



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:37 AM UTC

PDB ID : 9IS4 / pdb_00009is4
EMDB ID : EMD-60830
Title : Cryo-EM structure of a TEF30-associated intermediate C2S-type PSII-LHCII supercomplex from *Chlamydomonas reinhardtii*
Authors : Wang, Y.; Wang, C.; Li, A.; Liu, Z.
Deposited on : 2024-07-16
Resolution : 2.90 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

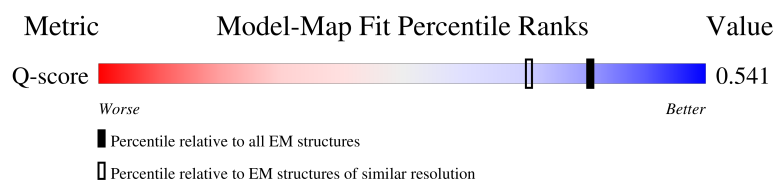
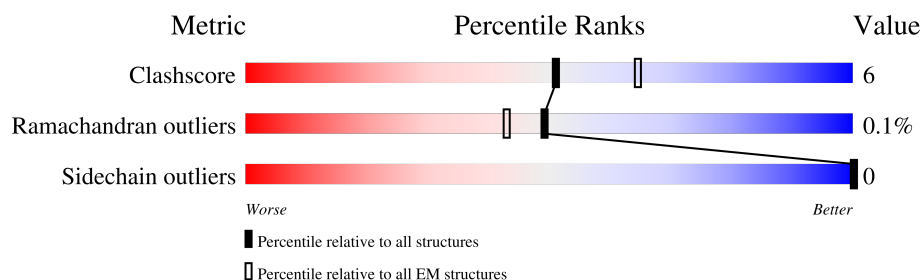
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



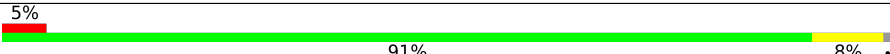
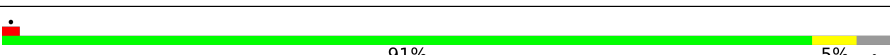
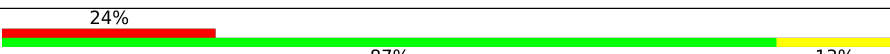
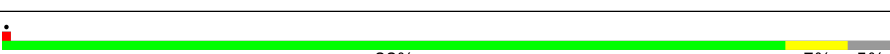
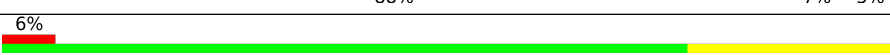
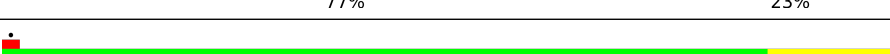
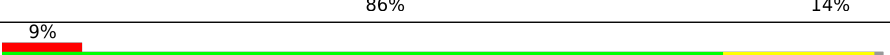
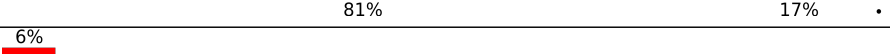
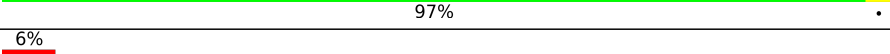
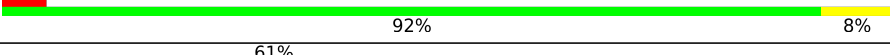
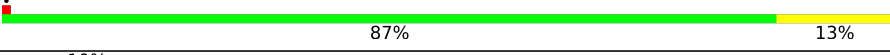
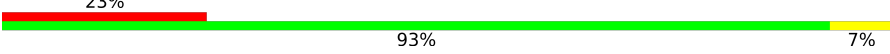
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	1	159	12% 84% 16%
2	A	335	7% 80% 14% 6%
2	a	335	• 82% 9% 9%
3	B	481	• 93% 7%

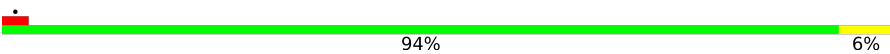
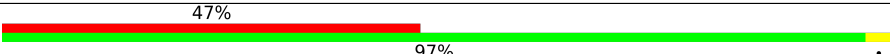
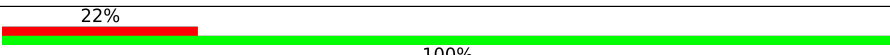
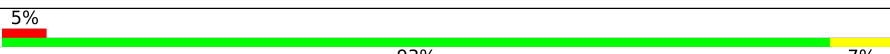
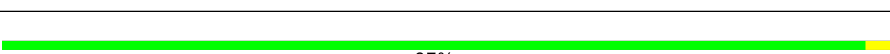
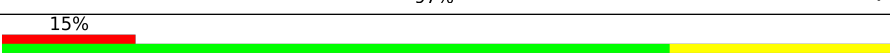
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Mol	Chain	Length	Quality of chain
3	b	481	
4	C	449	
4	c	449	
5	D	351	
5	d	351	
6	E	75	
6	e	75	
7	F	31	
7	f	31	
8	G	219	
9	H	69	
9	h	69	
10	I	35	
10	i	35	
11	K	37	
11	k	37	
12	L	37	
12	l	37	
13	M	31	
13	m	31	
14	N	219	
15	O	240	
16	S	250	
17	T	30	
17	t	30	

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Mol	Chain	Length	Quality of chain
18	V	32	
18	v	32	
19	W	56	
20	X	32	
20	x	32	
21	Y	220	
22	Z	61	
22	z	61	
23	r	201	

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
25	CLA	A	402	X	-	-	-
25	CLA	A	403	X	-	-	-
25	CLA	A	405	X	-	-	-
25	CLA	B	501	X	-	-	-
25	CLA	B	502	X	-	-	-
25	CLA	B	503	X	-	-	-
25	CLA	B	504	X	-	-	-
25	CLA	B	505	X	-	-	-
25	CLA	B	506	X	-	-	-
25	CLA	B	507	X	-	-	-
25	CLA	B	508	X	-	-	-
25	CLA	B	509	X	-	-	-
25	CLA	B	510	X	-	-	-
25	CLA	B	511	X	-	-	-
25	CLA	B	512	X	-	-	-
25	CLA	B	513	X	-	-	-
25	CLA	B	514	X	-	-	-
25	CLA	B	515	X	-	-	-
25	CLA	B	516	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	401	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	D	405	X	-	-	-
25	CLA	G	602	X	-	-	-
25	CLA	G	603	X	-	-	-
25	CLA	G	604	X	-	-	-
25	CLA	G	610	X	-	-	-
25	CLA	G	611	X	-	-	-
25	CLA	G	612	X	-	-	-
25	CLA	G	613	X	-	-	-
25	CLA	G	614	X	-	-	-
25	CLA	N	303	X	-	-	-
25	CLA	N	304	X	-	-	-
25	CLA	N	305	X	-	-	-
25	CLA	N	311	X	-	-	-
25	CLA	N	312	X	-	-	-
25	CLA	N	313	X	-	-	-
25	CLA	N	314	X	-	-	-
25	CLA	N	315	X	-	-	-
25	CLA	S	602	X	-	-	-
25	CLA	S	603	X	-	-	-
25	CLA	S	604	X	-	-	-
25	CLA	S	605	X	-	-	-
25	CLA	S	609	X	-	-	-
25	CLA	S	610	X	-	-	-
25	CLA	S	611	X	-	-	-
25	CLA	S	612	X	-	-	-
25	CLA	S	613	X	-	-	-
25	CLA	S	614	X	-	-	-
25	CLA	Y	304	X	-	-	-
25	CLA	Y	305	X	-	-	-
25	CLA	Y	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	Y	311	X	-	-	-
25	CLA	Y	312	X	-	-	-
25	CLA	Y	313	X	-	-	-
25	CLA	Y	314	X	-	-	-
25	CLA	Y	315	X	-	-	-
25	CLA	a	402	X	-	-	-
25	CLA	a	403	X	-	-	-
25	CLA	a	405	X	-	-	-
25	CLA	b	501	X	-	-	-
25	CLA	b	502	X	-	-	-
25	CLA	b	503	X	-	-	-
25	CLA	b	504	X	-	-	-
25	CLA	b	505	X	-	-	-
25	CLA	b	506	X	-	-	-
25	CLA	b	507	X	-	-	-
25	CLA	b	508	X	-	-	-
25	CLA	b	509	X	-	-	-
25	CLA	b	510	X	-	-	-
25	CLA	b	511	X	-	-	-
25	CLA	b	512	X	-	-	-
25	CLA	b	513	X	-	-	-
25	CLA	b	514	X	-	-	-
25	CLA	b	515	X	-	-	-
25	CLA	b	516	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-
25	CLA	r	301	X	-	-	-
25	CLA	r	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	r	303	X	-	-	-
25	CLA	r	307	X	-	-	-
25	CLA	r	308	X	-	-	-
33	BCT	a	409	-	-	X	-
36	CHL	G	601	X	-	-	-
36	CHL	G	605	X	-	-	-
36	CHL	G	606	X	-	-	-
36	CHL	G	607	X	-	-	-
36	CHL	G	608	X	-	-	-
36	CHL	G	609	X	-	-	-
36	CHL	G	619	X	-	-	-
36	CHL	N	302	X	-	-	-
36	CHL	N	306	X	-	-	-
36	CHL	N	307	X	-	-	-
36	CHL	N	308	X	-	-	-
36	CHL	N	309	X	-	-	-
36	CHL	N	310	X	-	-	-
36	CHL	S	601	X	-	-	-
36	CHL	S	606	X	-	-	-
36	CHL	S	607	X	-	-	-
36	CHL	S	608	X	-	-	-
36	CHL	Y	303	X	-	-	-
36	CHL	Y	307	X	-	-	-
36	CHL	Y	308	X	-	-	-
36	CHL	Y	309	X	-	-	-
36	CHL	Y	310	X	-	-	-
36	CHL	r	304	X	-	-	-
36	CHL	r	305	X	-	-	-
36	CHL	r	306	X	-	-	-

2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 55146 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 PDZ domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	159	Total	C	N	O	S	0	0
			1285	803	231	245	6		

- Molecule 2 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	315	Total	C	N	O	S	0	0
			2465	1620	407	423	15		
2	a	304	Total	C	N	O	S	0	0
			2375	1561	392	407	15		

- Molecule 3 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	480	Total	C	N	O	S	0	0
			3755	2462	630	651	12		
3	b	481	Total	C	N	O	S	0	0
			3763	2468	631	652	12		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3498	2288	584	609	17		
4	c	438	Total	C	N	O	S	0	0
			3431	2249	571	594	17		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2771	1828	456	475	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	337	Total	C	N	O	S	0	0
			2686	1777	439	458	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	75	Total	C	N	O		0	0
			610	399	101	110			
6	e	71	Total	C	N	O		0	0
			575	376	94	105			

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			251	171	42	37	1		
7	f	31	Total	C	N	O	S	0	0
			251	171	42	37	1		

- Molecule 8 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	219	Total	C	N	O	S	0	0
			1667	1082	272	308	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	68	Total	C	N	O	S	0	0
			519	347	77	93	2		
9	h	68	Total	C	N	O	S	0	0
			519	346	77	94	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	35	Total	C	N	O	S	0	0
			283	193	43	45	2		
10	i	34	Total	C	N	O	S	0	0
			275	189	41	43	2		

- 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
			297	209	43	45		
11	k	37	Total	C	N	O	0	0
			296	209	43	44		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	36	Total	C	N	O	0	0
			301	202	49	50		
12	l	37	Total	C	N	O	0	0
			306	205	50	51		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	30	Total	C	N	O	0	0
			230	158	32	40		
13	m	30	Total	C	N	O	0	0
			232	158	33	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	219	Total	C	N	O	S	0	0
			1672	1081	272	314	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	207	Total	C	N	O	S	0	0
			1565	1001	246	314	4		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	250	Total	C	N	O	S	0	0
			1894	1225	310	355	4		

- Molecule 17 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	30	Total	C	N	O	S	0	0
			247	171	36	38	2		
17	t	27	Total	C	N	O	S	0	0
			220	154	30	35	1		

- Molecule 18 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	32	Total	C	N	O		0	0
			224	147	37	40			
18	v	32	Total	C	N	O		0	0
			224	147	37	40			

- Molecule 19 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	56	Total	C	N	O	S	0	0
			434	281	70	81	2		

- Molecule 20 is a protein called Chloroplast photosystem II subunit X.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	32	Total	C	N	O		0	0
			214	140	35	39			
20	x	32	Total	C	N	O		0	0
			214	140	35	39			

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	220	Total	C	N	O	S	0	0
			1686	1100	271	310	5		

- Molecule 22 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		
22	z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		

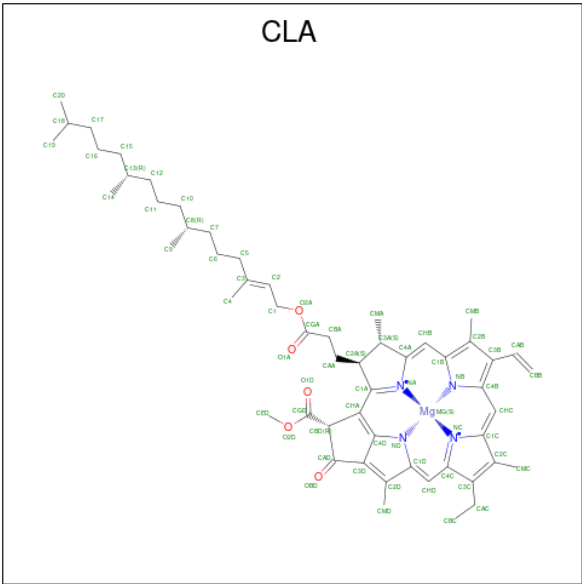
- Molecule 23 is a protein called Chlorophyll a-b binding protein CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	r	160	Total	C	N	O	S	0	0
			1235	795	208	227	5		

- Molecule 24 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	Fe	0
			1	1	
24	a	1	Total	Fe	0
			1	1	

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	G	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 49	C 39	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	S	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	S	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	S	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 54	C 44	Mg 1	N 4	O 5	0

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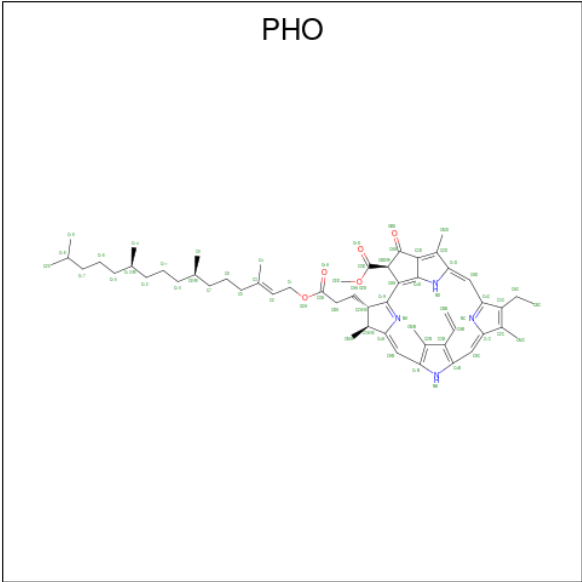
Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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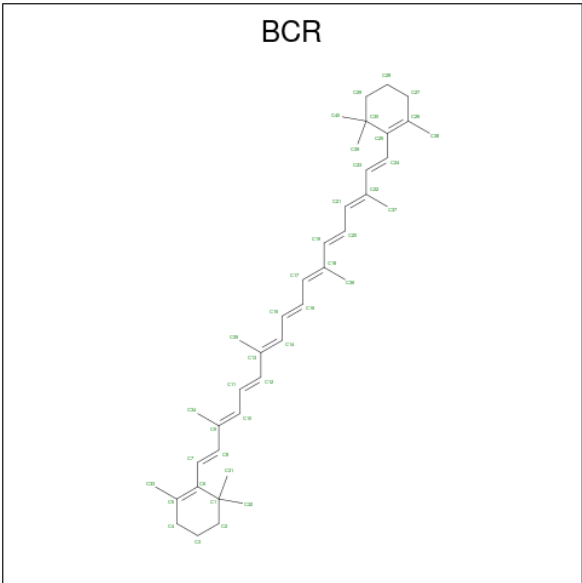
Mol	Chain	Residues	Atoms					AltConf
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Lig- and of Interest" by depositor).



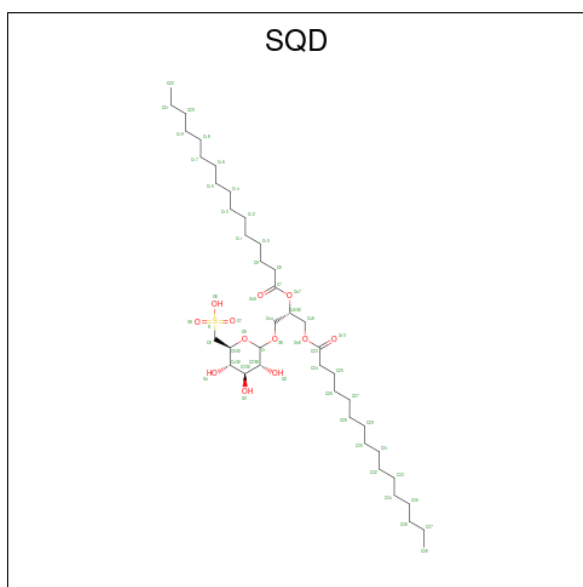
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	N	O	0
			64	55	4	5	
26	D	1	Total	C	N	O	0
			64	55	4	5	
26	a	1	Total	C	N	O	0
			64	55	4	5	
26	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



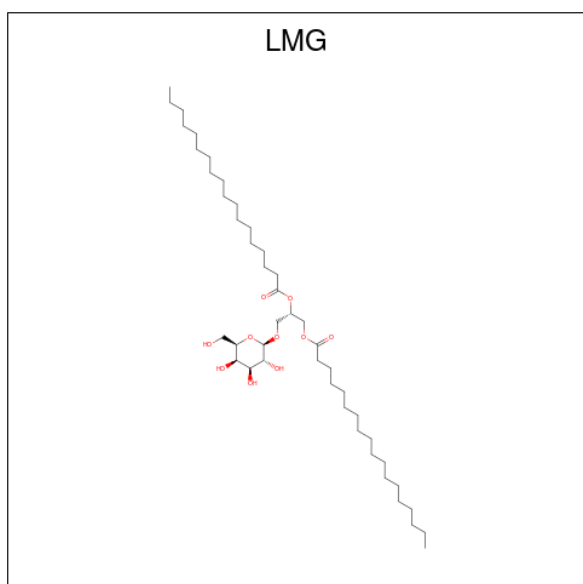
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	D	1	Total C 40 40	0
27	H	1	Total C 40 40	0
27	V	1	Total C 40 40	0
27	a	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	c	1	Total C 40 40	0
27	d	1	Total C 40 40	0
27	h	1	Total C 40 40	0
27	k	1	Total C 40 40	0
27	t	1	Total C 40 40	0
27	v	1	Total C 40 40	0
27	z	1	Total C 40 40	0

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



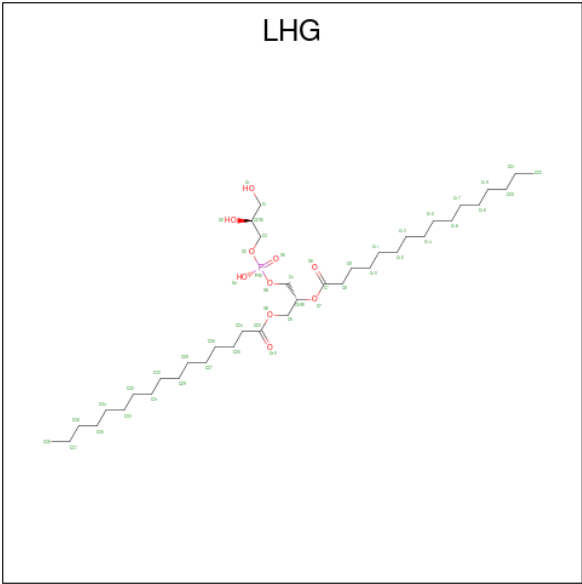
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	S	0
			51	38	12	1	
28	a	1	Total	C	O	S	0
			51	38	12	1	
28	t	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	C	O	0
			51	41	10	
29	C	1	Total	C	O	0
			51	41	10	
29	D	1	Total	C	O	0
			46	36	10	
29	H	1	Total	C	O	0
			48	38	10	
29	W	1	Total	C	O	0
			48	38	10	
29	a	1	Total	C	O	0
			46	36	10	
29	b	1	Total	C	O	0
			42	32	10	
29	c	1	Total	C	O	0
			40	30	10	
29	d	1	Total	C	O	0
			41	31	10	
29	d	1	Total	C	O	0
			48	38	10	

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



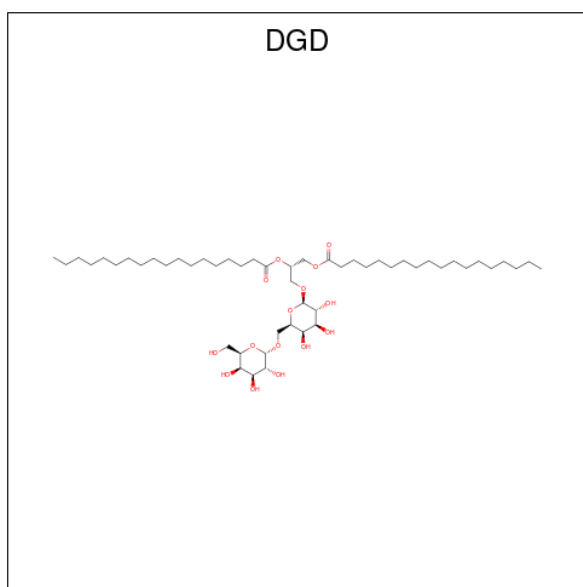
Mol	Chain	Residues	Atoms				AltConf
30	B	1	Total	C	O	P	0
			44	33	10	1	

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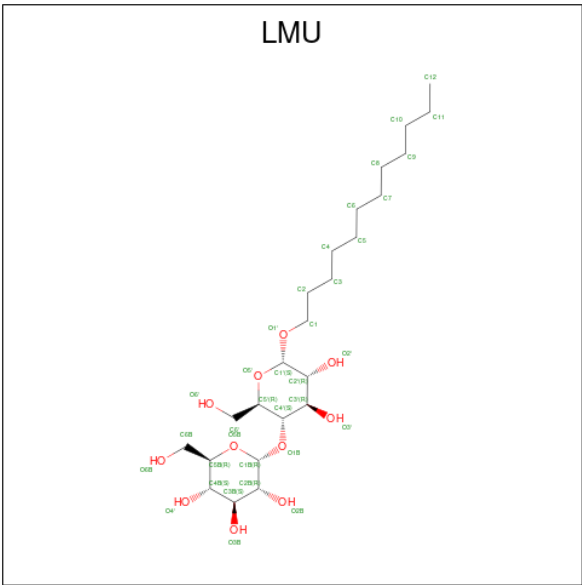
Mol	Chain	Residues	Atoms				AltConf
30	C	1	Total	C	O	P	0
			47	36	10	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			39	28	10	1	
30	G	1	Total	C	O	P	0
			49	38	10	1	
30	L	1	Total	C	O	P	0
			49	38	10	1	
30	N	1	Total	C	O	P	0
			49	38	10	1	
30	S	1	Total	C	O	P	0
			45	34	10	1	
30	Y	1	Total	C	O	P	0
			49	38	10	1	
30	a	1	Total	C	O	P	0
			43	32	10	1	
30	a	1	Total	C	O	P	0
			44	33	10	1	
30	b	1	Total	C	O	P	0
			49	38	10	1	
30	d	1	Total	C	O	P	0
			44	33	10	1	
30	d	1	Total	C	O	P	0
			49	38	10	1	
30	l	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



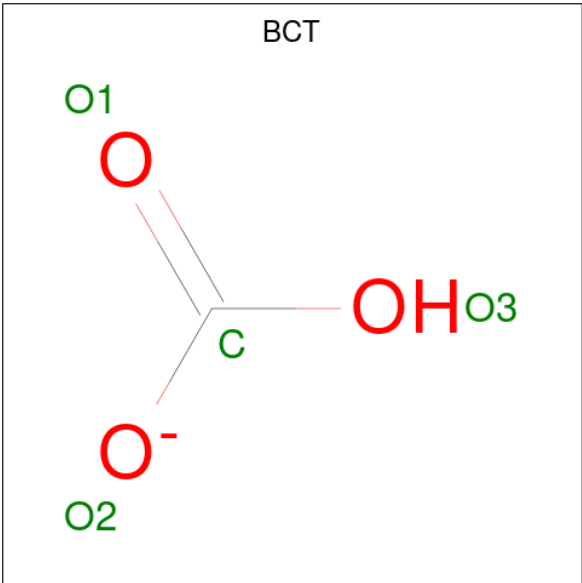
Mol	Chain	Residues	Atoms			AltConf
31	C	1	Total	C	O	0
			55	40	15	
31	C	1	Total	C	O	0
			62	47	15	
31	C	1	Total	C	O	0
			59	44	15	
31	W	1	Total	C	O	0
			66	51	15	
31	Y	1	Total	C	O	0
			66	51	15	
31	c	1	Total	C	O	0
			53	38	15	
31	c	1	Total	C	O	0
			49	34	15	
31	c	1	Total	C	O	0
			59	44	15	

- Molecule 32 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



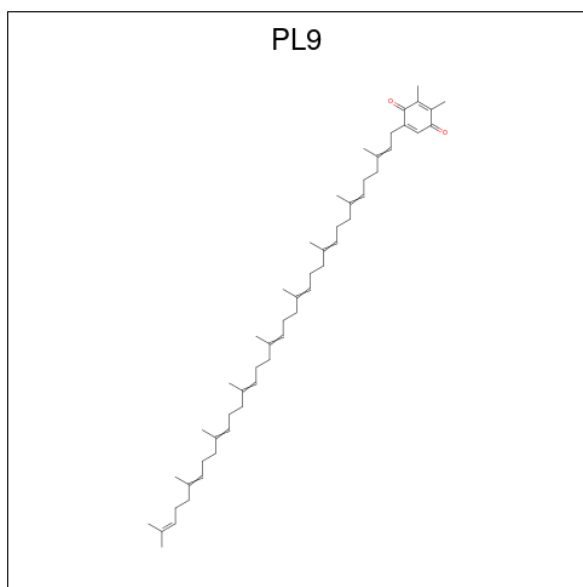
Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total	C	O	0
			35	24	11	
32	C	1	Total	C	O	0
			35	24	11	
32	S	1	Total	C	O	0
			35	24	11	
32	c	1	Total	C	O	0
			35	24	11	

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



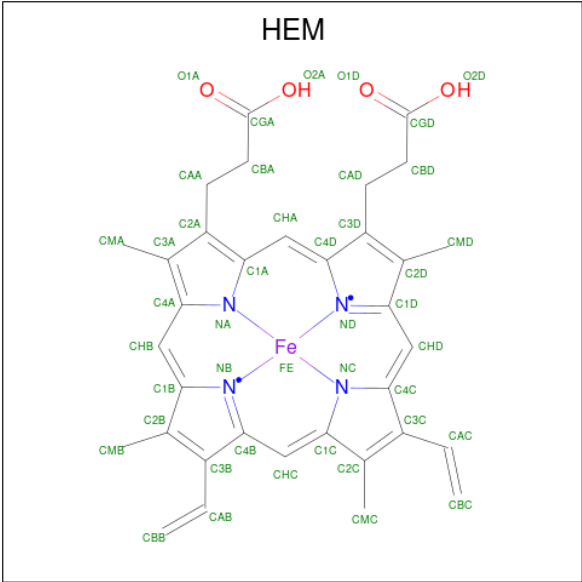
Mol	Chain	Residues	Atoms			AltConf
33	D	1	Total	C	O	0
			4	1	3	
33	a	1	Total	C	O	0
			4	1	3	

- Molecule 34 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: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



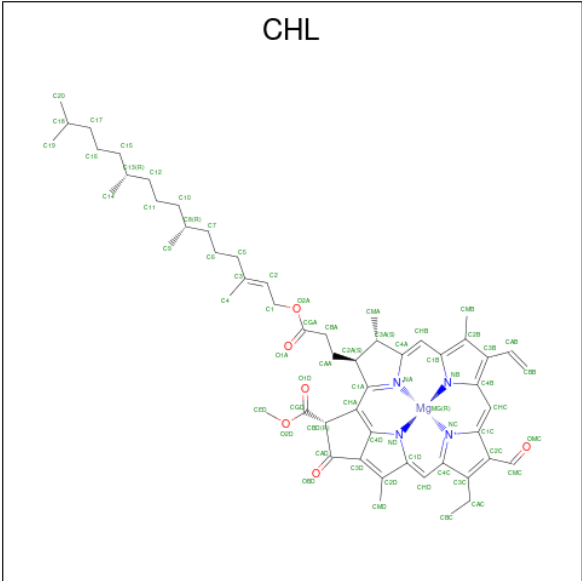
Mol	Chain	Residues	Atoms			AltConf
34	D	1	Total	C	O	0
			55	53	2	
34	d	1	Total	C	O	0
			55	53	2	

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
35	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
35	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 36 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
36	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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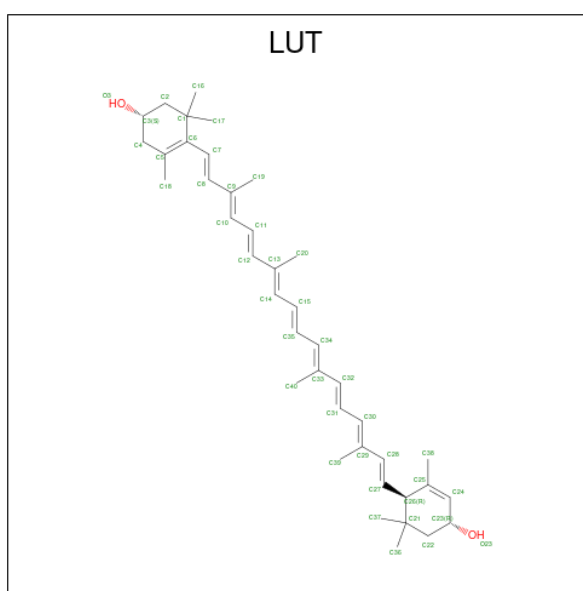
Mol	Chain	Residues	Atoms					AltConf
36	G	1	Total 43	C 34	Mg 1	N 4	O 4	0
36	G	1	Total 43	C 34	Mg 1	N 4	O 4	0
36	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
36	G	1	Total 44	C 35	Mg 1	N 4	O 4	0
36	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
36	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
36	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
36	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
36	N	1	Total 46	C 35	Mg 1	N 4	O 6	0
36	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
36	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
36	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
36	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
36	S	1	Total 44	C 35	Mg 1	N 4	O 4	0
36	S	1	Total 43	C 34	Mg 1	N 4	O 4	0
36	S	1	Total 49	C 38	Mg 1	N 4	O 6	0
36	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
36	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
36	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
36	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
36	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
36	r	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
36	r	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
36	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 37 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



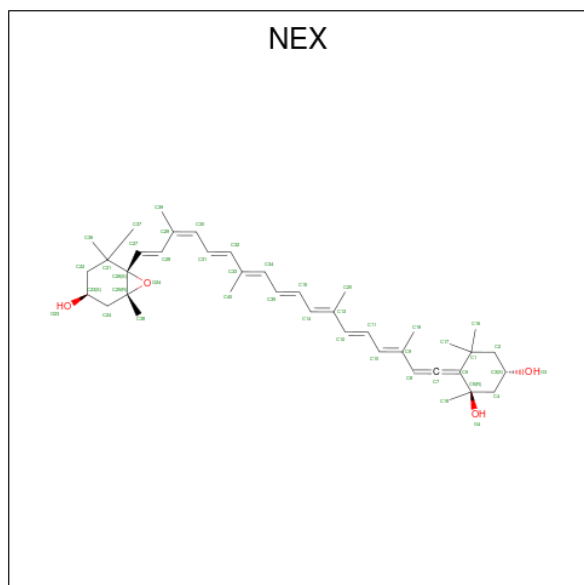
Mol	Chain	Residues	Atoms				AltConf
37	G	1	Total	C	O		0
			42	40	2		
37	G	1	Total	C	O		0
			42	40	2		
37	N	1	Total	C	O		0
			42	40	2		
37	N	1	Total	C	O		0
			42	40	2		
37	S	1	Total	C	O		0
			42	40	2		
37	S	1	Total	C	O		0
			42	40	2		
37	Y	1	Total	C	O		0
			42	40	2		

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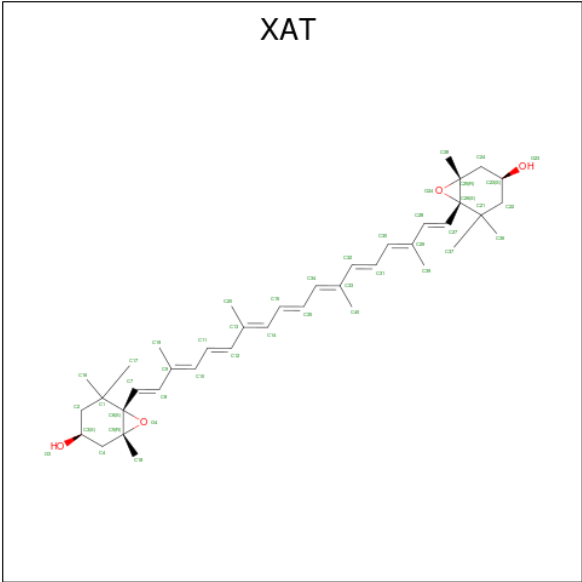
Mol	Chain	Residues	Atoms			AltConf
37	Y	1	Total	C	O	0
			42	40	2	

- Molecule 38 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
38	G	1	Total	C	O	0
			44	40	4	
38	N	1	Total	C	O	0
			44	40	4	
38	S	1	Total	C	O	0
			44	40	4	
38	Y	1	Total	C	O	0
			44	40	4	
38	r	1	Total	C	O	0
			44	40	4	

- Molecule 39 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).

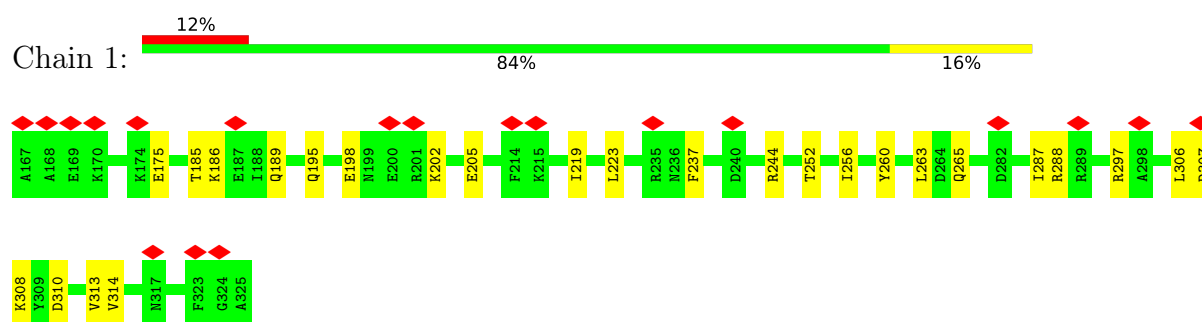


Mol	Chain	Residues	Atoms			AltConf
39	G	1	Total	C	O	0
			44	40	4	
39	N	1	Total	C	O	0
			44	40	4	
39	Y	1	Total	C	O	0
			44	40	4	
39	r	1	Total	C	O	0
			44	40	4	

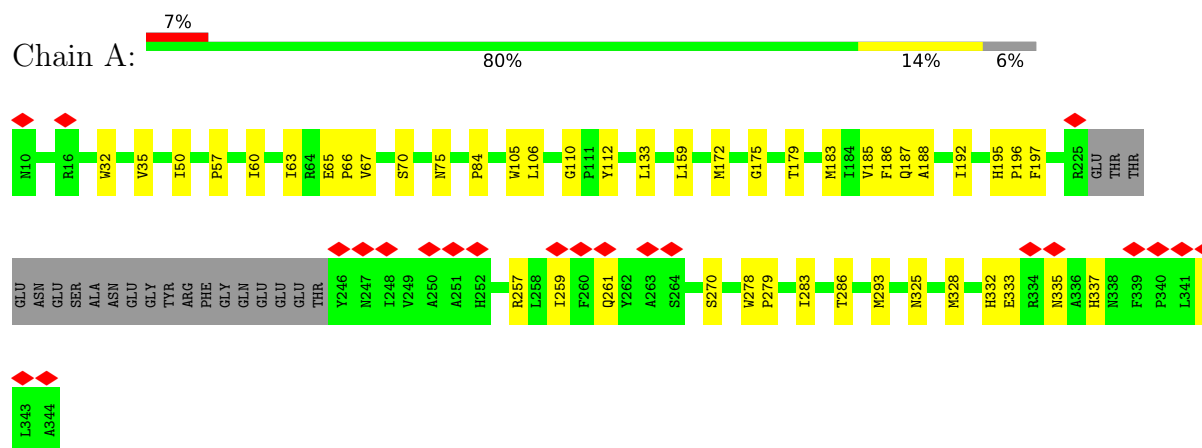
3 Residue-property plots [i](#)

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.

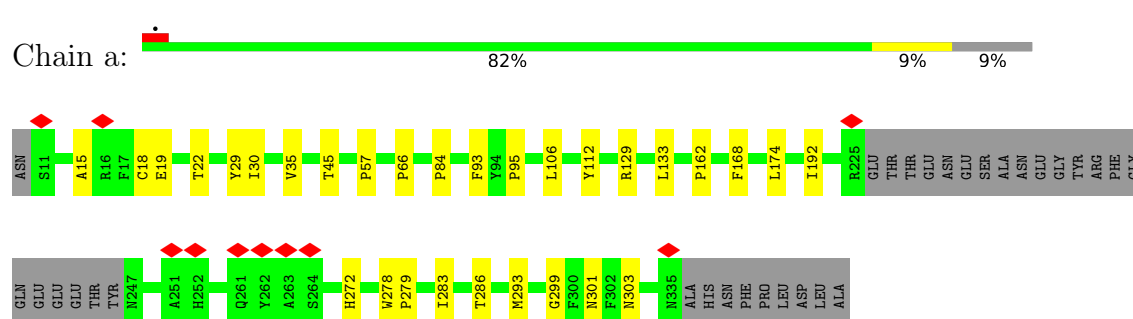
- Molecule 1: PDZ domain-containing protein



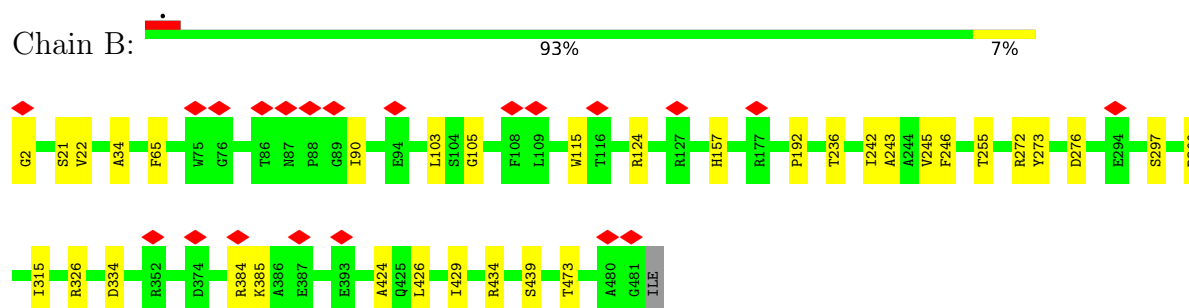
- Molecule 2: Photosystem II protein D1



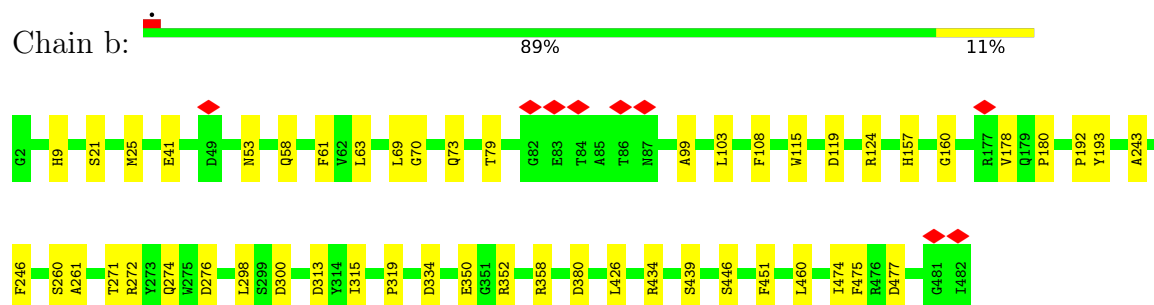
- Molecule 2: Photosystem II protein D1



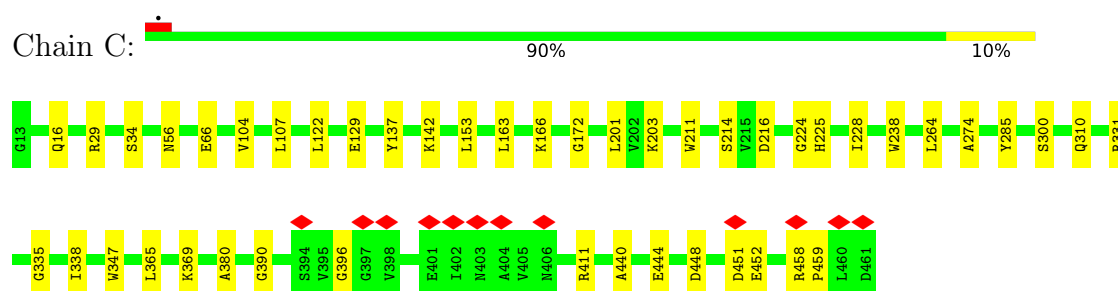
- Molecule 3: Photosystem II CP47 reaction center protein



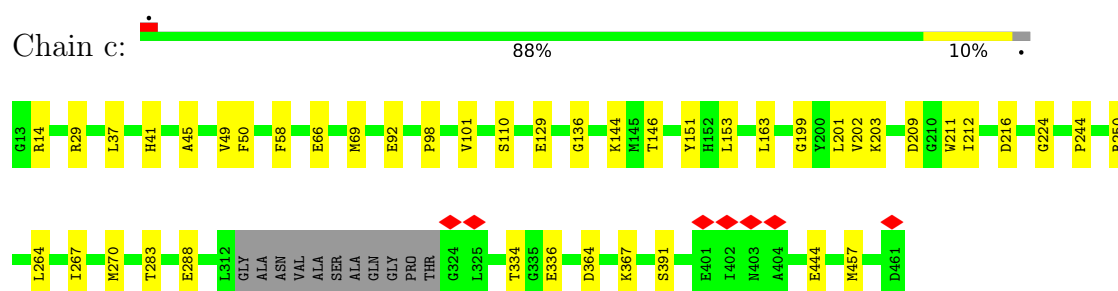
- Molecule 3: Photosystem II CP47 reaction center protein



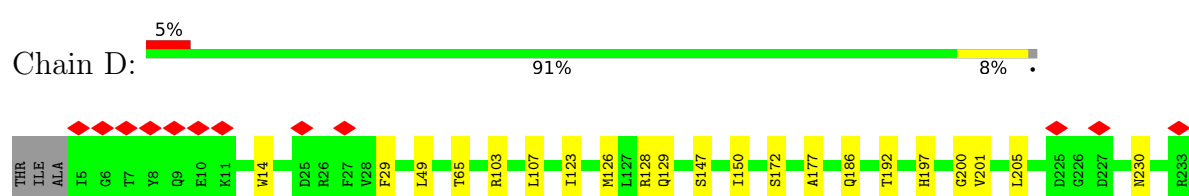
- Molecule 4: Photosystem II CP43 reaction center protein

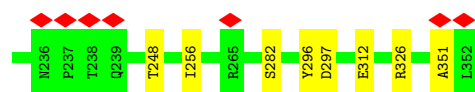


- Molecule 4: Photosystem II CP43 reaction center protein



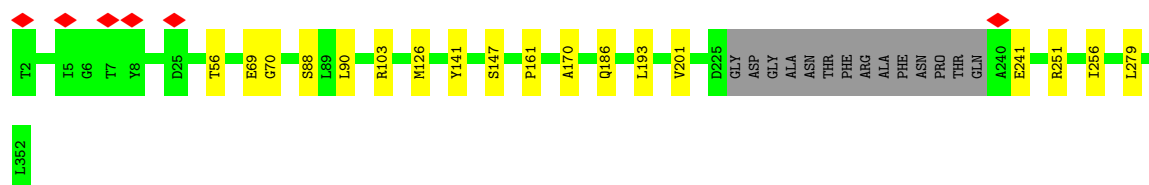
- Molecule 5: Photosystem II D2 protein





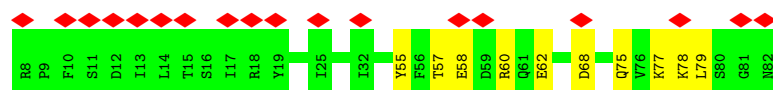
- Molecule 5: Photosystem II D2 protein

Chain d: 91% 5%



- Molecule 6: Cytochrome b559 subunit alpha

Chain E: 24% 87% 13%



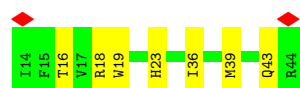
- Molecule 6: Cytochrome b559 subunit alpha

Chain e: 88% 7% 5%



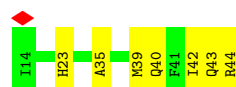
- Molecule 7: Cytochrome b559 subunit beta

Chain F: 6% 77% 23%



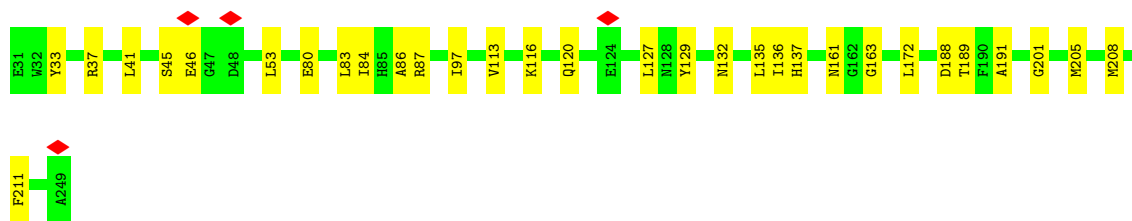
- Molecule 7: Cytochrome b559 subunit beta

Chain f: 77% 23%

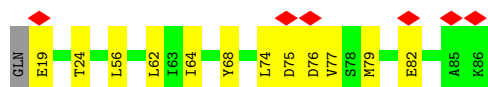
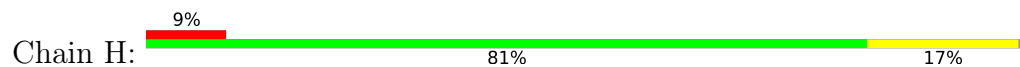


- Molecule 8: Chlorophyll a-b binding protein, chloroplastic

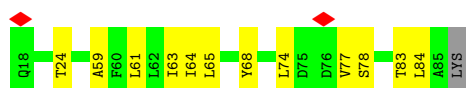
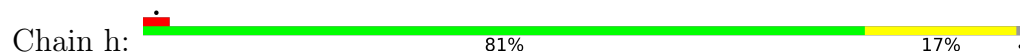
Chain G: 86% 14%



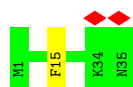
- Molecule 9: Photosystem II reaction center protein H



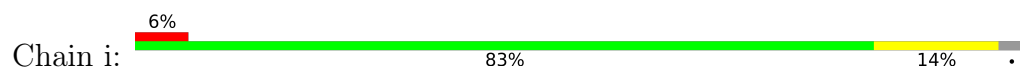
- Molecule 9: Photosystem II reaction center protein H



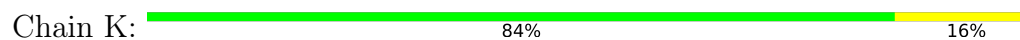
- Molecule 10: Photosystem II reaction center protein I



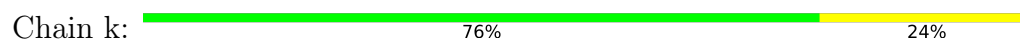
- Molecule 10: Photosystem II reaction center protein I



- Molecule 11: Photosystem II reaction center protein K

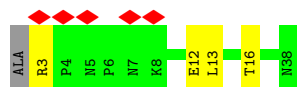
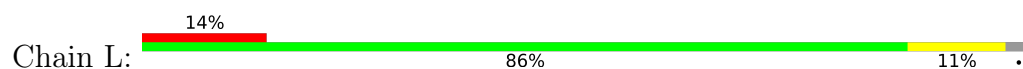


- Molecule 11: Photosystem II reaction center protein K

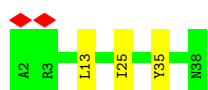




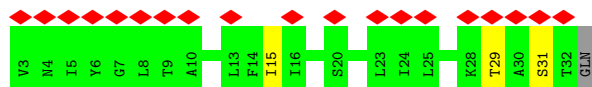
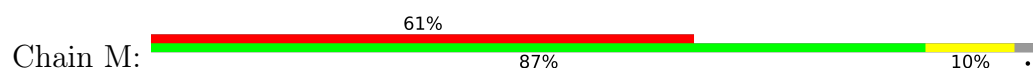
- Molecule 12: Photosystem II reaction center protein L



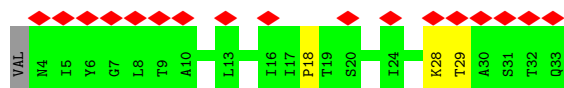
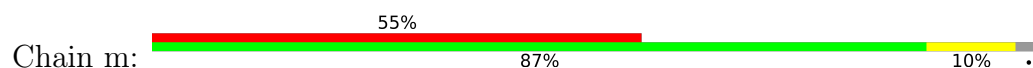
- Molecule 12: Photosystem II reaction center protein L



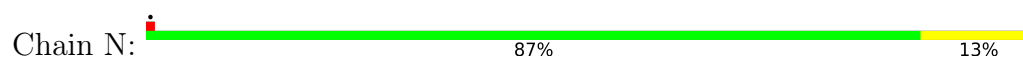
- Molecule 13: Photosystem II reaction center protein M



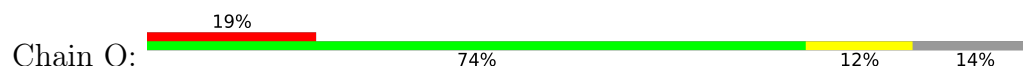
- Molecule 13: Photosystem II reaction center protein M

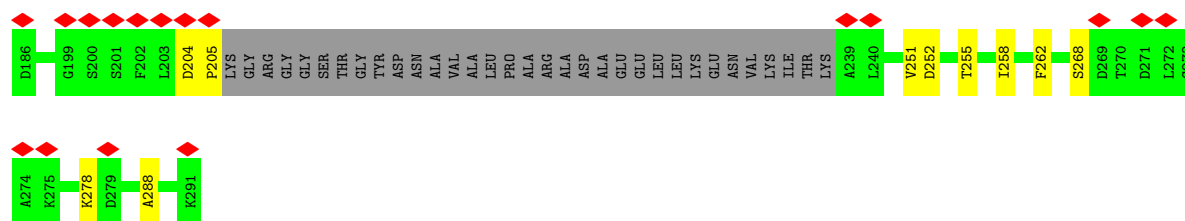


- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



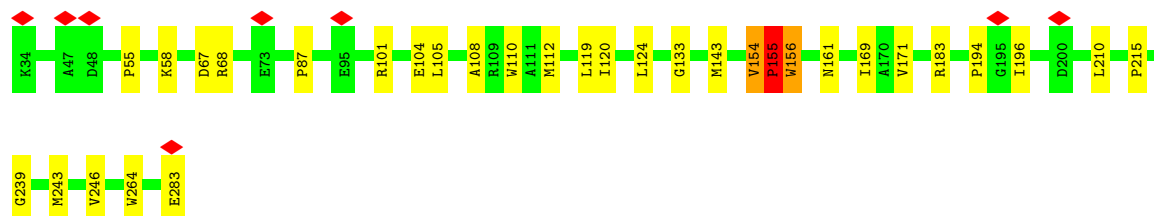
- Molecule 15: Oxygen-evolving enhancer protein 1, chloroplastic





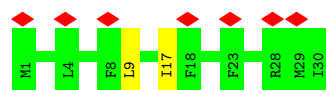
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain S: 87% 12%



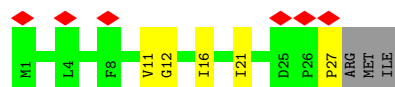
- Molecule 17: Photosystem II reaction center protein T

Chain T: 23% 93% 7%



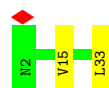
- Molecule 17: Photosystem II reaction center protein T

Chain t: 20% 73% 17% 10%



- Molecule 18: Photosystem II reaction center protein Psb30

Chain V: 94% 6%

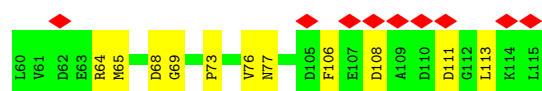
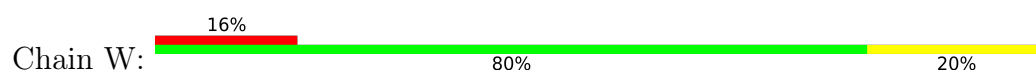


- Molecule 18: Photosystem II reaction center protein Psb30

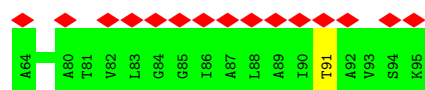
Chain v: 22% 72% 28%



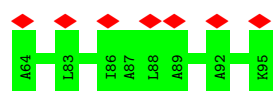
- Molecule 19: Photosystem II reaction center W protein, chloroplastic



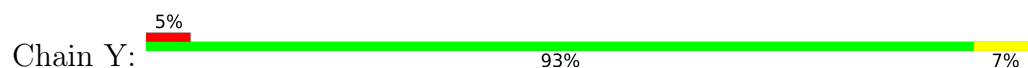
- Molecule 20: Chloroplast photosystem II subunit X



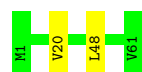
- Molecule 20: Chloroplast photosystem II subunit X



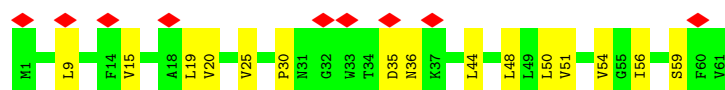
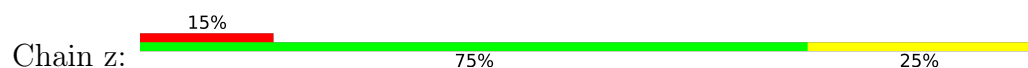
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic



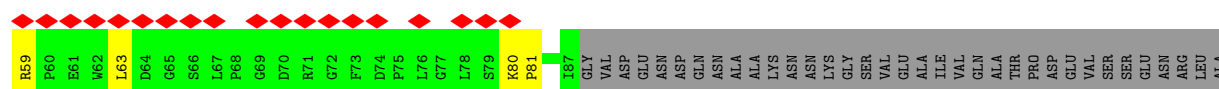
- Molecule 22: Photosystem II reaction center protein Z



- Molecule 22: Photosystem II reaction center protein Z



- Molecule 23: Chlorophyll a-b binding protein CP29



PRO	TYR	SER	GLU	VAL	PHE	G129	L130	A131	R132	F133	R134	E137	L138	G141	R142	W143	A144	M145	L146	G150	A151	L152	E155	A156	T157	T158	G159	W162	V163	E164	K167	V168	E169	L170	D171	G172	A173	G177	L178	P181	F182	S183	I184	T185	Q186	L187	I188	W189	I193	L194							
V195	G196	G197	A198	E199	F200	Y201	R202	N203	S204	E205	T206	N207	P208	E209	K210	R211	C212	Y213	P214	G215	G216	V217	F218	D219	P220	L221	K222	L223	A224	S225	E226	D227	E228	E229	R230	A231	F232	R233	L234	K235	T236	A237	E238	A242	R243	L244	F249	F250	G251	Y252	G253	V254	Q255	A256	L257	S258	T259

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97962	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	39.154	Depositor
Minimum map value	-20.689	Depositor
Average map value	0.008	Depositor
Map value standard deviation	1.163	Depositor
Recommended contour level	6.8	Depositor
Map size ($\text{\AA}$)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	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, CHL, BCR, DGD, LHG, HEM, LMU, NEX, XAT, LMG, FE2, BCT, PL9, PHO, SQD, LUT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.11	0/1307	0.29	0/1755
2	A	0.16	0/2544	0.28	0/3470
2	a	0.18	0/2450	0.29	0/3340
3	B	0.14	0/3883	0.27	0/5286
3	b	0.17	0/3891	0.29	0/5297
4	C	0.15	0/3619	0.27	0/4931
4	c	0.15	0/3550	0.31	0/4834
5	D	0.16	0/2866	0.29	0/3909
5	d	0.17	0/2777	0.28	0/3787
6	E	0.12	0/628	0.29	0/857
6	e	0.13	0/591	0.29	0/807
7	F	0.12	0/258	0.27	0/349
7	f	0.15	0/258	0.26	0/349
8	G	0.14	0/1717	0.29	0/2337
9	H	0.13	0/530	0.28	0/725
9	h	0.31	0/530	0.46	0/726
10	I	0.14	0/291	0.23	0/394
10	i	0.15	0/283	0.32	0/383
11	K	0.17	0/309	0.32	0/425
11	k	0.17	0/308	0.41	0/425
12	L	0.12	0/309	0.21	0/420
12	l	0.15	0/314	0.25	0/427
13	M	0.13	0/234	0.25	0/321
13	m	0.14	0/236	0.30	0/323
14	N	0.14	0/1720	0.28	0/2341
15	O	0.11	0/1593	0.29	0/2150
16	S	0.16	0/1948	0.42	3/2653 (0.1%)
17	T	0.10	0/254	0.22	0/343
17	t	0.13	0/227	0.24	0/308
18	V	0.10	0/224	0.22	0/307
18	v	0.13	0/224	0.34	0/307
19	W	0.12	0/445	0.27	0/603

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	X	0.11	0/215	0.22	0/292
20	x	0.13	0/215	0.24	0/292
21	Y	0.14	0/1739	0.26	0/2364
22	Z	0.13	0/469	0.26	0/644
22	z	0.13	0/469	0.34	0/644
23	r	0.16	0/1264	0.39	2/1711 (0.1%)
All	All	0.15	0/44689	0.30	5/60836 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
16	S	0	1
23	r	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	S	155	PRO	CA-N-CD	-6.95	102.27	112.00
16	S	155	PRO	CA-C-N	5.51	132.07	121.54
16	S	155	PRO	C-N-CA	5.51	132.07	121.54
23	r	225	SER	CB-CA-C	-5.21	110.55	116.54
23	r	199	GLU	CA-CB-CG	5.17	124.45	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	S	154	VAL	Peptide
23	r	199	GLU	Sidechain

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	l	1285	0	1254	16	0
2	A	2465	0	2396	34	0
2	a	2375	0	2316	20	0
3	B	3755	0	3642	29	0
3	b	3763	0	3653	35	0
4	C	3498	0	3372	36	0
4	c	3431	0	3308	34	0
5	D	2771	0	2655	28	0
5	d	2686	0	2585	15	0
6	E	610	0	599	8	0
6	e	575	0	565	4	0
7	F	251	0	263	5	0
7	f	251	0	263	7	0
8	G	1667	0	1606	22	0
9	H	519	0	549	13	0
9	h	519	0	544	9	0
10	I	283	0	293	1	0
10	i	275	0	287	4	0
11	K	297	0	308	5	0
11	k	296	0	308	8	0
12	L	301	0	310	4	0
12	l	306	0	315	3	0
13	M	230	0	252	3	0
13	m	232	0	251	3	0
14	N	1672	0	1611	18	0
15	O	1565	0	1562	20	0
16	S	1894	0	1838	30	0
17	T	247	0	260	2	0
17	t	220	0	227	4	0
18	V	224	0	256	3	0
18	v	224	0	256	7	0
19	W	434	0	411	9	0
20	X	214	0	240	1	0
20	x	214	0	240	0	0
21	Y	1686	0	1623	11	0
22	Z	458	0	490	2	0
22	z	458	0	490	11	0
23	r	1235	0	1221	17	0
24	A	1	0	0	0	0
24	a	1	0	0	0	0
25	A	174	0	170	1	0
25	B	1040	0	1152	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	C	845	0	936	12	0
25	D	195	0	216	4	0
25	G	432	0	416	2	0
25	N	461	0	463	5	0
25	S	471	0	363	9	0
25	Y	502	0	535	0	0
25	a	174	0	170	2	0
25	b	1000	0	1074	19	0
25	c	808	0	861	14	0
25	d	172	0	175	4	0
25	r	241	0	193	3	0
26	A	64	0	74	2	0
26	D	64	0	74	1	0
26	a	64	0	74	2	0
26	d	64	0	74	1	0
27	A	40	0	56	5	0
27	B	80	0	112	6	0
27	C	120	0	168	12	0
27	D	40	0	56	3	0
27	H	40	0	56	5	0
27	V	40	0	56	4	0
27	a	40	0	56	2	0
27	b	120	0	168	4	0
27	c	40	0	56	4	0
27	d	40	0	56	2	0
27	h	40	0	56	5	0
27	k	40	0	56	4	0
27	t	40	0	56	3	0
27	v	40	0	56	8	0
27	z	40	0	56	3	0
28	A	51	0	69	2	0
28	a	51	0	69	0	0
28	t	54	0	78	0	0
29	B	51	0	72	2	0
29	C	51	0	72	0	0
29	D	46	0	62	0	0
29	H	48	0	66	2	0
29	W	48	0	66	1	0
29	a	46	0	62	0	0
29	b	42	0	54	0	0
29	c	40	0	46	0	0
29	d	89	0	118	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	44	0	61	1	0
30	C	47	0	67	0	0
30	D	88	0	122	2	0
30	G	49	0	74	0	0
30	L	49	0	74	1	0
30	N	49	0	74	1	0
30	S	45	0	63	2	0
30	Y	49	0	74	2	0
30	a	87	0	117	1	0
30	b	49	0	74	1	0
30	d	93	0	135	4	0
30	l	49	0	74	4	0
31	C	176	0	226	1	0
31	W	66	0	96	0	0
31	Y	66	0	96	1	0
31	c	161	0	196	3	0
32	C	70	0	92	3	0
32	S	35	0	46	0	0
32	c	35	0	46	0	0
33	D	4	0	0	0	0
33	a	4	0	0	2	0
34	D	55	0	80	0	0
34	d	55	0	80	1	0
35	F	43	0	30	5	0
35	f	43	0	30	4	0
36	G	378	0	336	9	0
36	N	360	0	348	13	0
36	S	182	0	125	10	0
36	Y	274	0	239	8	0
36	r	133	0	91	4	0
37	G	84	0	112	4	0
37	N	84	0	112	4	0
37	S	84	0	112	8	0
37	Y	84	0	112	6	0
38	G	44	0	56	3	0
38	N	44	0	56	1	0
38	S	44	0	56	1	0
38	Y	44	0	56	4	0
38	r	44	0	56	3	0
39	G	44	0	56	2	0
39	N	44	0	56	3	0
39	Y	44	0	56	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	r	44	0	56	3	0
All	All	55146	0	55711	611	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 6.

All (611) 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)
8:G:208:MET:HE2	37:G:616:LUT:H10	1.55	0.89
2:A:185:VAL:HG13	2:A:332:HIS:HE1	1.37	0.89
35:f:101:HEM:HHC	35:f:101:HEM:HBB2	1.66	0.77
4:c:264:LEU:HD21	25:c:508:CLA:HAB	1.66	0.77
36:G:606:CHL:HHC	36:G:606:CHL:HBB1	1.66	0.76
9:h:78:SER:HB2	9:h:83:THR:HG22	1.68	0.76
36:G:608:CHL:HHC	36:G:608:CHL:HBB1	1.66	0.75
36:N:306:CHL:HHC	36:N:306:CHL:HBB1	1.68	0.75
5:D:186:GLN:HB2	25:D:404:CLA:HBC1	1.69	0.74
36:Y:310:CHL:HHC	36:Y:310:CHL:HBB1	1.68	0.74
14:N:152:THR:HG22	36:N:306:CHL:HAC1	1.69	0.73
21:Y:216:MET:HE2	37:Y:317:LUT:H10	1.70	0.73
5:d:186:GLN:HB2	25:d:403:CLA:HBC1	1.69	0.73
16:S:246:VAL:HG11	37:S:616:LUT:H12	1.70	0.73
2:A:133:LEU:HD23	5:D:256:ILE:HG12	1.70	0.71
4:C:264:LEU:HD21	25:C:508:CLA:HAB	1.72	0.70
6:E:60:ARG:NH1	6:E:79:LEU:O	2.25	0.70
3:B:384:ARG:NH2	15:O:204:ASP:O	2.25	0.70
5:D:192:THR:HG23	25:D:404:CLA:HBC2	1.73	0.70
36:Y:309:CHL:HHC	36:Y:309:CHL:HBB1	1.73	0.70
2:A:172:MET:HE3	2:A:179:THR:HG22	1.75	0.69
36:Y:308:CHL:HHC	36:Y:308:CHL:HBB1	1.74	0.69
3:B:192:PRO:HG3	9:H:68:TYR:CD1	2.27	0.69
4:C:310:GLN:HE22	4:C:369:LYS:HA	1.58	0.69
36:N:310:CHL:HBB1	36:N:310:CHL:HHC	1.73	0.69
4:c:153:LEU:HD21	25:c:506:CLA:HAB	1.74	0.69
36:r:304:CHL:HHC	36:r:304:CHL:HBB1	1.76	0.68
3:B:272:ARG:NH1	3:B:276:ASP:OD2	2.26	0.68
2:A:185:VAL:HG13	2:A:332:HIS:CE1	2.25	0.68
23:r:141:GLY:HA3	23:r:242:ALA:HB1	1.75	0.67
4:C:300:SER:OG	4:C:380:ALA:O	2.13	0.67
2:a:29:TYR:O	2:a:129:ARG:NH1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:G:609:CHL:HHC	36:G:609:CHL:HBB1	1.76	0.66
9:H:82:GLU:N	9:H:82:GLU:OE1	2.27	0.66
4:c:444:GLU:N	4:c:444:GLU:OE1	2.28	0.66
13:M:31:SER:OG	13:m:28:LYS:NZ	2.27	0.66
36:S:607:CHL:HHC	36:S:607:CHL:HBB1	1.77	0.66
25:b:504:CLA:HAA2	25:b:512:CLA:H141	1.78	0.66
16:S:58:LYS:NZ	30:S:618:LHG:O1	2.30	0.65
18:v:26:LEU:HD21	22:z:25:VAL:HA	1.79	0.65
1:1:287:ILE:O	1:1:297:ARG:NH2	2.30	0.65
4:C:142:LYS:NZ	19:W:111:ASP:O	2.31	0.63
9:h:74:LEU:HB2	9:h:77:VAL:HG22	1.81	0.63
2:a:299:GLY:O	4:c:391:SER:OG	2.17	0.63
18:v:15:VAL:HG23	27:v:101:BCR:HC8	1.81	0.63
36:r:305:CHL:HHC	36:r:305:CHL:HBB1	1.81	0.63
16:S:55:PRO:O	16:S:68:ARG:NH1	2.32	0.63
2:A:270:SER:OG	28:A:407:SQD:O49	2.16	0.62
25:b:505:CLA:H8	25:b:512:CLA:H203	1.81	0.62
23:r:80:LYS:NZ	23:r:81:PRO:O	2.31	0.62
3:b:243:ALA:HA	3:b:246:PHE:CE2	2.33	0.62
2:A:332:HIS:CD2	2:A:333:GLU:HG2	2.35	0.62
1:1:313:VAL:HG23	1:1:314:VAL:HG23	1.79	0.62
14:N:196:ASP:OD1	14:N:197:THR:N	2.33	0.62
25:b:502:CLA:H42	29:d:410:LMG:H112	1.81	0.61
18:V:15:VAL:HG13	27:V:101:BCR:H10C	1.82	0.61
3:B:124:ARG:NH1	9:H:19:GLU:O	2.33	0.61
3:b:272:ARG:NH1	3:b:276:ASP:OD2	2.33	0.61
5:d:279:LEU:HD22	26:d:402:PHO:HBC3	1.81	0.61
23:r:202:ARG:NH2	25:r:307:CLA:O1D	2.33	0.61
5:D:126:MET:HE3	5:D:150:ILE:HD12	1.83	0.61
36:S:606:CHL:HHC	36:S:606:CHL:HBB1	1.83	0.61
8:G:87:ARG:NH1	36:G:608:CHL:OBD	2.34	0.60
16:S:161:ASN:ND2	36:S:606:CHL:OBD	2.33	0.60
16:S:101:ARG:NH1	16:S:104:GLU:OE1	2.35	0.60
21:Y:94:ALA:HB1	21:Y:209:GLY:HA3	1.83	0.60
30:d:408:LHG:H322	17:t:21:ILE:HD11	1.82	0.60
16:S:108:ALA:O	16:S:112:MET:HG3	2.03	0.59
4:C:34:SER:OG	4:C:129:GLU:OE2	2.15	0.59
16:S:171:VAL:HG11	36:S:606:CHL:HED2	1.86	0.58
3:b:41:GLU:OE2	3:b:61:PHE:N	2.32	0.58
4:c:216:ASP:HA	4:c:283:THR:HG21	1.85	0.58
5:D:172:SER:HB2	5:D:177:ALA:HB1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:201:LEU:HD11	27:c:514:BCR:H373	1.85	0.58
36:N:309:CHL:HHC	36:N:309:CHL:HBB1	1.86	0.58
5:d:193:LEU:O	12:l:35:TYR:OH	2.15	0.58
11:K:13:GLU:OE1	11:K:13:GLU:N	2.29	0.57
15:O:251:VAL:HG23	15:O:258:ILE:HG22	1.84	0.57
3:b:434:ARG:HG3	3:b:439:SER:HB2	1.85	0.57
3:B:192:PRO:HG3	9:H:68:TYR:CE1	2.39	0.57
8:G:33:TYR:CE2	8:G:191:ALA:HB1	2.40	0.57
8:G:188:ASP:OD1	8:G:189:THR:N	2.37	0.57
14:N:135:LEU:HD21	25:N:305:CLA:HAA2	1.85	0.57
36:N:307:CHL:HHC	36:N:307:CHL:HBB1	1.85	0.57
35:F:101:HEM:HBC2	35:F:101:HEM:HHD	1.87	0.57
31:c:515:DGD:O4E	31:c:515:DGD:O5E	2.20	0.57
11:k:36:ALA:HB2	27:k:101:BCR:H391	1.87	0.57
12:l:13:LEU:N	13:m:29:THR:OG1	2.37	0.57
23:r:227:ASP:OD2	23:r:230:ARG:N	2.38	0.57
27:v:101:BCR:H382	27:v:101:BCR:H23C	1.86	0.57
12:L:13:LEU:N	13:M:29:THR:OG1	2.34	0.56
5:d:241:GLU:OE1	5:d:241:GLU:N	2.29	0.56
2:A:50:ILE:HG22	27:A:406:BCR:H271	1.86	0.56
3:b:350:GLU:OE1	3:b:352:ARG:NH1	2.37	0.56
1:1:306:LEU:O	1:1:310:ASP:N	2.37	0.56
25:b:516:CLA:OBD	9:h:24:THR:HG21	2.05	0.56
38:Y:318:NEX:H183	38:Y:318:NEX:H192	1.88	0.56
3:B:192:PRO:HG3	9:H:68:TYR:HD1	1.71	0.56
3:B:424:ALA:HB2	3:B:429:ILE:HD11	1.88	0.56
15:O:124:LEU:HD23	19:W:64:ARG:HH22	1.71	0.56
4:C:122:LEU:HD11	25:C:511:CLA:H92	1.88	0.56
4:C:153:LEU:HD21	25:C:506:CLA:HAB	1.85	0.56
4:C:444:GLU:OE1	4:C:444:GLU:N	2.31	0.56
14:N:94:ALA:HB1	14:N:209:GLY:HA3	1.86	0.56
15:O:252:ASP:OD1	15:O:255:THR:OG1	2.24	0.56
4:c:267:ILE:HA	4:c:270:MET:HE3	1.87	0.56
30:D:408:LHG:H291	17:T:17:ILE:HG23	1.88	0.56
35:f:101:HEM:HBC2	35:f:101:HEM:HMC2	1.87	0.56
4:C:107:LEU:HD23	27:C:516:BCR:HC8	1.88	0.55
6:E:58:GLU:N	6:E:58:GLU:OE1	2.39	0.55
4:c:199:GLY:HA2	4:c:202:VAL:HG12	1.87	0.55
16:S:133:GLY:HA3	25:S:604:CLA:HED3	1.88	0.55
23:r:142:ARG:NE	23:r:238:GLU:OE2	2.39	0.55
8:G:163:GLY:H	36:G:608:CHL:HMC	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:43:GLN:N	7:F:43:GLN:OE1	2.39	0.55
28:A:407:SQD:O8	5:D:230:ASN:ND2	2.35	0.55
3:B:326:ARG:NH2	5:D:297:ASP:OD2	2.39	0.55
27:V:101:BCR:H343	22:Z:20:VAL:HG21	1.87	0.55
4:c:334:THR:OG1	4:c:336:GLU:OE1	2.24	0.55
7:f:35:ALA:O	7:f:39:MET:HG3	2.06	0.55
2:a:30:ILE:O	2:a:30:ILE:HG13	2.07	0.55
2:a:133:LEU:HD23	5:d:256:ILE:HG12	1.88	0.55
22:z:9:LEU:HD13	22:z:54:VAL:HG21	1.89	0.55
35:F:101:HEM:HBB2	35:F:101:HEM:HMB1	1.89	0.54
2:a:272:HIS:CE1	33:a:409:BCT:O2	2.60	0.54
2:A:335:ASN:HA	5:D:351:ALA:HB2	1.88	0.54
14:N:216:MET:HG2	37:N:317:LUT:H12	1.88	0.54
16:S:143:MET:HE1	36:S:606:CHL:HMD3	1.89	0.54
36:S:608:CHL:HHC	36:S:608:CHL:HBB1	1.90	0.54
4:c:224:GLY:HA3	27:c:514:BCR:H402	1.90	0.54
14:N:95:ARG:NH1	36:N:309:CHL:OBD	2.33	0.54
2:A:187:GLN:HG2	2:A:192:ILE:HG22	1.89	0.54
16:S:169:ILE:HG12	36:S:607:CHL:HBC1	1.89	0.54
6:e:74:GLU:OE1	6:e:74:GLU:N	2.31	0.54
38:r:310:NEX:H192	38:r:310:NEX:H183	1.90	0.54
9:h:61:LEU:HD23	9:h:64:ILE:HD11	1.90	0.54
5:D:123:ILE:HD11	29:H:102:LMG:H402	1.90	0.53
16:S:154:VAL:HB	25:S:605:CLA:C4D	2.38	0.53
14:N:116:GLN:OE1	14:N:116:GLN:N	2.42	0.53
13:M:15:ILE:HD11	17:T:9:LEU:HD21	1.91	0.53
11:k:35:LEU:HB2	27:v:101:BCR:H351	1.90	0.53
22:z:56:ILE:O	22:z:59:SER:OG	2.26	0.53
1:1:175:GLU:OE2	1:1:185:THR:OG1	2.25	0.53
2:A:195:HIS:CD2	2:A:197:PHE:HB2	2.44	0.53
16:S:194:PRO:HG2	16:S:196:ILE:HB	1.90	0.53
4:c:14:ARG:O	4:c:29:ARG:NH1	2.41	0.53
23:r:141:GLY:O	23:r:145:MET:HG3	2.08	0.53
9:H:19:GLU:OE2	12:L:3:ARG:NH2	2.41	0.53
21:Y:167:ARG:NH2	36:Y:310:CHL:O1D	2.41	0.53
23:r:59:ARG:NH2	23:r:63:LEU:O	2.42	0.53
2:A:337:HIS:NE2	2:A:342:ASP:OD1	2.37	0.53
16:S:196:ILE:HD11	16:S:215:PRO:HA	1.91	0.53
4:c:129:GLU:OE1	4:c:129:GLU:N	2.41	0.53
8:G:86:ALA:HB1	8:G:201:GLY:HA3	1.91	0.53
27:B:517:BCR:H373	17:t:11:VAL:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:452:GLU:OE2	5:D:248:THR:OG1	2.27	0.52
9:H:75:ASP:OD1	9:H:76:ASP:N	2.43	0.52
15:O:133:ASP:OD1	15:O:134:ALA:N	2.42	0.52
4:C:104:VAL:HG21	27:C:514:BCR:HC42	1.90	0.52
3:b:70:GLY:HA2	3:b:178:VAL:HG11	1.91	0.52
18:v:20:PRO:HA	18:v:23:VAL:HG12	1.91	0.52
29:d:409:LMG:O6	7:f:40:GLN:NE2	2.43	0.52
1:1:288:ARG:NH2	1:1:310:ASP:OD2	2.41	0.52
8:G:113:VAL:HG23	8:G:116:LYS:HB2	1.92	0.52
16:S:154:VAL:HG12	16:S:155:PRO:HD2	1.92	0.52
39:Y:302:XAT:H10	30:Y:319:LHG:H211	1.90	0.52
4:c:66:GLU:N	4:c:66:GLU:OE1	2.39	0.52
18:v:15:VAL:CG2	27:v:101:BCR:HC8	2.40	0.52
30:a:410:LHG:O3	30:a:410:LHG:O1	2.28	0.52
3:b:157:HIS:HE1	25:b:506:CLA:NA	2.07	0.52
4:C:274:ALA:HB2	25:C:502:CLA:HMD1	1.92	0.51
32:C:522:LMU:H101	31:Y:301:DGD:HAH2	1.93	0.51
21:Y:91:LEU:HD23	21:Y:180:LEU:HD22	1.93	0.51
25:c:508:CLA:H2	25:c:510:CLA:H12	1.92	0.51
15:O:125:MET:HE2	15:O:163:GLN:HB3	1.92	0.51
3:b:73:GLN:HG2	3:b:79:THR:HG22	1.92	0.51
14:N:105:ILE:HD11	14:N:219:PHE:HZ	1.76	0.51
16:S:283:GLU:OE1	16:S:283:GLU:N	2.41	0.51
30:B:520:LHG:H111	30:L:101:LHG:HC92	1.91	0.51
5:D:312:GLU:HG2	15:O:205:PRO:HG3	1.93	0.51
36:N:308:CHL:HHC	36:N:308:CHL:HBB1	1.93	0.51
4:C:365:LEU:O	4:C:369:LYS:HG2	2.11	0.51
8:G:83:LEU:HD23	8:G:172:LEU:HD22	1.93	0.51
2:A:259:ILE:HG23	2:A:261:GLN:HG2	1.92	0.51
22:z:48:LEU:O	22:z:51:VAL:HG22	2.10	0.51
16:S:264:TRP:HB2	37:S:615:LUT:H22	1.93	0.50
2:a:162:PRO:HB3	2:a:168:PHE:HA	1.93	0.50
3:b:9:HIS:HB2	25:b:511:CLA:HBA1	1.93	0.50
2:A:185:VAL:CG1	2:A:332:HIS:HE1	2.19	0.50
25:b:510:CLA:HBB1	27:h:101:BCR:HC22	1.93	0.50
4:c:151:TYR:CD2	25:c:512:CLA:HAB	2.47	0.50
16:S:67:ASP:OD1	16:S:68:ARG:N	2.43	0.50
2:a:192:ILE:HD12	2:a:293:MET:HE1	1.93	0.50
30:D:408:LHG:HC62	12:L:16:THR:HG23	1.92	0.50
39:Y:302:XAT:H171	30:Y:319:LHG:H221	1.93	0.50
31:c:517:DGD:O3D	29:d:409:LMG:O3	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:250:ARG:NH1	10:i:26:ASN:O	2.45	0.50
21:Y:81:GLU:O	21:Y:85:ARG:HG2	2.12	0.50
4:c:136:GLY:O	4:c:144:LYS:NZ	2.45	0.50
4:C:29:ARG:NH1	25:C:511:CLA:OBD	2.44	0.49
5:d:161:PRO:HB3	5:d:170:ALA:HB2	1.93	0.49
15:O:268:SER:N	15:O:278:LYS:O	2.44	0.49
2:a:272:HIS:HE1	33:a:409:BCT:O2	1.96	0.49
25:N:305:CLA:H61	16:S:155:PRO:HG3	1.94	0.49
2:a:278:TRP:HB3	2:a:279:PRO:HD3	1.93	0.49
25:S:605:CLA:H2A	25:S:605:CLA:O2D	2.13	0.49
15:O:99:ILE:HD12	15:O:135:MET:HE1	1.94	0.49
25:c:511:CLA:H171	22:z:20:VAL:HG23	1.94	0.49
2:A:67:VAL:HG12	5:D:312:GLU:HB2	1.94	0.49
2:A:337:HIS:O	5:D:351:ALA:HB1	2.12	0.49
14:N:128:GLN:HG3	14:N:135:LEU:HD13	1.94	0.49
9:H:74:LEU:HB2	9:H:77:VAL:HG22	1.95	0.48
2:a:283:ILE:HA	2:a:286:THR:HG22	1.94	0.48
3:B:105:GLY:HA3	27:B:517:BCR:H271	1.95	0.48
4:C:331:ARG:NH1	4:C:335:GLY:O	2.46	0.48
5:D:296:TYR:OH	5:D:326:ARG:NH1	2.44	0.48
1:1:219:ILE:HG21	1:1:263:LEU:HD11	1.95	0.48
4:C:216:ASP:OD1	4:C:216:ASP:N	2.45	0.48
14:N:160:MET:HA	14:N:163:VAL:HG22	1.94	0.48
2:a:301:ASN:OD1	2:a:303:ASN:ND2	2.46	0.48
4:c:98:PRO:HA	4:c:101:VAL:HG22	1.95	0.48
4:c:163:LEU:HD22	25:c:501:CLA:C2D	2.43	0.48
25:c:501:CLA:HBA2	25:c:501:CLA:H3A	1.60	0.48
2:A:60:ILE:HD12	2:A:84:PRO:HD2	1.95	0.48
36:Y:303:CHL:HHC	36:Y:303:CHL:HBB1	1.95	0.48
25:b:511:CLA:H2A	25:b:511:CLA:O1D	2.13	0.48
36:G:605:CHL:HHC	36:G:605:CHL:HBB1	1.95	0.48
25:c:511:CLA:H93	27:k:101:BCR:H272	1.95	0.48
25:S:602:CLA:H3A	25:S:602:CLA:HBA2	1.50	0.48
4:C:224:GLY:C	27:C:515:BCR:H383	2.39	0.48
8:G:41:LEU:HB2	8:G:45:SER:HB2	1.96	0.48
25:b:502:CLA:H43	9:h:65:LEU:HA	1.95	0.48
2:A:32:TRP:O	2:A:35:VAL:HG12	2.14	0.48
3:B:385:LYS:NZ	15:O:204:ASP:OD1	2.38	0.48
2:a:84:PRO:HA	2:a:112:TYR:CG	2.48	0.48
25:b:501:CLA:HMD1	27:h:101:BCR:H272	1.95	0.48
7:F:18:ARG:NH2	35:F:101:HEM:O2A	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:r:249:PHE:CZ	39:r:309:XAT:H10	2.49	0.48
11:K:29:PRO:O	11:K:32:PHE:HB2	2.14	0.47
16:S:105:LEU:HD23	16:S:210:LEU:HB3	1.96	0.47
3:b:99:ALA:HB1	25:b:506:CLA:H51	1.96	0.47
30:d:407:LHG:H111	30:l:101:LHG:H102	1.95	0.47
5:D:129:GLN:NE2	26:D:402:PHO:OBD	2.47	0.47
7:F:23:HIS:NE2	35:F:101:HEM:C4B	2.81	0.47
1:l:237:PHE:O	1:l:244:ARG:NH1	2.47	0.47
2:A:278:TRP:HB3	2:A:279:PRO:HD3	1.97	0.47
3:B:236:THR:HB	3:B:473:THR:HG21	1.94	0.47
6:E:55:TYR:O	6:E:60:ARG:NH2	2.45	0.47
4:c:224:GLY:C	27:c:514:BCR:H383	2.39	0.47
25:c:506:CLA:H122	25:c:506:CLA:H162	1.50	0.47
2:A:257:ARG:O	5:D:128:ARG:NH2	2.48	0.47
25:S:605:CLA:HBD	25:S:605:CLA:HBA1	1.96	0.47
3:b:474:ILE:HD11	30:b:521:LHG:HC5	1.96	0.47
23:r:199:GLU:OE2	25:r:307:CLA:C4A	2.61	0.47
1:l:252:THR:O	1:l:256:ILE:HG12	2.14	0.47
5:D:29:PHE:O	5:D:128:ARG:NH1	2.47	0.47
21:Y:88:GLU:HA	21:Y:180:LEU:HD21	1.96	0.47
25:d:401:CLA:H3A	25:d:401:CLA:HBA2	1.54	0.47
11:k:37:PHE:HB3	27:v:101:BCR:H272	1.96	0.47
3:B:242:ILE:HA	3:B:245:VAL:HG22	1.97	0.47
5:D:126:MET:HE1	5:D:147:SER:HA	1.97	0.47
7:f:39:MET:O	7:f:42:ILE:HG22	2.14	0.47
2:A:106:LEU:HD11	27:A:406:BCR:H402	1.95	0.47
3:B:243:ALA:HA	3:B:246:PHE:CD2	2.50	0.47
25:C:513:CLA:H62	25:C:513:CLA:H41	1.69	0.47
5:D:65:THR:O	5:D:65:THR:OG1	2.33	0.47
6:E:57:THR:OG1	6:E:58:GLU:OE1	2.33	0.47
8:G:129:TYR:HB2	8:G:136:ILE:HD12	1.97	0.47
25:G:611:CLA:H3A	25:G:611:CLA:HBA2	1.46	0.47
16:S:154:VAL:CG1	16:S:155:PRO:HD2	2.44	0.47
36:Y:303:CHL:HBA1	36:Y:303:CHL:H3A	1.75	0.47
27:b:518:BCR:H351	27:b:518:BCR:H15C	1.73	0.47
3:B:103:LEU:HB2	25:B:506:CLA:H62	1.97	0.47
3:B:315:ILE:HG21	3:B:426:LEU:HD22	1.97	0.47
11:K:30:VAL:O	11:K:33:ILE:HG22	2.15	0.47
5:d:141:TYR:OH	30:d:407:LHG:O4	2.28	0.47
27:A:406:BCR:H15C	27:A:406:BCR:H351	1.78	0.47
4:C:129:GLU:OE1	4:C:137:TYR:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:G:617:NEX:H15	38:G:617:NEX:H201	1.73	0.47
18:V:15:VAL:CG1	27:V:101:BCR:H10C	2.44	0.47
7:f:23:HIS:HE1	35:f:101:HEM:C4D	2.32	0.47
18:v:13:VAL:HA	18:v:16:VAL:HG12	1.97	0.47
19:W:68:ASP:OD1	19:W:69:GLY:N	2.48	0.47
27:z:101:BCR:H15C	27:z:101:BCR:H351	1.78	0.47
27:v:101:BCR:H23C	27:v:101:BCR:H19C	1.96	0.46
35:F:101:HEM:HBC2	35:F:101:HEM:CHD	2.45	0.46
30:d:407:LHG:H111	30:l:101:LHG:HC81	1.96	0.46
4:C:225:HIS:HA	4:C:228:ILE:HG22	1.97	0.46
27:C:515:BCR:H382	27:C:515:BCR:H23C	1.97	0.46
5:d:126:MET:HE1	5:d:147:SER:HA	1.98	0.46
25:B:515:CLA:H61	25:B:515:CLA:H92	1.76	0.46
11:K:29:PRO:HA	11:K:32:PHE:HD2	1.80	0.46
27:a:406:BCR:H15C	27:a:406:BCR:H351	1.79	0.46
4:c:92:GLU:N	4:c:92:GLU:OE1	2.48	0.46
3:B:90:ILE:HD11	25:B:506:CLA:H202	1.97	0.46
3:b:41:GLU:OE1	3:b:63:LEU:N	2.45	0.46
3:b:334:ASP:OD1	3:b:334:ASP:N	2.46	0.46
27:h:101:BCR:H11C	27:h:101:BCR:H341	1.74	0.46
1:1:263:LEU:O	1:1:265:GLN:NE2	2.45	0.46
3:B:243:ALA:HA	3:B:246:PHE:CE2	2.51	0.46
25:N:312:CLA:HBD	25:N:313:CLA:OBD	2.16	0.46
27:C:515:BCR:H15C	27:C:515:BCR:H351	1.74	0.46
8:G:132:ASN:HB3	8:G:135:LEU:HD13	1.98	0.46
39:G:620:XAT:H202	21:Y:153:LEU:HD21	1.98	0.46
27:H:101:BCR:H341	27:H:101:BCR:H11C	1.77	0.46
36:S:601:CHL:HBB1	36:S:601:CHL:HHC	1.98	0.46
25:S:610:CLA:HAB	37:S:615:LUT:H32	1.98	0.46
27:z:101:BCR:HC8	27:z:101:BCR:H321	1.98	0.46
12:l:25:ILE:HD13	13:m:18:PRO:HB2	1.97	0.46
1:1:202:LYS:O	1:1:205:GLU:HG3	2.16	0.46
1:1:307:ASP:OD1	1:1:308:LYS:N	2.49	0.46
15:O:94:LEU:HD11	15:O:288:ALA:HB1	1.97	0.46
16:S:110:TRP:CD1	25:S:609:CLA:HMD3	2.51	0.46
27:C:514:BCR:H11C	27:C:514:BCR:H341	1.82	0.46
4:c:211:TRP:CE3	4:c:212:ILE:HG12	2.51	0.46
4:C:16:GLN:OE1	5:D:230:ASN:ND2	2.41	0.45
4:C:166:LYS:HD3	25:C:502:CLA:H192	1.98	0.45
2:a:15:ALA:O	2:a:19:GLU:HG2	2.16	0.45
3:b:451:PHE:HE2	25:b:504:CLA:HMA3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:405:BCR:H15C	27:d:405:BCR:H351	1.86	0.45
5:D:103:ARG:NH2	6:E:77:LYS:HG3	2.31	0.45
8:G:205:MET:HE2	25:G:602:CLA:HMC3	1.97	0.45
36:G:606:CHL:OMC	37:G:616:LUT:H163	2.16	0.45
21:Y:171:GLY:H	36:Y:309:CHL:HMC	1.80	0.45
4:c:457:MET:HE2	5:d:251:ARG:NH2	2.31	0.45
5:d:103:ARG:HG2	6:e:73:LEU:HD12	1.98	0.45
17:t:12:GLY:O	17:t:16:ILE:HG12	2.16	0.45
4:C:66:GLU:OE1	4:C:66:GLU:N	2.44	0.45
3:b:192:PRO:HG3	9:h:68:TYR:CD1	2.52	0.45
4:c:50:PHE:HB2	4:c:110:SER:OG	2.15	0.45
4:C:166:LYS:NZ	4:C:172:GLY:O	2.49	0.45
18:V:33:LEU:HD23	18:V:33:LEU:H	1.82	0.45
9:H:56:LEU:HB3	27:H:101:BCR:H14C	1.99	0.45
16:S:87:PRO:O	37:S:616:LUT:O23	2.28	0.45
16:S:155:PRO:O	16:S:156:TRP:CG	2.70	0.45
2:A:283:ILE:HA	2:A:286:THR:HG22	1.98	0.45
37:G:616:LUT:H15	37:G:616:LUT:H201	1.82	0.45
38:N:318:NEX:H35	38:N:318:NEX:H401	1.79	0.45
3:b:298:LEU:HD23	3:b:298:LEU:HA	1.86	0.45
23:r:230:ARG:HD2	23:r:233:ARG:HE	1.82	0.45
16:S:110:TRP:HD1	25:S:609:CLA:HMD3	1.82	0.45
5:d:56:THR:OG1	5:d:69:GLU:OE2	2.30	0.45
5:d:70:GLY:O	7:f:44:ARG:NH1	2.49	0.45
27:D:406:BCR:H20C	27:D:406:BCR:H361	1.81	0.45
36:N:302:CHL:H141	36:N:302:CHL:H161	1.72	0.45
16:S:108:ALA:HB1	16:S:239:GLY:HA3	1.98	0.45
39:Y:302:XAT:H31	39:Y:302:XAT:H391	1.80	0.45
25:B:513:CLA:H2	25:B:513:CLA:HED3	2.00	0.44
27:H:101:BCR:H20C	27:H:101:BCR:H361	1.86	0.44
15:O:116:GLU:N	15:O:116:GLU:OE1	2.50	0.44
21:Y:95:ARG:HA	21:Y:98:MET:HE3	1.99	0.44
3:b:271:THR:HB	3:b:274:GLN:HG3	2.00	0.44
25:b:503:CLA:H3A	25:b:503:CLA:HBA2	1.52	0.44
25:b:507:CLA:HBA2	25:b:507:CLA:H3A	1.62	0.44
6:e:55:TYR:O	6:e:60:ARG:NH2	2.50	0.44
27:t:101:BCR:H11C	27:t:101:BCR:H341	1.79	0.44
4:c:146:THR:HG21	4:c:244:PRO:HD3	1.99	0.44
4:c:203:LYS:HG2	4:c:209:ASP:HB3	1.99	0.44
39:N:301:XAT:H35	39:N:301:XAT:H401	1.82	0.44
37:Y:317:LUT:H15	37:Y:317:LUT:H201	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:53:ASN:OD1	3:b:58:GLN:NE2	2.50	0.44
3:b:380:ASP:OD1	3:b:380:ASP:N	2.50	0.44
1:l:186:LYS:HE2	17:t:27:PRO:HG2	1.99	0.44
27:B:517:BCR:H11C	27:B:517:BCR:H341	1.88	0.44
36:N:310:CHL:H91	36:N:310:CHL:H112	1.79	0.44
30:N:319:LHG:O3	30:N:319:LHG:O1	2.35	0.44
15:O:180:ASP:N	15:O:180:ASP:OD1	2.49	0.44
27:t:101:BCR:H15C	27:t:101:BCR:H351	1.74	0.44
38:S:617:NEX:H35	38:S:617:NEX:H401	1.74	0.44
9:h:59:ALA:O	9:h:63:ILE:HG12	2.18	0.44
2:A:186:PHE:HE1	2:A:293:MET:SD	2.41	0.44
25:B:504:CLA:H92	25:B:504:CLA:H61	1.77	0.44
25:B:508:CLA:HMB2	5:D:126:MET:SD	2.58	0.44
2:A:84:PRO:HA	2:A:112:TYR:CG	2.52	0.44
38:G:617:NEX:H35	38:G:617:NEX:H401	1.83	0.44
7:f:42:ILE:HG13	7:f:43:GLN:H	1.83	0.44
2:A:325:ASN:HA	2:A:328:MET:HE3	1.99	0.44
27:B:518:BCR:H331	27:B:518:BCR:HC8	2.00	0.44
4:C:390:GLY:HA2	4:C:396:GLY:HA2	1.98	0.44
27:C:515:BCR:H11C	27:C:515:BCR:H341	1.84	0.44
38:G:617:NEX:H11	38:G:617:NEX:H191	1.75	0.44
15:O:109:GLU:HG3	15:O:117:THR:HG22	1.99	0.44
37:Y:317:LUT:H11	37:Y:317:LUT:H191	1.88	0.44
34:d:406:PL9:H322	30:l:101:LHG:H211	2.00	0.44
23:r:155:GLU:OE2	23:r:162:TRP:N	2.51	0.44
27:v:101:BCR:H24C	27:v:101:BCR:H371	1.56	0.44
14:N:124:LYS:HA	36:N:308:CHL:HED2	2.00	0.44
25:N:303:CLA:H141	25:N:303:CLA:H162	1.79	0.44
38:Y:318:NEX:H15	38:Y:318:NEX:H201	1.75	0.44
3:b:21:SER:OG	3:b:115:TRP:HB2	2.17	0.44
8:G:120:GLN:HB2	8:G:127:LEU:HD12	1.99	0.43
37:G:615:LUT:H11	37:G:615:LUT:H191	1.84	0.43
14:N:81:GLU:O	14:N:85:ARG:HG2	2.18	0.43
14:N:210:ARG:HA	14:N:213:MET:HE3	2.00	0.43
19:W:108:ASP:OD1	19:W:108:ASP:N	2.47	0.43
25:a:402:CLA:HBD	25:d:401:CLA:HAC2	1.99	0.43
3:b:460:LEU:HD23	3:b:460:LEU:HA	1.90	0.43
31:c:515:DGD:HO5E	31:c:515:DGD:HO4E	1.63	0.43
23:r:214:PRO:HB3	36:r:306:CHL:HBC2	2.00	0.43
25:B:509:CLA:H92	25:B:509:CLA:H62	1.70	0.43
4:C:104:VAL:HG23	27:C:516:BCR:H332	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:68:ASP:OD1	6:E:68:ASP:N	2.46	0.43
39:Y:302:XAT:H11	39:Y:302:XAT:H191	1.88	0.43
4:c:58:PHE:HE1	25:c:504:CLA:HED3	1.84	0.43
25:B:501:CLA:HBB2	27:H:101:BCR:H351	1.99	0.43
4:C:203:LYS:NZ	4:C:214:SER:OG	2.40	0.43
25:C:504:CLA:H141	25:C:504:CLA:H161	1.77	0.43
25:C:509:CLA:H141	25:C:509:CLA:H161	1.77	0.43
8:G:37:ARG:NH2	8:G:53:LEU:O	2.51	0.43
29:H:102:LMG:H111	29:H:102:LMG:H142	1.69	0.43
16:S:183:ARG:HG3	36:S:608:CHL:CHD	2.48	0.43
19:W:106:PHE:HD2	19:W:111:ASP:HB3	1.83	0.43
2:a:18:CYS:O	2:a:22:THR:HG22	2.18	0.43
2:a:174:LEU:HD22	26:a:404:PHO:H143	2.00	0.43
27:b:519:BCR:H15C	27:b:519:BCR:H351	1.76	0.43
29:B:519:LMG:H421	29:B:519:LMG:H392	1.84	0.43
2:A:188:ALA:HB2	2:A:328:MET:HB3	2.01	0.43
5:D:200:GLY:HA3	5:D:282:SER:OG	2.18	0.43
11:K:38:VAL:HG21	27:V:101:BCR:H19C	2.01	0.43
19:W:65:MET:HE2	19:W:77:ASN:HD21	1.84	0.43
38:Y:318:NEX:H35	38:Y:318:NEX:H401	1.79	0.43
2:a:45:THR:HB	26:a:404:PHO:H93	2.00	0.43
27:b:517:BCR:H15C	27:b:517:BCR:H351	1.72	0.43
1:l:189:GLN:HG2	4:c:457:MET:O	2.18	0.43
2:a:93:PHE:CE2	2:a:95:PRO:HG3	2.54	0.43
18:v:7:LEU:HA	18:v:10:VAL:HG22	2.00	0.43
18:v:31:GLY:HA2	22:z:30:PRO:HD3	2.01	0.43
3:B:2:GLY:N	12:L:12:GLU:OE2	2.51	0.43
4:C:238:TRP:HE3	32:C:522:LMU:H61	1.83	0.43
25:C:502:CLA:H92	25:C:512:CLA:H42	2.00	0.43
27:C:514:BCR:H20C	27:C:514:BCR:H361	1.89	0.43
8:G:46:GLU:N	8:G:46:GLU:OE1	2.52	0.43
22:Z:48:LEU:HD23	22:Z:48:LEU:HA	1.87	0.43
3:b:193:TYR:O	9:h:84:LEU:HD23	2.19	0.43
5:d:201:VAL:HG22	25:d:403:CLA:C1B	2.49	0.43
29:d:410:LMG:H111	29:d:410:LMG:H141	1.80	0.43
2:A:159:LEU:HD23	31:C:517:DGD:HBT1	2.01	0.43
29:B:519:LMG:H392	29:B:519:LMG:H361	1.75	0.43
4:C:163:LEU:HD22	25:C:501:CLA:C2D	2.48	0.43
4:C:440:ALA:HB1	19:W:113:LEU:HG	2.01	0.43
36:N:306:CHL:HED3	16:S:124:LEU:HD21	2.01	0.43
29:W:201:LMG:O5	29:W:201:LMG:O4	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:25:MET:HE1	3:b:108:PHE:CD1	2.54	0.43
3:b:260:SER:OG	3:b:261:ALA:N	2.52	0.43
3:B:157:HIS:HE1	25:B:506:CLA:NA	2.17	0.43
4:C:338:ILE:HG21	4:C:347:TRP:HB2	2.01	0.43
8:G:97:ILE:HD11	8:G:211:PHE:CZ	2.54	0.43
37:N:317:LUT:H11	37:N:317:LUT:H191	1.88	0.43
38:Y:318:NEX:H11	38:Y:318:NEX:H191	1.82	0.43
7:f:23:HIS:HE1	35:f:101:HEM:ND	2.16	0.43
32:C:522:LMU:H61	32:C:522:LMU:H92	1.73	0.42
3:b:103:LEU:HD22	25:b:506:CLA:H41	2.00	0.42
25:c:506:CLA:H71	25:c:506:CLA:H111	1.80	0.42
11:k:18:PHE:CE2	22:z:9:LEU:HD23	2.54	0.42
1:l:195:GLN:O	1:l:198:GLU:HG3	2.19	0.42
2:A:195:HIS:ND1	2:A:196:PRO:HD2	2.34	0.42
3:B:297:SER:OG	3:B:300:ASP:OD2	2.32	0.42
7:F:16:THR:HG23	7:F:19:TRP:H	1.84	0.42
8:G:97:ILE:HD11	8:G:211:PHE:HZ	1.84	0.42
36:G:607:CHL:HHC	36:G:607:CHL:HBB1	2.01	0.42
14:N:60:TYR:OH	14:N:72:ASP:OD2	2.30	0.42
37:N:317:LUT:H15	37:N:317:LUT:H201	1.83	0.42
37:S:616:LUT:H15	37:S:616:LUT:H201	1.84	0.42
25:b:502:CLA:H143	25:b:502:CLA:H162	1.79	0.42
4:c:45:ALA:O	4:c:49:VAL:HG22	2.19	0.42
4:C:458:ARG:HG3	4:C:459:PRO:HD2	2.01	0.42
27:C:516:BCR:H24C	27:C:516:BCR:H371	1.70	0.42
15:O:144:ASP:OD1	15:O:145:GLY:N	2.53	0.42
2:a:106:LEU:HD21	27:a:406:BCR:H402	2.01	0.42
2:A:63:ILE:HG13	2:A:65:GLU:HG2	1.99	0.42
3:b:477:ASP:OD1	3:b:477:ASP:N	2.51	0.42
5:d:88:SER:OG	6:e:69:ARG:NH2	2.53	0.42
2:A:57:PRO:HB2	2:A:66:PRO:HB2	2.02	0.42
25:B:502:CLA:H43	9:H:64:ILE:HG22	2.01	0.42
27:B:517:BCR:H24C	27:B:517:BCR:H371	1.78	0.42
4:C:448:ASP:OD2	4:C:451:ASP:N	2.53	0.42
27:c:514:BCR:H341	27:c:514:BCR:H11C	1.80	0.42
27:h:101:BCR:H15C	27:h:101:BCR:H351	1.80	0.42
23:r:232:PHE:O	23:r:236:THR:HG23	2.19	0.42
3:B:21:SER:OG	3:B:115:TRP:HB2	2.19	0.42
4:C:201:LEU:O	4:C:211:TRP:NE1	2.46	0.42
36:N:302:CHL:HBA1	36:N:302:CHL:H3A	1.87	0.42
25:a:405:CLA:H42	10:i:9:TYR:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:r:233:ARG:O	23:r:236:THR:OG1	2.29	0.42
27:v:101:BCR:H20C	27:v:101:BCR:H361	1.44	0.42
25:D:405:CLA:O1D	25:D:405:CLA:H2A	2.19	0.42
10:i:2:LEU:O	10:i:6:ILE:HG12	2.20	0.42
23:r:249:PHE:CE1	39:r:309:XAT:H12	2.54	0.42
25:B:501:CLA:H142	25:B:501:CLA:H112	1.90	0.42
16:S:243:MET:HE3	25:S:602:CLA:HMC3	2.02	0.42
3:b:119:ASP:OD1	3:b:124:ARG:NH2	2.53	0.42
25:B:502:CLA:H122	25:B:502:CLA:H162	1.89	0.42
25:B:512:CLA:HBA1	25:B:512:CLA:H3A	1.91	0.42
21:Y:206:ILE:HD12	21:Y:206:ILE:HA	1.95	0.42
37:Y:317:LUT:H35	37:Y:317:LUT:H401	1.81	0.42
25:c:509:CLA:H93	25:c:509:CLA:H111	1.78	0.42
27:k:101:BCR:H11C	27:k:101:BCR:H341	1.91	0.42
27:t:101:BCR:H24C	27:t:101:BCR:H371	1.89	0.42
5:D:49:LEU:HD13	27:D:406:BCR:C15	2.50	0.42
7:F:36:ILE:HA	7:F:39:MET:HE3	2.02	0.42
23:r:143:TRP:CE2	36:r:306:CHL:HED2	2.55	0.42
25:B:503:CLA:H41	25:B:503:CLA:H61	1.88	0.41
27:C:515:BCR:H20C	27:C:515:BCR:H361	1.94	0.41
14:N:49:LEU:HB2	14:N:53:SER:HB3	2.02	0.41
15:O:79:SER:OG	15:O:80:GLY:N	2.53	0.41
16:S:119:LEU:HD23	16:S:119:LEU:HA	1.90	0.41
2:a:57:PRO:HB2	2:a:66:PRO:HB2	2.02	0.41
39:r:309:XAT:H401	39:r:309:XAT:H35	1.77	0.41
2:A:183:MET:HB3	25:A:402:CLA:HBC2	2.02	0.41
3:B:315:ILE:HG22	3:B:426:LEU:HB3	2.02	0.41
8:G:33:TYR:HE2	8:G:191:ALA:HB1	1.83	0.41
8:G:161:ASN:HD22	14:N:52:TYR:HA	1.85	0.41
3:b:313:ASP:OD1	3:b:358:ARG:NH1	2.53	0.41
27:b:519:BCR:H11C	27:b:519:BCR:H341	1.80	0.41
38:r:310:NEX:H11	38:r:310:NEX:H191	1.80	0.41
3:B:255:THR:HG21	25:B:502:CLA:HED1	2.03	0.41
4:C:56:ASN:C	4:C:56:ASN:HD22	2.28	0.41
39:G:620:XAT:H11	39:G:620:XAT:H191	1.87	0.41
15:O:72:ASN:ND2	15:O:128:LEU:HB3	2.36	0.41
37:Y:316:LUT:H35	37:Y:316:LUT:H401	1.77	0.41
2:A:261:GLN:OE1	2:A:261:GLN:HA	2.20	0.41
25:C:504:CLA:H93	25:C:504:CLA:H111	1.87	0.41
15:O:163:GLN:HA	15:O:169:ARG:HA	2.03	0.41
36:Y:310:CHL:H143	36:Y:310:CHL:H161	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:319:PRO:HB3	3:b:446:SER:HB3	2.02	0.41
27:h:101:BCR:H24C	27:h:101:BCR:H371	1.85	0.41
38:r:310:NEX:H15	38:r:310:NEX:H201	1.74	0.41
27:B:518:BCR:H11C	27:B:518:BCR:H341	1.87	0.41
5:D:14:TRP:NE1	20:X:91:THR:OG1	2.51	0.41
5:D:103:ARG:O	5:D:107:LEU:HB2	2.20	0.41
5:D:197:HIS:O	5:D:201:VAL:HG12	2.21	0.41
6:E:75:GLN:HA	6:E:78:LYS:HG2	2.01	0.41
8:G:83:LEU:HD12	8:G:83:LEU:HA	1.90	0.41
39:Y:302:XAT:H35	39:Y:302:XAT:H401	1.81	0.41
3:b:474:ILE:HG23	3:b:475:PHE:CD1	2.55	0.41
25:b:510:CLA:H2	25:b:510:CLA:H61	1.71	0.41
27:k:101:BCR:H371	27:k:101:BCR:H24C	1.66	0.41
14:N:91:LEU:HD12	14:N:91:LEU:HA	1.90	0.41
14:N:140:ASN:HB3	14:N:143:LEU:HD13	2.03	0.41
39:N:301:XAT:H31	39:N:301:XAT:H391	1.87	0.41
19:W:65:MET:HE2	19:W:65:MET:HB3	2.00	0.41
4:c:37:LEU:HD12	4:c:37:LEU:HA	1.86	0.41
25:c:506:CLA:H171	25:c:506:CLA:H51	2.03	0.41
27:d:405:BCR:H20C	27:d:405:BCR:H361	1.88	0.41
11:k:28:ILE:H	11:k:28:ILE:HD12	1.86	0.41
11:k:35:LEU:HA	11:k:38:VAL:HG12	2.02	0.41
22:z:15:VAL:HG11	22:z:50:LEU:HD12	2.02	0.41
27:z:101:BCR:H20C	27:z:101:BCR:H361	1.84	0.41
25:B:516:CLA:OBD	9:H:24:THR:HG21	2.21	0.41
8:G:80:GLU:O	8:G:84:ILE:HG12	2.21	0.41
36:N:306:CHL:H102	16:S:120:ILE:HD11	2.03	0.41
36:S:601:CHL:O1D	30:S:618:LHG:H121	2.21	0.41
19:W:73:PRO:O	19:W:76:VAL:HG22	2.21	0.41
3:b:193:TYR:HB2	9:h:83:THR:OG1	2.21	0.41
3:b:300:ASP:N	3:b:300:ASP:OD1	2.51	0.41
4:c:288:GLU:OE1	4:c:288:GLU:N	2.52	0.41
22:z:19:LEU:HD11	22:z:44:LEU:HD12	2.03	0.41
27:A:406:BCR:HC31	10:I:15:PHE:HE1	1.85	0.41
6:E:62:GLU:OE1	6:E:62:GLU:HA	2.20	0.41
37:S:615:LUT:H11	37:S:615:LUT:H191	1.89	0.41
22:z:35:ASP:OD1	22:z:36:ASN:N	2.53	0.41
1:1:223:LEU:HD21	1:1:260:TYR:CZ	2.56	0.41
2:A:175:GLY:O	2:A:179:THR:HG23	2.20	0.41
25:B:506:CLA:H112	25:B:506:CLA:H152	1.87	0.41
4:C:104:VAL:HG11	27:C:514:BCR:HC32	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:285:TYR:O	4:C:411:ARG:NH2	2.53	0.41
25:D:405:CLA:H42	9:H:62:LEU:HD11	2.03	0.41
27:H:101:BCR:H351	27:H:101:BCR:H15C	1.76	0.41
25:N:305:CLA:H92	25:N:305:CLA:H62	1.96	0.41
37:S:615:LUT:H15	37:S:615:LUT:H201	1.86	0.41
37:S:616:LUT:H401	37:S:616:LUT:H35	1.77	0.41
3:b:69:LEU:HD12	25:b:505:CLA:HBA1	2.03	0.41
4:c:37:LEU:HG	4:c:41:HIS:CE1	2.55	0.41
4:c:267:ILE:HG12	25:c:502:CLA:HAC1	2.02	0.41
11:k:19:ALA:N	11:k:20:PRO:HD2	2.36	0.41
27:D:406:BCR:H15C	27:D:406:BCR:H351	1.85	0.41
36:G:601:CHL:H62	36:G:601:CHL:H41	1.96	0.41
39:Y:302:XAT:H373	39:Y:302:XAT:H23	1.92	0.41
11:k:28:ILE:N	11:k:29:PRO:HD2	2.36	0.41
2:A:105:TRP:NE1	2:A:110:GLY:HA3	2.35	0.40
26:A:404:PHO:HAB	5:D:205:LEU:HD13	2.03	0.40
25:B:514:CLA:H112	25:B:514:CLA:H91	1.90	0.40
9:H:79:MET:HE2	9:H:79:MET:HA	2.02	0.40
37:N:316:LUT:H401	37:N:316:LUT:H35	1.79	0.40
21:Y:132:GLU:OE1	21:Y:132:GLU:N	2.50	0.40
5:d:90:LEU:HD12	5:d:90:LEU:HA	1.89	0.40
30:l:101:LHG:H141	30:l:101:LHG:H111	1.93	0.40
23:r:145:MET:HE3	25:r:308:CLA:HMC2	2.02	0.40
3:B:34:ALA:HB2	25:B:505:CLA:HMD2	2.04	0.40
2:a:35:VAL:HG11	10:i:18:LEU:HD23	2.02	0.40
4:c:364:ASP:HB3	4:c:367:LYS:HB2	2.03	0.40
22:z:50:LEU:HD23	22:z:50:LEU:HA	1.77	0.40
1:1:307:ASP:OD1	1:1:307:ASP:C	2.65	0.40
26:A:404:PHO:H61	26:A:404:PHO:H2	1.77	0.40
3:B:65:PHE:HE1	25:B:504:CLA:HED2	1.86	0.40
3:B:273:TYR:HA	3:B:276:ASP:HB2	2.03	0.40
3:B:334:ASP:OD1	3:B:334:ASP:C	2.65	0.40
25:B:516:CLA:H11	25:B:516:CLA:H52	1.75	0.40
8:G:135:LEU:O	8:G:137:HIS:N	2.51	0.40
25:b:506:CLA:HBA2	25:b:506:CLA:H3A	1.36	0.40
2:A:70:SER:O	2:A:75:ASN:HB2	2.21	0.40
3:B:22:VAL:HG13	25:B:514:CLA:HMB3	2.03	0.40
39:N:301:XAT:H201	39:N:301:XAT:H15	1.78	0.40
15:O:86:GLU:OE1	15:O:86:GLU:N	2.54	0.40
37:Y:316:LUT:H11	37:Y:316:LUT:H191	1.88	0.40
3:b:160:GLY:HA3	3:b:180:PRO:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:406:BCR:H20C	27:A:406:BCR:H361	1.90	0.40
3:B:434:ARG:HB2	3:B:439:SER:HB2	2.04	0.40
15:O:99:ILE:HG23	15:O:262:PHE:CE1	2.56	0.40
3:b:315:ILE:HG22	3:b:426:LEU:HB3	2.04	0.40
4:c:69:MET:HE3	4:c:69:MET:HB2	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
2	A	311/335 (93%)	304 (98%)	7 (2%)	0	100	100
2	a	300/335 (90%)	295 (98%)	5 (2%)	0	100	100
3	B	478/481 (99%)	472 (99%)	6 (1%)	0	100	100
3	b	479/481 (100%)	468 (98%)	11 (2%)	0	100	100
4	C	447/449 (100%)	440 (98%)	7 (2%)	0	100	100
4	c	434/449 (97%)	418 (96%)	16 (4%)	0	100	100
5	D	346/351 (99%)	341 (99%)	5 (1%)	0	100	100
5	d	333/351 (95%)	325 (98%)	8 (2%)	0	100	100
6	E	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
6	e	69/75 (92%)	67 (97%)	2 (3%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
7	f	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
8	G	217/219 (99%)	211 (97%)	6 (3%)	0	100	100
9	H	66/69 (96%)	66 (100%)	0	0	100	100
9	h	66/69 (96%)	63 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	I	33/35 (94%)	33 (100%)	0	0	100	100
10	i	32/35 (91%)	31 (97%)	1 (3%)	0	100	100
11	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k	35/37 (95%)	35 (100%)	0	0	100	100
12	L	34/37 (92%)	34 (100%)	0	0	100	100
12	l	35/37 (95%)	35 (100%)	0	0	100	100
13	M	28/31 (90%)	28 (100%)	0	0	100	100
13	m	28/31 (90%)	28 (100%)	0	0	100	100
14	N	217/219 (99%)	210 (97%)	6 (3%)	1 (0%)	24	54
15	O	203/240 (85%)	197 (97%)	6 (3%)	0	100	100
16	S	248/250 (99%)	235 (95%)	11 (4%)	2 (1%)	16	44
17	T	28/30 (93%)	28 (100%)	0	0	100	100
17	t	25/30 (83%)	25 (100%)	0	0	100	100
18	V	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
18	v	30/32 (94%)	30 (100%)	0	0	100	100
19	W	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
20	X	30/32 (94%)	30 (100%)	0	0	100	100
20	x	30/32 (94%)	30 (100%)	0	0	100	100
21	Y	218/220 (99%)	213 (98%)	5 (2%)	0	100	100
22	Z	59/61 (97%)	59 (100%)	0	0	100	100
22	z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
23	r	156/201 (78%)	148 (95%)	8 (5%)	0	100	100
All	All	5481/5736 (96%)	5351 (98%)	127 (2%)	3 (0%)	49	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	S	155	PRO
16	S	156	TRP
14	N	144	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	132/132 (100%)	132 (100%)	0	100	100
2	A	256/273 (94%)	256 (100%)	0	100	100
2	a	247/273 (90%)	247 (100%)	0	100	100
3	B	382/383 (100%)	382 (100%)	0	100	100
3	b	383/383 (100%)	383 (100%)	0	100	100
4	C	352/352 (100%)	352 (100%)	0	100	100
4	c	346/352 (98%)	346 (100%)	0	100	100
5	D	278/280 (99%)	278 (100%)	0	100	100
5	d	270/280 (96%)	270 (100%)	0	100	100
6	E	66/66 (100%)	66 (100%)	0	100	100
6	e	62/66 (94%)	62 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	f	25/25 (100%)	25 (100%)	0	100	100
8	G	164/164 (100%)	164 (100%)	0	100	100
9	H	58/59 (98%)	58 (100%)	0	100	100
9	h	58/59 (98%)	58 (100%)	0	100	100
10	I	32/32 (100%)	32 (100%)	0	100	100
10	i	31/32 (97%)	31 (100%)	0	100	100
11	K	31/31 (100%)	31 (100%)	0	100	100
11	k	31/31 (100%)	31 (100%)	0	100	100
12	L	34/34 (100%)	34 (100%)	0	100	100
12	l	34/34 (100%)	34 (100%)	0	100	100
13	M	26/27 (96%)	26 (100%)	0	100	100
13	m	26/27 (96%)	26 (100%)	0	100	100
14	N	169/169 (100%)	169 (100%)	0	100	100
15	O	171/195 (88%)	171 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	S	188/188 (100%)	188 (100%)	0	100	100
17	T	27/27 (100%)	27 (100%)	0	100	100
17	t	24/27 (89%)	24 (100%)	0	100	100
18	V	26/26 (100%)	26 (100%)	0	100	100
18	v	26/26 (100%)	26 (100%)	0	100	100
19	W	44/44 (100%)	44 (100%)	0	100	100
20	X	22/22 (100%)	22 (100%)	0	100	100
20	x	22/22 (100%)	22 (100%)	0	100	100
21	Y	169/169 (100%)	169 (100%)	0	100	100
22	Z	51/51 (100%)	51 (100%)	0	100	100
22	z	51/51 (100%)	51 (100%)	0	100	100
23	r	127/161 (79%)	127 (100%)	0	100	100
All	All	4466/4598 (97%)	4466 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	192	ASN
2	A	108	ASN
2	A	304	GLN
2	A	332	HIS
4	C	106	HIS
4	C	310	GLN
5	D	106	GLN
8	G	105	ASN
14	N	148	ASN
21	Y	147	GLN
2	a	322	ASN
2	a	332	HIS
3	b	179	GLN
4	c	370	ASN
5	d	164	GLN
7	f	43	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 223 ligands modelled in this entry, 2 are monoatomic - leaving 221 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	$\# Z > 2$
30	LHG	G	618	25	48,48,48	0.92	2 (4%)	51,54,54	1.06	3 (5%)
25	CLA	c	510	-	69,73,73	1.16	8 (11%)	82,113,113	1.15	4 (4%)
36	CHL	r	304	-	38,52,74	4.23	17 (44%)	31,87,114	3.27	14 (45%)
34	PL9	D	407	-	55,55,55	1.24	4 (7%)	68,69,69	1.51	12 (17%)
25	CLA	C	506	-	69,73,73	1.16	7 (10%)	82,113,113	1.16	6 (7%)
25	CLA	S	602	16	53,57,73	1.31	8 (15%)	61,93,113	1.21	6 (9%)
27	BCR	A	406	-	41,41,41	0.73	0	56,56,56	1.93	13 (23%)
27	BCR	a	406	-	41,41,41	0.77	1 (2%)	56,56,56	1.92	18 (32%)
25	CLA	B	508	-	69,73,73	1.16	6 (8%)	82,113,113	1.11	6 (7%)
25	CLA	S	605	16	54,58,73	1.30	6 (11%)	64,95,113	1.25	5 (7%)
25	CLA	b	508	-	69,73,73	1.17	6 (8%)	82,113,113	1.14	8 (9%)
27	BCR	B	517	-	41,41,41	0.72	0	56,56,56	2.64	21 (37%)
36	CHL	G	609	8	60,74,74	3.41	18 (30%)	58,114,114	2.45	16 (27%)
32	LMU	C	523	-	36,36,36	1.16	2 (5%)	47,47,47	0.99	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	D	409	-	38,38,48	1.03	2 (5%)	41,44,54	1.10	2 (4%)
25	CLA	b	501	-	69,73,73	1.16	6 (8%)	82,113,113	1.09	3 (3%)
25	CLA	B	504	-	69,73,73	1.15	6 (8%)	82,113,113	1.19	9 (10%)
36	CHL	r	306	-	40,54,74	4.19	18 (45%)	34,90,114	2.93	13 (38%)
33	BCT	D	403	24	3,3,3	1.13	0	2,3,3	4.18	2 (100%)
36	CHL	N	308	-	60,74,74	3.39	19 (31%)	58,114,114	2.50	17 (29%)
25	CLA	r	301	23	64,68,73	1.22	8 (12%)	76,107,113	1.14	4 (5%)
25	CLA	B	502	-	69,73,73	1.16	8 (11%)	82,113,113	1.15	7 (8%)
28	SQD	a	407	-	49,51,54	1.14	3 (6%)	59,62,65	1.08	4 (6%)
31	DGD	C	518	-	63,63,67	0.89	3 (4%)	77,77,81	0.99	4 (5%)
37	LUT	N	317	-	42,43,43	0.80	1 (2%)	51,60,60	1.80	14 (27%)
31	DGD	c	517	-	60,60,67	0.89	2 (3%)	74,74,81	1.01	3 (4%)
25	CLA	G	604	-	46,50,73	1.39	7 (15%)	53,85,113	1.25	5 (9%)
25	CLA	b	507	-	69,73,73	1.16	8 (11%)	82,113,113	1.12	6 (7%)
25	CLA	S	612	16	49,53,73	1.36	6 (12%)	58,89,113	1.25	3 (5%)
25	CLA	a	403	-	53,57,73	1.30	6 (11%)	61,93,113	1.25	5 (8%)
25	CLA	B	514	-	69,73,73	1.17	7 (10%)	82,113,113	1.13	6 (7%)
25	CLA	G	613	8	69,73,73	1.16	6 (8%)	82,113,113	1.14	4 (4%)
25	CLA	G	614	-	46,50,73	1.39	7 (15%)	53,85,113	1.21	3 (5%)
25	CLA	d	404	-	46,50,73	1.38	6 (13%)	53,85,113	1.28	3 (5%)
31	DGD	W	202	-	67,67,67	0.85	2 (2%)	81,81,81	0.97	5 (6%)
35	HEM	F	101	6,7	50,50,50	1.59	8 (16%)	67,82,82	0.99	0
39	XAT	Y	302	-	41,47,47	0.92	2 (4%)	54,74,74	2.64	20 (37%)
25	CLA	B	513	-	69,73,73	1.16	8 (11%)	82,113,113	1.18	7 (8%)
36	CHL	r	305	-	37,51,74	4.31	17 (45%)	30,86,114	3.22	13 (43%)
25	CLA	c	503	-	69,73,73	1.16	7 (10%)	82,113,113	1.16	6 (7%)
25	CLA	c	507	-	69,73,73	1.16	7 (10%)	82,113,113	1.20	6 (7%)
30	LHG	d	407	-	43,43,48	0.97	2 (4%)	46,49,54	1.10	4 (8%)
25	CLA	B	505	-	69,73,73	1.16	7 (10%)	82,113,113	1.13	4 (4%)
25	CLA	N	314	14	69,73,73	1.17	7 (10%)	82,113,113	1.15	5 (6%)
25	CLA	Y	304	21	69,73,73	1.16	7 (10%)	82,113,113	1.10	4 (4%)
26	PHO	a	404	-	58,69,69	2.10	10 (17%)	55,99,99	1.46	7 (12%)
25	CLA	a	402	-	69,73,73	1.16	7 (10%)	82,113,113	1.13	5 (6%)
38	NEX	r	310	-	40,46,46	1.12	3 (7%)	50,70,70	2.25	14 (28%)
36	CHL	N	310	14	60,74,74	3.41	19 (31%)	58,114,114	2.34	16 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C	512	-	69,73,73	1.17	7 (10%)	82,113,113	1.13	5 (6%)
25	CLA	b	515	-	69,73,73	1.16	6 (8%)	82,113,113	1.16	4 (4%)
27	BCR	C	515	-	41,41,41	0.79	2 (4%)	56,56,56	1.95	16 (28%)
30	LHG	B	520	-	43,43,48	0.98	2 (4%)	46,49,54	1.07	3 (6%)
38	NEX	Y	318	-	40,46,46	1.11	3 (7%)	50,70,70	2.25	13 (26%)
39	XAT	r	309	-	41,47,47	0.90	2 (4%)	54,74,74	2.63	21 (38%)
30	LHG	S	618	25	44,44,48	0.95	2 (4%)	47,50,54	1.13	4 (8%)
36	CHL	N	309	-	44,58,74	3.96	19 (43%)	37,94,114	3.03	14 (37%)
25	CLA	Y	305	-	69,73,73	1.16	6 (8%)	82,113,113	1.17	4 (4%)
25	CLA	r	308	23	45,49,73	1.43	6 (13%)	54,84,113	1.25	4 (7%)
25	CLA	N	303	14	69,73,73	1.16	8 (11%)	82,113,113	1.15	6 (7%)
27	BCR	b	519	-	41,41,41	0.74	0	56,56,56	2.00	15 (26%)
36	CHL	G	605	8	37,51,74	4.28	17 (45%)	30,86,114	3.31	13 (43%)
25	CLA	c	504	-	64,68,73	1.21	7 (10%)	76,107,113	1.14	4 (5%)
25	CLA	B	503	-	69,73,73	1.16	7 (10%)	82,113,113	1.13	5 (6%)
29	LMG	C	520	-	51,51,55	0.94	2 (3%)	59,59,63	0.98	3 (5%)
25	CLA	d	403	-	69,73,73	1.16	8 (11%)	82,113,113	1.21	6 (7%)
25	CLA	b	502	-	69,73,73	1.16	8 (11%)	82,113,113	1.13	7 (8%)
25	CLA	r	303	-	53,57,73	1.32	7 (13%)	61,93,113	1.22	4 (6%)
25	CLA	S	604	-	53,57,73	1.32	7 (13%)	61,93,113	1.22	4 (6%)
28	SQD	A	407	-	49,51,54	1.14	3 (6%)	59,62,65	1.15	3 (5%)
25	CLA	C	507	-	69,73,73	1.15	6 (8%)	82,113,113	1.21	6 (7%)
25	CLA	C	511	4	69,73,73	1.17	7 (10%)	82,113,113	1.19	6 (7%)
25	CLA	S	613	16	53,57,73	1.32	6 (11%)	61,93,113	1.22	5 (8%)
25	CLA	C	504	-	69,73,73	1.16	7 (10%)	82,113,113	1.11	4 (4%)
25	CLA	c	512	-	60,64,73	1.24	7 (11%)	71,102,113	1.23	5 (7%)
25	CLA	b	509	-	69,73,73	1.16	6 (8%)	82,113,113	1.17	6 (7%)
25	CLA	B	516	-	69,73,73	1.16	7 (10%)	82,113,113	1.17	4 (4%)
25	CLA	B	510	-	69,73,73	1.17	7 (10%)	82,113,113	1.20	5 (6%)
33	BCT	a	409	24	3,3,3	1.14	0	2,3,3	4.20	2 (100%)
37	LUT	S	615	-	42,43,43	0.76	1 (2%)	51,60,60	1.79	13 (25%)
25	CLA	Y	313	21	69,73,73	1.17	7 (10%)	82,113,113	1.15	3 (3%)
25	CLA	c	505	-	69,73,73	1.15	7 (10%)	82,113,113	1.06	6 (7%)
25	CLA	N	312	30	53,57,73	1.32	8 (15%)	61,93,113	1.23	4 (6%)
25	CLA	S	609	16	45,49,73	1.40	6 (13%)	54,84,113	1.24	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	509	-	69,73,73	1.16	7 (10%)	82,113,113	1.20	6 (7%)
35	HEM	f	101	6,7	50,50,50	1.45	6 (12%)	67,82,82	1.13	6 (8%)
25	CLA	G	612	8	47,51,73	1.37	6 (12%)	55,86,113	1.22	3 (5%)
36	CHL	Y	310	21	60,74,74	3.44	19 (31%)	58,114,114	2.26	16 (27%)
25	CLA	a	405	-	64,68,73	1.19	7 (10%)	76,107,113	1.18	6 (7%)
30	LHG	C	521	-	46,46,48	0.96	2 (4%)	49,52,54	1.02	3 (6%)
27	BCR	c	514	-	41,41,41	0.75	1 (2%)	56,56,56	1.98	13 (23%)
25	CLA	N	304	-	69,73,73	1.16	7 (10%)	82,113,113	1.15	4 (4%)
27	BCR	h	101	-	41,41,41	0.71	0	56,56,56	2.03	12 (21%)
29	LMG	c	518	-	39,39,55	1.06	2 (5%)	46,46,63	1.07	3 (6%)
37	LUT	G	616	-	42,43,43	0.78	1 (2%)	51,60,60	1.75	12 (23%)
27	BCR	V	101	-	41,41,41	0.77	1 (2%)	56,56,56	1.90	18 (32%)
25	CLA	r	302	-	50,54,73	1.36	6 (12%)	59,90,113	1.26	4 (6%)
25	CLA	Y	315	-	58,62,73	1.26	7 (12%)	68,99,113	1.18	6 (8%)
25	CLA	b	514	-	49,53,73	1.37	8 (16%)	58,89,113	1.24	4 (6%)
25	CLA	d	401	-	69,73,73	1.17	7 (10%)	82,113,113	1.18	6 (7%)
36	CHL	S	606	-	38,52,74	4.19	17 (44%)	31,87,114	3.36	14 (45%)
27	BCR	H	101	-	41,41,41	0.72	0	56,56,56	2.01	12 (21%)
25	CLA	D	405	-	69,73,73	1.16	6 (8%)	82,113,113	1.15	4 (4%)
25	CLA	G	602	8	69,73,73	1.16	7 (10%)	82,113,113	1.11	4 (4%)
25	CLA	b	505	-	69,73,73	1.16	8 (11%)	82,113,113	1.12	5 (6%)
36	CHL	G	619	-	60,74,74	3.40	19 (31%)	58,114,114	2.55	17 (29%)
27	BCR	D	406	-	41,41,41	0.74	0	56,56,56	2.08	21 (37%)
36	CHL	Y	307	21	40,54,74	4.17	18 (45%)	34,90,114	3.08	14 (41%)
31	DGD	Y	301	-	67,67,67	0.84	2 (2%)	81,81,81	0.91	3 (3%)
25	CLA	S	603	-	46,50,73	1.38	8 (17%)	53,85,113	1.27	3 (5%)
28	SQD	t	102	-	52,54,54	1.11	3 (5%)	62,65,65	1.02	2 (3%)
30	LHG	l	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.08	4 (7%)
36	CHL	S	607	-	37,51,74	4.29	17 (45%)	30,86,114	3.31	14 (46%)
25	CLA	C	502	-	69,73,73	1.17	7 (10%)	82,113,113	1.18	4 (4%)
25	CLA	N	305	-	69,73,73	1.16	8 (11%)	82,113,113	1.15	5 (6%)
25	CLA	B	509	-	69,73,73	1.16	7 (10%)	82,113,113	1.14	6 (7%)
37	LUT	Y	317	-	42,43,43	0.78	1 (2%)	51,60,60	1.78	14 (27%)
25	CLA	C	510	-	69,73,73	1.16	8 (11%)	82,113,113	1.19	6 (7%)
25	CLA	b	516	-	49,53,73	1.37	7 (14%)	58,89,113	1.34	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	LUT	N	316	-	42,43,43	0.74	0	51,60,60	1.76	11 (21%)
25	CLA	b	503	-	69,73,73	1.16	8 (11%)	82,113,113	1.13	5 (6%)
37	LUT	G	615	-	42,43,43	0.74	0	51,60,60	1.79	13 (25%)
37	LUT	S	616	-	42,43,43	0.78	1 (2%)	51,60,60	1.87	18 (35%)
25	CLA	r	307	23	49,53,73	1.42	6 (12%)	58,89,113	1.15	3 (5%)
25	CLA	A	403	-	53,57,73	1.31	6 (11%)	61,93,113	1.25	5 (8%)
25	CLA	D	404	-	69,73,73	1.16	8 (11%)	82,113,113	1.18	8 (9%)
26	PHO	D	402	-	58,69,69	2.11	10 (17%)	55,99,99	1.45	6 (10%)
32	LMU	C	522	-	36,36,36	1.15	2 (5%)	47,47,47	0.98	1 (2%)
29	LMG	b	520	-	42,42,55	1.00	2 (4%)	50,50,63	1.04	3 (6%)
25	CLA	b	504	-	69,73,73	1.15	6 (8%)	82,113,113	1.19	4 (4%)
27	BCR	C	516	-	41,41,41	0.72	0	56,56,56	2.05	20 (35%)
25	CLA	C	505	-	69,73,73	1.16	8 (11%)	82,113,113	1.08	5 (6%)
25	CLA	Y	314	21	69,73,73	1.17	6 (8%)	82,113,113	1.14	4 (4%)
25	CLA	Y	306	-	62,66,73	1.22	7 (11%)	73,104,113	1.21	8 (10%)
30	LHG	L	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.09	4 (7%)
32	LMU	c	519	-	36,36,36	1.16	2 (5%)	47,47,47	0.94	1 (2%)
37	LUT	Y	316	-	42,43,43	0.74	0	51,60,60	1.79	14 (27%)
38	NEX	N	318	-	40,46,46	1.10	4 (10%)	50,70,70	2.20	13 (26%)
25	CLA	b	510	-	69,73,73	1.16	8 (11%)	82,113,113	1.22	6 (7%)
25	CLA	c	506	-	69,73,73	1.16	8 (11%)	82,113,113	1.12	6 (7%)
27	BCR	C	514	-	41,41,41	0.79	1 (2%)	56,56,56	1.90	14 (25%)
38	NEX	G	617	-	40,46,46	1.11	3 (7%)	50,70,70	2.31	16 (32%)
27	BCR	b	518	-	41,41,41	0.72	0	56,56,56	1.93	19 (33%)
26	PHO	d	402	-	58,69,69	2.10	10 (17%)	55,99,99	1.43	7 (12%)
25	CLA	c	502	-	69,73,73	1.17	7 (10%)	82,113,113	1.22	5 (6%)
29	LMG	a	408	-	46,46,55	0.98	2 (4%)	54,54,63	1.07	3 (5%)
25	CLA	C	501	-	69,73,73	1.17	8 (11%)	82,113,113	1.12	5 (6%)
36	CHL	S	601	16	40,54,74	4.17	19 (47%)	34,90,114	3.05	14 (41%)
25	CLA	G	611	30	49,53,73	1.37	7 (14%)	58,89,113	1.28	4 (6%)
36	CHL	Y	309	-	44,58,74	4.02	19 (43%)	37,94,114	2.76	14 (37%)
29	LMG	D	410	-	46,46,55	0.98	2 (4%)	54,54,63	1.03	3 (5%)
25	CLA	B	512	-	69,73,73	1.15	7 (10%)	82,113,113	1.23	6 (7%)
29	LMG	d	409	-	41,41,55	1.03	2 (4%)	49,49,63	1.09	3 (6%)
25	CLA	G	610	8	69,73,73	1.15	7 (10%)	82,113,113	1.09	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	Y	319	25	48,48,48	0.92	2 (4%)	51,54,54	1.07	3 (5%)
25	CLA	b	513	-	69,73,73	1.16	8 (11%)	82,113,113	1.21	8 (9%)
34	PL9	d	406	-	55,55,55	1.26	5 (9%)	68,69,69	1.52	12 (17%)
36	CHL	G	601	8	60,74,74	3.40	19 (31%)	58,114,114	2.43	16 (27%)
30	LHG	D	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.03	3 (5%)
25	CLA	Y	311	21	69,73,73	1.16	8 (11%)	82,113,113	1.09	4 (4%)
36	CHL	G	608	-	38,52,74	4.22	18 (47%)	31,87,114	2.94	12 (38%)
25	CLA	C	508	-	69,73,73	1.16	8 (11%)	82,113,113	1.11	5 (6%)
27	BCR	z	101	-	41,41,41	0.72	0	56,56,56	2.09	14 (25%)
32	LMU	S	619	-	36,36,36	1.15	2 (5%)	47,47,47	0.93	1 (2%)
39	XAT	N	301	-	41,47,47	0.92	2 (4%)	54,74,74	2.61	21 (38%)
25	CLA	N	311	14	69,73,73	1.15	7 (10%)	82,113,113	1.06	5 (6%)
36	CHL	S	608	-	43,57,74	3.99	18 (41%)	37,93,114	2.96	14 (37%)
25	CLA	C	503	-	69,73,73	1.16	7 (10%)	82,113,113	1.14	4 (4%)
25	CLA	b	511	-	69,73,73	1.16	7 (10%)	82,113,113	1.15	6 (7%)
29	LMG	H	102	-	48,48,55	0.97	2 (4%)	56,56,63	1.05	3 (5%)
27	BCR	B	518	-	41,41,41	0.76	1 (2%)	56,56,56	1.93	13 (23%)
25	CLA	A	402	-	69,73,73	1.17	8 (11%)	82,113,113	1.13	6 (7%)
30	LHG	b	521	-	48,48,48	0.93	2 (4%)	51,54,54	0.96	2 (3%)
31	DGD	C	517	-	56,56,67	0.90	2 (3%)	70,70,81	1.04	4 (5%)
27	BCR	k	101	-	41,41,41	0.71	1 (2%)	56,56,56	2.09	14 (25%)
31	DGD	c	515	-	54,54,67	0.92	2 (3%)	68,68,81	1.04	4 (5%)
25	CLA	Y	312	30	69,73,73	1.16	8 (11%)	82,113,113	1.16	6 (7%)
25	CLA	b	506	-	69,73,73	1.15	7 (10%)	82,113,113	1.13	4 (4%)
36	CHL	N	302	14	60,74,74	3.39	19 (31%)	58,114,114	2.43	16 (27%)
25	CLA	B	507	-	69,73,73	1.16	7 (10%)	82,113,113	1.13	6 (7%)
27	BCR	d	405	-	41,41,41	0.75	1 (2%)	56,56,56	2.16	18 (32%)
29	LMG	W	201	-	48,48,55	0.95	2 (4%)	56,56,63	1.07	3 (5%)
38	NEX	S	617	-	40,46,46	1.10	3 (7%)	50,70,70	2.22	13 (26%)
30	LHG	N	319	25	48,48,48	0.92	2 (4%)	51,54,54	1.07	3 (5%)
25	CLA	A	405	-	64,68,73	1.20	7 (10%)	76,107,113	1.19	7 (9%)
25	CLA	c	501	-	69,73,73	1.17	8 (11%)	82,113,113	1.13	6 (7%)
29	LMG	B	519	-	51,51,55	0.93	2 (3%)	59,59,63	1.01	3 (5%)
27	BCR	t	101	-	41,41,41	0.73	1 (2%)	56,56,56	2.01	18 (32%)
39	XAT	G	620	-	41,47,47	0.92	2 (4%)	54,74,74	4.15	23 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PHO	A	404	-	58,69,69	2.12	10 (17%)	55,99,99	1.45	6 (10%)
25	CLA	B	511	-	69,73,73	1.16	8 (11%)	82,113,113	1.15	6 (7%)
30	LHG	a	411	-	43,43,48	0.99	2 (4%)	46,49,54	1.03	3 (6%)
30	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	1.09	4 (7%)
36	CHL	N	306	14	60,74,74	3.42	19 (31%)	58,114,114	2.42	16 (27%)
25	CLA	S	614	-	52,56,73	1.34	7 (13%)	61,92,113	1.18	5 (8%)
25	CLA	B	515	-	69,73,73	1.16	5 (7%)	82,113,113	1.12	3 (3%)
36	CHL	Y	303	21	60,74,74	3.39	19 (31%)	58,114,114	2.50	16 (27%)
25	CLA	S	611	30	53,57,73	1.31	7 (13%)	61,93,113	1.26	5 (8%)
25	CLA	B	501	-	69,73,73	1.16	6 (8%)	82,113,113	1.13	5 (6%)
25	CLA	N	313	14	49,53,73	1.38	8 (16%)	58,89,113	1.24	4 (6%)
27	BCR	v	101	-	41,41,41	0.77	0	56,56,56	2.51	20 (35%)
25	CLA	D	401	-	69,73,73	1.16	7 (10%)	82,113,113	1.19	6 (7%)
25	CLA	C	513	-	69,73,73	1.14	7 (10%)	82,113,113	1.14	6 (7%)
36	CHL	Y	308	-	40,54,74	4.18	19 (47%)	34,90,114	3.12	14 (41%)
30	LHG	a	410	-	42,42,48	1.00	2 (4%)	45,48,54	1.14	2 (4%)
25	CLA	c	511	4	69,73,73	1.17	7 (10%)	82,113,113	1.20	7 (8%)
27	BCR	b	517	-	41,41,41	0.74	1 (2%)	56,56,56	1.94	17 (30%)
36	CHL	G	607	-	44,58,74	3.97	19 (43%)	37,94,114	3.03	15 (40%)
36	CHL	G	606	-	37,51,74	4.25	18 (48%)	30,86,114	3.30	14 (46%)
36	CHL	N	307	-	40,54,74	4.17	19 (47%)	34,90,114	3.04	14 (41%)
25	CLA	S	610	16	53,57,73	1.31	8 (15%)	61,93,113	1.14	7 (11%)
25	CLA	B	506	-	69,73,73	1.16	8 (11%)	82,113,113	1.11	7 (8%)
25	CLA	c	508	-	69,73,73	1.16	8 (11%)	82,113,113	1.11	5 (6%)
25	CLA	c	513	-	46,50,73	1.37	6 (13%)	53,85,113	1.19	3 (5%)
29	LMG	d	410	-	48,48,55	0.95	2 (4%)	56,56,63	1.06	4 (7%)
25	CLA	G	603	-	69,73,73	1.16	6 (8%)	82,113,113	1.16	4 (4%)
31	DGD	C	519	-	60,60,67	0.90	2 (3%)	74,74,81	0.89	3 (4%)
31	DGD	c	516	-	50,50,67	0.97	2 (4%)	64,64,81	1.02	3 (4%)
25	CLA	C	509	-	69,73,73	1.16	7 (10%)	82,113,113	1.17	5 (6%)
25	CLA	N	315	-	46,50,73	1.39	7 (15%)	53,85,113	1.17	4 (7%)
25	CLA	b	512	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	7 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LHG	G	618	25	-	8/53/53/53	-
25	CLA	c	510	-	1/1/15/20	8/39/115/115	-
36	CHL	r	304	-	3/3/15/26	3/13/111/137	-
34	PL9	D	407	-	-	4/53/73/73	0/1/1/1
25	CLA	C	506	-	1/1/15/20	8/39/115/115	-
25	CLA	S	602	16	1/1/11/20	7/20/96/115	-
27	BCR	A	406	-	-	0/29/63/63	0/2/2/2
27	BCR	a	406	-	-	2/29/63/63	0/2/2/2
25	CLA	B	508	-	1/1/15/20	14/39/115/115	-
25	CLA	S	605	16	1/1/12/20	5/21/97/115	-
25	CLA	b	508	-	1/1/15/20	10/39/115/115	-
27	BCR	B	517	-	-	8/29/63/63	0/2/2/2
36	CHL	G	609	8	3/3/20/26	20/39/137/137	-
32	LMU	C	523	-	-	8/21/61/61	0/2/2/2
30	LHG	D	409	-	-	6/43/43/53	-
25	CLA	b	501	-	1/1/15/20	16/39/115/115	-
25	CLA	B	504	-	1/1/15/20	17/39/115/115	-
36	CHL	r	306	-	3/3/16/26	6/15/113/137	-
36	CHL	N	308	-	3/3/20/26	23/39/137/137	-
25	CLA	r	301	23	1/1/14/20	5/33/109/115	-
25	CLA	B	502	-	1/1/15/20	5/39/115/115	-
28	SQD	a	407	-	-	5/46/66/69	0/1/1/1
31	DGD	C	518	-	-	9/51/91/95	0/2/2/2
37	LUT	N	317	-	-	0/29/67/67	0/2/2/2
31	DGD	c	517	-	-	8/48/88/95	0/2/2/2
25	CLA	G	604	-	1/1/10/20	1/12/88/115	-
25	CLA	b	507	-	1/1/15/20	12/39/115/115	-
25	CLA	S	612	16	1/1/11/20	2/15/91/115	-
25	CLA	a	403	-	1/1/11/20	7/20/96/115	-
25	CLA	B	514	-	1/1/15/20	11/39/115/115	-
25	CLA	G	613	8	1/1/15/20	11/39/115/115	-
25	CLA	G	614	-	1/1/10/20	0/12/88/115	-
25	CLA	d	404	-	1/1/10/20	4/12/88/115	-
31	DGD	W	202	-	-	6/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HEM	F	101	6,7	-	1/14/54/54	-
39	XAT	Y	302	-	-	0/31/93/93	0/4/4/4
25	CLA	B	513	-	1/1/15/20	5/39/115/115	-
36	CHL	r	305	-	3/3/15/26	4/12/110/137	-
25	CLA	c	503	-	1/1/15/20	13/39/115/115	-
25	CLA	c	507	-	1/1/15/20	14/39/115/115	-
30	LHG	d	407	-	-	7/48/48/53	-
25	CLA	B	505	-	1/1/15/20	10/39/115/115	-
25	CLA	N	314	14	1/1/15/20	11/39/115/115	-
25	CLA	Y	304	21	1/1/15/20	8/39/115/115	-
26	PHO	a	404	-	-	9/37/103/103	0/5/6/6
25	CLA	a	402	-	1/1/15/20	8/39/115/115	-
38	NEX	r	310	-	-	3/27/83/83	0/3/3/3
36	CHL	N	310	14	3/3/20/26	14/39/137/137	-
25	CLA	C	512	-	1/1/15/20	8/39/115/115	-
25	CLA	b	515	-	1/1/15/20	14/39/115/115	-
27	BCR	C	515	-	-	6/29/63/63	0/2/2/2
30	LHG	B	520	-	-	12/48/48/53	-
38	NEX	Y	318	-	-	3/27/83/83	0/3/3/3
39	XAT	r	309	-	-	0/31/93/93	0/4/4/4
30	LHG	S	618	25	-	7/49/49/53	-
36	CHL	N	309	-	3/3/16/26	5/20/118/137	-
25	CLA	Y	305	-	1/1/15/20	17/39/115/115	-
25	CLA	r	308	23	1/1/10/20	4/10/86/115	-
25	CLA	N	303	14	1/1/15/20	9/39/115/115	-
27	BCR	b	519	-	-	4/29/63/63	0/2/2/2
36	CHL	G	605	8	3/3/15/26	4/12/110/137	-
25	CLA	c	504	-	1/1/14/20	10/33/109/115	-
25	CLA	B	503	-	1/1/15/20	7/39/115/115	-
29	LMG	C	520	-	-	5/46/66/70	0/1/1/1
25	CLA	d	403	-	1/1/15/20	10/39/115/115	-
25	CLA	b	502	-	1/1/15/20	10/39/115/115	-
25	CLA	r	303	-	1/1/11/20	9/20/96/115	-
25	CLA	S	604	-	1/1/11/20	5/20/96/115	-
28	SQD	A	407	-	-	7/46/66/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	507	-	1/1/15/20	5/39/115/115	-
25	CLA	C	511	4	1/1/15/20	6/39/115/115	-
25	CLA	S	613	16	1/1/11/20	8/20/96/115	-
25	CLA	C	504	-	1/1/15/20	8/39/115/115	-
25	CLA	c	512	-	1/1/13/20	3/29/105/115	-
25	CLA	b	509	-	1/1/15/20	15/39/115/115	-
25	CLA	B	516	-	1/1/15/20	12/39/115/115	-
25	CLA	B	510	-	1/1/15/20	13/39/115/115	-
37	LUT	S	615	-	-	0/29/67/67	0/2/2/2
25	CLA	Y	313	21	1/1/15/20	7/39/115/115	-
25	CLA	c	505	-	1/1/15/20	11/39/115/115	-
25	CLA	N	312	30	1/1/11/20	9/20/96/115	-
25	CLA	S	609	16	1/1/10/20	6/10/86/115	-
25	CLA	c	509	-	1/1/15/20	13/39/115/115	-
35	HEM	f	101	6,7	-	1/14/54/54	-
25	CLA	G	612	8	1/1/10/20	4/13/89/115	-
36	CHL	Y	310	21	3/3/20/26	20/39/137/137	-
25	CLA	a	405	-	1/1/14/20	5/33/109/115	-
30	LHG	C	521	-	-	10/51/51/53	-
27	BCR	c	514	-	-	4/29/63/63	0/2/2/2
25	CLA	N	304	-	1/1/15/20	11/39/115/115	-
27	BCR	h	101	-	-	2/29/63/63	0/2/2/2
29	LMG	c	518	-	-	5/32/52/70	0/1/1/1
37	LUT	G	616	-	-	0/29/67/67	0/2/2/2
27	BCR	V	101	-	-	4/29/63/63	0/2/2/2
25	CLA	r	302	-	1/1/11/20	3/17/93/115	-
25	CLA	Y	315	-	1/1/12/20	5/26/102/115	-
25	CLA	b	514	-	1/1/11/20	4/15/91/115	-
25	CLA	d	401	-	1/1/15/20	12/39/115/115	-
36	CHL	S	606	-	3/3/15/26	5/13/111/137	-
27	BCR	H	101	-	-	2/29/63/63	0/2/2/2
25	CLA	D	405	-	1/1/15/20	16/39/115/115	-
25	CLA	G	602	8	1/1/15/20	11/39/115/115	-
25	CLA	b	505	-	1/1/15/20	15/39/115/115	-
36	CHL	G	619	-	3/3/20/26	18/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	D	406	-	-	2/29/63/63	0/2/2/2
36	CHL	Y	307	21	3/3/16/26	3/15/113/137	-
31	DGD	Y	301	-	-	10/55/95/95	0/2/2/2
25	CLA	S	603	-	1/1/10/20	2/12/88/115	-
36	CHL	S	607	-	3/3/15/26	1/12/110/137	-
28	SQD	t	102	-	-	5/49/69/69	0/1/1/1
30	LHG	l	101	-	-	6/53/53/53	-
25	CLA	C	502	-	1/1/15/20	10/39/115/115	-
25	CLA	N	305	-	1/1/15/20	12/39/115/115	-
25	CLA	B	509	-	1/1/15/20	10/39/115/115	-
37	LUT	Y	317	-	-	0/29/67/67	0/2/2/2
25	CLA	C	510	-	1/1/15/20	14/39/115/115	-
25	CLA	b	516	-	1/1/11/20	3/15/91/115	-
37	LUT	N	316	-	-	0/29/67/67	0/2/2/2
25	CLA	b	503	-	1/1/15/20	11/39/115/115	-
37	LUT	G	615	-	-	0/29/67/67	0/2/2/2
37	LUT	S	616	-	-	0/29/67/67	0/2/2/2
25	CLA	r	307	23	1/1/11/20	6/15/91/115	-
25	CLA	A	403	-	1/1/11/20	3/20/96/115	-
25	CLA	D	404	-	1/1/15/20	9/39/115/115	-
26	PHO	D	402	-	-	10/37/103/103	0/5/6/6
32	LMU	C	522	-	-	8/21/61/61	0/2/2/2
29	LMG	b	520	-	-	5/37/57/70	0/1/1/1
25	CLA	b	504	-	1/1/15/20	14/39/115/115	-
27	BCR	C	516	-	-	1/29/63/63	0/2/2/2
25	CLA	C	505	-	1/1/15/20	8/39/115/115	-
25	CLA	Y	314	21	1/1/15/20	11/39/115/115	-
25	CLA	Y	306	-	1/1/13/20	5/31/107/115	-
30	LHG	L	101	-	-	8/53/53/53	-
32	LMU	c	519	-	-	5/21/61/61	0/2/2/2
37	LUT	Y	316	-	-	0/29/67/67	0/2/2/2
38	NEX	N	318	-	-	2/27/83/83	0/3/3/3
25	CLA	b	510	-	1/1/15/20	16/39/115/115	-
25	CLA	c	506	-	1/1/15/20	16/39/115/115	-
27	BCR	C	514	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	NEX	G	617	-	-	2/27/83/83	0/3/3/3
27	BCR	b	518	-	-	2/29/63/63	0/2/2/2
26	PHO	d	402	-	-	7/37/103/103	0/5/6/6
25	CLA	c	502	-	1/1/15/20	15/39/115/115	-
36	CHL	S	601	16	3/3/16/26	5/15/113/137	-
25	CLA	C	501	-	1/1/15/20	14/39/115/115	-
29	LMG	a	408	-	-	5/41/61/70	0/1/1/1
25	CLA	G	611	30	1/1/11/20	5/15/91/115	-
36	CHL	Y	309	-	3/3/16/26	6/20/118/137	-
29	LMG	D	410	-	-	6/41/61/70	0/1/1/1
25	CLA	B	512	-	1/1/15/20	10/39/115/115	-
29	LMG	d	409	-	-	7/36/56/70	0/1/1/1
25	CLA	G	610	8	1/1/15/20	7/39/115/115	-
30	LHG	Y	319	25	-	13/53/53/53	-
25	CLA	b	513	-	1/1/15/20	6/39/115/115	-
36	CHL	G	608	-	3/3/15/26	3/13/111/137	-
36	CHL	G	601	8	3/3/20/26	17/39/137/137	-
30	LHG	D	408	-	-	8/53/53/53	-
25	CLA	Y	311	21	1/1/15/20	6/39/115/115	-
34	PL9	d	406	-	-	5/53/73/73	0/1/1/1
25	CLA	C	508	-	1/1/15/20	9/39/115/115	-
27	BCR	z	101	-	-	6/29/63/63	0/2/2/2
32	LMU	S	619	-	-	6/21/61/61	0/2/2/2
39	XAT	N	301	-	-	0/31/93/93	0/4/4/4
25	CLA	N	311	14	1/1/15/20	6/39/115/115	-
36	CHL	S	608	-	3/3/16/26	8/19/117/137	-
25	CLA	C	503	-	1/1/15/20	8/39/115/115	-
25	CLA	b	511	-	1/1/15/20	18/39/115/115	-
29	LMG	H	102	-	-	8/43/63/70	0/1/1/1
27	BCR	B	518	-	-	2/29/63/63	0/2/2/2
25	CLA	A	402	-	1/1/15/20	9/39/115/115	-
30	LHG	b	521	-	-	9/53/53/53	-
31	DGD	C	517	-	-	6/44/84/95	0/2/2/2
27	BCR	k	101	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	c	515	-	-	3/42/82/95	0/2/2/2
25	CLA	Y	312	30	1/1/15/20	4/39/115/115	-
25	CLA	b	506	-	1/1/15/20	15/39/115/115	-
36	CHL	N	302	14	3/3/20/26	16/39/137/137	-
25	CLA	B	507	-	1/1/15/20	7/39/115/115	-
27	BCR	d	405	-	-	4/29/63/63	0/2/2/2
29	LMG	W	201	-	-	9/43/63/70	0/1/1/1
38	NEX	S	617	-	-	3/27/83/83	0/3/3/3
30	LHG	N	319	25	-	9/53/53/53	-
25	CLA	A	405	-	1/1/14/20	4/33/109/115	-
25	CLA	c	501	-	1/1/15/20	17/39/115/115	-
29	LMG	B	519	-	-	2/46/66/70	0/1/1/1
27	BCR	t	101	-	-	6/29/63/63	0/2/2/2
39	XAT	G	620	-	-	0/31/93/93	0/4/4/4
26	PHO	A	404	-	-	6/37/103/103	0/5/6/6
25	CLA	B	511	-	1/1/15/20	3/39/115/115	-
36	CHL	N	306	14	3/3/20/26	16/39/137/137	-
30	LHG	a	411	-	-	9/48/48/53	-
30	LHG	d	408	-	-	5/53/53/53	-
25	CLA	S	614	-	1/1/11/20	8/19/95/115	-
25	CLA	B	515	-	1/1/15/20	3/39/115/115	-
36	CHL	Y	303	21	3/3/20/26	15/39/137/137	-
25	CLA	S	611	30	1/1/11/20	4/20/96/115	-
25	CLA	B	501	-	1/1/15/20	9/39/115/115	-
25	CLA	N	313	14	1/1/11/20	4/15/91/115	-
27	BCR	v	101	-	-	5/29/63/63	0/2/2/2
25	CLA	D	401	-	1/1/15/20	5/39/115/115	-
25	CLA	C	513	-	1/1/15/20	15/39/115/115	-
36	CHL	Y	308	-	3/3/16/26	5/15/113/137	-
30	LHG	a	410	-	-	6/47/47/53	-
25	CLA	c	511	4	1/1/15/20	12/39/115/115	-
27	BCR	b	517	-	-	4/29/63/63	0/2/2/2
36	CHL	G	607	-	3/3/16/26	5/20/118/137	-
36	CHL	G	606	-	3/3/15/26	0/12/110/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CHL	N	307	-	3/3/16/26	7/15/113/137	-
25	CLA	S	610	16	1/1/11/20	5/20/96/115	-
25	CLA	B	506	-	1/1/15/20	6/39/115/115	-
25	CLA	c	508	-	1/1/15/20	12/39/115/115	-
25	CLA	c	513	-	1/1/10/20	4/12/88/115	-
29	LMG	d	410	-	-	12/43/63/70	0/1/1/1
25	CLA	G	603	-	1/1/15/20	19/39/115/115	-
31	DGD	C	519	-	-	3/48/88/95	0/2/2/2
31	DGD	c	516	-	-	6/38/78/95	0/2/2/2
25	CLA	C	509	-	1/1/15/20	10/39/115/115	-
25	CLA	N	315	-	1/1/10/20	6/12/88/115	-
25	CLA	b	512	-	1/1/15/20	13/39/115/115	-

