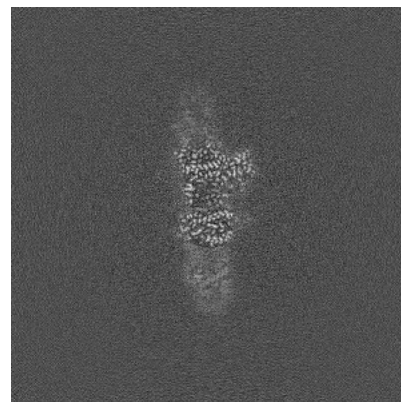
6.2.2 Raw map



X Index: 250



Y Index: 250

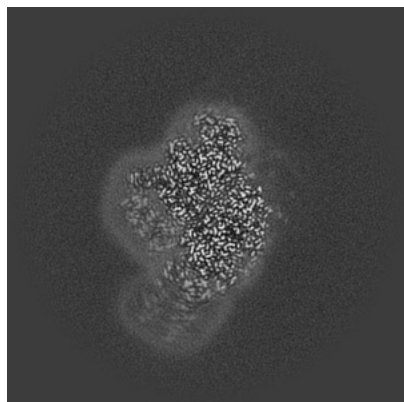


Z Index: 250

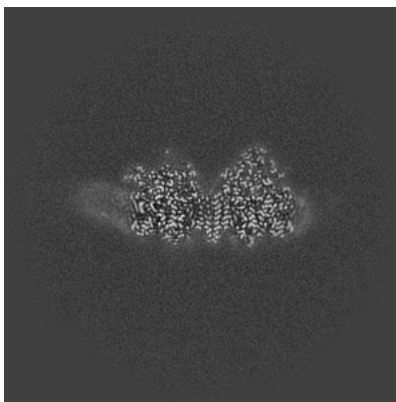
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

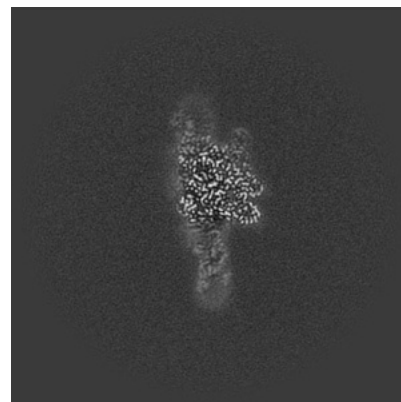
6.3.1 Primary map



X Index: 259

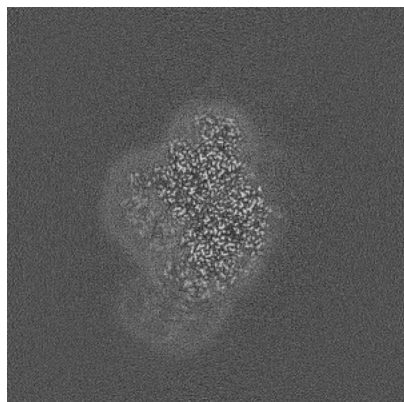


Y Index: 259

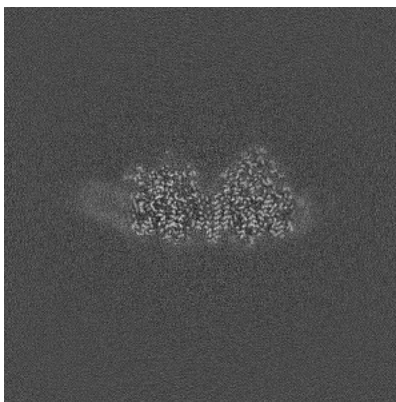


Z Index: 223

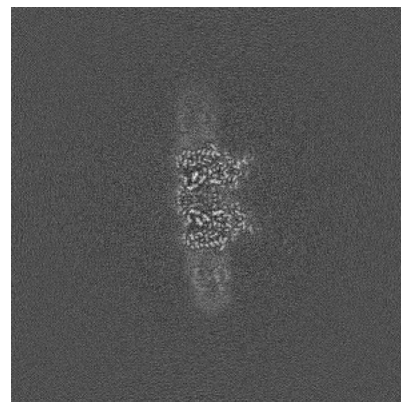
6.3.2 Raw map



X Index: 259



Y Index: 259

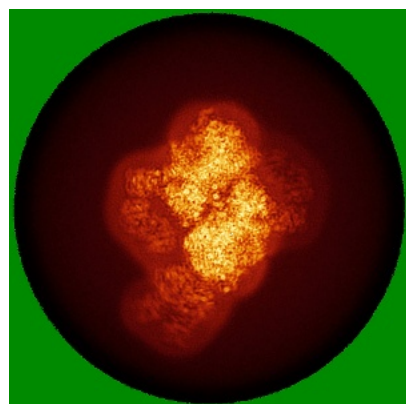


Z Index: 260

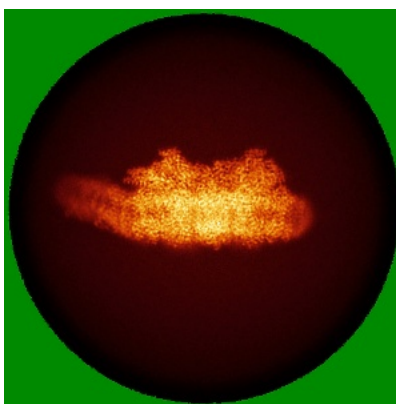
The images above show the largest variance slices of the map in three orthogonal directions.

