



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:27 AM UTC

PDB ID : 7PI0 / pdb_00007pi0
EMDB ID : EMD-13429
Title : Unstacked compact Dunaliella PSII
Authors : Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.
Deposited on : 2021-08-19
Resolution : 2.43 Å (reported)
Based on initial model : 6KAC

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

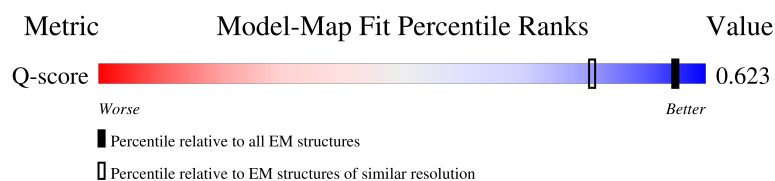
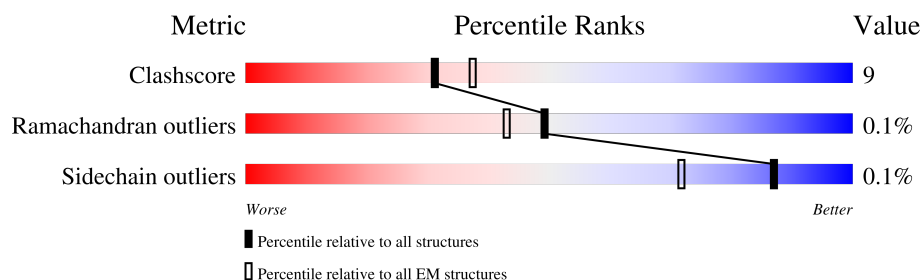
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.43 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.



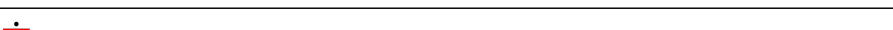
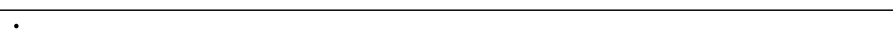
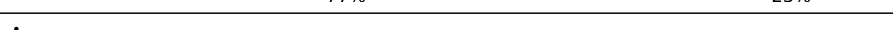
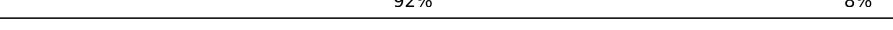
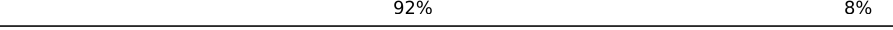
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5787 (1.94 - 2.93)

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

Mol	Chain	Length	Quality of chain
1	A	336	 76% 22% .
1	a	336	 79% 21%
2	B	484	 84% 16%
2	b	484	 80% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	V	32	 88% 12%
3	v	32	 88% 12%
4	C	449	 85% 15%
4	c	449	 85% 15%
5	D	348	 82% 17%
5	d	348	 86% 14%
6	E	76	 82% 18%
6	e	76	 83% 17%
7	F	31	 90% 10%
7	f	31	 74% 26%
8	H	67	 90% 10%
8	h	67	 90% 10%
9	I	35	 77% 23%
9	i	35	 77% 23%
10	J	36	 86% 14%
10	j	36	 92% 8%
11	K	37	 86% 14%
11	k	37	 86% 14%
12	L	38	 92% 8%
12	l	38	 87% 13%
13	M	31	 81% 19%
13	m	31	 77% 23%
14	O	238	 81% 19%
14	o	238	 79% 21%
15	P	187	 21% 78% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	p	187	 8% 81% 19%
16	T	30	 83% 17%
16	t	30	 80% 20%
17	W	44	 93% 7%
17	w	44	 82% 18%
18	X	30	 83% 17%
18	x	30	 80% 20%
19	Z	61	 93% 7%
19	z	61	 93% 7%
20	N	222	 83% 17%
20	n	222	 84% 16%
21	G	221	 90% 10%
21	g	221	 83% 17%
22	R	196	 85% 15%
22	r	196	 85% 15%
23	S	243	 88% 12%
23	s	243	 85% 15%
24	Y	222	 85% 15%
24	y	222	 86% 14%
25	U	27	 67% 33%
25	u	27	 63% 37%

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
29	CLA	A	405	X	-	-	-
29	CLA	A	406	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	A	407	X	-	-	-
29	CLA	B	501	X	-	-	-
29	CLA	B	502	X	-	-	-
29	CLA	B	503	X	-	-	-
29	CLA	B	504	X	-	-	-
29	CLA	B	505	X	-	-	-
29	CLA	B	506	X	-	-	-
29	CLA	B	507	X	-	-	-
29	CLA	B	508	X	-	-	-
29	CLA	B	509	X	-	-	-
29	CLA	B	510	X	-	-	-
29	CLA	B	512	X	-	-	-
29	CLA	B	513	X	-	-	-
29	CLA	B	514	X	-	-	-
29	CLA	B	515	X	-	-	-
29	CLA	B	516	X	-	-	-
29	CLA	C	503	X	-	-	-
29	CLA	C	505	X	-	-	-
29	CLA	C	506	X	-	-	-
29	CLA	C	508	X	-	-	-
29	CLA	C	509	X	-	-	-
29	CLA	C	510	X	-	-	-
29	CLA	C	511	X	-	-	-
29	CLA	C	512	X	-	-	-
29	CLA	C	513	X	-	-	-
29	CLA	D	404	X	-	-	-
29	CLA	D	405	X	-	-	-
29	CLA	G	602	X	-	-	-
29	CLA	G	603	X	-	-	-
29	CLA	G	604	X	-	-	-
29	CLA	G	610	X	-	-	-
29	CLA	G	611	X	-	-	-
29	CLA	G	612	X	-	-	-
29	CLA	G	613	X	-	-	-
29	CLA	G	614	X	-	-	-
29	CLA	N	602	X	-	-	-
29	CLA	N	603	X	-	-	-
29	CLA	N	604	X	-	-	-
29	CLA	N	610	X	-	-	-
29	CLA	N	611	X	-	-	-
29	CLA	N	612	X	-	-	-
29	CLA	N	613	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	N	614	X	-	-	-
29	CLA	R	301	X	-	-	-
29	CLA	R	303	X	-	-	-
29	CLA	R	306	X	-	-	-
29	CLA	R	307	X	-	-	-
29	CLA	R	308	X	-	-	-
29	CLA	R	309	X	-	-	-
29	CLA	S	303	X	-	-	-
29	CLA	S	304	X	-	-	-
29	CLA	S	305	X	-	-	-
29	CLA	S	306	X	-	-	-
29	CLA	S	310	X	-	-	-
29	CLA	S	311	X	-	-	-
29	CLA	S	312	X	-	-	-
29	CLA	S	313	X	-	-	-
29	CLA	S	314	X	-	-	-
29	CLA	S	315	X	-	-	-
29	CLA	S	316	X	-	-	-
29	CLA	Y	303	X	-	-	-
29	CLA	Y	304	X	-	-	-
29	CLA	Y	305	X	-	-	-
29	CLA	Y	309	X	-	-	-
29	CLA	Y	311	X	-	-	-
29	CLA	Y	312	X	-	-	-
29	CLA	Y	313	X	-	-	-
29	CLA	Y	314	X	-	-	-
29	CLA	Y	315	X	-	-	-
29	CLA	a	404	X	-	-	-
29	CLA	a	405	X	-	-	-
29	CLA	b	501	X	-	-	-
29	CLA	b	502	X	-	-	-
29	CLA	b	503	X	-	-	-
29	CLA	b	504	X	-	-	-
29	CLA	b	505	X	-	-	-
29	CLA	b	506	X	-	-	-
29	CLA	b	507	X	-	-	-
29	CLA	b	509	X	-	-	-
29	CLA	b	510	X	-	-	-
29	CLA	b	512	X	-	-	-
29	CLA	b	513	X	-	-	-
29	CLA	b	514	X	-	-	-
29	CLA	b	515	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	b	516	X	-	-	-
29	CLA	c	502	X	-	-	-
29	CLA	c	504	X	-	-	-
29	CLA	c	505	X	-	-	-
29	CLA	c	507	X	-	-	-
29	CLA	c	508	X	-	-	-
29	CLA	c	509	X	-	-	-
29	CLA	c	510	X	-	-	-
29	CLA	c	512	X	-	-	-
29	CLA	d	403	X	-	-	-
29	CLA	d	404	X	-	-	-
29	CLA	g	602	X	-	-	-
29	CLA	g	603	X	-	-	-
29	CLA	g	604	X	-	-	-
29	CLA	g	610	X	-	-	-
29	CLA	g	611	X	-	-	-
29	CLA	g	614	X	-	-	-
29	CLA	n	602	X	-	-	-
29	CLA	n	603	X	-	-	-
29	CLA	n	604	X	-	-	-
29	CLA	n	609	X	-	-	-
29	CLA	n	610	X	-	-	-
29	CLA	n	611	X	-	-	-
29	CLA	n	613	X	-	-	-
29	CLA	r	302	X	-	-	-
29	CLA	r	304	X	-	-	-
29	CLA	r	307	X	-	-	-
29	CLA	r	308	X	-	-	-
29	CLA	r	309	X	-	-	-
29	CLA	r	310	X	-	-	-
29	CLA	s	303	X	-	-	-
29	CLA	s	305	X	-	-	-
29	CLA	s	310	X	-	-	-
29	CLA	s	311	X	-	-	-
29	CLA	s	312	X	-	-	-
29	CLA	s	313	X	-	-	-
29	CLA	s	314	X	-	-	-
29	CLA	s	315	X	-	-	-
29	CLA	s	316	X	-	-	-
29	CLA	y	304	X	-	-	-
29	CLA	y	305	X	-	-	-
29	CLA	y	306	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	y	310	X	-	-	-
29	CLA	y	312	X	-	-	-
29	CLA	y	313	X	-	-	-
29	CLA	y	314	X	-	-	-
29	CLA	y	316	X	-	-	-
34	C7Z	B	519	X	-	-	-
34	C7Z	b	519	X	-	-	-
45	RRX	H	101	X	-	-	-
45	RRX	h	101	X	-	-	-
46	CHL	G	601	X	-	-	-
46	CHL	G	605	X	-	-	-
46	CHL	G	606	X	-	-	-
46	CHL	G	607	X	-	-	-
46	CHL	G	608	X	-	-	-
46	CHL	G	609	X	-	-	-
46	CHL	N	601	X	-	-	-
46	CHL	N	605	X	-	-	-
46	CHL	N	606	X	-	-	-
46	CHL	N	607	X	-	-	-
46	CHL	N	608	X	-	-	-
46	CHL	N	609	X	-	-	-
46	CHL	R	304	X	-	-	-
46	CHL	R	305	X	-	-	-
46	CHL	S	302	X	-	-	-
46	CHL	S	307	X	-	-	-
46	CHL	S	308	X	-	-	-
46	CHL	S	309	X	-	-	-
46	CHL	Y	302	X	-	-	-
46	CHL	Y	306	X	-	-	-
46	CHL	Y	307	X	-	-	-
46	CHL	Y	308	X	-	-	-
46	CHL	Y	310	X	-	-	-
46	CHL	g	601	X	-	-	-
46	CHL	g	605	X	-	-	-
46	CHL	g	606	X	-	-	-
46	CHL	g	607	X	-	-	-
46	CHL	g	608	X	-	-	-
46	CHL	g	609	X	-	-	-
46	CHL	n	601	X	-	-	-
46	CHL	n	605	X	-	-	-
46	CHL	n	606	X	-	-	-
46	CHL	n	607	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
46	CHL	n	608	X	-	-	-
46	CHL	r	305	X	-	-	-
46	CHL	r	306	X	-	-	-
46	CHL	s	302	X	-	-	-
46	CHL	s	307	X	-	-	-
46	CHL	s	308	X	-	-	-
46	CHL	s	309	X	-	-	-
46	CHL	y	301	X	-	-	-
46	CHL	y	303	X	-	-	-
46	CHL	y	307	X	-	-	-
46	CHL	y	308	X	-	-	-
46	CHL	y	309	X	-	-	-
46	CHL	y	311	X	-	-	-
49	XAT	G	619	X	-	-	-
49	XAT	N	619	X	-	-	-
49	XAT	R	311	X	-	-	-
49	XAT	Y	301	X	-	-	-
49	XAT	g	619	X	-	-	-
49	XAT	n	618	X	-	-	-
49	XAT	r	312	X	-	-	-
49	XAT	y	302	X	-	-	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 77465 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	336	Total	C	N	O	S	0	0
			2635	1719	432	468	16		
1	a	336	Total	C	N	O	S	0	0
			2635	1719	432	468	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3785	2480	630	665	10		
2	b	484	Total	C	N	O	S	0	0
			3785	2480	630	665	10		

- Molecule 3 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	32	Total	C	N	O	0	0
			227	152	37	38		
3	v	32	Total	C	N	O	0	0
			227	152	37	38		

- 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
			3483	2282	581	607	13		
4	c	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		

- 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
			2766	1824	454	477	11		
5	d	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	76	Total	C	N	O	S	0	0
			621	404	102	115			
6	e	76	Total	C	N	O	S	0	0
			621	404	102	115			

- 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
			252	172	42	37	1		
7	f	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h	67	Total	C	N	O	S	0	0
			503	334	76	92	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i	35	Total	C	N	O	S	0	0
			279	190	42	46	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	36	Total	C	N	O	0	0
			266	183	40	43		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	36	Total	C	N	O	0	0
			266	183	40	43		

- 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	207	43	47		
11	k	37	Total	C	N	O	0	0
			297	207	43	47		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	l	38	Total	C	N	O	S	0	0
			313	209	51	52	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	31	Total	C	N	O	0	0
			234	159	33	42		
13	m	31	Total	C	N	O	0	0
			234	159	33	42		

- Molecule 14 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	o	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t	30	Total	C	N	O	S	0	0
			247	171	36	39	1		

- Molecule 17 is a protein called PSII 6.1 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w	44	Total	C	N	O	S	0	0
			332	215	53	63	1		

- Molecule 18 is a protein called Hypothetical protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	30	Total	C	N	O	S	0	0
			201	132	32	37			
18	x	30	Total	C	N	O	S	0	0
			201	132	32	37			

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		
19	z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		

- Molecule 20 is a protein called Chlorophyll a-b binding protein of LHCII type 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		
20	n	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		

- Molecule 21 is a protein called Chlorophyll a-b binding protein of LHCII type 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		
21	g	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		

- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic, CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	196	Total	C	N	O	P S	0	0
			1490	943	251	292	1 3		
22	r	196	Total	C	N	O	P S	0	0
			1490	943	251	292	1 3		

- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic, CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	s	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		

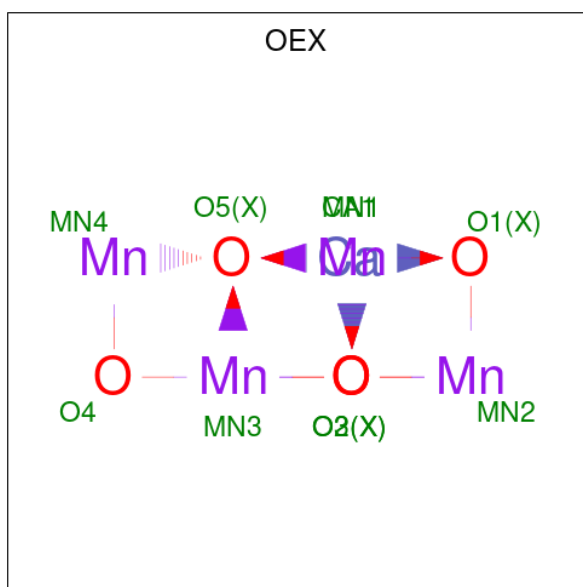
- Molecule 24 is a protein called Chlorophyll a-b binding protein of LHCII type 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		

- Molecule 25 is a protein called Photosystem II extrinsic protein U.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	u	27	Total	C	N	O	S	0	0
			224	134	42	47	1		

- Molecule 26 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

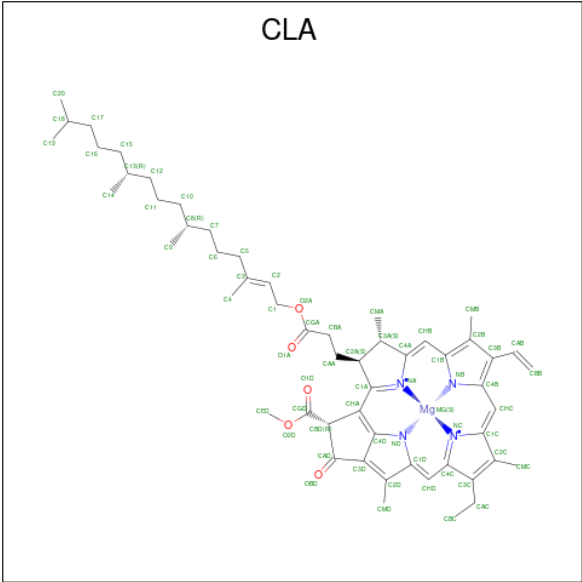
- Molecule 27 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total	Fe	0
			1	1	
27	d	1	Total	Fe	0
			1	1	

- Molecule 28 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
28	A	2	Total	Cl	0
			2	2	
28	a	2	Total	Cl	0
			2	2	

- Molecule 29 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	D	1	Total 60	C 50	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G	1	Total 43	C 35	Mg 1	N 4	O 3	0
29	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R	1	Total 46	C 36	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 57	C 47	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	n	1	Total 45	C 35	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

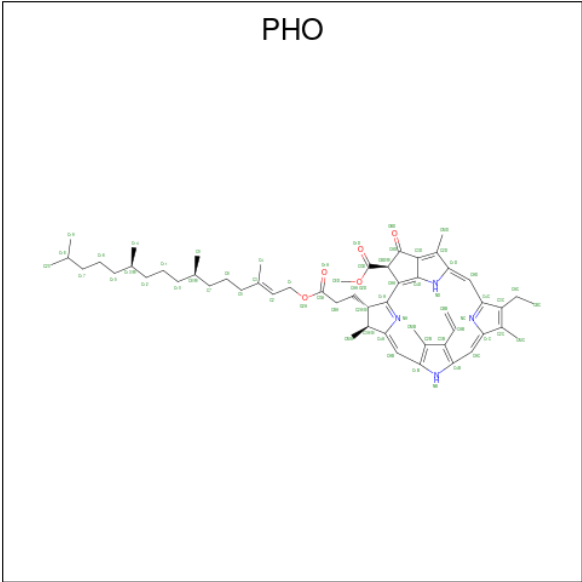
Mol	Chain	Residues	Atoms					AltConf
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 43	C 35	Mg 1	N 4	O 3	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	s	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	s	1	Total 50	C 40	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

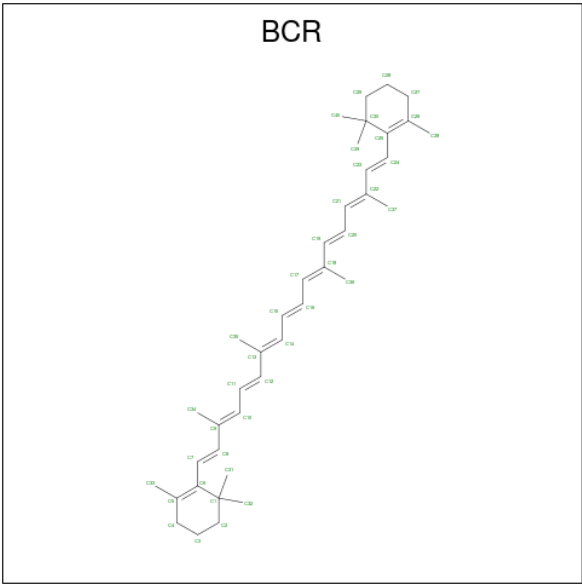
Mol	Chain	Residues	Atoms					AltConf
29	s	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 30 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).

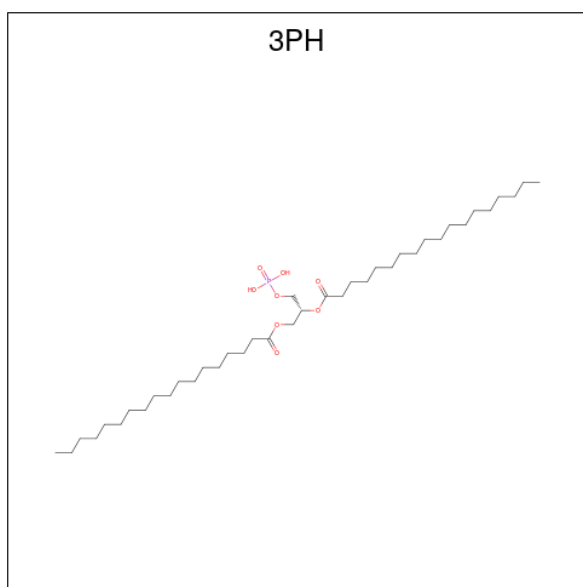


Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	F	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	v	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	f	1	Total C 40 40	0
31	z	1	Total C 40 40	0

- Molecule 32 is SODIUM ION (CCD ID: NA) (formula: Na).

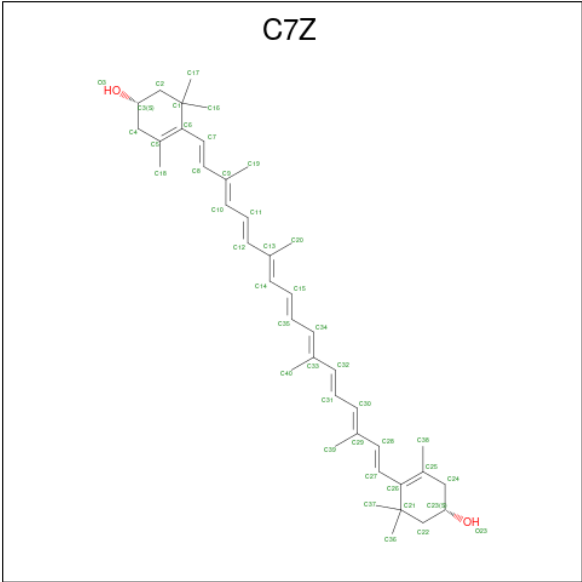
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total Na 1 1	0
32	a	1	Total Na 1 1	0

- Molecule 33 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P).



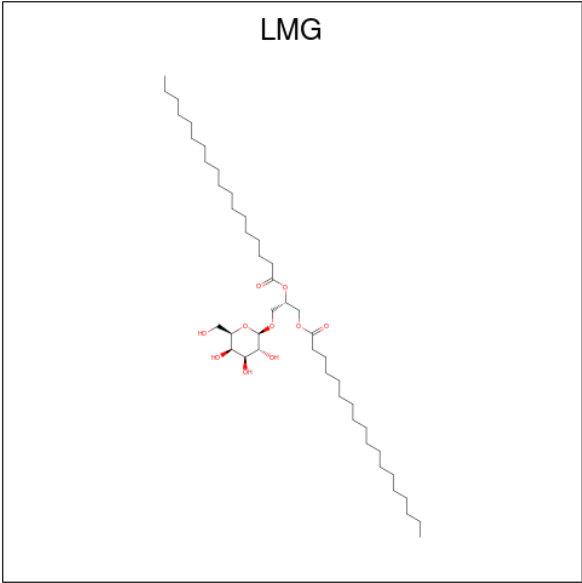
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	O	P	0
			48	39	8	1	
33	B	1	Total	C	O	P	0
			48	39	8	1	
33	S	1	Total	C	O	P	0
			30	21	8	1	
33	a	1	Total	C	O	P	0
			48	39	8	1	
33	b	1	Total	C	O	P	0
			39	30	8	1	
33	s	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 34 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			42	40	2	
34	b	1	Total	C	O	0
			42	40	2	

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



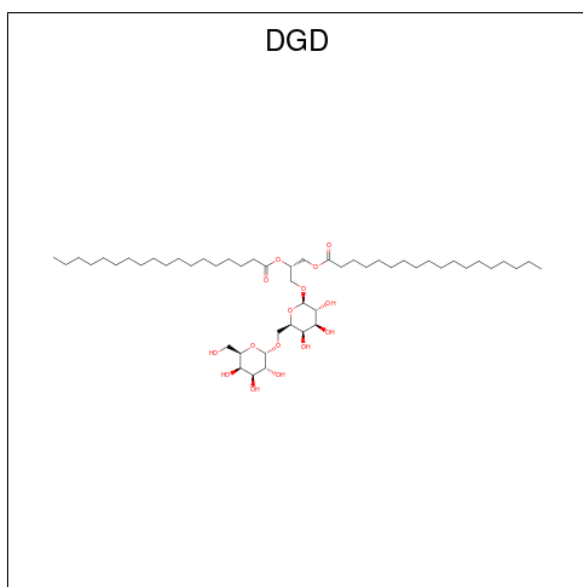
Mol	Chain	Residues	Atoms			AltConf
35	B	1	Total	C	O	0
			44	34	10	

Continued on next page...

Continued from previous page...

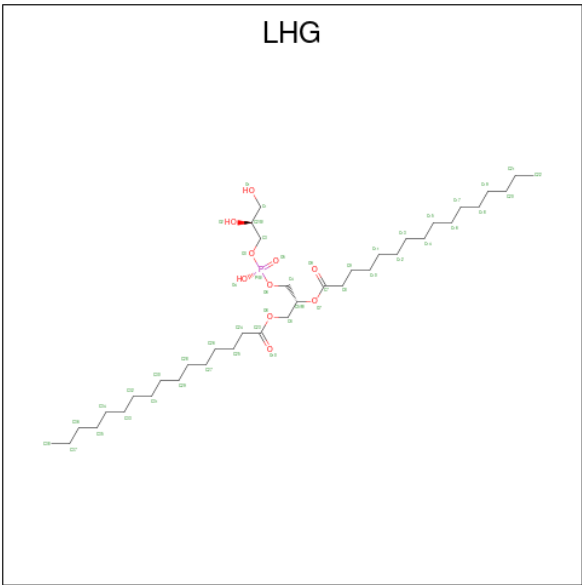
Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			47	37	10	
35	C	1	Total	C	O	0
			55	45	10	
35	C	1	Total	C	O	0
			42	32	10	
35	D	1	Total	C	O	0
			42	32	10	
35	D	1	Total	C	O	0
			48	38	10	
35	W	1	Total	C	O	0
			40	30	10	
35	W	1	Total	C	O	0
			39	29	10	
35	b	1	Total	C	O	0
			44	34	10	
35	c	1	Total	C	O	0
			51	41	10	
35	c	1	Total	C	O	0
			55	45	10	
35	d	1	Total	C	O	0
			46	36	10	
35	d	1	Total	C	O	0
			48	38	10	
35	i	1	Total	C	O	0
			48	38	10	
35	w	1	Total	C	O	0
			39	29	10	

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



Mol	Chain	Residues	Atoms			AltConf
36	B	1	Total	C	O	0
			43	28	15	
36	C	1	Total	C	O	0
			51	36	15	
36	C	1	Total	C	O	0
			53	38	15	
36	C	1	Total	C	O	0
			53	38	15	
36	c	1	Total	C	O	0
			55	40	15	
36	c	1	Total	C	O	0
			62	47	15	
36	c	1	Total	C	O	0
			59	44	15	
36	r	1	Total	C	O	0
			43	28	15	

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



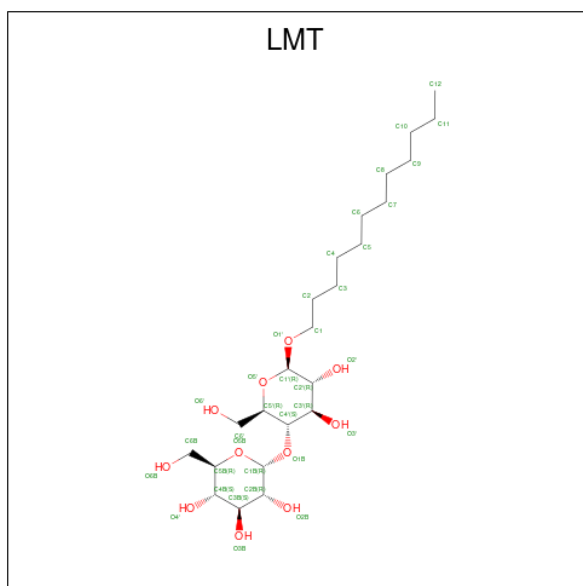
Mol	Chain	Residues	Atoms				AltConf
37	B	1	Total	C	O	P	0
			44	33	10	1	
37	D	1	Total	C	O	P	0
			49	38	10	1	
37	D	1	Total	C	O	P	0
			39	28	10	1	
37	L	1	Total	C	O	P	0
			49	38	10	1	
37	N	1	Total	C	O	P	0
			49	38	10	1	
37	G	1	Total	C	O	P	0
			49	38	10	1	
37	S	1	Total	C	O	P	0
			35	24	10	1	
37	S	1	Total	C	O	P	0
			45	34	10	1	
37	Y	1	Total	C	O	P	0
			49	38	10	1	
37	a	1	Total	C	O	P	0
			44	33	10	1	
37	a	1	Total	C	O	P	0
			39	28	10	1	
37	c	1	Total	C	O	P	0
			47	36	10	1	
37	d	1	Total	C	O	P	0
			49	38	10	1	
37	l	1	Total	C	O	P	0
			49	38	10	1	

Continued on next page...

Continued from previous page...

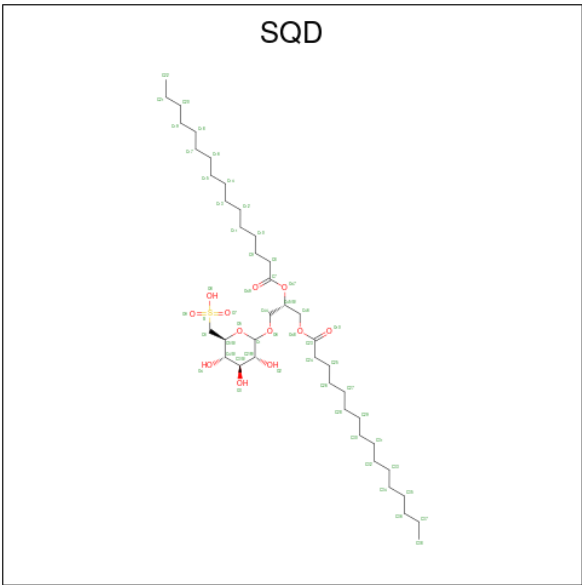
Mol	Chain	Residues	Atoms				AltConf
37	n	1	Total	C	O	P	0
			42	31	10	1	
37	g	1	Total	C	O	P	0
			49	38	10	1	
37	s	1	Total	C	O	P	0
			38	27	10	1	
37	s	1	Total	C	O	P	0
			45	34	10	1	
37	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 38 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



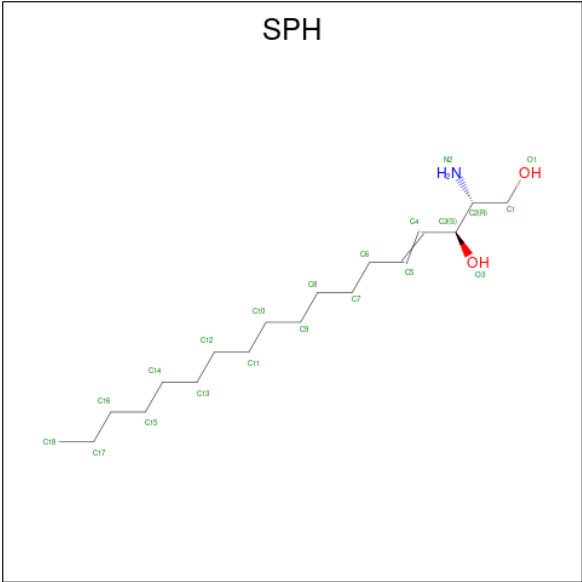
Mol	Chain	Residues	Atoms			AltConf
38	B	1	Total	C	O	0
			35	24	11	
38	b	1	Total	C	O	0
			35	24	11	

- Molecule 39 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



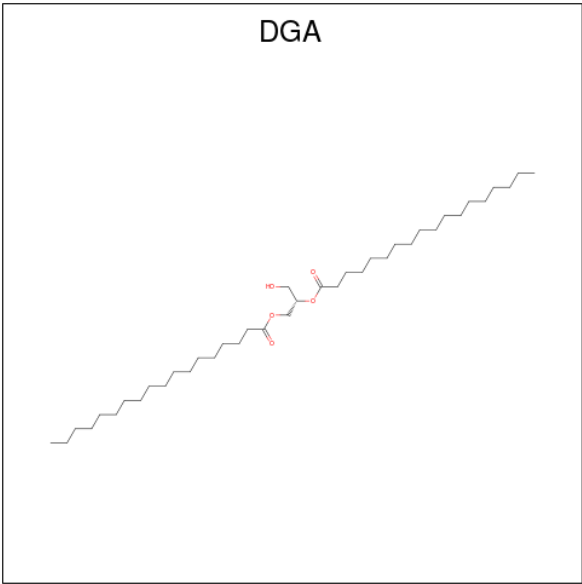
Mol	Chain	Residues	Atoms				AltConf
39	C	1	Total	C	O	S	0
			42	29	12	1	
39	C	1	Total	C	O	S	0
			36	23	12	1	
39	L	1	Total	C	O	S	0
			42	29	12	1	
39	M	1	Total	C	O	S	0
			42	29	12	1	
39	a	1	Total	C	O	S	0
			51	38	12	1	
39	b	1	Total	C	O	S	0
			54	41	12	1	
39	c	1	Total	C	O	S	0
			54	41	12	1	
39	l	1	Total	C	O	S	0
			42	29	12	1	
39	m	1	Total	C	O	S	0
			42	29	12	1	
39	o	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 40 is SPHINGOSINE (CCD ID: SPH) (formula: C₁₈H₃₇NO₂).



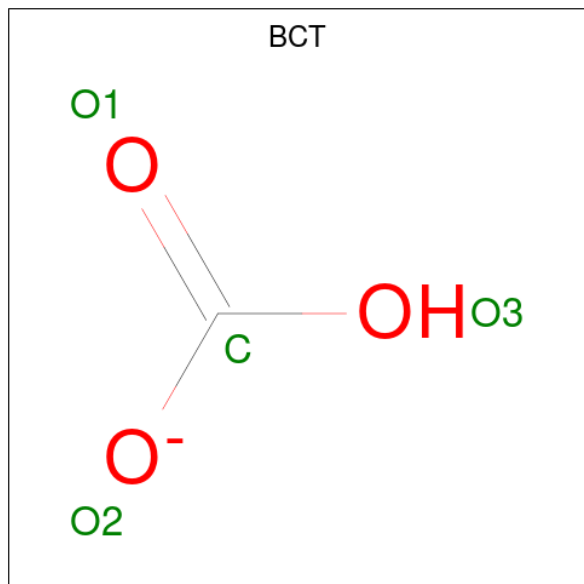
Mol	Chain	Residues	Atoms				AltConf
40	C	1	Total	C	N	O	0
			21	18	1	2	
40	I	1	Total	C	N	O	0
			21	18	1	2	
40	c	1	Total	C	N	O	0
			21	18	1	2	
40	i	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 41 is DIACYL GLYCEROL (CCD ID: DGA) (formula: C₃₉H₇₆O₅).



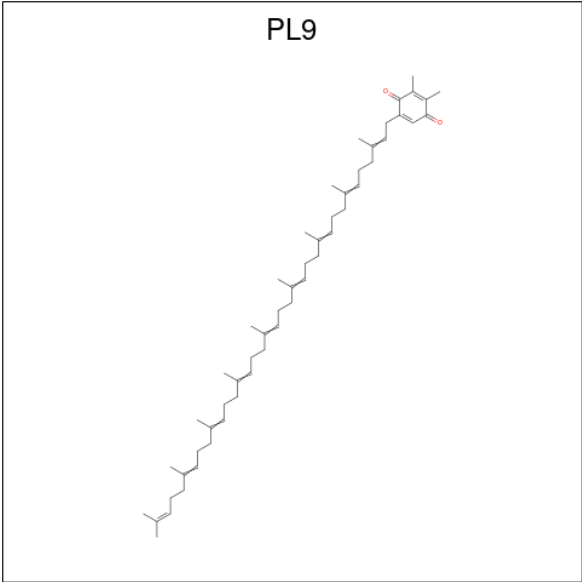
Mol	Chain	Residues	Atoms			AltConf
41	D	1	Total	C	O	0
			37	32	5	
41	J	1	Total	C	O	0
			29	24	5	
41	W	1	Total	C	O	0
			44	39	5	
41	b	1	Total	C	O	0
			44	39	5	
41	j	1	Total	C	O	0
			29	24	5	
41	w	1	Total	C	O	0
			44	39	5	

- Molecule 42 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



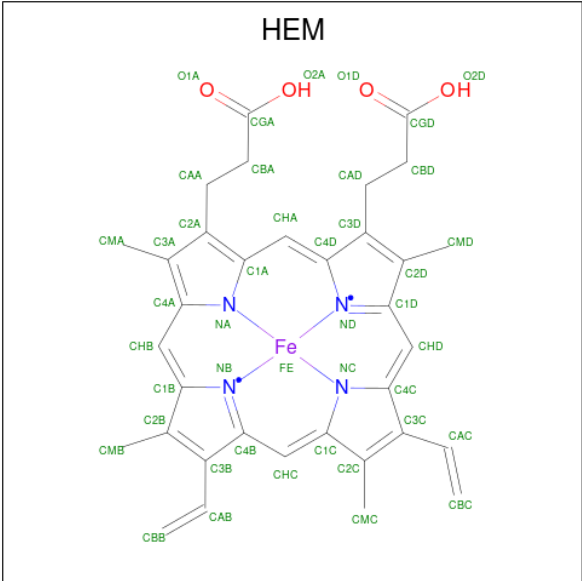
Mol	Chain	Residues	Atoms			AltConf
42	D	1	Total	C	O	0
			4	1	3	
42	a	1	Total	C	O	0
			4	1	3	

- Molecule 43 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: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



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

- Molecule 44 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



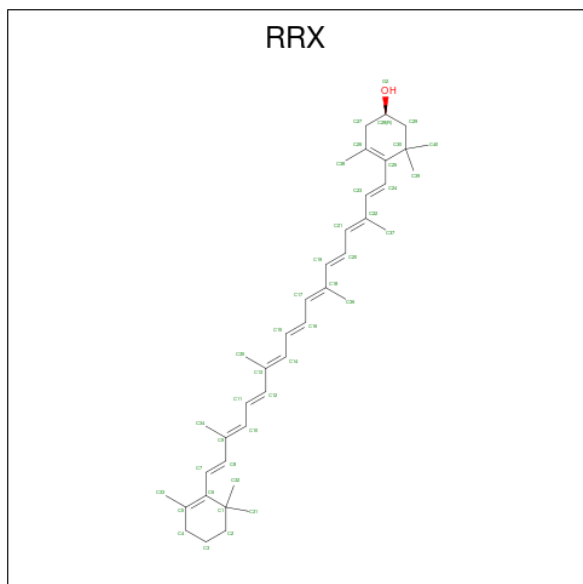
Mol	Chain	Residues	Atoms					AltConf
44	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

Continued on next page...

Continued from previous page...

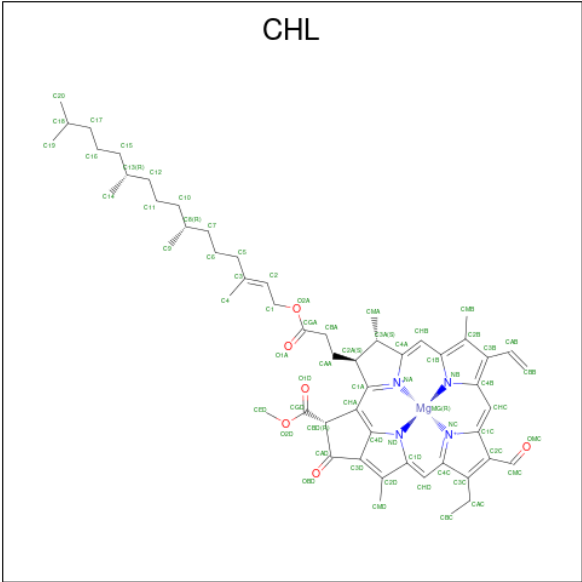
Mol	Chain	Residues	Atoms					AltConf
44	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 45 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



Mol	Chain	Residues	Atoms			AltConf
45	H	1	Total	C	O	0
			41	40	1	
45	h	1	Total	C	O	0
			41	40	1	

- Molecule 46 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
46	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
46	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	G	1	Total 48	C 37	Mg 1	N 4	O 6	0
46	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
46	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	G	1	Total 44	C 35	Mg 1	N 4	O 4	0
46	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	R	1	Total 44	C 35	Mg 1	N 4	O 4	0
46	R	1	Total 50	C 39	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

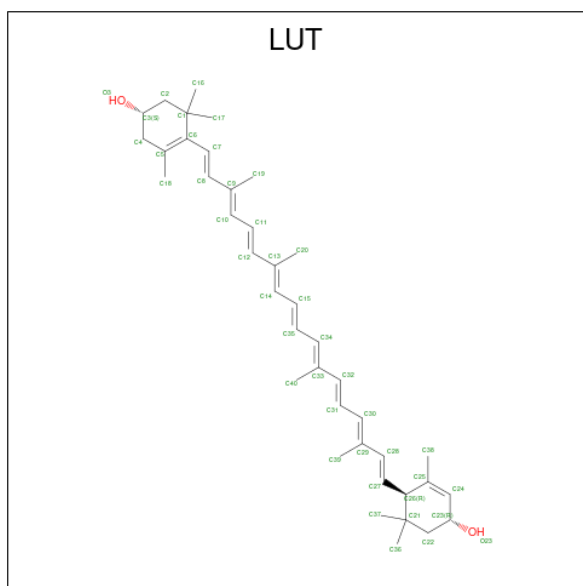
Mol	Chain	Residues	Atoms					AltConf
46	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
46	S	1	Total 44	C 35	Mg 1	N 4	O 4	0
46	S	1	Total 43	C 34	Mg 1	N 4	O 4	0
46	S	1	Total 61	C 50	Mg 1	N 4	O 6	0
46	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
46	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
46	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	g	1	Total 48	C 37	Mg 1	N 4	O 6	0
46	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
46	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	g	1	Total 44	C 35	Mg 1	N 4	O 4	0
46	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	r	1	Total 44	C 35	Mg 1	N 4	O 4	0

Continued on next page...

Continued from previous page...

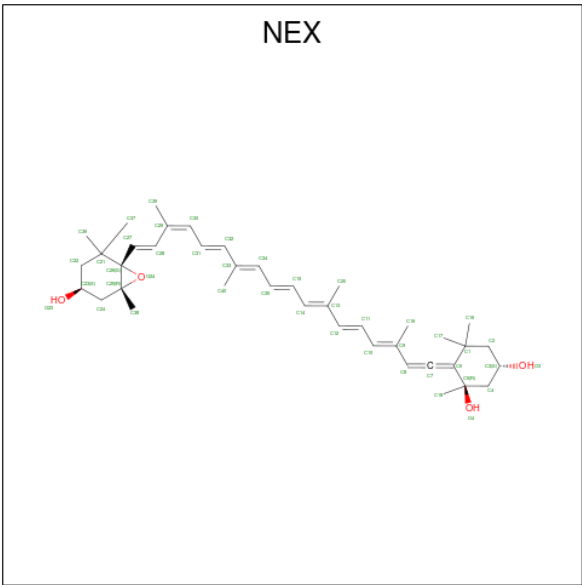
Mol	Chain	Residues	Atoms					AltConf
46	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
46	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
46	s	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
46	s	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
46	s	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
46	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
46	y	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
46	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 47 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



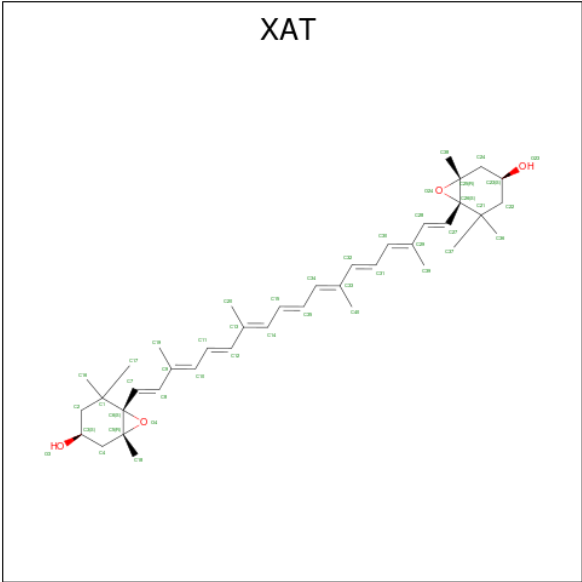
Mol	Chain	Residues	Atoms			AltConf
47	N	1	Total	C	O	0
			42	40	2	
47	N	1	Total	C	O	0
			42	40	2	
47	G	1	Total	C	O	0
			42	40	2	
47	G	1	Total	C	O	0
			42	40	2	
47	R	1	Total	C	O	0
			42	40	2	
47	S	1	Total	C	O	0
			42	40	2	
47	S	1	Total	C	O	0
			42	40	2	
47	Y	1	Total	C	O	0
			42	40	2	
47	Y	1	Total	C	O	0
			42	40	2	
47	n	1	Total	C	O	0
			42	40	2	
47	n	1	Total	C	O	0
			42	40	2	
47	g	1	Total	C	O	0
			42	40	2	
47	g	1	Total	C	O	0
			42	40	2	
47	r	1	Total	C	O	0
			42	40	2	
47	s	1	Total	C	O	0
			42	40	2	
47	s	1	Total	C	O	0
			42	40	2	
47	y	1	Total	C	O	0
			42	40	2	
47	y	1	Total	C	O	0
			42	40	2	

- Molecule 48 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



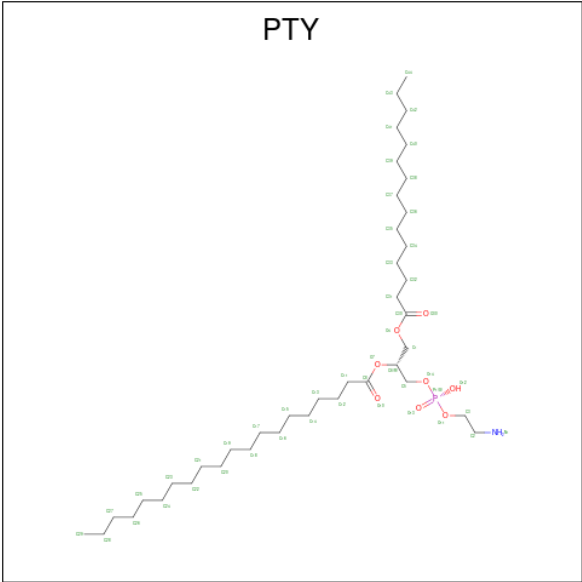
Mol	Chain	Residues	Atoms			AltConf
48	N	1	Total	C	O	0
			44	40	4	
48	G	1	Total	C	O	0
			44	40	4	
48	R	1	Total	C	O	0
			27	25	2	
48	S	1	Total	C	O	0
			44	40	4	
48	Y	1	Total	C	O	0
			44	40	4	
48	n	1	Total	C	O	0
			44	40	4	
48	g	1	Total	C	O	0
			44	40	4	
48	r	1	Total	C	O	0
			27	25	2	
48	s	1	Total	C	O	0
			44	40	4	
48	y	1	Total	C	O	0
			44	40	4	

- Molecule 49 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).



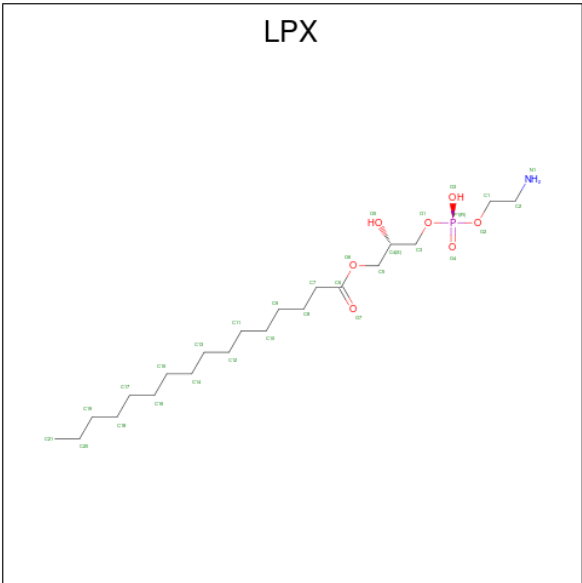
Mol	Chain	Residues	Atoms			AltConf
49	N	1	Total	C	O	0
			44	40	4	
49	G	1	Total	C	O	0
			44	40	4	
49	R	1	Total	C	O	0
			44	40	4	
49	Y	1	Total	C	O	0
			44	40	4	
49	n	1	Total	C	O	0
			44	40	4	
49	g	1	Total	C	O	0
			44	40	4	
49	r	1	Total	C	O	0
			44	40	4	
49	y	1	Total	C	O	0
			44	40	4	

- Molecule 50 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



Mol	Chain	Residues	Atoms					AltConf
50	N	1	Total	C	N	O	P	0
			50	40	1	8	1	
50	Y	1	Total	C	N	O	P	0
			19	9	1	8	1	
50	n	1	Total	C	N	O	P	0
			50	40	1	8	1	
50	y	1	Total	C	N	O	P	0
			19	9	1	8	1	

- Molecule 51 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: C₂₁H₄₄NO₇P).



Mol	Chain	Residues	Atoms					AltConf
51	S	1	Total	C	N	O	P	0
			20	11	1	7	1	
51	s	1	Total	C	N	O	P	0
			19	10	1	7	1	

- Molecule 52 is water.

Mol	Chain	Residues	Atoms		AltConf
52	A	93	Total	O	0
			93	93	
52	B	144	Total	O	0
			144	144	
52	V	7	Total	O	0
			7	7	
52	C	110	Total	O	0
			110	110	
52	D	74	Total	O	0
			74	74	
52	E	15	Total	O	0
			15	15	
52	F	2	Total	O	0
			2	2	
52	H	13	Total	O	0
			13	13	
52	I	9	Total	O	0
			9	9	
52	J	5	Total	O	0
			5	5	
52	K	9	Total	O	0
			9	9	
52	L	14	Total	O	0
			14	14	
52	M	9	Total	O	0
			9	9	
52	O	75	Total	O	0
			75	75	
52	P	22	Total	O	0
			22	22	
52	T	5	Total	O	0
			5	5	
52	W	9	Total	O	0
			9	9	
52	X	3	Total	O	0
			3	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
52	Z	4	Total 4	O 4	0
52	N	63	Total 63	O 63	0
52	G	60	Total 60	O 60	0
52	R	36	Total 36	O 36	0
52	S	33	Total 33	O 33	0
52	Y	55	Total 55	O 55	0
52	U	8	Total 8	O 8	0
52	a	91	Total 91	O 91	0
52	b	123	Total 123	O 123	0
52	v	3	Total 3	O 3	0
52	c	102	Total 102	O 102	0
52	d	68	Total 68	O 68	0
52	e	23	Total 23	O 23	0
52	f	3	Total 3	O 3	0
52	h	18	Total 18	O 18	0
52	i	11	Total 11	O 11	0
52	j	3	Total 3	O 3	0
52	k	9	Total 9	O 9	0
52	l	8	Total 8	O 8	0
52	m	6	Total 6	O 6	0
52	o	78	Total 78	O 78	0

Continued on next page...

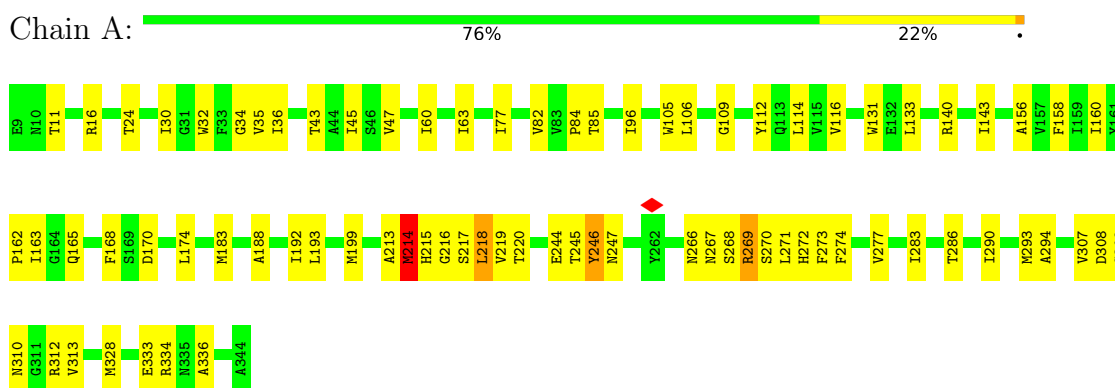
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
52	p	64	Total 64	O 64	0
52	t	2	Total 2	O 2	0
52	w	12	Total 12	O 12	0
52	x	9	Total 9	O 9	0
52	z	6	Total 6	O 6	0
52	n	36	Total 36	O 36	0
52	g	33	Total 33	O 33	0
52	r	33	Total 33	O 33	0
52	s	40	Total 40	O 40	0
52	y	61	Total 61	O 61	0
52	u	5	Total 5	O 5	0

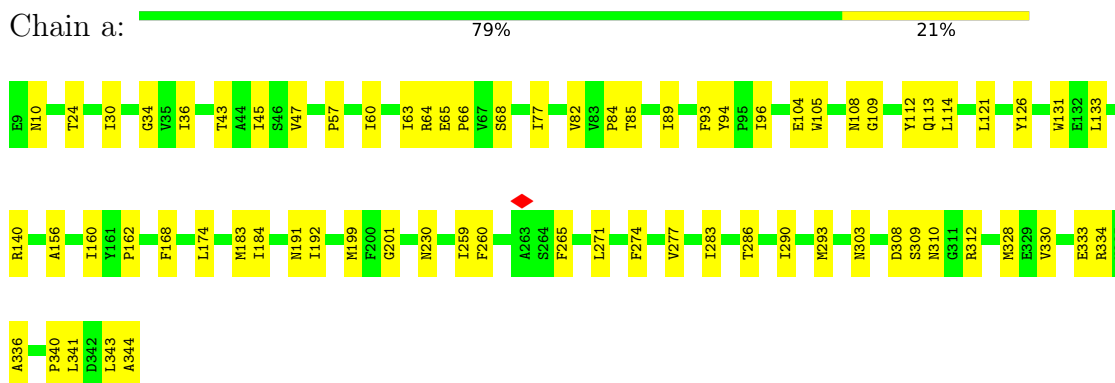
3 Residue-property plots

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

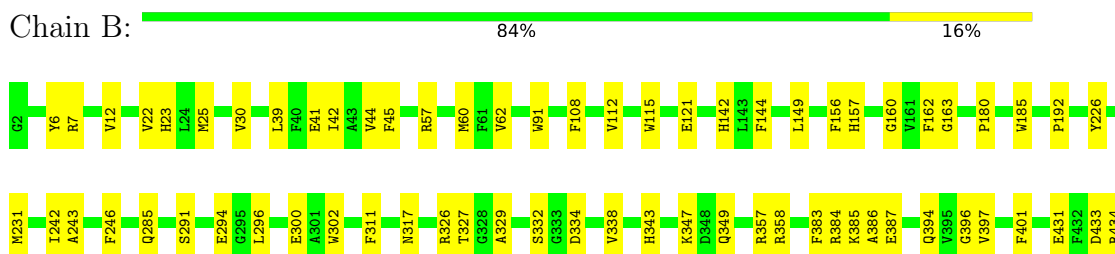
• Molecule 1: Photosystem II protein D1



• Molecule 1: Photosystem II protein D1



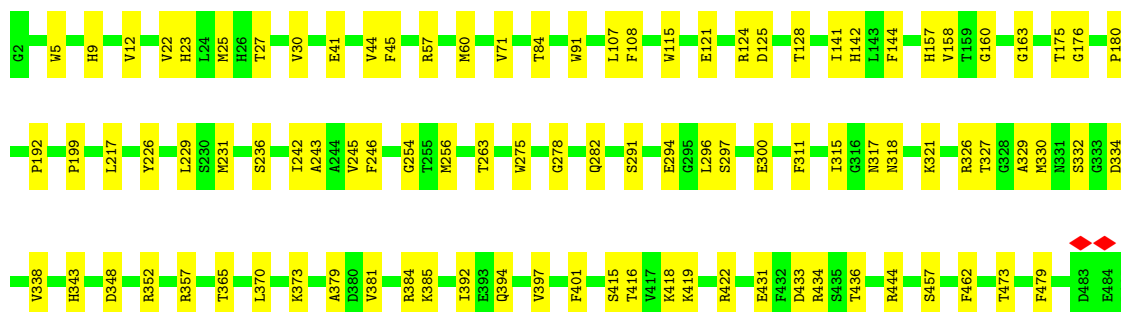
• Molecule 2: Photosystem II CP47 reaction center protein





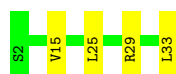
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 80% 20%



- Molecule 3: Photosystem II reaction center protein Ycf12

Chain V: 88% 12%



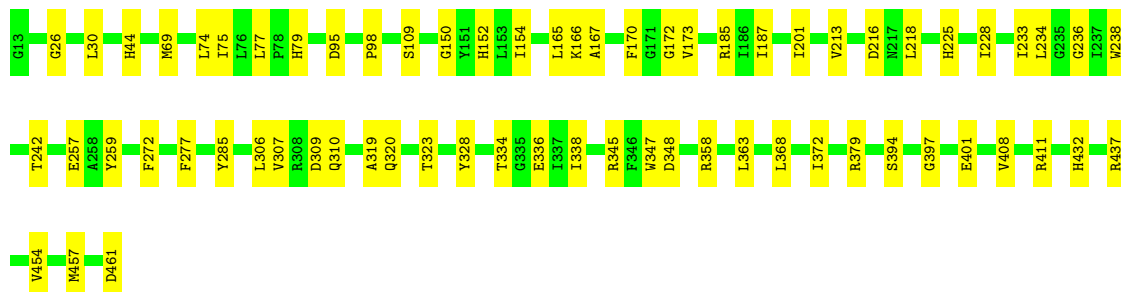
- Molecule 3: Photosystem II reaction center protein Ycf12

Chain v: 88% 12%



- Molecule 4: Photosystem II CP43 reaction center protein

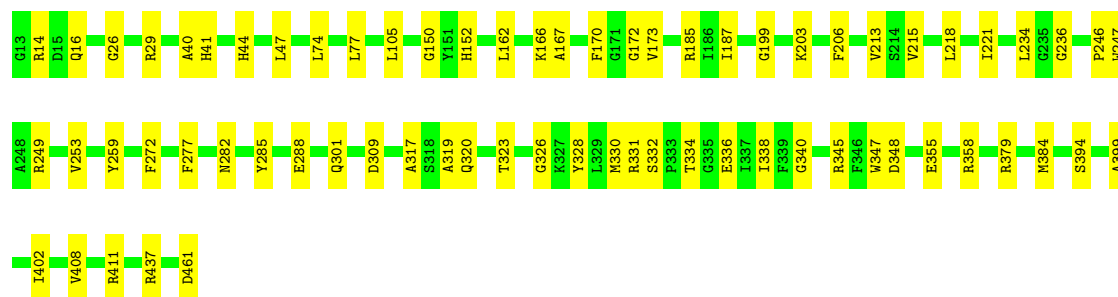
Chain C: 85% 15%



- Molecule 4: Photosystem II CP43 reaction center protein

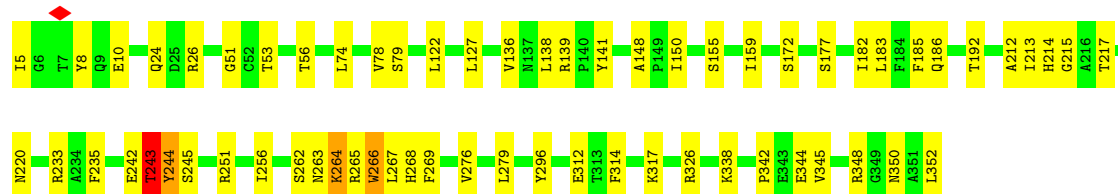
Chain c: 85% 15%





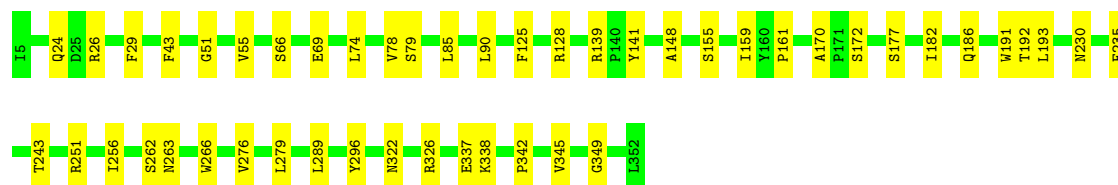
• Molecule 5: Photosystem II D2 protein

Chain D: 82% 17%



• Molecule 5: Photosystem II D2 protein

Chain d: 86% 14%



• Molecule 6: Cytochrome b559 subunit alpha

Chain E: 82% 18%



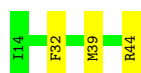
• Molecule 6: Cytochrome b559 subunit alpha

Chain e: 83% 17%



• Molecule 7: Cytochrome b559 subunit beta

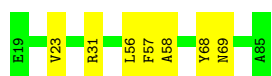
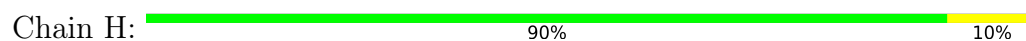
Chain F: 90% 10%



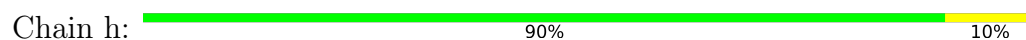
- Molecule 7: Cytochrome b559 subunit beta



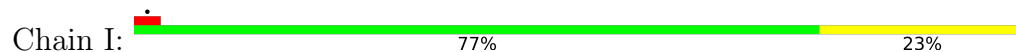
- Molecule 8: Photosystem II reaction center protein H



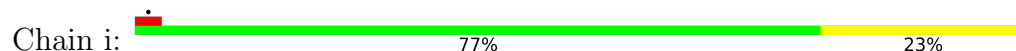
- Molecule 8: Photosystem II reaction center protein H



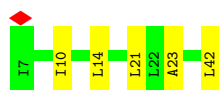
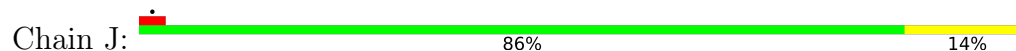
- Molecule 9: Photosystem II reaction center protein I



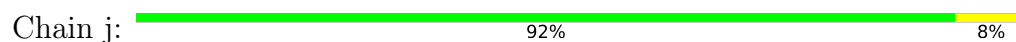
- Molecule 9: Photosystem II reaction center protein I



- Molecule 10: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein J





- Molecule 11: Photosystem II reaction center protein K

Chain K: 86% 14%



- Molecule 11: Photosystem II reaction center protein K

Chain k: 86% 14%



- Molecule 12: Photosystem II reaction center protein L

Chain L: 92% 8%



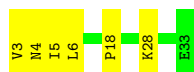
- Molecule 12: Photosystem II reaction center protein L

Chain l: 87% 13%



- Molecule 13: Photosystem II reaction center protein M

Chain M: 81% 19%



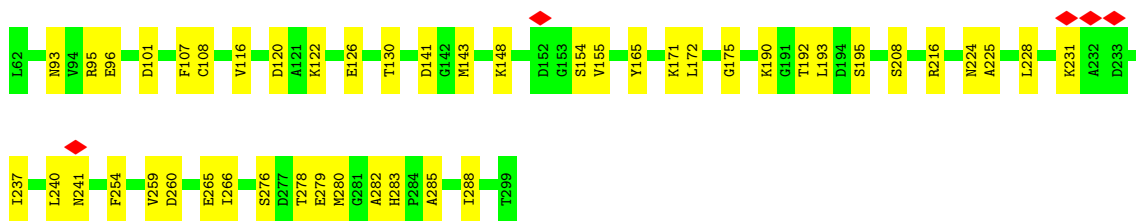
- Molecule 13: Photosystem II reaction center protein M

Chain m: 77% 23%



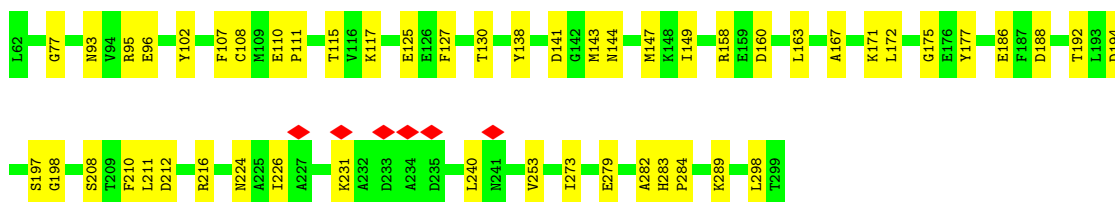
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain O: 81% 19%