All (1415) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	Y	309	CHL	C2C-C3C	10.64	1.46	1.36
36	Y	310	CHL	C2C-C3C	10.56	1.46	1.36
36	G	609	CHL	C2C-C3C	10.55	1.46	1.36
36	G	608	CHL	C2C-C3C	10.54	1.46	1.36
36	N	306	CHL	C2C-C3C	10.49	1.46	1.36
36	r	305	CHL	C2C-C3C	10.45	1.46	1.36
36	r	306	CHL	C2C-C3C	10.45	1.46	1.36
36	G	605	CHL	C2C-C3C	10.44	1.46	1.36
36	S	601	CHL	C2C-C3C	10.41	1.46	1.36
36	S	607	CHL	C2C-C3C	10.41	1.46	1.36
36	G	601	CHL	C2C-C3C	10.36	1.46	1.36
36	N	307	CHL	C2C-C3C	10.35	1.46	1.36
36	G	607	CHL	C2C-C3C	10.33	1.46	1.36
36	S	608	CHL	C2C-C3C	10.32	1.46	1.36
36	N	309	CHL	C2C-C3C	10.31	1.46	1.36
36	Y	307	CHL	C2C-C3C	10.31	1.46	1.36
36	G	619	CHL	C2C-C3C	10.30	1.46	1.36
36	Y	303	CHL	C2C-C3C	10.30	1.46	1.36
36	r	304	CHL	C1D-C2D	10.29	1.51	1.39
36	N	308	CHL	C2C-C3C	10.29	1.46	1.36
36	r	305	CHL	C1D-C2D	10.28	1.51	1.39
36	N	302	CHL	C2C-C3C	10.27	1.46	1.36
36	N	310	CHL	C2C-C3C	10.27	1.46	1.36
36	Y	308	CHL	C2C-C3C	10.25	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	r	304	CHL	C2C-C3C	10.25	1.46	1.36
36	r	306	CHL	C1D-C2D	10.23	1.51	1.39
36	Y	310	CHL	C1D-C2D	10.17	1.51	1.39
36	N	310	CHL	C1D-C2D	10.14	1.51	1.39
36	Y	303	CHL	C1D-C2D	10.11	1.51	1.39
36	G	601	CHL	C1D-C2D	10.11	1.51	1.39
36	G	605	CHL	C1D-C2D	10.09	1.51	1.39
36	N	302	CHL	C1D-C2D	10.09	1.51	1.39
36	G	609	CHL	C1D-C2D	10.07	1.51	1.39
36	G	606	CHL	C2C-C3C	10.06	1.46	1.36
36	S	601	CHL	C1D-C2D	10.04	1.51	1.39
36	Y	307	CHL	C1D-C2D	10.04	1.51	1.39
36	N	306	CHL	C1D-C2D	10.00	1.50	1.39
36	Y	308	CHL	C1D-C2D	9.99	1.50	1.39
36	S	607	CHL	C1D-C2D	9.99	1.50	1.39
36	S	606	CHL	C2C-C3C	9.97	1.46	1.36
36	Y	309	CHL	C1D-C2D	9.96	1.50	1.39
36	N	309	CHL	C1D-C2D	9.96	1.50	1.39
36	G	607	CHL	C1D-C2D	9.95	1.50	1.39
36	G	619	CHL	C1D-C2D	9.95	1.50	1.39
36	G	608	CHL	C1D-C2D	9.94	1.50	1.39
36	S	608	CHL	C1D-C2D	9.86	1.50	1.39
36	N	308	CHL	C1D-C2D	9.84	1.50	1.39
36	S	606	CHL	C1D-C2D	9.77	1.50	1.39
36	N	307	CHL	C1D-C2D	9.73	1.50	1.39
36	G	606	CHL	C1D-C2D	9.64	1.50	1.39
26	D	402	PHO	C1B-C2B	9.36	1.49	1.39
26	d	402	PHO	C1B-C2B	9.33	1.49	1.39
26	A	404	PHO	C1B-C2B	9.32	1.49	1.39
26	a	404	PHO	C1B-C2B	9.18	1.49	1.39
36	Y	308	CHL	C3B-C4B	8.46	1.49	1.41
26	A	404	PHO	C3B-C4B	8.44	1.50	1.41
36	G	606	CHL	C3B-C4B	8.42	1.49	1.41
26	D	402	PHO	C3B-C4B	8.40	1.50	1.41
26	a	404	PHO	C3B-C4B	8.36	1.49	1.41
36	Y	309	CHL	C3B-C4B	8.35	1.49	1.41
36	G	605	CHL	C1B-C2B	8.33	1.49	1.39
36	N	307	CHL	C3B-C4B	8.33	1.49	1.41
36	r	306	CHL	C1B-C2B	8.33	1.49	1.39
36	S	608	CHL	C1B-C2B	8.29	1.49	1.39
36	r	305	CHL	C1B-C2B	8.27	1.49	1.39
36	Y	307	CHL	C1B-C2B	8.24	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	r	304	CHL	C1B-C2B	8.24	1.48	1.39
36	N	306	CHL	C3B-C4B	8.23	1.49	1.41
36	S	601	CHL	C3B-C4B	8.23	1.49	1.41
36	G	608	CHL	C3B-C4B	8.22	1.49	1.41
36	S	606	CHL	C1B-C2B	8.21	1.48	1.39
36	S	607	CHL	C3B-C4B	8.20	1.49	1.41
26	d	402	PHO	C3B-C4B	8.20	1.49	1.41
36	G	619	CHL	C1B-C2B	8.20	1.48	1.39
36	S	606	CHL	C3B-C4B	8.19	1.49	1.41
36	N	308	CHL	C1B-C2B	8.19	1.48	1.39
36	Y	310	CHL	C3B-C4B	8.19	1.49	1.41
36	Y	309	CHL	C1B-C2B	8.18	1.48	1.39
36	G	609	CHL	C1B-C2B	8.15	1.48	1.39
36	G	601	CHL	C1B-C2B	8.15	1.48	1.39
36	G	606	CHL	C1B-C2B	8.14	1.48	1.39
36	r	304	CHL	C3B-C4B	8.14	1.49	1.41
36	S	607	CHL	C1B-C2B	8.13	1.48	1.39
36	G	607	CHL	C1B-C2B	8.12	1.48	1.39
36	N	302	CHL	C1B-C2B	8.11	1.48	1.39
36	Y	303	CHL	C1B-C2B	8.11	1.48	1.39
36	N	309	CHL	C1B-C2B	8.09	1.48	1.39
36	N	309	CHL	C3B-C4B	8.09	1.49	1.41
36	N	310	CHL	C1B-C2B	8.09	1.48	1.39
36	N	306	CHL	C1B-C2B	8.05	1.48	1.39
36	N	308	CHL	C1A-CHA	8.02	1.49	1.40
36	S	606	CHL	C1A-CHA	8.00	1.49	1.40
36	r	305	CHL	C3B-C4B	8.00	1.49	1.41
36	S	601	CHL	C1B-C2B	7.99	1.48	1.39
36	N	308	CHL	C3B-C4B	7.97	1.49	1.41
36	N	307	CHL	C1B-C2B	7.94	1.48	1.39
36	Y	310	CHL	C1B-C2B	7.94	1.48	1.39
36	G	608	CHL	C1B-C2B	7.93	1.48	1.39
36	Y	303	CHL	C3B-C4B	7.92	1.49	1.41
36	G	607	CHL	C1A-CHA	7.90	1.49	1.40
36	r	306	CHL	C3B-C4B	7.90	1.49	1.41
36	Y	308	CHL	C1B-C2B	7.88	1.48	1.39
36	N	310	CHL	C3B-C4B	7.88	1.49	1.41
36	r	306	CHL	C1A-CHA	7.88	1.49	1.40
36	G	619	CHL	C3B-C4B	7.87	1.49	1.41
36	G	607	CHL	C3B-C4B	7.85	1.49	1.41
36	Y	307	CHL	C1A-CHA	7.83	1.48	1.40
36	N	302	CHL	C3B-C4B	7.83	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	619	CHL	C1A-CHA	7.83	1.48	1.40
36	Y	307	CHL	C3B-C4B	7.81	1.49	1.41
36	Y	309	CHL	C1A-CHA	7.81	1.48	1.40
36	S	608	CHL	C3B-C4B	7.81	1.49	1.41
36	G	605	CHL	C3B-C4B	7.81	1.49	1.41
36	G	609	CHL	C3B-C4B	7.81	1.49	1.41
36	S	608	CHL	C1A-CHA	7.78	1.48	1.40
36	G	605	CHL	C1A-CHA	7.78	1.48	1.40
36	N	306	CHL	C1A-CHA	7.74	1.48	1.40
36	G	608	CHL	C1A-CHA	7.74	1.48	1.40
36	G	601	CHL	C1A-CHA	7.73	1.48	1.40
36	G	601	CHL	C3B-C4B	7.70	1.48	1.41
36	r	305	CHL	C1A-CHA	7.68	1.48	1.40
36	S	607	CHL	C1A-CHA	7.67	1.48	1.40
36	N	309	CHL	C1A-CHA	7.65	1.48	1.40
36	r	304	CHL	C1A-CHA	7.64	1.48	1.40
36	N	310	CHL	C1A-CHA	7.63	1.48	1.40
36	G	609	CHL	C1A-CHA	7.58	1.48	1.40
36	G	606	CHL	C1A-CHA	7.58	1.48	1.40
36	N	302	CHL	C1A-CHA	7.53	1.48	1.40
36	Y	310	CHL	C1A-CHA	7.50	1.48	1.40
36	Y	303	CHL	C1A-CHA	7.48	1.48	1.40
36	Y	308	CHL	C1A-CHA	7.45	1.48	1.40
36	S	601	CHL	C1A-CHA	7.43	1.48	1.40
36	N	307	CHL	C1A-CHA	7.41	1.48	1.40
36	Y	310	CHL	C3D-C4D	-5.57	1.33	1.41
36	N	307	CHL	C3D-C4D	-5.53	1.33	1.41
36	G	609	CHL	C3D-C4D	-5.52	1.33	1.41
36	N	310	CHL	C3D-C4D	-5.50	1.33	1.41
36	Y	303	CHL	C3D-C4D	-5.49	1.33	1.41
36	N	309	CHL	C3D-C4D	-5.48	1.33	1.41
36	Y	308	CHL	C3D-C4D	-5.46	1.33	1.41
36	N	302	CHL	C3D-C4D	-5.42	1.33	1.41
36	Y	309	CHL	C3D-C4D	-5.42	1.33	1.41
36	G	601	CHL	C3D-C4D	-5.42	1.33	1.41
36	S	601	CHL	C3D-C4D	-5.41	1.33	1.41
36	S	608	CHL	C3D-C4D	-5.40	1.33	1.41
36	G	608	CHL	C3D-C4D	-5.39	1.33	1.41
36	G	619	CHL	C3D-C4D	-5.39	1.33	1.41
36	S	607	CHL	C3D-C4D	-5.38	1.33	1.41
36	N	306	CHL	C3D-C4D	-5.38	1.33	1.41
36	G	606	CHL	C3D-C4D	-5.38	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	607	CHL	C3D-C4D	-5.37	1.33	1.41
36	r	305	CHL	C3D-C4D	-5.37	1.33	1.41
36	S	606	CHL	C3D-C4D	-5.34	1.33	1.41
36	Y	307	CHL	C3D-C4D	-5.34	1.33	1.41
36	N	307	CHL	CHC-C4B	5.30	1.48	1.39
36	N	308	CHL	C3D-C4D	-5.30	1.33	1.41
36	r	304	CHL	C3D-C4D	-5.29	1.33	1.41
36	r	306	CHL	C3D-C4D	-5.29	1.33	1.41
36	G	605	CHL	C3D-C4D	-5.29	1.33	1.41
36	Y	308	CHL	CHC-C4B	5.22	1.48	1.39
36	Y	309	CHL	CHC-C4B	5.16	1.48	1.39
36	r	305	CHL	O2D-CGD	5.13	1.45	1.33
36	Y	307	CHL	O2D-CGD	5.12	1.45	1.33
36	r	304	CHL	O2D-CGD	5.12	1.45	1.33
36	G	606	CHL	CHC-C4B	5.11	1.47	1.39
36	S	601	CHL	C3A-C2A	-5.11	1.50	1.54
36	G	605	CHL	O2D-CGD	5.10	1.45	1.33
36	S	606	CHL	CHC-C4B	5.10	1.47	1.39
36	G	601	CHL	O2D-CGD	5.09	1.45	1.33
36	G	606	CHL	O2D-CGD	5.08	1.45	1.33
36	S	607	CHL	O2D-CGD	5.08	1.45	1.33
36	G	607	CHL	O2D-CGD	5.08	1.45	1.33
36	N	308	CHL	O2D-CGD	5.08	1.45	1.33
36	G	609	CHL	O2D-CGD	5.07	1.45	1.33
36	Y	308	CHL	O2D-CGD	5.07	1.45	1.33
36	r	306	CHL	O2D-CGD	5.07	1.45	1.33
36	G	619	CHL	O2D-CGD	5.06	1.45	1.33
36	G	608	CHL	CHC-C4B	5.05	1.47	1.39
36	Y	310	CHL	C3B-C2B	5.05	1.47	1.40
36	N	310	CHL	O2D-CGD	5.05	1.45	1.33
36	N	302	CHL	O2D-CGD	5.05	1.45	1.33
36	Y	309	CHL	C3B-C2B	5.05	1.47	1.40
36	N	309	CHL	CHC-C4B	5.04	1.47	1.39
36	N	307	CHL	O2D-CGD	5.03	1.45	1.33
36	Y	309	CHL	O2D-CGD	5.03	1.45	1.33
36	S	601	CHL	CHC-C4B	5.03	1.47	1.39
36	r	306	CHL	OBD-CAD	5.03	1.28	1.22
36	S	601	CHL	O2D-CGD	5.03	1.45	1.33
36	S	607	CHL	CHC-C4B	5.03	1.47	1.39
36	r	305	CHL	C3B-C2B	5.02	1.47	1.40
36	N	310	CHL	C3B-C2B	5.02	1.47	1.40
36	Y	310	CHL	O2D-CGD	5.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	N	306	CHL	CHC-C4B	5.02	1.47	1.39
36	G	608	CHL	O2D-CGD	5.01	1.45	1.33
36	N	306	CHL	O2D-CGD	5.01	1.45	1.33
36	G	605	CHL	OBD-CAD	5.01	1.28	1.22
36	Y	303	CHL	O2D-CGD	5.01	1.45	1.33
36	r	305	CHL	OBD-CAD	5.00	1.28	1.22
36	N	309	CHL	O2D-CGD	4.99	1.45	1.33
36	Y	310	CHL	CHC-C4B	4.99	1.47	1.39
36	G	605	CHL	C3B-C2B	4.99	1.47	1.40
36	G	606	CHL	OBD-CAD	4.99	1.28	1.22
36	r	304	CHL	OBD-CAD	4.99	1.28	1.22
36	Y	308	CHL	OBD-CAD	4.98	1.28	1.22
36	G	607	CHL	C3A-C2A	-4.98	1.50	1.54
36	S	607	CHL	C3B-C2B	4.98	1.47	1.40
36	N	302	CHL	OBD-CAD	4.98	1.28	1.22
36	G	607	CHL	OBD-CAD	4.96	1.28	1.22
36	N	307	CHL	OBD-CAD	4.96	1.28	1.22
36	G	608	CHL	C3B-C2B	4.95	1.47	1.40
36	S	607	CHL	OBD-CAD	4.95	1.28	1.22
36	Y	303	CHL	CHC-C4B	4.95	1.47	1.39
36	S	606	CHL	OBD-CAD	4.95	1.28	1.22
36	N	310	CHL	OBD-CAD	4.95	1.28	1.22
36	Y	307	CHL	CHC-C4B	4.94	1.47	1.39
36	Y	308	CHL	C3A-C2A	-4.94	1.50	1.54
36	Y	307	CHL	OBD-CAD	4.94	1.28	1.22
36	G	619	CHL	CHC-C4B	4.93	1.47	1.39
36	N	306	CHL	C3A-C2A	-4.93	1.50	1.54
36	N	302	CHL	CHC-C4B	4.93	1.47	1.39
36	G	601	CHL	OBD-CAD	4.93	1.28	1.22
36	S	606	CHL	O2D-CGD	4.93	1.45	1.33
36	G	601	CHL	C3A-C2A	-4.93	1.50	1.54
36	r	305	CHL	CHC-C4B	4.92	1.47	1.39
36	G	609	CHL	C3B-C2B	4.92	1.47	1.40
36	r	306	CHL	C3B-C2B	4.91	1.47	1.40
36	N	308	CHL	CHC-C4B	4.91	1.47	1.39
36	N	306	CHL	OBD-CAD	4.91	1.28	1.22
36	S	608	CHL	CHC-C4B	4.91	1.47	1.39
36	G	619	CHL	OBD-CAD	4.91	1.28	1.22
36	G	605	CHL	CHC-C4B	4.91	1.47	1.39
36	G	607	CHL	CHC-C4B	4.90	1.47	1.39
36	Y	303	CHL	OBD-CAD	4.90	1.28	1.22
36	Y	307	CHL	C3B-C2B	4.90	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	619	CHL	C3A-C2A	-4.89	1.50	1.54
36	S	608	CHL	C3B-C2B	4.89	1.47	1.40
36	N	310	CHL	CHC-C4B	4.89	1.47	1.39
36	r	304	CHL	C3B-C2B	4.89	1.47	1.40
36	r	304	CHL	CHC-C4B	4.89	1.47	1.39
36	N	309	CHL	OBD-CAD	4.89	1.28	1.22
36	N	308	CHL	C3A-C2A	-4.88	1.50	1.54
36	r	306	CHL	CHC-C4B	4.88	1.47	1.39
36	Y	309	CHL	OBD-CAD	4.87	1.28	1.22
36	N	308	CHL	OBD-CAD	4.87	1.28	1.22
36	N	310	CHL	C3A-C2A	-4.87	1.50	1.54
36	Y	310	CHL	OBD-CAD	4.86	1.28	1.22
36	S	608	CHL	C3A-C2A	-4.86	1.50	1.54
36	G	605	CHL	C3A-C2A	-4.85	1.50	1.54
36	G	606	CHL	C3A-C2A	-4.85	1.50	1.54
36	N	306	CHL	C3B-C2B	4.84	1.46	1.40
36	G	608	CHL	OBD-CAD	4.84	1.28	1.22
36	G	609	CHL	OBD-CAD	4.83	1.28	1.22
36	S	608	CHL	O2D-CGD	4.83	1.45	1.33
36	N	302	CHL	C3A-C2A	-4.82	1.50	1.54
36	S	601	CHL	OBD-CAD	4.82	1.28	1.22
36	G	606	CHL	C3B-C2B	4.82	1.46	1.40
36	G	609	CHL	CHC-C4B	4.81	1.47	1.39
36	G	601	CHL	CHC-C4B	4.81	1.47	1.39
36	S	606	CHL	C3B-C2B	4.80	1.46	1.40
36	N	309	CHL	C3B-C2B	4.80	1.46	1.40
36	G	619	CHL	C3B-C2B	4.78	1.46	1.40
36	Y	307	CHL	C3A-C2A	-4.78	1.50	1.54
36	N	302	CHL	C3B-C2B	4.78	1.46	1.40
36	G	607	CHL	C3B-C2B	4.77	1.46	1.40
36	N	309	CHL	C3A-C2A	-4.76	1.50	1.54
36	S	607	CHL	C3A-C2A	-4.75	1.50	1.54
36	N	308	CHL	C3B-C2B	4.75	1.46	1.40
36	Y	303	CHL	C3B-C2B	4.74	1.46	1.40
36	N	307	CHL	CHC-C1C	4.72	1.48	1.39
36	r	304	CHL	C3A-C2A	-4.72	1.50	1.54
36	S	601	CHL	C3B-C2B	4.71	1.46	1.40
36	G	609	CHL	C3A-C2A	-4.71	1.50	1.54
36	N	307	CHL	C3B-C2B	4.71	1.46	1.40
36	Y	303	CHL	CHB-C4A	-4.70	1.33	1.38
36	N	307	CHL	C3A-C2A	-4.70	1.50	1.54
36	S	606	CHL	C3A-C2A	-4.70	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	N	307	CHL	CHB-C1B	4.70	1.47	1.39
36	G	601	CHL	C3B-C2B	4.69	1.46	1.40
36	N	310	CHL	CHB-C1B	4.68	1.47	1.39
36	Y	310	CHL	CHB-C1B	4.68	1.47	1.39
36	Y	308	CHL	C3B-C2B	4.67	1.46	1.40
36	Y	303	CHL	C3A-C2A	-4.67	1.50	1.54
36	G	608	CHL	C3A-C2A	-4.66	1.50	1.54
36	Y	308	CHL	CHC-C1C	4.64	1.48	1.39
36	S	601	CHL	CHB-C4A	-4.64	1.33	1.38
36	S	607	CHL	CHB-C1B	4.64	1.47	1.39
36	S	608	CHL	OBD-CAD	4.64	1.28	1.22
36	Y	310	CHL	C3A-C2A	-4.64	1.50	1.54
36	G	605	CHL	CHB-C1B	4.63	1.47	1.39
36	S	606	CHL	CHB-C1B	4.63	1.47	1.39
36	N	302	CHL	CHB-C4A	-4.63	1.33	1.38
36	G	601	CHL	CHB-C4A	-4.62	1.33	1.38
36	r	305	CHL	C3A-C2A	-4.60	1.50	1.54
36	Y	308	CHL	CHB-C1B	4.59	1.47	1.39
36	r	306	CHL	C3A-C2A	-4.58	1.50	1.54
36	N	308	CHL	CHB-C4A	-4.58	1.33	1.38
36	r	304	CHL	CHB-C1B	4.57	1.47	1.39
36	G	606	CHL	CHB-C1B	4.57	1.47	1.39
36	G	607	CHL	CHB-C4A	-4.56	1.33	1.38
36	r	305	CHL	CHB-C1B	4.56	1.47	1.39
36	Y	309	CHL	CHB-C1B	4.55	1.47	1.39
36	N	307	CHL	CHB-C4A	-4.55	1.33	1.38
36	Y	310	CHL	CHD-C4C	4.55	1.48	1.39
36	G	609	CHL	CHB-C1B	4.55	1.47	1.39
36	Y	307	CHL	O2A-CGA	4.55	1.45	1.30
36	G	608	CHL	CHB-C1B	4.55	1.47	1.39
36	G	609	CHL	CHB-C4A	-4.54	1.33	1.38
36	Y	308	CHL	O2A-CGA	4.54	1.45	1.30
36	Y	309	CHL	CHC-C1C	4.54	1.48	1.39
36	N	306	CHL	CHB-C1B	4.53	1.47	1.39
36	Y	310	CHL	CHB-C4A	-4.53	1.33	1.38
36	N	309	CHL	CHB-C1B	4.53	1.47	1.39
36	S	601	CHL	O2A-CGA	4.53	1.45	1.30
36	r	305	CHL	CHD-C4C	4.53	1.48	1.39
36	r	304	CHL	CHD-C4C	4.52	1.48	1.39
36	G	606	CHL	CHB-C4A	-4.52	1.33	1.38
36	r	306	CHL	CHB-C1B	4.52	1.46	1.39
36	N	307	CHL	O2A-CGA	4.52	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	619	CHL	CHB-C4A	-4.52	1.33	1.38
36	r	306	CHL	O2A-CGA	4.51	1.45	1.30
36	G	601	CHL	CHD-C4C	4.51	1.48	1.39
36	G	606	CHL	CHC-C1C	4.51	1.48	1.39
36	S	608	CHL	CHB-C1B	4.50	1.46	1.39
36	S	606	CHL	CHC-C1C	4.50	1.48	1.39
36	N	308	CHL	CHB-C1B	4.49	1.46	1.39
36	Y	310	CHL	CHD-C1D	4.49	1.46	1.39
36	G	608	CHL	CHB-C4A	-4.49	1.33	1.38
36	S	607	CHL	CHC-C1C	4.48	1.48	1.39
36	Y	307	CHL	CHB-C1B	4.48	1.46	1.39
36	r	306	CHL	CHD-C4C	4.48	1.48	1.39
36	Y	309	CHL	CHB-C4A	-4.48	1.33	1.38
36	Y	307	CHL	CHB-C4A	-4.48	1.33	1.38
36	Y	308	CHL	CHB-C4A	-4.48	1.33	1.38
36	G	607	CHL	CHB-C1B	4.47	1.46	1.39
36	N	309	CHL	CHC-C1C	4.47	1.48	1.39
36	S	607	CHL	CHB-C4A	-4.47	1.33	1.38
36	G	619	CHL	CHB-C1B	4.46	1.46	1.39
36	Y	310	CHL	CHC-C1C	4.46	1.47	1.39
36	N	302	CHL	CHD-C4C	4.46	1.47	1.39
36	N	306	CHL	CHB-C4A	-4.45	1.33	1.38
36	r	305	CHL	CHC-C1C	4.45	1.47	1.39
36	G	608	CHL	CHC-C1C	4.45	1.47	1.39
36	Y	303	CHL	CHD-C4C	4.44	1.47	1.39
36	Y	309	CHL	C3A-C2A	-4.44	1.50	1.54
36	N	309	CHL	CHB-C4A	-4.44	1.33	1.38
36	G	605	CHL	CHD-C4C	4.44	1.47	1.39
36	N	302	CHL	CHC-C1C	4.44	1.47	1.39
36	Y	309	CHL	CHD-C4C	4.44	1.47	1.39
36	Y	307	CHL	CHC-C1C	4.44	1.47	1.39
36	r	306	CHL	CHD-C1D	4.44	1.46	1.39
36	S	606	CHL	CHB-C4A	-4.43	1.33	1.38
36	r	305	CHL	CHD-C1D	4.43	1.46	1.39
36	G	619	CHL	CHC-C1C	4.43	1.47	1.39
36	G	609	CHL	CHD-C4C	4.43	1.47	1.39
36	Y	307	CHL	CHD-C4C	4.43	1.47	1.39
28	t	102	SQD	O8-S	4.43	1.63	1.47
28	A	407	SQD	O8-S	4.42	1.63	1.47
36	r	306	CHL	CHB-C4A	-4.42	1.33	1.38
36	S	601	CHL	CHD-C4C	4.42	1.47	1.39
36	N	310	CHL	CHD-C4C	4.41	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	S	601	CHL	CHC-C1C	4.41	1.47	1.39
36	G	607	CHL	CHC-C1C	4.41	1.47	1.39
36	S	608	CHL	CHD-C4C	4.41	1.47	1.39
28	a	407	SQD	O8-S	4.41	1.63	1.47
36	N	310	CHL	CHB-C4A	-4.40	1.33	1.38
36	G	608	CHL	CHD-C4C	4.40	1.47	1.39
36	Y	303	CHL	CHC-C1C	4.40	1.47	1.39
36	N	302	CHL	CHB-C1B	4.40	1.46	1.39
36	N	309	CHL	CHD-C4C	4.40	1.47	1.39
36	Y	308	CHL	CHD-C4C	4.39	1.47	1.39
36	G	601	CHL	CHD-C1D	4.39	1.46	1.39
36	S	608	CHL	CHC-C1C	4.39	1.47	1.39
36	N	308	CHL	CHC-C1C	4.39	1.47	1.39
36	G	609	CHL	CHD-C1D	4.39	1.46	1.39
36	r	305	CHL	CHB-C4A	-4.39	1.33	1.38
36	N	310	CHL	CHC-C1C	4.38	1.47	1.39
36	Y	303	CHL	CHD-C1D	4.38	1.46	1.39
36	G	607	CHL	CHD-C4C	4.38	1.47	1.39
36	N	306	CHL	CHC-C1C	4.37	1.47	1.39
36	S	608	CHL	CHB-C4A	-4.37	1.33	1.38
36	N	310	CHL	CHD-C1D	4.37	1.46	1.39
36	r	304	CHL	CHC-C1C	4.37	1.47	1.39
36	Y	309	CHL	CHD-C1D	4.36	1.46	1.39
36	G	608	CHL	CHD-C1D	4.36	1.46	1.39
36	G	609	CHL	O2A-CGA	4.36	1.46	1.33
36	G	619	CHL	CHD-C4C	4.36	1.47	1.39
36	S	607	CHL	CHD-C4C	4.36	1.47	1.39
36	N	302	CHL	CHD-C1D	4.36	1.46	1.39
36	r	304	CHL	CHD-C1D	4.35	1.46	1.39
36	r	306	CHL	CHC-C1C	4.34	1.47	1.39
36	N	307	CHL	CHD-C4C	4.34	1.47	1.39
36	S	607	CHL	CHD-C1D	4.34	1.46	1.39
35	F	101	HEM	FE-NB	4.33	2.08	1.94
36	S	601	CHL	CHD-C1D	4.33	1.46	1.39
36	Y	307	CHL	CHD-C1D	4.33	1.46	1.39
36	N	306	CHL	CHD-C4C	4.33	1.47	1.39
36	r	304	CHL	CHB-C4A	-4.33	1.33	1.38
36	G	601	CHL	O2A-CGA	4.30	1.45	1.33
36	G	605	CHL	CHC-C1C	4.30	1.47	1.39
36	G	607	CHL	O2A-CGA	4.30	1.45	1.33
36	G	605	CHL	CHB-C4A	-4.30	1.33	1.38
36	Y	310	CHL	O2A-CGA	4.30	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	N	308	CHL	CHD-C4C	4.29	1.47	1.39
31	C	519	DGD	O1G-C1A	4.29	1.45	1.33
36	G	607	CHL	CHD-C1D	4.29	1.46	1.39
36	G	601	CHL	CHB-C1B	4.29	1.46	1.39
29	C	520	LMG	O8-C28	4.29	1.45	1.33
36	G	601	CHL	CHC-C1C	4.28	1.47	1.39
36	G	609	CHL	CHC-C1C	4.27	1.47	1.39
36	S	606	CHL	CHD-C4C	4.27	1.47	1.39
36	S	601	CHL	CHB-C1B	4.27	1.46	1.39
36	N	310	CHL	O2A-CGA	4.27	1.45	1.33
30	a	411	LHG	O8-C23	4.27	1.45	1.33
36	S	608	CHL	O2A-CGA	4.27	1.45	1.33
31	c	516	DGD	O1G-C1A	4.26	1.45	1.33
28	t	102	SQD	O48-C23	4.26	1.45	1.33
29	d	409	LMG	O8-C28	4.26	1.45	1.33
36	Y	303	CHL	CHB-C1B	4.26	1.46	1.39
28	a	407	SQD	O48-C23	4.26	1.45	1.33
36	S	608	CHL	CHD-C1D	4.26	1.46	1.39
29	a	408	LMG	O8-C28	4.25	1.45	1.33
36	N	302	CHL	O2A-CGA	4.25	1.45	1.33
29	c	518	LMG	O8-C28	4.25	1.45	1.33
36	N	309	CHL	O2A-CGA	4.25	1.45	1.33
31	C	518	DGD	O1G-C1A	4.25	1.45	1.33
30	C	521	LHG	O8-C23	4.25	1.45	1.33
36	G	619	CHL	O2A-CGA	4.24	1.45	1.33
36	Y	309	CHL	O2A-CGA	4.24	1.45	1.33
36	N	307	CHL	CHD-C1D	4.24	1.46	1.39
36	N	306	CHL	O2A-CGA	4.24	1.45	1.33
36	N	308	CHL	O2A-CGA	4.24	1.45	1.33
36	N	309	CHL	CHD-C1D	4.23	1.46	1.39
29	D	410	LMG	O8-C28	4.23	1.45	1.33
30	B	520	LHG	O8-C23	4.23	1.45	1.33
36	G	606	CHL	CHD-C4C	4.23	1.47	1.39
36	G	605	CHL	CHD-C1D	4.23	1.46	1.39
36	Y	303	CHL	O2A-CGA	4.23	1.45	1.33
36	Y	308	CHL	CHD-C1D	4.23	1.46	1.39
29	H	102	LMG	O8-C28	4.22	1.45	1.33
36	S	606	CHL	CHD-C1D	4.22	1.46	1.39
29	B	519	LMG	O8-C28	4.22	1.45	1.33
31	Y	301	DGD	O1G-C1A	4.21	1.45	1.33
31	c	515	DGD	O1G-C1A	4.21	1.45	1.33
36	G	619	CHL	CHD-C1D	4.21	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	L	101	LHG	O8-C23	4.20	1.45	1.33
29	b	520	LMG	O8-C28	4.20	1.45	1.33
30	N	319	LHG	O8-C23	4.19	1.45	1.33
28	t	102	SQD	O47-C7	4.19	1.46	1.34
30	D	408	LHG	O8-C23	4.18	1.45	1.33
29	d	410	LMG	O8-C28	4.18	1.45	1.33
30	b	521	LHG	O8-C23	4.18	1.45	1.33
30	a	410	LHG	O8-C23	4.18	1.45	1.33
28	A	407	SQD	O48-C23	4.18	1.45	1.33
36	N	306	CHL	CHD-C1D	4.17	1.46	1.39
30	D	409	LHG	O8-C23	4.17	1.45	1.33
31	W	202	DGD	O1G-C1A	4.17	1.45	1.33
29	W	201	LMG	O8-C28	4.17	1.45	1.33
31	C	517	DGD	O1G-C1A	4.17	1.45	1.33
31	c	517	DGD	O1G-C1A	4.16	1.45	1.33
30	a	410	LHG	O7-C7	4.16	1.46	1.34
29	H	102	LMG	O7-C10	4.16	1.46	1.34
30	Y	319	LHG	O8-C23	4.16	1.45	1.33
29	D	410	LMG	O7-C10	4.16	1.46	1.34
29	C	520	LMG	O7-C10	4.15	1.46	1.34
35	F	101	HEM	FE-ND	4.15	2.07	1.94
30	l	101	LHG	O8-C23	4.14	1.45	1.33
30	G	618	LHG	O8-C23	4.14	1.45	1.33
30	d	407	LHG	O8-C23	4.13	1.45	1.33
30	d	408	LHG	O8-C23	4.13	1.45	1.33
30	C	521	LHG	O7-C7	4.12	1.45	1.34
28	a	407	SQD	O47-C7	4.11	1.45	1.34
36	N	308	CHL	CHD-C1D	4.10	1.46	1.39
30	S	618	LHG	O8-C23	4.09	1.45	1.33
29	a	408	LMG	O7-C10	4.09	1.45	1.34
29	B	519	LMG	O7-C10	4.09	1.45	1.34
30	b	521	LHG	O7-C7	4.08	1.45	1.34
30	D	409	LHG	O7-C7	4.08	1.45	1.34
30	a	411	LHG	O7-C7	4.07	1.45	1.34
29	W	201	LMG	O7-C10	4.07	1.45	1.34
28	A	407	SQD	O47-C7	4.06	1.45	1.34
29	c	518	LMG	O7-C10	4.06	1.45	1.34
31	C	519	DGD	O2G-C1B	4.06	1.45	1.34
31	Y	301	DGD	O2G-C1B	4.05	1.45	1.34
31	C	518	DGD	O2G-C1B	4.05	1.45	1.34
31	c	517	DGD	O2G-C1B	4.05	1.45	1.34
29	d	410	LMG	O7-C10	4.05	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	516	DGD	O2G-C1B	4.05	1.45	1.34
36	G	606	CHL	CHD-C1D	4.05	1.46	1.39
30	D	408	LHG	O7-C7	4.04	1.45	1.34
31	c	515	DGD	O2G-C1B	4.04	1.45	1.34
29	d	409	LMG	O7-C10	4.03	1.45	1.34
30	Y	319	LHG	O7-C7	4.01	1.45	1.34
31	W	202	DGD	O2G-C1B	4.01	1.45	1.34
31	C	517	DGD	O2G-C1B	4.01	1.45	1.34
30	S	618	LHG	O7-C7	4.01	1.45	1.34
30	B	520	LHG	O7-C7	4.01	1.45	1.34
30	L	101	LHG	O7-C7	4.01	1.45	1.34
30	N	319	LHG	O7-C7	4.00	1.45	1.34
30	l	101	LHG	O7-C7	4.00	1.45	1.34
30	G	618	LHG	O7-C7	3.99	1.45	1.34
36	r	305	CHL	C3D-C2D	3.97	1.46	1.39
36	S	606	CHL	C3D-C2D	3.96	1.46	1.39
29	b	520	LMG	O7-C10	3.96	1.45	1.34
36	r	304	CHL	C3D-C2D	3.96	1.46	1.39
30	d	407	LHG	O7-C7	3.95	1.45	1.34
30	d	408	LHG	O7-C7	3.95	1.45	1.34
36	Y	310	CHL	C3D-C2D	3.89	1.46	1.39
36	N	307	CHL	C3D-C2D	3.87	1.46	1.39
36	Y	307	CHL	C3D-C2D	3.86	1.46	1.39
36	S	607	CHL	C3D-C2D	3.85	1.46	1.39
36	G	609	CHL	C3D-C2D	3.85	1.46	1.39
36	G	606	CHL	C3D-C2D	3.84	1.46	1.39
36	r	306	CHL	C3D-C2D	3.84	1.46	1.39
36	G	607	CHL	C3D-C2D	3.83	1.46	1.39
26	d	402	PHO	C1D-C2D	3.81	1.43	1.39
35	F	101	HEM	FE-NA	3.81	2.07	1.95
36	N	302	CHL	C3D-C2D	3.81	1.46	1.39
36	G	601	CHL	C3D-C2D	3.80	1.46	1.39
36	G	608	CHL	C3D-C2D	3.79	1.46	1.39
36	Y	308	CHL	C3D-C2D	3.79	1.46	1.39
36	G	605	CHL	C3D-C2D	3.79	1.46	1.39
35	F	101	HEM	FE-NC	3.78	2.07	1.95
36	S	601	CHL	C3D-C2D	3.78	1.46	1.39
36	Y	303	CHL	C3D-C2D	3.78	1.46	1.39
36	N	308	CHL	C3D-C2D	3.77	1.46	1.39
36	G	619	CHL	C3D-C2D	3.76	1.46	1.39
36	N	310	CHL	C3D-C2D	3.76	1.46	1.39
25	r	307	CLA	C1D-ND	3.76	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	N	306	CHL	C3D-C2D	3.76	1.46	1.39
36	Y	309	CHL	C3D-C2D	3.75	1.46	1.39
38	Y	318	NEX	C7-C6	-3.75	1.26	1.30
36	S	608	CHL	C3D-C2D	3.75	1.46	1.39
34	d	406	PL9	C3-C4	-3.73	1.43	1.49
36	N	309	CHL	C3D-C2D	3.70	1.46	1.39
25	r	308	CLA	C1D-ND	3.69	1.42	1.37
26	D	402	PHO	C1D-C2D	3.69	1.43	1.39
26	A	404	PHO	C1D-C2D	3.69	1.43	1.39
26	A	404	PHO	C4D-CHA	3.67	1.45	1.39
35	f	101	HEM	FE-NB	3.64	2.06	1.94
34	D	407	PL9	C3-C4	-3.62	1.43	1.49
38	S	617	NEX	C7-C6	-3.62	1.26	1.30
26	a	404	PHO	C4D-CHA	3.62	1.45	1.39
25	r	301	CLA	C1D-ND	3.62	1.42	1.37
25	B	516	CLA	C1D-ND	3.62	1.42	1.37
25	r	308	CLA	C4B-NB	3.62	1.42	1.37
26	a	404	PHO	C1D-C2D	3.61	1.43	1.39
25	N	311	CLA	C1D-ND	3.60	1.42	1.37
25	b	507	CLA	C1D-ND	3.58	1.42	1.37
25	d	404	CLA	C1D-ND	3.57	1.42	1.37
25	B	507	CLA	C1D-ND	3.57	1.42	1.37
25	B	514	CLA	C1D-ND	3.56	1.42	1.37
25	Y	311	CLA	C1D-ND	3.56	1.42	1.37
25	S	605	CLA	C1D-ND	3.56	1.42	1.37
25	r	302	CLA	C1D-ND	3.56	1.42	1.37
25	Y	314	CLA	C1D-ND	3.55	1.42	1.37
38	G	617	NEX	C7-C6	-3.55	1.26	1.30
25	C	503	CLA	C1D-ND	3.54	1.42	1.37
25	D	405	CLA	C1D-ND	3.54	1.42	1.37
25	S	609	CLA	C1D-ND	3.54	1.42	1.37
25	r	307	CLA	C4B-NB	3.52	1.42	1.37
25	Y	313	CLA	C1D-ND	3.52	1.42	1.37
25	B	510	CLA	C1D-ND	3.51	1.42	1.37
25	S	614	CLA	C1D-ND	3.51	1.42	1.37
25	c	511	CLA	C1D-ND	3.51	1.42	1.37
25	N	314	CLA	C1D-ND	3.50	1.42	1.37
26	D	402	PHO	C4D-CHA	3.50	1.44	1.39
35	f	101	HEM	FE-ND	3.50	2.05	1.94
25	Y	304	CLA	C1D-ND	3.50	1.42	1.37
25	b	516	CLA	C1D-ND	3.50	1.42	1.37
25	G	613	CLA	C1D-ND	3.50	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	604	CLA	C1D-ND	3.50	1.42	1.37
25	A	403	CLA	C1D-ND	3.49	1.42	1.37
25	c	513	CLA	C1D-ND	3.49	1.42	1.37
25	D	401	CLA	C1D-ND	3.49	1.42	1.37
25	N	313	CLA	C1D-ND	3.49	1.42	1.37
25	c	504	CLA	C1D-ND	3.49	1.42	1.37
25	C	510	CLA	C1D-ND	3.49	1.42	1.37
25	c	508	CLA	C1D-ND	3.49	1.42	1.37
25	c	510	CLA	C1D-ND	3.48	1.42	1.37
25	G	612	CLA	C1D-ND	3.48	1.42	1.37
25	r	303	CLA	C1D-ND	3.48	1.42	1.37
25	c	506	CLA	C1D-ND	3.48	1.42	1.37
25	G	614	CLA	C1D-ND	3.48	1.42	1.37
25	Y	315	CLA	C1D-ND	3.48	1.42	1.37
25	G	610	CLA	C1D-ND	3.48	1.42	1.37
25	S	611	CLA	C1D-ND	3.48	1.42	1.37
25	G	602	CLA	C1D-ND	3.48	1.42	1.37
25	C	502	CLA	C1D-ND	3.48	1.42	1.37
25	S	613	CLA	C1D-ND	3.47	1.42	1.37
25	S	604	CLA	C1D-ND	3.47	1.42	1.37
25	b	501	CLA	C1D-ND	3.47	1.42	1.37
25	C	511	CLA	C1D-ND	3.47	1.42	1.37
25	C	509	CLA	C1D-ND	3.46	1.42	1.37
38	r	310	NEX	C7-C6	-3.46	1.26	1.30
25	Y	306	CLA	C1D-ND	3.46	1.42	1.37
25	N	315	CLA	C1D-ND	3.46	1.42	1.37
25	c	507	CLA	C1D-ND	3.46	1.42	1.37
25	B	509	CLA	C1D-ND	3.46	1.42	1.37
25	C	507	CLA	C1D-ND	3.45	1.42	1.37
25	a	405	CLA	C1D-ND	3.45	1.42	1.37
25	N	312	CLA	C1D-ND	3.45	1.42	1.37
25	b	515	CLA	C1D-ND	3.45	1.42	1.37
25	C	508	CLA	C1D-ND	3.45	1.42	1.37
25	C	506	CLA	C1D-ND	3.45	1.42	1.37
25	c	501	CLA	C1D-ND	3.45	1.42	1.37
25	B	506	CLA	C1D-ND	3.45	1.42	1.37
25	N	304	CLA	C1D-ND	3.45	1.42	1.37
26	d	402	PHO	C4D-CHA	3.45	1.44	1.39
25	G	603	CLA	C1D-ND	3.45	1.42	1.37
25	B	515	CLA	C1D-ND	3.44	1.42	1.37
25	d	401	CLA	C1D-ND	3.44	1.42	1.37
25	c	503	CLA	C1D-ND	3.44	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	402	CLA	C1D-ND	3.44	1.42	1.37
25	B	501	CLA	C1D-ND	3.44	1.42	1.37
25	b	504	CLA	C1D-ND	3.44	1.42	1.37
25	G	611	CLA	C1D-ND	3.43	1.42	1.37
25	C	501	CLA	C1D-ND	3.43	1.42	1.37
25	b	511	CLA	C1D-ND	3.43	1.42	1.37
25	c	509	CLA	C1D-ND	3.43	1.42	1.37
25	S	612	CLA	C1D-ND	3.43	1.42	1.37
25	S	602	CLA	C1D-ND	3.43	1.42	1.37
25	B	505	CLA	C1D-ND	3.43	1.42	1.37
25	Y	305	CLA	C1D-ND	3.43	1.42	1.37
25	r	301	CLA	C4B-NB	3.42	1.42	1.37
25	B	511	CLA	C1D-ND	3.42	1.42	1.37
25	N	303	CLA	C1D-ND	3.41	1.42	1.37
25	N	305	CLA	C1D-ND	3.41	1.42	1.37
25	A	405	CLA	C1D-ND	3.41	1.42	1.37
25	C	504	CLA	C1D-ND	3.41	1.42	1.37
25	S	610	CLA	C1D-ND	3.41	1.42	1.37
25	a	402	CLA	C1D-ND	3.41	1.42	1.37
25	b	509	CLA	C1D-ND	3.40	1.42	1.37
25	B	513	CLA	C1D-ND	3.40	1.42	1.37
25	b	513	CLA	C1D-ND	3.40	1.42	1.37
25	C	512	CLA	C1D-ND	3.40	1.42	1.37
25	b	505	CLA	C1D-ND	3.40	1.42	1.37
32	c	519	LMU	O5'-C1'	3.40	1.50	1.41
25	Y	312	CLA	C1D-ND	3.40	1.42	1.37
25	B	512	CLA	C1D-ND	3.40	1.42	1.37
38	G	617	NEX	C7-C8	-3.39	1.26	1.31
25	a	403	CLA	C1D-ND	3.39	1.42	1.37
25	S	603	CLA	C1D-ND	3.39	1.42	1.37
25	b	514	CLA	C1D-ND	3.38	1.42	1.37
25	B	502	CLA	C1D-ND	3.38	1.42	1.37
25	B	504	CLA	C1D-ND	3.37	1.42	1.37
25	b	506	CLA	C1D-ND	3.37	1.42	1.37
25	b	508	CLA	C1D-ND	3.37	1.42	1.37
25	b	510	CLA	C1D-ND	3.37	1.42	1.37
25	B	503	CLA	C1D-ND	3.37	1.42	1.37
38	N	318	NEX	C7-C6	-3.36	1.26	1.30
25	b	502	CLA	C1D-ND	3.36	1.42	1.37
38	S	617	NEX	C7-C8	-3.36	1.26	1.31
25	c	512	CLA	C1D-ND	3.36	1.42	1.37
25	c	502	CLA	C1D-ND	3.35	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	505	CLA	C1D-ND	3.34	1.42	1.37
25	r	303	CLA	C4B-NB	3.34	1.42	1.37
25	C	513	CLA	C1D-ND	3.33	1.42	1.37
32	S	619	LMU	O5B-C1B	3.33	1.50	1.41
25	d	401	CLA	C4B-NB	3.32	1.42	1.37
25	S	613	CLA	C4B-NB	3.31	1.42	1.37
25	b	512	CLA	C1D-ND	3.31	1.42	1.37
32	C	523	LMU	O5B-C1B	3.31	1.50	1.41
25	b	503	CLA	C1D-ND	3.30	1.42	1.37
38	Y	318	NEX	C7-C8	-3.28	1.26	1.31
32	C	522	LMU	O5B-C1B	3.28	1.50	1.41
32	S	619	LMU	O5'-C1'	3.28	1.50	1.41
25	d	403	CLA	C1D-ND	3.27	1.42	1.37
25	S	609	CLA	C4B-NB	3.27	1.42	1.37
25	r	302	CLA	C4B-NB	3.26	1.42	1.37
25	B	508	CLA	C1D-ND	3.26	1.42	1.37
25	c	501	CLA	C4B-NB	3.26	1.42	1.37
32	c	519	LMU	O5B-C1B	3.25	1.50	1.41
25	b	501	CLA	C4B-NB	3.25	1.42	1.37
32	C	522	LMU	O5'-C1'	3.24	1.50	1.41
25	S	614	CLA	C4B-NB	3.24	1.42	1.37
25	C	512	CLA	C4B-NB	3.24	1.42	1.37
25	D	404	CLA	C1D-ND	3.24	1.42	1.37
25	N	313	CLA	C4B-NB	3.23	1.42	1.37
25	C	501	CLA	C4B-NB	3.22	1.42	1.37
25	G	610	CLA	C4B-NB	3.22	1.42	1.37
25	G	603	CLA	C4B-NB	3.22	1.42	1.37
25	N	315	CLA	C4B-NB	3.22	1.42	1.37
25	d	404	CLA	C4B-NB	3.22	1.42	1.37
25	S	602	CLA	C4B-NB	3.21	1.42	1.37
25	S	603	CLA	C4B-NB	3.21	1.42	1.37
25	S	605	CLA	C4B-NB	3.21	1.42	1.37
38	r	310	NEX	C7-C8	-3.21	1.26	1.31
25	c	505	CLA	C1D-ND	3.20	1.42	1.37
32	C	523	LMU	O5'-C1'	3.20	1.50	1.41
25	N	314	CLA	C4B-NB	3.20	1.42	1.37
25	c	510	CLA	C4B-NB	3.19	1.42	1.37
25	D	405	CLA	C4B-NB	3.18	1.42	1.37
35	f	101	HEM	FE-NA	3.18	2.05	1.95
25	c	504	CLA	C4B-NB	3.18	1.42	1.37
25	N	312	CLA	C4B-NB	3.18	1.42	1.37
25	C	504	CLA	C4B-NB	3.17	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	604	CLA	C4B-NB	3.16	1.42	1.37
25	B	509	CLA	C4B-NB	3.16	1.42	1.37
38	N	318	NEX	C7-C8	-3.16	1.26	1.31
25	Y	314	CLA	C4B-NB	3.16	1.42	1.37
25	G	604	CLA	C4B-NB	3.16	1.42	1.37
25	N	305	CLA	C4B-NB	3.15	1.42	1.37
25	b	508	CLA	C4B-NB	3.15	1.42	1.37
25	Y	311	CLA	C4B-NB	3.15	1.42	1.37
25	B	514	CLA	C4B-NB	3.15	1.42	1.37
25	B	508	CLA	C4B-NB	3.15	1.42	1.37
25	B	506	CLA	C4B-NB	3.15	1.42	1.37
25	G	614	CLA	C4B-NB	3.15	1.42	1.37
25	S	610	CLA	C4B-NB	3.15	1.42	1.37
25	B	511	CLA	C4B-NB	3.14	1.42	1.37
25	G	612	CLA	C4B-NB	3.14	1.42	1.37
25	c	511	CLA	C4B-NB	3.14	1.42	1.37
25	c	512	CLA	C4B-NB	3.14	1.42	1.37
25	C	511	CLA	C4B-NB	3.14	1.42	1.37
25	G	613	CLA	C4B-NB	3.14	1.42	1.37
34	D	407	PL9	C7-C3	-3.14	1.47	1.51
25	C	508	CLA	C4B-NB	3.14	1.42	1.37
25	A	403	CLA	C4B-NB	3.13	1.42	1.37
25	B	504	CLA	C4B-NB	3.13	1.42	1.37
25	B	502	CLA	C4B-NB	3.13	1.42	1.37
25	N	303	CLA	C4B-NB	3.13	1.42	1.37
25	Y	312	CLA	C4B-NB	3.12	1.42	1.37
25	N	304	CLA	C4B-NB	3.12	1.42	1.37
25	B	515	CLA	C4B-NB	3.12	1.42	1.37
25	c	505	CLA	C4B-NB	3.12	1.42	1.37
25	b	509	CLA	C4B-NB	3.11	1.42	1.37
25	C	506	CLA	C4B-NB	3.11	1.42	1.37
25	D	404	CLA	C4B-NB	3.11	1.42	1.37
25	Y	313	CLA	C4B-NB	3.11	1.41	1.37
25	C	510	CLA	C4B-NB	3.11	1.41	1.37
25	B	510	CLA	C4B-NB	3.10	1.41	1.37
25	c	513	CLA	C4B-NB	3.09	1.41	1.37
25	c	503	CLA	C4B-NB	3.09	1.41	1.37
25	B	507	CLA	C4B-NB	3.09	1.41	1.37
34	d	406	PL9	C7-C3	-3.09	1.47	1.51
25	B	501	CLA	C4B-NB	3.09	1.41	1.37
25	b	514	CLA	C4B-NB	3.08	1.41	1.37
25	d	403	CLA	C4B-NB	3.08	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	515	CLA	C4B-NB	3.08	1.41	1.37
25	b	507	CLA	C4B-NB	3.08	1.41	1.37
25	c	508	CLA	C4B-NB	3.08	1.41	1.37
25	b	503	CLA	C4B-NB	3.08	1.41	1.37
25	C	505	CLA	C4B-NB	3.07	1.41	1.37
25	c	506	CLA	C4B-NB	3.07	1.41	1.37
25	B	503	CLA	C4B-NB	3.07	1.41	1.37
25	C	503	CLA	C4B-NB	3.07	1.41	1.37
25	B	513	CLA	C4B-NB	3.07	1.41	1.37
25	a	403	CLA	C4B-NB	3.07	1.41	1.37
25	S	612	CLA	C4B-NB	3.07	1.41	1.37
35	F	101	HEM	CAB-C3B	3.07	1.55	1.47
25	G	611	CLA	C4B-NB	3.06	1.41	1.37
25	b	511	CLA	C4B-NB	3.06	1.41	1.37
25	Y	306	CLA	C4B-NB	3.06	1.41	1.37
25	B	505	CLA	C4B-NB	3.05	1.41	1.37
25	b	506	CLA	C4B-NB	3.04	1.41	1.37
25	c	502	CLA	C4B-NB	3.04	1.41	1.37
25	C	509	CLA	C4B-NB	3.04	1.41	1.37
25	A	402	CLA	C4B-NB	3.03	1.41	1.37
25	D	401	CLA	C4B-NB	3.03	1.41	1.37
25	C	513	CLA	C4B-NB	3.03	1.41	1.37
25	N	311	CLA	C4B-NB	3.02	1.41	1.37
25	Y	305	CLA	C4B-NB	3.02	1.41	1.37
25	c	509	CLA	C4B-NB	3.02	1.41	1.37
25	B	516	CLA	C4B-NB	3.02	1.41	1.37
25	b	504	CLA	C4B-NB	3.02	1.41	1.37
25	b	502	CLA	C4B-NB	3.01	1.41	1.37
25	b	513	CLA	C4B-NB	3.01	1.41	1.37
25	b	505	CLA	C4B-NB	3.00	1.41	1.37
35	f	101	HEM	CAC-C3C	2.99	1.55	1.47
25	A	405	CLA	C4B-NB	2.98	1.41	1.37
25	c	507	CLA	C4B-NB	2.98	1.41	1.37
25	a	402	CLA	C4B-NB	2.97	1.41	1.37
25	G	602	CLA	C4B-NB	2.97	1.41	1.37
25	C	507	CLA	C4B-NB	2.97	1.41	1.37
25	Y	315	CLA	C4B-NB	2.96	1.41	1.37
35	F	101	HEM	CAC-C3C	2.96	1.55	1.47
25	B	512	CLA	C4B-NB	2.96	1.41	1.37
25	a	405	CLA	C4B-NB	2.95	1.41	1.37
25	S	611	CLA	C4B-NB	2.95	1.41	1.37
25	b	516	CLA	C4B-NB	2.94	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	502	CLA	C4B-NB	2.94	1.41	1.37
34	d	406	PL9	C6-C1	-2.94	1.43	1.48
25	b	512	CLA	C4B-NB	2.94	1.41	1.37
25	b	510	CLA	C4B-NB	2.92	1.41	1.37
35	f	101	HEM	CAB-C3B	2.89	1.55	1.47
25	Y	304	CLA	C4B-NB	2.87	1.41	1.37
25	r	307	CLA	MG-NA	2.78	2.12	2.06
26	A	404	PHO	CMC-C2C	-2.73	1.46	1.50
25	r	307	CLA	C1B-C2B	2.73	1.49	1.43
35	f	101	HEM	FE-NC	2.73	2.04	1.95
25	r	308	CLA	C1B-C2B	2.72	1.49	1.43
25	C	502	CLA	C1B-C2B	2.72	1.49	1.43
25	N	314	CLA	C1B-C2B	2.72	1.49	1.43
25	B	509	CLA	C1B-C2B	2.71	1.49	1.43
25	C	507	CLA	C1B-C2B	2.71	1.49	1.43
25	B	501	CLA	C1B-C2B	2.69	1.49	1.43
25	G	613	CLA	C1B-C2B	2.69	1.49	1.43
25	Y	314	CLA	C1B-C2B	2.69	1.49	1.43
26	D	402	PHO	CMC-C2C	-2.69	1.46	1.50
25	c	513	CLA	C1B-C2B	2.69	1.49	1.43
25	C	503	CLA	C1B-C2B	2.69	1.49	1.43
25	C	511	CLA	C1B-C2B	2.68	1.49	1.43
25	b	509	CLA	C1B-C2B	2.68	1.49	1.43
25	D	405	CLA	C1B-C2B	2.68	1.49	1.43
25	B	515	CLA	C1B-C2B	2.68	1.49	1.43
26	a	404	PHO	CMC-C2C	-2.68	1.46	1.50
25	C	501	CLA	C1B-C2B	2.67	1.49	1.43
25	G	611	CLA	C1B-C2B	2.67	1.49	1.43
25	Y	311	CLA	C1B-C2B	2.66	1.49	1.43
25	c	502	CLA	C1B-C2B	2.66	1.49	1.43
25	b	505	CLA	C1B-C2B	2.66	1.49	1.43
25	N	312	CLA	C1B-C2B	2.66	1.49	1.43
25	b	515	CLA	C1B-C2B	2.66	1.49	1.43
26	d	402	PHO	CMC-C2C	-2.66	1.46	1.50
25	S	611	CLA	C1B-C2B	2.65	1.49	1.43
25	r	301	CLA	C1B-C2B	2.65	1.49	1.43
25	B	516	CLA	C1B-C2B	2.65	1.49	1.43
25	Y	313	CLA	C1B-C2B	2.64	1.49	1.43
25	S	604	CLA	C1B-C2B	2.64	1.49	1.43
25	r	302	CLA	C1B-C2B	2.64	1.49	1.43
25	Y	312	CLA	C1B-C2B	2.64	1.49	1.43
25	r	303	CLA	C1B-C2B	2.64	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	614	CLA	C1B-C2B	2.64	1.49	1.43
25	N	303	CLA	C1B-C2B	2.64	1.49	1.43
25	b	512	CLA	C1B-C2B	2.64	1.49	1.43
26	d	402	PHO	CMD-C2D	-2.63	1.46	1.51
34	D	407	PL9	C6-C1	-2.63	1.44	1.48
25	c	511	CLA	C1B-C2B	2.63	1.49	1.43
25	N	305	CLA	C1B-C2B	2.63	1.49	1.43
25	B	505	CLA	C1B-C2B	2.63	1.49	1.43
25	G	612	CLA	C1B-C2B	2.63	1.49	1.43
25	S	613	CLA	C1B-C2B	2.62	1.49	1.43
25	S	602	CLA	C1B-C2B	2.62	1.49	1.43
25	N	315	CLA	C1B-C2B	2.62	1.49	1.43
26	D	402	PHO	CMD-C2D	-2.62	1.46	1.51
25	b	507	CLA	C1B-C2B	2.62	1.49	1.43
25	C	513	CLA	C1B-C2B	2.61	1.49	1.43
25	B	512	CLA	C1B-C2B	2.61	1.49	1.43
25	C	509	CLA	C1B-C2B	2.61	1.49	1.43
25	B	514	CLA	C1B-C2B	2.61	1.49	1.43
25	Y	304	CLA	C1B-C2B	2.61	1.49	1.43
25	D	404	CLA	C1B-C2B	2.61	1.49	1.43
25	Y	315	CLA	C1B-C2B	2.61	1.49	1.43
25	b	504	CLA	C1B-C2B	2.60	1.49	1.43
25	d	403	CLA	C1B-C2B	2.60	1.49	1.43
25	B	502	CLA	C1B-C2B	2.60	1.49	1.43
25	S	609	CLA	C1B-C2B	2.60	1.49	1.43
25	N	311	CLA	C1B-C2B	2.60	1.49	1.43
25	S	612	CLA	C1B-C2B	2.60	1.49	1.43
25	b	506	CLA	C1B-C2B	2.60	1.49	1.43
25	C	504	CLA	C1B-C2B	2.59	1.49	1.43
25	G	602	CLA	C1B-C2B	2.59	1.49	1.43
25	G	604	CLA	C1B-C2B	2.59	1.49	1.43
26	A	404	PHO	CMD-C2D	-2.59	1.46	1.51
25	A	405	CLA	C1B-C2B	2.59	1.49	1.43
25	S	605	CLA	C1B-C2B	2.59	1.49	1.43
25	D	401	CLA	C1B-C2B	2.59	1.49	1.43
25	c	507	CLA	C1B-C2B	2.59	1.49	1.43
25	d	404	CLA	C1B-C2B	2.59	1.49	1.43
25	B	511	CLA	C1B-C2B	2.59	1.49	1.43
25	Y	305	CLA	C1B-C2B	2.59	1.49	1.43
25	S	603	CLA	C1B-C2B	2.59	1.49	1.43
25	c	504	CLA	C1B-C2B	2.59	1.49	1.43
25	c	501	CLA	C1B-C2B	2.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	503	CLA	C1B-C2B	2.58	1.49	1.43
25	Y	306	CLA	C1B-C2B	2.58	1.49	1.43
25	B	510	CLA	C1B-C2B	2.58	1.49	1.43
25	a	405	CLA	C1B-C2B	2.58	1.49	1.43
25	b	501	CLA	C1B-C2B	2.58	1.49	1.43
25	A	403	CLA	C1B-C2B	2.58	1.49	1.43
25	B	504	CLA	C1B-C2B	2.57	1.49	1.43
25	d	401	CLA	C1B-C2B	2.57	1.49	1.43
25	N	313	CLA	C1B-C2B	2.57	1.49	1.43
25	G	603	CLA	C1B-C2B	2.56	1.49	1.43
25	b	511	CLA	C1B-C2B	2.56	1.49	1.43
25	c	509	CLA	C1B-C2B	2.56	1.49	1.43
25	b	514	CLA	C1B-C2B	2.56	1.49	1.43
25	B	513	CLA	C1B-C2B	2.55	1.49	1.43
25	G	610	CLA	C1B-C2B	2.55	1.49	1.43
25	b	502	CLA	C1B-C2B	2.55	1.49	1.43
25	C	510	CLA	C1B-C2B	2.55	1.49	1.43
26	a	404	PHO	CMD-C2D	-2.55	1.46	1.51
25	B	503	CLA	C1B-C2B	2.55	1.49	1.43
25	N	304	CLA	C1B-C2B	2.55	1.49	1.43
25	b	510	CLA	C1B-C2B	2.55	1.49	1.43
25	C	506	CLA	C1B-C2B	2.55	1.49	1.43
25	S	614	CLA	C1B-C2B	2.55	1.49	1.43
25	a	402	CLA	C1B-C2B	2.54	1.49	1.43
25	a	403	CLA	C1B-C2B	2.54	1.49	1.43
25	c	503	CLA	C1B-C2B	2.54	1.49	1.43
25	c	505	CLA	C1B-C2B	2.54	1.49	1.43
25	c	508	CLA	C1B-C2B	2.54	1.49	1.43
25	B	506	CLA	C1B-C2B	2.54	1.49	1.43
25	B	507	CLA	C1B-C2B	2.54	1.49	1.43
25	C	512	CLA	C1B-C2B	2.54	1.49	1.43
25	b	516	CLA	C1B-C2B	2.54	1.49	1.43
25	c	510	CLA	C1B-C2B	2.54	1.49	1.43
26	A	404	PHO	CMB-C2B	-2.54	1.46	1.51
25	C	508	CLA	C1B-C2B	2.54	1.49	1.43
25	C	505	CLA	C1B-C2B	2.53	1.49	1.43
25	S	610	CLA	C1B-C2B	2.52	1.49	1.43
26	a	404	PHO	CMB-C2B	-2.51	1.46	1.51
25	b	513	CLA	C1B-C2B	2.51	1.49	1.43
25	c	506	CLA	C1B-C2B	2.51	1.49	1.43
25	A	402	CLA	C1B-C2B	2.51	1.49	1.43
26	d	402	PHO	CMB-C2B	-2.50	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	512	CLA	C1B-C2B	2.49	1.49	1.43
26	D	402	PHO	CMB-C2B	-2.49	1.46	1.51
26	A	404	PHO	CAC-C3C	-2.47	1.47	1.51
25	b	508	CLA	CMB-C2B	-2.45	1.45	1.50
25	B	508	CLA	C1B-C2B	2.45	1.48	1.43
27	a	406	BCR	C30-C25	-2.43	1.50	1.53
25	d	403	CLA	CMC-C2C	-2.41	1.45	1.50
34	d	406	PL9	C53-C6	-2.41	1.45	1.50
26	a	404	PHO	CAC-C3C	-2.40	1.47	1.51
25	D	404	CLA	CMD-C2D	-2.38	1.45	1.50
26	d	402	PHO	CAC-C3C	-2.37	1.47	1.51
25	b	508	CLA	C1B-C2B	2.37	1.48	1.43
25	S	614	CLA	C3B-C4B	2.37	1.49	1.42
39	G	620	XAT	O24-C25	-2.36	1.43	1.46
25	S	610	CLA	C3B-C4B	2.35	1.49	1.42
26	a	404	PHO	C3D-C4D	2.35	1.44	1.41
27	C	515	BCR	C30-C25	-2.35	1.50	1.53
25	N	313	CLA	C3B-C4B	2.33	1.49	1.42
25	d	401	CLA	C3B-C4B	2.33	1.49	1.42
25	b	501	CLA	C3B-C4B	2.32	1.49	1.42
25	S	613	CLA	C3B-C4B	2.32	1.49	1.42
26	D	402	PHO	CAC-C3C	-2.32	1.47	1.51
25	N	312	CLA	C3B-C4B	2.31	1.49	1.42
25	c	505	CLA	CMD-C2D	-2.31	1.46	1.50
25	C	512	CLA	C3B-C4B	2.30	1.49	1.42
25	N	315	CLA	C3B-C4B	2.30	1.49	1.42
25	c	501	CLA	C3B-C4B	2.30	1.49	1.42
25	Y	304	CLA	C3B-C4B	2.30	1.49	1.42
25	N	304	CLA	C3B-C4B	2.30	1.49	1.42
25	G	610	CLA	C3B-C4B	2.30	1.49	1.42
25	G	604	CLA	C3B-C4B	2.30	1.49	1.42
25	C	505	CLA	CMD-C2D	-2.29	1.46	1.50
25	B	510	CLA	C3B-C4B	2.29	1.49	1.42
25	C	501	CLA	C3B-C4B	2.29	1.49	1.42
25	c	511	CLA	C3B-C4B	2.29	1.49	1.42
25	B	508	CLA	CMB-C2B	-2.29	1.46	1.50
25	N	303	CLA	C3B-C4B	2.29	1.49	1.42
25	c	505	CLA	C3B-C4B	2.29	1.49	1.42
25	G	602	CLA	C3B-C4B	2.29	1.49	1.42
34	D	407	PL9	C53-C6	-2.28	1.46	1.50
25	b	511	CLA	CMB-C2B	-2.28	1.46	1.50
25	B	514	CLA	C3B-C4B	2.28	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	505	CLA	C3B-C4B	2.28	1.49	1.42
25	C	510	CLA	C3B-C4B	2.28	1.49	1.42
25	A	402	CLA	CMC-C2C	-2.27	1.46	1.50
25	b	508	CLA	CMD-C2D	-2.27	1.46	1.50
25	b	516	CLA	CMC-C2C	-2.27	1.46	1.50
25	Y	311	CLA	C3B-C4B	2.27	1.49	1.42
39	N	301	XAT	O4-C5	-2.27	1.43	1.46
26	D	402	PHO	C3D-C4D	2.27	1.44	1.41
25	B	507	CLA	C3B-C4B	2.27	1.49	1.42
25	C	504	CLA	C3B-C4B	2.27	1.49	1.42
39	Y	302	XAT	O4-C5	-2.27	1.43	1.46
25	r	302	CLA	C3B-C4B	2.27	1.49	1.42
25	c	503	CLA	C3B-C4B	2.27	1.49	1.42
25	G	603	CLA	C3B-C4B	2.27	1.49	1.42
25	Y	306	CLA	C3B-C4B	2.26	1.49	1.42
25	b	503	CLA	CMD-C2D	-2.26	1.46	1.50
25	B	506	CLA	C3B-C4B	2.26	1.49	1.42
25	G	614	CLA	C3B-C4B	2.26	1.49	1.42
25	c	508	CLA	C3B-C4B	2.26	1.49	1.42
25	S	602	CLA	C3B-C4B	2.26	1.49	1.42
25	B	513	CLA	C3B-C4B	2.26	1.49	1.42
25	A	402	CLA	CMD-C2D	-2.26	1.46	1.50
25	d	403	CLA	CMD-C2D	-2.26	1.46	1.50
26	A	404	PHO	C3D-C4D	2.26	1.44	1.41
25	C	502	CLA	CMB-C2B	-2.26	1.46	1.50
27	V	101	BCR	C1-C6	-2.26	1.50	1.53
25	Y	312	CLA	C3B-C4B	2.26	1.49	1.42
25	r	301	CLA	C3B-C4B	2.25	1.49	1.42
25	r	308	CLA	C3B-C4B	2.25	1.49	1.42
25	B	503	CLA	C3B-C4B	2.25	1.49	1.42
25	b	502	CLA	C3B-C4B	2.25	1.49	1.42
25	b	509	CLA	CMB-C2B	-2.24	1.46	1.50
25	B	505	CLA	C3B-C4B	2.24	1.49	1.42
25	c	502	CLA	CMB-C2B	-2.24	1.46	1.50
25	a	402	CLA	CMC-C2C	-2.24	1.46	1.50
25	B	503	CLA	CMD-C2D	-2.24	1.46	1.50
36	N	308	CHL	CBD-CGD	-2.24	1.49	1.52
25	b	514	CLA	C3B-C4B	2.24	1.49	1.42
25	d	404	CLA	C3B-C4B	2.24	1.49	1.42
25	C	506	CLA	C3B-C4B	2.24	1.49	1.42
25	d	401	CLA	CMB-C2B	-2.24	1.46	1.50
25	Y	313	CLA	C3B-C4B	2.24	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	510	CLA	C3B-C4B	2.24	1.49	1.42
25	b	503	CLA	C3B-C4B	2.24	1.49	1.42
38	N	318	NEX	C1-C6	-2.23	1.50	1.54
25	b	507	CLA	C3B-C4B	2.23	1.49	1.42
25	N	311	CLA	C3B-C4B	2.23	1.49	1.42
25	A	402	CLA	C3B-C4B	2.23	1.49	1.42
25	b	516	CLA	C3B-C4B	2.23	1.49	1.42
25	c	506	CLA	C3B-C4B	2.23	1.49	1.42
25	B	512	CLA	CMD-C2D	-2.23	1.46	1.50
25	b	512	CLA	CMD-C2D	-2.23	1.46	1.50
25	r	303	CLA	C3B-C4B	2.23	1.49	1.42
25	B	504	CLA	CMD-C2D	-2.23	1.46	1.50
27	b	517	BCR	C30-C25	-2.23	1.50	1.53
25	c	512	CLA	C3B-C4B	2.23	1.49	1.42
25	B	509	CLA	C3B-C4B	2.22	1.49	1.42
27	c	514	BCR	C30-C25	-2.22	1.50	1.53
25	B	502	CLA	C3B-C4B	2.22	1.49	1.42
25	r	307	CLA	C3B-C4B	2.22	1.49	1.42
25	N	305	CLA	C3B-C4B	2.22	1.49	1.42
36	N	306	CHL	CBD-CGD	-2.22	1.49	1.52
25	B	515	CLA	C3B-C4B	2.22	1.49	1.42
25	c	513	CLA	C3B-C4B	2.22	1.49	1.42
25	c	504	CLA	C3B-C4B	2.21	1.49	1.42
36	N	302	CHL	CBD-CGD	-2.21	1.49	1.52
25	c	509	CLA	C3B-C4B	2.21	1.49	1.42
25	C	508	CLA	C3B-C4B	2.21	1.49	1.42
25	S	612	CLA	C3B-C4B	2.20	1.49	1.42
25	Y	314	CLA	C3B-C4B	2.20	1.49	1.42
25	C	501	CLA	CMD-C2D	-2.20	1.46	1.50
25	S	603	CLA	C3B-C4B	2.20	1.49	1.42
27	C	514	BCR	C30-C25	-2.20	1.51	1.53
25	b	512	CLA	C3B-C4B	2.20	1.49	1.42
25	A	405	CLA	C3B-C4B	2.20	1.49	1.42
25	b	513	CLA	C3B-C4B	2.20	1.49	1.42
25	G	611	CLA	C3B-C4B	2.20	1.49	1.42
25	D	404	CLA	CMC-C2C	-2.20	1.46	1.50
27	k	101	BCR	C1-C6	-2.20	1.51	1.53
25	G	613	CLA	C3B-C4B	2.20	1.49	1.42
25	B	511	CLA	C3B-C4B	2.19	1.49	1.42
25	B	508	CLA	C3B-C4B	2.19	1.49	1.42
25	C	506	CLA	CMB-C2B	-2.19	1.46	1.50
25	B	512	CLA	C3B-C4B	2.19	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	402	CLA	CMD-C2D	-2.19	1.46	1.50
25	b	506	CLA	CMD-C2D	-2.19	1.46	1.50
25	a	402	CLA	C3B-C4B	2.19	1.49	1.42
27	t	101	BCR	C30-C25	-2.19	1.51	1.53
39	G	620	XAT	O4-C5	-2.19	1.43	1.46
25	d	403	CLA	C3B-C4B	2.19	1.49	1.42
25	b	503	CLA	CMB-C2B	-2.19	1.46	1.50
36	Y	309	CHL	CBD-CGD	-2.19	1.49	1.52
25	Y	315	CLA	C3B-C4B	2.19	1.49	1.42
36	S	601	CHL	CBD-CGD	-2.19	1.49	1.52
25	a	405	CLA	C3B-C4B	2.19	1.49	1.42
25	S	604	CLA	C3B-C4B	2.19	1.49	1.42
25	C	513	CLA	C3B-C4B	2.18	1.49	1.42
25	c	506	CLA	CMB-C2B	-2.18	1.46	1.50
25	b	505	CLA	C3B-C4B	2.18	1.49	1.42
25	b	506	CLA	C3B-C4B	2.18	1.49	1.42
25	C	511	CLA	C3B-C4B	2.18	1.49	1.42
25	B	504	CLA	C3B-C4B	2.18	1.49	1.42
25	C	503	CLA	C3B-C4B	2.18	1.49	1.42
25	S	610	CLA	CMD-C2D	-2.18	1.46	1.50
25	D	405	CLA	C3B-C4B	2.18	1.49	1.42
25	S	605	CLA	C3B-C4B	2.18	1.49	1.42
25	N	314	CLA	C3B-C4B	2.18	1.49	1.42
25	G	612	CLA	C3B-C4B	2.18	1.49	1.42
25	S	609	CLA	C3B-C4B	2.18	1.49	1.42
25	d	401	CLA	CMD-C2D	-2.18	1.46	1.50
25	D	404	CLA	C3B-C4B	2.18	1.49	1.42
25	c	512	CLA	CMD-C2D	-2.17	1.46	1.50
26	d	402	PHO	C3D-C4D	2.17	1.44	1.41
25	S	611	CLA	C3B-C4B	2.17	1.49	1.42
25	B	503	CLA	CMB-C2B	-2.17	1.46	1.50
25	b	508	CLA	C3B-C4B	2.17	1.49	1.42
25	a	403	CLA	CMD-C2D	-2.17	1.46	1.50
25	Y	305	CLA	C3B-C4B	2.17	1.49	1.42
25	N	311	CLA	CMD-C2D	-2.17	1.46	1.50
27	d	405	BCR	C1-C6	-2.17	1.51	1.53
25	a	403	CLA	C3B-C4B	2.16	1.49	1.42
25	B	516	CLA	CMC-C2C	-2.16	1.46	1.50
25	B	508	CLA	CMD-C2D	-2.16	1.46	1.50
25	b	512	CLA	MG-NB	-2.16	2.01	2.05
25	C	512	CLA	CMD-C2D	-2.16	1.46	1.50
25	S	614	CLA	CMD-C2D	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	513	CLA	CMB-C2B	-2.16	1.46	1.50
25	b	511	CLA	C3B-C4B	2.16	1.49	1.42
25	D	401	CLA	C3B-C4B	2.16	1.49	1.42
25	S	605	CLA	CMB-C2B	-2.16	1.46	1.50
25	b	504	CLA	CMB-C2B	-2.16	1.46	1.50
25	a	403	CLA	CMB-C2B	-2.16	1.46	1.50
25	D	401	CLA	CMB-C2B	-2.16	1.46	1.50
25	c	507	CLA	CMD-C2D	-2.16	1.46	1.50
25	Y	313	CLA	CMD-C2D	-2.16	1.46	1.50
25	c	510	CLA	CMD-C2D	-2.16	1.46	1.50
25	N	305	CLA	CMD-C2D	-2.15	1.46	1.50
25	S	602	CLA	CHC-C1C	2.15	1.42	1.38
25	S	610	CLA	CHC-C1C	2.15	1.42	1.38
25	C	511	CLA	CMB-C2B	-2.15	1.46	1.50
25	C	513	CLA	CMD-C2D	-2.15	1.46	1.50
25	A	403	CLA	C3B-C4B	2.15	1.49	1.42
25	C	509	CLA	C3B-C4B	2.15	1.49	1.42
25	c	507	CLA	C3B-C4B	2.15	1.49	1.42
25	b	515	CLA	C3B-C4B	2.14	1.49	1.42
36	G	606	CHL	CBD-CGD	-2.14	1.49	1.52
25	Y	305	CLA	CMB-C2B	-2.14	1.46	1.50
25	N	312	CLA	CHC-C1C	2.14	1.42	1.38
35	F	101	HEM	CMB-C2B	2.14	1.55	1.50
25	G	614	CLA	CMD-C2D	-2.14	1.46	1.50
25	b	510	CLA	C3B-C4B	2.14	1.49	1.42
25	c	508	CLA	CMB-C2B	-2.14	1.46	1.50
25	B	501	CLA	C3B-C4B	2.14	1.49	1.42
27	C	515	BCR	C1-C6	-2.14	1.51	1.53
25	b	502	CLA	CMD-C2D	-2.14	1.46	1.50
36	N	307	CHL	CBD-CGD	-2.14	1.49	1.52
25	G	603	CLA	CMB-C2B	-2.13	1.46	1.50
25	N	315	CLA	CMD-C2D	-2.13	1.46	1.50
25	c	509	CLA	CMD-C2D	-2.13	1.46	1.50
25	b	506	CLA	CMB-C2B	-2.13	1.46	1.50
25	c	501	CLA	CMB-C2B	-2.13	1.46	1.50
25	B	516	CLA	C3B-C4B	2.13	1.49	1.42
25	A	405	CLA	CMD-C2D	-2.13	1.46	1.50
25	b	512	CLA	CHC-C1C	2.13	1.42	1.38
25	b	509	CLA	C3B-C4B	2.13	1.48	1.42
25	G	603	CLA	CMD-C2D	-2.13	1.46	1.50
25	b	505	CLA	CMD-C2D	-2.13	1.46	1.50
25	c	501	CLA	CMD-C2D	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	619	CHL	CBD-CGD	-2.13	1.49	1.52
25	Y	315	CLA	CMD-C2D	-2.13	1.46	1.50
25	b	501	CLA	CMD-C2D	-2.13	1.46	1.50
25	c	508	CLA	CMD-C2D	-2.13	1.46	1.50
26	A	404	PHO	C4D-ND	-2.13	1.35	1.38
25	b	512	CLA	CMC-C2C	-2.13	1.46	1.50
25	B	510	CLA	CMB-C2B	-2.13	1.46	1.50
25	C	511	CLA	CMD-C2D	-2.12	1.46	1.50
25	D	401	CLA	CMD-C2D	-2.12	1.46	1.50
25	b	510	CLA	CMD-C2D	-2.12	1.46	1.50
25	A	403	CLA	CMB-C2B	-2.12	1.46	1.50
25	G	610	CLA	CHC-C1C	2.12	1.42	1.38
39	r	309	XAT	O4-C5	-2.12	1.43	1.46
25	b	510	CLA	CMB-C2B	-2.12	1.46	1.50
36	Y	308	CHL	CBD-CGD	-2.12	1.49	1.52
25	A	403	CLA	CMD-C2D	-2.12	1.46	1.50
25	S	613	CLA	CMD-C2D	-2.12	1.46	1.50
25	b	515	CLA	CMD-C2D	-2.12	1.46	1.50
25	Y	312	CLA	CHC-C1C	2.12	1.42	1.38
25	b	505	CLA	CMB-C2B	-2.12	1.46	1.50
25	b	509	CLA	CMD-C2D	-2.12	1.46	1.50
25	S	604	CLA	CMB-C2B	-2.12	1.46	1.50
25	c	507	CLA	CMB-C2B	-2.12	1.46	1.50
25	N	312	CLA	CMD-C2D	-2.12	1.46	1.50
25	B	510	CLA	CMD-C2D	-2.11	1.46	1.50
25	C	510	CLA	CMD-C2D	-2.11	1.46	1.50
25	Y	305	CLA	CMD-C2D	-2.11	1.46	1.50
25	B	511	CLA	CMB-C2B	-2.11	1.46	1.50
25	b	504	CLA	CMD-C2D	-2.11	1.46	1.50
25	c	502	CLA	CMD-C2D	-2.11	1.46	1.50
37	N	317	LUT	C1-C6	-2.11	1.51	1.53
25	C	506	CLA	CMD-C2D	-2.11	1.46	1.50
25	S	602	CLA	CMD-C2D	-2.11	1.46	1.50
25	b	511	CLA	CMD-C2D	-2.11	1.46	1.50
25	c	505	CLA	CHC-C1C	2.11	1.42	1.38
25	B	501	CLA	CMD-C2D	-2.11	1.46	1.50
25	C	507	CLA	C3B-C4B	2.11	1.48	1.42
25	G	612	CLA	CMD-C2D	-2.11	1.46	1.50
26	D	402	PHO	C4D-ND	-2.11	1.35	1.38
25	b	513	CLA	CMD-C2D	-2.11	1.46	1.50
38	N	318	NEX	O24-C25	-2.11	1.43	1.46
25	N	304	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	515	CLA	CMB-C2B	-2.11	1.46	1.50
25	b	516	CLA	CMD-C2D	-2.11	1.46	1.50
25	C	508	CLA	CMD-C2D	-2.10	1.46	1.50
25	Y	304	CLA	CMD-C2D	-2.10	1.46	1.50
25	D	405	CLA	CMD-C2D	-2.10	1.46	1.50
25	b	514	CLA	CMB-C2B	-2.10	1.46	1.50
25	c	506	CLA	CMD-C2D	-2.10	1.46	1.50
25	c	509	CLA	CMB-C2B	-2.10	1.46	1.50
25	b	514	CLA	CMD-C2D	-2.10	1.46	1.50
25	N	315	CLA	CHC-C1C	2.10	1.42	1.38
25	B	513	CLA	CMD-C2D	-2.10	1.46	1.50
25	c	504	CLA	CMB-C2B	-2.10	1.46	1.50
25	B	506	CLA	CMD-C2D	-2.10	1.46	1.50
25	S	611	CLA	CMD-C2D	-2.10	1.46	1.50
25	G	611	CLA	CHC-C1C	2.10	1.42	1.38
36	N	309	CHL	CBD-CGD	-2.10	1.49	1.52
25	G	604	CLA	CHC-C1C	2.10	1.42	1.38
25	c	503	CLA	CMD-C2D	-2.10	1.46	1.50
25	S	604	CLA	CMD-C2D	-2.10	1.46	1.50
25	B	505	CLA	CMD-C2D	-2.10	1.46	1.50
25	S	612	CLA	CMD-C2D	-2.10	1.46	1.50
25	C	508	CLA	CMB-C2B	-2.10	1.46	1.50
25	C	504	CLA	CMB-C2B	-2.10	1.46	1.50
25	B	511	CLA	CMC-C2C	-2.10	1.46	1.50
25	B	507	CLA	CMD-C2D	-2.10	1.46	1.50
25	B	511	CLA	CMD-C2D	-2.09	1.46	1.50
25	S	603	CLA	CMB-C2B	-2.09	1.46	1.50
25	S	611	CLA	CHC-C1C	2.09	1.42	1.38
25	b	507	CLA	CHC-C1C	2.09	1.42	1.38
25	r	301	CLA	CHC-C1C	2.09	1.42	1.38
39	N	301	XAT	O24-C25	-2.09	1.43	1.46
25	N	313	CLA	CMB-C2B	-2.09	1.46	1.50
25	S	611	CLA	CMB-C2B	-2.09	1.46	1.50
25	b	502	CLA	CMB-C2B	-2.09	1.46	1.50
38	S	617	NEX	O24-C25	-2.09	1.43	1.46
25	C	512	CLA	CMB-C2B	-2.09	1.46	1.50
25	Y	312	CLA	CMD-C2D	-2.09	1.46	1.50
25	b	511	CLA	CMC-C2C	-2.09	1.46	1.50
25	B	502	CLA	CMD-C2D	-2.09	1.46	1.50
36	G	607	CHL	CBD-CGD	-2.09	1.49	1.52
36	Y	303	CHL	CBD-CGD	-2.09	1.49	1.52
25	C	502	CLA	C3B-C4B	2.09	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	302	CLA	CMD-C2D	-2.09	1.46	1.50
25	G	602	CLA	CMB-C2B	-2.09	1.46	1.50
25	G	602	CLA	CMD-C2D	-2.09	1.46	1.50
25	c	510	CLA	CMB-C2B	-2.09	1.46	1.50
25	d	404	CLA	CMD-C2D	-2.09	1.46	1.50
25	G	611	CLA	CMD-C2D	-2.09	1.46	1.50
25	b	507	CLA	CMB-C2B	-2.09	1.46	1.50
25	c	502	CLA	C3B-C4B	2.09	1.48	1.42
36	Y	310	CHL	CBD-CGD	-2.09	1.49	1.52
25	b	504	CLA	C3B-C4B	2.09	1.48	1.42
39	Y	302	XAT	O24-C25	-2.09	1.43	1.46
25	S	614	CLA	CHC-C1C	2.09	1.42	1.38
25	G	613	CLA	CMB-C2B	-2.09	1.46	1.50
25	r	301	CLA	CMB-C2B	-2.09	1.46	1.50
34	d	406	PL9	C52-C5	-2.09	1.46	1.50
25	B	503	CLA	CHC-C1C	2.08	1.42	1.38
25	B	507	CLA	CHC-C1C	2.08	1.42	1.38
25	S	613	CLA	CMB-C2B	-2.08	1.46	1.50
25	C	510	CLA	CHC-C1C	2.08	1.42	1.38
25	d	403	CLA	CMB-C2B	-2.08	1.46	1.50
27	B	518	BCR	C1-C6	-2.08	1.51	1.53
25	B	504	CLA	CMB-C2B	-2.08	1.46	1.50
26	a	404	PHO	C4D-ND	-2.08	1.35	1.38
25	C	501	CLA	CMB-C2B	-2.08	1.46	1.50
25	Y	304	CLA	CMB-C2B	-2.08	1.46	1.50
25	c	508	CLA	CMC-C2C	-2.08	1.46	1.50
25	C	505	CLA	CHC-C1C	2.08	1.42	1.38
25	c	508	CLA	CHC-C1C	2.08	1.42	1.38
25	N	314	CLA	CMD-C2D	-2.08	1.46	1.50
25	a	402	CLA	CMB-C2B	-2.08	1.46	1.50
25	B	513	CLA	CHC-C1C	2.08	1.42	1.38
25	C	509	CLA	CMB-C2B	-2.08	1.46	1.50
25	a	405	CLA	CMD-C2D	-2.08	1.46	1.50
25	b	513	CLA	CHC-C1C	2.08	1.42	1.38
38	Y	318	NEX	O24-C25	-2.08	1.43	1.46
25	C	507	CLA	CMD-C2D	-2.08	1.46	1.50
25	N	305	CLA	CMB-C2B	-2.08	1.46	1.50
25	B	514	CLA	CMD-C2D	-2.08	1.46	1.50
25	B	506	CLA	CMB-C2B	-2.08	1.46	1.50
25	C	508	CLA	CMC-C2C	-2.08	1.46	1.50
25	Y	315	CLA	CMB-C2B	-2.08	1.46	1.50
26	d	402	PHO	C4D-ND	-2.08	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	502	CLA	CMD-C2D	-2.08	1.46	1.50
25	C	504	CLA	CMD-C2D	-2.08	1.46	1.50
25	C	502	CLA	CMC-C2C	-2.07	1.46	1.50
25	c	501	CLA	CHC-C1C	2.07	1.42	1.38
25	B	506	CLA	CMC-C2C	-2.07	1.46	1.50
25	Y	314	CLA	CMD-C2D	-2.07	1.46	1.50
25	B	507	CLA	CMB-C2B	-2.07	1.46	1.50
25	S	605	CLA	CMD-C2D	-2.07	1.46	1.50
25	r	301	CLA	CMD-C2D	-2.07	1.46	1.50
25	D	404	CLA	CHC-C1C	2.07	1.42	1.38
25	Y	312	CLA	CMB-C2B	-2.07	1.46	1.50
25	N	304	CLA	CMB-C2B	-2.07	1.46	1.50
25	c	510	CLA	CHC-C1C	2.07	1.42	1.38
25	N	315	CLA	CMB-C2B	-2.07	1.46	1.50
25	N	303	CLA	CMD-C2D	-2.07	1.46	1.50
25	N	303	CLA	CHC-C1C	2.07	1.42	1.38
25	B	514	CLA	CMB-C2B	-2.07	1.46	1.50
25	S	614	CLA	CMB-C2B	-2.07	1.46	1.50
25	Y	314	CLA	CMB-C2B	-2.07	1.46	1.50
25	B	501	CLA	CMB-C2B	-2.07	1.46	1.50
25	b	516	CLA	CMB-C2B	-2.07	1.46	1.50
25	G	604	CLA	CMD-C2D	-2.07	1.46	1.50
25	r	308	CLA	CMD-C2D	-2.07	1.46	1.50
25	N	312	CLA	CMB-C2B	-2.07	1.46	1.50
25	Y	313	CLA	CMB-C2B	-2.07	1.46	1.50
25	b	507	CLA	CMD-C2D	-2.07	1.46	1.50
25	c	504	CLA	CMD-C2D	-2.07	1.46	1.50
38	G	617	NEX	O24-C25	-2.07	1.43	1.46
25	N	313	CLA	CMD-C2D	-2.07	1.46	1.50
25	c	511	CLA	CMD-C2D	-2.07	1.46	1.50
25	B	512	CLA	CMB-C2B	-2.07	1.46	1.50
25	S	602	CLA	CMB-C2B	-2.07	1.46	1.50
36	N	310	CHL	CBD-CGD	-2.06	1.49	1.52
25	S	603	CLA	CMD-C2D	-2.06	1.46	1.50
25	Y	311	CLA	CMD-C2D	-2.06	1.46	1.50
25	b	510	CLA	MG-NB	-2.06	2.01	2.05
25	b	501	CLA	CMB-C2B	-2.06	1.46	1.50
25	B	514	CLA	CHC-C1C	2.06	1.42	1.38
25	d	404	CLA	CMB-C2B	-2.06	1.46	1.50
25	A	402	CLA	CHC-C1C	2.06	1.42	1.38
25	S	609	CLA	CMD-C2D	-2.06	1.46	1.50
36	G	601	CHL	CBD-CGD	-2.06	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	513	CLA	CMB-C2B	-2.06	1.46	1.50
25	D	401	CLA	CMC-C2C	-2.06	1.46	1.50
25	D	405	CLA	CMB-C2B	-2.06	1.46	1.50
25	a	405	CLA	CMB-C2B	-2.06	1.46	1.50
25	c	506	CLA	CHC-C1C	2.06	1.42	1.38
25	A	402	CLA	CMB-C2B	-2.06	1.46	1.50
25	B	516	CLA	CMB-C2B	-2.06	1.46	1.50
25	Y	306	CLA	CHC-C1C	2.06	1.42	1.38
25	C	503	CLA	CMB-C2B	-2.06	1.46	1.50
25	b	503	CLA	CMC-C2C	-2.06	1.46	1.50
25	S	610	CLA	CMC-C2C	-2.06	1.46	1.50
25	r	303	CLA	CMD-C2D	-2.06	1.46	1.50
25	B	511	CLA	CHC-C1C	2.06	1.42	1.38
25	b	512	CLA	CMB-C2B	-2.06	1.46	1.50
25	C	506	CLA	CHC-C1C	2.06	1.42	1.38
35	F	101	HEM	CMD-C2D	2.05	1.55	1.50
39	r	309	XAT	O24-C25	-2.05	1.43	1.46
25	G	614	CLA	CMB-C2B	-2.05	1.46	1.50
25	c	503	CLA	CHC-C1C	2.05	1.42	1.38
25	r	303	CLA	CHC-C1C	2.05	1.42	1.38
25	G	613	CLA	CMD-C2D	-2.05	1.46	1.50
25	N	314	CLA	CMB-C2B	-2.05	1.46	1.50
25	d	403	CLA	CHC-C1C	2.05	1.42	1.38
25	C	503	CLA	CMD-C2D	-2.05	1.46	1.50
25	c	510	CLA	CMC-C2C	-2.05	1.46	1.50
25	B	515	CLA	CMD-C2D	-2.05	1.46	1.50
25	G	611	CLA	CMB-C2B	-2.05	1.46	1.50
25	N	305	CLA	CHC-C1C	2.05	1.42	1.38
25	Y	306	CLA	CMB-C2B	-2.05	1.46	1.50
25	r	303	CLA	CMB-C2B	-2.05	1.46	1.50
25	Y	311	CLA	CMC-C2C	-2.05	1.46	1.50
25	b	503	CLA	CHC-C1C	2.05	1.42	1.38
25	C	509	CLA	CMD-C2D	-2.05	1.46	1.50
25	c	502	CLA	CMC-C2C	-2.05	1.46	1.50
36	G	608	CHL	CBD-CGD	-2.05	1.49	1.52
25	c	511	CLA	CMB-C2B	-2.05	1.46	1.50
25	S	609	CLA	CMB-C2B	-2.05	1.46	1.50
25	B	502	CLA	CMB-C2B	-2.05	1.46	1.50
25	S	602	CLA	CMC-C2C	-2.05	1.46	1.50
25	b	510	CLA	CMC-C2C	-2.05	1.46	1.50
25	c	505	CLA	CMB-C2B	-2.05	1.46	1.50
25	Y	315	CLA	CHC-C1C	2.05	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	502	CLA	CHC-C1C	2.05	1.42	1.38
25	G	604	CLA	CMB-C2B	-2.04	1.46	1.50
25	d	401	CLA	CMC-C2C	-2.04	1.46	1.50
25	Y	311	CLA	CMB-C2B	-2.04	1.46	1.50
38	r	310	NEX	O24-C25	-2.04	1.43	1.46
25	C	507	CLA	CMB-C2B	-2.04	1.46	1.50
25	B	516	CLA	CMD-C2D	-2.04	1.46	1.50
25	B	509	CLA	CMD-C2D	-2.04	1.46	1.50
25	D	404	CLA	CMB-C2B	-2.04	1.46	1.50
25	B	505	CLA	CHC-C1C	2.04	1.42	1.38
25	c	504	CLA	CHC-C1C	2.04	1.42	1.38
25	N	311	CLA	CMC-C2C	-2.04	1.46	1.50
25	b	514	CLA	CMC-C2C	-2.04	1.46	1.50
25	Y	304	CLA	CMC-C2C	-2.04	1.46	1.50
25	Y	312	CLA	CMC-C2C	-2.03	1.46	1.50
25	b	513	CLA	CMC-C2C	-2.03	1.46	1.50
25	Y	306	CLA	CMD-C2D	-2.03	1.46	1.50
25	c	509	CLA	CMC-C2C	-2.03	1.46	1.50
37	G	616	LUT	C1-C6	-2.03	1.51	1.53
25	b	507	CLA	CMC-C2C	-2.03	1.46	1.50
25	Y	313	CLA	CMC-C2C	-2.03	1.46	1.50
25	r	307	CLA	CMD-C2D	-2.03	1.46	1.50
25	c	511	CLA	CMC-C2C	-2.03	1.46	1.50
25	C	510	CLA	CMC-C2C	-2.03	1.46	1.50
25	C	505	CLA	CMB-C2B	-2.03	1.46	1.50
25	G	614	CLA	CHC-C1C	2.03	1.42	1.38
25	S	604	CLA	CHC-C1C	2.03	1.42	1.38
25	G	610	CLA	CMD-C2D	-2.03	1.46	1.50
25	N	303	CLA	CMC-C2C	-2.03	1.46	1.50
25	r	302	CLA	CMB-C2B	-2.03	1.46	1.50
25	b	502	CLA	CHC-C1C	2.03	1.42	1.38
25	C	508	CLA	CHC-C1C	2.03	1.42	1.38
25	N	304	CLA	CHC-C1C	2.03	1.42	1.38
25	b	514	CLA	CHC-C1C	2.03	1.42	1.38
25	r	308	CLA	CMB-C2B	-2.03	1.46	1.50
25	A	405	CLA	CMB-C2B	-2.03	1.46	1.50
31	C	518	DGD	O5D-C1E	2.03	1.43	1.40
25	C	504	CLA	CHC-C1C	2.03	1.42	1.38
25	C	503	CLA	CMC-C2C	-2.02	1.46	1.50
25	C	509	CLA	CMC-C2C	-2.02	1.46	1.50
25	N	312	CLA	CMC-C2C	-2.02	1.46	1.50
25	B	510	CLA	CHC-C1C	2.02	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	314	CLA	CMC-C2C	-2.02	1.46	1.50
37	S	616	LUT	C1-C6	-2.02	1.51	1.53
25	S	603	CLA	CHC-C1C	2.02	1.42	1.38
25	B	509	CLA	CMB-C2B	-2.02	1.46	1.50
25	b	506	CLA	CMC-C2C	-2.02	1.46	1.50
25	B	513	CLA	CMC-C2C	-2.02	1.46	1.50
25	c	506	CLA	CMC-C2C	-2.02	1.46	1.50
25	c	512	CLA	CMB-C2B	-2.02	1.46	1.50
25	B	506	CLA	CHC-C1C	2.02	1.42	1.38
25	N	311	CLA	CMB-C2B	-2.02	1.46	1.50
25	C	501	CLA	CHC-C1C	2.02	1.42	1.38
25	C	512	CLA	CMC-C2C	-2.02	1.46	1.50
25	a	405	CLA	CHC-C1C	2.01	1.42	1.38
25	b	505	CLA	CHC-C1C	2.01	1.42	1.38
25	S	603	CLA	CMC-C2C	-2.01	1.46	1.50
25	c	513	CLA	CMD-C2D	-2.01	1.46	1.50
25	c	501	CLA	CMC-C2C	-2.01	1.46	1.50
25	r	301	CLA	CMC-C2C	-2.01	1.46	1.50
25	B	505	CLA	CMB-C2B	-2.01	1.46	1.50
25	G	602	CLA	CMC-C2C	-2.01	1.46	1.50
25	A	405	CLA	CHC-C1C	2.01	1.42	1.38
25	N	305	CLA	CMC-C2C	-2.01	1.46	1.50
25	S	612	CLA	CMC-C2C	-2.01	1.46	1.50
25	C	510	CLA	CMB-C2B	-2.01	1.46	1.50
25	C	513	CLA	CMC-C2C	-2.01	1.46	1.50
25	N	313	CLA	CMC-C2C	-2.01	1.46	1.50
25	G	612	CLA	CMB-C2B	-2.01	1.46	1.50
25	N	303	CLA	CMB-C2B	-2.01	1.46	1.50
25	C	513	CLA	CMB-C2B	-2.01	1.46	1.50
25	c	512	CLA	CMC-C2C	-2.01	1.46	1.50
25	B	509	CLA	CHC-C1C	2.01	1.42	1.38
25	c	507	CLA	CHC-C1C	2.01	1.42	1.38
25	b	502	CLA	CMC-C2C	-2.00	1.46	1.50
25	Y	311	CLA	CHC-C1C	2.00	1.42	1.38
25	G	610	CLA	CMC-C2C	-2.00	1.46	1.50
25	S	610	CLA	CMB-C2B	-2.00	1.46	1.50
25	N	313	CLA	CHC-C1C	2.00	1.42	1.38
37	S	615	LUT	C1-C6	-2.00	1.51	1.53
25	C	501	CLA	CMC-C2C	-2.00	1.46	1.50
25	c	503	CLA	CMB-C2B	-2.00	1.46	1.50
25	B	512	CLA	CHC-C1C	2.00	1.42	1.38
25	C	505	CLA	CMC-C2C	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	511	CLA	CMC-C2C	-2.00	1.46	1.50
25	b	505	CLA	CMC-C2C	-2.00	1.46	1.50
25	B	502	CLA	CMC-C2C	-2.00	1.46	1.50
25	c	513	CLA	CMB-C2B	-2.00	1.46	1.50
37	Y	317	LUT	C1-C6	-2.00	1.51	1.53