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

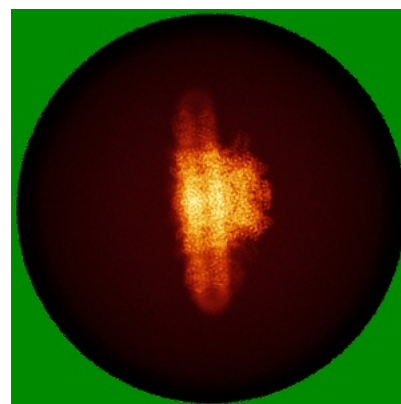
6.4.1 Primary map



X

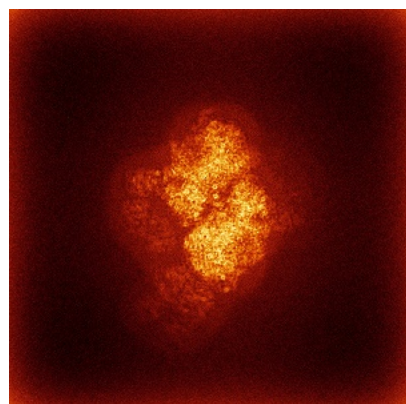


Y

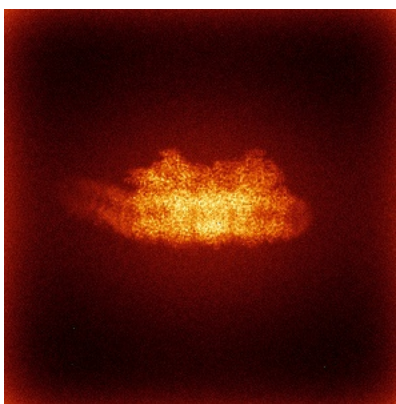


Z

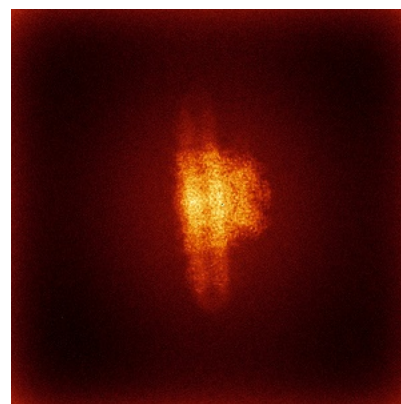
6.4.2 Raw map



X



Y

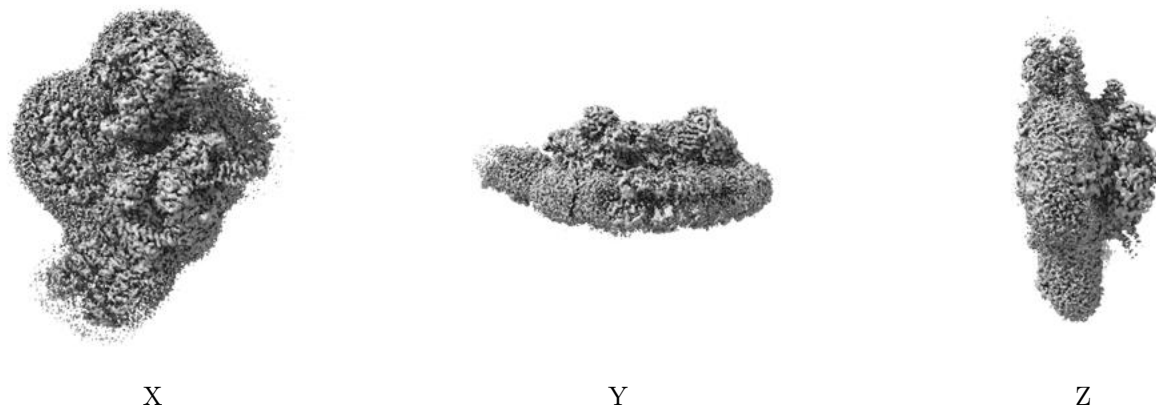


Z

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.