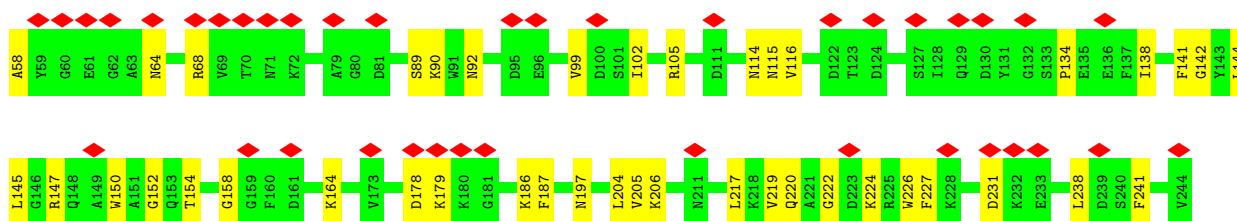
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain o: 79% 21%



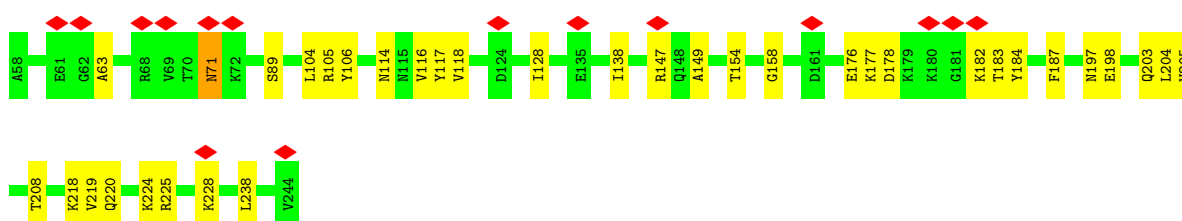
- Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

Chain P: 21% 78% 22%



- Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

Chain p: 8% 81% 19%



- Molecule 16: Photosystem II reaction center protein T

Chain T: 83% 17%



- Molecule 16: Photosystem II reaction center protein T

Chain t:  80% 20%



- Molecule 17: PSII 6.1 kDa protein

Chain W:  93% 7%



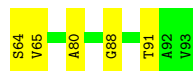
- Molecule 17: PSII 6.1 kDa protein

Chain w:  82% 18%



- Molecule 18: Hypothetical protein

Chain X:  83% 17%



- Molecule 18: Hypothetical protein

Chain x:  80% 20%



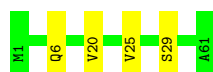
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  93% 7%



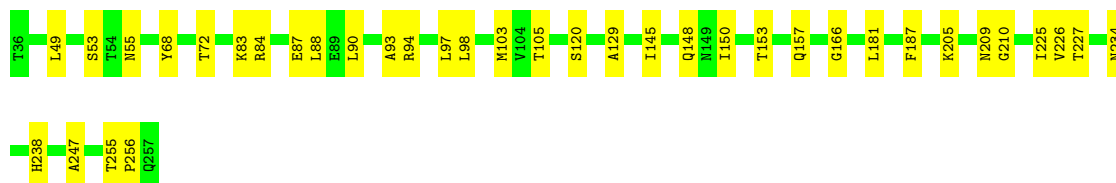
- Molecule 19: Photosystem II reaction center protein Z

Chain z:  93% 7%



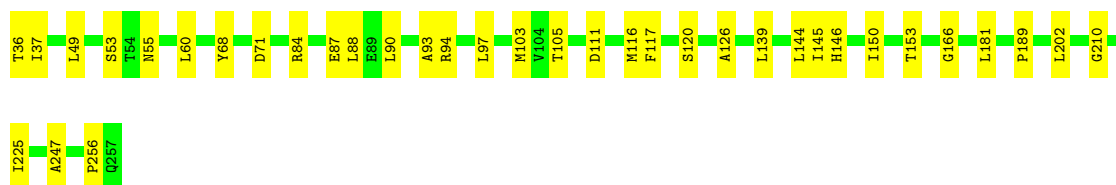
- Molecule 20: Chlorophyll a-b binding protein of LHCII type 3, chloroplastic

Chain N:  83% 17%



- Molecule 20: Chlorophyll a-b binding protein of LHCII type 3, chloroplastic

Chain n:  84% 16%



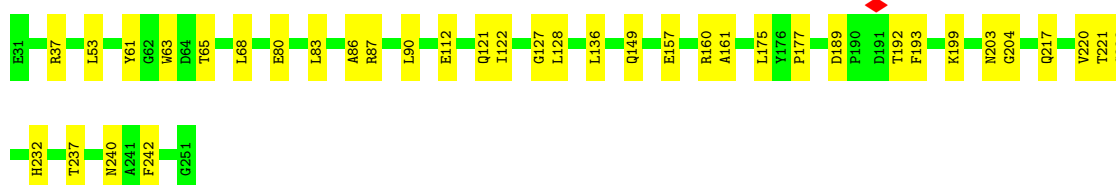
- Molecule 21: Chlorophyll a-b binding protein of LHCII type 2, chloroplastic

Chain G:  90% 10%



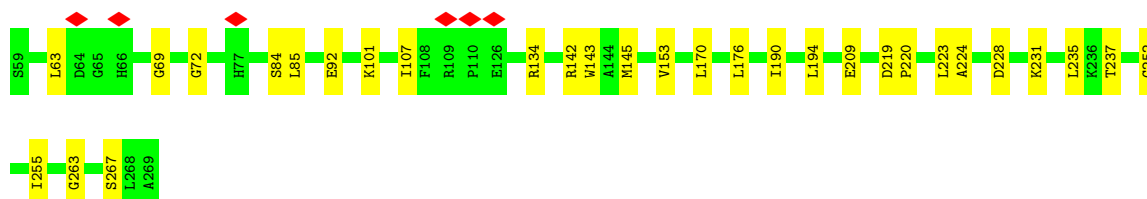
- Molecule 21: Chlorophyll a-b binding protein of LHCII type 2, chloroplastic

Chain g:  83% 17%



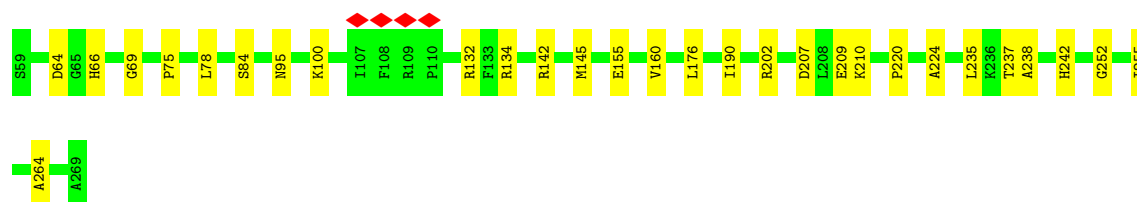
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic, CP29

Chain R:  85% 15%



- Molecule 22: Chlorophyll a-b binding protein, chloroplastic, CP29

Chain r:  85% 15%



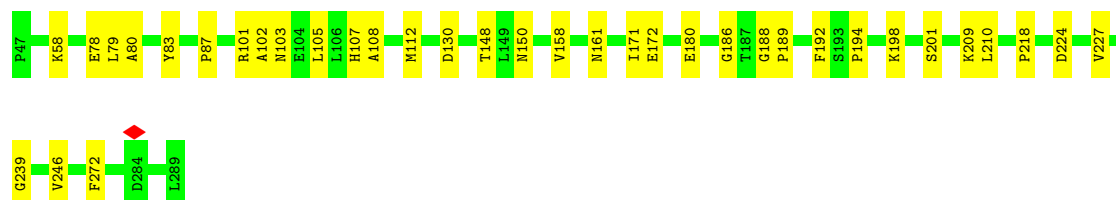
- Molecule 23: Chlorophyll a-b binding protein, chloroplastic, CP26

Chain S: 88% 12%



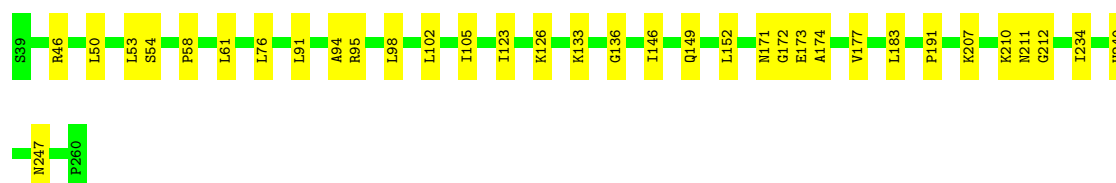
- Molecule 23: Chlorophyll a-b binding protein, chloroplastic, CP26

Chain s: 85% 15%



- Molecule 24: Chlorophyll a-b binding protein of LHCII type 1, chloroplastic

Chain Y: 85% 15%



- Molecule 24: Chlorophyll a-b binding protein of LHCII type 1, chloroplastic

Chain y: 86% 14%



- Molecule 25: Photosystem II extrinsic protein U

Chain U: 67% 33%



- Molecule 25: Photosystem II extrinsic protein U



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39357	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.81	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	39.371	Depositor
Minimum map value	-16.255	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.002	Depositor
Recommended contour level	2.5	Depositor
Map size ($\text{\AA}$)	448.0, 448.0, 448.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.896, 0.896, 0.896	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, NA, DGD, NEX, CL, PTY, LUT, HEM, SPH, 3PH, DGA, LMT, CLA, SQD, CSD, C7Z, LMG, OEX, BCT, SEP, RRX, XAT, LPX, PHO, LHG, FE2, PL9, CHL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.76	49/2717 (1.8%)	0.97	38/3707 (1.0%)
1	a	0.24	0/2717	0.42	0/3707
2	B	0.21	0/3906	0.37	0/5319
2	b	0.21	0/3906	0.38	0/5319
3	V	0.14	0/228	0.33	0/311
3	v	0.15	0/228	0.33	0/311
4	C	0.18	0/3602	0.37	0/4913
4	c	0.19	0/3602	0.35	0/4913
5	D	1.89	46/2860 (1.6%)	0.92	36/3899 (0.9%)
5	d	0.23	0/2860	0.38	0/3899
6	E	0.19	0/639	0.44	0/870
6	e	0.18	0/639	0.43	0/870
7	F	0.19	0/259	0.38	0/351
7	f	0.16	0/259	0.33	0/351
8	H	0.16	0/513	0.36	0/703
8	h	0.17	0/513	0.34	0/703
9	I	0.24	0/287	0.40	0/386
9	i	0.20	0/287	0.40	0/386
10	J	0.12	0/272	0.26	0/369
10	j	0.14	0/272	0.31	0/369
11	K	0.25	0/308	0.60	2/423 (0.5%)
11	k	0.25	0/308	0.49	0/423
12	L	0.19	0/321	0.33	0/435
12	l	0.21	0/321	0.31	0/435
13	M	0.24	0/237	0.48	0/323
13	m	0.25	0/237	0.51	0/323
14	O	0.16	0/1855	0.40	0/2505
14	o	0.17	0/1855	0.40	0/2505
15	P	0.15	0/1473	0.40	0/1988
15	p	0.15	0/1473	0.42	2/1988 (0.1%)
16	T	0.22	0/254	0.38	0/342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	t	0.21	0/254	0.32	0/342
17	W	0.17	0/339	0.38	0/460
17	w	0.21	0/339	0.39	0/460
18	X	0.19	0/202	0.42	0/276
18	x	0.17	0/202	0.38	0/276
19	Z	0.14	0/469	0.30	0/641
19	z	0.14	0/469	0.30	0/641
20	N	0.17	0/1751	0.36	0/2386
20	n	0.18	0/1751	0.36	0/2386
21	G	0.16	0/1725	0.34	0/2348
21	g	0.17	0/1725	0.35	0/2348
22	R	0.15	0/1506	0.33	0/2035
22	r	0.15	0/1506	0.33	0/2035
23	S	0.18	0/1903	0.39	0/2590
23	s	0.18	0/1903	0.38	0/2590
24	Y	0.18	0/1715	0.36	0/2338
24	y	0.19	0/1715	0.33	0/2338
25	U	0.19	0/224	0.41	0/298
25	u	0.30	0/224	0.67	0/298
All	All	0.59	95/59130 (0.2%)	0.46	78/80432 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	D	0	2

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	213	ILE	C-O	-30.87	0.88	1.24
1	A	216	GLY	C-O	-30.70	0.87	1.23
5	D	264	LYS	C-O	-30.20	0.88	1.24
5	D	268	HIS	C-O	-26.99	0.90	1.24
5	D	265	ARG	C-O	-26.81	0.93	1.24
5	D	263	ASN	C-O	-26.29	0.94	1.24
5	D	215	GLY	C-O	-24.13	0.94	1.23
1	A	269	ARG	C-O	-23.63	0.95	1.24
5	D	214	HIS	C-O	-23.02	0.97	1.24
1	A	214	MET	C-O	-22.62	0.97	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	269	PHE	C-O	-21.88	0.98	1.24
1	A	215	HIS	C-O	-21.17	0.99	1.24
1	A	218	LEU	C-O	-21.14	0.96	1.24
1	A	272	HIS	C-O	-20.50	1.00	1.24
5	D	245	SER	C-O	-20.27	0.99	1.24
1	A	273	PHE	C-O	-19.97	1.00	1.24
1	A	267	ASN	C-O	-19.91	1.01	1.24
1	A	219	VAL	C-O	-19.27	1.00	1.24
1	A	271	LEU	C-O	-18.60	1.02	1.24
5	D	267	LEU	C-O	-17.62	1.03	1.24
5	D	245	SER	CA-CB	-17.59	1.30	1.53
5	D	243	THR	C-O	-17.26	1.00	1.23
5	D	244	TYR	C-O	-16.75	1.02	1.23
1	A	220	THR	C-O	-16.20	1.04	1.24
1	A	215	HIS	C-N	-14.40	1.15	1.33
1	A	246	TYR	C-O	-13.89	1.06	1.23
5	D	265	ARG	C-N	-13.22	1.16	1.33
5	D	214	HIS	CE1-NE2	-13.15	1.19	1.32
5	D	262	SER	C-N	-12.31	1.17	1.33
1	A	218	LEU	C-N	-12.09	1.18	1.33
5	D	213	ILE	C-N	-11.95	1.19	1.33
5	D	268	HIS	CE1-NE2	-11.87	1.20	1.32
1	A	245	THR	C-O	-11.50	1.08	1.24
5	D	266	TRP	C-N	-11.36	1.19	1.33
1	A	272	HIS	CE1-NE2	-10.70	1.21	1.32
1	A	216	GLY	CA-C	-10.69	1.39	1.51
5	D	243	THR	C-N	-10.65	1.20	1.33
5	D	214	HIS	C-N	-10.39	1.19	1.33
1	A	269	ARG	C-N	-10.02	1.20	1.34
5	D	268	HIS	CD2-NE2	-9.98	1.26	1.37
1	A	268	SER	C-O	-9.92	1.11	1.24
5	D	268	HIS	ND1-CE1	-9.84	1.22	1.32
1	A	268	SER	CA-CB	-9.84	1.37	1.53
1	A	247	ASN	C-O	-9.75	1.10	1.23
5	D	244	TYR	CA-C	-9.62	1.40	1.52
5	D	268	HIS	C-N	-9.50	1.21	1.33
1	A	271	LEU	N-CA	-9.38	1.35	1.46
1	A	273	PHE	C-N	-9.20	1.21	1.33
5	D	215	GLY	N-CA	-9.05	1.33	1.45
1	A	217	SER	C-N	-8.82	1.21	1.33
1	A	272	HIS	ND1-CE1	-8.55	1.24	1.32
1	A	220	THR	C-N	-8.50	1.22	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	HIS	CA-C	-8.38	1.42	1.52
5	D	269	PHE	CA-C	-8.21	1.42	1.52
1	A	245	THR	C-N	-8.13	1.23	1.33
5	D	213	ILE	CA-C	-8.10	1.42	1.52
1	A	271	LEU	C-N	-8.04	1.23	1.33
1	A	219	VAL	C-N	-8.03	1.23	1.33
1	A	213	ALA	C-N	-7.97	1.23	1.33
5	D	212	ALA	C-N	-7.96	1.23	1.33
5	D	214	HIS	ND1-CE1	-7.77	1.24	1.32
1	A	214	MET	C-N	-7.69	1.24	1.33
5	D	244	TYR	C-N	-7.68	1.23	1.33
5	D	214	HIS	CG-ND1	-7.65	1.29	1.38
1	A	214	MET	CA-C	-7.20	1.43	1.52
1	A	267	ASN	C-N	-7.05	1.24	1.34
5	D	214	HIS	CD2-NE2	-7.04	1.30	1.37
1	A	216	GLY	N-CA	-7.02	1.37	1.45
1	A	216	GLY	C-N	-6.93	1.24	1.34
5	D	265	ARG	N-CA	-6.91	1.38	1.46
5	D	268	HIS	CG-ND1	-6.87	1.30	1.38
5	D	245	SER	C-N	-6.84	1.25	1.33
5	D	268	HIS	CG-CD2	-6.78	1.28	1.35
1	A	215	HIS	CE1-NE2	-6.63	1.25	1.32
1	A	272	HIS	CD2-NE2	-6.62	1.30	1.37
1	A	272	HIS	CG-ND1	-6.59	1.31	1.38
5	D	269	PHE	N-CA	-6.57	1.38	1.46
5	D	267	LEU	N-CA	-6.50	1.38	1.46
1	A	247	ASN	CA-C	-6.49	1.45	1.53
1	A	273	PHE	N-CA	-6.47	1.38	1.46
5	D	264	LYS	C-N	-6.47	1.26	1.33
1	A	215	HIS	ND1-CE1	-6.39	1.26	1.32
5	D	263	ASN	CA-C	-6.14	1.45	1.52
1	A	273	PHE	CA-C	-6.11	1.45	1.52
1	A	272	HIS	CA-C	-6.10	1.44	1.52
5	D	245	SER	CA-C	-5.85	1.45	1.52
5	D	214	HIS	CA-C	-5.84	1.45	1.52
5	D	265	ARG	CA-C	-5.56	1.45	1.52
1	A	272	HIS	CG-CD2	-5.53	1.29	1.35
5	D	268	HIS	N-CA	-5.44	1.39	1.46
1	A	215	HIS	CG-ND1	-5.37	1.32	1.38
5	D	268	HIS	CA-C	-5.26	1.45	1.52
1	A	219	VAL	CA-C	-5.19	1.45	1.52
1	A	215	HIS	N-CA	-5.13	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	SER	C-N	-5.11	1.27	1.33

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	MET	CA-C-O	-13.04	106.59	120.42
5	D	263	ASN	CA-CB-CG	11.75	124.35	112.60
1	A	269	ARG	CB-CA-C	11.29	131.37	110.70
5	D	267	LEU	N-CA-C	10.04	123.48	111.33
5	D	265	ARG	CB-CA-C	9.94	126.72	110.92
5	D	263	ASN	CA-C-N	9.75	133.35	120.28
5	D	263	ASN	C-N-CA	9.75	133.35	120.28
5	D	268	HIS	CA-C-N	9.23	133.00	120.44
5	D	268	HIS	C-N-CA	9.23	133.00	120.44
5	D	267	LEU	CA-C-O	-9.22	110.68	120.63
5	D	263	ASN	CA-C-O	-9.14	110.55	120.24
1	A	266	ASN	CA-C-N	9.12	135.85	123.00
1	A	266	ASN	C-N-CA	9.12	135.85	123.00
5	D	264	LYS	CA-C-N	8.78	133.00	120.79
5	D	264	LYS	C-N-CA	8.78	133.00	120.79
1	A	216	GLY	N-CA-C	8.54	122.97	112.64
1	A	267	ASN	CA-CB-CG	8.53	121.13	112.60
1	A	270	SER	CA-C-N	8.52	132.02	120.44
1	A	270	SER	C-N-CA	8.52	132.02	120.44
5	D	215	GLY	CA-C-O	-7.95	113.01	120.80
5	D	268	HIS	CB-CA-C	7.94	125.92	110.67
5	D	214	HIS	N-CA-C	7.72	119.38	110.97
5	D	242	GLU	CA-C-N	7.67	135.20	122.54
5	D	242	GLU	C-N-CA	7.67	135.20	122.54
1	A	267	ASN	CB-CA-C	7.65	122.85	110.16
1	A	268	SER	N-CA-CB	-7.46	98.74	110.22
1	A	271	LEU	CA-C-N	7.45	130.26	120.28
1	A	271	LEU	C-N-CA	7.45	130.26	120.28
1	A	272	HIS	CA-C-O	-7.43	112.67	120.55
1	A	218	LEU	CA-C-N	7.41	132.40	120.55
1	A	218	LEU	C-N-CA	7.41	132.40	120.55
1	A	219	VAL	CA-C-O	-7.18	113.03	120.71
5	D	266	TRP	O-C-N	-7.14	114.55	122.12
1	A	244	GLU	O-C-N	-6.97	114.36	122.93
5	D	266	TRP	CA-C-N	6.97	129.93	120.38
5	D	266	TRP	C-N-CA	6.97	129.93	120.38
1	A	272	HIS	CA-C-N	6.94	129.88	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	HIS	C-N-CA	6.94	129.88	120.44
5	D	268	HIS	CA-CB-CG	6.92	120.72	113.80
5	D	244	TYR	CA-CB-CG	6.90	126.31	113.90
1	A	214	MET	N-CA-C	6.80	118.77	111.36
1	A	269	ARG	N-CA-C	-6.52	103.67	111.69
1	A	266	ASN	O-C-N	-6.47	113.45	122.37
1	A	247	ASN	CA-CB-CG	6.42	119.02	112.60
1	A	270	SER	O-C-N	-6.40	114.40	122.27
5	D	264	LYS	CB-CA-C	6.34	121.31	110.79
5	D	269	PHE	CA-C-O	-6.25	114.26	120.70
1	A	215	HIS	CB-CA-C	6.22	120.55	110.96
5	D	214	HIS	CA-CB-CG	6.14	119.94	113.80
5	D	212	ALA	CA-C-N	6.13	128.85	120.46
5	D	212	ALA	C-N-CA	6.13	128.85	120.46
1	A	219	VAL	CA-C-N	6.12	128.97	120.29
1	A	219	VAL	C-N-CA	6.12	128.97	120.29
1	A	246	TYR	CA-C-O	-6.05	114.80	121.33
5	D	243	THR	CA-C-N	6.04	132.87	121.69
5	D	243	THR	C-N-CA	6.04	132.87	121.69
5	D	242	GLU	O-C-N	-5.95	116.00	122.79
5	D	215	GLY	O-C-N	5.92	127.91	122.17
1	A	272	HIS	CB-CA-C	5.88	120.55	110.79
1	A	219	VAL	CA-CB-CG2	5.79	120.25	110.40
1	A	216	GLY	CA-C-O	-5.72	115.16	121.05
1	A	269	ARG	CA-CB-CG	5.63	125.36	114.10
1	A	213	ALA	O-C-N	-5.59	116.19	122.12
1	A	246	TYR	CA-C-N	5.55	130.99	122.77
1	A	246	TYR	C-N-CA	5.55	130.99	122.77
1	A	271	LEU	CA-C-O	-5.54	114.99	120.70
11	K	27	ILE	CA-C-N	5.53	123.73	120.24
11	K	27	ILE	C-N-CA	5.53	123.73	120.24
5	D	213	ILE	CA-C-O	-5.36	115.38	120.95
5	D	245	SER	CA-C-O	-5.31	114.60	120.60
5	D	267	LEU	O-C-N	5.19	127.62	122.12
5	D	269	PHE	O-C-N	5.16	127.66	122.09
5	D	212	ALA	O-C-N	-5.15	116.77	122.07
1	A	244	GLU	CA-C-N	5.08	132.10	121.94
1	A	244	GLU	C-N-CA	5.08	132.10	121.94
15	p	71	ASN	CA-C-N	5.07	131.22	121.54
15	p	71	ASN	C-N-CA	5.07	131.22	121.54
5	D	214	HIS	CB-CA-C	5.03	118.70	110.96

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	D	243	THR	Mainchain
5	D	244	TYR	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2635	0	2535	50	0
1	a	2635	0	2536	52	0
2	B	3785	0	3663	64	0
2	b	3785	0	3663	74	0
3	V	227	0	261	3	0
3	v	227	0	261	4	0
4	C	3483	0	3376	49	0
4	c	3483	0	3376	51	0
5	D	2766	0	2654	41	0
5	d	2766	0	2655	36	0
6	E	621	0	605	11	0
6	e	621	0	605	10	0
7	F	252	0	265	5	0
7	f	252	0	265	8	0
8	H	503	0	532	8	0
8	h	503	0	532	8	0
9	I	279	0	288	8	0
9	i	279	0	288	7	0
10	J	266	0	286	4	0
10	j	266	0	286	3	0
11	K	297	0	312	3	0
11	k	297	0	312	4	0
12	L	313	0	325	3	0
12	l	313	0	325	5	0
13	M	234	0	258	6	0
13	m	234	0	258	6	0
14	O	1820	0	1776	32	0
14	o	1820	0	1776	35	0
15	P	1444	0	1403	39	0
15	p	1444	0	1403	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	T	247	0	260	6	0
16	t	247	0	260	6	0
17	W	332	0	323	3	0
17	w	332	0	323	7	0
18	X	201	0	224	4	0
18	x	201	0	224	4	0
19	Z	457	0	478	4	0
19	z	457	0	478	4	0
20	N	1703	0	1641	30	0
20	n	1703	0	1641	28	0
21	G	1680	0	1614	15	0
21	g	1680	0	1614	27	0
22	R	1490	0	1454	24	0
22	r	1490	0	1454	20	0
23	S	1856	0	1816	23	0
23	s	1856	0	1816	26	0
24	Y	1667	0	1624	22	0
24	y	1667	0	1624	21	0
25	U	224	0	226	8	0
25	u	224	0	226	9	0
26	A	10	0	0	1	0
26	a	10	0	0	1	0
27	A	1	0	0	0	0
27	d	1	0	0	0	0
28	A	2	0	0	0	0
28	a	2	0	0	0	0
29	A	240	0	242	19	0
29	B	1030	0	1129	41	0
29	C	830	0	900	27	0
29	D	125	0	131	9	0
29	G	466	0	471	20	0
29	N	468	0	471	17	0
29	R	385	0	347	14	0
29	S	620	0	582	29	0
29	Y	570	0	615	24	0
29	a	239	0	242	14	0
29	b	1032	0	1133	41	0
29	c	840	0	923	33	0
29	d	130	0	144	7	0
29	g	466	0	471	16	0
29	n	468	0	471	22	0
29	r	400	0	375	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	s	625	0	592	23	0
29	y	570	0	615	27	0
30	A	64	0	74	5	0
30	D	64	0	74	3	0
30	a	64	0	74	4	0
30	d	64	0	74	2	0
31	A	40	0	53	3	0
31	B	80	0	105	7	0
31	C	120	0	158	11	0
31	F	40	0	53	2	0
31	K	40	0	53	4	0
31	a	40	0	53	2	0
31	b	80	0	106	10	0
31	c	80	0	105	8	0
31	f	40	0	53	2	0
31	v	40	0	53	3	0
31	z	40	0	53	5	0
32	A	1	0	0	0	0
32	a	1	0	0	0	0
33	A	48	0	75	1	0
33	B	48	0	75	3	0
33	S	30	0	33	2	0
33	a	48	0	75	3	0
33	b	39	0	51	4	0
33	s	48	0	75	3	0
34	B	42	0	0	0	0
34	b	42	0	0	0	0
35	B	44	0	58	3	0
35	C	144	0	204	5	0
35	D	90	0	120	5	0
35	W	79	0	98	4	0
35	b	44	0	58	4	0
35	c	106	0	158	10	0
35	d	94	0	128	4	0
35	i	48	0	66	2	0
35	w	39	0	48	2	0
36	B	43	0	44	1	0
36	C	157	0	188	9	0
36	c	176	0	226	11	0
36	r	43	0	44	1	0
37	B	44	0	61	3	0
37	D	88	0	122	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	G	49	0	74	1	0
37	L	49	0	74	3	0
37	N	49	0	74	4	0
37	S	80	0	103	6	0
37	Y	49	0	74	8	0
37	a	83	0	109	5	0
37	c	47	0	67	7	0
37	d	49	0	74	5	0
37	g	49	0	74	4	0
37	l	49	0	74	3	0
37	n	42	0	57	5	0
37	s	83	0	109	6	0
37	y	49	0	74	3	0
38	B	35	0	44	2	0
38	b	35	0	44	4	0
39	C	78	0	82	2	0
39	L	42	0	47	5	0
39	M	42	0	47	2	0
39	a	51	0	68	1	0
39	b	54	0	77	4	0
39	c	54	0	77	3	0
39	l	42	0	47	3	0
39	m	42	0	47	1	0
39	o	54	0	77	1	0
40	C	21	0	37	1	0
40	I	21	0	37	3	0
40	c	21	0	37	4	0
40	i	21	0	37	1	0
41	D	37	0	56	3	0
41	J	29	0	40	2	0
41	W	44	0	76	4	0
41	b	44	0	76	2	0
41	j	29	0	40	3	0
41	w	44	0	76	6	0
42	D	4	0	0	1	0
42	a	4	0	0	0	0
43	D	55	0	80	2	0
43	d	55	0	80	2	0
44	E	43	0	30	1	0
44	e	43	0	30	3	0
45	H	41	0	56	3	0
45	h	41	0	56	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	G	340	0	305	12	0
46	N	380	0	382	20	0
46	R	94	0	66	3	0
46	S	194	0	144	12	0
46	Y	310	0	308	12	0
46	g	340	0	306	13	0
46	n	314	0	314	15	0
46	r	94	0	66	4	0
46	s	194	0	144	8	0
46	y	361	0	344	16	0
47	G	84	0	110	6	0
47	N	84	0	110	6	0
47	R	42	0	55	4	0
47	S	84	0	110	8	0
47	Y	84	0	110	6	0
47	g	84	0	110	6	0
47	n	84	0	110	7	0
47	r	42	0	55	3	0
47	s	84	0	110	6	0
47	y	84	0	110	4	0
48	G	44	0	54	3	0
48	N	44	0	54	3	0
48	R	27	0	32	3	0
48	S	44	0	54	4	0
48	Y	44	0	54	3	0
48	g	44	0	55	2	0
48	n	44	0	54	1	0
48	r	27	0	32	1	0
48	s	44	0	54	3	0
48	y	44	0	54	3	0
49	G	44	0	56	3	0
49	N	44	0	56	5	0
49	R	44	0	56	1	0
49	Y	44	0	56	3	0
49	g	44	0	56	2	0
49	n	44	0	56	4	0
49	r	44	0	56	4	0
49	y	44	0	56	4	0
50	N	50	0	79	8	0
50	Y	19	0	11	0	0
50	n	50	0	79	5	0
50	y	19	0	11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	S	20	0	20	3	0
51	s	19	0	18	0	0
52	A	93	0	0	0	0
52	B	144	0	0	3	0
52	C	110	0	0	3	0
52	D	74	0	0	0	0
52	E	15	0	0	1	0
52	F	2	0	0	0	0
52	G	60	0	0	0	0
52	H	13	0	0	0	0
52	I	9	0	0	1	0
52	J	5	0	0	0	0
52	K	9	0	0	0	0
52	L	14	0	0	0	0
52	M	9	0	0	1	0
52	N	63	0	0	1	0
52	O	75	0	0	0	0
52	P	22	0	0	1	0
52	R	36	0	0	0	0
52	S	33	0	0	0	0
52	T	5	0	0	0	0
52	U	8	0	0	1	0
52	V	7	0	0	0	0
52	W	9	0	0	0	0
52	X	3	0	0	1	0
52	Y	55	0	0	0	0
52	Z	4	0	0	1	0
52	a	91	0	0	2	0
52	b	123	0	0	1	0
52	c	102	0	0	1	0
52	d	68	0	0	0	0
52	e	23	0	0	0	0
52	f	3	0	0	1	0
52	g	33	0	0	0	0
52	h	18	0	0	0	0
52	i	11	0	0	0	0
52	j	3	0	0	0	0
52	k	9	0	0	0	0
52	l	8	0	0	0	0
52	m	6	0	0	0	0
52	n	36	0	0	0	0
52	o	78	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	p	64	0	0	1	0
52	r	33	0	0	1	0
52	s	40	0	0	1	0
52	t	2	0	0	0	0
52	u	5	0	0	0	0
52	v	3	0	0	0	0
52	w	12	0	0	0	0
52	x	9	0	0	0	0
52	y	61	0	0	0	0
52	z	6	0	0	1	0
All	All	77465	0	76472	1333	0