All (1695) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	620	XAT	C37-C21-C36	-16.40	83.54	107.37
39	G	620	XAT	C37-C21-C22	-13.59	85.08	108.97
36	S	606	CHL	O2D-CGD-CBD	10.22	122.18	110.95
36	N	308	CHL	C1B-CHB-C4A	10.13	127.84	121.32
36	G	607	CHL	C1B-CHB-C4A	10.05	127.79	121.32
36	r	304	CHL	C1B-CHB-C4A	10.00	127.75	121.32
36	G	619	CHL	C1B-CHB-C4A	9.95	127.73	121.32
36	G	606	CHL	C1B-CHB-C4A	9.87	127.67	121.32
36	N	309	CHL	C1B-CHB-C4A	9.83	127.65	121.32
27	B	517	BCR	C16-C17-C18	-9.77	113.57	127.28
36	G	605	CHL	C1B-CHB-C4A	9.73	127.58	121.32
36	Y	308	CHL	C1B-CHB-C4A	9.52	127.45	121.32
36	S	607	CHL	C1B-CHB-C4A	9.49	127.43	121.32
36	Y	307	CHL	C1B-CHB-C4A	9.47	127.42	121.32
36	S	608	CHL	C1B-CHB-C4A	9.38	127.36	121.32
36	S	606	CHL	C1B-CHB-C4A	9.33	127.33	121.32
36	r	305	CHL	C1B-CHB-C4A	9.33	127.32	121.32
36	N	306	CHL	C1B-CHB-C4A	9.18	127.23	121.32
36	Y	303	CHL	C1B-CHB-C4A	9.04	127.14	121.32
36	S	601	CHL	C1B-CHB-C4A	8.98	127.10	121.32
36	Y	310	CHL	O2D-CGD-CBD	8.80	120.62	110.95
36	G	609	CHL	O2D-CGD-CBD	8.69	120.49	110.95
36	N	307	CHL	O2D-CGD-CBD	8.66	120.46	110.95
36	r	306	CHL	C1B-CHB-C4A	8.64	126.88	121.32
36	S	607	CHL	O2D-CGD-CBD	8.61	120.41	110.95
36	G	601	CHL	C1B-CHB-C4A	8.58	126.84	121.32
36	N	310	CHL	O2D-CGD-CBD	8.58	120.38	110.95
36	G	609	CHL	C1B-CHB-C4A	8.52	126.80	121.32
36	S	608	CHL	O2D-CGD-CBD	8.47	120.25	110.95
36	N	307	CHL	C1B-CHB-C4A	8.42	126.74	121.32
36	N	302	CHL	O2D-CGD-CBD	8.41	120.19	110.95
36	Y	308	CHL	O2D-CGD-CBD	8.30	120.06	110.95
36	r	304	CHL	O2D-CGD-CBD	8.28	120.04	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	Y	303	CHL	O2D-CGD-CBD	8.23	119.99	110.95
36	N	309	CHL	O2D-CGD-CBD	8.22	119.98	110.95
36	r	305	CHL	O2D-CGD-CBD	8.21	119.97	110.95
27	v	101	BCR	C16-C17-C18	-8.20	115.77	127.28
36	G	619	CHL	O2D-CGD-CBD	8.16	119.92	110.95
36	Y	307	CHL	O2D-CGD-CBD	8.11	119.85	110.95
36	G	606	CHL	O2D-CGD-CBD	8.08	119.82	110.95
36	G	605	CHL	O2D-CGD-CBD	8.07	119.81	110.95
36	Y	309	CHL	O2D-CGD-CBD	7.96	119.69	110.95
36	G	601	CHL	O2D-CGD-CBD	7.93	119.66	110.95
36	G	608	CHL	O2D-CGD-CBD	7.91	119.64	110.95
36	G	607	CHL	O2D-CGD-CBD	7.88	119.60	110.95
36	N	302	CHL	C1B-CHB-C4A	7.81	126.34	121.32
36	N	308	CHL	O2D-CGD-CBD	7.72	119.43	110.95
36	S	601	CHL	O2D-CGD-CBD	7.72	119.43	110.95
36	N	306	CHL	O2D-CGD-CBD	7.70	119.41	110.95
36	r	306	CHL	O2D-CGD-CBD	7.63	119.33	110.95
36	G	608	CHL	C1B-CHB-C4A	7.50	126.15	121.32
27	B	517	BCR	C24-C23-C22	-7.43	115.25	126.23
36	Y	309	CHL	C1B-CHB-C4A	7.42	126.10	121.32
39	G	620	XAT	C37-C21-C26	-7.13	90.80	110.05
36	G	605	CHL	C4D-ND-C1D	-6.97	99.93	105.22
39	N	301	XAT	O24-C25-C24	6.92	119.98	113.49
39	G	620	XAT	C18-C5-C6	-6.85	111.03	122.30
36	S	601	CHL	C4D-ND-C1D	-6.84	100.03	105.22
38	N	318	NEX	C38-C25-C26	-6.83	111.06	122.30
38	r	310	NEX	C38-C25-C26	-6.81	111.09	122.30
36	N	306	CHL	C4D-ND-C1D	-6.81	100.05	105.22
38	G	617	NEX	C38-C25-C26	-6.76	111.17	122.30
38	S	617	NEX	C38-C25-C26	-6.71	111.25	122.30
39	r	309	XAT	C18-C5-C6	-6.71	111.25	122.30
39	N	301	XAT	C18-C5-C6	-6.70	111.28	122.30
36	G	619	CHL	C4D-ND-C1D	-6.69	100.14	105.22
36	G	606	CHL	C4D-ND-C1D	-6.68	100.15	105.22
39	Y	302	XAT	O24-C25-C24	6.68	119.75	113.49
39	r	309	XAT	C38-C25-C26	-6.68	111.31	122.30
36	G	607	CHL	C4D-ND-C1D	-6.67	100.16	105.22
38	Y	318	NEX	C38-C25-C26	-6.65	111.35	122.30
36	N	309	CHL	C4D-ND-C1D	-6.65	100.17	105.22
36	Y	307	CHL	C4D-ND-C1D	-6.65	100.17	105.22
39	Y	302	XAT	C18-C5-C6	-6.62	111.41	122.30
39	G	620	XAT	C36-C21-C22	6.61	120.59	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	N	308	CHL	C4D-ND-C1D	-6.61	100.20	105.22
36	Y	308	CHL	C4D-ND-C1D	-6.60	100.21	105.22
39	G	620	XAT	C38-C25-C26	-6.59	111.45	122.30
36	r	304	CHL	C4D-ND-C1D	-6.59	100.22	105.22
36	N	302	CHL	C4D-ND-C1D	-6.58	100.23	105.22
39	N	301	XAT	C38-C25-C26	-6.57	111.49	122.30
39	Y	302	XAT	C38-C25-C26	-6.56	111.51	122.30
36	S	607	CHL	C4D-ND-C1D	-6.51	100.28	105.22
36	Y	303	CHL	C4D-ND-C1D	-6.51	100.28	105.22
36	G	601	CHL	C4D-ND-C1D	-6.50	100.29	105.22
36	r	306	CHL	C4D-ND-C1D	-6.47	100.31	105.22
36	Y	309	CHL	C4D-ND-C1D	-6.45	100.33	105.22
36	r	305	CHL	C4D-ND-C1D	-6.44	100.33	105.22
36	N	307	CHL	C4D-ND-C1D	-6.43	100.34	105.22
36	G	608	CHL	C4D-ND-C1D	-6.42	100.35	105.22
36	N	310	CHL	C4D-ND-C1D	-6.42	100.35	105.22
36	G	609	CHL	C4D-ND-C1D	-6.40	100.36	105.22
38	S	617	NEX	O24-C25-C24	6.36	119.45	113.49
39	G	620	XAT	O24-C25-C24	6.35	119.44	113.49
26	A	404	PHO	C4D-CHA-CBD	-6.34	105.41	108.45
36	S	606	CHL	C4D-ND-C1D	-6.34	100.41	105.22
25	b	512	CLA	C4A-NA-C1A	6.33	109.57	106.68
38	Y	318	NEX	O24-C25-C24	6.33	119.42	113.49
38	G	617	NEX	O24-C25-C24	6.30	119.40	113.49
36	S	608	CHL	C4D-ND-C1D	-6.24	100.48	105.22
36	S	601	CHL	CHA-C1A-C2A	-6.24	118.66	133.31
38	r	310	NEX	O24-C25-C24	6.22	119.32	113.49
36	Y	308	CHL	CHA-C1A-C2A	-6.15	118.87	133.31
36	N	302	CHL	CHA-C1A-C2A	-6.15	118.88	133.31
27	v	101	BCR	C24-C23-C22	-6.14	117.15	126.23
36	G	605	CHL	CHA-C1A-C2A	-6.13	118.92	133.31
36	G	609	CHL	CHA-C1A-C2A	-6.13	118.92	133.31
36	G	606	CHL	CHA-C1A-C2A	-6.09	119.00	133.31
36	N	307	CHL	CHA-C1A-C2A	-6.06	119.07	133.31
36	Y	303	CHL	CHA-C1A-C2A	-6.06	119.08	133.31
36	G	601	CHL	CHA-C1A-C2A	-6.06	119.09	133.31
36	r	304	CHL	CHA-C1A-C2A	-6.02	119.17	133.31
39	r	309	XAT	O24-C25-C24	6.02	119.13	113.49
36	N	309	CHL	CHA-C1A-C2A	-6.01	119.20	133.31
36	N	306	CHL	CHA-C1A-C2A	-6.00	119.21	133.31
36	G	619	CHL	CHA-C1A-C2A	-5.98	119.26	133.31
36	r	305	CHL	CHA-C1A-C2A	-5.98	119.26	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	S	607	CHL	CHA-C1A-C2A	-5.98	119.28	133.31
36	S	608	CHL	CHA-C1A-C2A	-5.97	119.29	133.31
36	Y	307	CHL	CHA-C1A-C2A	-5.96	119.31	133.31
36	N	310	CHL	CHA-C1A-C2A	-5.96	119.32	133.31
36	N	310	CHL	C1B-CHB-C4A	5.94	125.15	121.32
36	Y	310	CHL	C4D-ND-C1D	-5.93	100.72	105.22
36	Y	310	CHL	CHA-C1A-C2A	-5.90	119.46	133.31
36	r	306	CHL	CHA-C1A-C2A	-5.89	119.47	133.31
36	G	607	CHL	CHA-C1A-C2A	-5.89	119.48	133.31
36	S	606	CHL	CHA-C1A-C2A	-5.87	119.52	133.31
26	D	402	PHO	C4D-CHA-CBD	-5.87	105.64	108.45
39	r	309	XAT	O4-C5-C4	5.79	118.91	113.49
36	N	308	CHL	CHA-C1A-C2A	-5.75	119.80	133.31
38	N	318	NEX	O24-C25-C24	5.75	118.88	113.49
26	a	404	PHO	C4D-CHA-CBD	-5.75	105.70	108.45
25	c	502	CLA	C4A-NA-C1A	5.72	109.29	106.68
27	d	405	BCR	C28-C27-C26	-5.69	103.91	114.06
36	G	608	CHL	CHA-C1A-C2A	-5.67	120.00	133.31
25	C	511	CLA	C4A-NA-C1A	5.67	109.26	106.68
36	Y	309	CHL	CHA-C1A-C2A	-5.64	120.06	133.31
25	C	502	CLA	C4A-NA-C1A	5.64	109.25	106.68
27	k	101	BCR	C20-C21-C22	-5.64	119.37	127.28
27	h	101	BCR	C7-C8-C9	-5.60	117.95	126.23
25	B	512	CLA	C4A-NA-C1A	5.59	109.23	106.68
33	a	409	BCT	O2-C-O1	5.58	133.94	119.68
27	h	101	BCR	C11-C10-C9	-5.57	119.46	127.28
25	d	403	CLA	C4A-NA-C1A	5.54	109.21	106.68
33	D	403	BCT	O2-C-O1	5.53	133.81	119.68
36	Y	310	CHL	C1B-CHB-C4A	5.52	124.87	121.32
25	b	510	CLA	C4A-NA-C1A	5.50	109.19	106.68
25	B	513	CLA	C4A-NA-C1A	5.50	109.19	106.68
27	k	101	BCR	C24-C23-C22	-5.47	118.14	126.23
39	Y	302	XAT	O4-C5-C4	5.46	118.61	113.49
25	c	509	CLA	C4A-NA-C1A	5.46	109.17	106.68
25	b	513	CLA	C4A-NA-C1A	5.43	109.16	106.68
25	G	611	CLA	C4A-NA-C1A	5.33	109.11	106.68
26	d	402	PHO	C4D-CHA-CBD	-5.33	105.90	108.45
27	C	516	BCR	C24-C23-C22	-5.28	118.43	126.23
27	H	101	BCR	C11-C10-C9	-5.27	119.89	127.28
25	c	507	CLA	C4A-NA-C1A	5.27	109.08	106.68
39	N	301	XAT	O4-C5-C4	5.25	118.41	113.49
25	Y	312	CLA	C4A-NA-C1A	5.24	109.07	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	507	CLA	C4A-NA-C1A	5.24	109.07	106.68
27	C	516	BCR	C20-C21-C22	-5.24	119.93	127.28
25	C	509	CLA	C4A-NA-C1A	5.24	109.07	106.68
27	c	514	BCR	C15-C14-C13	-5.22	119.96	127.28
25	B	510	CLA	C4A-NA-C1A	5.21	109.06	106.68
25	D	404	CLA	C4A-NA-C1A	5.18	109.04	106.68
25	S	611	CLA	C4A-NA-C1A	5.13	109.02	106.68
27	v	101	BCR	C20-C19-C18	-5.12	112.31	126.36
27	b	517	BCR	C15-C14-C13	-5.09	120.14	127.28
27	H	101	BCR	C7-C8-C9	-5.08	118.72	126.23
39	G	620	XAT	O4-C5-C4	5.08	118.25	113.49
38	G	617	NEX	C15-C14-C13	-5.08	120.16	127.28
25	b	516	CLA	C4A-NA-C1A	5.07	108.99	106.68
27	z	101	BCR	C11-C10-C9	-5.04	120.21	127.28
25	C	510	CLA	C4A-NA-C1A	5.03	108.97	106.68
25	c	511	CLA	C4A-NA-C1A	5.03	108.97	106.68
25	D	401	CLA	C4A-NA-C1A	5.02	108.97	106.68
25	b	509	CLA	C4A-NA-C1A	5.01	108.96	106.68
25	N	314	CLA	C4A-NA-C1A	4.97	108.95	106.68
25	r	301	CLA	C4A-NA-C1A	4.96	108.94	106.68
25	r	308	CLA	C4A-NA-C1A	4.94	108.93	106.68
38	r	310	NEX	C15-C14-C13	-4.94	120.36	127.28
27	z	101	BCR	C16-C17-C18	-4.93	120.36	127.28
25	B	516	CLA	C4A-NA-C1A	4.93	108.93	106.68
25	S	604	CLA	C4A-NA-C1A	4.93	108.93	106.68
25	d	404	CLA	C4A-NA-C1A	4.93	108.93	106.68
25	c	510	CLA	C4A-NA-C1A	4.91	108.92	106.68
25	b	515	CLA	C4A-NA-C1A	4.91	108.92	106.68
25	G	613	CLA	C4A-NA-C1A	4.91	108.92	106.68
39	G	620	XAT	C15-C14-C13	-4.91	120.39	127.28
27	D	406	BCR	C7-C8-C9	4.90	133.49	126.23
25	Y	314	CLA	C4A-NA-C1A	4.90	108.91	106.68
27	b	518	BCR	C15-C14-C13	-4.90	120.41	127.28
25	C	506	CLA	C4A-NA-C1A	4.89	108.91	106.68
25	B	505	CLA	C4A-NA-C1A	4.89	108.91	106.68
39	G	620	XAT	O4-C5-C18	4.87	120.49	115.05
27	k	101	BCR	C11-C10-C9	-4.86	120.46	127.28
25	C	501	CLA	C4A-NA-C1A	4.84	108.89	106.68
25	r	303	CLA	C4A-NA-C1A	4.84	108.89	106.68
39	r	309	XAT	C6-C7-C8	-4.84	115.77	125.99
27	V	101	BCR	C16-C17-C18	-4.83	120.51	127.28
25	b	505	CLA	C4A-NA-C1A	4.81	108.87	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	405	CLA	C4A-NA-C1A	4.80	108.87	106.68
25	N	312	CLA	C4A-NA-C1A	4.80	108.87	106.68
34	d	406	PL9	C7-C3-C4	4.80	120.86	116.91
25	C	513	CLA	C4A-NA-C1A	4.79	108.86	106.68
25	S	603	CLA	C4A-NA-C1A	4.78	108.86	106.68
34	D	407	PL9	C7-C3-C4	4.78	120.84	116.91
27	C	515	BCR	C15-C14-C13	-4.77	120.59	127.28
25	N	305	CLA	C4A-NA-C1A	4.76	108.85	106.68
25	Y	305	CLA	C4A-NA-C1A	4.76	108.85	106.68
25	B	501	CLA	C4A-NA-C1A	4.75	108.84	106.68
39	N	301	XAT	O4-C5-C18	4.75	120.35	115.05
38	N	318	NEX	O24-C25-C38	4.74	120.35	115.05
25	d	401	CLA	C4A-NA-C1A	4.73	108.84	106.68
38	Y	318	NEX	C15-C14-C13	-4.73	120.65	127.28
39	r	309	XAT	O4-C5-C18	4.73	120.33	115.05
25	c	512	CLA	C4A-NA-C1A	4.73	108.83	106.68
25	b	511	CLA	C4A-NA-C1A	4.72	108.83	106.68
25	B	509	CLA	C4A-NA-C1A	4.71	108.83	106.68
25	a	405	CLA	C4A-NA-C1A	4.71	108.83	106.68
27	B	517	BCR	C16-C15-C14	-4.71	113.88	123.52
25	N	304	CLA	C4A-NA-C1A	4.71	108.83	106.68
27	H	101	BCR	C16-C17-C18	-4.71	120.67	127.28
27	t	101	BCR	C15-C14-C13	-4.71	120.67	127.28
25	C	504	CLA	C4A-NA-C1A	4.71	108.83	106.68
25	A	405	CLA	C4A-NA-C1A	4.66	108.81	106.68
25	c	506	CLA	C4A-NA-C1A	4.66	108.81	106.68
25	G	603	CLA	C4A-NA-C1A	4.64	108.79	106.68
38	G	617	NEX	C11-C10-C9	-4.63	120.78	127.28
38	S	617	NEX	C35-C34-C33	-4.62	120.80	127.28
25	c	504	CLA	C4A-NA-C1A	4.61	108.78	106.68
25	N	303	CLA	C4A-NA-C1A	4.61	108.78	106.68
25	b	504	CLA	C4A-NA-C1A	4.61	108.78	106.68
25	Y	306	CLA	C4A-NA-C1A	4.58	108.77	106.68
25	Y	313	CLA	C4A-NA-C1A	4.58	108.77	106.68
25	a	403	CLA	C4A-NA-C1A	4.58	108.77	106.68
39	Y	302	XAT	C15-C14-C13	-4.55	120.89	127.28
25	S	613	CLA	C4A-NA-C1A	4.55	108.76	106.68
27	B	517	BCR	C19-C18-C17	4.55	126.17	119.01
39	r	309	XAT	O24-C25-C38	4.55	120.13	115.05
25	B	515	CLA	C4A-NA-C1A	4.54	108.75	106.68
39	r	309	XAT	C35-C34-C33	-4.54	120.92	127.28
25	c	501	CLA	C4A-NA-C1A	4.52	108.74	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	514	CLA	C4A-NA-C1A	4.51	108.74	106.68
25	C	512	CLA	C4A-NA-C1A	4.51	108.74	106.68
27	b	519	BCR	C16-C17-C18	-4.50	120.97	127.28
25	A	402	CLA	C4A-NA-C1A	4.50	108.73	106.68
27	d	405	BCR	C27-C26-C25	-4.49	116.63	122.70
25	b	503	CLA	C4A-NA-C1A	4.49	108.73	106.68
25	A	403	CLA	C4A-NA-C1A	4.48	108.72	106.68
25	B	502	CLA	C4A-NA-C1A	4.47	108.72	106.68
27	b	519	BCR	C15-C14-C13	-4.47	121.02	127.28
25	S	602	CLA	C4A-NA-C1A	4.46	108.72	106.68
25	b	501	CLA	C4A-NA-C1A	4.46	108.72	106.68
27	A	406	BCR	C11-C10-C9	-4.46	121.02	127.28
39	Y	302	XAT	O4-C5-C18	4.46	120.03	115.05
27	z	101	BCR	C33-C5-C6	-4.45	119.62	124.48
27	t	101	BCR	C30-C25-C26	-4.45	116.55	122.64
27	c	514	BCR	C24-C23-C22	-4.45	119.65	126.23
27	V	101	BCR	C33-C5-C6	-4.45	119.63	124.48
25	b	507	CLA	C4A-NA-C1A	4.44	108.70	106.68
38	G	617	NEX	O24-C25-C38	4.43	120.00	115.05
25	b	506	CLA	C4A-NA-C1A	4.43	108.70	106.68
27	B	518	BCR	C16-C17-C18	-4.42	121.08	127.28
25	B	503	CLA	C4A-NA-C1A	4.41	108.69	106.68
25	C	503	CLA	C4A-NA-C1A	4.41	108.69	106.68
39	N	301	XAT	C6-C7-C8	-4.40	116.69	125.99
39	G	620	XAT	C6-C7-C8	-4.40	116.70	125.99
27	d	405	BCR	C16-C17-C18	-4.40	121.11	127.28
25	c	508	CLA	C4A-NA-C1A	4.39	108.68	106.68
27	h	101	BCR	C16-C17-C18	-4.39	121.12	127.28
25	C	508	CLA	C4A-NA-C1A	4.39	108.68	106.68
25	B	511	CLA	C4A-NA-C1A	4.39	108.68	106.68
37	S	616	LUT	C26-C27-C28	-4.38	117.76	124.58
38	r	310	NEX	O24-C25-C38	4.38	119.94	115.05
37	S	616	LUT	C35-C34-C33	-4.36	121.17	127.28
29	d	410	LMG	O7-C10-C11	4.35	120.89	111.48
39	Y	302	XAT	C6-C7-C8	-4.35	116.80	125.99
25	Y	304	CLA	C4A-NA-C1A	4.34	108.66	106.68
25	B	506	CLA	C4A-NA-C1A	4.34	108.66	106.68
27	H	101	BCR	C15-C14-C13	-4.34	121.19	127.28
38	r	310	NEX	C27-C28-C29	-4.34	118.80	125.53
25	b	514	CLA	C4A-NA-C1A	4.33	108.65	106.68
31	W	202	DGD	O2G-C1B-C2B	4.30	120.79	111.48
37	Y	316	LUT	C35-C34-C33	-4.30	121.25	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	513	CLA	C4A-NA-C1A	4.29	108.64	106.68
27	a	406	BCR	C16-C17-C18	-4.29	121.27	127.28
27	t	101	BCR	C11-C10-C9	-4.28	121.28	127.28
25	G	604	CLA	C4A-NA-C1A	4.27	108.62	106.68
25	S	612	CLA	C4A-NA-C1A	4.26	108.62	106.68
39	r	309	XAT	C26-C27-C28	-4.26	116.99	125.99
38	G	617	NEX	C27-C28-C29	-4.26	118.92	125.53
30	S	618	LHG	O7-C7-C8	4.26	120.69	111.48
27	D	406	BCR	C16-C17-C18	-4.25	121.32	127.28
27	B	518	BCR	C1-C6-C5	-4.25	116.83	122.64
27	A	406	BCR	C15-C14-C13	-4.24	121.33	127.28
29	D	410	LMG	O7-C10-C11	4.23	120.64	111.48
25	B	507	CLA	C4A-NA-C1A	4.22	108.61	106.68
30	L	101	LHG	O7-C7-C8	4.22	120.61	111.48
25	N	313	CLA	C4A-NA-C1A	4.22	108.60	106.68
25	G	602	CLA	C4A-NA-C1A	4.22	108.60	106.68
38	S	617	NEX	O24-C25-C38	4.22	119.76	115.05
39	N	301	XAT	C15-C14-C13	-4.21	121.38	127.28
27	A	406	BCR	C16-C17-C18	-4.20	121.39	127.28
25	b	502	CLA	C4A-NA-C1A	4.19	108.59	106.68
31	C	518	DGD	O2G-C1B-C2B	4.19	120.55	111.48
25	B	508	CLA	C4A-NA-C1A	4.19	108.59	106.68
27	t	101	BCR	C3-C4-C5	-4.18	106.61	114.06
27	z	101	BCR	C20-C21-C22	-4.18	121.42	127.28
27	a	406	BCR	C24-C23-C22	-4.17	120.06	126.23
38	Y	318	NEX	O24-C25-C38	4.16	119.70	115.05
38	Y	318	NEX	C27-C28-C29	-4.16	119.08	125.53
30	a	410	LHG	O7-C7-C8	4.16	120.47	111.48
27	z	101	BCR	C24-C23-C22	-4.15	120.10	126.23
25	G	614	CLA	C4A-NA-C1A	4.14	108.57	106.68
27	A	406	BCR	C7-C8-C9	-4.14	120.10	126.23
38	N	318	NEX	C27-C28-C29	-4.14	119.10	125.53
31	c	517	DGD	O2G-C1B-C2B	4.14	120.44	111.48
27	t	101	BCR	C33-C5-C6	-4.14	119.97	124.48
29	a	408	LMG	O7-C10-C11	4.13	120.42	111.48
37	N	316	LUT	C35-C34-C33	-4.13	121.49	127.28
25	Y	315	CLA	C4A-NA-C1A	4.13	108.56	106.68
27	A	406	BCR	C24-C23-C22	-4.12	120.14	126.23
28	A	407	SQD	O47-C7-C8	4.12	120.39	111.48
25	G	612	CLA	C4A-NA-C1A	4.11	108.56	106.68
38	Y	318	NEX	C35-C34-C33	-4.11	121.52	127.28
27	D	406	BCR	C34-C9-C8	4.11	124.36	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	620	XAT	C35-C34-C33	-4.11	121.52	127.28
27	k	101	BCR	C7-C8-C9	-4.11	120.16	126.23
38	S	617	NEX	C27-C28-C29	-4.10	119.17	125.53
37	S	615	LUT	C35-C34-C33	-4.10	121.53	127.28
37	G	615	LUT	C35-C34-C33	-4.10	121.53	127.28
27	a	406	BCR	C15-C14-C13	-4.09	121.54	127.28
39	Y	302	XAT	C31-C30-C29	-4.09	121.54	127.28
29	W	201	LMG	O7-C10-C11	4.08	120.30	111.48
25	a	402	CLA	C4A-NA-C1A	4.07	108.54	106.68
27	B	518	BCR	C15-C14-C13	-4.07	121.57	127.28
30	N	319	LHG	O7-C7-C8	4.07	120.29	111.48
27	C	514	BCR	C7-C8-C9	-4.07	120.22	126.23
25	r	302	CLA	C4A-NA-C1A	4.07	108.53	106.68
29	d	409	LMG	O7-C10-C11	4.07	120.28	111.48
27	b	518	BCR	C16-C17-C18	-4.06	121.59	127.28
27	h	101	BCR	C20-C21-C22	-4.05	121.59	127.28
27	C	514	BCR	C30-C25-C26	-4.05	117.10	122.64
27	c	514	BCR	C7-C8-C9	-4.05	120.24	126.23
27	B	517	BCR	C21-C20-C19	-4.05	111.48	123.20
27	B	517	BCR	C27-C26-C25	-4.05	117.24	122.70
30	d	408	LHG	O7-C7-C8	4.04	120.22	111.48
29	B	519	LMG	O7-C10-C11	4.04	120.22	111.48
39	Y	302	XAT	O24-C25-C38	4.04	119.56	115.05
37	G	615	LUT	C26-C27-C28	-4.03	118.31	124.58
31	C	517	DGD	O2G-C1B-C2B	4.02	120.17	111.48
27	z	101	BCR	C15-C14-C13	-4.01	121.65	127.28
29	H	102	LMG	O7-C10-C11	4.01	120.16	111.48
27	v	101	BCR	C23-C22-C21	4.01	125.32	119.01
27	b	519	BCR	C11-C10-C9	-4.00	121.66	127.28
27	C	514	BCR	C16-C17-C18	-4.00	121.67	127.28
27	b	519	BCR	C20-C21-C22	-3.99	121.68	127.28
31	c	516	DGD	O2G-C1B-C2B	3.98	120.10	111.48
27	C	515	BCR	C24-C23-C22	-3.98	120.34	126.23
27	B	517	BCR	C23-C22-C21	3.98	125.27	119.01
27	v	101	BCR	C19-C18-C17	3.97	125.25	119.01
30	D	408	LHG	O7-C7-C8	3.96	120.05	111.48
37	Y	316	LUT	C26-C27-C28	-3.96	118.41	124.58
29	C	520	LMG	O7-C10-C11	3.96	120.05	111.48
25	b	508	CLA	C4A-NA-C1A	3.96	108.49	106.68
30	C	521	LHG	O7-C7-C8	3.95	120.02	111.48
30	G	618	LHG	O7-C7-C8	3.92	119.96	111.48
38	N	318	NEX	C15-C14-C13	-3.92	121.78	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	409	LHG	O7-C7-C8	3.92	119.95	111.48
27	h	101	BCR	C15-C14-C13	-3.91	121.79	127.28
31	c	515	DGD	O2G-C1B-C2B	3.91	119.95	111.48
25	B	504	CLA	C4A-NA-C1A	3.91	108.46	106.68
39	Y	302	XAT	C35-C34-C33	-3.91	121.79	127.28
27	C	516	BCR	C11-C10-C9	-3.91	121.80	127.28
30	B	520	LHG	O7-C7-C8	3.90	119.92	111.48
29	b	520	LMG	O7-C10-C11	3.90	119.92	111.48
27	b	518	BCR	C11-C10-C9	-3.90	121.81	127.28
30	Y	319	LHG	O7-C7-C8	3.88	119.88	111.48
25	S	605	CLA	C4A-NA-C1A	3.88	108.45	106.68
31	C	519	DGD	O2G-C1B-C2B	3.88	119.86	111.48
37	N	316	LUT	C26-C27-C28	-3.87	118.55	124.58
25	S	609	CLA	C4A-NA-C1A	3.87	108.44	106.68
37	G	616	LUT	C26-C27-C28	-3.87	118.56	124.58
39	N	301	XAT	O24-C25-C38	3.86	119.36	115.05
27	c	514	BCR	C16-C17-C18	-3.86	121.86	127.28
39	N	301	XAT	C35-C34-C33	-3.86	121.87	127.28
27	H	101	BCR	C20-C21-C22	-3.84	121.89	127.28
30	d	407	LHG	O7-C7-C8	3.84	119.80	111.48
29	c	518	LMG	O7-C10-C11	3.84	119.78	111.48
25	Y	311	CLA	C4A-NA-C1A	3.84	108.43	106.68
30	l	101	LHG	O7-C7-C8	3.83	119.77	111.48
38	N	318	NEX	C35-C34-C33	-3.83	121.90	127.28
28	t	102	SQD	O47-C7-C8	3.83	119.77	111.48
25	c	503	CLA	C4A-NA-C1A	3.82	108.42	106.68
38	r	310	NEX	C35-C34-C33	-3.82	121.92	127.28
39	G	620	XAT	C31-C30-C29	-3.82	121.92	127.28
27	v	101	BCR	C16-C15-C14	-3.82	115.71	123.52
27	b	519	BCR	C24-C23-C22	-3.81	120.60	126.23
27	B	517	BCR	C33-C5-C6	-3.81	120.33	124.48
27	b	518	BCR	C20-C21-C22	-3.80	121.94	127.28
37	Y	317	LUT	C35-C34-C33	-3.80	121.94	127.28
30	a	411	LHG	O7-C7-C8	3.80	119.70	111.48
38	Y	318	NEX	C11-C10-C9	-3.79	121.96	127.28
27	v	101	BCR	C30-C25-C26	-3.79	117.46	122.64
27	z	101	BCR	C3-C4-C5	-3.79	107.30	114.06
34	D	407	PL9	C7-C3-C2	-3.78	118.93	123.39
27	C	514	BCR	C11-C10-C9	-3.77	121.98	127.28
27	c	514	BCR	C11-C10-C9	-3.77	121.99	127.28
27	C	514	BCR	C24-C23-C22	-3.77	120.67	126.23
27	z	101	BCR	C7-C8-C9	-3.76	120.67	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Y	301	DGD	O2G-C1B-C2B	3.76	119.61	111.48
38	S	617	NEX	C15-C14-C13	-3.75	122.02	127.28
25	G	610	CLA	C4A-NA-C1A	3.75	108.39	106.68
27	v	101	BCR	C3-C4-C5	-3.75	107.37	114.06
27	d	405	BCR	C20-C21-C22	-3.73	122.05	127.28
27	B	518	BCR	C24-C23-C22	-3.73	120.72	126.23
37	Y	317	LUT	C26-C27-C28	-3.72	118.79	124.58
34	d	406	PL9	C7-C3-C2	-3.72	119.00	123.39
27	v	101	BCR	C37-C22-C21	-3.72	116.79	122.82
37	N	317	LUT	C26-C27-C28	-3.72	118.79	124.58
36	N	302	CHL	C1-C2-C3	-3.70	120.13	126.20
27	B	518	BCR	C20-C21-C22	-3.70	122.09	127.28
37	S	615	LUT	C21-C26-C27	-3.70	108.57	112.83
37	S	615	LUT	C26-C27-C28	-3.69	118.83	124.58
27	b	519	BCR	C7-C8-C9	-3.68	120.79	126.23
28	a	407	SQD	O47-C7-C8	3.68	119.44	111.48
37	G	615	LUT	C11-C10-C9	-3.67	122.12	127.28
37	G	616	LUT	C35-C34-C33	-3.67	122.13	127.28
37	G	616	LUT	C15-C14-C13	-3.66	122.14	127.28
27	b	517	BCR	C16-C17-C18	-3.66	122.14	127.28
27	v	101	BCR	C33-C5-C6	-3.65	120.50	124.48
27	B	517	BCR	C28-C27-C26	-3.65	107.54	114.06
36	Y	303	CHL	C1-C2-C3	-3.65	120.22	126.20
27	d	405	BCR	C24-C23-C22	-3.64	120.85	126.23
27	k	101	BCR	C28-C27-C26	-3.64	107.56	114.06
27	C	516	BCR	C7-C8-C9	-3.64	120.86	126.23
37	S	616	LUT	C15-C14-C13	-3.63	122.18	127.28
27	b	517	BCR	C3-C4-C5	-3.63	107.58	114.06
25	N	311	CLA	C4A-NA-C1A	3.63	108.34	106.68
25	N	315	CLA	C4A-NA-C1A	3.63	108.33	106.68
36	G	605	CHL	C3D-C4D-ND	3.62	118.75	112.94
27	B	518	BCR	C38-C26-C25	-3.62	120.53	124.48
27	c	514	BCR	C3-C4-C5	-3.62	107.60	114.06
27	d	405	BCR	C1-C6-C5	-3.62	117.69	122.64
36	S	601	CHL	C3D-C4D-ND	3.62	118.74	112.94
37	Y	317	LUT	C15-C14-C13	-3.62	122.21	127.28
36	N	307	CHL	C3D-C4D-ND	3.61	118.73	112.94
27	C	514	BCR	C15-C14-C13	-3.61	122.22	127.28
36	r	304	CHL	C3D-C4D-ND	3.60	118.72	112.94
27	b	517	BCR	C11-C10-C9	-3.60	122.23	127.28
27	B	518	BCR	C4-C5-C6	-3.59	117.85	122.70
27	C	515	BCR	C16-C17-C18	-3.59	122.25	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	620	XAT	O24-C25-C38	3.58	119.05	115.05
36	Y	308	CHL	C3D-C4D-ND	3.57	118.67	112.94
26	A	404	PHO	C2B-C1B-NB	-3.57	106.85	109.43
27	D	406	BCR	C20-C21-C22	-3.57	122.27	127.28
37	S	615	LUT	C18-C5-C6	-3.57	120.59	124.48
27	C	515	BCR	C11-C10-C9	-3.57	122.28	127.28
26	a	404	PHO	C2B-C1B-NB	-3.56	106.86	109.43
30	b	521	LHG	O7-C7-C8	3.55	119.16	111.48
27	h	101	BCR	C24-C23-C22	-3.55	120.98	126.23
36	r	305	CHL	C3D-C4D-ND	3.53	118.60	112.94
37	N	317	LUT	C7-C8-C9	-3.53	121.01	126.23
36	N	302	CHL	C3D-C4D-ND	3.53	118.60	112.94
36	G	606	CHL	C3D-C4D-ND	3.53	118.60	112.94
39	r	309	XAT	C15-C14-C13	-3.52	122.34	127.28
27	d	405	BCR	C11-C10-C9	-3.52	122.34	127.28
27	A	406	BCR	C33-C5-C6	-3.52	120.65	124.48
36	Y	303	CHL	C3D-C4D-ND	3.52	118.58	112.94
27	A	406	BCR	C20-C21-C22	-3.51	122.35	127.28
36	S	607	CHL	C3D-C4D-ND	3.51	118.57	112.94
36	N	306	CHL	C3D-C4D-ND	3.51	118.57	112.94
39	Y	302	XAT	C26-C27-C28	-3.51	118.58	125.99
36	G	601	CHL	C3D-C4D-ND	3.51	118.56	112.94
37	N	317	LUT	C35-C34-C33	-3.51	122.36	127.28
39	N	301	XAT	C26-C27-C28	-3.50	118.58	125.99
27	t	101	BCR	C27-C26-C25	-3.50	117.97	122.70
36	G	619	CHL	C3D-C4D-ND	3.50	118.56	112.94
27	a	406	BCR	C7-C8-C9	-3.50	121.06	126.23
36	N	309	CHL	C3D-C4D-ND	3.50	118.55	112.94
36	N	310	CHL	C3D-C4D-ND	3.50	118.55	112.94
39	G	620	XAT	C26-C27-C28	-3.50	118.60	125.99
27	C	514	BCR	C20-C21-C22	-3.50	122.38	127.28
36	r	306	CHL	C3D-C4D-ND	3.50	118.55	112.94
27	d	405	BCR	C15-C14-C13	-3.49	122.38	127.28
27	C	515	BCR	C30-C25-C26	-3.49	117.87	122.64
27	H	101	BCR	C3-C4-C5	-3.48	107.84	114.06
27	D	406	BCR	C24-C23-C22	-3.48	121.09	126.23
37	N	317	LUT	C15-C14-C13	-3.47	122.41	127.28
36	G	609	CHL	C3D-C4D-ND	3.47	118.51	112.94
27	h	101	BCR	C3-C4-C5	-3.47	107.87	114.06
26	D	402	PHO	C2B-C1B-NB	-3.47	106.92	109.43
37	G	616	LUT	C7-C8-C9	-3.46	121.11	126.23
25	b	511	CLA	O2D-CGD-O1D	-3.46	117.11	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	G	607	CHL	C3D-C4D-ND	3.46	118.49	112.94
27	a	406	BCR	C30-C25-C26	-3.46	117.91	122.64
27	c	514	BCR	C30-C25-C26	-3.46	117.91	122.64
26	d	402	PHO	C2B-C1B-NB	-3.45	106.93	109.43
38	r	310	NEX	C11-C10-C9	-3.45	122.44	127.28
38	G	617	NEX	C35-C34-C33	-3.45	122.44	127.28
37	G	615	LUT	C21-C26-C27	-3.44	108.87	112.83
36	Y	307	CHL	C3D-C4D-ND	3.44	118.45	112.94
27	b	517	BCR	C24-C23-C22	-3.44	121.15	126.23
27	d	405	BCR	C7-C8-C9	-3.42	121.17	126.23
27	b	518	BCR	C7-C8-C9	-3.41	121.19	126.23
27	V	101	BCR	C7-C8-C9	-3.41	121.20	126.23
37	Y	317	LUT	C7-C8-C9	-3.40	121.20	126.23
36	Y	309	CHL	C3D-C4D-ND	3.39	118.38	112.94
37	N	316	LUT	C21-C26-C27	-3.38	108.94	112.83
27	C	516	BCR	C10-C11-C12	-3.37	113.44	123.20
36	Y	310	CHL	C3D-C4D-ND	3.37	118.34	112.94
36	G	608	CHL	C3D-C4D-ND	3.35	118.32	112.94
27	b	517	BCR	C20-C21-C22	-3.35	122.58	127.28
37	G	615	LUT	C7-C8-C9	-3.35	121.28	126.23
36	S	606	CHL	C3D-C4D-ND	3.35	118.31	112.94
37	S	615	LUT	C15-C14-C13	-3.35	122.58	127.28
36	Y	303	CHL	CBC-CAC-C3C	-3.34	108.08	112.87
25	d	401	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
37	N	316	LUT	C15-C14-C13	-3.34	122.59	127.28
37	Y	316	LUT	C7-C8-C9	-3.34	121.29	126.23
25	c	511	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
37	Y	316	LUT	C21-C26-C27	-3.33	108.99	112.83
27	D	406	BCR	C15-C14-C13	-3.33	122.60	127.28
36	G	606	CHL	C1C-CHC-C4B	3.33	127.98	116.07
27	k	101	BCR	C33-C5-C6	-3.32	120.86	124.48
36	N	308	CHL	C3D-C4D-ND	3.32	118.26	112.94
27	C	515	BCR	C33-C5-C6	-3.32	120.86	124.48
25	a	403	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
37	S	615	LUT	C7-C8-C9	-3.31	121.33	126.23
27	a	406	BCR	C11-C10-C9	-3.31	122.63	127.28
37	Y	316	LUT	C15-C14-C13	-3.31	122.63	127.28
37	N	316	LUT	C7-C8-C9	-3.31	121.34	126.23
37	N	316	LUT	C18-C5-C6	-3.31	120.87	124.48
27	D	406	BCR	C3-C4-C5	-3.31	108.16	114.06
36	N	310	CHL	C1-C2-C3	-3.31	120.78	126.20
37	G	616	LUT	C18-C5-C6	-3.30	120.88	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	614	CLA	C4A-NA-C1A	3.30	108.18	106.68
36	S	607	CHL	CBC-CAC-C3C	-3.29	108.16	112.87
25	A	403	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
36	G	609	CHL	C1C-CHC-C4B	3.28	127.82	116.07
39	G	620	XAT	C36-C21-C26	3.28	118.91	110.05
27	v	101	BCR	C20-C21-C22	3.28	131.88	127.28
27	c	514	BCR	C33-C5-C6	-3.28	120.91	124.48
25	b	506	CLA	O2D-CGD-O1D	-3.27	117.47	123.85
27	C	516	BCR	C28-C27-C26	-3.27	108.22	114.06
37	N	316	LUT	C11-C10-C9	-3.27	122.69	127.28
36	N	306	CHL	C1C-CHC-C4B	3.27	127.76	116.07
36	N	309	CHL	C1C-CHC-C4B	3.26	127.74	116.07
36	Y	308	CHL	C1C-CHC-C4B	3.26	127.73	116.07
37	S	616	LUT	C21-C26-C27	-3.25	109.08	112.83
36	S	608	CHL	C1C-CHC-C4B	3.25	127.72	116.07
27	b	517	BCR	C30-C25-C26	-3.25	118.20	122.64
27	V	101	BCR	C24-C23-C22	-3.25	121.43	126.23
27	B	517	BCR	C7-C8-C9	-3.25	121.43	126.23
36	S	608	CHL	C3D-C4D-ND	3.24	118.14	112.94
36	N	310	CHL	C1C-CHC-C4B	3.24	127.67	116.07
27	b	518	BCR	C33-C5-C6	-3.24	120.95	124.48
26	d	402	PHO	O1D-CGD-CBD	3.23	129.62	124.72
25	C	505	CLA	C4A-NA-C1A	3.23	108.15	106.68
37	Y	316	LUT	C11-C10-C9	-3.23	122.75	127.28
36	Y	310	CHL	C1C-CHC-C4B	3.23	127.63	116.07
36	r	304	CHL	C1C-CHC-C4B	3.23	127.62	116.07
37	G	615	LUT	C15-C14-C13	-3.22	122.76	127.28
36	Y	309	CHL	C1C-CHC-C4B	3.22	127.60	116.07
27	b	519	BCR	C38-C26-C25	-3.22	120.97	124.48
36	N	308	CHL	C1C-CHC-C4B	3.22	127.58	116.07
36	N	307	CHL	C1C-CHC-C4B	3.22	127.57	116.07
27	a	406	BCR	C33-C5-C6	-3.21	120.98	124.48
36	r	305	CHL	C1C-CHC-C4B	3.21	127.57	116.07
25	D	405	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
27	b	518	BCR	C24-C23-C22	-3.20	121.50	126.23
36	S	606	CHL	C1C-CHC-C4B	3.20	127.52	116.07
27	a	406	BCR	C3-C4-C5	-3.19	108.36	114.06
37	Y	317	LUT	C18-C5-C6	-3.19	121.00	124.48
36	S	606	CHL	O2D-CGD-O1D	-3.19	117.65	123.85
27	t	101	BCR	C16-C17-C18	-3.18	122.81	127.28
36	G	605	CHL	C1C-CHC-C4B	3.18	127.46	116.07
27	H	101	BCR	C24-C23-C22	-3.18	121.53	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	G	608	CHL	C1C-CHC-C4B	3.18	127.45	116.07
36	G	607	CHL	C1C-CHC-C4B	3.18	127.45	116.07
36	S	601	CHL	C1C-CHC-C4B	3.18	127.45	116.07
27	b	519	BCR	C33-C5-C6	-3.18	121.02	124.48
39	N	301	XAT	C31-C30-C29	-3.18	122.82	127.28
36	S	607	CHL	C1C-CHC-C4B	3.18	127.43	116.07
27	C	516	BCR	C33-C5-C6	-3.17	121.02	124.48
38	S	617	NEX	C31-C30-C29	-3.17	122.84	127.28
36	N	302	CHL	C1C-CHC-C4B	3.16	127.39	116.07
25	S	614	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
37	Y	316	LUT	C18-C5-C6	-3.16	121.03	124.48
36	G	619	CHL	C1C-CHC-C4B	3.16	127.38	116.07
25	c	507	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
27	v	101	BCR	C27-C26-C25	-3.16	118.44	122.70
27	B	518	BCR	C11-C10-C9	-3.15	122.85	127.28
25	S	605	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
36	G	601	CHL	C1C-CHC-C4B	3.15	127.33	116.07
36	Y	307	CHL	C1C-CHC-C4B	3.15	127.33	116.07
27	k	101	BCR	C15-C16-C17	-3.14	117.09	123.52
34	d	406	PL9	C7-C8-C9	-3.14	121.42	126.83
37	Y	317	LUT	C16-C1-C6	-3.14	105.32	110.24
27	z	101	BCR	C30-C25-C26	-3.13	118.35	122.64
37	Y	317	LUT	C21-C26-C27	-3.13	109.23	112.83
27	D	406	BCR	C30-C25-C26	-3.13	118.36	122.64
27	B	517	BCR	C38-C26-C27	3.12	120.26	113.60
36	G	601	CHL	CBC-CAC-C3C	-3.12	108.40	112.87
27	C	515	BCR	C3-C4-C5	-3.12	108.49	114.06
36	G	619	CHL	C1-C2-C3	-3.12	121.09	126.20
25	d	404	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
36	r	306	CHL	C1C-CHC-C4B	3.12	127.22	116.07
27	C	514	BCR	C27-C26-C25	-3.12	118.49	122.70
25	b	502	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
36	Y	303	CHL	C1C-CHC-C4B	3.09	127.14	116.07
25	c	508	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
25	S	602	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
32	C	522	LMU	C1B-O1B-C4'	-3.09	110.66	117.98
27	k	101	BCR	C15-C14-C13	-3.09	122.95	127.28
38	N	318	NEX	C11-C10-C9	-3.09	122.95	127.28
30	l	101	LHG	O8-C23-C24	3.09	121.24	111.83
37	N	317	LUT	C11-C10-C9	-3.08	122.96	127.28
27	C	516	BCR	C16-C17-C18	-3.08	122.96	127.28
27	c	514	BCR	C20-C21-C22	-3.08	122.96	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	v	101	BCR	C21-C20-C19	3.08	132.12	123.20
39	Y	302	XAT	C11-C10-C9	-3.08	122.96	127.28
25	C	512	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
27	k	101	BCR	C16-C17-C18	-3.07	122.97	127.28
25	A	405	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
39	G	620	XAT	C11-C10-C9	-3.07	122.97	127.28
36	G	601	CHL	C4-C3-C5	3.06	120.54	115.23
39	r	309	XAT	C10-C11-C12	-3.06	114.34	123.20
27	C	515	BCR	C8-C7-C6	-3.06	118.83	127.00
27	h	101	BCR	C38-C26-C25	-3.06	121.15	124.48
37	G	615	LUT	C18-C5-C6	-3.05	121.16	124.48
27	b	517	BCR	C7-C8-C9	-3.04	121.73	126.23
27	V	101	BCR	C16-C15-C14	-3.04	117.30	123.52
26	A	404	PHO	O1D-CGD-CBD	3.03	129.32	124.72
26	a	404	PHO	O1D-CGD-CBD	3.03	129.32	124.72
25	N	312	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
25	C	508	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
25	c	501	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
36	N	308	CHL	C4-C3-C5	3.02	120.48	115.23
37	N	317	LUT	C18-C5-C4	3.02	119.98	114.42
25	S	613	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
25	b	514	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
27	b	519	BCR	C3-C4-C5	-3.01	108.68	114.06
27	B	518	BCR	C3-C4-C5	-3.01	108.69	114.06
29	W	201	LMG	C8-O7-C10	-3.01	110.59	117.80
25	C	507	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
25	D	401	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
25	b	510	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
25	D	404	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
26	d	402	PHO	C1-C2-C3	-3.00	121.28	126.20
36	S	606	CHL	O1D-CGD-CBD	-3.00	120.17	124.72
28	a	407	SQD	O7-S-C6	3.00	111.23	106.76
38	S	617	NEX	C26-C27-C28	-3.00	119.66	125.99
25	B	510	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
27	C	515	BCR	C33-C5-C4	2.99	119.98	113.60
27	b	519	BCR	C28-C27-C26	-2.99	108.72	114.06
37	N	317	LUT	C18-C5-C6	-2.99	121.22	124.48
27	D	406	BCR	C33-C5-C6	-2.99	121.22	124.48
27	b	518	BCR	C28-C27-C26	-2.99	108.72	114.06
31	c	517	DGD	O1G-C1A-C2A	2.98	120.93	111.83
36	N	310	CHL	CBC-CAC-C3C	-2.98	108.61	112.87
27	d	405	BCR	C29-C30-C25	2.98	114.77	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	517	BCR	C36-C18-C17	-2.98	118.00	122.82
29	c	518	LMG	O8-C28-C29	2.97	120.90	111.83
25	G	613	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
27	k	101	BCR	C10-C11-C12	-2.97	114.59	123.20
25	C	510	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
27	C	515	BCR	C1-C6-C5	-2.97	118.58	122.64
25	B	511	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
25	S	609	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
25	Y	315	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
30	d	407	LHG	O8-C23-C24	2.96	120.86	111.83
25	B	502	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
27	C	516	BCR	C15-C14-C13	-2.96	123.13	127.28
25	b	508	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
25	B	514	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
27	v	101	BCR	C36-C18-C17	-2.96	118.03	122.82
27	D	406	BCR	C8-C9-C10	-2.95	114.36	119.01
26	a	404	PHO	C1-C2-C3	-2.95	121.36	126.20
31	W	202	DGD	C2G-O2G-C1B	-2.95	110.73	117.80
25	C	511	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
25	C	501	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
25	d	403	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
27	C	515	BCR	C7-C8-C9	-2.95	121.87	126.23
27	b	517	BCR	C33-C5-C6	-2.95	121.27	124.48
26	d	402	PHO	CMB-C2B-C3B	2.95	130.58	124.68
27	H	101	BCR	C38-C26-C25	-2.95	121.27	124.48
28	A	407	SQD	O7-S-C6	2.94	111.15	106.76
26	D	402	PHO	CMB-C2B-C3B	2.94	130.56	124.68
25	C	513	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
38	S	617	NEX	C11-C10-C9	-2.94	123.15	127.28
27	v	101	BCR	C28-C27-C26	-2.94	108.81	114.06
29	d	409	LMG	C8-O7-C10	-2.94	110.76	117.80
36	S	601	CHL	CBC-CAC-C3C	-2.94	108.67	112.87
27	B	517	BCR	C11-C10-C9	-2.94	123.16	127.28
39	N	301	XAT	C11-C10-C9	-2.94	123.16	127.28
36	G	605	CHL	CBC-CAC-C3C	-2.94	108.67	112.87
31	c	516	DGD	O1G-C1A-C2A	2.94	120.07	111.15
26	D	402	PHO	O1D-CGD-CBD	2.94	129.18	124.72
25	G	614	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
25	N	314	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
25	Y	314	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
27	V	101	BCR	C10-C11-C12	-2.92	114.73	123.20
25	N	305	CLA	O2D-CGD-O1D	-2.92	118.16	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	306	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
37	S	615	LUT	C11-C10-C9	-2.92	123.18	127.28
25	S	610	CLA	C4A-NA-C1A	2.92	108.01	106.68
25	B	512	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
36	S	608	CHL	O2D-CGD-O1D	-2.92	118.17	123.85
29	a	408	LMG	O8-C28-C29	2.92	120.73	111.83
25	B	503	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
37	Y	317	LUT	C11-C10-C9	-2.91	123.19	127.28
37	S	616	LUT	C7-C8-C9	-2.91	121.92	126.23
27	d	405	BCR	C38-C26-C27	2.91	119.81	113.60
36	N	306	CHL	C1-C2-C3	-2.91	121.42	126.20
25	C	509	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
25	b	504	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
27	B	517	BCR	C30-C25-C26	-2.91	118.66	122.64
25	B	501	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
38	Y	318	NEX	C26-C27-C28	-2.90	119.85	125.99
25	N	315	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
25	c	512	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
25	d	401	CLA	C1-C2-C3	-2.90	121.44	126.20
38	N	318	NEX	C24-C23-C22	-2.90	105.37	110.79
37	S	616	LUT	C16-C1-C6	-2.90	105.70	110.24
25	a	405	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
27	D	406	BCR	C10-C11-C12	-2.90	114.81	123.20
25	b	503	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
25	B	507	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
27	B	517	BCR	C37-C22-C21	-2.89	118.13	122.82
25	C	506	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
27	V	101	BCR	C33-C5-C4	2.88	119.75	113.60
25	r	303	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
25	C	503	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
37	G	616	LUT	C21-C26-C27	-2.88	109.51	112.83
25	r	302	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
25	b	516	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
29	H	102	LMG	O8-C28-C29	2.88	120.62	111.83
25	b	512	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
25	c	510	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
25	G	612	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
34	D	407	PL9	C7-C8-C9	-2.88	121.87	126.83
31	C	517	DGD	O1G-C1A-C2A	2.88	120.61	111.83
38	Y	318	NEX	C24-C23-C22	-2.88	105.41	110.79
31	C	518	DGD	O1G-C1A-C2A	2.88	120.60	111.83
25	N	304	CLA	O2D-CGD-O1D	-2.88	118.25	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	515	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
30	B	520	LHG	O8-C23-C24	2.87	120.60	111.83
25	N	303	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
27	d	405	BCR	C30-C25-C26	-2.87	118.71	122.64
25	Y	305	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
25	c	504	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
25	c	505	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
25	c	501	CLA	C1-C2-C3	-2.87	121.50	126.20
30	S	618	LHG	C5-O7-C7	-2.87	110.94	117.80
25	B	508	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
25	C	505	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
25	G	610	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
34	D	407	PL9	C22-C23-C24	-2.86	121.07	127.62
30	Y	319	LHG	O8-C23-C24	2.86	120.55	111.83
25	S	603	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
27	B	518	BCR	C7-C8-C9	-2.86	122.01	126.23
26	a	404	PHO	CMB-C2B-C3B	2.86	130.39	124.68
36	N	309	CHL	O2A-CGA-CBA	2.85	120.54	111.83
27	C	516	BCR	C3-C4-C5	-2.85	108.97	114.06
38	S	617	NEX	C24-C23-C22	-2.85	105.45	110.79
38	Y	318	NEX	C31-C30-C29	-2.85	123.28	127.28
39	r	309	XAT	C31-C30-C29	-2.85	123.28	127.28
27	d	405	BCR	C4-C5-C6	-2.85	118.85	122.70
30	d	408	LHG	O8-C23-C24	2.85	120.52	111.83
36	G	619	CHL	O2A-CGA-CBA	2.84	120.51	111.83
37	N	317	LUT	C21-C26-C27	-2.84	109.56	112.83
25	c	509	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
25	r	307	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
25	N	313	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
34	D	407	PL9	C40-C39-C41	2.84	120.16	115.23
30	L	101	LHG	C5-O7-C7	-2.84	111.01	117.80
34	d	406	PL9	C40-C39-C41	2.84	120.15	115.23
25	b	513	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
36	S	608	CHL	O2A-CGA-CBA	2.83	120.47	111.83
25	G	602	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
28	t	102	SQD	O48-C23-C24	2.83	120.47	111.83
25	r	308	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
25	c	505	CLA	C4A-NA-C1A	2.82	107.97	106.68
36	S	606	CHL	OMC-CMC-C2C	-2.82	120.22	125.12
27	C	516	BCR	C15-C16-C17	-2.82	117.74	123.52
36	Y	310	CHL	O1D-CGD-CBD	-2.82	120.44	124.72
29	C	520	LMG	O8-C28-C29	2.82	120.44	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	304	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
38	r	310	NEX	C26-C27-C28	-2.82	120.03	125.99
25	B	505	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
25	Y	313	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
36	N	310	CHL	O2A-CGA-CBA	2.81	120.40	111.83
36	G	607	CHL	O2A-CGA-CBA	2.81	120.40	111.83
25	b	507	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
31	W	202	DGD	O1G-C1A-C2A	2.81	120.39	111.83
25	G	611	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
37	S	616	LUT	C18-C5-C6	-2.80	121.42	124.48
25	Y	311	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
36	N	302	CHL	CBC-CAC-C3C	-2.80	108.86	112.87
25	c	502	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
30	a	410	LHG	O8-C23-C24	2.80	120.37	111.83
27	D	406	BCR	C38-C26-C25	-2.80	121.43	124.48
25	b	501	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
26	A	404	PHO	CMB-C2B-C3B	2.79	130.26	124.68
25	b	509	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
25	C	504	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
27	C	514	BCR	C1-C6-C5	-2.79	118.82	122.64
25	B	509	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
25	B	506	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
34	d	406	PL9	C22-C23-C24	-2.79	121.24	127.62
27	b	518	BCR	C38-C26-C25	-2.79	121.44	124.48
25	B	504	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
25	B	515	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
25	B	516	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
25	S	611	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
36	N	307	CHL	O1D-CGD-CBD	-2.78	120.51	124.72
31	C	517	DGD	C2G-O2G-C1B	-2.78	111.14	117.80
27	D	406	BCR	C33-C5-C4	2.78	119.52	113.60
31	Y	301	DGD	O1G-C1A-C2A	2.78	120.30	111.83
25	Y	306	CLA	C1-C2-C3	-2.78	121.65	126.20
37	N	317	LUT	C16-C1-C6	-2.78	105.89	110.24
36	G	609	CHL	O2A-CGA-CBA	2.77	120.30	111.83
26	D	402	PHO	O2D-CGD-O1D	-2.77	118.45	123.85
39	Y	302	XAT	C4-C3-C2	-2.77	105.61	110.79
25	S	612	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
31	c	515	DGD	O1G-C1A-C2A	2.77	120.28	111.83
25	N	311	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
36	Y	310	CHL	C4-C3-C5	2.77	120.03	115.23
25	c	506	CLA	O2D-CGD-O1D	-2.77	118.46	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	511	CLA	C1-C2-C3	-2.77	121.66	126.20
36	G	608	CHL	CBC-CAC-C3C	-2.77	108.91	112.87
25	G	603	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
25	G	604	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
38	r	310	NEX	C31-C30-C29	-2.76	123.40	127.28
38	G	617	NEX	C24-C23-C22	-2.76	105.62	110.79
37	S	615	LUT	C35-C15-C14	-2.76	117.87	123.52
28	a	407	SQD	O48-C23-C24	2.76	120.25	111.83
30	L	101	LHG	O8-C23-C24	2.76	120.24	111.83
25	S	604	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
25	S	610	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
38	N	318	NEX	C26-C27-C28	-2.75	120.17	125.99
36	r	304	CHL	CBC-CAC-C3C	-2.75	108.93	112.87
27	v	101	BCR	C8-C7-C6	-2.75	119.65	127.00
36	Y	309	CHL	O2A-CGA-CBA	2.75	120.22	111.83
39	G	620	XAT	C4-C3-C2	-2.75	105.65	110.79
32	C	523	LMU	C1B-O1B-C4'	-2.75	111.46	117.98
36	N	302	CHL	O1D-CGD-CBD	-2.75	120.56	124.72
36	N	309	CHL	CBC-CAC-C3C	-2.75	108.94	112.87
36	Y	303	CHL	O2A-CGA-CBA	2.75	120.21	111.83
27	t	101	BCR	C28-C27-C26	-2.75	109.16	114.06
25	r	302	CLA	CHB-C4A-NA	2.74	128.36	124.40
26	d	402	PHO	O2D-CGD-O1D	-2.74	118.51	123.85
36	G	609	CHL	C1-C2-C3	-2.74	121.71	126.20
25	C	502	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
30	N	319	LHG	O8-C23-C24	2.73	120.17	111.83
27	a	406	BCR	C20-C21-C22	-2.73	123.44	127.28
36	G	601	CHL	O2A-CGA-CBA	2.73	120.16	111.83
30	G	618	LHG	O8-C23-C24	2.73	120.16	111.83
27	V	101	BCR	C38-C26-C25	-2.73	121.51	124.48
27	c	514	BCR	C27-C26-C25	-2.73	119.02	122.70
25	b	515	CLA	CHB-C4A-NA	2.73	128.33	124.40
38	N	318	NEX	C31-C30-C29	-2.73	123.46	127.28
25	a	402	CLA	O2D-CGD-O1D	-2.72	118.54	123.85
25	Y	312	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
36	N	302	CHL	C4-C3-C5	2.72	119.94	115.23
27	V	101	BCR	C8-C7-C6	-2.71	119.75	127.00
27	t	101	BCR	C20-C21-C22	-2.71	123.47	127.28
29	a	408	LMG	C8-O7-C10	-2.71	111.30	117.80
25	r	301	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
37	S	616	LUT	C18-C5-C4	2.71	119.41	114.42
25	c	503	CLA	O2D-CGD-O1D	-2.71	118.58	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	G	609	CHL	O1D-CGD-CBD	-2.71	120.61	124.72
36	Y	310	CHL	CMB-C2B-C3B	2.71	130.09	124.68
36	r	304	CHL	O1D-CGD-CBD	-2.70	120.62	124.72
36	N	308	CHL	O2A-CGA-CBA	2.70	120.08	111.83
36	S	607	CHL	O1D-CGD-CBD	-2.70	120.62	124.72
36	Y	308	CHL	O1D-CGD-CBD	-2.70	120.62	124.72
30	D	409	LHG	O8-C23-C24	2.70	120.06	111.83
36	N	306	CHL	O2A-CGA-CBA	2.70	120.06	111.83
26	a	404	PHO	O2D-CGD-O1D	-2.70	118.60	123.85
39	Y	302	XAT	C27-C28-C29	-2.69	121.35	125.53
31	C	519	DGD	O1G-C1A-C2A	2.69	120.03	111.83
31	c	515	DGD	C2G-O2G-C1B	-2.69	111.37	117.80
25	b	512	CLA	C3B-C4B-NB	-2.69	108.13	110.53
36	G	609	CHL	C4-C3-C5	2.68	119.89	115.23
38	r	310	NEX	C24-C23-C22	-2.68	105.77	110.79
29	d	409	LMG	O8-C28-C29	2.68	120.01	111.83
36	N	302	CHL	O2A-CGA-CBA	2.68	120.00	111.83
36	N	310	CHL	O1D-CGD-CBD	-2.68	120.66	124.72
25	c	512	CLA	CHB-C4A-NA	2.68	128.26	124.40
37	G	615	LUT	C35-C15-C14	-2.68	118.04	123.52
35	f	101	HEM	C3B-C2B-C1B	2.68	108.42	106.41
28	A	407	SQD	O48-C23-C24	2.68	119.99	111.83
25	C	507	CLA	CHB-C4A-NA	2.67	128.26	124.40
34	d	406	PL9	C27-C28-C29	-2.67	121.51	127.62
39	r	309	XAT	C24-C23-C22	-2.67	105.80	110.79
30	S	618	LHG	O8-C23-C24	2.66	119.95	111.83
36	G	619	CHL	C4-C3-C5	2.66	119.85	115.23
30	D	408	LHG	O8-C23-C24	2.66	119.95	111.83
36	Y	307	CHL	CBC-CAC-C3C	-2.66	109.06	112.87
36	S	601	CHL	OMC-CMC-C2C	-2.66	120.50	125.12
25	c	513	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
37	N	316	LUT	C35-C15-C14	-2.65	118.09	123.52
30	a	411	LHG	O8-C23-C24	2.65	119.92	111.83
36	G	619	CHL	CBC-CAC-C3C	-2.65	109.08	112.87
27	z	101	BCR	C27-C26-C25	-2.65	119.12	122.70
38	G	617	NEX	C26-C27-C28	-2.65	120.39	125.99
26	A	404	PHO	O2D-CGD-O1D	-2.65	118.69	123.85
29	d	410	LMG	O8-C28-C29	2.65	119.91	111.83
25	B	504	CLA	C1-C2-C3	-2.65	121.86	126.20
36	r	305	CHL	CMB-C2B-C3B	2.65	129.97	124.68
25	c	507	CLA	CHB-C4A-NA	2.64	128.22	124.40
27	h	101	BCR	C28-C27-C26	-2.64	109.34	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	407	PL9	C27-C28-C29	-2.64	121.58	127.62
30	C	521	LHG	O8-C23-C24	2.64	119.88	111.83
27	v	101	BCR	C33-C5-C4	2.64	119.22	113.60
29	b	520	LMG	O8-C28-C29	2.64	119.88	111.83
37	Y	316	LUT	C35-C15-C14	-2.64	118.12	123.52
27	C	515	BCR	C4-C5-C6	-2.63	119.15	122.70
25	B	513	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
39	Y	302	XAT	C18-C5-C4	2.63	117.20	114.24
25	c	509	CLA	CHB-C4A-NA	2.63	128.19	124.40
27	t	101	BCR	C38-C26-C27	2.63	119.20	113.60
36	G	619	CHL	CMB-C2B-C3B	2.63	129.93	124.68
36	Y	303	CHL	CMB-C2B-C3B	2.63	129.93	124.68
27	C	516	BCR	C33-C5-C4	2.63	119.19	113.60
36	G	609	CHL	CMB-C2B-C3B	2.63	129.93	124.68
30	d	408	LHG	C5-O7-C7	-2.62	111.51	117.80
36	G	607	CHL	CMB-C2B-C3B	2.62	129.91	124.68
31	C	518	DGD	C2G-O2G-C1B	-2.61	111.54	117.80
25	c	502	CLA	C1-C2-C3	-2.61	121.91	126.20
37	S	615	LUT	C30-C31-C32	-2.61	115.64	123.20
36	G	601	CHL	C1-C2-C3	-2.61	121.93	126.20
39	G	620	XAT	C18-C5-C4	2.60	117.17	114.24
36	N	308	CHL	C1-C2-C3	-2.60	121.93	126.20
27	C	515	BCR	C20-C21-C22	-2.60	123.63	127.28
36	N	307	CHL	OMC-CMC-C2C	-2.60	120.60	125.12
27	D	406	BCR	C28-C27-C26	-2.60	109.43	114.06
25	b	516	CLA	CHB-C4A-NA	2.59	128.14	124.40
36	r	305	CHL	O1D-CGD-CBD	-2.59	120.79	124.72
39	G	620	XAT	C38-C25-C24	2.59	117.15	114.24
36	G	606	CHL	O1D-CGD-CBD	-2.59	120.79	124.72
36	G	619	CHL	O1D-CGD-CBD	-2.59	120.79	124.72
27	V	101	BCR	C28-C27-C26	-2.59	109.44	114.06
25	G	603	CLA	CHB-C4A-NA	2.59	128.14	124.40
39	N	301	XAT	C4-C3-C2	-2.59	105.94	110.79
25	B	510	CLA	CHB-C4A-NA	2.59	128.14	124.40
25	B	512	CLA	CHB-C4A-NA	2.59	128.14	124.40
36	N	302	CHL	CMB-C2B-C3B	2.59	129.85	124.68
36	r	304	CHL	CMB-C2B-C3B	2.59	129.85	124.68
36	S	601	CHL	CMB-C2B-C3B	2.58	129.85	124.68
25	N	313	CLA	CHB-C4A-NA	2.58	128.13	124.40
32	c	519	LMU	C1B-O1B-C4'	-2.58	111.86	117.98
37	G	616	LUT	C16-C1-C6	-2.58	106.19	110.24
27	D	406	BCR	C4-C5-C6	-2.58	119.22	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	612	CLA	CHB-C4A-NA	2.58	128.12	124.40
27	D	406	BCR	C38-C26-C27	2.58	119.09	113.60
27	d	405	BCR	C33-C5-C4	2.58	119.09	113.60
30	l	101	LHG	C5-O7-C7	-2.58	111.63	117.80
27	b	519	BCR	C33-C5-C4	2.57	119.09	113.60
25	S	603	CLA	CHB-C4A-NA	2.57	128.11	124.40
37	G	616	LUT	C18-C5-C4	2.57	119.14	114.42
27	b	517	BCR	C27-C26-C25	-2.57	119.23	122.70
36	G	619	CHL	OMC-CMC-C2C	-2.57	120.67	125.12
25	G	612	CLA	CHB-C4A-NA	2.56	128.10	124.40
27	A	406	BCR	C33-C5-C4	2.56	119.06	113.60
36	N	309	CHL	O1D-CGD-CBD	-2.56	120.84	124.72
27	H	101	BCR	C28-C27-C26	-2.56	109.49	114.06
27	d	405	BCR	C10-C11-C12	-2.56	115.78	123.20
36	Y	303	CHL	C4-C3-C5	2.56	119.67	115.23
29	d	410	LMG	C8-O7-C10	-2.56	111.67	117.80
36	Y	303	CHL	O1D-CGD-CBD	-2.56	120.84	124.72
25	B	516	CLA	CHB-C4A-NA	2.56	128.09	124.40
36	S	601	CHL	O1D-CGD-CBD	-2.56	120.85	124.72
27	D	406	BCR	C1-C6-C5	-2.56	119.14	122.64
36	N	308	CHL	CMB-C2B-C3B	2.55	129.79	124.68
25	Y	313	CLA	CHB-C4A-NA	2.55	128.09	124.40
25	b	510	CLA	CHB-C4A-NA	2.55	128.08	124.40
38	G	617	NEX	C31-C30-C29	-2.55	123.70	127.28
27	C	514	BCR	C3-C4-C5	-2.55	109.50	114.06
37	G	616	LUT	C11-C10-C9	-2.55	123.70	127.28
36	Y	307	CHL	CMB-C2B-C3B	2.55	129.77	124.68
37	Y	317	LUT	C18-C5-C4	2.55	119.10	114.42
36	G	609	CHL	O2D-CGD-O1D	-2.55	118.89	123.85
39	r	309	XAT	C19-C9-C8	2.54	121.97	118.09
25	Y	305	CLA	CHB-C4A-NA	2.54	128.07	124.40
25	A	402	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
36	r	306	CHL	CMB-C2B-C3B	2.54	129.76	124.68
36	Y	309	CHL	CMB-C2B-C3B	2.54	129.76	124.68
31	c	517	DGD	C2G-O2G-C1B	-2.54	111.72	117.80
30	B	520	LHG	C5-O7-C7	-2.54	111.72	117.80
25	c	503	CLA	C1-C2-C3	-2.54	122.04	126.20
37	G	616	LUT	C31-C30-C29	-2.53	123.72	127.28
27	z	101	BCR	C33-C5-C4	2.53	118.99	113.60
36	G	605	CHL	CMB-C2B-C3B	2.53	129.74	124.68
36	N	309	CHL	CMB-C2B-C3B	2.53	129.74	124.68
36	r	306	CHL	CBC-CAC-C3C	-2.53	109.25	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	518	BCR	C38-C26-C27	2.53	118.98	113.60
25	B	515	CLA	CHB-C4A-NA	2.53	128.04	124.40
25	C	512	CLA	CHB-C4A-NA	2.52	128.04	124.40
36	Y	310	CHL	O2D-CGD-O1D	-2.52	118.94	123.85
36	G	601	CHL	CMB-C2B-C3B	2.52	129.72	124.68
29	b	520	LMG	C8-O7-C10	-2.52	111.76	117.80
27	t	101	BCR	C24-C23-C22	-2.52	122.51	126.23
36	G	608	CHL	O1D-CGD-CBD	-2.52	120.90	124.72
27	t	101	BCR	C33-C5-C4	2.52	118.97	113.60
37	S	615	LUT	C8-C7-C6	-2.52	120.27	127.00
36	G	608	CHL	CMB-C2B-C3B	2.52	129.71	124.68
30	d	407	LHG	C5-O7-C7	-2.52	111.77	117.80
36	N	310	CHL	C4-C3-C5	2.52	119.60	115.23
25	B	504	CLA	CAA-C2A-C3A	-2.52	106.20	113.00
29	D	410	LMG	O8-C28-C29	2.51	119.50	111.83
25	b	513	CLA	C1-C2-C3	-2.51	122.08	126.20
25	b	508	CLA	CMB-C2B-C1B	-2.51	121.59	125.42
36	Y	310	CHL	O2A-CGA-CBA	2.51	119.50	111.83
36	S	607	CHL	CMB-C2B-C3B	2.51	129.70	124.68
36	N	310	CHL	O2D-CGD-O1D	-2.51	118.96	123.85
36	S	607	CHL	O2D-CGD-O1D	-2.51	118.96	123.85
25	b	504	CLA	CHB-C4A-NA	2.51	128.02	124.40
36	Y	307	CHL	O1D-CGD-CBD	-2.51	120.92	124.72
39	N	301	XAT	C27-C28-C29	-2.51	121.64	125.53
25	b	513	CLA	CHB-C4A-NA	2.50	128.01	124.40
38	G	617	NEX	C39-C29-C30	-2.50	118.76	122.82
27	B	517	BCR	C33-C5-C4	2.50	118.94	113.60
27	C	514	BCR	C28-C27-C26	-2.50	109.59	114.06
37	Y	316	LUT	C30-C31-C32	-2.50	115.95	123.20
25	r	307	CLA	C4A-NA-C1A	2.50	107.82	106.68
29	D	410	LMG	C8-O7-C10	-2.50	111.81	117.80
36	Y	309	CHL	O1D-CGD-CBD	-2.50	120.93	124.72
25	C	513	CLA	C1-C2-C3	-2.50	122.10	126.20
36	N	306	CHL	CMB-C2B-C3B	2.50	129.68	124.68
37	S	616	LUT	C11-C10-C9	-2.50	123.77	127.28
36	Y	308	CHL	CBC-CAC-C3C	-2.50	109.30	112.87
27	A	406	BCR	C3-C4-C5	-2.50	109.61	114.06
25	N	304	CLA	CHB-C4A-NA	2.49	128.00	124.40
25	D	404	CLA	C1-C2-C3	-2.49	122.11	126.20
27	V	101	BCR	C3-C4-C5	-2.49	109.61	114.06
27	d	405	BCR	C16-C15-C14	-2.49	118.42	123.52
27	C	516	BCR	C27-C26-C25	-2.49	119.34	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	519	LMG	O8-C28-C29	2.49	119.43	111.83
39	N	301	XAT	C18-C5-C4	2.49	117.04	114.24
39	r	309	XAT	C35-C15-C14	-2.49	118.43	123.52
27	V	101	BCR	C15-C14-C13	-2.49	123.79	127.28
30	b	521	LHG	O8-C23-C24	2.49	119.42	111.83
36	S	608	CHL	CMB-C2B-C3B	2.49	129.65	124.68
36	G	606	CHL	CBC-CAC-C3C	-2.49	109.31	112.87
27	v	101	BCR	C38-C26-C27	2.48	118.89	113.60
36	G	607	CHL	O1D-CGD-CBD	-2.48	120.95	124.72
28	a	407	SQD	O9-S-C6	2.48	110.47	106.76
36	Y	310	CHL	C1-C2-C3	-2.48	122.13	126.20
27	C	515	BCR	C21-C20-C19	-2.48	116.02	123.20
27	b	517	BCR	C15-C16-C17	-2.48	118.45	123.52
36	N	310	CHL	CMB-C2B-C3B	2.48	129.63	124.68
36	N	307	CHL	CMB-C2B-C3B	2.48	129.63	124.68
39	r	309	XAT	C4-C3-C2	-2.47	106.16	110.79
36	N	307	CHL	O2D-CGD-O1D	-2.47	119.03	123.85
27	t	101	BCR	C7-C8-C9	-2.47	122.58	126.23
25	B	503	CLA	C3B-C4B-NB	-2.47	108.33	110.53
25	B	504	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
36	G	605	CHL	O1D-CGD-CBD	-2.46	120.99	124.72
25	Y	312	CLA	C3B-C4B-NB	-2.46	108.33	110.53
25	C	506	CLA	C1-C2-C3	-2.46	122.17	126.20
25	B	513	CLA	CHB-C4A-NA	2.46	127.95	124.40
29	H	102	LMG	C8-O7-C10	-2.46	111.92	117.80
36	Y	308	CHL	OMC-CMC-C2C	-2.46	120.86	125.12
36	G	606	CHL	CMB-C2B-C3B	2.46	129.59	124.68
25	c	512	CLA	C1-C2-C3	-2.45	122.17	126.20
34	d	406	PL9	C20-C19-C21	2.45	119.49	115.23
25	D	405	CLA	CHB-C4A-NA	2.45	127.94	124.40
36	G	606	CHL	OMC-CMC-C2C	-2.45	120.87	125.12
36	Y	310	CHL	OMC-CMC-C2C	-2.45	120.87	125.12
27	B	518	BCR	C38-C26-C27	2.45	118.82	113.60
36	N	308	CHL	O1D-CGD-CBD	-2.45	121.02	124.72
27	a	406	BCR	C40-C30-C25	-2.44	106.41	110.24
25	C	509	CLA	CHB-C4A-NA	2.44	127.92	124.40
36	r	305	CHL	CMA-C3A-C4A	-2.44	109.36	114.61
37	Y	317	LUT	C31-C30-C29	-2.44	123.86	127.28
27	b	518	BCR	C33-C5-C4	2.44	118.79	113.60
36	G	601	CHL	O1D-CGD-CBD	-2.44	121.03	124.72
25	B	504	CLA	CHB-C4A-NA	2.44	127.91	124.40
27	C	514	BCR	C38-C26-C27	2.43	118.79	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	G	618	LHG	C5-O7-C7	-2.43	111.97	117.80
25	S	602	CLA	C3B-C4B-NB	-2.43	108.36	110.53
27	C	515	BCR	C27-C26-C25	-2.43	119.42	122.70
27	D	406	BCR	C8-C7-C6	2.43	133.49	127.00
27	B	517	BCR	C3-C4-C5	-2.43	109.72	114.06
36	r	306	CHL	O1D-CGD-CBD	-2.43	121.04	124.72
27	D	406	BCR	C27-C26-C25	-2.43	119.42	122.70
36	Y	309	CHL	CBC-CAC-C3C	-2.42	109.40	112.87
36	N	310	CHL	CMA-C3A-C4A	-2.42	109.39	114.61
27	a	406	BCR	C27-C26-C25	-2.42	119.43	122.70
37	S	616	LUT	C10-C11-C12	-2.42	116.18	123.20
27	c	514	BCR	C15-C16-C17	-2.42	118.57	123.52
30	D	408	LHG	C5-O7-C7	-2.42	112.01	117.80
37	N	317	LUT	C1-C2-C3	2.42	118.90	113.59
25	N	312	CLA	C3B-C4B-NB	-2.42	108.37	110.53
39	G	620	XAT	C27-C28-C29	-2.42	121.78	125.53
36	G	607	CHL	CBC-CAC-C3C	-2.42	109.42	112.87
25	S	605	CLA	CHB-C4A-NA	2.41	127.88	124.40
25	b	505	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
27	b	517	BCR	C38-C26-C27	2.41	118.74	113.60
31	C	519	DGD	C2G-O2G-C1B	-2.41	112.02	117.80
34	D	407	PL9	C20-C19-C21	2.41	119.42	115.23
27	k	101	BCR	C35-C13-C12	2.41	121.77	118.09
36	N	308	CHL	OMC-CMC-C2C	-2.41	120.93	125.12
27	B	517	BCR	C8-C7-C6	-2.41	120.56	127.00
27	b	519	BCR	C38-C26-C27	2.41	118.74	113.60
25	A	405	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
36	Y	303	CHL	O2D-CGD-O1D	-2.41	119.16	123.85
36	Y	308	CHL	CMB-C2B-C3B	2.41	129.49	124.68
39	Y	302	XAT	C15-C35-C34	-2.40	118.60	123.52
27	d	405	BCR	C3-C4-C5	-2.40	109.77	114.06
25	d	401	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
36	N	309	CHL	O2D-CGD-O1D	-2.40	119.18	123.85
34	d	406	PL9	O2-C1-C6	2.40	124.29	120.48
38	Y	318	NEX	C38-C25-C24	2.39	116.93	114.24
25	A	405	CLA	C1-C2-C3	-2.39	122.28	126.20
37	N	317	LUT	C10-C11-C12	-2.39	116.26	123.20
36	N	306	CHL	O2D-CGD-O1D	-2.39	119.19	123.85
25	N	305	CLA	C1-C2-C3	-2.39	122.28	126.20
34	D	407	PL9	O2-C1-C6	2.39	124.28	120.48
27	C	516	BCR	C36-C18-C19	2.39	121.74	118.09
39	Y	302	XAT	C24-C23-C22	-2.39	106.33	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	G	605	CHL	O2D-CGD-O1D	-2.39	119.20	123.85
25	b	501	CLA	CHB-C4A-NA	2.39	127.84	124.40
25	B	507	CLA	CHB-C4A-NA	2.38	127.83	124.40
36	S	606	CHL	CMB-C2B-C3B	2.38	129.44	124.68
36	Y	307	CHL	O2D-CGD-O1D	-2.38	119.22	123.85
25	c	511	CLA	C1-C2-C3	-2.38	122.30	126.20
25	d	403	CLA	C1-C2-C3	-2.38	122.31	126.20
25	G	602	CLA	C1-C2-C3	-2.37	122.31	126.20
25	c	502	CLA	CHB-C4A-NA	2.37	127.82	124.40
38	N	318	NEX	C39-C29-C30	-2.37	118.97	122.82
25	A	403	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
25	a	405	CLA	CHB-C4A-NA	2.37	127.82	124.40
38	G	617	NEX	C15-C35-C34	-2.37	118.67	123.52
36	r	305	CHL	O2D-CGD-O1D	-2.37	119.24	123.85
25	b	504	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
25	Y	312	CLA	CHB-C4A-NA	2.37	127.81	124.40
29	B	519	LMG	C8-O7-C10	-2.37	112.14	117.80
25	S	611	CLA	C3B-C4B-NB	-2.36	108.42	110.53
37	G	615	LUT	C30-C31-C32	-2.36	116.36	123.20
25	b	503	CLA	CHB-C4A-NA	2.36	127.81	124.40
25	Y	312	CLA	C1-C2-C3	-2.36	122.33	126.20
36	N	302	CHL	O2D-CGD-O1D	-2.36	119.26	123.85
25	D	401	CLA	CHB-C4A-NA	2.36	127.80	124.40
38	N	318	NEX	C38-C25-C24	2.36	116.89	114.24
27	a	406	BCR	C38-C26-C25	-2.36	121.91	124.48
27	C	515	BCR	C15-C16-C17	-2.36	118.70	123.52
25	b	503	CLA	C3B-C4B-NB	-2.36	108.43	110.53
27	H	101	BCR	C23-C24-C25	-2.36	120.71	127.00
25	Y	304	CLA	CHB-C4A-NA	2.35	127.80	124.40
25	d	404	CLA	CHB-C4A-NA	2.35	127.80	124.40
27	z	101	BCR	C28-C27-C26	-2.35	109.86	114.06
27	B	517	BCR	C15-C16-C17	2.35	128.33	123.52
37	S	616	LUT	C8-C7-C6	-2.35	120.72	127.00
34	d	406	PL9	C12-C13-C14	-2.35	122.25	127.62
25	C	506	CLA	CHB-C4A-NA	2.35	127.79	124.40
36	G	607	CHL	OMC-CMC-C2C	-2.35	121.05	125.12
25	N	305	CLA	CHB-C4A-NA	2.35	127.79	124.40
25	c	511	CLA	CHB-C4A-NA	2.35	127.78	124.40
25	C	510	CLA	C1-C2-C3	-2.35	122.35	126.20
27	a	406	BCR	C21-C20-C19	-2.34	116.41	123.20
37	Y	316	LUT	C8-C7-C6	-2.34	120.74	127.00
25	B	507	CLA	CMB-C2B-C1B	-2.34	121.85	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	501	CLA	CHB-C4A-NA	2.34	127.78	124.40
39	G	620	XAT	C15-C35-C34	-2.34	118.72	123.52
36	G	619	CHL	O2D-CGD-O1D	-2.34	119.29	123.85
25	S	614	CLA	C3B-C4B-NB	-2.34	108.44	110.53
37	G	615	LUT	C8-C7-C6	-2.34	120.75	127.00
27	a	406	BCR	C38-C26-C27	2.34	118.58	113.60
25	C	510	CLA	CHB-C4A-NA	2.34	127.77	124.40
25	b	502	CLA	CHB-C4A-NA	2.34	127.77	124.40
27	k	101	BCR	C33-C5-C4	2.34	118.58	113.60
25	C	513	CLA	CHB-C4A-NA	2.34	127.77	124.40
27	b	518	BCR	C30-C25-C26	-2.33	119.44	122.64
25	c	503	CLA	CHB-C4A-NA	2.33	127.77	124.40
38	S	617	NEX	C38-C25-C24	2.33	116.86	114.24
27	B	518	BCR	C33-C5-C4	2.33	118.57	113.60
25	G	614	CLA	CHB-C4A-NA	2.33	127.77	124.40
36	G	601	CHL	O2D-CGD-O1D	-2.33	119.31	123.85
37	N	316	LUT	C30-C31-C32	-2.33	116.44	123.20
37	Y	316	LUT	C10-C11-C12	-2.33	116.45	123.20
36	Y	308	CHL	O2D-CGD-O1D	-2.33	119.31	123.85
26	D	402	PHO	C1-C2-C3	-2.33	122.38	126.20
25	b	506	CLA	CHB-C4A-NA	2.33	127.76	124.40
27	V	101	BCR	C37-C22-C23	2.33	121.64	118.09
25	c	505	CLA	C3B-C4B-NB	-2.33	108.45	110.53
25	b	508	CLA	C1-C2-C3	-2.33	122.38	126.20
25	S	602	CLA	CHB-C4A-NA	2.33	127.76	124.40
37	N	317	LUT	C31-C30-C29	-2.33	124.02	127.28
27	b	518	BCR	C27-C26-C25	-2.33	119.56	122.70
36	S	606	CHL	CBC-CAC-C3C	-2.32	109.55	112.87
25	C	502	CLA	C1-C2-C3	-2.32	122.39	126.20
25	B	514	CLA	CHB-C4A-NA	2.32	127.75	124.40
25	N	314	CLA	CHB-C4A-NA	2.32	127.75	124.40
37	S	616	LUT	C35-C15-C14	-2.32	118.77	123.52
34	d	406	PL9	O1-C4-C3	-2.32	118.28	120.73
27	a	406	BCR	C8-C7-C6	-2.32	120.80	127.00
25	B	508	CLA	CHB-C4A-NA	2.32	127.75	124.40
25	C	511	CLA	CHB-C4A-NA	2.32	127.75	124.40
36	r	304	CHL	O2D-CGD-O1D	-2.32	119.34	123.85
25	b	507	CLA	CHB-C4A-NA	2.32	127.74	124.40
25	G	602	CLA	CHB-C4A-NA	2.32	127.74	124.40
25	b	514	CLA	CHB-C4A-NA	2.32	127.74	124.40
25	c	506	CLA	CHB-C4A-NA	2.31	127.74	124.40
25	a	403	CLA	CHB-C4A-NA	2.31	127.74	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	611	CLA	CHB-C4A-NA	2.31	127.73	124.40
36	S	606	CHL	CAC-C3C-C4C	2.31	129.97	124.03
25	a	402	CLA	CHB-C4A-NA	2.31	127.73	124.40
25	C	502	CLA	CHB-C4A-NA	2.31	127.73	124.40
25	b	510	CLA	C3B-C4B-NB	-2.31	108.47	110.53
27	b	517	BCR	C38-C26-C25	-2.31	121.97	124.48
25	A	405	CLA	CHB-C4A-NA	2.31	127.73	124.40
27	t	101	BCR	C8-C7-C6	-2.31	120.83	127.00
27	C	516	BCR	C8-C7-C6	-2.31	120.83	127.00
25	B	509	CLA	CHB-C4A-NA	2.30	127.73	124.40
30	N	319	LHG	C5-O7-C7	-2.30	112.28	117.80
36	N	306	CHL	C4-C3-C5	2.30	119.23	115.23
25	G	604	CLA	C3B-C4B-NB	-2.30	108.47	110.53
36	G	606	CHL	O2D-CGD-O1D	-2.30	119.37	123.85
25	N	312	CLA	CHB-C4A-NA	2.30	127.72	124.40
36	Y	309	CHL	O2D-CGD-O1D	-2.30	119.37	123.85
25	B	510	CLA	C3B-C4B-NB	-2.30	108.48	110.53
25	B	505	CLA	CHB-C4A-NA	2.30	127.72	124.40
25	B	502	CLA	CHB-C4A-NA	2.30	127.72	124.40
29	W	201	LMG	O8-C28-C29	2.30	118.84	111.83
27	c	514	BCR	C21-C20-C19	-2.30	116.55	123.20
27	H	101	BCR	C38-C26-C27	2.30	118.49	113.60
39	N	301	XAT	C15-C35-C34	-2.30	118.82	123.52
25	G	610	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
25	r	307	CLA	CHB-C4A-NA	2.30	127.71	124.40
34	D	407	PL9	O1-C4-C3	-2.30	118.31	120.73
25	A	402	CLA	C3B-C4B-NB	-2.30	108.48	110.53
25	S	610	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
37	Y	316	LUT	C18-C5-C4	2.29	118.64	114.42
34	D	407	PL9	C12-C13-C14	-2.29	122.37	127.62
25	C	506	CLA	C3B-C4B-NB	-2.29	108.48	110.53
36	S	608	CHL	OMC-CMC-C2C	-2.29	121.14	125.12
36	N	307	CHL	CMA-C3A-C4A	-2.29	109.68	114.61
25	Y	306	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
25	B	503	CLA	CHB-C4A-NA	2.29	127.70	124.40
25	B	511	CLA	CHB-C4A-NA	2.29	127.70	124.40
37	N	316	LUT	C8-C7-C6	-2.29	120.89	127.00
25	c	509	CLA	C1-C2-C3	-2.29	122.45	126.20
29	C	520	LMG	C8-O7-C10	-2.29	112.32	117.80
25	d	403	CLA	C3B-C4B-NB	-2.28	108.49	110.53
25	B	514	CLA	C1-C2-C3	-2.28	122.46	126.20
25	C	505	CLA	C3B-C4B-NB	-2.28	108.49	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	611	CLA	C3B-C4B-NB	-2.28	108.49	110.53
25	B	512	CLA	CMB-C2B-C1B	-2.28	121.94	125.42
27	v	101	BCR	C1-C6-C5	-2.28	119.52	122.64
27	h	101	BCR	C38-C26-C27	2.28	118.46	113.60
38	r	310	NEX	C38-C25-C24	2.28	116.80	114.24
25	G	611	CLA	CHB-C4A-NA	2.28	127.69	124.40
39	N	301	XAT	C24-C23-C22	-2.28	106.53	110.79
25	C	508	CLA	CHB-C4A-NA	2.28	127.69	124.40
25	Y	306	CLA	CHB-C4A-NA	2.28	127.69	124.40
36	N	302	CHL	OMC-CMC-C2C	-2.28	121.17	125.12
25	b	511	CLA	CHB-C4A-NA	2.28	127.69	124.40
27	b	518	BCR	C3-C4-C5	-2.27	110.01	114.06
36	Y	309	CHL	OMC-CMC-C2C	-2.27	121.18	125.12
25	S	613	CLA	CHB-C4A-NA	2.27	127.67	124.40
31	Y	301	DGD	O6D-C5D-C6D	2.27	111.19	106.69
36	S	608	CHL	CMA-C3A-C4A	-2.27	109.72	114.61
27	d	405	BCR	C33-C5-C6	-2.27	122.01	124.48
27	a	406	BCR	C33-C5-C4	2.27	118.43	113.60
27	A	406	BCR	C8-C7-C6	-2.27	120.94	127.00
25	Y	314	CLA	CHB-C4A-NA	2.27	127.67	124.40
25	B	501	CLA	CHB-C4A-NA	2.27	127.67	124.40
25	A	403	CLA	CHB-C4A-NA	2.26	127.67	124.40
36	G	607	CHL	O2D-CGD-O1D	-2.26	119.44	123.85
25	c	504	CLA	CHB-C4A-NA	2.26	127.66	124.40
36	S	607	CHL	OMC-CMC-C2C	-2.26	121.19	125.12
27	k	101	BCR	C27-C26-C25	-2.26	119.65	122.70
25	C	511	CLA	C1-C2-C3	-2.26	122.49	126.20
25	c	510	CLA	C1-C2-C3	-2.26	122.49	126.20
39	G	620	XAT	C10-C11-C12	-2.26	116.65	123.20
25	G	613	CLA	CHB-C4A-NA	2.26	127.66	124.40
25	d	403	CLA	CHB-C4A-NA	2.26	127.66	124.40
36	N	310	CHL	OMC-CMC-C2C	-2.26	121.20	125.12
25	S	609	CLA	CHB-C4A-NA	2.26	127.66	124.40
25	c	502	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
25	B	504	CLA	CAA-CBA-CGA	-2.26	106.80	113.21
36	G	608	CHL	O2D-CGD-O1D	-2.26	119.46	123.85
25	c	508	CLA	CHB-C4A-NA	2.26	127.66	124.40
27	b	517	BCR	C8-C7-C6	-2.26	120.97	127.00
27	b	517	BCR	C28-C27-C26	-2.26	110.03	114.06
27	a	406	BCR	C16-C15-C14	-2.25	118.91	123.52
25	B	506	CLA	CHB-C4A-NA	2.25	127.65	124.40
25	C	504	CLA	CHB-C4A-NA	2.25	127.65	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	401	CLA	CHB-C4A-NA	2.25	127.65	124.40
27	C	516	BCR	C35-C13-C12	2.25	121.53	118.09
25	S	602	CLA	O2D-CGD-CBD	2.25	115.17	111.23
25	b	509	CLA	C1-C2-C3	-2.25	122.51	126.20
25	b	512	CLA	CHB-C4A-NA	2.25	127.65	124.40
36	G	609	CHL	CMA-C3A-C4A	-2.25	109.76	114.61
38	Y	318	NEX	C39-C29-C30	-2.25	119.17	122.82
25	c	501	CLA	CHB-C4A-NA	2.25	127.64	124.40
36	Y	308	CHL	CMA-C3A-C4A	-2.25	109.77	114.61
27	b	519	BCR	C8-C7-C6	-2.25	121.00	127.00
37	G	616	LUT	C10-C11-C12	-2.24	116.70	123.20
25	N	303	CLA	C1-C2-C3	-2.24	122.52	126.20
38	N	318	NEX	C8-C7-C6	-2.24	175.02	177.66
25	c	510	CLA	CHB-C4A-NA	2.24	127.63	124.40
25	A	402	CLA	CHB-C4A-NA	2.24	127.63	124.40
27	C	516	BCR	C21-C20-C19	-2.24	116.71	123.20
37	S	615	LUT	C10-C11-C12	-2.24	116.71	123.20
25	Y	315	CLA	CHB-C4A-NA	2.24	127.63	124.40
29	c	518	LMG	C8-O7-C10	-2.24	112.44	117.80
25	b	516	CLA	CMB-C2B-C1B	-2.24	122.02	125.42
25	N	303	CLA	CHB-C4A-NA	2.24	127.63	124.40
25	r	303	CLA	CHB-C4A-NA	2.23	127.62	124.40
27	C	516	BCR	C38-C26-C27	2.23	118.36	113.60
25	B	511	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
25	N	315	CLA	CHB-C4A-NA	2.23	127.62	124.40
27	k	101	BCR	C36-C18-C19	2.23	121.50	118.09
36	Y	303	CHL	CMA-C3A-C4A	-2.23	109.81	114.61
36	N	306	CHL	CBC-CAC-C3C	-2.23	109.68	112.87
25	b	508	CLA	CHB-C4A-NA	2.23	127.62	124.40
32	C	523	LMU	O5'-C5'-C4'	2.23	114.33	109.72
38	r	310	NEX	C39-C29-C30	-2.23	119.21	122.82
25	C	503	CLA	CHB-C4A-NA	2.23	127.61	124.40
25	B	504	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
25	B	508	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
26	a	404	PHO	O2A-CGA-O1A	-2.23	118.06	123.63
25	D	404	CLA	CHB-C4A-NA	2.23	127.61	124.40
36	Y	310	CHL	CMA-C3A-C4A	-2.23	109.81	114.61
25	d	401	CLA	O2D-CGD-CBD	2.23	115.12	111.23
25	c	513	CLA	CHB-C4A-NA	2.23	127.61	124.40
27	h	101	BCR	C23-C24-C25	-2.22	121.06	127.00
39	N	301	XAT	C30-C31-C32	-2.22	116.76	123.20
25	S	614	CLA	CHB-C4A-NA	2.22	127.61	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	518	BCR	C8-C7-C6	-2.22	121.06	127.00
25	a	405	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
25	B	509	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
31	c	515	DGD	O6D-C5D-C6D	2.22	111.10	106.69
25	S	609	CLA	CAA-C2A-C3A	-2.22	111.14	116.23
25	D	401	CLA	C1-C2-C3	-2.22	122.56	126.20
25	G	604	CLA	CHB-C4A-NA	2.22	127.60	124.40
25	r	308	CLA	CAA-C2A-C3A	-2.22	111.15	116.23
36	Y	310	CHL	CBC-CAC-C3C	-2.22	109.70	112.87
30	a	411	LHG	C5-O7-C7	-2.22	112.49	117.80
36	G	609	CHL	OMC-CMC-C2C	-2.22	121.27	125.12
36	S	607	CHL	CMA-C3A-C4A	-2.21	109.84	114.61
25	D	404	CLA	C3B-C4B-NB	-2.21	108.56	110.53
36	N	307	CHL	CBC-CAC-C3C	-2.21	109.71	112.87
39	N	301	XAT	C10-C11-C12	-2.21	116.79	123.20
25	Y	315	CLA	C3B-C4B-NB	-2.21	108.56	110.53
36	N	308	CHL	O2D-CGD-O1D	-2.21	119.55	123.85
36	Y	303	CHL	OMC-CMC-C2C	-2.21	121.28	125.12
27	H	101	BCR	C33-C5-C6	-2.21	122.07	124.48
25	C	506	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
25	A	403	CLA	O2D-CGD-CBD	2.21	115.09	111.23
38	G	617	NEX	C17-C1-C6	-2.21	108.50	110.47
25	S	604	CLA	CHB-C4A-NA	2.21	127.58	124.40
36	G	601	CHL	CAC-C3C-C4C	2.21	129.70	124.03
35	f	101	HEM	C1B-NB-C4B	2.21	107.82	105.21
37	S	616	LUT	C31-C30-C29	-2.21	124.19	127.28
37	N	317	LUT	C8-C7-C6	-2.20	121.11	127.00
25	B	502	CLA	C3B-C4B-NB	-2.20	108.56	110.53
30	C	521	LHG	C5-O7-C7	-2.20	112.53	117.80
25	N	311	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
25	b	509	CLA	CHB-C4A-NA	2.20	127.57	124.40
36	N	306	CHL	O1D-CGD-CBD	-2.20	121.39	124.72
36	G	601	CHL	OMC-CMC-C2C	-2.20	121.30	125.12
35	f	101	HEM	C3B-C4B-NB	-2.20	107.89	109.47
25	b	513	CLA	CMB-C2B-C1B	-2.20	122.08	125.42
37	Y	317	LUT	C30-C31-C32	-2.19	116.84	123.20
36	N	306	CHL	OMC-CMC-C2C	-2.19	121.31	125.12
32	S	619	LMU	C1B-O1B-C4'	-2.19	112.78	117.98
36	Y	303	CHL	C4C-CHD-C1D	2.19	123.91	116.07
25	c	507	CLA	C3B-C4B-NB	-2.19	108.57	110.53
25	Y	311	CLA	CHB-C4A-NA	2.19	127.56	124.40
36	r	304	CHL	CAC-C3C-C4C	2.19	129.66	124.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	508	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
25	N	315	CLA	C3B-C4B-NB	-2.19	108.58	110.53
25	b	505	CLA	C3B-C4B-NB	-2.19	108.58	110.53
37	G	615	LUT	C18-C5-C4	2.18	118.44	114.42
37	G	616	LUT	C30-C31-C32	-2.18	116.87	123.20
27	A	406	BCR	C38-C26-C25	-2.18	122.10	124.48
36	N	309	CHL	CMA-C3A-C4A	-2.18	109.91	114.61
35	f	101	HEM	C4D-ND-C1D	2.18	107.79	105.21
25	b	508	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
25	Y	311	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
36	r	304	CHL	CMA-C3A-C4A	-2.18	109.92	114.61
38	G	617	NEX	C30-C31-C32	-2.18	116.89	123.20
27	C	516	BCR	C4-C5-C6	-2.18	119.76	122.70
34	d	406	PL9	C37-C38-C39	-2.18	122.64	127.62
37	S	616	LUT	C30-C31-C32	-2.17	116.90	123.20
39	r	309	XAT	C38-C25-C24	2.17	116.68	114.24
25	A	405	CLA	CMB-C2B-C3B	2.17	131.66	126.55
25	G	610	CLA	CHB-C4A-NA	2.17	127.54	124.40
25	B	508	CLA	C3B-C4B-NB	-2.17	108.59	110.53
30	Y	319	LHG	C5-O7-C7	-2.17	112.59	117.80
25	a	403	CLA	O2D-CGD-CBD	2.17	115.03	111.23
27	b	519	BCR	C1-C6-C5	-2.17	119.67	122.64
31	C	518	DGD	O6D-C5D-C6D	2.17	111.00	106.69
36	r	306	CHL	O2D-CGD-O1D	-2.17	119.62	123.85
25	B	505	CLA	C3B-C4B-NB	-2.17	108.59	110.53
25	b	502	CLA	O2D-CGD-CBD	2.17	115.02	111.23
36	G	605	CHL	OMC-CMC-C2C	-2.17	121.35	125.12
25	C	505	CLA	CHB-C4A-NA	2.17	127.53	124.40
25	N	311	CLA	CHB-C4A-NA	2.17	127.53	124.40
36	G	605	CHL	CMA-C3A-C4A	-2.17	109.94	114.61
36	G	619	CHL	CMA-C3A-C4A	-2.17	109.94	114.61
25	b	512	CLA	C16-C15-C13	-2.17	108.77	115.97
25	B	513	CLA	C1-C2-C3	-2.17	122.65	126.20
27	A	406	BCR	C16-C15-C14	-2.17	119.09	123.52
36	S	606	CHL	CMA-C3A-C4A	-2.16	109.95	114.61
25	B	508	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
36	Y	307	CHL	CMA-C3A-C4A	-2.16	109.95	114.61
36	S	601	CHL	CMA-C3A-C4A	-2.16	109.96	114.61
38	S	617	NEX	C35-C15-C14	-2.16	119.10	123.52
38	G	617	NEX	C38-C25-C24	2.16	116.67	114.24
25	G	603	CLA	C1-C2-C3	-2.16	122.66	126.20
37	N	316	LUT	C10-C11-C12	-2.16	116.94	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	610	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
36	S	608	CHL	CAC-C3C-C4C	2.16	129.58	124.03
27	V	101	BCR	C20-C21-C22	-2.16	124.25	127.28
27	b	518	BCR	C15-C16-C17	-2.16	119.11	123.52
29	d	410	LMG	O7-C10-O9	-2.15	118.67	123.70
39	Y	302	XAT	C10-C11-C12	-2.15	116.96	123.20
27	t	101	BCR	C15-C16-C17	-2.15	119.11	123.52
25	S	610	CLA	C3B-C4B-NB	-2.15	108.61	110.53
25	r	301	CLA	CHB-C4A-NA	2.15	127.51	124.40
25	B	503	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
25	b	507	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
36	Y	309	CHL	C4C-CHD-C1D	2.15	123.75	116.07
36	G	608	CHL	C4C-CHD-C1D	2.15	123.75	116.07
36	Y	307	CHL	OMC-CMC-C2C	-2.15	121.39	125.12
25	C	512	CLA	C3B-C4B-NB	-2.15	108.61	110.53
25	b	507	CLA	C1-C2-C3	-2.14	122.68	126.20
31	W	202	DGD	O6D-C5D-C6D	2.14	110.94	106.69
25	b	507	CLA	C3B-C4B-NB	-2.14	108.62	110.53
25	c	501	CLA	C3B-C4B-NB	-2.14	108.62	110.53
25	c	507	CLA	C1-C2-C3	-2.14	122.69	126.20
25	B	501	CLA	C1-C2-C3	-2.14	122.69	126.20
31	c	516	DGD	C2G-O2G-C1B	-2.14	112.67	117.80
25	B	506	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
25	B	512	CLA	CMB-C2B-C3B	2.14	131.59	126.55
36	G	607	CHL	CMA-C3A-C4A	-2.14	110.00	114.61
25	C	508	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
38	S	617	NEX	C39-C29-C30	-2.14	119.35	122.82
36	N	308	CHL	CMA-C3A-C4A	-2.14	110.01	114.61
25	r	302	CLA	C2A-C1A-CHA	2.14	127.58	123.87
36	N	310	CHL	CAC-C3C-C4C	2.14	129.52	124.03
36	r	305	CHL	CAC-C3C-C4C	2.14	129.52	124.03
25	N	305	CLA	C3B-C4B-NB	-2.14	108.62	110.53
25	Y	314	CLA	C1-C2-C3	-2.14	122.70	126.20
25	Y	306	CLA	C3B-C4B-NB	-2.13	108.62	110.53
25	B	513	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
36	G	619	CHL	C4C-CHD-C1D	2.13	123.70	116.07
36	N	308	CHL	CBC-CAC-C3C	-2.13	109.82	112.87
25	c	505	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
31	W	202	DGD	O2G-C1B-O1B	-2.13	118.72	123.70
27	b	517	BCR	C33-C5-C4	2.13	118.14	113.60
36	N	309	CHL	OMC-CMC-C2C	-2.13	121.42	125.12
36	r	306	CHL	OMC-CMC-C2C	-2.13	121.42	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	605	CLA	C1-C2-C3	-2.13	123.31	126.76
25	B	507	CLA	CMB-C2B-C3B	2.13	131.56	126.55
27	h	101	BCR	C33-C5-C6	-2.13	122.16	124.48
25	C	513	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
25	C	510	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
36	G	607	CHL	C4C-CHD-C1D	2.13	123.68	116.07
36	S	601	CHL	C4C-CHD-C1D	2.13	123.68	116.07
25	b	509	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
27	V	101	BCR	C38-C26-C27	2.13	118.13	113.60
25	c	509	CLA	CMB-C2B-C3B	2.13	131.56	126.55
25	b	513	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
36	r	304	CHL	C4C-CHD-C1D	2.13	123.68	116.07
27	t	101	BCR	C2-C1-C6	2.13	113.53	110.44
36	G	608	CHL	OMC-CMC-C2C	-2.12	121.43	125.12
30	d	407	LHG	O8-C23-O10	-2.12	118.31	123.63
25	b	508	CLA	C3B-C4B-NB	-2.12	108.63	110.53
25	D	401	CLA	O2D-CGD-CBD	2.12	114.94	111.23
36	r	306	CHL	CMA-C3A-C4A	-2.12	110.04	114.61
36	r	305	CHL	C4C-CHD-C1D	2.12	123.65	116.07
25	B	514	CLA	C3B-C4B-NB	-2.12	108.64	110.53
25	S	613	CLA	C3B-C4B-NB	-2.12	108.64	110.53
37	N	317	LUT	C30-C31-C32	-2.12	117.06	123.20
25	N	303	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
25	b	502	CLA	C3B-C4B-NB	-2.12	108.64	110.53
27	C	514	BCR	C33-C5-C6	-2.12	122.17	124.48
36	S	601	CHL	O2D-CGD-O1D	-2.12	119.73	123.85
36	r	305	CHL	CBC-CAC-C3C	-2.11	109.84	112.87
25	a	403	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
37	Y	317	LUT	C10-C11-C12	-2.11	117.08	123.20
25	N	304	CLA	C3B-C4B-NB	-2.11	108.64	110.53
25	S	610	CLA	CMB-C2B-C3B	2.11	131.51	126.55
25	A	402	CLA	C1-C2-C3	-2.11	122.74	126.20
36	G	609	CHL	CAC-C3C-C4C	2.11	129.46	124.03
25	G	610	CLA	CMB-C2B-C3B	2.11	131.51	126.55
25	D	404	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
25	S	602	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
27	t	101	BCR	C21-C20-C19	-2.11	117.09	123.20
27	A	406	BCR	C21-C20-C19	-2.11	117.09	123.20
36	G	601	CHL	C4C-CHD-C1D	2.11	123.61	116.07
36	G	607	CHL	CAC-C3C-C4C	2.11	129.45	124.03
34	D	407	PL9	O2-C1-C2	-2.11	117.04	121.83
34	D	407	PL9	C37-C38-C39	-2.11	122.80	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	S	615	LUT	C18-C5-C4	2.11	118.29	114.42
25	a	402	CLA	C3B-C4B-NB	-2.10	108.65	110.53
25	d	403	CLA	O2D-CGD-CBD	2.10	114.91	111.23
37	S	615	LUT	C27-C28-C29	-2.10	121.80	126.32
36	G	605	CHL	C4C-CHD-C1D	2.10	123.59	116.07
36	N	302	CHL	C4C-CHD-C1D	2.10	123.59	116.07
25	B	506	CLA	C1-C2-C3	-2.10	122.75	126.20
25	b	512	CLA	C1-C2-C3	-2.10	122.75	126.20
36	S	608	CHL	O1D-CGD-CBD	-2.10	121.53	124.72
25	c	509	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
25	a	405	CLA	CMB-C2B-C3B	2.10	131.49	126.55
25	b	505	CLA	CHB-C4A-NA	2.10	127.43	124.40
25	b	511	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
34	d	406	PL9	O2-C1-C2	-2.10	117.06	121.83
25	G	610	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
38	r	310	NEX	C15-C35-C34	-2.10	119.23	123.52
36	N	306	CHL	C4C-CHD-C1D	2.10	123.57	116.07
25	N	313	CLA	C3B-C4B-NB	-2.10	108.66	110.53
39	Y	302	XAT	C38-C25-C24	2.10	116.59	114.24
25	S	611	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
27	b	517	BCR	C21-C20-C19	-2.09	117.13	123.20
36	Y	310	CHL	CAC-C3C-C4C	2.09	129.41	124.03
25	C	505	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
25	S	605	CLA	O2D-CGD-CBD	2.09	114.89	111.23
25	A	405	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
25	S	613	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
27	b	519	BCR	C4-C5-C6	-2.09	119.88	122.70
38	Y	318	NEX	C30-C31-C32	-2.09	117.14	123.20
25	B	502	CLA	O2D-CGD-CBD	2.09	114.89	111.23
25	B	509	CLA	C1-C2-C3	-2.09	122.77	126.20
36	G	606	CHL	CAC-C3C-C4C	2.09	129.41	124.03
25	B	506	CLA	C3B-C4B-NB	-2.09	108.66	110.53
25	c	505	CLA	CHB-C4A-NA	2.09	127.41	124.40
27	V	101	BCR	C35-C13-C12	2.09	121.28	118.09
37	S	616	LUT	C3-C4-C5	-2.09	106.98	112.18
27	z	101	BCR	C20-C19-C18	-2.09	120.64	126.36
25	G	604	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
36	r	306	CHL	C4C-CHD-C1D	2.09	123.53	116.07
39	r	309	XAT	C18-C5-C4	2.09	116.58	114.24
25	N	311	CLA	C1-C2-C3	-2.08	122.78	126.20
33	D	403	BCT	O3-C-O1	-2.08	114.34	119.68
25	C	503	CLA	O2A-CGA-O1A	-2.08	118.41	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	Y	307	CHL	CAC-C3C-C4C	2.08	129.39	124.03
25	b	516	CLA	CMB-C2B-C3B	2.08	131.45	126.55
25	b	502	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
25	A	402	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
25	Y	312	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
25	c	504	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
25	D	404	CLA	O2D-CGD-CBD	2.08	114.87	111.23
36	Y	307	CHL	C4C-CHD-C1D	2.08	123.52	116.07
25	B	507	CLA	C3B-C4B-NB	-2.08	108.67	110.53
25	c	506	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
25	S	604	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
25	D	405	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
39	r	309	XAT	C20-C13-C12	2.08	121.26	118.09
27	B	517	BCR	C10-C11-C12	-2.08	117.18	123.20
36	N	308	CHL	CAC-C3C-C4C	2.08	129.37	124.03
36	N	308	CHL	C4C-CHD-C1D	2.08	123.49	116.07
25	S	614	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
37	G	615	LUT	C31-C30-C29	-2.07	124.37	127.28
25	c	506	CLA	C3B-C4B-NB	-2.07	108.68	110.53
25	N	314	CLA	C1-C2-C3	-2.07	122.80	126.20
36	N	307	CHL	CAC-C3C-C4C	2.07	129.36	124.03
25	C	504	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
25	a	405	CLA	C1-C2-C3	-2.07	122.80	126.20
36	N	309	CHL	C4C-CHD-C1D	2.07	123.47	116.07
25	S	610	CLA	CHB-C4A-NA	2.07	127.39	124.40
27	c	514	BCR	C33-C5-C4	2.07	118.01	113.60
25	c	501	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
36	G	609	CHL	CBC-CAC-C3C	-2.07	109.91	112.87
36	Y	308	CHL	C4C-CHD-C1D	2.07	123.46	116.07
25	Y	304	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
25	C	507	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
25	b	514	CLA	C3B-C4B-NB	-2.07	108.69	110.53
27	B	518	BCR	C28-C27-C26	-2.07	110.37	114.06
37	G	615	LUT	C39-C29-C28	2.07	121.24	118.09
36	G	606	CHL	CMA-C3A-C4A	-2.07	110.16	114.61
39	r	309	XAT	C30-C31-C32	-2.06	117.22	123.20
25	r	303	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
25	b	506	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
27	a	406	BCR	C10-C11-C12	-2.06	117.22	123.20
39	N	301	XAT	C19-C9-C8	2.06	121.24	118.09
25	C	507	CLA	C3B-C4B-NB	-2.06	108.69	110.53
25	b	516	CLA	C3B-C4B-NB	-2.06	108.69	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	402	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
25	B	506	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
37	S	616	LUT	C39-C29-C28	2.06	121.23	118.09
25	r	301	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
27	z	101	BCR	C16-C15-C14	-2.06	119.31	123.52
25	c	507	CLA	O2D-CGD-CBD	2.05	114.82	111.23
25	c	512	CLA	C3B-C4B-NB	-2.05	108.70	110.53
25	C	513	CLA	CMB-C2B-C3B	2.05	131.38	126.55
25	c	511	CLA	CAA-CBA-CGA	-2.05	107.38	113.21
27	v	101	BCR	C10-C11-C12	-2.05	117.26	123.20
31	C	517	DGD	O1G-C1A-O1A	-2.05	118.50	123.63
37	Y	316	LUT	C16-C1-C6	-2.05	107.03	110.24
36	N	302	CHL	CAC-C3C-C4C	2.05	129.30	124.03
25	B	513	CLA	CMB-C2B-C3B	2.05	131.37	126.55
25	c	503	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
25	G	613	CLA	C1-C2-C3	-2.05	122.84	126.20
25	Y	306	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
25	B	504	CLA	CMB-C2B-C3B	2.05	131.37	126.55
37	S	616	LUT	C15-C35-C34	-2.05	119.33	123.52
25	C	508	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
27	D	406	BCR	C16-C15-C14	-2.05	119.33	123.52
36	S	607	CHL	C4C-CHD-C1D	2.04	123.39	116.07
30	S	618	LHG	O7-C7-O9	-2.04	118.92	123.70
30	l	101	LHG	O8-C23-O10	-2.04	118.52	123.63
25	N	303	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
25	D	404	CLA	CHC-C4B-NB	2.04	127.11	124.05
26	A	404	PHO	O2A-CGA-O1A	-2.04	118.52	123.63
33	a	409	BCT	O3-C-O1	-2.04	114.45	119.68
25	b	509	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
25	D	401	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
25	B	509	CLA	C3B-C4B-NB	-2.03	108.71	110.53
25	b	510	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
30	L	101	LHG	O7-C7-O9	-2.03	118.95	123.70
25	c	506	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
36	G	619	CHL	CAC-C3C-C4C	2.03	129.25	124.03
36	G	606	CHL	C4C-CHD-C1D	2.03	123.34	116.07
25	c	508	CLA	C3B-C4B-NB	-2.03	108.72	110.53
25	b	502	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
27	B	517	BCR	C35-C13-C12	2.03	121.19	118.09
27	t	101	BCR	C11-C12-C13	-2.03	120.80	126.36
25	B	510	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
39	N	301	XAT	C38-C25-C24	2.03	116.52	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	308	CLA	CMA-C3A-C2A	-2.03	111.58	116.23
39	r	309	XAT	C39-C29-C28	2.03	121.19	118.09
25	Y	315	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
38	r	310	NEX	C30-C31-C32	-2.03	117.33	123.20
35	f	101	HEM	C2A-C1A-NA	-2.03	107.90	110.15
27	D	406	BCR	C23-C24-C25	-2.03	121.59	127.00
35	f	101	HEM	C3D-C4D-ND	-2.03	107.95	110.17
25	b	508	CLA	CHB-C1B-NB	2.03	127.09	124.05
36	Y	308	CHL	CAC-C3C-C4C	2.02	129.24	124.03
27	V	101	BCR	C11-C10-C9	-2.02	124.44	127.28
25	b	513	CLA	CMB-C2B-C3B	2.02	131.31	126.55
38	G	617	NEX	C11-C12-C13	-2.02	120.81	126.36
25	C	509	CLA	CMB-C2B-C3B	2.02	131.31	126.55
25	C	507	CLA	C1-C2-C3	-2.02	122.88	126.20
25	C	510	CLA	CMB-C2B-C3B	2.02	131.31	126.55
27	C	514	BCR	C4-C5-C6	-2.02	119.97	122.70
25	C	512	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
25	B	514	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
25	b	515	CLA	C3B-C4B-NB	-2.02	108.73	110.53
25	C	509	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
25	Y	315	CLA	C1-C2-C3	-2.02	122.89	126.20
25	C	511	CLA	C3B-C4B-NB	-2.02	108.73	110.53
25	c	505	CLA	CHB-C1B-NB	2.02	127.08	124.05
25	b	511	CLA	C1-C2-C3	-2.02	122.89	126.20
25	C	501	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
25	B	512	CLA	C3B-C4B-NB	-2.02	108.73	110.53
25	c	511	CLA	C3B-C4B-NB	-2.02	108.73	110.53
36	S	608	CHL	C4C-CHD-C1D	2.02	123.29	116.07
25	N	314	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
25	B	511	CLA	C3B-C4B-NB	-2.02	108.73	110.53
25	B	516	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
25	b	512	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
25	c	511	CLA	O2D-CGD-CBD	2.02	114.75	111.23
25	b	510	CLA	C1-C2-C3	-2.02	122.89	126.20
37	Y	317	LUT	C27-C28-C29	-2.02	121.99	126.32
25	Y	306	CLA	CMB-C2B-C3B	2.01	131.29	126.55
27	C	516	BCR	C38-C26-C25	-2.01	122.29	124.48
37	Y	316	LUT	C20-C13-C12	2.01	121.17	118.09
30	d	408	LHG	O7-C7-O9	-2.01	119.00	123.70
25	c	503	CLA	CAA-CBA-CGA	-2.01	107.49	113.21
25	b	503	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
36	S	607	CHL	CAC-C3C-C4C	2.01	129.20	124.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	Y	309	CHL	CMA-C3A-C4A	-2.01	110.28	114.61
26	d	402	PHO	CAA-CBA-CGA	-2.01	107.50	113.21
36	N	307	CHL	C4C-CHD-C1D	2.01	123.26	116.07
27	V	101	BCR	C30-C25-C26	-2.01	119.89	122.64
25	B	501	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
25	B	502	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
25	C	501	CLA	C1-C2-C3	-2.01	122.91	126.20
25	B	513	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
27	b	518	BCR	C23-C24-C25	-2.01	121.64	127.00
25	C	511	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
36	N	306	CHL	CMA-C3A-C4A	-2.01	110.29	114.61
36	r	304	CHL	OMC-CMC-C2C	-2.00	121.64	125.12
27	b	518	BCR	C1-C6-C5	-2.00	119.90	122.64
37	S	616	LUT	C38-C25-C24	-2.00	118.62	123.36
36	S	606	CHL	C4C-CHD-C1D	2.00	123.24	116.07
25	b	513	CLA	C3B-C4B-NB	-2.00	108.74	110.53
36	S	601	CHL	CAC-C3C-C4C	2.00	129.18	124.03
25	B	502	CLA	C1-C2-C3	-2.00	122.92	126.20
37	Y	317	LUT	C35-C15-C14	-2.00	119.42	123.52
39	Y	302	XAT	C19-C9-C8	2.00	121.15	118.09
25	b	511	CLA	O1D-CGD-CBD	2.00	128.47	124.52
25	b	505	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
27	b	518	BCR	C11-C12-C13	-2.00	120.88	126.36
25	Y	305	CLA	O2A-CGA-O1A	-2.00	118.62	123.63