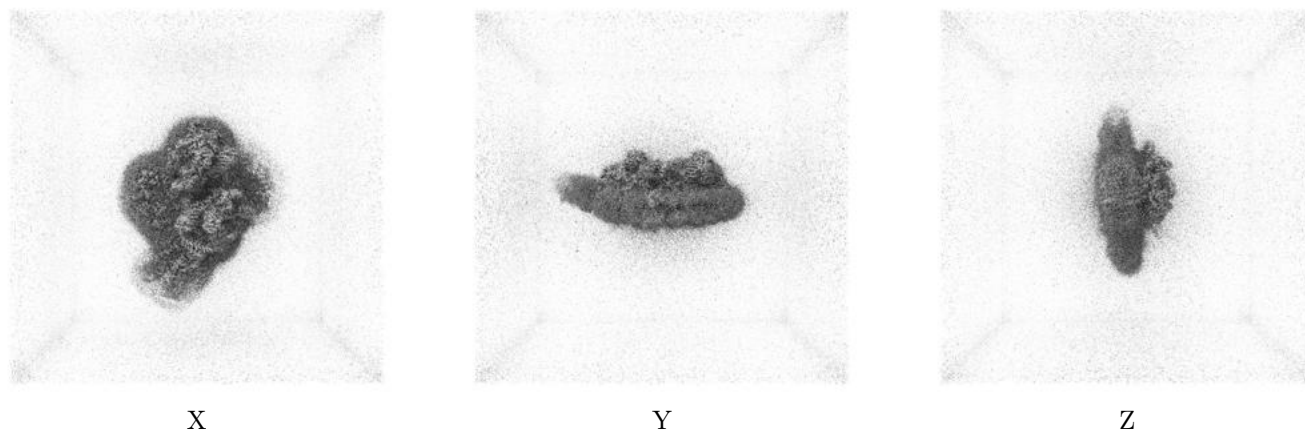
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.088. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

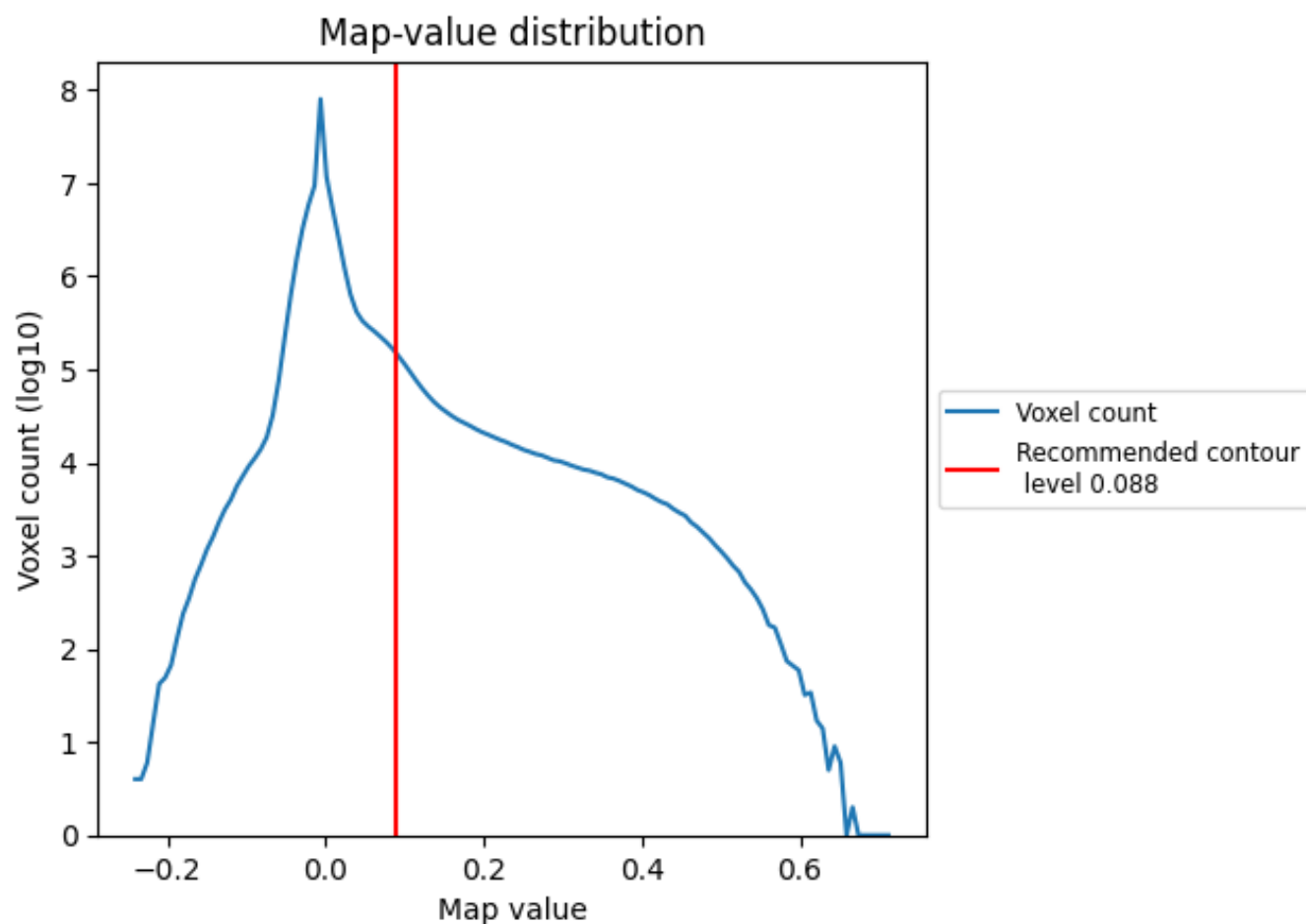
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