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

All (1333) 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)
29:R:306:CLA:HMB2	48:R:312:NEX:H35	1.60	0.83
29:C:507:CLA:H91	31:C:516:BCR:H14C	1.63	0.80
29:r:309:CLA:H2	47:r:311:LUT:H28	1.63	0.80
29:n:603:CLA:H2	29:n:603:CLA:HMA2	1.65	0.77
29:c:503:CLA:H172	29:c:510:CLA:HBB2	1.67	0.76
23:s:246:VAL:HG11	47:s:318:LUT:H12	1.66	0.76
20:N:49:LEU:HB2	20:N:53:SER:HB3	1.67	0.75
29:S:303:CLA:H72	47:S:318:LUT:H28	1.70	0.74
22:r:69:GLY:H	22:r:237:THR:HG22	1.53	0.73
29:S:303:CLA:H71	29:S:304:CLA:HMD1	1.69	0.73
35:c:520:LMG:H392	29:y:313:CLA:HBB2	1.70	0.72
1:A:140:ARG:NH2	37:D:408:LHG:O5	2.23	0.72
15:P:105:ARG:HH21	15:P:115:ASN:HD22	1.36	0.72
23:S:95:GLU:OE2	23:S:96:GLN:NE2	2.24	0.71
23:S:108:ALA:HB1	23:S:239:GLY:HA3	1.72	0.71
39:L:102:SQD:H442	2:b:115:TRP:HE1	1.56	0.70
29:b:507:CLA:HBC1	31:b:517:BCR:H10C	1.74	0.69
20:n:49:LEU:HB2	20:n:53:SER:HB3	1.75	0.69
23:S:246:VAL:HG11	47:S:318:LUT:H12	1.74	0.69
5:d:26:ARG:HD3	7:f:17:VAL:HG21	1.73	0.69
23:s:108:ALA:HB1	23:s:239:GLY:HA3	1.75	0.69
29:c:506:CLA:H62	31:c:514:BCR:H14C	1.75	0.69
4:c:74:LEU:HD13	4:c:77:LEU:HD12	1.73	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:88:LEU:HD11	29:N:603:CLA:HBD	1.74	0.68
4:C:167:ALA:HB1	4:C:187:ILE:HD13	1.74	0.68
15:P:204:LEU:HD12	15:P:238:LEU:HD22	1.76	0.68
14:O:228:LEU:HB3	14:O:231:LYS:HB3	1.75	0.68
2:b:394:GLN:HB3	15:p:147:ARG:HE	1.57	0.68
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.76	0.67
31:a:409:BCR:H19C	39:o:301:SQD:H191	1.75	0.67
6:e:12:ASP:OD1	10:j:7:ILE:N	2.27	0.67
29:Y:304:CLA:HAC1	46:Y:308:CHL:HBB2	1.75	0.67
31:c:515:BCR:H391	11:k:36:ALA:HB2	1.77	0.66
5:d:279:LEU:HD22	30:d:402:PHO:HBC3	1.77	0.66
41:J:101:DGA:HB31	41:J:101:DGA:HA31	1.77	0.66
35:d:408:LMG:O10	8:h:69:ASN:ND2	2.29	0.66
37:c:521:LHG:H141	29:s:312:CLA:HBB2	1.77	0.66
15:P:114:ASN:HA	15:P:220:GLN:O	1.96	0.66
4:c:259:TYR:O	52:c:601:HOH:O	2.14	0.66
23:s:224:ASP:HB3	23:s:227:VAL:HG22	1.78	0.66
2:B:285:GLN:HB3	25:U:97:MET:HE1	1.78	0.65
20:N:103:MET:HE2	47:N:616:LUT:H8	1.77	0.65
29:A:405:CLA:H191	37:D:407:LHG:H181	1.77	0.65
2:B:434:ARG:HH22	14:O:231:LYS:HD3	1.62	0.65
22:R:220:PRO:HB3	24:y:191:PRO:HB3	1.78	0.65
20:N:93:ALA:HB1	20:N:210:GLY:HA3	1.79	0.65
29:A:405:CLA:H122	30:A:408:PHO:H3A	1.77	0.65
2:b:44:VAL:HG23	2:b:60:MET:HE1	1.79	0.65
2:B:23:HIS:ND1	29:B:515:CLA:OBD	2.28	0.65
15:P:206:LYS:HD3	15:P:241:PHE:HB3	1.79	0.65
29:c:506:CLA:H12	31:c:514:BCR:H10C	1.78	0.65
31:v:101:BCR:H361	10:j:21:LEU:HD21	1.78	0.64
22:R:134:ARG:NH1	22:R:209:GLU:OE2	2.31	0.64
4:C:234:LEU:HB3	40:C:525:SPH:H151	1.78	0.64
21:G:86:ALA:HB1	21:G:204:GLY:HA3	1.79	0.64
35:D:410:LMG:O10	8:H:69:ASN:ND2	2.30	0.64
15:P:204:LEU:HB3	15:P:238:LEU:HD13	1.80	0.64
2:b:434:ARG:HH12	14:o:231:LYS:HD3	1.63	0.64
29:y:315:CLA:H122	37:y:320:LHG:H361	1.79	0.64
1:A:170:ASP:OD2	4:C:345:ARG:NH1	2.31	0.64
1:a:82:VAL:HB	1:a:174:LEU:HB2	1.79	0.64
21:g:86:ALA:HB1	21:g:204:GLY:HA3	1.80	0.64
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.80	0.64
4:c:246:PRO:HG3	4:c:249:ARG:HH21	1.63	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:d:407:LMG:H371	31:f:101:BCR:H21C	1.80	0.64
20:n:93:ALA:HB1	20:n:210:GLY:HA3	1.79	0.63
46:g:607:CHL:HMA2	46:g:607:CHL:H2	1.79	0.63
2:B:121:GLU:OE1	8:H:31:ARG:NH1	2.31	0.63
5:D:279:LEU:HD22	30:D:401:PHO:HBC3	1.77	0.63
24:Y:191:PRO:HB3	22:r:220:PRO:HB3	1.79	0.63
2:b:415:SER:HA	2:b:418:LYS:HB2	1.80	0.63
29:b:504:CLA:HBD	29:b:504:CLA:HBA1	1.81	0.63
29:g:610:CLA:H52	47:g:615:LUT:H30	1.81	0.63
4:C:259:TYR:O	52:C:1001:HOH:O	2.15	0.63
1:a:45:ILE:HD11	30:a:407:PHO:H51	1.80	0.63
2:B:327:THR:HB	35:B:520:LMG:HC8	1.81	0.63
15:p:114:ASN:HA	15:p:220:GLN:O	1.99	0.63
29:G:602:CLA:H91	29:Y:304:CLA:H102	1.81	0.63
22:R:85:LEU:HG	22:R:107:ILE:HG12	1.79	0.63
24:y:94:ALA:HB1	24:y:212:GLY:HA3	1.80	0.63
2:b:338:VAL:HB	2:b:431:GLU:HG3	1.80	0.62
4:c:461:ASP:OD1	16:t:24:ARG:NH2	2.32	0.62
4:C:30:LEU:HD21	29:C:512:CLA:H2A	1.81	0.62
24:Y:94:ALA:HB1	24:Y:212:GLY:HA3	1.82	0.62
29:S:304:CLA:H11	29:S:310:CLA:H2	1.81	0.62
46:S:309:CHL:H72	29:S:316:CLA:H2	1.82	0.62
15:p:178:ASP:OD1	15:p:182:LYS:N	2.32	0.62
14:o:158:ARG:NH2	14:o:186:GLU:OE1	2.31	0.62
4:c:331:ARG:NH2	14:o:141:ASP:OD2	2.30	0.62
29:r:309:CLA:H52	47:r:311:LUT:H30	1.81	0.62
14:O:237:ILE:HG13	14:O:241:ASN:HB2	1.82	0.62
29:S:311:CLA:H51	29:S:313:CLA:H3A	1.80	0.62
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.82	0.62
2:b:381:VAL:HG11	2:b:422:ARG:HH22	1.65	0.62
10:J:21:LEU:HD21	31:K:101:BCR:H361	1.81	0.61
14:o:171:LYS:HE2	14:o:175:GLY:HA2	1.82	0.61
5:d:338:LYS:HB2	25:u:103:GLU:HG2	1.82	0.61
20:N:55:ASN:ND2	21:G:161:ALA:O	2.33	0.61
29:n:603:CLA:HAC1	46:y:301:CHL:HBB2	1.80	0.61
46:n:605:CHL:H172	29:s:311:CLA:H101	1.82	0.61
46:g:601:CHL:H152	37:g:618:LHG:H223	1.83	0.61
29:g:602:CLA:H91	29:y:305:CLA:H102	1.80	0.61
2:b:236:SER:HB2	2:b:473:THR:HG21	1.82	0.61
29:N:603:CLA:H11	24:Y:76:LEU:HD11	1.83	0.61
5:d:79:SER:HA	5:d:172:SER:HB3	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:327:THR:HB	35:b:520:LMG:HC8	1.81	0.60
46:y:309:CHL:H143	46:y:311:CHL:H101	1.82	0.60
29:N:610:CLA:H51	47:N:615:LUT:H30	1.81	0.60
4:c:167:ALA:HB1	4:c:187:ILE:HD13	1.82	0.60
14:o:208:SER:HB3	15:p:154:THR:HG21	1.83	0.60
6:E:75:GLN:HB2	25:U:113:ILE:HG22	1.81	0.60
2:B:434:ARG:NH1	52:B:611:HOH:O	2.35	0.60
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.84	0.60
6:E:57:THR:O	6:E:61:GLN:NE2	2.33	0.60
1:a:140:ARG:HH22	37:a:414:LHG:HC42	1.66	0.60
4:C:272:PHE:HB3	36:C:518:DGD:HB62	1.82	0.60
46:g:601:CHL:H12	46:y:311:CHL:H43	1.83	0.60
23:s:148:THR:OG1	23:s:161:ASN:O	2.19	0.60
2:B:7:ARG:NH2	52:B:609:HOH:O	2.34	0.60
2:b:23:HIS:ND1	29:b:515:CLA:OBD	2.28	0.60
5:d:24:GLN:OE1	5:d:26:ARG:NH2	2.34	0.60
12:L:27:VAL:HG11	37:L:101:LHG:H201	1.84	0.59
4:c:247:TRP:NE1	35:c:520:LMG:O10	2.34	0.59
23:S:189:PRO:HD2	46:S:309:CHL:HBB2	1.83	0.59
46:n:606:CHL:HED1	46:n:606:CHL:H71	1.84	0.59
15:P:187:PHE:HB2	15:P:205:VAL:HB	1.84	0.59
7:f:44:ARG:NH2	52:f:201:HOH:O	2.35	0.59
29:g:603:CLA:HAC1	46:g:607:CHL:HBB2	1.84	0.59
2:B:44:VAL:HG23	2:B:60:MET:HE1	1.82	0.59
29:N:614:CLA:HBC1	47:N:615:LUT:H162	1.84	0.59
23:S:268:LEU:HD12	51:S:321:LPX:H9A	1.84	0.59
2:b:121:GLU:O	8:h:31:ARG:NH1	2.36	0.59
24:y:46:ARG:NH2	24:y:61:LEU:O	2.36	0.59
5:D:24:GLN:OE1	5:D:26:ARG:NH2	2.35	0.59
29:R:308:CLA:H52	47:R:310:LUT:H30	1.85	0.59
29:b:512:CLA:H171	29:b:513:CLA:HBB2	1.84	0.59
29:C:512:CLA:H143	19:Z:20:VAL:HG13	1.84	0.59
46:G:607:CHL:H143	46:G:609:CHL:H92	1.84	0.59
29:G:610:CLA:H52	47:G:615:LUT:H30	1.84	0.59
24:y:79:ASP:HB3	24:y:82:THR:HG22	1.83	0.59
29:S:311:CLA:H61	47:S:317:LUT:H30	1.85	0.59
6:e:57:THR:O	6:e:61:GLN:NE2	2.35	0.59
20:n:202:LEU:HB3	29:n:609:CLA:H3A	1.83	0.59
4:C:379:ARG:NH1	52:C:1007:HOH:O	2.36	0.58
29:B:512:CLA:H171	29:B:513:CLA:HBB2	1.85	0.58
4:C:238:TRP:O	4:C:242:THR:OG1	2.20	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:G:611:CLA:HAB	49:G:619:XAT:H221	1.84	0.58
29:y:305:CLA:HAC1	46:y:309:CHL:HBB2	1.85	0.58
29:S:312:CLA:H161	29:S:313:CLA:HMC3	1.85	0.58
4:c:355:GLU:OE2	4:c:358:ARG:NH1	2.35	0.58
31:B:518:BCR:HC42	35:B:520:LMG:H341	1.85	0.58
29:a:404:CLA:H122	30:a:407:PHO:H3A	1.85	0.58
29:s:312:CLA:H162	29:s:313:CLA:HAB	1.84	0.58
23:s:172:GLU:OE1	52:s:401:HOH:O	2.17	0.58
14:O:171:LYS:HE2	14:O:175:GLY:HA2	1.86	0.58
21:g:80:GLU:HA	21:g:175:LEU:HD21	1.85	0.58
23:s:58:LYS:HE3	37:s:320:LHG:HC11	1.85	0.58
29:d:404:CLA:H102	18:x:80:ALA:HB2	1.86	0.58
3:V:33:LEU:O	11:K:39:TRP:NE1	2.28	0.58
7:F:44:ARG:NH2	10:J:42:LEU:O	2.37	0.58
14:O:225:ALA:H	14:O:240:LEU:HD22	1.69	0.58
41:W:202:DGA:HAF1	35:W:203:LMG:H351	1.86	0.58
46:N:605:CHL:H61	29:S:306:CLA:HED1	1.84	0.58
1:a:64:ARG:NH1	14:o:167:ALA:O	2.37	0.58
14:O:107:PHE:HB3	14:O:143:MET:HB2	1.85	0.58
5:d:192:THR:HG23	29:d:403:CLA:HBC2	1.86	0.58
29:s:303:CLA:H71	29:s:304:CLA:HMD1	1.85	0.58
20:N:84:ARG:HH22	24:Y:58:PRO:HB3	1.68	0.58
1:A:43:THR:HG23	31:A:410:BCR:H362	1.86	0.57
52:a:501:HOH:O	4:c:345:ARG:NH1	2.37	0.57
46:y:309:CHL:H121	46:y:311:CHL:H121	1.85	0.57
37:n:617:LHG:H202	49:n:618:XAT:H12	1.86	0.57
4:C:225:HIS:HA	4:C:228:ILE:HG22	1.86	0.57
4:C:348:ASP:OD2	36:C:518:DGD:O3D	2.21	0.57
4:c:166:LYS:HA	4:c:170:PHE:HB2	1.84	0.57
37:d:406:LHG:H322	16:t:21:ILE:HD11	1.85	0.57
20:n:103:MET:HE2	47:n:615:LUT:H8	1.87	0.57
23:s:189:PRO:HD2	46:s:309:CHL:HBB2	1.85	0.57
23:s:105:LEU:HD23	23:s:210:LEU:HB3	1.85	0.57
2:b:297:SER:OG	2:b:300:GLU:OE1	2.21	0.57
14:o:212:ASP:OD1	14:o:216:ARG:N	2.36	0.57
15:p:177:LYS:HA	15:p:183:THR:HA	1.86	0.57
4:C:166:LYS:HA	4:C:170:PHE:HB2	1.86	0.57
5:D:5:ILE:N	5:D:10:GLU:OE1	2.37	0.57
20:n:94:ARG:HA	20:n:97:LEU:HD12	1.85	0.57
36:C:519:DGD:HA32	41:J:101:DGA:HA92	1.86	0.57
31:K:101:BCR:H10C	19:Z:20:VAL:HG11	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:p:203:GLN:OE1	15:p:218:LYS:NZ	2.38	0.57
21:g:157:GLU:OE1	21:g:160:ARG:NH2	2.33	0.57
21:g:220:VAL:HG23	21:g:221:THR:HG23	1.86	0.57
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.87	0.57
4:C:98:PRO:HB3	35:C:524:LMG:H291	1.86	0.57
9:I:5:LYS:NZ	17:W:77:ASN:OD1	2.33	0.57
29:c:513:CLA:H52	37:c:521:LHG:H351	1.86	0.57
29:C:507:CLA:HBA2	29:C:508:CLA:H202	1.87	0.57
37:D:407:LHG:H322	16:T:21:ILE:HD11	1.85	0.57
2:b:416:THR:HA	2:b:419:LYS:HG2	1.87	0.57
22:r:64:ASP:OD1	22:r:66:HIS:ND1	2.38	0.57
46:r:305:CHL:HHC	46:r:305:CHL:HBB1	1.87	0.57
1:a:30:ILE:O	1:a:34:GLY:HA3	2.06	0.56
29:c:505:CLA:H172	36:c:516:DGD:HA71	1.86	0.56
15:p:176:GLU:O	15:p:184:TYR:N	2.32	0.56
22:r:207:ASP:HB3	22:r:210:LYS:HB2	1.87	0.56
5:D:186:GLN:HB2	29:D:404:CLA:HBC1	1.87	0.56
20:N:68:TYR:HB2	29:N:602:CLA:HMD1	1.87	0.56
2:b:385:LYS:HB2	15:p:149:ALA:HB3	1.87	0.56
5:d:263:ASN:HB3	5:d:266:TRP:HB3	1.85	0.56
14:o:192:THR:OG1	14:o:194:ASP:OD1	2.21	0.56
50:N:620:PTY:H182	50:N:620:PTY:H381	1.87	0.56
29:G:603:CLA:H11	29:G:603:CLA:HED2	1.87	0.56
23:s:78:GLU:HG2	23:s:79:LEU:HG	1.87	0.56
1:A:63:ILE:HB	4:C:323:THR:HG21	1.86	0.56
14:o:107:PHE:HB3	14:o:143:MET:HB2	1.86	0.56
50:n:619:PTY:H442	29:y:316:CLA:HBC2	1.88	0.56
29:g:603:CLA:H51	29:g:603:CLA:HMA2	1.87	0.56
25:U:108:GLU:OE1	25:U:108:GLU:N	2.39	0.56
15:p:116:VAL:HG23	15:p:219:VAL:HG22	1.88	0.56
6:E:45:ASP:HB3	15:P:58:ALA:HA	1.87	0.56
4:c:152:HIS:ND1	29:c:507:CLA:OBD	2.30	0.56
46:R:304:CHL:HHC	46:R:304:CHL:HBB1	1.87	0.56
4:C:285:TYR:O	4:C:411:ARG:NH2	2.37	0.56
41:W:202:DGA:HBT1	35:W:203:LMG:H371	1.88	0.56
20:N:94:ARG:HA	20:N:97:LEU:HD12	1.88	0.56
37:N:618:LHG:H202	49:N:619:XAT:H12	1.88	0.56
2:B:479:PHE:O	5:D:139:ARG:NH2	2.39	0.56
29:c:513:CLA:HAB	31:z:101:BCR:H24C	1.88	0.56
29:n:602:CLA:HBA1	47:n:615:LUT:H382	1.88	0.56
4:C:358:ARG:NH1	52:C:1008:HOH:O	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:19:TYR:O	6:E:23:HIS:ND1	2.23	0.55
20:n:189:PRO:O	47:n:614:LUT:O23	2.24	0.55
21:g:177:PRO:HB3	46:g:608:CHL:HBC2	1.88	0.55
1:A:24:THR:O	5:D:251:ARG:NH2	2.36	0.55
37:d:406:LHG:H291	16:t:17:ILE:HD12	1.86	0.55
21:g:83:LEU:HD23	21:g:175:LEU:HD22	1.89	0.55
46:g:608:CHL:HHC	46:g:608:CHL:HBB1	1.88	0.55
46:s:309:CHL:HHC	46:s:309:CHL:HBB1	1.88	0.55
29:C:503:CLA:H61	29:C:513:CLA:H42	1.88	0.55
1:A:30:ILE:O	1:A:34:GLY:HA3	2.06	0.55
14:O:260:ASP:HB2	14:O:265:GLU:HG2	1.89	0.55
20:N:226:VAL:HG23	20:N:227:THR:HG23	1.88	0.55
4:c:234:LEU:HB3	40:c:523:SPH:H151	1.87	0.55
46:N:601:CHL:HHC	46:N:601:CHL:HBB1	1.89	0.55
1:A:45:ILE:HD11	30:A:408:PHO:H51	1.88	0.55
9:I:5:LYS:HD2	17:W:65:MET:HE1	1.87	0.55
21:G:220:VAL:HG23	21:G:221:THR:HG23	1.87	0.55
2:B:296:LEU:HD23	2:B:300:GLU:HG3	1.88	0.55
6:E:18:ARG:NH2	52:E:201:HOH:O	2.40	0.55
46:S:309:CHL:HHC	46:S:309:CHL:HBB1	1.89	0.55
38:b:524:LMT:H32	29:r:303:CLA:H102	1.89	0.55
46:n:601:CHL:HHC	46:n:601:CHL:HBB1	1.89	0.55
46:y:311:CHL:HHC	46:y:311:CHL:HBB1	1.89	0.55
4:C:437:ARG:NH2	9:I:27:ASP:OD2	2.40	0.55
29:a:408:CLA:H12	35:i:101:LMG:H112	1.88	0.55
29:a:408:CLA:H141	35:i:101:LMG:H292	1.89	0.55
4:c:320:GLN:HA	4:c:326:GLY:HA2	1.88	0.55
5:d:66:SER:HB3	5:d:69:GLU:HG3	1.88	0.55
6:e:23:HIS:NE2	44:e:101:HEM:ND	2.54	0.55
14:o:279:GLU:HB2	14:o:282:ALA:HB3	1.88	0.55
15:p:198:GLU:HG2	15:p:224:LYS:HE2	1.89	0.55
20:n:117:PHE:O	20:n:120:SER:OG	2.20	0.55
20:n:225:ILE:HG12	46:y:301:CHL:H41	1.88	0.55
2:b:192:PRO:HG2	8:h:68:TYR:CD1	2.41	0.55
5:d:172:SER:HB2	5:d:177:SER:HB2	1.89	0.55
23:s:130:ASP:HB3	23:s:158:VAL:HG21	1.89	0.55
4:C:461:ASP:OD1	16:T:24:ARG:NH2	2.40	0.55
15:p:71:ASN:ND2	15:p:89:SER:OG	2.39	0.55
15:p:128:ILE:HD13	15:p:208:THR:HA	1.88	0.55
23:S:194:PRO:HG2	29:S:316:CLA:HBB1	1.89	0.54
1:a:330:VAL:O	5:d:349:GLY:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:148:ALA:HB2	5:d:276:VAL:HG13	1.89	0.54
22:r:145:MET:SD	29:r:309:CLA:HAB	2.48	0.54
5:D:148:ALA:HB2	5:D:276:VAL:HG13	1.89	0.54
5:D:348:ARG:NH2	15:P:197:ASN:OD1	2.40	0.54
16:T:4:LEU:HD22	33:b:521:3PH:H3A1	1.88	0.54
22:R:176:LEU:O	24:y:142:ASN:ND2	2.39	0.54
46:n:608:CHL:H101	46:y:301:CHL:H143	1.87	0.54
2:B:62:VAL:HB	29:B:505:CLA:HED3	1.90	0.54
29:S:315:CLA:HBC1	37:S:320:LHG:H371	1.89	0.54
37:S:320:LHG:H121	37:S:320:LHG:H312	1.89	0.54
49:Y:301:XAT:H30	37:Y:319:LHG:H371	1.88	0.54
2:B:121:GLU:HG2	8:H:23:VAL:HG22	1.89	0.54
29:G:602:CLA:H92	29:G:603:CLA:HMA1	1.89	0.54
29:c:513:CLA:H72	31:z:101:BCR:H23C	1.87	0.54
17:w:76:VAL:HG13	17:w:81:LEU:HB2	1.89	0.54
33:B:522:3PH:H341	16:t:1:MET:HB2	1.90	0.54
22:R:190:ILE:HG21	46:R:304:CHL:HED2	1.89	0.54
2:B:25:MET:HG2	31:B:517:BCR:H23C	1.90	0.54
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.42	0.54
2:B:349:GLN:HG2	2:B:396:GLY:HA3	1.88	0.54
21:G:199:LYS:O	21:G:203:ASN:ND2	2.31	0.54
1:a:265:PHE:HB3	1:a:271:LEU:HB2	1.90	0.54
4:c:199:GLY:O	4:c:203:LYS:HG3	2.08	0.54
20:n:36:THR:OG1	20:n:37:ILE:N	2.39	0.54
21:g:199:LYS:O	21:g:203:ASN:ND2	2.28	0.54
25:U:102:LYS:NZ	52:U:202:HOH:O	2.40	0.54
2:b:392:ILE:HG23	2:b:397:VAL:HB	1.89	0.54
6:e:19:TYR:O	6:e:23:HIS:ND1	2.41	0.54
35:C:522:LMG:HC72	29:Y:312:CLA:HBA1	1.89	0.54
2:B:311:PHE:O	2:B:317:ASN:ND2	2.41	0.54
29:G:614:CLA:HAA1	24:Y:152:LEU:HD12	1.90	0.54
22:R:69:GLY:H	22:R:237:THR:HG22	1.73	0.54
1:a:308:ASP:OD1	1:a:312:ARG:N	2.41	0.54
4:C:173:VAL:HG23	4:C:218:LEU:HD13	1.90	0.53
39:L:102:SQD:H271	39:M:101:SQD:H132	1.89	0.53
37:c:521:LHG:HC91	31:z:101:BCR:H281	1.89	0.53
15:p:187:PHE:HB2	15:p:205:VAL:HB	1.90	0.53
24:y:210:LYS:NZ	37:y:320:LHG:O4	2.40	0.53
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.90	0.53
2:B:476:ARG:NH1	22:R:92:GLU:OE1	2.41	0.53
9:I:4:LEU:HD22	40:I:101:SPH:H62	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:194:LEU:HD22	48:R:312:NEX:H15	1.90	0.53
46:S:307:CHL:HHC	46:S:307:CHL:HBB1	1.90	0.53
20:n:166:GLY:HA3	24:y:53:LEU:HD13	1.90	0.53
29:n:609:CLA:H42	29:n:611:CLA:HBA1	1.90	0.53
37:B:523:LHG:O4	5:D:141:TYR:OH	2.24	0.53
23:S:224:ASP:HB3	23:S:227:VAL:HG22	1.90	0.53
24:Y:210:LYS:NZ	37:Y:319:LHG:O4	2.37	0.53
46:Y:310:CHL:HHC	46:Y:310:CHL:HBB1	1.90	0.53
4:c:309:ASP:OD2	4:c:328:TYR:OH	2.21	0.53
14:o:188:ASP:O	14:o:198:GLY:HA3	2.08	0.53
29:c:504:CLA:H112	29:c:508:CLA:H202	1.90	0.53
29:A:409:CLA:H101	9:I:16:VAL:HG11	1.89	0.53
2:B:192:PRO:HG3	8:H:68:TYR:HD1	1.72	0.53
29:G:603:CLA:HAC1	46:G:607:CHL:HBB2	1.89	0.53
29:Y:314:CLA:H143	37:Y:319:LHG:H361	1.90	0.53
15:p:147:ARG:HH12	15:p:149:ALA:HA	1.73	0.53
46:N:605:CHL:H51	29:S:312:CLA:H151	1.91	0.53
29:c:512:CLA:H143	39:c:522:SQD:H342	1.91	0.53
5:d:51:GLY:HA3	5:d:78:VAL:HG22	1.91	0.53
13:M:5:ILE:HG21	13:m:5:ILE:HG21	1.91	0.53
50:N:620:PTY:H182	50:N:620:PTY:H362	1.90	0.53
37:a:414:LHG:O3	37:a:414:LHG:O1	2.27	0.53
3:v:33:LEU:HA	29:c:511:CLA:H42	1.90	0.53
24:Y:50:LEU:HB2	24:Y:54:SER:HA	1.90	0.53
24:Y:123:ILE:HD11	24:Y:126:LYS:HD2	1.91	0.53
22:r:100:LYS:NZ	52:r:404:HOH:O	2.42	0.53
29:s:312:CLA:H161	29:s:313:CLA:HMC3	1.91	0.53
46:g:609:CHL:HHC	46:g:609:CHL:HBB1	1.90	0.53
2:B:347:LYS:O	2:B:397:VAL:HA	2.09	0.52
24:Y:174:ALA:HB3	24:Y:177:VAL:HB	1.91	0.52
2:b:433:ASP:OD2	2:b:436:THR:OG1	2.24	0.52
23:s:103:ASN:O	23:s:107:HIS:ND1	2.25	0.52
29:B:510:CLA:H11	29:B:512:CLA:H191	1.92	0.52
23:S:112:MET:SD	29:S:311:CLA:HAB	2.49	0.52
6:e:71:ASN:HB2	25:u:113:ILE:HG21	1.91	0.52
15:p:104:LEU:HD11	15:p:106:TYR:HE1	1.74	0.52
4:C:358:ARG:HG2	4:C:363:LEU:HD23	1.92	0.52
5:D:172:SER:HB2	5:D:177:SER:HB2	1.92	0.52
39:L:102:SQD:H252	31:b:517:BCR:H383	1.91	0.52
46:G:609:CHL:HHC	46:G:609:CHL:HBB1	1.91	0.52
46:Y:307:CHL:HBB2	46:Y:308:CHL:HAB	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:134:ARG:NH1	22:r:209:GLU:OE2	2.40	0.52
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.91	0.52
5:D:296:TYR:OH	5:D:326:ARG:NH1	2.41	0.52
20:N:148:GLN:O	50:N:620:PTY:N1	2.41	0.52
25:U:106:VAL:HG22	25:U:110:ARG:HE	1.75	0.52
14:o:110:GLU:OE2	17:w:60:LEU:N	2.42	0.52
1:A:283:ILE:HA	1:A:286:THR:HG22	1.92	0.52
2:B:115:TRP:HE1	39:l:101:SQD:H442	1.75	0.52
31:B:517:BCR:H24C	39:l:101:SQD:H261	1.92	0.52
31:C:517:BCR:H391	11:K:36:ALA:HB2	1.91	0.52
36:C:520:DGD:HA42	35:D:409:LMG:H141	1.92	0.52
4:c:348:ASP:OD2	36:c:516:DGD:O3D	2.23	0.52
29:c:511:CLA:H143	19:z:20:VAL:HG13	1.92	0.52
11:k:12:PRO:HB2	11:k:15:TYR:HD2	1.75	0.52
4:C:309:ASP:OD2	4:C:328:TYR:OH	2.20	0.52
4:C:334:THR:OG1	4:C:336:GLU:OE1	2.24	0.52
1:A:36:ILE:HG23	29:A:409:CLA:HBB1	1.92	0.52
1:A:193:LEU:HD21	29:A:405:CLA:HMC3	1.91	0.52
4:C:95:ASP:OD2	23:S:285:ARG:NH1	2.38	0.52
46:G:605:CHL:HHC	46:G:605:CHL:HBB1	1.91	0.52
22:R:145:MET:SD	29:R:308:CLA:HAB	2.50	0.52
1:a:89:ILE:HD11	1:a:108:ASN:HB3	1.92	0.52
1:a:183:MET:HA	29:a:404:CLA:HMD2	1.92	0.52
31:v:101:BCR:H10C	19:z:20:VAL:HG11	1.91	0.52
37:c:521:LHG:H311	37:s:320:LHG:H101	1.89	0.52
46:y:307:CHL:HHC	46:y:307:CHL:HBB1	1.92	0.52
1:A:310:ASN:O	15:P:89:SER:OG	2.28	0.52
31:A:410:BCR:H19C	39:b:523:SQD:H191	1.92	0.52
14:O:278:THR:HG22	14:O:285:ALA:HB2	1.92	0.52
1:a:43:THR:HG23	31:a:409:BCR:H362	1.91	0.52
2:B:142:HIS:ND1	29:B:510:CLA:OBD	2.36	0.52
22:R:263:GLY:O	22:R:267:SER:N	2.37	0.52
1:a:77:ILE:HD13	12:l:30:VAL:HG13	1.92	0.52
1:a:85:THR:HA	1:a:109:GLY:HA3	1.92	0.52
20:n:55:ASN:ND2	21:g:161:ALA:O	2.43	0.52
1:A:85:THR:HA	1:A:109:GLY:HA3	1.92	0.51
9:I:21:PHE:HA	9:I:24:LEU:HB2	1.92	0.51
15:P:105:ARG:NH2	15:P:115:ASN:HD22	2.06	0.51
1:a:63:ILE:HB	4:c:323:THR:HG21	1.92	0.51
2:b:243:ALA:HA	2:b:246:PHE:CE1	2.45	0.51
9:i:5:LYS:NZ	17:w:77:ASN:OD1	2.33	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:C:505:CLA:H62	36:C:520:DGD:HB71	1.92	0.51
39:L:102:SQD:O3	39:M:101:SQD:O8	2.25	0.51
14:O:208:SER:HB3	15:P:154:THR:HG21	1.92	0.51
15:P:204:LEU:HB2	15:P:219:VAL:HB	1.92	0.51
29:g:603:CLA:HMA2	29:g:603:CLA:H12	1.90	0.51
2:B:192:PRO:HG3	8:H:68:TYR:CD1	2.46	0.51
2:B:338:VAL:HG23	2:B:431:GLU:HG3	1.91	0.51
19:z:6:GLN:NE2	52:z:202:HOH:O	2.44	0.51
33:A:412:3PH:H2H1	33:A:412:3PH:H2C1	1.92	0.51
46:N:605:CHL:H151	29:S:311:CLA:H91	1.92	0.51
1:a:191:ASN:HB2	4:c:399:ALA:HB1	1.93	0.51
29:c:502:CLA:H61	29:c:512:CLA:H42	1.93	0.51
4:C:109:SER:HA	31:C:515:BCR:H16C	1.93	0.51
15:P:134:PRO:HB3	15:P:187:PHE:HE1	1.75	0.51
46:Y:306:CHL:HHC	46:Y:306:CHL:HBB1	1.92	0.51
36:c:517:DGD:HB72	35:c:519:LMG:H401	1.92	0.51
7:f:36:ILE:HA	7:f:39:MET:HG2	1.92	0.51
23:s:80:ALA:O	23:s:101:ARG:NH2	2.39	0.51
29:s:311:CLA:H71	47:s:317:LUT:H30	1.93	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.46	0.51
4:C:307:VAL:HA	4:C:310:GLN:HG2	1.93	0.51
22:R:142:ARG:NH1	29:R:306:CLA:OBD	2.40	0.51
20:N:166:GLY:HA3	24:Y:53:LEU:HD13	1.92	0.51
1:a:333:GLU:HB3	1:a:336:ALA:HB3	1.93	0.51
29:c:513:CLA:H91	37:c:521:LHG:H162	1.93	0.51
35:c:520:LMG:H122	29:y:313:CLA:H43	1.91	0.51
46:n:605:CHL:HHC	46:n:605:CHL:HBB1	1.93	0.51
1:A:47:VAL:HG21	1:A:114:LEU:HD22	1.93	0.51
43:D:406:PL9:H111	37:D:407:LHG:H102	1.92	0.51
2:b:57:ARG:NH2	2:b:334:ASP:OD1	2.40	0.51
9:i:5:LYS:HD2	17:w:65:MET:HE1	1.92	0.51
4:C:166:LYS:NZ	4:C:172:GLY:O	2.40	0.51
15:P:105:ARG:NH2	52:P:304:HOH:O	2.44	0.51
29:N:610:CLA:H43	29:N:612:CLA:HBA1	1.93	0.51
29:g:602:CLA:H52	47:g:616:LUT:H28	1.92	0.51
2:B:458:PHE:HB3	29:B:504:CLA:HBC2	1.92	0.50
1:a:10:ASN:ND2	17:w:102:ASP:O	2.44	0.50
19:z:25:VAL:O	19:z:29:SER:OG	2.26	0.50
22:r:75:PRO:HD2	49:r:312:XAT:H222	1.93	0.50
1:A:333:GLU:HB3	1:A:336:ALA:HB3	1.93	0.50
46:N:609:CHL:HHC	46:N:609:CHL:HBB1	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Y:307:CHL:HHC	46:Y:307:CHL:HBB1	1.94	0.50
39:a:410:SQD:H301	29:c:508:CLA:H71	1.93	0.50
2:b:370:LEU:HB2	2:b:379:ALA:HB3	1.93	0.50
1:A:163:ILE:HD11	36:C:518:DGD:HA31	1.92	0.50
10:j:7:ILE:HG23	10:j:9:ARG:HG2	1.93	0.50
29:r:303:CLA:H51	29:r:308:CLA:H43	1.92	0.50
2:B:22:VAL:HG11	29:B:514:CLA:HMA1	1.94	0.50
20:n:68:TYR:HB2	29:n:602:CLA:HMD1	1.93	0.50
21:g:87:ARG:HA	21:g:90:LEU:HD12	1.93	0.50
46:g:601:CHL:HHC	46:g:601:CHL:HBB1	1.94	0.50
29:y:306:CLA:H12	48:y:319:NEX:H241	1.93	0.50
1:A:77:ILE:HD13	12:L:30:VAL:HG13	1.94	0.50
46:N:606:CHL:HMB2	46:N:609:CHL:HMC	1.92	0.50
37:S:301:LHG:H251	29:S:312:CLA:HAB	1.93	0.50
5:d:235:PHE:HD1	5:d:243:THR:HG21	1.76	0.50
14:O:259:VAL:HG13	14:O:266:ILE:HG22	1.94	0.50
1:a:156:ALA:HA	1:a:160:ILE:HB	1.94	0.50
15:p:105:ARG:NH2	52:p:304:HOH:O	2.43	0.50
29:n:603:CLA:HMC3	46:y:301:CHL:H122	1.94	0.50
46:y:303:CHL:HHC	46:y:303:CHL:HBB1	1.92	0.50
2:B:343:HIS:O	2:B:401:PHE:HA	2.12	0.50
14:O:108:CYS:HA	14:O:141:ASP:HA	1.94	0.50
46:G:607:CHL:HMA2	46:G:607:CHL:H2	1.93	0.50
29:G:612:CLA:H2A	29:G:612:CLA:HED2	1.93	0.50
20:n:247:ALA:HB3	49:n:618:XAT:H193	1.94	0.50
46:g:605:CHL:HBB1	46:g:605:CHL:HHC	1.93	0.50
23:s:194:PRO:HB2	23:s:218:PRO:HB3	1.92	0.50
1:a:259:ILE:HG13	1:a:260:PHE:H	1.76	0.50
1:a:283:ILE:HA	1:a:286:THR:HG22	1.93	0.50
20:n:88:LEU:HD13	29:n:603:CLA:HBA1	1.92	0.50
1:A:269:ARG:HD2	5:D:235:PHE:HB2	1.94	0.49
29:C:514:CLA:H101	31:C:515:BCR:H21C	1.94	0.49
20:N:225:ILE:HG12	46:N:607:CHL:H41	1.94	0.49
21:G:227:GLN:NE2	21:G:231:ASP:OD1	2.43	0.49
15:P:205:VAL:HA	15:P:217:LEU:O	2.11	0.49
29:Y:313:CLA:H121	29:Y:313:CLA:HMB3	1.94	0.49
22:r:155:GLU:HG3	22:r:264:ALA:HB3	1.93	0.49
24:y:130:GLU:HA	24:y:133:LYS:HD3	1.94	0.49
29:s:304:CLA:H203	29:s:304:CLA:HMB1	1.93	0.49
2:B:57:ARG:NH2	2:B:334:ASP:OD1	2.41	0.49
2:B:291:SER:HA	2:B:294:GLU:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:74:LEU:HD13	4:C:77:LEU:HD12	1.94	0.49
25:U:91:VAL:HA	25:U:94:VAL:HG12	1.94	0.49
2:b:25:MET:HE1	2:b:108:PHE:HD1	1.77	0.49
29:r:304:CLA:HBA1	46:r:305:CHL:C1D	2.41	0.49
24:y:172:GLY:HA2	29:y:310:CLA:HAC1	1.94	0.49
37:B:523:LHG:H102	37:B:523:LHG:H352	1.94	0.49
5:D:51:GLY:HA3	5:D:78:VAL:HG22	1.94	0.49
20:N:87:GLU:HA	20:N:181:LEU:HD11	1.94	0.49
21:g:112:GLU:N	21:g:121:GLN:OE1	2.46	0.49
22:r:78:LEU:HD22	49:r:312:XAT:H23	1.93	0.49
29:S:304:CLA:HMB1	29:S:304:CLA:H203	1.93	0.49
24:Y:207:LYS:O	24:Y:211:ASN:ND2	2.46	0.49
2:b:121:GLU:OE2	8:h:21:GLY:N	2.45	0.49
2:b:125:ASP:OD2	2:b:128:THR:OG1	2.30	0.49
2:B:384:ARG:HH12	15:P:197:ASN:ND2	2.10	0.49
1:a:47:VAL:HG21	1:a:114:LEU:HD22	1.94	0.49
22:r:142:ARG:NH1	29:r:307:CLA:OBD	2.39	0.49
29:B:507:CLA:H41	29:B:507:CLA:H62	1.58	0.49
4:C:26:GLY:HA3	29:C:512:CLA:HMD2	1.94	0.49
1:a:65:GLU:HG3	14:o:210:PHE:HZ	1.78	0.49
13:m:3:VAL:HG22	13:m:4:ASN:H	1.78	0.49
24:y:102:LEU:HD13	29:y:314:CLA:HBB2	1.95	0.49
4:C:152:HIS:ND1	29:C:508:CLA:OBD	2.31	0.49
20:N:90:LEU:HD23	20:N:181:LEU:HD22	1.94	0.49
2:b:291:SER:HA	2:b:294:GLU:HB2	1.94	0.49
29:c:513:CLA:HMC2	31:z:101:BCR:H372	1.95	0.49
20:n:111:ASP:HB2	20:n:116:MET:HB2	1.93	0.49
21:g:68:LEU:HD21	29:y:305:CLA:H42	1.95	0.49
24:y:91:LEU:HD23	24:y:183:LEU:HG	1.95	0.49
2:B:384:ARG:HH12	15:P:197:ASN:HD22	1.61	0.49
5:D:185:PHE:CD2	29:D:404:CLA:HMD3	2.47	0.49
46:Y:308:CHL:H143	46:Y:310:CHL:H101	1.94	0.49
29:b:506:CLA:HMD2	36:r:301:DGD:HG11	1.95	0.49
3:v:15:VAL:O	31:v:101:BCR:H14C	2.13	0.49
23:s:83:TYR:HB2	29:s:303:CLA:HMD1	1.95	0.49
2:B:357:ARG:NH1	2:B:358:ARG:O	2.46	0.48
20:N:83:LYS:NZ	20:N:87:GLU:OE2	2.45	0.48
23:S:234:LYS:HD3	29:S:313:CLA:HAA2	1.94	0.48
29:c:508:CLA:HAC2	29:c:510:CLA:H71	1.94	0.48
5:d:266:TRP:HH2	37:l:102:LHG:H112	1.76	0.48
21:G:65:THR:HG21	46:Y:310:CHL:HAA2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:95:ARG:HA	24:Y:98:LEU:HD12	1.95	0.48
1:a:84:PRO:HA	1:a:112:TYR:CG	2.48	0.48
26:A:401:OEX:O2	4:C:345:ARG:NH2	2.46	0.48
46:G:601:CHL:HHC	46:G:601:CHL:HBB1	1.94	0.48
29:G:603:CLA:H12	29:G:603:CLA:HMA2	1.96	0.48
38:b:524:LMT:H101	29:r:308:CLA:H101	1.95	0.48
4:c:172:GLY:HA3	4:c:185:ARG:O	2.13	0.48
14:o:144:ASN:O	14:o:160:ASP:N	2.41	0.48
20:n:60:LEU:HD11	20:n:71:ASP:HB2	1.96	0.48
14:O:116:VAL:HB	14:O:172:LEU:HD21	1.95	0.48
1:a:133:LEU:HD23	5:d:256:ILE:HG12	1.95	0.48
14:o:147:MET:HE2	14:o:149:ILE:HD11	1.96	0.48
23:s:194:PRO:HG2	29:s:316:CLA:HBB1	1.95	0.48
5:d:296:TYR:OH	5:d:326:ARG:NH1	2.38	0.48
23:s:186:GLY:HA2	46:s:309:CHL:HAC1	1.96	0.48
29:A:406:CLA:HBB1	30:A:408:PHO:H141	1.95	0.48
37:D:407:LHG:H121	37:D:407:LHG:H281	1.95	0.48
51:S:321:LPX:H9	33:S:322:3PH:H272	1.94	0.48
37:Y:319:LHG:H331	37:Y:319:LHG:H112	1.96	0.48
2:b:192:PRO:HG2	8:h:68:TYR:HD1	1.79	0.48
2:b:357:ARG:NH2	5:d:337:GLU:OE1	2.46	0.48
2:B:473:THR:O	22:R:101:LYS:NZ	2.46	0.48
4:C:397:GLY:HA3	4:C:401:GLU:HG3	1.95	0.48
14:O:228:LEU:HD13	14:O:231:LYS:HG2	1.94	0.48
29:G:604:CLA:H12	48:G:617:NEX:H241	1.95	0.48
33:S:322:3PH:H361	33:S:322:3PH:H231	1.96	0.48
4:c:162:LEU:HD22	29:c:502:CLA:H202	1.95	0.48
46:g:606:CHL:HHC	46:g:606:CHL:HBB1	1.96	0.48
1:A:156:ALA:HA	1:A:160:ILE:HB	1.95	0.48
1:A:165:GLN:NE2	1:A:294:ALA:O	2.46	0.48
3:V:25:LEU:O	3:V:29:ARG:HB2	2.13	0.48
4:C:454:VAL:HA	4:C:457:MET:HG3	1.94	0.48
5:D:314:PHE:HA	5:D:317:LYS:HD2	1.95	0.48
14:O:224:ASN:HA	14:O:240:LEU:HB2	1.95	0.48
20:N:238:HIS:CG	29:N:613:CLA:HAA2	2.49	0.48
1:a:309:SER:HA	7:f:44:ARG:HG3	1.96	0.48
41:w:201:DGA:HBT2	35:w:202:LMG:H371	1.95	0.48
29:r:307:CLA:H41	29:r:307:CLA:H61	1.59	0.48
29:y:314:CLA:HMB3	29:y:314:CLA:H121	1.96	0.48
2:B:385:LYS:O	52:B:601:HOH:O	2.20	0.48
4:C:257:GLU:OE2	4:C:432:HIS:ND1	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:C:514:CLA:H72	31:C:515:BCR:H23C	1.95	0.48
5:D:79:SER:HA	5:D:172:SER:HB3	1.94	0.48
1:a:303:ASN:HB2	4:c:402:ILE:HA	1.96	0.48
1:a:310:ASN:O	15:p:89:SER:OG	2.32	0.48
29:c:508:CLA:HMB2	29:c:510:CLA:HBA1	1.95	0.48
46:s:308:CHL:HHC	46:s:308:CHL:HBB1	1.96	0.48
36:B:521:DGD:HD61	22:R:170:LEU:HD11	1.96	0.48
4:C:172:GLY:HA3	4:C:185:ARG:O	2.14	0.48
29:c:501:CLA:H193	29:c:506:CLA:HMB2	1.95	0.48
14:o:273:ILE:HG12	14:o:289:LYS:HG3	1.95	0.48
2:B:157:HIS:HA	2:B:163:GLY:HA3	1.96	0.47
29:G:613:CLA:H152	49:G:619:XAT:H34	1.95	0.47
37:S:301:LHG:HC92	29:S:312:CLA:HMB1	1.96	0.47
37:S:320:LHG:H121	37:S:320:LHG:HC92	1.66	0.47
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.96	0.47
4:c:105:LEU:HD21	37:s:301:LHG:H121	1.96	0.47
4:C:368:LEU:HD12	4:C:372:ILE:HD11	1.96	0.47
45:H:101:RRX:H26	45:H:101:RRX:H22	1.71	0.47
1:a:57:PRO:HB2	1:a:66:PRO:HB2	1.96	0.47
4:c:285:TYR:O	4:c:411:ARG:NH2	2.40	0.47
14:o:216:ARG:NH2	52:o:415:HOH:O	2.47	0.47
49:g:619:XAT:H15	49:g:619:XAT:H201	1.69	0.47
13:M:3:VAL:HG22	13:M:4:ASN:H	1.79	0.47
23:S:212:PRO:HB3	46:S:309:CHL:HBC2	1.96	0.47
2:b:343:HIS:O	2:b:401:PHE:HA	2.15	0.47
41:b:522:DGA:HAV1	18:x:83:LEU:HD21	1.95	0.47
23:s:188:GLY:O	23:s:201:SER:OG	2.30	0.47
29:B:509:CLA:O2A	45:H:101:RRX:O2	2.31	0.47
24:Y:91:LEU:HD23	24:Y:183:LEU:HG	1.96	0.47
2:B:41:GLU:O	2:B:45:PHE:HB2	2.14	0.47
2:B:144:PHE:HZ	38:B:524:LMT:H3'	1.80	0.47
4:C:306:LEU:HD12	4:C:328:TYR:HB3	1.95	0.47
11:K:12:PRO:HB2	11:K:15:TYR:HD2	1.80	0.47
21:G:142:ILE:HA	21:G:145:THR:HG22	1.97	0.47
22:R:228:ASP:OD2	22:R:231:LYS:N	2.41	0.47
1:a:334:ARG:HB2	14:o:211:LEU:HD12	1.96	0.47
37:a:414:LHG:H291	37:a:414:LHG:H322	1.72	0.47
22:r:190:ILE:HG21	46:r:305:CHL:HED2	1.95	0.47
24:y:50:LEU:HB2	24:y:54:SER:HA	1.95	0.47
29:y:315:CLA:H61	29:y:315:CLA:H2	1.64	0.47
2:B:156:PHE:HB3	2:B:162:PHE:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:C:514:CLA:H91	29:C:514:CLA:H112	1.74	0.47
40:I:101:SPH:H131	39:b:523:SQD:H202	1.96	0.47
29:Y:314:CLA:H121	37:Y:319:LHG:H332	1.97	0.47
18:x:64:SER:OG	18:x:65:VAL:N	2.45	0.47
49:n:618:XAT:H15	49:n:618:XAT:H201	1.67	0.47
23:s:112:MET:SD	29:s:311:CLA:HAB	2.54	0.47
24:y:241:LEU:HD21	29:y:316:CLA:HMC3	1.97	0.47
2:B:329:ALA:O	2:B:332:SER:OG	2.30	0.47
2:B:394:GLN:HG2	15:P:147:ARG:HH11	1.79	0.47
5:D:122:LEU:HD21	29:D:404:CLA:H92	1.96	0.47
15:P:116:VAL:HG23	15:P:219:VAL:HG22	1.96	0.47
29:N:604:CLA:H121	48:N:617:NEX:H402	1.96	0.47
29:N:610:CLA:HBA2	29:N:610:CLA:H3A	1.61	0.47
47:G:616:LUT:H363	29:Y:304:CLA:HED3	1.97	0.47
22:R:63:LEU:HD13	22:R:72:GLY:HA2	1.96	0.47
22:R:219:ASP:OD1	47:R:310:LUT:O23	2.25	0.47
23:S:215:PRO:HB2	29:S:316:CLA:HBC2	1.96	0.47
23:S:264:ILE:HB	47:S:317:LUT:H22	1.94	0.47
29:Y:305:CLA:H12	48:Y:318:NEX:H241	1.96	0.47
29:Y:314:CLA:H102	37:Y:319:LHG:H132	1.97	0.47
1:a:184:ILE:HG23	1:a:328:MET:HE3	1.97	0.47
29:n:612:CLA:H2	29:n:612:CLA:H61	1.68	0.47
37:s:320:LHG:H321	37:s:320:LHG:H292	1.67	0.47
1:A:11:THR:O	1:A:16:ARG:NH2	2.48	0.47
2:B:12:VAL:HG23	29:B:512:CLA:HMC2	1.97	0.47
20:N:247:ALA:HB3	49:N:619:XAT:H193	1.97	0.47
29:N:602:CLA:H151	29:N:602:CLA:H18	1.68	0.47
29:R:306:CLA:H3A	29:R:306:CLA:HBA2	1.50	0.47
33:s:322:3PH:H221	33:s:322:3PH:H372	1.97	0.47
2:B:456:LEU:HD21	35:D:410:LMG:H201	1.97	0.47
29:C:511:CLA:H112	29:C:511:CLA:H152	1.68	0.47
46:N:605:CHL:H143	47:S:317:LUT:H403	1.97	0.47
22:R:153:VAL:HG21	29:R:303:CLA:HAC2	1.97	0.47
2:b:318:ASN:HB3	2:b:321:LYS:HG2	1.97	0.47
35:c:520:LMG:H371	40:c:523:SPH:H182	1.96	0.47
9:i:1:MET:HE2	40:i:102:SPH:H11	1.96	0.47
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.96	0.47
1:A:246:TYR:HE2	42:D:403:BCT:O3	1.97	0.47
36:C:519:DGD:HB22	35:C:521:LMG:H322	1.95	0.47
1:a:199:MET:HE1	5:d:74:LEU:HD13	1.97	0.47
2:b:479:PHE:O	5:d:139:ARG:NH2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:162:LEU:HD21	29:s:315:CLA:H51	1.96	0.47
1:A:133:LEU:HD23	5:D:256:ILE:HG12	1.96	0.46
46:G:606:CHL:HBB2	46:G:607:CHL:HAB	1.96	0.46
49:Y:301:XAT:C34	29:Y:314:CLA:H111	2.45	0.46
3:v:33:LEU:OXT	11:k:39:TRP:NE1	2.30	0.46
4:c:40:ALA:HB1	29:c:509:CLA:HBB1	1.97	0.46
5:d:186:GLN:NE2	5:d:322:ASN:OD1	2.41	0.46
21:g:65:THR:HG21	46:y:311:CHL:HAA2	1.97	0.46
46:s:302:CHL:HHC	46:s:302:CHL:HBB1	1.97	0.46
29:s:304:CLA:HBA1	29:s:304:CLA:H3A	1.35	0.46
29:n:609:CLA:H2	47:n:614:LUT:H373	1.96	0.46
1:A:116:VAL:HG13	1:A:158:PHE:HB3	1.98	0.46
1:A:290:ILE:HG13	29:A:405:CLA:HED3	1.96	0.46
2:B:149:LEU:HD13	29:B:504:CLA:H172	1.97	0.46
5:D:122:LEU:HB3	5:D:150:ILE:HG12	1.98	0.46
7:F:44:ARG:OXT	15:P:64:ASN:ND2	2.47	0.46
24:Y:171:ASN:ND2	24:Y:173:GLU:OE2	2.48	0.46
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.51	0.46
29:b:507:CLA:H203	12:l:36:ILE:HG13	1.96	0.46
9:i:21:PHE:HA	9:i:24:LEU:HB2	1.97	0.46
17:w:90:GLY:HA3	41:w:201:DGA:HBH2	1.97	0.46
29:n:603:CLA:H102	29:y:304:CLA:H91	1.97	0.46
29:n:610:CLA:C4C	37:n:617:LHG:HC62	2.46	0.46
29:r:309:CLA:H92	47:r:311:LUT:H371	1.96	0.46
23:s:102:ALA:HA	23:s:210:LEU:HD11	1.97	0.46
24:y:105:ILE:HD12	24:y:234:ILE:HD11	1.97	0.46
5:D:53:THR:HG22	7:F:39:MET:HE1	1.98	0.46
5:D:350:ASN:O	5:D:352:LEU:N	2.48	0.46
4:c:301:GLN:HB2	4:c:384:MET:HG3	1.98	0.46
4:c:338:ILE:HG21	4:c:347:TRP:HB2	1.96	0.46
36:c:517:DGD:HA62	41:j:101:DGA:HA92	1.98	0.46
14:o:115:THR:HB	14:o:127:PHE:HB3	1.97	0.46
29:s:306:CLA:H42	46:s:309:CHL:H142	1.98	0.46
29:C:505:CLA:H41	29:C:505:CLA:H61	1.70	0.46
36:C:520:DGD:HA32	5:D:74:LEU:HG	1.97	0.46
37:D:408:LHG:O3	37:D:408:LHG:O1	2.33	0.46
46:G:608:CHL:HHC	46:G:608:CHL:HBB1	1.97	0.46
1:a:94:TYR:OH	1:a:104:GLU:OE2	2.33	0.46
36:c:517:DGD:HG31	41:j:101:DGA:HA21	1.98	0.46
4:C:319:ALA:O	14:O:165:TYR:OH	2.34	0.46
20:N:120:SER:HB3	20:N:129:ALA:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:83:LEU:HD23	21:G:175:LEU:HB3	1.97	0.46
29:b:507:CLA:H193	12:l:29:ALA:HA	1.98	0.46
20:n:105:THR:HG21	29:n:604:CLA:HAC2	1.98	0.46
29:A:409:CLA:H11	9:I:9:TYR:CZ	2.51	0.46
31:C:517:BCR:H351	31:C:517:BCR:H15C	1.81	0.46
40:I:101:SPH:H72	39:b:523:SQD:H141	1.98	0.46
2:b:311:PHE:O	2:b:317:ASN:ND2	2.48	0.46
4:c:330:MET:HG2	4:c:340:GLY:HA2	1.97	0.46
14:o:93:ASN:O	14:o:95:ARG:N	2.44	0.46
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.50	0.46
29:A:406:CLA:H3A	29:A:406:CLA:HBA2	1.64	0.46
4:C:150:GLY:HA2	4:C:236:GLY:HA2	1.96	0.46
2:b:12:VAL:HG23	29:b:512:CLA:HMC2	1.97	0.46
5:d:155:SER:HA	5:d:159:ILE:HB	1.98	0.46
37:g:618:LHG:H301	37:g:618:LHG:H112	1.98	0.46
2:b:41:GLU:O	2:b:45:PHE:HB2	2.16	0.46
4:c:173:VAL:HG23	4:c:218:LEU:HD13	1.98	0.46
20:n:84:ARG:HH21	24:y:58:PRO:HB3	1.81	0.46
33:s:322:3PH:H321	33:s:322:3PH:H351	1.60	0.46
1:A:334:ARG:NH2	5:D:312:GLU:OE1	2.38	0.46
29:B:505:CLA:H92	29:B:505:CLA:H61	1.79	0.46
5:D:182:ILE:CG2	29:D:404:CLA:HAC1	2.46	0.46
46:N:607:CHL:HHC	46:N:607:CHL:HBB1	1.97	0.46
46:S:307:CHL:HBB1	47:S:318:LUT:H161	1.97	0.46
2:b:330:MET:HA	2:b:444:ARG:HB2	1.98	0.46
29:d:404:CLA:H92	29:d:404:CLA:H62	1.82	0.46
14:o:102:TYR:CD2	14:o:298:LEU:HB3	2.51	0.46
48:s:319:NEX:H161	48:s:319:NEX:H193	1.97	0.46
49:y:302:XAT:H391	49:y:302:XAT:H31	1.67	0.46
1:A:131:TRP:CH2	29:C:506:CLA:HAA2	2.50	0.45
1:A:143:ILE:HD11	5:D:217:THR:HA	1.98	0.45
20:N:98:LEU:HB3	29:N:604:CLA:HAB	1.98	0.45
24:Y:105:ILE:HD12	24:Y:234:ILE:HD11	1.98	0.45
1:a:24:THR:O	5:d:251:ARG:NH2	2.45	0.45
29:c:504:CLA:H41	29:c:504:CLA:H62	1.75	0.45
29:c:505:CLA:HAC1	31:c:514:BCR:H341	1.97	0.45
5:d:342:PRO:O	5:d:345:VAL:HG12	2.16	0.45
14:o:108:CYS:HA	14:o:141:ASP:HA	1.97	0.45
48:S:319:NEX:H15	48:S:319:NEX:H201	1.80	0.45
26:a:401:OEX:O2	4:c:345:ARG:NH2	2.49	0.45
35:c:520:LMG:H171	29:y:314:CLA:HBC1	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:HB2	5:D:220:ASN:HA	1.98	0.45
29:C:508:CLA:H41	29:C:508:CLA:H62	1.69	0.45
29:C:514:CLA:H101	31:C:515:BCR:H23C	1.99	0.45
29:a:405:CLA:HBB1	30:a:407:PHO:H141	1.97	0.45
33:a:415:3PH:H2C1	33:a:415:3PH:H2H1	1.99	0.45
5:d:262:SER:OG	37:d:406:LHG:O4	2.27	0.45
41:w:201:DGA:HAW2	35:w:202:LMG:H381	1.98	0.45
46:n:606:CHL:HBB2	46:y:301:CHL:HAB	1.97	0.45
29:A:406:CLA:H62	29:A:406:CLA:H92	1.79	0.45
7:F:32:PHE:HB3	31:F:101:BCR:H363	1.98	0.45
46:N:601:CHL:H41	46:N:601:CHL:H61	1.74	0.45
29:G:610:CLA:H43	29:G:612:CLA:HBA1	1.98	0.45
46:Y:302:CHL:HMA2	46:Y:302:CHL:H2	1.99	0.45
37:a:413:LHG:H382	29:b:513:CLA:H43	1.98	0.45
2:b:384:ARG:HH12	15:p:197:ASN:HD22	1.64	0.45
37:g:618:LHG:H172	37:g:618:LHG:H201	1.76	0.45
33:s:322:3PH:H342	33:s:322:3PH:H371	1.64	0.45
1:A:308:ASP:OD1	1:A:312:ARG:N	2.49	0.45
5:D:338:LYS:HB2	25:U:103:GLU:HG2	1.98	0.45
15:P:68:ARG:HD3	15:P:68:ARG:HA	1.79	0.45
15:P:231:ASP:OD1	15:P:231:ASP:N	2.49	0.45
19:Z:31:ASN:ND2	52:Z:102:HOH:O	2.47	0.45
2:b:22:VAL:HG11	29:b:514:CLA:HMA1	1.98	0.45
2:b:256:MET:HA	2:b:263:THR:HG21	1.99	0.45
5:d:29:PHE:O	5:d:128:ARG:NH1	2.43	0.45
14:o:197:SER:HB3	14:o:253:VAL:HG22	1.98	0.45
23:s:150:ASN:HB3	23:s:158:VAL:HG13	1.99	0.45
1:A:307:VAL:HG12	1:A:313:VAL:HA	1.99	0.45
29:A:407:CLA:H3A	29:A:407:CLA:HBA2	1.71	0.45
29:B:507:CLA:H93	29:B:507:CLA:H61	1.76	0.45
18:X:64:SER:N	52:X:101:HOH:O	2.49	0.45
22:R:176:LEU:HD22	24:y:145:LEU:HD21	1.98	0.45
2:b:157:HIS:HA	2:b:163:GLY:HA3	1.99	0.45
2:b:226:TYR:CD1	2:b:231:MET:HB2	2.51	0.45
2:b:315:ILE:HG12	2:b:321:LYS:HG3	1.98	0.45
2:b:373:LYS:HD2	25:u:96:ASP:HB3	1.98	0.45
4:c:16:GLN:OE1	5:d:230:ASN:ND2	2.38	0.45
4:c:334:THR:HG21	14:o:77:GLY:HA2	1.99	0.45
46:n:606:CHL:H141	46:n:606:CHL:H161	1.71	0.45
2:B:433:ASP:OD2	2:B:436:THR:OG1	2.23	0.45
14:O:282:ALA:O	14:O:283:HIS:ND1	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:S:304:CLA:H3A	29:S:304:CLA:HBA1	1.57	0.45
2:b:282:GLN:HG3	25:u:107:LYS:NZ	2.32	0.45
29:b:514:CLA:H52	31:b:517:BCR:H372	1.98	0.45
33:b:521:3PH:H2D2	33:b:521:3PH:H2A2	1.75	0.45
37:c:521:LHG:H192	37:c:521:LHG:H161	1.72	0.45
29:n:610:CLA:HBA2	29:n:610:CLA:H3A	1.70	0.45
22:r:224:ALA:HB2	22:r:235:LEU:HD12	1.98	0.45
1:A:183:MET:HA	29:A:405:CLA:HMD2	1.98	0.45
5:D:127:LEU:HD13	41:D:402:DGA:HA81	1.97	0.45
14:O:130:THR:HG22	14:O:172:LEU:HD23	1.99	0.45
46:N:605:CHL:H141	46:N:605:CHL:H161	1.73	0.45
23:S:169:THR:HB	46:S:308:CHL:HBC1	1.98	0.45
2:b:327:THR:HG22	29:b:507:CLA:H12	1.98	0.45
29:y:304:CLA:H13	29:y:304:CLA:H102	1.78	0.45
29:B:509:CLA:H61	29:B:509:CLA:H41	1.74	0.45
29:S:311:CLA:H91	29:S:311:CLA:H111	1.79	0.45
1:a:131:TRP:CH2	29:c:505:CLA:HAA2	2.52	0.45
46:n:606:CHL:HHC	46:n:606:CHL:HBB1	1.98	0.45
1:A:199:MET:HE1	5:D:74:LEU:HD13	1.99	0.45
43:D:406:PL9:H401	37:D:407:LHG:H211	1.99	0.45
15:P:142:GLY:O	15:P:145:LEU:HB2	2.17	0.45
15:p:138:ILE:HD11	15:p:187:PHE:CG	2.52	0.45
29:A:405:CLA:HBB1	29:A:405:CLA:HMB1	1.99	0.44
4:C:69:MET:HB2	4:C:74:LEU:HD12	1.99	0.44
4:C:461:ASP:OD2	5:D:251:ARG:HA	2.16	0.44
10:J:10:ILE:HD11	10:J:14:LEU:HD23	1.99	0.44
16:T:28:ARG:HA	16:T:28:ARG:HD3	1.65	0.44
21:G:217:GLN:O	21:G:221:THR:OG1	2.28	0.44
29:a:404:CLA:H42	29:a:405:CLA:HMC2	1.99	0.44
2:b:25:MET:HG2	31:b:517:BCR:H23C	1.98	0.44
29:b:509:CLA:H141	29:b:509:CLA:H161	1.71	0.44
29:b:515:CLA:H3A	29:b:515:CLA:HBA1	1.77	0.44
41:w:201:DGA:HBN2	41:w:201:DGA:HBG2	1.75	0.44
21:g:122:ILE:HA	21:g:127:GLY:HA2	1.98	0.44
29:s:312:CLA:H62	29:s:312:CLA:H41	1.86	0.44
25:u:91:VAL:HA	25:u:94:VAL:HG12	1.99	0.44
46:N:605:CHL:HHC	46:N:605:CHL:HBB1	1.99	0.44
46:N:606:CHL:HHC	46:N:606:CHL:HBB1	1.98	0.44
47:N:616:LUT:H363	29:G:603:CLA:HED3	1.98	0.44
21:G:128:LEU:HD21	29:G:604:CLA:HAA1	1.98	0.44
29:b:509:CLA:O2A	45:h:101:RRX:O2	2.35	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:150:GLY:HA2	4:c:236:GLY:HA2	1.99	0.44
46:s:307:CHL:HBB2	46:s:308:CHL:CBB	2.46	0.44
29:y:305:CLA:HAC1	46:y:309:CHL:CBB	2.48	0.44
1:A:214:MET:O	1:A:218:LEU:HG	2.18	0.44
2:B:39:LEU:HD23	2:B:39:LEU:HA	1.84	0.44
23:S:186:GLY:HA2	46:S:309:CHL:HAC1	1.99	0.44
1:a:344:ALA:O	52:a:501:HOH:O	2.21	0.44
29:b:502:CLA:H112	29:b:502:CLA:H151	1.82	0.44
4:c:47:LEU:HD21	11:k:32:PHE:CD2	2.52	0.44
29:s:305:CLA:HMD2	29:s:306:CLA:HMD1	1.99	0.44
2:B:115:TRP:HE1	39:l:101:SQD:C44	2.30	0.44
2:B:383:PHE:N	5:D:344:GLU:O	2.49	0.44
19:Z:1:MET:HE2	19:Z:60:PHE:HB2	1.98	0.44
37:N:618:LHG:H223	49:N:619:XAT:H10	1.99	0.44
21:G:63:TRP:CE3	47:G:616:LUT:H383	2.53	0.44
47:G:616:LUT:H35	47:G:616:LUT:H401	1.83	0.44
2:b:9:HIS:ND1	29:b:513:CLA:O1A	2.35	0.44
2:b:242:ILE:HA	2:b:245:VAL:HG22	1.98	0.44
29:b:501:CLA:H8	29:b:501:CLA:H51	1.79	0.44
1:A:309:SER:HA	7:F:44:ARG:HD3	2.00	0.44
29:B:509:CLA:H61	29:B:509:CLA:H93	1.80	0.44
29:B:514:CLA:H52	31:B:517:BCR:H372	1.99	0.44
3:V:15:VAL:O	31:K:101:BCR:H14C	2.17	0.44
14:O:276:SER:HB3	14:O:288:ILE:HD11	2.00	0.44
29:Y:312:CLA:H111	29:Y:312:CLA:H72	1.83	0.44
1:a:93:PHE:HB2	4:c:206:PHE:CG	2.53	0.44
2:b:30:VAL:HG12	29:b:505:CLA:HHD	2.00	0.44
4:c:26:GLY:O	4:c:29:ARG:HB2	2.17	0.44
4:c:272:PHE:HB3	36:c:516:DGD:HB61	2.00	0.44
21:g:232:HIS:CG	29:g:613:CLA:HAA2	2.53	0.44
47:y:317:LUT:H15	47:y:317:LUT:H201	1.84	0.44
2:B:30:VAL:HG12	29:B:505:CLA:HHD	2.00	0.44
29:B:514:CLA:H101	31:B:517:BCR:H362	1.99	0.44
5:D:56:THR:HG21	6:E:50:PRO:HD3	1.99	0.44
6:E:8:ARG:HE	6:E:13:ILE:HG12	1.82	0.44
31:F:101:BCR:H381	10:J:23:ALA:HB1	1.99	0.44
47:Y:317:LUT:H35	47:Y:317:LUT:H401	1.83	0.44
2:b:282:GLN:HG3	25:u:107:LYS:HZ3	1.83	0.44
35:c:520:LMG:H411	40:c:523:SPH:H101	2.00	0.44
14:o:95:ARG:HH12	14:o:194:ASP:HB3	1.82	0.44
50:n:619:PTY:H201	50:n:619:PTY:H372	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:238:ALA:O	22:r:242:HIS:ND1	2.45	0.44
4:C:213:VAL:HG13	4:C:277:PHE:HA	2.00	0.44
4:C:320:GLN:H	15:P:158:GLY:HA3	1.83	0.44
29:C:508:CLA:H91	29:C:508:CLA:H112	1.76	0.44
39:L:102:SQD:H261	31:b:517:BCR:H24C	1.99	0.44
23:S:103:ASN:O	23:S:107:HIS:ND1	2.41	0.44
2:b:44:VAL:HG12	33:b:521:3PH:H351	1.99	0.44
46:n:605:CHL:H141	46:n:605:CHL:H161	1.78	0.44
21:g:128:LEU:HD21	46:g:606:CHL:HAC1	2.00	0.44
29:y:304:CLA:H142	47:y:318:LUT:H361	1.99	0.44
29:C:505:CLA:H61	29:C:505:CLA:H93	1.79	0.44
29:C:514:CLA:HMC2	31:C:515:BCR:H372	2.00	0.44
5:D:266:TRP:HH2	37:L:101:LHG:H111	1.81	0.44
29:D:405:CLA:H102	18:X:80:ALA:HB2	2.00	0.44
48:N:617:NEX:H35	48:N:617:NEX:H401	1.84	0.44
50:N:620:PTY:H212	50:N:620:PTY:H401	1.99	0.44
49:G:619:XAT:H31	49:G:619:XAT:H391	1.67	0.44
47:Y:317:LUT:H15	47:Y:317:LUT:H201	1.82	0.44
1:a:290:ILE:HG13	29:a:404:CLA:HED3	2.00	0.44
2:b:158:VAL:HG23	2:b:199:PRO:HB3	2.00	0.44
4:c:44:HIS:HB2	29:c:509:CLA:HMB2	1.99	0.44
35:c:520:LMG:H292	41:w:201:DGA:HA51	2.00	0.44
44:e:101:HEM:HMC2	7:f:30:ILE:HG13	1.99	0.44
13:m:23:LEU:HD11	39:m:101:SQD:H162	2.00	0.44
20:n:256:PRO:HB2	21:g:222:GLY:HA2	1.99	0.44
37:s:320:LHG:H272	37:s:320:LHG:H242	1.76	0.44
29:B:504:CLA:H41	29:B:504:CLA:H61	1.68	0.44
33:B:522:3PH:H3I1	16:t:8:PHE:HB2	1.99	0.44
15:P:141:PHE:HB3	15:P:144:LEU:HD13	1.98	0.44
29:N:603:CLA:H91	46:N:609:CHL:H142	1.98	0.44
50:N:620:PTY:H351	50:N:620:PTY:H322	1.75	0.44
29:G:604:CLA:C1C	48:G:617:NEX:H222	2.48	0.44
23:S:227:VAL:HA	23:S:230:GLU:HG3	2.00	0.44
29:S:305:CLA:C1C	48:S:319:NEX:H222	2.48	0.44
29:a:404:CLA:H111	29:a:404:CLA:H72	1.75	0.44
2:b:229:LEU:HD21	29:b:509:CLA:H43	2.00	0.44
29:b:510:CLA:H102	29:b:515:CLA:HAA1	1.99	0.44
39:b:523:SQD:H162	39:b:523:SQD:H131	1.84	0.44
29:g:611:CLA:H142	29:g:611:CLA:H112	1.80	0.44
4:C:338:ILE:HG21	4:C:347:TRP:HB2	1.99	0.43
6:E:41:GLY:HA2	6:E:44:TYR:HD2	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:S:312:CLA:H3A	29:S:312:CLA:HBA2	1.50	0.43
29:b:515:CLA:H172	8:h:26:LEU:HD21	2.01	0.43
14:o:224:ASN:HA	14:o:240:LEU:HB2	2.00	0.43
21:g:237:THR:O	21:g:240:ASN:ND2	2.51	0.43
23:s:87:PRO:HD2	47:s:318:LUT:H23	1.99	0.43
1:A:328:MET:HE1	5:D:183:LEU:HD22	2.01	0.43
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.53	0.43
15:P:134:PRO:HB3	15:P:187:PHE:CE1	2.52	0.43
15:P:150:TRP:NE1	15:P:152:GLY:O	2.51	0.43
24:Y:46:ARG:NH2	24:Y:61:LEU:O	2.51	0.43
1:a:230:ASN:ND2	22:r:95:ASN:OD1	2.50	0.43
33:a:415:3PH:H3B1	33:a:415:3PH:H2F1	1.99	0.43
5:d:161:PRO:HB3	5:d:170:ALA:HB2	2.00	0.43
14:o:111:PRO:HD2	14:o:138:TYR:HD1	1.83	0.43
14:o:216:ARG:HH11	14:o:240:LEU:HB3	1.82	0.43
21:g:37:ARG:NH2	21:g:53:LEU:O	2.51	0.43
29:g:614:CLA:H12	29:g:614:CLA:HBA1	1.74	0.43
29:r:303:CLA:H92	29:r:303:CLA:H62	1.88	0.43
5:D:342:PRO:O	5:D:345:VAL:HG22	2.18	0.43
20:N:153:THR:HB	46:N:605:CHL:HAC1	2.00	0.43
49:N:619:XAT:H11	49:N:619:XAT:H191	1.83	0.43
24:Y:240:HIS:CG	29:Y:314:CLA:HAA2	2.54	0.43
29:Y:311:CLA:H52	47:Y:316:LUT:H30	1.99	0.43
48:Y:318:NEX:H15	48:Y:318:NEX:H201	1.82	0.43
2:b:329:ALA:O	2:b:332:SER:OG	2.29	0.43
5:d:85:LEU:HD13	5:d:90:LEU:HD21	2.00	0.43
5:d:191:TRP:CE3	5:d:289:LEU:HD11	2.52	0.43
29:n:609:CLA:H51	29:n:609:CLA:H8	1.76	0.43
1:A:274:PHE:HD1	39:C:501:SQD:H112	1.83	0.43
4:C:44:HIS:HB2	29:C:510:CLA:HMB1	2.01	0.43
36:C:518:DGD:HB61	36:C:518:DGD:HB92	1.85	0.43
20:N:72:THR:N	47:N:616:LUT:O23	2.49	0.43
29:R:308:CLA:H93	29:R:308:CLA:H61	1.86	0.43
47:Y:316:LUT:H15	47:Y:316:LUT:H201	1.81	0.43
37:a:413:LHG:O4	5:d:141:TYR:OH	2.28	0.43
29:b:508:CLA:H151	29:b:509:CLA:H172	1.99	0.43
35:d:407:LMG:HC61	7:f:39:MET:HG3	2.00	0.43
29:s:310:CLA:H93	29:s:310:CLA:H111	1.79	0.43
29:s:312:CLA:H62	29:s:312:CLA:H92	1.79	0.43
2:B:25:MET:HE1	2:B:108:PHE:CD1	2.54	0.43
4:C:75:ILE:O	4:C:79:HIS:ND1	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:N:620:PTY:H371	50:N:620:PTY:H342	1.70	0.43
48:G:617:NEX:H35	48:G:617:NEX:H401	1.86	0.43
29:a:408:CLA:HMB2	9:i:12:VAL:HG13	2.00	0.43
2:b:71:VAL:HG23	29:b:506:CLA:HMA2	2.00	0.43
2:b:254:GLY:HA2	35:d:408:LMG:H202	2.01	0.43
29:b:511:CLA:H112	29:b:511:CLA:H72	1.77	0.43
35:c:520:LMG:H452	49:y:302:XAT:H382	1.99	0.43
15:p:128:ILE:HG21	15:p:208:THR:HA	1.99	0.43
29:n:604:CLA:H143	29:n:604:CLA:H161	1.85	0.43
46:n:607:CHL:H12	47:n:614:LUT:H383	2.01	0.43
2:B:42:ILE:HD13	2:B:42:ILE:HA	1.87	0.43
35:C:522:LMG:H131	35:C:522:LMG:H352	2.00	0.43
30:D:401:PHO:H72	30:D:401:PHO:H112	1.76	0.43
25:U:106:VAL:O	25:U:110:ARG:HB2	2.19	0.43
2:b:25:MET:HE1	2:b:108:PHE:CD1	2.53	0.43
2:b:141:ILE:HG13	2:b:217:LEU:HD21	2.01	0.43
2:b:365:THR:HG21	14:o:226:ILE:HD12	2.00	0.43
37:c:521:LHG:HC92	29:s:312:CLA:HMB1	2.01	0.43
43:d:405:PL9:H221	37:l:102:LHG:H171	2.00	0.43
46:n:601:CHL:H61	46:n:601:CHL:H41	1.74	0.43
29:C:502:CLA:C2D	29:C:504:CLA:H2	2.49	0.43
14:O:93:ASN:HD22	14:O:96:GLU:HB2	1.83	0.43
22:R:223:LEU:HD23	22:R:223:LEU:H	1.84	0.43
1:a:36:ILE:HG23	29:a:408:CLA:HBB1	2.01	0.43
29:b:505:CLA:H92	29:b:505:CLA:H61	1.77	0.43
15:p:104:LEU:HB3	15:p:118:VAL:HG22	2.01	0.43
48:n:616:NEX:H11	48:n:616:NEX:H191	1.84	0.43
50:n:619:PTY:H352	50:n:619:PTY:H181	2.00	0.43
29:y:313:CLA:C4C	37:y:320:LHG:HC62	2.49	0.43
31:C:515:BCR:C10	35:C:524:LMG:H172	2.49	0.43
49:R:311:XAT:H31	49:R:311:XAT:H391	1.74	0.43
29:a:405:CLA:H3A	29:a:405:CLA:HBA2	1.63	0.43
29:a:408:CLA:H11	9:i:9:TYR:CZ	2.53	0.43
4:c:282:ASN:OD1	36:c:516:DGD:O5E	2.36	0.43
39:c:522:SQD:H2	39:c:522:SQD:H441	1.84	0.43
20:n:153:THR:HB	46:n:605:CHL:HAC1	2.01	0.43
29:r:308:CLA:H111	29:r:308:CLA:H91	1.74	0.43
24:y:201:PHE:CZ	24:y:205:LYS:HE3	2.54	0.43
1:A:312:ARG:NH2	15:P:92:ASN:OD1	2.42	0.43
29:B:508:CLA:H193	29:D:405:CLA:HAA2	2.01	0.43
37:L:101:LHG:H312	13:M:18:PRO:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:186:LYS:HA	15:P:205:VAL:O	2.19	0.43
21:G:80:GLU:OE1	46:G:609:CHL:HED2	2.19	0.43
47:G:615:LUT:H15	47:G:615:LUT:H201	1.85	0.43
1:a:121:LEU:HD21	29:c:505:CLA:H162	2.00	0.43
2:b:291:SER:O	2:b:296:LEU:HB2	2.19	0.43
2:b:326:ARG:HB3	2:b:444:ARG:HD3	2.01	0.43
29:b:502:CLA:H61	29:b:502:CLA:H41	1.74	0.43
4:c:215:VAL:HG21	31:c:514:BCR:H291	2.00	0.43
29:y:314:CLA:H142	29:y:314:CLA:H111	1.77	0.43
1:A:106:LEU:HD11	31:A:410:BCR:H292	2.01	0.43
2:B:91:TRP:CD2	29:B:506:CLA:HBA2	2.54	0.43
5:D:136:VAL:HG23	5:D:138:LEU:HG	2.01	0.43
20:N:105:THR:HG21	29:N:604:CLA:HAC2	2.00	0.43
29:N:611:CLA:H3A	29:N:611:CLA:HBA2	1.65	0.43
24:Y:102:LEU:HG	29:Y:305:CLA:HAC1	2.01	0.43
4:c:213:VAL:HG13	4:c:277:PHE:HA	2.00	0.43
20:n:84:ARG:HG3	24:y:75:GLY:HA3	2.01	0.43
21:g:61:TYR:HB2	29:g:602:CLA:HMD1	2.01	0.43
29:B:501:CLA:HBA2	29:B:501:CLA:HBD	2.00	0.42
29:C:502:CLA:H193	29:C:507:CLA:HMB2	2.01	0.42
9:I:27:ASP:HA	9:I:30:ARG:HG3	2.01	0.42
29:G:602:CLA:H41	29:G:603:CLA:HAA1	2.01	0.42
46:G:606:CHL:HHC	46:G:606:CHL:HBB1	2.01	0.42
29:Y:303:CLA:H111	29:Y:303:CLA:H91	1.78	0.42
29:a:406:CLA:HMB3	29:d:403:CLA:H102	2.01	0.42
35:b:520:LMG:H152	35:b:520:LMG:H121	1.86	0.42
20:n:87:GLU:HA	20:n:181:LEU:HD21	2.00	0.42
48:g:617:NEX:H15	48:g:617:NEX:H201	1.86	0.42
29:A:405:CLA:H192	29:A:406:CLA:H111	2.00	0.42
8:H:56:LEU:HB3	45:H:101:RRX:H31	2.00	0.42
20:N:150:ILE:HA	20:N:153:THR:HG22	2.01	0.42
20:N:234:ASN:ND2	52:N:711:HOH:O	2.42	0.42
2:b:348:ASP:OD2	2:b:352:ARG:NH1	2.52	0.42
29:b:502:CLA:H143	29:b:502:CLA:H162	1.82	0.42
29:b:504:CLA:H112	29:b:515:CLA:H42	2.00	0.42
4:c:319:ALA:HA	15:p:158:GLY:HA3	2.01	0.42
29:c:513:CLA:HMB3	31:z:101:BCR:H402	2.01	0.42
14:o:117:LYS:HG2	14:o:125:GLU:OE2	2.19	0.42
49:r:312:XAT:H391	49:r:312:XAT:H31	1.73	0.42
1:A:32:TRP:O	1:A:35:VAL:HG22	2.19	0.42
2:B:327:THR:HG22	29:B:507:CLA:H11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:E:101:HEM:HBC2	44:E:101:HEM:HMC2	2.01	0.42
14:O:216:ARG:HH11	14:O:240:LEU:HB3	1.83	0.42
15:P:142:GLY:HA2	15:P:145:LEU:HD13	2.01	0.42
50:N:620:PTY:H411	29:Y:315:CLA:H71	2.02	0.42
46:S:308:CHL:HHC	46:S:308:CHL:HBB1	2.00	0.42
48:Y:318:NEX:H35	48:Y:318:NEX:H401	1.95	0.42
1:a:340:PRO:HB2	15:p:224:LYS:HD3	2.00	0.42
2:b:457:SER:HB2	35:b:520:LMG:H231	2.01	0.42
4:c:14:ARG:O	4:c:29:ARG:NH1	2.52	0.42
20:n:90:LEU:HD23	20:n:181:LEU:HD22	2.01	0.42
29:y:304:CLA:H91	29:y:304:CLA:H111	1.81	0.42
29:A:409:CLA:H122	35:W:201:LMG:H202	2.01	0.42
29:C:513:CLA:H92	29:C:513:CLA:H61	1.75	0.42
14:O:93:ASN:O	14:O:95:ARG:N	2.47	0.42
14:O:120:ASP:OD2	14:O:122:LYS:NZ	2.43	0.42
21:G:80:GLU:HB2	21:G:175:LEU:HD21	2.02	0.42
29:R:302:CLA:HBD	29:R:302:CLA:HAA1	2.01	0.42
2:b:175:THR:OG1	2:b:176:GLY:N	2.52	0.42
29:b:515:CLA:H91	29:b:515:CLA:H111	1.80	0.42
4:c:394:SER:HA	4:c:408:VAL:HG23	2.01	0.42
29:c:512:CLA:H92	29:c:512:CLA:H61	1.75	0.42
5:d:43:PHE:HD1	31:f:101:BCR:H342	1.85	0.42
43:d:405:PL9:H412	37:d:406:LHG:H212	2.01	0.42
50:n:619:PTY:H362	50:n:619:PTY:H331	1.90	0.42
47:g:616:LUT:H11	47:g:616:LUT:H191	1.91	0.42
29:y:313:CLA:H142	29:y:313:CLA:H112	1.84	0.42
29:B:516:CLA:HBB1	29:B:516:CLA:HMB1	2.02	0.42
30:D:401:PHO:H3A	30:D:401:PHO:HBA1	1.50	0.42
41:D:402:DGA:HAF1	41:D:402:DGA:HAE2	1.85	0.42
37:D:407:LHG:H291	16:T:17:ILE:HG23	2.02	0.42
14:O:154:SER:HA	14:O:192:THR:HA	2.00	0.42
15:P:222:GLY:O	15:P:226:TRP:N	2.50	0.42
1:a:126:TYR:CZ	30:a:407:PHO:HBA1	2.54	0.42
1:a:341:LEU:HD13	1:a:343:LEU:HD21	2.01	0.42
4:c:317:ALA:HB1	14:o:163:LEU:HD22	2.02	0.42
29:g:604:CLA:H11	46:g:606:CHL:HBA2	2.01	0.42
47:g:615:LUT:H35	47:g:615:LUT:H401	1.82	0.42
22:r:252:GLY:HA2	22:r:255:ILE:HG12	2.02	0.42
2:B:474:ILE:HG23	41:D:402:DGA:HG2	2.02	0.42
18:X:88:GLY:HA2	18:X:91:THR:HG22	2.02	0.42
20:N:187:PHE:HD1	46:N:608:CHL:H11	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:b:513:CLA:H2	29:b:513:CLA:HED3	2.02	0.42
35:c:520:LMG:H251	29:y:316:CLA:HMC1	2.02	0.42
40:c:523:SPH:H102	40:c:523:SPH:H131	1.89	0.42
14:o:171:LYS:HE3	14:o:177:TYR:HE1	1.85	0.42
20:n:117:PHE:HZ	20:n:139:LEU:HD23	1.84	0.42
46:n:601:CHL:HED2	37:n:617:LHG:H141	2.02	0.42
29:n:603:CLA:HED3	47:y:318:LUT:H363	2.00	0.42
29:n:609:CLA:H62	29:n:609:CLA:H41	1.88	0.42
29:n:612:CLA:H202	29:n:613:CLA:HBA2	2.01	0.42
47:n:615:LUT:H15	47:n:615:LUT:H201	1.85	0.42
29:g:602:CLA:H122	29:y:305:CLA:H121	2.01	0.42
1:A:274:PHE:HA	1:A:277:VAL:HG12	2.02	0.42
2:B:112:VAL:HA	31:B:517:BCR:H282	2.01	0.42
31:K:101:BCR:H351	31:K:101:BCR:H15C	1.88	0.42
29:Y:315:CLA:H143	29:Y:315:CLA:H161	1.82	0.42
2:b:124:ARG:HD2	52:b:650:HOH:O	2.20	0.42
29:b:509:CLA:H2	29:b:509:CLA:H62	1.84	0.42
39:c:522:SQD:H241	39:c:522:SQD:H461	1.82	0.42
14:o:130:THR:HG22	14:o:172:LEU:HD23	2.02	0.42
15:p:117:TYR:CE1	15:p:218:LYS:HE3	2.54	0.42
29:s:305:CLA:C1C	48:s:319:NEX:H222	2.50	0.42
2:B:386:ALA:O	2:B:387:GLU:HG2	2.20	0.42
29:B:504:CLA:H101	29:B:504:CLA:H13	1.90	0.42
37:D:407:LHG:H182	16:T:17:ILE:HD11	2.00	0.42
35:D:410:LMG:H111	35:D:410:LMG:H291	2.02	0.42
14:O:195:SER:HA	14:O:254:PHE:O	2.20	0.42
29:N:611:CLA:C4C	37:N:618:LHG:HC62	2.50	0.42
29:N:613:CLA:H91	29:N:613:CLA:H112	1.77	0.42
47:R:310:LUT:H191	47:R:310:LUT:H11	1.81	0.42
23:S:276:LEU:HD13	29:S:314:CLA:HMD3	2.02	0.42
47:S:317:LUT:H15	47:S:317:LUT:H201	1.87	0.42
29:Y:313:CLA:H142	29:Y:313:CLA:H111	1.79	0.42
1:a:274:PHE:HA	1:a:277:VAL:HG12	2.01	0.42
5:d:186:GLN:HB2	29:d:403:CLA:HBC1	2.01	0.42
14:o:93:ASN:ND2	14:o:96:GLU:HB2	2.34	0.42
21:g:63:TRP:CE3	47:g:616:LUT:H383	2.55	0.42
49:g:619:XAT:H391	49:g:619:XAT:H31	1.64	0.42
46:r:306:CHL:HBC2	46:r:306:CHL:HHD	2.02	0.42
47:s:318:LUT:H35	47:s:318:LUT:H401	1.82	0.42
2:B:6:TYR:OH	37:B:523:LHG:HC31	2.19	0.42
20:N:87:GLU:HA	20:N:181:LEU:HD21	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N:609:CHL:HMB2	46:Y:302:CHL:HHB	2.00	0.42
23:S:284:ASP:OD1	23:S:285:ARG:N	2.51	0.42
1:a:60:ILE:HD12	1:a:84:PRO:HD2	2.02	0.42
2:b:278:GLY:HA3	25:u:105:THR:HG23	2.02	0.42
31:b:517:BCR:H351	31:b:517:BCR:H15C	1.84	0.42
4:c:221:ILE:HG12	31:c:514:BCR:H282	2.02	0.42
4:c:253:VAL:HG21	4:c:437:ARG:HD2	2.02	0.42
5:d:193:LEU:O	12:l:35:TYR:OH	2.28	0.42
44:e:101:HEM:HMC2	44:e:101:HEM:HBC2	2.01	0.42
41:w:201:DGA:HAW1	41:w:201:DGA:HAN2	1.83	0.42
47:s:317:LUT:H11	47:s:317:LUT:H191	1.93	0.42
46:y:309:CHL:H102	46:y:309:CHL:H13	1.93	0.42
5:D:182:ILE:HG23	29:D:404:CLA:CHD	2.50	0.42
13:M:4:ASN:ND2	52:M:202:HOH:O	2.52	0.42
14:O:120:ASP:OD1	2:b:84:THR:OG1	2.28	0.42
14:O:190:LYS:HD2	14:O:190:LYS:HA	1.82	0.42
50:N:620:PTY:H441	29:Y:314:CLA:H151	2.02	0.42
29:G:613:CLA:H122	29:G:613:CLA:H8	1.93	0.42
48:S:319:NEX:H35	48:S:319:NEX:H401	1.93	0.42
37:Y:319:LHG:H321	37:Y:319:LHG:H351	1.83	0.42
2:b:25:MET:HE3	31:b:517:BCR:H23C	2.02	0.42
29:c:507:CLA:H171	29:c:507:CLA:H13	1.96	0.42
14:o:283:HIS:HA	14:o:284:PRO:HD3	1.87	0.42
21:g:136:LEU:HD23	21:g:136:LEU:HA	1.86	0.42
49:y:302:XAT:H15	49:y:302:XAT:H201	1.71	0.42
14:O:126:GLU:N	14:O:126:GLU:OE1	2.53	0.41
20:N:157:GLN:NE2	46:N:607:CHL:OMC	2.46	0.41
46:N:607:CHL:H141	46:N:607:CHL:H161	1.77	0.41
48:N:617:NEX:H15	48:N:617:NEX:H201	1.93	0.41
24:Y:133:LYS:HA	24:Y:133:LYS:HD3	1.95	0.41
24:Y:240:HIS:ND1	24:Y:247:ASN:O	2.36	0.41
2:b:144:PHE:HZ	38:b:524:LMT:H3'	1.85	0.41
31:b:517:BCR:H332	13:m:13:LEU:HD12	2.01	0.41
4:c:332:SER:OG	4:c:336:GLU:OE1	2.38	0.41
29:n:602:CLA:H201	37:n:617:LHG:H182	2.02	0.41
47:g:616:LUT:H15	47:g:616:LUT:H201	1.80	0.41
29:B:510:CLA:H102	29:B:515:CLA:HAA1	2.01	0.41
29:B:515:CLA:H2	29:B:516:CLA:CBB	2.50	0.41
4:C:154:ILE:HA	4:C:233:ILE:HD13	2.01	0.41
4:C:394:SER:HA	4:C:408:VAL:HG23	2.01	0.41
29:C:504:CLA:H61	29:C:504:CLA:H101	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:155:SER:HA	5:D:159:ILE:HB	2.02	0.41
18:X:64:SER:OG	18:X:65:VAL:N	2.49	0.41
46:G:601:CHL:C4D	37:G:618:LHG:HC91	2.50	0.41
22:R:143:TRP:CD1	29:R:307:CLA:HMD3	2.56	0.41
29:S:312:CLA:H162	29:S:313:CLA:HAB	2.01	0.41
46:Y:307:CHL:H203	46:Y:307:CHL:H161	1.92	0.41
29:b:515:CLA:H92	29:b:515:CLA:H61	1.91	0.41
8:h:56:LEU:HB3	45:h:101:RRX:H31	2.02	0.41
18:x:88:GLY:HA2	18:x:91:THR:HG22	2.02	0.41
49:y:302:XAT:H11	49:y:302:XAT:H191	1.87	0.41
4:C:216:ASP:N	4:C:216:ASP:OD1	2.53	0.41
5:D:192:THR:HG23	29:D:404:CLA:HBC2	2.02	0.41
15:P:115:ASN:OD1	15:P:220:GLN:HB3	2.20	0.41
29:N:613:CLA:H171	37:N:618:LHG:H331	2.01	0.41
47:N:616:LUT:H35	47:N:616:LUT:H401	1.81	0.41
49:N:619:XAT:H15	49:N:619:XAT:H201	1.72	0.41
22:R:224:ALA:HB3	29:R:308:CLA:HAA2	2.02	0.41
29:R:306:CLA:H62	29:R:306:CLA:H92	1.85	0.41
23:S:78:GLU:HG2	23:S:79:LEU:HD12	2.01	0.41
29:S:312:CLA:H92	29:S:312:CLA:H61	1.75	0.41
1:a:201:GLY:HA3	1:a:286:THR:HB	2.02	0.41
7:f:19:TRP:O	7:f:23:HIS:ND1	2.53	0.41
20:n:120:SER:HB2	20:n:126:ALA:HA	2.02	0.41
20:n:202:LEU:HD13	29:n:609:CLA:HAA2	2.02	0.41
23:s:171:ILE:HG21	46:s:307:CHL:HED3	2.02	0.41
29:y:306:CLA:H43	48:y:319:NEX:H23	2.01	0.41
2:B:185:TRP:HB3	29:B:501:CLA:HMA3	2.02	0.41
29:B:513:CLA:H202	29:B:513:CLA:H162	1.90	0.41
29:C:514:CLA:H93	31:C:515:BCR:H393	2.02	0.41
5:D:8:TYR:CD1	22:R:85:LEU:HD21	2.55	0.41
15:P:224:LYS:HA	15:P:227:PHE:CZ	2.55	0.41
22:R:252:GLY:HA2	22:R:255:ILE:HG12	2.02	0.41
29:S:311:CLA:H141	29:S:311:CLA:H161	1.81	0.41
1:a:121:LEU:HD23	1:a:121:LEU:HA	1.92	0.41
33:a:415:3PH:H362	33:a:415:3PH:H2A1	2.02	0.41
46:n:601:CHL:HED1	37:n:617:LHG:H272	2.01	0.41
29:g:604:CLA:H43	48:g:617:NEX:H23	2.02	0.41
29:r:303:CLA:HBA2	29:r:303:CLA:H3A	1.78	0.41
29:r:310:CLA:H11	29:r:310:CLA:HBA2	1.42	0.41
24:y:77:SER:OG	29:y:304:CLA:O1A	2.33	0.41
29:A:405:CLA:H42	29:A:406:CLA:HMC2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:GLU:C	2:B:302:TRP:H	2.29	0.41
29:B:502:CLA:HMD2	8:H:57:PHE:HZ	1.85	0.41
29:B:505:CLA:H61	29:B:505:CLA:H41	1.92	0.41
29:B:512:CLA:HBB1	29:B:512:CLA:HMB1	2.01	0.41
4:C:165:LEU:HD13	51:S:321:LPX:H7A	2.02	0.41
39:C:501:SQD:H62	5:D:233:ARG:HD3	2.02	0.41
15:P:164:LYS:HD3	15:P:164:LYS:HA	1.85	0.41
29:R:303:CLA:C1C	48:R:312:NEX:H222	2.50	0.41
23:S:284:ASP:CG	23:S:285:ARG:H	2.28	0.41
29:b:508:CLA:H143	29:b:508:CLA:H161	1.80	0.41
4:c:288:GLU:HG3	4:c:379:ARG:HH12	1.85	0.41
22:r:235:LEU:HD13	29:r:309:CLA:O1A	2.20	0.41
29:A:405:CLA:H72	29:A:405:CLA:H111	1.86	0.41
2:B:441:GLY:HA3	14:O:231:LYS:HB2	2.03	0.41
15:P:138:ILE:HD13	15:P:187:PHE:CD2	2.56	0.41
41:W:202:DGA:HB52	29:Y:312:CLA:H52	2.02	0.41
21:G:232:HIS:CG	29:G:613:CLA:HAA2	2.55	0.41
29:S:303:CLA:H101	29:S:303:CLA:H13	1.97	0.41
1:a:85:THR:OG1	1:a:113:GLN:HG3	2.20	0.41
29:b:512:CLA:HMB1	29:b:512:CLA:HBB1	2.02	0.41
21:g:61:TYR:OH	37:g:618:LHG:O5	2.35	0.41
21:g:189:ASP:OD2	21:g:192:THR:OG1	2.32	0.41
48:s:319:NEX:H35	48:s:319:NEX:H401	1.90	0.41
2:B:326:ARG:HB3	2:B:444:ARG:HD3	2.02	0.41
29:B:513:CLA:H143	29:B:513:CLA:H111	1.78	0.41
31:C:515:BCR:H281	37:S:301:LHG:HC91	2.02	0.41
20:N:88:LEU:HG	46:N:609:CHL:OBD	2.21	0.41
47:R:310:LUT:H15	47:R:310:LUT:H201	1.79	0.41
46:S:309:CHL:H101	48:S:319:NEX:H35	2.02	0.41
24:Y:172:GLY:HA2	29:Y:309:CLA:HAC1	2.02	0.41
31:b:517:BCR:HC42	13:m:10:ALA:HB2	2.02	0.41
29:c:506:CLA:H91	29:c:506:CLA:H112	1.91	0.41
36:c:518:DGD:HA51	36:c:518:DGD:HA22	1.98	0.41
17:w:89:LEU:HD23	17:w:89:LEU:HA	1.90	0.41
17:W:89:LEU:HB3	35:W:203:LMG:H401	2.03	0.41
23:S:240:ARG:HA	23:S:243:MET:HE3	2.02	0.41
29:S:314:CLA:H52	29:S:314:CLA:H11	1.75	0.41
29:S:314:CLA:HBB1	47:S:317:LUT:H181	2.02	0.41
24:Y:136:GLY:HA3	24:Y:149:GLN:HE21	1.86	0.41
36:c:517:DGD:HAE2	36:c:517:DGD:HA81	1.85	0.41
5:d:51:GLY:HA2	5:d:55:VAL:HB	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:s:303:CLA:H92	29:s:303:CLA:H62	1.92	0.41
25:u:106:VAL:HG22	25:u:110:ARG:HE	1.84	0.41
1:A:32:TRP:NE1	52:I:202:HOH:O	2.42	0.41
30:A:408:PHO:H192	30:A:408:PHO:H162	1.88	0.41
29:A:409:CLA:H102	29:A:409:CLA:H13	1.89	0.41
2:B:25:MET:HE3	31:B:517:BCR:H23C	2.03	0.41
29:B:514:CLA:H3A	29:B:514:CLA:HBA2	1.89	0.41
33:B:522:3PH:H3A1	16:t:4:LEU:HD22	2.03	0.41
6:E:23:HIS:HA	6:E:26:THR:OG1	2.21	0.41
14:O:101:ASP:OD2	14:O:148:LYS:NZ	2.50	0.41
14:O:279:GLU:HB2	14:O:280:MET:H	1.66	0.41
20:N:205:LYS:O	20:N:209:ASN:ND2	2.42	0.41
21:G:87:ARG:HA	21:G:90:LEU:HD12	2.02	0.41
29:G:602:CLA:H3A	29:G:602:CLA:HBA2	1.68	0.41
29:R:308:CLA:H62	29:R:308:CLA:H41	1.76	0.41
46:S:302:CHL:HHC	46:S:302:CHL:HBB1	2.02	0.41
46:S:307:CHL:HBB2	46:S:308:CHL:CBB	2.51	0.41
49:Y:301:XAT:H15	49:Y:301:XAT:H201	1.73	0.41
29:Y:303:CLA:H142	47:Y:317:LUT:H361	2.02	0.41
1:a:57:PRO:HB3	1:a:68:SER:HA	2.02	0.41
29:a:405:CLA:H122	29:a:405:CLA:H162	1.79	0.41
2:b:5:TRP:NE1	37:l:102:LHG:O10	2.52	0.41
29:b:505:CLA:H141	29:b:505:CLA:H162	1.87	0.41
35:b:520:LMG:H171	35:b:520:LMG:H142	1.85	0.41
38:b:524:LMT:H121	38:b:524:LMT:H91	1.83	0.41
36:c:517:DGD:HA32	41:j:101:DGA:HA72	2.03	0.41
5:d:182:ILE:HG23	29:d:403:CLA:CHD	2.50	0.41
20:n:150:ILE:HA	20:n:153:THR:HG22	2.03	0.41
46:n:606:CHL:HMB2	46:n:608:CHL:HMC	2.03	0.41
49:n:618:XAT:H35	49:n:618:XAT:H401	1.92	0.41
21:g:149:GLN:OE1	46:g:607:CHL:HMC	2.21	0.41
29:r:304:CLA:C1C	48:r:313:NEX:H222	2.50	0.41
49:r:312:XAT:H201	49:r:312:XAT:H15	1.81	0.41
23:s:192:PHE:H	23:s:198:LYS:HA	1.85	0.41
23:s:209:LYS:HE2	23:s:209:LYS:HB2	1.90	0.41
47:s:317:LUT:H15	47:s:317:LUT:H201	1.91	0.41
48:y:319:NEX:H15	48:y:319:NEX:H201	1.83	0.41
2:B:454:GLY:HA2	35:B:520:LMG:H192	2.02	0.41
15:P:178:ASP:OD1	15:P:179:LYS:N	2.45	0.41
20:N:255:THR:HA	20:N:256:PRO:HD3	1.88	0.41
29:Y:315:CLA:H61	29:Y:315:CLA:H41	1.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:315:CLA:H142	29:Y:315:CLA:H112	1.89	0.41
2:b:27:THR:HG22	2:b:107:LEU:HD13	2.03	0.41
29:b:508:CLA:H91	41:b:522:DGA:HBS1	2.03	0.41
29:b:514:CLA:H112	31:b:517:BCR:H362	2.02	0.41
3:v:25:LEU:O	3:v:29:ARG:HB3	2.21	0.41
6:e:35:TRP:HA	7:f:38:ALA:HB2	2.03	0.41
9:i:28:PRO:O	9:i:31:ASN:ND2	2.54	0.41
15:p:117:TYR:HE1	15:p:218:LYS:HE3	1.85	0.41
20:n:144:LEU:O	20:n:146:HIS:N	2.54	0.41
47:n:615:LUT:H11	47:n:615:LUT:H191	1.92	0.41
21:g:242:PHE:HB3	24:y:132:PHE:HZ	1.86	0.41
29:B:515:CLA:H2	29:B:516:CLA:HBB2	2.03	0.40
14:O:172:LEU:HD23	14:O:172:LEU:HA	1.85	0.40
4:c:41:HIS:CG	29:c:512:CLA:HMD1	2.56	0.40
31:c:515:BCR:H351	31:c:515:BCR:H15C	1.81	0.40
6:e:26:THR:O	6:e:29:SER:OG	2.36	0.40
29:n:602:CLA:H151	29:n:602:CLA:H18	1.64	0.40
22:r:202:ARG:HG3	29:r:307:CLA:HMD3	2.04	0.40
29:s:304:CLA:H193	29:s:304:CLA:H161	1.92	0.40
29:B:507:CLA:H203	12:L:36:ILE:HG13	2.02	0.40
4:C:201:ILE:HD12	29:C:507:CLA:H161	2.02	0.40
29:C:506:CLA:H112	29:C:506:CLA:H72	1.92	0.40
46:R:305:CHL:HHC	46:R:305:CHL:HBB1	2.03	0.40
37:Y:319:LHG:H371	37:Y:319:LHG:H342	1.67	0.40
2:b:91:TRP:CD2	29:b:506:CLA:HBA2	2.56	0.40
2:b:121:GLU:HG3	8:h:23:VAL:HG22	2.02	0.40
2:b:142:HIS:ND1	29:b:510:CLA:OBD	2.38	0.40
6:e:78:LYS:HG3	6:e:79:LEU:HD12	2.04	0.40
15:p:225:ARG:HA	15:p:228:LYS:HG3	2.02	0.40
29:g:611:CLA:H93	29:g:611:CLA:H111	1.91	0.40
22:r:160:VAL:HG21	29:r:304:CLA:HED2	2.03	0.40
23:s:180:GLU:HG3	29:s:310:CLA:NB	2.37	0.40
29:B:502:CLA:H101	29:B:502:CLA:H13	1.90	0.40
29:B:503:CLA:H201	8:H:58:ALA:HB2	2.03	0.40
29:B:508:CLA:H141	29:D:405:CLA:H12	2.04	0.40
6:E:62:ASP:OD1	6:E:62:ASP:N	2.53	0.40
13:M:3:VAL:HG12	13:M:6:LEU:HB3	2.03	0.40
14:O:155:VAL:HG13	14:O:193:LEU:HD22	2.03	0.40
41:W:202:DGA:HAT2	41:W:202:DGA:HAH1	1.80	0.40
29:G:602:CLA:H161	46:Y:310:CHL:H42	2.02	0.40
47:G:616:LUT:H201	47:G:616:LUT:H15	1.80	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:242:ILE:HG23	2:b:462:PHE:HD2	1.86	0.40
33:b:521:3PH:H362	33:b:521:3PH:H332	1.81	0.40
4:c:105:LEU:HD23	4:c:105:LEU:HA	1.87	0.40
29:c:505:CLA:H151	36:c:516:DGD:HA82	2.03	0.40
29:d:404:CLA:H172	29:d:404:CLA:H13	1.94	0.40
21:g:193:PHE:CZ	29:g:610:CLA:HED3	2.56	0.40
29:g:611:CLA:H141	29:g:611:CLA:H162	1.76	0.40
29:s:304:CLA:H3A	29:s:310:CLA:H12	2.02	0.40
46:y:308:CHL:HBB2	46:y:309:CHL:HAB	2.03	0.40
1:A:312:ARG:NH1	6:E:61:GLN:O	2.37	0.40
1:A:313:VAL:HG23	15:P:90:LYS:HB3	2.02	0.40
29:A:406:CLA:H71	30:A:408:PHO:HMB2	2.02	0.40
2:B:242:ILE:HG23	2:B:462:PHE:HD2	1.86	0.40
38:B:524:LMT:H32	29:R:302:CLA:H102	2.03	0.40
35:D:409:LMG:H181	35:D:409:LMG:H152	1.77	0.40
15:P:99:VAL:HB	15:P:102:ILE:HG13	2.04	0.40
15:P:186:LYS:HD2	15:P:238:LEU:HD21	2.04	0.40
22:R:235:LEU:HA	22:R:235:LEU:HD23	1.86	0.40
46:Y:308:CHL:H92	46:Y:308:CHL:H62	1.85	0.40
47:Y:316:LUT:H35	47:Y:316:LUT:H401	1.90	0.40
2:b:275:TRP:O	25:u:102:LYS:HE3	2.20	0.40
29:c:511:CLA:HBA2	31:c:515:BCR:H271	2.04	0.40
15:p:204:LEU:HB3	15:p:238:LEU:HD22	2.03	0.40
23:s:272:PHE:HB3	37:s:301:LHG:HC62	2.03	0.40
29:B:511:CLA:H112	29:B:511:CLA:H72	1.86	0.40
29:B:516:CLA:H52	29:B:516:CLA:H11	1.90	0.40
13:M:28:LYS:HB2	13:m:27:VAL:HG12	2.02	0.40
46:G:607:CHL:H101	46:G:607:CHL:H13	1.90	0.40
23:S:236:ILE:HD12	23:S:236:ILE:HA	1.95	0.40
29:b:501:CLA:H2	29:b:501:CLA:H112	2.04	0.40
5:d:125:PHE:HB2	30:d:402:PHO:H11	2.03	0.40
37:d:406:LHG:H242	12:l:20:TRP:CE2	2.57	0.40
6:e:44:TYR:HE2	15:p:63:ALA:HB2	1.85	0.40
6:e:64:PRO:HB3	6:e:79:LEU:HD23	2.03	0.40
50:n:619:PTY:H391	50:n:619:PTY:H422	1.84	0.40
21:g:217:GLN:O	21:g:221:THR:OG1	2.26	0.40
22:r:132:ARG:HH12	29:r:303:CLA:HAA2	1.86	0.40
24:y:255:LYS:HE3	24:y:255:LYS:HB3	1.93	0.40
29:y:304:CLA:CAB	47:y:318:LUT:H32	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/336 (99%)	327 (98%)	7 (2%)	0	100	100
1	a	334/336 (99%)	327 (98%)	7 (2%)	0	100	100
2	B	481/484 (99%)	470 (98%)	11 (2%)	0	100	100
2	b	481/484 (99%)	468 (97%)	13 (3%)	0	100	100
3	V	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	v	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
4	C	447/449 (100%)	434 (97%)	13 (3%)	0	100	100
4	c	447/449 (100%)	434 (97%)	13 (3%)	0	100	100
5	D	346/348 (99%)	338 (98%)	8 (2%)	0	100	100
5	d	346/348 (99%)	340 (98%)	6 (2%)	0	100	100
6	E	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
6	e	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
7	f	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
8	h	65/67 (97%)	65 (100%)	0	0	100	100
9	I	33/35 (94%)	33 (100%)	0	0	100	100
9	i	33/35 (94%)	33 (100%)	0	0	100	100
10	J	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
10	j	34/36 (94%)	34 (100%)	0	0	100	100
11	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	L	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
12	l	36/38 (95%)	36 (100%)	0	0	100	100
13	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	m	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
14	O	236/238 (99%)	228 (97%)	8 (3%)	0	100	100
14	o	236/238 (99%)	218 (92%)	18 (8%)	0	100	100
15	P	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
15	p	185/187 (99%)	173 (94%)	12 (6%)	0	100	100
16	T	28/30 (93%)	28 (100%)	0	0	100	100
16	t	28/30 (93%)	28 (100%)	0	0	100	100
17	W	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
17	w	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
18	X	28/30 (93%)	28 (100%)	0	0	100	100
18	x	28/30 (93%)	28 (100%)	0	0	100	100
19	Z	59/61 (97%)	59 (100%)	0	0	100	100
19	z	59/61 (97%)	59 (100%)	0	0	100	100
20	N	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	24	29
20	n	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	24	29
21	G	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
21	g	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
22	R	191/196 (97%)	178 (93%)	13 (7%)	0	100	100
22	r	191/196 (97%)	174 (91%)	16 (8%)	1 (0%)	24	29
23	S	241/243 (99%)	228 (95%)	13 (5%)	0	100	100
23	s	241/243 (99%)	220 (91%)	21 (9%)	0	100	100
24	Y	220/222 (99%)	213 (97%)	6 (3%)	1 (0%)	24	29
24	y	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	24	29
25	U	25/27 (93%)	25 (100%)	0	0	100	100
25	u	25/27 (93%)	23 (92%)	2 (8%)	0	100	100
All	All	7334/7442 (98%)	7065 (96%)	264 (4%)	5 (0%)	49	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	r	176	LEU
24	y	146	ILE
24	Y	146	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	n	145	ILE
20	N	145	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/275 (100%)	274 (100%)	1 (0%)	84	89
1	a	275/275 (100%)	275 (100%)	0	100	100
2	B	387/387 (100%)	387 (100%)	0	100	100
2	b	387/387 (100%)	387 (100%)	0	100	100
3	V	25/25 (100%)	25 (100%)	0	100	100
3	v	25/25 (100%)	25 (100%)	0	100	100
4	C	350/350 (100%)	350 (100%)	0	100	100
4	c	350/350 (100%)	350 (100%)	0	100	100
5	D	279/279 (100%)	277 (99%)	2 (1%)	76	83
5	d	279/279 (100%)	279 (100%)	0	100	100
6	E	68/68 (100%)	68 (100%)	0	100	100
6	e	68/68 (100%)	68 (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	H	56/56 (100%)	56 (100%)	0	100	100
8	h	56/56 (100%)	56 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
10	J	27/27 (100%)	27 (100%)	0	100	100
10	j	27/27 (100%)	27 (100%)	0	100	100
11	K	33/33 (100%)	33 (100%)	0	100	100
11	k	33/33 (100%)	33 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	26/26 (100%)	26 (100%)	0	100	100
13	m	26/26 (100%)	26 (100%)	0	100	100
14	O	195/195 (100%)	195 (100%)	0	100	100
14	o	195/195 (100%)	195 (100%)	0	100	100
15	P	151/151 (100%)	151 (100%)	0	100	100
15	p	151/151 (100%)	151 (100%)	0	100	100
16	T	26/26 (100%)	26 (100%)	0	100	100
16	t	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	34 (100%)	0	100	100
17	w	34/34 (100%)	34 (100%)	0	100	100
18	X	21/21 (100%)	21 (100%)	0	100	100
18	x	21/21 (100%)	21 (100%)	0	100	100
19	Z	50/50 (100%)	50 (100%)	0	100	100
19	z	50/50 (100%)	50 (100%)	0	100	100
20	N	171/171 (100%)	171 (100%)	0	100	100
20	n	171/171 (100%)	171 (100%)	0	100	100
21	G	168/168 (100%)	168 (100%)	0	100	100
21	g	168/168 (100%)	168 (100%)	0	100	100
22	R	151/151 (100%)	151 (100%)	0	100	100
22	r	151/151 (100%)	151 (100%)	0	100	100
23	S	190/190 (100%)	190 (100%)	0	100	100
23	s	190/190 (100%)	190 (100%)	0	100	100
24	Y	167/167 (100%)	167 (100%)	0	100	100
24	y	167/167 (100%)	167 (100%)	0	100	100
25	U	26/26 (100%)	26 (100%)	0	100	100
25	u	26/26 (100%)	26 (100%)	0	100	100
All	All	5934/5934 (100%)	5931 (100%)	3 (0%)	87	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	MET
5	D	243	THR
5	D	264	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	198	HIS
2	B	179	GLN
2	B	343	HIS
2	B	349	GLN
2	B	394	GLN
5	D	83	ASN
5	D	350	ASN
14	O	93	ASN
15	P	71	ASN
15	P	115	ASN
15	P	153	GLN
15	P	203	GLN
15	P	220	GLN
20	N	46	ASN
20	N	241	ASN
22	R	86	GLN
23	S	96	GLN
23	S	150	ASN
23	S	238	ASN
1	a	75	ASN
1	a	108	ASN
1	a	198	HIS
2	b	277	GLN
2	b	394	GLN
2	b	438	GLN
4	c	315	ASN
4	c	403	ASN
5	d	83	ASN
5	d	186	GLN
5	d	236	ASN
5	d	322	ASN
15	p	71	ASN
15	p	121	GLN
19	z	36	ASN
20	n	39	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	n	149	ASN
20	n	241	ASN
21	g	129	ASN
21	g	227	GLN
22	r	204	ASN
24	y	236	ASN
24	y	238	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CSD	b	218	2	4,7,8	1.05	0	1,8,10	0.57	0
22	SEP	R	84	22	8,9,10	1.56	1 (12%)	7,12,14	1.35	1 (14%)
22	SEP	r	84	22	8,9,10	1.58	1 (12%)	7,12,14	1.41	1 (14%)
2	CSD	B	218	2	4,7,8	0.97	0	1,8,10	0.56	0