All (184) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	402	CLA	ND
25	A	403	CLA	ND
25	A	405	CLA	ND
25	B	501	CLA	ND
25	B	502	CLA	ND
25	B	503	CLA	ND
25	B	504	CLA	ND
25	B	505	CLA	ND
25	B	506	CLA	ND
25	B	507	CLA	ND
25	B	508	CLA	ND
25	B	509	CLA	ND
25	B	510	CLA	ND
25	B	511	CLA	ND

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Mol	Chain	Res	Type	Atom
25	B	512	CLA	ND
25	B	513	CLA	ND
25	B	514	CLA	ND
25	B	515	CLA	ND
25	B	516	CLA	ND
25	C	501	CLA	ND
25	C	502	CLA	ND
25	C	503	CLA	ND
25	C	504	CLA	ND
25	C	505	CLA	ND
25	C	506	CLA	ND
25	C	507	CLA	ND
25	C	508	CLA	ND
25	C	509	CLA	ND
25	C	510	CLA	ND
25	C	511	CLA	ND
25	C	512	CLA	ND
25	C	513	CLA	ND
25	D	401	CLA	ND
25	D	404	CLA	ND
25	D	405	CLA	ND
25	G	602	CLA	ND
25	G	603	CLA	ND
25	G	604	CLA	ND
25	G	610	CLA	ND
25	G	611	CLA	ND
25	G	612	CLA	ND
25	G	613	CLA	ND
25	G	614	CLA	ND
25	N	303	CLA	ND
25	N	304	CLA	ND
25	N	305	CLA	ND
25	N	311	CLA	ND
25	N	312	CLA	ND
25	N	313	CLA	ND
25	N	314	CLA	ND
25	N	315	CLA	ND
25	S	602	CLA	ND
25	S	603	CLA	ND
25	S	604	CLA	ND
25	S	605	CLA	ND
25	S	609	CLA	ND

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Mol	Chain	Res	Type	Atom
25	S	610	CLA	ND
25	S	611	CLA	ND
25	S	612	CLA	ND
25	S	613	CLA	ND
25	S	614	CLA	ND
25	Y	304	CLA	ND
25	Y	305	CLA	ND
25	Y	306	CLA	ND
25	Y	311	CLA	ND
25	Y	312	CLA	ND
25	Y	313	CLA	ND
25	Y	314	CLA	ND
25	Y	315	CLA	ND
25	a	402	CLA	ND
25	a	403	CLA	ND
25	a	405	CLA	ND
25	b	501	CLA	ND
25	b	502	CLA	ND
25	b	503	CLA	ND
25	b	504	CLA	ND
25	b	505	CLA	ND
25	b	506	CLA	ND
25	b	507	CLA	ND
25	b	508	CLA	ND
25	b	509	CLA	ND
25	b	510	CLA	ND
25	b	511	CLA	ND
25	b	512	CLA	ND
25	b	513	CLA	ND
25	b	514	CLA	ND
25	b	515	CLA	ND
25	b	516	CLA	ND
25	c	501	CLA	ND
25	c	502	CLA	ND
25	c	503	CLA	ND
25	c	504	CLA	ND
25	c	505	CLA	ND
25	c	506	CLA	ND
25	c	507	CLA	ND
25	c	508	CLA	ND
25	c	509	CLA	ND
25	c	510	CLA	ND

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Mol	Chain	Res	Type	Atom
25	c	511	CLA	ND
25	c	512	CLA	ND
25	c	513	CLA	ND
25	d	401	CLA	ND
25	d	403	CLA	ND
25	d	404	CLA	ND
25	r	301	CLA	ND
25	r	302	CLA	ND
25	r	303	CLA	ND
25	r	307	CLA	ND
25	r	308	CLA	ND
36	G	601	CHL	NA
36	G	601	CHL	ND
36	G	601	CHL	NC
36	G	605	CHL	NA
36	G	605	CHL	ND
36	G	605	CHL	NC
36	G	606	CHL	NA
36	G	606	CHL	ND
36	G	606	CHL	NC
36	G	607	CHL	NA
36	G	607	CHL	ND
36	G	607	CHL	NC
36	G	608	CHL	NA
36	G	608	CHL	ND
36	G	608	CHL	NC
36	G	609	CHL	NA
36	G	609	CHL	ND
36	G	609	CHL	NC
36	G	619	CHL	NA
36	G	619	CHL	ND
36	G	619	CHL	NC
36	N	302	CHL	NA
36	N	302	CHL	ND
36	N	302	CHL	NC
36	N	306	CHL	NA
36	N	306	CHL	ND
36	N	306	CHL	NC
36	N	307	CHL	NA
36	N	307	CHL	ND
36	N	307	CHL	NC
36	N	308	CHL	NA

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Mol	Chain	Res	Type	Atom
36	N	308	CHL	ND
36	N	308	CHL	NC
36	N	309	CHL	NA
36	N	309	CHL	ND
36	N	309	CHL	NC
36	N	310	CHL	NA
36	N	310	CHL	ND
36	N	310	CHL	NC
36	S	601	CHL	NA
36	S	601	CHL	ND
36	S	601	CHL	NC
36	S	606	CHL	NA
36	S	606	CHL	ND
36	S	606	CHL	NC
36	S	607	CHL	NA
36	S	607	CHL	ND
36	S	607	CHL	NC
36	S	608	CHL	NA
36	S	608	CHL	ND
36	S	608	CHL	NC
36	Y	303	CHL	NA
36	Y	303	CHL	ND
36	Y	303	CHL	NC
36	Y	307	CHL	NA
36	Y	307	CHL	ND
36	Y	307	CHL	NC
36	Y	308	CHL	NA
36	Y	308	CHL	ND
36	Y	308	CHL	NC
36	Y	309	CHL	NA
36	Y	309	CHL	ND
36	Y	309	CHL	NC
36	Y	310	CHL	NA
36	Y	310	CHL	ND
36	Y	310	CHL	NC
36	r	304	CHL	NA
36	r	304	CHL	ND
36	r	304	CHL	NC
36	r	305	CHL	NA
36	r	305	CHL	ND
36	r	305	CHL	NC
36	r	306	CHL	NA

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Mol	Chain	Res	Type	Atom
36	r	306	CHL	ND
36	r	306	CHL	NC

All (1603) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	501	CLA	CAD-CBD-CGD-O1D
25	B	501	CLA	CAD-CBD-CGD-O2D
25	B	504	CLA	C1A-C2A-CAA-CBA
25	B	507	CLA	CBD-CGD-O2D-CED
25	B	509	CLA	C1A-C2A-CAA-CBA
25	B	509	CLA	C3A-C2A-CAA-CBA
25	B	510	CLA	CHA-CBD-CGD-O1D
25	B	510	CLA	CHA-CBD-CGD-O2D
25	B	512	CLA	C1A-C2A-CAA-CBA
25	B	514	CLA	CAD-CBD-CGD-O1D
25	B	514	CLA	CAD-CBD-CGD-O2D
25	C	501	CLA	CAD-CBD-CGD-O1D
25	C	501	CLA	CAD-CBD-CGD-O2D
25	C	502	CLA	CAD-CBD-CGD-O2D
25	C	503	CLA	CHA-CBD-CGD-O1D
25	C	503	CLA	CHA-CBD-CGD-O2D
25	C	503	CLA	CBD-CGD-O2D-CED
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	510	CLA	CHA-CBD-CGD-O1D
25	C	510	CLA	CHA-CBD-CGD-O2D
25	C	513	CLA	C1A-C2A-CAA-CBA
25	C	513	CLA	C11-C12-C13-C14
25	D	404	CLA	C1A-C2A-CAA-CBA
25	D	404	CLA	C3A-C2A-CAA-CBA
25	D	405	CLA	CAD-CBD-CGD-O1D
25	D	405	CLA	CAD-CBD-CGD-O2D
25	D	405	CLA	C11-C12-C13-C14
25	G	603	CLA	C1A-C2A-CAA-CBA
25	G	603	CLA	C3A-C2A-CAA-CBA
25	G	603	CLA	CHA-CBD-CGD-O1D
25	G	603	CLA	CHA-CBD-CGD-O2D
25	G	603	CLA	C14-C13-C15-C16
25	G	611	CLA	C3A-C2A-CAA-CBA
25	N	304	CLA	CHA-CBD-CGD-O1D
25	N	304	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	N	305	CLA	CAD-CBD-CGD-O1D
25	N	305	CLA	CAD-CBD-CGD-O2D
25	N	305	CLA	CBD-CGD-O2D-CED
25	N	311	CLA	CBD-CGD-O2D-CED
25	N	312	CLA	C1A-C2A-CAA-CBA
25	N	312	CLA	C3A-C2A-CAA-CBA
25	N	315	CLA	C1A-C2A-CAA-CBA
25	S	602	CLA	C3A-C2A-CAA-CBA
25	S	602	CLA	C2B-C3B-CAB-CBB
25	S	602	CLA	C4B-C3B-CAB-CBB
25	S	603	CLA	CHA-CBD-CGD-O1D
25	S	603	CLA	CHA-CBD-CGD-O2D
25	S	605	CLA	C1A-C2A-CAA-CBA
25	S	609	CLA	C2B-C3B-CAB-CBB
25	S	609	CLA	C4B-C3B-CAB-CBB
25	S	613	CLA	CBD-CGD-O2D-CED
25	Y	305	CLA	CHA-CBD-CGD-O1D
25	Y	305	CLA	CHA-CBD-CGD-O2D
25	a	403	CLA	C1A-C2A-CAA-CBA
25	a	403	CLA	C3A-C2A-CAA-CBA
25	b	501	CLA	C1A-C2A-CAA-CBA
25	b	501	CLA	CBD-CGD-O2D-CED
25	b	503	CLA	C3A-C2A-CAA-CBA
25	b	504	CLA	C1A-C2A-CAA-CBA
25	b	504	CLA	CAD-CBD-CGD-O1D
25	b	504	CLA	CAD-CBD-CGD-O2D
25	b	505	CLA	C1A-C2A-CAA-CBA
25	b	505	CLA	CBD-CGD-O2D-CED
25	b	506	CLA	C3A-C2A-CAA-CBA
25	b	506	CLA	CAD-CBD-CGD-O1D
25	b	506	CLA	CAD-CBD-CGD-O2D
25	b	507	CLA	C1A-C2A-CAA-CBA
25	b	507	CLA	C3A-C2A-CAA-CBA
25	b	509	CLA	C1A-C2A-CAA-CBA
25	b	509	CLA	C3A-C2A-CAA-CBA
25	b	509	CLA	CBD-CGD-O2D-CED
25	b	510	CLA	CHA-CBD-CGD-O1D
25	b	510	CLA	CHA-CBD-CGD-O2D
25	b	511	CLA	CAD-CBD-CGD-O1D
25	b	511	CLA	CAD-CBD-CGD-O2D
25	b	512	CLA	C1A-C2A-CAA-CBA
25	b	512	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	b	513	CLA	CHA-CBD-CGD-O1D
25	b	513	CLA	CHA-CBD-CGD-O2D
25	c	501	CLA	C3A-C2A-CAA-CBA
25	c	501	CLA	CHA-CBD-CGD-O1D
25	c	501	CLA	CHA-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CAD-CBD-CGD-O2D
25	c	503	CLA	C1A-C2A-CAA-CBA
25	c	503	CLA	CBD-CGD-O2D-CED
25	c	504	CLA	C4B-C3B-CAB-CBB
25	c	505	CLA	C1A-C2A-CAA-CBA
25	c	506	CLA	C1A-C2A-CAA-CBA
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	511	CLA	CAD-CBD-CGD-O1D
25	c	511	CLA	CAD-CBD-CGD-O2D
25	d	401	CLA	C1A-C2A-CAA-CBA
25	d	401	CLA	C3A-C2A-CAA-CBA
25	d	403	CLA	C1A-C2A-CAA-CBA
25	d	404	CLA	CAD-CBD-CGD-O1D
25	d	404	CLA	CAD-CBD-CGD-O2D
25	r	302	CLA	CBD-CGD-O2D-CED
25	r	303	CLA	CHA-CBD-CGD-O1D
25	r	303	CLA	CHA-CBD-CGD-O2D
25	r	307	CLA	CBD-CGD-O2D-CED
25	r	308	CLA	CBD-CGD-O2D-CED
27	B	517	BCR	C21-C22-C23-C24
27	B	517	BCR	C23-C24-C25-C26
27	B	518	BCR	C7-C8-C9-C10
27	B	518	BCR	C7-C8-C9-C34
27	C	514	BCR	C23-C24-C25-C26
27	C	515	BCR	C21-C22-C23-C24
27	C	515	BCR	C37-C22-C23-C24
27	C	515	BCR	C23-C24-C25-C26
27	D	406	BCR	C7-C8-C9-C10
27	V	101	BCR	C21-C22-C23-C24
27	V	101	BCR	C37-C22-C23-C24
27	b	517	BCR	C7-C8-C9-C10
27	b	517	BCR	C7-C8-C9-C34
27	c	514	BCR	C21-C22-C23-C24
27	t	101	BCR	C5-C6-C7-C8
27	t	101	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
27	z	101	BCR	C1-C6-C7-C8
27	z	101	BCR	C5-C6-C7-C8
27	z	101	BCR	C21-C22-C23-C24
29	W	201	LMG	O1-C7-C8-O7
29	a	408	LMG	O6-C1-O1-C7
29	c	518	LMG	C19-C20-C21-C22
29	d	410	LMG	O7-C8-C9-O8
30	B	520	LHG	C3-O3-P-O4
30	B	520	LHG	C3-O3-P-O5
30	B	520	LHG	C3-O3-P-O6
30	B	520	LHG	C4-O6-P-O3
30	B	520	LHG	C4-O6-P-O4
30	C	521	LHG	C4-O6-P-O3
30	C	521	LHG	C4-O6-P-O4
30	D	409	LHG	C4-O6-P-O3
30	D	409	LHG	C4-O6-P-O5
30	G	618	LHG	C4-O6-P-O3
30	G	618	LHG	C4-O6-P-O4
30	G	618	LHG	C4-O6-P-O5
30	L	101	LHG	C3-O3-P-O6
30	L	101	LHG	C4-O6-P-O3
30	L	101	LHG	C4-O6-P-O4
30	L	101	LHG	C4-O6-P-O5
30	N	319	LHG	C4-O6-P-O3
30	N	319	LHG	C4-O6-P-O4
30	N	319	LHG	C4-O6-P-O5
30	S	618	LHG	C4-O6-P-O3
30	S	618	LHG	C4-O6-P-O4
30	Y	319	LHG	C3-O3-P-O4
30	Y	319	LHG	C3-O3-P-O6
30	Y	319	LHG	C4-O6-P-O3
30	Y	319	LHG	C4-O6-P-O4
30	Y	319	LHG	C4-O6-P-O5
30	a	411	LHG	C3-O3-P-O4
30	a	411	LHG	C3-O3-P-O6
30	a	411	LHG	C4-O6-P-O4
30	b	521	LHG	C3-O3-P-O5
30	b	521	LHG	C4-O6-P-O3
30	b	521	LHG	C4-O6-P-O4
30	d	407	LHG	C3-O3-P-O4
30	d	407	LHG	C3-O3-P-O6
30	d	407	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
30	d	407	LHG	C4-O6-P-O4
30	d	408	LHG	C3-O3-P-O5
30	l	101	LHG	C3-O3-P-O4
30	l	101	LHG	C3-O3-P-O6
31	C	519	DGD	C4D-C5D-C6D-O5D
32	S	619	LMU	O5B-C1B-O1B-C4'
36	G	609	CHL	C4C-C3C-CAC-CBC
36	G	619	CHL	C1C-C2C-CMC-OMC
36	G	619	CHL	C3C-C2C-CMC-OMC
36	N	308	CHL	C1C-C2C-CMC-OMC
36	S	601	CHL	C1C-C2C-CMC-OMC
36	S	606	CHL	C1C-C2C-CMC-OMC
36	S	606	CHL	C3C-C2C-CMC-OMC
36	S	606	CHL	CAD-CBD-CGD-O2D
36	S	608	CHL	CAD-CBD-CGD-O1D
36	S	608	CHL	CAD-CBD-CGD-O2D
36	Y	310	CHL	C4C-C3C-CAC-CBC
25	r	303	CLA	O1D-CGD-O2D-CED
25	B	505	CLA	O1D-CGD-O2D-CED
25	G	612	CLA	O1D-CGD-O2D-CED
25	B	501	CLA	CBD-CGD-O2D-CED
25	B	505	CLA	CBD-CGD-O2D-CED
25	B	509	CLA	CBD-CGD-O2D-CED
25	C	506	CLA	CBD-CGD-O2D-CED
25	G	612	CLA	CBD-CGD-O2D-CED
25	N	314	CLA	CBD-CGD-O2D-CED
25	b	507	CLA	CBD-CGD-O2D-CED
25	b	511	CLA	CBD-CGD-O2D-CED
25	c	501	CLA	CBD-CGD-O2D-CED
25	c	502	CLA	CBD-CGD-O2D-CED
25	c	504	CLA	CBD-CGD-O2D-CED
25	c	506	CLA	CBD-CGD-O2D-CED
25	d	404	CLA	CBD-CGD-O2D-CED
25	r	303	CLA	CBD-CGD-O2D-CED
26	d	402	PHO	CBD-CGD-O2D-CED
36	S	608	CHL	CBD-CGD-O2D-CED
36	r	306	CHL	CBD-CGD-O2D-CED
25	A	402	CLA	O1A-CGA-O2A-C1
25	B	513	CLA	O1A-CGA-O2A-C1
25	r	302	CLA	O1D-CGD-O2D-CED
25	C	506	CLA	O1D-CGD-O2D-CED
25	c	506	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B	513	CLA	CBA-CGA-O2A-C1
25	b	508	CLA	CBA-CGA-O2A-C1
25	D	405	CLA	CBD-CGD-O2D-CED
25	B	516	CLA	O1A-CGA-O2A-C1
25	C	513	CLA	O1A-CGA-O2A-C1
25	N	312	CLA	O1A-CGA-O2A-C1
25	S	613	CLA	O1A-CGA-O2A-C1
25	Y	312	CLA	O1A-CGA-O2A-C1
25	b	508	CLA	O1A-CGA-O2A-C1
25	c	508	CLA	O1A-CGA-O2A-C1
25	d	401	CLA	O1A-CGA-O2A-C1
25	r	303	CLA	O1A-CGA-O2A-C1
26	a	404	PHO	O1A-CGA-O2A-C1
25	B	507	CLA	O1D-CGD-O2D-CED
25	C	503	CLA	O1D-CGD-O2D-CED
25	N	311	CLA	O1D-CGD-O2D-CED
25	b	505	CLA	O1D-CGD-O2D-CED
25	r	308	CLA	O1D-CGD-O2D-CED
25	S	613	CLA	O1D-CGD-O2D-CED
25	b	501	CLA	O1D-CGD-O2D-CED
25	c	503	CLA	O1D-CGD-O2D-CED
25	r	307	CLA	O1D-CGD-O2D-CED
25	G	613	CLA	C3-C5-C6-C7
25	Y	314	CLA	C3-C5-C6-C7
25	b	502	CLA	C3-C5-C6-C7
25	b	503	CLA	C3-C5-C6-C7
25	c	512	CLA	C3-C5-C6-C7
26	A	404	PHO	C3-C5-C6-C7
26	a	404	PHO	C3-C5-C6-C7
25	A	402	CLA	CBA-CGA-O2A-C1
25	B	516	CLA	CBA-CGA-O2A-C1
25	C	510	CLA	CBA-CGA-O2A-C1
25	C	512	CLA	CBA-CGA-O2A-C1
25	N	312	CLA	CBA-CGA-O2A-C1
25	Y	305	CLA	CBA-CGA-O2A-C1
25	d	401	CLA	CBA-CGA-O2A-C1
26	a	404	PHO	CBA-CGA-O2A-C1
25	B	514	CLA	CBD-CGD-O2D-CED
25	C	511	CLA	CBD-CGD-O2D-CED
25	G	602	CLA	CBD-CGD-O2D-CED
25	G	613	CLA	CBD-CGD-O2D-CED
25	S	609	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	Y	314	CLA	CBD-CGD-O2D-CED
25	b	515	CLA	CBD-CGD-O2D-CED
25	c	511	CLA	CBD-CGD-O2D-CED
25	N	305	CLA	O1D-CGD-O2D-CED
25	b	507	CLA	O1D-CGD-O2D-CED
25	b	509	CLA	O1D-CGD-O2D-CED
25	c	501	CLA	O1D-CGD-O2D-CED
25	c	504	CLA	O1D-CGD-O2D-CED
25	c	506	CLA	O1A-CGA-O2A-C1
25	c	502	CLA	O1D-CGD-O2D-CED
25	b	505	CLA	C4-C3-C5-C6
25	b	515	CLA	C4-C3-C5-C6
36	N	309	CHL	CBD-CGD-O2D-CED
25	N	314	CLA	O1D-CGD-O2D-CED
36	r	306	CHL	O1D-CGD-O2D-CED
25	c	502	CLA	C2A-CAA-CBA-CGA
25	b	508	CLA	C3-C5-C6-C7
26	D	402	PHO	C3-C5-C6-C7
25	C	513	CLA	CBA-CGA-O2A-C1
25	S	613	CLA	CBA-CGA-O2A-C1
25	Y	312	CLA	CBA-CGA-O2A-C1
25	b	502	CLA	CBA-CGA-O2A-C1
25	b	505	CLA	CBA-CGA-O2A-C1
25	b	509	CLA	CBA-CGA-O2A-C1
25	b	511	CLA	CBA-CGA-O2A-C1
25	c	508	CLA	CBA-CGA-O2A-C1
25	r	303	CLA	CBA-CGA-O2A-C1
27	v	101	BCR	C19-C20-C21-C22
25	B	510	CLA	O1A-CGA-O2A-C1
25	C	509	CLA	O1A-CGA-O2A-C1
25	C	512	CLA	O1A-CGA-O2A-C1
25	S	611	CLA	O1A-CGA-O2A-C1
25	Y	305	CLA	O1A-CGA-O2A-C1
25	b	502	CLA	O1A-CGA-O2A-C1
25	b	505	CLA	O1A-CGA-O2A-C1
25	b	509	CLA	O1A-CGA-O2A-C1
25	b	511	CLA	O1A-CGA-O2A-C1
25	B	504	CLA	C3-C5-C6-C7
25	C	502	CLA	CBD-CGD-O2D-CED
25	C	504	CLA	CBD-CGD-O2D-CED
25	Y	304	CLA	CBD-CGD-O2D-CED
36	G	605	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	G	608	CHL	CBD-CGD-O2D-CED
25	B	509	CLA	O1D-CGD-O2D-CED
26	d	402	PHO	O1D-CGD-O2D-CED
36	S	608	CHL	O1D-CGD-O2D-CED
25	C	509	CLA	CBA-CGA-O2A-C1
25	S	611	CLA	CBA-CGA-O2A-C1
26	A	404	PHO	CBA-CGA-O2A-C1
26	d	402	PHO	CBA-CGA-O2A-C1
25	C	510	CLA	O1A-CGA-O2A-C1
25	N	312	CLA	CBD-CGD-O2D-CED
36	S	601	CHL	CBD-CGD-O2D-CED
29	a	408	LMG	C11-C10-O7-C8
29	d	409	LMG	C11-C10-O7-C8
32	C	523	LMU	O5'-C5'-C6'-O6'
25	B	501	CLA	O1D-CGD-O2D-CED
25	b	511	CLA	O1D-CGD-O2D-CED
25	G	610	CLA	CBD-CGD-O2D-CED
25	d	404	CLA	O1D-CGD-O2D-CED
25	B	510	CLA	CBA-CGA-O2A-C1
25	c	504	CLA	CBA-CGA-O2A-C1
25	c	505	CLA	CBA-CGA-O2A-C1
25	c	506	CLA	CBA-CGA-O2A-C1
25	B	505	CLA	C4-C3-C5-C6
25	b	505	CLA	C2-C3-C5-C6
26	A	404	PHO	O1A-CGA-O2A-C1
29	a	408	LMG	O9-C10-O7-C8
34	D	407	PL9	C39-C41-C42-C43
25	b	506	CLA	CBD-CGD-O2D-CED
25	b	508	CLA	CBD-CGD-O2D-CED
31	C	518	DGD	O6D-C5D-C6D-O5D
25	b	511	CLA	C2A-CAA-CBA-CGA
36	Y	307	CHL	C2A-CAA-CBA-CGA
25	c	504	CLA	O1A-CGA-O2A-C1
25	c	505	CLA	O1A-CGA-O2A-C1
26	d	402	PHO	O1A-CGA-O2A-C1
29	W	201	LMG	O6-C1-O1-C7
32	C	522	LMU	O5'-C5'-C6'-O6'
25	S	604	CLA	CBD-CGD-O2D-CED
25	Y	311	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	CBD-CGD-O2D-CED
26	D	402	PHO	CBD-CGD-O2D-CED
36	r	304	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	D	405	CLA	O1D-CGD-O2D-CED
29	d	409	LMG	O9-C10-O7-C8
25	G	603	CLA	CBA-CGA-O2A-C1
25	N	314	CLA	CBA-CGA-O2A-C1
25	a	403	CLA	CBA-CGA-O2A-C1
25	a	405	CLA	CBA-CGA-O2A-C1
25	b	510	CLA	CBA-CGA-O2A-C1
25	a	403	CLA	CBD-CGD-O2D-CED
31	C	519	DGD	O6D-C5D-C6D-O5D
25	B	514	CLA	O1D-CGD-O2D-CED
25	b	515	CLA	C2-C3-C5-C6
36	Y	309	CHL	CBD-CGD-O2D-CED
25	B	504	CLA	C6-C7-C8-C9
25	B	506	CLA	C6-C7-C8-C9
25	B	508	CLA	C11-C10-C8-C9
25	C	504	CLA	C11-C12-C13-C14
25	C	512	CLA	C6-C7-C8-C9
25	b	509	CLA	C6-C7-C8-C9
25	b	510	CLA	C11-C12-C13-C14
25	b	511	CLA	C11-C12-C13-C14
25	b	515	CLA	C6-C7-C8-C9
25	c	507	CLA	C14-C13-C15-C16
36	N	302	CHL	C14-C13-C15-C16
36	N	306	CHL	C6-C7-C8-C9
36	N	308	CHL	C6-C7-C8-C9
36	N	308	CHL	C14-C13-C15-C16
36	Y	310	CHL	C14-C13-C15-C16
25	G	613	CLA	O1D-CGD-O2D-CED
31	c	516	DGD	C2E-C1E-O5D-C6D
30	b	521	LHG	O2-C2-C3-O3
25	S	614	CLA	CBA-CGA-O2A-C1
36	G	607	CHL	CBD-CGD-O2D-CED
27	B	517	BCR	C36-C18-C19-C20
27	B	517	BCR	C37-C22-C23-C24
27	C	515	BCR	C7-C8-C9-C34
27	D	406	BCR	C7-C8-C9-C34
27	H	101	BCR	C7-C8-C9-C34
27	b	519	BCR	C7-C8-C9-C34
27	c	514	BCR	C37-C22-C23-C24
27	d	405	BCR	C37-C22-C23-C24
27	h	101	BCR	C7-C8-C9-C34
27	t	101	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
27	z	101	BCR	C37-C22-C23-C24
27	B	517	BCR	C17-C18-C19-C20
27	H	101	BCR	C7-C8-C9-C10
27	h	101	BCR	C7-C8-C9-C10
27	t	101	BCR	C7-C8-C9-C10
32	C	522	LMU	C4'-C5'-C6'-O6'
25	B	516	CLA	C2A-CAA-CBA-CGA
25	C	509	CLA	C2A-CAA-CBA-CGA
25	c	508	CLA	C2A-CAA-CBA-CGA
25	G	603	CLA	O1A-CGA-O2A-C1
25	S	610	CLA	CBA-CGA-O2A-C1
25	B	506	CLA	C8-C10-C11-C12
25	d	401	CLA	C2-C1-O2A-CGA
25	b	515	CLA	O1D-CGD-O2D-CED
25	B	501	CLA	C8-C10-C11-C12
31	c	517	DGD	C4D-C5D-C6D-O5D
31	C	517	DGD	C1B-C2B-C3B-C4B
25	c	511	CLA	O1D-CGD-O2D-CED
25	C	505	CLA	CBA-CGA-O2A-C1
25	b	513	CLA	CBA-CGA-O2A-C1
36	G	601	CHL	C4-C3-C5-C6
31	C	518	DGD	C1B-C2B-C3B-C4B
25	S	609	CLA	O1D-CGD-O2D-CED
34	d	406	PL9	C39-C41-C42-C43
25	B	516	CLA	C8-C10-C11-C12
25	a	405	CLA	C10-C11-C12-C13
25	b	502	CLA	C8-C10-C11-C12
36	Y	310	CHL	C13-C15-C16-C17
30	B	520	LHG	C23-C24-C25-C26
25	a	403	CLA	O1A-CGA-O2A-C1
36	Y	308	CHL	CBD-CGD-O2D-CED
36	N	302	CHL	C15-C16-C17-C18
36	Y	310	CHL	C8-C10-C11-C12
32	c	519	LMU	C3'-C4'-O1B-C1B
25	B	506	CLA	C2A-CAA-CBA-CGA
25	B	513	CLA	C2A-CAA-CBA-CGA
25	b	506	CLA	C2A-CAA-CBA-CGA
25	c	506	CLA	C2A-CAA-CBA-CGA
36	G	619	CHL	C2A-CAA-CBA-CGA
36	N	306	CHL	C2A-CAA-CBA-CGA
36	N	307	CHL	C2A-CAA-CBA-CGA
36	S	601	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
36	Y	308	CHL	C2A-CAA-CBA-CGA
25	B	510	CLA	C15-C16-C17-C18
25	B	514	CLA	C8-C10-C11-C12
25	C	503	CLA	C15-C16-C17-C18
25	Y	311	CLA	C5-C6-C7-C8
25	b	502	CLA	C13-C15-C16-C17
36	N	302	CHL	C5-C6-C7-C8
36	N	306	CHL	C8-C10-C11-C12
25	N	314	CLA	O1A-CGA-O2A-C1
25	b	510	CLA	O1A-CGA-O2A-C1
36	N	306	CHL	C3-C5-C6-C7
31	c	516	DGD	O6E-C1E-O5D-C6D
25	Y	314	CLA	O1D-CGD-O2D-CED
25	C	504	CLA	C10-C11-C12-C13
25	C	507	CLA	C13-C15-C16-C17
25	G	613	CLA	C8-C10-C11-C12
25	b	502	CLA	C5-C6-C7-C8
36	G	609	CHL	C15-C16-C17-C18
36	G	619	CHL	C8-C10-C11-C12
36	Y	303	CHL	C5-C6-C7-C8
30	B	520	LHG	O2-C2-C3-O3
25	a	405	CLA	O1A-CGA-O2A-C1
25	B	509	CLA	C5-C6-C7-C8
36	G	601	CHL	C8-C10-C11-C12
25	C	504	CLA	O1D-CGD-O2D-CED
36	G	609	CHL	C3-C5-C6-C7
25	C	511	CLA	O1D-CGD-O2D-CED
36	N	309	CHL	O1D-CGD-O2D-CED
25	C	506	CLA	C13-C15-C16-C17
25	a	402	CLA	C13-C15-C16-C17
25	S	614	CLA	O1A-CGA-O2A-C1
25	B	505	CLA	C2-C3-C5-C6
30	d	408	LHG	C7-C8-C9-C10
25	G	602	CLA	O1D-CGD-O2D-CED
25	Y	304	CLA	O1D-CGD-O2D-CED
36	G	608	CHL	O1D-CGD-O2D-CED
25	B	504	CLA	C8-C10-C11-C12
36	N	310	CHL	C8-C10-C11-C12
36	Y	303	CHL	C8-C10-C11-C12
36	S	608	CHL	O2A-C1-C2-C3
25	C	505	CLA	O1A-CGA-O2A-C1
25	D	405	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
36	S	606	CHL	C2A-CAA-CBA-CGA
36	r	304	CHL	C2A-CAA-CBA-CGA
25	C	510	CLA	C15-C16-C17-C18
25	b	513	CLA	O1A-CGA-O2A-C1
30	B	520	LHG	C1-C2-C3-O3
25	A	402	CLA	C2A-CAA-CBA-CGA
36	G	607	CHL	C2A-CAA-CBA-CGA
36	N	306	CHL	C13-C15-C16-C17
36	N	310	CHL	C15-C16-C17-C18
25	b	504	CLA	CBD-CGD-O2D-CED
36	N	302	CHL	CBD-CGD-O2D-CED
25	C	502	CLA	O1D-CGD-O2D-CED
36	G	605	CHL	O1D-CGD-O2D-CED
25	B	515	CLA	C5-C6-C7-C8
36	G	619	CHL	C10-C11-C12-C13
36	S	601	CHL	O1D-CGD-O2D-CED
25	B	503	CLA	C13-C15-C16-C17
25	b	511	CLA	C5-C6-C7-C8
25	c	509	CLA	C8-C10-C11-C12
25	N	312	CLA	O1D-CGD-O2D-CED
25	B	514	CLA	CBA-CGA-O2A-C1
31	c	517	DGD	O6D-C5D-C6D-O5D
36	G	608	CHL	C2A-CAA-CBA-CGA
34	d	406	PL9	C47-C48-C49-C51
25	b	507	CLA	C3-C5-C6-C7
31	C	517	DGD	O6E-C5E-C6E-O5E
25	G	610	CLA	O1D-CGD-O2D-CED
25	B	501	CLA	C13-C15-C16-C17
25	N	304	CLA	C15-C16-C17-C18
30	d	408	LHG	O2-C2-C3-O3
25	c	509	CLA	CBA-CGA-O2A-C1
36	G	609	CHL	C16-C17-C18-C19
36	Y	303	CHL	C16-C17-C18-C19
25	S	610	CLA	O1A-CGA-O2A-C1
36	G	609	CHL	C10-C11-C12-C13
27	b	519	BCR	C37-C22-C23-C24
27	z	101	BCR	C7-C8-C9-C34
27	b	519	BCR	C7-C8-C9-C10
27	z	101	BCR	C7-C8-C9-C10
25	C	510	CLA	C2A-CAA-CBA-CGA
25	S	614	CLA	C2A-CAA-CBA-CGA
25	b	505	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	r	302	CLA	C2A-CAA-CBA-CGA
36	N	308	CHL	C2A-CAA-CBA-CGA
25	b	508	CLA	O1D-CGD-O2D-CED
25	C	501	CLA	C16-C17-C18-C19
36	G	601	CHL	C16-C17-C18-C20
36	G	619	CHL	C16-C17-C18-C20
36	N	302	CHL	C16-C17-C18-C20
36	N	310	CHL	C16-C17-C18-C20
36	Y	310	CHL	C16-C17-C18-C20
25	G	602	CLA	C3-C5-C6-C7
25	b	505	CLA	C13-C15-C16-C17
25	c	510	CLA	C8-C10-C11-C12
36	G	619	CHL	C15-C16-C17-C18
25	b	506	CLA	O1D-CGD-O2D-CED
25	b	506	CLA	CBA-CGA-O2A-C1
36	G	601	CHL	CBD-CGD-O2D-CED
25	C	509	CLA	C2-C1-O2A-CGA
25	c	506	CLA	C2-C1-O2A-CGA
25	c	508	CLA	C2-C1-O2A-CGA
25	A	405	CLA	C11-C12-C13-C14
25	C	501	CLA	C16-C17-C18-C20
25	D	401	CLA	C16-C17-C18-C20
36	G	601	CHL	C16-C17-C18-C19
36	N	302	CHL	C16-C17-C18-C19
36	N	306	CHL	C16-C17-C18-C19
31	c	517	DGD	C3B-C4B-C5B-C6B
30	C	521	LHG	C32-C33-C34-C35
32	C	523	LMU	C4-C5-C6-C7
36	N	310	CHL	C13-C15-C16-C17
36	Y	303	CHL	C13-C15-C16-C17
30	N	319	LHG	C33-C34-C35-C36
28	t	102	SQD	C31-C32-C33-C34
25	S	604	CLA	O1D-CGD-O2D-CED
25	Y	311	CLA	O1D-CGD-O2D-CED
25	C	512	CLA	C4B-C3B-CAB-CBB
25	G	603	CLA	C4B-C3B-CAB-CBB
25	G	612	CLA	C4B-C3B-CAB-CBB
25	N	312	CLA	C4B-C3B-CAB-CBB
25	N	315	CLA	C4B-C3B-CAB-CBB
25	S	613	CLA	C4B-C3B-CAB-CBB
25	A	405	CLA	C11-C12-C13-C15
25	D	405	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	G	602	CLA	C16-C17-C18-C19
25	G	602	CLA	C16-C17-C18-C20
25	G	613	CLA	C16-C17-C18-C20
25	N	303	CLA	C16-C17-C18-C19
25	N	303	CLA	C16-C17-C18-C20
25	r	301	CLA	C11-C12-C13-C14
25	r	301	CLA	C11-C12-C13-C15
36	G	609	CHL	C16-C17-C18-C20
36	G	619	CHL	C16-C17-C18-C19
36	N	310	CHL	C16-C17-C18-C19
36	Y	310	CHL	C16-C17-C18-C19
25	S	613	CLA	C2A-CAA-CBA-CGA
25	B	513	CLA	C15-C16-C17-C18
36	G	609	CHL	C5-C6-C7-C8
25	C	501	CLA	C11-C10-C8-C7
25	G	603	CLA	C6-C7-C8-C10
25	c	506	CLA	C12-C13-C15-C16
32	S	619	LMU	O1'-C1-C2-C3
32	c	519	LMU	C5'-C4'-O1B-C1B
25	A	402	CLA	C3A-C2A-CAA-CBA
25	B	516	CLA	C3A-C2A-CAA-CBA
25	C	513	CLA	C3A-C2A-CAA-CBA
25	N	304	CLA	C3A-C2A-CAA-CBA
25	S	605	CLA	C3A-C2A-CAA-CBA
25	Y	305	CLA	C3A-C2A-CAA-CBA
25	b	501	CLA	C3A-C2A-CAA-CBA
25	b	504	CLA	C3A-C2A-CAA-CBA
25	c	507	CLA	C3A-C2A-CAA-CBA
25	d	403	CLA	C3A-C2A-CAA-CBA
25	b	509	CLA	C5-C6-C7-C8
36	r	304	CHL	O1D-CGD-O2D-CED
25	D	405	CLA	C16-C17-C18-C20
25	G	613	CLA	C16-C17-C18-C19
36	G	619	CHL	CBD-CGD-O2D-CED
36	r	305	CHL	CBD-CGD-O2D-CED
29	d	410	LMG	C15-C16-C17-C18
25	B	507	CLA	CBA-CGA-O2A-C1
25	Y	315	CLA	CBA-CGA-O2A-C1
29	H	102	LMG	C29-C30-C31-C32
30	B	520	LHG	C28-C29-C30-C31
30	C	521	LHG	C12-C13-C14-C15
25	Y	313	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	c	518	LMG	C10-C11-C12-C13
29	b	520	LMG	C11-C12-C13-C14
31	W	202	DGD	C2A-C3A-C4A-C5A
25	B	514	CLA	O1A-CGA-O2A-C1
25	c	509	CLA	O1A-CGA-O2A-C1
26	D	402	PHO	O1D-CGD-O2D-CED
32	c	519	LMU	C1-C2-C3-C4
32	C	523	LMU	C4'-C5'-C6'-O6'
25	c	513	CLA	O1D-CGD-O2D-CED
25	D	401	CLA	C16-C17-C18-C19
30	D	408	LHG	C7-C8-C9-C10
25	C	512	CLA	C2B-C3B-CAB-CBB
25	G	603	CLA	C2B-C3B-CAB-CBB
25	N	304	CLA	C2B-C3B-CAB-CBB
25	N	312	CLA	C2B-C3B-CAB-CBB
25	N	315	CLA	C2B-C3B-CAB-CBB
25	c	504	CLA	C2B-C3B-CAB-CBB
27	B	517	BCR	C23-C24-C25-C30
27	C	514	BCR	C1-C6-C7-C8
27	C	514	BCR	C5-C6-C7-C8
27	C	514	BCR	C23-C24-C25-C30
27	C	515	BCR	C23-C24-C25-C30
27	a	406	BCR	C23-C24-C25-C26
27	c	514	BCR	C23-C24-C25-C26
27	c	514	BCR	C23-C24-C25-C30
27	d	405	BCR	C23-C24-C25-C26
27	t	101	BCR	C1-C6-C7-C8
27	t	101	BCR	C23-C24-C25-C30
27	v	101	BCR	C23-C24-C25-C26
27	v	101	BCR	C23-C24-C25-C30
25	b	503	CLA	CBD-CGD-O2D-CED
28	a	407	SQD	C8-C7-O47-C45
25	d	401	CLA	C15-C16-C17-C18
25	B	514	CLA	C2A-CAA-CBA-CGA
25	N	314	CLA	C2A-CAA-CBA-CGA
25	b	507	CLA	C2A-CAA-CBA-CGA
25	b	506	CLA	O1A-CGA-O2A-C1
25	C	513	CLA	C4-C3-C5-C6
36	G	601	CHL	C2-C3-C5-C6
25	D	405	CLA	C14-C13-C15-C16
25	b	504	CLA	C11-C12-C13-C14
31	C	518	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
36	N	302	CHL	C13-C15-C16-C17
36	Y	303	CHL	C15-C16-C17-C18
32	C	523	LMU	C6-C7-C8-C9
25	B	504	CLA	CBD-CGD-O2D-CED
25	b	510	CLA	C15-C16-C17-C18
26	a	404	PHO	C8-C10-C11-C12
36	G	619	CHL	C13-C15-C16-C17
30	d	407	LHG	C29-C30-C31-C32
32	C	523	LMU	C7-C8-C9-C10
26	d	402	PHO	C3-C5-C6-C7
36	N	306	CHL	C16-C17-C18-C20
28	A	407	SQD	C8-C7-O47-C45
29	b	520	LMG	C11-C10-O7-C8
29	d	409	LMG	C28-C29-C30-C31
29	W	201	LMG	C29-C30-C31-C32
29	b	520	LMG	O9-C10-O7-C8
28	a	407	SQD	C33-C34-C35-C36
36	G	609	CHL	C2C-C3C-CAC-CBC
25	A	405	CLA	C3-C5-C6-C7
25	c	508	CLA	C3-C5-C6-C7
31	c	517	DGD	C5D-C6D-O5D-C1E
36	G	601	CHL	C2A-CAA-CBA-CGA
36	N	308	CHL	CBD-CGD-O2D-CED
25	B	508	CLA	C13-C15-C16-C17
30	d	407	LHG	C23-C24-C25-C26
29	D	410	LMG	O6-C5-C6-O5
29	b	520	LMG	O6-C5-C6-O5
29	W	201	LMG	C11-C10-O7-C8
30	C	521	LHG	C8-C7-O7-C5
30	l	101	LHG	C8-C7-O7-C5
36	Y	303	CHL	C16-C17-C18-C20
25	B	507	CLA	O1A-CGA-O2A-C1
25	Y	315	CLA	O1A-CGA-O2A-C1
29	B	519	LMG	C10-C11-C12-C13
29	a	408	LMG	C10-C11-C12-C13
29	a	408	LMG	O6-C5-C6-O5
25	Y	305	CLA	C3-C5-C6-C7
29	C	520	LMG	O7-C8-C9-O8
29	H	102	LMG	O7-C8-C9-O8
25	Y	305	CLA	C13-C15-C16-C17
29	c	518	LMG	O6-C5-C6-O5
36	Y	309	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	S	619	LMU	O5'-C5'-C6'-O6'
28	A	407	SQD	O49-C7-O47-C45
25	C	505	CLA	C2A-CAA-CBA-CGA
25	b	508	CLA	C2A-CAA-CBA-CGA
36	Y	310	CHL	CBD-CGD-O2D-CED
36	G	607	CHL	O1D-CGD-O2D-CED
31	C	518	DGD	O6E-C5E-C6E-O5E
25	A	402	CLA	C1A-C2A-CAA-CBA
25	B	516	CLA	C1A-C2A-CAA-CBA
25	C	503	CLA	C1A-C2A-CAA-CBA
25	G	611	CLA	C1A-C2A-CAA-CBA
25	N	304	CLA	C1A-C2A-CAA-CBA
25	S	602	CLA	C1A-C2A-CAA-CBA
25	Y	305	CLA	C1A-C2A-CAA-CBA
25	Y	306	CLA	C1A-C2A-CAA-CBA
25	Y	315	CLA	C1A-C2A-CAA-CBA
25	b	503	CLA	C1A-C2A-CAA-CBA
25	b	506	CLA	C1A-C2A-CAA-CBA
25	b	514	CLA	C1A-C2A-CAA-CBA
25	c	501	CLA	C1A-C2A-CAA-CBA
25	c	507	CLA	C1A-C2A-CAA-CBA
25	c	511	CLA	C1A-C2A-CAA-CBA
25	r	303	CLA	C1A-C2A-CAA-CBA
29	d	410	LMG	O6-C5-C6-O5
32	S	619	LMU	O5B-C5B-C6B-O6B
25	C	503	CLA	C8-C10-C11-C12
29	H	102	LMG	O6-C5-C6-O5
31	C	517	DGD	C3A-C4A-C5A-C6A
25	N	303	CLA	C3-C5-C6-C7
25	B	508	CLA	C6-C7-C8-C10
25	B	508	CLA	C11-C10-C8-C7
25	B	515	CLA	C12-C13-C15-C16
25	C	510	CLA	C12-C13-C15-C16
25	C	512	CLA	C6-C7-C8-C10
25	D	401	CLA	C11-C12-C13-C15
25	G	613	CLA	C12-C13-C15-C16
25	Y	313	CLA	C11-C12-C13-C15
25	b	506	CLA	C11-C10-C8-C7
25	b	508	CLA	C11-C12-C13-C15
25	b	512	CLA	C11-C10-C8-C7
25	b	513	CLA	C6-C7-C8-C10
25	c	505	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	c	509	CLA	C6-C7-C8-C10
36	Y	310	CHL	C11-C12-C13-C15
32	C	522	LMU	C3-C4-C5-C6
25	N	304	CLA	C16-C17-C18-C20
25	b	503	CLA	C8-C10-C11-C12
31	Y	301	DGD	O6E-C5E-C6E-O5E
25	C	506	CLA	C5-C6-C7-C8
36	G	601	CHL	C15-C16-C17-C18
26	A	404	PHO	C2-C3-C5-C6
32	c	519	LMU	O5'-C5'-C6'-O6'
25	B	512	CLA	C10-C11-C12-C13
25	G	603	CLA	C2A-CAA-CBA-CGA
25	G	611	CLA	C2A-CAA-CBA-CGA
25	Y	314	CLA	C2A-CAA-CBA-CGA
25	b	516	CLA	C2A-CAA-CBA-CGA
25	C	501	CLA	C11-C10-C8-C9
25	C	506	CLA	C6-C7-C8-C9
25	C	510	CLA	C14-C13-C15-C16
25	C	511	CLA	C6-C7-C8-C9
25	D	404	CLA	C11-C10-C8-C9
25	G	613	CLA	C14-C13-C15-C16
25	Y	305	CLA	C11-C12-C13-C14
25	Y	314	CLA	C14-C13-C15-C16
25	b	506	CLA	C11-C10-C8-C9
25	b	512	CLA	C11-C10-C8-C9
25	b	513	CLA	C6-C7-C8-C9
25	c	501	CLA	C6-C7-C8-C9
25	c	503	CLA	C11-C10-C8-C9
25	c	509	CLA	C6-C7-C8-C9
25	c	510	CLA	C11-C12-C13-C14
26	a	404	PHO	C11-C12-C13-C14
36	G	619	CHL	C6-C7-C8-C9
36	Y	310	CHL	C11-C12-C13-C14
36	G	601	CHL	CBA-CGA-O2A-C1
36	N	302	CHL	CBA-CGA-O2A-C1
25	Y	313	CLA	C8-C10-C11-C12
36	Y	310	CHL	C2C-C3C-CAC-CBC
25	a	403	CLA	O1D-CGD-O2D-CED
28	A	407	SQD	C10-C11-C12-C13
29	d	409	LMG	C10-C11-C12-C13
29	H	102	LMG	C7-C8-C9-O8
29	W	201	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	C	521	LHG	C4-C5-C6-O8
25	c	506	CLA	C5-C6-C7-C8
36	N	310	CHL	C5-C6-C7-C8
25	B	504	CLA	CBA-CGA-O2A-C1
36	Y	308	CHL	O1D-CGD-O2D-CED
26	D	402	PHO	CHA-CBD-CGD-O1D
26	D	402	PHO	CHA-CBD-CGD-O2D
36	G	605	CHL	CHA-CBD-CGD-O1D
36	G	605	CHL	CHA-CBD-CGD-O2D
36	G	609	CHL	CHA-CBD-CGD-O1D
36	r	305	CHL	CHA-CBD-CGD-O2D
26	A	404	PHO	C4-C3-C5-C6
25	N	315	CLA	CBD-CGD-O2D-CED
34	d	406	PL9	C13-C14-C16-C17
25	B	504	CLA	C5-C6-C7-C8
27	C	514	BCR	C7-C8-C9-C34
30	N	319	LHG	C25-C26-C27-C28
29	d	409	LMG	O6-C5-C6-O5
27	d	405	BCR	C21-C22-C23-C24
36	N	302	CHL	O1A-CGA-O2A-C1
25	C	510	CLA	C8-C10-C11-C12
36	Y	310	CHL	C15-C16-C17-C18
25	c	511	CLA	CBA-CGA-O2A-C1
29	W	201	LMG	C29-C28-O8-C9
25	C	509	CLA	O2A-C1-C2-C3
25	B	506	CLA	C5-C6-C7-C8
28	A	407	SQD	C25-C26-C27-C28
36	G	607	CHL	C3C-C2C-CMC-OMC
36	N	307	CHL	C3C-C2C-CMC-OMC
36	N	308	CHL	C3C-C2C-CMC-OMC
36	S	601	CHL	C3C-C2C-CMC-OMC
25	N	304	CLA	C16-C17-C18-C19
30	a	410	LHG	O6-C4-C5-O7
25	C	501	CLA	CBA-CGA-O2A-C1
25	S	604	CLA	CBA-CGA-O2A-C1
25	c	512	CLA	CBA-CGA-O2A-C1
25	B	508	CLA	C2-C3-C5-C6
30	a	411	LHG	C14-C15-C16-C17
32	c	519	LMU	C3-C4-C5-C6
29	H	102	LMG	C10-C11-C12-C13
36	G	609	CHL	C8-C10-C11-C12
25	A	403	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	N	305	CLA	CBA-CGA-O2A-C1
25	Y	306	CLA	CBA-CGA-O2A-C1
25	a	402	CLA	CBA-CGA-O2A-C1
36	N	307	CHL	C1C-C2C-CMC-OMC
36	G	609	CHL	CBD-CGD-O2D-CED
25	C	501	CLA	C8-C10-C11-C12
36	G	609	CHL	C13-C15-C16-C17
25	B	503	CLA	C16-C17-C18-C20
26	a	404	PHO	C4-C3-C5-C6
25	B	509	CLA	CBA-CGA-O2A-C1
36	N	310	CHL	CBA-CGA-O2A-C1
28	a	407	SQD	O49-C7-O47-C45
25	B	508	CLA	C6-C7-C8-C9
25	B	508	CLA	C11-C12-C13-C14
25	B	510	CLA	C11-C12-C13-C14
25	B	515	CLA	C14-C13-C15-C16
25	B	516	CLA	C14-C13-C15-C16
25	D	401	CLA	C11-C12-C13-C14
25	N	305	CLA	C11-C12-C13-C14
25	Y	313	CLA	C11-C12-C13-C14
25	b	502	CLA	C11-C10-C8-C9
25	b	504	CLA	C14-C13-C15-C16
25	b	508	CLA	C11-C12-C13-C14
25	c	501	CLA	C11-C12-C13-C14
25	c	505	CLA	C14-C13-C15-C16
25	c	508	CLA	C11-C10-C8-C9
25	c	511	CLA	C14-C13-C15-C16
25	d	401	CLA	C11-C12-C13-C14
36	G	601	CHL	C11-C12-C13-C14
36	N	302	CHL	C11-C12-C13-C14
36	Y	310	CHL	C6-C7-C8-C9
25	C	501	CLA	C4B-C3B-CAB-CBB
25	N	304	CLA	C4B-C3B-CAB-CBB
36	N	302	CHL	O1D-CGD-O2D-CED
28	A	407	SQD	O47-C7-C8-C9
25	B	507	CLA	C5-C6-C7-C8
25	C	501	CLA	C2A-CAA-CBA-CGA
28	A	407	SQD	C28-C29-C30-C31
36	Y	303	CHL	C3-C5-C6-C7
30	C	521	LHG	O6-C4-C5-C6
30	a	411	LHG	O6-C4-C5-C6
25	B	516	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	C	506	CLA	C6-C7-C8-C10
25	C	508	CLA	C6-C7-C8-C10
25	C	511	CLA	C6-C7-C8-C10
25	C	513	CLA	C11-C12-C13-C15
25	D	404	CLA	C11-C10-C8-C7
25	G	603	CLA	C12-C13-C15-C16
25	Y	305	CLA	C11-C12-C13-C15
25	Y	314	CLA	C12-C13-C15-C16
25	b	502	CLA	C11-C10-C8-C7
25	b	503	CLA	C11-C12-C13-C15
25	b	504	CLA	C12-C13-C15-C16
25	b	509	CLA	C6-C7-C8-C10
25	c	501	CLA	C6-C7-C8-C10
25	c	501	CLA	C11-C12-C13-C15
25	c	503	CLA	C11-C10-C8-C7
25	c	507	CLA	C6-C7-C8-C10
25	c	510	CLA	C11-C12-C13-C15
25	c	511	CLA	C12-C13-C15-C16
25	d	401	CLA	C11-C12-C13-C15
26	a	404	PHO	C11-C12-C13-C15
26	d	402	PHO	C11-C10-C8-C7
36	G	601	CHL	C11-C12-C13-C15
36	N	302	CHL	C11-C12-C13-C15
36	N	308	CHL	C6-C7-C8-C10
36	Y	303	CHL	C12-C13-C15-C16
36	Y	310	CHL	C6-C7-C8-C10
36	N	308	CHL	C13-C15-C16-C17
25	B	504	CLA	O1A-CGA-O2A-C1
25	B	508	CLA	C4-C3-C5-C6
25	B	512	CLA	C3A-C2A-CAA-CBA
25	b	505	CLA	C3A-C2A-CAA-CBA
25	c	505	CLA	C3A-C2A-CAA-CBA
25	c	506	CLA	C3A-C2A-CAA-CBA
25	c	511	CLA	C4-C3-C5-C6
25	G	613	CLA	C2-C3-C5-C6
25	c	511	CLA	C2-C3-C5-C6
34	D	407	PL9	C13-C14-C16-C17
36	G	601	CHL	O1A-CGA-O2A-C1
25	b	504	CLA	O1D-CGD-O2D-CED
29	d	410	LMG	C12-C13-C14-C15
25	c	511	CLA	O1A-CGA-O2A-C1
36	G	619	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	C	503	CLA	C5-C6-C7-C8
32	C	523	LMU	C3-C4-C5-C6
30	C	521	LHG	O9-C7-O7-C5
36	N	309	CHL	C2A-CAA-CBA-CGA
32	C	522	LMU	C4-C5-C6-C7
28	t	102	SQD	O6-C44-C45-C46
29	C	520	LMG	C7-C8-C9-O8
32	C	522	LMU	C9-C10-C11-C12
25	B	503	CLA	C16-C17-C18-C19
25	B	516	CLA	C5-C6-C7-C8
25	G	613	CLA	C4-C3-C5-C6
26	a	404	PHO	C2-C3-C5-C6
36	N	308	CHL	O1D-CGD-O2D-CED
36	G	601	CHL	O1D-CGD-O2D-CED
30	D	409	LHG	O6-C4-C5-O7
25	C	501	CLA	C2B-C3B-CAB-CBB
25	N	313	CLA	C2B-C3B-CAB-CBB
27	a	406	BCR	C23-C24-C25-C30
27	b	517	BCR	C23-C24-C25-C26
32	S	619	LMU	C4-C5-C6-C7
25	d	403	CLA	C8-C10-C11-C12
25	C	504	CLA	C15-C16-C17-C18
30	N	319	LHG	O7-C5-C6-O8
31	Y	301	DGD	O2G-C2G-C3G-O3G
31	C	518	DGD	C1A-C2A-C3A-C4A
25	C	501	CLA	O1A-CGA-O2A-C1
25	C	510	CLA	C4-C3-C5-C6
34	D	407	PL9	C15-C14-C16-C17
34	d	406	PL9	C15-C14-C16-C17
29	B	519	LMG	C37-C38-C39-C40
25	C	510	CLA	C2-C3-C5-C6
30	S	618	LHG	C23-C24-C25-C26
30	b	521	LHG	C23-C24-C25-C26
29	W	201	LMG	O10-C28-O8-C9
25	C	507	CLA	C11-C10-C8-C9
25	C	508	CLA	C6-C7-C8-C9
25	c	507	CLA	C6-C7-C8-C9
26	d	402	PHO	C11-C10-C8-C9
36	Y	303	CHL	C14-C13-C15-C16
36	r	305	CHL	O1D-CGD-O2D-CED
25	S	602	CLA	O2A-C1-C2-C3
25	r	303	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
31	c	515	DGD	C4B-C5B-C6B-C7B
26	D	402	PHO	C2C-C3C-CAC-CBC
30	G	618	LHG	C32-C33-C34-C35
29	d	410	LMG	C33-C34-C35-C36
27	k	101	BCR	C9-C10-C11-C12
25	b	515	CLA	C3-C5-C6-C7
36	Y	303	CHL	CBA-CGA-O2A-C1
30	L	101	LHG	O6-C4-C5-C6
30	a	410	LHG	O6-C4-C5-C6
25	B	508	CLA	C16-C17-C18-C20
25	A	402	CLA	CBD-CGD-O2D-CED
25	B	502	CLA	C13-C15-C16-C17
25	B	502	CLA	C11-C10-C8-C7
25	B	507	CLA	C11-C12-C13-C15
25	C	507	CLA	C11-C10-C8-C7
25	C	508	CLA	C11-C12-C13-C15
25	N	304	CLA	C6-C7-C8-C10
25	N	311	CLA	C12-C13-C15-C16
25	N	314	CLA	C12-C13-C15-C16
25	b	506	CLA	C12-C13-C15-C16
25	b	511	CLA	C6-C7-C8-C10
25	b	515	CLA	C12-C13-C15-C16
25	c	509	CLA	C12-C13-C15-C16
26	D	402	PHO	C6-C7-C8-C10
36	G	619	CHL	C11-C12-C13-C15
36	N	306	CHL	C11-C12-C13-C15
25	A	405	CLA	C5-C6-C7-C8
27	C	515	BCR	C7-C8-C9-C10
27	b	519	BCR	C21-C22-C23-C24
25	b	501	CLA	CBA-CGA-O2A-C1
25	c	502	CLA	CBA-CGA-O2A-C1
25	c	507	CLA	CBA-CGA-O2A-C1
25	B	509	CLA	O1A-CGA-O2A-C1
25	S	604	CLA	O1A-CGA-O2A-C1
25	a	402	CLA	O1A-CGA-O2A-C1
25	c	512	CLA	O1A-CGA-O2A-C1
32	C	522	LMU	C6-C7-C8-C9
25	b	511	CLA	C16-C17-C18-C19
25	B	504	CLA	O1D-CGD-O2D-CED
29	W	201	LMG	O9-C10-O7-C8
30	l	101	LHG	O9-C7-O7-C5
36	N	310	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	Y	306	CLA	O1A-CGA-O2A-C1
25	B	514	CLA	C16-C17-C18-C20
25	A	403	CLA	O1A-CGA-O2A-C1
25	N	305	CLA	O1A-CGA-O2A-C1
36	N	302	CHL	C3-C5-C6-C7
28	t	102	SQD	O47-C7-C8-C9
30	a	411	LHG	O6-C4-C5-O7
25	S	604	CLA	O2A-C1-C2-C3
29	d	410	LMG	C7-C8-C9-O8
30	N	319	LHG	C23-C24-C25-C26
25	C	508	CLA	C13-C15-C16-C17
25	D	404	CLA	C10-C11-C12-C13
25	D	405	CLA	C10-C11-C12-C13
25	Y	314	CLA	C8-C10-C11-C12
35	F	101	HEM	C4C-C3C-CAC-CBC
35	f	101	HEM	C4B-C3B-CAB-CBB
25	C	509	CLA	C4-C3-C5-C6
25	b	503	CLA	C4-C3-C5-C6
36	Y	309	CHL	C2A-CAA-CBA-CGA
25	C	513	CLA	C2-C3-C5-C6
31	W	202	DGD	O1G-C1G-C2G-O2G
25	B	502	CLA	C11-C10-C8-C9
25	B	507	CLA	C11-C12-C13-C14
25	C	513	CLA	C11-C10-C8-C9
25	N	304	CLA	C6-C7-C8-C9
25	N	311	CLA	C14-C13-C15-C16
25	N	314	CLA	C11-C12-C13-C14
25	b	515	CLA	C14-C13-C15-C16
25	c	501	CLA	C14-C13-C15-C16
25	c	509	CLA	C14-C13-C15-C16
26	A	404	PHO	C6-C7-C8-C9
36	G	609	CHL	C11-C10-C8-C9
25	b	508	CLA	C16-C17-C18-C20
36	Y	303	CHL	O1A-CGA-O2A-C1
36	N	306	CHL	C15-C16-C17-C18
25	b	503	CLA	O1D-CGD-O2D-CED
36	N	307	CHL	CBD-CGD-O2D-CED
25	b	511	CLA	C2-C1-O2A-CGA
25	S	614	CLA	O2A-C1-C2-C3
36	Y	310	CHL	O1D-CGD-O2D-CED
25	G	603	CLA	C16-C17-C18-C20
25	c	502	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	c	504	CLA	C11-C12-C13-C14
31	Y	301	DGD	C6A-C7A-C8A-C9A
30	L	101	LHG	C28-C29-C30-C31
25	Y	315	CLA	C4-C3-C5-C6
25	b	510	CLA	C3-C5-C6-C7
29	H	102	LMG	C11-C12-C13-C14
25	G	613	CLA	C2A-CAA-CBA-CGA
25	b	512	CLA	CBA-CGA-O2A-C1
25	B	504	CLA	C16-C17-C18-C19
25	B	508	CLA	C16-C17-C18-C19
25	b	501	CLA	O1A-CGA-O2A-C1
31	Y	301	DGD	CAA-CBA-CCA-CDA
31	W	202	DGD	C3A-C4A-C5A-C6A
36	G	601	CHL	C4C-C3C-CAC-CBC
36	N	306	CHL	O1D-CGD-O2D-CED
31	C	517	DGD	C7B-C8B-C9B-CAB
29	d	409	LMG	C11-C12-C13-C14
25	B	510	CLA	C4B-C3B-CAB-CBB
25	B	511	CLA	C1A-C2A-CAA-CBA
25	C	508	CLA	C1A-C2A-CAA-CBA
25	N	313	CLA	C4B-C3B-CAB-CBB
25	S	614	CLA	C4B-C3B-CAB-CBB
25	b	501	CLA	C4B-C3B-CAB-CBB
25	c	501	CLA	C4B-C3B-CAB-CBB
25	r	308	CLA	C4B-C3B-CAB-CBB
29	H	102	LMG	C29-C28-O8-C9
27	C	514	BCR	C7-C8-C9-C10
25	b	512	CLA	C16-C17-C18-C20
32	S	619	LMU	C2-C3-C4-C5
25	c	502	CLA	O1A-CGA-O2A-C1
25	c	507	CLA	O1A-CGA-O2A-C1
36	Y	303	CHL	CBD-CGD-O2D-CED
25	B	504	CLA	C12-C13-C15-C16
25	B	506	CLA	C6-C7-C8-C10
25	C	506	CLA	C11-C10-C8-C7
25	G	602	CLA	C6-C7-C8-C10
25	G	610	CLA	C11-C10-C8-C7
25	N	314	CLA	C11-C12-C13-C15
25	b	510	CLA	C6-C7-C8-C10
25	b	510	CLA	C11-C12-C13-C15
25	d	403	CLA	C11-C12-C13-C15
25	r	301	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
36	G	609	CHL	C11-C12-C13-C15
36	G	619	CHL	C12-C13-C15-C16
36	N	310	CHL	C11-C12-C13-C15
25	B	512	CLA	C16-C17-C18-C19
25	b	511	CLA	C16-C17-C18-C20
25	A	402	CLA	O1D-CGD-O2D-CED
36	G	609	CHL	O1D-CGD-O2D-CED
29	D	410	LMG	C12-C13-C14-C15
25	c	503	CLA	C3A-C2A-CAA-CBA
25	b	508	CLA	C16-C17-C18-C19
30	C	521	LHG	O6-C4-C5-O7
30	L	101	LHG	O6-C4-C5-O7
36	N	306	CHL	CBD-CGD-O2D-CED
25	C	508	CLA	C11-C12-C13-C14
25	b	506	CLA	C14-C13-C15-C16
25	b	511	CLA	C6-C7-C8-C9
36	N	306	CHL	C11-C12-C13-C14
25	B	508	CLA	C15-C16-C17-C18
27	C	516	BCR	C9-C10-C11-C12
25	N	315	CLA	O1D-CGD-O2D-CED
36	N	307	CHL	O1D-CGD-O2D-CED
25	Y	306	CLA	C8-C10-C11-C12
31	C	517	DGD	C2A-C3A-C4A-C5A
25	S	602	CLA	C1-C2-C3-C4
25	S	610	CLA	C1-C2-C3-C4
25	S	611	CLA	C1-C2-C3-C4
25	S	613	CLA	C1-C2-C3-C4
36	N	309	CHL	C1-C2-C3-C4
28	t	102	SQD	O6-C44-C45-O47
31	c	516	DGD	O2G-C2G-C3G-O3G
30	d	408	LHG	C1-C2-C3-O3
29	d	410	LMG	C19-C20-C21-C22
25	N	312	CLA	O2A-C1-C2-C3
25	a	403	CLA	O2A-C1-C2-C3
25	N	305	CLA	C5-C6-C7-C8
25	b	506	CLA	C8-C10-C11-C12
29	D	410	LMG	C16-C17-C18-C19
36	N	308	CHL	C16-C17-C18-C20
30	N	319	LHG	C4-C5-C6-O8
31	W	202	DGD	O1G-C1G-C2G-C3G
31	Y	301	DGD	C1G-C2G-C3G-O3G
25	Y	305	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
32	C	523	LMU	C5-C6-C7-C8
25	B	504	CLA	CAD-CBD-CGD-O2D
25	B	509	CLA	CAD-CBD-CGD-O2D
25	S	609	CLA	CAD-CBD-CGD-O2D
25	S	614	CLA	CAD-CBD-CGD-O2D
25	b	509	CLA	CAD-CBD-CGD-O2D
25	c	503	CLA	CAD-CBD-CGD-O2D
25	c	513	CLA	CAD-CBD-CGD-O2D
36	Y	303	CHL	O1D-CGD-O2D-CED
25	D	405	CLA	CBA-CGA-O2A-C1
25	b	504	CLA	CBA-CGA-O2A-C1
25	c	509	CLA	C2A-CAA-CBA-CGA
25	c	504	CLA	C10-C11-C12-C13
29	H	102	LMG	O10-C28-O8-C9
31	c	517	DGD	C9B-CAB-CBB-CCB
25	B	503	CLA	CHA-CBD-CGD-O1D
25	B	504	CLA	CAD-CBD-CGD-O1D
25	B	505	CLA	CHA-CBD-CGD-O1D
25	B	505	CLA	CHA-CBD-CGD-O2D
25	B	509	CLA	CAD-CBD-CGD-O1D
25	B	516	CLA	CHA-CBD-CGD-O1D
25	B	516	CLA	CHA-CBD-CGD-O2D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O2D
25	C	512	CLA	CHA-CBD-CGD-O1D
25	C	512	CLA	CHA-CBD-CGD-O2D
25	N	315	CLA	CHA-CBD-CGD-O1D
25	S	609	CLA	CAD-CBD-CGD-O1D
25	S	614	CLA	CAD-CBD-CGD-O1D
25	b	509	CLA	CAD-CBD-CGD-O1D
25	c	503	CLA	CAD-CBD-CGD-O1D
25	c	505	CLA	CAD-CBD-CGD-O1D
25	c	509	CLA	CHA-CBD-CGD-O1D
25	c	509	CLA	CHA-CBD-CGD-O2D
25	c	513	CLA	CAD-CBD-CGD-O1D
30	D	408	LHG	C3-O3-P-O5
30	L	101	LHG	C3-O3-P-O5
30	S	618	LHG	C3-O3-P-O5
30	S	618	LHG	C4-O6-P-O5
30	a	411	LHG	C4-O6-P-O3
30	b	521	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
30	b	521	LHG	C4-O6-P-O5
36	G	601	CHL	CHA-CBD-CGD-O2D
36	G	609	CHL	CHA-CBD-CGD-O2D
36	S	606	CHL	CAD-CBD-CGD-O1D
36	Y	310	CHL	CHA-CBD-CGD-O2D
36	r	305	CHL	CHA-CBD-CGD-O1D
36	r	306	CHL	CHA-CBD-CGD-O2D
25	S	605	CLA	O1A-CGA-O2A-C1
36	G	619	CHL	C4-C3-C5-C6
25	G	612	CLA	C2B-C3B-CAB-CBB
25	S	613	CLA	C2B-C3B-CAB-CBB
25	b	501	CLA	C2B-C3B-CAB-CBB
25	c	501	CLA	C2B-C3B-CAB-CBB
25	r	308	CLA	C2B-C3B-CAB-CBB
30	a	410	LHG	C33-C34-C35-C36
27	b	518	BCR	C7-C8-C9-C34
30	G	618	LHG	C17-C18-C19-C20
25	C	505	CLA	C8-C10-C11-C12
25	B	514	CLA	C16-C17-C18-C19
25	b	512	CLA	O1A-CGA-O2A-C1
31	W	202	DGD	C2B-C3B-C4B-C5B
25	B	512	CLA	O1A-CGA-O2A-C1
25	D	405	CLA	O1A-CGA-O2A-C1
25	B	503	CLA	C10-C11-C12-C13
25	D	401	CLA	C15-C16-C17-C18
25	B	504	CLA	C16-C17-C18-C20
25	b	505	CLA	C8-C10-C11-C12
25	c	501	CLA	C8-C10-C11-C12
25	C	509	CLA	C2-C3-C5-C6
25	c	502	CLA	C16-C17-C18-C19
36	N	308	CHL	C16-C17-C18-C19
25	B	512	CLA	CBA-CGA-O2A-C1
25	S	605	CLA	CBA-CGA-O2A-C1
25	B	509	CLA	C6-C7-C8-C9
25	G	602	CLA	C11-C12-C13-C14
25	Y	304	CLA	C14-C13-C15-C16
25	Y	306	CLA	C6-C7-C8-C9
25	Y	311	CLA	C11-C12-C13-C14
25	b	503	CLA	C11-C12-C13-C14
25	c	509	CLA	C11-C12-C13-C14
36	G	609	CHL	C11-C12-C13-C14
36	G	619	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
36	N	308	CHL	C11-C10-C8-C9
25	G	602	CLA	C11-C12-C13-C15
31	C	518	DGD	O6D-C1D-O3G-C3G
31	C	518	DGD	O6E-C1E-O5D-C6D
25	G	603	CLA	C16-C17-C18-C19
25	B	511	CLA	C13-C15-C16-C17
36	N	310	CHL	C4-C3-C5-C6
25	b	504	CLA	O1A-CGA-O2A-C1
25	C	510	CLA	C13-C15-C16-C17
30	C	521	LHG	O7-C5-C6-O8
36	Y	309	CHL	O1A-CGA-O2A-C1
36	Y	309	CHL	CBA-CGA-O2A-C1
25	B	512	CLA	C16-C17-C18-C20
25	B	501	CLA	C2A-CAA-CBA-CGA
25	b	509	CLA	C2-C1-O2A-CGA
25	c	505	CLA	C2-C1-O2A-CGA
25	A	403	CLA	O2A-C1-C2-C3
25	C	513	CLA	C16-C17-C18-C19
31	c	516	DGD	C1G-C2G-C3G-O3G
25	N	303	CLA	C2A-CAA-CBA-CGA
25	S	602	CLA	C2A-CAA-CBA-CGA
25	Y	304	CLA	C2A-CAA-CBA-CGA
25	b	501	CLA	C2A-CAA-CBA-CGA
25	b	504	CLA	C2A-CAA-CBA-CGA
25	b	515	CLA	C16-C17-C18-C20
25	Y	315	CLA	C2-C3-C5-C6
36	G	619	CHL	C2-C3-C5-C6
25	B	504	CLA	C14-C13-C15-C16
25	C	504	CLA	C14-C13-C15-C16
25	D	404	CLA	C11-C12-C13-C14
25	Y	314	CLA	C11-C10-C8-C9
36	N	308	CHL	C11-C12-C13-C14
25	D	404	CLA	C4B-C3B-CAB-CBB
25	b	510	CLA	C4B-C3B-CAB-CBB
25	A	402	CLA	C15-C16-C17-C18
25	b	507	CLA	C16-C17-C18-C20
25	G	602	CLA	C2A-CAA-CBA-CGA
25	S	611	CLA	O2A-C1-C2-C3
25	d	403	CLA	C3-C5-C6-C7
25	C	510	CLA	C6-C7-C8-C10
25	C	513	CLA	C6-C7-C8-C10
25	Y	314	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	b	512	CLA	C6-C7-C8-C10
25	b	515	CLA	C6-C7-C8-C10
25	c	505	CLA	C11-C12-C13-C15
36	N	308	CHL	C11-C12-C13-C15
36	Y	310	CHL	C12-C13-C15-C16
25	b	512	CLA	C16-C17-C18-C19
25	b	515	CLA	C16-C17-C18-C19
25	C	502	CLA	C13-C15-C16-C17
25	Y	304	CLA	C13-C15-C16-C17
25	c	510	CLA	C10-C11-C12-C13
25	B	504	CLA	C3A-C2A-CAA-CBA
25	N	305	CLA	C3A-C2A-CAA-CBA
36	N	308	CHL	C4-C3-C5-C6
29	D	410	LMG	C18-C19-C20-C21
26	a	404	PHO	C5-C6-C7-C8
27	B	517	BCR	C20-C21-C22-C37
27	v	101	BCR	C20-C21-C22-C37
38	G	617	NEX	C39-C29-C30-C31
38	N	318	NEX	C39-C29-C30-C31
38	S	617	NEX	C39-C29-C30-C31
38	Y	318	NEX	C39-C29-C30-C31
38	r	310	NEX	C39-C29-C30-C31
28	A	407	SQD	O49-C7-C8-C9
25	b	515	CLA	C13-C15-C16-C17
31	Y	301	DGD	CDA-CEA-CFA-CGA
25	N	303	CLA	C8-C10-C11-C12
36	N	306	CHL	C5-C6-C7-C8
30	Y	319	LHG	C27-C28-C29-C30
25	b	504	CLA	C5-C6-C7-C8
25	c	502	CLA	C4-C3-C5-C6
30	d	407	LHG	C7-C8-C9-C10
25	Y	305	CLA	C2-C3-C5-C6
36	N	310	CHL	C2-C3-C5-C6
30	b	521	LHG	C1-C2-C3-O3
25	N	314	CLA	C10-C11-C12-C13
25	S	610	CLA	C2A-CAA-CBA-CGA
25	B	505	CLA	C6-C7-C8-C9
25	C	513	CLA	C6-C7-C8-C9
25	G	610	CLA	C11-C12-C13-C14
25	b	504	CLA	C11-C10-C8-C9
25	b	510	CLA	C6-C7-C8-C9
25	b	515	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	c	508	CLA	C11-C12-C13-C14
25	d	403	CLA	C11-C12-C13-C14
36	G	609	CHL	C14-C13-C15-C16
36	N	302	CHL	C11-C10-C8-C9
36	N	310	CHL	C11-C12-C13-C14
25	B	505	CLA	C13-C15-C16-C17
36	r	306	CHL	C1A-C2A-CAA-CBA
30	B	520	LHG	C31-C32-C33-C34
31	c	515	DGD	C4E-C5E-C6E-O5E
25	G	602	CLA	C8-C10-C11-C12
25	Y	305	CLA	C2A-CAA-CBA-CGA
25	N	305	CLA	C1A-C2A-CAA-CBA
25	r	307	CLA	C1A-C2A-CAA-CBA
27	B	517	BCR	C20-C21-C22-C23
27	v	101	BCR	C20-C21-C22-C23
38	G	617	NEX	C28-C29-C30-C31
38	N	318	NEX	C28-C29-C30-C31
38	S	617	NEX	C28-C29-C30-C31
38	Y	318	NEX	C28-C29-C30-C31
38	r	310	NEX	C28-C29-C30-C31
25	C	513	CLA	C16-C17-C18-C20
29	b	520	LMG	C17-C18-C19-C20
31	c	516	DGD	CCB-CDB-CEB-CFB
25	D	404	CLA	C2B-C3B-CAB-CBB
25	S	614	CLA	C2B-C3B-CAB-CBB
25	b	510	CLA	C2B-C3B-CAB-CBB
27	V	101	BCR	C23-C24-C25-C26
27	V	101	BCR	C23-C24-C25-C30
25	B	508	CLA	O1D-CGD-O2D-CED
25	Y	313	CLA	C10-C11-C12-C13
25	C	508	CLA	CBD-CGD-O2D-CED
25	a	405	CLA	C4-C3-C5-C6
25	b	507	CLA	C4-C3-C5-C6
25	B	508	CLA	CBD-CGD-O2D-CED
25	C	502	CLA	C11-C12-C13-C15
25	D	404	CLA	C11-C12-C13-C15
25	N	303	CLA	C6-C7-C8-C10
25	Y	311	CLA	C11-C12-C13-C15
25	b	501	CLA	C6-C7-C8-C10
25	b	511	CLA	C11-C12-C13-C15
25	c	507	CLA	C11-C12-C13-C15
25	c	508	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
36	G	609	CHL	C12-C13-C15-C16
36	N	302	CHL	C11-C10-C8-C7
25	B	508	CLA	C2A-CAA-CBA-CGA
25	c	501	CLA	C2A-CAA-CBA-CGA
25	d	401	CLA	C2A-CAA-CBA-CGA
30	Y	319	LHG	O7-C5-C6-O8
36	r	306	CHL	CAA-CBA-CGA-O2A
25	Y	304	CLA	C10-C11-C12-C13
30	D	408	LHG	C14-C15-C16-C17
25	Y	313	CLA	C15-C16-C17-C18
25	d	403	CLA	C10-C11-C12-C13
36	N	307	CHL	CAA-CBA-CGA-O2A
25	c	502	CLA	C2-C3-C5-C6
25	N	313	CLA	CAA-CBA-CGA-O2A
25	a	402	CLA	C15-C16-C17-C18
25	B	503	CLA	C2A-CAA-CBA-CGA
36	N	307	CHL	CAA-CBA-CGA-O1A
25	B	505	CLA	C11-C12-C13-C14
25	B	510	CLA	C14-C13-C15-C16
25	C	510	CLA	C6-C7-C8-C9
25	G	603	CLA	C11-C12-C13-C14
25	b	512	CLA	C6-C7-C8-C9
26	D	402	PHO	C15-C16-C17-C18
25	d	401	CLA	C2C-C3C-CAC-CBC
25	b	503	CLA	C2-C3-C5-C6
25	N	311	CLA	C8-C10-C11-C12
36	N	310	CHL	C10-C11-C12-C13
36	G	607	CHL	O2A-C1-C2-C3
36	N	309	CHL	O2A-C1-C2-C3
36	Y	309	CHL	O2A-C1-C2-C3
30	G	618	LHG	C16-C17-C18-C19
30	Y	319	LHG	C4-C5-C6-O8
25	G	604	CLA	C1A-C2A-CAA-CBA
36	S	608	CHL	C2A-CAA-CBA-CGA
25	b	501	CLA	C16-C17-C18-C20
25	C	505	CLA	C13-C15-C16-C17
30	N	319	LHG	C11-C10-C9-C8
30	G	618	LHG	O6-C4-C5-O7
29	c	518	LMG	C11-C12-C13-C14
25	B	501	CLA	C4B-C3B-CAB-CBB
25	c	507	CLA	C4B-C3B-CAB-CBB
25	S	612	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	b	501	CLA	C16-C17-C18-C19
36	G	601	CHL	CHA-CBD-CGD-O1D
36	Y	303	CHL	CHA-CBD-CGD-O1D
36	Y	303	CHL	CHA-CBD-CGD-O2D
36	Y	310	CHL	CHA-CBD-CGD-O1D
25	c	501	CLA	C15-C16-C17-C18
25	N	313	CLA	CAA-CBA-CGA-O1A
25	C	509	CLA	C13-C15-C16-C17
30	G	618	LHG	O6-C4-C5-C6
31	Y	301	DGD	O6D-C5D-C6D-O5D
25	a	402	CLA	C16-C17-C18-C20
25	C	508	CLA	O1D-CGD-O2D-CED
25	c	501	CLA	C10-C11-C12-C13
25	G	610	CLA	C11-C12-C13-C15
25	c	507	CLA	C12-C13-C15-C16
36	Y	307	CHL	CAA-CBA-CGA-O2A
25	C	502	CLA	C8-C10-C11-C12
25	C	506	CLA	C11-C10-C8-C9
25	C	508	CLA	C11-C10-C8-C9
25	D	405	CLA	C11-C10-C8-C9
25	G	602	CLA	C6-C7-C8-C9
25	G	610	CLA	C11-C10-C8-C9
25	b	501	CLA	C14-C13-C15-C16
25	b	505	CLA	C11-C12-C13-C14
25	c	502	CLA	C14-C13-C15-C16
25	c	506	CLA	C14-C13-C15-C16
25	c	508	CLA	C6-C7-C8-C9
25	Y	314	CLA	O1A-CGA-O2A-C1
31	Y	301	DGD	C5D-C6D-O5D-C1E
36	Y	308	CHL	CAA-CBA-CGA-O2A
25	c	510	CLA	C2-C1-O2A-CGA
31	c	515	DGD	O6D-C5D-C6D-O5D
25	r	307	CLA	C3A-C2A-CAA-CBA
36	N	308	CHL	C3A-C2A-CAA-CBA
25	S	612	CLA	CAA-CBA-CGA-O1A
36	r	306	CHL	CAA-CBA-CGA-O1A
25	C	511	CLA	O1A-CGA-O2A-C1
29	c	518	LMG	C12-C13-C14-C15
25	b	516	CLA	CAA-CBA-CGA-O2A
30	b	521	LHG	C25-C26-C27-C28
25	C	504	CLA	C13-C15-C16-C17
36	S	607	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
36	Y	310	CHL	C3C-C2C-CMC-OMC
25	r	307	CLA	CAA-CBA-CGA-O2A
32	C	523	LMU	C1-C2-C3-C4
25	c	506	CLA	C10-C11-C12-C13
30	a	411	LHG	C25-C26-C27-C28
25	C	511	CLA	CBA-CGA-O2A-C1
29	d	410	LMG	C29-C28-O8-C9
31	C	519	DGD	C7A-C8A-C9A-CAA
25	c	504	CLA	C11-C12-C13-C15
38	S	617	NEX	O24-C26-C27-C28
38	Y	318	NEX	O24-C26-C27-C28
38	r	310	NEX	O24-C26-C27-C28
36	Y	307	CHL	CAA-CBA-CGA-O1A
36	Y	308	CHL	CAA-CBA-CGA-O1A
25	G	611	CLA	CAA-CBA-CGA-O2A
30	D	408	LHG	C33-C34-C35-C36
25	N	303	CLA	O1A-CGA-O2A-C1
32	C	522	LMU	O1'-C1-C2-C3
31	Y	301	DGD	C2A-C3A-C4A-C5A
25	N	303	CLA	CBA-CGA-O2A-C1
25	c	506	CLA	CAA-CBA-CGA-O2A
25	a	402	CLA	C16-C17-C18-C19
30	l	101	LHG	C14-C15-C16-C17
25	A	402	CLA	C13-C15-C16-C17
25	G	611	CLA	CAA-CBA-CGA-O1A
25	b	516	CLA	CAA-CBA-CGA-O1A
25	Y	314	CLA	CBA-CGA-O2A-C1
36	N	308	CHL	O1A-CGA-O2A-C1
30	d	408	LHG	C23-C24-C25-C26
36	S	608	CHL	CAA-CBA-CGA-O2A
30	S	618	LHG	C11-C12-C13-C14
25	c	506	CLA	C3-C5-C6-C7
25	b	510	CLA	C11-C10-C8-C9
25	c	502	CLA	C11-C10-C8-C9
25	c	506	CLA	C11-C12-C13-C14
25	r	301	CLA	C6-C7-C8-C9
26	D	402	PHO	C6-C7-C8-C9
36	G	619	CHL	C11-C12-C13-C14
25	N	305	CLA	C16-C17-C18-C19
25	d	401	CLA	CAA-CBA-CGA-O2A
29	D	410	LMG	O7-C10-C11-C12
25	c	503	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	D	409	LHG	O6-C4-C5-C6
30	D	408	LHG	C12-C13-C14-C15
29	d	410	LMG	O10-C28-O8-C9
25	b	509	CLA	CAA-CBA-CGA-O2A
29	C	520	LMG	C35-C36-C37-C38
25	B	505	CLA	C11-C12-C13-C15
25	B	510	CLA	C12-C13-C15-C16
25	B	512	CLA	C11-C10-C8-C7
25	C	504	CLA	C11-C12-C13-C15
25	D	405	CLA	C11-C10-C8-C7
25	G	603	CLA	C11-C12-C13-C15
25	Y	305	CLA	C12-C13-C15-C16
25	Y	312	CLA	C11-C10-C8-C7
25	b	505	CLA	C11-C12-C13-C15
25	b	515	CLA	C11-C10-C8-C7
25	c	502	CLA	C12-C13-C15-C16
25	c	508	CLA	C6-C7-C8-C10
25	c	511	CLA	C6-C7-C8-C10
36	G	609	CHL	C6-C7-C8-C10
25	c	507	CLA	C2B-C3B-CAB-CBB
27	b	517	BCR	C23-C24-C25-C30
27	d	405	BCR	C23-C24-C25-C30
25	d	403	CLA	CAA-CBA-CGA-O2A
36	N	310	CHL	C2-C1-O2A-CGA
25	Y	304	CLA	O1A-CGA-O2A-C1
25	S	610	CLA	O2A-C1-C2-C3
25	Y	311	CLA	C16-C17-C18-C20
29	d	410	LMG	C32-C33-C34-C35
25	b	511	CLA	CAA-CBA-CGA-O2A
29	C	520	LMG	O7-C10-C11-C12
25	c	510	CLA	C4-C3-C5-C6
25	Y	305	CLA	CAA-CBA-CGA-O2A
25	c	510	CLA	C2-C3-C5-C6
25	N	311	CLA	C2A-CAA-CBA-CGA
25	b	503	CLA	C2A-CAA-CBA-CGA
25	b	509	CLA	C2A-CAA-CBA-CGA
30	D	409	LHG	O8-C23-C24-C25
31	c	517	DGD	O2G-C1B-C2B-C3B
36	N	308	CHL	CAA-CBA-CGA-O2A
34	D	407	PL9	C4-C3-C7-C8
30	B	520	LHG	C9-C10-C11-C12
25	Y	304	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	G	603	CLA	CAA-CBA-CGA-O2A
30	Y	319	LHG	C23-C24-C25-C26
25	B	502	CLA	C3-C5-C6-C7
28	a	407	SQD	C4-C5-C6-S
36	Y	310	CHL	C4-C3-C5-C6
25	b	512	CLA	CAA-CBA-CGA-O2A
25	c	508	CLA	CAA-CBA-CGA-O2A
36	N	308	CHL	C2-C3-C5-C6
25	B	512	CLA	C2A-CAA-CBA-CGA
30	Y	319	LHG	C11-C10-C9-C8
25	r	307	CLA	CAA-CBA-CGA-O1A
25	b	514	CLA	CBD-CGD-O2D-CED
25	b	511	CLA	C8-C10-C11-C12
25	B	512	CLA	C11-C10-C8-C9
25	N	303	CLA	C6-C7-C8-C9
25	N	314	CLA	C14-C13-C15-C16
25	b	501	CLA	C6-C7-C8-C9
25	b	505	CLA	C6-C7-C8-C9
25	b	501	CLA	CAA-CBA-CGA-O2A
25	b	502	CLA	CAA-CBA-CGA-O2A
25	c	503	CLA	CAA-CBA-CGA-O2A
31	W	202	DGD	O2G-C1B-C2B-C3B
25	B	510	CLA	C1A-C2A-CAA-CBA
25	B	516	CLA	C4B-C3B-CAB-CBB
25	S	605	CLA	C4B-C3B-CAB-CBB
36	N	308	CHL	CBA-CGA-O2A-C1
25	B	503	CLA	C4-C3-C5-C6
25	C	513	CLA	C13-C15-C16-C17
25	c	509	CLA	CAA-CBA-CGA-O2A
25	b	507	CLA	C2-C3-C5-C6
30	D	408	LHG	C13-C14-C15-C16
27	b	518	BCR	C7-C8-C9-C10
25	B	506	CLA	C13-C15-C16-C17
26	D	402	PHO	C16-C17-C18-C19
28	t	102	SQD	O49-C7-C8-C9
25	a	402	CLA	CAA-CBA-CGA-O2A
25	b	507	CLA	CAA-CBA-CGA-O2A
30	a	410	LHG	O8-C23-C24-C25
31	C	518	DGD	O1G-C1A-C2A-C3A
25	d	403	CLA	C16-C17-C18-C19
25	b	510	CLA	CAA-CBA-CGA-O2A
36	N	306	CHL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	B	510	CLA	C2-C1-O2A-CGA
25	B	513	CLA	C2-C1-O2A-CGA
25	C	505	CLA	C2-C1-O2A-CGA
25	b	506	CLA	C2-C1-O2A-CGA
25	c	507	CLA	C2-C1-O2A-CGA
25	B	504	CLA	C6-C7-C8-C10
25	D	405	CLA	C11-C12-C13-C15
25	D	405	CLA	C12-C13-C15-C16
25	b	507	CLA	C11-C12-C13-C15
25	b	510	CLA	C11-C10-C8-C7
36	N	306	CHL	C6-C7-C8-C10
30	Y	319	LHG	C30-C31-C32-C33
30	S	618	LHG	C13-C14-C15-C16
25	G	610	CLA	C2A-CAA-CBA-CGA
25	Y	312	CLA	C16-C17-C18-C19
29	d	410	LMG	O7-C10-C11-C12
25	C	502	CLA	O1A-CGA-O2A-C1
25	B	502	CLA	C4-C3-C5-C6
25	B	510	CLA	C3A-C2A-CAA-CBA
25	r	303	CLA	C3A-C2A-CAA-CBA
34	d	406	PL9	C45-C44-C46-C47
25	C	505	CLA	C16-C17-C18-C19
32	C	522	LMU	C7-C8-C9-C10
25	b	511	CLA	CAA-CBA-CGA-O1A
25	d	403	CLA	CAA-CBA-CGA-O1A
28	a	407	SQD	C10-C11-C12-C13
36	N	308	CHL	C5-C6-C7-C8
25	b	514	CLA	O1D-CGD-O2D-CED
25	B	501	CLA	CAA-CBA-CGA-O2A
25	Y	313	CLA	CAA-CBA-CGA-O2A
25	Y	305	CLA	CAA-CBA-CGA-O1A
25	b	509	CLA	CAA-CBA-CGA-O1A
31	c	517	DGD	O1B-C1B-C2B-C3B
25	c	503	CLA	CBA-CGA-O2A-C1
25	C	502	CLA	C11-C12-C13-C14
25	G	603	CLA	C6-C7-C8-C9
25	Y	305	CLA	C14-C13-C15-C16
25	b	507	CLA	C11-C12-C13-C14
25	c	505	CLA	C11-C12-C13-C14
36	G	601	CHL	C11-C10-C8-C9
30	a	410	LHG	C29-C30-C31-C32
25	c	503	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	c	506	CLA	CAA-CBA-CGA-O1A
25	c	508	CLA	CAA-CBA-CGA-O1A
36	N	308	CHL	CAA-CBA-CGA-O1A
30	Y	319	LHG	C17-C18-C19-C20
36	Y	310	CHL	C5-C6-C7-C8
31	c	517	DGD	C7A-C8A-C9A-CAA
25	B	511	CLA	C2-C3-C5-C6
25	a	402	CLA	CAA-CBA-CGA-O1A
25	b	501	CLA	CAA-CBA-CGA-O1A
25	b	510	CLA	CAA-CBA-CGA-O1A
25	b	512	CLA	CAA-CBA-CGA-O1A
25	d	401	CLA	CAA-CBA-CGA-O1A
30	B	520	LHG	C7-C8-C9-C10
25	b	505	CLA	CAA-CBA-CGA-O2A
29	D	410	LMG	O9-C10-C11-C12
30	D	409	LHG	O10-C23-C24-C25
36	S	608	CHL	CAA-CBA-CGA-O1A
29	d	410	LMG	C36-C37-C38-C39
25	B	514	CLA	C13-C15-C16-C17
25	c	503	CLA	C13-C15-C16-C17
29	C	520	LMG	O9-C10-C11-C12
25	c	510	CLA	CAA-CBA-CGA-O2A
36	N	306	CHL	CAA-CBA-CGA-O2A
30	Y	319	LHG	C26-C27-C28-C29
30	a	411	LHG	C4-C5-C6-O8
25	G	603	CLA	CAA-CBA-CGA-O1A
25	b	502	CLA	CAA-CBA-CGA-O1A
30	a	410	LHG	O10-C23-C24-C25
25	b	512	CLA	C8-C10-C11-C12
25	c	505	CLA	C10-C11-C12-C13
31	C	517	DGD	O1G-C1A-C2A-C3A
31	Y	301	DGD	O1G-C1A-C2A-C3A
31	C	518	DGD	O1A-C1A-C2A-C3A
29	W	201	LMG	C28-C29-C30-C31
25	C	505	CLA	CAD-CBD-CGD-O2D
25	C	513	CLA	CAD-CBD-CGD-O2D
25	a	405	CLA	CAD-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O2D
25	c	509	CLA	CAA-CBA-CGA-O1A
25	c	502	CLA	C5-C6-C7-C8
31	c	516	DGD	O6D-C5D-C6D-O5D
25	C	502	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	N	314	CLA	C2-C1-O2A-CGA
25	b	514	CLA	CAA-CBA-CGA-O2A
25	C	501	CLA	CAA-CBA-CGA-O2A
25	N	305	CLA	C16-C17-C18-C20
25	r	301	CLA	C2A-CAA-CBA-CGA
36	N	308	CHL	C12-C13-C15-C16
30	D	408	LHG	O8-C23-C24-C25
25	C	501	CLA	CAA-CBA-CGA-O1A
25	B	510	CLA	CAA-CBA-CGA-O2A
30	l	101	LHG	O8-C23-C24-C25
29	d	409	LMG	C29-C30-C31-C32
36	N	302	CHL	C8-C10-C11-C12
30	D	408	LHG	O10-C23-C24-C25

There are no ring outliers.

152 monomers are involved in 298 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	510	CLA	1	0
36	r	304	CHL	1	0
25	C	506	CLA	1	0
25	S	602	CLA	2	0
27	A	406	BCR	5	0
27	a	406	BCR	2	0
25	B	508	CLA	1	0
25	S	605	CLA	3	0
27	B	517	BCR	4	0
36	G	609	CHL	1	0
25	b	501	CLA	1	0
25	B	504	CLA	2	0
36	r	306	CHL	2	0
36	N	308	CHL	2	0
25	B	502	CLA	3	0
37	N	317	LUT	3	0
31	c	517	DGD	1	0
25	b	507	CLA	1	0
25	B	514	CLA	2	0
35	F	101	HEM	5	0
39	Y	302	XAT	6	0
25	B	513	CLA	1	0
36	r	305	CHL	1	0
30	d	407	LHG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	505	CLA	1	0
26	a	404	PHO	2	0
25	a	402	CLA	1	0
38	r	310	NEX	3	0
36	N	310	CHL	2	0
25	C	512	CLA	1	0
27	C	515	BCR	5	0
30	B	520	LHG	1	0
38	Y	318	NEX	4	0
39	r	309	XAT	3	0
30	S	618	LHG	2	0
36	N	309	CHL	2	0
25	r	308	CLA	1	0
25	N	303	CLA	1	0
27	b	519	BCR	2	0
36	G	605	CHL	1	0
25	c	504	CLA	1	0
25	B	503	CLA	1	0
25	d	403	CLA	2	0
25	b	502	CLA	3	0
25	S	604	CLA	1	0
28	A	407	SQD	2	0
25	C	511	CLA	2	0
25	C	504	CLA	2	0
25	c	512	CLA	1	0
25	B	516	CLA	2	0
33	a	409	BCT	2	0
37	S	615	LUT	4	0
25	N	312	CLA	1	0
25	S	609	CLA	2	0
25	c	509	CLA	1	0
35	f	101	HEM	4	0
36	Y	310	CHL	3	0
25	a	405	CLA	1	0
27	c	514	BCR	4	0
27	h	101	BCR	5	0
37	G	616	LUT	3	0
27	V	101	BCR	4	0
25	d	401	CLA	2	0
36	S	606	CHL	4	0
27	H	101	BCR	5	0
25	D	405	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	G	602	CLA	1	0
25	b	505	CLA	2	0
27	D	406	BCR	3	0
31	Y	301	DGD	1	0
30	l	101	LHG	4	0
36	S	607	CHL	2	0
25	C	502	CLA	3	0
25	N	305	CLA	3	0
25	B	509	CLA	1	0
37	Y	317	LUT	4	0
25	b	516	CLA	1	0
37	N	316	LUT	1	0
25	b	503	CLA	1	0
37	G	615	LUT	1	0
37	S	616	LUT	4	0
25	r	307	CLA	2	0
25	D	404	CLA	2	0
26	D	402	PHO	1	0
32	C	522	LMU	3	0
25	b	504	CLA	2	0
27	C	516	BCR	3	0
30	L	101	LHG	1	0
37	Y	316	LUT	2	0
38	N	318	NEX	1	0
25	b	510	CLA	2	0
25	c	506	CLA	4	0
27	C	514	BCR	4	0
38	G	617	NEX	3	0
27	b	518	BCR	1	0
26	d	402	PHO	1	0
25	c	502	CLA	1	0
25	C	501	CLA	1	0
36	S	601	CHL	2	0
25	G	611	CLA	1	0
36	Y	309	CHL	2	0
25	B	512	CLA	1	0
29	d	409	LMG	2	0
30	Y	319	LHG	2	0
34	d	406	PL9	1	0
36	G	601	CHL	1	0
30	D	408	LHG	2	0
36	G	608	CHL	3	0

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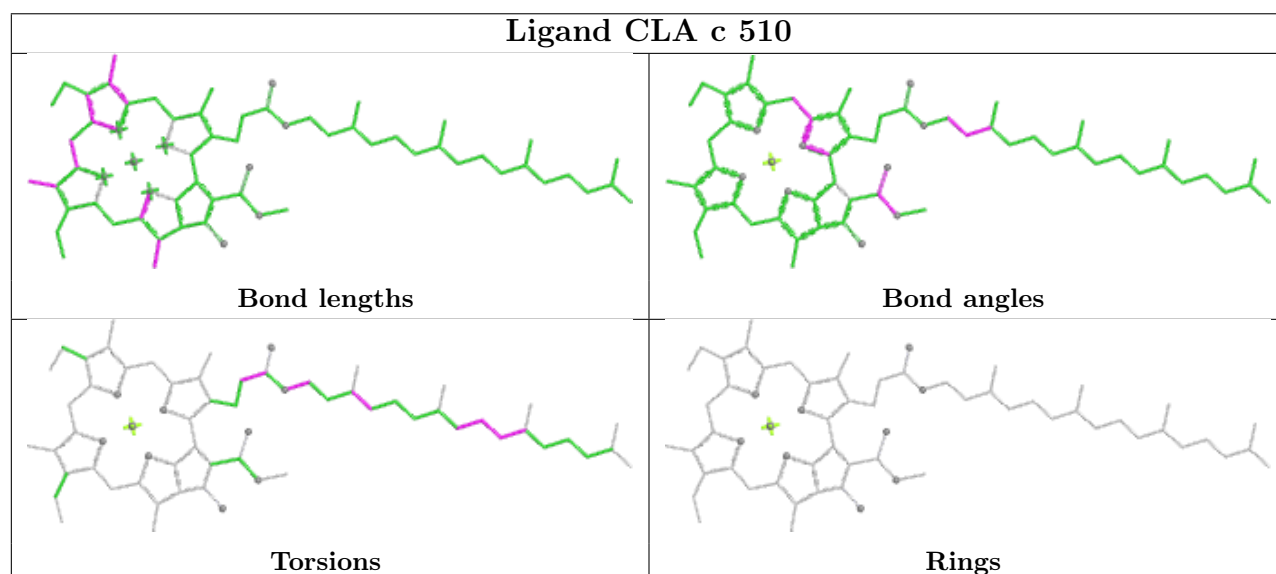
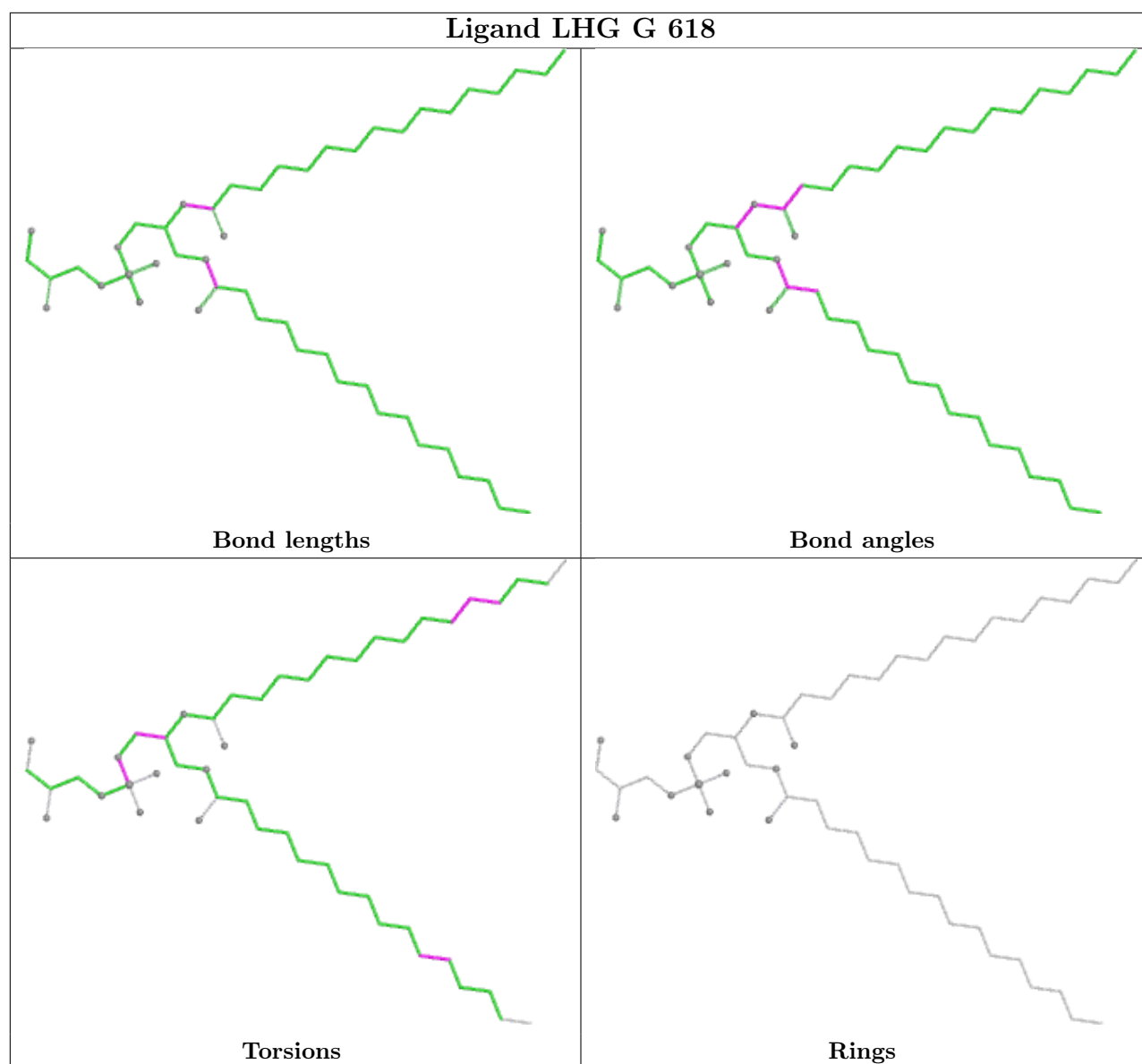
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	508	CLA	1	0
27	z	101	BCR	3	0
39	N	301	XAT	3	0
36	S	608	CHL	2	0
25	b	511	CLA	2	0
29	H	102	LMG	2	0
27	B	518	BCR	2	0
25	A	402	CLA	1	0
30	b	521	LHG	1	0
31	C	517	DGD	1	0
27	k	101	BCR	4	0
31	c	515	DGD	2	0
25	b	506	CLA	4	0
36	N	302	CHL	2	0
27	d	405	BCR	2	0
29	W	201	LMG	1	0
38	S	617	NEX	1	0
30	N	319	LHG	1	0
25	c	501	CLA	2	0
29	B	519	LMG	2	0
27	t	101	BCR	3	0
39	G	620	XAT	2	0
26	A	404	PHO	2	0
30	d	408	LHG	1	0
36	N	306	CHL	4	0
25	B	515	CLA	1	0
36	Y	303	CHL	2	0
25	B	501	CLA	2	0
25	N	313	CLA	1	0
27	v	101	BCR	8	0
25	C	513	CLA	1	0
36	Y	308	CHL	1	0
30	a	410	LHG	1	0
25	c	511	CLA	2	0
27	b	517	BCR	1	0
36	G	607	CHL	1	0
36	G	606	CHL	2	0
36	N	307	CHL	1	0
25	S	610	CLA	1	0
25	B	506	CLA	4	0
25	c	508	CLA	2	0
29	d	410	LMG	2	0

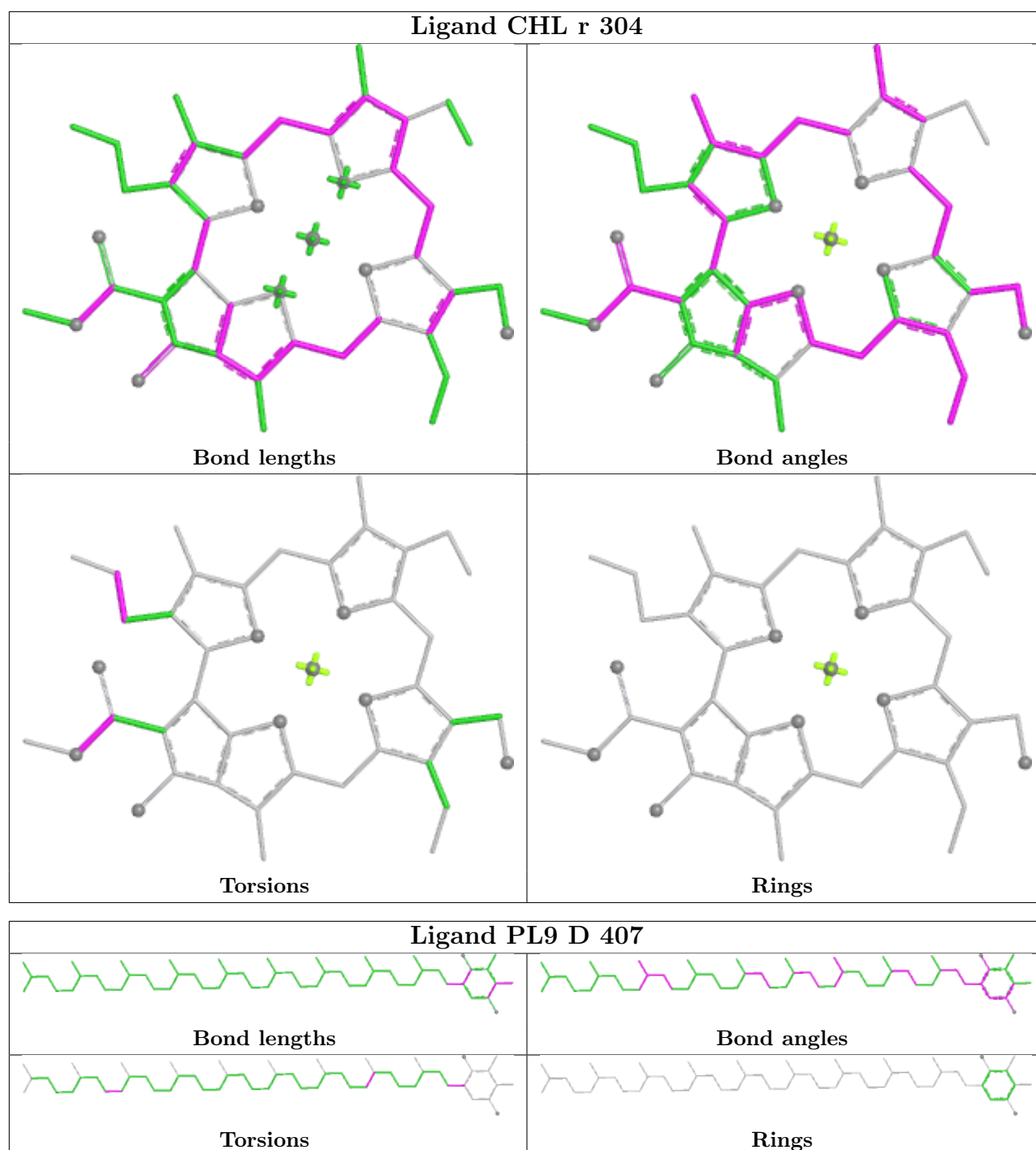
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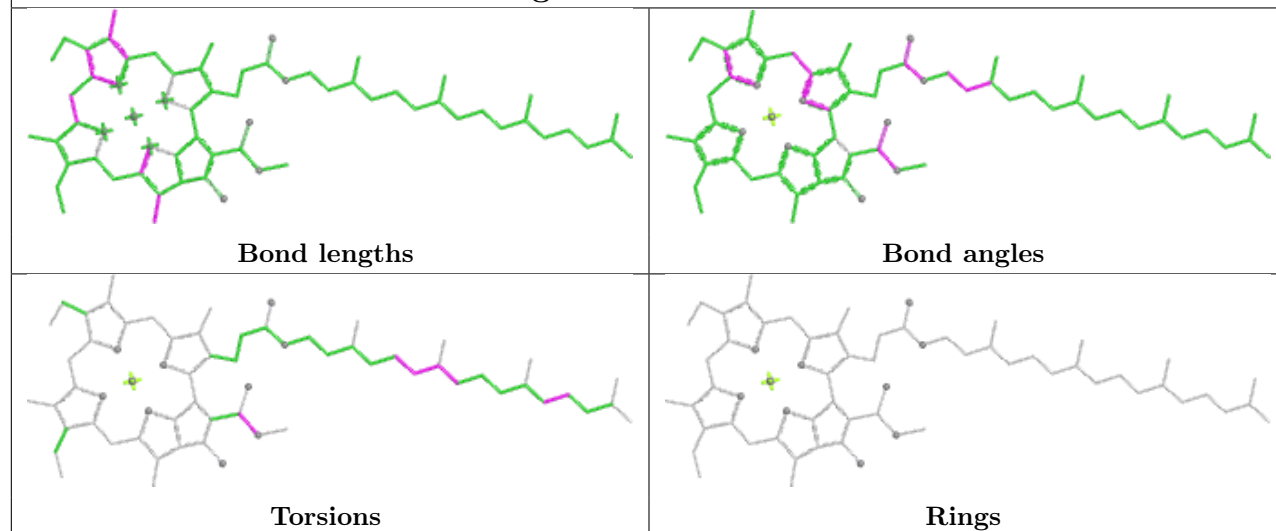
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	509	CLA	1	0
25	b	512	CLA	2	0

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.