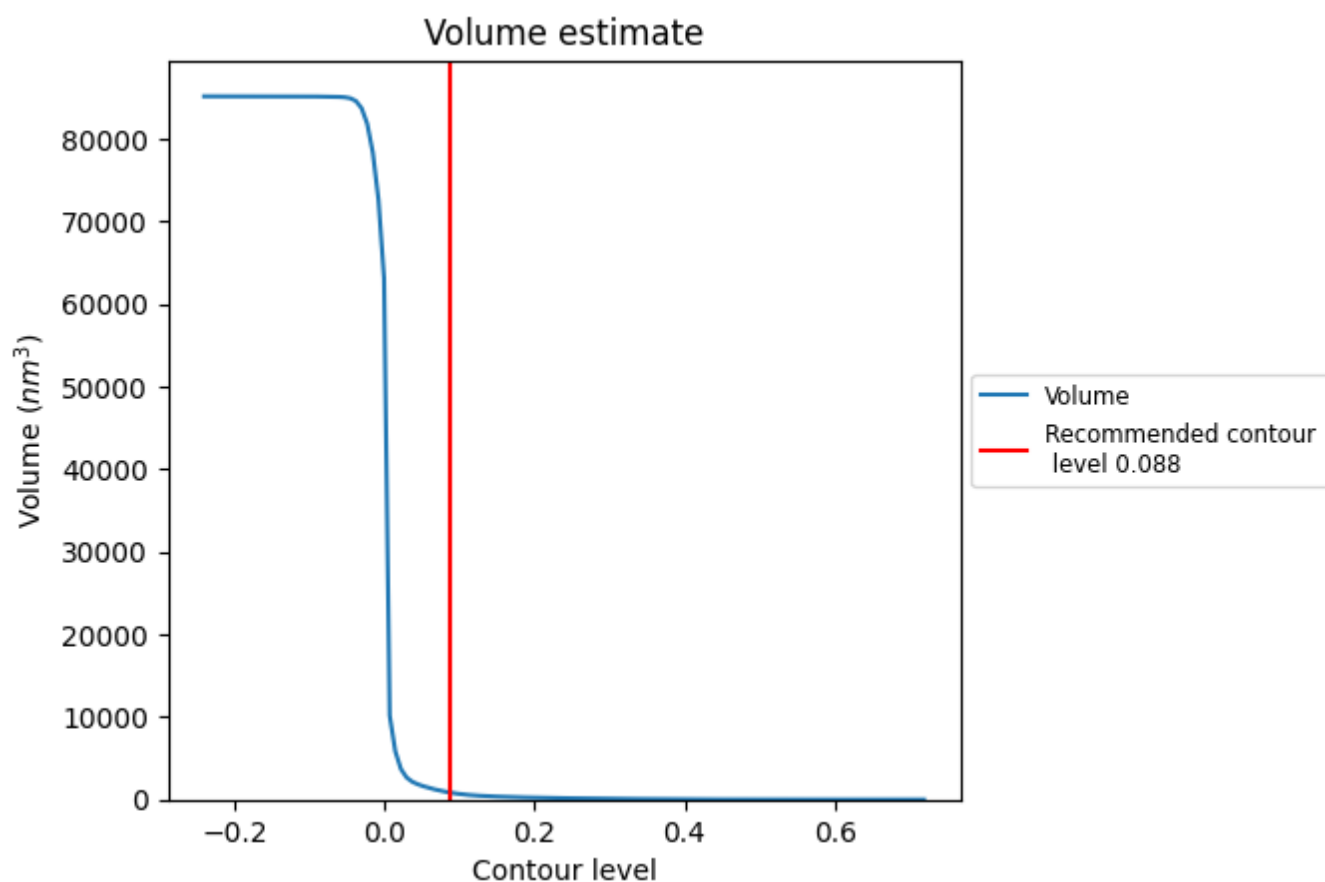
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