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
2	CSD	b	218	2	-	1/2/6/8	-
22	SEP	R	84	22	-	2/6/8/10	-
22	SEP	r	84	22	-	4/6/8/10	-
2	CSD	B	218	2	-	1/2/6/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	84	SEP	P-O1P	3.50	1.61	1.50
22	r	84	SEP	P-O1P	3.48	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	r	84	SEP	OG-CB-CA	2.94	111.00	108.14
22	R	84	SEP	OG-CB-CA	2.94	111.00	108.14

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	R	84	SEP	N-CA-CB-OG
22	R	84	SEP	C-CA-CB-OG
22	r	84	SEP	N-CA-CB-OG
22	r	84	SEP	CB-OG-P-O1P
22	r	84	SEP	CB-OG-P-O2P
22	r	84	SEP	CB-OG-P-O3P
2	B	218	CSD	N-CA-CB-SG
2	b	218	CSD	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 354 ligands modelled in this entry, 8 are monoatomic - leaving 346 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
29	CLA	B	515	-	69,73,73	0.99	4 (5%)	82,113,113	0.94	4 (4%)
39	SQD	l	101	-	40,42,54	0.86	0	50,53,65	0.93	3 (6%)
29	CLA	B	511	-	69,73,73	0.98	5 (7%)	82,113,113	1.06	3 (3%)
29	CLA	y	313	37	69,73,73	0.98	4 (5%)	82,113,113	0.97	5 (6%)
46	CHL	y	307	24	40,54,74	1.73	9 (22%)	34,90,114	2.07	10 (29%)
29	CLA	c	511	4	69,73,73	1.00	4 (5%)	82,113,113	1.10	3 (3%)
51	LPX	S	321	-	19,19,29	1.22	2 (10%)	21,23,33	1.06	1 (4%)
29	CLA	C	508	52	69,73,73	0.98	4 (5%)	82,113,113	1.07	3 (3%)
30	PHO	a	407	-	58,69,69	2.05	10 (17%)	55,99,99	1.47	6 (10%)
41	DGA	D	402	-	36,36,43	1.21	2 (5%)	38,38,45	1.33	3 (7%)
36	DGD	c	516	-	56,56,67	1.05	4 (7%)	70,70,81	0.95	2 (2%)
37	LHG	a	414	-	38,38,48	0.42	0	41,44,54	1.10	2 (4%)
29	CLA	b	503	-	69,73,73	0.98	5 (7%)	82,113,113	1.11	5 (6%)
33	3PH	B	522	-	47,47,47	0.87	4 (8%)	50,52,52	1.13	2 (4%)
29	CLA	s	310	-	64,68,73	1.03	4 (6%)	76,107,113	1.04	3 (3%)
29	CLA	c	510	-	69,73,73	0.97	3 (4%)	82,113,113	0.97	5 (6%)
30	PHO	d	402	-	58,69,69	2.11	10 (17%)	55,99,99	1.61	7 (12%)
29	CLA	R	301	22	64,68,73	1.01	4 (6%)	76,107,113	1.09	5 (6%)
35	LMG	C	521	-	47,47,55	1.08	4 (8%)	55,55,63	1.13	4 (7%)
31	BCR	C	515	-	41,41,41	1.62	4 (9%)	56,56,56	4.37	13 (23%)
29	CLA	s	313	23	49,53,73	1.17	4 (8%)	58,89,113	1.10	4 (6%)
29	CLA	s	305	-	59,63,73	1.05	5 (8%)	70,101,113	1.20	3 (4%)
48	NEX	G	617	-	40,46,46	2.67	11 (27%)	50,70,70	1.77	13 (26%)
29	CLA	a	404	-	69,73,73	0.99	4 (5%)	82,113,113	1.10	3 (3%)
29	CLA	C	512	4	69,73,73	1.00	4 (5%)	82,113,113	1.00	5 (6%)
29	CLA	r	304	-	53,57,73	1.11	4 (7%)	61,93,113	1.02	2 (3%)
39	SQD	c	522	-	52,54,54	0.78	0	62,65,65	0.83	2 (3%)
29	CLA	S	306	23	54,58,73	1.12	5 (9%)	64,95,113	1.29	5 (7%)
31	BCR	f	101	-	41,41,41	1.60	4 (9%)	56,56,56	4.44	18 (32%)
29	CLA	a	408	-	64,68,73	1.01	6 (9%)	76,107,113	1.11	5 (6%)
29	CLA	R	303	-	53,57,73	1.11	4 (7%)	61,93,113	0.97	1 (1%)
46	CHL	G	609	21	60,74,74	1.45	9 (15%)	58,114,114	1.62	13 (22%)
29	CLA	b	516	-	69,73,73	1.00	6 (8%)	82,113,113	1.02	5 (6%)
48	NEX	s	319	-	40,46,46	2.70	11 (27%)	50,70,70	1.54	8 (16%)
29	CLA	b	501	-	69,73,73	0.98	4 (5%)	82,113,113	1.00	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	b	515	-	69,73,73	0.99	4 (5%)	82,113,113	0.96	4 (4%)
31	BCR	c	514	-	41,41,41	1.62	5 (12%)	56,56,56	4.33	19 (33%)
29	CLA	R	309	-	54,58,73	1.13	5 (9%)	64,95,113	1.14	6 (9%)
31	BCR	K	101	-	41,41,41	1.60	4 (9%)	56,56,56	4.41	14 (25%)
29	CLA	d	403	-	69,73,73	0.97	5 (7%)	82,113,113	1.03	3 (3%)
29	CLA	R	307	22	50,54,73	1.13	4 (8%)	59,90,113	1.13	6 (10%)
47	LUT	n	615	-	42,43,43	2.42	1 (2%)	51,60,60	1.68	10 (19%)
29	CLA	s	304	-	69,73,73	1.05	7 (10%)	82,113,113	1.24	6 (7%)
29	CLA	G	604	-	53,57,73	1.13	4 (7%)	61,93,113	1.05	5 (8%)
46	CHL	S	302	23	40,54,74	1.82	8 (20%)	34,90,114	2.17	11 (32%)
29	CLA	Y	304	-	69,73,73	0.98	4 (5%)	82,113,113	0.99	5 (6%)
41	DGA	W	202	-	43,43,43	1.15	3 (6%)	45,45,45	1.50	3 (6%)
46	CHL	R	305	-	44,58,74	1.62	9 (20%)	37,94,114	2.12	11 (29%)
29	CLA	Y	315	-	69,73,73	0.97	4 (5%)	82,113,113	1.08	6 (7%)
29	CLA	C	502	-	69,73,73	0.97	4 (5%)	82,113,113	1.01	5 (6%)
29	CLA	G	603	-	69,73,73	0.99	4 (5%)	82,113,113	0.99	5 (6%)
29	CLA	c	501	-	69,73,73	0.97	4 (5%)	82,113,113	1.05	6 (7%)
29	CLA	B	505	-	69,73,73	0.99	4 (5%)	82,113,113	1.15	4 (4%)
29	CLA	G	612	21	47,51,73	1.16	4 (8%)	55,86,113	1.07	3 (5%)
37	LHG	B	523	-	43,43,48	0.41	0	46,49,54	1.04	2 (4%)
47	LUT	g	616	-	42,43,43	2.47	1 (2%)	51,60,60	1.93	12 (23%)
38	LMT	B	524	-	36,36,36	1.19	6 (16%)	47,47,47	1.19	5 (10%)
49	XAT	N	619	-	41,47,47	0.69	1 (2%)	54,74,74	1.98	13 (24%)
29	CLA	b	507	52	69,73,73	0.98	4 (5%)	82,113,113	1.08	2 (2%)
43	PL9	D	406	-	55,55,55	1.31	5 (9%)	68,69,69	1.44	11 (16%)
34	C7Z	b	519	-	43,43,43	5.37	26 (60%)	56,60,60	2.47	23 (41%)
35	LMG	C	522	-	55,55,55	1.27	6 (10%)	63,63,63	1.06	2 (3%)
29	CLA	c	504	-	69,73,73	0.96	5 (7%)	82,113,113	1.04	4 (4%)
49	XAT	y	302	-	41,47,47	0.68	1 (2%)	54,74,74	2.04	13 (24%)
46	CHL	S	308	-	37,51,74	1.65	8 (21%)	30,86,114	2.29	10 (33%)
31	BCR	C	516	-	41,41,41	1.61	4 (9%)	56,56,56	4.39	14 (25%)
39	SQD	a	410	-	49,51,54	0.79	0	59,62,65	0.87	2 (3%)
37	LHG	D	407	-	48,48,48	0.41	0	51,54,54	1.01	3 (5%)
40	SPH	c	523	-	19,20,20	0.66	0	18,21,21	1.12	1 (5%)
29	CLA	S	313	23	49,53,73	1.17	4 (8%)	58,89,113	1.03	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	DGD	c	517	-	63,63,67	1.22	7 (11%)	77,77,81	0.95	3 (3%)
29	CLA	g	604	-	53,57,73	1.11	5 (9%)	61,93,113	1.07	3 (4%)
48	NEX	g	617	-	40,46,46	2.65	11 (27%)	50,70,70	1.81	11 (22%)
29	CLA	b	509	-	69,73,73	0.99	5 (7%)	82,113,113	1.07	6 (7%)
46	CHL	Y	302	24	60,74,74	1.17	9 (15%)	58,114,114	1.79	12 (20%)
46	CHL	N	608	-	44,58,74	1.51	7 (15%)	37,94,114	2.04	12 (32%)
29	CLA	N	604	-	69,73,73	0.99	5 (7%)	82,113,113	1.02	5 (6%)
35	LMG	c	520	-	55,55,55	1.28	6 (10%)	63,63,63	1.03	2 (3%)
29	CLA	g	603	-	69,73,73	0.99	5 (7%)	82,113,113	1.04	4 (4%)
29	CLA	c	502	-	69,73,73	0.98	4 (5%)	82,113,113	1.08	5 (6%)
46	CHL	Y	306	24	40,54,74	1.72	9 (22%)	34,90,114	2.06	10 (29%)
29	CLA	y	316	-	69,73,73	0.98	4 (5%)	82,113,113	1.02	5 (6%)
49	XAT	G	619	-	41,47,47	0.67	1 (2%)	54,74,74	3.77	17 (31%)
29	CLA	g	610	21	69,73,73	0.99	6 (8%)	82,113,113	1.25	6 (7%)
29	CLA	N	612	20	49,53,73	1.17	4 (8%)	58,89,113	1.08	4 (6%)
46	CHL	N	601	20	60,74,74	1.28	8 (13%)	58,114,114	1.79	12 (20%)
47	LUT	S	317	-	42,43,43	2.33	1 (2%)	51,60,60	1.79	12 (23%)
29	CLA	c	505	-	69,73,73	1.00	5 (7%)	82,113,113	1.09	5 (6%)
29	CLA	S	315	-	54,58,73	1.11	4 (7%)	64,95,113	1.07	5 (7%)
29	CLA	Y	303	24	69,73,73	0.99	4 (5%)	82,113,113	1.06	6 (7%)
31	BCR	v	101	-	41,41,41	1.60	4 (9%)	56,56,56	4.45	19 (33%)
29	CLA	R	306	-	64,68,73	1.03	6 (9%)	76,107,113	1.03	2 (2%)
29	CLA	B	512	-	69,73,73	0.98	4 (5%)	82,113,113	1.01	2 (2%)
29	CLA	b	506	-	61,65,73	1.03	5 (8%)	72,103,113	1.11	5 (6%)
29	CLA	y	306	52	69,73,73	0.98	5 (7%)	82,113,113	1.09	5 (6%)
29	CLA	C	504	-	69,73,73	0.99	4 (5%)	82,113,113	0.99	3 (3%)
29	CLA	s	303	23	64,68,73	1.01	4 (6%)	76,107,113	1.13	5 (6%)
29	CLA	G	613	21	69,73,73	0.98	4 (5%)	82,113,113	0.95	2 (2%)
29	CLA	g	613	21	69,73,73	1.00	4 (5%)	82,113,113	0.97	3 (3%)
46	CHL	g	605	21	42,56,74	1.71	9 (21%)	36,92,114	2.15	11 (30%)
37	LHG	y	320	29	48,48,48	0.39	0	51,54,54	1.12	4 (7%)
29	CLA	n	611	20	49,53,73	1.17	4 (8%)	58,89,113	1.14	5 (8%)
46	CHL	s	309	-	55,69,74	1.37	9 (16%)	52,108,114	1.69	9 (17%)
29	CLA	C	513	-	69,73,73	0.99	4 (5%)	82,113,113	0.93	3 (3%)
29	CLA	A	405	-	69,73,73	0.98	4 (5%)	82,113,113	1.00	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	b	511	-	69,73,73	0.98	5 (7%)	82,113,113	1.08	5 (6%)
29	CLA	c	512	-	69,73,73	0.98	4 (5%)	82,113,113	0.99	5 (6%)
46	CHL	n	601	20	60,74,74	1.34	8 (13%)	58,114,114	1.78	12 (20%)
29	CLA	g	602	21	69,73,73	0.97	4 (5%)	82,113,113	1.00	4 (4%)
37	LHG	n	617	-	41,41,48	0.42	0	44,47,54	1.17	4 (9%)
50	PTY	y	321	-	18,18,49	1.33	3 (16%)	21,23,54	1.47	2 (9%)
29	CLA	s	315	-	59,63,73	1.08	5 (8%)	70,101,113	1.05	4 (5%)
29	CLA	a	405	52	69,73,73	0.98	5 (7%)	82,113,113	1.04	6 (7%)
29	CLA	d	404	-	69,73,73	0.99	4 (5%)	82,113,113	1.10	7 (8%)
42	BCT	D	403	27	3,3,3	1.05	0	2,3,3	1.24	0
46	CHL	G	601	21	60,74,74	1.35	9 (15%)	58,114,114	1.71	11 (18%)
29	CLA	N	614	-	53,57,73	1.13	4 (7%)	61,93,113	1.07	6 (9%)
35	LMG	i	101	-	48,48,55	1.11	5 (10%)	56,56,63	1.08	3 (5%)
29	CLA	S	304	-	69,73,73	1.03	6 (8%)	82,113,113	1.21	10 (12%)
37	LHG	Y	319	29	48,48,48	0.40	0	51,54,54	1.00	2 (3%)
31	BCR	B	517	-	41,41,41	1.66	5 (12%)	56,56,56	4.38	19 (33%)
36	DGD	C	519	-	54,54,67	1.07	4 (7%)	68,68,81	0.92	3 (4%)
46	CHL	s	308	-	37,51,74	1.72	9 (24%)	30,86,114	2.34	11 (36%)
48	NEX	r	313	-	25,28,46	2.60	7 (28%)	32,42,70	1.78	6 (18%)
47	LUT	Y	316	-	42,43,43	2.46	1 (2%)	51,60,60	1.77	16 (31%)
37	LHG	D	408	-	38,38,48	0.42	0	41,44,54	1.06	3 (7%)
46	CHL	G	607	-	60,74,74	1.19	7 (11%)	58,114,114	1.77	12 (20%)
46	CHL	g	609	21	60,74,74	1.47	10 (16%)	58,114,114	1.62	12 (20%)
49	XAT	r	312	-	41,47,47	0.65	1 (2%)	54,74,74	1.88	12 (22%)
29	CLA	R	302	-	64,68,73	1.05	6 (9%)	76,107,113	1.12	6 (7%)
50	PTY	Y	320	-	18,18,49	1.33	3 (16%)	21,23,54	1.50	2 (9%)
46	CHL	n	605	20	60,74,74	1.66	9 (15%)	58,114,114	1.66	11 (18%)
46	CHL	g	608	-	38,52,74	1.73	9 (23%)	31,87,114	2.17	10 (32%)
46	CHL	y	303	24	60,74,74	1.38	10 (16%)	58,114,114	1.74	12 (20%)
37	LHG	S	320	29	44,44,48	0.41	0	47,50,54	1.05	3 (6%)
46	CHL	y	301	-	60,74,74	1.26	7 (11%)	58,114,114	1.73	12 (20%)
29	CLA	y	304	24	69,73,73	1.00	4 (5%)	82,113,113	1.10	6 (7%)
29	CLA	c	506	-	64,68,73	1.01	3 (4%)	76,107,113	1.10	6 (7%)
30	PHO	A	408	-	58,69,69	2.10	10 (17%)	55,99,99	1.50	7 (12%)
47	LUT	r	311	-	42,43,43	2.54	2 (4%)	51,60,60	1.84	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	SQD	L	102	-	40,42,54	0.85	0	50,53,65	0.89	2 (4%)
35	LMG	d	407	-	46,46,55	1.03	4 (8%)	54,54,63	1.06	2 (3%)
29	CLA	n	610	-	53,57,73	1.14	5 (9%)	61,93,113	1.04	4 (6%)
29	CLA	G	614	-	53,57,73	1.12	4 (7%)	61,93,113	1.06	3 (4%)
29	CLA	r	309	22	64,68,73	1.02	4 (6%)	76,107,113	1.17	7 (9%)
41	DGA	J	101	-	28,28,43	1.31	3 (10%)	30,30,45	1.26	2 (6%)
29	CLA	A	407	-	54,58,73	1.09	4 (7%)	64,95,113	1.09	6 (9%)
29	CLA	S	312	37	69,73,73	1.00	4 (5%)	82,113,113	1.07	4 (4%)
37	LHG	l	102	-	48,48,48	0.40	0	51,54,54	1.01	2 (3%)
46	CHL	y	309	-	60,74,74	1.10	7 (11%)	58,114,114	1.80	12 (20%)
29	CLA	B	504	-	69,73,73	1.00	3 (4%)	82,113,113	1.24	6 (7%)
29	CLA	B	514	-	69,73,73	0.99	4 (5%)	82,113,113	1.07	5 (6%)
37	LHG	d	406	-	48,48,48	0.40	0	51,54,54	1.02	3 (5%)
29	CLA	y	305	-	69,73,73	0.98	4 (5%)	82,113,113	1.00	4 (4%)
46	CHL	y	308	52	45,59,74	1.61	8 (17%)	40,96,114	1.91	12 (30%)
29	CLA	C	510	-	69,73,73	0.99	4 (5%)	82,113,113	1.02	4 (4%)
47	LUT	S	318	-	42,43,43	2.40	1 (2%)	51,60,60	1.82	13 (25%)
46	CHL	Y	307	-	60,74,74	1.58	10 (16%)	58,114,114	1.63	10 (17%)
42	BCT	a	412	27	3,3,3	0.59	0	2,3,3	5.12	2 (100%)
29	CLA	C	506	-	64,68,73	1.03	6 (9%)	76,107,113	1.06	4 (5%)
29	CLA	r	302	22	64,68,73	1.01	4 (6%)	76,107,113	1.10	5 (6%)
29	CLA	y	312	24	69,73,73	0.99	6 (8%)	82,113,113	1.08	5 (6%)
31	BCR	z	101	-	41,41,41	1.61	4 (9%)	56,56,56	4.45	11 (19%)
29	CLA	g	614	-	53,57,73	1.12	4 (7%)	61,93,113	1.09	4 (6%)
47	LUT	Y	317	-	42,43,43	2.45	1 (2%)	51,60,60	1.84	13 (25%)
37	LHG	G	618	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
35	LMG	d	408	-	48,48,55	1.12	5 (10%)	56,56,63	1.13	2 (3%)
37	LHG	N	618	29	48,48,48	0.40	0	51,54,54	1.07	5 (9%)
47	LUT	N	615	-	42,43,43	2.45	1 (2%)	51,60,60	1.74	13 (25%)
29	CLA	s	314	23	59,63,73	1.08	5 (8%)	70,101,113	1.11	4 (5%)
47	LUT	g	615	-	42,43,43	2.41	1 (2%)	51,60,60	1.82	15 (29%)
29	CLA	Y	305	52	69,73,73	0.98	4 (5%)	82,113,113	0.99	5 (6%)
48	NEX	y	319	-	40,46,46	2.67	12 (30%)	50,70,70	1.74	11 (22%)
41	DGA	j	101	-	28,28,43	1.30	3 (10%)	30,30,45	1.29	2 (6%)
47	LUT	n	614	-	42,43,43	2.44	1 (2%)	51,60,60	1.80	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	SQD	m	101	-	40,42,54	0.88	0	50,53,65	0.88	2 (4%)
29	CLA	C	503	-	69,73,73	0.98	4 (5%)	82,113,113	1.08	4 (4%)
49	XAT	R	311	-	41,47,47	0.66	1 (2%)	54,74,74	1.86	13 (24%)
47	LUT	s	318	-	42,43,43	2.38	1 (2%)	51,60,60	1.81	11 (21%)
29	CLA	y	314	24	69,73,73	0.98	5 (7%)	82,113,113	1.03	6 (7%)
36	DGD	C	520	-	54,54,67	1.00	4 (7%)	68,68,81	0.91	2 (2%)
35	LMG	W	203	-	39,39,55	0.94	2 (5%)	47,47,63	1.17	3 (6%)
29	CLA	C	505	52	59,63,73	1.04	4 (6%)	70,101,113	1.07	2 (2%)
29	CLA	B	508	-	69,73,73	1.01	5 (7%)	82,113,113	0.99	4 (4%)
50	PTY	N	620	-	49,49,49	0.89	4 (8%)	52,54,54	1.06	2 (3%)
29	CLA	s	311	23	69,73,73	1.00	6 (8%)	82,113,113	1.08	6 (7%)
46	CHL	r	305	-	38,52,74	1.72	9 (23%)	31,87,114	2.19	11 (35%)
35	LMG	W	201	-	40,40,55	0.84	2 (5%)	48,48,63	1.16	4 (8%)
30	PHO	D	401	-	58,69,69	2.13	10 (17%)	55,99,99	1.54	7 (12%)
29	CLA	C	511	-	69,73,73	0.97	4 (5%)	82,113,113	0.94	2 (2%)
29	CLA	B	509	-	69,73,73	0.98	6 (8%)	82,113,113	1.03	5 (6%)
29	CLA	D	405	-	64,68,73	1.03	4 (6%)	76,107,113	1.14	6 (7%)
45	RRX	h	101	-	42,42,42	5.01	24 (57%)	56,58,58	2.53	21 (37%)
29	CLA	B	506	-	69,73,73	0.99	4 (5%)	82,113,113	1.07	5 (6%)
44	HEM	E	101	7,6	50,50,50	1.41	7 (14%)	67,82,82	1.06	1 (1%)
35	LMG	D	409	-	42,42,55	0.84	2 (4%)	50,50,63	0.98	2 (4%)
47	LUT	R	310	-	42,43,43	2.48	1 (2%)	51,60,60	1.96	14 (27%)
29	CLA	n	603	-	69,73,73	0.98	4 (5%)	82,113,113	1.01	5 (6%)
48	NEX	n	616	-	40,46,46	2.70	11 (27%)	50,70,70	1.50	9 (18%)
47	LUT	N	616	-	42,43,43	2.44	1 (2%)	51,60,60	1.74	12 (23%)
29	CLA	s	306	23	54,58,73	1.10	5 (9%)	64,95,113	1.22	8 (12%)
29	CLA	N	610	-	69,73,73	0.99	5 (7%)	82,113,113	1.10	4 (4%)
29	CLA	b	508	-	69,73,73	0.99	5 (7%)	82,113,113	1.00	4 (4%)
37	LHG	L	101	-	48,48,48	0.39	0	51,54,54	1.24	3 (5%)
47	LUT	G	615	-	42,43,43	2.46	1 (2%)	51,60,60	1.75	12 (23%)
35	LMG	B	520	-	44,44,55	0.96	3 (6%)	52,52,63	1.09	3 (5%)
31	BCR	B	518	-	41,41,41	1.66	5 (12%)	56,56,56	4.29	13 (23%)
41	DGA	w	201	-	43,43,43	1.15	3 (6%)	45,45,45	1.51	3 (6%)
35	LMG	D	410	-	48,48,55	1.11	5 (10%)	56,56,63	1.10	2 (3%)
46	CHL	G	608	-	38,52,74	1.86	9 (23%)	31,87,114	2.21	11 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	CHL	R	304	-	38,52,74	1.70	9 (23%)	31,87,114	2.25	11 (35%)
26	OEX	a	401	52,1,4	0,15,15	-	-	-		
36	DGD	c	518	-	60,60,67	1.16	6 (10%)	74,74,81	0.97	2 (2%)
46	CHL	Y	308	-	60,74,74	1.14	7 (11%)	58,114,114	1.80	12 (20%)
29	CLA	N	611	37	53,57,73	1.14	5 (9%)	61,93,113	1.11	6 (9%)
29	CLA	s	312	37	69,73,73	0.99	5 (7%)	82,113,113	1.11	5 (6%)
29	CLA	b	512	-	69,73,73	0.98	5 (7%)	82,113,113	0.99	4 (4%)
29	CLA	C	507	-	69,73,73	0.98	4 (5%)	82,113,113	0.99	3 (3%)
46	CHL	s	307	-	38,52,74	1.62	8 (21%)	31,87,114	2.26	11 (35%)
29	CLA	Y	312	37	69,73,73	0.97	4 (5%)	82,113,113	1.00	6 (7%)
44	HEM	e	101	7,6	50,50,50	1.39	8 (16%)	67,82,82	1.05	1 (1%)
49	XAT	n	618	-	41,47,47	0.70	1 (2%)	54,74,74	2.02	12 (22%)
46	CHL	g	601	21	60,74,74	1.35	9 (15%)	58,114,114	1.66	11 (18%)
29	CLA	c	508	-	69,73,73	0.97	5 (7%)	82,113,113	1.02	5 (6%)
39	SQD	o	301	-	52,54,54	0.79	0	62,65,65	0.85	2 (3%)
31	BCR	F	101	-	41,41,41	1.61	4 (9%)	56,56,56	4.30	13 (23%)
29	CLA	S	303	23	64,68,73	1.02	4 (6%)	76,107,113	0.99	5 (6%)
39	SQD	M	101	-	40,42,54	0.87	0	50,53,65	0.88	2 (4%)
29	CLA	y	315	24	69,73,73	0.98	4 (5%)	82,113,113	0.95	3 (3%)
46	CHL	y	311	24	60,74,74	1.27	8 (13%)	58,114,114	1.74	13 (22%)
46	CHL	g	607	-	60,74,74	1.33	7 (11%)	58,114,114	1.75	12 (20%)
37	LHG	c	521	-	46,46,48	0.40	0	49,52,54	1.05	2 (4%)
29	CLA	n	613	-	53,57,73	1.10	4 (7%)	61,93,113	1.16	3 (4%)
47	LUT	y	318	-	42,43,43	2.45	1 (2%)	51,60,60	1.86	12 (23%)
31	BCR	c	515	-	41,41,41	1.62	4 (9%)	56,56,56	4.43	20 (35%)
29	CLA	A	406	52	69,73,73	0.98	4 (5%)	82,113,113	1.10	6 (7%)
48	NEX	N	617	-	40,46,46	2.67	11 (27%)	50,70,70	1.52	9 (18%)
29	CLA	g	611	37	69,73,73	1.00	5 (7%)	82,113,113	1.07	6 (7%)
29	CLA	G	611	-	69,73,73	1.01	5 (7%)	82,113,113	1.09	5 (6%)
29	CLA	a	406	52	53,57,73	1.08	5 (9%)	61,93,113	1.16	5 (8%)
29	CLA	B	502	-	69,73,73	0.97	4 (5%)	82,113,113	1.06	5 (6%)
29	CLA	N	602	20	69,73,73	0.98	5 (7%)	82,113,113	0.99	7 (8%)
38	LMT	b	524	-	36,36,36	1.22	6 (16%)	47,47,47	1.17	4 (8%)
29	CLA	b	502	-	69,73,73	0.96	4 (5%)	82,113,113	1.02	5 (6%)
46	CHL	r	306	-	44,58,74	1.58	9 (20%)	37,94,114	2.15	11 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	NEX	Y	318	-	40,46,46	2.67	11 (27%)	50,70,70	1.81	11 (22%)
36	DGD	B	521	-	44,44,67	0.86	1 (2%)	58,58,81	1.15	5 (8%)
46	CHL	Y	310	24	60,74,74	1.37	9 (15%)	58,114,114	1.67	12 (20%)
29	CLA	b	513	-	69,73,73	0.98	5 (7%)	82,113,113	0.97	3 (3%)
29	CLA	y	310	-	54,58,73	1.11	5 (9%)	64,95,113	1.10	5 (7%)
40	SPH	i	102	-	19,20,20	0.66	0	18,21,21	1.09	1 (5%)
47	LUT	s	317	-	42,43,43	2.45	1 (2%)	51,60,60	1.88	15 (29%)
37	LHG	a	413	-	43,43,48	0.41	0	46,49,54	1.06	2 (4%)
48	NEX	R	312	-	25,28,46	2.61	6 (24%)	32,42,70	1.71	7 (21%)
29	CLA	c	509	-	69,73,73	0.99	4 (5%)	82,113,113	1.06	4 (4%)
29	CLA	B	501	-	69,73,73	0.98	4 (5%)	82,113,113	1.01	5 (6%)
47	LUT	y	317	-	42,43,43	2.47	1 (2%)	51,60,60	1.74	15 (29%)
31	BCR	A	410	-	41,41,41	1.64	5 (12%)	56,56,56	4.45	14 (25%)
50	PTY	n	619	-	49,49,49	0.89	4 (8%)	52,54,54	1.06	2 (3%)
31	BCR	b	517	-	41,41,41	1.63	4 (9%)	56,56,56	4.39	13 (23%)
36	DGD	r	301	-	44,44,67	0.86	1 (2%)	58,58,81	1.20	5 (8%)
46	CHL	N	607	-	60,74,74	1.44	9 (15%)	58,114,114	1.67	10 (17%)
29	CLA	R	308	22	64,68,73	1.02	4 (6%)	76,107,113	1.09	6 (7%)
46	CHL	N	609	20	60,74,74	1.32	8 (13%)	58,114,114	1.75	13 (22%)
29	CLA	n	612	20	69,73,73	0.99	4 (5%)	82,113,113	1.02	2 (2%)
51	LPX	s	321	-	18,18,29	1.26	2 (11%)	20,22,33	1.05	1 (5%)
46	CHL	S	307	-	38,52,74	1.86	9 (23%)	31,87,114	2.16	10 (32%)
29	CLA	Y	311	24	69,73,73	0.98	5 (7%)	82,113,113	1.08	5 (6%)
49	XAT	Y	301	-	41,47,47	0.68	1 (2%)	54,74,74	2.02	12 (22%)
49	XAT	g	619	-	41,47,47	0.68	1 (2%)	54,74,74	3.76	16 (29%)
29	CLA	r	303	-	64,68,73	1.05	5 (7%)	76,107,113	1.15	7 (9%)
29	CLA	c	507	52	69,73,73	0.99	5 (7%)	82,113,113	1.06	4 (4%)
29	CLA	G	602	21	69,73,73	0.98	4 (5%)	82,113,113	0.96	5 (6%)
33	3PH	s	322	-	47,47,47	0.87	4 (8%)	50,52,52	1.12	2 (4%)
37	LHG	g	618	29	48,48,48	0.39	0	51,54,54	1.05	4 (7%)
29	CLA	b	514	-	69,73,73	0.99	4 (5%)	82,113,113	1.06	6 (7%)
29	CLA	B	516	-	59,63,73	1.08	6 (10%)	70,101,113	1.11	5 (7%)
37	LHG	s	320	29	44,44,48	0.42	0	47,50,54	1.04	3 (6%)
39	SQD	b	523	-	52,54,54	0.79	0	62,65,65	0.83	2 (3%)
46	CHL	N	606	-	60,74,74	1.44	8 (13%)	58,114,114	1.76	13 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	3PH	a	415	-	47,47,47	0.86	4 (8%)	50,52,52	1.20	2 (4%)
31	BCR	C	517	-	41,41,41	1.61	4 (9%)	56,56,56	4.41	17 (30%)
46	CHL	n	606	-	60,74,74	1.53	10 (16%)	58,114,114	1.77	11 (18%)
43	PL9	d	405	-	55,55,55	1.27	5 (9%)	68,69,69	1.47	12 (17%)
31	BCR	a	409	-	41,41,41	1.64	5 (12%)	56,56,56	4.43	13 (23%)
29	CLA	n	609	20	69,73,73	0.99	6 (8%)	82,113,113	1.16	6 (7%)
37	LHG	S	301	-	34,34,48	0.44	0	37,40,54	1.19	2 (5%)
29	CLA	b	504	-	69,73,73	1.01	5 (7%)	82,113,113	1.24	6 (7%)
41	DGA	b	522	-	43,43,43	1.13	2 (4%)	45,45,45	1.53	3 (6%)
29	CLA	r	310	-	55,59,73	1.14	4 (7%)	64,96,113	1.22	6 (9%)
29	CLA	C	509	-	69,73,73	0.96	5 (7%)	82,113,113	1.04	6 (7%)
29	CLA	Y	309	52	54,58,73	1.09	5 (9%)	64,95,113	1.11	4 (6%)
35	LMG	b	520	-	44,44,55	0.97	3 (6%)	52,52,63	1.08	2 (3%)
29	CLA	g	612	21	47,51,73	1.16	5 (10%)	55,86,113	1.12	3 (5%)
35	LMG	w	202	-	39,39,55	0.95	2 (5%)	47,47,63	1.07	2 (4%)
29	CLA	c	503	-	69,73,73	0.99	5 (7%)	82,113,113	1.04	4 (4%)
39	SQD	C	523	-	34,36,54	0.93	0	44,47,65	0.96	2 (4%)
29	CLA	B	513	-	69,73,73	0.98	5 (7%)	82,113,113	0.95	3 (3%)
29	CLA	S	310	23	64,68,73	1.03	4 (6%)	76,107,113	1.10	5 (6%)
34	C7Z	B	519	-	43,43,43	5.38	26 (60%)	56,60,60	2.51	22 (39%)
35	LMG	c	519	-	51,51,55	1.21	6 (11%)	59,59,63	1.13	3 (5%)
45	RRX	H	101	-	42,42,42	5.00	24 (57%)	56,58,58	2.62	21 (37%)
37	LHG	s	301	-	37,37,48	0.44	0	40,43,54	1.18	4 (10%)
29	CLA	D	404	-	69,73,73	3.26	29 (42%)	82,113,113	3.77	34 (41%)
33	3PH	A	412	-	47,47,47	0.85	4 (8%)	50,52,52	1.14	2 (4%)
29	CLA	r	308	22	64,68,73	1.04	3 (4%)	76,107,113	1.02	4 (5%)
46	CHL	g	606	-	44,58,74	1.86	10 (22%)	37,94,114	2.08	13 (35%)
29	CLA	s	316	23	54,58,73	1.13	5 (9%)	64,95,113	1.21	7 (10%)
26	OEX	A	401	52,1,4	0,15,15	-	-	-	-	-
46	CHL	S	309	-	55,69,74	1.48	10 (18%)	52,108,114	1.77	12 (23%)
40	SPH	C	525	-	19,20,20	0.65	0	18,21,21	1.10	1 (5%)
29	CLA	n	604	-	69,73,73	0.99	5 (7%)	82,113,113	0.96	5 (6%)
29	CLA	S	314	23	59,63,73	1.08	4 (6%)	70,101,113	1.16	5 (7%)
29	CLA	S	305	-	59,63,73	1.07	5 (8%)	70,101,113	1.04	2 (2%)
29	CLA	Y	313	24	69,73,73	0.98	4 (5%)	82,113,113	0.97	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	b	505	-	69,73,73	0.99	4 (5%)	82,113,113	1.13	4 (4%)
46	CHL	s	302	23	40,54,74	1.76	9 (22%)	34,90,114	2.11	11 (32%)
29	CLA	A	409	-	64,68,73	1.01	6 (9%)	76,107,113	1.13	5 (6%)
29	CLA	B	507	52	69,73,73	0.97	4 (5%)	82,113,113	1.02	2 (2%)
47	LUT	G	616	-	42,43,43	2.44	1 (2%)	51,60,60	1.78	10 (19%)
46	CHL	N	605	20	60,74,74	1.34	8 (13%)	58,114,114	1.73	10 (17%)
31	BCR	b	518	-	41,41,41	1.66	5 (12%)	56,56,56	4.29	13 (23%)
46	CHL	n	608	20	60,74,74	1.28	8 (13%)	58,114,114	1.72	12 (20%)
29	CLA	r	307	-	64,68,73	1.01	5 (7%)	76,107,113	1.09	4 (5%)
29	CLA	c	513	-	69,73,73	0.97	4 (5%)	82,113,113	1.04	3 (3%)
29	CLA	n	602	20	69,73,73	0.99	4 (5%)	82,113,113	1.08	7 (8%)
29	CLA	B	503	-	69,73,73	0.98	5 (7%)	82,113,113	1.10	5 (6%)
33	3PH	S	322	-	29,29,47	1.10	4 (13%)	32,34,52	1.28	2 (6%)
46	CHL	G	606	-	44,58,74	1.67	8 (18%)	37,94,114	2.17	12 (32%)
29	CLA	Y	314	24	69,73,73	0.98	4 (5%)	82,113,113	0.93	3 (3%)
29	CLA	N	603	-	69,73,73	1.01	4 (5%)	82,113,113	0.95	3 (3%)
46	CHL	n	607	-	44,58,74	1.57	7 (15%)	37,94,114	2.03	12 (32%)
36	DGD	C	518	-	52,52,67	1.10	4 (7%)	66,66,81	0.94	2 (3%)
29	CLA	S	311	23	69,73,73	0.98	4 (5%)	82,113,113	1.05	5 (6%)
46	CHL	G	605	21	42,56,74	1.53	8 (19%)	36,92,114	2.22	12 (33%)
35	LMG	C	524	-	42,42,55	0.86	2 (4%)	50,50,63	1.19	4 (8%)
39	SQD	C	501	-	40,42,54	0.86	0	50,53,65	0.92	2 (4%)
48	NEX	S	319	-	40,46,46	2.68	11 (27%)	50,70,70	1.77	13 (26%)
40	SPH	I	101	-	19,20,20	0.66	0	18,21,21	1.08	1 (5%)
29	CLA	B	510	52	69,73,73	0.98	4 (5%)	82,113,113	0.99	5 (6%)
29	CLA	G	610	21	69,73,73	0.99	5 (7%)	82,113,113	1.19	6 (7%)
29	CLA	C	514	-	69,73,73	0.98	4 (5%)	82,113,113	1.00	2 (2%)
29	CLA	b	510	52	69,73,73	0.98	3 (4%)	82,113,113	0.96	3 (3%)
29	CLA	S	316	23	54,58,73	1.14	5 (9%)	64,95,113	1.27	7 (10%)
33	3PH	b	521	-	38,38,47	0.97	4 (10%)	41,43,52	1.20	2 (4%)
29	CLA	N	613	20	69,73,73	1.01	5 (7%)	82,113,113	1.01	4 (4%)