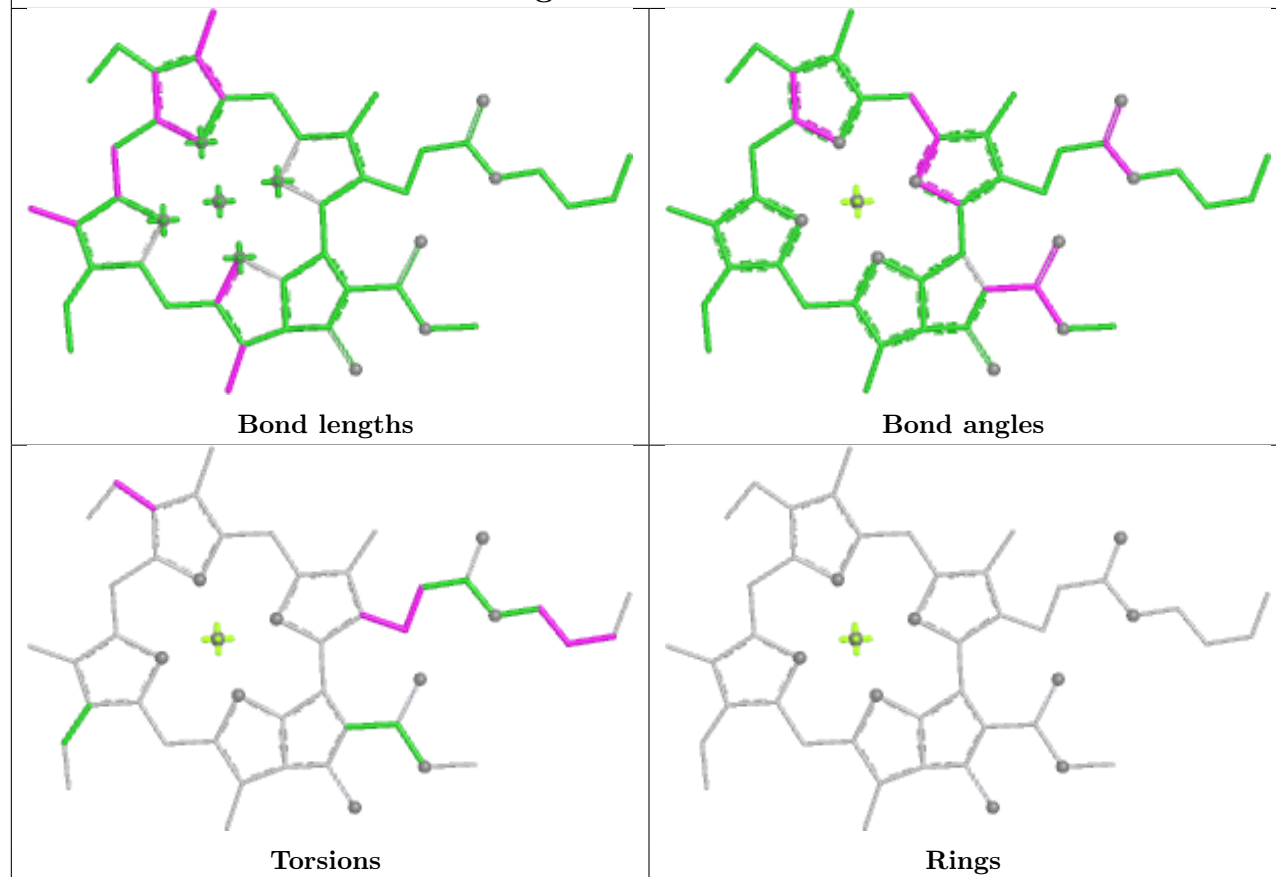


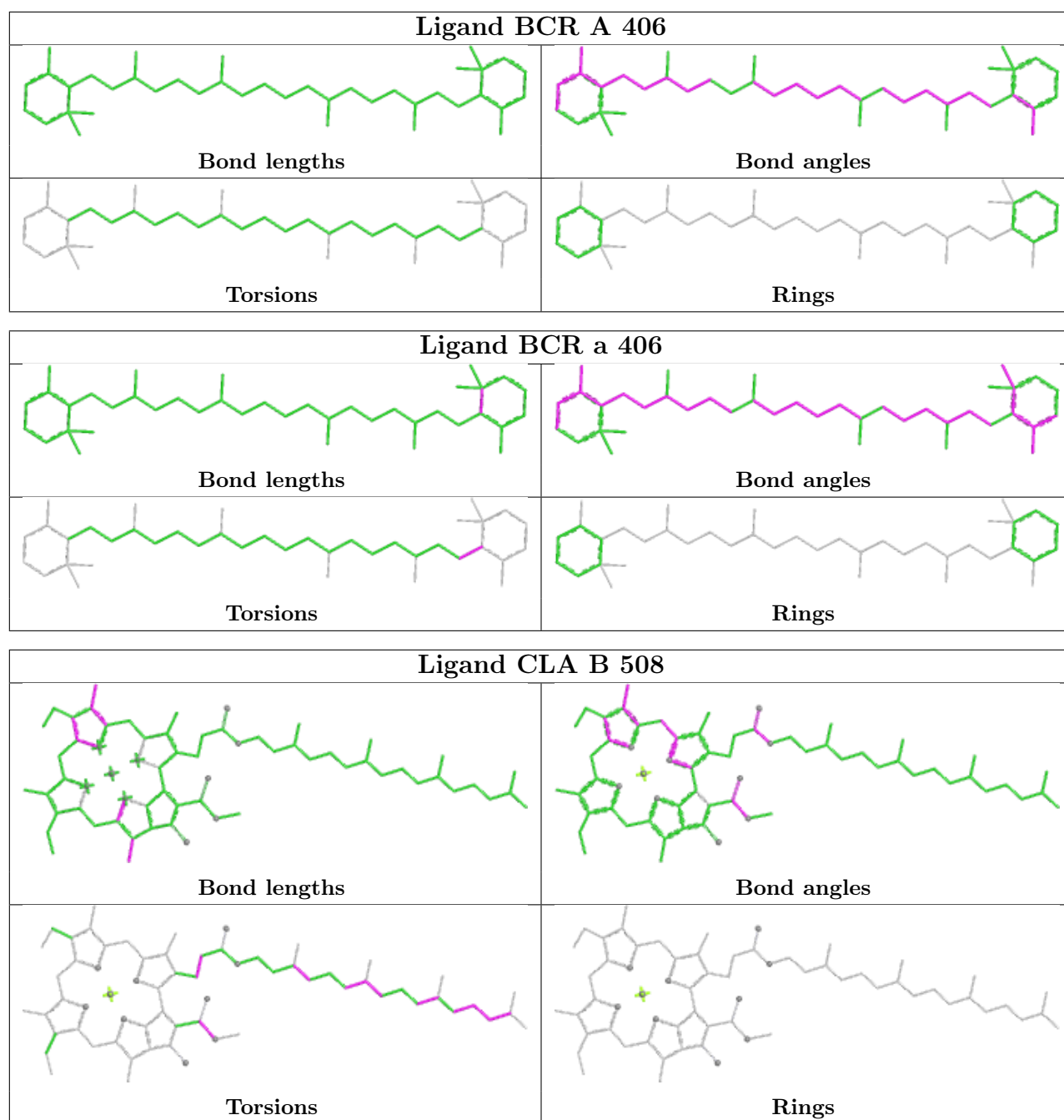


Ligand CLA C 506

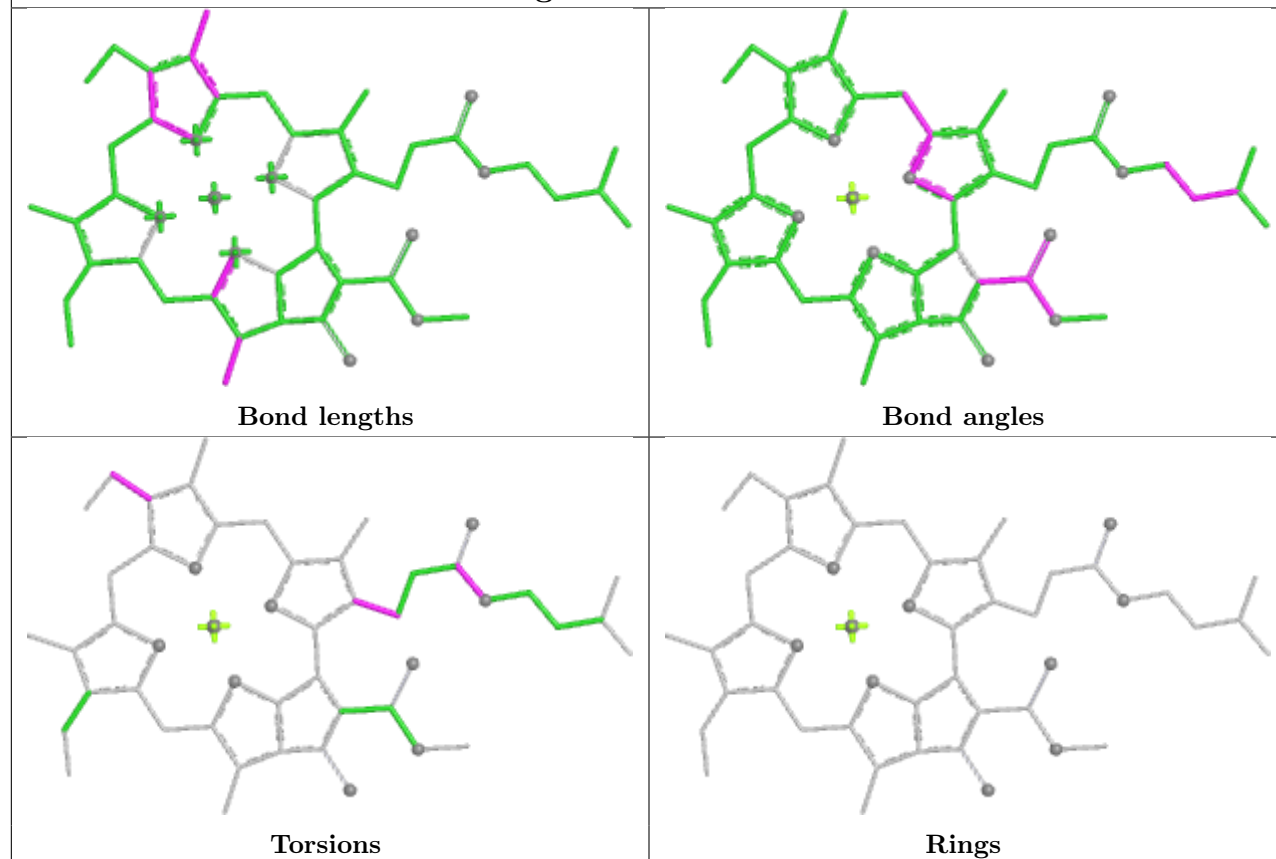


Ligand CLA S 602

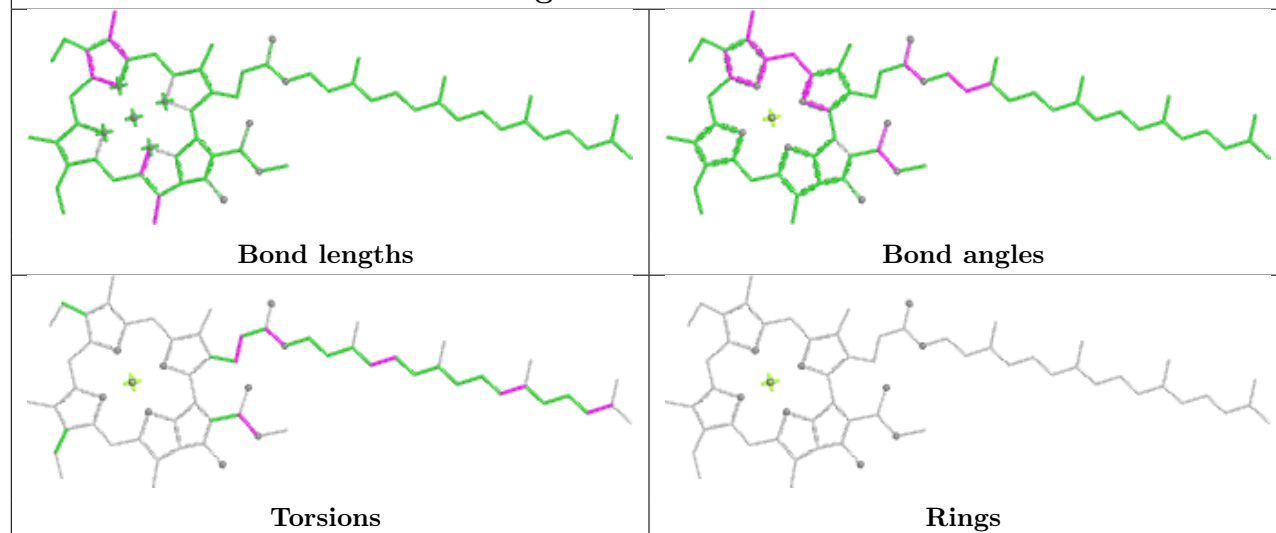


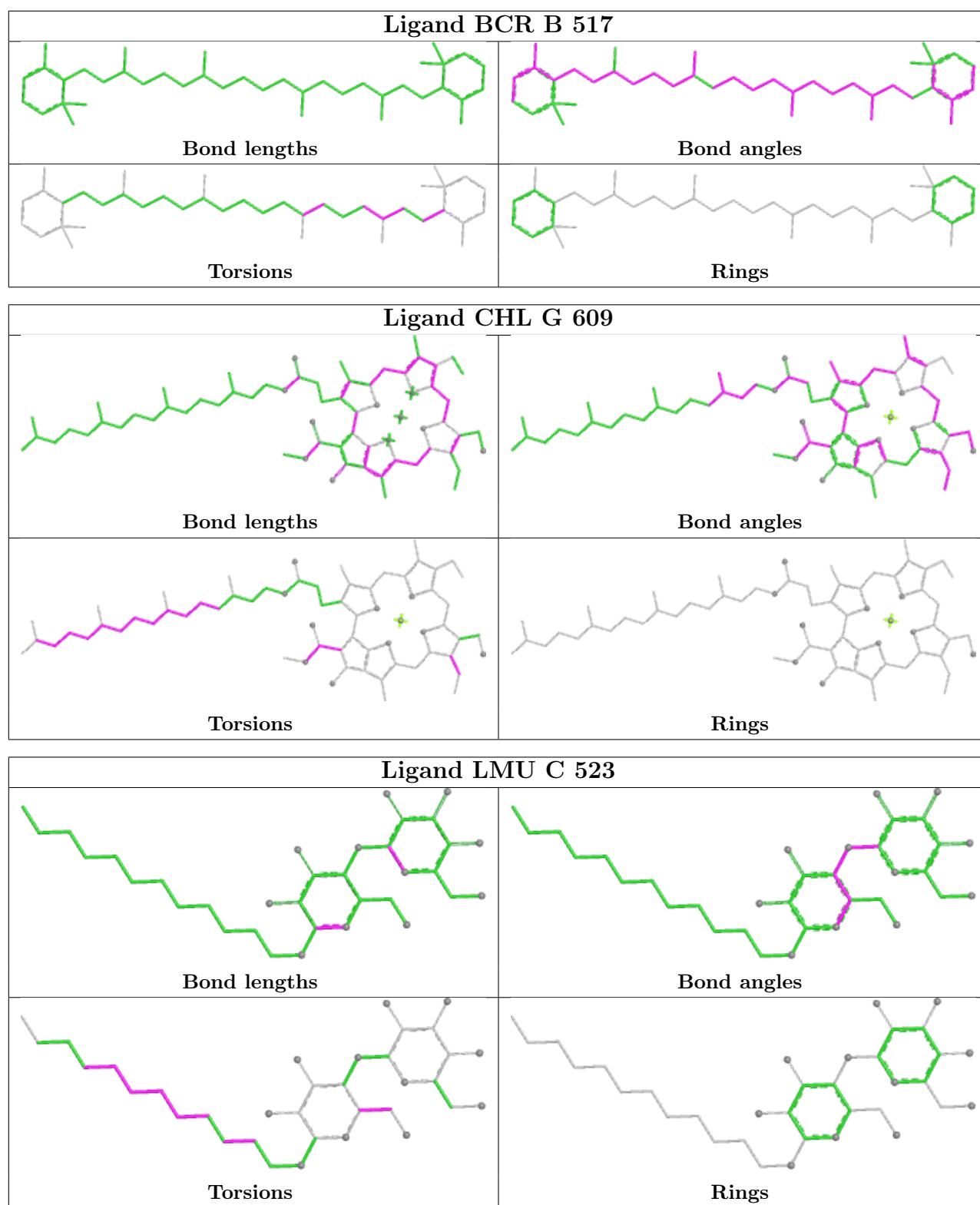


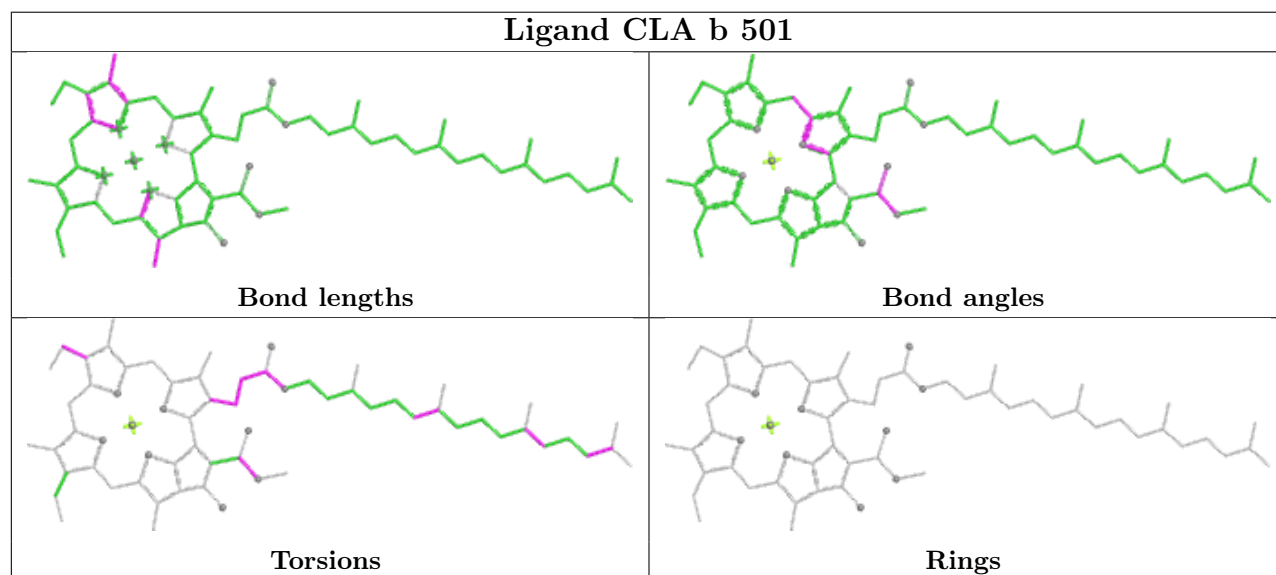
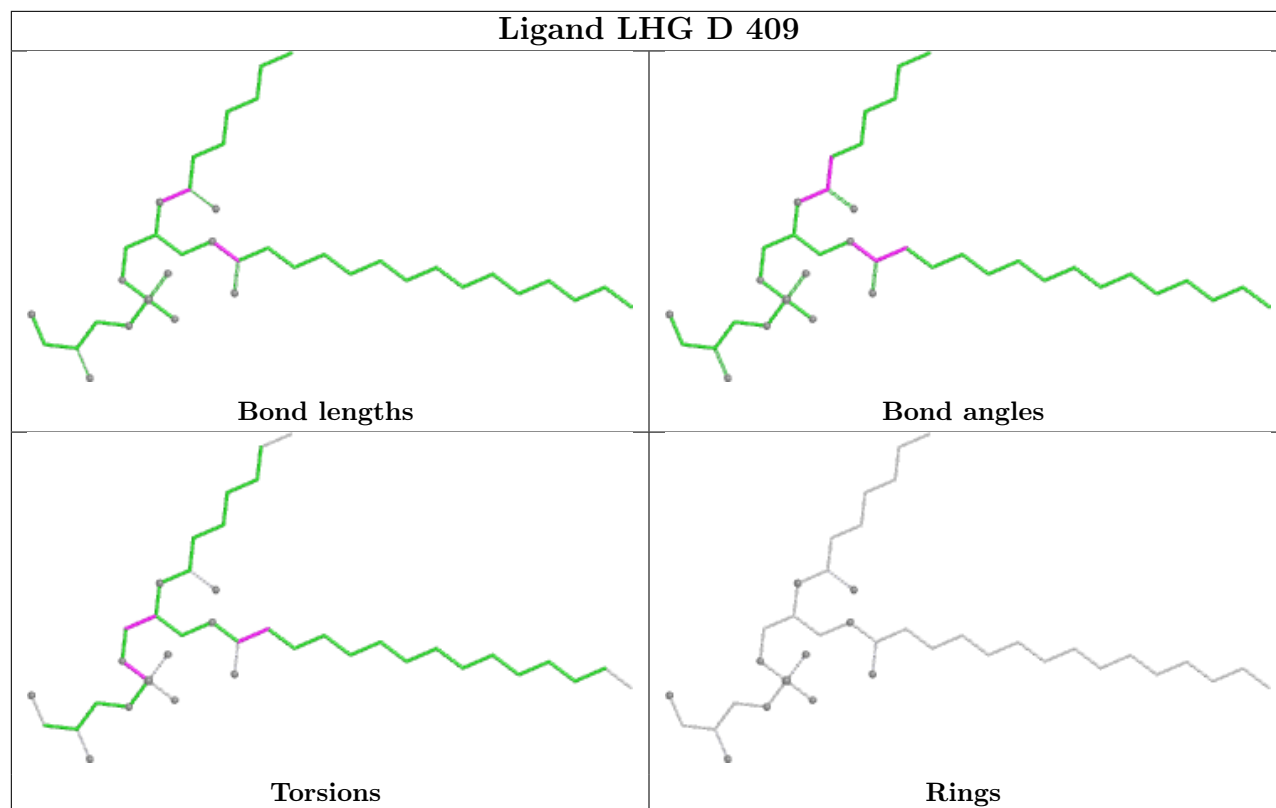
Ligand CLA S 605



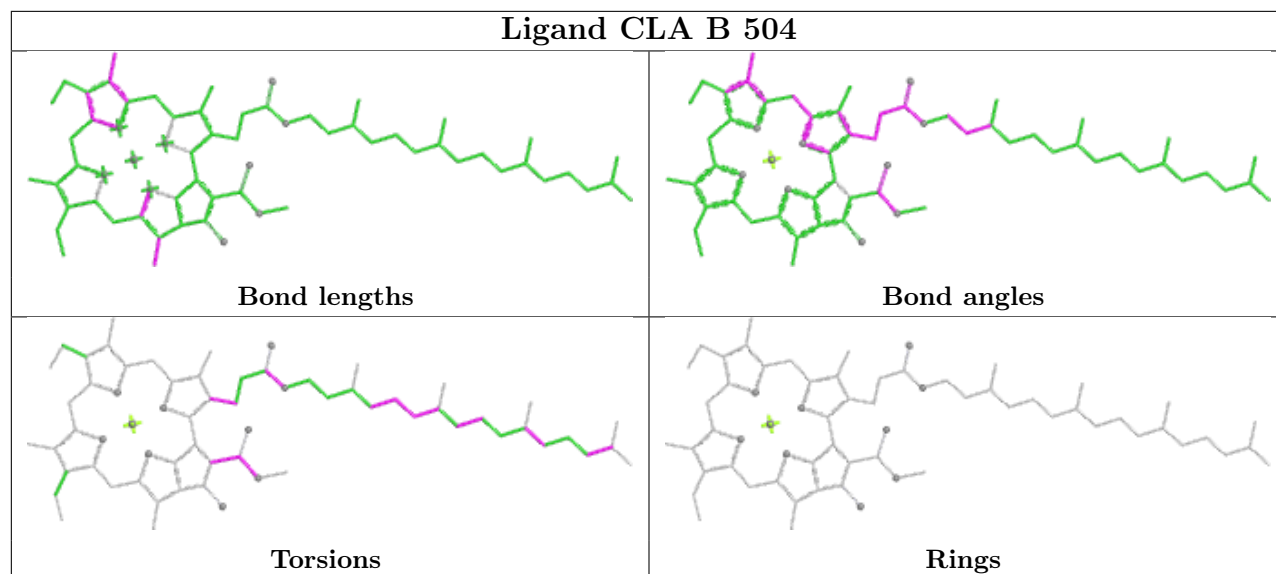
Ligand CLA b 508



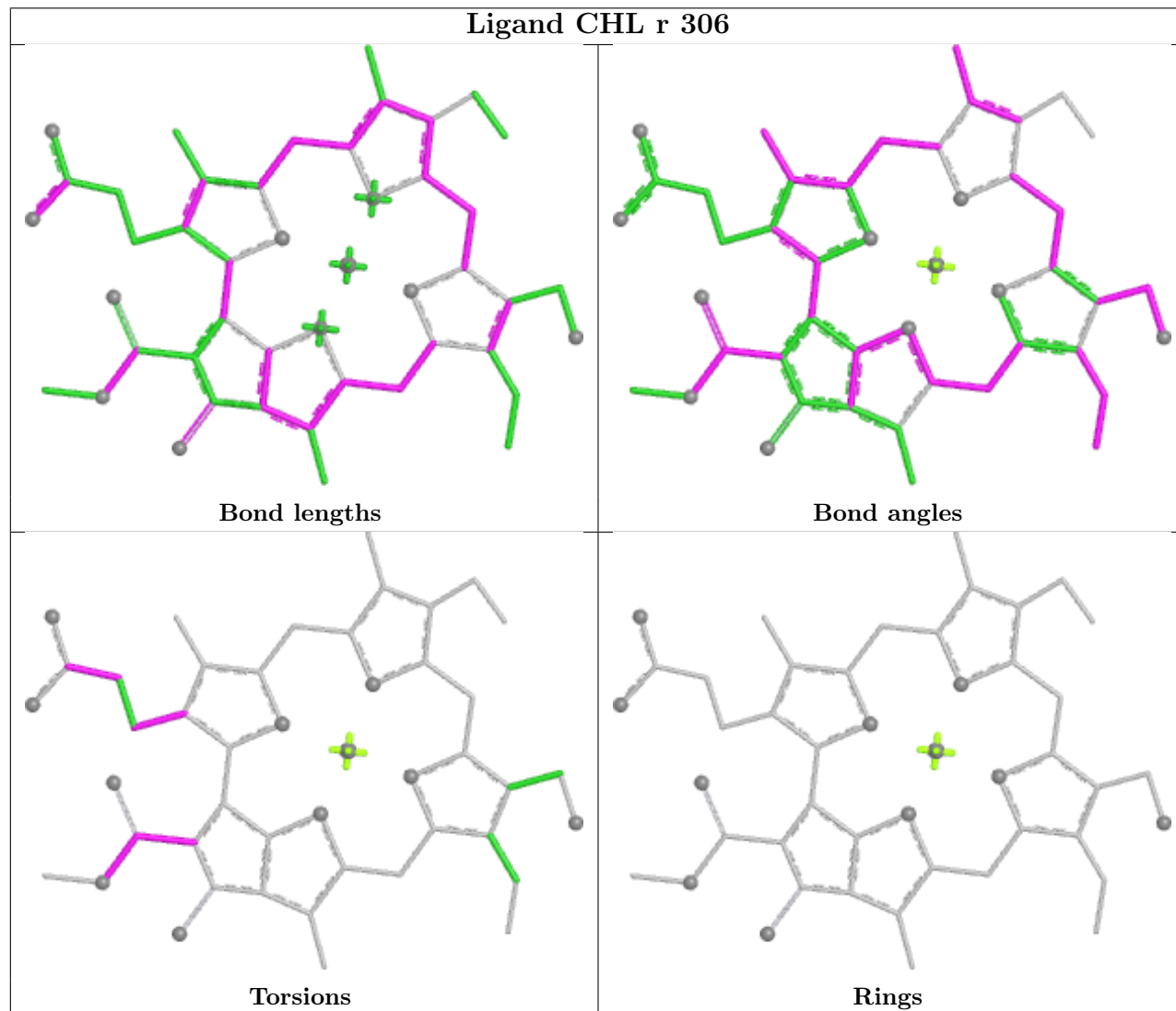


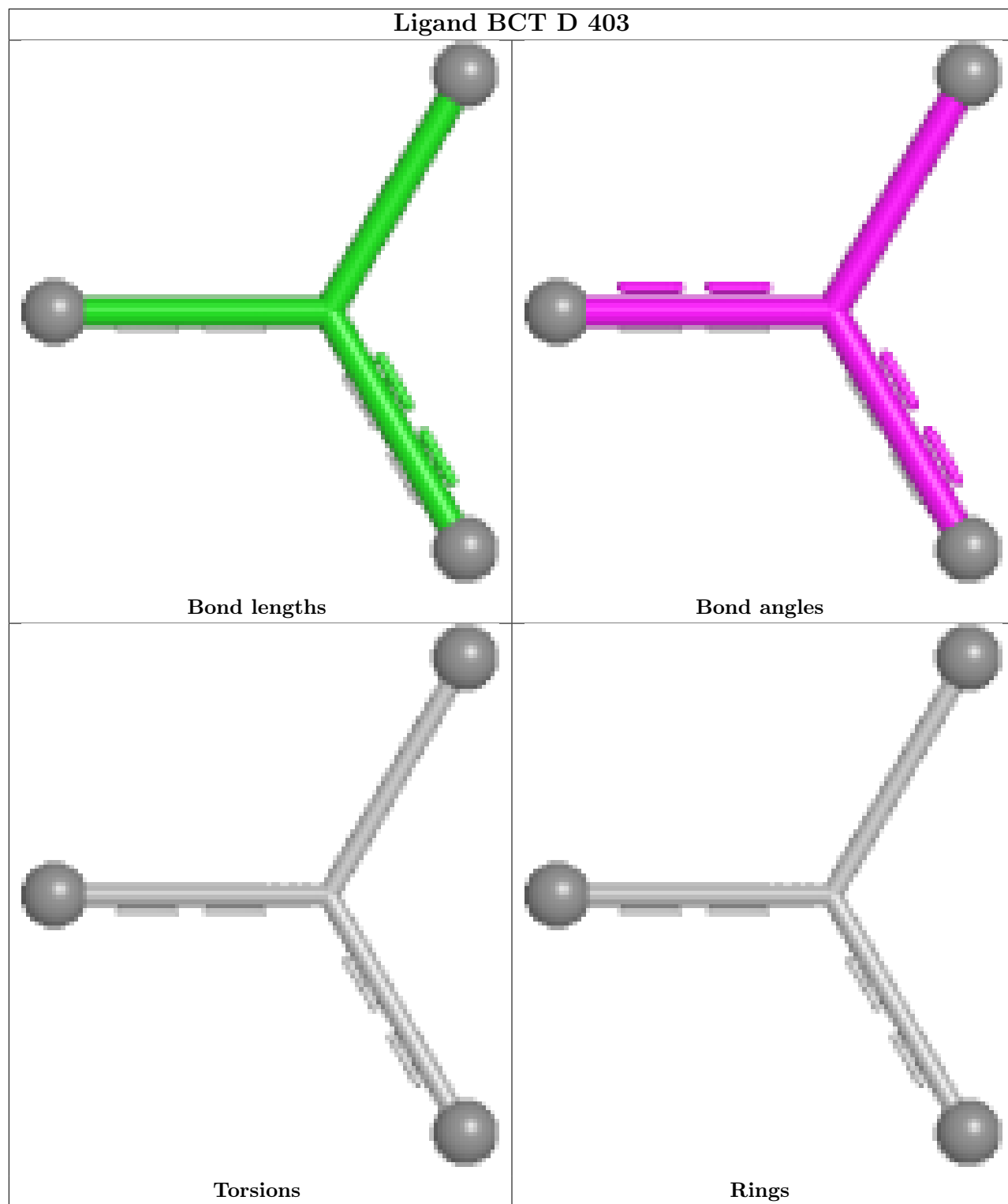


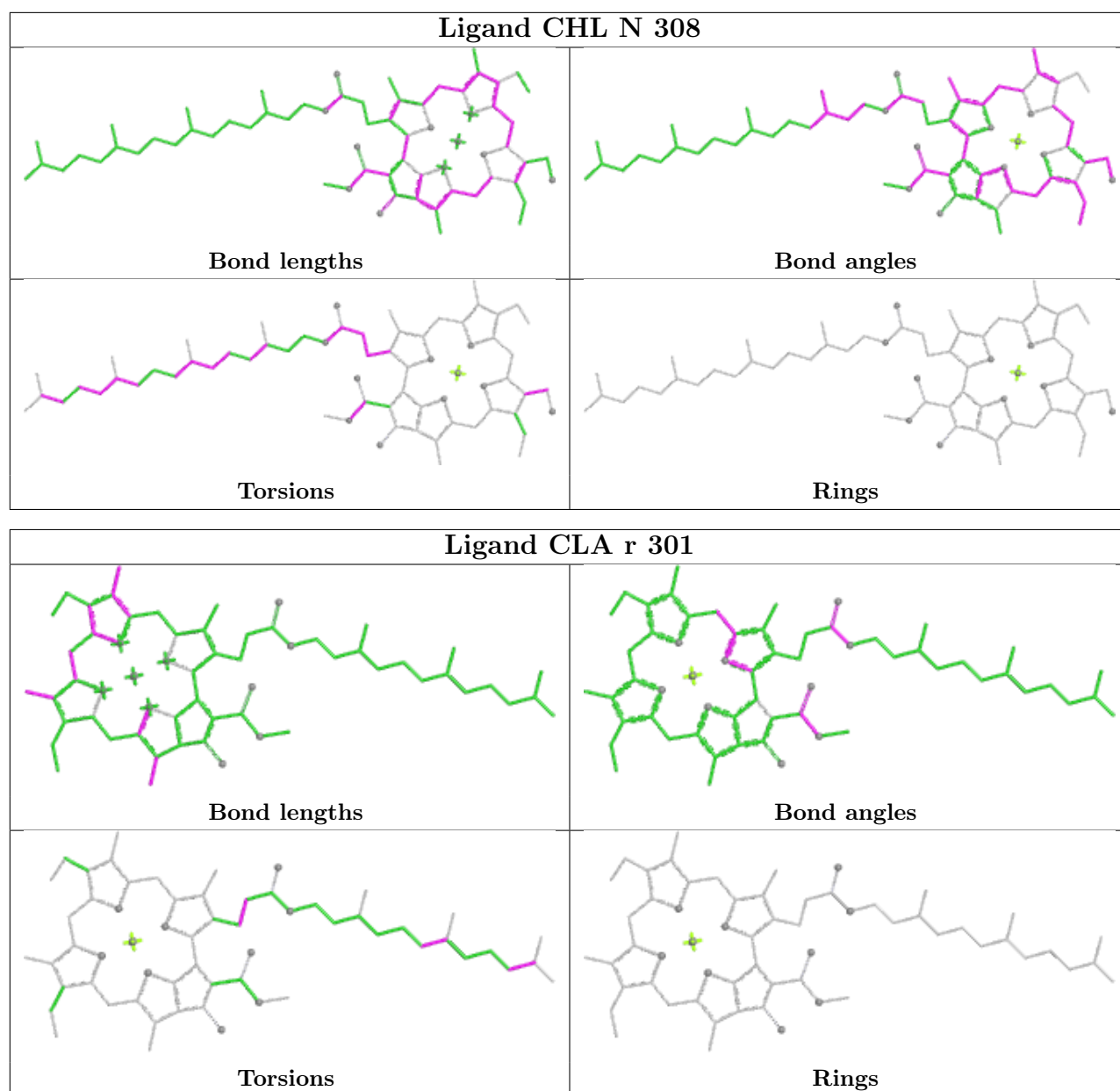
Ligand CLA B 504

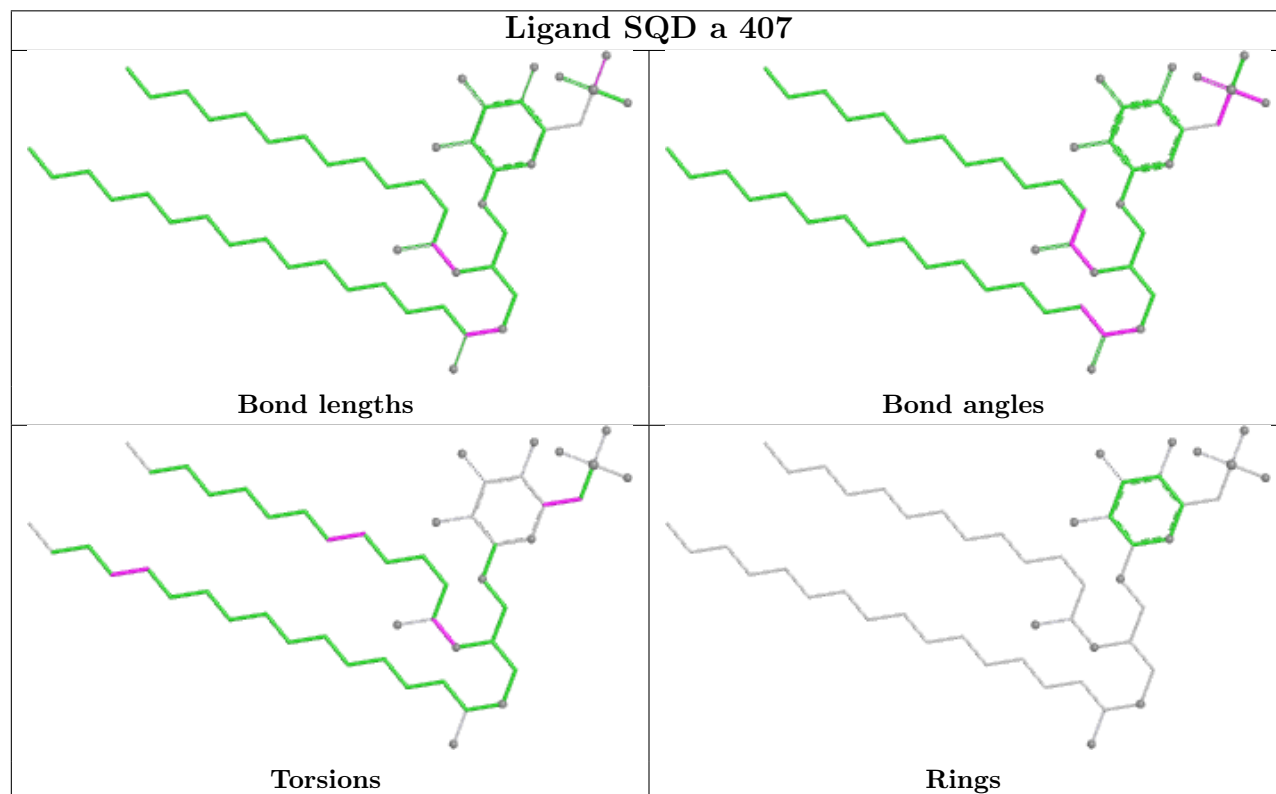
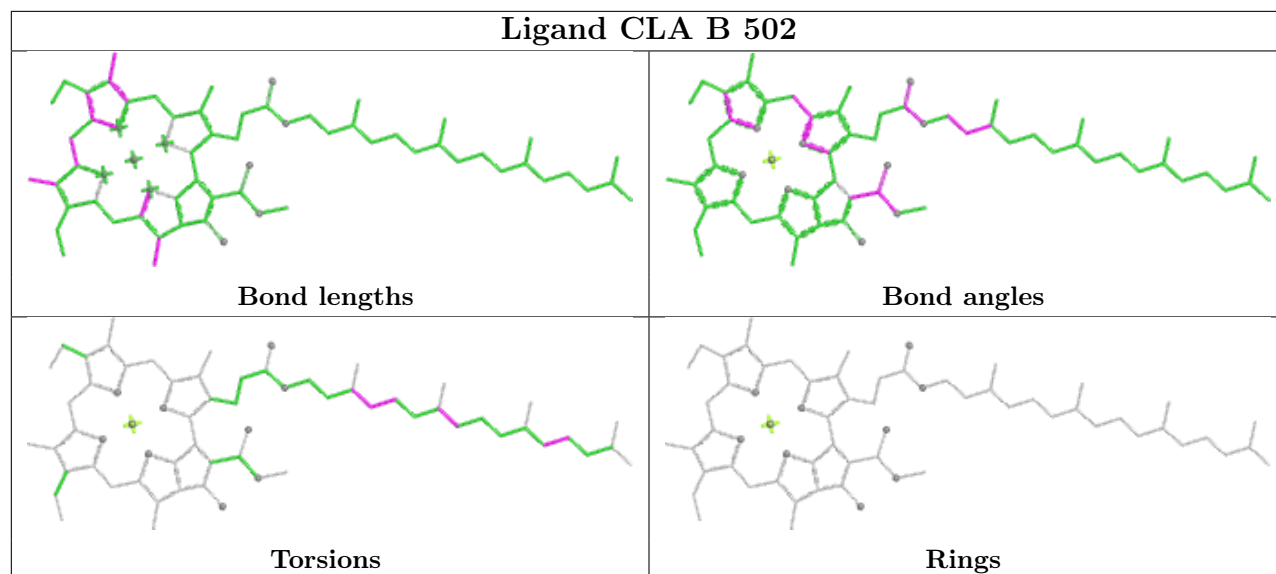


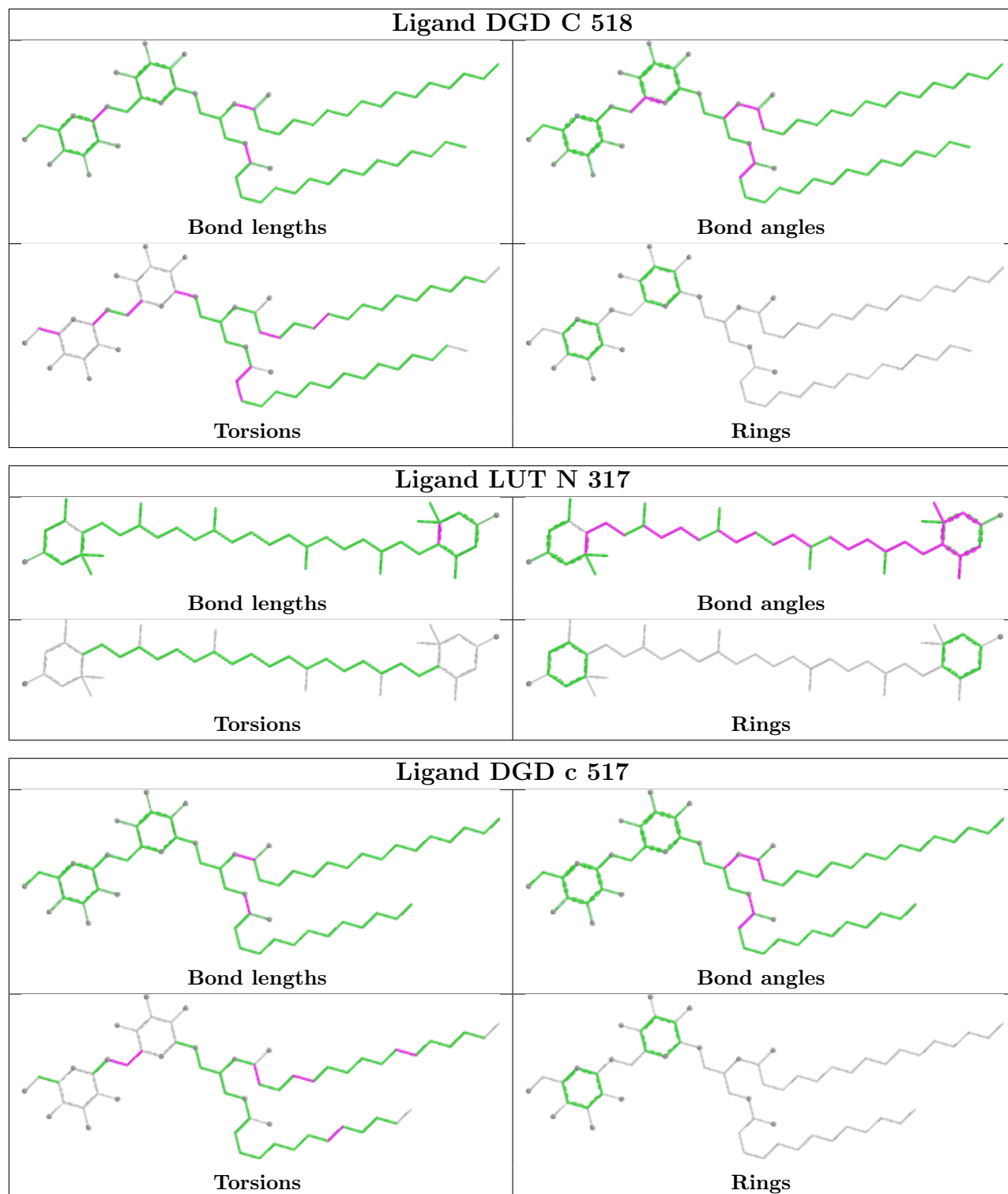
Ligand CHL r 306



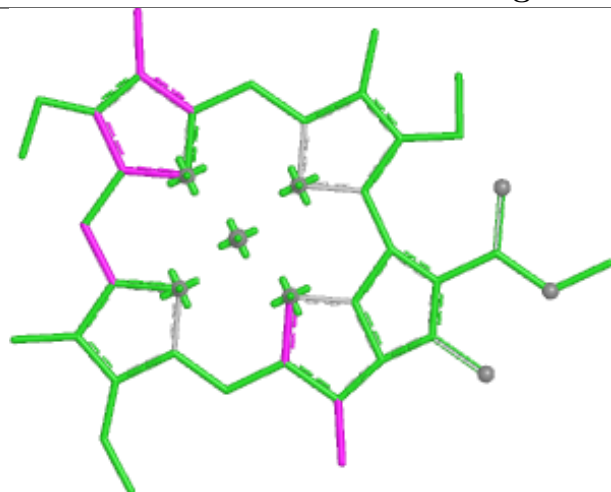








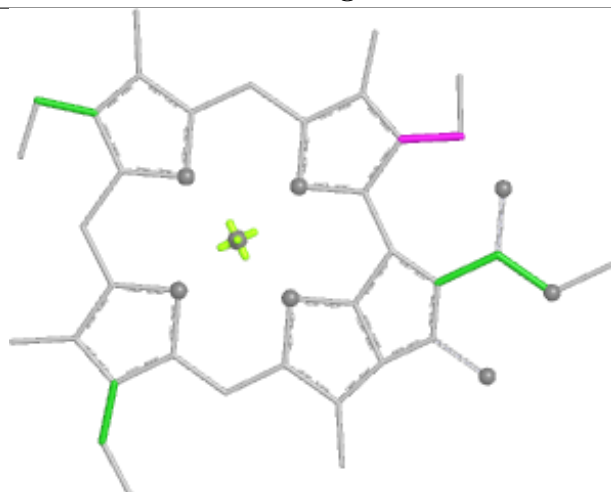
Ligand CLA G 604



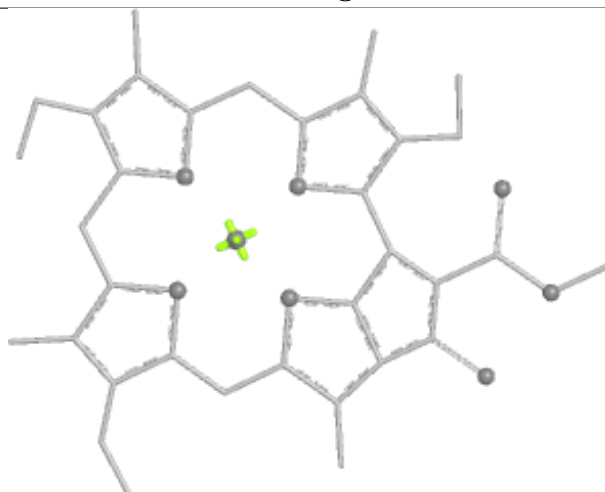
Bond lengths



Bond angles

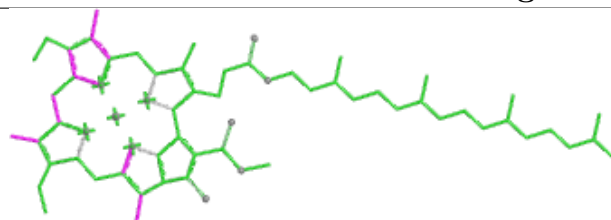


Torsions

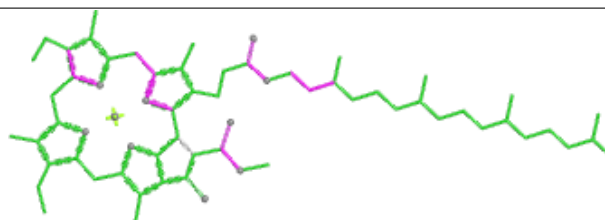


Rings

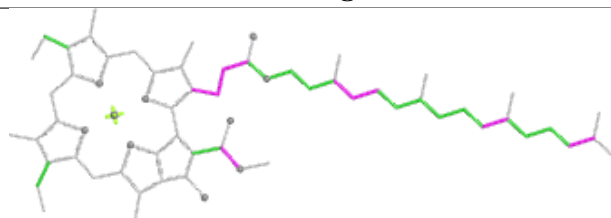
Ligand CLA b 507



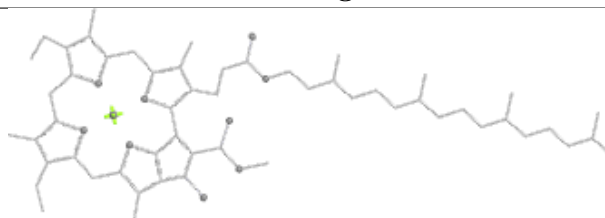
Bond lengths



Bond angles

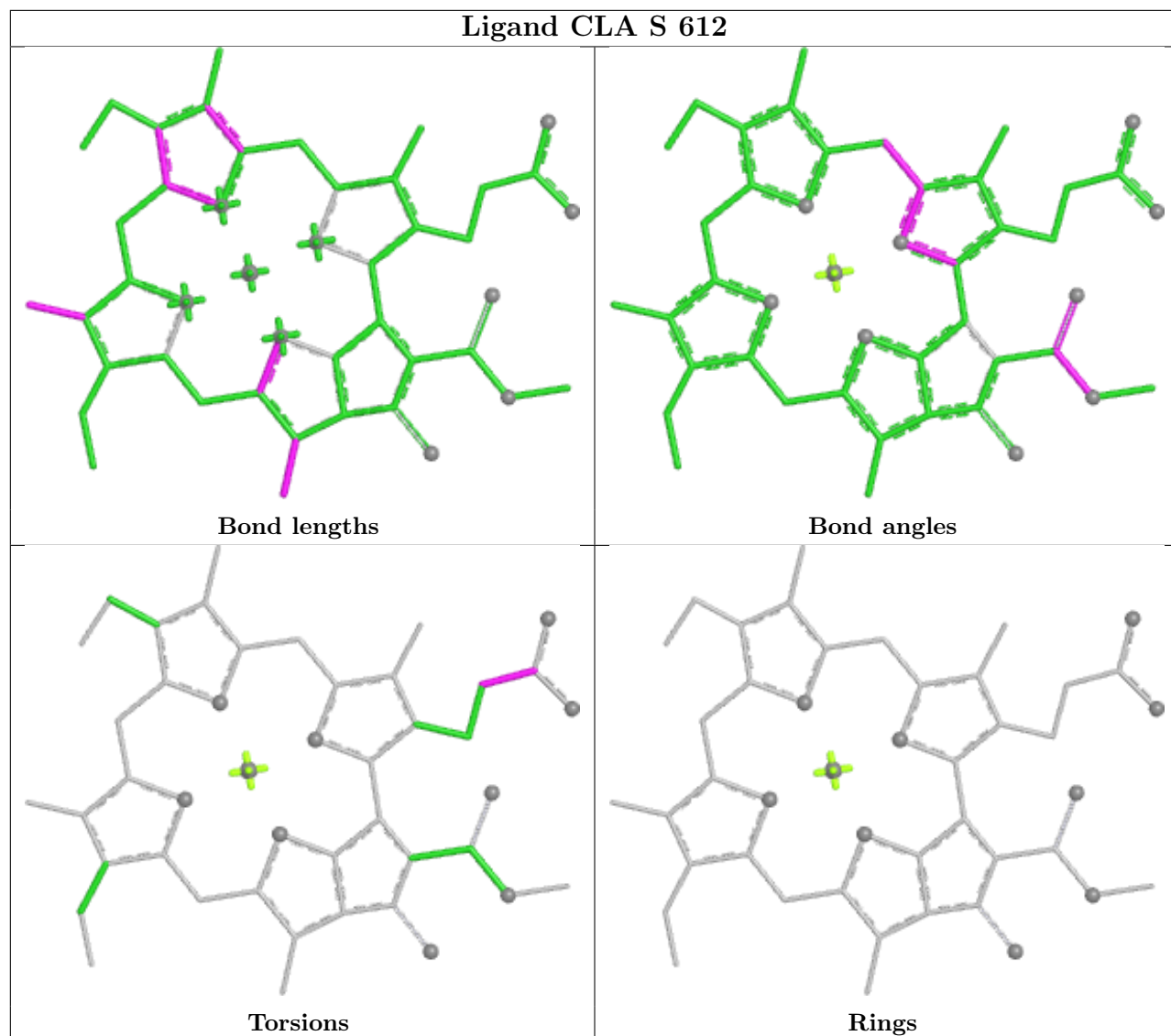


Torsions

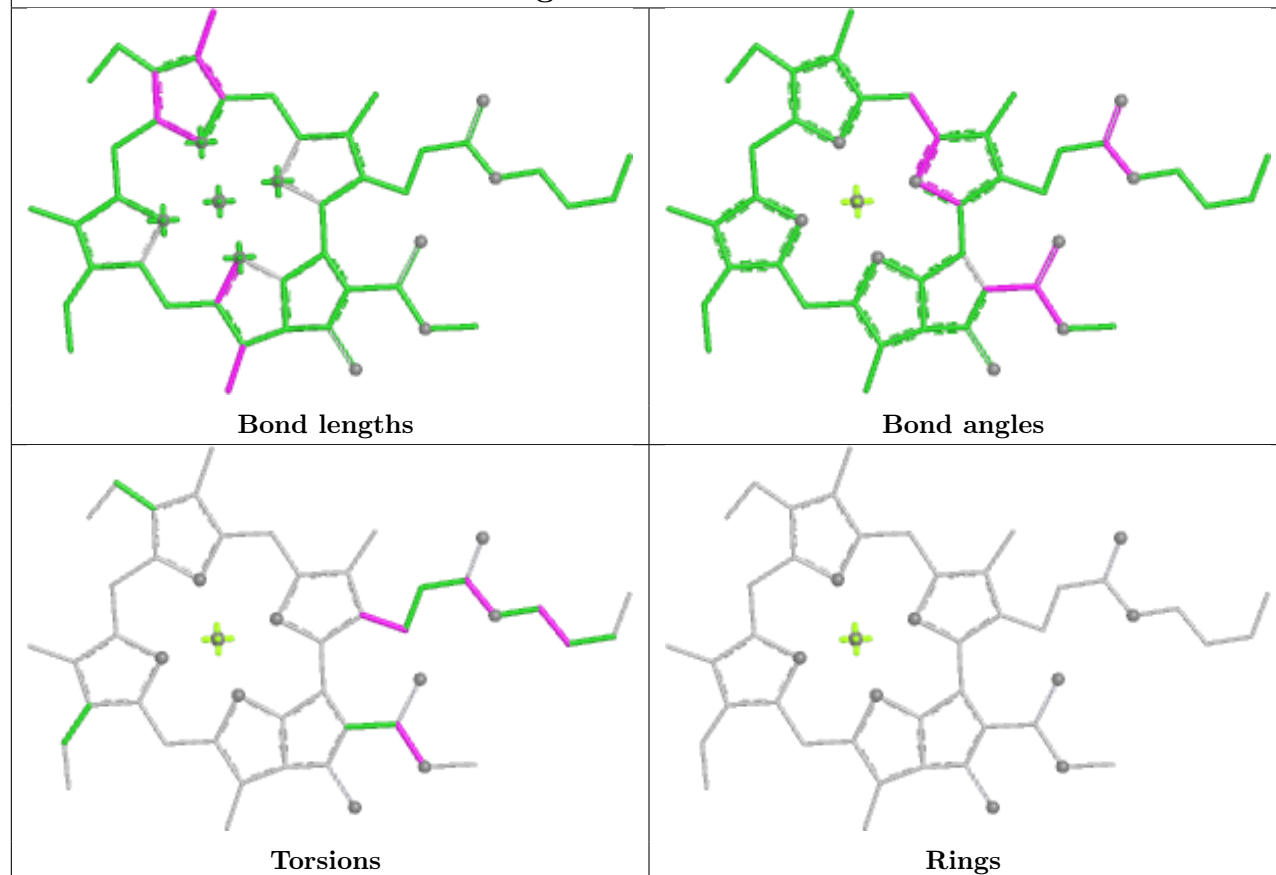


Rings

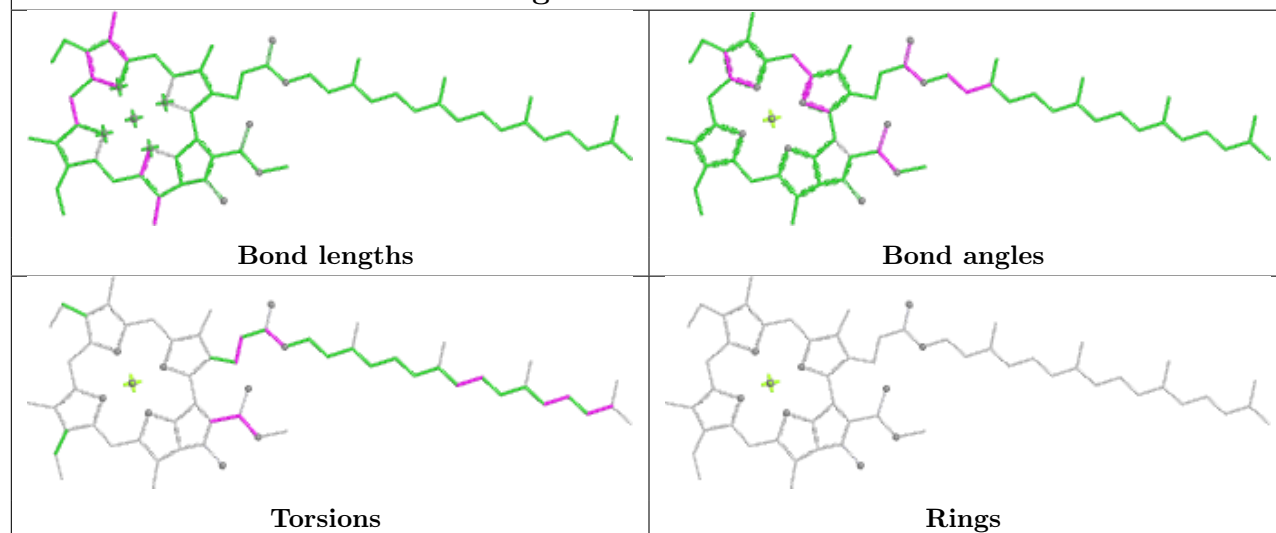
Ligand CLA S 612



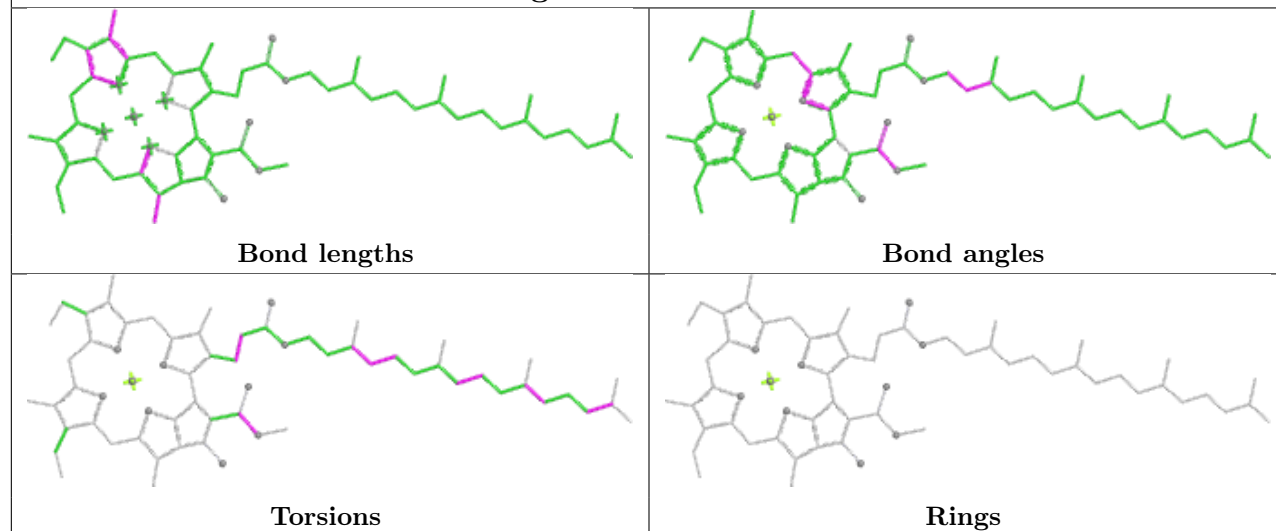
Ligand CLA a 403



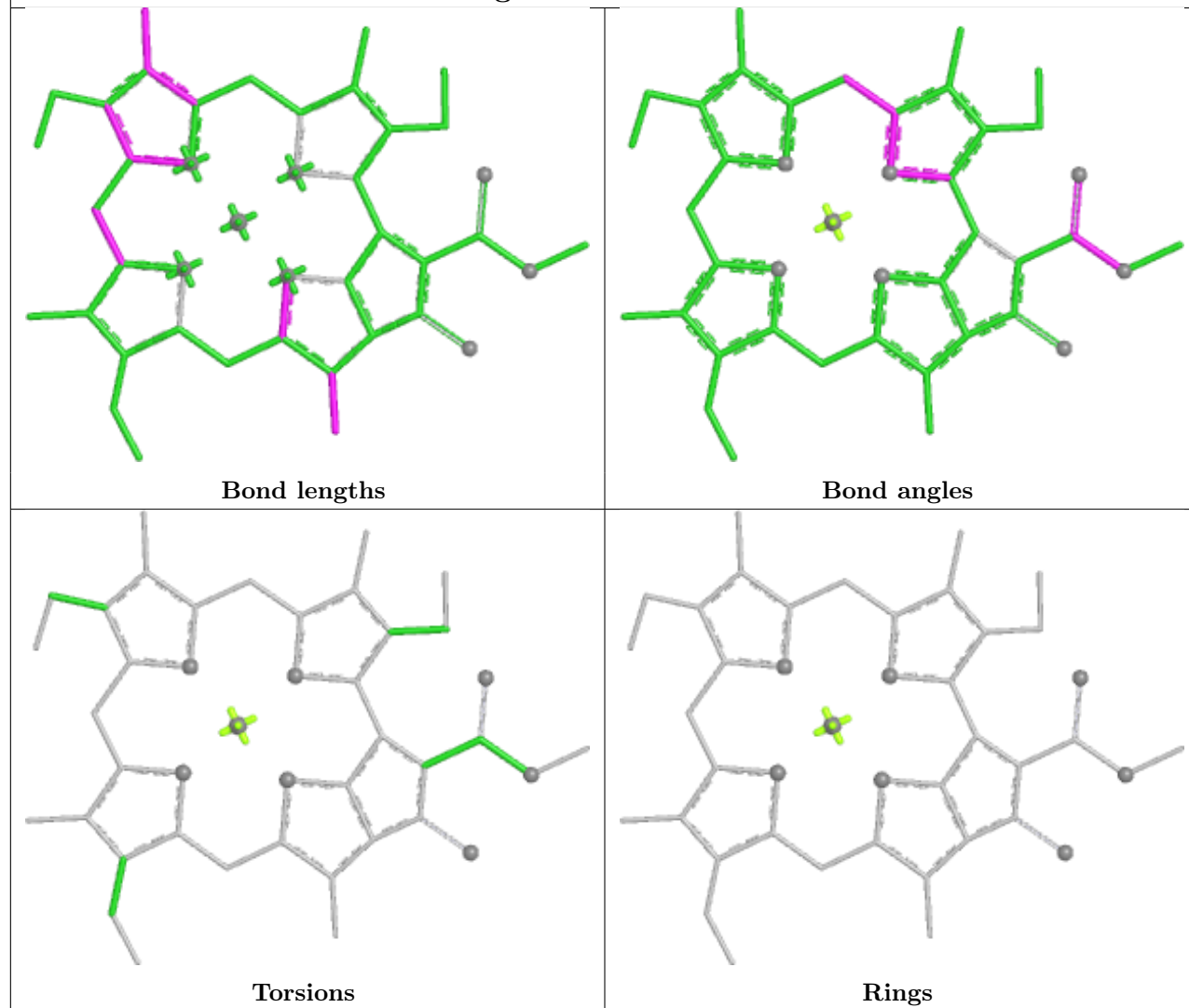
Ligand CLA B 514



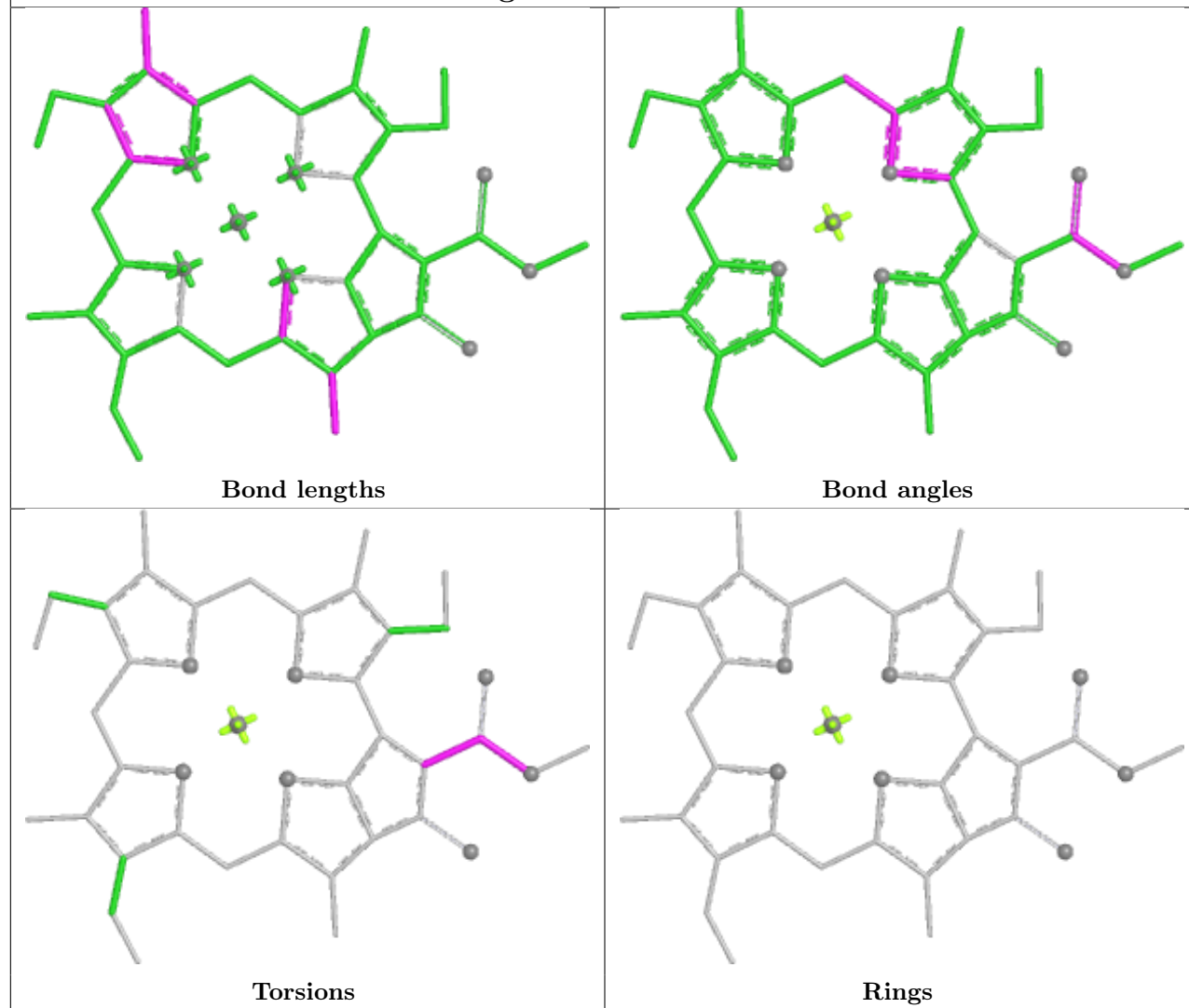
Ligand CLA G 613



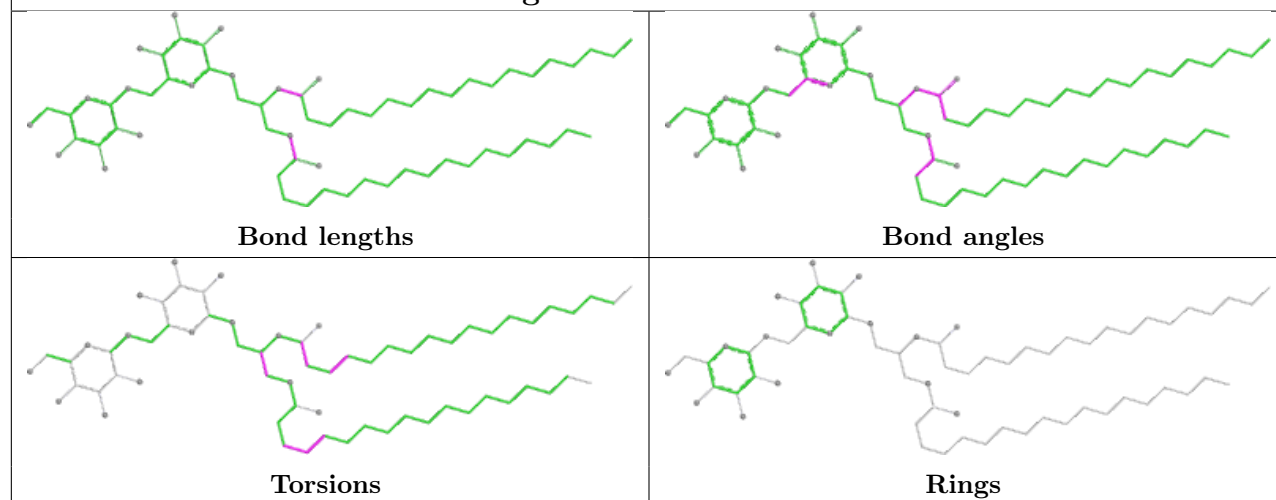
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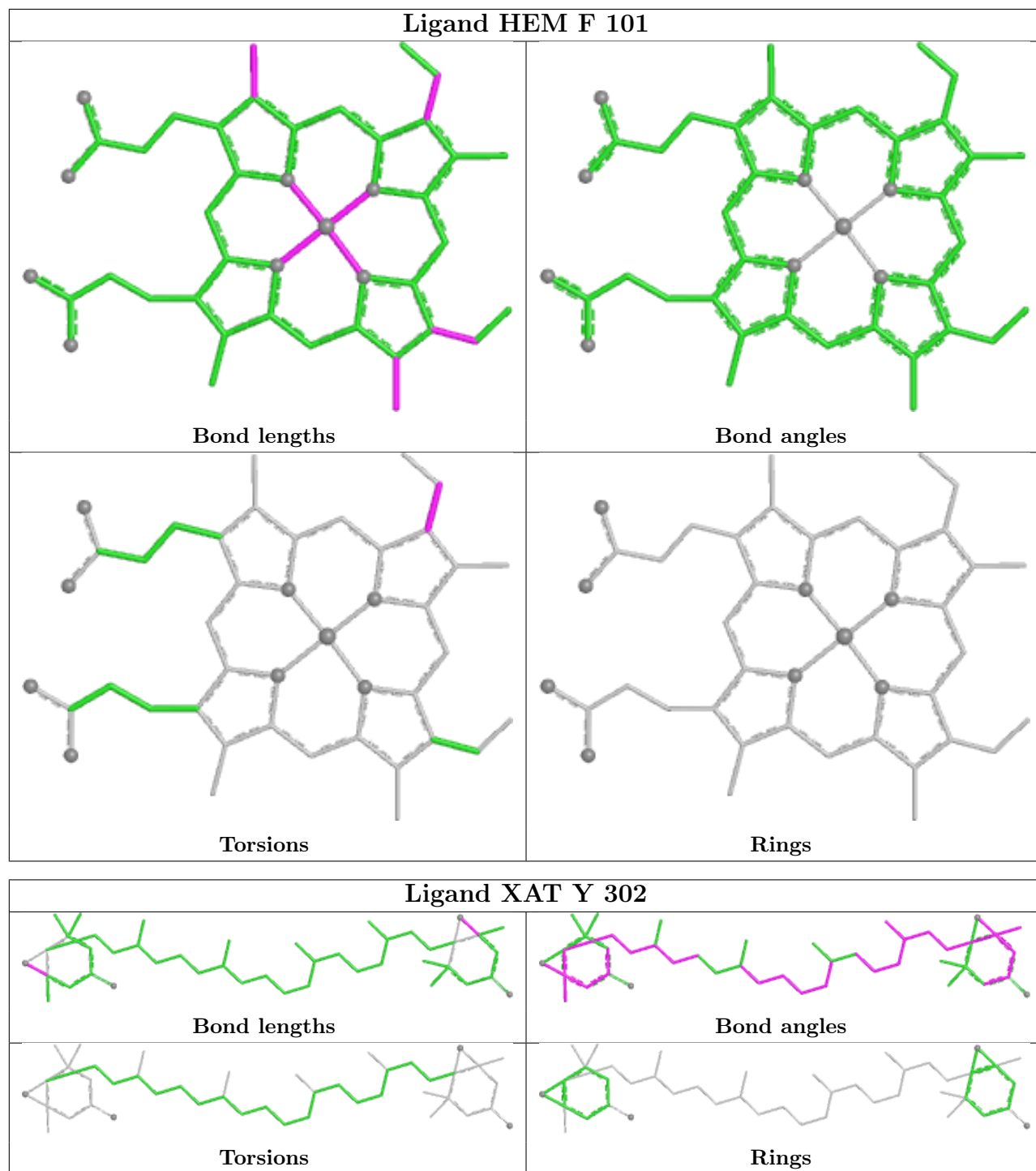


Ligand CLA d 404

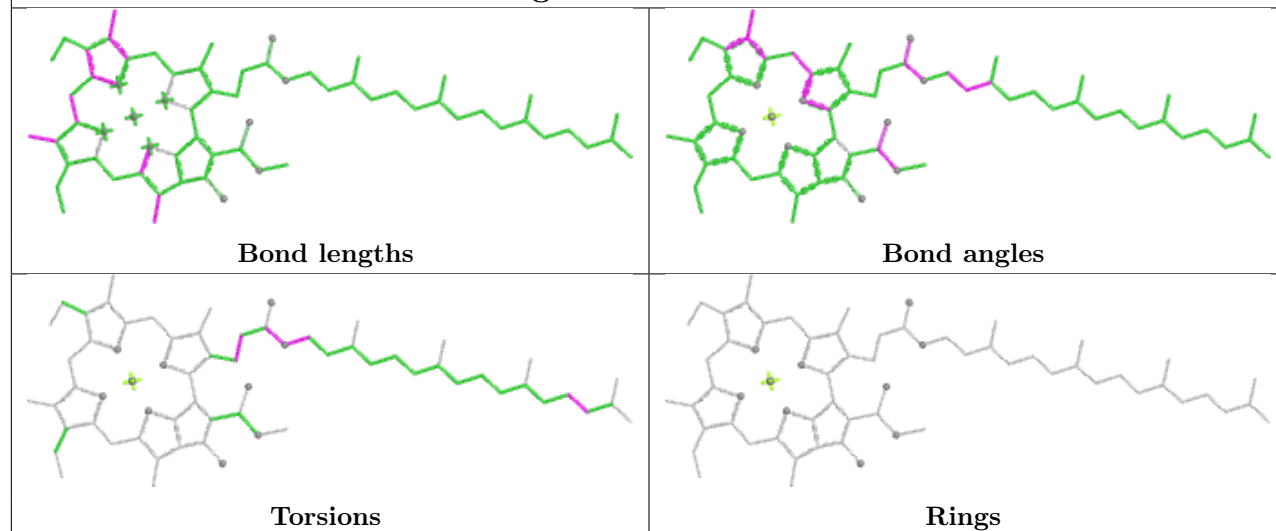


Ligand DGD W 202

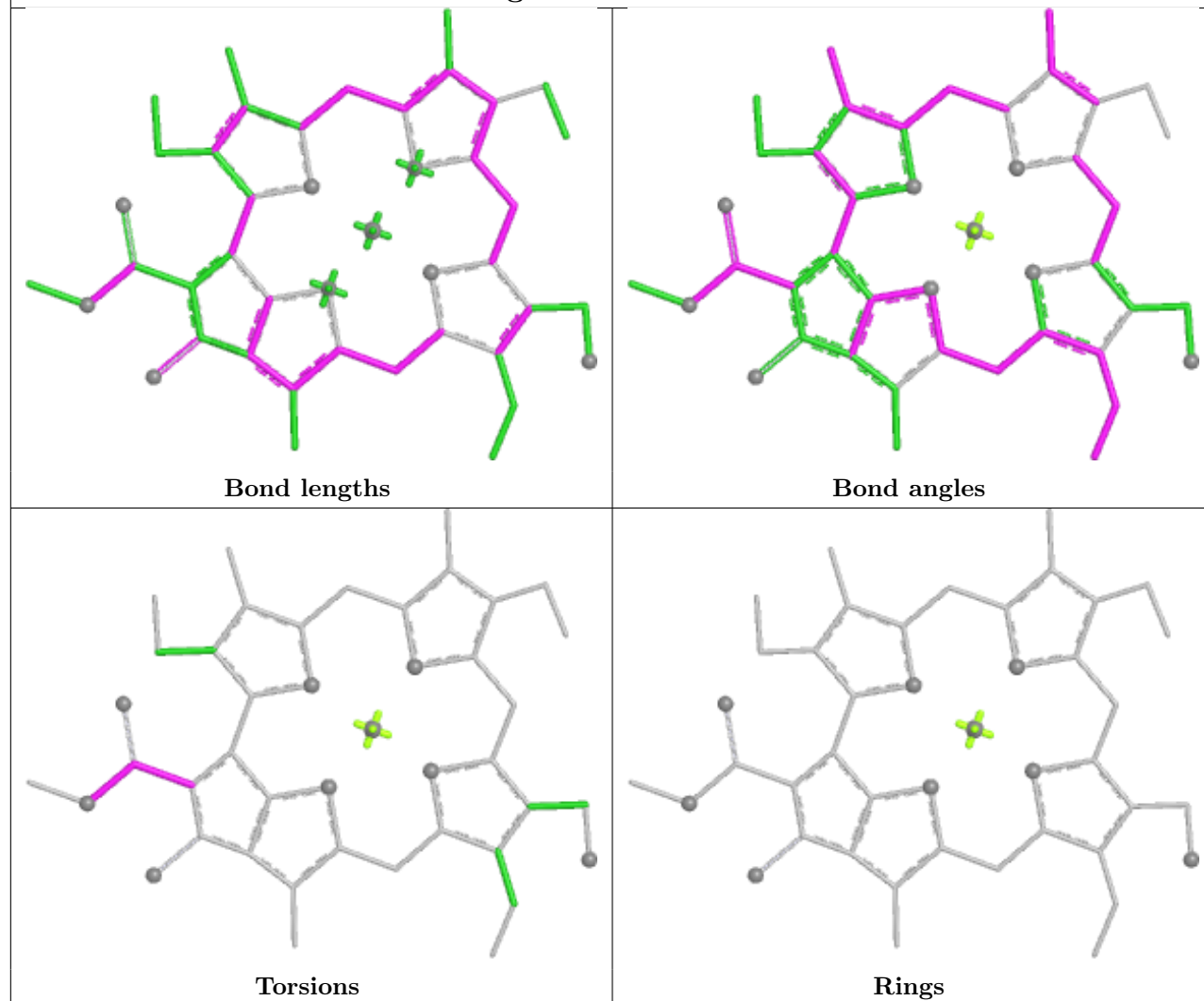


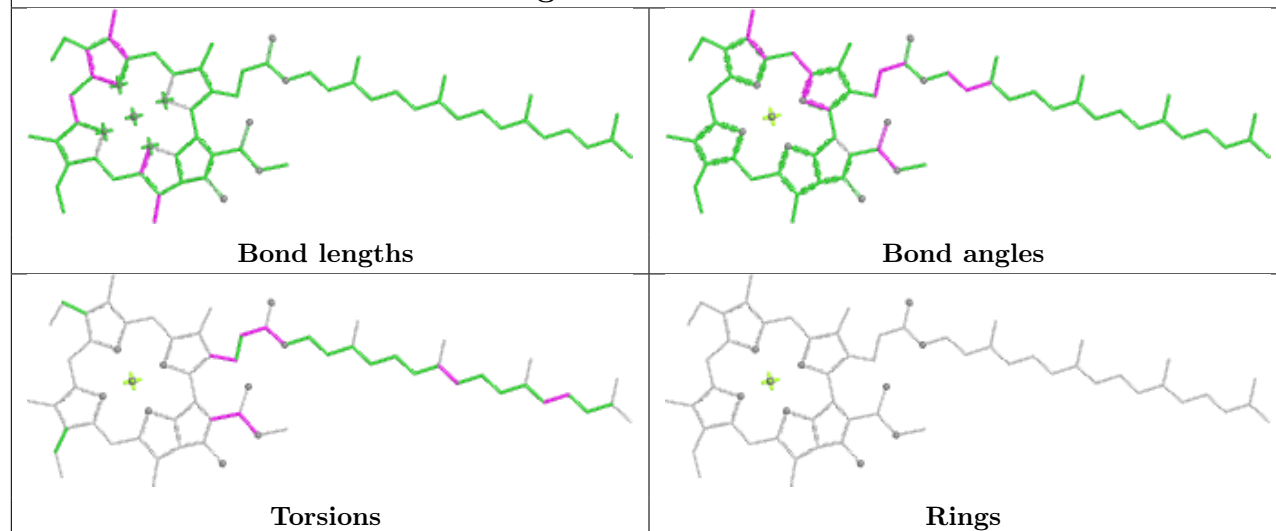
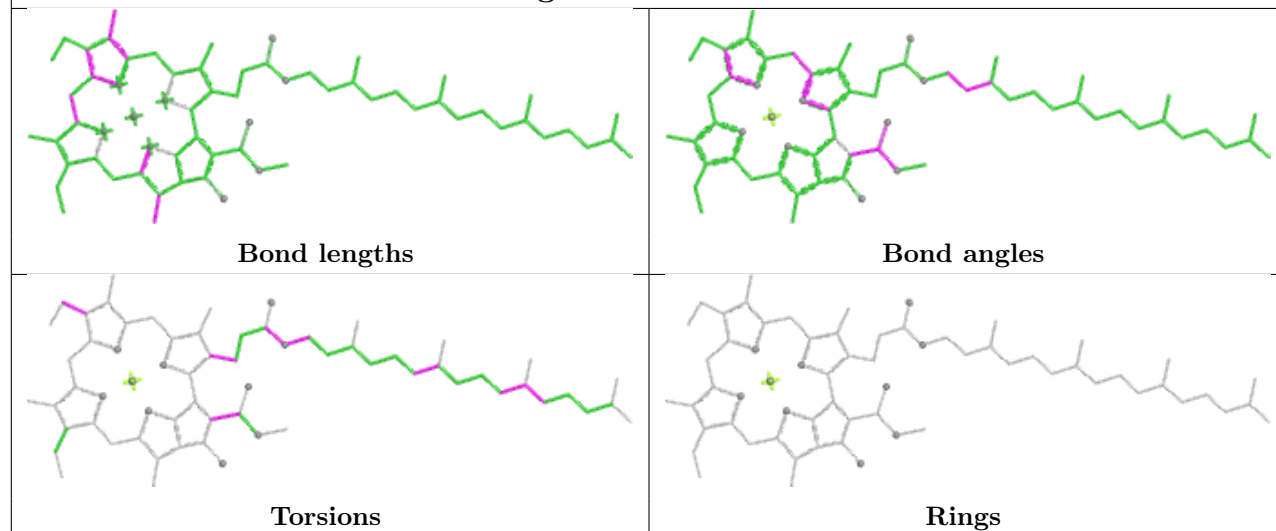


Ligand CLA B 513

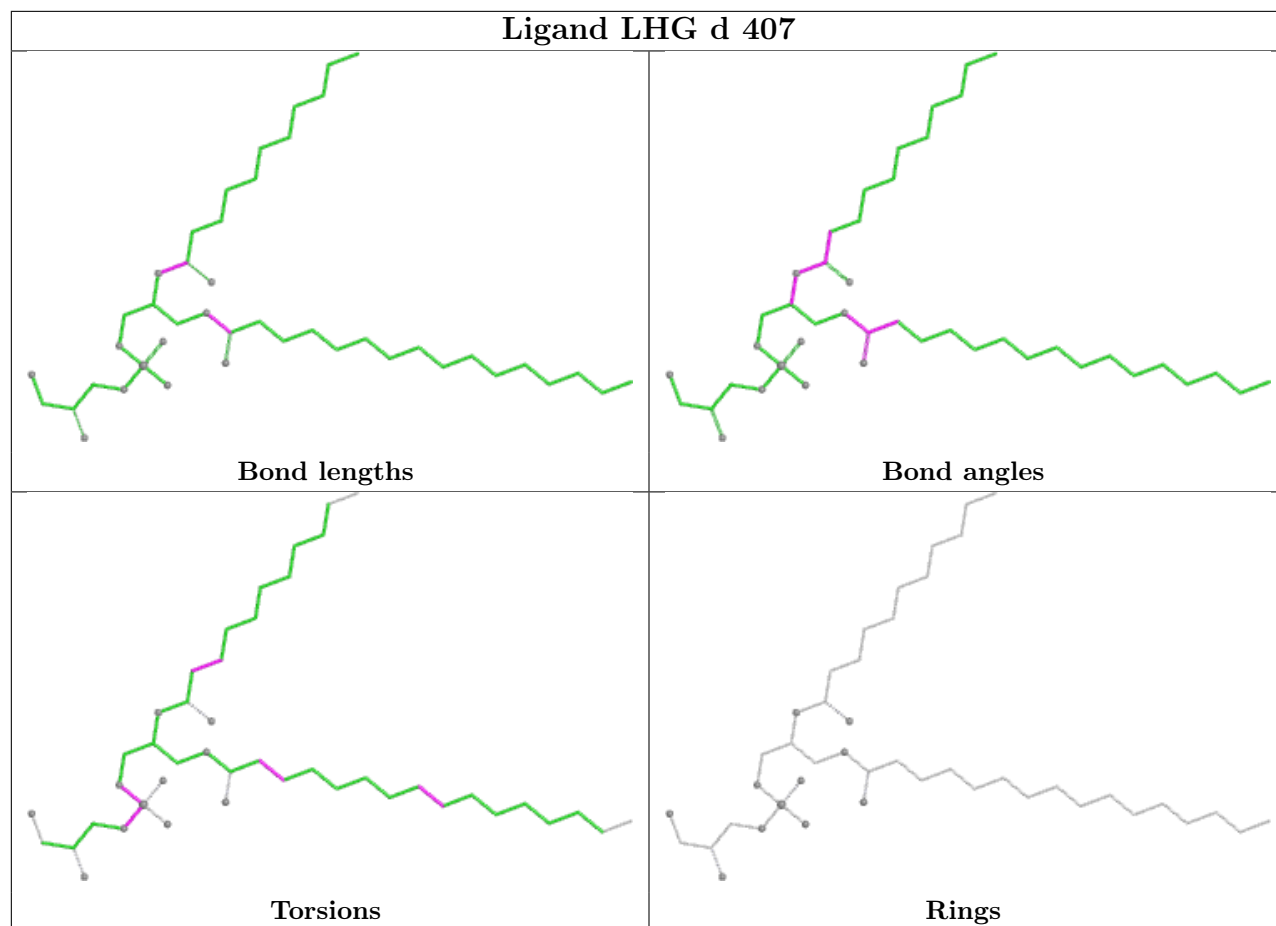


Ligand CHL r 305

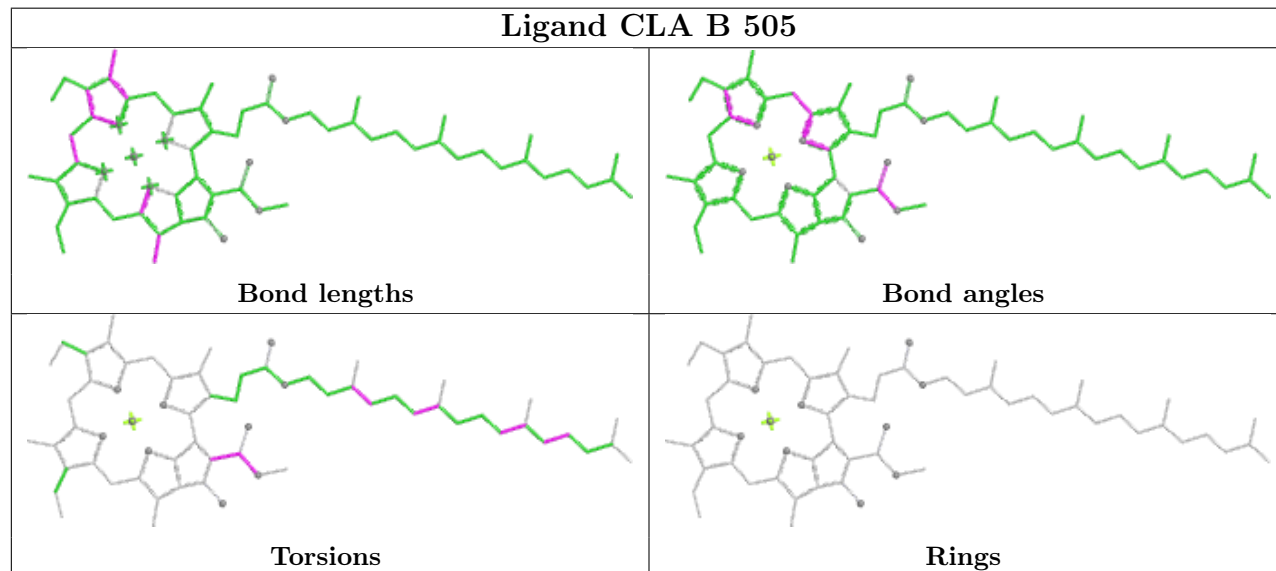


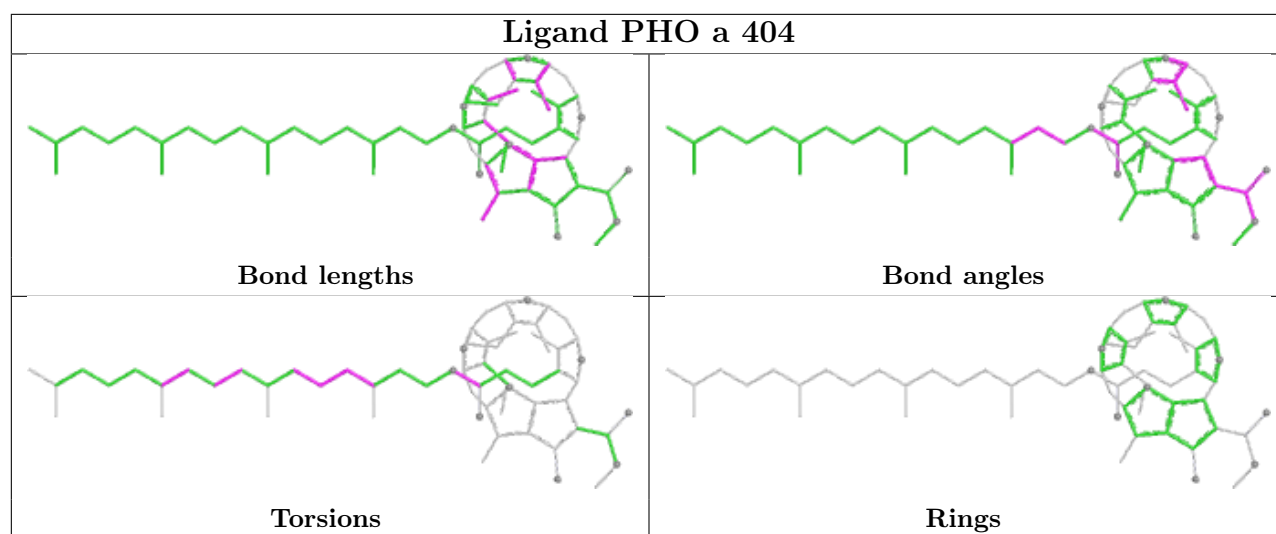
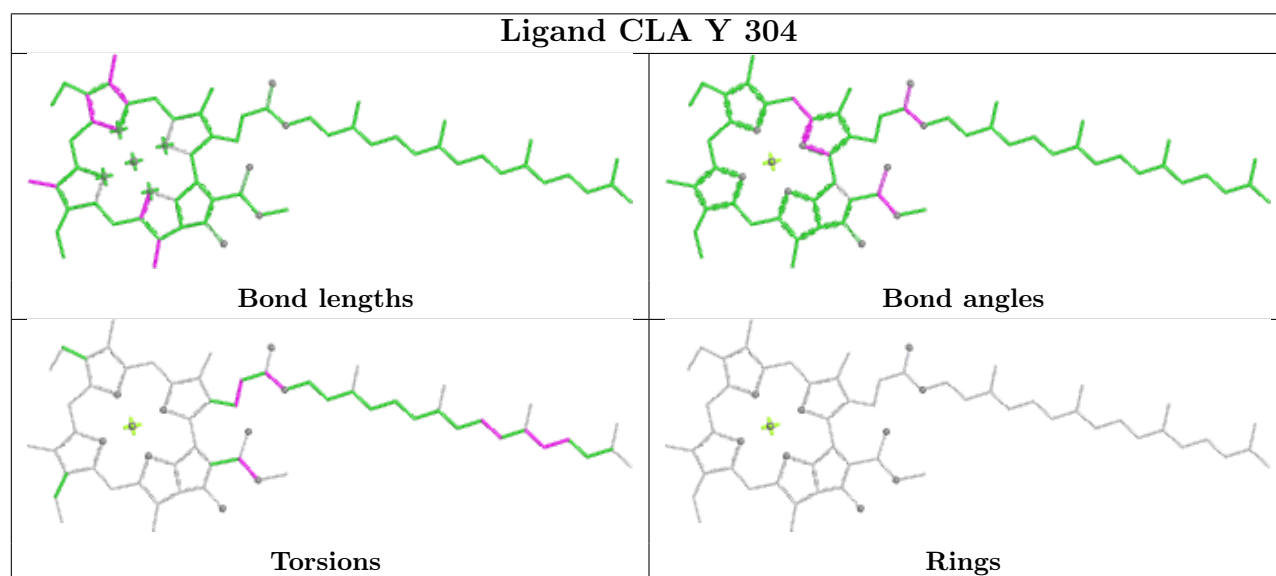
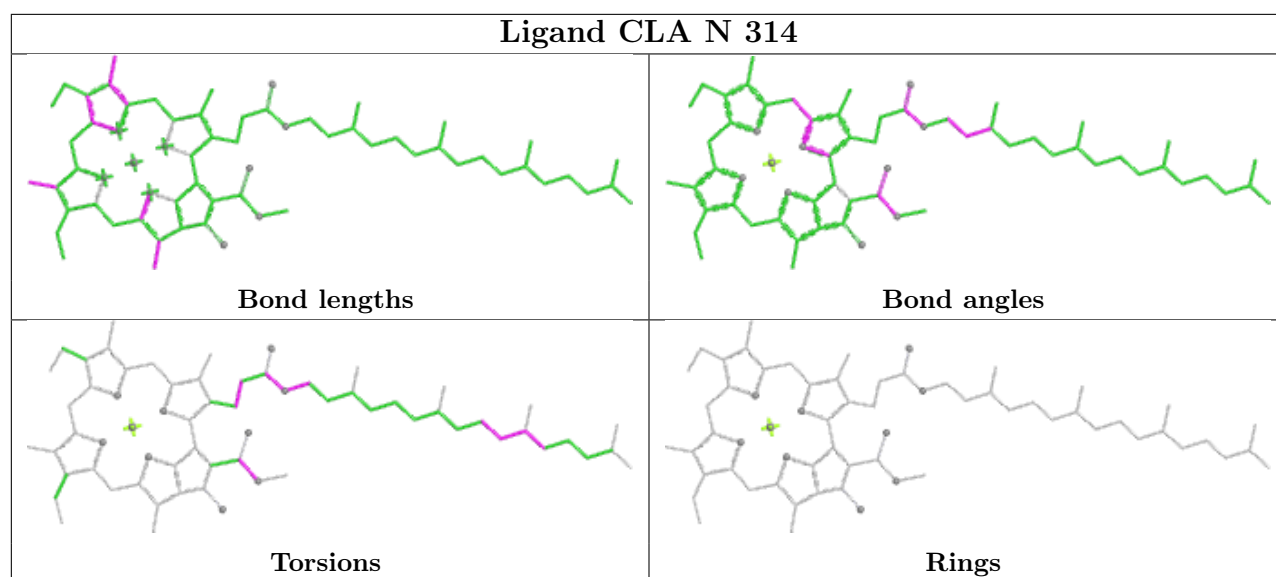
Ligand CLA c 503**Ligand CLA c 507**

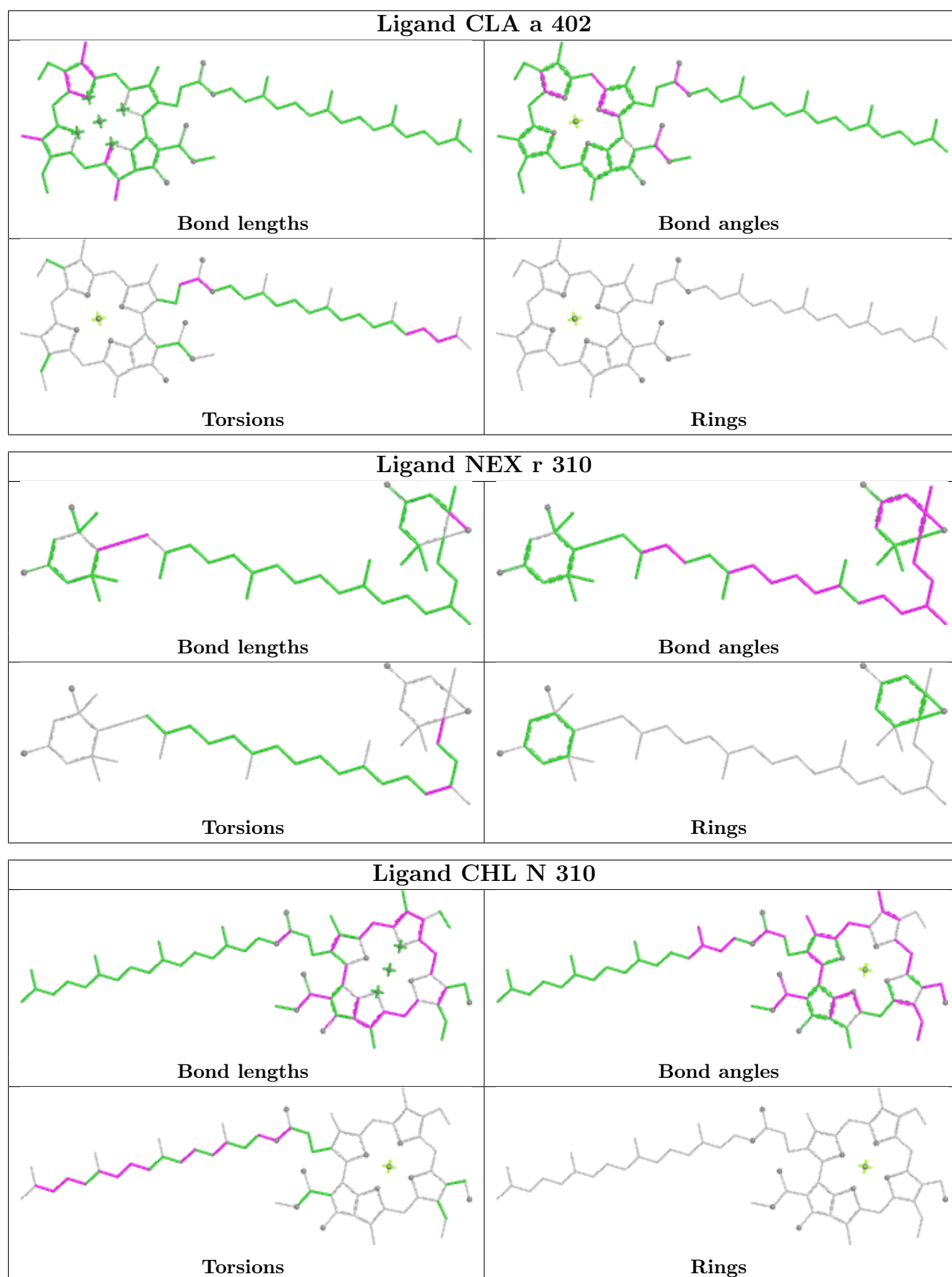
Ligand LHG d 407

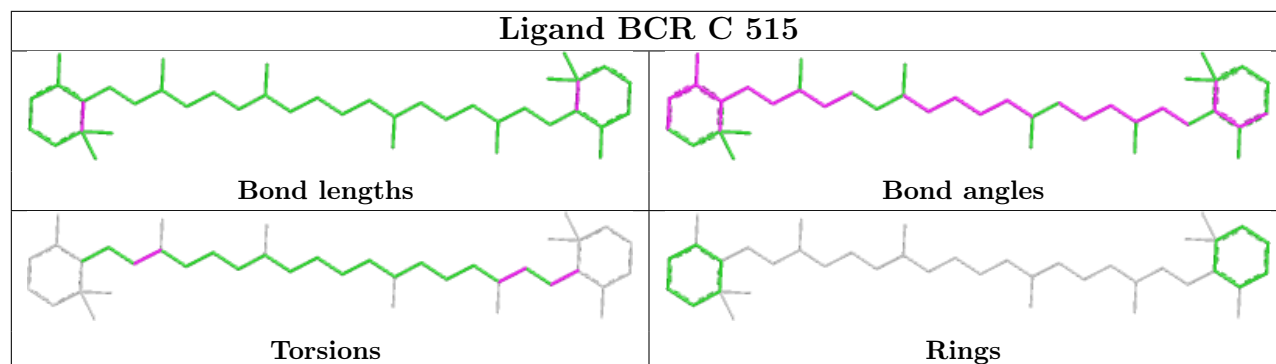
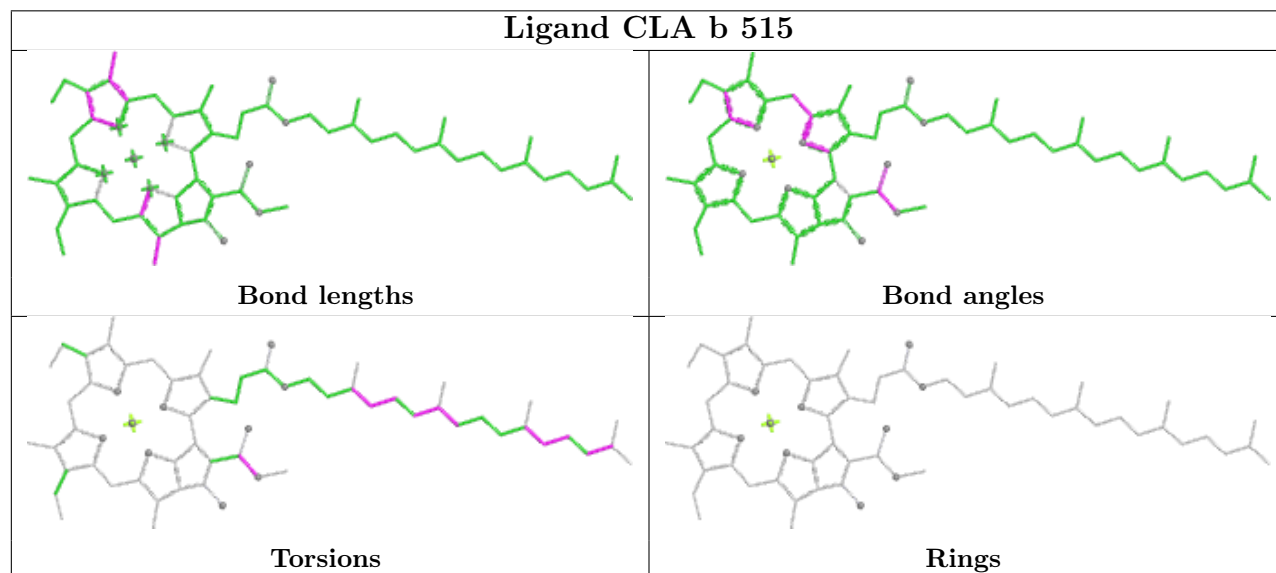
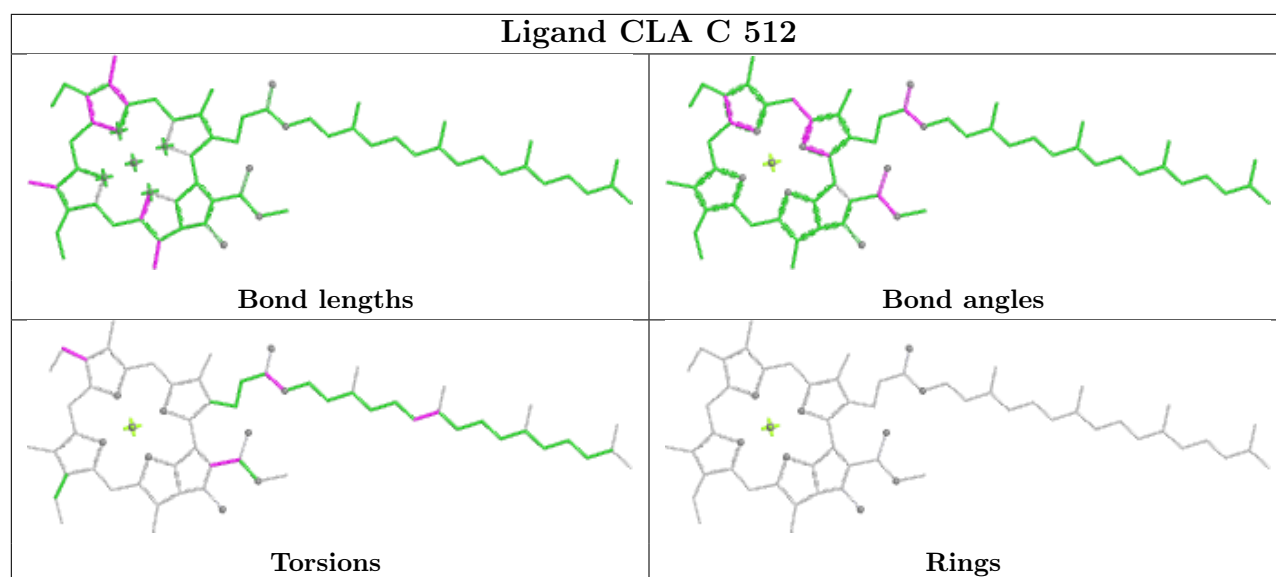


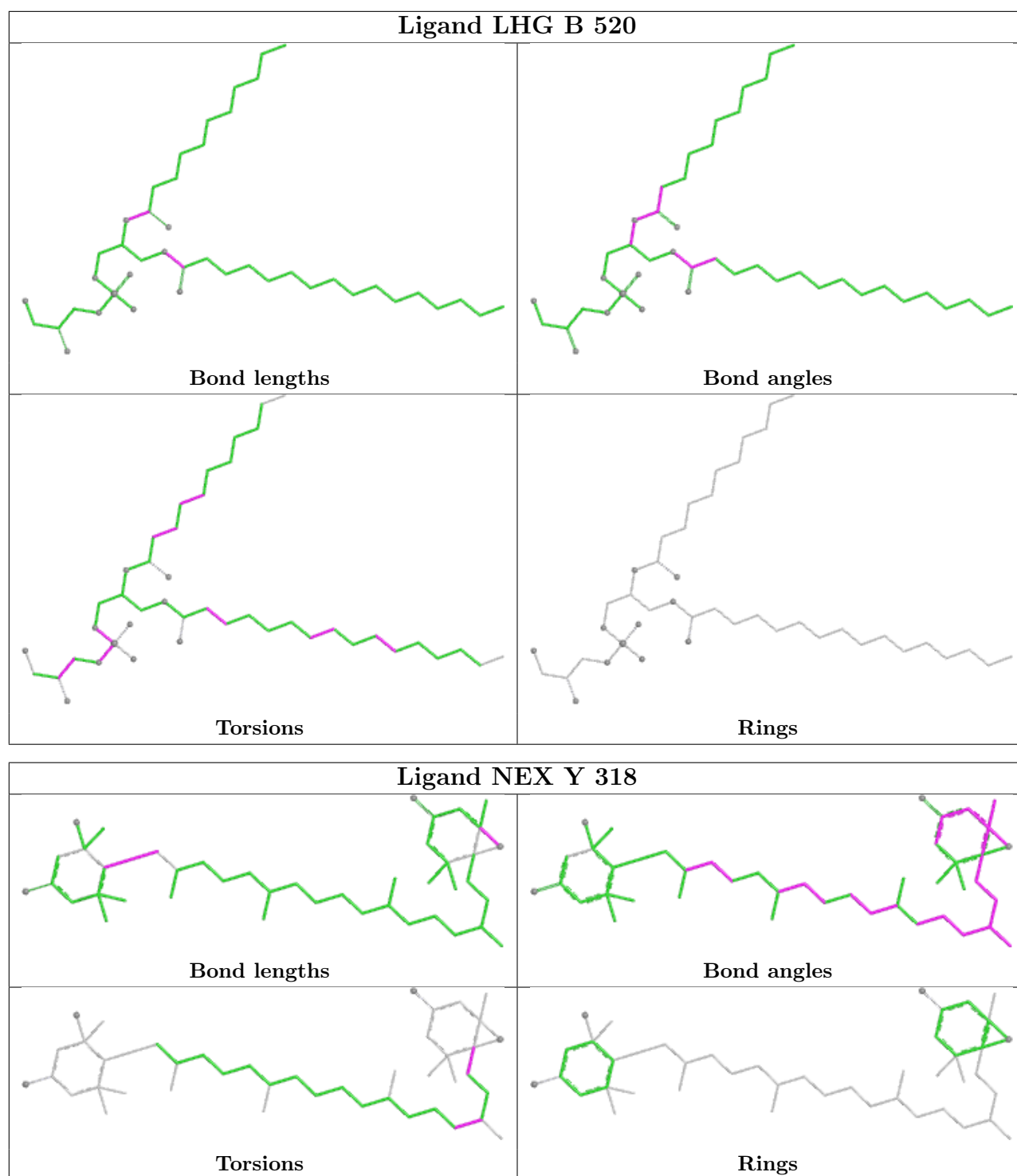
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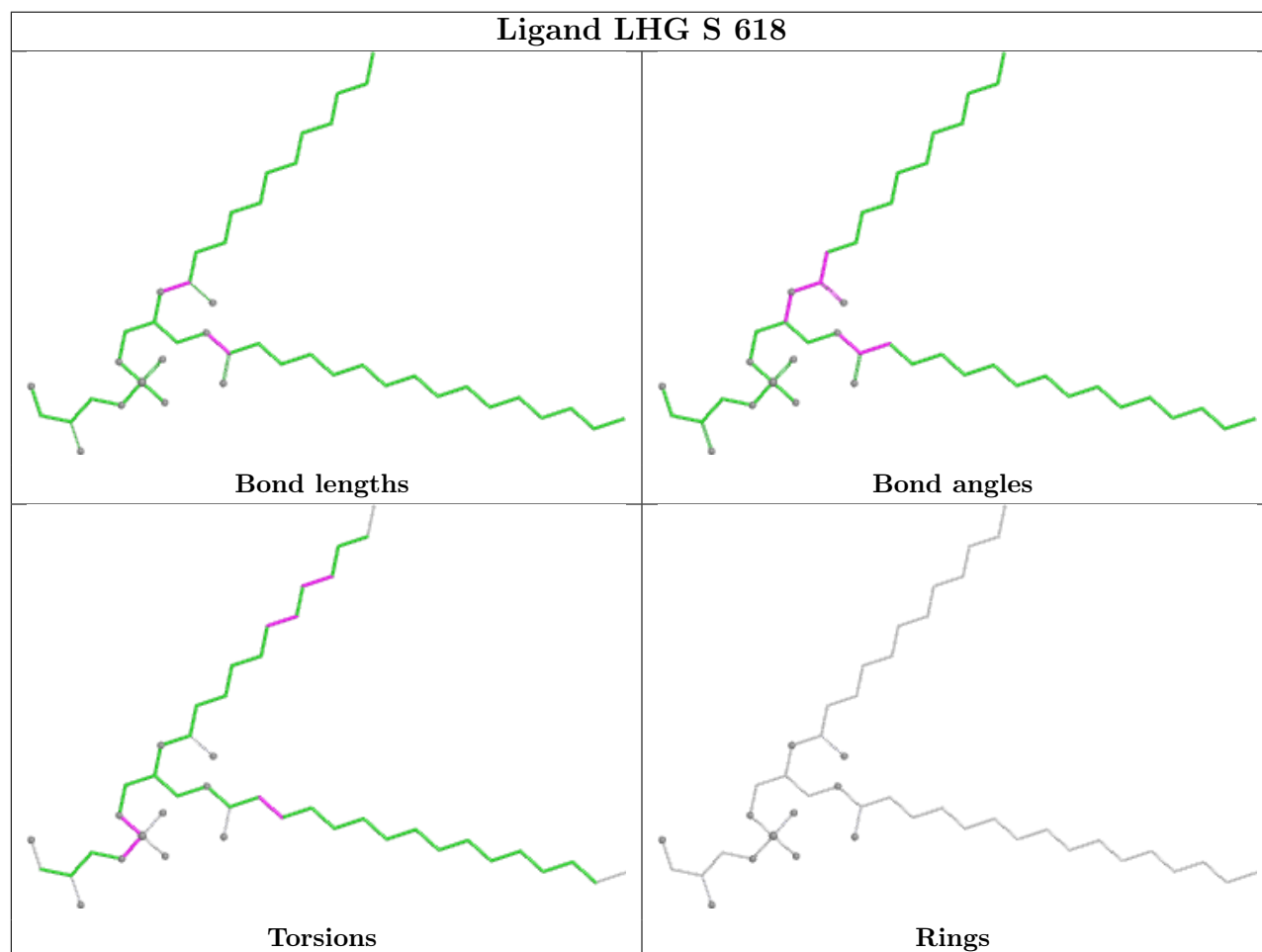
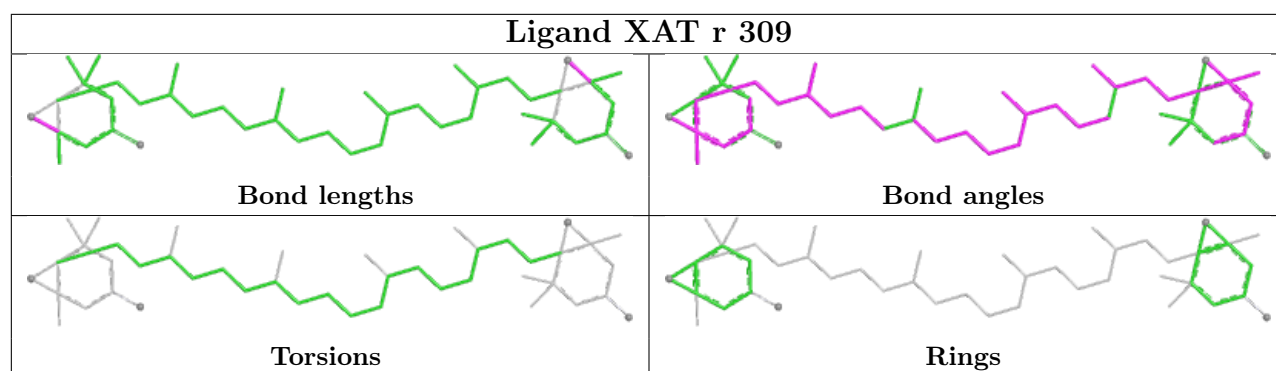


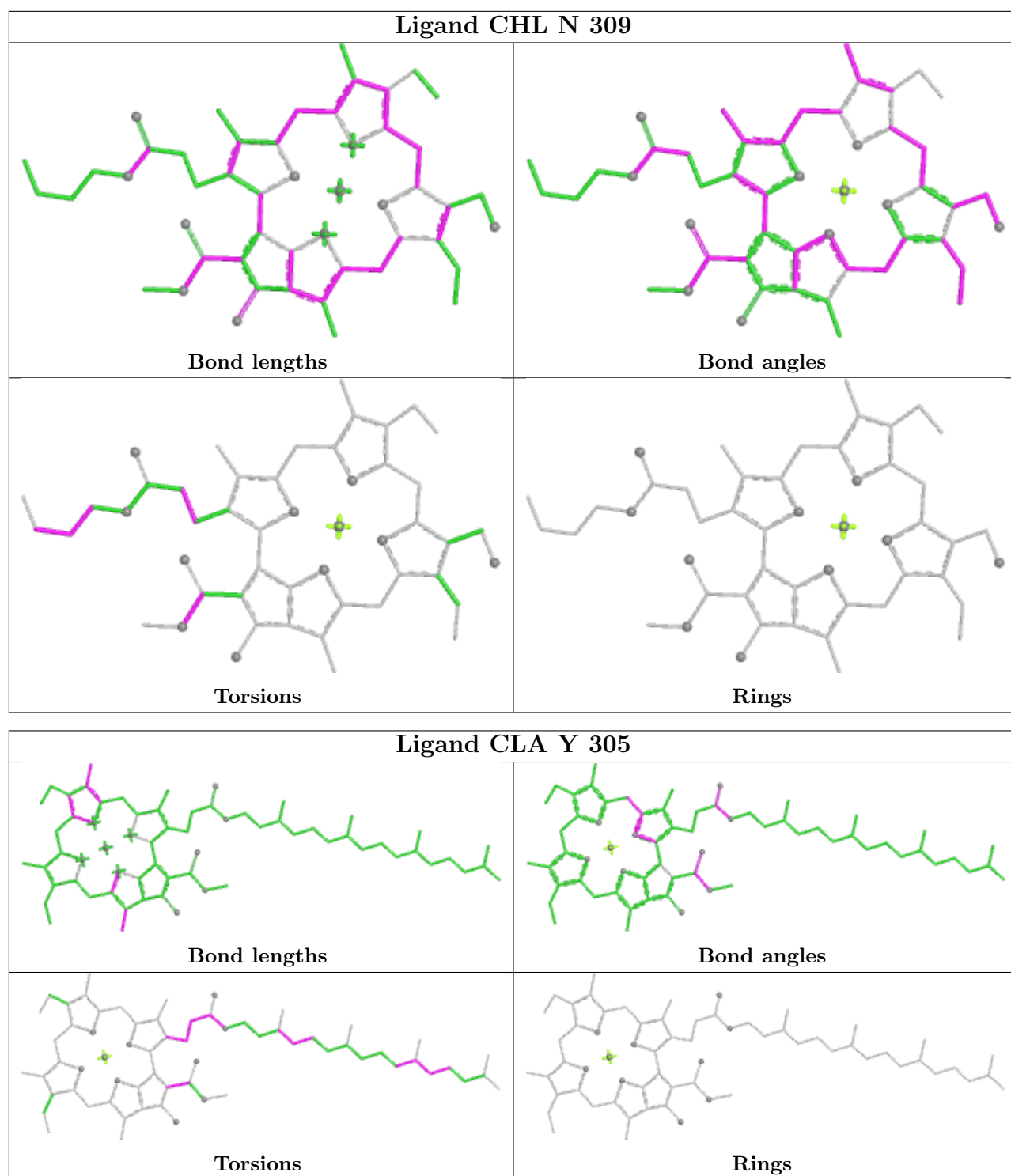




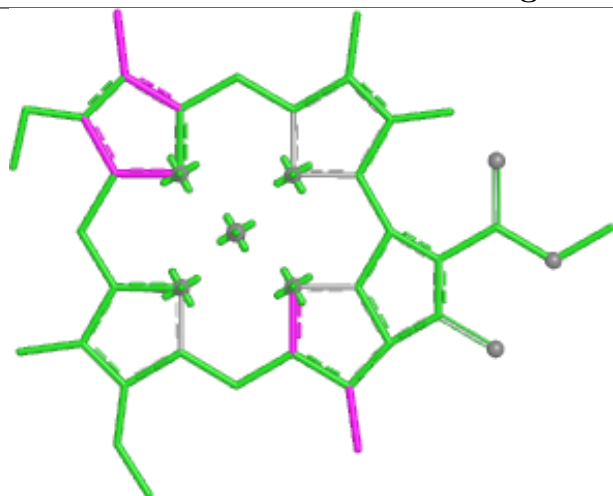




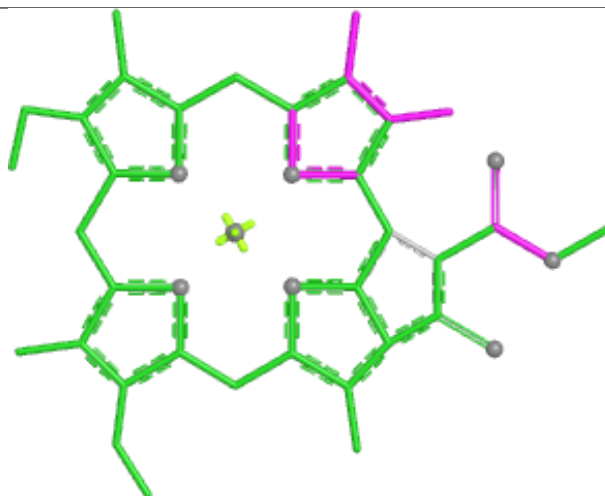




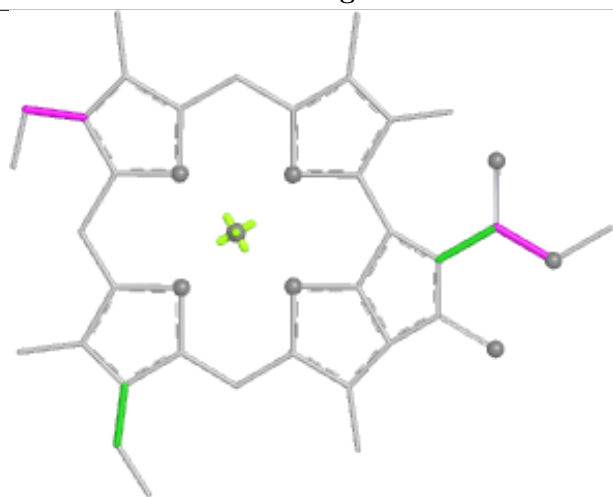
Ligand CLA r 308



Bond lengths



Bond angles

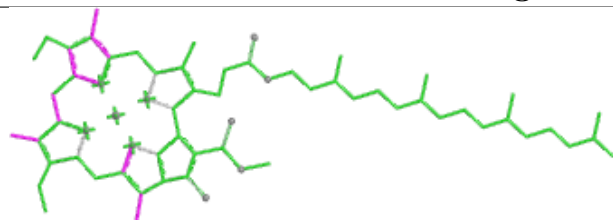


Torsions

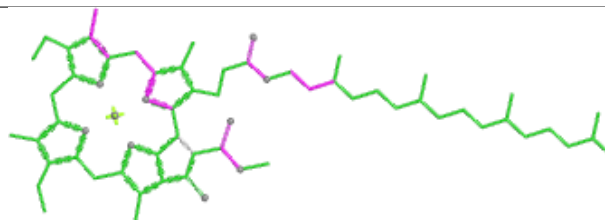


Rings

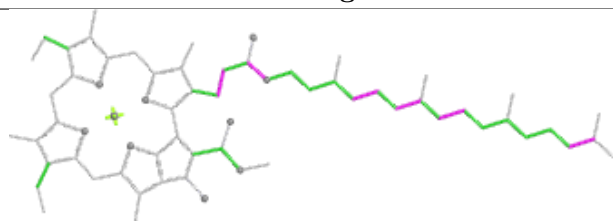
Ligand CLA N 303



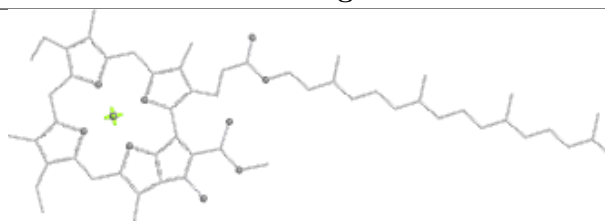
Bond lengths



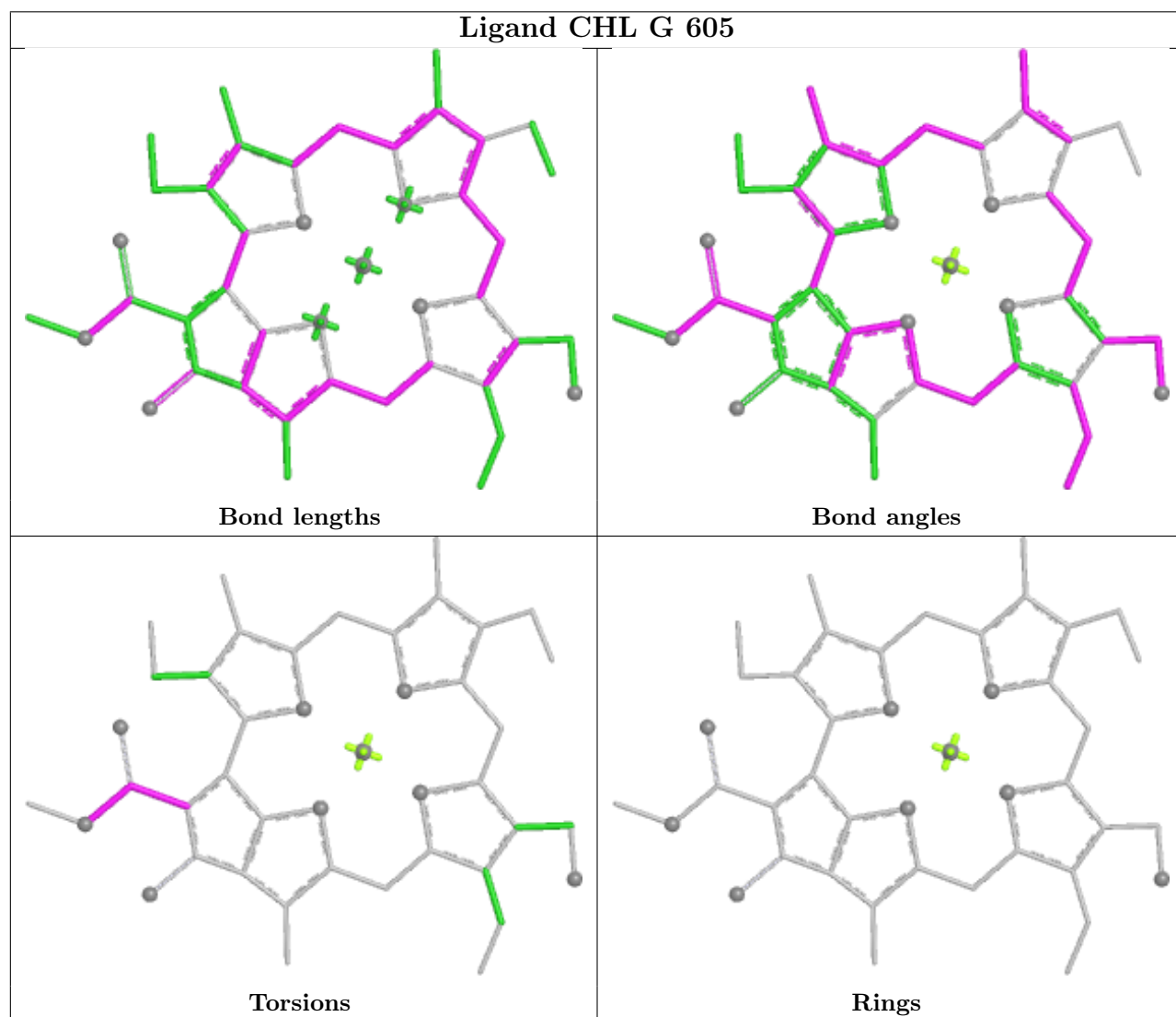
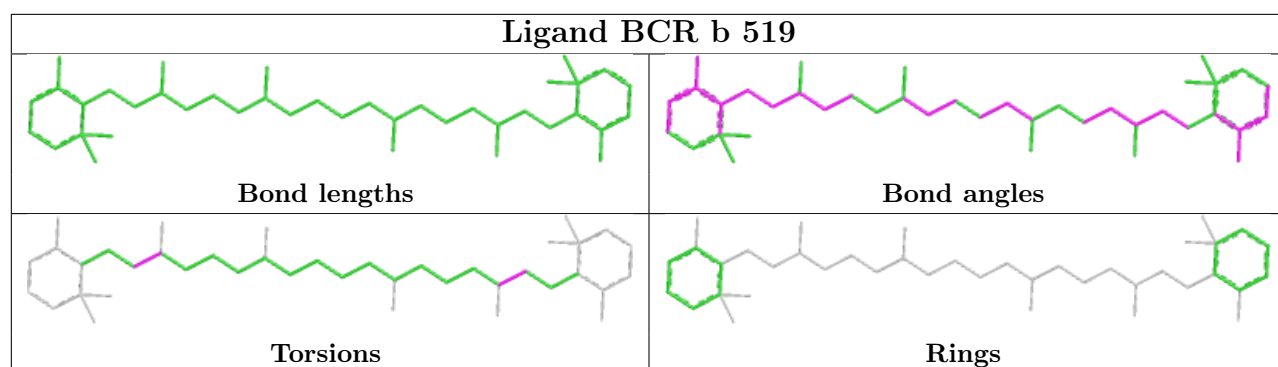
Bond angles

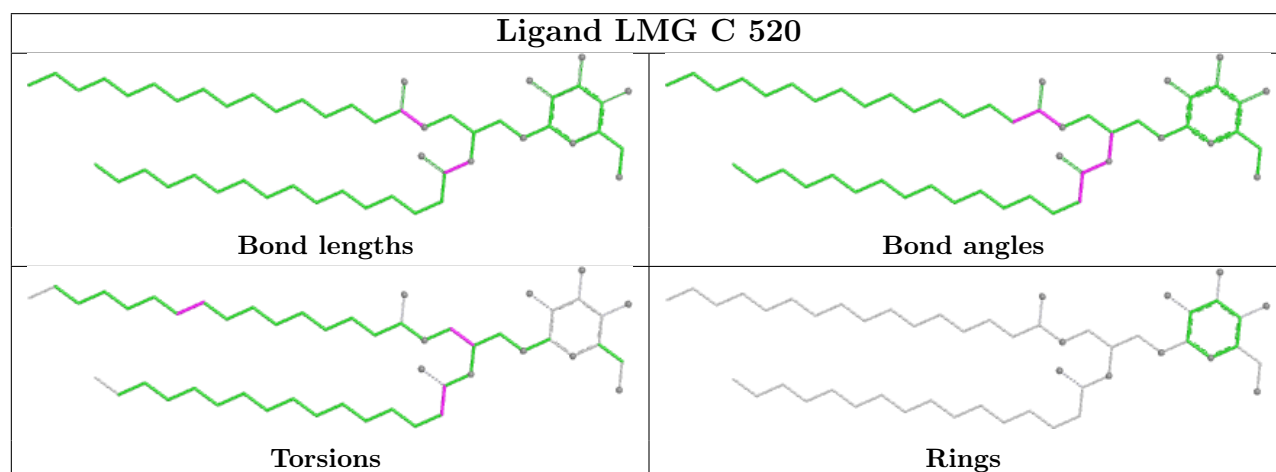
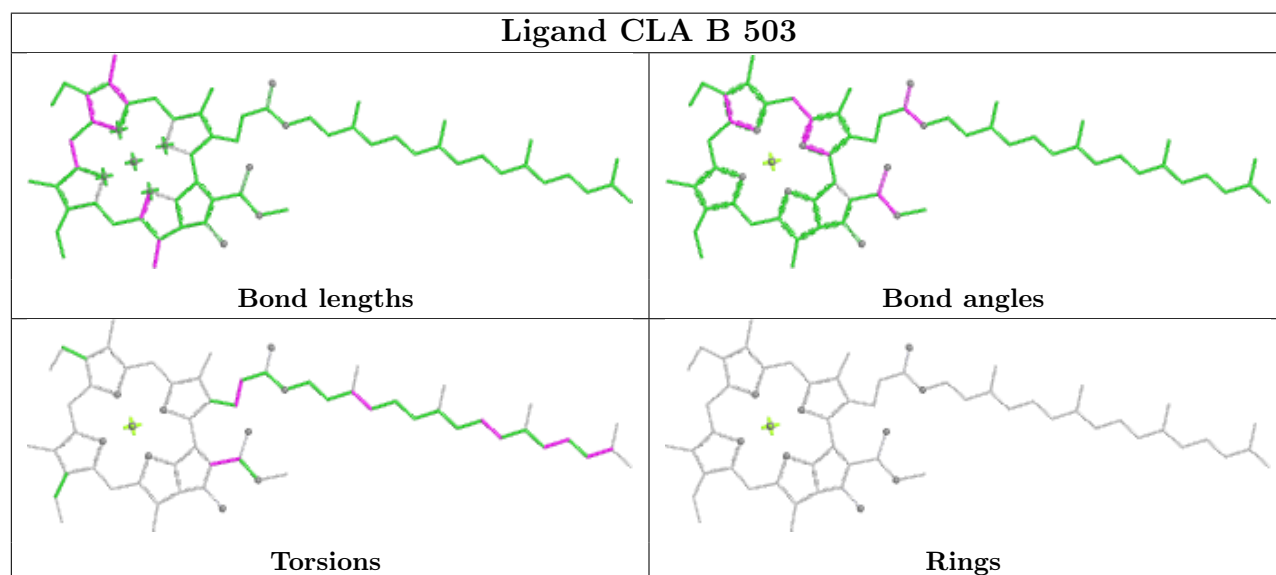
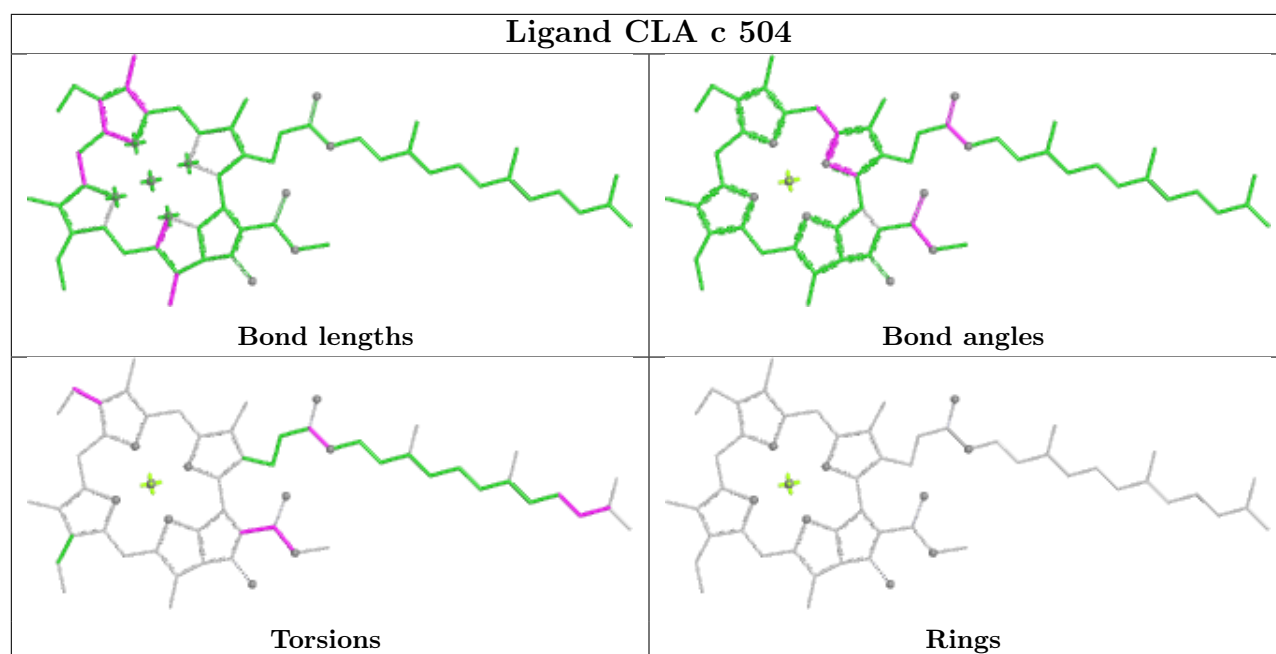


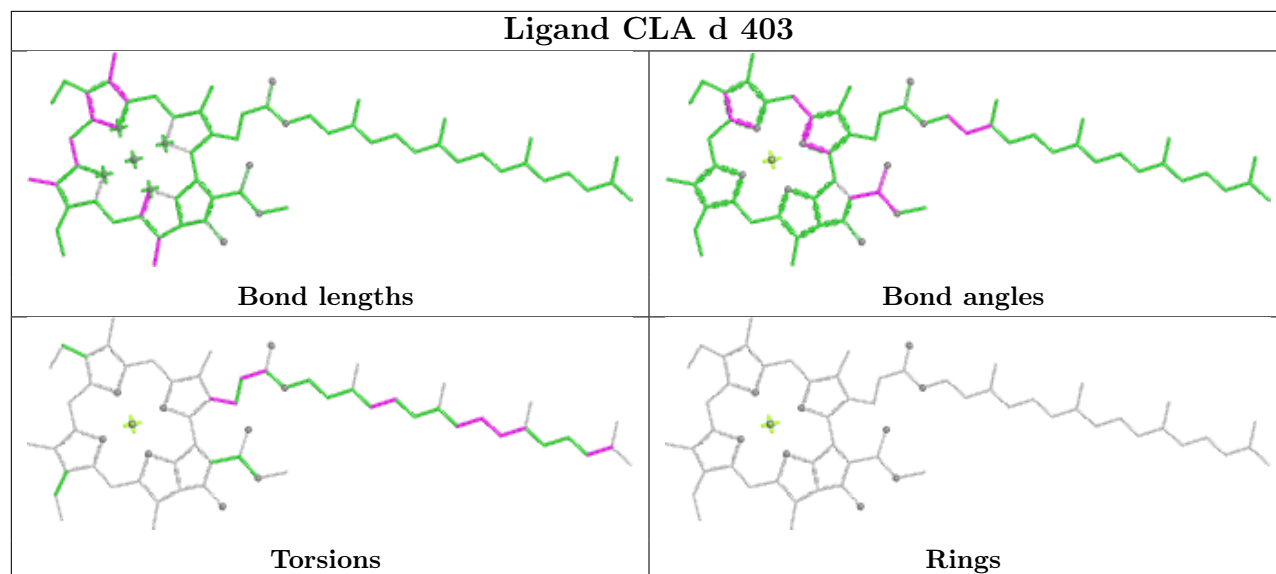
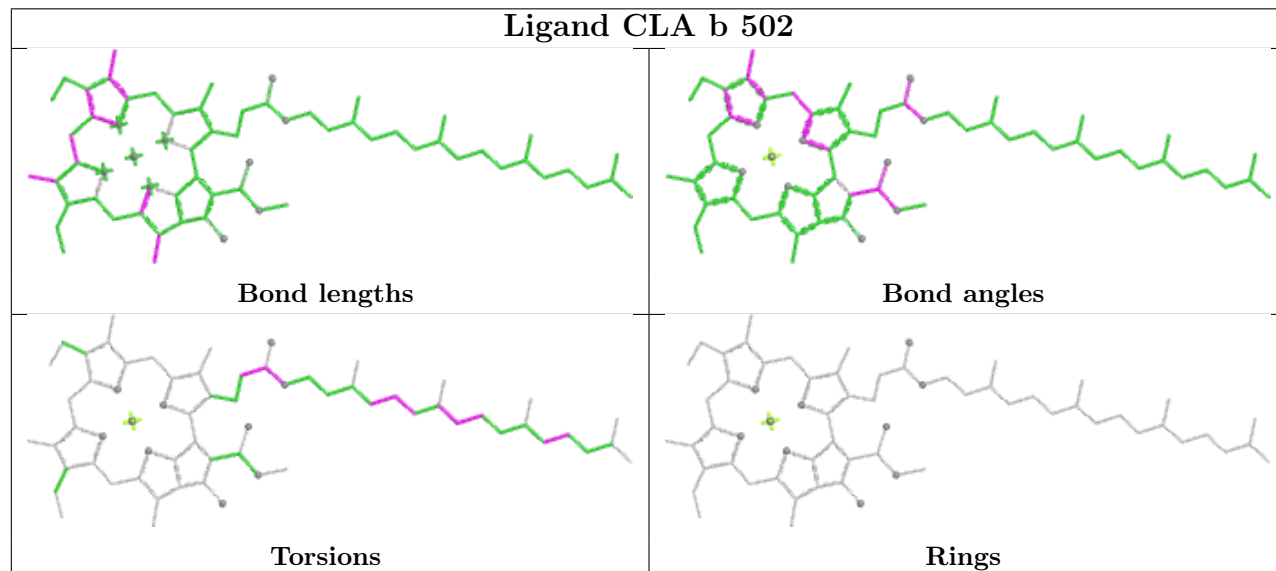
Torsions