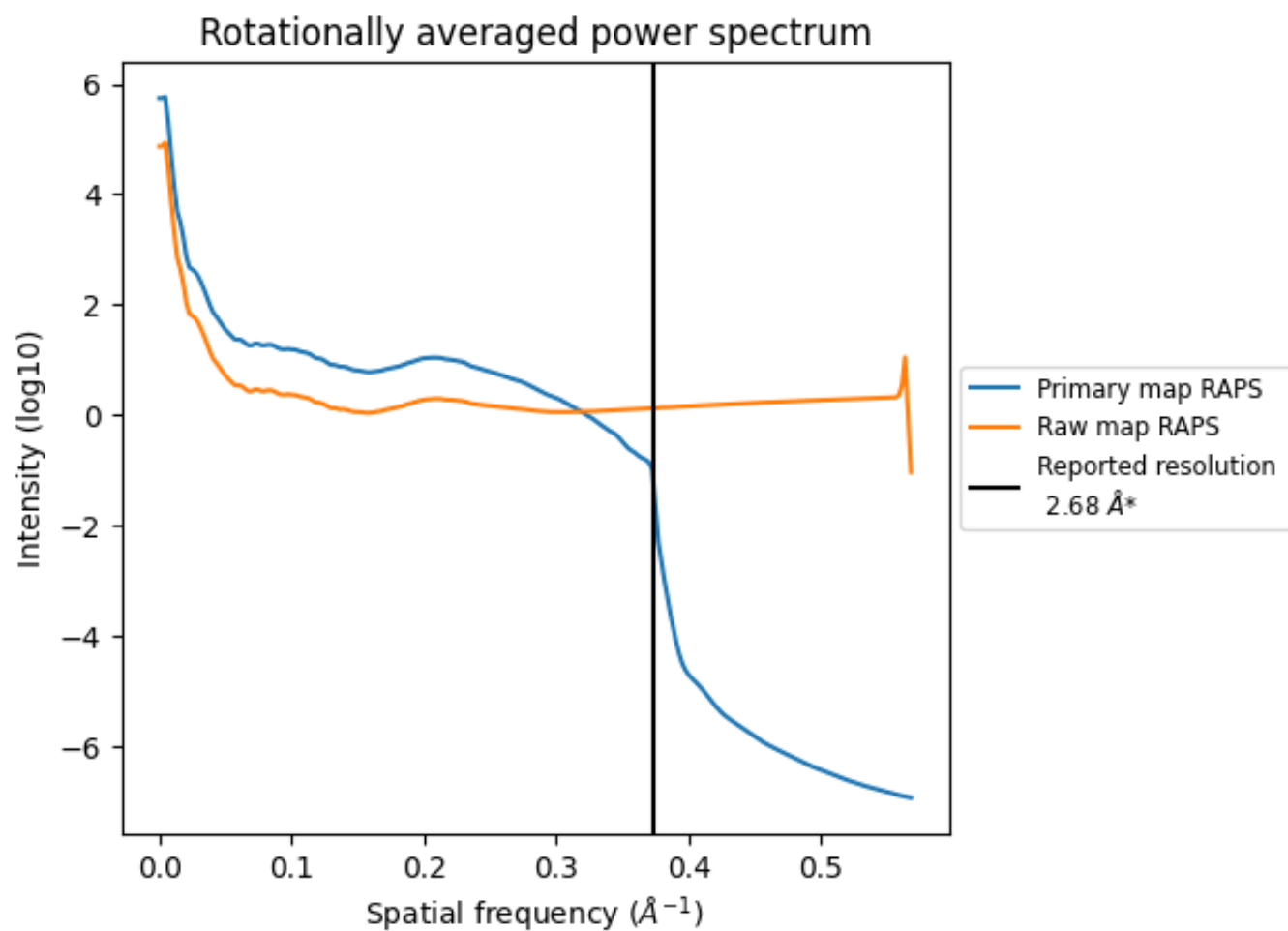
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 833 nm³; this corresponds to an approximate mass of 752 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 ⓘ