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
29	CLA	B	515	-	1/1/15/20	10/39/115/115	-
39	SQD	l	101	-	-	14/37/57/69	0/1/1/1
29	CLA	B	511	-	-	11/39/115/115	-
29	CLA	y	313	37	1/1/15/20	7/39/115/115	-
46	CHL	y	307	24	3/3/16/26	3/15/113/137	-
29	CLA	c	511	4	-	10/39/115/115	-
51	LPX	S	321	-	-	6/21/21/31	-
29	CLA	C	508	52	1/1/15/20	11/39/115/115	-
30	PHO	a	407	-	-	5/37/103/103	0/5/6/6
41	DGA	D	402	-	-	19/38/38/45	-
36	DGD	c	516	-	-	10/44/84/95	0/2/2/2
37	LHG	a	414	-	-	21/43/43/53	-
29	CLA	b	503	-	1/1/15/20	9/39/115/115	-
33	3PH	B	522	-	-	20/49/49/49	-
29	CLA	s	310	-	1/1/14/20	16/33/109/115	-
29	CLA	c	510	-	1/1/15/20	9/39/115/115	-
30	PHO	d	402	-	-	5/37/103/103	0/5/6/6
29	CLA	R	301	22	1/1/14/20	6/33/109/115	-
35	LMG	C	521	-	-	9/42/62/70	0/1/1/1
31	BCR	C	515	-	-	13/29/63/63	0/2/2/2
29	CLA	s	313	23	1/1/11/20	2/15/91/115	-
29	CLA	s	305	-	1/1/13/20	14/27/103/115	-
48	NEX	G	617	-	-	4/27/83/83	0/3/3/3
29	CLA	a	404	-	1/1/15/20	12/39/115/115	-
29	CLA	C	512	4	1/1/15/20	6/39/115/115	-
29	CLA	r	304	-	1/1/11/20	11/20/96/115	-
39	SQD	c	522	-	-	15/49/69/69	0/1/1/1
29	CLA	S	306	23	1/1/12/20	8/21/97/115	-
31	BCR	f	101	-	-	11/29/63/63	0/2/2/2
29	CLA	a	408	-	-	8/33/109/115	-
29	CLA	R	303	-	1/1/11/20	8/20/96/115	-
46	CHL	G	609	21	4/4/20/26	9/39/137/137	-
29	CLA	b	516	-	1/1/15/20	14/39/115/115	-
48	NEX	s	319	-	-	2/27/83/83	0/3/3/3
29	CLA	b	501	-	1/1/15/20	21/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	b	515	-	1/1/15/20	10/39/115/115	-
31	BCR	c	514	-	-	13/29/63/63	0/2/2/2
29	CLA	R	309	-	1/1/12/20	9/21/97/115	-
31	BCR	K	101	-	-	11/29/63/63	0/2/2/2
29	CLA	d	403	-	1/1/15/20	7/39/115/115	-
29	CLA	R	307	22	1/1/11/20	8/17/93/115	-
47	LUT	n	615	-	-	2/29/67/67	0/2/2/2
29	CLA	s	304	-	-	17/39/115/115	-
29	CLA	G	604	-	1/1/11/20	9/20/96/115	-
46	CHL	S	302	23	3/3/16/26	3/15/113/137	-
29	CLA	Y	304	-	1/1/15/20	15/39/115/115	-
41	DGA	W	202	-	-	22/45/45/45	-
46	CHL	R	305	-	3/3/16/26	3/20/118/137	-
29	CLA	Y	315	-	1/1/15/20	14/39/115/115	-
29	CLA	G	603	-	1/1/15/20	9/39/115/115	-
29	CLA	C	502	-	-	14/39/115/115	-
29	CLA	c	501	-	-	14/39/115/115	-
29	CLA	B	505	-	1/1/15/20	7/39/115/115	-
29	CLA	G	612	21	1/1/10/20	3/13/89/115	-
37	LHG	B	523	-	-	15/48/48/53	-
47	LUT	g	616	-	-	2/29/67/67	0/2/2/2
38	LMT	B	524	-	-	2/21/61/61	0/2/2/2
49	XAT	N	619	-	2/2/12/26	1/31/93/93	0/4/4/4
29	CLA	b	507	52	1/1/15/20	6/39/115/115	-
43	PL9	D	406	-	-	10/53/73/73	0/1/1/1
34	C7Z	b	519	-	1/1/12/26	7/29/67/67	0/2/2/2
35	LMG	C	522	-	-	21/50/70/70	0/1/1/1
29	CLA	c	504	-	1/1/15/20	11/39/115/115	-
49	XAT	y	302	-	1/1/12/26	0/31/93/93	0/4/4/4
46	CHL	S	308	-	3/3/15/26	2/12/110/137	-
31	BCR	C	516	-	-	10/29/63/63	0/2/2/2
39	SQD	a	410	-	-	16/46/66/69	0/1/1/1
37	LHG	D	407	-	-	18/53/53/53	-
40	SPH	c	523	-	-	4/21/21/21	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	S	313	23	1/1/11/20	2/15/91/115	-
36	DGD	c	517	-	-	18/51/91/95	0/2/2/2
29	CLA	g	604	-	1/1/11/20	7/20/96/115	-
48	NEX	g	617	-	-	5/27/83/83	0/3/3/3
29	CLA	b	509	-	1/1/15/20	7/39/115/115	-
46	CHL	Y	302	24	4/4/20/26	3/39/137/137	-
46	CHL	N	608	-	3/3/16/26	4/20/118/137	-
29	CLA	N	604	-	1/1/15/20	8/39/115/115	-
35	LMG	c	520	-	-	13/50/70/70	0/1/1/1
29	CLA	g	603	-	1/1/15/20	19/39/115/115	-
29	CLA	c	502	-	1/1/15/20	9/39/115/115	-
46	CHL	Y	306	24	3/3/16/26	5/15/113/137	-
29	CLA	y	316	-	1/1/15/20	15/39/115/115	-
49	XAT	G	619	-	1/1/12/26	0/31/93/93	0/4/4/4
29	CLA	g	610	21	1/1/15/20	7/39/115/115	-
29	CLA	N	612	20	1/1/11/20	5/15/91/115	-
46	CHL	N	601	20	4/4/20/26	8/39/137/137	-
47	LUT	S	317	-	-	3/29/67/67	0/2/2/2
29	CLA	c	505	-	1/1/15/20	16/39/115/115	-
29	CLA	S	315	-	1/1/12/20	8/21/97/115	-
29	CLA	Y	303	24	1/1/15/20	14/39/115/115	-
31	BCR	v	101	-	-	10/29/63/63	0/2/2/2
29	CLA	R	306	-	1/1/14/20	12/33/109/115	-
29	CLA	B	512	-	1/1/15/20	8/39/115/115	-
29	CLA	b	506	-	1/1/13/20	11/30/106/115	-
29	CLA	y	306	52	1/1/15/20	13/39/115/115	-
29	CLA	C	504	-	-	10/39/115/115	-
29	CLA	s	303	23	1/1/14/20	7/33/109/115	-
29	CLA	G	613	21	1/1/15/20	9/39/115/115	-
29	CLA	g	613	21	-	15/39/115/115	-
46	CHL	g	605	21	3/3/16/26	2/18/116/137	-
37	LHG	y	320	29	-	27/53/53/53	-
29	CLA	n	611	20	1/1/11/20	7/15/91/115	-
46	CHL	s	309	-	4/4/19/26	6/33/131/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	C	513	-	1/1/15/20	16/39/115/115	-
29	CLA	A	405	-	1/1/15/20	12/39/115/115	-
29	CLA	c	512	-	1/1/15/20	15/39/115/115	-
29	CLA	b	511	-	-	13/39/115/115	-
46	CHL	n	601	20	4/4/20/26	10/39/137/137	-
29	CLA	g	602	21	1/1/15/20	16/39/115/115	-
37	LHG	n	617	-	-	29/46/46/53	-
50	PTY	y	321	-	-	13/20/20/53	-
29	CLA	s	315	-	1/1/13/20	4/27/103/115	-
29	CLA	a	405	52	1/1/15/20	12/39/115/115	-
29	CLA	d	404	-	1/1/15/20	11/39/115/115	-
46	CHL	G	601	21	4/4/20/26	9/39/137/137	-
29	CLA	N	614	-	1/1/11/20	8/20/96/115	-
35	LMG	i	101	-	-	19/43/63/70	0/1/1/1
29	CLA	S	304	-	1/1/15/20	18/39/115/115	-
37	LHG	Y	319	29	-	27/53/53/53	-
31	BCR	B	517	-	-	6/29/63/63	0/2/2/2
36	DGD	C	519	-	-	11/42/82/95	0/2/2/2
46	CHL	s	308	-	3/3/15/26	0/12/110/137	-
48	NEX	r	313	-	-	5/19/50/83	0/2/2/3
47	LUT	Y	316	-	-	2/29/67/67	0/2/2/2
37	LHG	D	408	-	-	18/43/43/53	-
46	CHL	G	607	-	4/4/20/26	15/39/137/137	-
46	CHL	g	609	21	4/4/20/26	10/39/137/137	-
49	XAT	r	312	-	1/1/12/26	0/31/93/93	0/4/4/4
29	CLA	R	302	-	-	12/33/109/115	-
50	PTY	Y	320	-	-	11/20/20/53	-
46	CHL	n	605	20	4/4/20/26	10/39/137/137	-
46	CHL	g	608	-	3/3/15/26	0/13/111/137	-
46	CHL	y	303	24	4/4/20/26	6/39/137/137	-
37	LHG	S	320	29	-	14/49/49/53	-
46	CHL	y	301	-	4/4/20/26	9/39/137/137	-
29	CLA	y	304	24	1/1/15/20	7/39/115/115	-
29	CLA	c	506	-	-	6/33/109/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PHO	A	408	-	-	5/37/103/103	0/5/6/6
47	LUT	r	311	-	-	4/29/67/67	0/2/2/2
39	SQD	L	102	-	-	13/37/57/69	0/1/1/1
35	LMG	d	407	-	-	7/41/61/70	0/1/1/1
29	CLA	n	610	-	1/1/11/20	6/20/96/115	-
29	CLA	G	614	-	1/1/11/20	7/20/96/115	-
29	CLA	r	309	22	1/1/14/20	7/33/109/115	-
41	DGA	J	101	-	-	12/30/30/45	-
29	CLA	A	407	-	1/1/12/20	8/21/97/115	-
29	CLA	S	312	37	1/1/15/20	17/39/115/115	-
37	LHG	l	102	-	-	31/53/53/53	-
46	CHL	y	309	-	4/4/20/26	12/39/137/137	-
29	CLA	B	504	-	1/1/15/20	17/39/115/115	-
29	CLA	B	514	-	1/1/15/20	11/39/115/115	-
46	CHL	y	308	52	3/3/17/26	2/21/119/137	-
29	CLA	y	305	-	1/1/15/20	16/39/115/115	-
37	LHG	d	406	-	-	21/53/53/53	-
29	CLA	C	510	-	1/1/15/20	16/39/115/115	-
47	LUT	S	318	-	-	2/29/67/67	0/2/2/2
46	CHL	Y	307	-	4/4/20/26	16/39/137/137	-
29	CLA	C	506	-	1/1/14/20	11/33/109/115	-
29	CLA	r	302	22	1/1/14/20	8/33/109/115	-
29	CLA	y	312	24	1/1/15/20	6/39/115/115	-
31	BCR	z	101	-	-	13/29/63/63	0/2/2/2
29	CLA	g	614	-	1/1/11/20	8/20/96/115	-
47	LUT	Y	317	-	-	2/29/67/67	0/2/2/2
37	LHG	G	618	-	-	28/53/53/53	-
35	LMG	d	408	-	-	13/43/63/70	0/1/1/1
37	LHG	N	618	29	-	29/53/53/53	-
47	LUT	N	615	-	-	3/29/67/67	0/2/2/2
29	CLA	s	314	23	1/1/13/20	10/27/103/115	-
47	LUT	g	615	-	-	2/29/67/67	0/2/2/2
29	CLA	Y	305	52	1/1/15/20	13/39/115/115	-
48	NEX	y	319	-	-	7/27/83/83	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	DGA	j	101	-	-	16/30/30/45	-
47	LUT	n	614	-	-	1/29/67/67	0/2/2/2
39	SQD	m	101	-	-	20/37/57/69	0/1/1/1
29	CLA	C	503	-	1/1/15/20	9/39/115/115	-
49	XAT	R	311	-	2/2/12/26	0/31/93/93	0/4/4/4
47	LUT	s	318	-	-	1/29/67/67	0/2/2/2
29	CLA	y	314	24	1/1/15/20	13/39/115/115	-
36	DGD	C	520	-	-	5/42/82/95	0/2/2/2
35	LMG	W	203	-	-	16/34/54/70	0/1/1/1
29	CLA	C	505	52	1/1/13/20	9/27/103/115	-
29	CLA	B	508	-	1/1/15/20	7/39/115/115	-
50	PTY	N	620	-	-	17/53/53/53	-
29	CLA	s	311	23	1/1/15/20	11/39/115/115	-
46	CHL	r	305	-	3/3/15/26	3/13/111/137	-
35	LMG	W	201	-	-	10/35/55/70	0/1/1/1
30	PHO	D	401	-	-	4/37/103/103	0/5/6/6
29	CLA	C	511	-	1/1/15/20	13/39/115/115	-
29	CLA	B	509	-	1/1/15/20	12/39/115/115	-
29	CLA	D	405	-	1/1/14/20	11/33/109/115	-
45	RRX	h	101	-	1/1/11/25	13/29/65/65	0/2/2/2
29	CLA	B	506	-	1/1/15/20	15/39/115/115	-
44	HEM	E	101	7,6	-	1/14/54/54	-
35	LMG	D	409	-	-	4/37/57/70	0/1/1/1
47	LUT	R	310	-	-	4/29/67/67	0/2/2/2
29	CLA	n	603	-	1/1/15/20	12/39/115/115	-
48	NEX	n	616	-	-	2/27/83/83	1/3/3/3
47	LUT	N	616	-	-	2/29/67/67	0/2/2/2
29	CLA	s	306	23	-	5/21/97/115	-
29	CLA	N	610	-	1/1/15/20	13/39/115/115	-
29	CLA	b	508	-	-	2/39/115/115	-
37	LHG	L	101	-	-	33/53/53/53	-
47	LUT	G	615	-	-	1/29/67/67	0/2/2/2
35	LMG	B	520	-	-	12/39/59/70	0/1/1/1
31	BCR	B	518	-	-	13/29/63/63	0/2/2/2
41	DGA	w	201	-	-	27/45/45/45	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	CHL	G	608	-	3/3/15/26	2/13/111/137	-
35	LMG	D	410	-	-	17/43/63/70	0/1/1/1
46	CHL	R	304	-	3/3/15/26	3/13/111/137	-
36	DGD	c	518	-	-	8/48/88/95	0/2/2/2
46	CHL	Y	308	-	4/4/20/26	12/39/137/137	-
29	CLA	N	611	37	1/1/11/20	5/20/96/115	-
29	CLA	s	312	37	1/1/15/20	15/39/115/115	-
29	CLA	b	512	-	1/1/15/20	8/39/115/115	-
29	CLA	C	507	-	-	8/39/115/115	-
46	CHL	s	307	-	3/3/15/26	3/13/111/137	-
29	CLA	Y	312	37	1/1/15/20	10/39/115/115	-
49	XAT	n	618	-	2/2/12/26	1/31/93/93	0/4/4/4
44	HEM	e	101	7,6	-	1/14/54/54	-
46	CHL	g	601	21	4/4/20/26	8/39/137/137	-
29	CLA	c	508	-	1/1/15/20	3/39/115/115	-
39	SQD	o	301	-	-	14/49/69/69	0/1/1/1
31	BCR	F	101	-	-	12/29/63/63	0/2/2/2
29	CLA	S	303	23	1/1/14/20	12/33/109/115	-
39	SQD	M	101	-	-	20/37/57/69	0/1/1/1
29	CLA	y	315	24	-	10/39/115/115	-
46	CHL	y	311	24	4/4/20/26	8/39/137/137	-
46	CHL	g	607	-	4/4/20/26	12/39/137/137	-
37	LHG	c	521	-	-	28/51/51/53	-
29	CLA	n	613	-	1/1/11/20	2/20/96/115	-
47	LUT	y	318	-	-	2/29/67/67	0/2/2/2
31	BCR	c	515	-	-	7/29/63/63	0/2/2/2
29	CLA	A	406	52	1/1/15/20	15/39/115/115	-
48	NEX	N	617	-	-	2/27/83/83	1/3/3/3
29	CLA	g	611	37	1/1/15/20	9/39/115/115	-
29	CLA	G	611	-	1/1/15/20	12/39/115/115	-
29	CLA	a	406	52	-	6/20/96/115	-
29	CLA	B	502	-	1/1/15/20	4/39/115/115	-
29	CLA	N	602	20	1/1/15/20	15/39/115/115	-
38	LMT	b	524	-	-	13/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	b	502	-	1/1/15/20	9/39/115/115	-
46	CHL	r	306	-	3/3/16/26	4/20/118/137	-
48	NEX	Y	318	-	-	7/27/83/83	0/3/3/3
36	DGD	B	521	-	-	13/32/72/95	0/2/2/2
46	CHL	Y	310	24	4/4/20/26	8/39/137/137	-
29	CLA	b	513	-	1/1/15/20	11/39/115/115	-
29	CLA	y	310	-	1/1/12/20	8/21/97/115	-
40	SPH	i	102	-	-	11/21/21/21	-
47	LUT	s	317	-	-	2/29/67/67	0/2/2/2
37	LHG	a	413	-	-	21/48/48/53	-
48	NEX	R	312	-	-	9/19/50/83	0/2/2/3
29	CLA	c	509	-	1/1/15/20	15/39/115/115	-
29	CLA	B	501	-	1/1/15/20	17/39/115/115	-
47	LUT	y	317	-	-	0/29/67/67	0/2/2/2
31	BCR	A	410	-	-	7/29/63/63	0/2/2/2
50	PTY	n	619	-	-	27/53/53/53	-
31	BCR	b	517	-	-	10/29/63/63	0/2/2/2
36	DGD	r	301	-	-	9/32/72/95	0/2/2/2
46	CHL	N	607	-	4/4/20/26	12/39/137/137	-
29	CLA	R	308	22	1/1/14/20	12/33/109/115	-
46	CHL	N	609	20	4/4/20/26	5/39/137/137	-
29	CLA	n	612	20	-	13/39/115/115	-
51	LPX	s	321	-	-	9/20/20/31	-
46	CHL	S	307	-	3/3/15/26	3/13/111/137	-
29	CLA	Y	311	24	1/1/15/20	5/39/115/115	-
49	XAT	Y	301	-	1/1/12/26	0/31/93/93	0/4/4/4
49	XAT	g	619	-	1/1/12/26	1/31/93/93	0/4/4/4
29	CLA	r	303	-	-	11/33/109/115	-
29	CLA	c	507	52	1/1/15/20	14/39/115/115	-
29	CLA	G	602	21	1/1/15/20	15/39/115/115	-
33	3PH	s	322	-	-	23/49/49/49	-
37	LHG	g	618	29	-	29/53/53/53	-
29	CLA	b	514	-	1/1/15/20	13/39/115/115	-
29	CLA	B	516	-	1/1/13/20	10/27/103/115	-
37	LHG	s	320	29	-	21/49/49/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	SQD	b	523	-	-	19/49/69/69	0/1/1/1
46	CHL	N	606	-	4/4/20/26	8/39/137/137	-
33	3PH	a	415	-	-	25/49/49/49	-
31	BCR	C	517	-	-	10/29/63/63	0/2/2/2
46	CHL	n	606	-	4/4/20/26	11/39/137/137	-
43	PL9	d	405	-	-	11/53/73/73	0/1/1/1
31	BCR	a	409	-	-	7/29/63/63	0/2/2/2
29	CLA	n	609	20	1/1/15/20	12/39/115/115	-
37	LHG	S	301	-	-	23/39/39/53	-
29	CLA	b	504	-	1/1/15/20	13/39/115/115	-
41	DGA	b	522	-	-	19/45/45/45	-
29	CLA	r	310	-	1/1/12/20	10/23/99/115	-
29	CLA	C	509	-	1/1/15/20	3/39/115/115	-
29	CLA	Y	309	52	1/1/12/20	10/21/97/115	-
35	LMG	b	520	-	-	11/39/59/70	0/1/1/1
29	CLA	g	612	21	-	3/13/89/115	-
35	LMG	w	202	-	-	17/34/54/70	0/1/1/1
29	CLA	c	503	-	-	14/39/115/115	-
39	SQD	C	523	-	-	13/31/51/69	0/1/1/1
29	CLA	B	513	-	1/1/15/20	11/39/115/115	-
29	CLA	S	310	23	1/1/14/20	10/33/109/115	-
34	C7Z	B	519	-	1/1/12/26	8/29/67/67	0/2/2/2
35	LMG	c	519	-	-	21/46/66/70	0/1/1/1
45	RRX	H	101	-	1/1/11/25	8/29/65/65	0/2/2/2
37	LHG	s	301	-	-	18/42/42/53	-
29	CLA	D	404	-	1/1/15/20	11/39/115/115	-
33	3PH	A	412	-	-	27/49/49/49	-
29	CLA	r	308	22	1/1/14/20	11/33/109/115	-
46	CHL	g	606	-	3/3/16/26	2/20/118/137	-
29	CLA	s	316	23	1/1/12/20	5/21/97/115	-
46	CHL	S	309	-	4/4/19/26	7/33/131/137	-
40	SPH	C	525	-	-	11/21/21/21	-
29	CLA	n	604	-	1/1/15/20	14/39/115/115	-
29	CLA	S	314	23	1/1/13/20	13/27/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	S	305	-	1/1/13/20	7/27/103/115	-
29	CLA	Y	313	24	1/1/15/20	12/39/115/115	-
29	CLA	b	505	-	1/1/15/20	7/39/115/115	-
46	CHL	s	302	23	3/3/16/26	5/15/113/137	-
29	CLA	B	507	52	1/1/15/20	21/39/115/115	-
29	CLA	A	409	-	-	8/33/109/115	-
47	LUT	G	616	-	-	2/29/67/67	0/2/2/2
46	CHL	N	605	20	4/4/20/26	15/39/137/137	-
31	BCR	b	518	-	-	9/29/63/63	0/2/2/2
46	CHL	n	608	20	4/4/20/26	6/39/137/137	-
29	CLA	r	307	-	1/1/14/20	13/33/109/115	-
29	CLA	c	513	-	-	11/39/115/115	-
29	CLA	n	602	20	1/1/15/20	13/39/115/115	-
29	CLA	B	503	-	1/1/15/20	9/39/115/115	-
33	3PH	S	322	-	-	7/31/31/49	-
46	CHL	G	606	-	3/3/16/26	5/20/118/137	-
29	CLA	Y	314	24	1/1/15/20	18/39/115/115	-
29	CLA	N	603	-	1/1/15/20	23/39/115/115	-
46	CHL	n	607	-	3/3/16/26	5/20/118/137	-
36	DGD	C	518	-	-	9/40/80/95	0/2/2/2
29	CLA	S	311	23	1/1/15/20	10/39/115/115	-
46	CHL	G	605	21	3/3/16/26	4/18/116/137	-
35	LMG	C	524	-	-	20/37/57/70	0/1/1/1
39	SQD	C	501	-	-	9/37/57/69	0/1/1/1
48	NEX	S	319	-	-	2/27/83/83	0/3/3/3
40	SPH	I	101	-	-	10/21/21/21	-
29	CLA	B	510	52	1/1/15/20	7/39/115/115	-
29	CLA	G	610	21	1/1/15/20	6/39/115/115	-
29	CLA	b	510	52	1/1/15/20	5/39/115/115	-
29	CLA	C	514	-	-	11/39/115/115	-
29	CLA	S	316	23	1/1/12/20	5/21/97/115	-
33	3PH	b	521	-	-	26/40/40/49	-
29	CLA	N	613	20	1/1/15/20	13/39/115/115	-