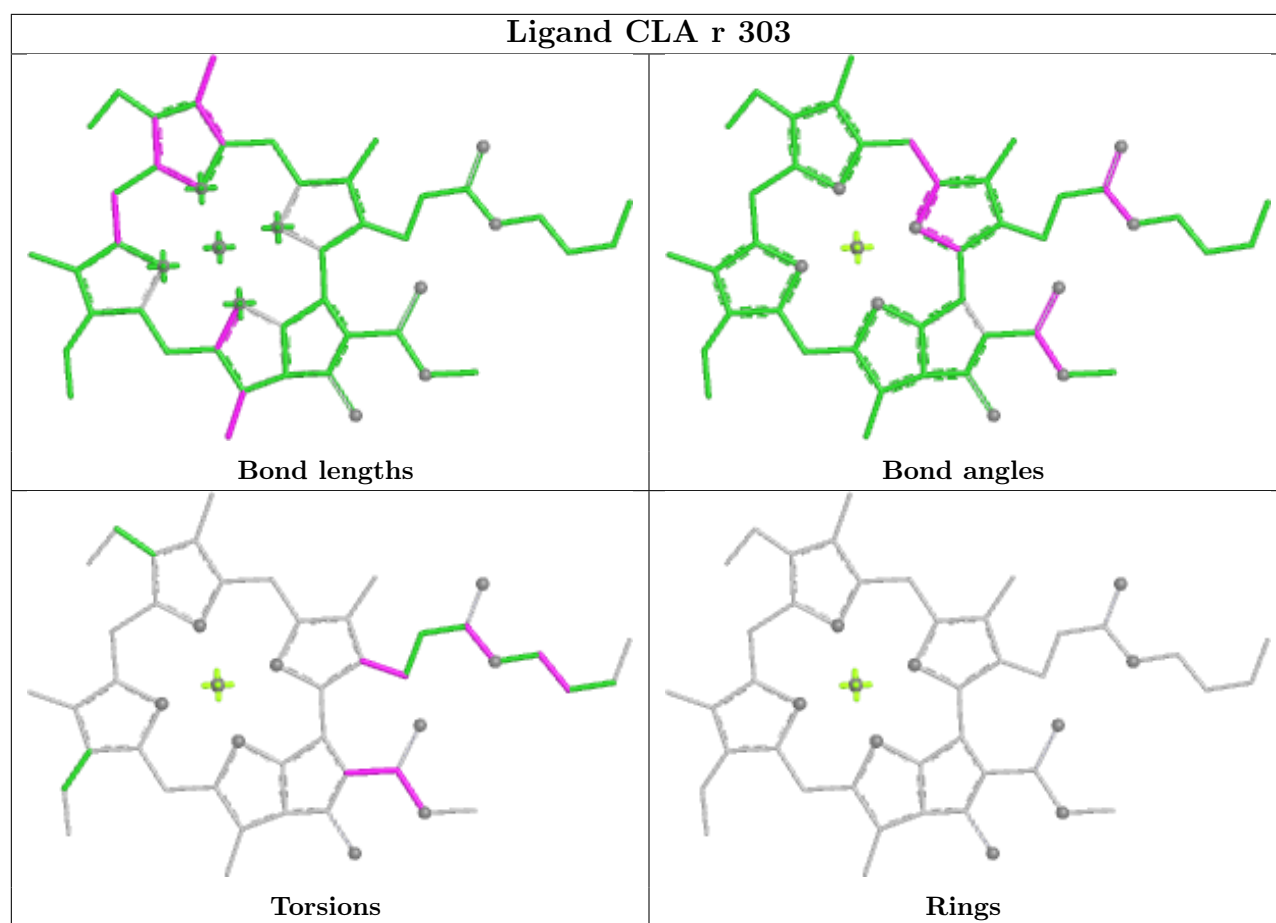


Rings

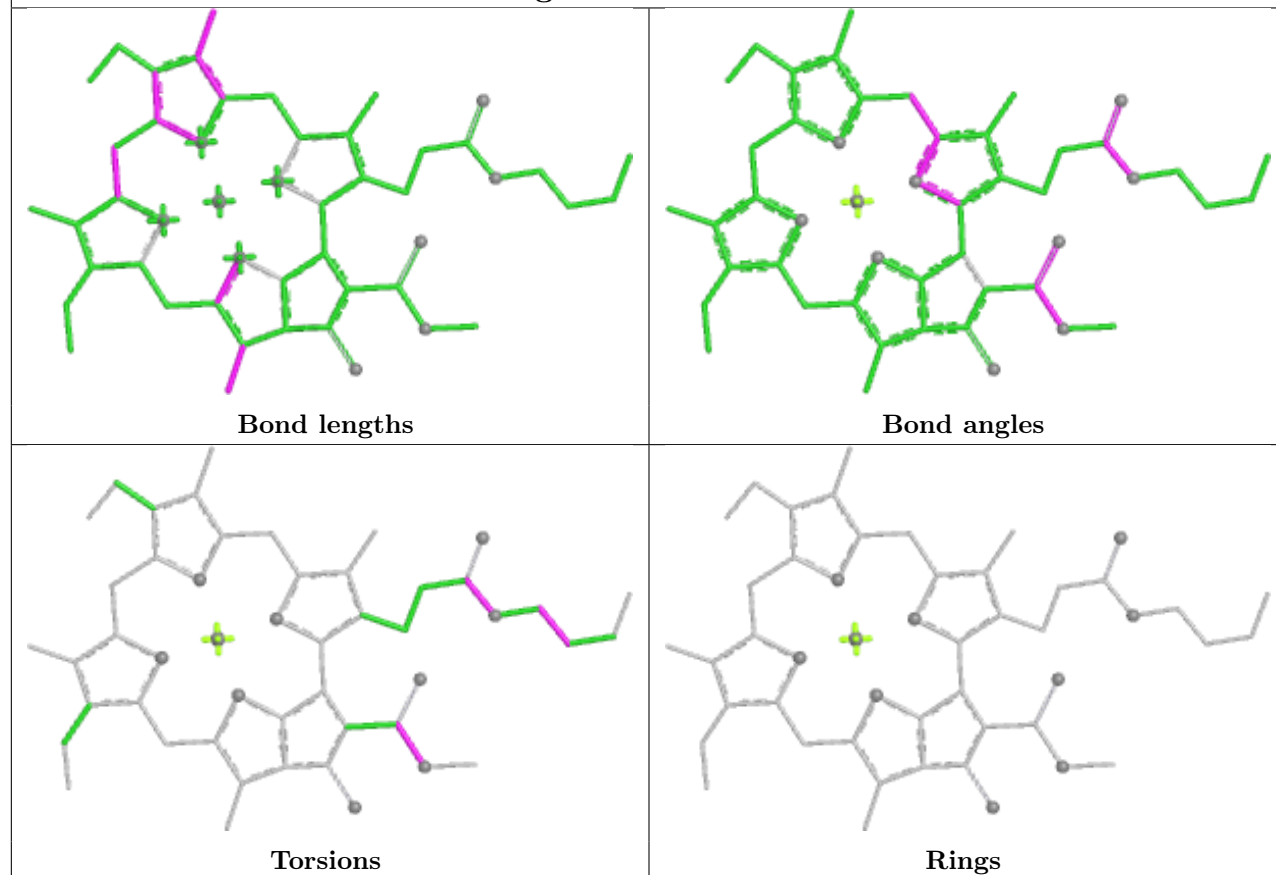




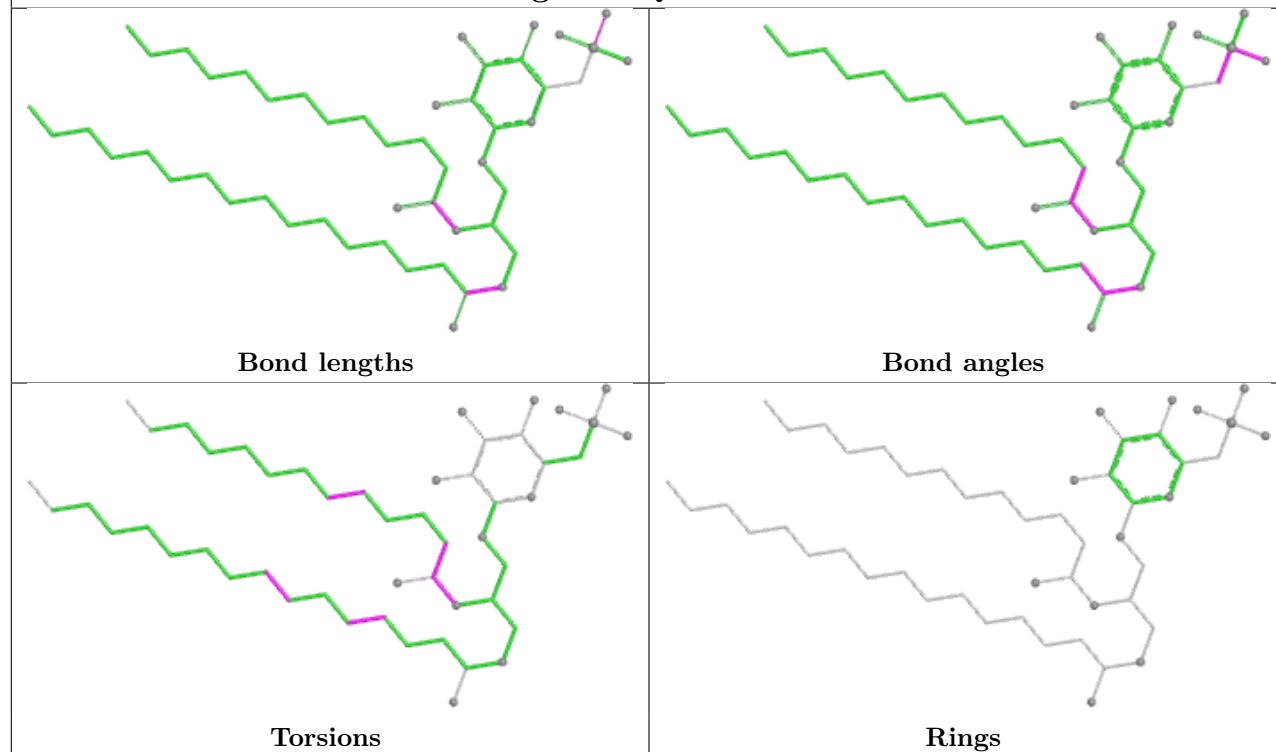
Ligand CLA d 403**Ligand CLA b 502**

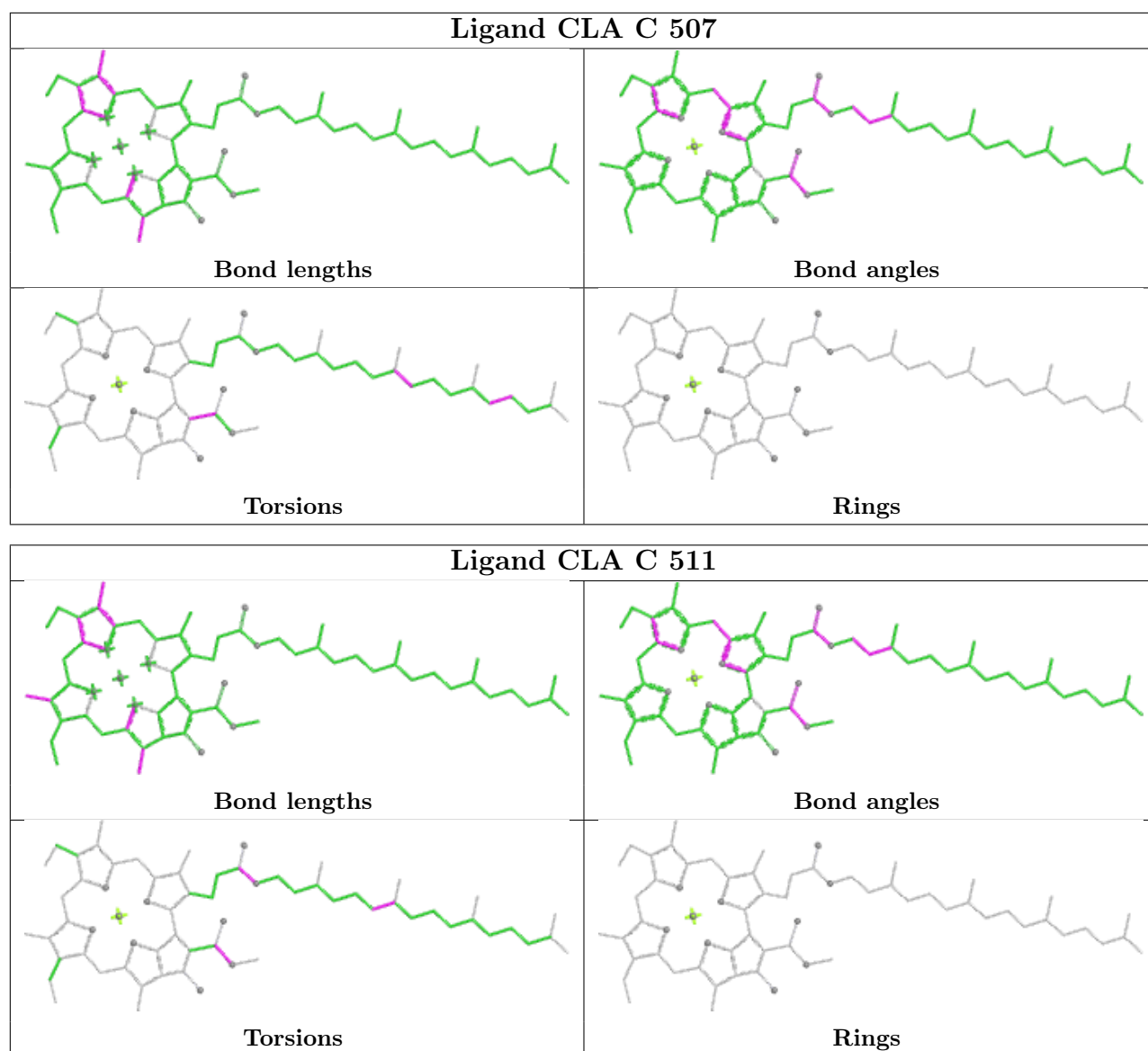


Ligand CLA S 604

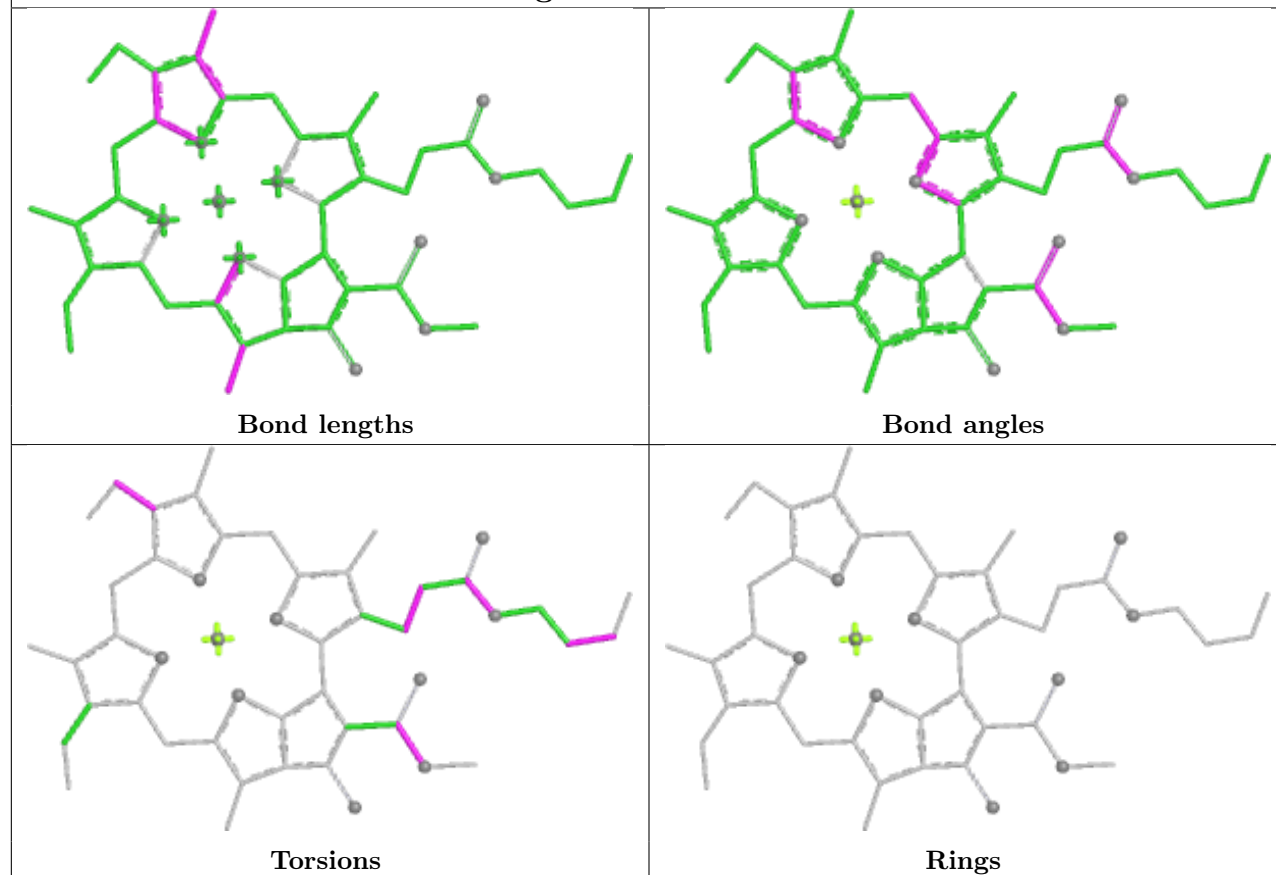


Ligand SQD A 407

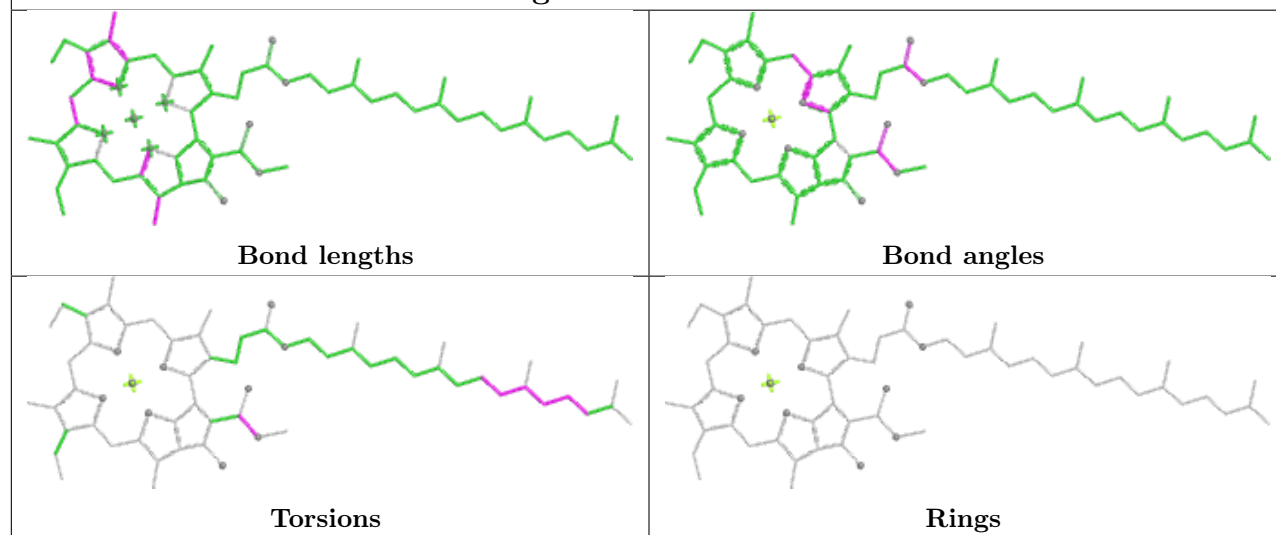




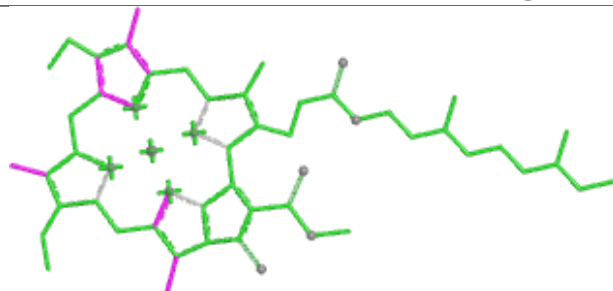
Ligand CLA S 613



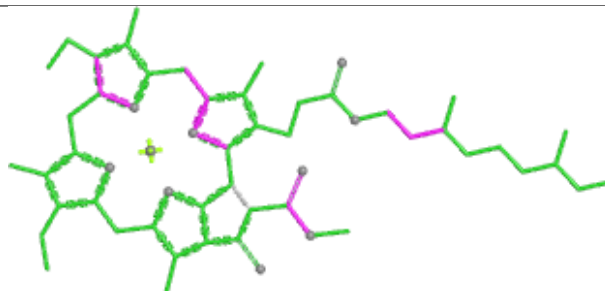
Ligand CLA C 504



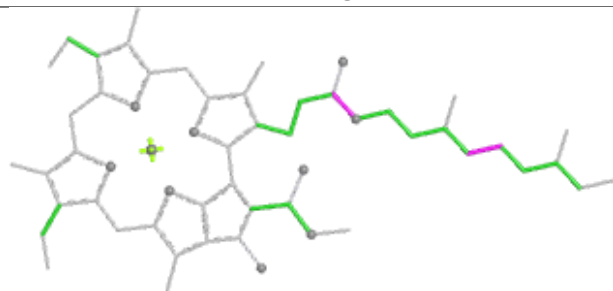
Ligand CLA c 512



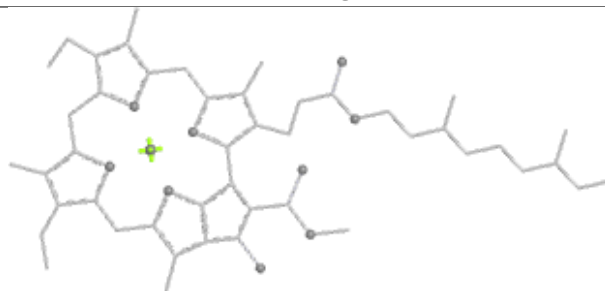
Bond lengths



Bond angles

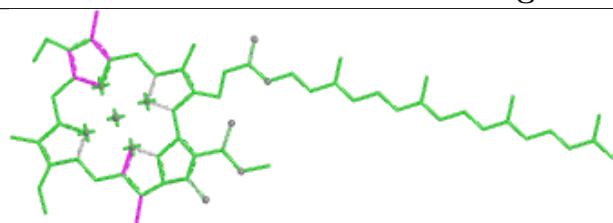


Torsions

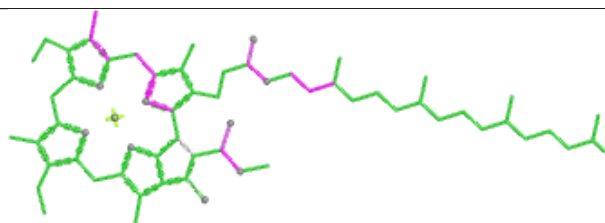


Rings

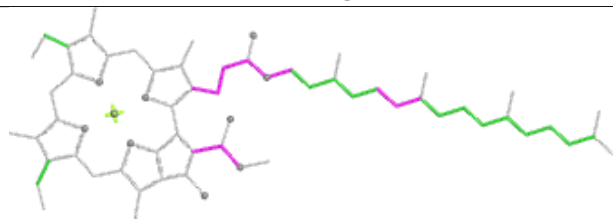
Ligand CLA b 509



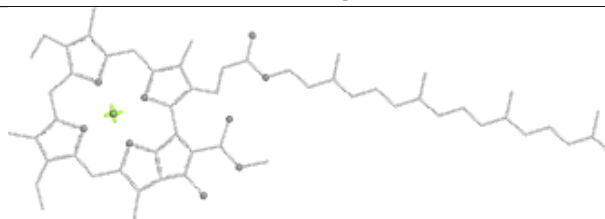
Bond lengths



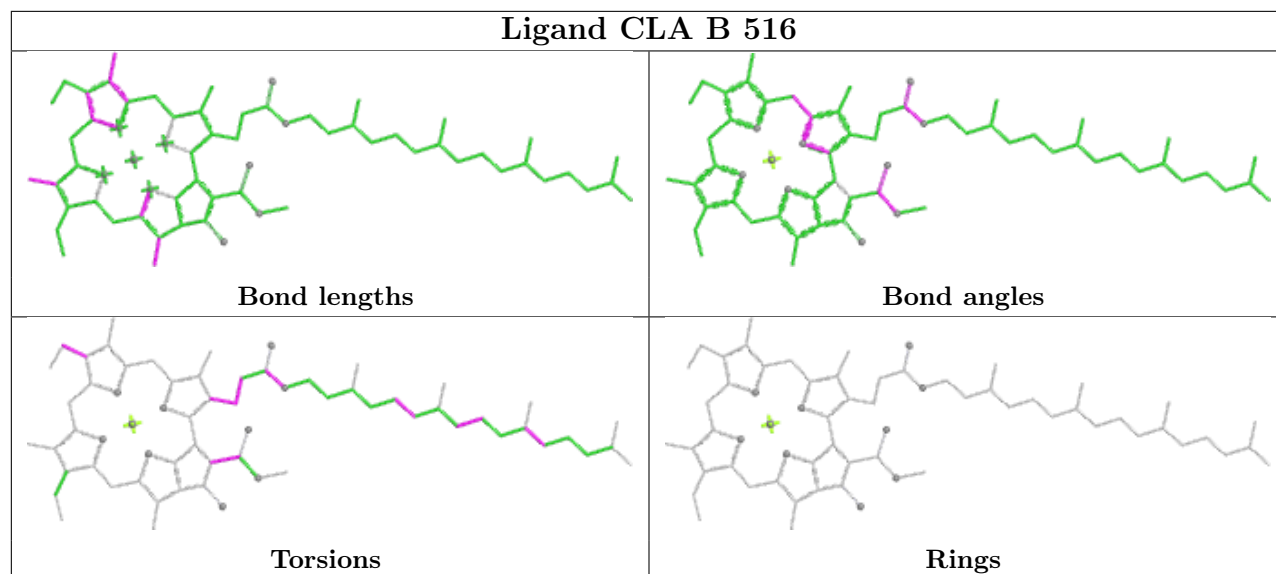
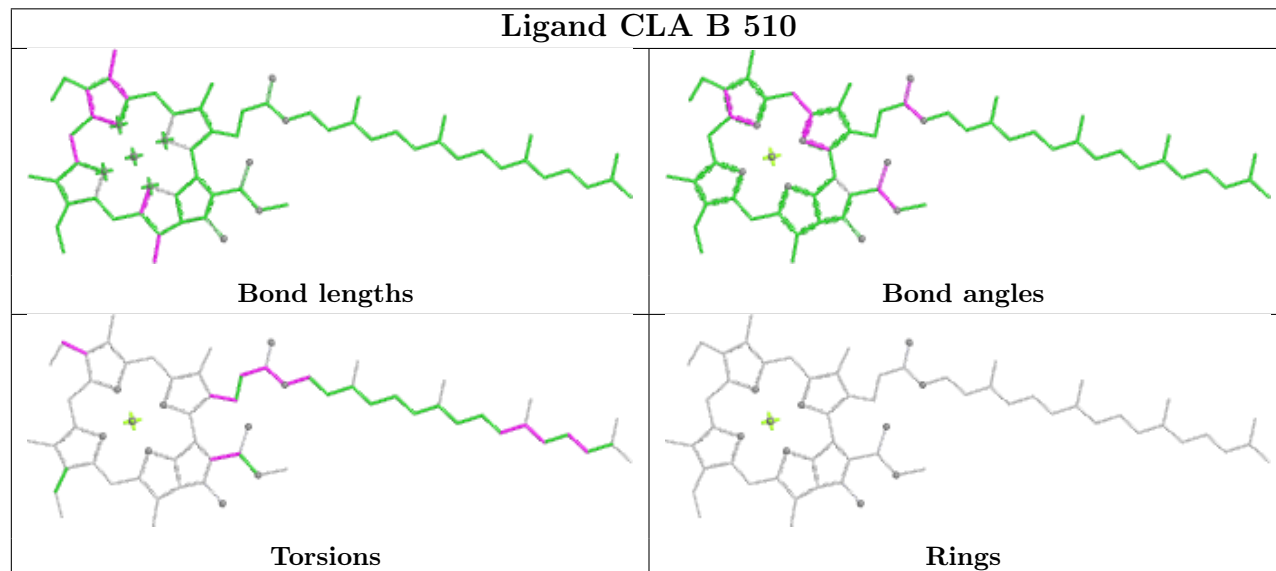
Bond angles

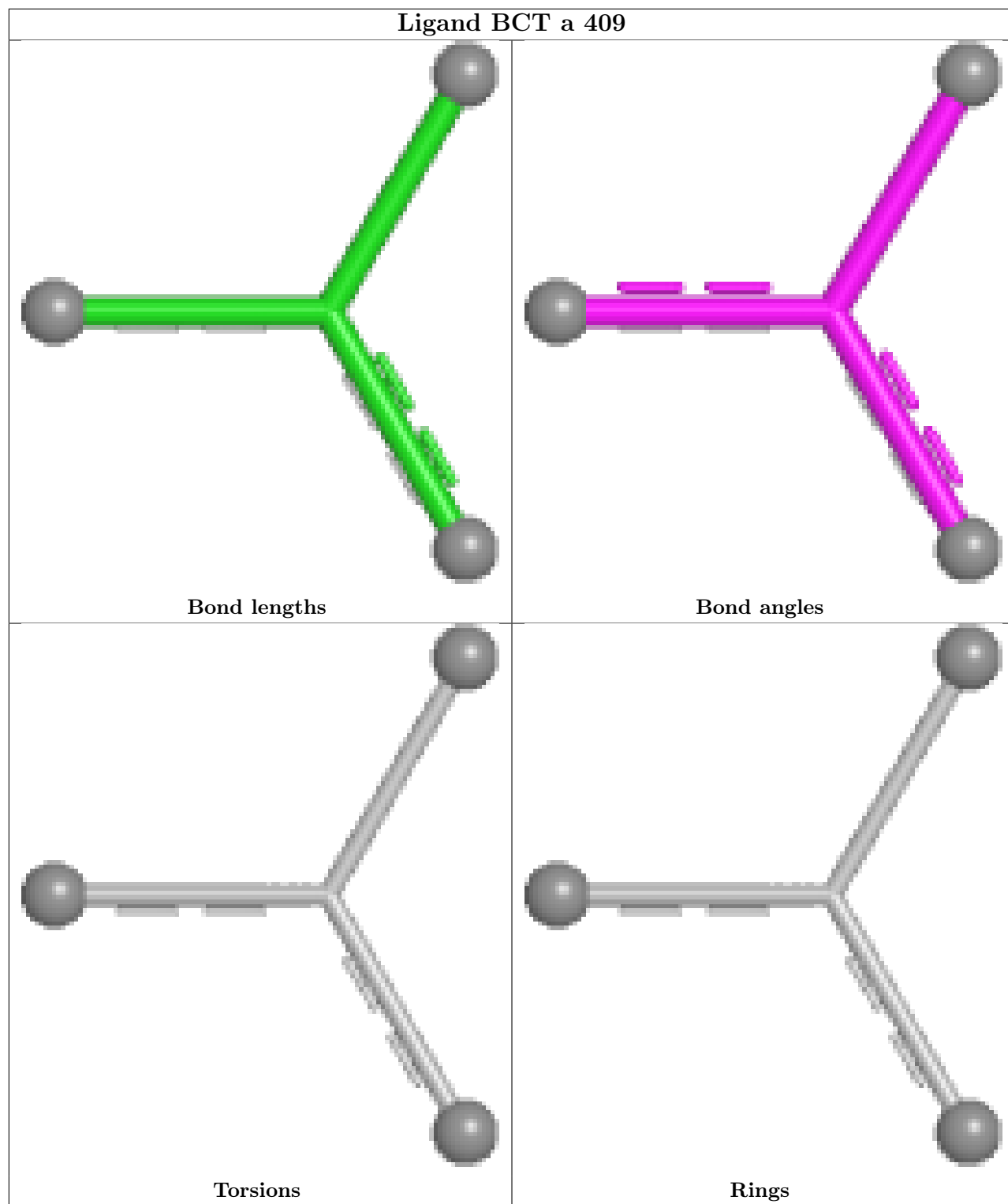


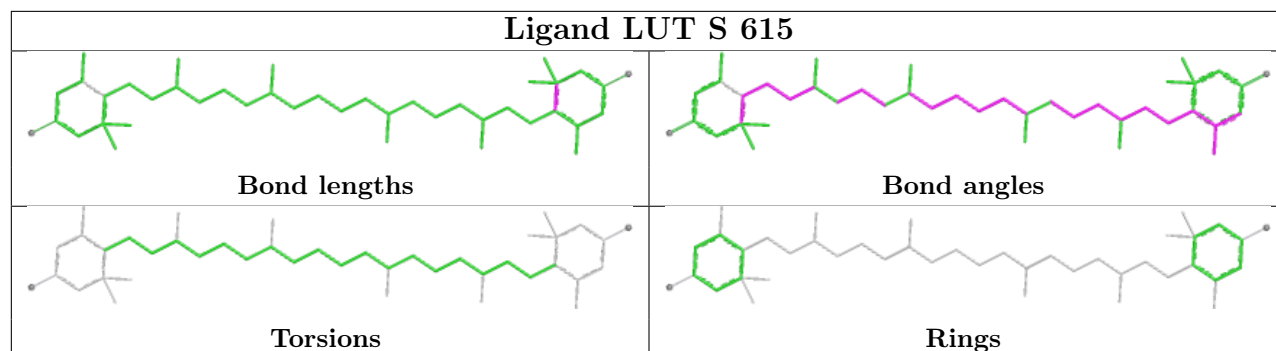
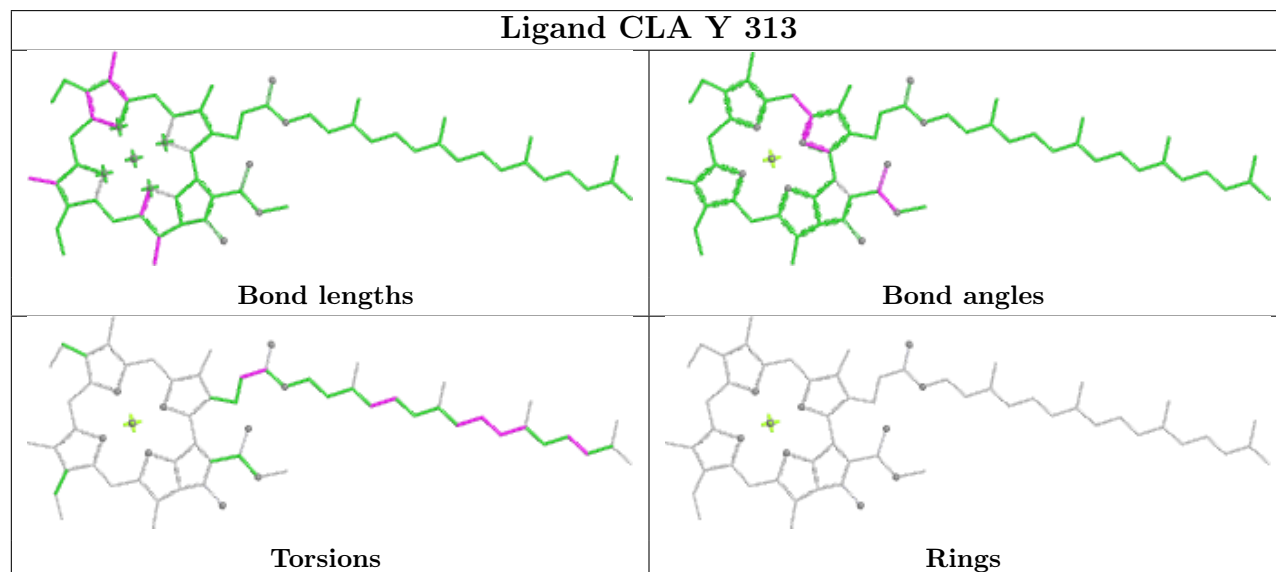
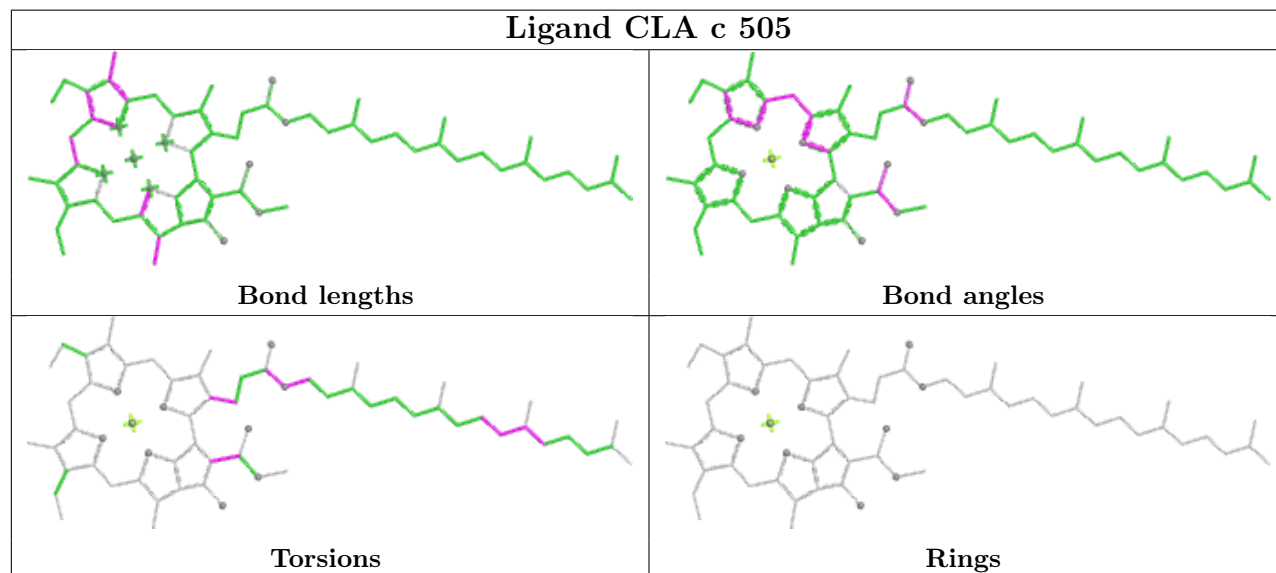
Torsions

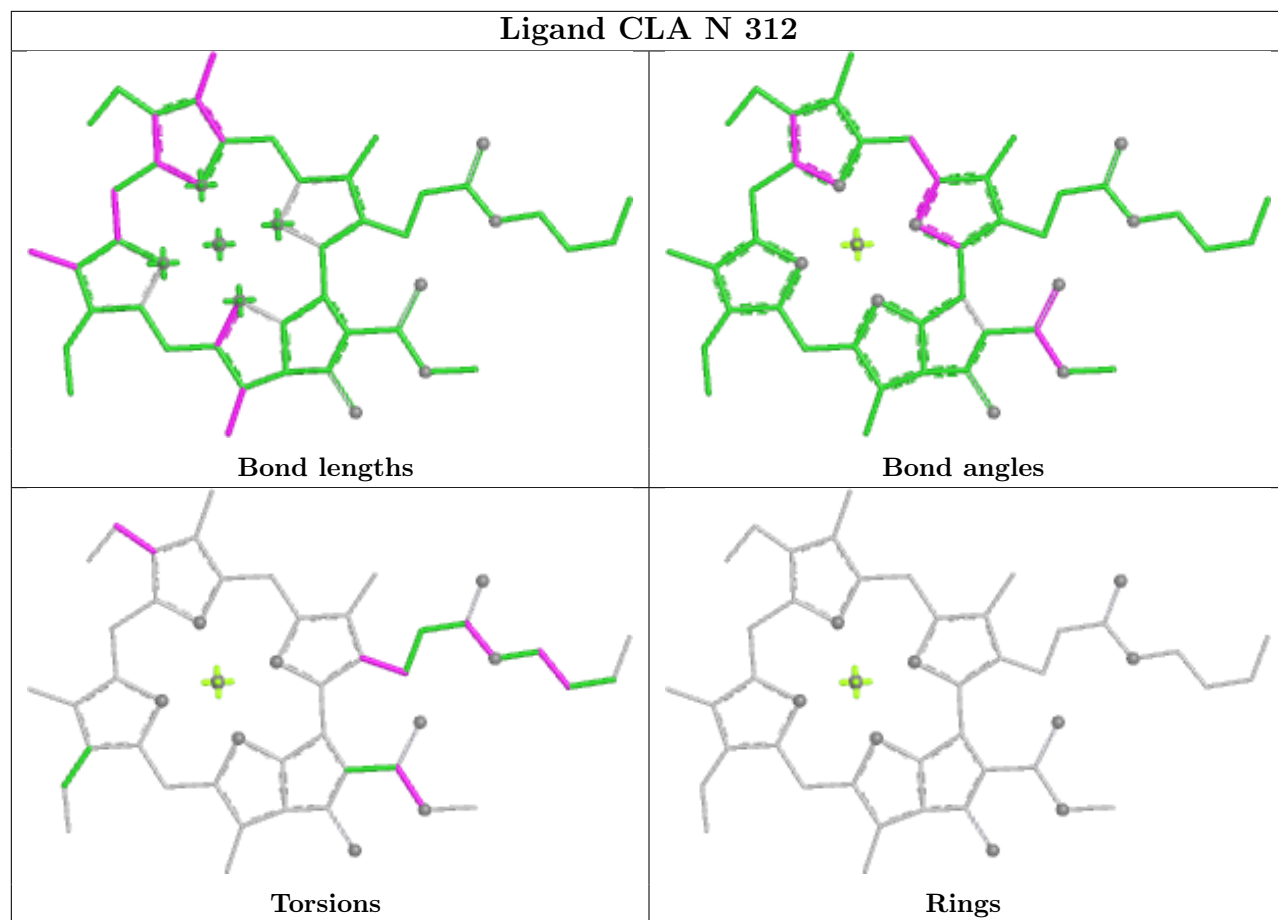


Rings

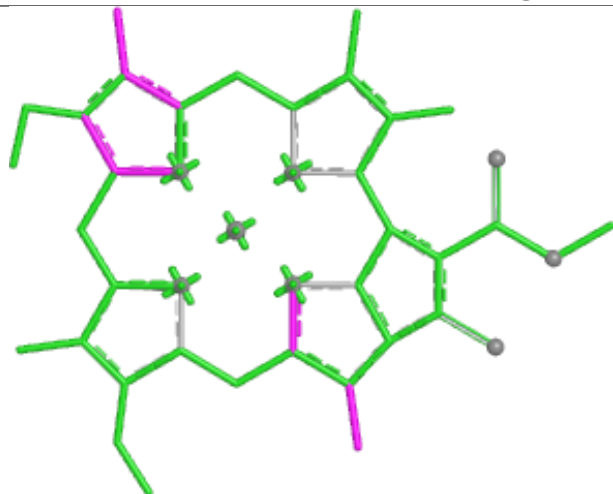
Ligand CLA B 516**Ligand CLA B 510**



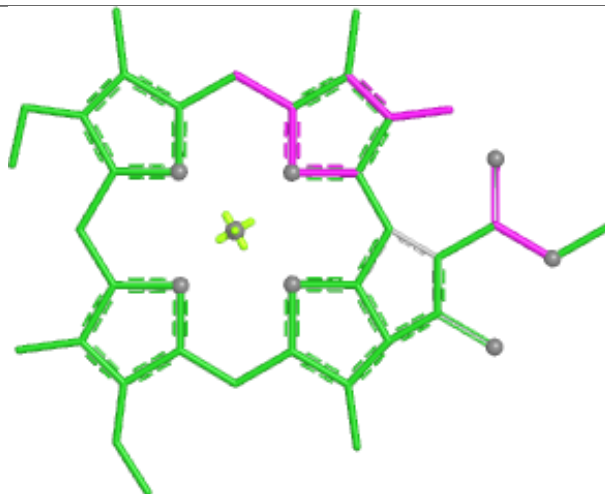
Ligand LUT S 615**Ligand CLA Y 313****Ligand CLA c 505**



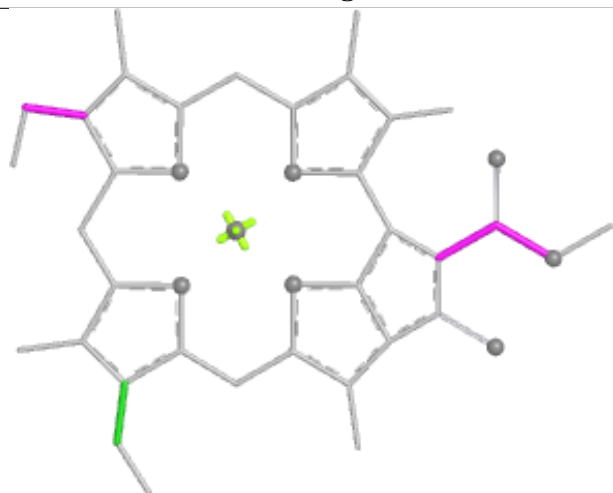
Ligand CLA S 609



Bond lengths



Bond angles

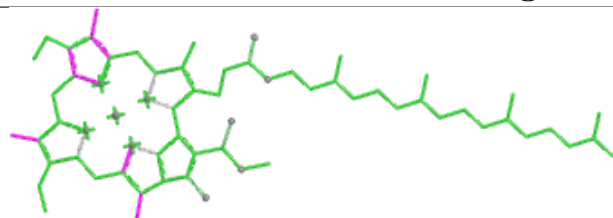


Torsions

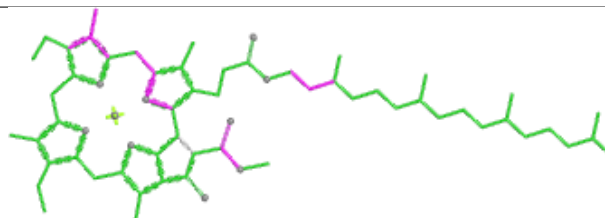


Rings

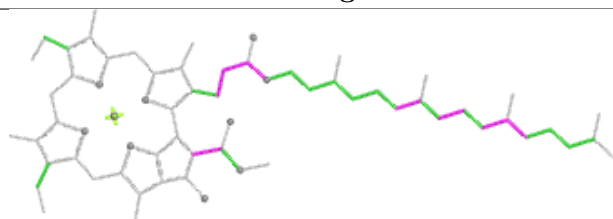
Ligand CLA c 509



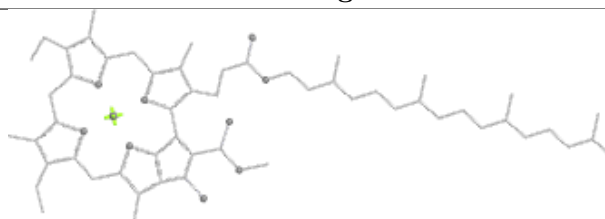
Bond lengths



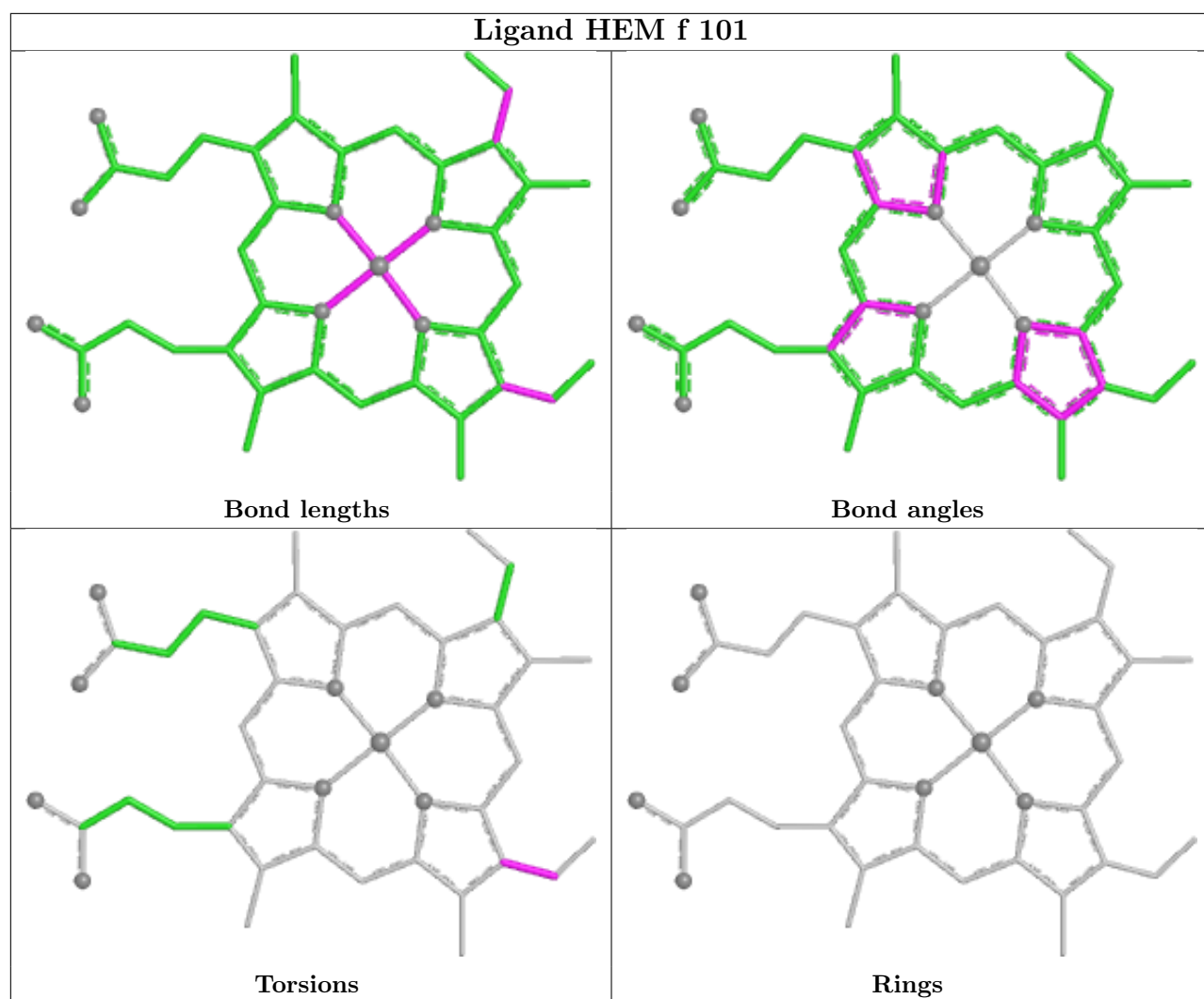
Bond angles



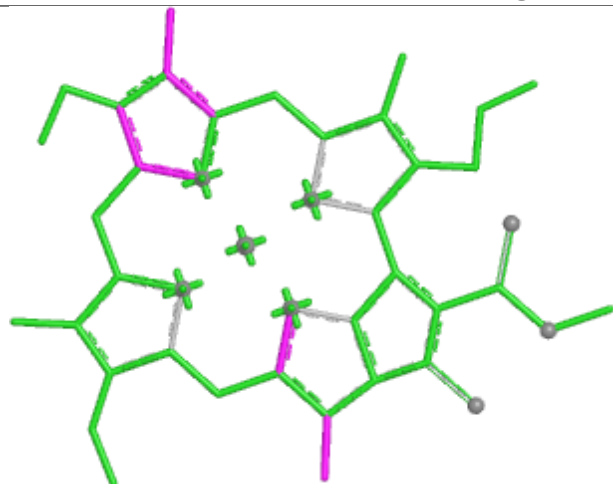
Torsions



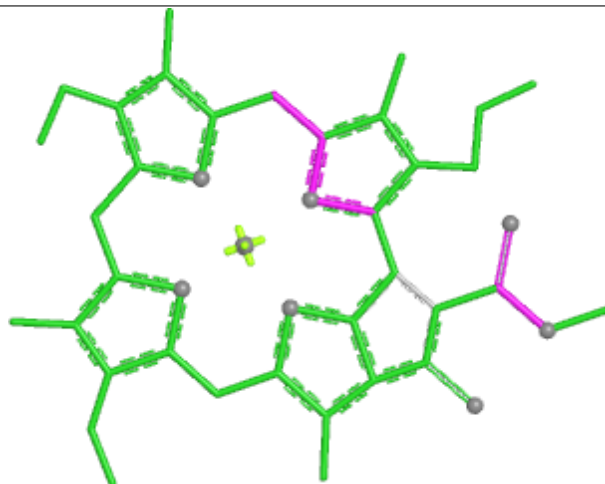
Rings



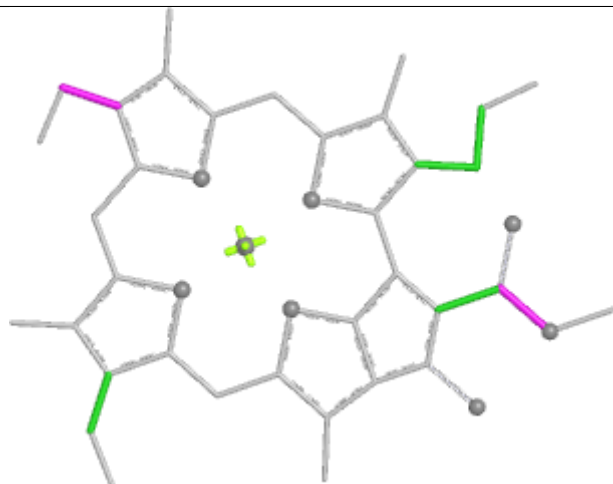
Ligand CLA G 612



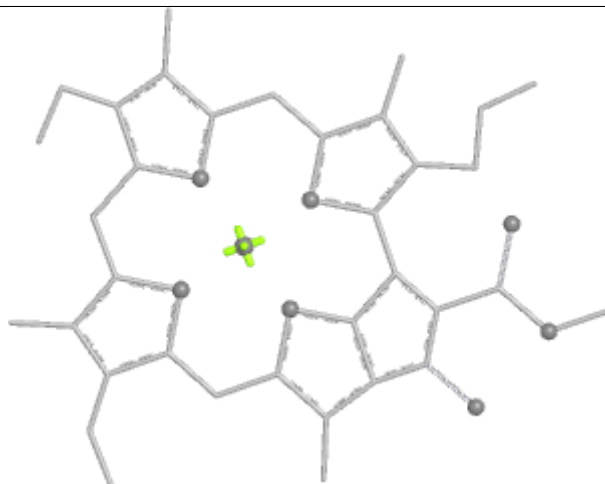
Bond lengths



Bond angles

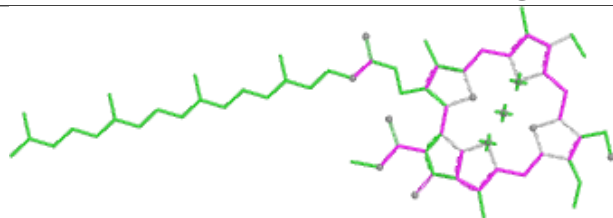


Torsions

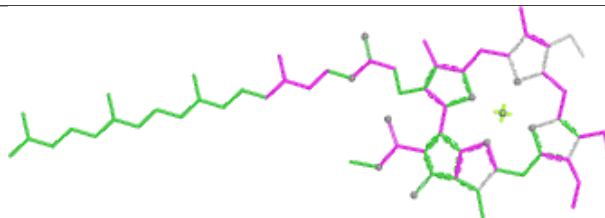


Rings

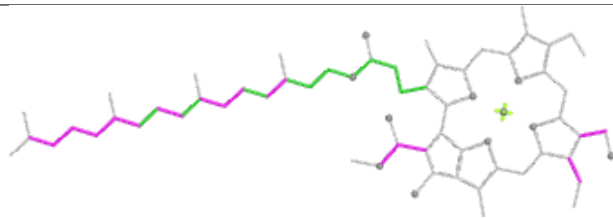
Ligand CHL Y 310



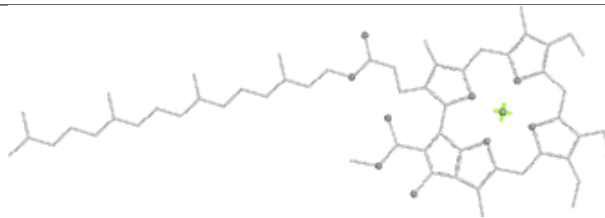
Bond lengths



Bond angles

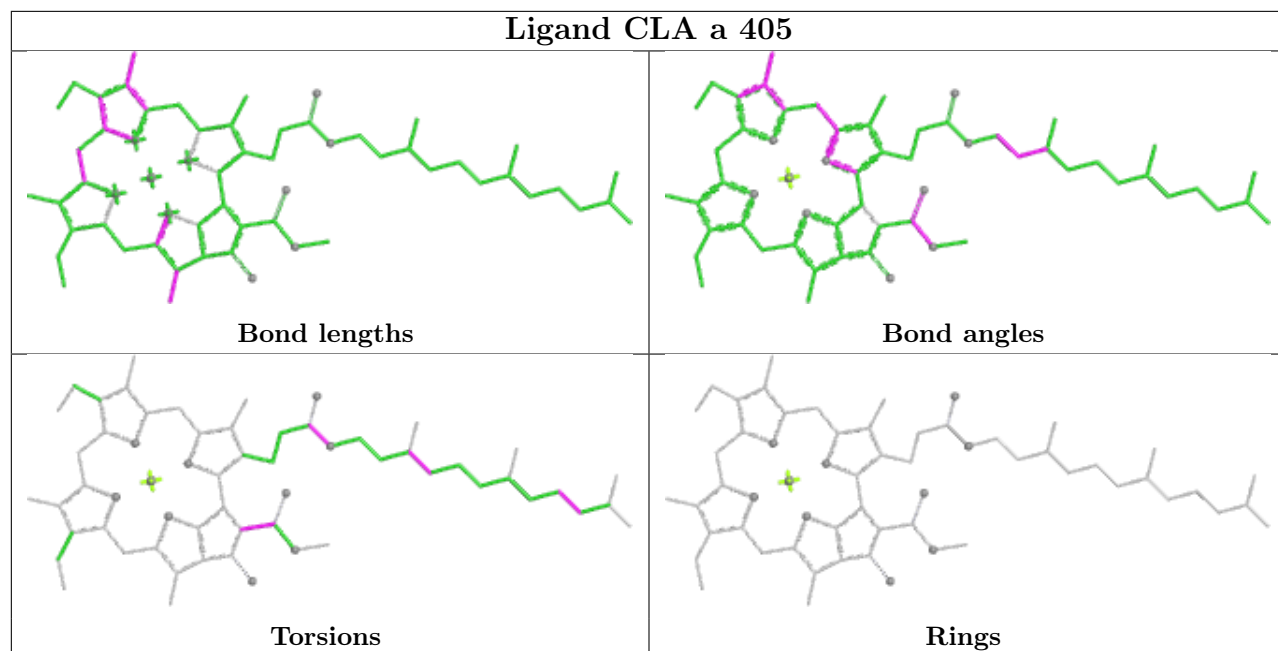


Torsions

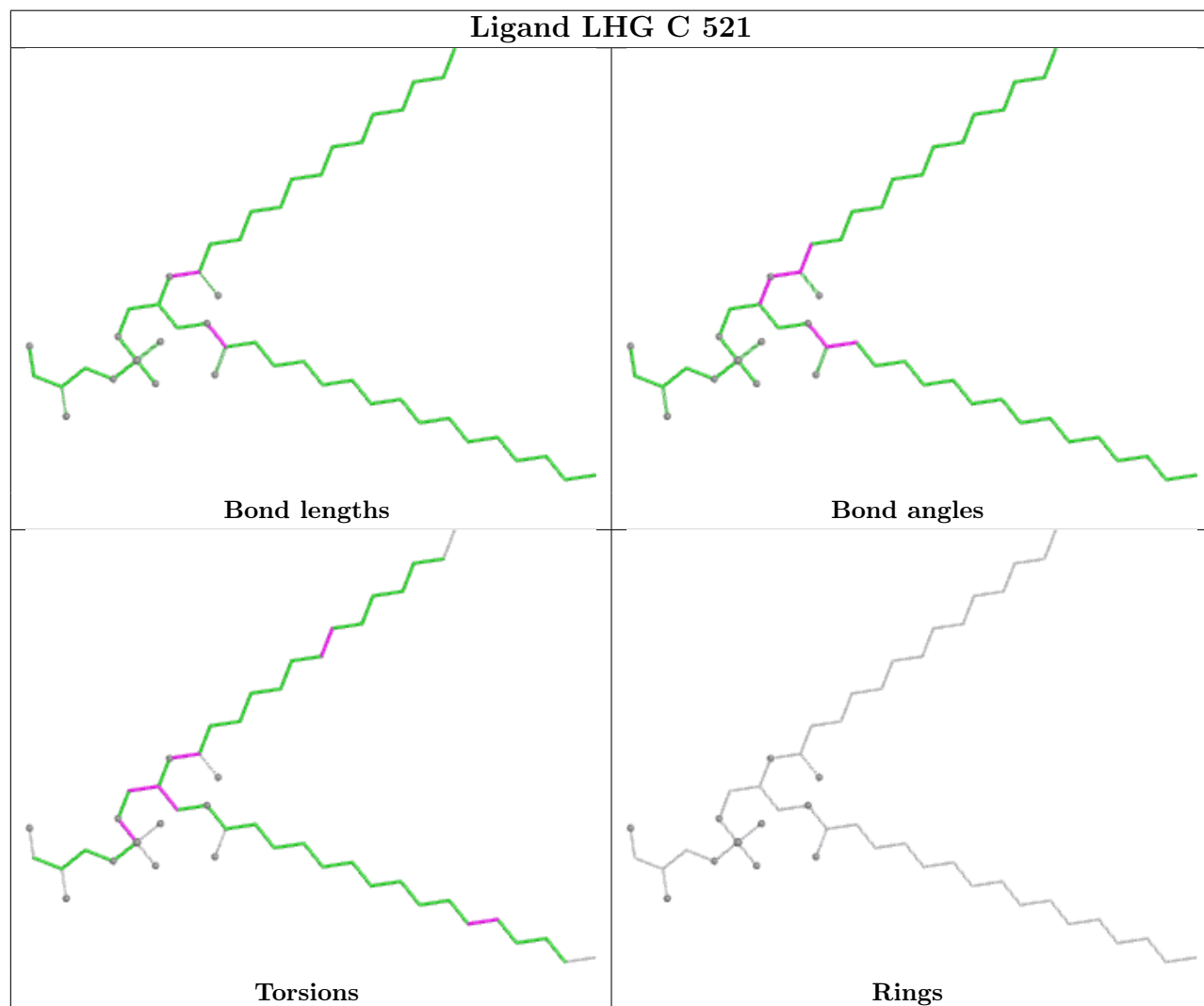


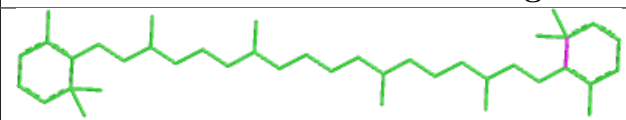
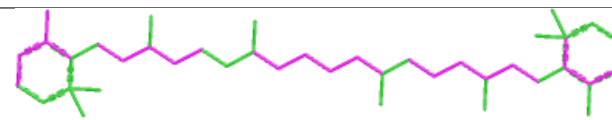
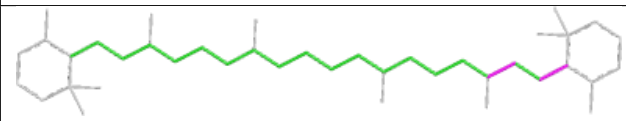
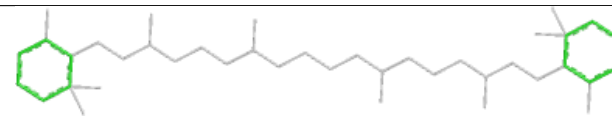
Rings

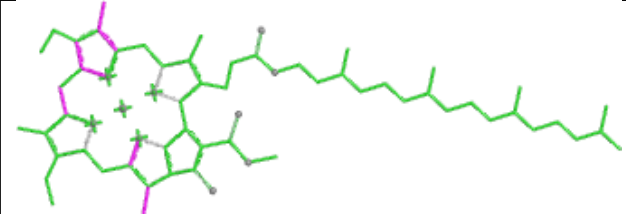
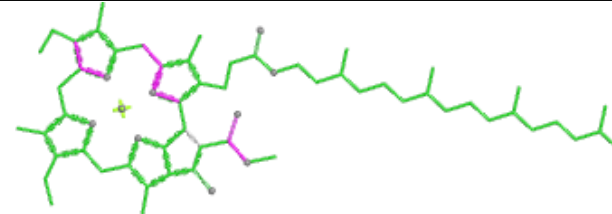
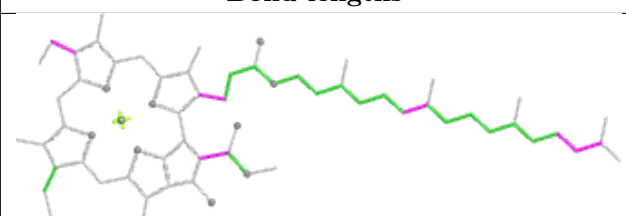
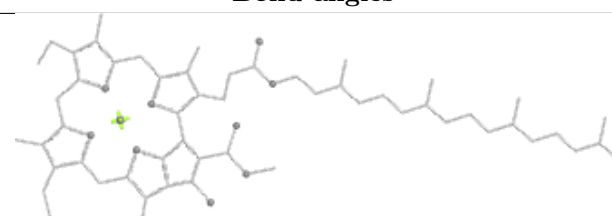
Ligand CLA a 405

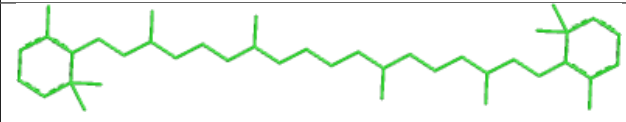
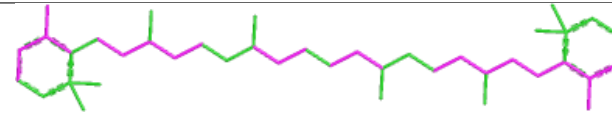
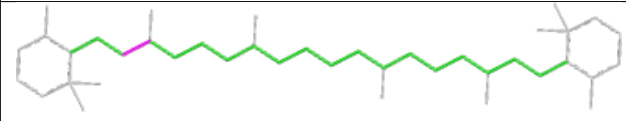
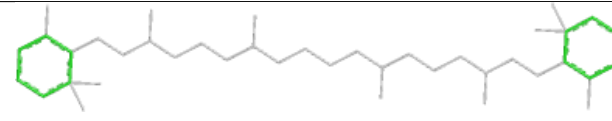


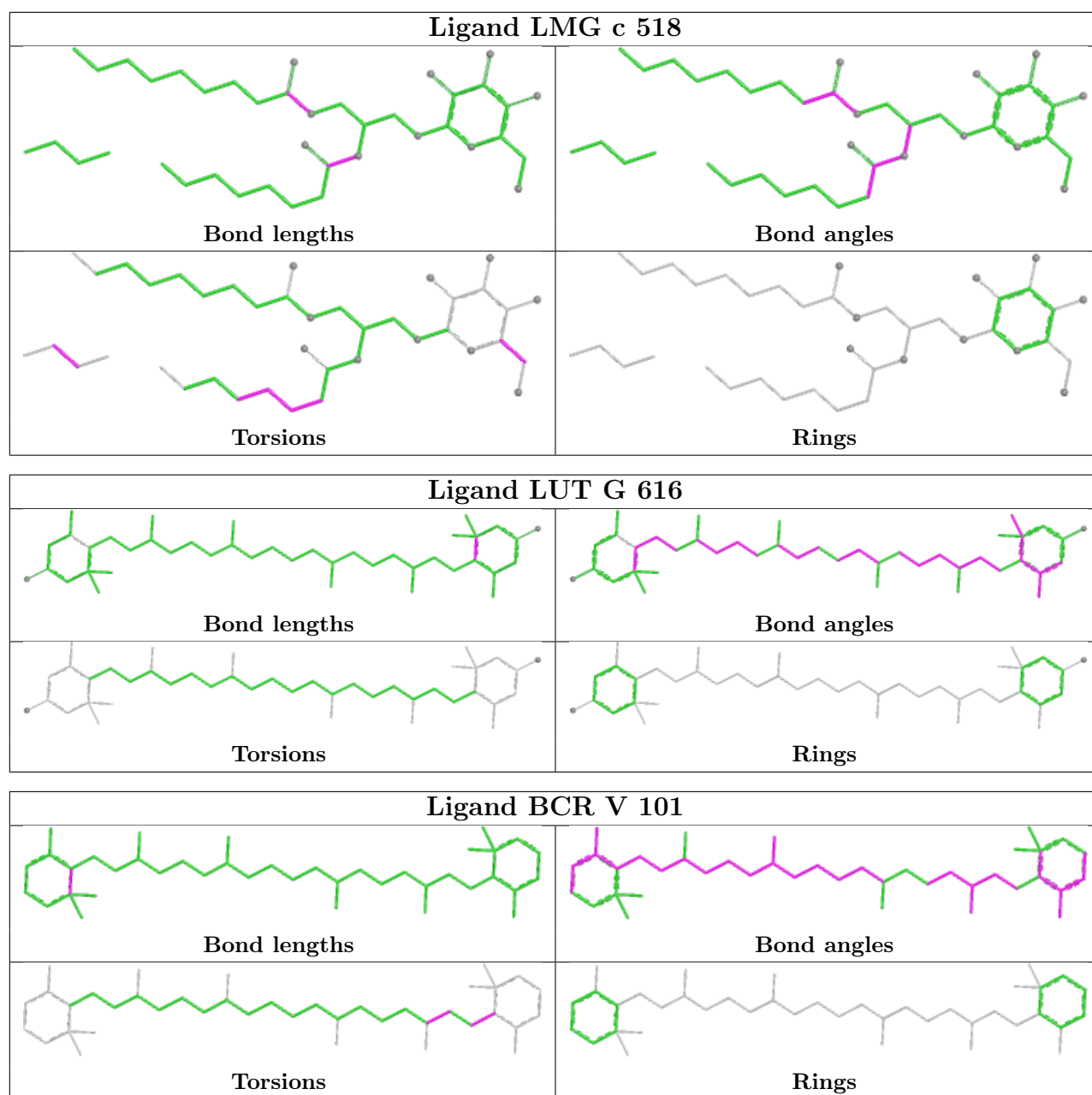
Ligand LHG C 521



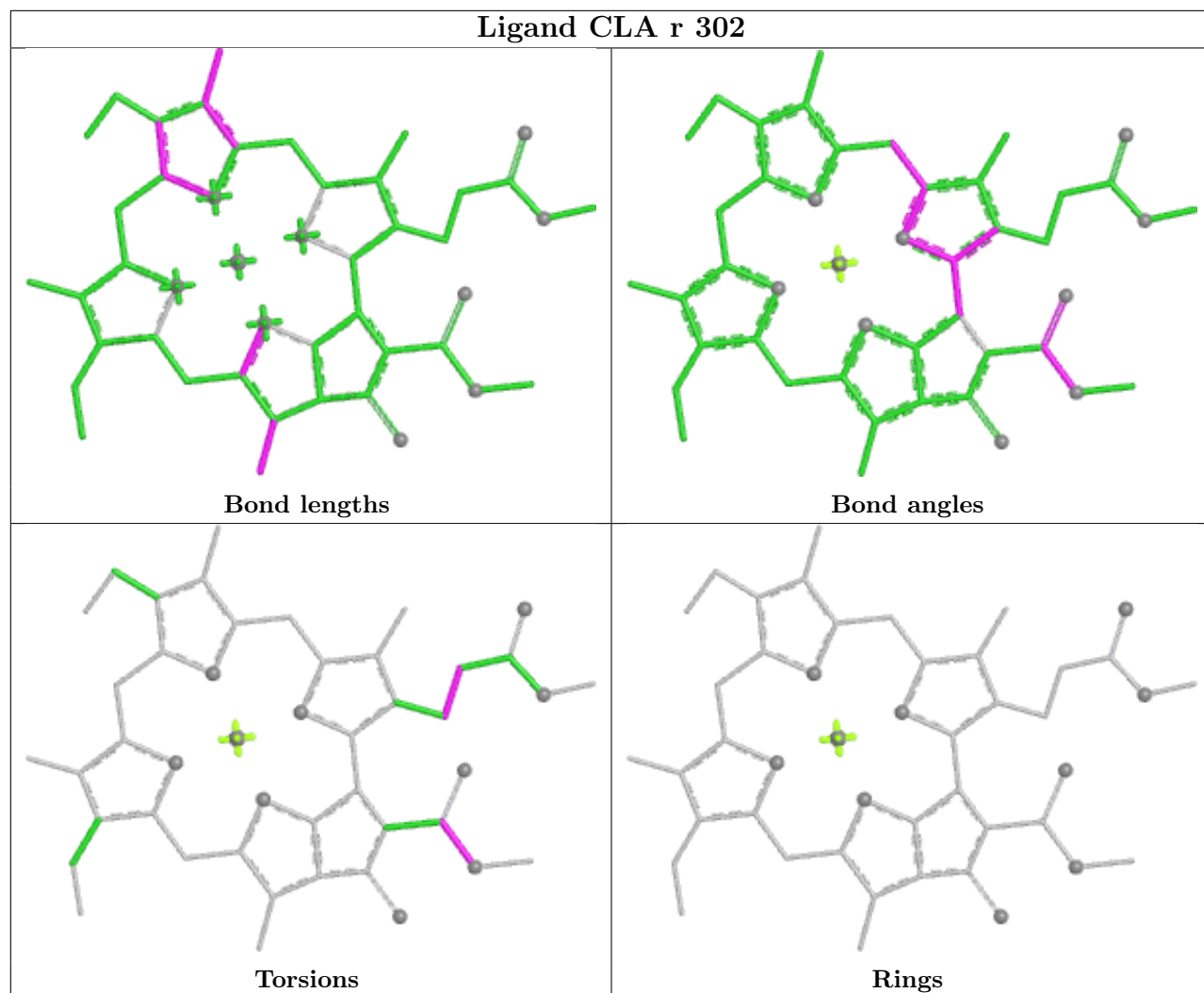
Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

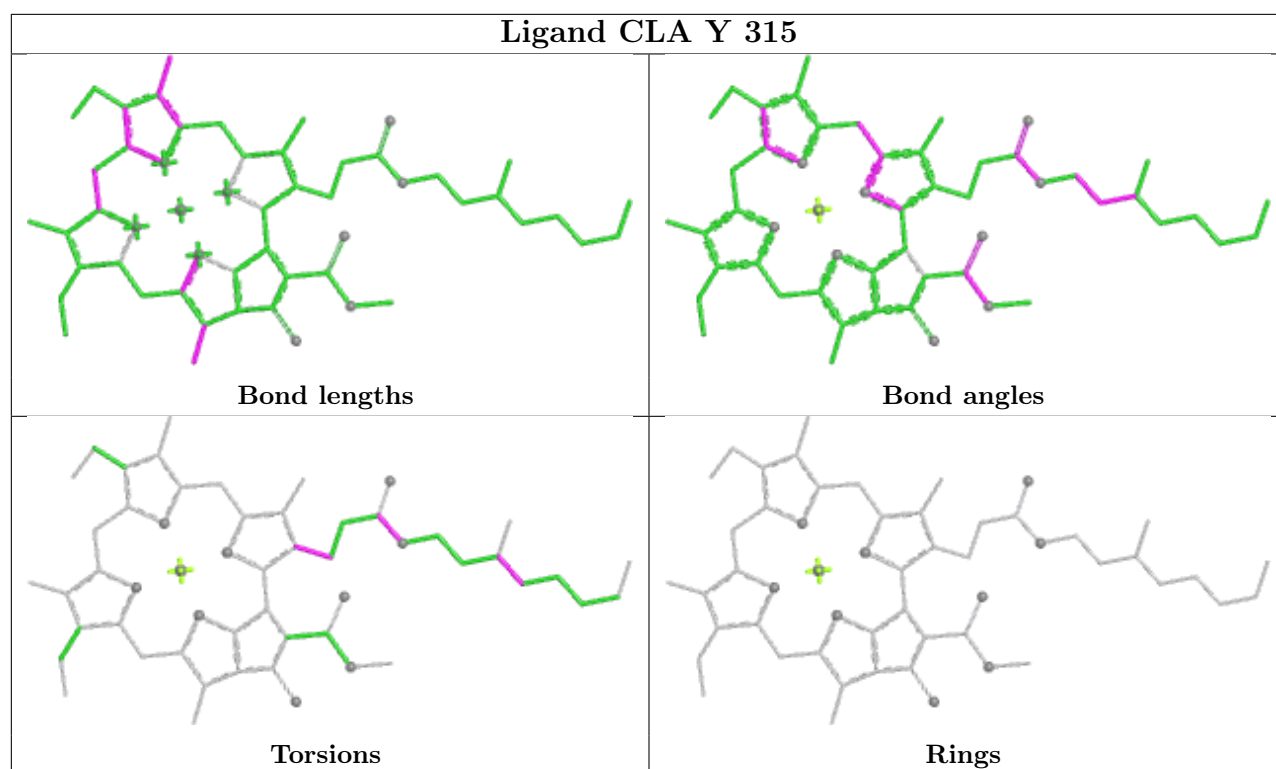
Ligand CLA N 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

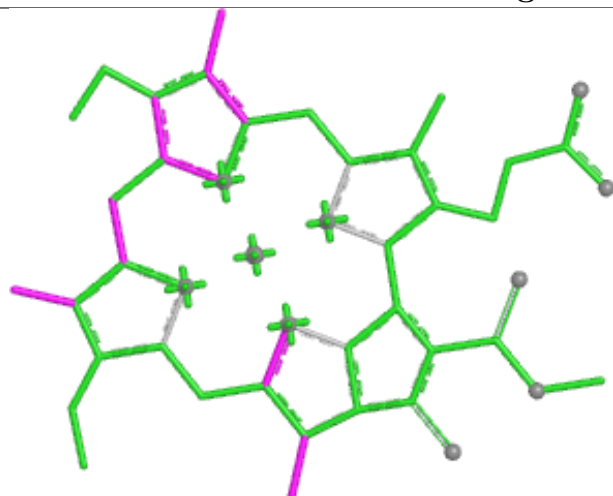


Ligand CLA r 302

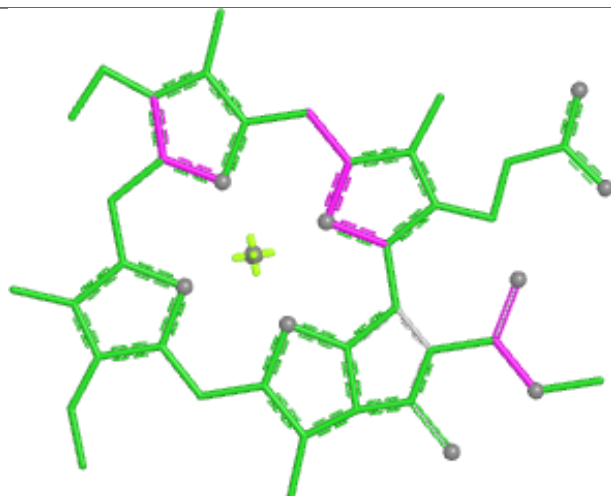




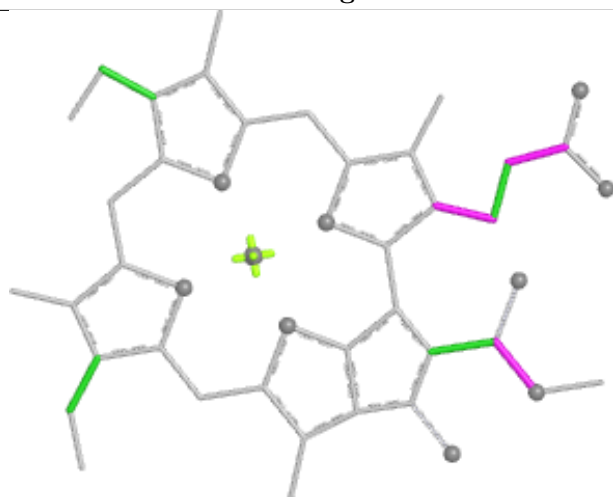
Ligand CLA b 514



Bond lengths



Bond angles

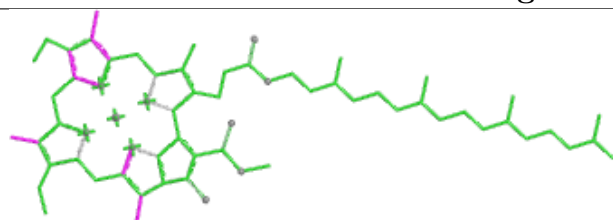


Torsions

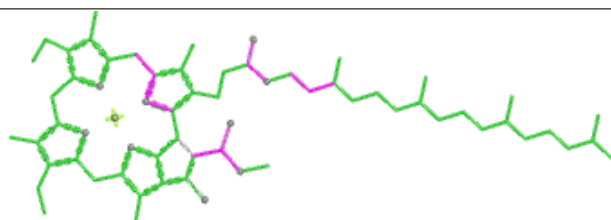


Rings

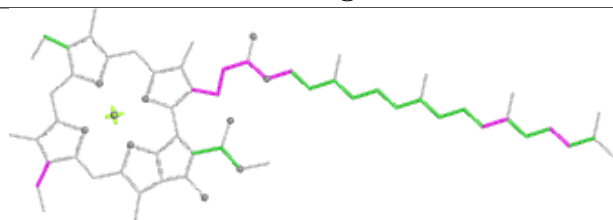
Ligand CLA d 401



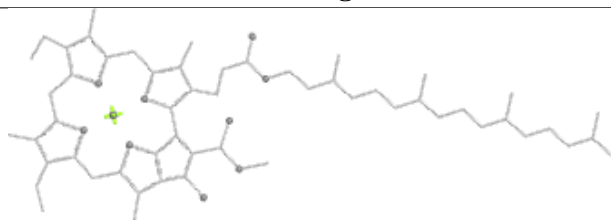
Bond lengths



Bond angles

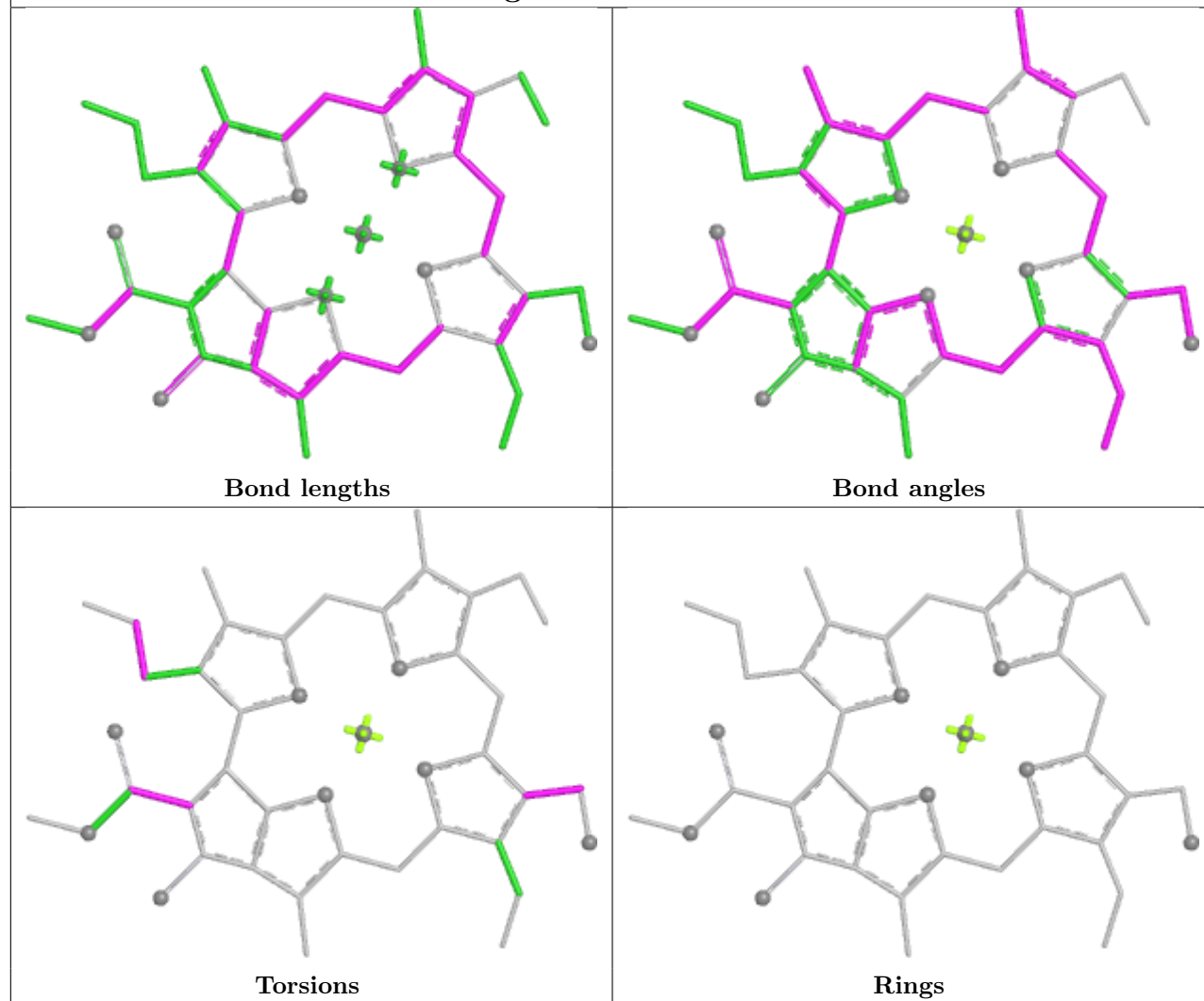


Torsions

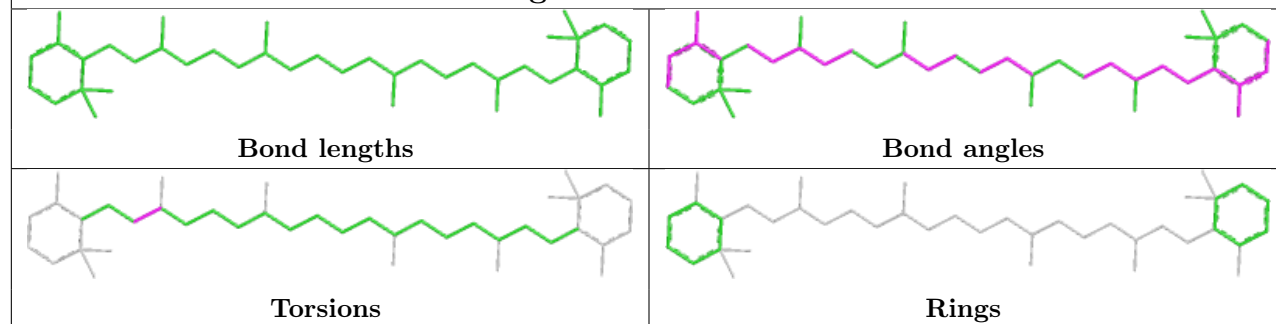


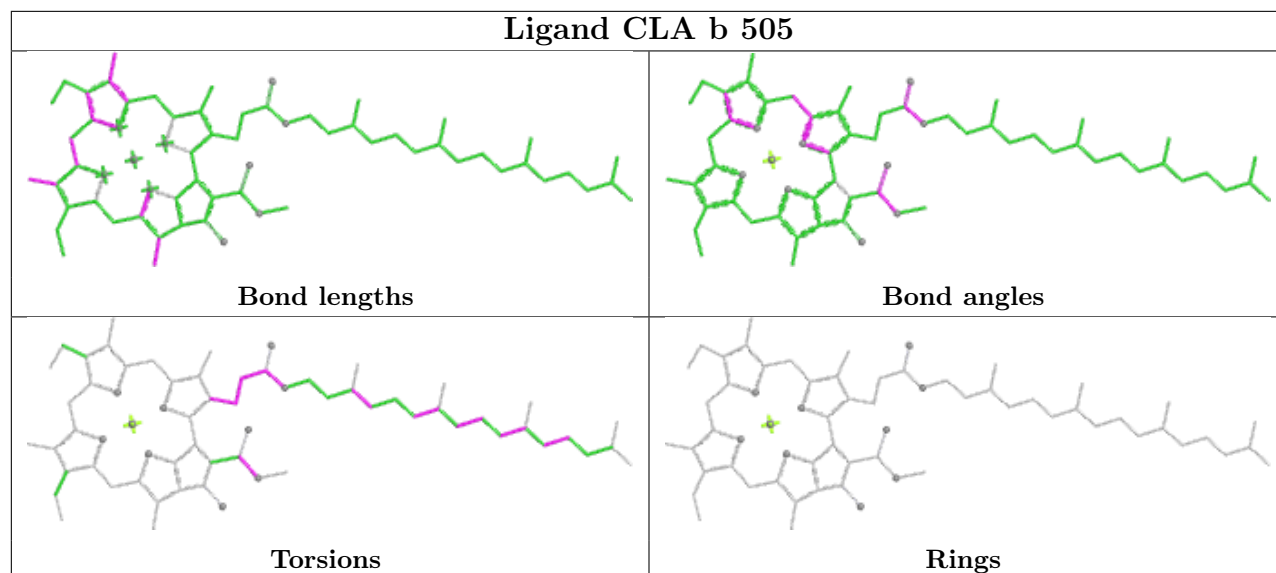
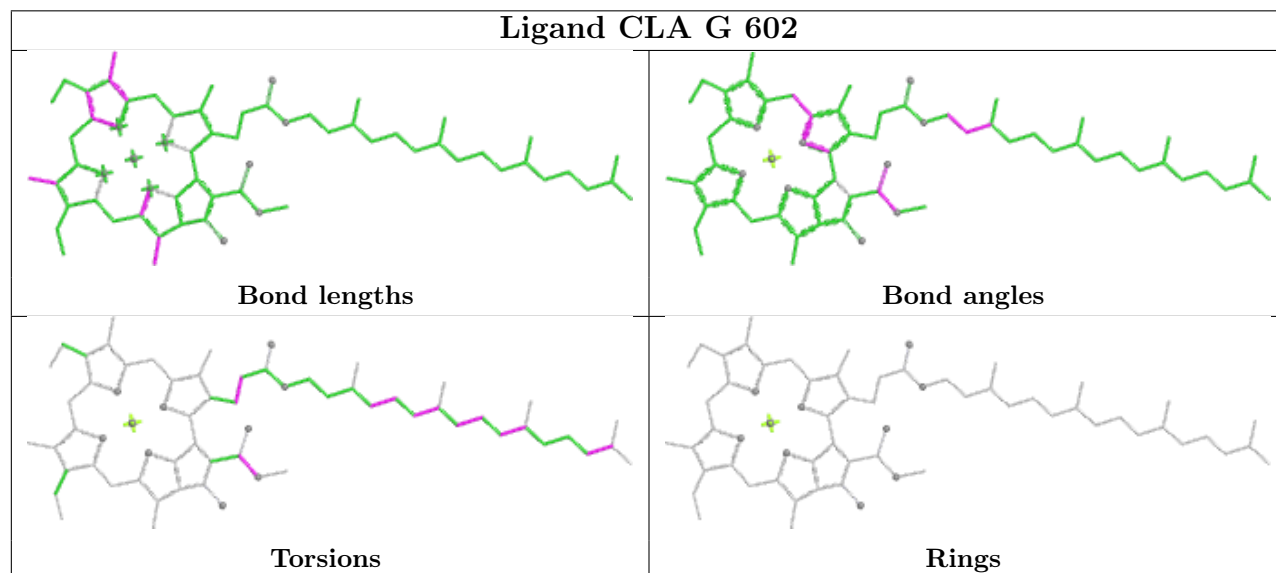
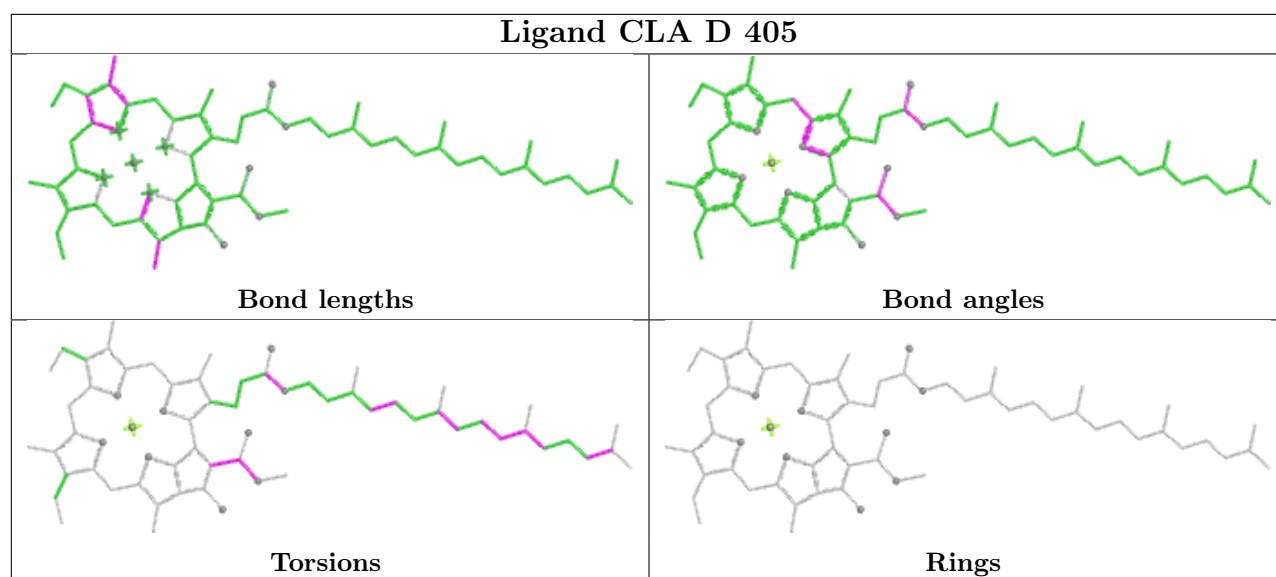
Rings

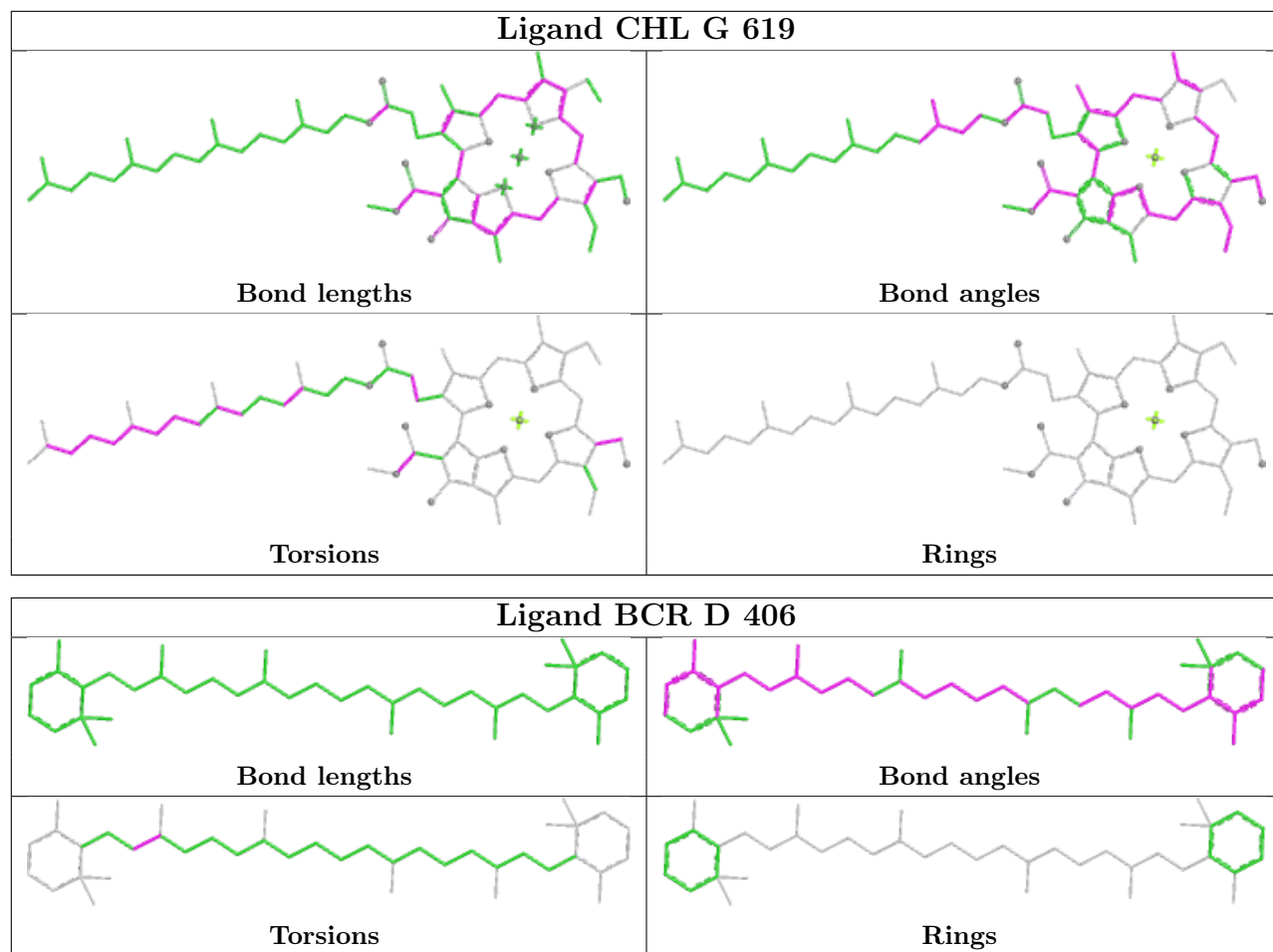
Ligand CHL S 606

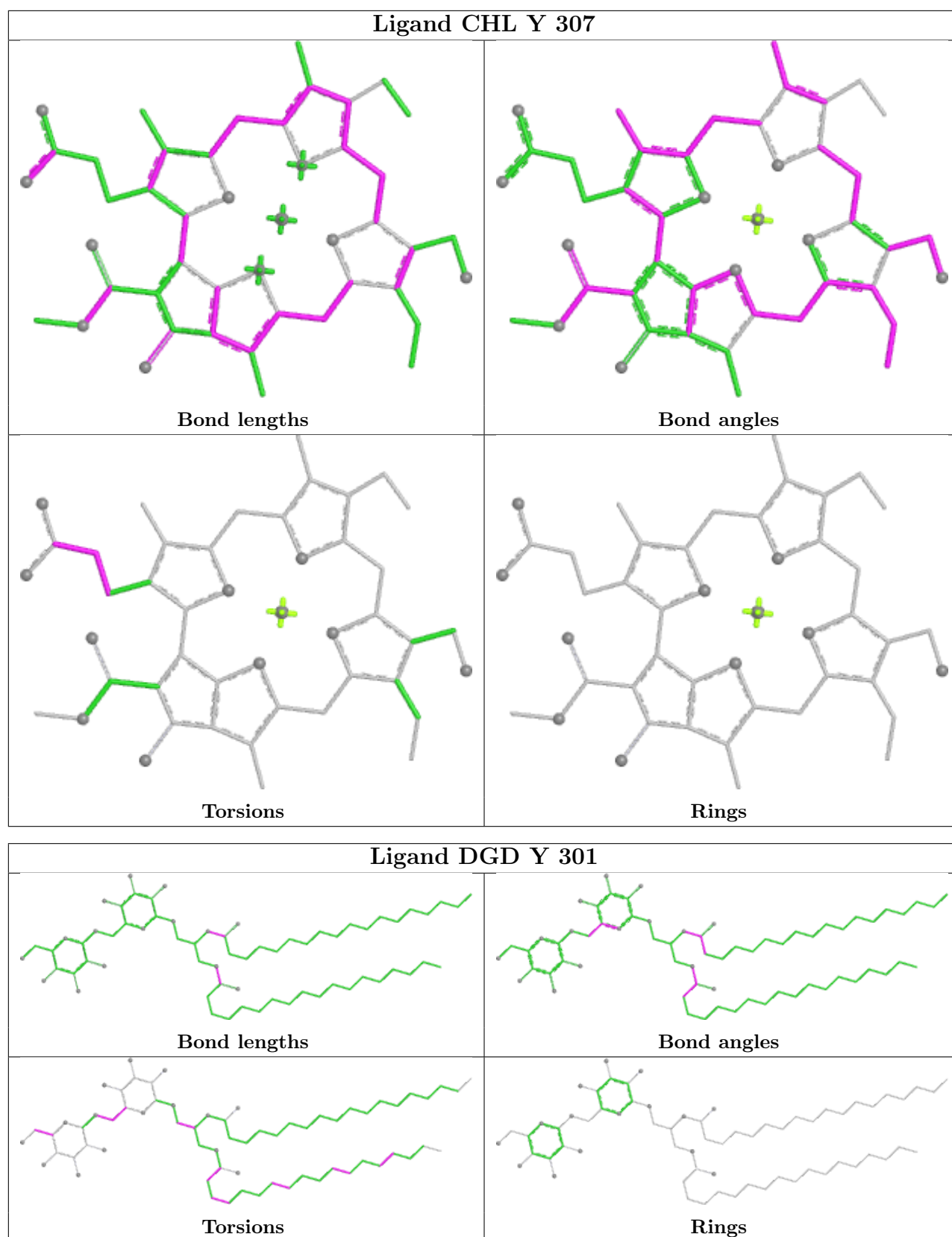


Ligand BCR H 101

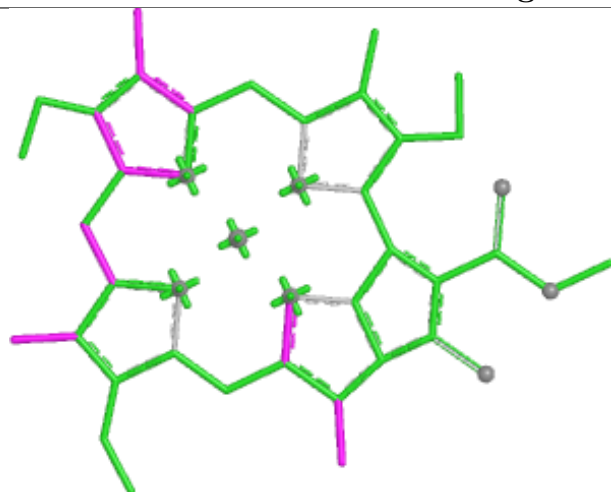




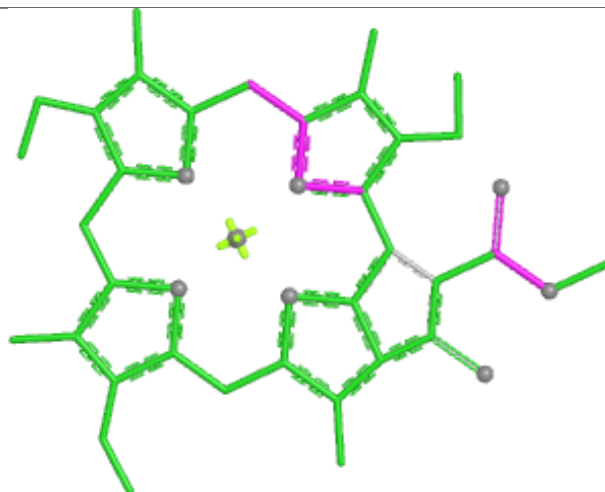




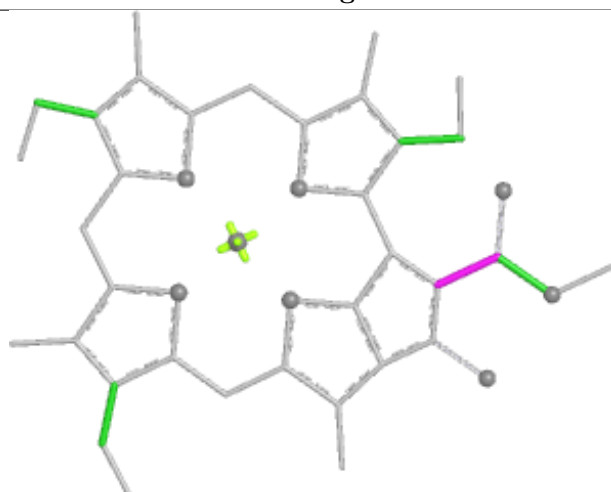
Ligand CLA S 603



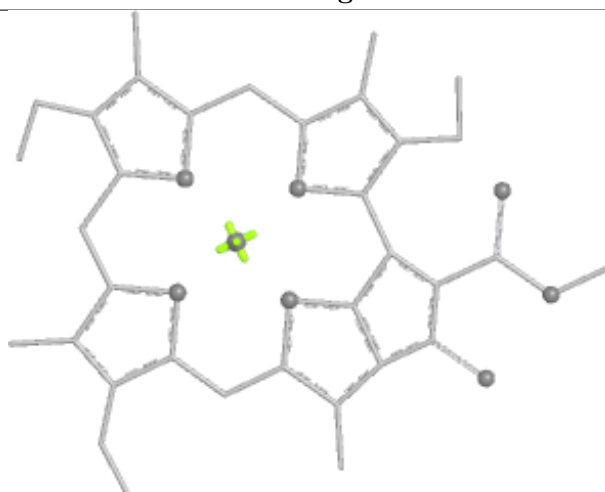
Bond lengths



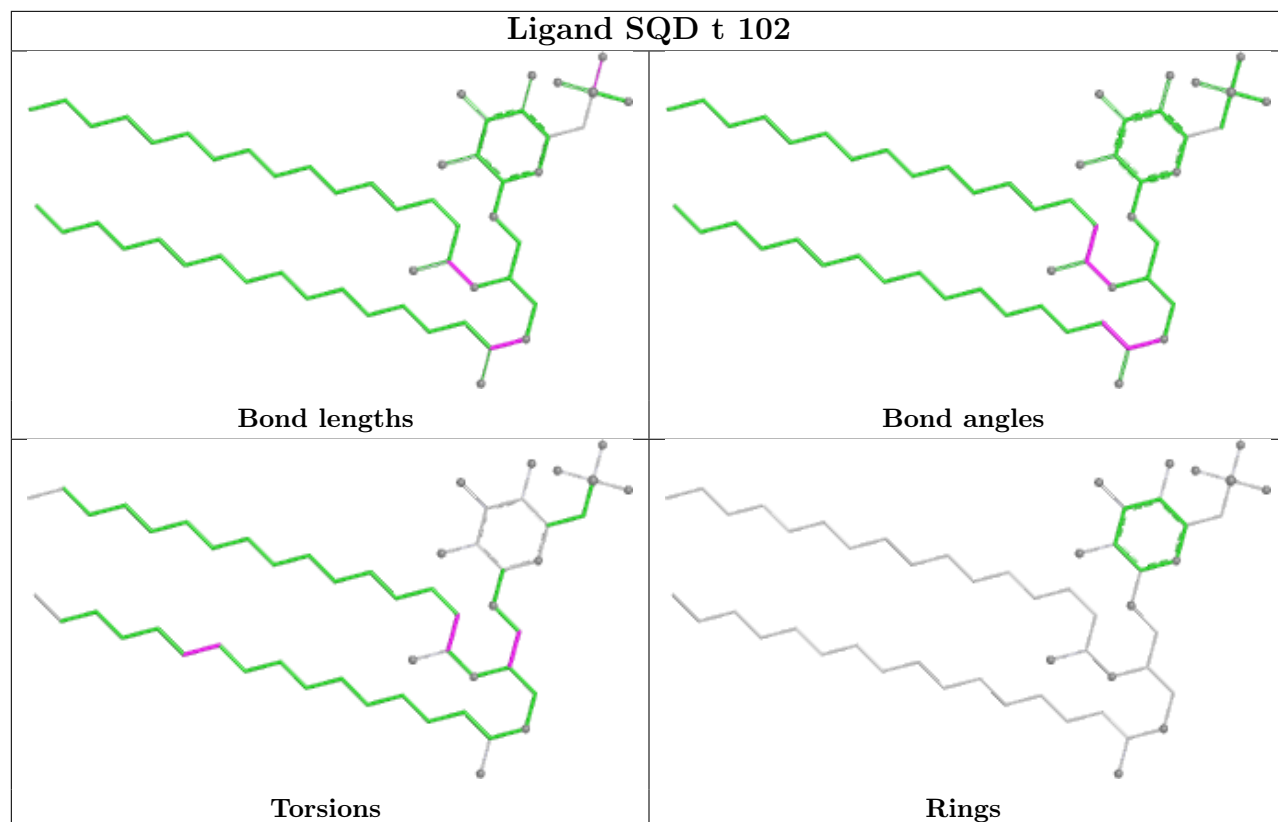
Bond angles

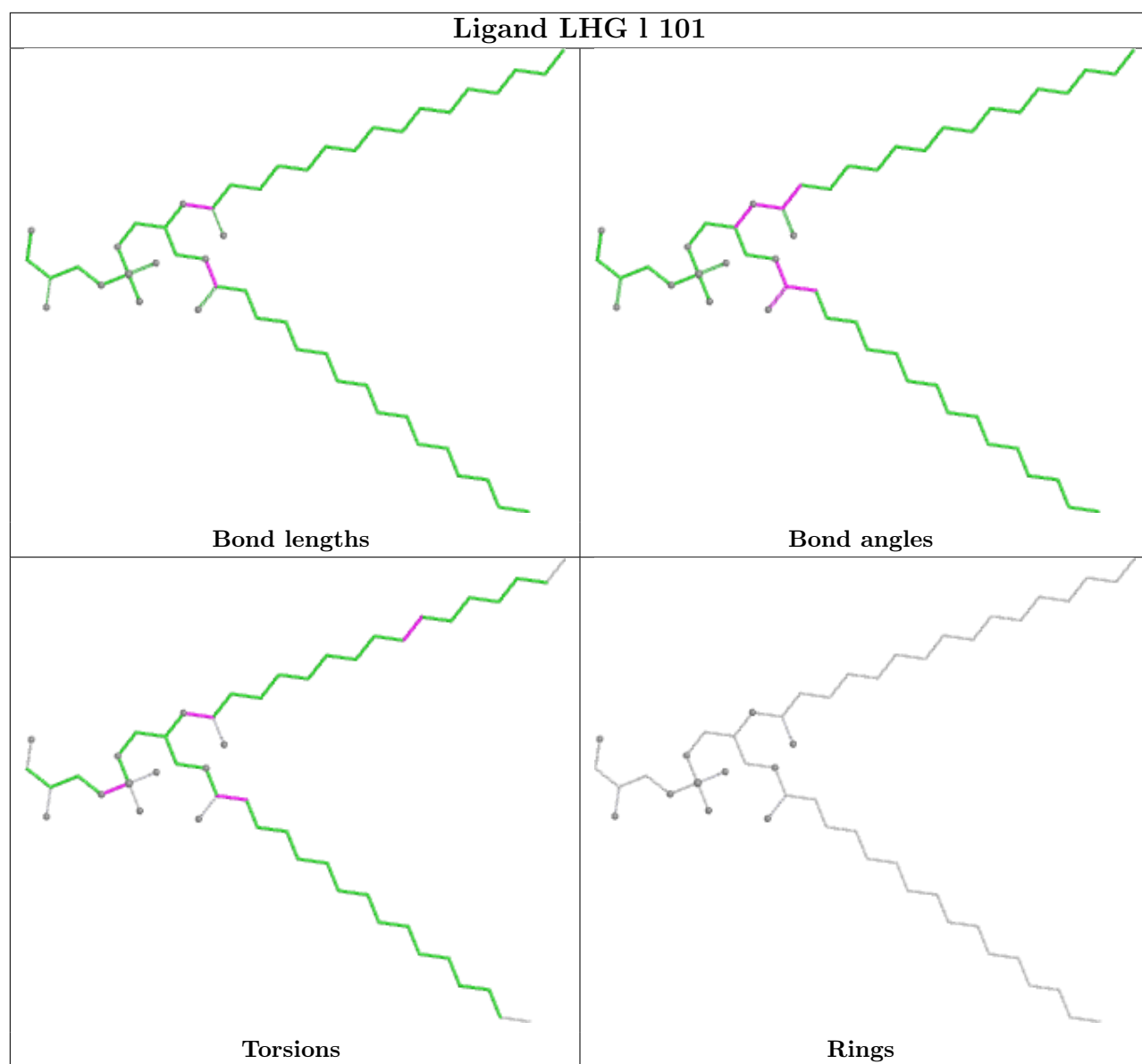


Torsions

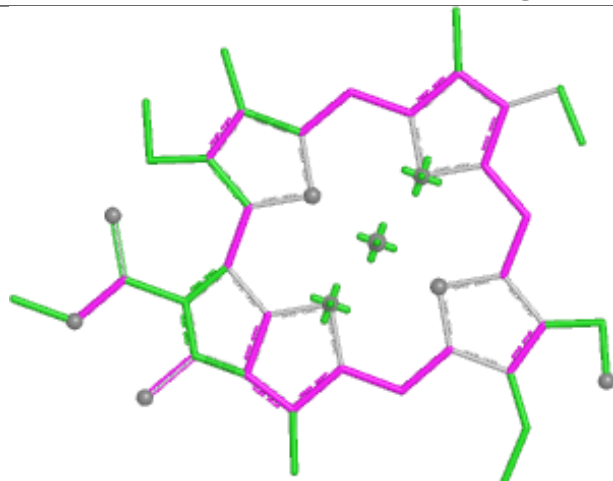


Rings

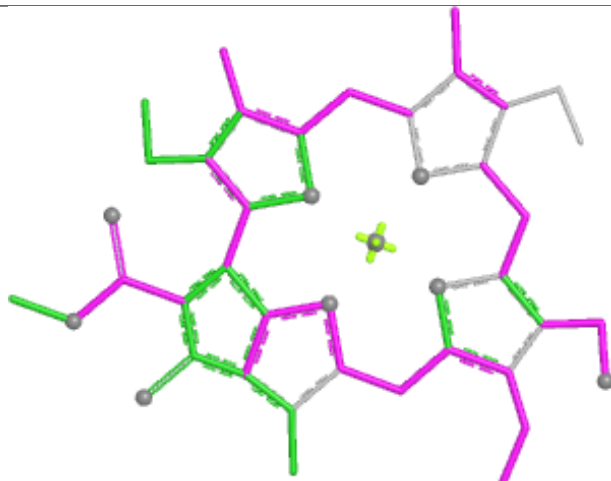




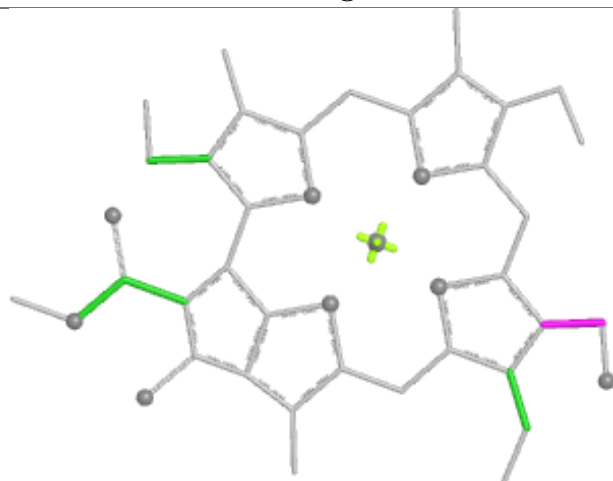
Ligand CHL S 607



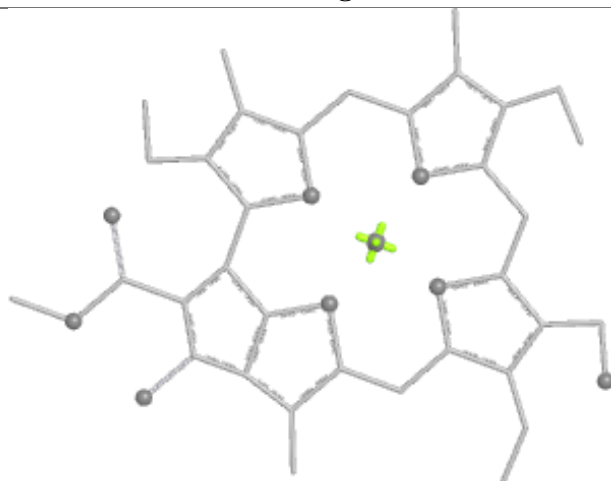
Bond lengths



Bond angles

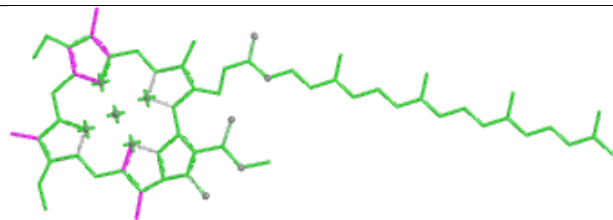


Torsions

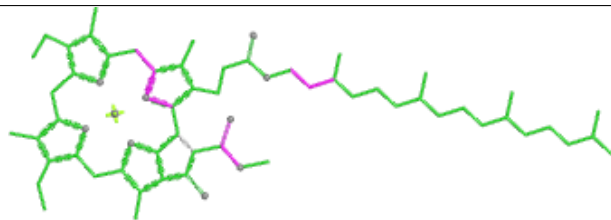


Rings

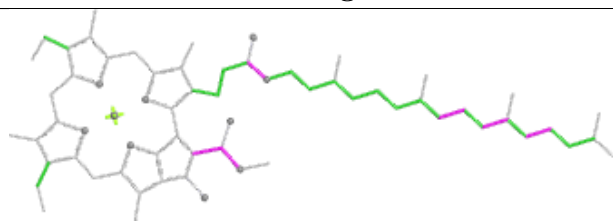
Ligand CLA C 502



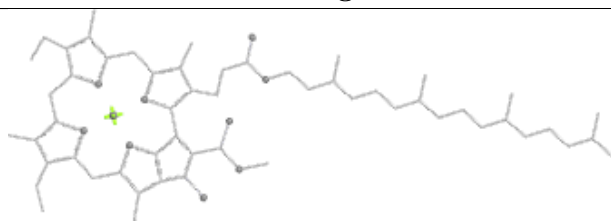
Bond lengths



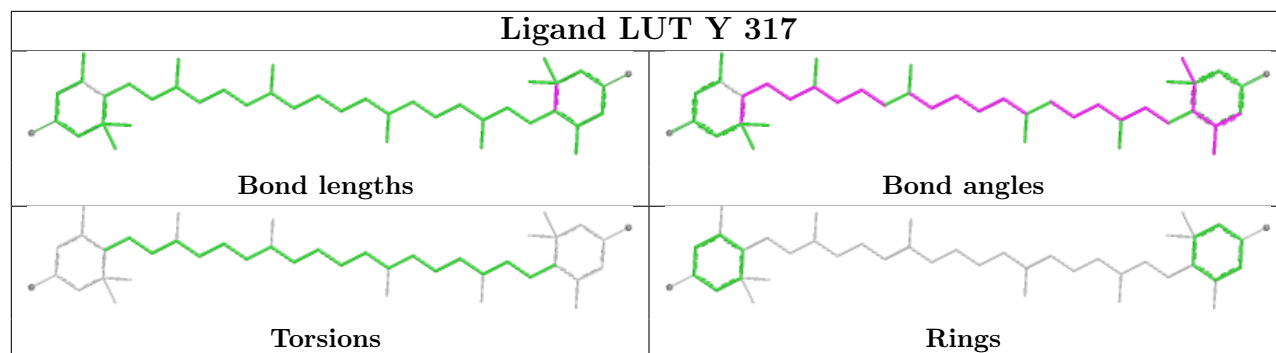
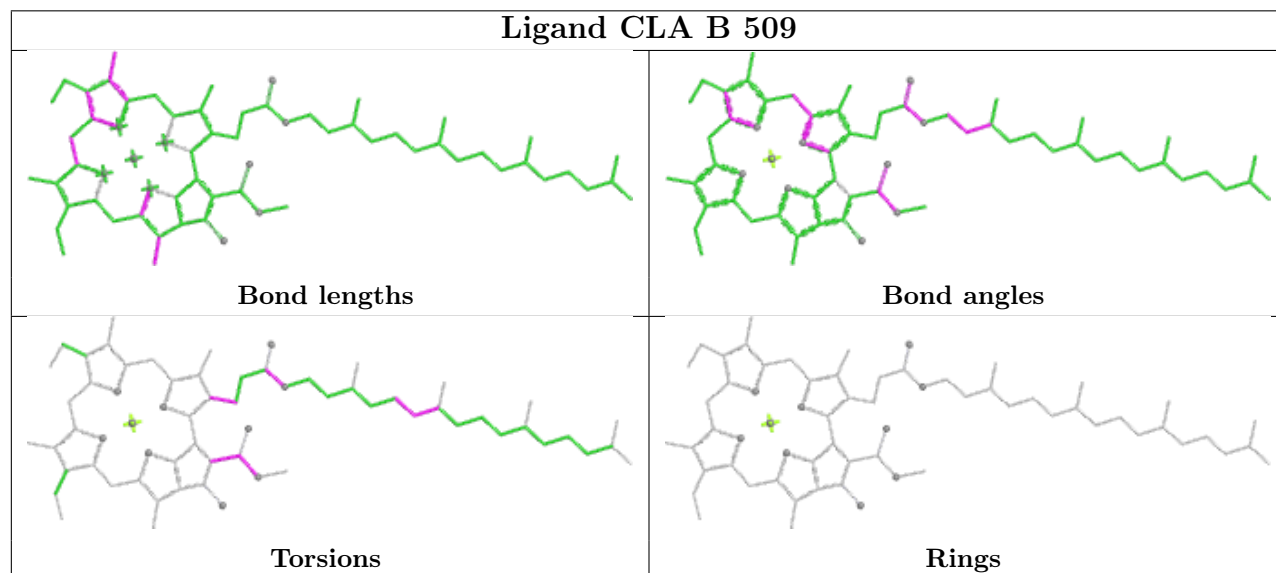
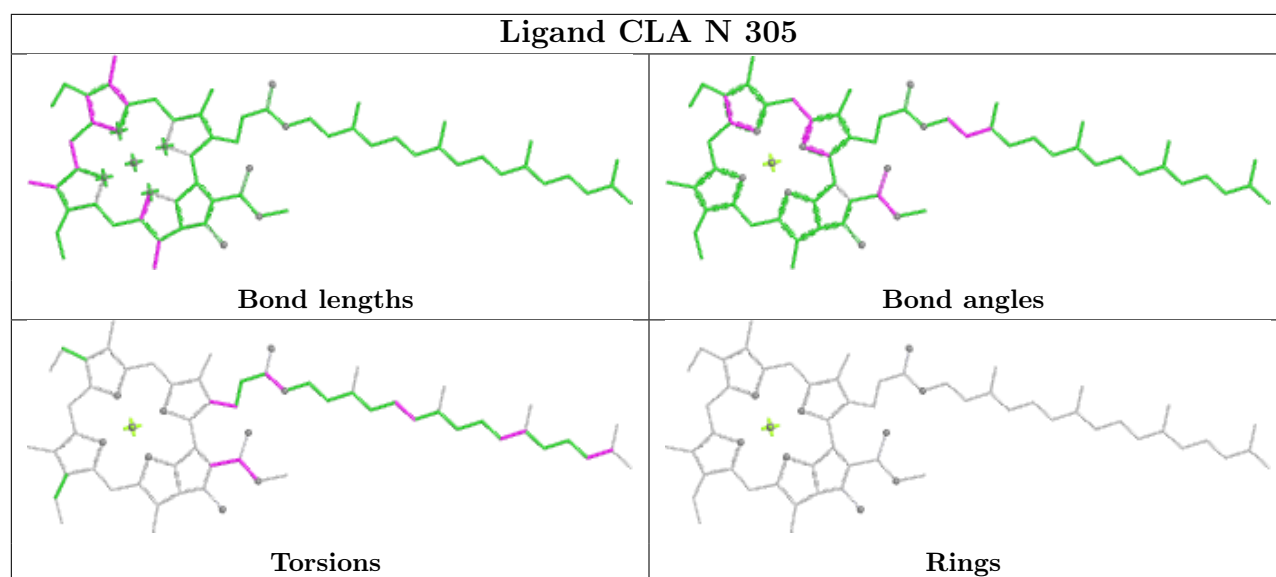
Bond angles

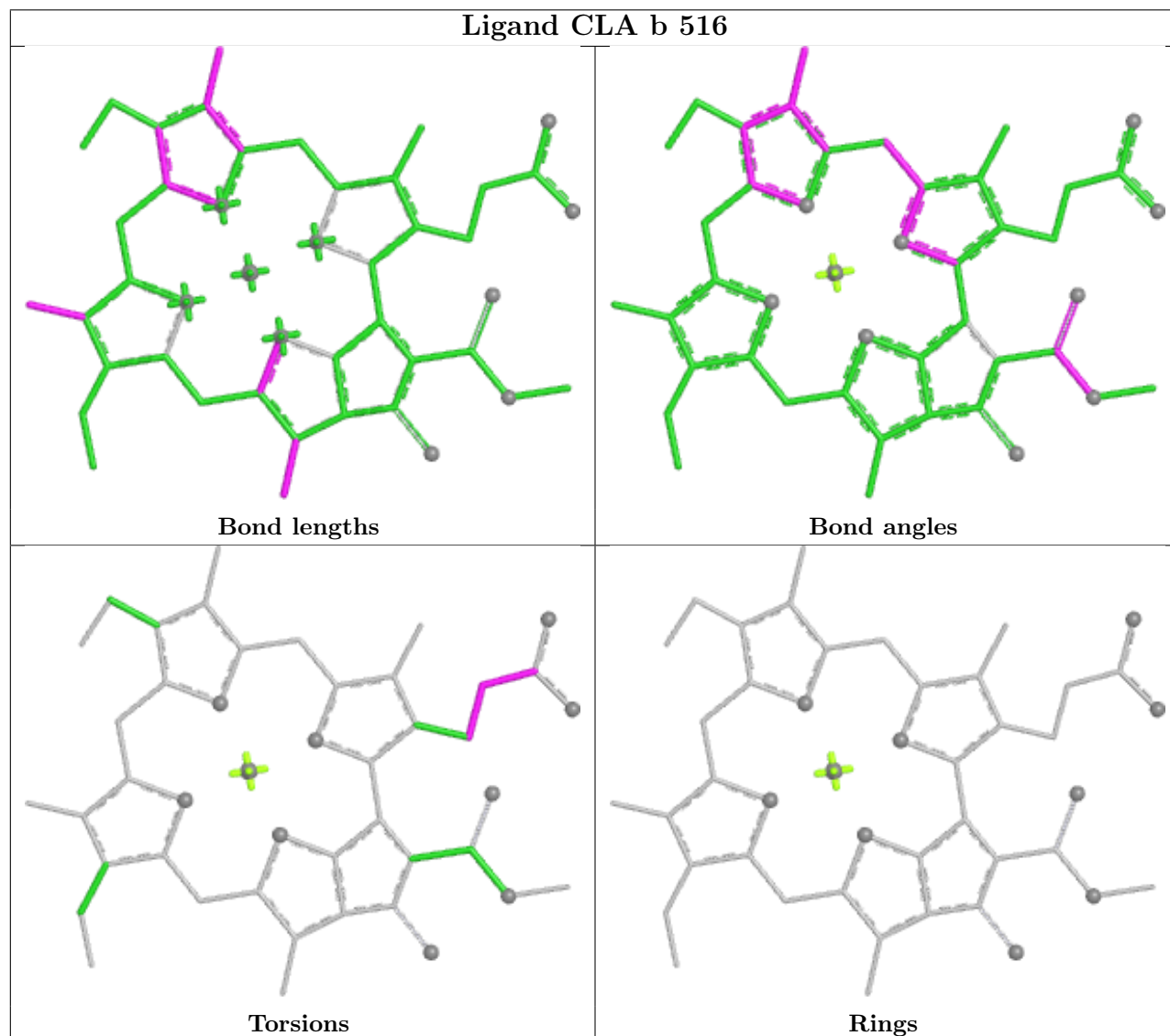
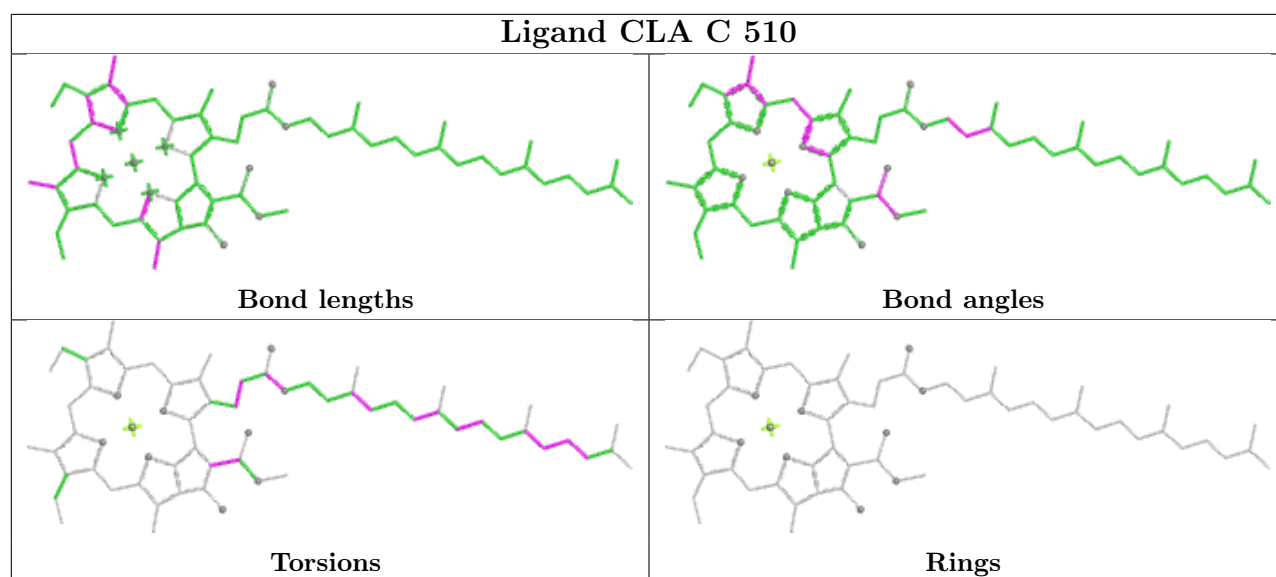