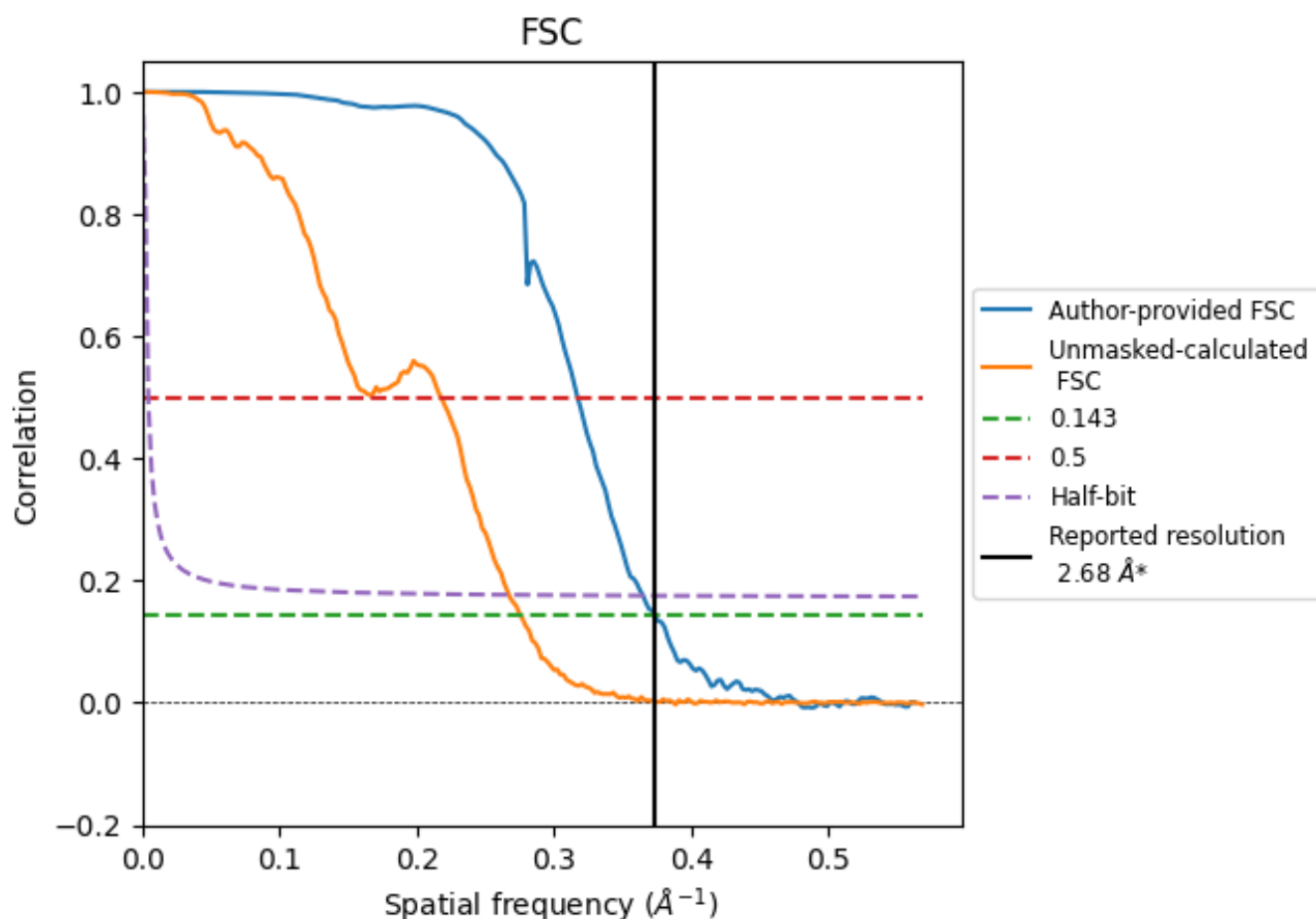


*Reported resolution corresponds to spatial frequency of 0.373 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.373 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

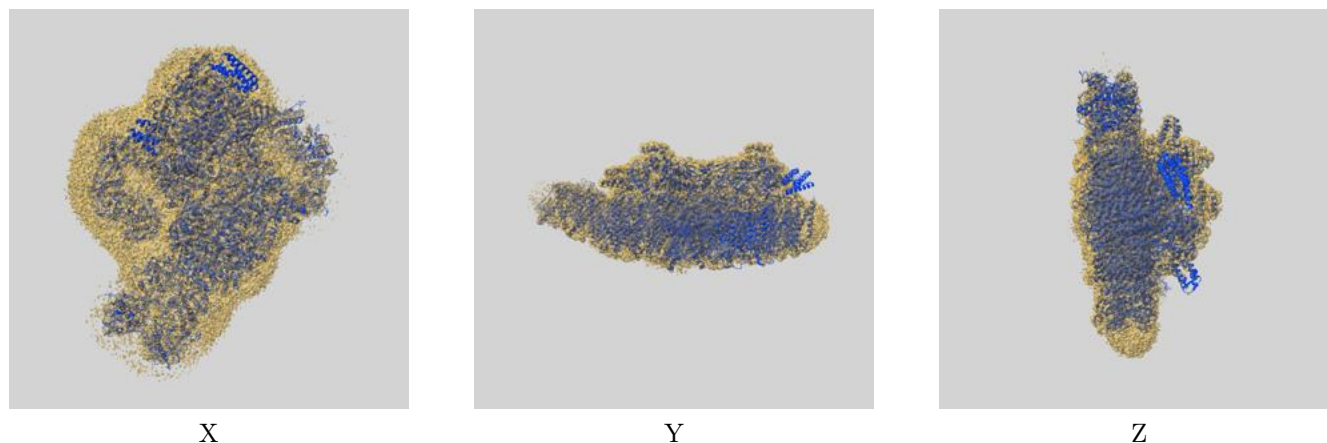
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	2.68	3.15	2.74
Unmasked-calculated*	3.63	4.59	3.74

*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 3.63 differs from the reported value 2.68 by more than 10 %