All (1639) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	H	101	RRX	C26-C25	16.09	1.61	1.34
45	h	101	RRX	C26-C25	15.99	1.61	1.34
34	B	519	C7Z	C25-C26	15.86	1.61	1.34
34	b	519	C7Z	C25-C26	15.83	1.61	1.34
47	r	311	LUT	C24-C25	15.43	1.51	1.33
34	B	519	C7Z	C5-C6	15.28	1.60	1.34
47	G	615	LUT	C24-C25	15.27	1.51	1.33
47	y	317	LUT	C24-C25	15.25	1.51	1.33
47	Y	316	LUT	C24-C25	15.24	1.51	1.33
34	b	519	C7Z	C5-C6	15.23	1.60	1.34
45	h	101	RRX	C5-C6	15.22	1.60	1.34
45	H	101	RRX	C5-C6	15.21	1.60	1.34
47	N	615	LUT	C24-C25	15.21	1.51	1.33
47	g	616	LUT	C24-C25	15.20	1.51	1.33
47	Y	317	LUT	C24-C25	15.17	1.51	1.33
47	s	317	LUT	C24-C25	15.14	1.51	1.33
47	R	310	LUT	C24-C25	15.13	1.51	1.33
47	y	318	LUT	C24-C25	15.10	1.51	1.33
47	N	616	LUT	C24-C25	15.09	1.51	1.33
47	G	616	LUT	C24-C25	15.09	1.51	1.33
47	n	614	LUT	C24-C25	15.04	1.51	1.33
47	n	615	LUT	C24-C25	14.93	1.50	1.33
47	g	615	LUT	C24-C25	14.86	1.50	1.33
47	S	318	LUT	C24-C25	14.79	1.50	1.33
47	s	318	LUT	C24-C25	14.68	1.50	1.33
47	S	317	LUT	C24-C25	14.44	1.50	1.33
34	B	519	C7Z	C24-C23	11.44	1.72	1.52
34	b	519	C7Z	C24-C23	11.32	1.72	1.52
29	D	404	CLA	C3D-C4D	-11.06	1.19	1.44
29	D	404	CLA	C4B-NB	-11.00	1.23	1.37
34	B	519	C7Z	C2-C3	-10.81	1.37	1.52
34	b	519	C7Z	C22-C23	-10.76	1.37	1.52
34	B	519	C7Z	C22-C23	-10.66	1.37	1.52
45	H	101	RRX	C29-C28	-10.63	1.37	1.52
45	h	101	RRX	C29-C28	-10.56	1.37	1.52
34	b	519	C7Z	C2-C3	-10.54	1.37	1.52
30	d	402	PHO	C1B-C2B	9.27	1.49	1.39
30	D	401	PHO	C1B-C2B	9.24	1.49	1.39
30	A	408	PHO	C1B-C2B	9.15	1.49	1.39
29	D	404	CLA	C1B-NB	-9.10	1.25	1.37
30	a	407	PHO	C1B-C2B	8.81	1.49	1.39
30	D	401	PHO	C3B-C4B	8.78	1.50	1.41
46	n	605	CHL	C3A-C2A	-8.62	1.47	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	408	PHO	C3B-C4B	8.52	1.50	1.41
30	d	402	PHO	C3B-C4B	8.51	1.50	1.41
30	a	407	PHO	C3B-C4B	8.28	1.49	1.41
34	b	519	C7Z	C4-C3	8.25	1.66	1.52
34	B	519	C7Z	C4-C3	8.20	1.66	1.52
45	h	101	RRX	C27-C28	7.87	1.66	1.52
45	H	101	RRX	C27-C28	7.84	1.66	1.52
29	D	404	CLA	O1D-CGD	-7.31	1.02	1.21
46	g	606	CHL	C3A-C2A	-7.10	1.48	1.54
46	y	308	CHL	C3A-C2A	-7.08	1.48	1.54
45	H	101	RRX	C2-C3	-6.78	1.36	1.52
45	h	101	RRX	C2-C3	-6.75	1.36	1.52
48	n	616	NEX	C35-C15	-6.59	1.18	1.36
48	s	319	NEX	C35-C15	-6.54	1.18	1.36
48	R	312	NEX	C35-C15	-6.54	1.18	1.36
48	N	617	NEX	C35-C15	-6.52	1.18	1.36
48	r	313	NEX	C35-C15	-6.50	1.18	1.36
48	S	319	NEX	C35-C15	-6.50	1.18	1.36
48	g	617	NEX	C35-C15	-6.48	1.18	1.36
46	n	607	CHL	C3A-C2A	-6.48	1.49	1.54
48	Y	318	NEX	C35-C15	-6.46	1.18	1.36
48	G	617	NEX	C35-C15	-6.46	1.18	1.36
48	y	319	NEX	C35-C15	-6.46	1.18	1.36
45	H	101	RRX	C1-C6	-6.40	1.45	1.53
45	h	101	RRX	C1-C6	-6.34	1.45	1.53
48	n	616	NEX	C11-C12	-6.28	1.18	1.34
48	s	319	NEX	C11-C12	-6.28	1.18	1.34
48	s	319	NEX	C31-C32	-6.27	1.18	1.34
48	n	616	NEX	C31-C32	-6.25	1.18	1.34
48	S	319	NEX	C31-C32	-6.25	1.18	1.34
48	R	312	NEX	C31-C32	-6.24	1.18	1.34
46	G	606	CHL	C3B-C4B	6.23	1.47	1.41
46	y	307	CHL	C3A-C2A	-6.21	1.49	1.54
46	Y	307	CHL	C3A-C2A	-6.20	1.49	1.54
48	G	617	NEX	C11-C12	-6.20	1.18	1.34
48	Y	318	NEX	C31-C32	-6.19	1.18	1.34
48	y	319	NEX	C31-C32	-6.19	1.18	1.34
48	r	313	NEX	C31-C32	-6.18	1.18	1.34
48	y	319	NEX	C11-C12	-6.18	1.18	1.34
46	S	302	CHL	C3B-C4B	6.18	1.47	1.41
48	g	617	NEX	C31-C32	-6.17	1.18	1.34
48	g	617	NEX	C11-C12	-6.17	1.18	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	N	617	NEX	C11-C12	-6.17	1.18	1.34
46	g	607	CHL	C3A-C2A	-6.16	1.49	1.54
48	N	617	NEX	C31-C32	-6.16	1.18	1.34
48	S	319	NEX	C11-C12	-6.15	1.18	1.34
48	Y	318	NEX	C11-C12	-6.15	1.18	1.34
46	G	608	CHL	C3A-C2A	-6.13	1.49	1.54
48	G	617	NEX	C31-C32	-6.09	1.18	1.34
46	g	609	CHL	C3A-C2A	-6.04	1.49	1.54
46	S	302	CHL	C3A-C2A	-5.97	1.49	1.54
29	D	404	CLA	C1C-C2C	-5.90	1.32	1.44
46	G	609	CHL	C3A-C2A	-5.84	1.49	1.54
46	S	307	CHL	C3A-C2A	-5.82	1.49	1.54
31	F	101	BCR	C24-C23	5.81	1.50	1.33
31	v	101	BCR	C24-C23	5.80	1.50	1.33
48	s	319	NEX	C7-C8	5.80	1.41	1.31
45	H	101	RRX	C30-C25	-5.79	1.46	1.53
46	s	302	CHL	C3B-C4B	5.78	1.47	1.41
46	s	307	CHL	C3A-C2A	-5.78	1.49	1.54
31	K	101	BCR	C24-C23	5.77	1.50	1.33
46	n	606	CHL	C3A-C2A	-5.77	1.49	1.54
31	b	518	BCR	C24-C23	5.75	1.50	1.33
29	D	404	CLA	C1C-NC	-5.75	1.28	1.37
31	f	101	BCR	C24-C23	5.75	1.50	1.33
31	B	518	BCR	C24-C23	5.74	1.50	1.33
45	h	101	RRX	C30-C25	-5.73	1.46	1.53
46	N	606	CHL	C3B-C4B	5.72	1.47	1.41
46	Y	306	CHL	C3A-C2A	-5.70	1.49	1.54
31	c	515	BCR	C24-C23	5.67	1.50	1.33
34	b	519	C7Z	C1-C6	-5.66	1.46	1.53
48	S	319	NEX	C7-C8	5.65	1.41	1.31
31	C	517	BCR	C24-C23	5.65	1.49	1.33
48	N	617	NEX	C7-C8	5.65	1.41	1.31
46	s	302	CHL	C3A-C2A	-5.64	1.49	1.54
48	Y	318	NEX	C7-C8	5.63	1.41	1.31
48	y	319	NEX	C7-C8	5.63	1.41	1.31
31	C	515	BCR	C24-C23	5.61	1.49	1.33
31	z	101	BCR	C24-C23	5.61	1.49	1.33
46	Y	307	CHL	C3B-C4B	5.59	1.46	1.41
31	A	410	BCR	C24-C23	5.57	1.49	1.33
31	a	409	BCR	C24-C23	5.56	1.49	1.33
31	C	516	BCR	C24-C23	5.55	1.49	1.33
34	b	519	C7Z	C12-C13	5.54	1.57	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	G	617	NEX	C7-C8	5.54	1.40	1.31
31	b	518	BCR	C11-C12	-5.53	1.20	1.34
31	B	518	BCR	C11-C12	-5.52	1.20	1.34
46	G	608	CHL	C3B-C4B	5.52	1.46	1.41
31	a	409	BCR	C11-C12	-5.51	1.20	1.34
46	N	606	CHL	C3A-C2A	-5.50	1.50	1.54
31	c	514	BCR	C11-C12	-5.48	1.20	1.34
34	B	519	C7Z	C12-C13	5.47	1.57	1.46
48	n	616	NEX	C7-C8	5.47	1.40	1.31
46	n	608	CHL	C3A-C2A	-5.47	1.50	1.54
46	N	608	CHL	C3A-C2A	-5.46	1.50	1.54
31	A	410	BCR	C11-C12	-5.44	1.20	1.34
31	c	514	BCR	C24-C23	5.44	1.49	1.33
34	B	519	C7Z	C1-C6	-5.43	1.46	1.53
31	B	517	BCR	C11-C12	-5.42	1.20	1.34
31	B	517	BCR	C24-C23	5.42	1.49	1.33
46	g	605	CHL	C3A-C2A	-5.41	1.50	1.54
46	Y	310	CHL	C3A-C2A	-5.39	1.50	1.54
46	g	606	CHL	C3B-C4B	5.39	1.46	1.41
31	c	515	BCR	C11-C12	-5.38	1.20	1.34
31	C	517	BCR	C11-C12	-5.38	1.20	1.34
31	b	517	BCR	C11-C12	-5.35	1.20	1.34
48	S	319	NEX	C28-C29	-5.35	1.34	1.46
31	C	515	BCR	C11-C12	-5.35	1.20	1.34
31	b	517	BCR	C24-C23	5.35	1.49	1.33
46	g	608	CHL	C3A-C2A	-5.33	1.50	1.54
34	b	519	C7Z	C24-C25	-5.30	1.42	1.51
48	s	319	NEX	C28-C29	-5.30	1.34	1.46
48	r	313	NEX	C28-C29	-5.29	1.34	1.46
46	y	301	CHL	C3A-C2A	-5.29	1.50	1.54
48	R	312	NEX	C28-C29	-5.29	1.34	1.46
31	C	516	BCR	C11-C12	-5.27	1.20	1.34
46	g	601	CHL	C3B-C4B	5.26	1.46	1.41
31	z	101	BCR	C11-C12	-5.26	1.21	1.34
48	g	617	NEX	C28-C29	-5.26	1.34	1.46
48	Y	318	NEX	C28-C29	-5.25	1.34	1.46
34	B	519	C7Z	C24-C25	-5.24	1.42	1.51
46	S	307	CHL	C3B-C4B	5.24	1.46	1.41
46	n	605	CHL	C3B-C4B	5.23	1.46	1.41
31	f	101	BCR	C11-C12	-5.22	1.21	1.34
48	n	616	NEX	C28-C29	-5.20	1.34	1.46
45	h	101	RRX	C2-C1	5.20	1.66	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S	308	CHL	C3B-C4B	5.18	1.46	1.41
48	G	617	NEX	C28-C29	-5.18	1.34	1.46
48	y	319	NEX	C28-C29	-5.17	1.34	1.46
31	F	101	BCR	C11-C12	-5.17	1.21	1.34
46	n	606	CHL	C3B-C4B	5.16	1.46	1.41
46	Y	306	CHL	C3B-C4B	5.15	1.46	1.41
45	H	101	RRX	C2-C1	5.15	1.65	1.54
46	G	601	CHL	C3B-C4B	5.14	1.46	1.41
46	G	605	CHL	C3B-C4B	5.14	1.46	1.41
31	K	101	BCR	C11-C12	-5.14	1.21	1.34
46	R	305	CHL	C3B-C4B	5.13	1.46	1.41
48	N	617	NEX	C28-C29	-5.12	1.35	1.46
31	v	101	BCR	C11-C12	-5.11	1.21	1.34
46	n	601	CHL	C3A-C2A	-5.09	1.50	1.54
29	D	404	CLA	C4C-C3C	-5.08	1.36	1.45
45	h	101	RRX	C19-C18	5.06	1.56	1.46
29	D	404	CLA	C2A-C1A	-5.05	1.40	1.52
48	g	617	NEX	C7-C8	5.05	1.40	1.31
46	R	305	CHL	C3A-C2A	-5.05	1.50	1.54
46	N	609	CHL	C3A-C2A	-5.04	1.50	1.54
46	N	607	CHL	C3B-C4B	5.01	1.46	1.41
46	s	308	CHL	C3B-C4B	4.99	1.46	1.41
45	H	101	RRX	C19-C18	4.98	1.56	1.46
46	N	605	CHL	C3B-C4B	4.96	1.46	1.41
46	S	309	CHL	C3A-C2A	-4.93	1.50	1.54
46	N	605	CHL	C3A-C2A	-4.90	1.50	1.54
46	S	309	CHL	C3B-C4B	4.86	1.46	1.41
46	R	304	CHL	C3B-C4B	4.84	1.46	1.41
46	s	309	CHL	C3B-C4B	4.84	1.46	1.41
46	G	601	CHL	C3A-C2A	-4.84	1.50	1.54
46	r	306	CHL	C3A-C2A	-4.82	1.50	1.54
46	n	601	CHL	C3B-C4B	4.79	1.46	1.41
46	r	306	CHL	C3B-C4B	4.78	1.46	1.41
46	N	607	CHL	C3A-C2A	-4.77	1.50	1.54
46	g	605	CHL	C3B-C4B	4.77	1.46	1.41
46	y	307	CHL	C3B-C4B	4.73	1.46	1.41
46	N	601	CHL	C3B-C4B	4.73	1.46	1.41
45	h	101	RRX	C8-C9	4.73	1.56	1.46
46	r	305	CHL	C3B-C4B	4.72	1.46	1.41
29	D	404	CLA	O2D-CED	-4.72	1.34	1.45
34	b	519	C7Z	C28-C29	4.72	1.56	1.46
46	g	601	CHL	C3A-C2A	-4.71	1.50	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	s	308	CHL	C3A-C2A	-4.71	1.50	1.54
46	Y	310	CHL	C3B-C4B	4.68	1.45	1.41
34	B	519	C7Z	C28-C29	4.66	1.55	1.46
46	g	608	CHL	C3B-C4B	4.66	1.45	1.41
45	H	101	RRX	C8-C9	4.64	1.55	1.46
46	G	606	CHL	C3A-C2A	-4.60	1.50	1.54
31	a	409	BCR	C16-C17	-4.56	1.29	1.43
46	G	609	CHL	C3B-C4B	4.55	1.45	1.41
31	A	410	BCR	C16-C17	-4.54	1.29	1.43
31	c	514	BCR	C16-C17	-4.54	1.29	1.43
46	y	303	CHL	C3A-C2A	-4.53	1.50	1.54
34	b	519	C7Z	C32-C33	4.51	1.55	1.46
46	r	305	CHL	C3A-C2A	-4.51	1.50	1.54
31	B	517	BCR	C16-C17	-4.48	1.29	1.43
34	B	519	C7Z	C32-C33	4.48	1.55	1.46
29	D	404	CLA	OBD-CAD	-4.48	1.14	1.22
31	B	518	BCR	C16-C17	-4.47	1.29	1.43
46	y	311	CHL	C3A-C2A	-4.46	1.50	1.54
45	h	101	RRX	C12-C13	4.45	1.55	1.46
31	b	518	BCR	C16-C17	-4.45	1.29	1.43
34	B	519	C7Z	C4-C5	-4.45	1.44	1.51
34	b	519	C7Z	C4-C5	-4.42	1.44	1.51
31	C	517	BCR	C16-C17	-4.41	1.29	1.43
31	c	515	BCR	C16-C17	-4.41	1.29	1.43
31	C	516	BCR	C16-C17	-4.41	1.29	1.43
31	b	517	BCR	C16-C17	-4.40	1.29	1.43
48	R	312	NEX	C30-C29	-4.38	1.25	1.35
48	g	617	NEX	C10-C9	-4.38	1.25	1.35
46	y	303	CHL	C3B-C4B	4.37	1.45	1.41
46	s	309	CHL	C3A-C2A	-4.36	1.50	1.54
48	n	616	NEX	C34-C33	-4.35	1.25	1.35
48	n	616	NEX	C14-C13	-4.35	1.25	1.35
31	C	515	BCR	C16-C17	-4.35	1.29	1.43
48	s	319	NEX	C14-C13	-4.34	1.25	1.35
45	h	101	RRX	C27-C26	-4.33	1.44	1.51
31	F	101	BCR	C16-C17	-4.32	1.29	1.43
45	H	101	RRX	C12-C13	4.31	1.55	1.46
31	z	101	BCR	C16-C17	-4.31	1.29	1.43
48	n	616	NEX	C10-C9	-4.31	1.25	1.35
48	Y	318	NEX	C30-C29	-4.29	1.25	1.35
36	B	521	DGD	O1G-C1A	4.29	1.45	1.33
48	s	319	NEX	C34-C33	-4.29	1.25	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	N	617	NEX	C14-C13	-4.29	1.25	1.35
48	r	313	NEX	C34-C33	-4.29	1.25	1.35
48	r	313	NEX	C30-C29	-4.29	1.25	1.35
48	S	319	NEX	C14-C13	-4.28	1.25	1.35
48	N	617	NEX	C34-C33	-4.28	1.25	1.35
31	v	101	BCR	C16-C17	-4.27	1.29	1.43
48	g	617	NEX	C14-C13	-4.27	1.25	1.35
48	n	616	NEX	C30-C29	-4.27	1.25	1.35
29	D	404	CLA	CHB-C4A	-4.26	1.27	1.37
36	C	518	DGD	O1G-C1A	4.26	1.45	1.33
48	R	312	NEX	C34-C33	-4.26	1.25	1.35
45	H	101	RRX	C27-C26	-4.26	1.44	1.51
48	N	617	NEX	C30-C29	-4.26	1.26	1.35
46	N	601	CHL	C3A-C2A	-4.26	1.51	1.54
36	c	516	DGD	O1G-C1A	4.25	1.45	1.33
36	r	301	DGD	O1G-C1A	4.25	1.45	1.33
48	s	319	NEX	C30-C29	-4.25	1.26	1.35
48	s	319	NEX	C10-C9	-4.25	1.26	1.35
45	H	101	RRX	C3-C4	4.24	1.65	1.52
34	b	519	C7Z	C31-C30	4.24	1.56	1.43
46	g	609	CHL	C3B-C4B	4.24	1.45	1.41
45	h	101	RRX	C3-C4	4.24	1.65	1.52
48	G	617	NEX	C34-C33	-4.24	1.26	1.35
48	Y	318	NEX	C34-C33	-4.23	1.26	1.35
48	S	319	NEX	C30-C29	-4.23	1.26	1.35
48	g	617	NEX	C30-C29	-4.23	1.26	1.35
48	G	617	NEX	C14-C13	-4.22	1.26	1.35
48	S	319	NEX	C34-C33	-4.22	1.26	1.35
46	R	304	CHL	C3A-C2A	-4.22	1.51	1.54
48	Y	318	NEX	C14-C13	-4.22	1.26	1.35
48	G	617	NEX	C10-C9	-4.22	1.26	1.35
46	S	308	CHL	C3A-C2A	-4.21	1.51	1.54
31	K	101	BCR	C16-C17	-4.21	1.30	1.43
48	y	319	NEX	C14-C13	-4.21	1.26	1.35
48	y	319	NEX	C34-C33	-4.21	1.26	1.35
48	y	319	NEX	C30-C29	-4.20	1.26	1.35
36	C	520	DGD	O1G-C1A	4.20	1.45	1.33
48	S	319	NEX	C10-C9	-4.20	1.26	1.35
48	N	617	NEX	C10-C9	-4.20	1.26	1.35
48	G	617	NEX	C30-C29	-4.19	1.26	1.35
48	y	319	NEX	C10-C9	-4.18	1.26	1.35
34	B	519	C7Z	C31-C30	4.18	1.56	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	519	C7Z	C11-C10	4.18	1.56	1.43
46	N	608	CHL	C3B-C4B	4.17	1.45	1.41
31	f	101	BCR	C16-C17	-4.16	1.30	1.43
36	C	519	DGD	O1G-C1A	4.15	1.45	1.33
48	Y	318	NEX	C10-C9	-4.15	1.26	1.35
48	g	617	NEX	C34-C33	-4.14	1.26	1.35
30	D	401	PHO	C1D-C2D	4.13	1.44	1.39
48	g	617	NEX	C7-C6	-4.12	1.25	1.30
34	B	519	C7Z	C11-C10	4.11	1.55	1.43
29	D	404	CLA	CBD-CAD	-4.11	1.38	1.56
46	N	609	CHL	C3B-C4B	4.10	1.45	1.41
36	c	518	DGD	O1G-C1A	4.10	1.45	1.33
45	h	101	RRX	C20-C21	4.09	1.55	1.43
43	D	406	PL9	C3-C4	-4.09	1.43	1.49
34	b	519	C7Z	C8-C9	4.08	1.54	1.46
36	c	517	DGD	O1G-C1A	4.07	1.45	1.33
46	G	607	CHL	C3A-C2A	-4.06	1.51	1.54
34	b	519	C7Z	C22-C21	4.05	1.67	1.54
31	v	101	BCR	C10-C9	4.05	1.45	1.35
31	K	101	BCR	C10-C9	4.05	1.45	1.35
34	B	519	C7Z	C8-C9	4.04	1.54	1.46
34	B	519	C7Z	C22-C21	4.02	1.66	1.54
31	F	101	BCR	C10-C9	4.00	1.45	1.35
45	H	101	RRX	C20-C21	3.99	1.55	1.43
46	y	311	CHL	C3B-C4B	3.97	1.45	1.41
30	d	402	PHO	C1D-C2D	3.97	1.43	1.39
31	z	101	BCR	C10-C9	3.96	1.44	1.35
30	A	408	PHO	C1D-C2D	3.94	1.43	1.39
46	G	607	CHL	C3B-C4B	3.94	1.45	1.41
31	f	101	BCR	C10-C9	3.91	1.44	1.35
45	h	101	RRX	C15-C14	3.88	1.55	1.43
48	G	617	NEX	C7-C6	-3.86	1.26	1.30
31	b	517	BCR	C10-C9	3.85	1.44	1.35
46	G	605	CHL	C3A-C2A	-3.84	1.51	1.54
31	C	517	BCR	C10-C9	3.83	1.44	1.35
29	D	404	CLA	O2A-C1	-3.83	1.35	1.46
45	H	101	RRX	C15-C14	3.83	1.55	1.43
35	b	520	LMG	C22-C21	-3.82	1.32	1.51
31	c	515	BCR	C10-C9	3.81	1.44	1.35
46	Y	307	CHL	C2C-C3C	3.81	1.40	1.36
46	G	609	CHL	C2C-C3C	3.79	1.40	1.36
36	c	518	DGD	CAB-C9B	-3.76	1.33	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	515	BCR	C10-C9	3.75	1.44	1.35
44	E	101	HEM	FE-NA	3.75	2.07	1.95
45	h	101	RRX	C23-C22	3.75	1.54	1.46
35	B	520	LMG	C22-C21	-3.75	1.33	1.51
31	C	516	BCR	C10-C9	3.74	1.44	1.35
48	n	616	NEX	C7-C6	-3.74	1.26	1.30
36	c	517	DGD	CAB-C9B	-3.74	1.33	1.51
43	d	405	PL9	C3-C4	-3.74	1.43	1.49
35	c	520	LMG	C40-C39	-3.73	1.33	1.51
31	B	517	BCR	C10-C9	3.73	1.44	1.35
35	b	520	LMG	C19-C18	-3.73	1.33	1.51
35	B	520	LMG	C19-C18	-3.72	1.33	1.51
35	c	519	LMG	C40-C39	-3.72	1.33	1.51
48	Y	318	NEX	C7-C6	-3.72	1.26	1.30
35	C	521	LMG	C40-C39	-3.72	1.33	1.51
36	c	517	DGD	CDA-CCA	-3.72	1.33	1.51
35	D	410	LMG	C19-C18	-3.71	1.33	1.51
35	d	408	LMG	C19-C18	-3.71	1.33	1.51
35	c	519	LMG	C22-C21	-3.70	1.33	1.51
35	C	521	LMG	C19-C18	-3.70	1.33	1.51
36	C	518	DGD	CDB-CCB	-3.70	1.33	1.51
35	c	519	LMG	C37-C36	-3.69	1.33	1.51
36	C	519	DGD	CAB-C9B	-3.69	1.33	1.51
35	c	520	LMG	C37-C36	-3.69	1.33	1.51
35	c	519	LMG	C19-C18	-3.69	1.33	1.51
35	D	409	LMG	C19-C18	-3.69	1.33	1.51
35	C	521	LMG	C37-C36	-3.68	1.33	1.51
35	C	522	LMG	C25-C24	-3.68	1.33	1.51
36	C	520	DGD	CAA-C9A	-3.68	1.33	1.51
36	c	516	DGD	CDB-CCB	-3.68	1.33	1.51
34	b	519	C7Z	C2-C1	3.68	1.65	1.54
31	A	410	BCR	C10-C9	3.68	1.44	1.35
46	g	605	CHL	C2C-C3C	3.68	1.39	1.36
36	c	518	DGD	CAA-C9A	-3.68	1.33	1.51
35	C	522	LMG	C22-C21	-3.68	1.33	1.51
36	c	516	DGD	CAB-C9B	-3.67	1.33	1.51
36	c	517	DGD	CDB-CCB	-3.67	1.33	1.51
31	B	518	BCR	C10-C9	3.67	1.44	1.35
35	C	524	LMG	C37-C36	-3.67	1.33	1.51
31	b	518	BCR	C10-C9	3.67	1.44	1.35
46	Y	308	CHL	C3A-C2A	-3.67	1.51	1.54
35	c	520	LMG	C43-C42	-3.67	1.33	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	c	520	LMG	C19-C18	-3.66	1.33	1.51
35	i	101	LMG	C37-C36	-3.66	1.33	1.51
34	B	519	C7Z	C7-C6	3.66	1.57	1.45
35	C	522	LMG	C40-C39	-3.66	1.33	1.51
35	C	522	LMG	C37-C36	-3.66	1.33	1.51
36	C	519	DGD	CDB-CCB	-3.66	1.33	1.51
35	c	520	LMG	C22-C21	-3.66	1.33	1.51
30	a	407	PHO	C1D-C2D	3.66	1.43	1.39
35	d	407	LMG	C19-C18	-3.66	1.33	1.51
36	C	518	DGD	CAB-C9B	-3.65	1.33	1.51
35	c	520	LMG	C25-C24	-3.65	1.33	1.51
35	i	101	LMG	C40-C39	-3.65	1.33	1.51
36	c	517	DGD	CAA-C9A	-3.65	1.33	1.51
35	w	202	LMG	C37-C36	-3.65	1.33	1.51
45	H	101	RRX	C23-C22	3.65	1.53	1.46
35	W	203	LMG	C37-C36	-3.65	1.33	1.51
34	b	519	C7Z	C15-C14	3.64	1.54	1.43
46	g	607	CHL	C3B-C4B	3.64	1.44	1.41
35	i	101	LMG	C19-C18	-3.64	1.33	1.51
46	s	307	CHL	C3B-C4B	3.64	1.44	1.41
35	C	522	LMG	C43-C42	-3.64	1.33	1.51
35	D	410	LMG	C40-C39	-3.63	1.33	1.51
34	B	519	C7Z	C2-C1	3.63	1.65	1.54
35	D	410	LMG	C37-C36	-3.63	1.33	1.51
36	c	518	DGD	CDB-CCB	-3.63	1.33	1.51
43	D	406	PL9	C7-C3	-3.62	1.46	1.51
35	d	408	LMG	C37-C36	-3.62	1.33	1.51
31	c	514	BCR	C10-C9	3.62	1.44	1.35
35	W	201	LMG	C19-C18	-3.62	1.33	1.51
35	d	408	LMG	C40-C39	-3.61	1.33	1.51
48	y	319	NEX	C7-C6	-3.61	1.26	1.30
48	S	319	NEX	C7-C6	-3.60	1.26	1.30
46	n	606	CHL	C2C-C3C	3.60	1.39	1.36
35	d	407	LMG	C22-C21	-3.60	1.33	1.51
41	D	402	DGA	OG2-CB1	3.59	1.44	1.34
34	b	519	C7Z	C7-C6	3.59	1.57	1.45
35	W	203	LMG	C40-C39	-3.59	1.33	1.51
35	w	202	LMG	C40-C39	-3.59	1.33	1.51
31	a	409	BCR	C10-C9	3.58	1.44	1.35
46	g	609	CHL	C2C-C3C	3.58	1.39	1.36
35	C	522	LMG	C19-C18	-3.58	1.34	1.51
46	G	607	CHL	CBB-CAB	3.57	1.51	1.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	G	603	CLA	C1D-ND	3.57	1.42	1.37
41	b	522	DGA	OG2-CB1	3.56	1.44	1.34
48	N	617	NEX	C7-C6	-3.56	1.26	1.30
46	Y	302	CHL	CBB-CAB	3.56	1.51	1.29
44	E	101	HEM	FE-NB	3.56	2.05	1.94
46	G	605	CHL	CBB-CAB	3.56	1.51	1.29
46	n	608	CHL	CBB-CAB	3.56	1.51	1.29
45	h	101	RRX	C11-C10	3.55	1.54	1.43
34	B	519	C7Z	C15-C14	3.55	1.54	1.43
34	b	519	C7Z	C27-C26	3.55	1.57	1.45
29	N	614	CLA	C1D-ND	3.55	1.42	1.37
29	D	404	CLA	CAA-CBA	-3.55	1.42	1.52
46	g	605	CHL	CBB-CAB	3.54	1.51	1.29
46	N	608	CHL	CBB-CAB	3.54	1.51	1.29
34	B	519	C7Z	C27-C26	3.54	1.57	1.45
46	g	607	CHL	CBB-CAB	3.53	1.51	1.29
46	g	608	CHL	CBB-CAB	3.52	1.51	1.29
46	y	303	CHL	CBB-CAB	3.52	1.51	1.29
46	Y	306	CHL	CBB-CAB	3.51	1.51	1.29
46	y	307	CHL	CBB-CAB	3.51	1.51	1.29
46	n	601	CHL	CBB-CAB	3.51	1.51	1.29
46	N	609	CHL	CBB-CAB	3.51	1.51	1.29
45	H	101	RRX	C11-C10	3.51	1.54	1.43
46	s	307	CHL	CBB-CAB	3.51	1.51	1.29
46	y	311	CHL	CBB-CAB	3.51	1.51	1.29
46	N	601	CHL	CBB-CAB	3.51	1.51	1.29
46	g	601	CHL	CBB-CAB	3.51	1.51	1.29
46	Y	310	CHL	CBB-CAB	3.50	1.51	1.29
46	n	607	CHL	CBB-CAB	3.50	1.51	1.29
29	N	603	CLA	C1D-ND	3.50	1.42	1.37
30	d	402	PHO	C4D-CHA	3.50	1.44	1.39
46	G	601	CHL	CBB-CAB	3.50	1.51	1.29
46	G	609	CHL	CBB-CAB	3.49	1.51	1.29
41	J	101	DGA	OG2-CB1	3.49	1.44	1.34
46	n	607	CHL	C3B-C4B	3.49	1.44	1.41
46	N	607	CHL	C2C-C3C	3.49	1.39	1.36
46	g	609	CHL	CBB-CAB	3.49	1.51	1.29
46	S	308	CHL	CBB-CAB	3.49	1.51	1.29
46	Y	308	CHL	C3B-C4B	3.48	1.44	1.41
46	N	605	CHL	CBB-CAB	3.48	1.51	1.29
34	b	519	C7Z	C35-C34	3.47	1.54	1.43
34	B	519	C7Z	C21-C26	-3.47	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D	401	PHO	C4D-CHA	3.47	1.44	1.39
29	C	514	CLA	C1D-ND	3.47	1.42	1.37
46	y	303	CHL	C2C-C3C	3.47	1.39	1.36
46	n	605	CHL	CBB-CAB	3.45	1.50	1.29
29	N	611	CLA	C1D-ND	3.45	1.42	1.37
30	A	408	PHO	C4D-CHA	3.45	1.44	1.39
46	S	309	CHL	CBB-CAB	3.45	1.50	1.29
46	Y	308	CHL	CBB-CAB	3.45	1.50	1.29
29	s	316	CLA	C1D-ND	3.44	1.42	1.37
29	S	316	CLA	C1D-ND	3.43	1.42	1.37
46	S	307	CHL	C2C-C3C	3.43	1.39	1.36
41	j	101	DGA	OG2-CB1	3.42	1.43	1.34
46	s	309	CHL	CBB-CAB	3.42	1.50	1.29
46	y	301	CHL	CBB-CAB	3.42	1.50	1.29
29	G	604	CLA	C1D-ND	3.41	1.42	1.37
34	B	519	C7Z	C35-C34	3.41	1.53	1.43
29	y	313	CLA	C1D-ND	3.41	1.42	1.37
44	e	101	HEM	FE-NA	3.41	2.06	1.95
46	R	304	CHL	CBB-CAB	3.40	1.50	1.29
46	y	309	CHL	CBB-CAB	3.40	1.50	1.29
29	g	614	CLA	C1D-ND	3.40	1.42	1.37
29	g	611	CLA	C1D-ND	3.40	1.42	1.37
29	S	314	CLA	C1D-ND	3.39	1.42	1.37
46	R	305	CHL	CBB-CAB	3.39	1.50	1.29
41	W	202	DGA	OG2-CB1	3.39	1.43	1.34
29	r	304	CLA	C1D-ND	3.38	1.42	1.37
41	w	201	DGA	OG2-CB1	3.38	1.43	1.34
44	e	101	HEM	FE-ND	3.38	2.05	1.94
46	S	307	CHL	CBB-CAB	3.38	1.50	1.29
29	G	612	CLA	C1D-ND	3.38	1.42	1.37
45	h	101	RRX	C16-C17	3.38	1.53	1.43
46	r	305	CHL	CBB-CAB	3.37	1.50	1.29
46	y	301	CHL	C3B-C4B	3.37	1.44	1.41
29	C	512	CLA	C1D-ND	3.37	1.42	1.37
46	G	608	CHL	CBB-CAB	3.36	1.50	1.29
29	C	502	CLA	C1D-ND	3.36	1.42	1.37
46	s	308	CHL	CBB-CAB	3.36	1.50	1.29
46	r	306	CHL	CBB-CAB	3.36	1.50	1.29
29	G	611	CLA	C1D-ND	3.36	1.42	1.37
29	s	310	CLA	C1D-ND	3.36	1.42	1.37
29	r	310	CLA	C1D-ND	3.36	1.42	1.37
29	y	304	CLA	C1D-ND	3.36	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	g	606	CHL	CBB-CAB	3.35	1.50	1.29
29	Y	304	CLA	C1D-ND	3.35	1.42	1.37
29	s	312	CLA	C1D-ND	3.34	1.42	1.37
48	s	319	NEX	C7-C6	-3.34	1.26	1.30
41	w	201	DGA	OG1-CA1	3.34	1.43	1.33
45	H	101	RRX	C4-C5	-3.34	1.44	1.51
29	n	603	CLA	C1D-ND	3.33	1.42	1.37
29	y	315	CLA	C1D-ND	3.33	1.42	1.37
29	S	312	CLA	C1D-ND	3.33	1.42	1.37
29	S	305	CLA	C1D-ND	3.33	1.42	1.37
29	s	314	CLA	C1D-ND	3.32	1.42	1.37
46	n	606	CHL	CBB-CAB	3.32	1.50	1.29
34	b	519	C7Z	C21-C26	-3.32	1.49	1.53
46	y	309	CHL	C3A-C2A	-3.31	1.51	1.54
29	R	309	CLA	C1D-ND	3.31	1.42	1.37
46	N	607	CHL	CBB-CAB	3.31	1.50	1.29
29	b	514	CLA	C1D-ND	3.31	1.42	1.37
29	B	514	CLA	C1D-ND	3.30	1.42	1.37
29	Y	312	CLA	C1D-ND	3.30	1.42	1.37
29	n	612	CLA	C1D-ND	3.30	1.42	1.37
29	B	508	CLA	C1D-ND	3.30	1.42	1.37
29	C	504	CLA	C1D-ND	3.30	1.42	1.37
29	Y	314	CLA	C1D-ND	3.30	1.42	1.37
46	G	606	CHL	CBB-CAB	3.30	1.50	1.29
45	H	101	RRX	C16-C17	3.30	1.53	1.43
34	B	519	C7Z	C38-C25	3.30	1.56	1.50
29	c	513	CLA	C1D-ND	3.29	1.42	1.37
46	y	308	CHL	C2C-C3C	3.29	1.39	1.36
29	n	610	CLA	C1D-ND	3.29	1.42	1.37
41	J	101	DGA	OG1-CA1	3.29	1.42	1.33
41	W	202	DGA	OG1-CA1	3.29	1.42	1.33
46	s	302	CHL	CBB-CAB	3.29	1.49	1.29
29	N	613	CLA	C1D-ND	3.29	1.42	1.37
29	b	515	CLA	C1D-ND	3.29	1.42	1.37
41	D	402	DGA	OG1-CA1	3.29	1.42	1.33
45	h	101	RRX	C24-C25	3.28	1.56	1.45
29	g	613	CLA	C1D-ND	3.28	1.42	1.37
29	D	405	CLA	C1D-ND	3.28	1.42	1.37
46	Y	307	CHL	CBB-CAB	3.28	1.49	1.29
29	c	511	CLA	C1D-ND	3.28	1.42	1.37
41	j	101	DGA	OG1-CA1	3.27	1.42	1.33
29	Y	303	CLA	C1D-ND	3.27	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	N	606	CHL	CBB-CAB	3.27	1.49	1.29
29	n	602	CLA	C1D-ND	3.27	1.42	1.37
45	h	101	RRX	C4-C5	-3.27	1.44	1.51
29	G	602	CLA	C1D-ND	3.27	1.42	1.37
29	C	505	CLA	C1D-ND	3.26	1.42	1.37
29	G	610	CLA	C1D-ND	3.26	1.42	1.37
46	Y	302	CHL	C2C-C3C	3.26	1.39	1.36
29	B	506	CLA	C1D-ND	3.26	1.42	1.37
29	R	302	CLA	C1D-ND	3.26	1.42	1.37
29	g	603	CLA	C1D-ND	3.25	1.42	1.37
29	S	306	CLA	C1D-ND	3.25	1.42	1.37
29	B	504	CLA	C1D-ND	3.25	1.42	1.37
29	d	404	CLA	C1D-ND	3.25	1.42	1.37
29	B	515	CLA	C1D-ND	3.25	1.42	1.37
29	S	313	CLA	C1D-ND	3.25	1.42	1.37
29	r	303	CLA	C1D-ND	3.25	1.42	1.37
34	b	519	C7Z	C38-C25	3.25	1.56	1.50
29	n	611	CLA	C1D-ND	3.25	1.42	1.37
46	S	302	CHL	CBB-CAB	3.24	1.49	1.29
29	A	406	CLA	C1D-ND	3.24	1.42	1.37
29	g	602	CLA	C1D-ND	3.24	1.42	1.37
30	a	407	PHO	C4D-CHA	3.24	1.44	1.39
29	y	305	CLA	C1D-ND	3.24	1.42	1.37
29	S	310	CLA	C1D-ND	3.24	1.42	1.37
41	b	522	DGA	OG1-CA1	3.23	1.42	1.33
44	E	101	HEM	CAC-C3C	3.23	1.56	1.47
46	Y	302	CHL	C3A-C2A	-3.23	1.51	1.54
29	R	301	CLA	C1D-ND	3.23	1.42	1.37
29	C	510	CLA	C1D-ND	3.23	1.42	1.37
29	s	306	CLA	C1D-ND	3.22	1.42	1.37
29	S	311	CLA	C1D-ND	3.22	1.42	1.37
29	g	612	CLA	C1D-ND	3.22	1.42	1.37
29	b	508	CLA	C1D-ND	3.22	1.42	1.37
29	G	614	CLA	C1D-ND	3.22	1.42	1.37
29	c	501	CLA	C1D-ND	3.22	1.42	1.37
29	r	308	CLA	C1D-ND	3.21	1.42	1.37
45	H	101	RRX	C24-C25	3.21	1.56	1.45
29	D	404	CLA	CAA-C2A	-3.21	1.48	1.54
29	y	310	CLA	C1D-ND	3.21	1.42	1.37
29	N	612	CLA	C1D-ND	3.21	1.42	1.37
45	h	101	RRX	C29-C30	3.20	1.64	1.54
46	y	308	CHL	CBB-CAB	3.20	1.49	1.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	N	610	CLA	C1D-ND	3.20	1.42	1.37
29	b	510	CLA	C1D-ND	3.20	1.42	1.37
29	n	604	CLA	C1D-ND	3.20	1.42	1.37
29	B	501	CLA	C1D-ND	3.19	1.42	1.37
29	C	503	CLA	C1D-ND	3.19	1.42	1.37
29	c	509	CLA	C1D-ND	3.19	1.42	1.37
29	s	315	CLA	C1D-ND	3.19	1.42	1.37
46	g	606	CHL	C2C-C3C	3.19	1.39	1.36
29	c	503	CLA	C1D-ND	3.18	1.42	1.37
29	s	313	CLA	C1D-ND	3.18	1.42	1.37
29	G	613	CLA	C1D-ND	3.18	1.42	1.37
29	s	311	CLA	C1D-ND	3.18	1.42	1.37
29	c	505	CLA	C1D-ND	3.18	1.42	1.37
29	r	309	CLA	C1D-ND	3.17	1.42	1.37
29	S	303	CLA	C1D-ND	3.17	1.42	1.37
46	n	606	CHL	C3B-C2B	-3.17	1.36	1.40
29	D	404	CLA	O2A-CGA	3.17	1.42	1.33
29	s	303	CLA	C1D-ND	3.17	1.42	1.37
29	B	510	CLA	C1D-ND	3.16	1.42	1.37
44	e	101	HEM	CAC-C3C	3.16	1.55	1.47
29	Y	305	CLA	C1D-ND	3.16	1.42	1.37
29	b	511	CLA	C1D-ND	3.16	1.42	1.37
29	A	407	CLA	C1D-ND	3.16	1.42	1.37
29	N	604	CLA	C1D-ND	3.15	1.42	1.37
29	Y	313	CLA	C1D-ND	3.15	1.42	1.37
29	C	507	CLA	C1D-ND	3.15	1.42	1.37
29	r	302	CLA	C1D-ND	3.15	1.42	1.37
29	c	508	CLA	C1D-ND	3.14	1.42	1.37
29	C	508	CLA	C1D-ND	3.14	1.42	1.37
44	E	101	HEM	CAB-C3B	3.14	1.55	1.47
29	b	501	CLA	C1D-ND	3.13	1.42	1.37
44	e	101	HEM	CAB-C3B	3.13	1.55	1.47
29	C	513	CLA	C1D-ND	3.13	1.42	1.37
43	d	405	PL9	C6-C1	-3.13	1.43	1.48
29	R	307	CLA	C1D-ND	3.13	1.42	1.37
29	Y	315	CLA	C1D-ND	3.13	1.42	1.37
29	c	506	CLA	C1D-ND	3.13	1.42	1.37
29	y	306	CLA	C1D-ND	3.12	1.42	1.37
45	H	101	RRX	C29-C30	3.12	1.64	1.54
29	R	306	CLA	C1D-ND	3.12	1.42	1.37
29	c	507	CLA	C1D-ND	3.11	1.42	1.37
29	y	316	CLA	C1D-ND	3.11	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	R	308	CLA	C1D-ND	3.11	1.41	1.37
46	N	607	CHL	C3B-C2B	-3.11	1.36	1.40
29	r	307	CLA	C1D-ND	3.10	1.41	1.37
29	n	609	CLA	C1D-ND	3.10	1.41	1.37
29	n	613	CLA	C1D-ND	3.10	1.41	1.37
29	N	602	CLA	C1D-ND	3.10	1.41	1.37
29	A	409	CLA	C1D-ND	3.10	1.41	1.37
29	C	511	CLA	C1D-ND	3.10	1.41	1.37
29	s	304	CLA	C1D-ND	3.10	1.41	1.37
29	g	610	CLA	C1D-ND	3.10	1.41	1.37
29	g	604	CLA	C1D-ND	3.09	1.41	1.37
46	Y	307	CHL	C3B-C2B	-3.09	1.36	1.40
45	h	101	RRX	C7-C6	3.08	1.55	1.45
29	C	509	CLA	C1D-ND	3.08	1.41	1.37
29	a	405	CLA	C1D-ND	3.08	1.41	1.37
29	s	305	CLA	C1D-ND	3.08	1.41	1.37
29	B	502	CLA	C1D-ND	3.07	1.41	1.37
43	D	406	PL9	C6-C1	-3.06	1.43	1.48
29	Y	309	CLA	C1D-ND	3.06	1.41	1.37
29	a	408	CLA	C1D-ND	3.06	1.41	1.37
29	c	502	CLA	C1D-ND	3.05	1.41	1.37
29	c	512	CLA	C1D-ND	3.05	1.41	1.37
48	r	313	NEX	C14-C13	-3.05	1.26	1.34
29	b	505	CLA	C1D-ND	3.05	1.41	1.37
45	H	101	RRX	C7-C6	3.05	1.55	1.45
48	R	312	NEX	C14-C13	-3.04	1.26	1.34
29	B	511	CLA	C1D-ND	3.04	1.41	1.37
29	Y	311	CLA	C1D-ND	3.04	1.41	1.37
46	G	606	CHL	C3B-C2B	-3.03	1.36	1.40
29	B	516	CLA	C1D-ND	3.03	1.41	1.37
29	S	315	CLA	C1D-ND	3.03	1.41	1.37
46	r	305	CHL	C3B-C2B	-3.03	1.36	1.40
29	C	506	CLA	C1D-ND	3.03	1.41	1.37
29	y	312	CLA	C1D-ND	3.03	1.41	1.37
29	c	504	CLA	C1D-ND	3.02	1.41	1.37
46	n	606	CHL	CHB-C4A	-3.01	1.35	1.38
29	R	303	CLA	C1D-ND	3.01	1.41	1.37
29	B	509	CLA	C1D-ND	3.01	1.41	1.37
29	b	504	CLA	C1D-ND	3.00	1.41	1.37
29	y	314	CLA	C1D-ND	3.00	1.41	1.37
29	b	509	CLA	C1D-ND	3.00	1.41	1.37
29	b	516	CLA	C1D-ND	2.99	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	d	405	PL9	C7-C3	-2.99	1.47	1.51
29	a	406	CLA	C1D-ND	2.99	1.41	1.37
29	b	502	CLA	C1D-ND	2.99	1.41	1.37
46	N	607	CHL	CHB-C4A	-2.98	1.35	1.38
35	C	524	LMG	C40-C39	-2.97	1.33	1.51
46	G	608	CHL	CHB-C4A	-2.97	1.35	1.38
29	B	503	CLA	C1D-ND	2.96	1.41	1.37
29	B	507	CLA	C1D-ND	2.96	1.41	1.37
29	b	512	CLA	C1D-ND	2.96	1.41	1.37
46	s	308	CHL	CHB-C4A	-2.96	1.35	1.38
46	G	606	CHL	CHB-C4A	-2.96	1.35	1.38
29	c	510	CLA	C1D-ND	2.96	1.41	1.37
46	R	304	CHL	C2C-C3C	2.96	1.39	1.36
29	B	505	CLA	C1D-ND	2.95	1.41	1.37
35	d	407	LMG	C37-C36	-2.95	1.33	1.51
29	b	506	CLA	C1D-ND	2.94	1.41	1.37
46	s	302	CHL	CHB-C4A	-2.94	1.35	1.38
29	b	503	CLA	C1D-ND	2.94	1.41	1.37
35	D	409	LMG	C37-C36	-2.93	1.33	1.51
46	S	302	CHL	CHB-C4A	-2.93	1.35	1.38
29	D	404	CLA	CMC-C2C	-2.93	1.44	1.50
29	b	513	CLA	C1D-ND	2.92	1.41	1.37
29	A	405	CLA	C1D-ND	2.92	1.41	1.37
46	r	305	CHL	C2C-C3C	2.91	1.39	1.36
29	b	507	CLA	C1D-ND	2.91	1.41	1.37
46	r	306	CHL	C3B-C2B	-2.90	1.36	1.40
46	Y	310	CHL	CHB-C4A	-2.90	1.35	1.38
46	S	309	CHL	C3D-C2D	-2.90	1.34	1.39
46	S	302	CHL	C3B-C2B	-2.90	1.36	1.40
51	s	321	LPX	P1-O1	2.89	1.70	1.59
46	n	605	CHL	CHB-C4A	-2.88	1.35	1.38
46	g	606	CHL	CHB-C4A	-2.88	1.35	1.38
29	B	512	CLA	C1D-ND	2.88	1.41	1.37
46	Y	307	CHL	CHB-C4A	-2.88	1.35	1.38
46	g	606	CHL	C3B-C2B	-2.88	1.36	1.40
46	R	305	CHL	C3B-C2B	-2.87	1.36	1.40
29	B	513	CLA	C1D-ND	2.87	1.41	1.37
46	s	308	CHL	C3B-C2B	-2.86	1.36	1.40
46	N	606	CHL	CHB-C4A	-2.84	1.35	1.38
46	y	303	CHL	C3B-C2B	-2.84	1.36	1.40
29	D	404	CLA	CHB-C1B	2.83	1.45	1.39
29	a	404	CLA	C1D-ND	2.83	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	y	301	CHL	CHB-C4A	-2.82	1.35	1.38
30	a	407	PHO	CMC-C2C	-2.82	1.46	1.50
46	N	606	CHL	C3B-C2B	-2.82	1.36	1.40
46	y	311	CHL	CHB-C4A	-2.82	1.35	1.38
46	S	308	CHL	CHB-C4A	-2.82	1.35	1.38
45	H	101	RRX	C32-C1	2.81	1.59	1.53
46	n	608	CHL	CHB-C4A	-2.81	1.35	1.38
46	N	607	CHL	C1D-C2D	2.81	1.42	1.39
46	s	302	CHL	C3B-C2B	-2.81	1.36	1.40
46	Y	307	CHL	C1A-CHA	-2.80	1.36	1.40
46	R	304	CHL	C3B-C2B	-2.80	1.36	1.40
46	G	608	CHL	C3B-C2B	-2.80	1.36	1.40
46	g	609	CHL	CHB-C4A	-2.79	1.35	1.38
46	s	309	CHL	CHB-C4A	-2.79	1.35	1.38
46	g	607	CHL	CHB-C4A	-2.79	1.35	1.38
46	s	307	CHL	CHB-C4A	-2.79	1.35	1.38
46	Y	302	CHL	C3B-C4B	2.79	1.44	1.41
46	r	305	CHL	CHB-C4A	-2.78	1.35	1.38
46	n	608	CHL	C3B-C4B	2.78	1.44	1.41
45	h	101	RRX	C32-C1	2.78	1.59	1.53
46	Y	310	CHL	C1D-C2D	2.78	1.42	1.39
46	S	307	CHL	C3B-C2B	-2.78	1.36	1.40
46	Y	302	CHL	C1B-C2B	2.77	1.42	1.39
46	R	304	CHL	CHB-C4A	-2.77	1.35	1.38
30	d	402	PHO	CMC-C2C	-2.77	1.46	1.50
46	G	609	CHL	CHB-C4A	-2.77	1.35	1.38
46	r	306	CHL	CHB-C4A	-2.77	1.35	1.38
46	S	309	CHL	C1D-C2D	2.77	1.42	1.39
46	Y	302	CHL	C1D-C2D	2.76	1.42	1.39
46	n	608	CHL	C1D-C2D	2.76	1.42	1.39
46	R	305	CHL	C1D-C2D	2.75	1.42	1.39
46	G	601	CHL	C1D-C2D	2.75	1.42	1.39
46	G	605	CHL	C1B-C2B	2.75	1.42	1.39
46	G	607	CHL	C1B-C2B	2.75	1.42	1.39
46	S	307	CHL	CHB-C4A	-2.75	1.35	1.38
46	g	608	CHL	CHB-C4A	-2.74	1.35	1.38
51	S	321	LPX	P1-O1	2.74	1.70	1.59
46	R	305	CHL	CHB-C4A	-2.74	1.35	1.38
46	N	609	CHL	CHB-C4A	-2.74	1.35	1.38
46	N	601	CHL	CHB-C4A	-2.74	1.35	1.38
46	g	601	CHL	CHB-C4A	-2.74	1.35	1.38
46	G	605	CHL	C1D-C2D	2.73	1.42	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S	316	CLA	C1B-C2B	2.73	1.49	1.43
46	Y	308	CHL	CHB-C4A	-2.73	1.35	1.38
46	g	601	CHL	C1D-C2D	2.72	1.42	1.39
46	G	609	CHL	C1D-C2D	2.72	1.42	1.39
46	g	609	CHL	C3B-C2B	-2.72	1.36	1.40
46	n	601	CHL	C1D-C2D	2.72	1.42	1.39
46	n	601	CHL	CHB-C4A	-2.72	1.35	1.38
46	y	303	CHL	C1D-C2D	2.72	1.42	1.39
46	N	601	CHL	C1D-C2D	2.71	1.42	1.39
29	N	613	CLA	C1B-C2B	2.71	1.49	1.43
38	b	524	LMT	O3'-C3'	-2.71	1.36	1.43
46	S	307	CHL	C1D-C2D	2.71	1.42	1.39
46	s	302	CHL	C1D-C2D	2.71	1.42	1.39
29	s	316	CLA	C1B-C2B	2.71	1.49	1.43
46	N	608	CHL	C1B-C2B	2.70	1.42	1.39
46	G	606	CHL	C1D-C2D	2.70	1.42	1.39
29	r	310	CLA	C1B-C2B	2.70	1.49	1.43
46	N	605	CHL	C1D-C2D	2.70	1.42	1.39
46	g	605	CHL	C1D-C2D	2.70	1.42	1.39
30	D	401	PHO	CMC-C2C	-2.70	1.46	1.50
29	D	404	CLA	C3B-C4B	-2.70	1.35	1.42
46	S	309	CHL	CHB-C4A	-2.69	1.35	1.38
46	r	306	CHL	C1D-C2D	2.69	1.42	1.39
46	N	605	CHL	CHB-C4A	-2.69	1.35	1.38
46	R	304	CHL	C1B-C2B	2.69	1.42	1.39
29	n	612	CLA	C1B-C2B	2.68	1.49	1.43
46	y	307	CHL	C1D-C2D	2.68	1.42	1.39
29	S	304	CLA	C1D-ND	2.68	1.41	1.37
46	g	605	CHL	C1B-C2B	2.68	1.42	1.39
46	y	309	CHL	CHB-C4A	-2.67	1.35	1.38
33	B	522	3PH	O21-C2	-2.67	1.40	1.46
46	n	607	CHL	CHB-C4A	-2.67	1.35	1.38
46	r	305	CHL	C1B-C2B	2.67	1.42	1.39
46	G	601	CHL	CHB-C4A	-2.67	1.35	1.38
46	N	605	CHL	C1B-C2B	2.67	1.42	1.39
46	g	606	CHL	C1D-C2D	2.67	1.42	1.39
46	g	601	CHL	C1B-C2B	2.67	1.42	1.39
46	s	307	CHL	C1D-C2D	2.67	1.42	1.39
50	y	321	PTY	O7-C6	-2.67	1.40	1.46
46	s	308	CHL	C1D-C2D	2.66	1.42	1.39
46	n	605	CHL	C1D-C2D	2.66	1.42	1.39
29	s	315	CLA	C1B-C2B	2.66	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S	308	CHL	C1D-C2D	2.66	1.42	1.39
46	G	607	CHL	CHB-C4A	-2.66	1.35	1.38
50	n	619	PTY	O7-C6	-2.66	1.40	1.46
46	R	305	CHL	C1B-C2B	2.66	1.42	1.39
46	Y	306	CHL	CHB-C4A	-2.65	1.35	1.38
46	S	307	CHL	C1B-C2B	2.65	1.42	1.39
46	S	302	CHL	C1D-C2D	2.65	1.42	1.39
33	b	521	3PH	O21-C2	-2.65	1.40	1.46
46	y	303	CHL	CHB-C4A	-2.65	1.35	1.38
46	Y	308	CHL	C1B-C2B	2.65	1.42	1.39
46	n	607	CHL	C1B-C2B	2.65	1.42	1.39
46	n	607	CHL	C1D-C2D	2.65	1.42	1.39
46	n	608	CHL	C1A-CHA	-2.65	1.37	1.40
46	S	309	CHL	C1B-C2B	2.65	1.42	1.39
46	y	308	CHL	CHB-C4A	-2.65	1.35	1.38
46	Y	306	CHL	C1D-C2D	2.65	1.42	1.39
46	N	608	CHL	C1D-C2D	2.64	1.42	1.39
46	G	608	CHL	C1D-C2D	2.64	1.42	1.39
46	Y	308	CHL	C1D-C2D	2.64	1.42	1.39
46	n	605	CHL	C3B-C2B	-2.64	1.36	1.40
46	y	308	CHL	C1B-C2B	2.64	1.42	1.39
38	B	524	LMT	O3'-C3'	-2.64	1.36	1.43
46	R	304	CHL	C1D-C2D	2.64	1.42	1.39
46	g	609	CHL	C1D-C2D	2.64	1.42	1.39
46	y	307	CHL	CHB-C4A	-2.64	1.35	1.38
46	Y	306	CHL	C1B-C2B	2.64	1.42	1.39
29	B	505	CLA	C1B-C2B	2.64	1.49	1.43
46	G	601	CHL	C1B-C2B	2.64	1.42	1.39
46	y	309	CHL	C1B-C2B	2.64	1.42	1.39
46	y	311	CHL	C1B-C2B	2.64	1.42	1.39
30	A	408	PHO	CMC-C2C	-2.63	1.46	1.50
46	g	607	CHL	C1B-C2B	2.63	1.42	1.39
46	r	305	CHL	C1D-C2D	2.63	1.42	1.39
46	N	609	CHL	C1D-C2D	2.63	1.42	1.39
46	Y	307	CHL	C1D-C2D	2.63	1.42	1.39
29	N	614	CLA	C1B-C2B	2.63	1.49	1.43
46	y	311	CHL	C1D-C2D	2.63	1.42	1.39
46	N	601	CHL	C1B-C2B	2.62	1.42	1.39
46	y	301	CHL	C1B-C2B	2.62	1.42	1.39
46	y	303	CHL	C1B-C2B	2.62	1.42	1.39
29	R	309	CLA	C1B-C2B	2.62	1.49	1.43
50	Y	320	PTY	O7-C6	-2.62	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S	314	CLA	C1B-C2B	2.62	1.49	1.43
46	y	307	CHL	C1B-C2B	2.62	1.42	1.39
46	g	609	CHL	C1B-C2B	2.61	1.42	1.39
46	G	605	CHL	CHB-C4A	-2.61	1.35	1.38
29	s	314	CLA	C1B-C2B	2.61	1.49	1.43
46	s	309	CHL	C1B-C2B	2.61	1.42	1.39
29	g	613	CLA	C1B-C2B	2.61	1.49	1.43
44	E	101	HEM	FE-ND	2.61	2.02	1.94
46	n	608	CHL	C1B-C2B	2.61	1.42	1.39
46	g	608	CHL	C1B-C2B	2.61	1.42	1.39
46	Y	310	CHL	C1B-C2B	2.60	1.42	1.39
50	N	620	PTY	O7-C6	-2.60	1.40	1.46
46	y	301	CHL	C1D-C2D	2.59	1.42	1.39
29	s	306	CLA	C1B-C2B	2.59	1.49	1.43
29	b	505	CLA	C1B-C2B	2.59	1.49	1.43
46	n	606	CHL	C1D-C2D	2.59	1.42	1.39
46	g	605	CHL	CHB-C4A	-2.59	1.35	1.38
33	S	322	3PH	O21-C2	-2.59	1.40	1.46
46	g	607	CHL	C1D-C2D	2.59	1.42	1.39
46	n	601	CHL	C1B-C2B	2.59	1.42	1.39
29	S	303	CLA	C1B-C2B	2.59	1.49	1.43
46	N	607	CHL	C1B-C2B	2.59	1.42	1.39
46	N	608	CHL	CHB-C4A	-2.58	1.35	1.38
30	a	407	PHO	C4D-ND	-2.58	1.34	1.38
49	n	618	XAT	O24-C25	-2.58	1.42	1.46
46	N	605	CHL	C3B-C2B	-2.58	1.36	1.40
46	Y	302	CHL	CHB-C4A	-2.58	1.35	1.38
30	a	407	PHO	CMD-C2D	-2.58	1.46	1.51
29	B	515	CLA	C3B-C4B	2.58	1.50	1.42
29	r	302	CLA	C1B-C2B	2.58	1.49	1.43
29	S	306	CLA	C1B-C2B	2.57	1.49	1.43
46	G	607	CHL	C1D-C2D	2.57	1.42	1.39
29	y	310	CLA	C1B-C2B	2.57	1.49	1.43
29	n	613	CLA	C1B-C2B	2.57	1.49	1.43
29	g	614	CLA	C1B-C2B	2.57	1.49	1.43
46	G	609	CHL	C1B-C2B	2.56	1.42	1.39
29	G	614	CLA	C1B-C2B	2.56	1.49	1.43
46	N	609	CHL	C1B-C2B	2.56	1.42	1.39
46	r	306	CHL	C1B-C2B	2.56	1.42	1.39
43	D	406	PL9	C52-C5	-2.56	1.45	1.50
29	G	612	CLA	C1B-C2B	2.55	1.49	1.43
29	N	611	CLA	C1B-C2B	2.55	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	s	307	CHL	C1B-C2B	2.55	1.42	1.39
46	s	309	CHL	C1D-C2D	2.55	1.42	1.39
29	s	304	CLA	MG-NB	-2.55	2.00	2.05
46	s	309	CHL	C3B-C2B	-2.55	1.36	1.40
29	C	508	CLA	C1B-C2B	2.55	1.49	1.43
46	S	309	CHL	C1A-CHA	-2.55	1.37	1.40
49	y	302	XAT	O24-C25	-2.55	1.42	1.46
29	N	612	CLA	C1B-C2B	2.54	1.49	1.43
29	c	511	CLA	C1B-C2B	2.54	1.49	1.43
33	s	322	3PH	O21-C2	-2.54	1.40	1.46
30	A	408	PHO	CMD-C2D	-2.53	1.46	1.51
29	r	308	CLA	C1B-C2B	2.53	1.49	1.43
46	g	608	CHL	C1D-C2D	2.53	1.42	1.39
29	G	613	CLA	C1B-C2B	2.53	1.49	1.43
29	S	304	CLA	C1B-C2B	2.53	1.49	1.43
29	Y	314	CLA	C1B-C2B	2.53	1.49	1.43
29	s	303	CLA	C1B-C2B	2.53	1.49	1.43
29	S	315	CLA	C1B-C2B	2.53	1.49	1.43
49	g	619	XAT	O24-C25	-2.52	1.43	1.46
29	C	511	CLA	C1B-C2B	2.52	1.49	1.43
29	b	501	CLA	C1B-C2B	2.52	1.49	1.43
46	N	609	CHL	C3B-C2B	-2.52	1.37	1.40
46	y	309	CHL	C1D-C2D	2.52	1.42	1.39
29	s	304	CLA	C1B-C2B	2.52	1.49	1.43
29	g	611	CLA	C1B-C2B	2.52	1.49	1.43
29	C	513	CLA	C1B-C2B	2.51	1.49	1.43
29	n	610	CLA	C1B-C2B	2.51	1.49	1.43
29	C	512	CLA	C1B-C2B	2.51	1.49	1.43
46	G	609	CHL	C3B-C2B	-2.51	1.37	1.40
29	c	506	CLA	C1B-C2B	2.50	1.49	1.43
29	b	515	CLA	C3B-C4B	2.50	1.50	1.42
46	S	308	CHL	C1B-C2B	2.50	1.42	1.39
49	N	619	XAT	O24-C25	-2.50	1.43	1.46
29	G	611	CLA	C1B-C2B	2.50	1.49	1.43
29	R	307	CLA	C1B-C2B	2.50	1.49	1.43
29	Y	312	CLA	C1B-C2B	2.50	1.49	1.43
29	A	407	CLA	C1B-C2B	2.50	1.49	1.43
29	S	313	CLA	C1B-C2B	2.50	1.49	1.43
45	H	101	RRX	C35-C13	2.50	1.55	1.50
46	y	308	CHL	C1D-C2D	2.49	1.42	1.39
30	d	402	PHO	CMD-C2D	-2.49	1.46	1.51
29	y	305	CLA	C1B-C2B	2.49	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	R	301	CLA	C1B-C2B	2.49	1.49	1.43
49	G	619	XAT	O24-C25	-2.49	1.43	1.46
29	B	509	CLA	C1B-C2B	2.49	1.49	1.43
49	R	311	XAT	O24-C25	-2.49	1.43	1.46
46	Y	307	CHL	C1B-C2B	2.49	1.42	1.39
34	B	519	C7Z	C20-C13	2.49	1.55	1.50
29	c	507	CLA	C1B-C2B	2.49	1.49	1.43
29	y	313	CLA	C1B-C2B	2.49	1.49	1.43
46	N	606	CHL	C1A-CHA	-2.49	1.37	1.40
29	b	509	CLA	C1B-C2B	2.49	1.49	1.43
29	g	603	CLA	C1B-C2B	2.49	1.49	1.43
46	s	302	CHL	C1B-C2B	2.49	1.42	1.39
29	S	312	CLA	C1B-C2B	2.49	1.49	1.43
29	Y	315	CLA	C1B-C2B	2.49	1.49	1.43
29	B	502	CLA	C1B-C2B	2.49	1.49	1.43
29	b	502	CLA	C1B-C2B	2.48	1.49	1.43
30	D	401	PHO	CMD-C2D	-2.48	1.46	1.51
29	B	506	CLA	C1B-C2B	2.48	1.49	1.43
46	S	302	CHL	C1B-C2B	2.48	1.42	1.39
29	Y	304	CLA	C1B-C2B	2.48	1.48	1.43
29	d	404	CLA	C1B-C2B	2.48	1.48	1.43
29	D	405	CLA	C1B-C2B	2.48	1.48	1.43
29	s	313	CLA	C1B-C2B	2.48	1.48	1.43
29	s	312	CLA	C1B-C2B	2.48	1.48	1.43
45	h	101	RRX	C35-C13	2.48	1.55	1.50
29	B	504	CLA	C1B-C2B	2.47	1.48	1.43
29	n	602	CLA	C1B-C2B	2.47	1.48	1.43
29	c	505	CLA	C1B-C2B	2.47	1.48	1.43
29	c	512	CLA	C1B-C2B	2.47	1.48	1.43
33	b	521	3PH	O31-C31	2.47	1.40	1.33
46	G	608	CHL	C1B-C2B	2.47	1.42	1.39
29	S	310	CLA	C3B-C4B	2.47	1.49	1.42
46	s	308	CHL	C1B-C2B	2.46	1.42	1.39
46	n	605	CHL	C1B-C2B	2.46	1.42	1.39
29	A	405	CLA	C1B-C2B	2.46	1.48	1.43
30	a	407	PHO	CMB-C2B	-2.46	1.46	1.51
49	Y	301	XAT	O24-C25	-2.46	1.43	1.46
29	r	307	CLA	C3B-C4B	2.46	1.49	1.42
29	G	603	CLA	C1B-C2B	2.46	1.48	1.43
29	C	514	CLA	C1B-C2B	2.46	1.48	1.43
46	G	606	CHL	C1B-C2B	2.46	1.42	1.39
34	b	519	C7Z	C20-C13	2.45	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	r	312	XAT	O24-C25	-2.45	1.43	1.46
29	C	506	CLA	C1B-C2B	2.45	1.48	1.43
46	N	606	CHL	C1D-C2D	2.45	1.42	1.39
29	N	603	CLA	C1B-C2B	2.45	1.48	1.43
30	A	408	PHO	CMB-C2B	-2.45	1.46	1.51
29	g	612	CLA	C1B-C2B	2.45	1.48	1.43
46	g	606	CHL	C1B-C2B	2.45	1.42	1.39
29	B	508	CLA	C1B-C2B	2.45	1.48	1.43
29	C	502	CLA	C1B-C2B	2.45	1.48	1.43
29	B	501	CLA	C3B-C4B	2.44	1.49	1.42
29	r	309	CLA	CHC-C1C	2.44	1.43	1.38
29	D	404	CLA	C1D-C2D	-2.44	1.40	1.45
29	N	612	CLA	C3B-C4B	2.44	1.49	1.42
46	r	306	CHL	C1A-CHA	-2.43	1.37	1.40
29	n	604	CLA	C1B-C2B	2.43	1.48	1.43
29	r	304	CLA	C1B-C2B	2.43	1.48	1.43
29	r	309	CLA	C3B-C4B	2.43	1.49	1.42
29	C	504	CLA	C1B-C2B	2.43	1.48	1.43
29	y	316	CLA	C1B-C2B	2.43	1.48	1.43
29	y	315	CLA	C1B-C2B	2.43	1.48	1.43
33	a	415	3PH	O21-C2	-2.43	1.40	1.46
29	Y	313	CLA	C1B-C2B	2.43	1.48	1.43
46	y	309	CHL	C3B-C4B	2.43	1.43	1.41
29	C	507	CLA	C1B-C2B	2.43	1.48	1.43
29	D	404	CLA	CHC-C1C	2.43	1.43	1.38
33	B	522	3PH	O31-C31	2.43	1.40	1.33
29	G	603	CLA	C3B-C4B	2.42	1.49	1.42
29	Y	309	CLA	C1B-C2B	2.42	1.48	1.43
29	c	510	CLA	C1B-C2B	2.42	1.48	1.43
29	s	312	CLA	C3B-C4B	2.42	1.49	1.42
29	G	610	CLA	C3B-C4B	2.42	1.49	1.42
29	Y	303	CLA	C3B-C4B	2.42	1.49	1.42
29	n	611	CLA	C1B-C2B	2.42	1.48	1.43
29	S	310	CLA	C1B-C2B	2.42	1.48	1.43
29	B	501	CLA	C1B-C2B	2.42	1.48	1.43
50	y	321	PTY	O7-C8	2.42	1.40	1.35
29	d	403	CLA	C1D-ND	2.41	1.41	1.37
38	b	524	LMT	O2'-C2'	-2.41	1.37	1.43
33	S	322	3PH	O31-C31	2.41	1.40	1.33
46	S	309	CHL	C3B-C2B	-2.41	1.37	1.40
29	N	604	CLA	C1B-C2B	2.41	1.48	1.43
35	D	410	LMG	C22-C21	-2.41	1.33	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	y	303	CHL	C1A-CHA	-2.41	1.37	1.40
29	n	610	CLA	C3B-C4B	2.41	1.49	1.42
44	e	101	HEM	FE-NB	2.41	2.02	1.94
29	C	510	CLA	C1B-C2B	2.41	1.48	1.43
35	d	408	LMG	C22-C21	-2.41	1.33	1.50
29	N	611	CLA	C3B-C4B	2.41	1.49	1.42
29	b	508	CLA	C1B-C2B	2.41	1.48	1.43
50	N	620	PTY	O4-C30	2.40	1.40	1.33
29	b	513	CLA	C1B-C2B	2.40	1.48	1.43
29	g	610	CLA	CHC-C1C	2.40	1.43	1.38
29	R	308	CLA	CHC-C1C	2.40	1.43	1.38
29	g	610	CLA	C1B-C2B	2.40	1.48	1.43
29	G	602	CLA	C1B-C2B	2.40	1.48	1.43
29	R	303	CLA	C1B-C2B	2.40	1.48	1.43
33	s	322	3PH	O31-C31	2.40	1.40	1.33
29	S	311	CLA	C3B-C4B	2.40	1.49	1.42
36	C	519	DGD	CGB-CFB	-2.40	1.33	1.50
36	c	516	DGD	CGB-CFB	-2.40	1.33	1.50
29	c	501	CLA	C1B-C2B	2.40	1.48	1.43
29	R	306	CLA	C1B-C2B	2.40	1.48	1.43
29	s	310	CLA	C1B-C2B	2.40	1.48	1.43
35	c	519	LMG	C43-C42	-2.40	1.33	1.50
50	n	619	PTY	O4-C30	2.40	1.40	1.33
29	B	510	CLA	C3B-C4B	2.40	1.49	1.42
29	G	604	CLA	C3B-C4B	2.40	1.49	1.42
29	S	312	CLA	C3B-C4B	2.40	1.49	1.42
29	b	504	CLA	C1B-C2B	2.40	1.48	1.43
29	N	610	CLA	C1B-C2B	2.39	1.48	1.43
29	Y	305	CLA	C1B-C2B	2.39	1.48	1.43
38	B	524	LMT	O2'-C2'	-2.39	1.37	1.43
29	S	305	CLA	C1B-C2B	2.39	1.48	1.43
29	n	603	CLA	C3B-C4B	2.39	1.49	1.42
36	c	518	DGD	CDA-CCA	-2.39	1.33	1.50
29	C	503	CLA	C1B-C2B	2.39	1.48	1.43
29	y	304	CLA	C1B-C2B	2.39	1.48	1.43
29	c	513	CLA	C1B-C2B	2.39	1.48	1.43
29	R	308	CLA	C3B-C4B	2.39	1.49	1.42
29	n	609	CLA	CHC-C1C	2.39	1.43	1.38
36	C	520	DGD	CAB-C9B	-2.39	1.33	1.50
29	b	506	CLA	C1B-C2B	2.39	1.48	1.43
29	n	609	CLA	C3B-C4B	2.39	1.49	1.42
29	G	611	CLA	C3B-C4B	2.39	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S	306	CLA	C3B-C4B	2.39	1.49	1.42
29	n	611	CLA	C3B-C4B	2.39	1.49	1.42
29	y	304	CLA	C3B-C4B	2.39	1.49	1.42
36	c	517	DGD	CGB-CFB	-2.39	1.33	1.50
29	g	611	CLA	C3B-C4B	2.39	1.49	1.42
50	Y	320	PTY	O7-C8	2.39	1.40	1.35
29	d	403	CLA	C3B-C4B	2.39	1.49	1.42
29	S	304	CLA	MG-NB	-2.39	2.01	2.05
29	D	404	CLA	O1A-CGA	-2.39	1.15	1.22
29	s	311	CLA	CHC-C1C	2.39	1.43	1.38
35	c	519	LMG	C25-C24	-2.38	1.33	1.50
29	G	610	CLA	CHC-C1C	2.38	1.43	1.38
29	C	505	CLA	C3B-C4B	2.38	1.49	1.42
29	N	602	CLA	C3B-C4B	2.38	1.49	1.42
36	C	518	DGD	CGB-CFB	-2.38	1.33	1.50
29	Y	304	CLA	C3B-C4B	2.38	1.49	1.42
35	C	521	LMG	C43-C42	-2.38	1.33	1.50
35	B	520	LMG	C25-C24	-2.38	1.33	1.50
29	C	514	CLA	C3B-C4B	2.38	1.49	1.42
29	c	502	CLA	C1B-C2B	2.38	1.48	1.43
46	S	308	CHL	C3B-C2B	-2.38	1.37	1.40
36	c	518	DGD	CGB-CFB	-2.38	1.33	1.50
46	n	606	CHL	C1A-CHA	-2.38	1.37	1.40
29	b	507	CLA	C1B-C2B	2.38	1.48	1.43
29	s	304	CLA	C3B-C4B	2.38	1.49	1.42
29	n	602	CLA	C3B-C4B	2.37	1.49	1.42
29	B	513	CLA	C1B-C2B	2.37	1.48	1.43
35	i	101	LMG	C22-C21	-2.37	1.33	1.50
29	d	403	CLA	CHC-C1C	2.37	1.43	1.38
46	Y	310	CHL	C3B-C2B	-2.37	1.37	1.40
29	G	614	CLA	C3B-C4B	2.37	1.49	1.42
29	B	507	CLA	C1B-C2B	2.37	1.48	1.43
29	n	603	CLA	C1B-C2B	2.37	1.48	1.43
29	y	316	CLA	C3B-C4B	2.37	1.49	1.42
29	G	604	CLA	C1B-C2B	2.37	1.48	1.43
29	G	610	CLA	C1B-C2B	2.37	1.48	1.43
29	S	304	CLA	MG-ND	-2.37	2.01	2.05
36	C	520	DGD	CDA-CCA	-2.37	1.33	1.50
46	g	601	CHL	C3B-C2B	-2.37	1.37	1.40
29	N	611	CLA	CHC-C1C	2.37	1.43	1.38
29	g	602	CLA	CHC-C1C	2.37	1.43	1.38
29	B	503	CLA	C1B-C2B	2.37	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	i	101	LMG	C43-C42	-2.37	1.33	1.50
29	c	503	CLA	C1B-C2B	2.37	1.48	1.43
29	b	516	CLA	C1B-C2B	2.37	1.48	1.43
35	W	201	LMG	C22-C21	-2.37	1.33	1.50
36	c	517	DGD	CGA-CFA	-2.37	1.33	1.50
46	y	311	CHL	C3B-C2B	-2.37	1.37	1.40
29	a	406	CLA	C1B-C2B	2.37	1.48	1.43
29	g	602	CLA	C1B-C2B	2.37	1.48	1.43
29	Y	303	CLA	CHC-C1C	2.36	1.43	1.38
29	g	614	CLA	C3B-C4B	2.36	1.49	1.42
29	r	307	CLA	C1B-C2B	2.36	1.48	1.43
29	y	314	CLA	C1B-C2B	2.36	1.48	1.43
29	g	603	CLA	C3B-C4B	2.36	1.49	1.42
35	b	520	LMG	C25-C24	-2.36	1.33	1.50
29	r	309	CLA	C1B-C2B	2.36	1.48	1.43
29	N	614	CLA	C3B-C4B	2.36	1.49	1.42
35	d	407	LMG	C25-C24	-2.36	1.33	1.50
33	A	412	3PH	O31-C31	2.36	1.40	1.33
29	A	406	CLA	C1B-C2B	2.36	1.48	1.43
29	b	515	CLA	C1B-C2B	2.36	1.48	1.43
46	N	606	CHL	C1B-C2B	2.36	1.42	1.39
46	g	605	CHL	C3B-C2B	-2.36	1.37	1.40
29	b	501	CLA	C3B-C4B	2.36	1.49	1.42
29	s	311	CLA	C1B-C2B	2.36	1.48	1.43
29	D	405	CLA	C3B-C4B	2.36	1.49	1.42
29	b	503	CLA	C1B-C2B	2.36	1.48	1.43
33	A	412	3PH	O21-C21	2.35	1.40	1.34
29	A	409	CLA	C1B-C2B	2.35	1.48	1.43
30	A	408	PHO	C4D-ND	-2.35	1.35	1.38
29	C	503	CLA	C3B-C4B	2.35	1.49	1.42
29	B	503	CLA	C3B-C4B	2.35	1.49	1.42
35	D	410	LMG	C43-C42	-2.35	1.33	1.50
35	d	408	LMG	C43-C42	-2.35	1.33	1.50
29	G	612	CLA	C3B-C4B	2.35	1.49	1.42
29	n	613	CLA	C3B-C4B	2.35	1.49	1.42
29	S	311	CLA	C1B-C2B	2.35	1.48	1.43
29	B	512	CLA	C3B-C4B	2.35	1.49	1.42
29	s	311	CLA	C3B-C4B	2.35	1.49	1.42
29	s	310	CLA	C3B-C4B	2.35	1.49	1.42
29	R	306	CLA	C3B-C4B	2.35	1.49	1.42
29	b	508	CLA	C3B-C4B	2.35	1.49	1.42
33	a	415	3PH	O31-C31	2.35	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	G	602	CLA	CHC-C1C	2.35	1.43	1.38
29	G	611	CLA	CHC-C1C	2.35	1.43	1.38
29	b	512	CLA	C3B-C4B	2.34	1.49	1.42
46	G	605	CHL	CHA-CBD	2.34	1.54	1.51
29	C	505	CLA	C1B-C2B	2.34	1.48	1.43
29	c	509	CLA	C1B-C2B	2.34	1.48	1.43
46	Y	306	CHL	C3B-C2B	-2.34	1.37	1.40
41	w	201	DGA	OG2-CG2	-2.34	1.41	1.46
29	B	516	CLA	C1B-C2B	2.34	1.48	1.43
29	S	316	CLA	CHC-C1C	2.34	1.43	1.38
29	B	510	CLA	C1B-C2B	2.34	1.48	1.43
30	d	402	PHO	CMB-C2B	-2.34	1.46	1.51
46	n	606	CHL	C1B-C2B	2.34	1.42	1.39
29	Y	311	CLA	C3B-C4B	2.34	1.49	1.42
29	c	501	CLA	C3B-C4B	2.34	1.49	1.42
46	G	601	CHL	C1A-CHA	-2.34	1.37	1.40
29	R	308	CLA	C1B-C2B	2.33	1.48	1.43
34	b	519	C7Z	C18-C5	2.33	1.54	1.50
29	N	603	CLA	C3B-C4B	2.33	1.49	1.42
29	S	315	CLA	C3B-C4B	2.33	1.49	1.42
51	s	321	LPX	P1-O2	2.33	1.68	1.59
29	g	610	CLA	C3B-C4B	2.33	1.49	1.42
29	r	310	CLA	C3B-C4B	2.33	1.49	1.42
29	n	609	CLA	C1B-C2B	2.33	1.48	1.43
51	S	321	LPX	P1-O2	2.33	1.68	1.59
46	s	309	CHL	C1A-CHA	-2.33	1.37	1.40
29	b	510	CLA	C1B-C2B	2.33	1.48	1.43
29	c	513	CLA	C3B-C4B	2.32	1.49	1.42
29	b	514	CLA	C1B-C2B	2.32	1.48	1.43
46	r	305	CHL	CHA-CBD	2.32	1.54	1.51
41	j	101	DGA	OG2-CG2	-2.32	1.41	1.46
29	B	512	CLA	C1B-C2B	2.32	1.48	1.43
29	N	610	CLA	CHC-C1C	2.32	1.43	1.38
46	n	605	CHL	C1A-CHA	-2.32	1.37	1.40
29	B	515	CLA	C1B-C2B	2.32	1.48	1.43
46	R	304	CHL	CHA-CBD	2.32	1.54	1.51
29	s	305	CLA	C1B-C2B	2.32	1.48	1.43
29	y	306	CLA	C1B-C2B	2.32	1.48	1.43
33	S	322	3PH	O21-C21	2.32	1.40	1.34
29	b	510	CLA	C3B-C4B	2.32	1.49	1.42
29	g	604	CLA	C1B-C2B	2.32	1.48	1.43
29	N	610	CLA	C3B-C4B	2.32	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	y	304	CLA	CHC-C1C	2.31	1.43	1.38
29	c	513	CLA	CHC-C1C	2.31	1.43	1.38
29	B	514	CLA	C1B-C2B	2.31	1.48	1.43
29	g	602	CLA	C3B-C4B	2.31	1.49	1.42
29	g	612	CLA	C3B-C4B	2.31	1.49	1.42
29	b	503	CLA	CHC-C1C	2.31	1.43	1.38
29	S	304	CLA	C3B-C4B	2.31	1.49	1.42
41	W	202	DGA	OG2-CG2	-2.31	1.41	1.46
29	c	507	CLA	C3B-C4B	2.31	1.49	1.42
29	G	602	CLA	C3B-C4B	2.31	1.49	1.42
46	y	307	CHL	C3B-C2B	-2.31	1.37	1.40
29	B	503	CLA	CHC-C1C	2.31	1.43	1.38
29	G	604	CLA	CHC-C1C	2.31	1.43	1.38
29	g	604	CLA	C3B-C4B	2.31	1.49	1.42
29	S	311	CLA	CHC-C1C	2.31	1.43	1.38
29	b	503	CLA	C3B-C4B	2.31	1.49	1.42
29	y	315	CLA	C3B-C4B	2.31	1.49	1.42
30	a	407	PHO	CAC-C3C	-2.30	1.47	1.51
29	Y	314	CLA	C3B-C4B	2.30	1.49	1.42
29	b	512	CLA	C1B-C2B	2.30	1.48	1.43
29	S	312	CLA	CHC-C1C	2.30	1.43	1.38
46	G	609	CHL	CHA-CBD	2.30	1.54	1.51
29	y	312	CLA	C1B-C2B	2.30	1.48	1.43
46	n	601	CHL	C3B-C2B	-2.30	1.37	1.40
29	B	513	CLA	C3B-C4B	2.30	1.49	1.42
29	C	514	CLA	CHC-C1C	2.30	1.43	1.38
29	B	506	CLA	C3B-C4B	2.30	1.49	1.42
29	y	305	CLA	C3B-C4B	2.30	1.49	1.42
33	s	322	3PH	O21-C21	2.30	1.40	1.34
29	C	502	CLA	C3B-C4B	2.30	1.49	1.42
30	d	402	PHO	C4D-ND	-2.30	1.35	1.38
29	d	404	CLA	C3B-C4B	2.30	1.49	1.42
29	S	305	CLA	C3B-C4B	2.30	1.49	1.42
38	b	524	LMT	O2B-C2B	-2.30	1.37	1.43
29	Y	303	CLA	C1B-C2B	2.30	1.48	1.43
38	B	524	LMT	O2B-C2B	-2.30	1.37	1.43
29	A	407	CLA	C3B-C4B	2.30	1.49	1.42
29	n	610	CLA	CHC-C1C	2.30	1.43	1.38
29	b	502	CLA	C3B-C4B	2.29	1.49	1.42
29	S	313	CLA	C3B-C4B	2.29	1.49	1.42
29	N	602	CLA	C1B-C2B	2.29	1.48	1.43
29	a	404	CLA	C1B-C2B	2.29	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	512	CLA	C3B-C4B	2.29	1.49	1.42
29	a	408	CLA	C1B-C2B	2.29	1.48	1.43
46	s	308	CHL	C1A-CHA	-2.29	1.37	1.40
29	s	303	CLA	C3B-C4B	2.29	1.49	1.42
29	D	404	CLA	CMD-C2D	-2.29	1.46	1.50
29	g	611	CLA	CHC-C1C	2.29	1.43	1.38
29	N	612	CLA	CHC-C1C	2.29	1.43	1.38
29	y	312	CLA	C3B-C4B	2.29	1.49	1.42
29	N	602	CLA	CHC-C1C	2.29	1.43	1.38
46	S	309	CHL	CHA-CBD	2.29	1.54	1.51
30	D	401	PHO	CAC-C3C	-2.28	1.47	1.51
29	R	307	CLA	C3B-C4B	2.28	1.49	1.42
30	D	401	PHO	CMB-C2B	-2.28	1.47	1.51
29	B	502	CLA	C3B-C4B	2.28	1.49	1.42
29	S	303	CLA	C3B-C4B	2.28	1.49	1.42
29	Y	305	CLA	C3B-C4B	2.28	1.49	1.42
29	n	604	CLA	C3B-C4B	2.28	1.49	1.42
33	a	415	3PH	O21-C21	2.28	1.40	1.34
29	s	312	CLA	CHC-C1C	2.28	1.43	1.38
29	c	504	CLA	C1B-C2B	2.28	1.48	1.43
29	b	506	CLA	C3B-C4B	2.28	1.49	1.42
46	g	601	CHL	C1A-CHA	-2.28	1.37	1.40
29	b	513	CLA	C3B-C4B	2.28	1.49	1.42
29	s	315	CLA	C3B-C4B	2.28	1.49	1.42
34	B	519	C7Z	C18-C5	2.28	1.54	1.50
29	S	316	CLA	C3B-C4B	2.27	1.49	1.42
29	R	302	CLA	C3B-C4B	2.27	1.49	1.42
29	N	604	CLA	C3B-C4B	2.27	1.49	1.42
29	A	406	CLA	C3B-C4B	2.27	1.49	1.42
29	B	508	CLA	C3B-C4B	2.27	1.49	1.42
29	Y	311	CLA	C1B-C2B	2.27	1.48	1.43
29	B	506	CLA	CHC-C1C	2.27	1.43	1.38
46	N	601	CHL	C3B-C2B	-2.27	1.37	1.40
29	a	404	CLA	C3B-C4B	2.27	1.49	1.42
46	Y	306	CHL	C1A-CHA	-2.27	1.37	1.40
29	C	510	CLA	C3B-C4B	2.27	1.49	1.42
29	a	406	CLA	C3B-C4B	2.26	1.49	1.42
29	G	613	CLA	C3B-C4B	2.26	1.49	1.42
29	c	504	CLA	C3B-C4B	2.26	1.49	1.42
29	c	512	CLA	C3B-C4B	2.26	1.49	1.42
46	G	608	CHL	C1A-CHA	-2.26	1.37	1.40
46	G	605	CHL	C3B-C2B	-2.26	1.37	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	G	607	CHL	CHA-CBD	2.26	1.54	1.51
29	s	311	CLA	MG-NB	-2.26	2.01	2.05
29	C	504	CLA	C3B-C4B	2.26	1.49	1.42
29	Y	309	CLA	C3B-C4B	2.26	1.49	1.42
29	b	512	CLA	CHC-C1C	2.26	1.43	1.38
46	g	605	CHL	CHA-CBD	2.26	1.54	1.51
29	R	309	CLA	C3B-C4B	2.26	1.49	1.42
46	G	601	CHL	C3B-C2B	-2.26	1.37	1.40
46	N	609	CHL	CHA-CBD	2.26	1.54	1.51
29	a	405	CLA	C3B-C4B	2.26	1.49	1.42
30	d	402	PHO	CAC-C3C	-2.26	1.47	1.51
30	D	401	PHO	C4D-ND	-2.26	1.35	1.38
29	C	513	CLA	C3B-C4B	2.26	1.49	1.42
29	B	501	CLA	CHC-C1C	2.26	1.43	1.38
29	r	303	CLA	MG-ND	-2.26	2.01	2.05
29	B	515	CLA	CHC-C1C	2.25	1.43	1.38
29	C	506	CLA	C3B-C4B	2.25	1.49	1.42
29	c	509	CLA	C3B-C4B	2.25	1.49	1.42
29	s	316	CLA	CHC-C1C	2.25	1.43	1.38
30	A	408	PHO	C3D-C4D	2.25	1.44	1.41
29	Y	312	CLA	C3B-C4B	2.25	1.49	1.42
29	c	511	CLA	C3B-C4B	2.25	1.49	1.42
29	R	301	CLA	C3B-C4B	2.25	1.49	1.42
30	A	408	PHO	CAC-C3C	-2.25	1.47	1.51
29	y	313	CLA	C3B-C4B	2.25	1.49	1.42
43	d	405	PL9	C52-C5	-2.25	1.46	1.50
29	d	403	CLA	C1B-C2B	2.25	1.48	1.43
29	C	509	CLA	C3B-C4B	2.25	1.49	1.42
30	D	401	PHO	C3D-C4D	2.25	1.44	1.41
29	a	408	CLA	C3B-C4B	2.24	1.49	1.42
30	d	402	PHO	C3D-C4D	2.24	1.44	1.41
46	y	309	CHL	CHA-CBD	2.24	1.54	1.51
29	R	303	CLA	C3B-C4B	2.24	1.49	1.42
29	s	303	CLA	CHC-C1C	2.24	1.43	1.38
29	c	507	CLA	CHC-C1C	2.24	1.43	1.38
29	s	316	CLA	C3B-C4B	2.24	1.49	1.42
29	c	505	CLA	C3B-C4B	2.24	1.49	1.42
29	A	407	CLA	CHC-C1C	2.24	1.43	1.38
46	y	307	CHL	C1A-CHA	-2.24	1.37	1.40
29	C	506	CLA	CHC-C1C	2.24	1.43	1.38
29	C	508	CLA	C3B-C4B	2.24	1.49	1.42
48	y	319	NEX	O24-C25	-2.24	1.43	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	405	CLA	CHC-C1C	2.24	1.43	1.38
46	g	607	CHL	CHA-CBD	2.23	1.54	1.51
29	b	502	CLA	CHC-C1C	2.23	1.43	1.38
29	G	614	CLA	CHC-C1C	2.23	1.43	1.38
29	Y	315	CLA	C3B-C4B	2.23	1.49	1.42
29	r	304	CLA	C3B-C4B	2.23	1.49	1.42
46	s	302	CHL	C1A-CHA	-2.23	1.37	1.40
29	c	505	CLA	CHC-C1C	2.23	1.42	1.38
46	R	305	CHL	CHA-CBD	2.23	1.54	1.51
29	s	306	CLA	C3B-C4B	2.23	1.49	1.42
29	N	613	CLA	C3B-C4B	2.23	1.49	1.42
29	Y	313	CLA	C3B-C4B	2.22	1.49	1.42
29	c	512	CLA	CHC-C1C	2.22	1.42	1.38
29	d	404	CLA	CHC-C1C	2.22	1.42	1.38
29	R	309	CLA	CHC-C1C	2.22	1.42	1.38
29	g	613	CLA	C3B-C4B	2.22	1.49	1.42
29	n	611	CLA	CHC-C1C	2.22	1.42	1.38
46	G	608	CHL	CHA-CBD	2.22	1.54	1.51
29	b	505	CLA	C3B-C4B	2.22	1.49	1.42
29	D	404	CLA	C3A-C2A	-2.22	1.48	1.54
29	S	313	CLA	CHC-C1C	2.22	1.42	1.38
46	N	607	CHL	CHA-CBD	2.22	1.54	1.51
46	g	608	CHL	C3B-C2B	-2.22	1.37	1.40
46	S	302	CHL	CHA-CBD	2.22	1.54	1.51
29	n	602	CLA	CHC-C1C	2.22	1.42	1.38
33	S	322	3PH	O31-C3	-2.22	1.40	1.45
29	B	512	CLA	CHC-C1C	2.22	1.42	1.38
29	B	513	CLA	CHC-C1C	2.21	1.42	1.38
29	b	509	CLA	C3B-C4B	2.21	1.49	1.42
46	Y	308	CHL	CHA-CBD	2.21	1.54	1.51
29	y	310	CLA	C3B-C4B	2.21	1.49	1.42
29	S	310	CLA	CHC-C1C	2.21	1.42	1.38
29	D	404	CLA	C3D-CAD	-2.21	1.37	1.45
33	B	522	3PH	O31-C3	-2.21	1.40	1.45
29	R	301	CLA	CHC-C1C	2.21	1.42	1.38
43	d	405	PL9	C53-C6	-2.21	1.46	1.50
29	y	312	CLA	MG-NB	-2.21	2.01	2.05
29	c	509	CLA	CHC-C1C	2.21	1.42	1.38
29	b	501	CLA	CHC-C1C	2.21	1.42	1.38
46	N	601	CHL	CHA-CBD	2.21	1.54	1.51
29	A	409	CLA	C3B-C4B	2.21	1.49	1.42
46	y	307	CHL	CHA-CBD	2.21	1.54	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	r	302	CLA	C3B-C4B	2.20	1.49	1.42
29	C	513	CLA	CHC-C1C	2.20	1.42	1.38
29	a	405	CLA	C1B-C2B	2.20	1.48	1.43
46	N	608	CHL	CHA-CBD	2.20	1.54	1.51
29	N	604	CLA	CHC-C1C	2.20	1.42	1.38
29	B	505	CLA	C3B-C4B	2.20	1.49	1.42
46	Y	302	CHL	CHA-CBD	2.20	1.54	1.51
50	n	619	PTY	O4-C1	-2.20	1.40	1.45
46	G	601	CHL	CHA-CBD	2.20	1.54	1.51
29	n	613	CLA	CHC-C1C	2.20	1.42	1.38
29	S	306	CLA	CHC-C1C	2.20	1.42	1.38
29	C	505	CLA	CHC-C1C	2.20	1.42	1.38
29	y	312	CLA	CHC-C1C	2.20	1.42	1.38
29	g	610	CLA	MG-NB	-2.20	2.01	2.05
46	n	607	CHL	CHA-CBD	2.20	1.54	1.51
29	s	314	CLA	C3B-C4B	2.20	1.49	1.42
29	R	302	CLA	C1B-C2B	2.20	1.48	1.43
29	b	504	CLA	MG-ND	-2.20	2.01	2.05
46	y	303	CHL	CHA-CBD	2.20	1.54	1.51
29	G	612	CLA	CHC-C1C	2.19	1.42	1.38
29	Y	314	CLA	CHC-C1C	2.19	1.42	1.38
29	s	315	CLA	CHC-C1C	2.19	1.42	1.38
29	s	313	CLA	C3B-C4B	2.19	1.49	1.42
29	c	502	CLA	C3B-C4B	2.19	1.49	1.42
46	r	306	CHL	CHA-CBD	2.19	1.54	1.51
29	s	305	CLA	C3B-C4B	2.19	1.49	1.42
29	S	315	CLA	CHC-C1C	2.19	1.42	1.38
46	R	305	CHL	C1A-CHA	-2.19	1.37	1.40
46	g	608	CHL	C1A-CHA	-2.19	1.37	1.40
29	Y	311	CLA	CHC-C1C	2.19	1.42	1.38
47	r	311	LUT	C22-C21	-2.19	1.52	1.54
29	b	511	CLA	C3B-C4B	2.19	1.49	1.42
29	r	303	CLA	C3B-C4B	2.19	1.49	1.42
29	B	516	CLA	C4B-NB	-2.18	1.35	1.37
46	S	307	CHL	CHA-CBD	2.18	1.54	1.51
50	N	620	PTY	O7-C8	2.18	1.40	1.34
46	y	311	CHL	CHA-CBD	2.18	1.54	1.51
41	J	101	DGA	OG2-CG2	-2.18	1.41	1.46
29	c	503	CLA	C3B-C4B	2.18	1.49	1.42
29	b	515	CLA	CHC-C1C	2.18	1.42	1.38
29	n	604	CLA	CHC-C1C	2.18	1.42	1.38
29	r	304	CLA	CHC-C1C	2.18	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	511	CLA	C3B-C4B	2.18	1.49	1.42
29	C	507	CLA	C3B-C4B	2.18	1.49	1.42
29	b	508	CLA	CHC-C1C	2.18	1.42	1.38
29	B	502	CLA	CHC-C1C	2.18	1.42	1.38
29	r	303	CLA	MG-NB	-2.18	2.01	2.05
46	n	601	CHL	CHA-CBD	2.18	1.54	1.51
34	b	519	C7Z	C40-C33	2.18	1.55	1.50
29	C	502	CLA	CHC-C1C	2.18	1.42	1.38
29	B	509	CLA	C3B-C4B	2.18	1.49	1.42
29	g	614	CLA	CHC-C1C	2.18	1.42	1.38
29	B	508	CLA	CHC-C1C	2.17	1.42	1.38
29	A	409	CLA	CHC-C1C	2.17	1.42	1.38
46	n	605	CHL	CHA-CBD	2.17	1.54	1.51
29	C	503	CLA	CHC-C1C	2.17	1.42	1.38
46	N	605	CHL	CHA-CBD	2.17	1.54	1.51
29	b	514	CLA	CHC-C1C	2.17	1.42	1.38
29	b	506	CLA	CHC-C1C	2.17	1.42	1.38
29	r	308	CLA	C3B-C4B	2.17	1.49	1.42
33	s	322	3PH	O31-C3	-2.17	1.40	1.45
29	b	503	CLA	MG-NB	-2.17	2.01	2.05
46	y	301	CHL	CHA-CBD	2.17	1.54	1.51
29	s	314	CLA	CHC-C1C	2.17	1.42	1.38
29	n	612	CLA	C3B-C4B	2.17	1.49	1.42
50	n	619	PTY	O7-C8	2.17	1.40	1.34
29	y	315	CLA	CHC-C1C	2.16	1.42	1.38
29	g	603	CLA	CHC-C1C	2.16	1.42	1.38
29	y	316	CLA	CHC-C1C	2.16	1.42	1.38
46	s	308	CHL	CHA-CBD	2.16	1.54	1.51
48	Y	318	NEX	O24-C25	-2.16	1.43	1.46
46	Y	307	CHL	CHA-CBD	2.16	1.54	1.51
29	C	504	CLA	CHC-C1C	2.16	1.42	1.38
29	b	509	CLA	CHC-C1C	2.16	1.42	1.38
29	S	314	CLA	C3B-C4B	2.16	1.49	1.42
29	r	303	CLA	C1B-C2B	2.16	1.48	1.43
29	Y	315	CLA	CHC-C1C	2.16	1.42	1.38
29	Y	305	CLA	CHC-C1C	2.16	1.42	1.38
30	a	407	PHO	C3D-C4D	2.16	1.44	1.41
29	D	404	CLA	C1B-C2B	-2.16	1.38	1.43
29	C	508	CLA	CHC-C1C	2.16	1.42	1.38
29	a	406	CLA	CHC-C1C	2.16	1.42	1.38
29	g	604	CLA	CHC-C1C	2.16	1.42	1.38
29	D	404	CLA	C3A-C4A	-2.16	1.44	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	501	CLA	CHC-C1C	2.16	1.42	1.38
29	S	303	CLA	CHC-C1C	2.16	1.42	1.38
29	b	514	CLA	C3B-C4B	2.15	1.49	1.42
46	y	308	CHL	CHA-CBD	2.15	1.54	1.51
29	S	304	CLA	CHC-C1C	2.15	1.42	1.38
33	A	412	3PH	O31-C3	-2.15	1.40	1.45
43	D	406	PL9	C53-C6	-2.15	1.46	1.50
31	B	518	BCR	C12-C13	-2.15	1.41	1.46
46	g	609	CHL	CHA-CBD	2.15	1.54	1.51
38	b	524	LMT	O3B-C3B	-2.15	1.37	1.43
29	B	503	CLA	MG-NB	-2.15	2.01	2.05
29	Y	312	CLA	CHC-C1C	2.15	1.42	1.38
46	g	608	CHL	CHA-CBD	2.15	1.54	1.51
29	y	306	CLA	C3B-C4B	2.15	1.49	1.42
29	C	510	CLA	CHC-C1C	2.15	1.42	1.38
29	C	511	CLA	C3B-C4B	2.15	1.49	1.42
29	b	511	CLA	C1B-C2B	2.14	1.48	1.43
29	y	313	CLA	CHC-C1C	2.14	1.42	1.38
33	b	521	3PH	O21-C21	2.14	1.40	1.34
29	c	508	CLA	C3B-C4B	2.14	1.49	1.42
46	s	307	CHL	CHA-CBD	2.14	1.54	1.51
29	A	405	CLA	C3B-C4B	2.14	1.49	1.42
29	B	514	CLA	CHC-C1C	2.14	1.42	1.38
29	C	512	CLA	CHC-C1C	2.14	1.42	1.38
29	s	305	CLA	MG-NB	-2.14	2.01	2.05
29	R	302	CLA	MG-ND	-2.14	2.01	2.05
29	a	408	CLA	CHC-C1C	2.14	1.42	1.38
29	G	603	CLA	CHC-C1C	2.14	1.42	1.38
29	S	314	CLA	CHC-C1C	2.14	1.42	1.38
29	R	302	CLA	MG-NB	-2.14	2.01	2.05
34	B	519	C7Z	C40-C33	2.14	1.55	1.50
29	N	613	CLA	CHC-C1C	2.14	1.42	1.38
29	R	306	CLA	CHC-C1C	2.14	1.42	1.38
29	c	511	CLA	CHC-C1C	2.14	1.42	1.38
29	b	513	CLA	CHC-C1C	2.14	1.42	1.38
29	R	307	CLA	CHC-C1C	2.13	1.42	1.38
29	n	609	CLA	MG-NB	-2.13	2.01	2.05
29	y	314	CLA	C3B-C4B	2.13	1.48	1.42
29	N	614	CLA	CHC-C1C	2.13	1.42	1.38
29	R	303	CLA	CHC-C1C	2.13	1.42	1.38
29	s	313	CLA	CHC-C1C	2.13	1.42	1.38
46	s	309	CHL	CHA-CBD	2.13	1.54	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	508	CLA	MG-NB	-2.13	2.01	2.05
33	b	521	3PH	O31-C3	-2.13	1.40	1.45
29	B	514	CLA	C3B-C4B	2.13	1.48	1.42
33	A	412	3PH	O21-C2	-2.13	1.41	1.46
29	y	306	CLA	MG-NB	-2.13	2.01	2.05
29	B	509	CLA	CHC-C1C	2.13	1.42	1.38
50	Y	320	PTY	O4-C1	-2.12	1.40	1.45
29	G	610	CLA	MG-NB	-2.12	2.01	2.05
29	B	507	CLA	C3B-C4B	2.12	1.48	1.42
38	b	524	LMT	O1'-C1'	-2.12	1.36	1.40
46	Y	306	CHL	CHA-CBD	2.12	1.54	1.51
29	D	404	CLA	C4-C3	-2.12	1.45	1.50
29	b	516	CLA	C3B-C4B	2.12	1.48	1.42
31	c	514	BCR	C12-C13	-2.12	1.41	1.46
29	s	315	CLA	MG-NB	-2.12	2.01	2.05
29	A	409	CLA	C4B-NB	-2.12	1.35	1.37
29	g	612	CLA	MG-NB	-2.12	2.01	2.05
48	S	319	NEX	O24-C25	-2.12	1.43	1.46
29	B	516	CLA	C3B-C4B	2.12	1.48	1.42
29	a	408	CLA	C4B-NB	-2.12	1.35	1.37
29	Y	304	CLA	CHC-C1C	2.12	1.42	1.38
46	S	308	CHL	CHA-CBD	2.12	1.54	1.51
33	a	415	3PH	O31-C3	-2.12	1.40	1.45
29	G	611	CLA	MG-NB	-2.12	2.01	2.05
29	s	306	CLA	CHC-C1C	2.11	1.42	1.38
29	g	612	CLA	CHC-C1C	2.11	1.42	1.38
29	Y	311	CLA	MG-NB	-2.11	2.01	2.05
29	s	304	CLA	MG-ND	-2.11	2.01	2.05
48	s	319	NEX	O24-C25	-2.11	1.43	1.46
31	b	518	BCR	C12-C13	-2.11	1.41	1.46
46	g	601	CHL	CHA-CBD	2.11	1.54	1.51
46	G	606	CHL	CHA-CBD	2.11	1.54	1.51
46	Y	310	CHL	C1A-CHA	-2.11	1.37	1.40
44	e	101	HEM	CMB-C2B	2.11	1.55	1.50
29	A	406	CLA	CHC-C1C	2.11	1.42	1.38
29	Y	309	CLA	CHC-C1C	2.10	1.42	1.38
46	s	302	CHL	CHA-CBD	2.10	1.54	1.51
29	r	302	CLA	CHC-C1C	2.10	1.42	1.38
48	N	617	NEX	O24-C25	-2.10	1.43	1.46
29	s	304	CLA	C4B-NB	-2.10	1.35	1.37
29	s	310	CLA	CHC-C1C	2.10	1.42	1.38
29	C	509	CLA	MG-NB	-2.10	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	g	609	CHL	C1A-CHA	-2.10	1.37	1.40
29	b	509	CLA	MG-NB	-2.10	2.01	2.05
33	B	522	3PH	O21-C21	2.10	1.40	1.34
29	c	506	CLA	C3B-C4B	2.10	1.48	1.42
29	N	611	CLA	MG-NB	-2.10	2.01	2.05
29	n	609	CLA	MG-ND	-2.10	2.01	2.05
50	y	321	PTY	O4-C1	-2.10	1.40	1.45
29	c	508	CLA	C1B-C2B	2.09	1.48	1.43
29	B	513	CLA	MG-NB	-2.09	2.01	2.05
46	n	606	CHL	CHA-CBD	2.09	1.54	1.51
29	b	507	CLA	C3B-C4B	2.09	1.48	1.42
46	y	308	CHL	C1A-CHA	-2.09	1.37	1.40
38	B	524	LMT	O3B-C3B	-2.09	1.37	1.43
46	Y	310	CHL	CHA-CBD	2.09	1.54	1.51
29	C	506	CLA	MG-NB	-2.09	2.01	2.05
29	r	310	CLA	CHC-C1C	2.09	1.42	1.38
29	S	316	CLA	MG-NB	-2.09	2.01	2.05
29	B	516	CLA	MG-NB	-2.09	2.01	2.05
29	N	610	CLA	MG-NB	-2.09	2.01	2.05
29	N	603	CLA	CHC-C1C	2.08	1.42	1.38
46	g	606	CHL	CHA-CBD	2.08	1.54	1.51
29	r	307	CLA	CHC-C1C	2.08	1.42	1.38
48	n	616	NEX	O24-C25	-2.08	1.43	1.46
29	n	603	CLA	CHC-C1C	2.08	1.42	1.38
29	A	409	CLA	MG-NB	-2.08	2.01	2.05
29	D	404	CLA	CMB-C2B	-2.08	1.46	1.50
29	b	516	CLA	MG-NB	-2.08	2.01	2.05
29	g	604	CLA	MG-NB	-2.08	2.01	2.05
29	S	306	CLA	MG-NB	-2.08	2.01	2.05
38	B	524	LMT	O4'-C4B	-2.08	1.37	1.43
31	B	517	BCR	C12-C13	-2.08	1.41	1.46
29	R	306	CLA	MG-ND	-2.08	2.01	2.05
29	B	511	CLA	C1B-C2B	2.07	1.48	1.43
29	g	613	CLA	CHC-C1C	2.07	1.42	1.38
29	B	511	CLA	CHC-C1C	2.07	1.42	1.38
46	Y	302	CHL	C1A-CHA	-2.07	1.37	1.40
29	Y	313	CLA	CHC-C1C	2.07	1.42	1.38
29	n	604	CLA	MG-NB	-2.07	2.01	2.05
29	Y	309	CLA	MG-NB	-2.07	2.01	2.05
29	N	602	CLA	MG-NB	-2.07	2.01	2.05
29	C	511	CLA	CHC-C1C	2.07	1.42	1.38
29	y	306	CLA	CHC-C1C	2.06	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	s	304	CLA	CHC-C1C	2.06	1.42	1.38
48	g	617	NEX	O24-C25	-2.06	1.43	1.46
29	y	305	CLA	CHC-C1C	2.06	1.42	1.38
29	A	405	CLA	CHC-C1C	2.06	1.42	1.38
29	N	613	CLA	MG-NB	-2.06	2.01	2.05
29	y	314	CLA	MG-NB	-2.06	2.01	2.05
48	y	319	NEX	C1-C6	-2.06	1.51	1.54
44	e	101	HEM	C2A-C3A	-2.06	1.33	1.38
29	R	306	CLA	MG-NB	-2.06	2.01	2.05
29	b	507	CLA	MG-NB	-2.06	2.01	2.05
46	s	307	CHL	C1A-CHA	-2.06	1.37	1.40
50	N	620	PTY	O4-C1	-2.06	1.40	1.45
29	y	310	CLA	CHC-C1C	2.06	1.42	1.38
29	n	610	CLA	MG-NB	-2.06	2.01	2.05
29	B	509	CLA	MG-ND	-2.05	2.01	2.05
44	e	101	HEM	FE-NC	2.05	2.01	1.95
48	r	313	NEX	O24-C25	-2.05	1.43	1.46
29	y	312	CLA	MG-ND	-2.05	2.01	2.05
38	b	524	LMT	O4'-C4B	-2.05	1.37	1.43
29	b	506	CLA	MG-NB	-2.05	2.01	2.05
29	b	505	CLA	C4B-NB	-2.05	1.35	1.37
29	B	505	CLA	C4B-NB	-2.05	1.35	1.37
29	S	305	CLA	CHC-C1C	2.05	1.42	1.38
29	a	405	CLA	MG-NB	-2.05	2.01	2.05
29	G	613	CLA	CHC-C1C	2.05	1.42	1.38
29	a	408	CLA	MG-NB	-2.04	2.01	2.05
31	a	409	BCR	C12-C13	-2.04	1.41	1.46
29	c	508	CLA	CHC-C1C	2.04	1.42	1.38
29	c	510	CLA	C3B-C4B	2.04	1.48	1.42
29	B	504	CLA	C3B-C4B	2.04	1.48	1.42
29	C	506	CLA	MG-ND	-2.04	2.01	2.05
29	R	302	CLA	CHC-C1C	2.04	1.42	1.38
44	E	101	HEM	CMB-C2B	2.04	1.55	1.50
29	g	610	CLA	MG-ND	-2.04	2.01	2.05
29	B	516	CLA	MG-ND	-2.04	2.01	2.05
29	B	509	CLA	MG-NB	-2.04	2.01	2.05
29	C	509	CLA	CHC-C1C	2.04	1.42	1.38
29	a	406	CLA	MG-NB	-2.04	2.01	2.05
29	c	502	CLA	MG-NB	-2.04	2.01	2.05
29	a	404	CLA	CHC-C1C	2.04	1.42	1.38
38	B	524	LMT	O1'-C1'	-2.03	1.36	1.40
29	c	503	CLA	CHC-C1C	2.03	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	507	CLA	CHC-C1C	2.03	1.42	1.38
46	g	606	CHL	C1A-CHA	-2.03	1.37	1.40
29	s	306	CLA	MG-NB	-2.03	2.01	2.05
31	A	410	BCR	C12-C13	-2.03	1.41	1.46
29	N	604	CLA	MG-NB	-2.03	2.01	2.05
29	s	311	CLA	MG-ND	-2.03	2.01	2.05
29	B	507	CLA	MG-NB	-2.03	2.01	2.05
29	c	503	CLA	MG-NB	-2.03	2.01	2.05
29	a	405	CLA	CHC-C1C	2.03	1.42	1.38
29	s	312	CLA	MG-NB	-2.03	2.01	2.05
48	G	617	NEX	O24-C25	-2.03	1.43	1.46
29	c	504	CLA	MG-NB	-2.03	2.01	2.05
29	g	611	CLA	MG-NB	-2.03	2.01	2.05
29	c	504	CLA	CHC-C1C	2.03	1.42	1.38
29	B	511	CLA	MG-NB	-2.02	2.01	2.05
29	r	307	CLA	MG-ND	-2.02	2.01	2.05
29	b	516	CLA	MG-ND	-2.02	2.01	2.05
29	R	309	CLA	MG-NB	-2.02	2.01	2.05
29	y	310	CLA	MG-NB	-2.02	2.01	2.05
46	n	608	CHL	CHA-CBD	2.02	1.54	1.51
29	d	403	CLA	MG-ND	-2.02	2.01	2.05
29	b	512	CLA	MG-NB	-2.02	2.01	2.05
29	s	305	CLA	CHC-C1C	2.02	1.42	1.38
29	C	509	CLA	C1B-C2B	2.01	1.47	1.43
29	b	513	CLA	MG-NB	-2.01	2.01	2.05
29	b	511	CLA	CHC-C1C	2.01	1.42	1.38
29	g	603	CLA	MG-NB	-2.01	2.01	2.05
29	c	505	CLA	MG-ND	-2.01	2.01	2.05
29	s	314	CLA	MG-NB	-2.01	2.01	2.05
29	b	508	CLA	MG-NB	-2.01	2.01	2.05
29	c	507	CLA	MG-ND	-2.01	2.01	2.05
29	y	314	CLA	CHC-C1C	2.01	1.42	1.38
29	b	504	CLA	C3B-C4B	2.01	1.48	1.42
44	E	101	HEM	C2A-C3A	-2.01	1.33	1.38
29	s	316	CLA	MG-NB	-2.01	2.01	2.05
29	S	305	CLA	MG-NB	-2.00	2.01	2.05
29	b	511	CLA	MG-NB	-2.00	2.01	2.05
29	B	510	CLA	CHC-C1C	2.00	1.42	1.38
29	b	516	CLA	C4B-NB	-2.00	1.35	1.37
29	b	504	CLA	MG-NB	-2.00	2.01	2.05
29	n	612	CLA	MG-NB	-2.00	2.01	2.05
29	B	508	CLA	MG-NB	-2.00	2.01	2.05