Torsions

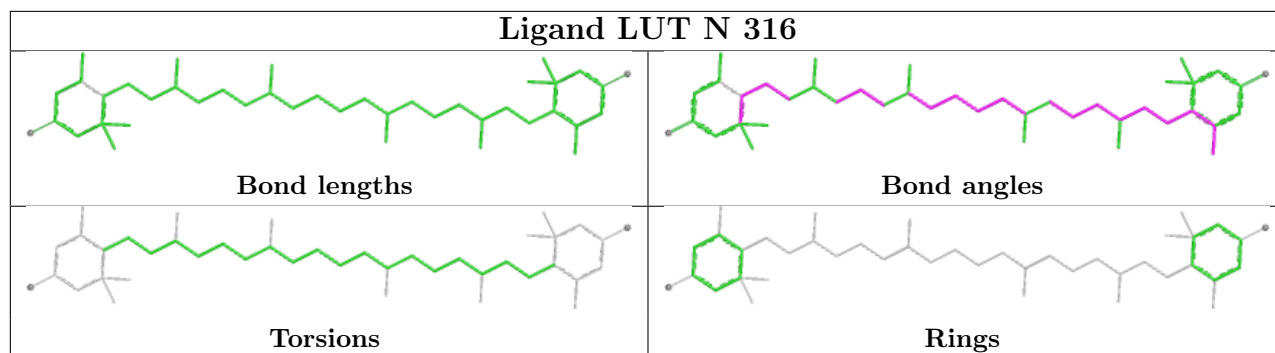


Rings

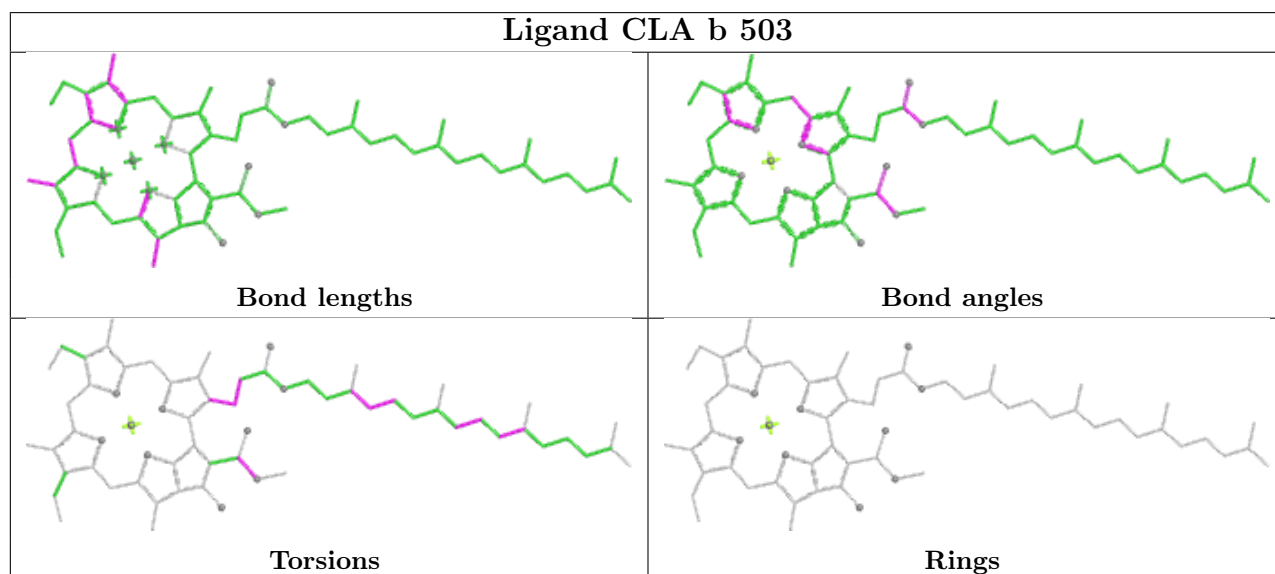




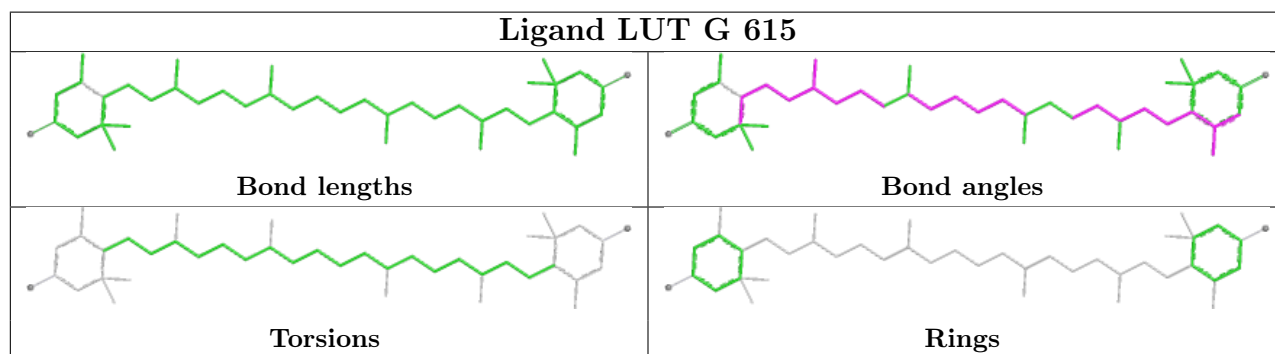
Ligand LUT N 316



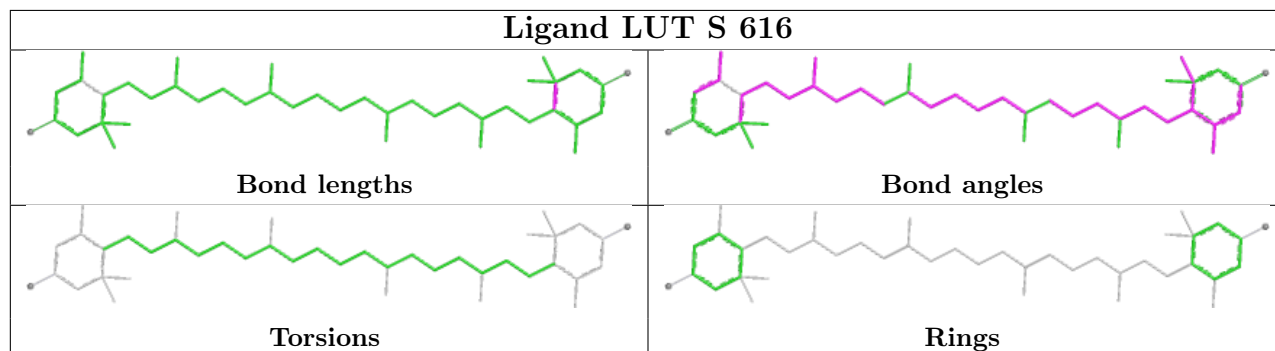
Ligand CLA b 503



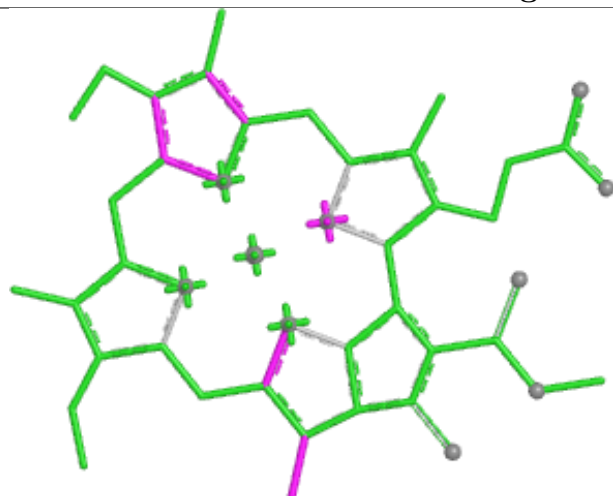
Ligand LUT G 615



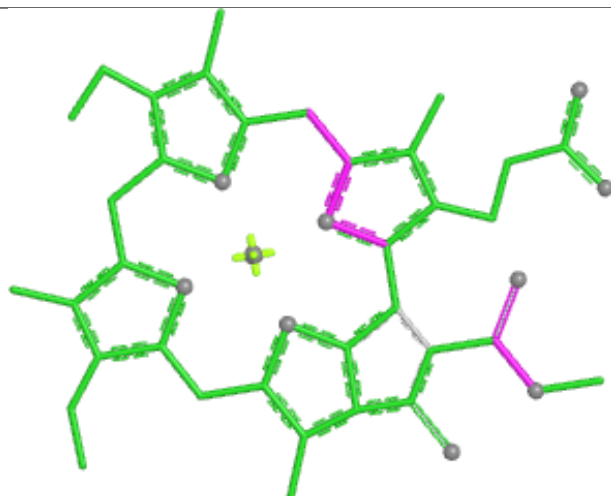
Ligand LUT S 616



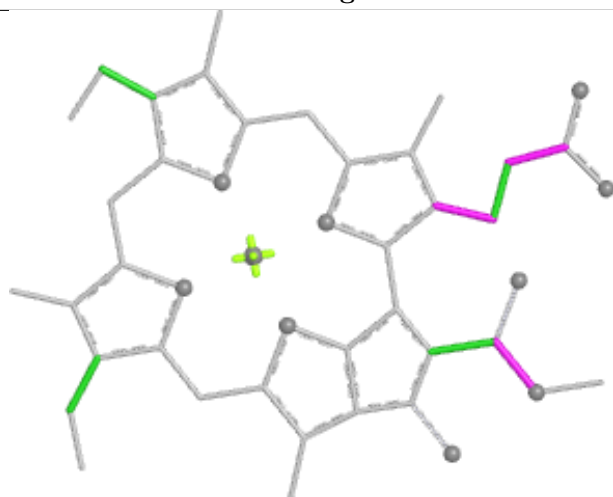
Ligand CLA r 307



Bond lengths



Bond angles

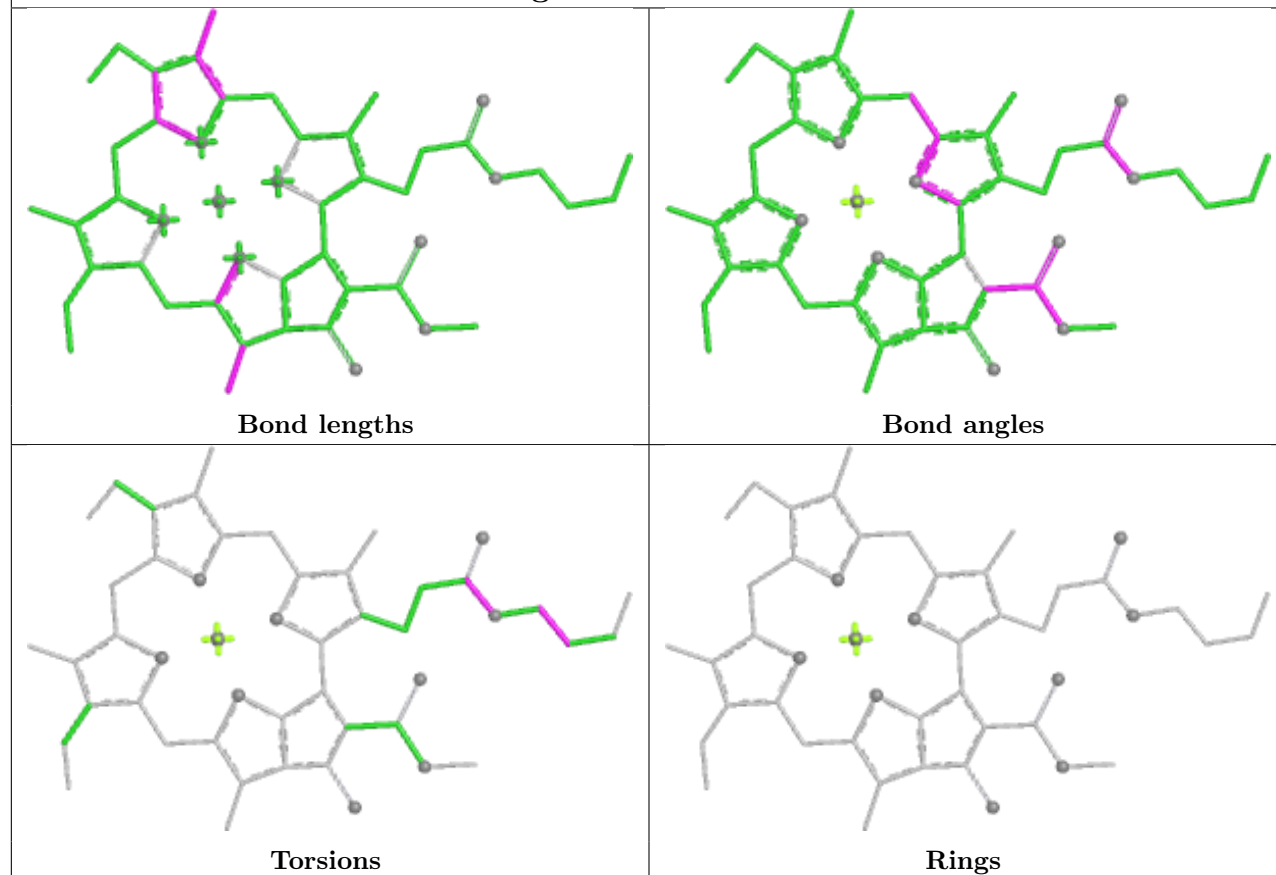


Torsions

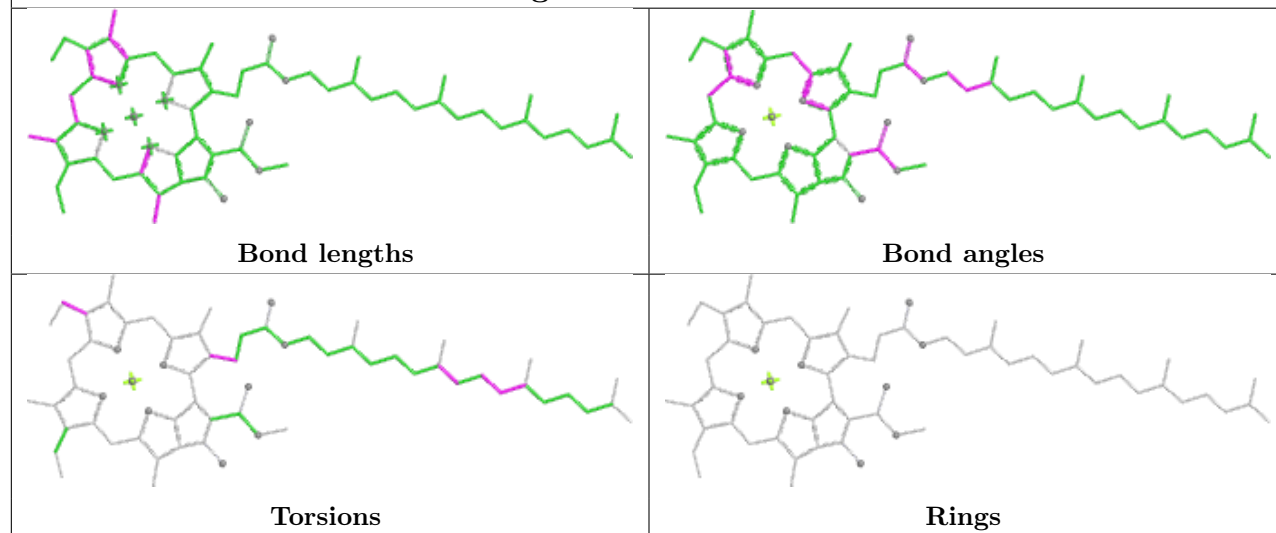


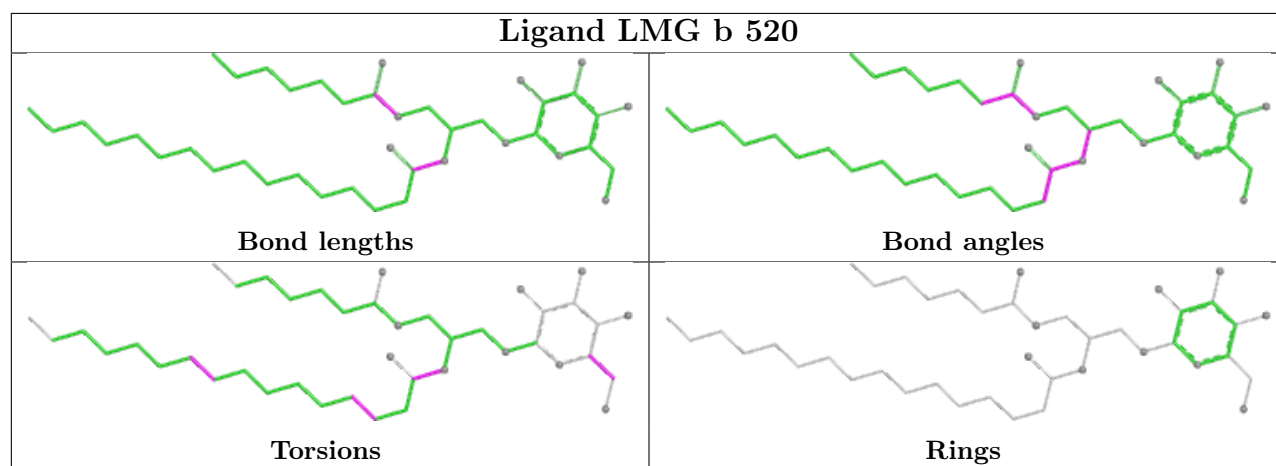
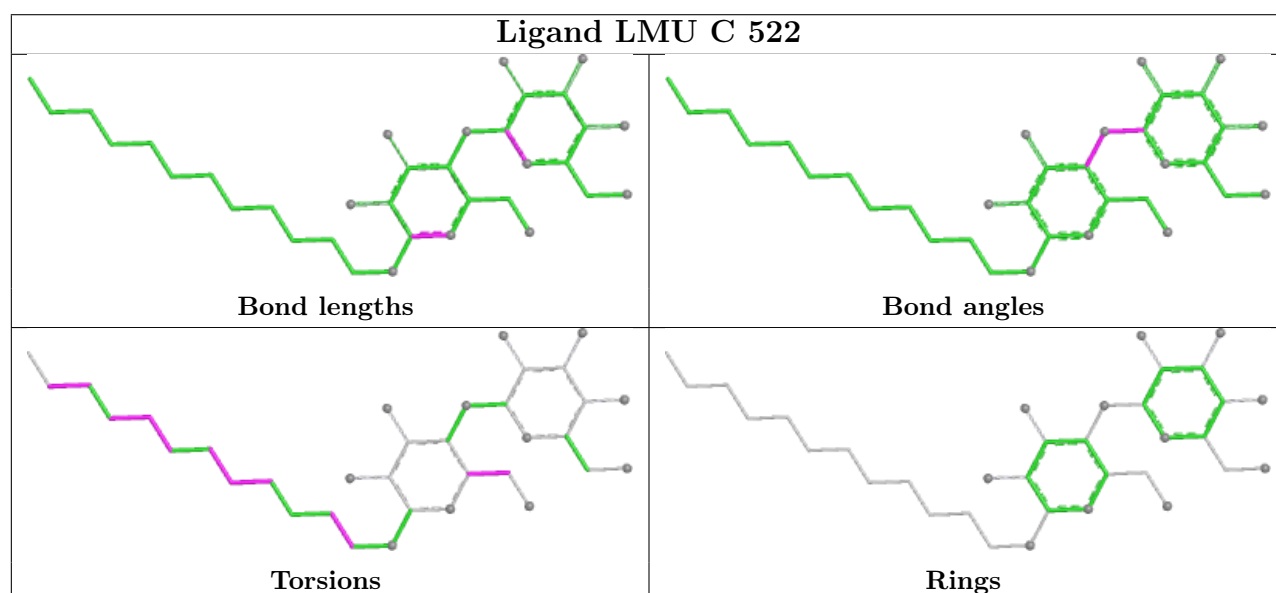
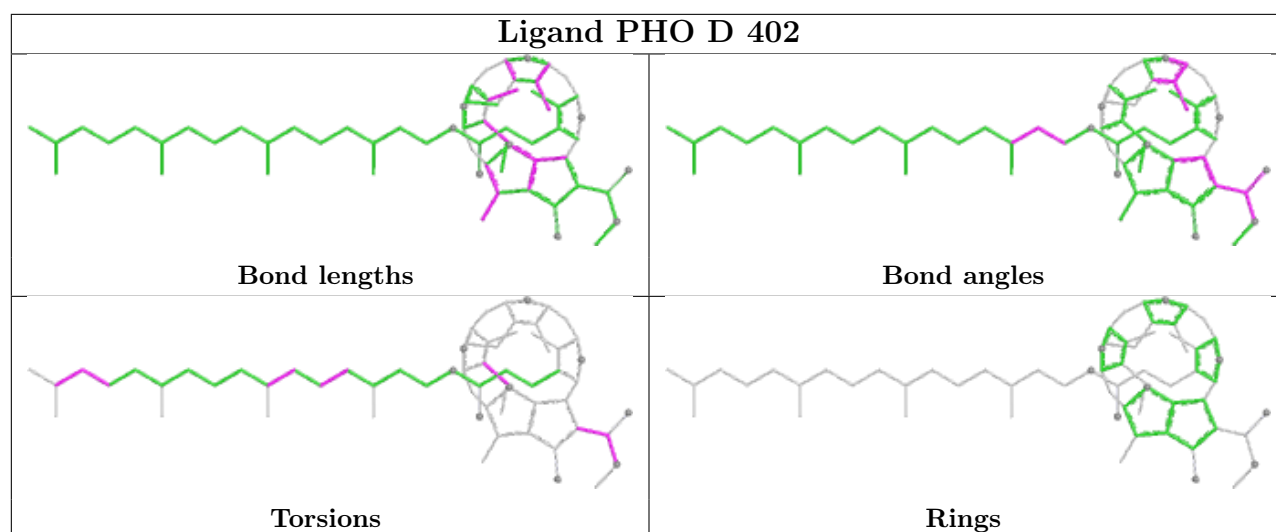
Rings

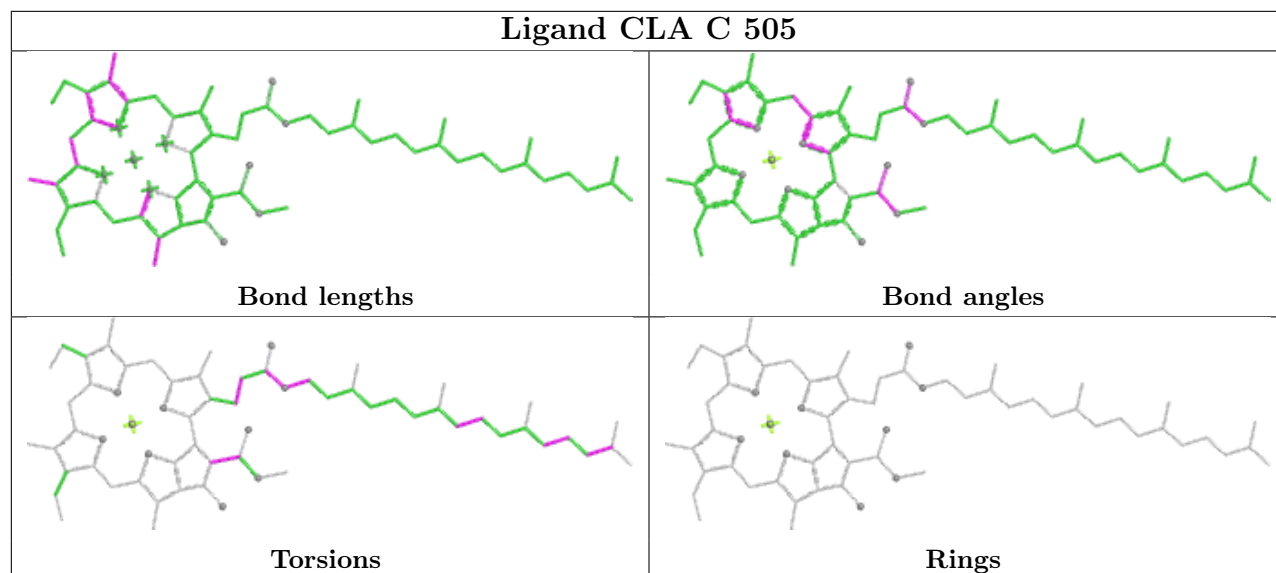
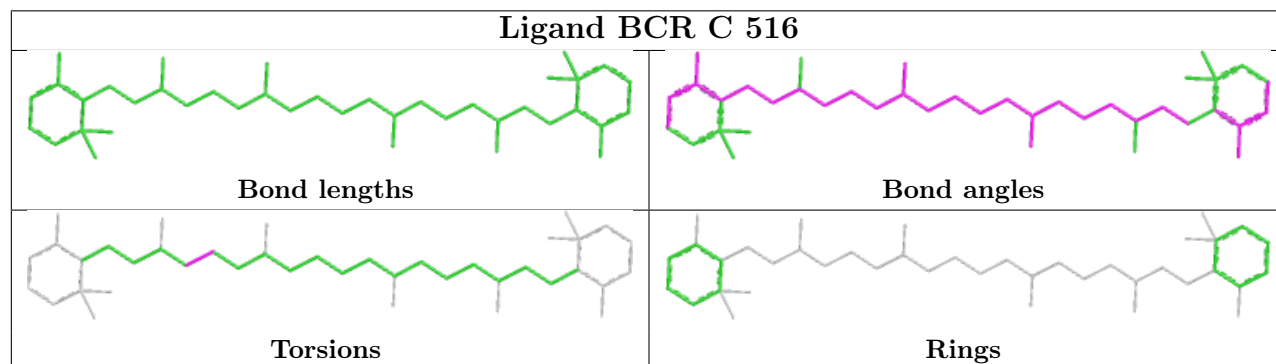
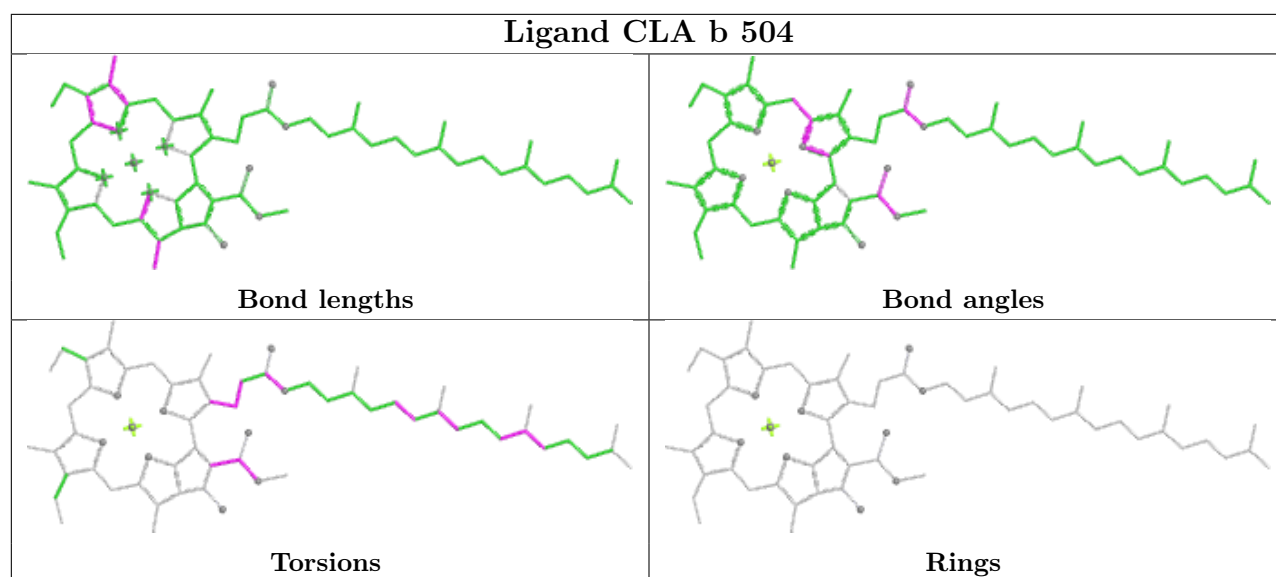
Ligand CLA A 403



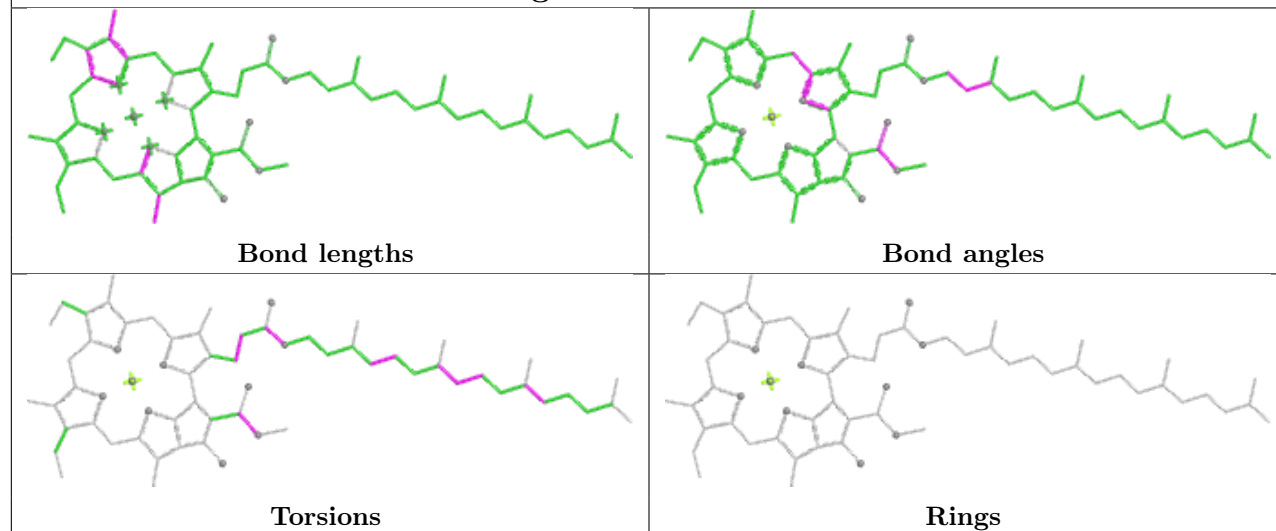
Ligand CLA D 404



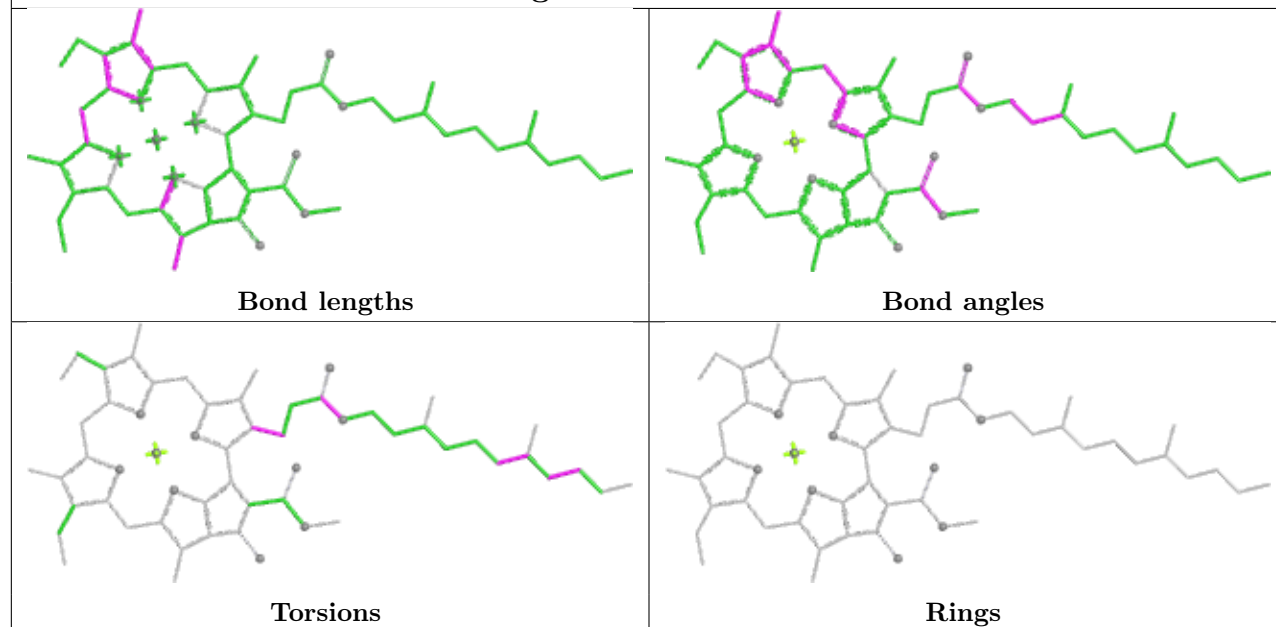


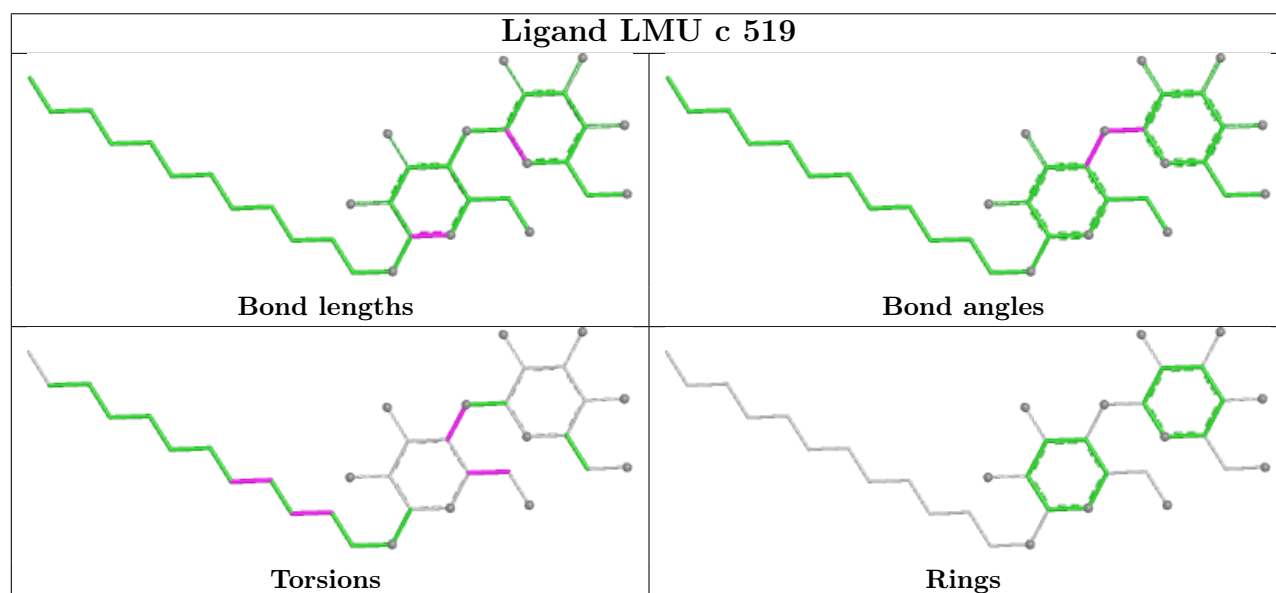
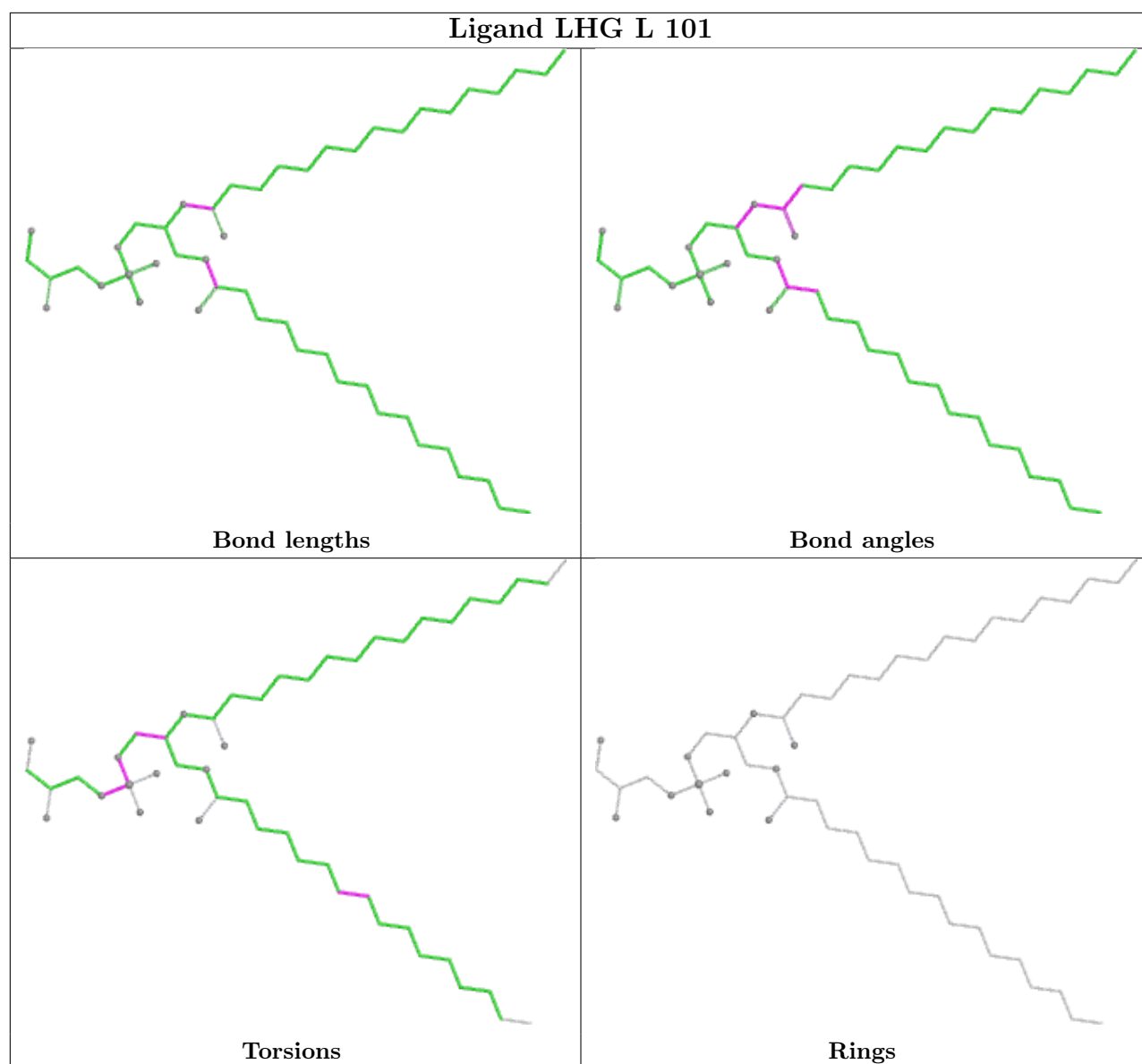


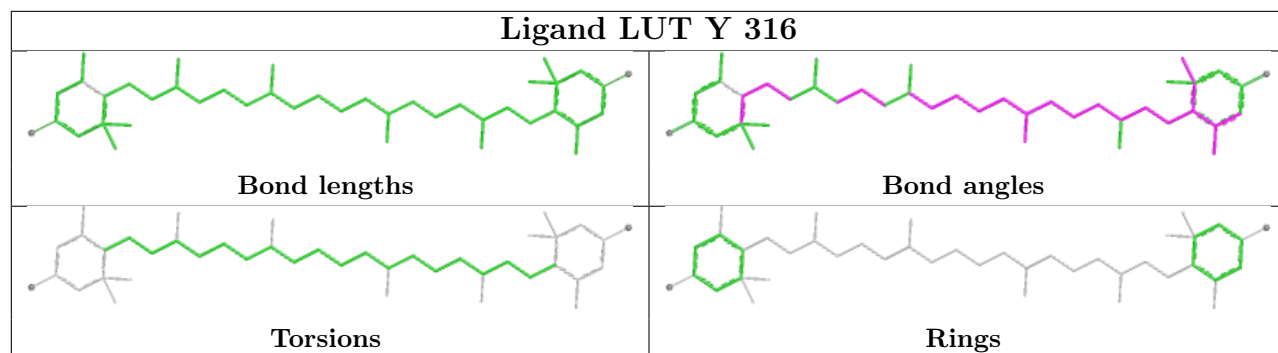
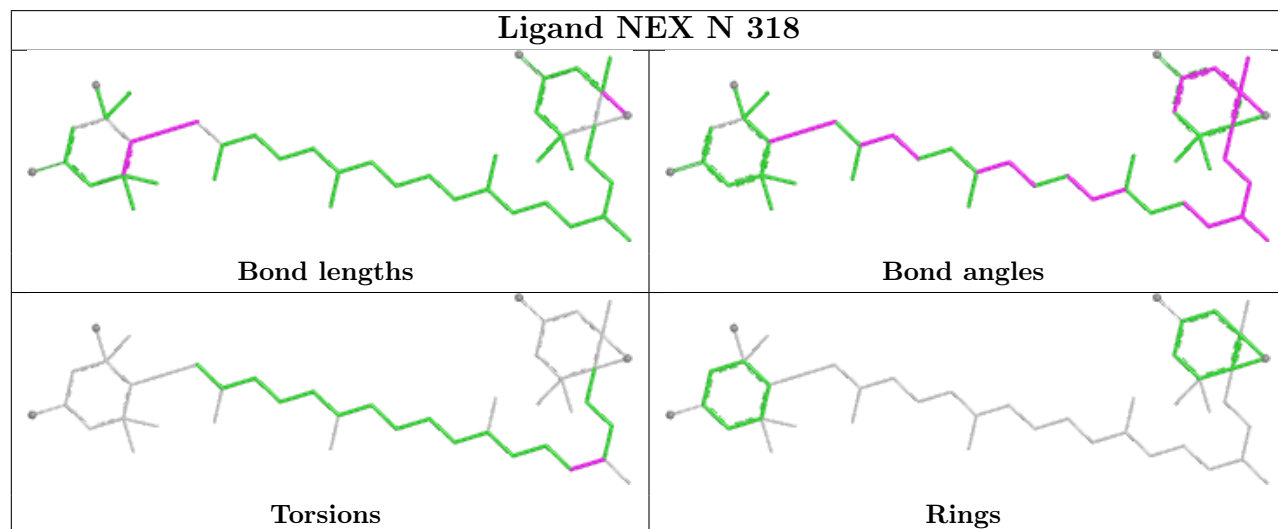
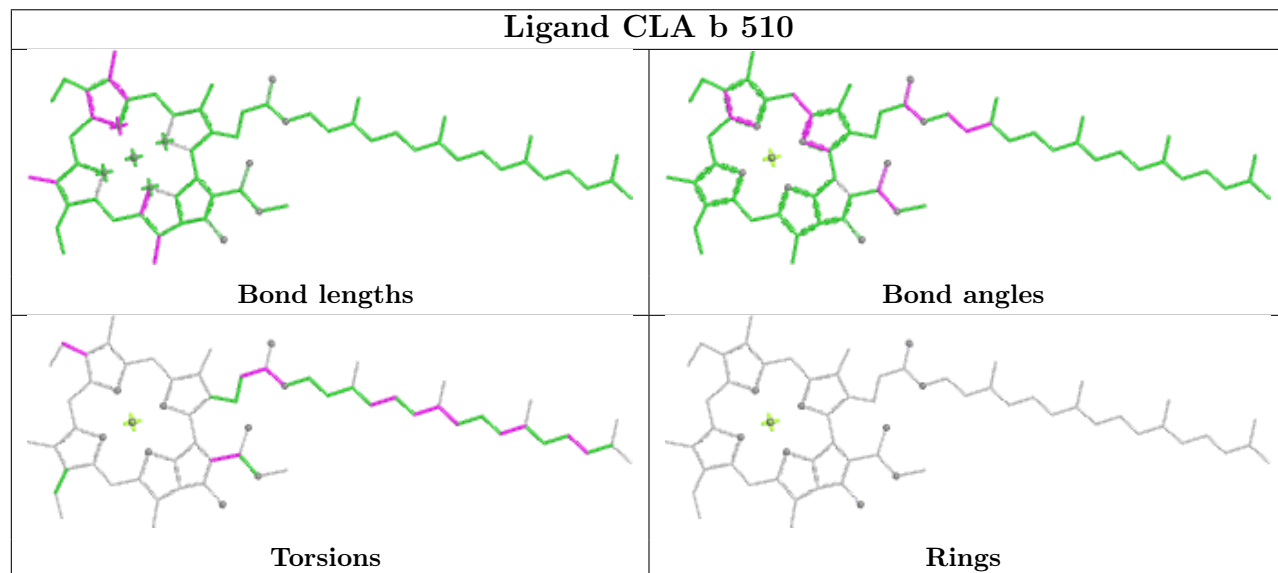
Ligand CLA Y 314

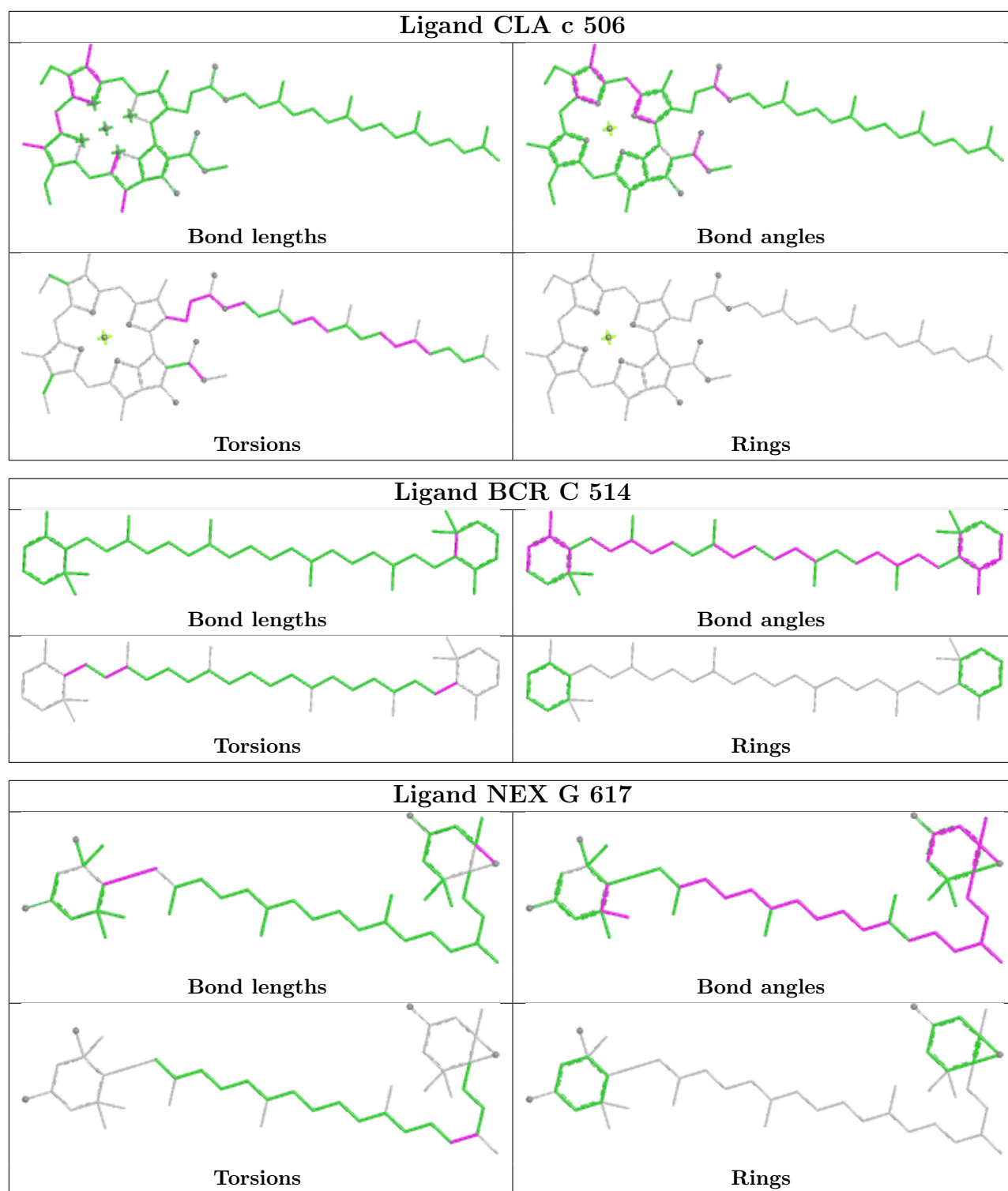


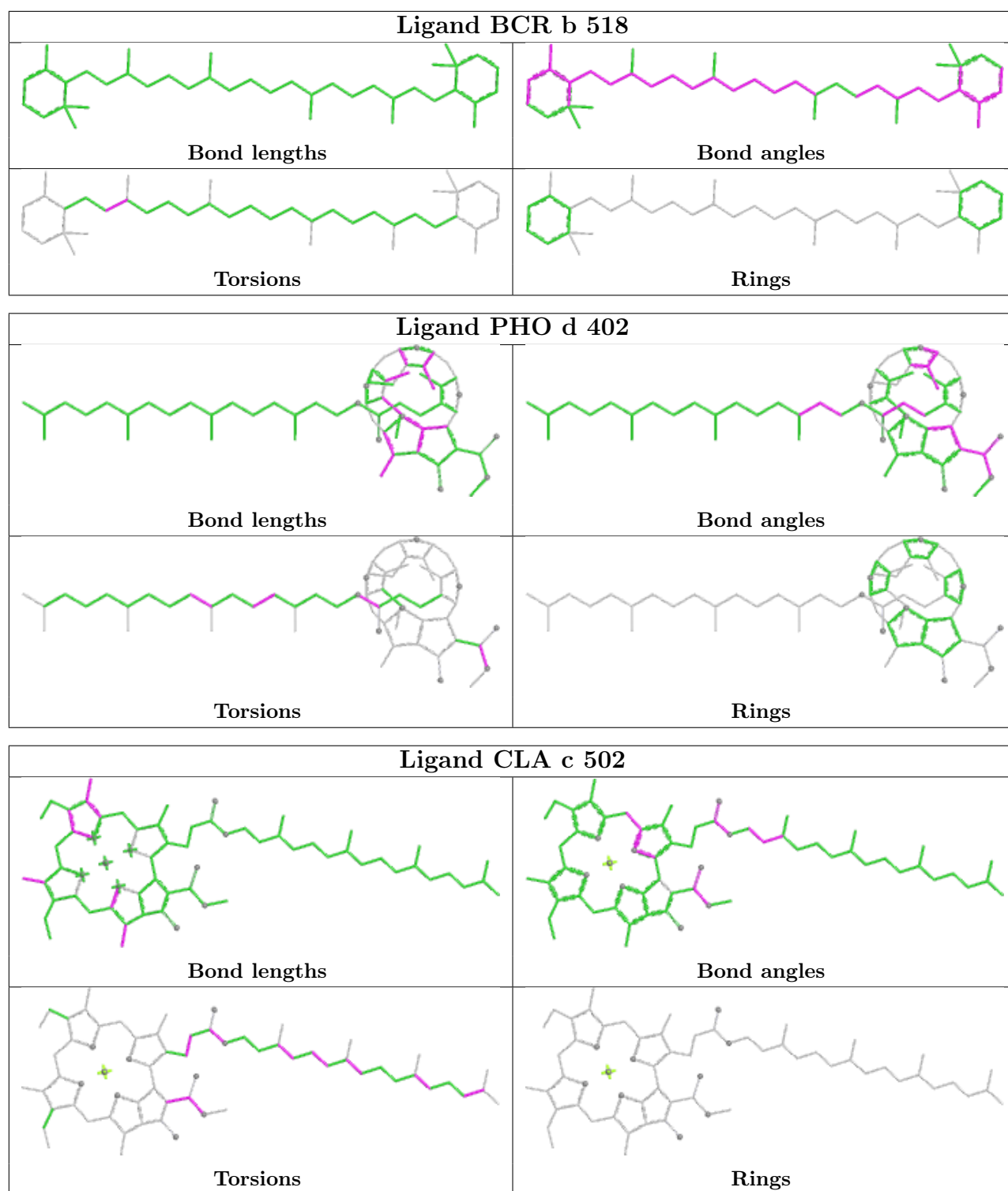
Ligand CLA Y 306

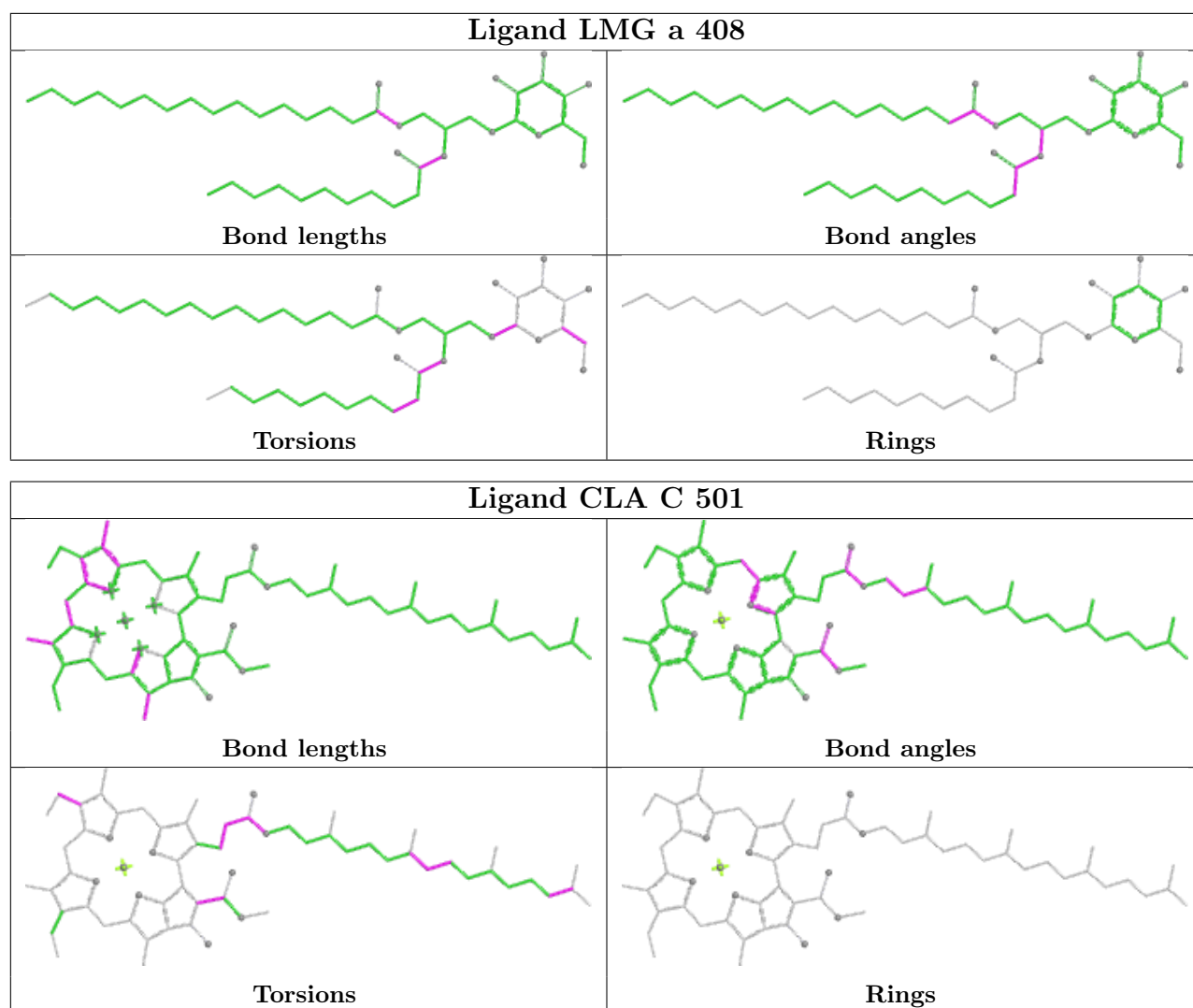




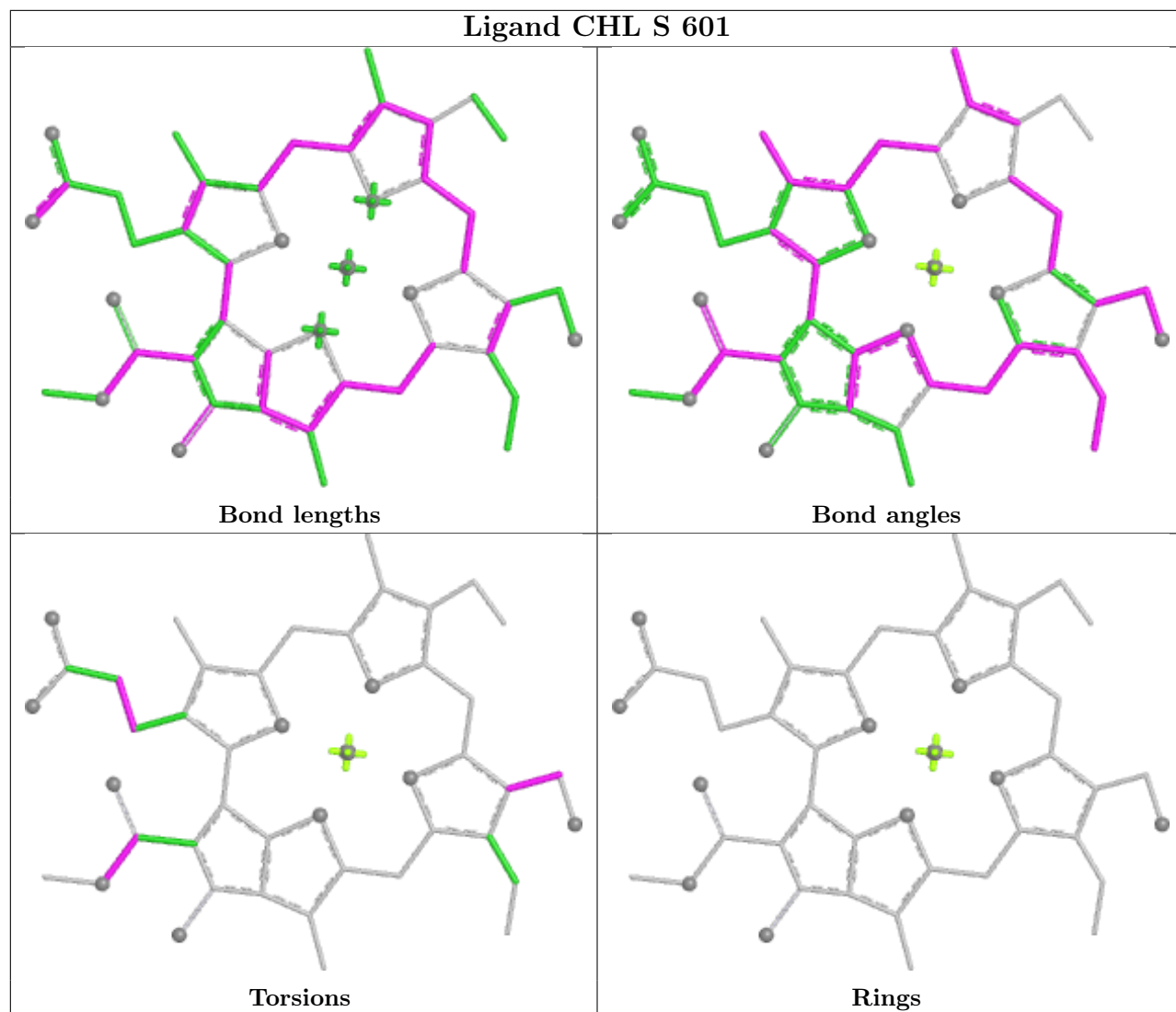
Ligand LUT Y 316**Ligand NEX N 318****Ligand CLA b 510**

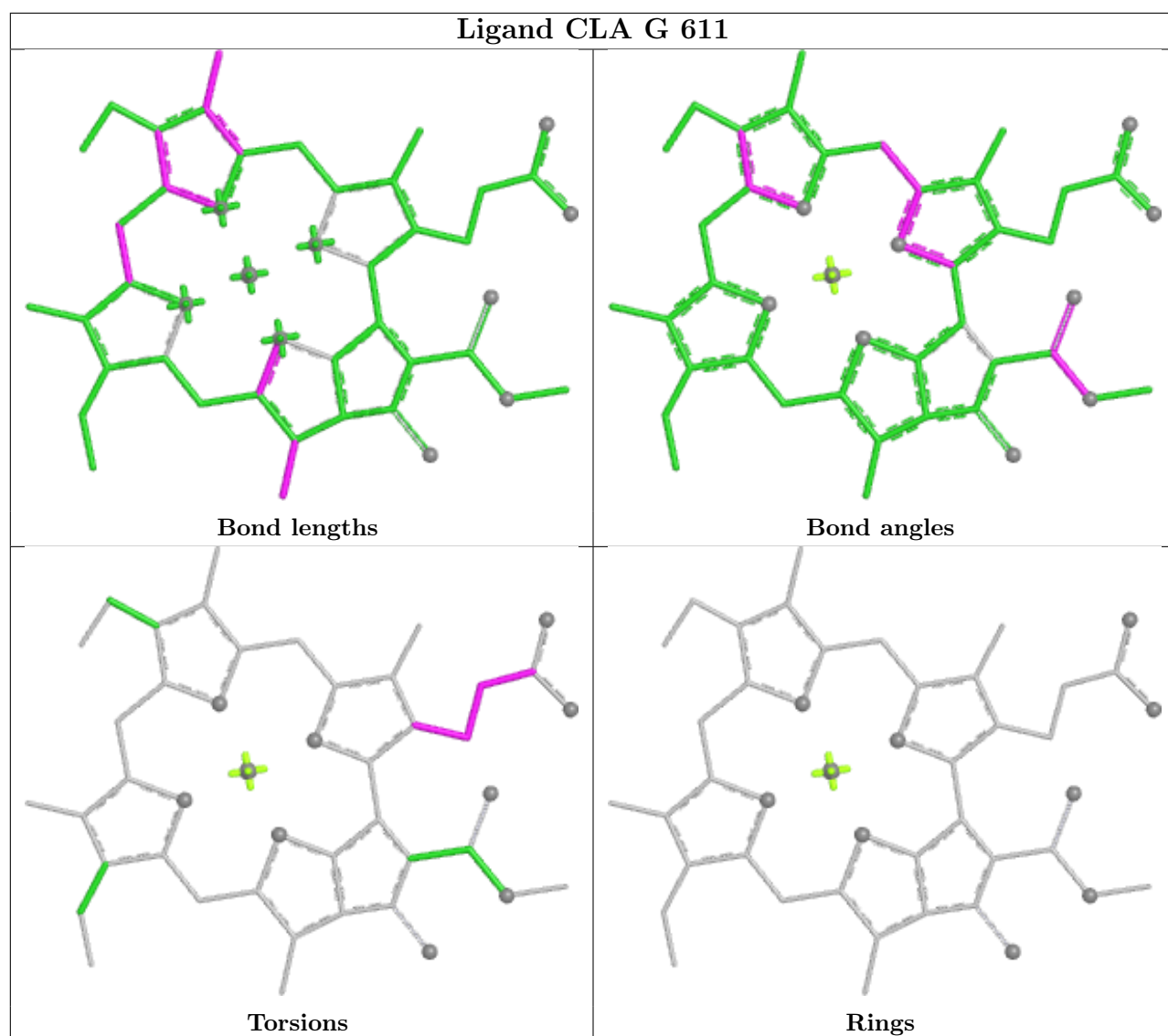


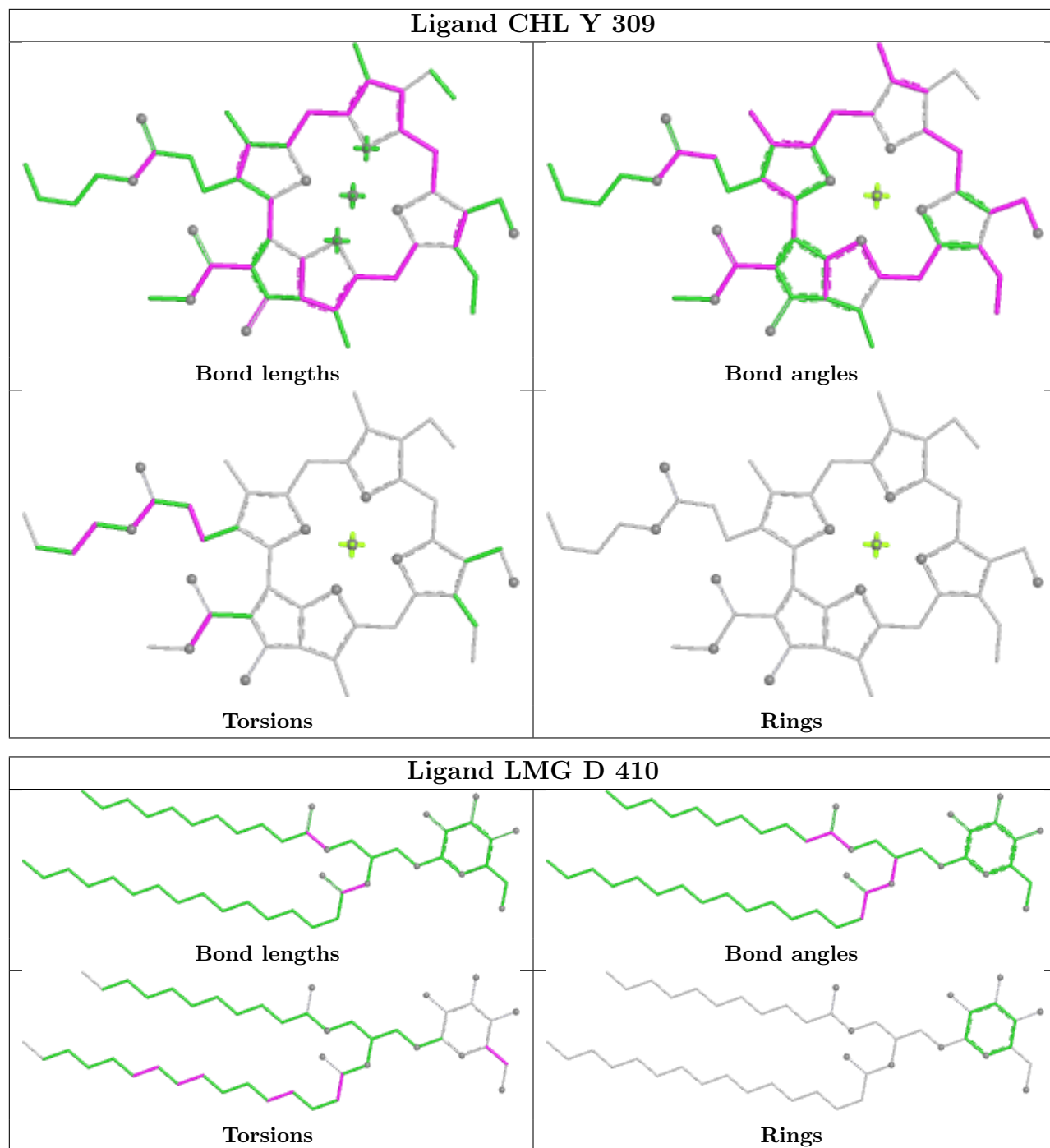


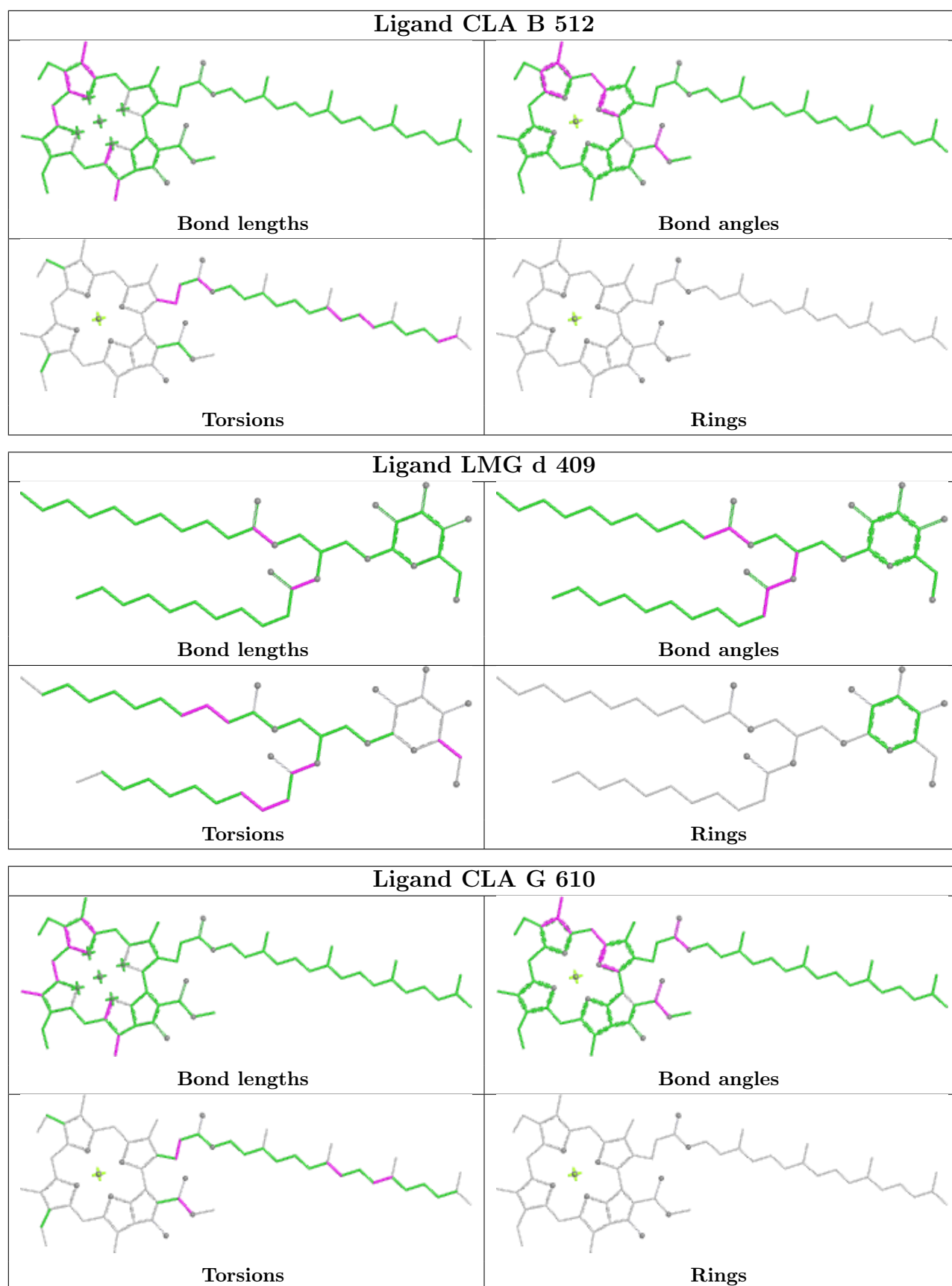


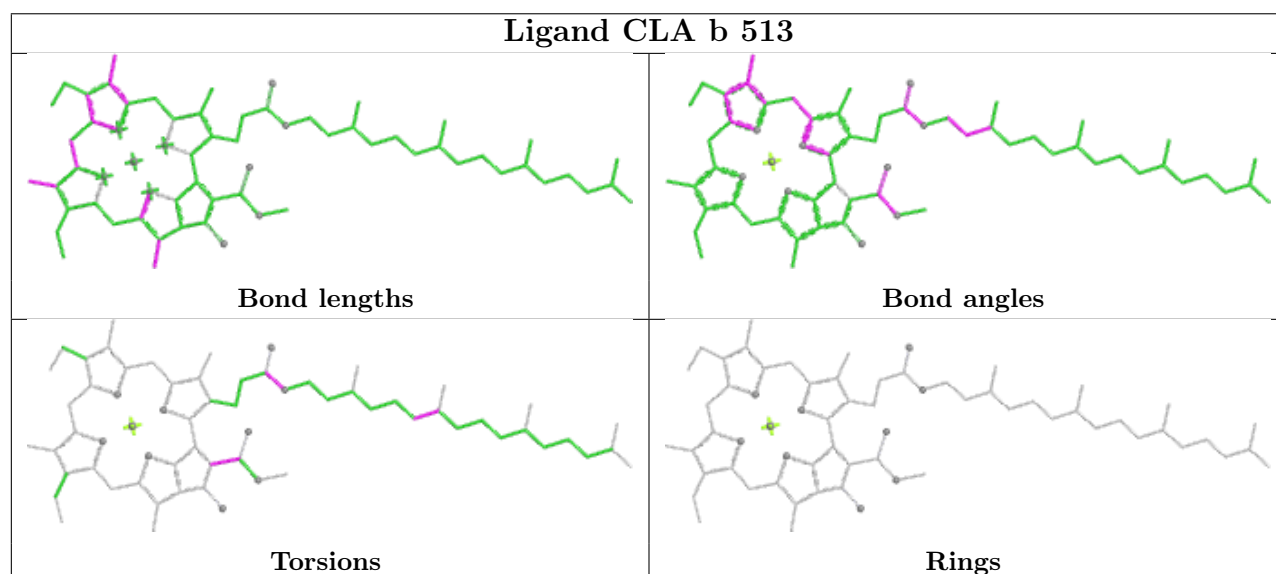
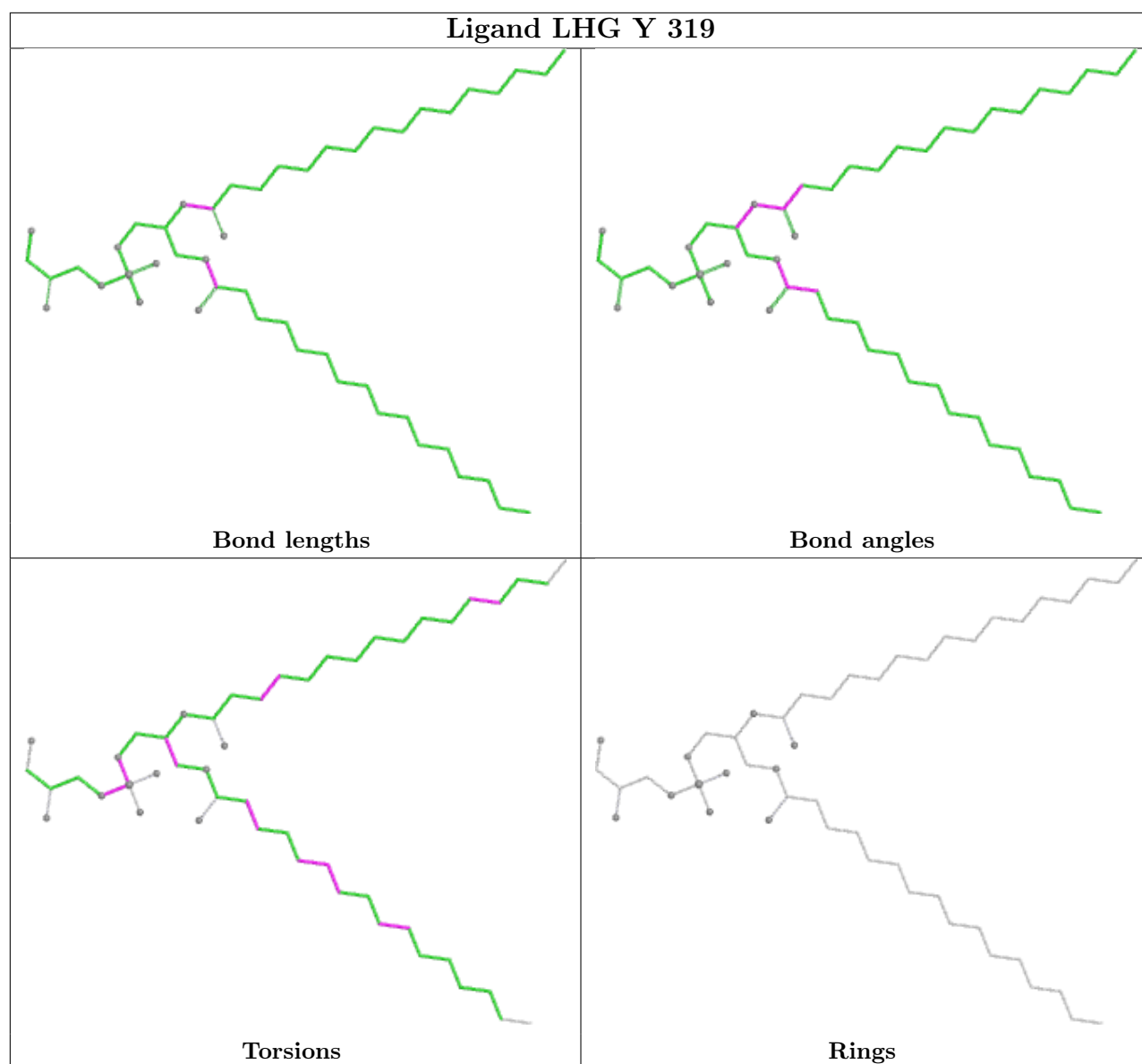
Ligand CHL S 601

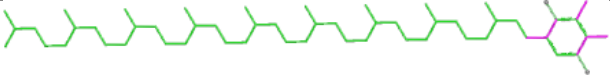
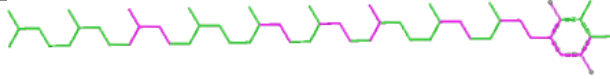
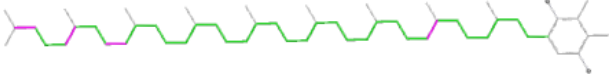
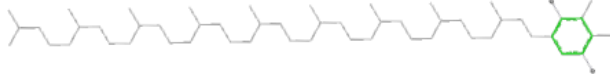
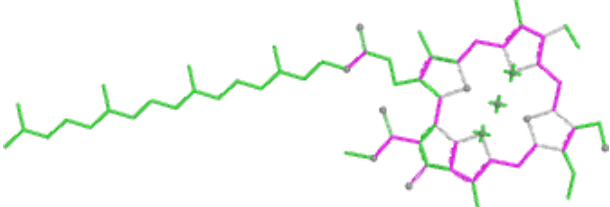
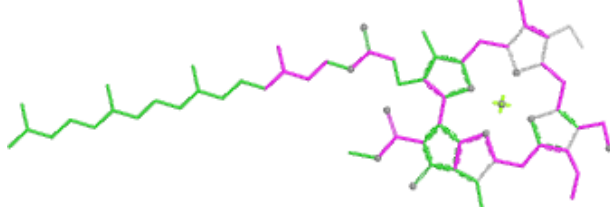
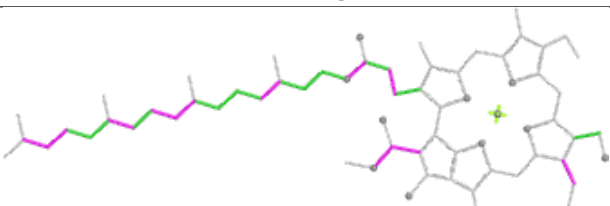
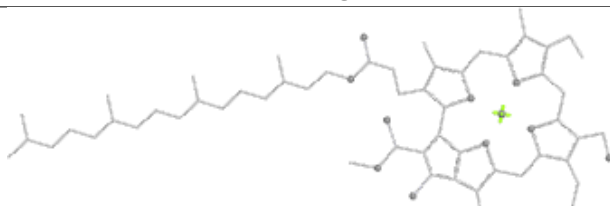


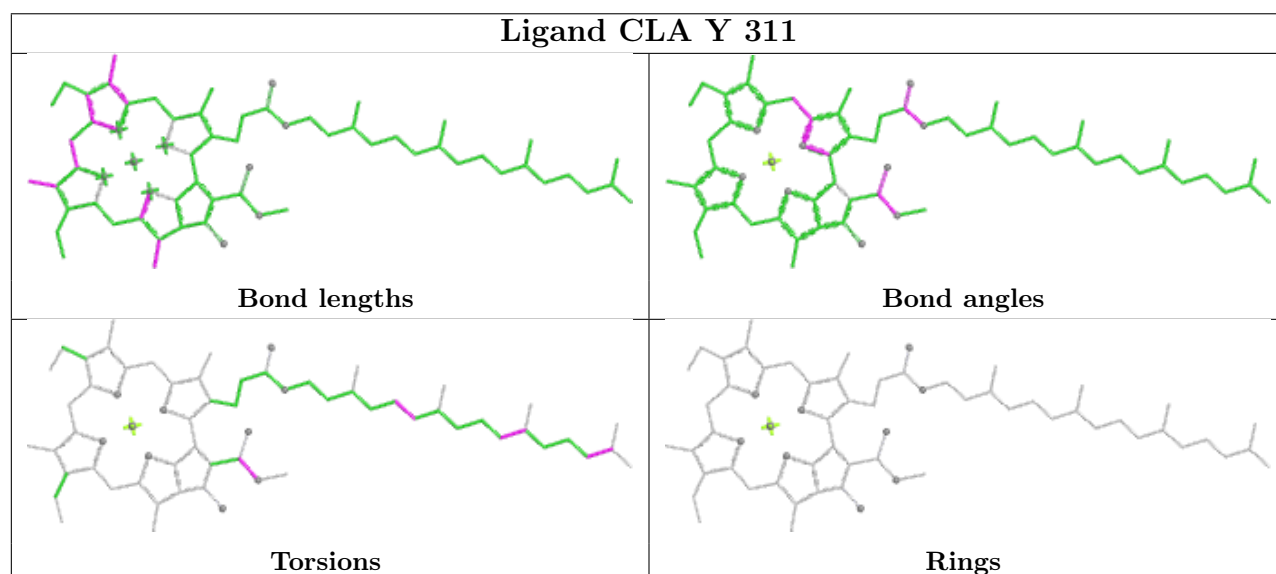
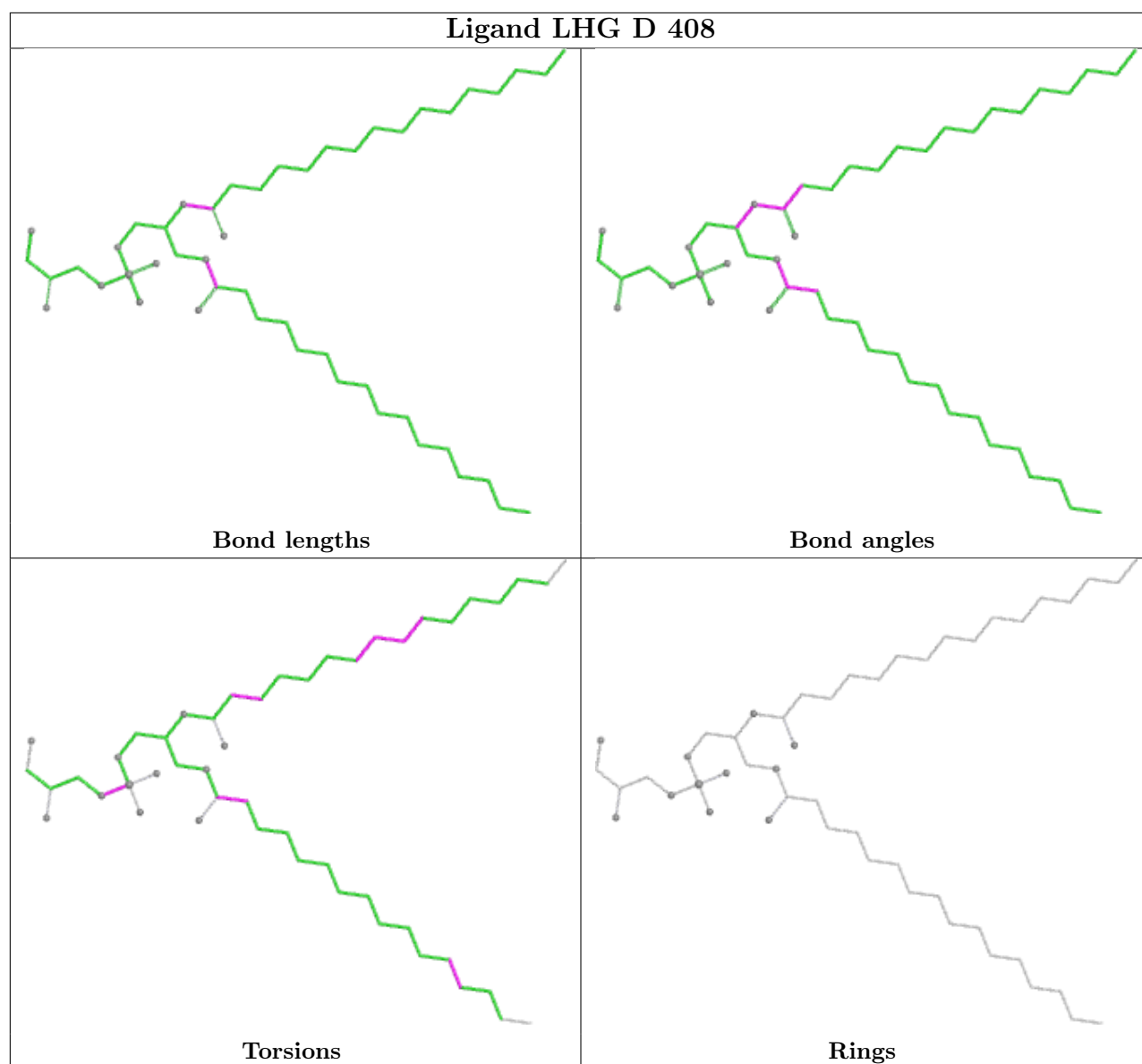


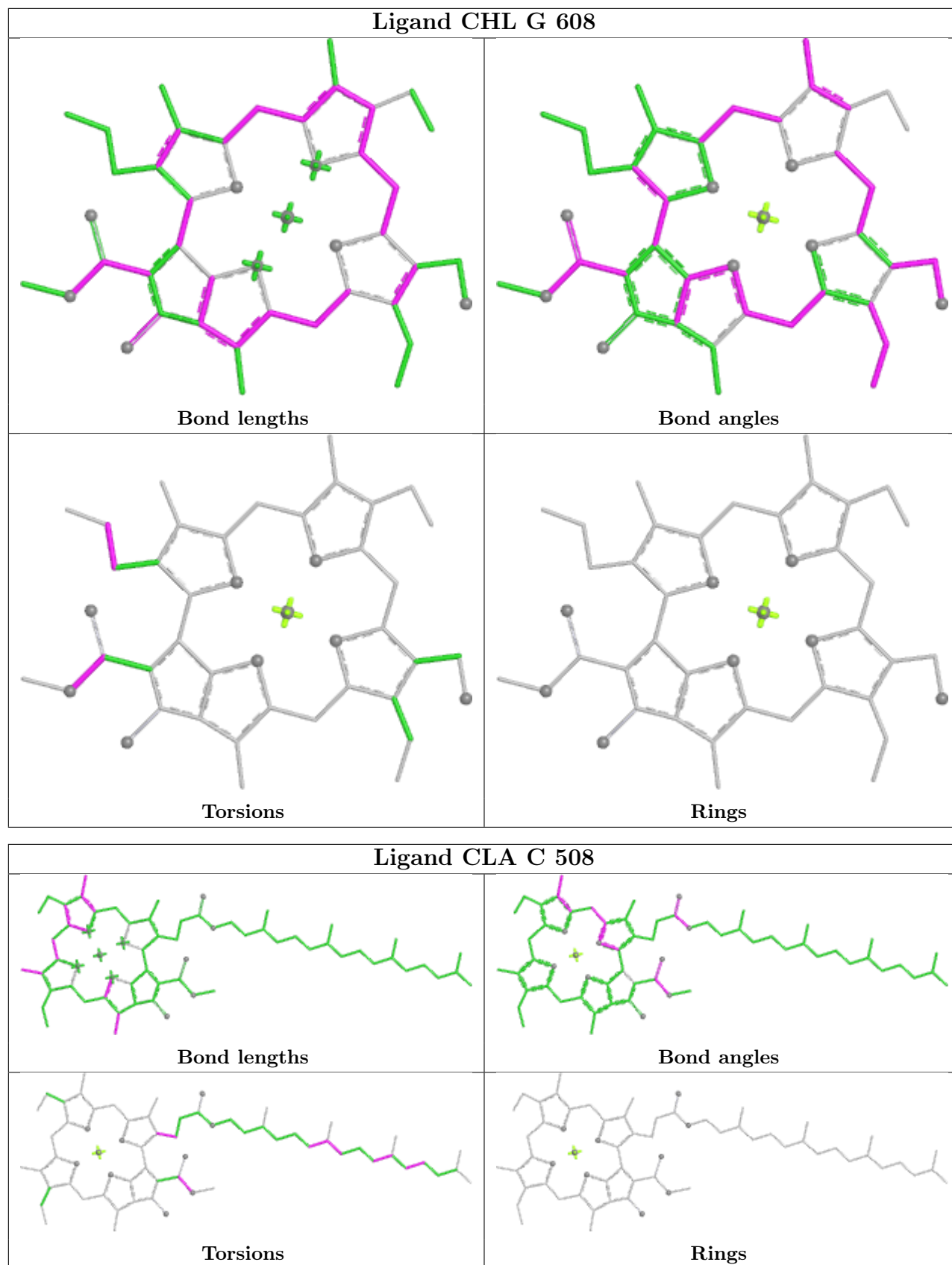


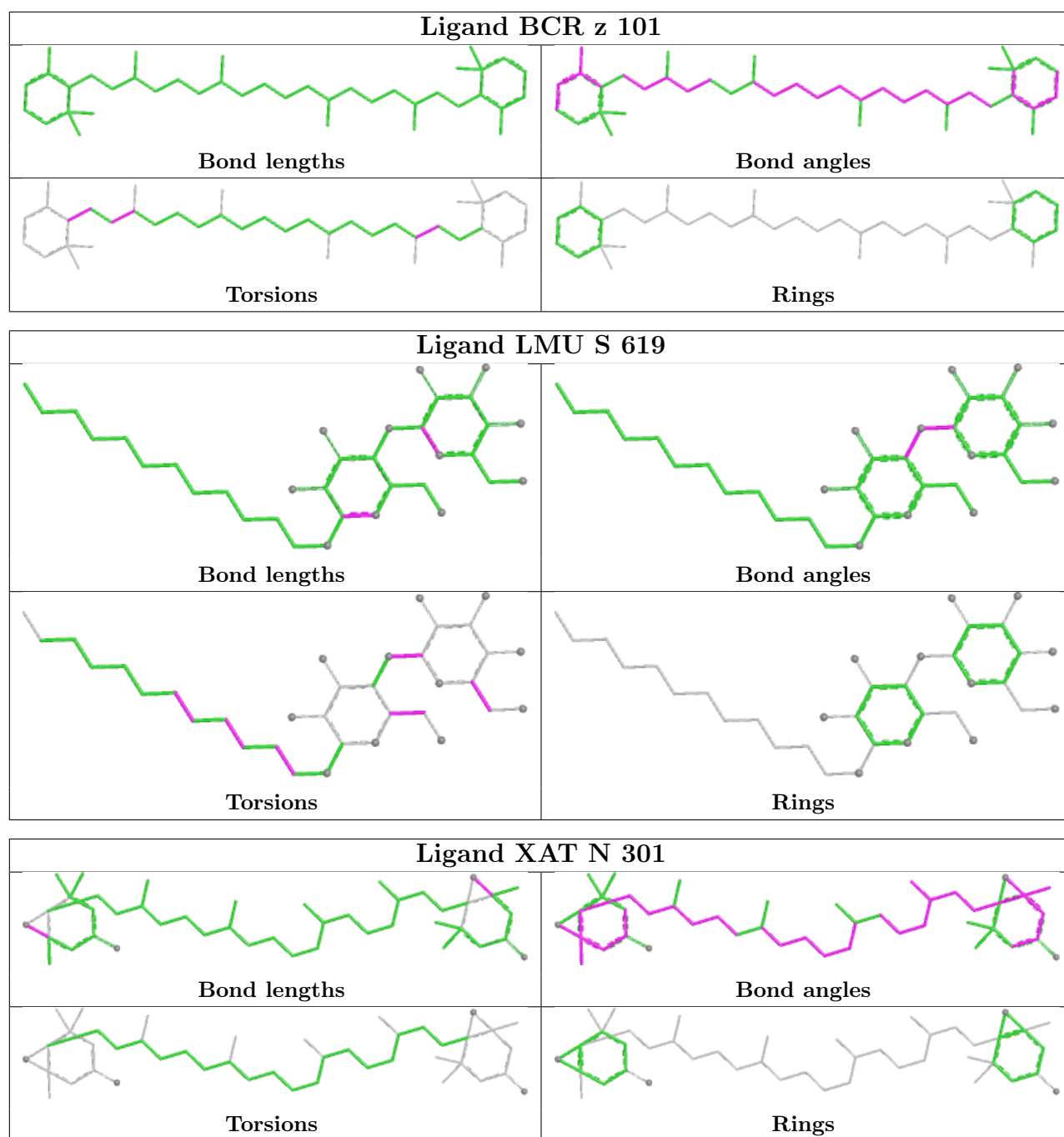


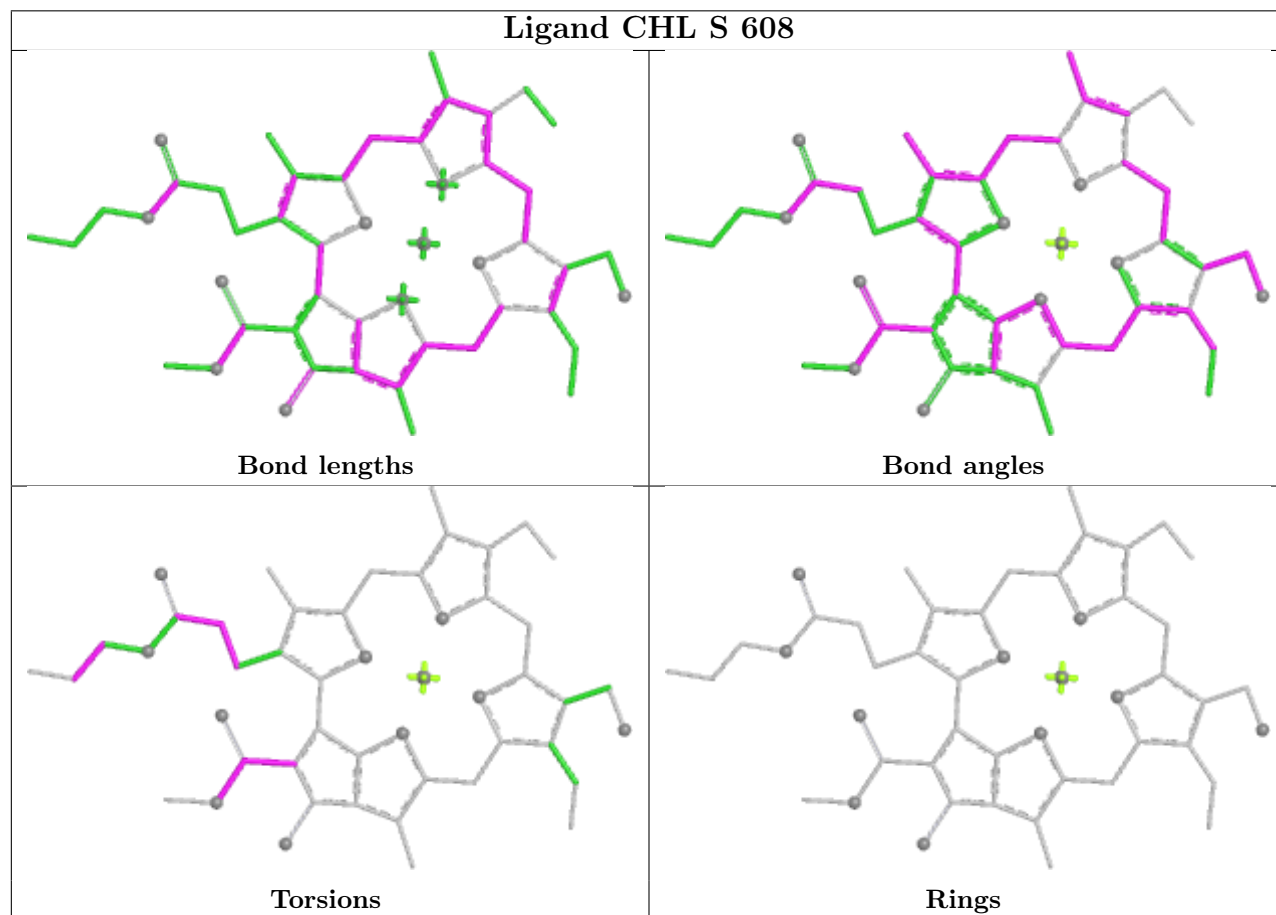
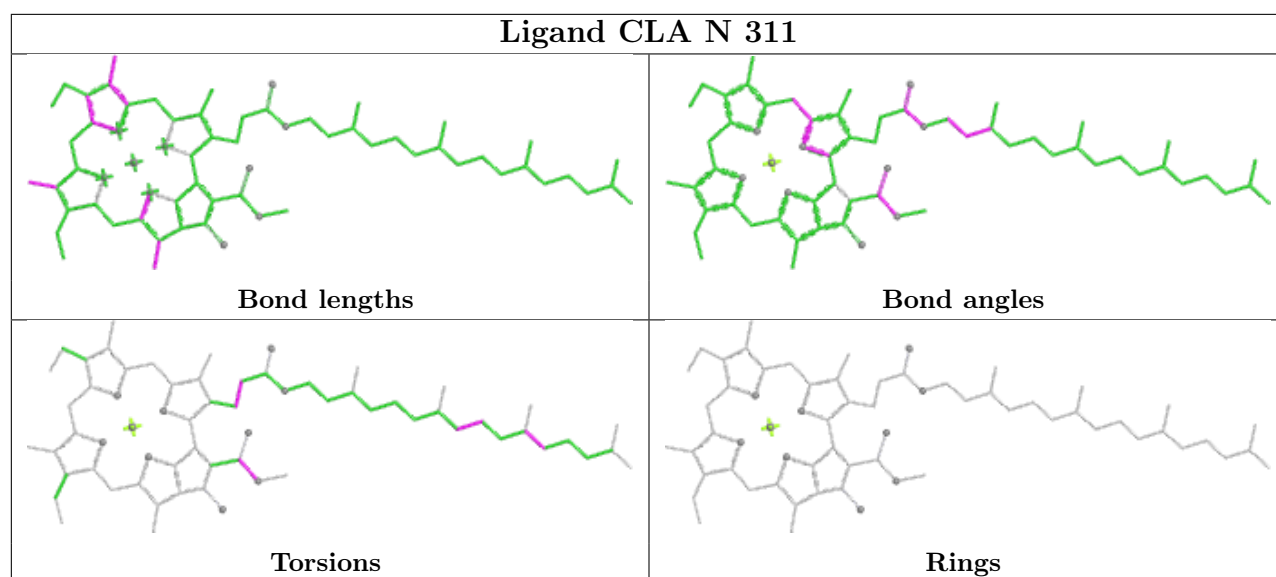


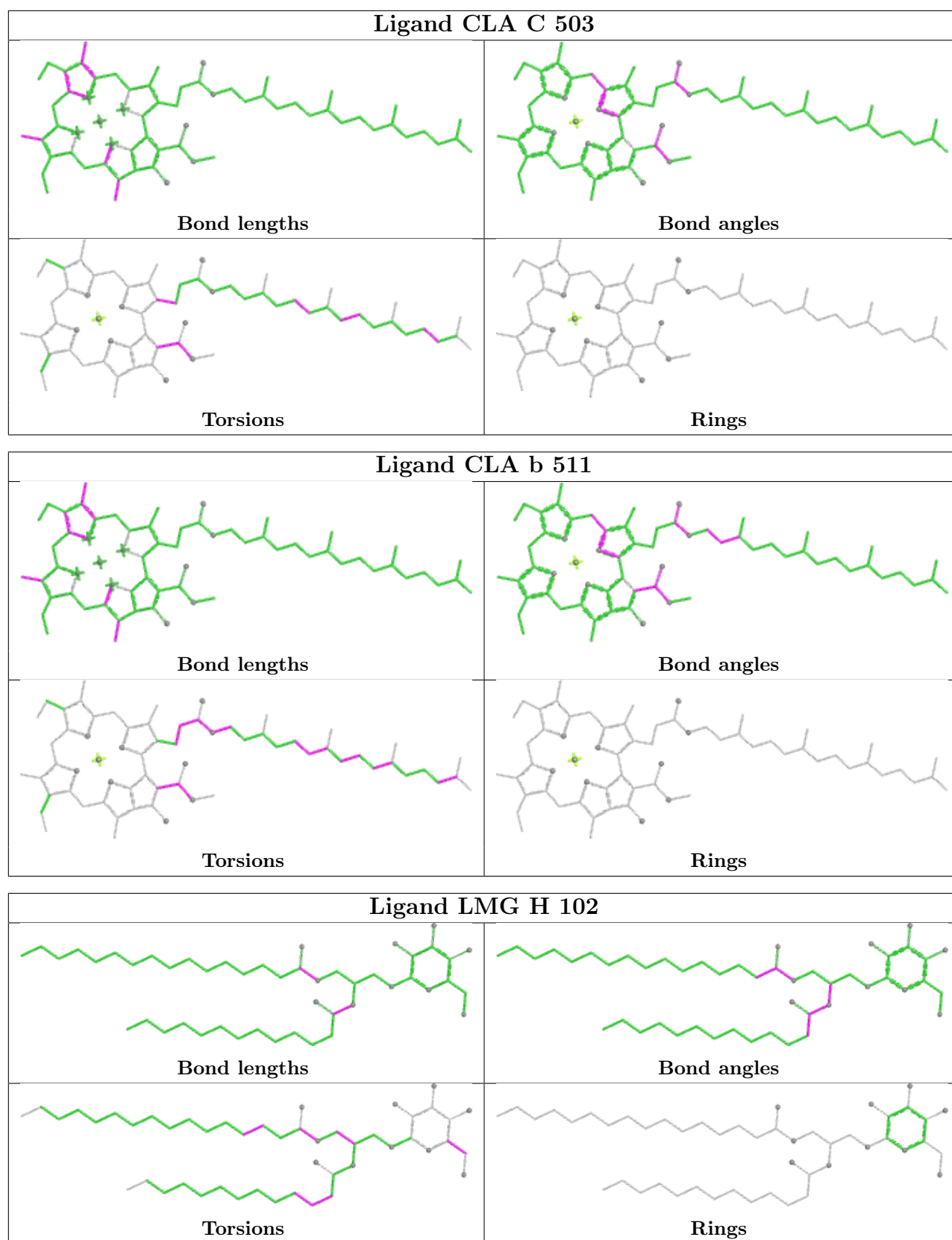
Ligand PL9 d 406	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CHL G 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

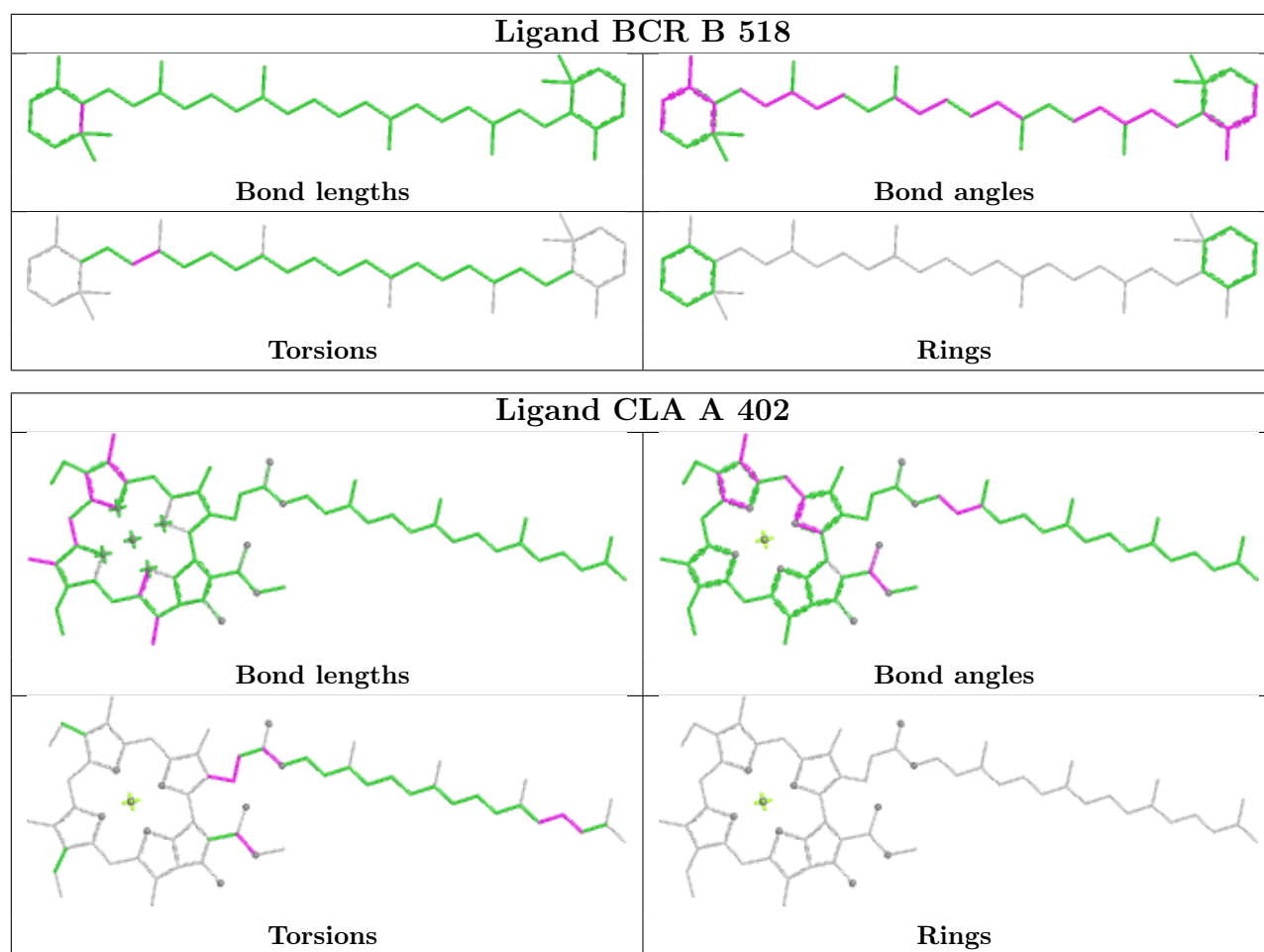


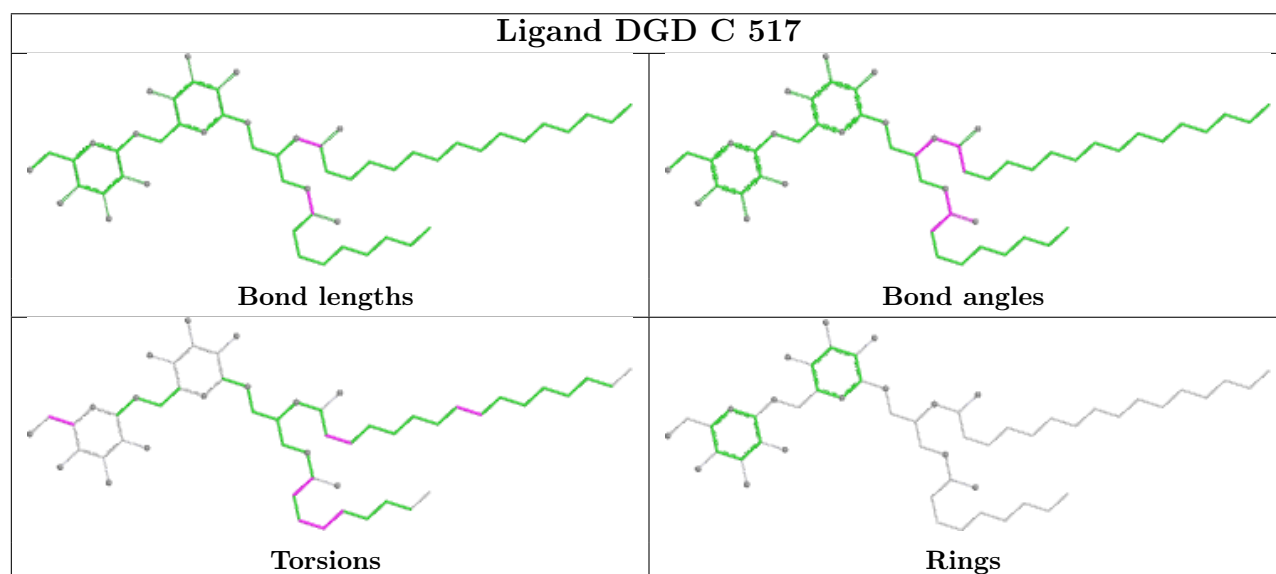
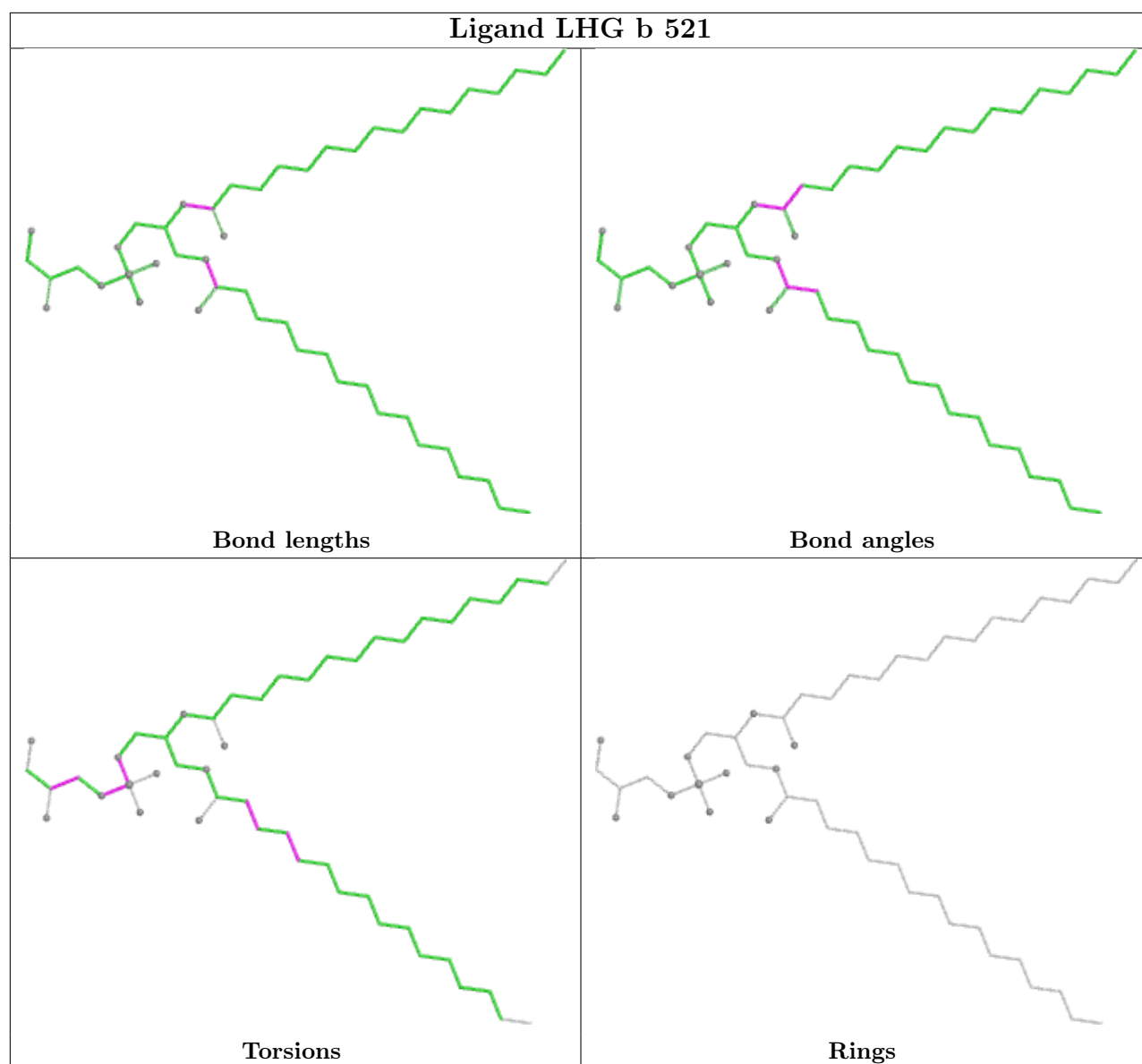




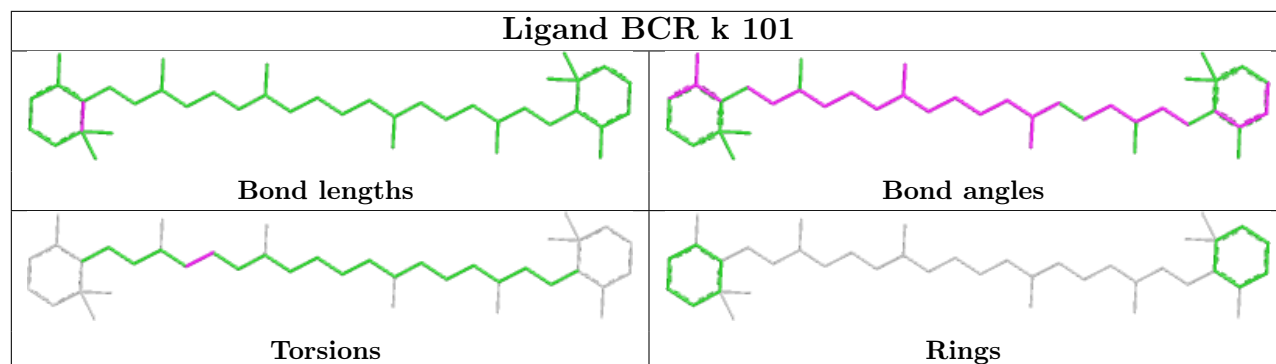




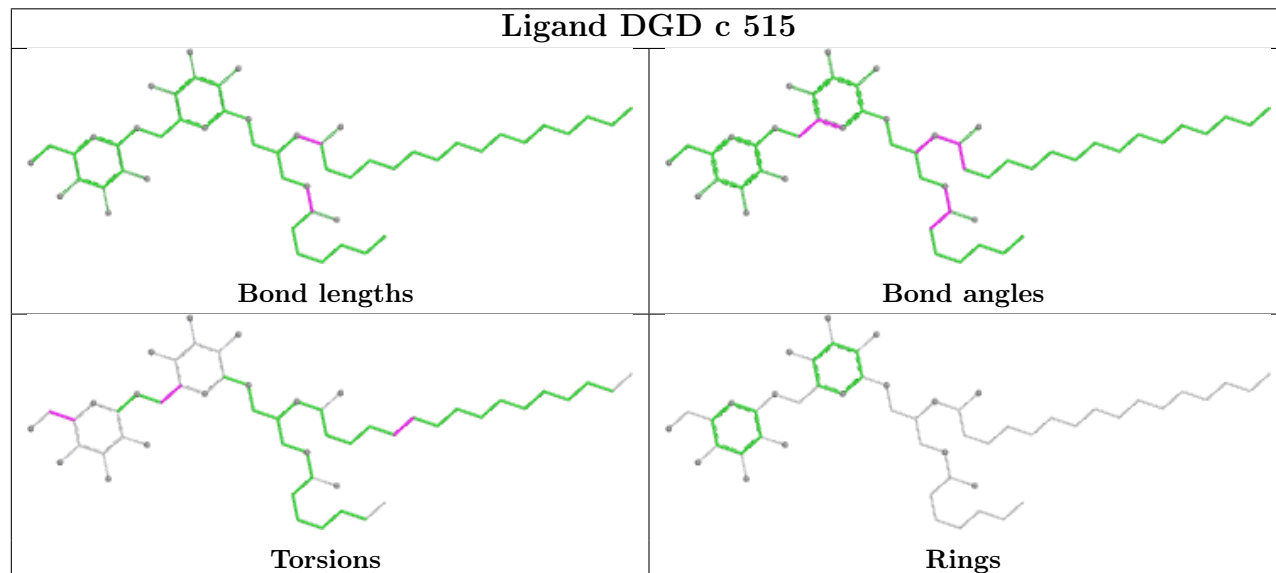




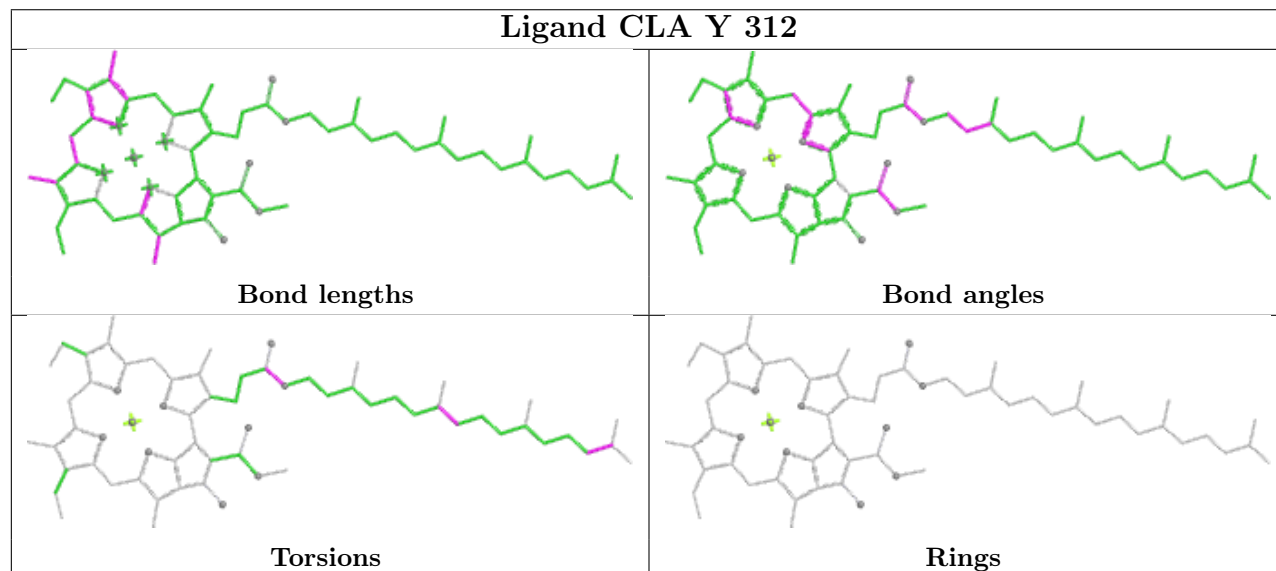
Ligand BCR k 101

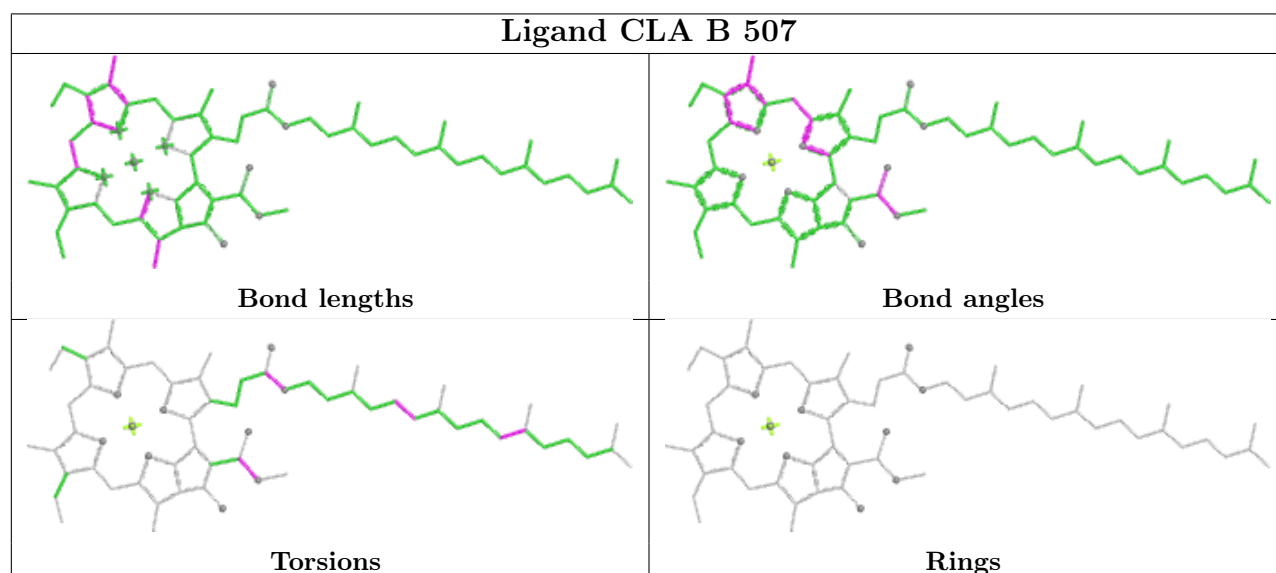
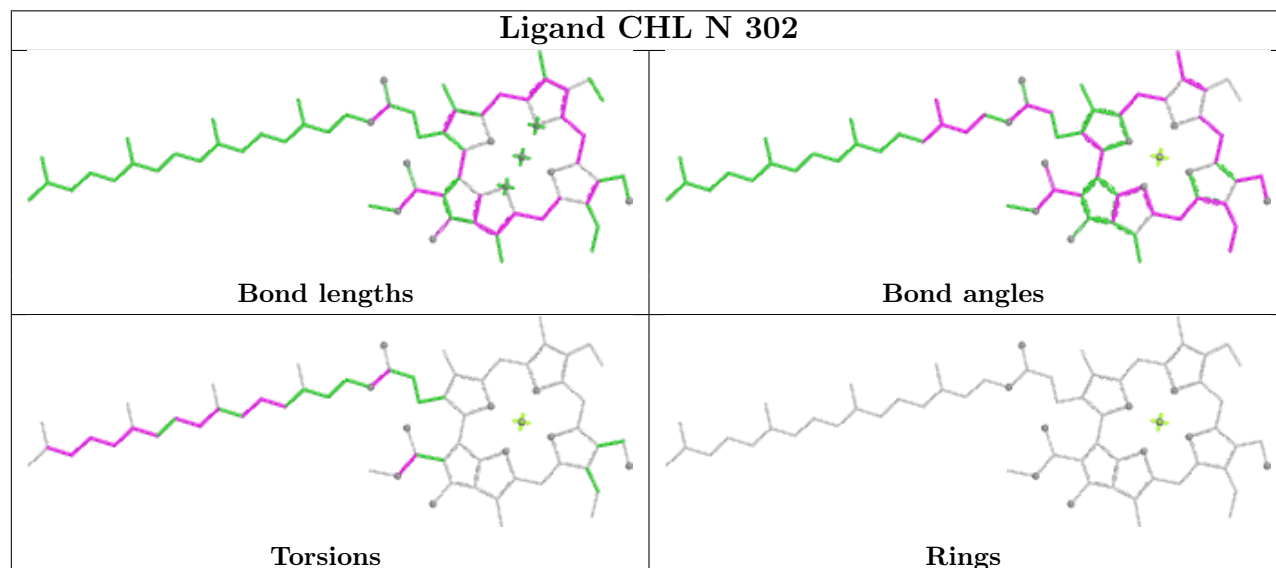
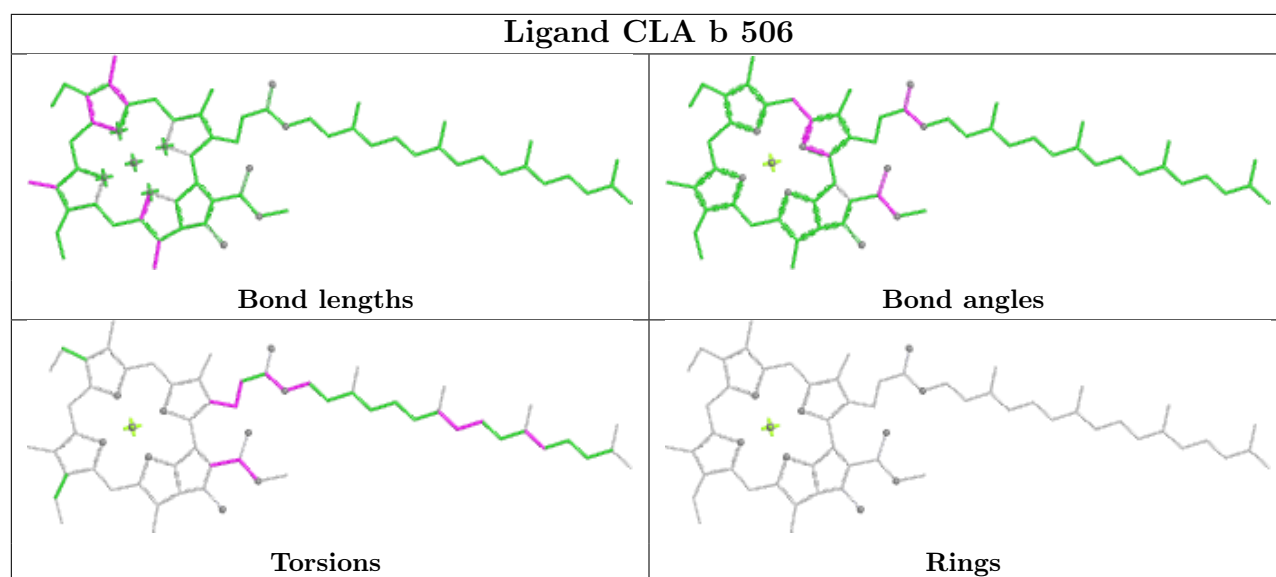