9 Map-model fit [i](#)

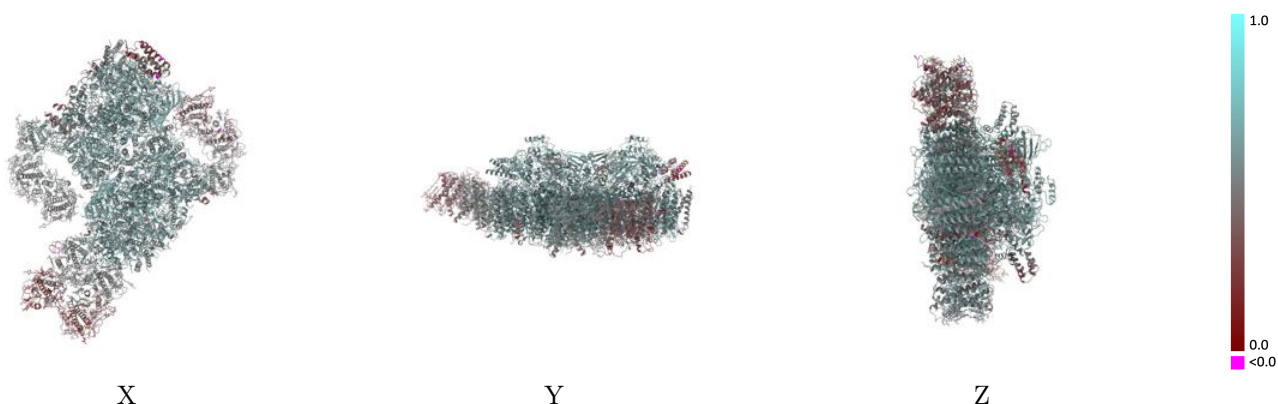
This section contains information regarding the fit between EMDB map EMD-35766 and PDB model 8IWH. Per-residue inclusion information can be found in section 3 on page 41.

9.1 Map-model overlay [i](#)



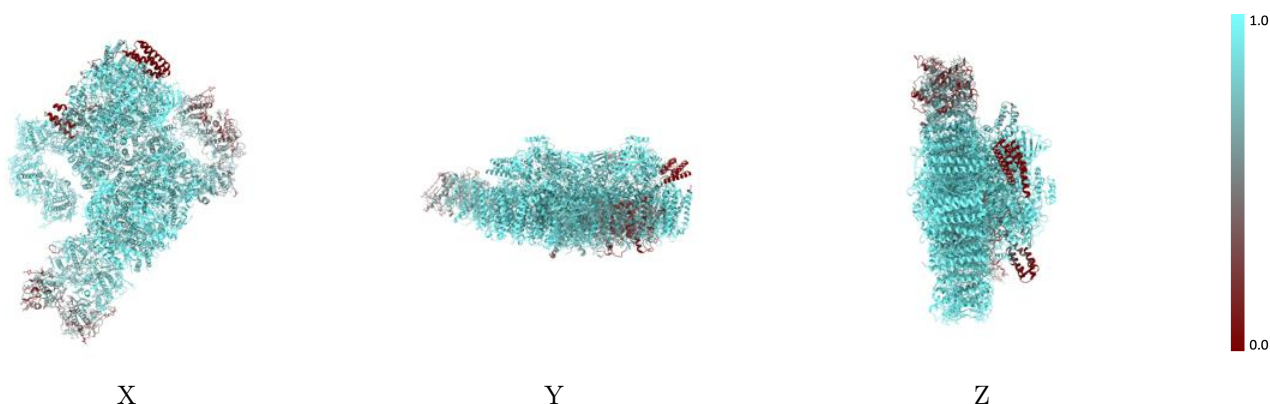
The images above show the 3D surface view of the map at the recommended contour level 0.088 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