All (2285) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	f	101	BCR	C10-C11-C12	19.02	178.32	123.20
31	C	517	BCR	C10-C11-C12	18.86	177.86	123.20
31	c	515	BCR	C10-C11-C12	18.79	177.64	123.20
31	b	517	BCR	C10-C11-C12	18.73	177.47	123.20
31	b	518	BCR	C10-C11-C12	18.70	177.38	123.20
31	B	518	BCR	C10-C11-C12	18.54	176.91	123.20
31	F	101	BCR	C10-C11-C12	18.53	176.89	123.20
31	v	101	BCR	C10-C11-C12	18.44	176.63	123.20
31	K	101	BCR	C10-C11-C12	18.26	176.10	123.20
31	C	515	BCR	C10-C11-C12	18.24	176.05	123.20
31	c	514	BCR	C10-C11-C12	18.21	175.95	123.20
31	z	101	BCR	C10-C11-C12	18.21	175.95	123.20
31	C	516	BCR	C10-C11-C12	18.00	175.35	123.20
31	B	517	BCR	C10-C11-C12	17.93	175.15	123.20
31	a	409	BCR	C10-C11-C12	17.82	174.83	123.20
31	A	410	BCR	C10-C11-C12	17.76	174.65	123.20
29	D	404	CLA	O2D-CGD-O1D	-17.15	90.46	123.85
49	G	619	XAT	C37-C21-C36	-17.08	82.56	107.37
49	g	619	XAT	C37-C21-C36	-16.92	82.78	107.37
31	z	101	BCR	C11-C10-C9	14.71	147.90	127.28
31	f	101	BCR	C21-C20-C19	14.15	164.21	123.20
31	v	101	BCR	C11-C10-C9	13.85	146.70	127.28
31	K	101	BCR	C11-C10-C9	13.85	146.70	127.28
29	D	404	CLA	O2D-CGD-CBD	13.54	134.91	111.23
31	a	409	BCR	C11-C10-C9	13.48	146.19	127.28
31	A	410	BCR	C11-C10-C9	13.47	146.17	127.28
31	C	515	BCR	C11-C10-C9	13.41	146.09	127.28
31	b	517	BCR	C11-C10-C9	13.29	145.91	127.28
31	A	410	BCR	C21-C20-C19	13.09	161.13	123.20
31	a	409	BCR	C21-C20-C19	12.98	160.82	123.20
31	c	515	BCR	C21-C20-C19	12.97	160.78	123.20
31	C	517	BCR	C21-C20-C19	12.96	160.75	123.20
31	B	517	BCR	C11-C10-C9	12.76	145.17	127.28
31	A	410	BCR	C11-C12-C13	12.60	160.91	126.36
31	a	409	BCR	C11-C12-C13	12.56	160.81	126.36
31	B	517	BCR	C11-C12-C13	12.45	160.51	126.36
31	C	516	BCR	C11-C12-C13	12.43	160.44	126.36
31	C	516	BCR	C11-C10-C9	12.38	144.65	127.28
31	c	515	BCR	C11-C10-C9	12.36	144.61	127.28
49	g	619	XAT	C37-C21-C22	-12.34	87.28	108.97
31	v	101	BCR	C21-C20-C19	12.23	158.65	123.20
31	C	517	BCR	C11-C10-C9	12.16	144.33	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	G	619	XAT	C37-C21-C22	-12.12	87.67	108.97
31	C	515	BCR	C16-C15-C14	12.05	148.18	123.52
31	z	101	BCR	C21-C20-C19	12.04	158.10	123.20
31	b	518	BCR	C21-C20-C19	12.04	158.08	123.20
31	F	101	BCR	C21-C20-C19	11.96	157.85	123.20
31	c	514	BCR	C11-C10-C9	11.94	144.03	127.28
31	F	101	BCR	C11-C12-C13	11.93	159.08	126.36
31	B	518	BCR	C11-C10-C9	11.92	143.99	127.28
31	K	101	BCR	C21-C20-C19	11.91	157.72	123.20
31	z	101	BCR	C16-C15-C14	11.77	147.60	123.52
31	C	515	BCR	C21-C20-C19	11.76	157.28	123.20
31	K	101	BCR	C11-C12-C13	11.72	158.51	126.36
31	C	516	BCR	C16-C15-C14	11.68	147.41	123.52
31	f	101	BCR	C16-C15-C14	11.66	147.38	123.52
31	b	518	BCR	C11-C10-C9	11.65	143.62	127.28
31	F	101	BCR	C11-C10-C9	11.64	143.60	127.28
31	B	518	BCR	C21-C20-C19	11.63	156.89	123.20
31	b	517	BCR	C21-C20-C19	11.60	156.80	123.20
31	v	101	BCR	C11-C12-C13	11.49	157.87	126.36
31	f	101	BCR	C11-C10-C9	11.44	143.32	127.28
31	B	517	BCR	C21-C20-C19	11.34	156.05	123.20
31	c	515	BCR	C16-C15-C14	11.33	146.71	123.52
31	z	101	BCR	C11-C12-C13	11.26	157.24	126.36
31	c	514	BCR	C16-C15-C14	11.23	146.51	123.52
31	b	517	BCR	C16-C15-C14	11.16	146.36	123.52
31	b	518	BCR	C11-C12-C13	11.15	156.93	126.36
31	C	517	BCR	C16-C15-C14	11.14	146.31	123.52
31	B	518	BCR	C11-C12-C13	11.12	156.84	126.36
31	b	518	BCR	C16-C15-C14	11.10	146.22	123.52
31	C	516	BCR	C21-C20-C19	11.08	155.30	123.20
31	c	515	BCR	C11-C12-C13	11.06	156.69	126.36
31	C	517	BCR	C11-C12-C13	11.03	156.61	126.36
31	f	101	BCR	C11-C12-C13	10.97	156.44	126.36
31	c	514	BCR	C11-C12-C13	10.94	156.35	126.36
31	c	514	BCR	C21-C20-C19	10.78	154.42	123.20
31	B	518	BCR	C16-C15-C14	10.76	145.53	123.52
31	b	517	BCR	C11-C12-C13	10.66	155.60	126.36
31	A	410	BCR	C16-C15-C14	10.54	145.09	123.52
31	K	101	BCR	C16-C15-C14	10.46	144.91	123.52
31	v	101	BCR	C16-C15-C14	10.45	144.90	123.52
31	a	409	BCR	C16-C15-C14	10.33	144.66	123.52
31	F	101	BCR	C16-C15-C14	10.30	144.60	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	515	BCR	C11-C12-C13	10.28	154.54	126.36
31	c	514	BCR	C20-C19-C18	9.82	153.29	126.36
31	B	517	BCR	C16-C15-C14	9.65	143.25	123.52
31	C	516	BCR	C20-C19-C18	9.49	152.37	126.36
31	B	517	BCR	C20-C19-C18	8.81	150.52	126.36
29	D	404	CLA	CED-O2D-CGD	8.79	135.86	115.92
31	C	515	BCR	C20-C19-C18	8.72	150.28	126.36
31	b	517	BCR	C20-C19-C18	8.59	149.93	126.36
31	B	518	BCR	C20-C19-C18	8.53	149.74	126.36
31	z	101	BCR	C20-C19-C18	8.42	149.45	126.36
31	v	101	BCR	C20-C19-C18	8.33	149.20	126.36
31	K	101	BCR	C20-C19-C18	8.31	149.15	126.36
46	n	606	CHL	C1B-CHB-C4A	8.30	126.66	121.32
31	F	101	BCR	C20-C19-C18	8.27	149.04	126.36
31	b	518	BCR	C20-C19-C18	8.21	148.88	126.36
46	G	605	CHL	C1B-CHB-C4A	8.19	126.59	121.32
46	Y	302	CHL	C1B-CHB-C4A	8.16	126.57	121.32
46	g	605	CHL	C1B-CHB-C4A	7.92	126.42	121.32
31	c	515	BCR	C20-C19-C18	7.83	147.84	126.36
46	n	601	CHL	C1B-CHB-C4A	7.82	126.35	121.32
31	C	517	BCR	C20-C19-C18	7.80	147.74	126.36
46	N	601	CHL	C1B-CHB-C4A	7.79	126.33	121.32
46	s	308	CHL	C1B-CHB-C4A	7.77	126.32	121.32
45	H	101	RRX	C20-C21-C22	-7.75	116.41	127.28
46	Y	308	CHL	C1B-CHB-C4A	7.74	126.30	121.32
46	N	606	CHL	C1B-CHB-C4A	7.66	126.25	121.32
46	y	309	CHL	C1B-CHB-C4A	7.63	126.23	121.32
46	r	306	CHL	C1B-CHB-C4A	7.62	126.22	121.32
29	D	404	CLA	C3B-C2B-C1B	-7.61	98.20	107.17
31	A	410	BCR	C20-C19-C18	7.61	147.24	126.36
29	D	404	CLA	C3D-C2D-C1D	-7.61	95.44	105.83
31	a	409	BCR	C20-C19-C18	7.60	147.19	126.36
46	y	303	CHL	C1B-CHB-C4A	7.59	126.20	121.32
46	G	606	CHL	C1B-CHB-C4A	7.58	126.20	121.32
46	N	605	CHL	C1B-CHB-C4A	7.57	126.19	121.32
46	S	302	CHL	C1B-CHB-C4A	7.39	126.08	121.32
29	D	404	CLA	C1D-ND-C4D	-7.38	101.13	106.31
49	G	619	XAT	C36-C21-C22	7.38	121.94	108.97
46	R	304	CHL	C1B-CHB-C4A	7.29	126.01	121.32
46	N	609	CHL	C1B-CHB-C4A	7.28	126.00	121.32
49	G	619	XAT	C37-C21-C26	-7.26	90.45	110.05
49	g	619	XAT	C37-C21-C26	-7.25	90.48	110.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S	308	CHL	C1B-CHB-C4A	7.23	125.97	121.32
46	R	305	CHL	C1B-CHB-C4A	7.20	125.95	121.32
46	G	607	CHL	C1B-CHB-C4A	7.19	125.95	121.32
46	y	301	CHL	C1B-CHB-C4A	7.13	125.91	121.32
49	g	619	XAT	C36-C21-C22	7.13	121.50	108.97
45	h	101	RRX	C11-C10-C9	-7.12	117.30	127.28
45	h	101	RRX	C20-C21-C22	-7.02	117.44	127.28
46	G	601	CHL	C1B-CHB-C4A	7.00	125.82	121.32
30	d	402	PHO	C4D-CHA-CBD	-6.96	105.12	108.45
45	H	101	RRX	C11-C10-C9	-6.95	117.53	127.28
46	G	608	CHL	C1B-CHB-C4A	6.90	125.76	121.32
34	B	519	C7Z	C11-C10-C9	-6.87	117.64	127.28
29	D	404	CLA	O2A-CGA-O1A	-6.84	106.51	123.63
41	b	522	DGA	CDB-CCB-CBB	-6.84	79.81	114.37
46	r	305	CHL	C1B-CHB-C4A	6.70	125.63	121.32
46	y	311	CHL	C1B-CHB-C4A	6.69	125.63	121.32
45	H	101	RRX	C15-C14-C13	-6.68	117.91	127.28
29	g	610	CLA	C4A-NA-C1A	6.64	109.71	106.68
41	W	202	DGA	CDB-CCB-CBB	-6.64	80.82	114.37
41	w	201	DGA	CDB-CCB-CBB	-6.63	80.83	114.37
46	s	307	CHL	C1B-CHB-C4A	6.62	125.58	121.32
46	s	302	CHL	C1B-CHB-C4A	6.59	125.56	121.32
46	n	608	CHL	C1B-CHB-C4A	6.58	125.55	121.32
49	Y	301	XAT	C31-C30-C29	-6.56	118.08	127.28
46	g	601	CHL	C1B-CHB-C4A	6.54	125.53	121.32
30	D	401	PHO	C4D-CHA-CBD	-6.50	105.34	108.45
31	f	101	BCR	C20-C19-C18	6.48	144.14	126.36
46	N	607	CHL	C1B-CHB-C4A	6.46	125.48	121.32
46	y	307	CHL	C1B-CHB-C4A	6.44	125.47	121.32
45	h	101	RRX	C16-C17-C18	-6.41	118.30	127.28
34	b	519	C7Z	C11-C10-C9	-6.32	118.41	127.28
46	g	606	CHL	C1B-CHB-C4A	6.25	125.34	121.32
46	Y	306	CHL	C1B-CHB-C4A	6.21	125.32	121.32
49	g	619	XAT	C31-C30-C29	-6.19	118.60	127.28
49	n	618	XAT	C15-C14-C13	-6.15	118.65	127.28
29	G	610	CLA	C4A-NA-C1A	6.14	109.48	106.68
49	N	619	XAT	C31-C30-C29	-6.13	118.69	127.28
45	h	101	RRX	C15-C14-C13	-6.12	118.70	127.28
45	H	101	RRX	C24-C23-C22	-6.10	117.20	126.23
46	S	309	CHL	C1B-CHB-C4A	6.10	125.25	121.32
49	G	619	XAT	C31-C30-C29	-6.08	118.75	127.28
46	S	307	CHL	C1B-CHB-C4A	6.08	125.23	121.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	408	PHO	C4D-CHA-CBD	-6.08	105.54	108.45
29	b	504	CLA	C4A-NA-C1A	6.01	109.42	106.68
29	D	404	CLA	CAC-C3C-C4C	5.98	132.57	124.79
46	Y	307	CHL	C1B-CHB-C4A	5.94	125.14	121.32
49	n	618	XAT	C31-C30-C29	-5.91	118.99	127.28
46	g	608	CHL	C1B-CHB-C4A	5.89	125.11	121.32
46	n	605	CHL	C1B-CHB-C4A	5.87	125.10	121.32
30	a	407	PHO	C4D-CHA-CBD	-5.84	105.66	108.45
29	S	306	CLA	C4A-NA-C1A	5.82	109.34	106.68
46	N	608	CHL	C1B-CHB-C4A	5.82	125.07	121.32
49	y	302	XAT	C31-C30-C29	-5.71	119.27	127.28
34	B	519	C7Z	C18-C5-C6	-5.70	118.26	124.48
29	s	304	CLA	C4A-NA-C1A	5.68	109.27	106.68
29	D	404	CLA	O2A-CGA-CBA	5.66	129.08	111.83
46	n	607	CHL	C1B-CHB-C4A	5.64	124.95	121.32
34	b	519	C7Z	C18-C5-C6	-5.63	118.34	124.48
46	g	607	CHL	C1B-CHB-C4A	5.59	124.92	121.32
46	Y	310	CHL	C1B-CHB-C4A	5.57	124.91	121.32
37	L	101	LHG	O7-C7-C8	5.57	123.53	111.48
34	B	519	C7Z	C35-C34-C33	-5.52	119.54	127.28
29	C	508	CLA	C4A-NA-C1A	5.52	109.20	106.68
29	N	610	CLA	C4A-NA-C1A	5.49	109.19	106.68
49	N	619	XAT	C15-C14-C13	-5.49	119.58	127.28
45	H	101	RRX	C16-C17-C18	-5.46	119.62	127.28
29	b	507	CLA	C4A-NA-C1A	5.43	109.16	106.68
42	a	412	BCT	O2-C-O1	5.40	133.49	119.68
47	S	317	LUT	C21-C26-C27	5.39	119.02	112.83
49	G	619	XAT	C15-C14-C13	-5.39	119.72	127.28
49	y	302	XAT	C15-C14-C13	-5.31	119.83	127.28
29	D	404	CLA	C1-O2A-CGA	5.29	129.46	116.65
49	r	312	XAT	C31-C30-C29	-5.29	119.86	127.28
29	D	404	CLA	CMD-C2D-C1D	5.22	133.91	124.73
49	Y	301	XAT	C15-C14-C13	-5.22	119.96	127.28
34	b	519	C7Z	C35-C34-C33	-5.18	120.02	127.28
29	y	312	CLA	C4A-NA-C1A	5.17	109.04	106.68
46	g	609	CHL	C1B-CHB-C4A	5.16	124.64	121.32
49	g	619	XAT	C15-C14-C13	-5.14	120.07	127.28
50	Y	320	PTY	O7-C8-C11	5.13	120.23	111.09
50	y	321	PTY	O7-C8-C11	5.12	120.22	111.09
49	R	311	XAT	C31-C30-C29	-5.10	120.13	127.28
29	s	305	CLA	C4A-NA-C1A	5.09	109.00	106.68
29	B	504	CLA	C4A-NA-C1A	5.08	109.00	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S	319	NEX	C2-C1-C6	5.06	114.13	109.21
29	D	404	CLA	O1D-CGD-CBD	5.05	134.48	124.52
46	s	309	CHL	C1C-CHC-C4B	5.05	134.14	116.07
47	n	615	LUT	C21-C26-C27	5.01	118.58	112.83
47	n	614	LUT	C21-C26-C27	5.00	118.57	112.83
46	G	609	CHL	C1B-CHB-C4A	4.99	124.53	121.32
46	y	308	CHL	C1C-CHC-C4B	4.99	133.93	116.07
29	r	302	CLA	C4A-NA-C1A	4.98	108.95	106.68
47	r	311	LUT	C21-C26-C27	4.97	118.54	112.83
34	b	519	C7Z	C1-C6-C5	-4.97	115.84	122.64
29	B	505	CLA	C4A-NA-C1A	4.96	108.94	106.68
29	c	507	CLA	C4A-NA-C1A	4.96	108.94	106.68
29	b	505	CLA	C4A-NA-C1A	4.96	108.94	106.68
47	y	318	LUT	C21-C26-C27	4.95	118.52	112.83
46	Y	310	CHL	C1C-CHC-C4B	4.93	133.70	116.07
34	B	519	C7Z	C38-C25-C26	-4.93	119.11	124.48
47	N	616	LUT	C21-C26-C27	4.92	118.48	112.83
29	R	301	CLA	C4A-NA-C1A	4.92	108.92	106.68
46	S	309	CHL	C1C-CHC-C4B	4.91	133.63	116.07
29	r	307	CLA	C4A-NA-C1A	4.90	108.91	106.68
46	g	608	CHL	C1C-CHC-C4B	4.90	133.59	116.07
48	Y	318	NEX	C2-C1-C6	4.88	113.96	109.21
43	d	405	PL9	C7-C3-C4	4.87	120.92	116.91
29	c	502	CLA	C4A-NA-C1A	4.86	108.89	106.68
46	g	607	CHL	C1C-CHC-C4B	4.84	133.39	116.07
46	g	609	CHL	C1C-CHC-C4B	4.84	133.38	116.07
46	G	609	CHL	C1C-CHC-C4B	4.83	133.37	116.07
42	a	412	BCT	O3-C-O1	-4.83	107.32	119.68
46	s	309	CHL	C1B-CHB-C4A	4.83	124.43	121.32
46	S	307	CHL	C1C-CHC-C4B	4.82	133.33	116.07
46	n	605	CHL	C1C-CHC-C4B	4.82	133.31	116.07
29	Y	311	CLA	C4A-NA-C1A	4.82	108.88	106.68
29	d	404	CLA	C4A-NA-C1A	4.80	108.87	106.68
47	g	616	LUT	C21-C26-C27	4.79	118.33	112.83
29	B	507	CLA	C4A-NA-C1A	4.79	108.86	106.68
29	b	503	CLA	C4A-NA-C1A	4.79	108.86	106.68
34	b	519	C7Z	C38-C25-C26	-4.79	119.26	124.48
29	B	503	CLA	C4A-NA-C1A	4.78	108.86	106.68
29	c	511	CLA	C4A-NA-C1A	4.78	108.86	106.68
46	N	607	CHL	C1C-CHC-C4B	4.77	133.14	116.07
36	r	301	DGD	O2G-C1B-C2B	4.77	121.79	111.48
46	y	307	CHL	C1C-CHC-C4B	4.76	133.11	116.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	r	313	NEX	C38-C25-C24	4.76	119.59	114.24
46	n	607	CHL	C1C-CHC-C4B	4.76	133.10	116.07
46	N	608	CHL	C1C-CHC-C4B	4.76	133.09	116.07
46	Y	306	CHL	C1C-CHC-C4B	4.76	133.09	116.07
46	r	305	CHL	C1C-CHC-C4B	4.75	133.08	116.07
49	y	302	XAT	C38-C25-C24	4.75	119.58	114.24
29	G	611	CLA	C4A-NA-C1A	4.75	108.85	106.68
29	C	503	CLA	C4A-NA-C1A	4.75	108.84	106.68
47	R	310	LUT	C21-C26-C27	4.75	118.28	112.83
46	Y	307	CHL	C1C-CHC-C4B	4.74	133.03	116.07
29	D	405	CLA	C4A-NA-C1A	4.72	108.83	106.68
49	y	302	XAT	C18-C5-C4	4.72	119.54	114.24
46	R	304	CHL	C1C-CHC-C4B	4.71	132.92	116.07
48	S	319	NEX	C38-C25-C24	4.71	119.53	114.24
46	g	601	CHL	C1C-CHC-C4B	4.70	132.89	116.07
46	y	311	CHL	C1C-CHC-C4B	4.69	132.86	116.07
49	G	619	XAT	C18-C5-C4	4.68	119.50	114.24
46	n	608	CHL	C1C-CHC-C4B	4.68	132.82	116.07
29	s	316	CLA	C4A-NA-C1A	4.67	108.81	106.68
48	Y	318	NEX	C38-C25-C24	4.67	119.49	114.24
46	N	601	CHL	C1C-CHC-C4B	4.67	132.78	116.07
46	g	606	CHL	C1C-CHC-C4B	4.67	132.77	116.07
48	y	319	NEX	C38-C25-C24	4.66	119.48	114.24
46	R	305	CHL	C1C-CHC-C4B	4.66	132.74	116.07
47	s	317	LUT	C21-C26-C27	4.64	118.16	112.83
48	s	319	NEX	C38-C25-C24	4.64	119.45	114.24
29	n	609	CLA	C4A-NA-C1A	4.64	108.80	106.68
46	G	607	CHL	C1C-CHC-C4B	4.64	132.67	116.07
29	s	303	CLA	C4A-NA-C1A	4.63	108.79	106.68
46	s	307	CHL	C1C-CHC-C4B	4.63	132.65	116.07
48	R	312	NEX	C38-C25-C24	4.63	119.44	114.24
34	B	519	C7Z	C1-C6-C5	-4.63	116.31	122.64
29	c	505	CLA	C4A-NA-C1A	4.62	108.79	106.68
46	N	609	CHL	C1C-CHC-C4B	4.62	132.59	116.07
46	G	601	CHL	C1C-CHC-C4B	4.62	132.59	116.07
35	W	201	LMG	O7-C10-C11	4.61	121.46	111.48
29	S	314	CLA	C4A-NA-C1A	4.61	108.78	106.68
46	n	601	CHL	C1C-CHC-C4B	4.61	132.56	116.07
29	s	311	CLA	C4A-NA-C1A	4.60	108.78	106.68
34	B	519	C7Z	C7-C8-C9	-4.60	119.44	126.23
29	y	304	CLA	C4A-NA-C1A	4.60	108.78	106.68
46	y	301	CHL	C1C-CHC-C4B	4.60	132.52	116.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	G	619	XAT	C38-C25-C24	4.59	119.40	114.24
43	D	406	PL9	C7-C3-C4	4.59	120.69	116.91
48	G	617	NEX	C38-C25-C24	4.58	119.39	114.24
29	g	612	CLA	C4A-NA-C1A	4.58	108.77	106.68
46	S	308	CHL	C1C-CHC-C4B	4.58	132.46	116.07
35	W	203	LMG	O7-C10-C11	4.58	121.38	111.48
48	g	617	NEX	C27-C28-C29	-4.57	118.44	125.53
46	s	302	CHL	C1C-CHC-C4B	4.57	132.43	116.07
46	r	306	CHL	C1C-CHC-C4B	4.56	132.38	116.07
49	Y	301	XAT	C18-C5-C4	4.56	119.36	114.24
49	Y	301	XAT	C38-C25-C24	4.56	119.36	114.24
48	n	616	NEX	C27-C28-C29	-4.55	118.47	125.53
46	y	303	CHL	C1C-CHC-C4B	4.54	132.31	116.07
29	s	306	CLA	C4A-NA-C1A	4.54	108.75	106.68
29	y	306	CLA	C4A-NA-C1A	4.53	108.75	106.68
46	Y	308	CHL	C1C-CHC-C4B	4.53	132.27	116.07
48	G	617	NEX	C27-C28-C29	-4.53	118.50	125.53
33	a	415	3PH	O21-C21-C22	4.52	121.26	111.48
46	y	309	CHL	C1C-CHC-C4B	4.52	132.25	116.07
31	K	101	BCR	C33-C5-C6	-4.52	119.55	124.48
29	s	310	CLA	C4A-NA-C1A	4.52	108.74	106.68
29	B	506	CLA	C4A-NA-C1A	4.51	108.74	106.68
46	G	608	CHL	C1C-CHC-C4B	4.51	132.20	116.07
49	N	619	XAT	C18-C5-C4	4.50	119.30	114.24
46	g	605	CHL	C1C-CHC-C4B	4.50	132.17	116.07
47	Y	317	LUT	C21-C26-C27	4.50	117.99	112.83
46	N	605	CHL	C1C-CHC-C4B	4.49	132.15	116.07
34	b	519	C7Z	C15-C14-C13	-4.49	120.99	127.28
29	B	516	CLA	C4A-NA-C1A	4.48	108.72	106.68
46	S	302	CHL	C1C-CHC-C4B	4.48	132.10	116.07
46	Y	302	CHL	C1C-CHC-C4B	4.46	132.04	116.07
46	s	308	CHL	C1C-CHC-C4B	4.46	132.02	116.07
48	N	617	NEX	C38-C25-C24	4.45	119.25	114.24
48	r	313	NEX	C27-C28-C29	-4.45	118.62	125.53
46	N	606	CHL	C1C-CHC-C4B	4.45	132.00	116.07
47	N	615	LUT	C21-C26-C27	4.44	117.93	112.83
29	S	311	CLA	C4A-NA-C1A	4.43	108.70	106.68
33	S	322	3PH	O21-C21-C22	4.43	121.06	111.48
49	n	618	XAT	C18-C5-C4	4.41	119.20	114.24
49	n	618	XAT	C7-C8-C9	-4.41	118.69	125.53
48	g	617	NEX	C38-C25-C24	4.41	119.19	114.24
46	G	605	CHL	C1C-CHC-C4B	4.41	131.84	116.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	404	CLA	C4A-NA-C1A	4.41	108.69	106.68
29	b	509	CLA	C4A-NA-C1A	4.41	108.69	106.68
48	n	616	NEX	C38-C25-C24	4.40	119.18	114.24
29	Y	315	CLA	C4A-NA-C1A	4.39	108.68	106.68
49	R	311	XAT	C38-C25-C24	4.39	119.18	114.24
46	G	606	CHL	C1C-CHC-C4B	4.39	131.78	116.07
49	N	619	XAT	C7-C8-C9	-4.38	118.73	125.53
29	S	316	CLA	C4A-NA-C1A	4.38	108.68	106.68
36	B	521	DGD	O2G-C1B-C2B	4.38	120.95	111.48
49	g	619	XAT	C18-C5-C4	4.37	119.15	114.24
34	B	519	C7Z	C15-C14-C13	-4.36	121.16	127.28
29	D	404	CLA	C4A-NA-C1A	4.36	108.67	106.68
46	y	309	CHL	C3D-C4D-CHA	4.35	115.15	108.54
29	r	309	CLA	C4A-NA-C1A	4.34	108.66	106.68
46	n	606	CHL	C1C-CHC-C4B	4.34	131.59	116.07
29	b	506	CLA	C4A-NA-C1A	4.33	108.66	106.68
47	S	318	LUT	C35-C34-C33	-4.32	121.21	127.28
35	C	524	LMG	O7-C10-C11	4.32	120.82	111.48
49	r	312	XAT	C18-C5-C4	4.31	119.08	114.24
34	b	519	C7Z	C7-C8-C9	-4.30	119.88	126.23
29	n	613	CLA	C4A-NA-C1A	4.30	108.64	106.68
48	y	319	NEX	C27-C28-C29	-4.30	118.86	125.53
29	c	504	CLA	C4A-NA-C1A	4.29	108.64	106.68
37	N	618	LHG	O7-C7-C8	4.28	120.74	111.48
49	g	619	XAT	C7-C8-C9	-4.27	118.90	125.53
45	h	101	RRX	C24-C23-C22	-4.27	119.91	126.23
48	Y	318	NEX	C27-C28-C29	-4.27	118.90	125.53
33	b	521	3PH	O21-C21-C22	4.26	120.71	111.48
46	N	609	CHL	C3D-C4D-CHA	4.26	115.02	108.54
49	g	619	XAT	C38-C25-C24	4.26	119.03	114.24
29	g	611	CLA	C4A-NA-C1A	4.26	108.62	106.68
37	n	617	LHG	O7-C7-C8	4.26	120.69	111.48
29	s	314	CLA	C4A-NA-C1A	4.25	108.62	106.68
37	S	301	LHG	O7-C7-C8	4.25	120.68	111.48
46	Y	308	CHL	C3D-C4D-CHA	4.24	114.98	108.54
47	G	615	LUT	C21-C26-C27	4.24	117.70	112.83
29	g	614	CLA	C4A-NA-C1A	4.23	108.61	106.68
48	N	617	NEX	C27-C28-C29	-4.23	118.96	125.53
48	R	312	NEX	C27-C28-C29	-4.23	118.97	125.53
46	S	302	CHL	C3D-C4D-CHA	4.22	114.96	108.54
46	G	605	CHL	C3D-C4D-CHA	4.22	114.95	108.54
47	r	311	LUT	C1-C6-C5	-4.21	116.89	122.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	g	616	LUT	C15-C14-C13	-4.20	121.38	127.28
46	N	601	CHL	C3D-C4D-CHA	4.20	114.93	108.54
46	N	606	CHL	C3D-C4D-CHA	4.20	114.92	108.54
46	s	307	CHL	C3D-C4D-CHA	4.19	114.92	108.54
46	n	606	CHL	C3D-C4D-CHA	4.19	114.91	108.54
47	s	318	LUT	C21-C26-C27	4.19	117.64	112.83
47	g	616	LUT	C35-C34-C33	-4.19	121.41	127.28
46	G	609	CHL	C3D-C4D-CHA	4.18	114.90	108.54
46	N	605	CHL	C3D-C4D-CHA	4.18	114.90	108.54
46	S	307	CHL	C3D-C4D-CHA	4.18	114.89	108.54
47	g	615	LUT	C35-C34-C33	-4.18	121.42	127.28
47	Y	316	LUT	C15-C14-C13	-4.17	121.43	127.28
29	D	404	CLA	C2C-C1C-NC	4.17	114.36	109.98
34	b	519	C7Z	C27-C28-C29	-4.17	120.07	126.23
29	S	312	CLA	C4A-NA-C1A	4.17	108.58	106.68
46	r	305	CHL	C3D-C4D-CHA	4.16	114.87	108.54
46	R	304	CHL	C3D-C4D-CHA	4.16	114.87	108.54
29	S	304	CLA	C4A-NA-C1A	4.15	108.57	106.68
49	r	312	XAT	C38-C25-C24	4.15	118.90	114.24
35	C	521	LMG	O7-C10-C11	4.15	120.46	111.48
46	g	605	CHL	C3D-C4D-CHA	4.15	114.84	108.54
46	G	607	CHL	C3D-C4D-CHA	4.14	114.83	108.54
46	Y	302	CHL	C3D-C4D-CHA	4.14	114.83	108.54
46	n	601	CHL	C3D-C4D-CHA	4.13	114.81	108.54
47	S	318	LUT	C21-C26-C27	4.12	117.56	112.83
46	y	308	CHL	C3D-C4D-CHA	4.12	114.80	108.54
29	D	404	CLA	C2B-C1B-NB	4.12	114.59	110.33
48	g	617	NEX	C17-C1-C6	-4.11	106.80	110.47
46	g	607	CHL	C3D-C4D-CHA	4.10	114.78	108.54
47	G	616	LUT	C21-C26-C27	4.10	117.54	112.83
46	S	308	CHL	C3D-C4D-CHA	4.10	114.77	108.54
46	G	608	CHL	C3D-C4D-CHA	4.10	114.77	108.54
29	B	509	CLA	C4A-NA-C1A	4.10	108.55	106.68
37	s	301	LHG	O7-C7-C8	4.10	120.34	111.48
46	g	606	CHL	C3D-C4D-CHA	4.09	114.76	108.54
46	s	308	CHL	C3D-C4D-CHA	4.09	114.76	108.54
46	R	305	CHL	C3D-C4D-CHA	4.09	114.76	108.54
47	R	310	LUT	C15-C14-C13	-4.09	121.54	127.28
46	G	606	CHL	C3D-C4D-CHA	4.09	114.75	108.54
37	c	521	LHG	O7-C7-C8	4.09	120.33	111.48
37	S	320	LHG	O7-C7-C8	4.09	120.32	111.48
47	R	310	LUT	C18-C5-C6	-4.09	120.03	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	y	320	LHG	O7-C7-C8	4.08	120.32	111.48
47	s	318	LUT	C35-C34-C33	-4.08	121.55	127.28
46	n	607	CHL	C3D-C4D-CHA	4.08	114.74	108.54
46	y	303	CHL	C3D-C4D-CHA	4.07	114.73	108.54
46	y	311	CHL	C3D-C4D-CHA	4.07	114.73	108.54
33	s	322	3PH	O21-C21-C22	4.07	120.28	111.48
35	i	101	LMG	O7-C10-C11	4.06	120.27	111.48
49	g	619	XAT	C36-C21-C26	4.06	121.00	110.05
46	n	605	CHL	C3D-C4D-CHA	4.06	114.70	108.54
47	G	616	LUT	C15-C14-C13	-4.05	121.59	127.28
46	s	302	CHL	C3D-C4D-CHA	4.05	114.70	108.54
37	G	618	LHG	O7-C7-C8	4.05	120.24	111.48
47	R	310	LUT	C11-C10-C9	-4.05	121.60	127.28
46	N	608	CHL	C3D-C4D-CHA	4.04	114.69	108.54
46	y	301	CHL	C3D-C4D-CHA	4.04	114.68	108.54
46	s	309	CHL	C3D-C4D-CHA	4.04	114.68	108.54
29	B	502	CLA	C4A-NA-C1A	4.04	108.52	106.68
29	R	306	CLA	C4A-NA-C1A	4.04	108.52	106.68
46	r	306	CHL	C3D-C4D-CHA	4.03	114.67	108.54
46	g	609	CHL	C3D-C4D-CHA	4.03	114.67	108.54
29	S	310	CLA	C4A-NA-C1A	4.03	108.52	106.68
29	B	512	CLA	C4A-NA-C1A	4.02	108.51	106.68
29	A	406	CLA	C4A-NA-C1A	4.01	108.51	106.68
29	s	304	CLA	C3B-C4B-NB	-4.01	106.95	110.53
46	N	607	CHL	C3D-C4D-CHA	4.01	114.63	108.54
49	r	312	XAT	C15-C14-C13	-3.99	121.68	127.28
29	n	602	CLA	C4A-NA-C1A	3.99	108.50	106.68
34	B	519	C7Z	C27-C28-C29	-3.98	120.34	126.23
46	G	601	CHL	C3D-C4D-CHA	3.98	114.58	108.54
41	D	402	DGA	CDB-CCB-CBB	-3.97	80.40	115.25
29	c	513	CLA	C4A-NA-C1A	3.97	108.49	106.68
33	A	412	3PH	O21-C21-C22	3.97	120.07	111.48
33	B	522	3PH	O21-C21-C22	3.97	120.07	111.48
45	h	101	RRX	C38-C26-C25	-3.97	120.15	124.48
35	d	408	LMG	O7-C10-C11	3.97	120.06	111.48
37	g	618	LHG	O7-C7-C8	3.97	120.06	111.48
46	y	307	CHL	C3D-C4D-CHA	3.96	114.56	108.54
37	a	414	LHG	O7-C7-C8	3.96	120.05	111.48
47	Y	317	LUT	C15-C14-C13	-3.96	121.72	127.28
48	S	319	NEX	C17-C1-C6	-3.96	106.93	110.47
46	Y	306	CHL	C3D-C4D-CHA	3.96	114.56	108.54
49	G	619	XAT	C36-C21-C26	3.96	120.73	110.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	G	617	NEX	C31-C30-C29	3.96	132.83	127.28
49	R	311	XAT	C18-C5-C4	3.96	118.69	114.24
37	s	320	LHG	O7-C7-C8	3.95	120.03	111.48
46	Y	310	CHL	C3D-C4D-CHA	3.95	114.55	108.54
34	b	519	C7Z	C31-C30-C29	-3.95	121.74	127.28
46	Y	307	CHL	C3D-C4D-CHA	3.95	114.54	108.54
47	Y	317	LUT	C7-C8-C9	-3.94	120.40	126.23
34	B	519	C7Z	C31-C30-C29	-3.94	121.75	127.28
46	g	601	CHL	C3D-C4D-CHA	3.94	114.53	108.54
48	S	319	NEX	C27-C28-C29	-3.94	119.42	125.53
47	Y	316	LUT	C21-C26-C27	3.93	117.35	112.83
46	n	608	CHL	C3D-C4D-CHA	3.93	114.51	108.54
29	N	614	CLA	C4A-NA-C1A	3.92	108.47	106.68
41	J	101	DGA	OG2-CB1-CB2	3.92	119.97	111.48
29	C	505	CLA	C4A-NA-C1A	3.90	108.46	106.68
49	R	311	XAT	C15-C14-C13	-3.90	121.81	127.28
41	w	201	DGA	OG2-CB1-CB2	3.89	119.91	111.48
47	y	318	LUT	C15-C14-C13	-3.89	121.82	127.28
47	g	616	LUT	C7-C8-C9	-3.89	120.48	126.23
35	C	522	LMG	O7-C10-C11	3.89	119.89	111.48
46	g	608	CHL	C3D-C4D-CHA	3.89	114.45	108.54
29	g	602	CLA	C4A-NA-C1A	3.89	108.45	106.68
37	D	408	LHG	O7-C7-C8	3.88	119.89	111.48
47	y	318	LUT	C35-C34-C33	-3.88	121.83	127.28
47	Y	317	LUT	C35-C34-C33	-3.88	121.83	127.28
48	s	319	NEX	C27-C28-C29	-3.87	119.52	125.53
41	D	402	DGA	OG2-CB1-CB2	3.87	119.85	111.48
41	b	522	DGA	OG2-CB1-CB2	3.86	119.84	111.48
29	G	612	CLA	C4A-NA-C1A	3.86	108.44	106.68
35	b	520	LMG	O7-C10-C11	3.86	119.83	111.48
50	n	619	PTY	O7-C8-C11	3.85	119.81	111.48
50	N	620	PTY	O7-C8-C11	3.85	119.81	111.48
47	G	616	LUT	C35-C34-C33	-3.84	121.89	127.28
47	n	615	LUT	C35-C34-C33	-3.84	121.90	127.28
35	c	519	LMG	O7-C10-C11	3.83	119.78	111.48
41	W	202	DGA	OG2-CB1-CB2	3.83	119.77	111.48
41	j	101	DGA	OG2-CB1-CB2	3.83	119.76	111.48
47	s	317	LUT	C35-C34-C33	-3.83	121.91	127.28
29	b	514	CLA	C4A-NA-C1A	3.82	108.42	106.68
47	y	317	LUT	C15-C14-C13	-3.81	121.94	127.28
47	y	317	LUT	C21-C26-C27	3.81	117.20	112.83
29	B	514	CLA	C4A-NA-C1A	3.80	108.41	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	y	314	CLA	C4A-NA-C1A	3.80	108.41	106.68
49	n	618	XAT	C38-C25-C24	3.80	118.51	114.24
47	N	616	LUT	C35-C34-C33	-3.80	121.95	127.28
46	g	607	CHL	C1-O2A-CGA	3.79	125.84	116.65
36	c	516	DGD	O2G-C1B-C2B	3.79	119.69	111.48
34	B	519	C7Z	C1-C6-C7	3.79	125.93	115.65
36	C	520	DGD	O2G-C1B-C2B	3.79	119.67	111.48
49	G	619	XAT	C7-C8-C9	-3.79	119.66	125.53
29	S	305	CLA	C4A-NA-C1A	3.78	108.41	106.68
35	D	410	LMG	O7-C10-C11	3.78	119.66	111.48
29	D	404	CLA	CBC-CAC-C3C	-3.78	102.18	112.42
37	a	413	LHG	O7-C7-C8	3.78	119.65	111.48
46	g	607	CHL	C1-C2-C3	-3.78	120.01	126.20
29	R	308	CLA	C4A-NA-C1A	3.77	108.40	106.68
47	R	310	LUT	C35-C34-C33	-3.77	121.99	127.28
31	b	517	BCR	C23-C24-C25	-3.76	116.95	127.00
45	h	101	RRX	C33-C5-C6	-3.76	120.38	124.48
31	B	517	BCR	C33-C5-C6	-3.76	120.38	124.48
37	Y	319	LHG	O7-C7-C8	3.76	119.61	111.48
49	N	619	XAT	C38-C25-C24	3.76	118.46	114.24
29	s	312	CLA	C4A-NA-C1A	3.75	108.39	106.68
36	c	518	DGD	O2G-C1B-C2B	3.75	119.60	111.48
47	S	317	LUT	C15-C14-C13	-3.75	122.02	127.28
47	g	615	LUT	C15-C14-C13	-3.75	122.02	127.28
48	g	617	NEX	C31-C30-C29	3.74	132.53	127.28
37	B	523	LHG	O7-C7-C8	3.73	119.56	111.48
49	r	312	XAT	C6-C7-C8	-3.73	118.11	125.99
46	y	308	CHL	C1B-CHB-C4A	3.73	123.72	121.32
29	R	307	CLA	C4A-NA-C1A	3.72	108.37	106.68
31	A	410	BCR	C12-C13-C14	-3.71	113.18	119.01
29	Y	303	CLA	C4A-NA-C1A	3.70	108.37	106.68
35	B	520	LMG	O7-C10-C11	3.70	119.48	111.48
47	y	318	LUT	C7-C8-C9	-3.69	120.77	126.23
29	s	312	CLA	C3B-C4B-NB	-3.69	107.24	110.53
47	g	615	LUT	C21-C26-C27	3.68	117.06	112.83
46	y	309	CHL	C4D-CHA-CBD	-3.68	105.26	108.97
30	A	408	PHO	C2B-C1B-NB	-3.68	106.77	109.43
29	b	513	CLA	C4A-NA-C1A	3.68	108.36	106.68
31	A	410	BCR	C33-C5-C6	-3.67	120.48	124.48
29	d	403	CLA	C4A-NA-C1A	3.67	108.35	106.68
43	d	405	PL9	C7-C3-C2	-3.67	119.07	123.39
47	R	310	LUT	C7-C8-C9	-3.67	120.81	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	D	406	PL9	C7-C3-C2	-3.66	119.07	123.39
45	H	101	RRX	C33-C5-C6	-3.66	120.49	124.48
29	s	313	CLA	C4A-NA-C1A	3.66	108.35	106.68
46	y	308	CHL	C1A-CHA-C4D	3.66	125.08	118.98
35	d	407	LMG	O7-C10-C11	3.65	119.39	111.48
47	r	311	LUT	C11-C10-C9	-3.65	122.16	127.28
31	C	516	BCR	C23-C24-C25	-3.65	117.25	127.00
48	g	617	NEX	C2-C1-C6	3.65	112.76	109.21
31	a	409	BCR	C12-C13-C14	-3.64	113.28	119.01
29	c	509	CLA	C4A-NA-C1A	3.64	108.34	106.68
47	s	318	LUT	C15-C14-C13	-3.63	122.18	127.28
46	s	309	CHL	CHA-C1A-C2A	-3.63	124.79	133.31
46	y	308	CHL	CHA-C1A-C2A	-3.63	124.79	133.31
47	G	615	LUT	C35-C34-C33	-3.63	122.19	127.28
47	g	616	LUT	C11-C10-C9	-3.62	122.20	127.28
47	S	318	LUT	C18-C5-C6	-3.62	120.53	124.48
47	N	615	LUT	C35-C34-C33	-3.62	122.21	127.28
35	c	520	LMG	O7-C10-C11	3.61	119.30	111.48
31	c	514	BCR	C23-C24-C25	-3.60	117.38	127.00
48	g	617	NEX	C5-C6-C1	3.60	123.27	119.70
48	G	617	NEX	C2-C1-C6	3.60	112.71	109.21
31	a	409	BCR	C23-C24-C25	-3.59	117.41	127.00
30	D	401	PHO	C2B-C1B-NB	-3.59	106.84	109.43
49	y	302	XAT	C6-C7-C8	-3.59	118.41	125.99
37	d	406	LHG	O7-C7-C8	3.58	119.24	111.48
49	y	302	XAT	C7-C8-C9	-3.58	119.97	125.53
29	Y	309	CLA	C4A-NA-C1A	3.58	108.31	106.68
29	C	510	CLA	C4A-NA-C1A	3.58	108.31	106.68
31	a	409	BCR	C33-C5-C6	-3.58	120.58	124.48
48	r	313	NEX	C31-C30-C29	3.58	132.29	127.28
29	Y	305	CLA	C4A-NA-C1A	3.58	108.31	106.68
31	C	517	BCR	C28-C27-C26	-3.57	107.69	114.06
49	Y	301	XAT	C6-C7-C8	-3.57	118.45	125.99
29	B	513	CLA	C4A-NA-C1A	3.57	108.31	106.68
47	G	615	LUT	C15-C14-C13	-3.56	122.28	127.28
29	S	316	CLA	C3B-C4B-NB	-3.56	107.35	110.53
47	s	318	LUT	C7-C8-C9	-3.56	120.97	126.23
29	n	612	CLA	C4A-NA-C1A	3.56	108.30	106.68
29	B	511	CLA	C4A-NA-C1A	3.55	108.30	106.68
46	Y	307	CHL	CHA-C1A-C2A	-3.55	124.97	133.31
47	s	317	LUT	C26-C27-C28	-3.55	119.06	124.58
48	Y	318	NEX	C17-C1-C6	-3.55	107.30	110.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	y	307	CHL	CHA-C1A-C2A	-3.54	124.99	133.31
29	r	308	CLA	C4A-NA-C1A	3.54	108.30	106.68
35	w	202	LMG	O7-C10-C11	3.54	119.14	111.48
47	s	317	LUT	C7-C8-C9	-3.54	121.00	126.23
46	Y	306	CHL	CHA-C1A-C2A	-3.54	125.00	133.31
47	g	615	LUT	C7-C8-C9	-3.53	121.01	126.23
31	v	101	BCR	C33-C5-C6	-3.53	120.63	124.48
31	c	514	BCR	C2-C1-C6	3.53	115.56	110.44
48	y	319	NEX	C31-C30-C29	3.52	132.22	127.28
31	B	517	BCR	C12-C13-C14	-3.52	113.47	119.01
46	g	609	CHL	CHA-C1A-C2A	-3.51	125.06	133.31
29	c	501	CLA	C4A-NA-C1A	3.51	108.28	106.68
47	g	615	LUT	C26-C27-C28	-3.51	119.12	124.58
30	d	402	PHO	C2B-C1B-NB	-3.51	106.89	109.43
29	R	309	CLA	C3B-C4B-NB	-3.51	107.40	110.53
29	a	408	CLA	C4A-NA-C1A	3.50	108.28	106.68
47	G	616	LUT	C7-C8-C9	-3.50	121.06	126.23
35	C	524	LMG	O8-C28-C29	3.49	122.49	111.83
46	Y	310	CHL	CHA-C1A-C2A	-3.49	125.11	133.31
31	A	410	BCR	C23-C24-C25	-3.49	117.67	127.00
34	B	519	C7Z	C28-C27-C26	-3.49	117.68	127.00
29	C	506	CLA	C4A-NA-C1A	3.48	108.27	106.68
29	y	310	CLA	C4A-NA-C1A	3.48	108.27	106.68
46	S	309	CHL	C3D-C4D-CHA	3.48	113.83	108.54
46	y	311	CHL	C3C-C4C-NC	-3.48	106.14	114.65
47	n	614	LUT	C15-C14-C13	-3.48	122.40	127.28
49	N	619	XAT	C38-C25-C26	-3.48	116.58	122.30
36	C	519	DGD	O2G-C1B-C2B	3.48	119.00	111.48
36	C	518	DGD	O2G-C1B-C2B	3.47	118.99	111.48
31	B	517	BCR	C23-C24-C25	-3.47	117.72	127.00
49	n	618	XAT	C38-C25-C26	-3.47	116.59	122.30
46	g	601	CHL	CHA-C1A-C2A	-3.47	125.17	133.31
29	S	304	CLA	C3B-C4B-NB	-3.46	107.44	110.53
47	N	616	LUT	C7-C8-C9	-3.46	121.11	126.23
47	S	317	LUT	C35-C34-C33	-3.46	122.42	127.28
46	S	309	CHL	CHA-C1A-C2A	-3.46	125.19	133.31
47	n	615	LUT	C7-C8-C9	-3.46	121.12	126.23
35	D	409	LMG	O7-C10-C11	3.45	118.94	111.48
29	C	514	CLA	C4A-NA-C1A	3.44	108.25	106.68
29	b	511	CLA	C4A-NA-C1A	3.43	108.25	106.68
46	S	307	CHL	CHA-C1A-C2A	-3.43	125.25	133.31
49	R	311	XAT	C6-C7-C8	-3.43	118.74	125.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S	318	LUT	C15-C14-C13	-3.43	122.47	127.28
45	H	101	RRX	C38-C26-C25	-3.42	120.75	124.48
46	G	601	CHL	CHA-C1A-C2A	-3.42	125.27	133.31
47	n	615	LUT	C15-C14-C13	-3.42	122.48	127.28
30	d	402	PHO	CMB-C2B-C3B	3.42	131.52	124.68
29	b	501	CLA	C4A-NA-C1A	3.42	108.24	106.68
46	s	309	CHL	C1A-CHA-C4D	3.42	124.68	118.98
29	D	404	CLA	C2A-C1A-CHA	-3.41	117.95	123.87
46	n	608	CHL	CHA-C1A-C2A	-3.41	125.31	133.31
46	R	305	CHL	CHA-C1A-C2A	-3.40	125.31	133.31
45	h	101	RRX	C4-C5-C6	-3.40	118.11	122.70
45	H	101	RRX	C4-C5-C6	-3.40	118.11	122.70
30	D	401	PHO	CMB-C2B-C3B	3.40	131.47	124.68
46	g	608	CHL	C1A-CHA-C4D	3.40	124.65	118.98
31	B	517	BCR	C33-C5-C4	3.40	120.84	113.60
47	N	615	LUT	C15-C14-C13	-3.40	122.52	127.28
46	s	307	CHL	C1A-CHA-C4D	3.39	124.65	118.98
46	N	608	CHL	CHA-C1A-C2A	-3.39	125.34	133.31
47	n	614	LUT	C35-C34-C33	-3.39	122.53	127.28
48	G	617	NEX	C17-C1-C6	-3.38	107.44	110.47
47	y	317	LUT	C35-C34-C33	-3.38	122.53	127.28
31	a	409	BCR	C35-C13-C12	3.38	123.25	118.09
31	A	410	BCR	C35-C13-C12	3.38	123.25	118.09
29	y	316	CLA	C4A-NA-C1A	3.38	108.22	106.68
47	s	317	LUT	C15-C14-C13	-3.37	122.55	127.28
37	l	102	LHG	O7-C7-C8	3.37	118.77	111.48
46	r	306	CHL	CHA-C1A-C2A	-3.37	125.39	133.31
46	Y	308	CHL	C4D-CHA-CBD	-3.37	105.57	108.97
46	r	306	CHL	C3C-C4C-NC	-3.37	106.42	114.65
46	Y	302	CHL	CHA-C1A-C2A	-3.37	125.40	133.31
46	g	607	CHL	CHA-C1A-C2A	-3.36	125.41	133.31
46	Y	310	CHL	C1A-CHA-C4D	3.36	124.59	118.98
47	G	616	LUT	C31-C30-C29	-3.36	122.57	127.28
47	G	616	LUT	C27-C28-C29	-3.36	119.10	126.32
46	N	608	CHL	C1A-CHA-C4D	3.35	124.58	118.98
31	B	517	BCR	C35-C13-C12	3.35	123.21	118.09
47	g	616	LUT	C18-C5-C6	-3.35	120.83	124.48
48	N	617	NEX	C31-C30-C29	3.35	131.98	127.28
29	N	604	CLA	C4A-NA-C1A	3.35	108.21	106.68
31	f	101	BCR	C19-C18-C17	3.35	124.28	119.01
46	y	303	CHL	CHA-C1A-C2A	-3.35	125.44	133.31
47	s	317	LUT	C35-C15-C14	-3.34	116.68	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	b	519	C7Z	C28-C27-C26	-3.34	118.07	127.00
47	r	311	LUT	C15-C14-C13	-3.34	122.59	127.28
46	G	601	CHL	C3C-C4C-NC	-3.34	106.48	114.65
29	N	611	CLA	C4A-NA-C1A	3.34	108.20	106.68
34	b	519	C7Z	C1-C6-C7	3.34	124.70	115.65
31	F	101	BCR	C33-C5-C6	-3.34	120.84	124.48
47	Y	316	LUT	C35-C34-C33	-3.34	122.60	127.28
31	C	516	BCR	C33-C5-C6	-3.33	120.84	124.48
29	D	404	CLA	C4D-CHA-C1A	-3.33	117.27	121.24
36	c	517	DGD	O2G-C1B-C2B	3.33	118.69	111.48
46	S	308	CHL	CHA-C1A-C2A	-3.33	125.49	133.31
29	Y	313	CLA	C4A-NA-C1A	3.32	108.19	106.68
46	G	605	CHL	CHA-C1A-C2A	-3.32	125.52	133.31
46	n	608	CHL	C3C-C4C-NC	-3.31	106.55	114.65
46	n	601	CHL	C3C-C4C-NC	-3.31	106.57	114.65
49	Y	301	XAT	C7-C8-C9	-3.31	120.40	125.53
46	n	607	CHL	C1A-CHA-C4D	3.31	124.50	118.98
47	n	614	LUT	C10-C11-C12	-3.30	113.63	123.20
29	B	504	CLA	C1-C2-C3	-3.30	120.79	126.20
46	n	605	CHL	C3C-C4C-NC	-3.30	106.58	114.65
29	C	509	CLA	C4A-NA-C1A	3.30	108.19	106.68
29	N	613	CLA	C4A-NA-C1A	3.30	108.19	106.68
46	n	607	CHL	CHA-C1A-C2A	-3.30	125.56	133.31
31	c	514	BCR	C12-C13-C14	-3.30	113.82	119.01
46	S	309	CHL	C1-O2A-CGA	3.30	124.63	116.65
31	b	518	BCR	C33-C5-C6	-3.29	120.89	124.48
46	n	605	CHL	CHA-C1A-C2A	-3.29	125.58	133.31
46	N	606	CHL	CHA-C1A-C2A	-3.29	125.59	133.31
47	s	317	LUT	C18-C5-C6	-3.28	120.90	124.48
46	S	307	CHL	C1A-CHA-C4D	3.28	124.45	118.98
30	A	408	PHO	CMB-C2B-C3B	3.27	131.23	124.68
29	r	309	CLA	C1-C2-C3	-3.27	120.84	126.20
46	S	302	CHL	C3C-C4C-NC	-3.27	106.66	114.65
30	a	407	PHO	C2B-C1B-NB	-3.27	107.07	109.43
46	g	601	CHL	C3C-C4C-NC	-3.27	106.66	114.65
29	A	409	CLA	C4A-NA-C1A	3.27	108.17	106.68
46	y	301	CHL	C4D-CHA-CBD	-3.26	105.68	108.97
46	g	608	CHL	CHA-C1A-C2A	-3.25	125.67	133.31
46	y	311	CHL	CHA-C1A-C2A	-3.25	125.67	133.31
46	N	609	CHL	C3C-C4C-NC	-3.25	106.70	114.65
47	S	318	LUT	C7-C8-C9	-3.25	121.43	126.23
45	h	101	RRX	C1-C6-C5	-3.25	118.20	122.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S	313	CLA	C4A-NA-C1A	3.25	108.16	106.68
29	b	512	CLA	C4A-NA-C1A	3.25	108.16	106.68
31	C	515	BCR	C23-C24-C25	-3.25	118.32	127.00
29	A	406	CLA	C1-C2-C3	-3.25	120.88	126.20
29	g	603	CLA	C3B-C4B-NB	-3.24	107.64	110.53
47	G	616	LUT	C11-C10-C9	-3.24	122.73	127.28
46	G	605	CHL	C3C-C4C-NC	-3.24	106.73	114.65
47	S	317	LUT	C7-C8-C9	-3.24	121.44	126.23
46	G	609	CHL	C1A-CHA-C4D	3.24	124.38	118.98
46	G	607	CHL	C4D-CHA-CBD	-3.23	105.71	108.97
29	b	508	CLA	C3B-C4B-NB	-3.23	107.64	110.53
49	y	302	XAT	C38-C25-C26	-3.23	116.98	122.30
49	Y	301	XAT	C38-C25-C26	-3.23	116.99	122.30
29	r	310	CLA	C4A-NA-C1A	3.23	108.15	106.68
46	s	302	CHL	CHA-C1A-C2A	-3.22	125.74	133.31
45	H	101	RRX	C1-C6-C5	-3.22	118.24	122.64
46	G	609	CHL	CHA-C1A-C2A	-3.22	125.75	133.31
46	N	605	CHL	C3C-C4C-NC	-3.22	106.79	114.65
30	a	407	PHO	CMB-C2B-C3B	3.22	131.11	124.68
46	S	309	CHL	C1-C2-C3	-3.21	120.93	126.20
46	R	305	CHL	C3C-C4C-NC	-3.21	106.79	114.65
29	R	308	CLA	C1-C2-C3	-3.21	120.93	126.20
47	y	318	LUT	C22-C23-C24	-3.21	106.41	111.18
46	G	608	CHL	CHA-C1A-C2A	-3.21	125.77	133.31
46	s	307	CHL	CHA-C1A-C2A	-3.21	125.77	133.31
46	s	308	CHL	CHA-C1A-C2A	-3.21	125.77	133.31
46	y	301	CHL	C3C-C4C-NC	-3.21	106.81	114.65
46	n	601	CHL	CHA-C1A-C2A	-3.21	125.78	133.31
49	r	312	XAT	O4-C5-C4	-3.21	110.49	113.49
37	D	407	LHG	O7-C7-C8	3.21	118.42	111.48
29	B	508	CLA	C3B-C4B-NB	-3.21	107.67	110.53
46	s	302	CHL	C3C-C4C-NC	-3.21	106.82	114.65
31	B	518	BCR	C23-C24-C25	-3.20	118.44	127.00
46	Y	310	CHL	C3C-C4C-NC	-3.20	106.82	114.65
47	S	318	LUT	C26-C27-C28	-3.20	119.59	124.58
46	g	607	CHL	C4D-CHA-CBD	-3.20	105.74	108.97
46	y	311	CHL	C1A-CHA-C4D	3.20	124.32	118.98
48	y	319	NEX	C17-C1-C6	-3.20	107.61	110.47
47	g	616	LUT	C31-C30-C29	-3.19	122.80	127.28
29	B	501	CLA	C4A-NA-C1A	3.18	108.13	106.68
46	S	309	CHL	C3C-C4C-NC	-3.18	106.87	114.65
46	S	308	CHL	C3C-C4C-NC	-3.18	106.88	114.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	N	601	CHL	C3C-C4C-NC	-3.18	106.88	114.65
29	D	404	CLA	C4D-C3D-CAD	-3.18	104.66	108.11
46	s	308	CHL	C3C-C4C-NC	-3.18	106.89	114.65
46	g	609	CHL	C1A-CHA-C4D	3.17	124.28	118.98
46	R	304	CHL	C4D-CHA-CBD	-3.17	105.77	108.97
46	N	605	CHL	CHA-C1A-C2A	-3.17	125.86	133.31
46	N	609	CHL	CHA-C1A-C2A	-3.17	125.86	133.31
49	R	311	XAT	C38-C25-C26	-3.17	117.08	122.30
31	B	518	BCR	C33-C5-C6	-3.17	121.03	124.48
47	s	318	LUT	C26-C27-C28	-3.16	119.66	124.58
46	y	307	CHL	C3C-C4C-NC	-3.16	106.92	114.65
46	N	607	CHL	C1A-CHA-C4D	3.16	124.25	118.98
46	g	607	CHL	C3C-C4C-NC	-3.16	106.93	114.65
46	g	606	CHL	C1A-CHA-C4D	3.15	124.24	118.98
38	b	524	LMT	O5B-C1B-C2B	3.15	116.85	110.37
47	N	616	LUT	C15-C14-C13	-3.15	122.86	127.28
49	Y	301	XAT	O4-C6-C7	-3.15	107.85	116.88
47	G	615	LUT	C7-C8-C9	-3.15	121.57	126.23
38	B	524	LMT	O5B-C1B-C2B	3.15	116.84	110.37
30	D	401	PHO	O1D-CGD-CBD	3.15	129.49	124.72
46	g	607	CHL	C1A-CHA-C4D	3.14	124.22	118.98
31	K	101	BCR	C19-C18-C17	3.14	123.94	119.01
46	G	608	CHL	C3C-C4C-NC	-3.14	106.98	114.65
46	r	305	CHL	C4D-CHA-CBD	-3.13	105.81	108.97
31	B	518	BCR	C37-C22-C23	3.13	122.87	118.09
46	g	608	CHL	C4D-CHA-CBD	-3.13	105.81	108.97
46	N	601	CHL	CHA-C1A-C2A	-3.13	125.95	133.31
46	n	606	CHL	C1-C2-C3	-3.13	121.07	126.20
46	G	606	CHL	C3C-C4C-NC	-3.13	107.00	114.65
49	y	302	XAT	O4-C6-C7	-3.13	107.92	116.88
47	r	311	LUT	C35-C34-C33	-3.12	122.90	127.28
47	n	615	LUT	C11-C10-C9	-3.12	122.90	127.28
29	B	511	CLA	C1-C2-C3	-3.12	121.08	126.20
31	c	515	BCR	C28-C27-C26	-3.12	108.49	114.06
46	N	601	CHL	C1-C2-C3	-3.12	121.09	126.20
31	B	518	BCR	C12-C13-C14	-3.12	114.11	119.01
46	y	309	CHL	C3C-C4C-NC	-3.12	107.03	114.65
29	d	403	CLA	CHD-C1D-ND	-3.12	120.42	124.80
46	G	607	CHL	CHA-C1A-C2A	-3.11	126.00	133.31
29	n	609	CLA	CHA-C1A-NA	-3.11	119.34	126.39
46	n	601	CHL	C1-C2-C3	-3.11	121.10	126.20
46	Y	306	CHL	C3C-C4C-NC	-3.11	107.06	114.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	g	606	CHL	C1-O2A-CGA	3.11	124.17	116.65
47	S	317	LUT	C35-C15-C14	-3.10	117.17	123.52
46	g	609	CHL	C1-O2A-CGA	3.10	124.15	116.65
45	h	101	RRX	C23-C24-C25	-3.10	118.72	127.00
46	n	606	CHL	C4D-CHA-CBD	-3.09	105.85	108.97
46	g	605	CHL	CHA-C1A-C2A	-3.09	126.05	133.31
48	y	319	NEX	C2-C1-C6	3.09	112.21	109.21
31	b	518	BCR	C23-C24-C25	-3.09	118.75	127.00
31	K	101	BCR	C36-C18-C17	-3.09	117.81	122.82
31	C	516	BCR	C35-C13-C12	3.08	122.80	118.09
29	A	409	CLA	C1-C2-C3	-3.08	121.15	126.20
46	n	607	CHL	C4D-CHA-CBD	-3.08	105.86	108.97
46	N	608	CHL	C3C-C4C-NC	-3.08	107.12	114.65
46	g	606	CHL	C4D-CHA-CBD	-3.08	105.86	108.97
46	s	307	CHL	C3C-C4C-NC	-3.08	107.13	114.65
46	n	607	CHL	C3C-C4C-NC	-3.08	107.13	114.65
29	n	611	CLA	C4A-NA-C1A	3.08	108.08	106.68
31	B	518	BCR	C23-C22-C21	-3.07	114.17	119.01
29	D	404	CLA	CMB-C2B-C3B	3.07	133.78	126.55
31	C	515	BCR	C33-C5-C6	-3.07	121.13	124.48
29	D	404	CLA	CMC-C2C-C1C	3.07	129.84	125.03