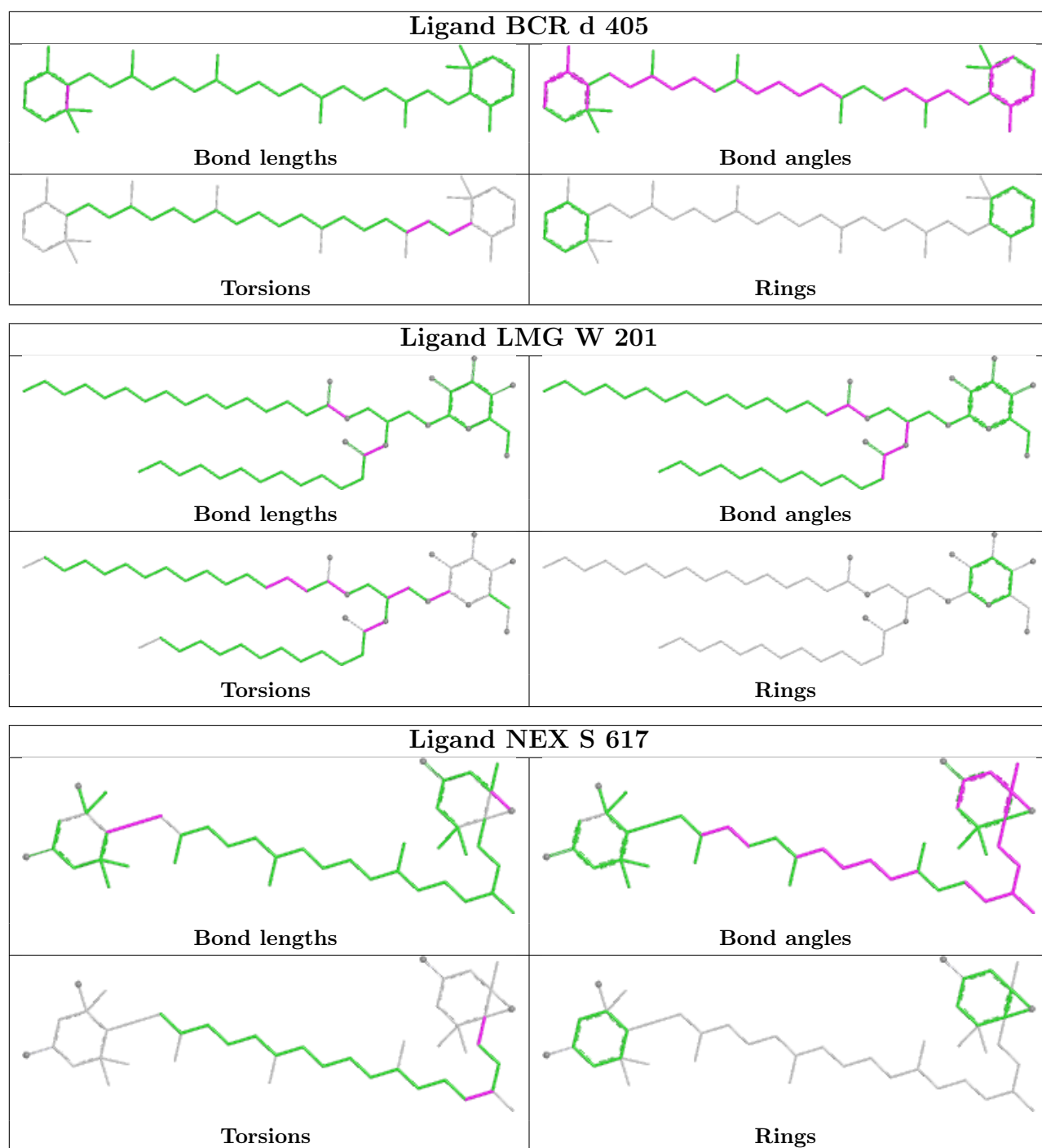
Ligand DGD c 515

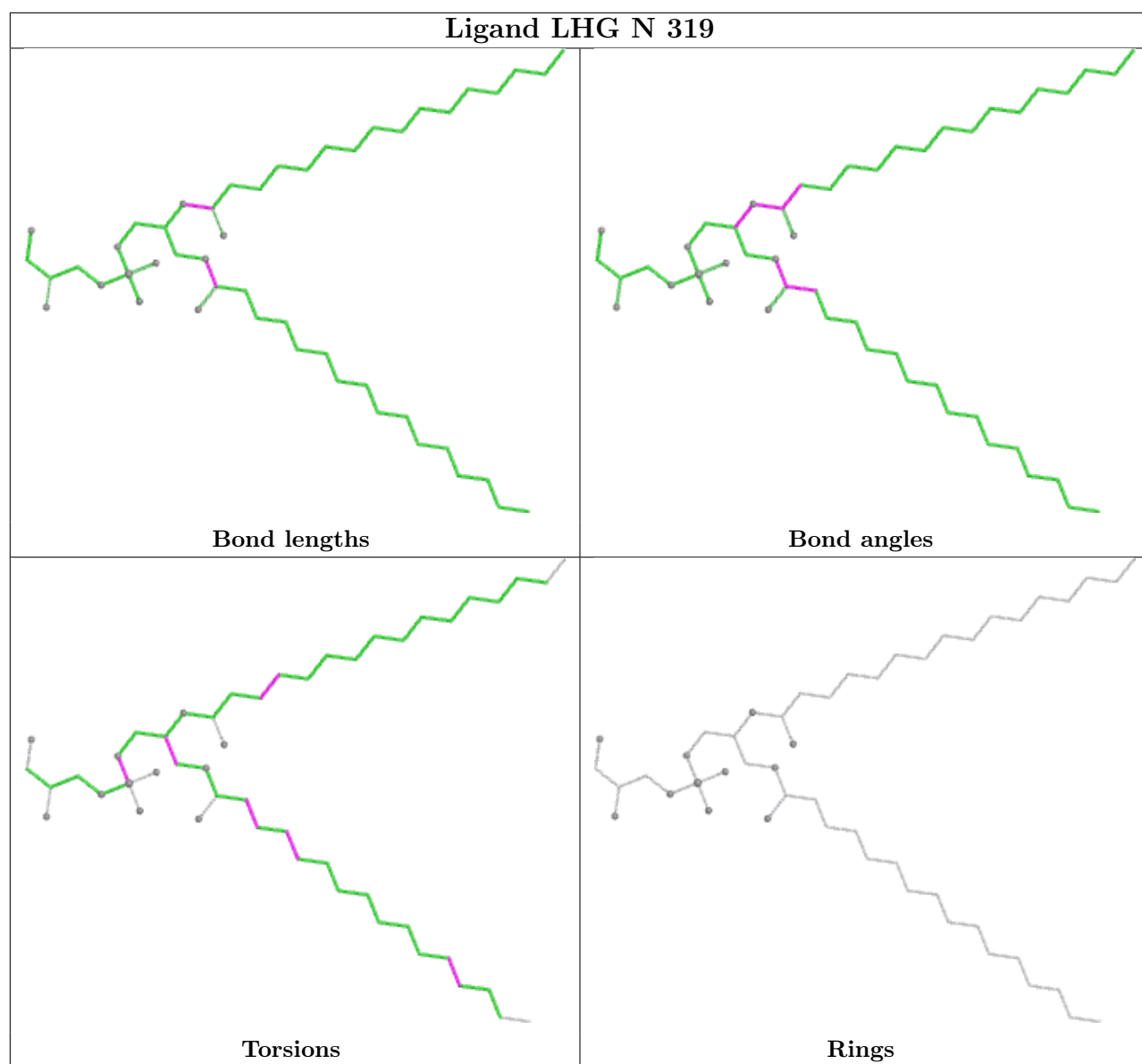


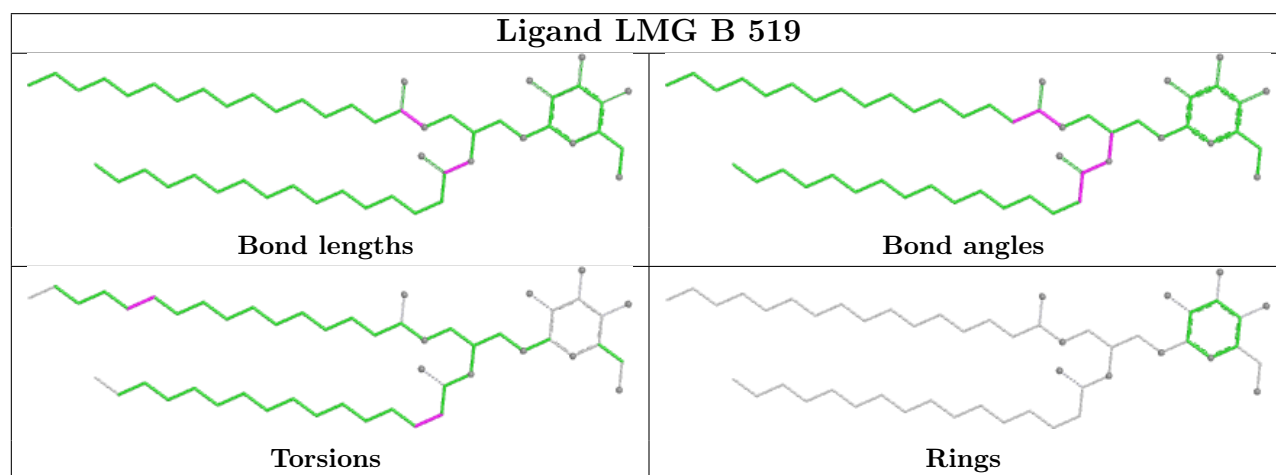
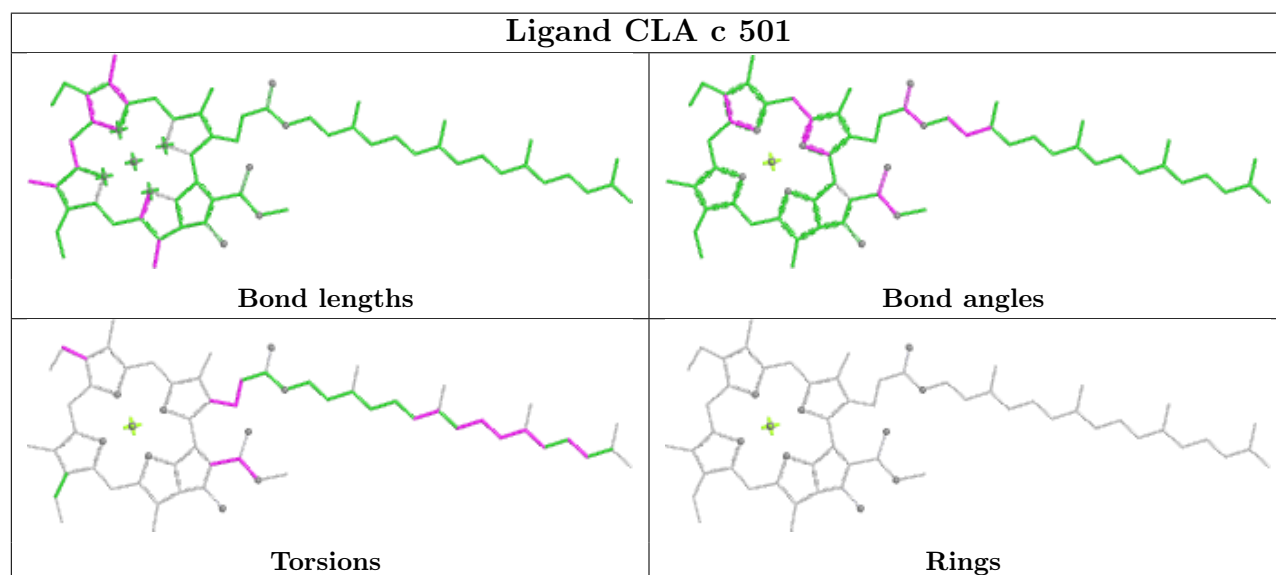
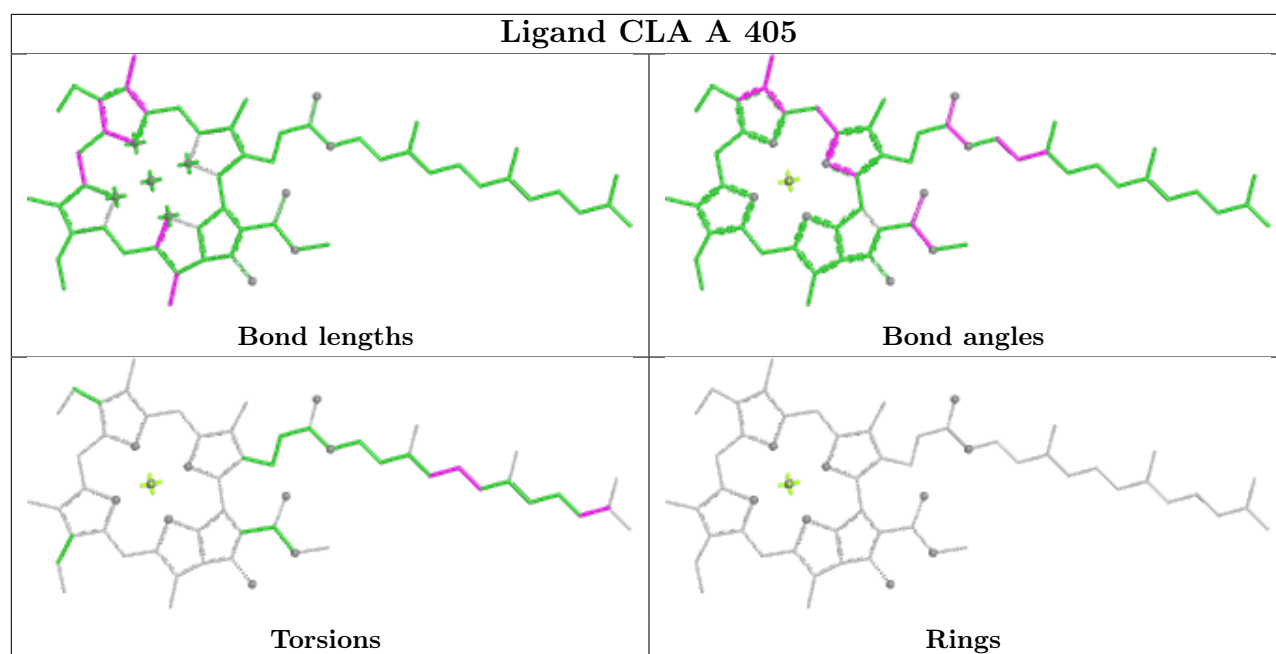
Ligand CLA Y 312

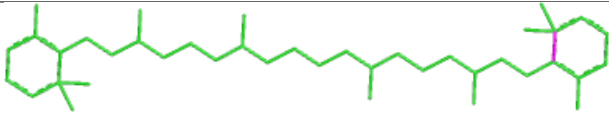
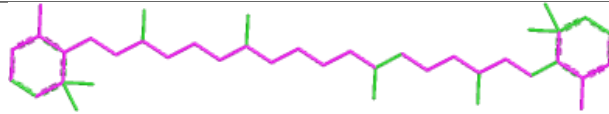
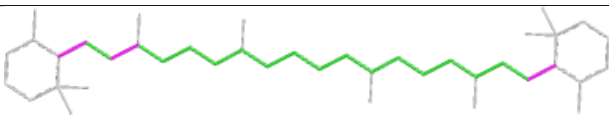
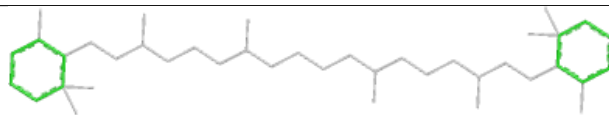


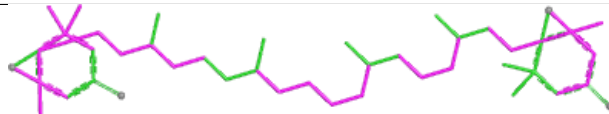
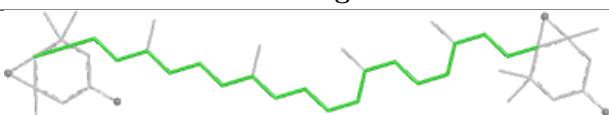
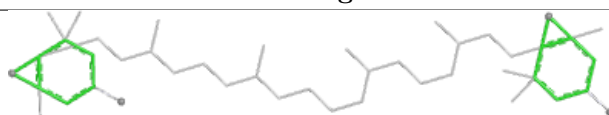


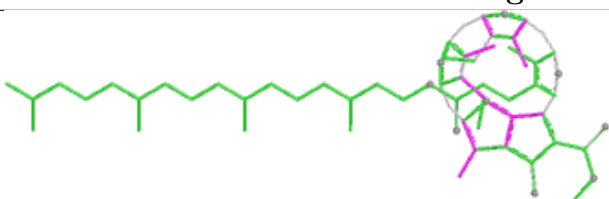
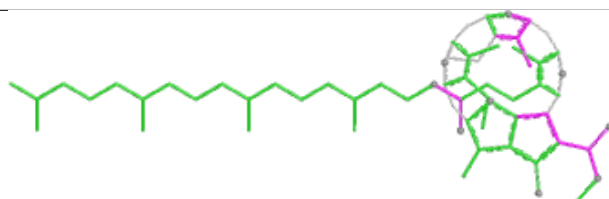
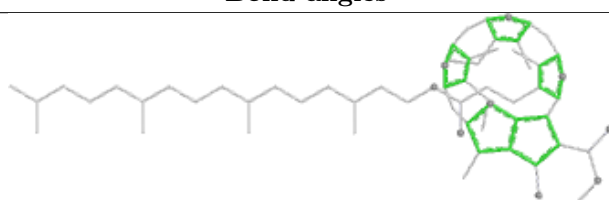


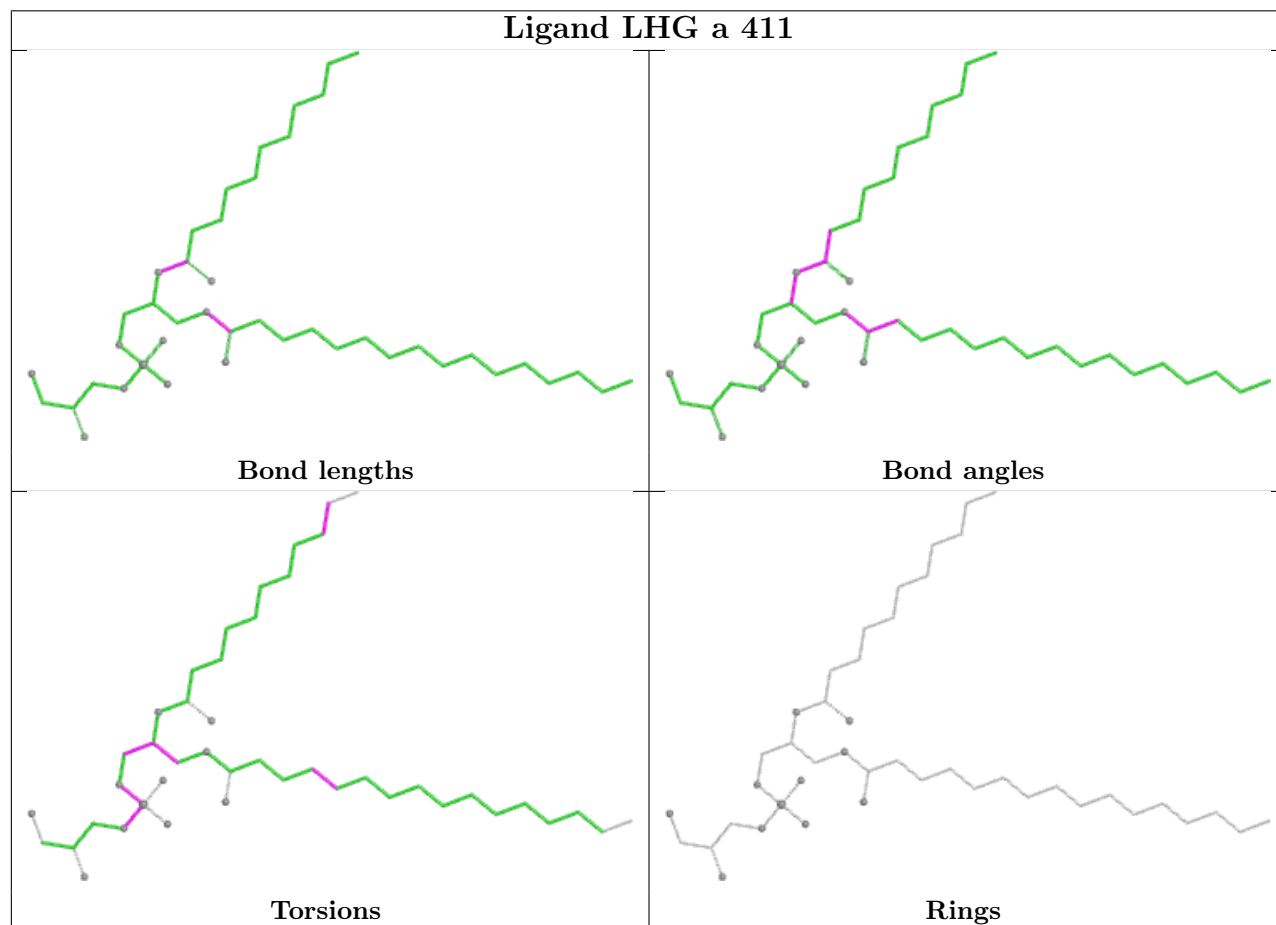
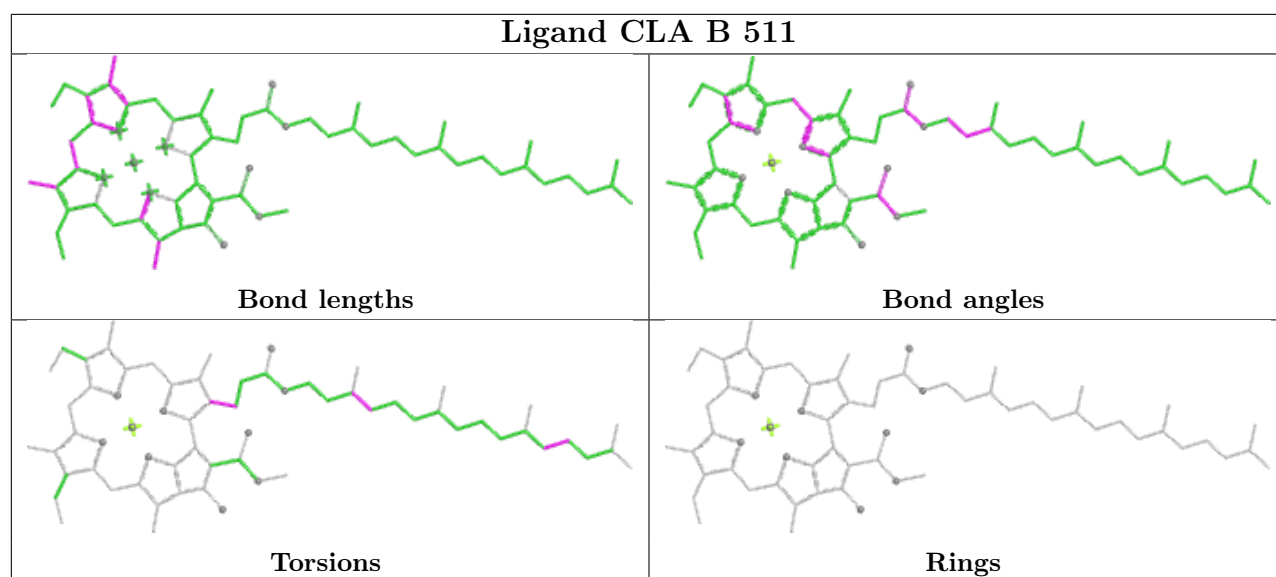




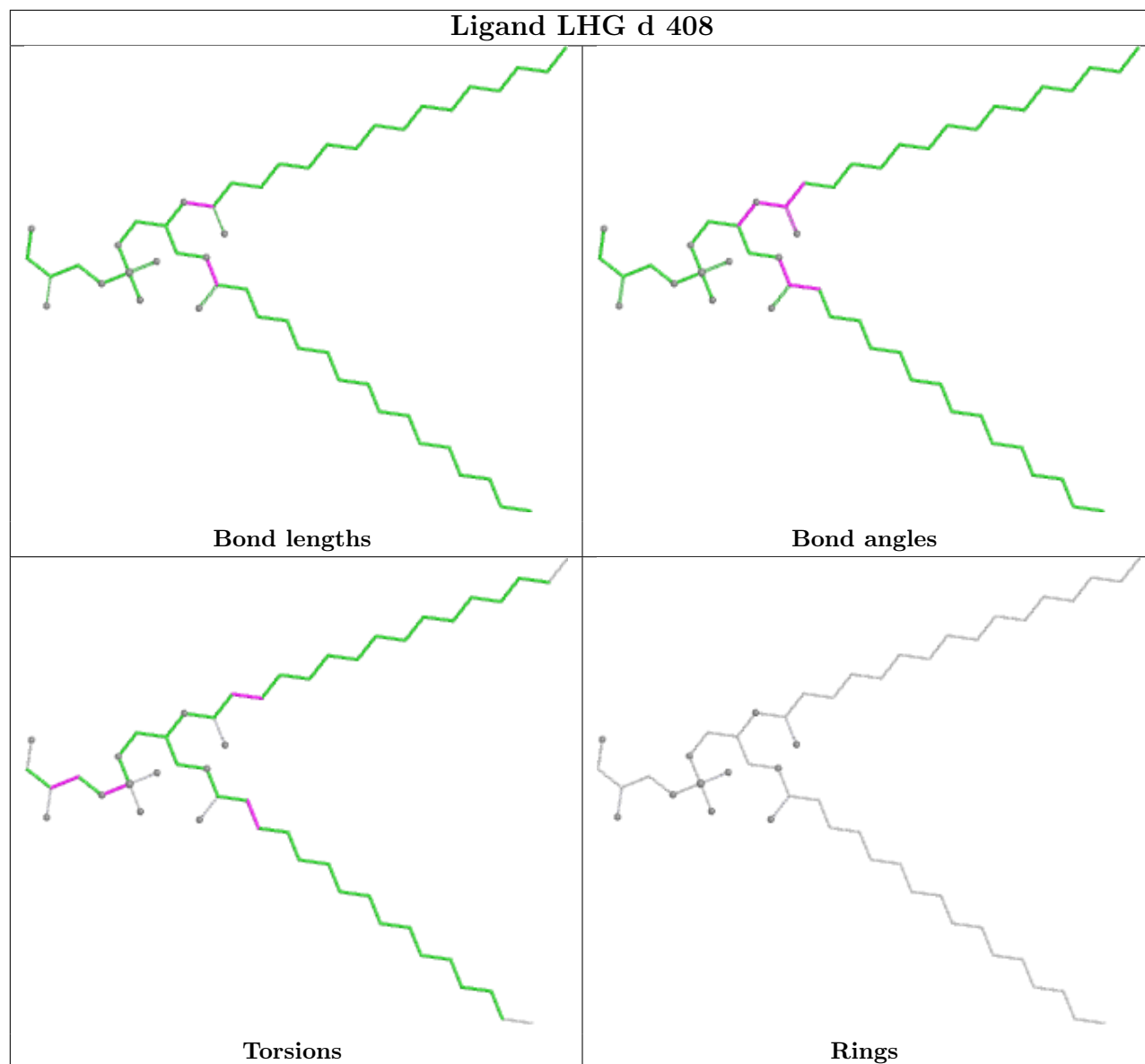
Ligand BCR t 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand XAT G 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

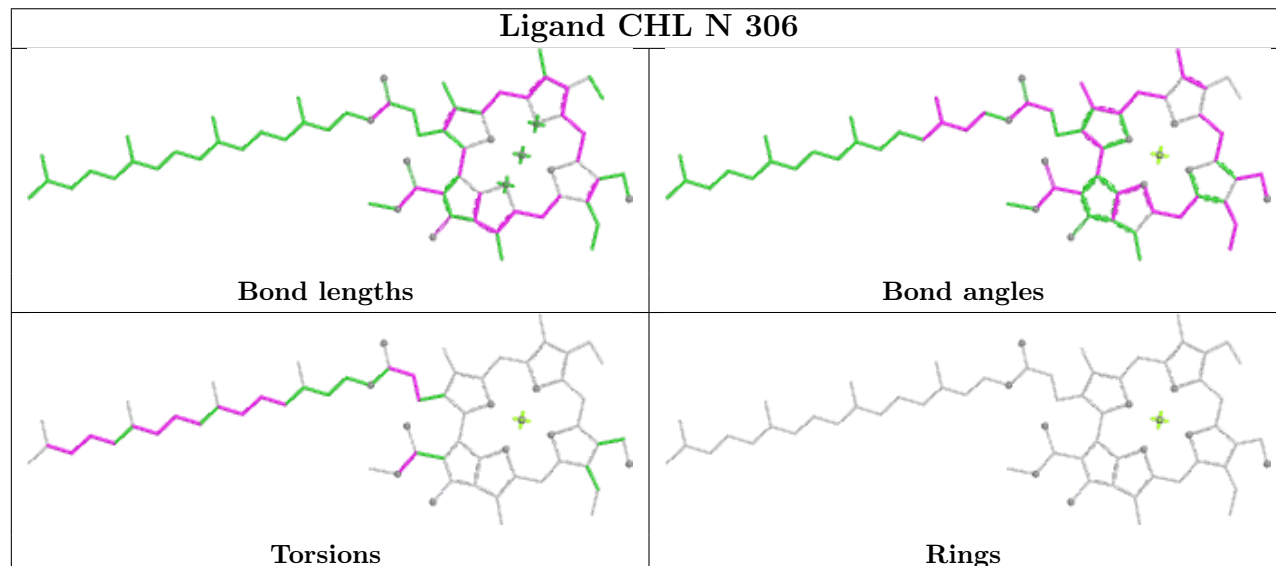
Ligand PHO A 404	
	
Bond lengths	Bond angles
	
Torsions	Rings



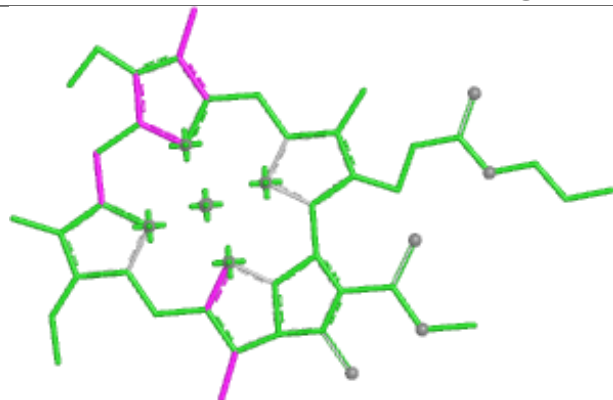
Ligand LHG d 408



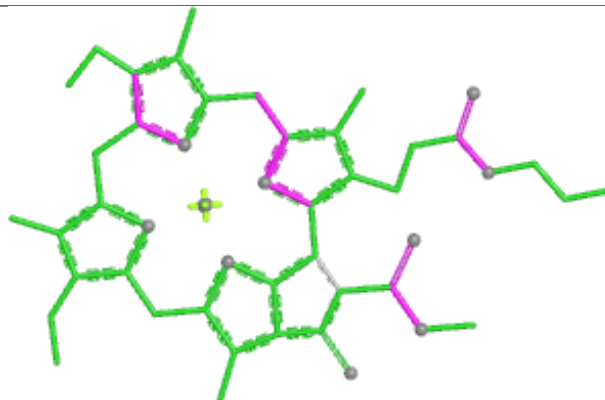
Ligand CHL N 306



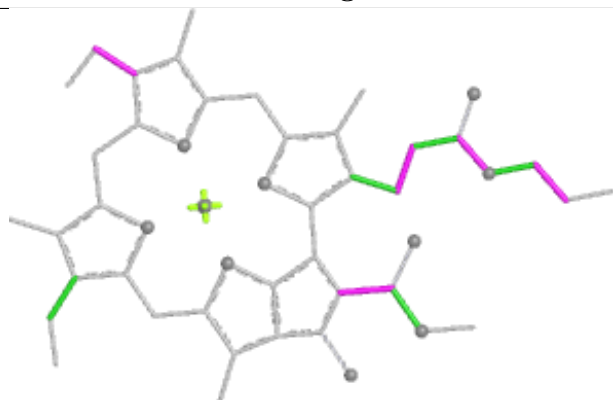
Ligand CLA S 614



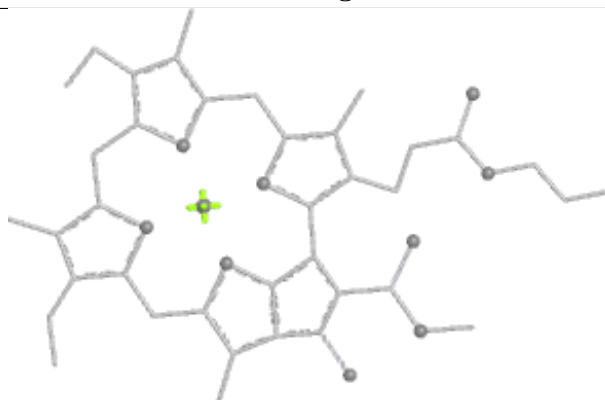
Bond lengths



Bond angles

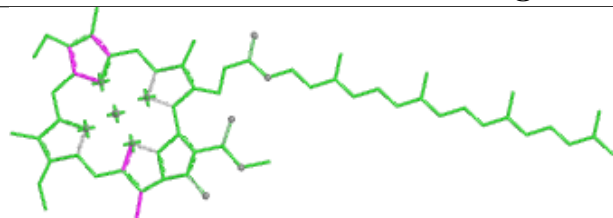


Torsions

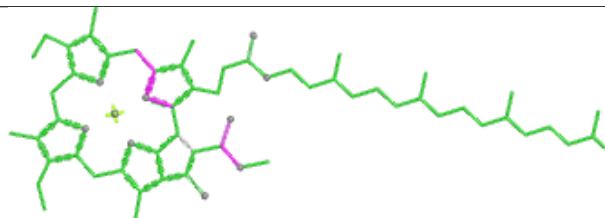


Rings

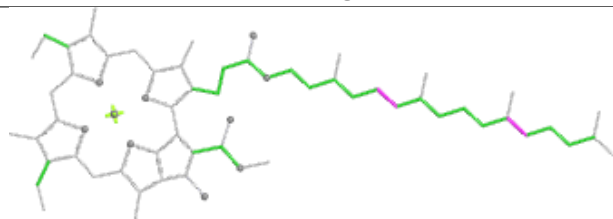
Ligand CLA B 515



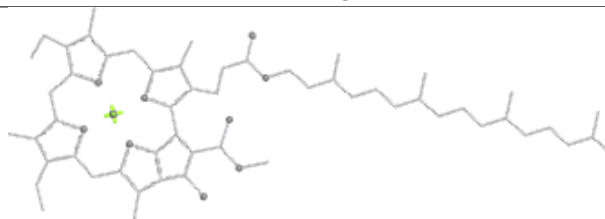
Bond lengths



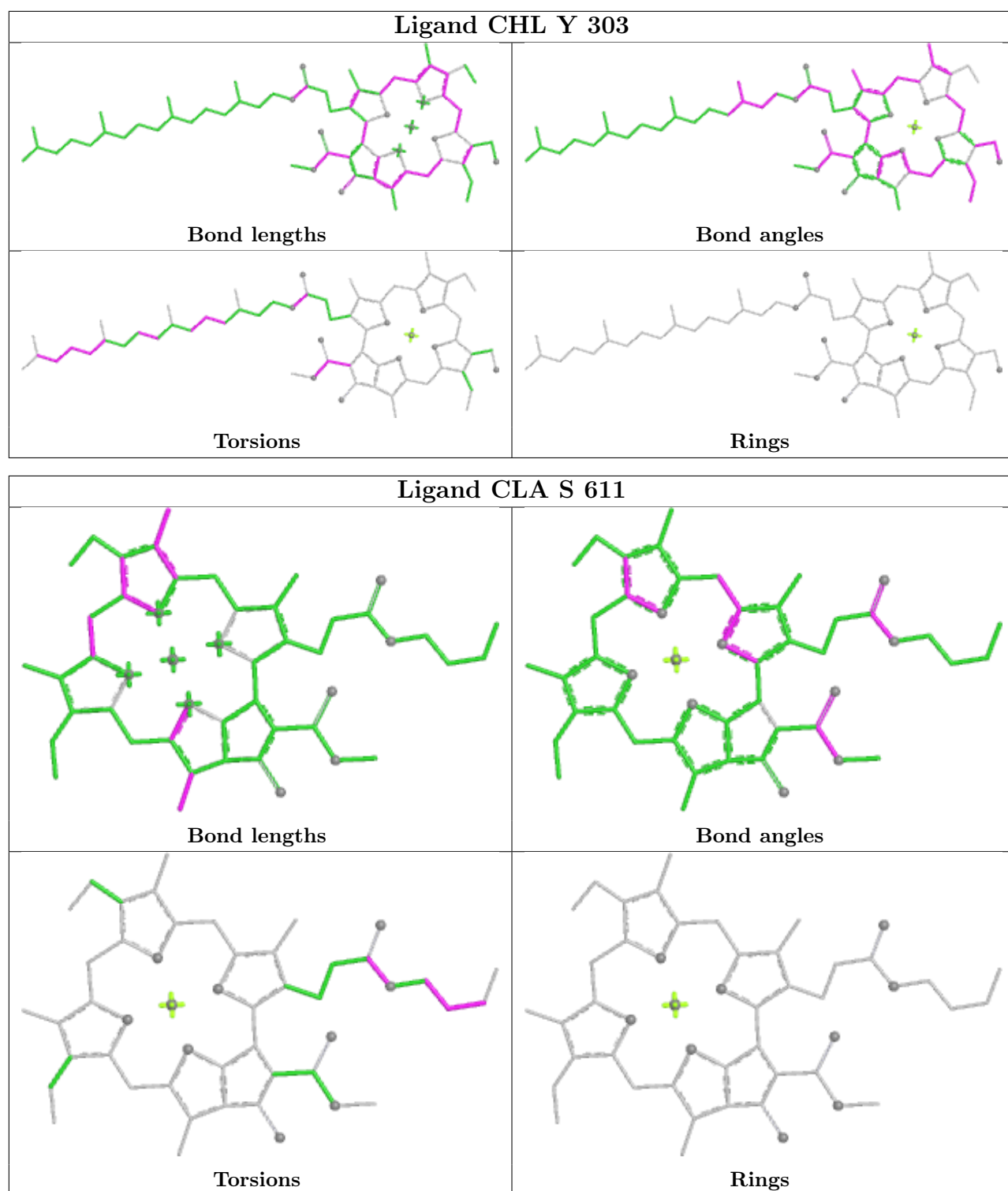
Bond angles



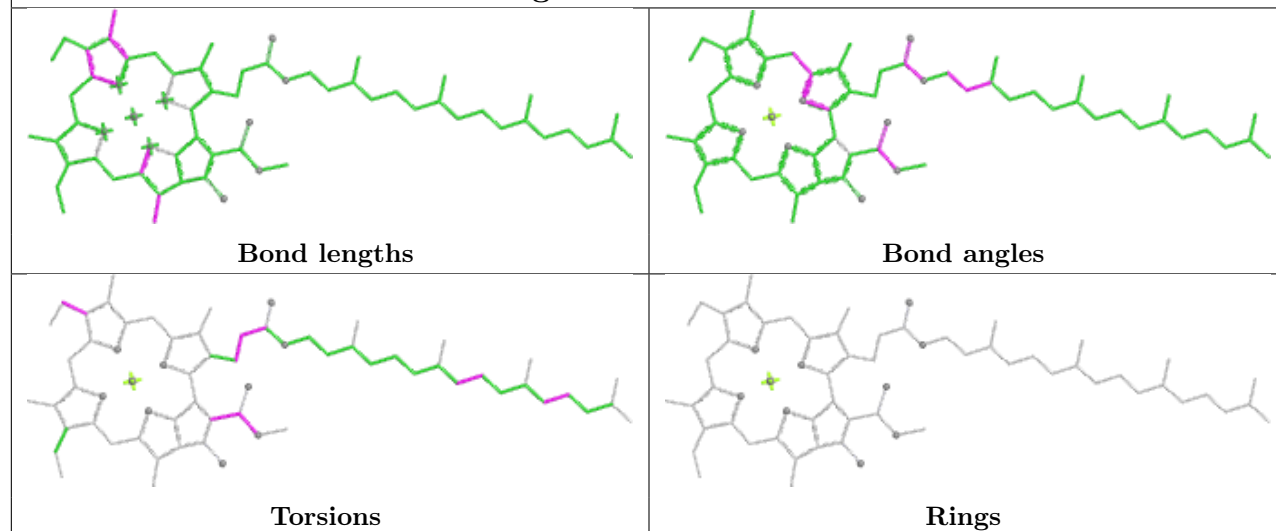
Torsions



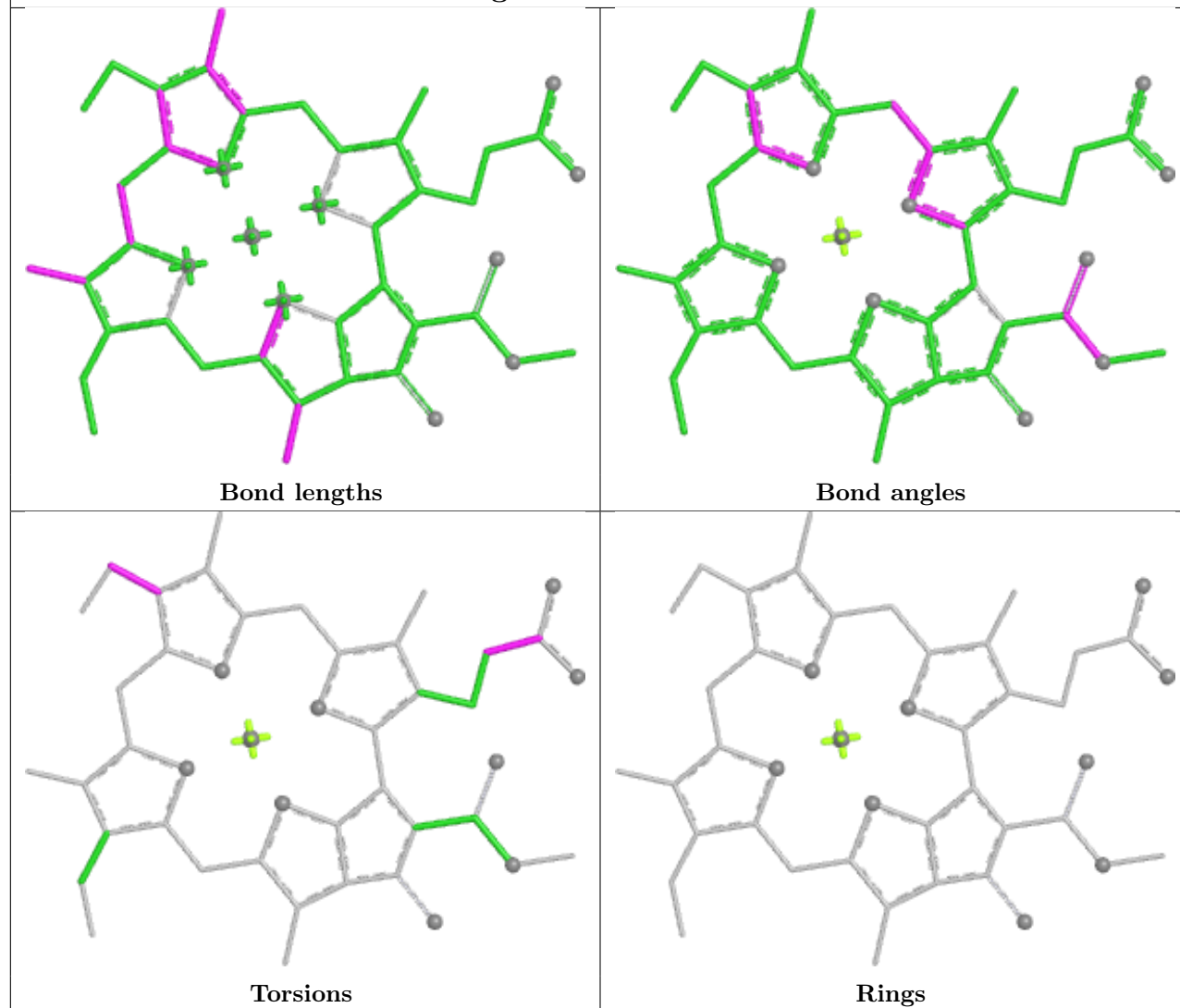
Rings

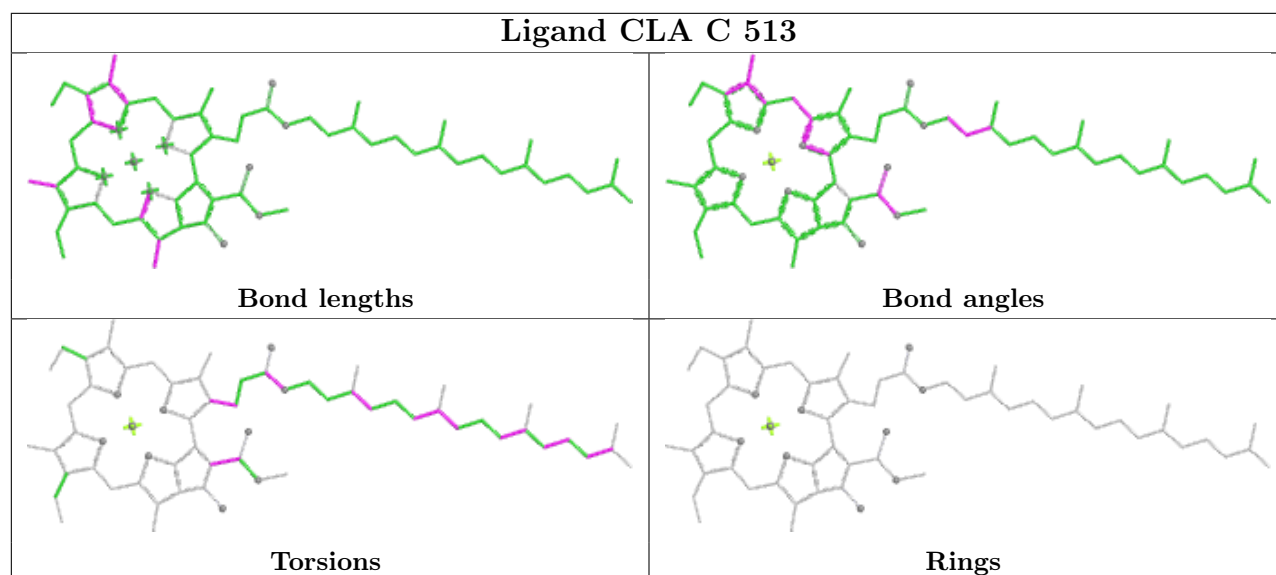
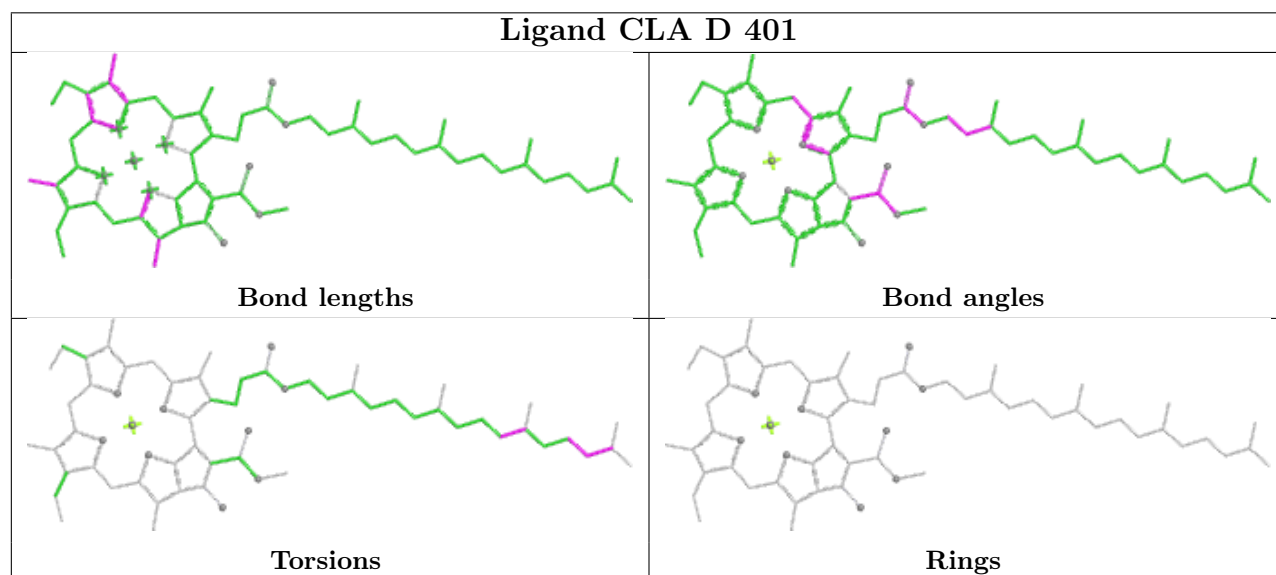
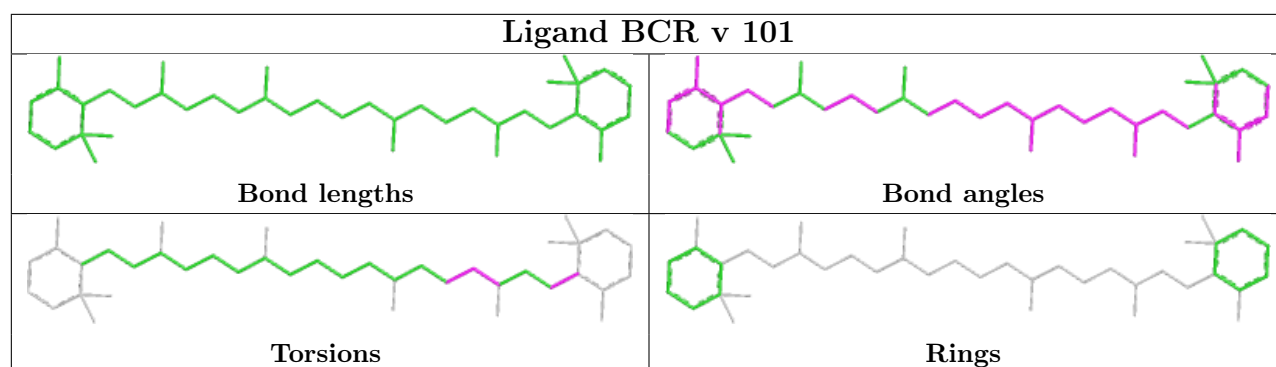


Ligand CLA B 501

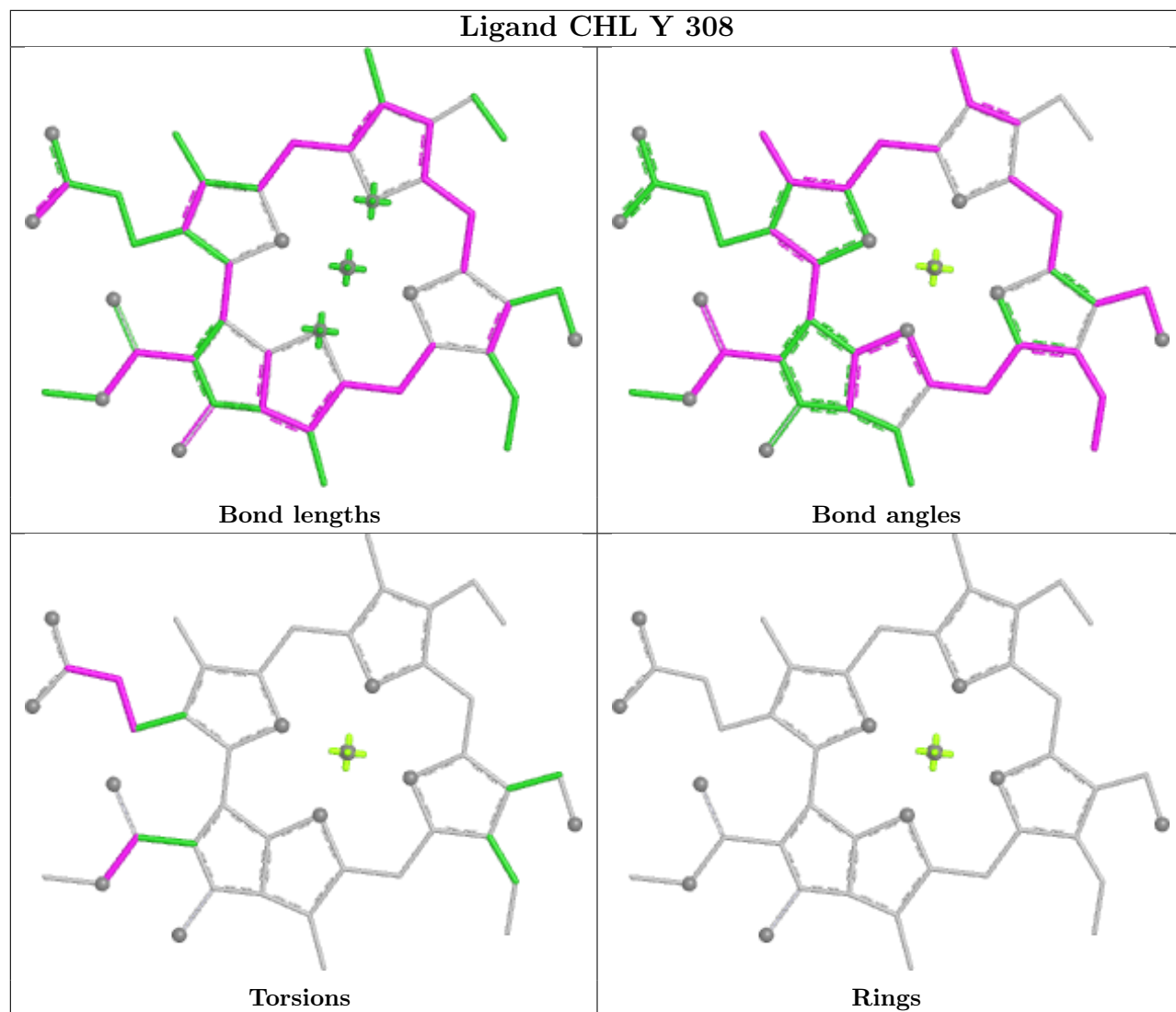


Ligand CLA N 313

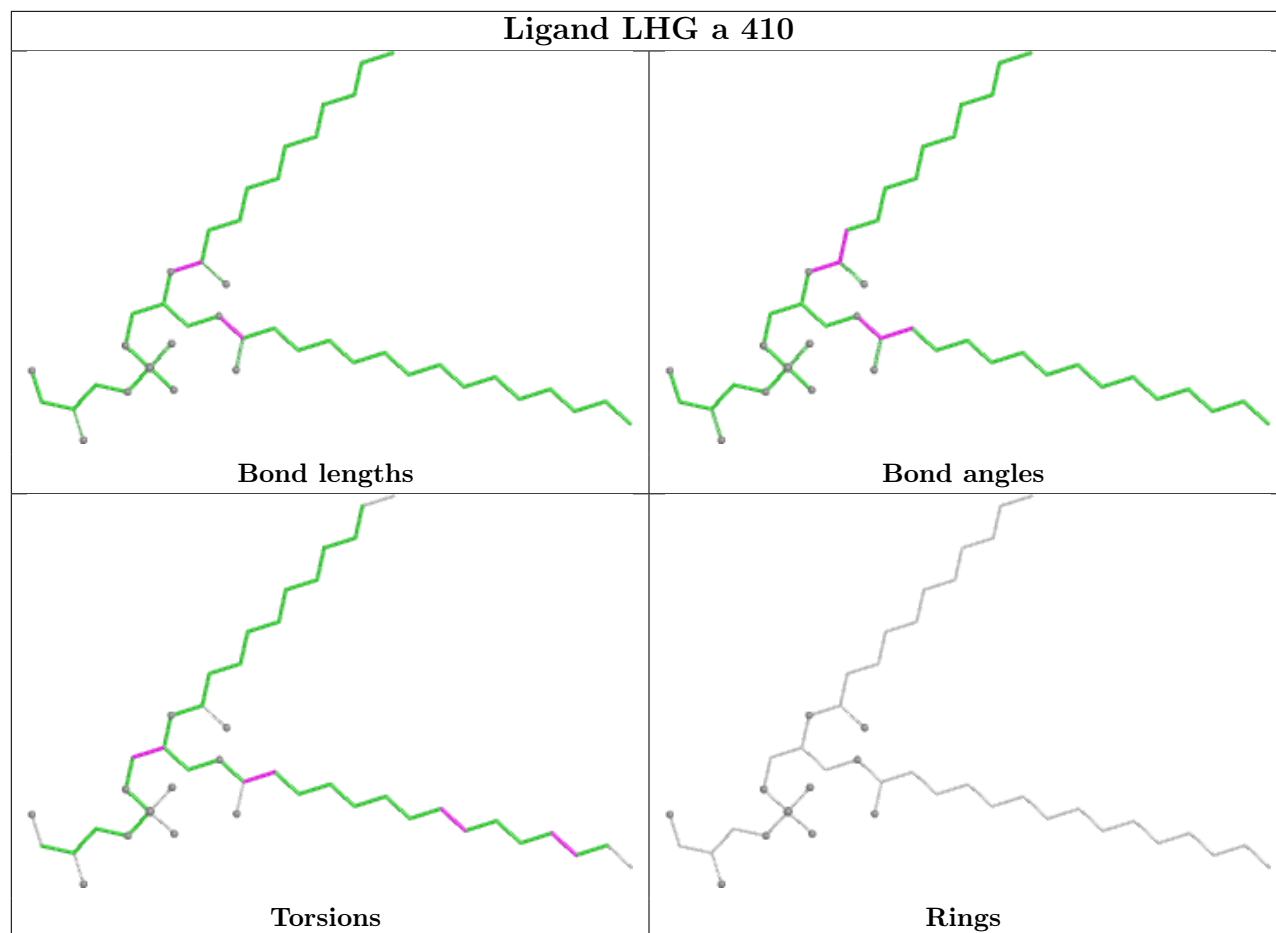




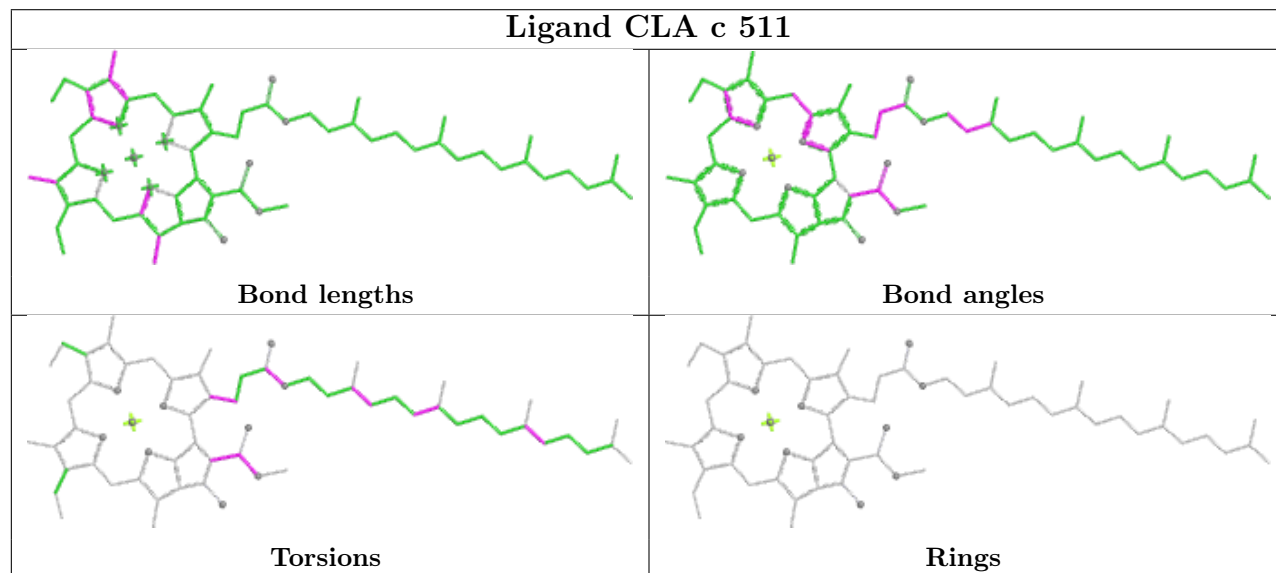
Ligand CHL Y 308

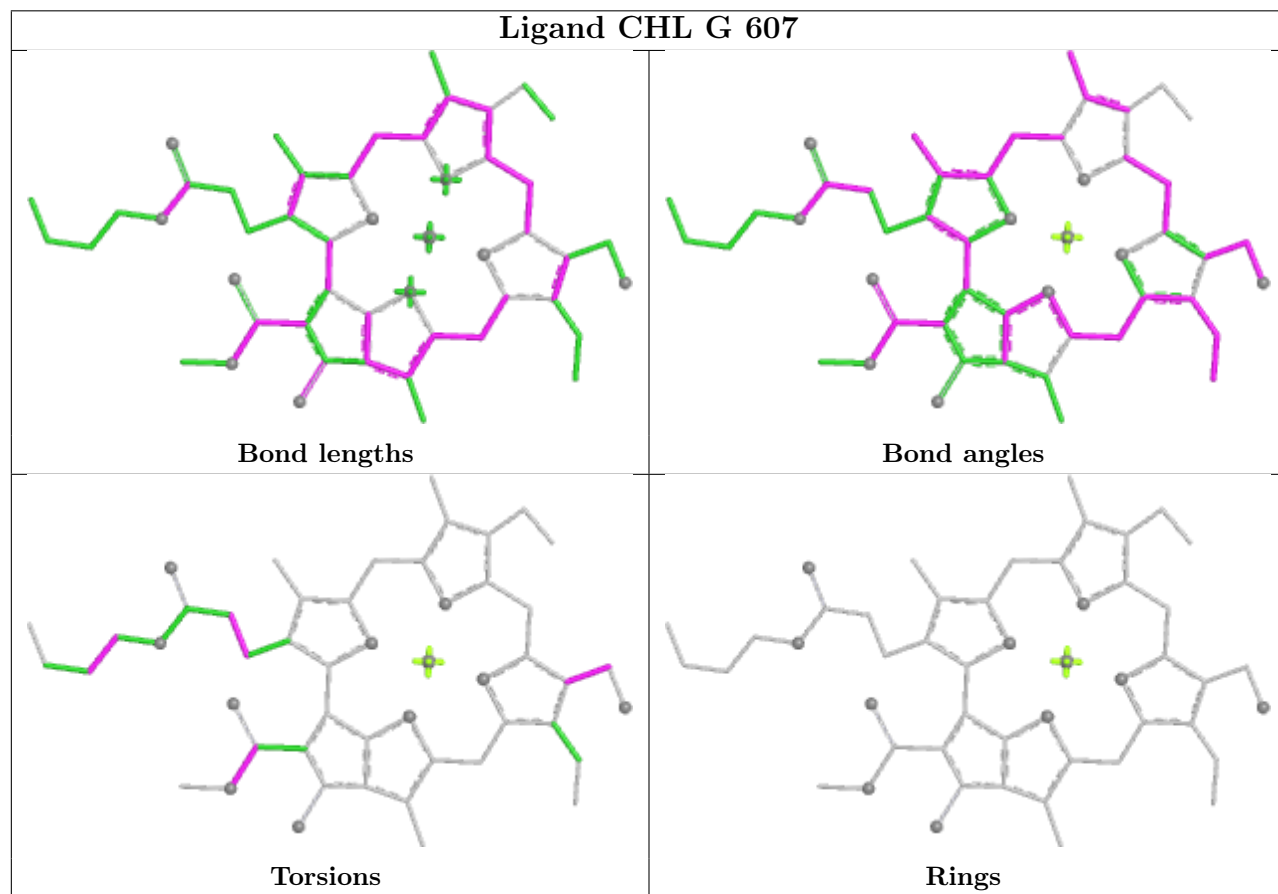
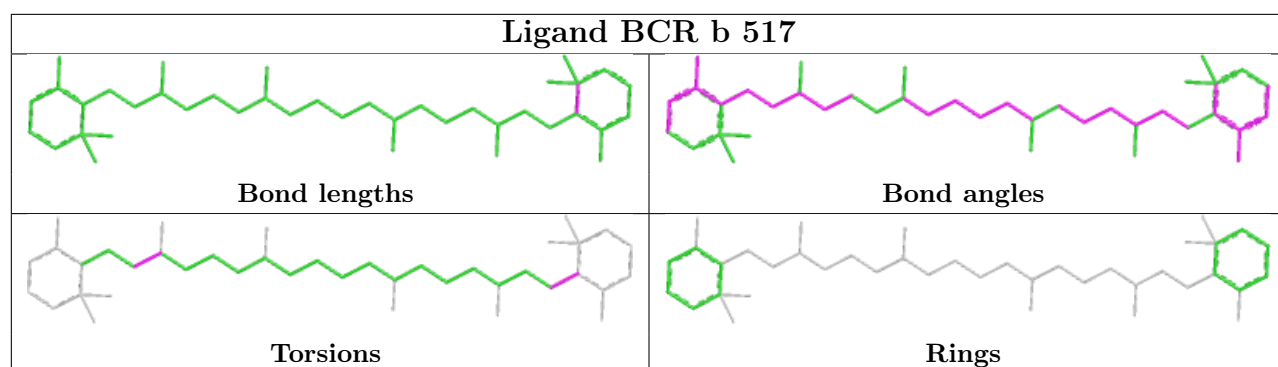


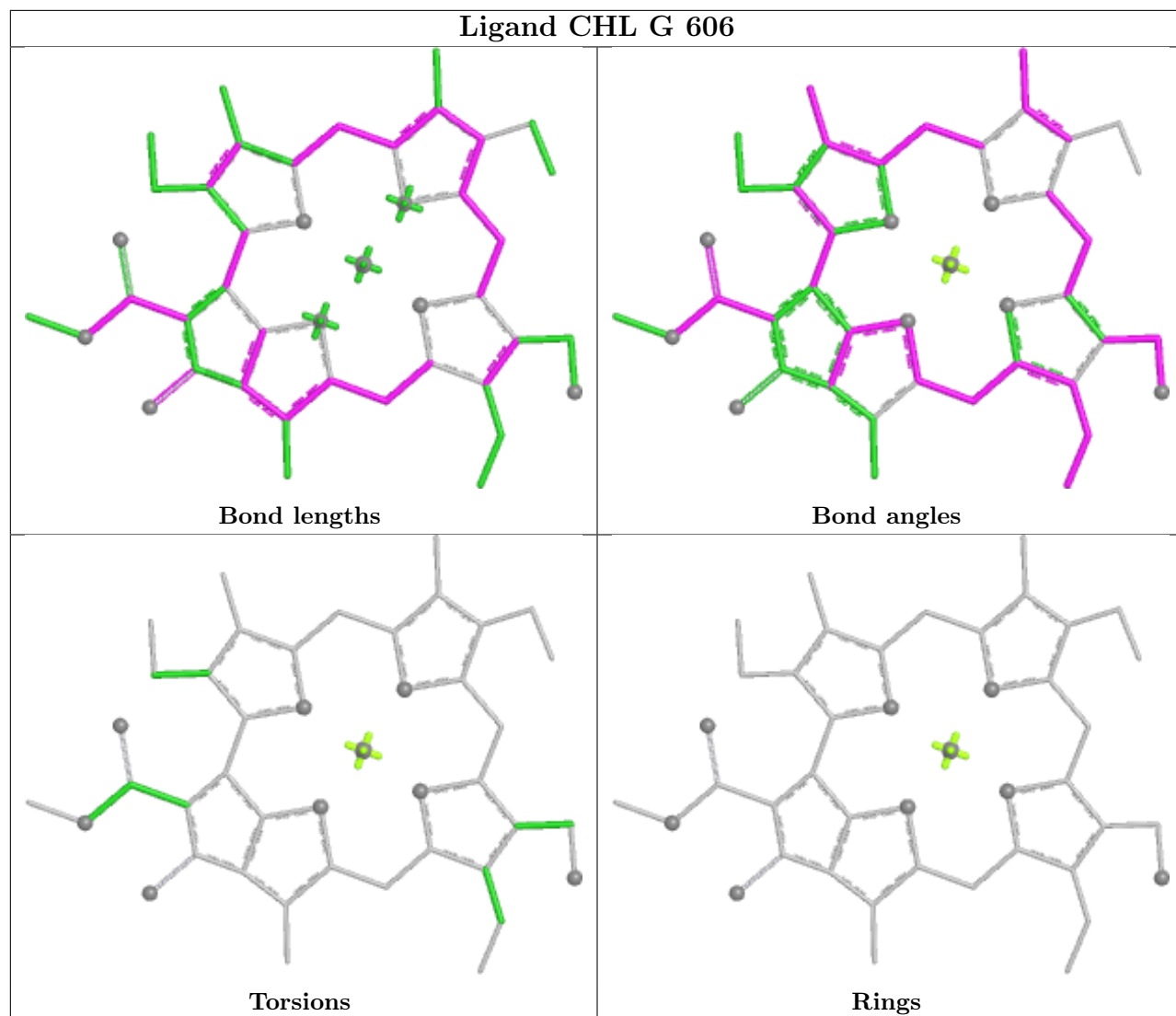
Ligand LHG a 410

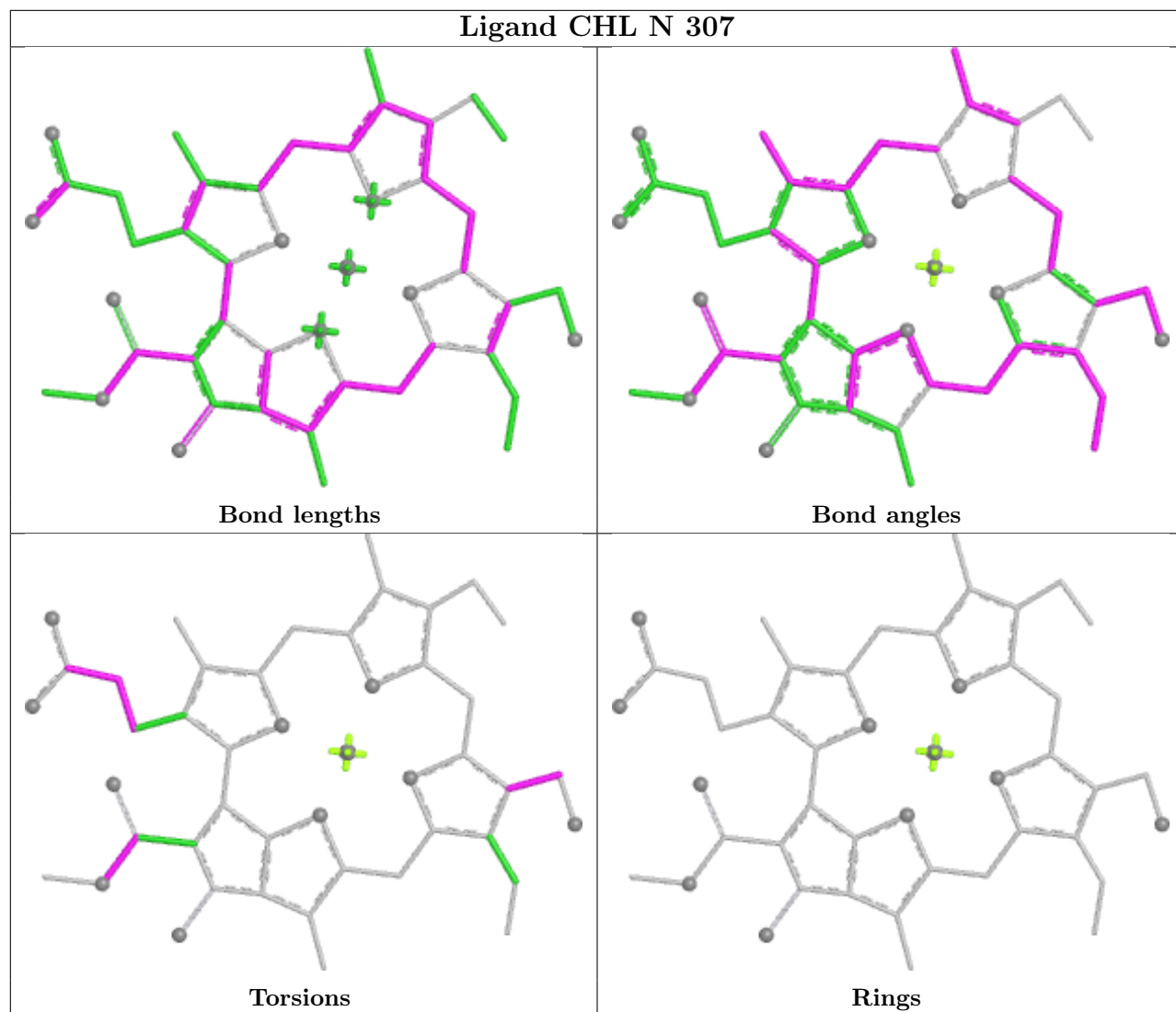


Ligand CLA c 511

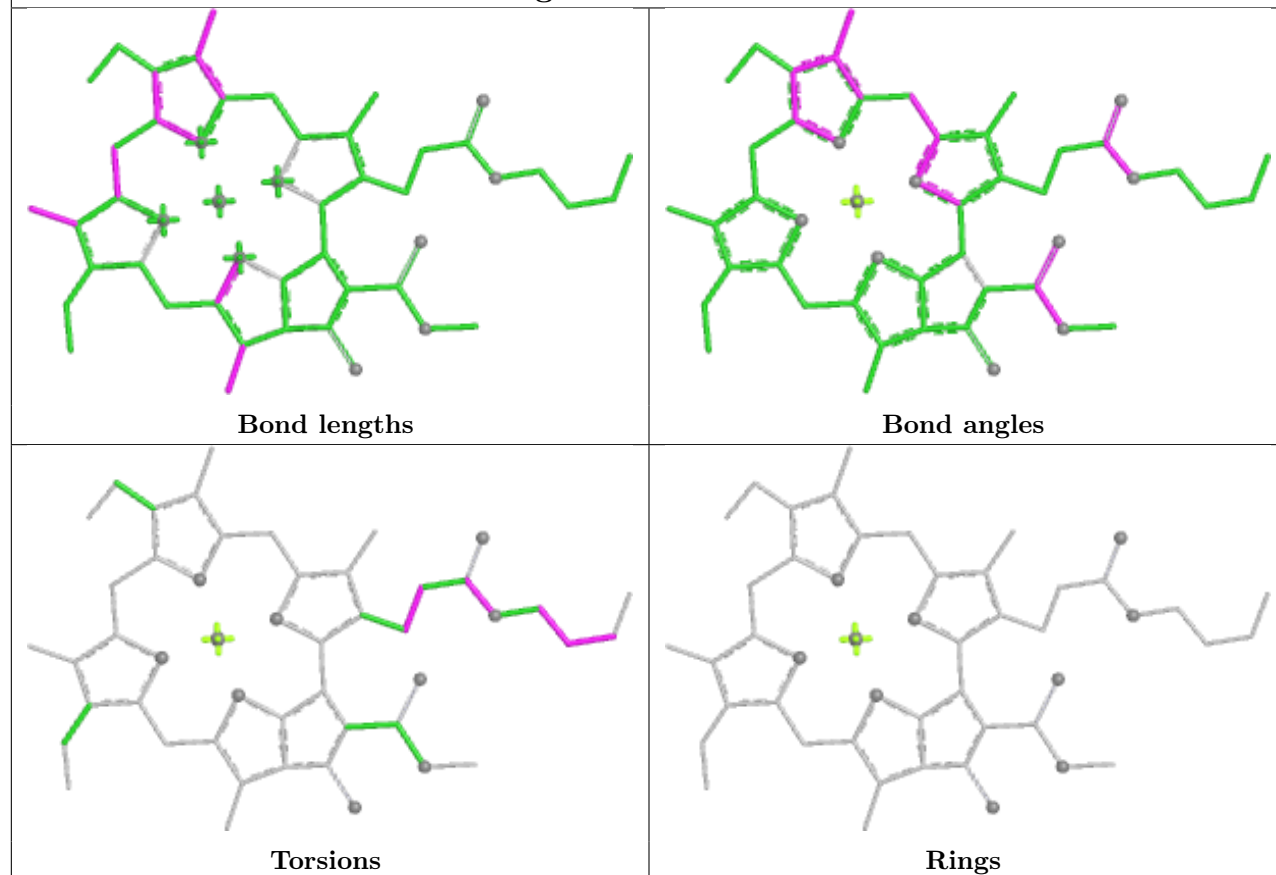




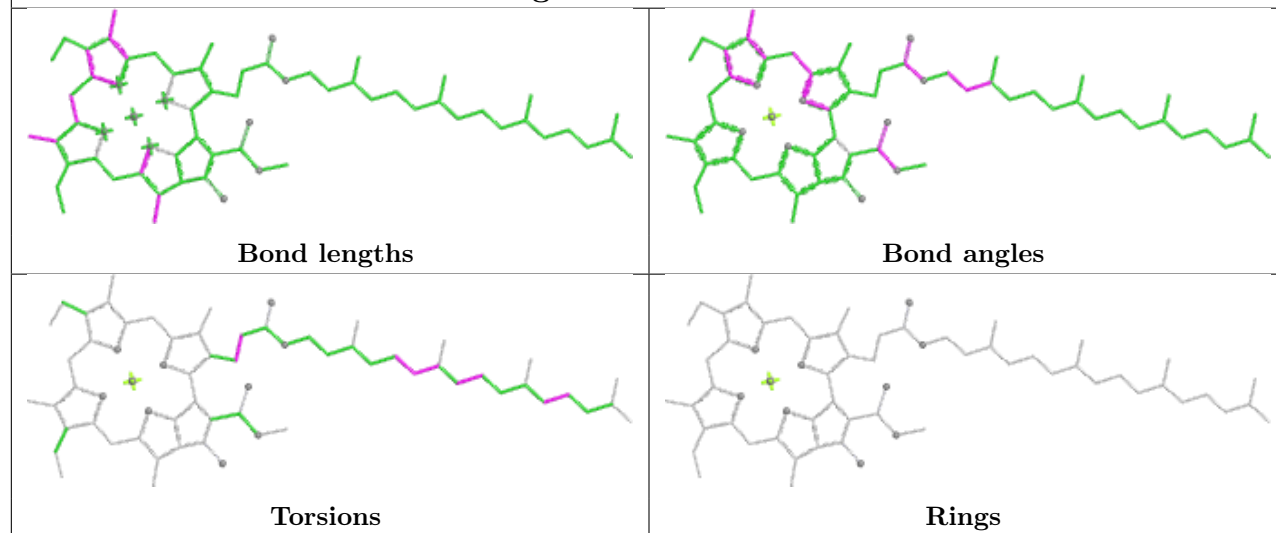




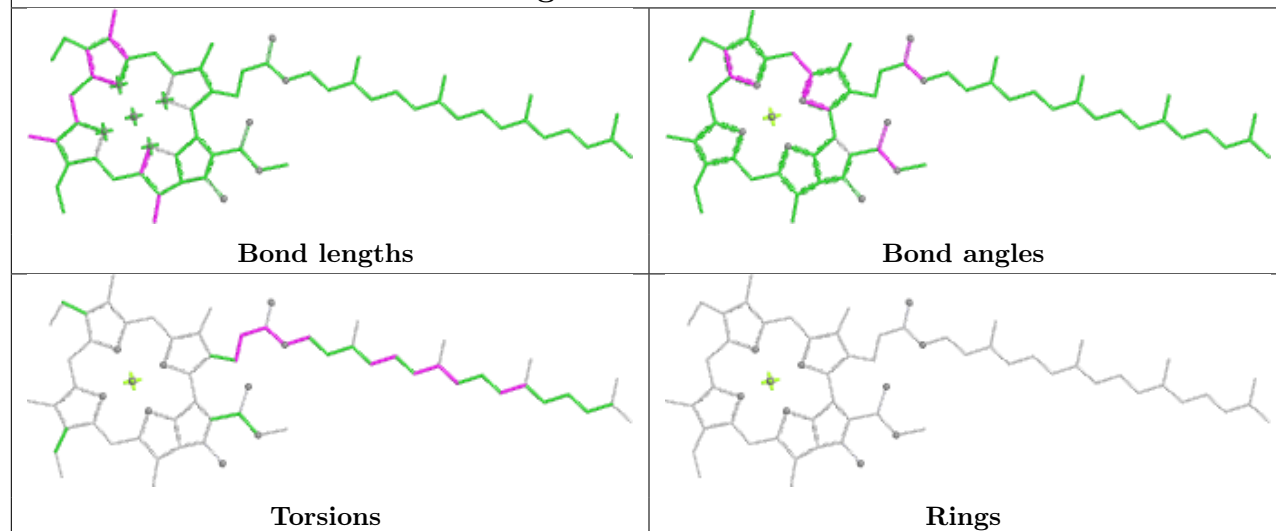
Ligand CLA S 610



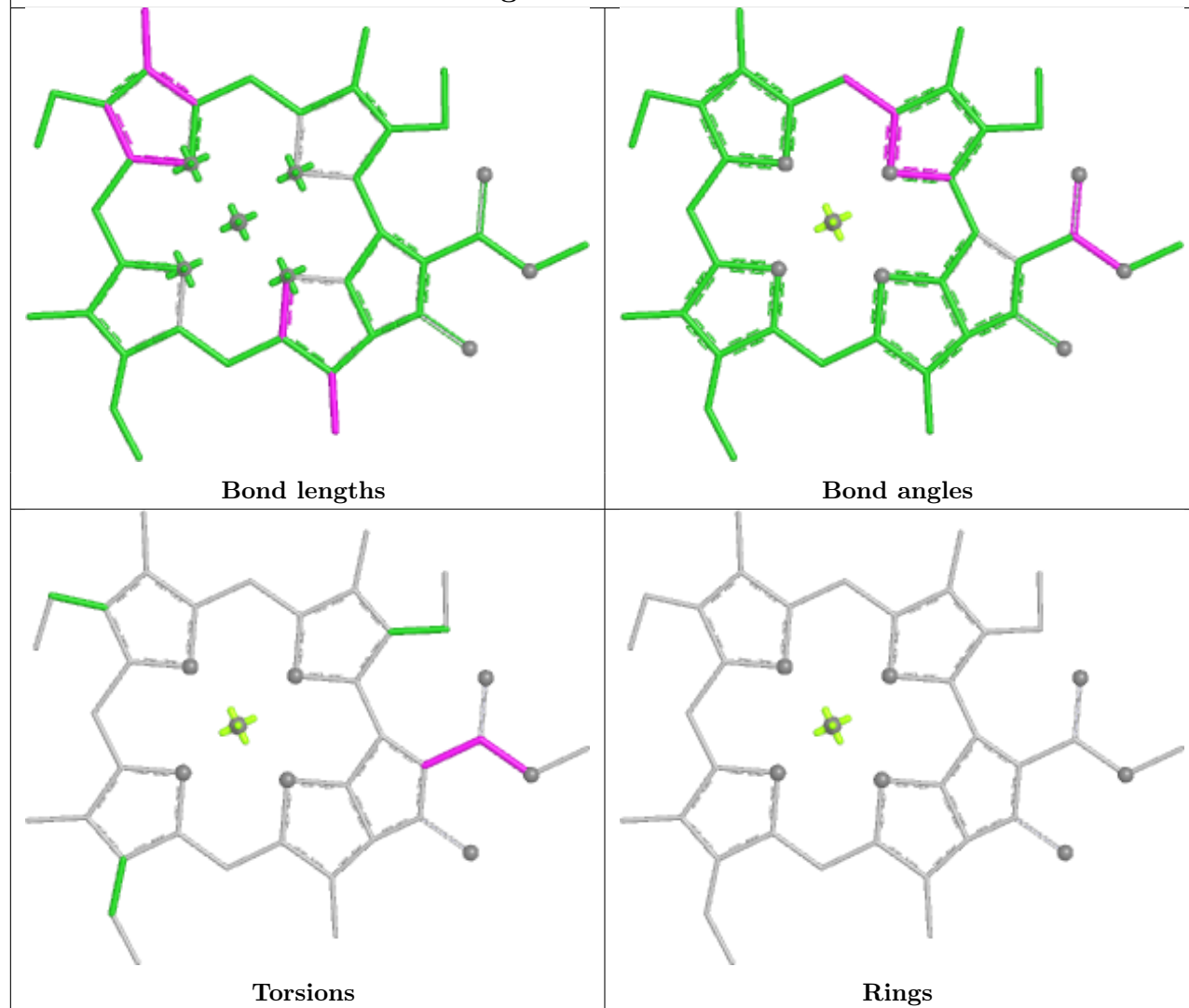
Ligand CLA B 506

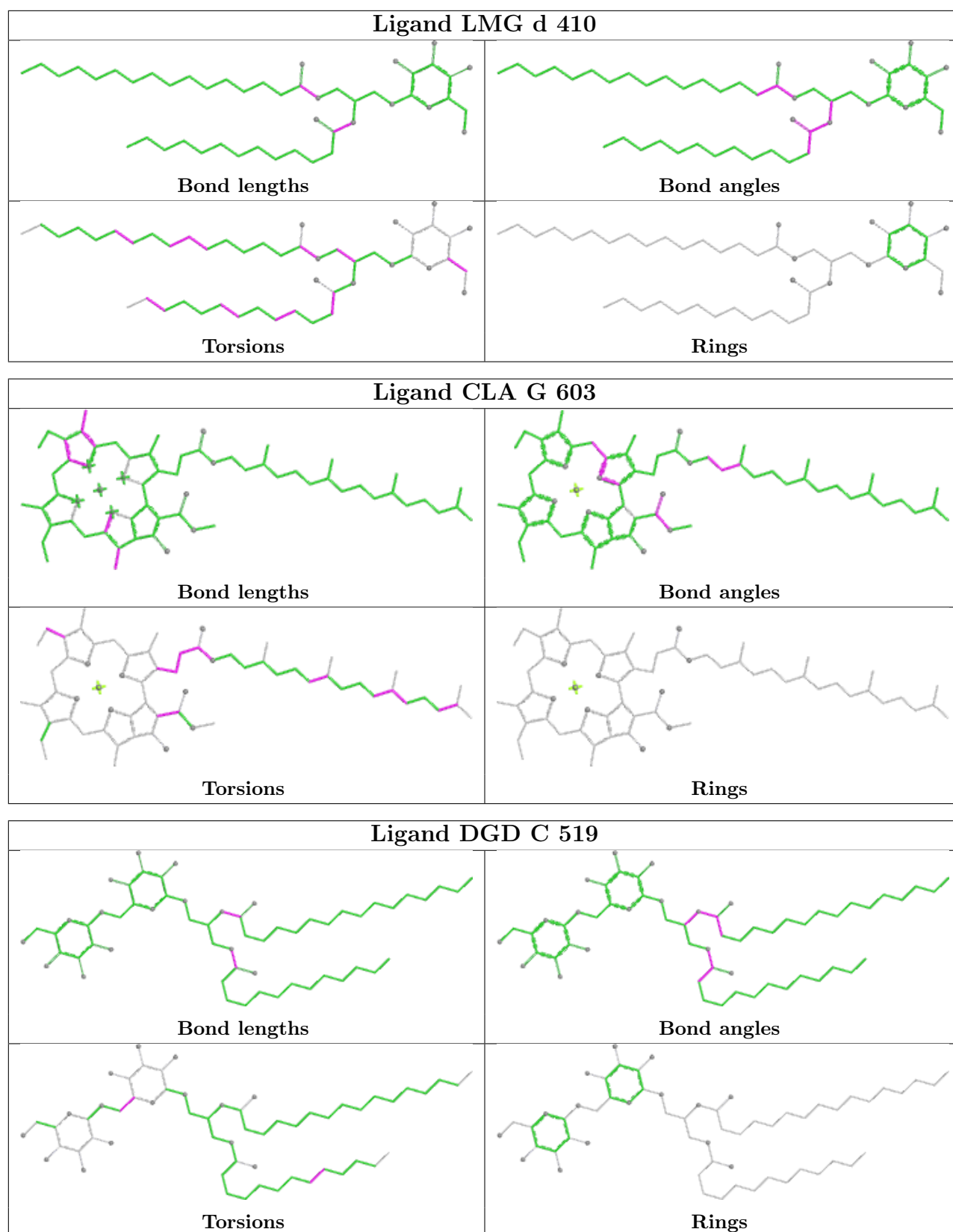


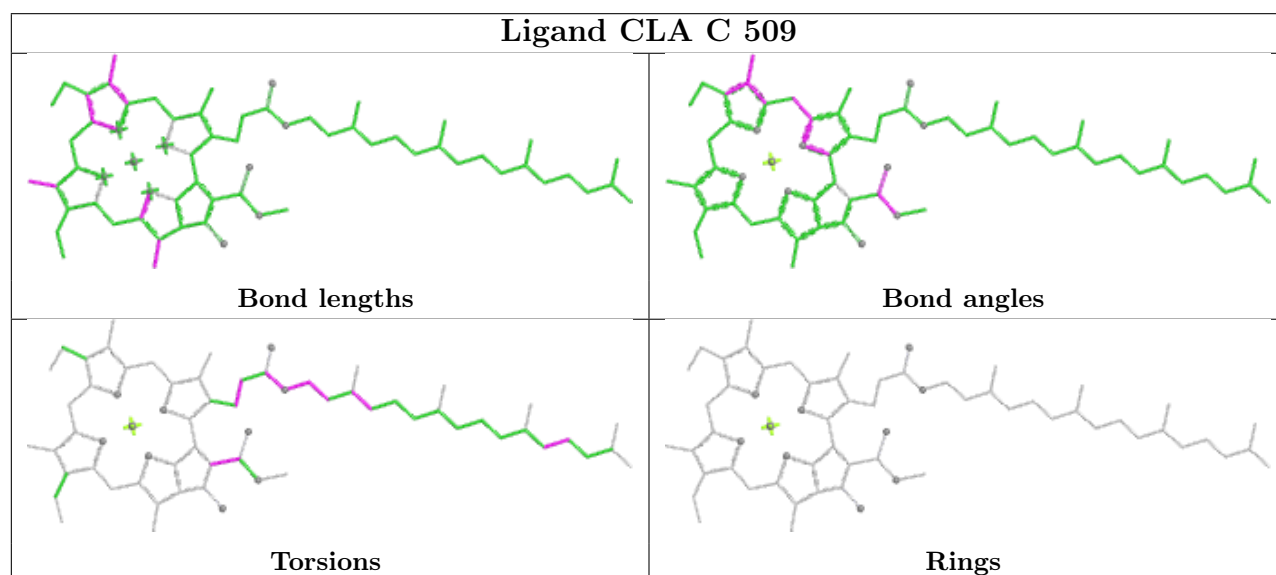
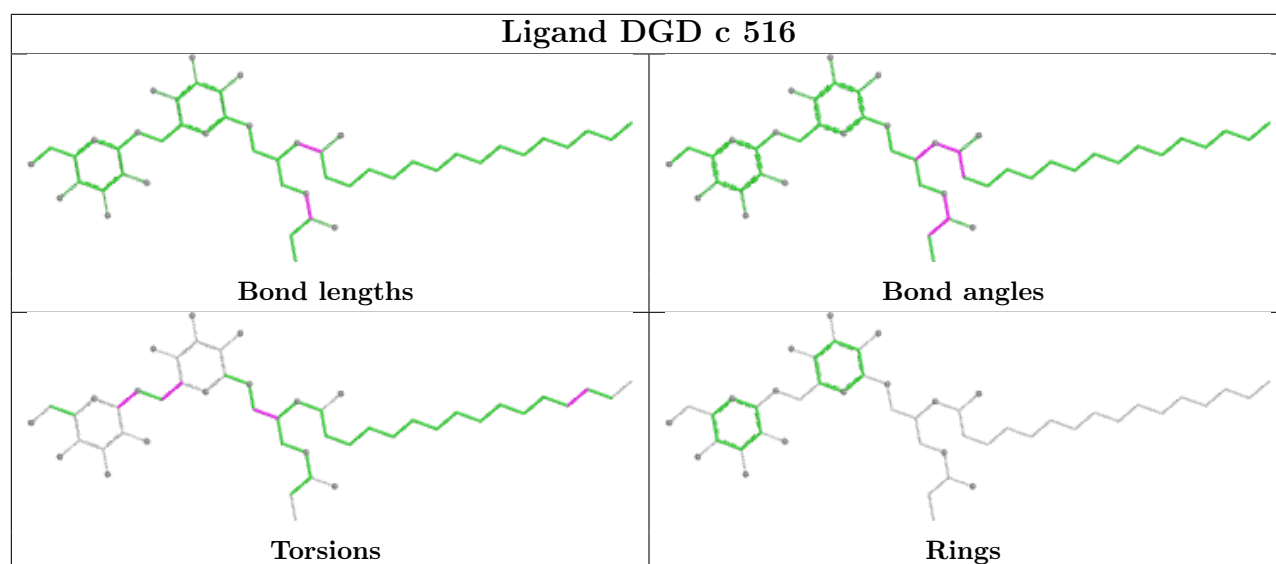
Ligand CLA c 508



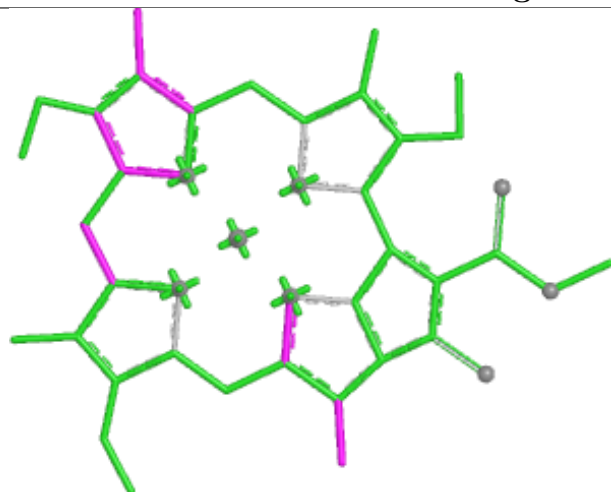
Ligand CLA c 513



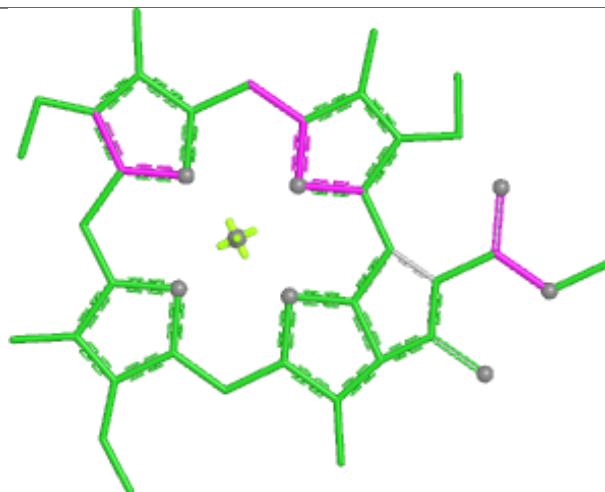




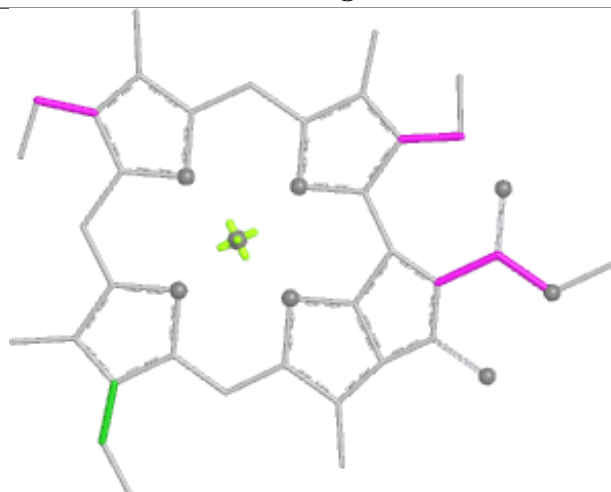
Ligand CLA N 315



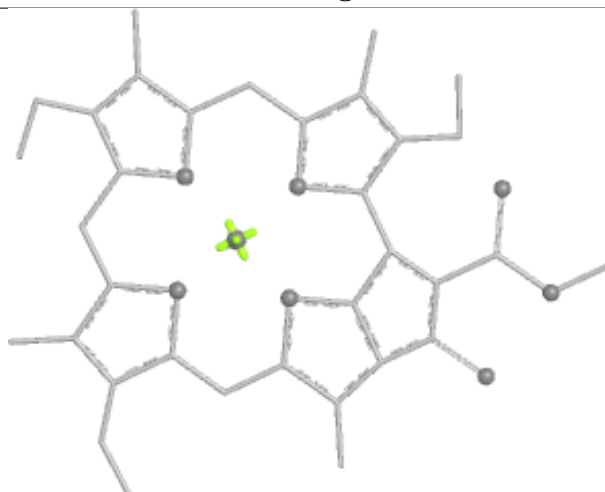
Bond lengths



Bond angles

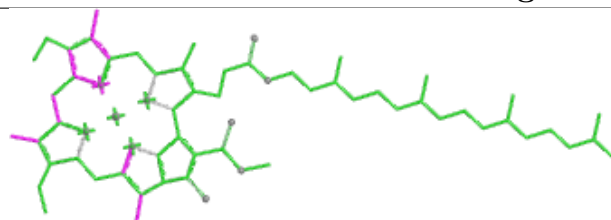


Torsions

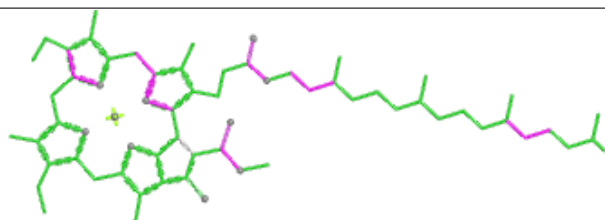


Rings

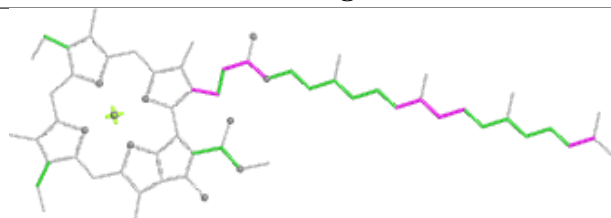
Ligand CLA b 512



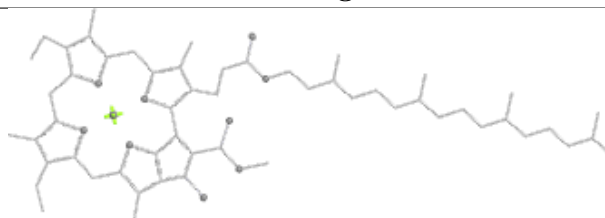
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

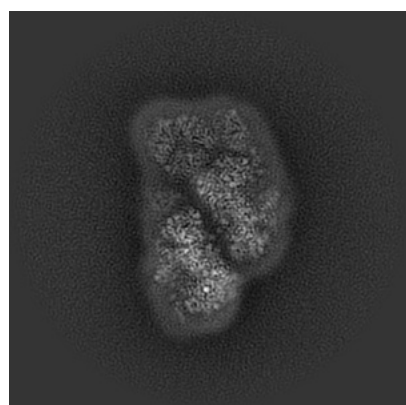
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60830. These allow visual inspection of the internal detail of the map and identification of artifacts.

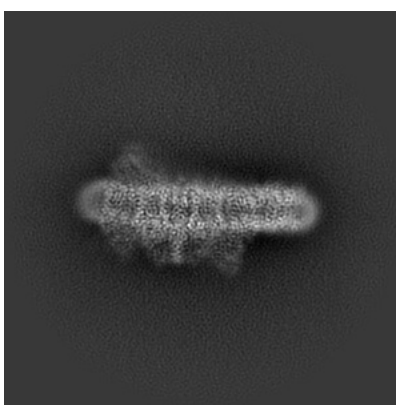
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

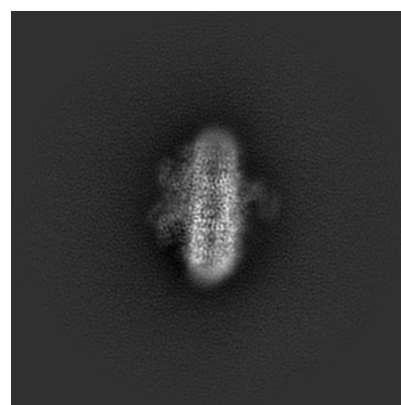
6.1.1 Primary map



X



Y

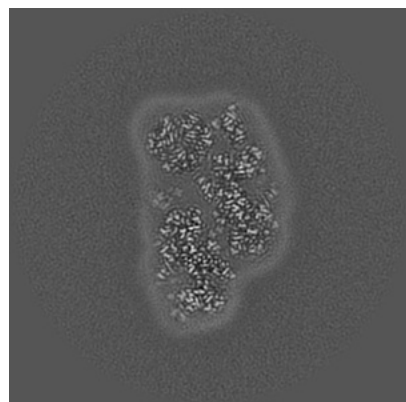


Z

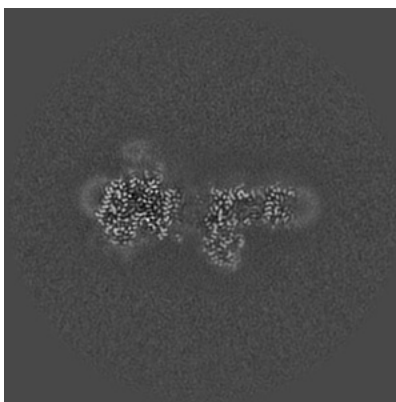
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

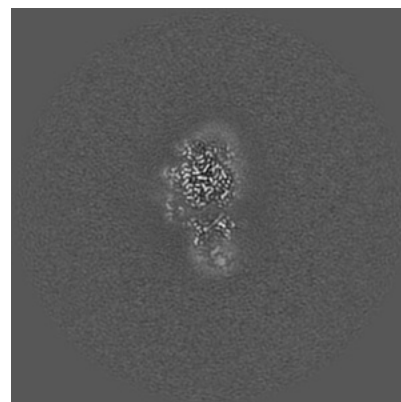
6.2.1 Primary map



X Index: 200



Y Index: 200

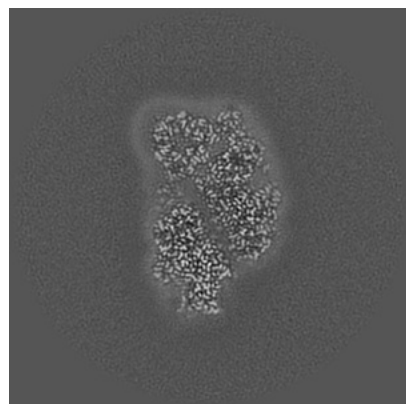


Z Index: 200

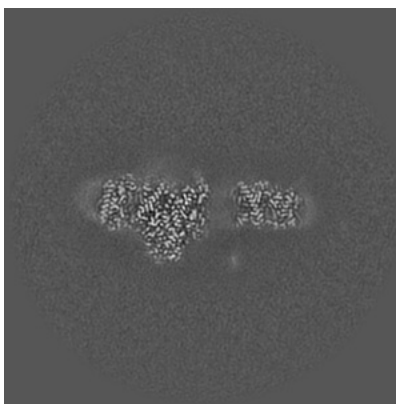
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

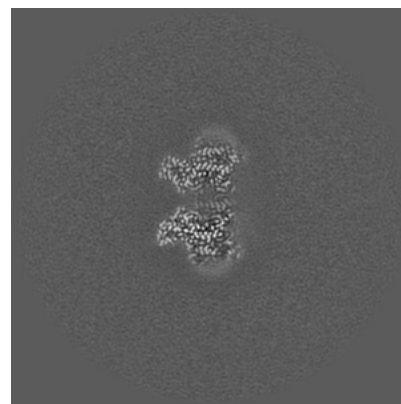
6.3.1 Primary map



X Index: 188



Y Index: 181

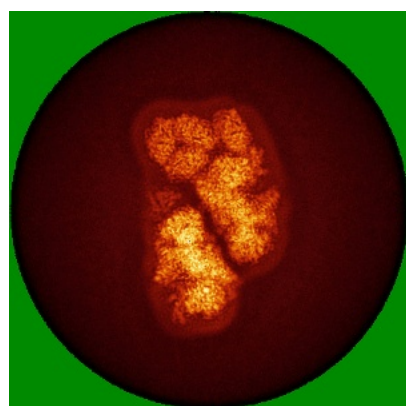


Z Index: 174

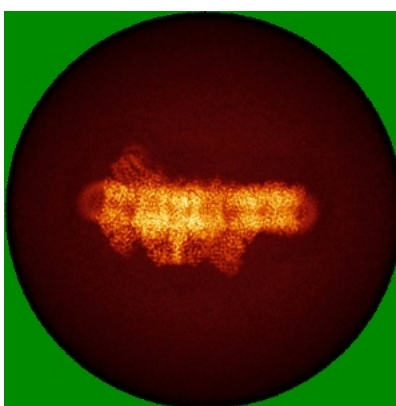
The images above show the largest variance slices of the map in three orthogonal directions.

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

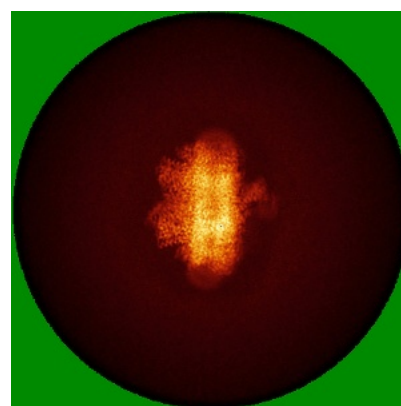
6.4.1 Primary map



X



Y

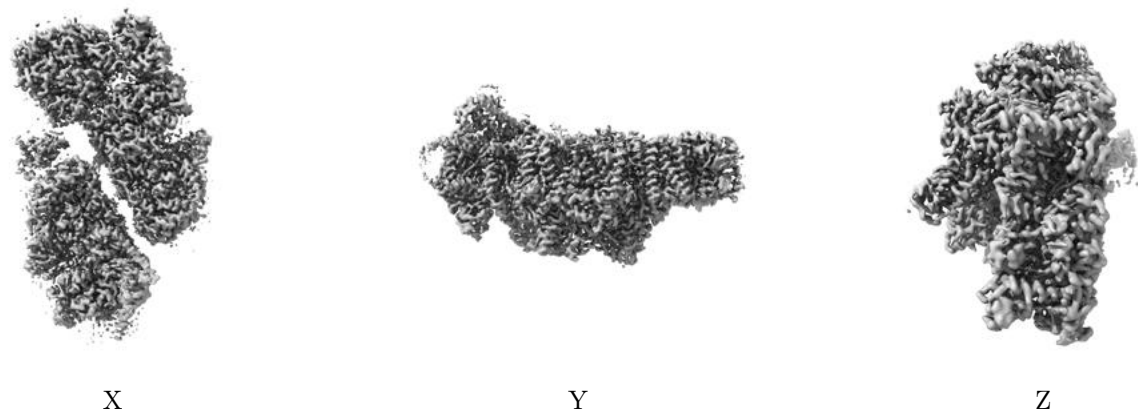


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

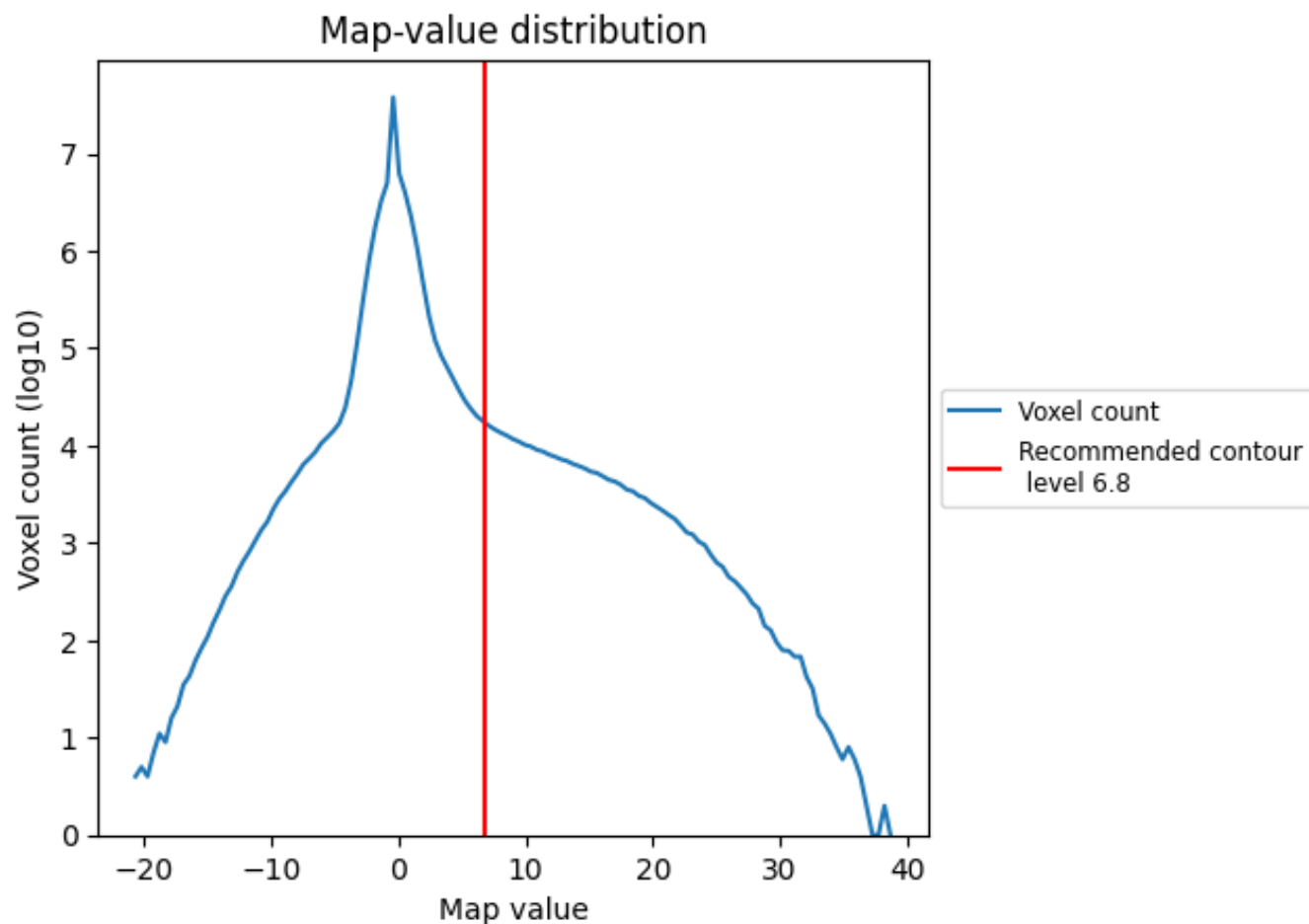
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

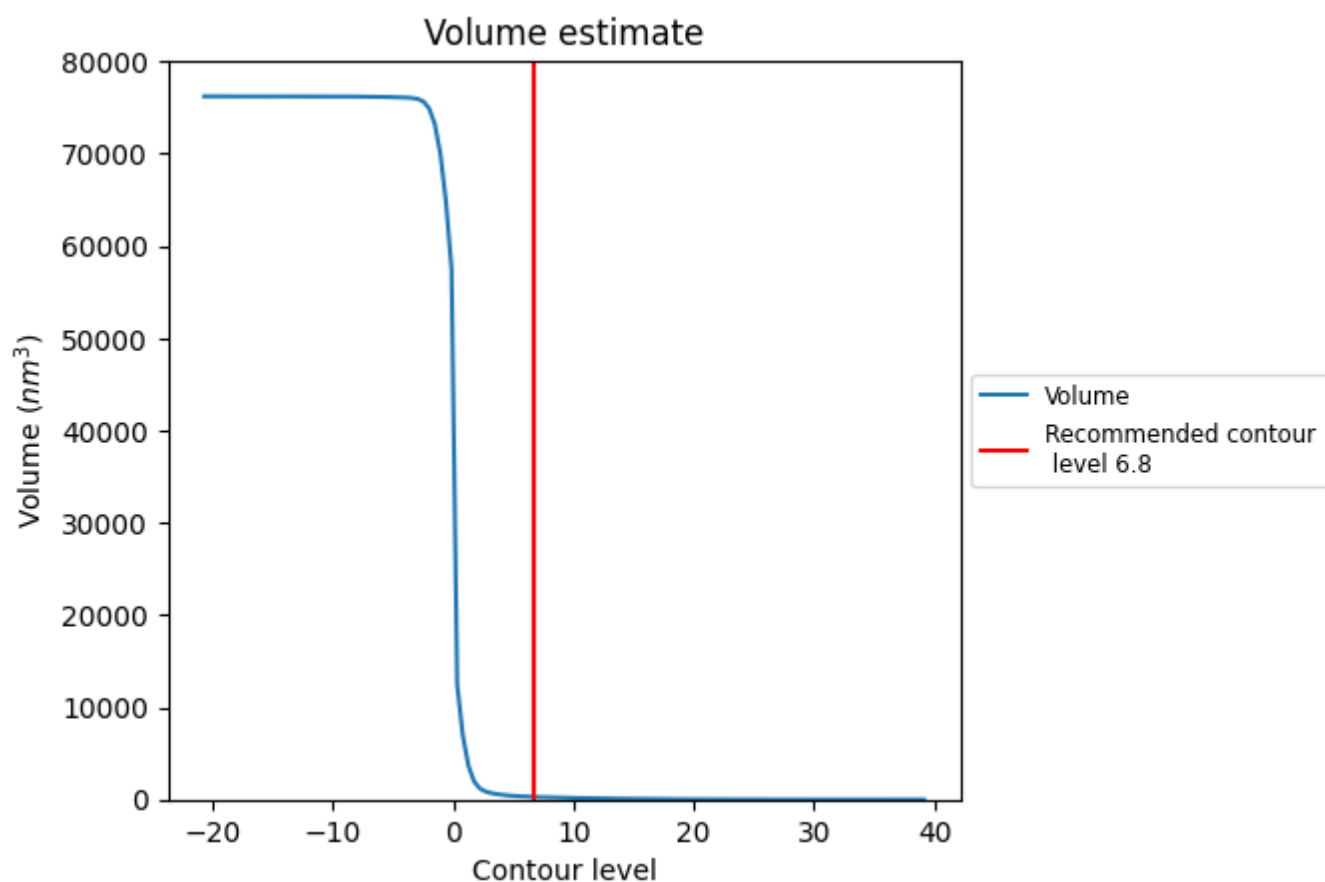
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

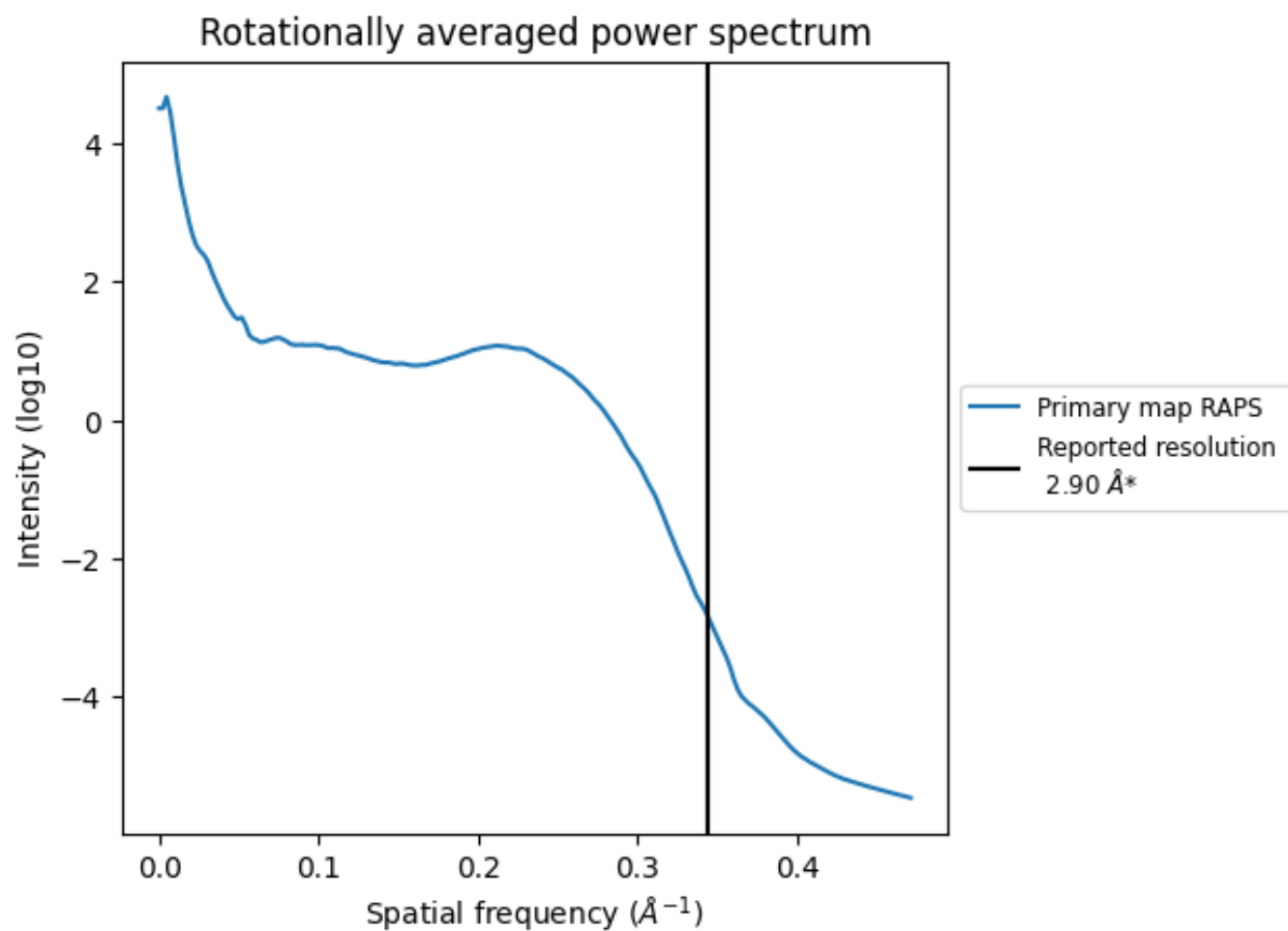
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 285 nm³; this corresponds to an approximate mass of 258 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 0.345 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

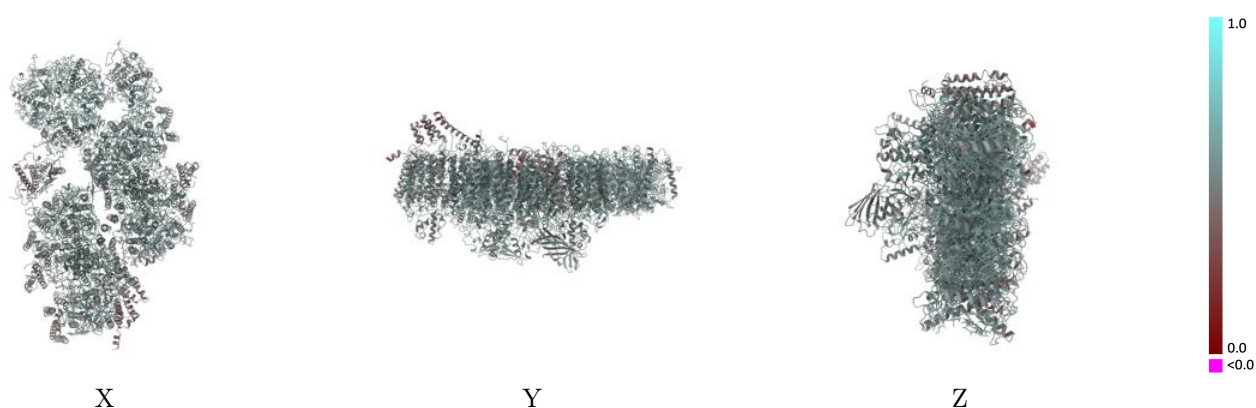
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60830 and PDB model 9IS4. Per-residue inclusion information can be found in section 3 on page 31.

9.1 Map-model overlay [i](#)

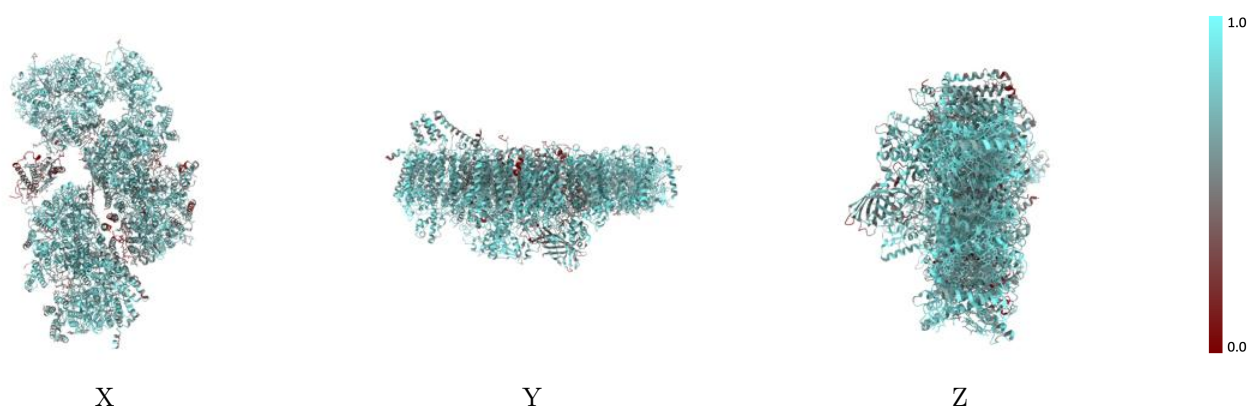
This section was not generated.

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



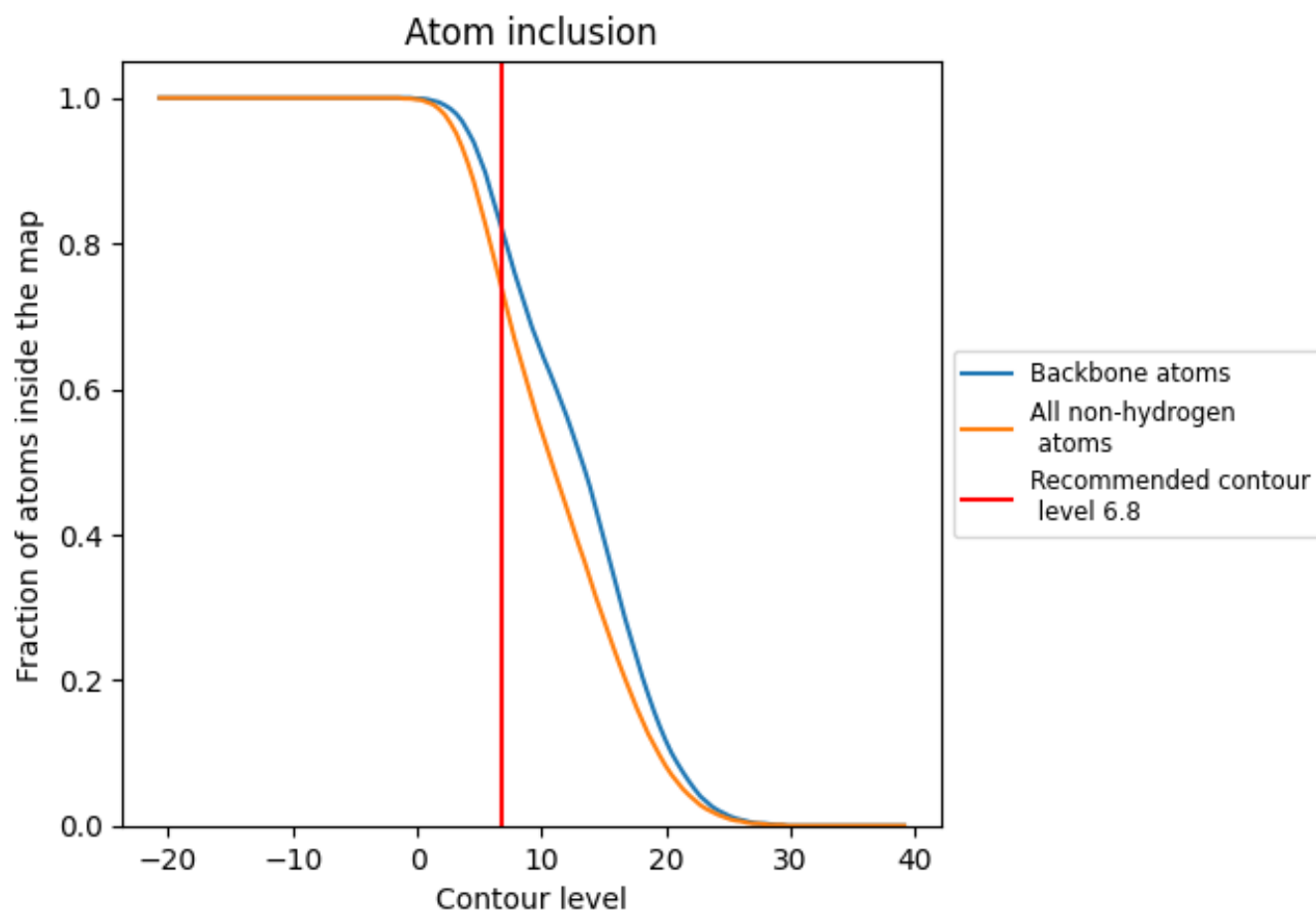
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 74% 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 (6.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7390	 0.5410
1	 0.6550	 0.4420
A	 0.7560	 0.5570
B	 0.7390	 0.5550
C	 0.7710	 0.5630
D	 0.7740	 0.5590
E	 0.5850	 0.4840
F	 0.6420	 0.4700
G	 0.7610	 0.5440
H	 0.6610	 0.5350
I	 0.7790	 0.5600
K	 0.7990	 0.5520
L	 0.6360	 0.5600
M	 0.3420	 0.4950
N	 0.7790	 0.5590
O	 0.5660	 0.5080
S	 0.7790	 0.5390
T	 0.5450	 0.5260
V	 0.5990	 0.4990
W	 0.6120	 0.5410
X	 0.3970	 0.4580
Y	 0.7480	 0.5640
Z	 0.7150	 0.5180
a	 0.7870	 0.5550
b	 0.8230	 0.5630
c	 0.8060	 0.5390
d	 0.8450	 0.5650
e	 0.7830	 0.4830
f	 0.7330	 0.4730
h	 0.7960	 0.5390
i	 0.7130	 0.5000
k	 0.7500	 0.5230
l	 0.7300	 0.5610
m	 0.3480	 0.5110
r	 0.3650	 0.4400



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Chain	Atom inclusion	Q-score
t	 0.4210	 0.5210
v	 0.5080	 0.4330
x	 0.6220	 0.4900
z	 0.5690	 0.4530