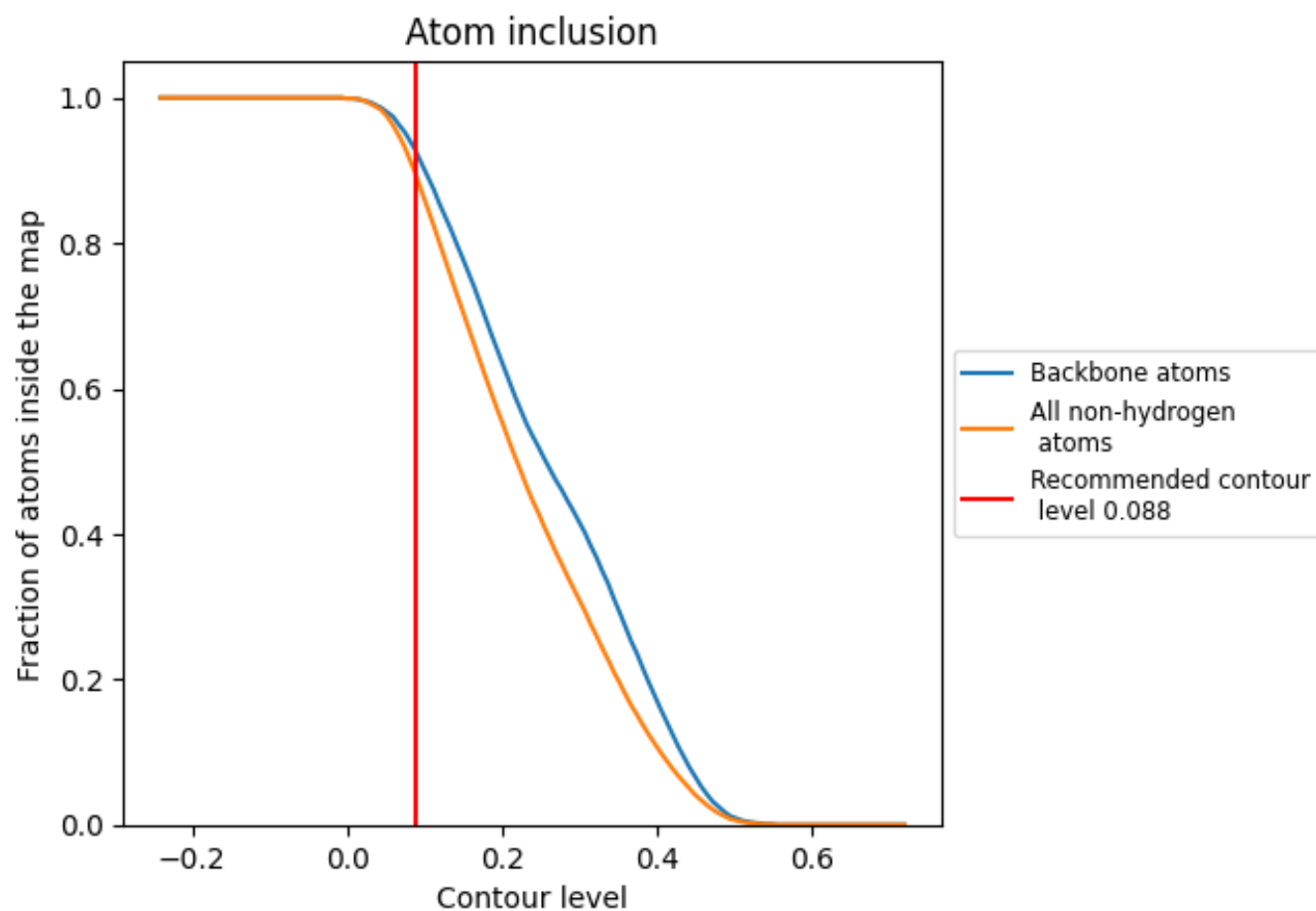
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.088).

9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.088) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8960	 0.5410
0	 0.7820	 0.5060
1	 0.4420	 0.4020
2	 0.5170	 0.3360
3	 0.9120	 0.4840
4	 0.9310	 0.4850
5	 0.5590	 0.3090
6	 0.5250	 0.2970
7	 0.9750	 0.5430
8	 0.9550	 0.4950
9	 0.9390	 0.4550
A	 0.9800	 0.5990
B	 0.9920	 0.6150
C	 0.9920	 0.6110
D	 0.9880	 0.6130
E	 0.9710	 0.5170
F	 0.9930	 0.5420
G	 0.7830	 0.5380
H	 0.9830	 0.5900
I	 0.9930	 0.6130
J	 0.9410	 0.5150
K	 0.9840	 0.5810
L	 0.9970	 0.6040
M	 0.9940	 0.6050
N	 0.9600	 0.4960
O	 0.9680	 0.6000
Q	 0.9690	 0.5810
T	 0.9860	 0.5800
U	 0.9870	 0.5970
V	 0.9890	 0.5950
W	 0.9620	 0.5820
X	 0.9840	 0.5500
Y	 0.9760	 0.5170
Z	 0.9760	 0.5180
a	 0.9740	 0.5910



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	 0.9910	 0.6160
c	 0.9870	 0.5950
d	 0.9920	 0.6130
e	 0.9720	 0.5010
f	 0.9640	 0.5140
g	 0.3360	 0.4630
h	 0.9850	 0.6030
i	 0.9900	 0.5840
j	 0.9160	 0.4460
k	 0.9810	 0.5700
l	 0.9940	 0.6040
m	 0.9920	 0.5980
n	 0.9600	 0.4800
o	 0.9480	 0.5870
q	 0.1580	 0.3360
t	 0.9870	 0.5710
u	 0.9740	 0.5960
v	 0.9680	 0.5730
w	 0.9360	 0.5310
x	 0.9760	 0.5460
y	 0.8920	 0.4190
z	 0.9220	 0.4740