31	C	516	BCR	C12-C13-C14	-3.07	114.18	119.01
46	Y	308	CHL	C3C-C4C-NC	-3.07	107.16	114.65
46	N	607	CHL	CHA-C1A-C2A	-3.06	126.11	133.31
46	N	607	CHL	C4D-CHA-CBD	-3.06	105.88	108.97
46	Y	307	CHL	C1A-CHA-C4D	3.06	124.09	118.98
37	B	523	LHG	O8-C23-C24	3.06	121.16	111.83
29	Y	303	CLA	C1-C2-C3	-3.06	121.19	126.20
45	H	101	RRX	C20-C19-C18	-3.06	117.98	126.36
49	R	311	XAT	C26-C27-C28	-3.06	119.53	125.99
47	y	318	LUT	C10-C11-C12	-3.05	114.35	123.20
46	G	607	CHL	C3C-C4C-NC	-3.05	107.20	114.65
46	Y	302	CHL	C3C-C4C-NC	-3.05	107.20	114.65
47	y	317	LUT	C10-C11-C12	-3.05	114.37	123.20
47	s	318	LUT	C18-C5-C6	-3.05	121.16	124.48
47	N	615	LUT	C10-C11-C12	-3.05	114.38	123.20
46	y	301	CHL	CHA-C1A-C2A	-3.04	126.16	133.31
46	n	605	CHL	C1-O2A-CGA	3.04	124.02	116.65
46	s	309	CHL	C3C-C4C-NC	-3.04	107.22	114.65
47	S	317	LUT	C10-C11-C12	-3.04	114.39	123.20
29	S	312	CLA	C3B-C4B-NB	-3.04	107.82	110.53
49	R	311	XAT	O4-C5-C4	-3.04	110.64	113.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	g	608	CHL	C3C-C4C-NC	-3.04	107.22	114.65
46	n	608	CHL	C1A-CHA-C4D	3.04	124.05	118.98
30	d	402	PHO	O1D-CGD-CBD	3.04	129.33	124.72
47	R	310	LUT	C18-C5-C4	3.04	120.00	114.42
46	R	304	CHL	CHA-C1A-C2A	-3.03	126.19	133.31
45	h	101	RRX	C8-C7-C6	-3.03	118.90	127.00
46	s	302	CHL	C1A-CHA-C4D	3.03	124.04	118.98
46	Y	306	CHL	C1A-CHA-C4D	3.03	124.03	118.98
29	a	405	CLA	C1-C2-C3	-3.02	121.24	126.20
29	A	409	CLA	C3B-C4B-NB	-3.02	107.83	110.53
46	r	305	CHL	CHA-C1A-C2A	-3.02	126.22	133.31
34	b	519	C7Z	C24-C25-C26	-3.02	114.56	120.76
47	Y	316	LUT	C10-C11-C12	-3.02	114.46	123.20
46	G	606	CHL	C4D-CHA-CBD	-3.01	105.93	108.97
46	S	302	CHL	CHA-C1A-C2A	-3.01	126.23	133.31
29	y	304	CLA	C1-C2-C3	-3.01	121.26	126.20
31	A	410	BCR	C37-C22-C23	3.01	122.68	118.09
35	C	521	LMG	O8-C28-C29	3.01	121.01	111.83
45	H	101	RRX	C8-C7-C6	-3.01	118.96	127.00
48	G	617	NEX	C39-C29-C30	-3.01	117.94	122.82
46	N	607	CHL	C3C-C4C-NC	-3.01	107.30	114.65
47	G	616	LUT	C18-C5-C6	-3.01	121.20	124.48
46	S	308	CHL	C1A-CHA-C4D	3.01	124.00	118.98
31	B	517	BCR	C8-C7-C6	-3.00	118.97	127.00
31	c	514	BCR	C35-C13-C12	3.00	122.68	118.09
48	s	319	NEX	C17-C1-C6	-3.00	107.78	110.47
46	s	307	CHL	C4D-CHA-CBD	-3.00	105.94	108.97
35	C	522	LMG	O8-C28-C29	3.00	120.98	111.83
46	N	606	CHL	C3C-C4C-NC	-3.00	107.32	114.65
29	G	614	CLA	C4A-NA-C1A	3.00	108.05	106.68
46	y	311	CHL	C4D-CHA-CBD	-3.00	105.95	108.97
29	R	303	CLA	CHD-C1D-ND	-2.99	120.59	124.80
46	Y	307	CHL	C1-O2A-CGA	2.99	123.90	116.65
46	r	305	CHL	C1A-CHA-C4D	2.99	123.98	118.98
46	g	605	CHL	C3C-C4C-NC	-2.99	107.34	114.65
46	Y	308	CHL	CHA-C1A-C2A	-2.99	126.28	133.31
31	A	410	BCR	C38-C26-C25	-2.99	121.22	124.48
48	R	312	NEX	C31-C30-C29	2.99	131.47	127.28
49	y	302	XAT	O4-C5-C4	-2.99	110.69	113.49
31	a	409	BCR	C37-C22-C23	2.99	122.66	118.09
48	Y	318	NEX	C31-C30-C29	2.99	131.47	127.28
30	d	402	PHO	O2D-CGD-O1D	-2.99	118.04	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	y	303	CHL	C1-C2-C3	-2.98	121.31	126.20
37	a	413	LHG	O8-C23-C24	2.98	120.93	111.83
48	y	319	NEX	C39-C29-C30	-2.98	117.99	122.82
29	n	613	CLA	CHD-C1D-ND	-2.98	120.61	124.80
31	C	517	BCR	C27-C26-C25	-2.98	118.68	122.70
29	c	506	CLA	C1D-ND-C4D	-2.98	104.22	106.31
49	r	312	XAT	C26-C27-C28	-2.98	119.70	125.99
46	y	303	CHL	C3C-C4C-NC	-2.98	107.37	114.65
46	G	607	CHL	C1-C2-C3	-2.98	121.32	126.20
29	C	506	CLA	C3B-C4B-NB	-2.98	107.87	110.53
47	Y	317	LUT	C11-C10-C9	-2.98	123.10	127.28
46	G	606	CHL	C1A-CHA-C4D	2.98	123.95	118.98
29	S	303	CLA	C4A-NA-C1A	2.97	108.04	106.68
29	c	508	CLA	C4A-NA-C1A	2.97	108.03	106.68
29	r	304	CLA	C4A-NA-C1A	2.97	108.03	106.68
46	y	311	CHL	C1-O2A-CGA	2.97	123.84	116.65
34	b	519	C7Z	C11-C12-C13	-2.97	118.21	126.36
48	g	617	NEX	C39-C29-C30	-2.97	118.00	122.82
45	H	101	RRX	C7-C8-C9	-2.97	121.84	126.23
47	g	615	LUT	C10-C11-C12	-2.97	114.60	123.20
34	B	519	C7Z	C24-C25-C26	-2.96	114.67	120.76
46	G	609	CHL	C4D-CHA-CBD	-2.96	105.98	108.97
46	n	605	CHL	C4D-CHA-CBD	-2.96	105.98	108.97
31	v	101	BCR	C36-C18-C17	-2.96	118.02	122.82
46	g	609	CHL	C3C-C4C-NC	-2.96	107.41	114.65
29	B	516	CLA	C3B-C4B-NB	-2.96	107.89	110.53
31	v	101	BCR	C19-C18-C17	2.96	123.67	119.01
46	G	601	CHL	C1-C2-C3	-2.96	121.35	126.20
46	N	608	CHL	C4D-CHA-CBD	-2.96	105.98	108.97
29	Y	315	CLA	C3B-C4B-NB	-2.96	107.89	110.53
47	n	614	LUT	C7-C8-C9	-2.96	121.86	126.23
47	S	318	LUT	C35-C15-C14	-2.96	117.47	123.52
46	G	607	CHL	C1A-CHA-C4D	2.95	123.91	118.98
29	g	610	CLA	C1-C2-C3	-2.95	121.36	126.20
29	c	506	CLA	C4A-NA-C1A	2.95	108.03	106.68
49	g	619	XAT	O4-C6-C7	-2.95	108.42	116.88
46	R	304	CHL	C1A-CHA-C4D	2.95	123.91	118.98
47	r	311	LUT	C18-C5-C4	2.95	119.85	114.42
29	S	304	CLA	CHD-C1D-ND	-2.95	120.65	124.80
46	Y	310	CHL	C1-O2A-CGA	2.95	123.79	116.65
30	A	408	PHO	O1D-CGD-CBD	2.95	129.20	124.72
46	N	601	CHL	C4D-CHA-CBD	-2.95	105.99	108.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	F	101	BCR	C35-C13-C12	2.95	122.59	118.09
48	n	616	NEX	C31-C30-C29	2.95	131.41	127.28
46	G	606	CHL	CHA-C1A-C2A	-2.95	126.38	133.31
47	n	614	LUT	C18-C5-C6	-2.94	121.27	124.48
46	G	609	CHL	C3C-C4C-NC	-2.94	107.46	114.65
46	y	308	CHL	C4D-CHA-CBD	-2.94	106.00	108.97
31	K	101	BCR	C35-C13-C12	2.94	122.57	118.09
51	s	321	LPX	O3-P1-O4	2.93	126.08	112.44
49	n	618	XAT	C26-C27-C28	-2.93	119.81	125.99
46	n	606	CHL	CHA-C1A-C2A	-2.93	126.44	133.31
49	g	619	XAT	C38-C25-C26	-2.92	117.49	122.30
46	y	309	CHL	C1A-CHA-C4D	2.92	123.86	118.98
29	b	504	CLA	CHA-C1A-NA	-2.92	119.77	126.39
46	y	301	CHL	C1A-CHA-C4D	2.92	123.86	118.98
29	c	503	CLA	C3B-C4B-NB	-2.92	107.92	110.53
46	N	605	CHL	C4D-CHA-CBD	-2.92	106.02	108.97
49	r	312	XAT	O4-C6-C7	-2.92	108.52	116.88
46	N	609	CHL	C4D-CHA-CBD	-2.92	106.03	108.97
29	D	404	CLA	C1C-C2C-C3C	-2.92	103.91	106.98
29	s	305	CLA	C1-C2-C3	-2.92	121.42	126.20
46	S	307	CHL	C4D-CHA-CBD	-2.92	106.03	108.97
47	n	614	LUT	C31-C30-C29	-2.91	123.19	127.28
30	a	407	PHO	O2D-CGD-O1D	-2.91	118.18	123.85
41	j	101	DGA	OG1-CA1-CA2	2.91	120.71	111.83
46	n	605	CHL	C1A-CHA-C4D	2.91	123.84	118.98
29	a	408	CLA	C1-C2-C3	-2.91	121.43	126.20
46	y	308	CHL	C1-C2-C3	-2.91	122.06	126.76
49	G	619	XAT	C38-C25-C26	-2.91	117.52	122.30
46	n	607	CHL	C1-O2A-CGA	2.91	123.68	116.65
47	s	318	LUT	C35-C15-C14	-2.91	117.57	123.52
31	B	517	BCR	C4-C5-C6	-2.91	118.78	122.70
43	d	405	PL9	C7-C8-C9	-2.91	121.83	126.83
49	g	619	XAT	C6-C7-C8	-2.90	119.85	125.99
46	N	606	CHL	C1A-CHA-C4D	2.90	123.82	118.98
46	g	601	CHL	C1A-CHA-C4D	2.90	123.82	118.98
37	S	301	LHG	O8-C23-C24	2.90	120.67	111.83
46	N	608	CHL	C1-O2A-CGA	2.89	123.66	116.65
31	z	101	BCR	C33-C5-C6	-2.89	121.33	124.48
29	b	511	CLA	C1-C2-C3	-2.89	121.46	126.20
29	Y	305	CLA	C1-C2-C3	-2.89	121.46	126.20
46	y	307	CHL	C1A-CHA-C4D	2.89	123.81	118.98
35	d	408	LMG	O8-C28-C29	2.89	120.65	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	s	308	CHL	C1A-CHA-C4D	2.89	123.81	118.98
46	Y	308	CHL	C1A-CHA-C4D	2.89	123.80	118.98
47	N	616	LUT	C11-C10-C9	-2.89	123.23	127.28
48	s	319	NEX	C38-C25-C26	-2.89	117.55	122.30
37	L	101	LHG	O8-C23-C24	2.89	120.64	111.83
37	l	102	LHG	O8-C23-C24	2.89	120.64	111.83
34	B	519	C7Z	C11-C12-C13	-2.89	118.45	126.36
45	h	101	RRX	C38-C26-C27	2.88	119.72	114.42
30	a	407	PHO	O1D-CGD-CBD	2.88	129.09	124.72
29	S	316	CLA	CHD-C1D-ND	-2.88	120.75	124.80
46	G	609	CHL	C1-O2A-CGA	2.88	123.62	116.65
31	b	517	BCR	C33-C5-C4	2.88	119.73	113.60
51	S	321	LPX	O3-P1-O4	2.88	125.83	112.44
46	N	606	CHL	C4D-CHA-CBD	-2.88	106.07	108.97
48	R	312	NEX	C39-C29-C30	-2.88	118.16	122.82
46	g	606	CHL	CHA-C1A-C2A	-2.88	126.55	133.31
47	Y	317	LUT	C10-C11-C12	-2.87	114.87	123.20
29	C	504	CLA	C3B-C2B-C1B	-2.87	103.78	107.17
48	N	617	NEX	C39-C29-C30	-2.87	118.17	122.82
35	W	203	LMG	O8-C28-C29	2.87	120.58	111.83
47	Y	317	LUT	C22-C23-C24	-2.87	106.93	111.18
29	a	406	CLA	C4A-NA-C1A	2.87	107.99	106.68
47	g	615	LUT	C11-C10-C9	-2.87	123.26	127.28
47	s	317	LUT	C39-C29-C28	2.87	122.47	118.09
29	r	303	CLA	C4A-NA-C1A	2.86	107.99	106.68
46	S	302	CHL	C4D-CHA-CBD	-2.86	106.08	108.97
46	y	309	CHL	C1-C2-C3	-2.86	121.51	126.20
46	G	606	CHL	C1-O2A-CGA	2.86	123.57	116.65
47	g	615	LUT	C18-C5-C6	-2.86	121.37	124.48
31	b	517	BCR	C4-C5-C6	-2.86	118.84	122.70
48	r	313	NEX	C39-C29-C30	-2.86	118.19	122.82
49	G	619	XAT	C6-C7-C8	-2.86	119.96	125.99
36	c	517	DGD	O1G-C1A-C2A	2.85	120.53	111.83
46	N	609	CHL	C1-O2A-CGA	2.85	123.56	116.65
36	C	519	DGD	O1G-C1A-C2A	2.85	120.52	111.83
37	s	301	LHG	O8-C23-C24	2.85	120.52	111.83
46	G	607	CHL	C1-O2A-CGA	2.85	123.55	116.65
47	y	317	LUT	C18-C5-C6	-2.85	121.38	124.48
29	g	604	CLA	C4A-NA-C1A	2.85	107.98	106.68
47	y	318	LUT	C11-C10-C9	-2.85	123.29	127.28
46	n	608	CHL	C1-O2A-CGA	2.84	123.53	116.65
46	Y	310	CHL	C4D-CHA-CBD	-2.84	106.11	108.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	518	DGD	O1G-C1A-C2A	2.84	120.48	111.83
46	G	605	CHL	C4D-CHA-CBD	-2.84	106.11	108.97
30	A	408	PHO	O2D-CGD-O1D	-2.84	118.33	123.85
49	Y	301	XAT	O4-C5-C4	-2.83	110.83	113.49
29	n	603	CLA	C4A-NA-C1A	-2.83	105.39	106.68
33	b	521	3PH	O31-C31-C32	2.83	120.46	111.83
29	a	406	CLA	CHD-C1D-ND	-2.83	120.82	124.80
46	G	608	CHL	C1A-CHA-C4D	2.83	123.70	118.98
46	Y	308	CHL	C1-C2-C3	-2.83	121.57	126.20
35	B	520	LMG	O8-C28-C29	2.83	120.45	111.83
46	R	305	CHL	C4D-CHA-CBD	-2.82	106.12	108.97
43	D	406	PL9	C7-C8-C9	-2.82	121.97	126.83
47	s	318	LUT	C11-C10-C9	-2.82	123.32	127.28
46	y	303	CHL	C1-O2A-CGA	2.82	123.48	116.65
50	N	620	PTY	O4-C30-C31	2.82	120.44	111.83
29	C	509	CLA	CHD-C1D-ND	-2.82	120.83	124.80
46	N	605	CHL	C1-C2-C3	-2.82	121.58	126.20
30	D	401	PHO	O2D-CGD-O1D	-2.82	118.36	123.85
47	S	317	LUT	C18-C5-C6	-2.82	121.41	124.48
46	G	608	CHL	C4D-CHA-CBD	-2.82	106.13	108.97
47	G	615	LUT	C10-C11-C12	-2.82	115.04	123.20
39	a	410	SQD	O7-S-C6	-2.82	102.55	106.76
31	B	517	BCR	C1-C6-C5	-2.81	118.79	122.64
48	n	616	NEX	C39-C29-C30	-2.81	118.26	122.82
31	b	517	BCR	C33-C5-C6	-2.81	121.42	124.48
46	N	606	CHL	C1-C2-C3	-2.81	121.60	126.20
48	Y	318	NEX	C39-C29-C30	-2.81	118.27	122.82
46	N	601	CHL	C1A-CHA-C4D	2.80	123.66	118.98
48	S	319	NEX	C38-C25-C26	-2.80	117.69	122.30
46	S	309	CHL	C1A-CHA-C4D	2.80	123.66	118.98
47	s	317	LUT	C30-C31-C32	-2.80	115.09	123.20
49	R	311	XAT	O4-C6-C7	-2.80	108.86	116.88
35	c	519	LMG	O8-C28-C29	2.80	120.36	111.83
45	H	101	RRX	C33-C5-C4	2.80	119.56	113.60
46	s	309	CHL	C4D-CHA-CBD	-2.80	106.15	108.97
49	r	312	XAT	C38-C25-C26	-2.79	117.70	122.30
46	S	309	CHL	C4D-CHA-CBD	-2.79	106.15	108.97
46	n	601	CHL	C4D-CHA-CBD	-2.79	106.15	108.97
29	B	505	CLA	C3B-C2B-C1B	-2.79	103.88	107.17
39	o	301	SQD	O7-S-C6	-2.79	102.59	106.76
47	s	317	LUT	C10-C11-C12	-2.79	115.11	123.20
31	f	101	BCR	C36-C18-C17	-2.79	118.30	122.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	S	322	3PH	O31-C31-C32	2.79	120.34	111.83
47	Y	317	LUT	C31-C30-C29	-2.79	123.37	127.28
46	r	306	CHL	C4D-CHA-CBD	-2.79	106.16	108.97
47	R	310	LUT	C8-C7-C6	-2.79	119.55	127.00
29	c	501	CLA	C1-C2-C3	-2.79	121.63	126.20
39	C	501	SQD	O7-S-C6	-2.79	102.60	106.76
46	G	601	CHL	C1A-CHA-C4D	2.78	123.62	118.98
31	z	101	BCR	C23-C24-C25	-2.78	119.57	127.00
29	g	611	CLA	C3B-C2B-C1B	-2.78	103.89	107.17
37	c	521	LHG	O8-C23-C24	2.78	120.31	111.83
46	R	305	CHL	C1A-CHA-C4D	2.78	123.62	118.98
46	g	606	CHL	C3C-C4C-NC	-2.78	107.86	114.65
46	g	601	CHL	C1-C2-C3	-2.78	121.64	126.20
33	B	522	3PH	O31-C31-C32	2.78	120.31	111.83
29	c	503	CLA	C3B-C2B-C1B	-2.78	103.89	107.17
46	S	308	CHL	C4D-CHA-CBD	-2.78	106.17	108.97
47	y	317	LUT	C7-C8-C9	-2.78	122.13	126.23
46	s	308	CHL	C4D-CHA-CBD	-2.78	106.17	108.97
29	a	404	CLA	C1-C2-C3	2.77	130.74	126.20
47	G	615	LUT	C11-C10-C9	-2.77	123.39	127.28
47	G	615	LUT	C26-C27-C28	-2.77	120.27	124.58
29	D	404	CLA	CHC-C1C-C2C	-2.77	119.07	126.95
46	y	307	CHL	C4D-CHA-CBD	-2.77	106.17	108.97
31	F	101	BCR	C23-C24-C25	-2.77	119.60	127.00
29	r	310	CLA	CHD-C1D-ND	-2.77	120.91	124.80
31	C	517	BCR	C2-C1-C6	2.77	114.46	110.44
47	r	311	LUT	C7-C8-C9	-2.77	122.14	126.23
48	s	319	NEX	C19-C9-C10	-2.77	118.33	122.82
46	y	308	CHL	C3C-C4C-NC	-2.77	107.89	114.65
35	b	520	LMG	O8-C28-C29	2.77	120.27	111.83
46	g	605	CHL	C4D-CHA-CBD	-2.77	106.18	108.97
36	c	518	DGD	O1G-C1A-C2A	2.76	120.26	111.83
37	d	406	LHG	O8-C23-C24	2.76	120.26	111.83
29	s	315	CLA	C3B-C4B-NB	-2.76	108.06	110.53
37	g	618	LHG	O8-C23-C24	2.76	120.25	111.83
31	b	518	BCR	C37-C22-C23	2.76	122.31	118.09
46	n	606	CHL	C3C-C4C-NC	-2.76	107.90	114.65
45	H	101	RRX	C38-C26-C27	2.76	119.50	114.42
46	Y	306	CHL	C4D-CHA-CBD	-2.76	106.19	108.97
29	R	307	CLA	CHD-C1D-ND	-2.76	120.92	124.80
29	C	502	CLA	C1-C2-C3	-2.76	121.68	126.20
50	n	619	PTY	O4-C30-C31	2.76	120.24	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	518	BCR	C35-C13-C12	2.76	122.30	118.09
46	y	309	CHL	CHA-C1A-C2A	-2.75	126.84	133.31
47	n	615	LUT	C18-C5-C6	-2.75	121.48	124.48
29	S	314	CLA	CHD-C1D-ND	-2.75	120.94	124.80
39	c	522	SQD	O7-S-C6	-2.75	102.65	106.76
46	Y	307	CHL	C3C-C4C-NC	-2.75	107.94	114.65
47	R	310	LUT	C27-C28-C29	-2.74	120.42	126.32
29	b	503	CLA	C3B-C4B-NB	-2.74	108.08	110.53
33	a	415	3PH	O31-C31-C32	2.74	120.20	111.83
46	Y	302	CHL	C1-O2A-CGA	2.74	123.28	116.65
37	G	618	LHG	O8-C23-C24	2.73	120.17	111.83
47	Y	316	LUT	C18-C5-C6	-2.73	121.50	124.48
29	b	502	CLA	C3B-C4B-NB	-2.73	108.09	110.53
39	M	101	SQD	O7-S-C6	-2.73	102.68	106.76
29	S	303	CLA	CHD-C1D-ND	-2.73	120.96	124.80
41	w	201	DGA	OG1-CA1-CA2	2.73	120.15	111.83
29	s	316	CLA	C3B-C4B-NB	-2.73	108.10	110.53
31	v	101	BCR	C35-C13-C12	2.73	122.25	118.09
36	C	520	DGD	O1G-C1A-C2A	2.72	120.14	111.83
47	N	616	LUT	C18-C5-C6	-2.72	121.51	124.48
31	a	409	BCR	C38-C26-C25	-2.72	121.51	124.48
36	r	301	DGD	O6E-C5E-C4E	2.72	114.60	109.70
29	S	315	CLA	CHD-C1D-ND	-2.72	120.98	124.80
49	G	619	XAT	O4-C6-C7	-2.72	109.09	116.88
29	B	514	CLA	CHD-C1D-ND	-2.72	120.98	124.80
29	C	510	CLA	CHD-C1D-ND	-2.72	120.98	124.80
29	c	512	CLA	C4A-NA-C1A	2.72	107.92	106.68
47	G	615	LUT	C18-C5-C6	-2.71	121.52	124.48
31	F	101	BCR	C12-C13-C14	-2.71	114.74	119.01
35	i	101	LMG	O8-C28-C29	2.71	120.10	111.83
29	y	306	CLA	C1-C2-C3	-2.71	121.76	126.20
47	N	615	LUT	C18-C5-C6	-2.71	121.53	124.48
35	W	201	LMG	C8-O7-C10	-2.71	111.31	117.80
46	R	304	CHL	C3C-C4C-NC	-2.71	108.03	114.65
46	r	305	CHL	C3C-C4C-NC	-2.71	108.03	114.65
47	n	614	LUT	C27-C28-C29	-2.70	120.51	126.32
29	s	315	CLA	C4A-NA-C1A	2.70	107.91	106.68
31	v	101	BCR	C2-C1-C6	2.70	114.37	110.44
46	S	302	CHL	C1A-CHA-C4D	2.70	123.50	118.98
29	s	303	CLA	CHD-C1D-ND	-2.70	121.00	124.80
46	r	306	CHL	C1-O2A-CGA	2.70	123.20	116.65
45	H	101	RRX	C11-C12-C13	-2.70	118.95	126.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	g	609	CHL	C4D-CHA-CBD	-2.70	106.24	108.97
47	Y	316	LUT	C26-C27-C28	-2.70	120.37	124.58
46	s	302	CHL	C4D-CHA-CBD	-2.70	106.24	108.97
34	b	519	C7Z	C18-C5-C4	2.70	119.39	114.42
38	B	524	LMT	C1B-C2B-C3B	2.70	115.69	110.01
46	r	306	CHL	C4C-CHD-C1D	2.70	125.73	116.07
31	f	101	BCR	C34-C9-C10	-2.70	118.44	122.82
39	m	101	SQD	O7-S-C6	-2.70	102.72	106.76
29	A	405	CLA	C4A-NA-C1A	2.70	107.91	106.68
29	R	302	CLA	C4A-NA-C1A	2.70	107.91	106.68
29	a	405	CLA	CHD-C1D-ND	-2.70	121.00	124.80
29	C	502	CLA	C4A-NA-C1A	2.70	107.91	106.68
29	g	610	CLA	C3B-C4B-NB	-2.69	108.12	110.53
47	N	615	LUT	C26-C27-C28	-2.69	120.39	124.58
46	G	606	CHL	C1C-C2C-CMC	2.69	131.66	126.80
46	S	307	CHL	C3C-C4C-NC	-2.69	108.07	114.65
47	G	615	LUT	C22-C23-C24	-2.69	107.19	111.18
29	A	407	CLA	CHD-C1D-ND	-2.69	121.01	124.80
29	a	406	CLA	CHA-C1A-NA	-2.69	120.30	126.39
35	c	520	LMG	O8-C28-C29	2.69	120.04	111.83
29	y	305	CLA	CHD-C1D-ND	-2.69	121.02	124.80
29	s	316	CLA	CHA-C1A-NA	-2.69	120.30	126.39
47	Y	317	LUT	C18-C5-C6	-2.69	121.55	124.48
46	N	605	CHL	C1A-CHA-C4D	2.69	123.47	118.98
29	N	612	CLA	C3B-C4B-NB	-2.68	108.13	110.53
31	b	518	BCR	C12-C13-C14	-2.68	114.79	119.01
29	C	511	CLA	CHD-C1D-ND	-2.68	121.03	124.80
31	C	517	BCR	C23-C24-C25	-2.68	119.83	127.00
47	R	310	LUT	C1-C6-C5	-2.68	118.97	122.64
34	B	519	C7Z	C35-C15-C14	-2.68	118.03	123.52
29	Y	312	CLA	CHD-C1D-ND	-2.68	121.03	124.80
29	c	512	CLA	C3B-C4B-NB	-2.68	108.14	110.53
45	h	101	RRX	C33-C5-C4	2.68	119.31	113.60
33	A	412	3PH	O31-C31-C32	2.68	120.00	111.83
29	s	312	CLA	CHD-C1D-ND	-2.68	121.03	124.80
49	N	619	XAT	C26-C27-C28	-2.68	120.33	125.99
29	r	310	CLA	CHA-C1A-NA	-2.68	120.33	126.39
29	B	512	CLA	CHD-C1D-ND	-2.67	121.04	124.80
39	b	523	SQD	O7-S-C6	-2.67	102.77	106.76
49	N	619	XAT	C18-C5-C6	-2.67	117.91	122.30
29	b	514	CLA	CHD-C1D-ND	-2.67	121.05	124.80
29	G	610	CLA	CHA-C1A-NA	-2.67	120.35	126.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	505	CLA	C3B-C2B-C1B	-2.67	104.02	107.17
46	n	608	CHL	C4D-CHA-CBD	-2.67	106.28	108.97
46	Y	302	CHL	C1-C2-C3	-2.67	121.83	126.20
29	S	315	CLA	C4A-NA-C1A	2.67	107.90	106.68
29	N	603	CLA	C3B-C4B-NB	-2.66	108.15	110.53
29	B	506	CLA	C3B-C4B-NB	-2.66	108.15	110.53
29	y	310	CLA	C3B-C4B-NB	-2.66	108.15	110.53
35	W	201	LMG	O8-C28-C29	2.66	119.95	111.83
46	R	305	CHL	C1-O2A-CGA	2.66	123.08	116.65
31	C	515	BCR	C35-C13-C12	2.66	122.14	118.09
47	N	616	LUT	C22-C23-C24	-2.66	107.24	111.18
48	Y	318	NEX	C1-C2-C3	2.65	119.41	113.59
47	y	318	LUT	C18-C5-C6	-2.65	121.59	124.48
37	D	407	LHG	C5-O7-C7	-2.65	111.45	117.80
49	y	302	XAT	O24-C25-C24	2.65	115.97	113.49
29	b	504	CLA	CAA-C2A-C3A	-2.65	105.84	113.00
39	C	523	SQD	O7-S-C6	-2.65	102.80	106.76
31	c	514	BCR	C3-C4-C5	-2.65	109.34	114.06
47	y	317	LUT	C26-C27-C28	-2.65	120.46	124.58
41	J	101	DGA	OG1-CA1-CA2	2.64	119.90	111.83
29	c	509	CLA	CHD-C1D-ND	-2.64	121.08	124.80
31	c	515	BCR	C23-C24-C25	-2.64	119.94	127.00
33	s	322	3PH	O31-C31-C32	2.64	119.89	111.83
29	G	602	CLA	CHD-C1D-ND	-2.64	121.08	124.80
46	Y	307	CHL	C4D-CHA-CBD	-2.64	106.30	108.97
31	c	515	BCR	C31-C1-C6	-2.64	106.10	110.24
29	R	302	CLA	CHA-C1A-NA	-2.64	120.41	126.39
47	g	616	LUT	C22-C23-C24	-2.64	107.26	111.18
29	y	315	CLA	C3B-C4B-NB	-2.64	108.17	110.53
29	r	303	CLA	CHA-C1A-NA	-2.63	120.43	126.39
35	w	202	LMG	O8-C28-C29	2.63	119.86	111.83
46	n	601	CHL	C1A-CHA-C4D	2.63	123.37	118.98
31	F	101	BCR	C34-C9-C10	-2.63	118.55	122.82
37	a	414	LHG	O8-C23-C24	2.63	119.86	111.83
29	g	611	CLA	C3B-C4B-NB	-2.63	108.18	110.53
29	s	311	CLA	CHD-C1D-ND	-2.63	121.10	124.80
29	c	508	CLA	CHD-C1D-ND	-2.63	121.10	124.80
37	s	320	LHG	O8-C23-C24	2.63	119.84	111.83
38	B	524	LMT	C3B-C4B-C5B	-2.63	105.47	110.23
29	d	404	CLA	C3B-C4B-NB	-2.63	108.19	110.53
29	R	306	CLA	CHD-C1D-ND	-2.63	121.11	124.80
37	L	101	LHG	O7-C7-O9	-2.62	117.57	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y	304	CLA	C3B-C4B-NB	-2.62	108.19	110.53
37	N	618	LHG	O8-C23-C24	2.62	119.83	111.83
46	n	606	CHL	C1A-CHA-C4D	2.62	123.36	118.98
29	G	602	CLA	C1-C2-C3	-2.62	121.90	126.20
29	s	314	CLA	CHD-C1D-ND	-2.62	121.12	124.80
39	l	101	SQD	O7-S-C6	-2.62	102.85	106.76
46	N	609	CHL	C1A-CHA-C4D	2.62	123.35	118.98
46	G	601	CHL	C4D-CHA-CBD	-2.62	106.33	108.97
48	G	617	NEX	O24-C25-C38	-2.62	112.12	115.05
46	y	308	CHL	CMA-C3A-C4A	2.62	120.25	114.61
46	Y	302	CHL	C4D-CHA-CBD	-2.62	106.33	108.97
29	R	302	CLA	C2A-C1A-CHA	2.61	128.40	123.87
29	C	507	CLA	C3B-C4B-NB	-2.61	108.20	110.53
46	Y	308	CHL	C1-O2A-CGA	2.60	122.96	116.65
29	Y	312	CLA	C4A-NA-C1A	2.60	107.87	106.68
46	y	303	CHL	C4D-CHA-CBD	-2.60	106.34	108.97
38	b	524	LMT	C1B-C2B-C3B	2.60	115.48	110.01
29	y	313	CLA	CHD-C1D-ND	-2.60	121.14	124.80
43	d	405	PL9	C22-C23-C24	-2.60	121.67	127.62
41	W	202	DGA	OG1-CA1-CA2	2.60	119.76	111.83
35	C	521	LMG	C8-O7-C10	-2.60	111.58	117.80
29	n	611	CLA	CHD-C1D-ND	-2.60	121.15	124.80
29	B	509	CLA	CHD-C1D-ND	-2.60	121.15	124.80
35	D	409	LMG	O8-C28-C29	2.59	119.75	111.83
29	N	611	CLA	CHD-C1D-ND	-2.59	121.15	124.80
29	Y	303	CLA	C3B-C2B-C1B	-2.59	104.11	107.17
39	L	102	SQD	O7-S-C6	-2.59	102.88	106.76
29	G	604	CLA	C4A-NA-C1A	2.59	107.86	106.68
47	Y	316	LUT	C7-C8-C9	-2.59	122.41	126.23
37	S	320	LHG	O8-C23-C24	2.58	119.72	111.83
29	s	315	CLA	CHD-C1D-ND	-2.58	121.17	124.80
29	S	306	CLA	CHD-C1D-ND	-2.58	121.17	124.80
46	g	605	CHL	C4C-CHD-C1D	2.58	125.31	116.07
31	C	516	BCR	C33-C5-C4	2.58	119.10	113.60
29	Y	309	CLA	CHD-C1D-ND	-2.58	121.17	124.80
46	G	605	CHL	C4C-CHD-C1D	2.58	125.30	116.07
41	D	402	DGA	OG1-CA1-CA2	2.58	119.69	111.83
47	y	318	LUT	C38-C25-C24	-2.58	117.26	123.36
37	s	301	LHG	C5-O7-C7	-2.58	111.63	117.80
48	S	319	NEX	C31-C30-C29	2.58	130.89	127.28
46	Y	307	CHL	CMA-C3A-C4A	2.57	120.16	114.61
29	D	405	CLA	C3B-C4B-NB	-2.57	108.23	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	N	611	CLA	C3B-C4B-NB	-2.57	108.23	110.53
47	S	317	LUT	C27-C28-C29	-2.57	120.79	126.32
29	c	509	CLA	O2A-CGA-O1A	-2.57	117.19	123.63
37	n	617	LHG	O8-C23-C24	2.57	119.67	111.83
47	s	317	LUT	C11-C10-C9	-2.57	123.67	127.28
29	b	508	CLA	CHD-C1D-ND	-2.57	121.18	124.80
29	s	313	CLA	CHD-C1D-ND	-2.57	121.19	124.80
29	n	602	CLA	C1-C2-C3	-2.57	121.99	126.20
36	B	521	DGD	C1E-O6E-C5E	2.57	118.74	113.72
37	n	617	LHG	C5-O7-C7	-2.57	111.65	117.80
29	d	403	CLA	C3B-C4B-NB	-2.57	108.24	110.53
29	g	602	CLA	C1-C2-C3	-2.57	121.99	126.20
34	b	519	C7Z	C38-C25-C24	2.57	119.14	114.42
46	N	609	CHL	CMA-C3A-C4A	2.57	120.14	114.61
29	s	311	CLA	C3B-C4B-NB	-2.57	108.24	110.53
37	y	320	LHG	O8-C23-C24	2.57	119.66	111.83
29	b	504	CLA	CAA-C2A-C1A	2.57	120.39	111.97
46	N	601	CHL	C1-O2A-CGA	2.57	122.86	116.65
29	y	316	CLA	CHD-C1D-ND	-2.56	121.19	124.80
30	d	402	PHO	C1-C2-C3	-2.56	122.00	126.20
46	S	307	CHL	CMA-C3A-C4A	2.56	120.14	114.61
47	N	616	LUT	C10-C11-C12	-2.56	115.77	123.20
49	n	618	XAT	C6-C7-C8	-2.56	120.58	125.99
31	c	515	BCR	C35-C13-C12	2.56	122.00	118.09
46	y	303	CHL	C4C-CHD-C1D	2.56	125.23	116.07
29	g	604	CLA	CHA-C1A-NA	-2.56	120.59	126.39
46	g	601	CHL	C4D-CHA-CBD	-2.56	106.39	108.97
36	B	521	DGD	O1G-C1A-C2A	2.56	119.64	111.83
29	g	604	CLA	CHD-C1D-ND	-2.56	121.20	124.80
29	B	502	CLA	C3B-C4B-NB	-2.56	108.25	110.53
37	Y	319	LHG	O8-C23-C24	2.56	119.63	111.83
36	r	301	DGD	O1G-C1A-C2A	2.56	119.63	111.83
29	D	404	CLA	CMA-C3A-C4A	2.55	118.64	111.77
29	y	306	CLA	O2A-CGA-O1A	-2.55	117.24	123.63
46	Y	310	CHL	C1-C2-C3	-2.55	122.01	126.20
29	G	611	CLA	C3B-C4B-NB	-2.55	108.25	110.53
29	C	510	CLA	CHA-C1A-NA	-2.55	120.61	126.39
29	S	310	CLA	CHD-C1D-ND	-2.55	121.21	124.80
29	Y	303	CLA	CHD-C1D-ND	-2.55	121.21	124.80
47	n	615	LUT	C10-C11-C12	-2.55	115.81	123.20
46	Y	302	CHL	C4C-CHD-C1D	2.55	125.19	116.07
46	R	305	CHL	C4C-CHD-C1D	2.55	125.19	116.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	507	CLA	CHD-C1D-ND	-2.55	121.22	124.80
38	b	524	LMT	C3'-C4'-C5'	-2.55	105.28	110.93
29	c	505	CLA	C1-C2-C3	-2.55	122.02	126.20
29	b	502	CLA	CHD-C1D-ND	-2.55	121.22	124.80
29	n	602	CLA	CHD-C1D-ND	-2.55	121.22	124.80
29	D	404	CLA	CHD-C4C-NC	-2.55	120.28	124.23
31	C	515	BCR	C12-C13-C14	-2.55	115.00	119.01
48	s	319	NEX	C39-C29-C30	-2.55	118.69	122.82
46	r	306	CHL	C1A-CHA-C4D	2.55	123.23	118.98
40	I	101	SPH	C3-C4-C5	-2.54	119.42	124.69
46	n	606	CHL	C4C-CHD-C1D	2.54	125.17	116.07
36	c	516	DGD	O1G-C1A-C2A	2.54	119.59	111.83
47	g	616	LUT	C10-C11-C12	-2.54	115.83	123.20
29	B	505	CLA	CHD-C1D-ND	-2.54	121.22	124.80
49	G	619	XAT	O4-C5-C4	-2.54	111.11	113.49
31	c	515	BCR	C33-C5-C6	-2.54	121.71	124.48
29	c	505	CLA	C3B-C4B-NB	-2.54	108.26	110.53
40	c	523	SPH	C3-C4-C5	-2.54	119.43	124.69
29	n	603	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
48	G	617	NEX	C16-C1-C6	-2.54	108.20	110.47
47	N	615	LUT	C38-C25-C24	-2.54	117.36	123.36
31	v	101	BCR	C31-C1-C6	-2.53	106.27	110.24
29	R	302	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
47	y	318	LUT	C35-C15-C14	-2.53	118.34	123.52
31	c	515	BCR	C2-C1-C6	2.53	114.12	110.44
31	b	518	BCR	C35-C13-C12	2.53	121.96	118.09
49	n	618	XAT	O4-C6-C7	-2.53	109.62	116.88
49	y	302	XAT	C26-C27-C28	-2.53	120.64	125.99
47	Y	316	LUT	C31-C30-C29	-2.53	123.73	127.28
29	a	408	CLA	C3B-C4B-NB	-2.53	108.27	110.53
29	r	308	CLA	CHD-C1D-ND	-2.53	121.24	124.80
29	s	316	CLA	CHD-C1D-ND	-2.53	121.24	124.80
29	C	506	CLA	CHD-C1D-ND	-2.53	121.25	124.80
29	r	309	CLA	O2A-CGA-O1A	-2.53	117.31	123.63
46	n	601	CHL	C1-O2A-CGA	2.53	122.77	116.65
29	s	304	CLA	CHA-C1A-NA	-2.53	120.67	126.39
29	c	509	CLA	CHA-C1A-NA	-2.52	120.67	126.39
48	g	617	NEX	C38-C25-C26	-2.52	118.15	122.30
46	n	608	CHL	C1-C2-C3	-2.52	122.06	126.20
47	S	317	LUT	C30-C31-C32	-2.52	115.89	123.20
34	B	519	C7Z	C38-C25-C24	2.52	119.06	114.42
45	H	101	RRX	C2-C1-C6	2.52	114.10	110.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	y	312	CLA	CHD-C1D-ND	-2.52	121.26	124.80
29	n	609	CLA	C3B-C4B-NB	-2.52	108.28	110.53
47	G	616	LUT	C10-C11-C12	-2.52	115.91	123.20
29	y	310	CLA	CHD-C1D-ND	-2.52	121.26	124.80
29	C	503	CLA	C1-C2-C3	-2.52	122.08	126.20
40	i	102	SPH	C3-C4-C5	-2.51	119.48	124.69
29	S	316	CLA	C2D-C1D-ND	-2.51	107.64	110.13
38	B	524	LMT	C3'-C4'-C5'	-2.51	105.36	110.93
43	D	406	PL9	C27-C28-C29	-2.51	121.87	127.62
29	R	309	CLA	C1D-ND-C4D	-2.51	104.55	106.31
37	y	320	LHG	C5-O7-C7	-2.51	111.79	117.80
29	n	609	CLA	CHD-C1D-ND	-2.51	121.27	124.80
29	D	404	CLA	C6-C5-C3	-2.51	107.36	113.47
29	S	304	CLA	C4B-C3B-C2B	-2.51	104.18	107.30
46	R	305	CHL	CMA-C3A-C4A	2.51	120.01	114.61
29	n	604	CLA	C4A-NA-C1A	2.51	107.82	106.68
31	v	101	BCR	C37-C22-C23	2.51	121.92	118.09
48	N	617	NEX	C38-C25-C26	-2.50	118.18	122.30
29	s	305	CLA	CHD-C1D-ND	-2.50	121.28	124.80
46	Y	302	CHL	C1A-CHA-C4D	2.50	123.16	118.98
29	b	516	CLA	C3B-C4B-NB	-2.50	108.30	110.53
46	y	303	CHL	C1A-CHA-C4D	2.50	123.16	118.98
48	S	319	NEX	C1-C2-C3	2.50	119.08	113.59
48	n	616	NEX	C38-C25-C26	-2.50	118.19	122.30
49	Y	301	XAT	C18-C5-C6	-2.50	118.19	122.30
46	y	309	CHL	C1-O2A-CGA	2.50	122.69	116.65
35	d	407	LMG	O8-C28-C29	2.50	119.45	111.83
29	B	503	CLA	CHD-C1D-ND	-2.50	121.29	124.80
29	B	502	CLA	CHD-C1D-ND	-2.50	121.29	124.80
29	r	309	CLA	CHD-C1D-ND	-2.49	121.29	124.80
47	Y	317	LUT	C38-C25-C24	-2.49	117.46	123.36
29	C	510	CLA	O2A-CGA-O1A	-2.49	117.39	123.63
35	D	410	LMG	O8-C28-C29	2.49	119.44	111.83
29	G	610	CLA	C1-C2-C3	-2.49	122.11	126.20
29	r	309	CLA	C3B-C2B-C1B	-2.49	104.23	107.17
29	Y	304	CLA	CHD-C1D-ND	-2.49	121.30	124.80
29	b	512	CLA	CHD-C1D-ND	-2.49	121.30	124.80
46	G	609	CHL	C1-C2-C3	-2.49	122.12	126.20
46	G	605	CHL	CMA-C3A-C4A	2.49	119.97	114.61
29	b	505	CLA	CHD-C1D-ND	-2.49	121.31	124.80
38	b	524	LMT	C3B-C4B-C5B	-2.49	105.73	110.23
31	z	101	BCR	C36-C18-C17	-2.48	118.79	122.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	503	CLA	CHD-C1D-ND	-2.48	121.31	124.80
29	b	516	CLA	C4A-NA-C1A	2.48	107.81	106.68
31	v	101	BCR	C3-C4-C5	-2.48	109.63	114.06
29	g	611	CLA	CHD-C1D-ND	-2.48	121.31	124.80
41	b	522	DGA	OG1-CA1-CA2	2.48	119.39	111.83
40	C	525	SPH	C3-C4-C5	-2.48	119.55	124.69
45	H	101	RRX	C30-C29-C28	-2.48	108.16	113.59
29	r	303	CLA	C2A-C1A-CHA	2.48	128.16	123.87
30	D	401	PHO	C1-C2-C3	-2.47	122.14	126.20
31	B	517	BCR	C37-C22-C23	2.47	121.87	118.09
29	s	306	CLA	C2A-C1A-CHA	2.47	128.16	123.87
29	D	404	CLA	CAC-C3C-C2C	-2.47	123.02	127.56
48	G	617	NEX	C38-C25-C26	-2.47	118.23	122.30
29	y	305	CLA	C3B-C4B-NB	-2.47	108.32	110.53
34	b	519	C7Z	C35-C15-C14	-2.47	118.46	123.52
29	G	604	CLA	CHD-C1D-ND	-2.47	121.33	124.80
29	r	310	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
29	Y	314	CLA	C3B-C4B-NB	-2.47	108.33	110.53
29	r	309	CLA	C3B-C4B-NB	-2.47	108.33	110.53
29	s	311	CLA	C1-C2-C3	-2.47	122.15	126.20
29	B	503	CLA	C3B-C4B-NB	-2.47	108.33	110.53
46	y	308	CHL	C1-O2A-CGA	2.47	122.62	116.65
43	d	405	PL9	C27-C28-C29	-2.47	121.98	127.62
29	N	612	CLA	C4A-NA-C1A	2.47	107.80	106.68
46	N	606	CHL	CMA-C3A-C4A	2.47	119.92	114.61
29	n	611	CLA	C3B-C4B-NB	-2.47	108.33	110.53
49	R	311	XAT	C7-C8-C9	-2.47	121.70	125.53
45	H	101	RRX	C23-C24-C25	-2.46	120.41	127.00
31	C	517	BCR	C29-C30-C25	2.46	114.02	110.44
46	G	609	CHL	CMA-C3A-C4A	2.46	119.92	114.61
43	D	406	PL9	C22-C23-C24	-2.46	121.99	127.62
47	Y	317	LUT	C36-C21-C26	-2.46	105.82	109.55
34	b	519	C7Z	C7-C6-C5	-2.46	115.89	121.56
48	y	319	NEX	C38-C25-C26	-2.46	118.26	122.30
29	Y	311	CLA	CHA-C1A-NA	-2.46	120.83	126.39
29	d	404	CLA	CHD-C1D-ND	-2.45	121.35	124.80
47	N	616	LUT	C38-C25-C24	-2.45	117.55	123.36
29	A	409	CLA	CHD-C1D-ND	-2.45	121.35	124.80
29	D	405	CLA	CHD-C1D-ND	-2.45	121.35	124.80
29	c	502	CLA	CHD-C1D-ND	-2.45	121.35	124.80
29	C	512	CLA	C4A-NA-C1A	2.45	107.80	106.68
29	G	604	CLA	CHA-C1A-NA	-2.45	120.84	126.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	g	617	NEX	O24-C25-C38	-2.45	112.31	115.05
31	C	517	BCR	C33-C5-C6	-2.45	121.81	124.48
29	b	513	CLA	CHD-C1D-ND	-2.45	121.35	124.80
29	N	603	CLA	CHA-C1A-NA	-2.45	120.84	126.39
29	n	603	CLA	C3B-C4B-NB	-2.45	108.34	110.53
29	r	307	CLA	CHD-C1D-ND	-2.45	121.36	124.80
46	N	608	CHL	CMA-C3A-C4A	2.45	119.89	114.61
29	A	406	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
31	c	515	BCR	C27-C26-C25	-2.45	119.39	122.70
47	R	310	LUT	C26-C27-C28	-2.45	120.77	124.58
29	A	407	CLA	C4A-NA-C1A	2.45	107.80	106.68
34	B	519	C7Z	C7-C6-C5	-2.45	115.92	121.56
31	C	516	BCR	C38-C26-C25	-2.45	121.82	124.48
46	N	606	CHL	C1C-C2C-CMC	2.44	131.21	126.80
46	N	605	CHL	C4C-CHD-C1D	2.44	124.81	116.07
35	i	101	LMG	C8-O7-C10	-2.44	111.95	117.80
47	y	317	LUT	C38-C25-C24	-2.44	117.58	123.36
29	s	314	CLA	C3B-C4B-NB	-2.44	108.35	110.53
29	A	406	CLA	CHD-C1D-ND	-2.44	121.37	124.80
29	Y	311	CLA	CHD-C1D-ND	-2.44	121.37	124.80
29	b	510	CLA	CHD-C1D-ND	-2.44	121.37	124.80
31	f	101	BCR	C33-C5-C6	-2.44	121.82	124.48
29	N	610	CLA	CHA-C1A-NA	-2.44	120.88	126.39
45	h	101	RRX	C2-C1-C6	2.44	113.98	110.44
31	C	515	BCR	C36-C18-C17	-2.43	118.87	122.82
47	S	318	LUT	C38-C25-C24	-2.43	117.60	123.36
29	G	611	CLA	C3B-C2B-C1B	-2.43	104.30	107.17
46	N	607	CHL	C1-O2A-CGA	2.43	122.54	116.65
46	n	601	CHL	C4C-CHD-C1D	2.43	124.77	116.07
29	G	610	CLA	CHD-C1D-ND	-2.43	121.38	124.80
35	C	524	LMG	O8-C28-O10	-2.43	117.55	123.63
29	A	405	CLA	C1-C2-C3	2.43	130.18	126.20
29	B	515	CLA	C3B-C4B-NB	-2.43	108.36	110.53
29	B	503	CLA	C1-C2-C3	-2.43	122.22	126.20
29	s	304	CLA	C2B-C1B-NB	-2.43	107.81	110.33
31	c	514	BCR	C4-C5-C6	-2.43	119.42	122.70
46	S	308	CHL	CMA-C3A-C4A	2.43	119.84	114.61
29	G	614	CLA	CHD-C1D-ND	-2.42	121.39	124.80
29	g	610	CLA	CHA-C1A-NA	-2.42	120.91	126.39
29	R	308	CLA	C3B-C2B-C1B	-2.42	104.31	107.17
29	R	309	CLA	C1-C2-C3	-2.42	122.84	126.76
29	s	306	CLA	C3B-C2B-C1B	-2.42	104.31	107.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	N	615	LUT	C7-C8-C9	-2.42	122.65	126.23
29	g	613	CLA	CHD-C1D-ND	-2.42	121.40	124.80
29	B	510	CLA	CHD-C1D-ND	-2.42	121.40	124.80
29	Y	305	CLA	O2A-CGA-O1A	-2.42	117.58	123.63
47	y	318	LUT	C31-C30-C29	-2.42	123.89	127.28
47	s	318	LUT	C10-C11-C12	-2.42	116.19	123.20
29	C	513	CLA	C4A-NA-C1A	2.42	107.78	106.68
29	C	504	CLA	C3B-C4B-NB	-2.42	108.37	110.53
49	N	619	XAT	C6-C7-C8	-2.42	120.88	125.99
29	c	504	CLA	CHD-C1D-ND	-2.41	121.40	124.80
30	A	408	PHO	C1-C2-C3	-2.41	122.24	126.20
29	c	510	CLA	C1D-ND-C4D	-2.41	104.62	106.31
29	G	603	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
29	g	612	CLA	CHD-C1D-ND	-2.41	121.41	124.80
29	G	603	CLA	CMB-C2B-C1B	2.41	129.09	125.42
46	y	301	CHL	C1-O2A-CGA	2.41	122.48	116.65
29	s	306	CLA	C3B-C4B-NB	-2.41	108.38	110.53
29	g	610	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
29	N	613	CLA	C3B-C4B-NB	-2.41	108.38	110.53
34	B	519	C7Z	C18-C5-C4	2.41	118.84	114.42
46	s	308	CHL	C4C-CHD-C1D	2.41	124.67	116.07
37	y	320	LHG	C6-C5-C4	-2.40	106.18	111.78
29	n	611	CLA	CMB-C2B-C1B	2.40	129.08	125.42
29	y	304	CLA	C3B-C2B-C1B	-2.40	104.34	107.17
46	g	608	CHL	CMA-C3A-C4A	2.40	119.78	114.61
29	Y	313	CLA	CHD-C1D-ND	-2.40	121.42	124.80
46	n	608	CHL	CMA-C3A-C4A	2.40	119.78	114.61
29	r	303	CLA	C3B-C4B-NB	-2.40	108.39	110.53
29	G	610	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
46	g	606	CHL	CMA-C3A-C4A	2.40	119.78	114.61
43	d	405	PL9	O1-C4-C3	-2.40	118.20	120.73
29	c	506	CLA	C3B-C4B-NB	-2.40	108.39	110.53
29	b	514	CLA	C1-C2-C3	-2.40	122.27	126.20
49	N	619	XAT	C19-C9-C10	-2.40	118.93	122.82
29	c	511	CLA	CHA-C1A-NA	-2.40	120.96	126.39
31	C	517	BCR	C35-C13-C12	2.40	121.75	118.09
29	c	510	CLA	CHD-C1D-ND	-2.40	121.43	124.80
29	b	502	CLA	C4A-NA-C1A	2.40	107.77	106.68
47	S	318	LUT	C10-C11-C12	-2.40	116.26	123.20
48	Y	318	NEX	C38-C25-C26	-2.39	118.36	122.30
46	Y	310	CHL	CMA-C3A-C4A	2.39	119.77	114.61
31	c	514	BCR	C33-C5-C6	-2.39	121.87	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	408	CLA	CHD-C1D-ND	-2.39	121.43	124.80
31	b	517	BCR	C1-C6-C5	-2.39	119.36	122.64
36	r	301	DGD	C1E-O6E-C5E	2.39	118.39	113.72
46	g	607	CHL	CMA-C3A-C4A	2.39	119.77	114.61
46	Y	302	CHL	CMA-C3A-C4A	2.39	119.76	114.61
29	g	614	CLA	CHD-C1D-ND	-2.39	121.44	124.80
37	d	406	LHG	C5-O7-C7	-2.39	112.07	117.80
29	R	308	CLA	C3B-C4B-NB	-2.39	108.40	110.53
29	S	311	CLA	CHD-C1D-ND	-2.39	121.44	124.80
29	n	610	CLA	CHD-C1D-ND	-2.39	121.44	124.80
29	N	602	CLA	C4A-NA-C1A	2.39	107.77	106.68
29	g	602	CLA	CHD-C1D-ND	-2.39	121.44	124.80
48	S	319	NEX	C39-C29-C30	-2.39	118.95	122.82
29	b	506	CLA	C3B-C4B-NB	-2.39	108.40	110.53
46	R	304	CHL	CMA-C3A-C4A	2.39	119.75	114.61
46	S	302	CHL	C4C-CHD-C1D	2.39	124.61	116.07
29	r	302	CLA	CHD-C1D-ND	-2.39	121.44	124.80
29	n	613	CLA	CHA-C1A-NA	-2.39	120.99	126.39
31	c	514	BCR	C33-C5-C4	2.39	118.68	113.60
47	y	317	LUT	C31-C30-C29	-2.39	123.93	127.28
29	s	310	CLA	CHD-C1D-ND	-2.38	121.45	124.80
29	b	514	CLA	C3B-C4B-NB	-2.38	108.40	110.53
49	y	302	XAT	C18-C5-C6	-2.38	118.38	122.30
46	g	609	CHL	C1-C2-C3	-2.38	122.29	126.20
47	N	615	LUT	C22-C23-C24	-2.38	107.65	111.18
29	b	515	CLA	C3B-C4B-NB	-2.38	108.40	110.53
31	f	101	BCR	C33-C5-C4	2.38	118.67	113.60
29	b	502	CLA	C3B-C2B-C1B	-2.38	104.36	107.17
31	C	517	BCR	C31-C1-C6	-2.38	106.51	110.24
46	n	607	CHL	CMA-C3A-C4A	2.38	119.74	114.61
46	g	601	CHL	CMA-C3A-C4A	2.38	119.74	114.61
29	r	310	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
46	g	606	CHL	CAA-C2A-C3A	-2.38	106.57	113.00
29	y	312	CLA	CHA-C1A-NA	-2.38	121.01	126.39
29	B	515	CLA	CMB-C2B-C1B	2.38	129.04	125.42
46	s	307	CHL	CMA-C3A-C4A	2.38	119.73	114.61
29	S	311	CLA	C1-C2-C3	-2.37	122.31	126.20
31	b	518	BCR	C23-C22-C21	-2.37	115.28	119.01
29	G	611	CLA	CHD-C1D-ND	-2.37	121.46	124.80
46	N	609	CHL	C1-C2-C3	-2.37	122.31	126.20
29	R	308	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
29	y	316	CLA	C1-C2-C3	-2.37	122.31	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	506	CLA	CHD-C1D-ND	-2.37	121.47	124.80
31	f	101	BCR	C28-C27-C26	-2.37	109.83	114.06
29	C	505	CLA	CHD-C1D-ND	-2.37	121.47	124.80
31	f	101	BCR	C4-C5-C6	-2.37	119.50	122.70
29	y	313	CLA	C3B-C2B-C1B	-2.37	104.38	107.17
31	c	514	BCR	C38-C26-C25	-2.37	121.90	124.48
29	r	302	CLA	C3B-C4B-NB	-2.37	108.42	110.53
37	D	408	LHG	O8-C23-C24	2.37	119.05	111.83
45	H	101	RRX	C23-C22-C21	2.36	122.73	119.01
48	y	319	NEX	C4-C3-C2	2.36	115.21	110.79
49	n	618	XAT	O24-C26-C27	-2.36	110.10	116.88
29	B	501	CLA	CHD-C1D-ND	-2.36	121.47	124.80
29	R	309	CLA	CHD-C1D-ND	-2.36	121.48	124.80
29	c	505	CLA	CHD-C1D-ND	-2.36	121.48	124.80
47	Y	316	LUT	C38-C25-C24	-2.36	117.77	123.36
29	Y	314	CLA	CMB-C2B-C1B	2.36	129.01	125.42
29	r	304	CLA	CHD-C1D-ND	-2.36	121.48	124.80
31	v	101	BCR	C29-C28-C27	2.36	116.47	111.28
50	Y	320	PTY	C6-O7-C8	-2.36	113.68	117.85
29	B	501	CLA	C3B-C4B-NB	-2.36	108.42	110.53
29	y	314	CLA	C3B-C4B-NB	-2.36	108.42	110.53
29	S	316	CLA	C3B-C2B-C1B	-2.36	104.39	107.17
29	S	310	CLA	C3B-C2B-C1B	-2.36	104.39	107.17
31	c	515	BCR	C29-C30-C25	2.36	113.86	110.44
31	C	515	BCR	C38-C26-C25	-2.36	121.91	124.48
29	n	604	CLA	CHA-C1A-NA	-2.36	121.06	126.39
47	g	616	LUT	C27-C28-C29	-2.35	121.26	126.32
29	B	508	CLA	CHD-C1D-ND	-2.35	121.49	124.80
29	C	514	CLA	CHD-C1D-ND	-2.35	121.49	124.80
46	G	601	CHL	C4C-CHD-C1D	2.35	124.48	116.07
46	G	606	CHL	C4C-CHD-C1D	2.35	124.48	116.07
39	l	101	SQD	O3-C3-C2	-2.35	104.83	110.38
48	Y	318	NEX	C16-C1-C6	-2.35	108.37	110.47
48	r	313	NEX	C38-C25-C26	-2.35	118.43	122.30
48	s	319	NEX	C31-C30-C29	2.35	130.57	127.28
29	c	512	CLA	C1-C2-C3	-2.35	122.35	126.20
29	N	602	CLA	C3B-C4B-NB	-2.35	108.43	110.53
49	r	312	XAT	C7-C8-C9	-2.35	121.89	125.53
47	n	615	LUT	C27-C28-C29	-2.35	121.28	126.32
43	d	405	PL9	C40-C39-C41	2.35	119.30	115.23
29	n	602	CLA	C3B-C4B-NB	-2.35	108.44	110.53
31	A	410	BCR	C23-C22-C21	-2.35	115.32	119.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	N	617	NEX	C17-C1-C6	-2.35	108.37	110.47
37	N	618	LHG	C5-O7-C7	-2.35	112.18	117.80
44	E	101	HEM	C4D-ND-C1D	2.35	107.98	105.21
29	C	512	CLA	C3B-C2B-C1B	-2.34	104.41	107.17
47	N	616	LUT	C35-C15-C14	-2.34	118.72	123.52
29	n	612	CLA	C3B-C4B-NB	-2.34	108.44	110.53
29	b	509	CLA	CHD-C1D-ND	-2.34	121.50	124.80
29	N	614	CLA	CHD-C1D-ND	-2.34	121.50	124.80
29	S	305	CLA	CHD-C1D-ND	-2.34	121.50	124.80
48	G	617	NEX	C4-C3-C2	2.34	115.17	110.79
29	Y	303	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
29	B	510	CLA	CMB-C2B-C1B	2.34	128.99	125.42
29	C	508	CLA	CHD-C1D-ND	-2.34	121.51	124.80
31	F	101	BCR	C37-C22-C23	2.34	121.67	118.09
31	B	517	BCR	C1-C6-C7	2.34	122.00	115.65
31	b	517	BCR	C35-C13-C12	2.34	121.66	118.09
31	c	515	BCR	C3-C4-C5	-2.34	109.89	114.06
47	G	615	LUT	C38-C25-C24	-2.34	117.83	123.36
47	r	311	LUT	C37-C21-C26	2.34	113.08	109.55
29	Y	311	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
31	f	101	BCR	C23-C24-C25	-2.33	120.76	127.00
43	D	406	PL9	O1-C4-C3	-2.33	118.27	120.73
29	B	515	CLA	CHD-C1D-ND	-2.33	121.52	124.80
46	G	607	CHL	CMA-C3A-C4A	2.33	119.64	114.61
29	N	602	CLA	CHA-C1A-NA	-2.33	121.11	126.39
31	C	517	BCR	C3-C4-C5	-2.33	109.89	114.06
46	N	606	CHL	C4C-CHD-C1D	2.33	124.42	116.07
29	B	505	CLA	C1-C2-C3	-2.33	122.38	126.20
29	s	303	CLA	CHA-C1A-NA	-2.33	121.11	126.39
29	G	603	CLA	CHA-C1A-NA	-2.33	121.11	126.39
29	S	303	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
29	C	512	CLA	CHD-C1D-ND	-2.33	121.52	124.80
29	a	405	CLA	C1-O2A-CGA	2.33	122.29	116.65
46	g	608	CHL	C3D-C4D-ND	-2.33	109.20	112.94
34	B	519	C7Z	C30-C31-C32	-2.33	116.45	123.20
29	S	306	CLA	CHA-C1A-NA	-2.33	121.12	126.39
31	a	409	BCR	C23-C22-C21	-2.33	115.35	119.01
46	r	305	CHL	CMA-C3A-C4A	2.33	119.62	114.61
29	N	604	CLA	CHD-C1D-ND	-2.33	121.53	124.80
29	R	308	CLA	CHD-C1D-ND	-2.33	121.53	124.80
29	b	501	CLA	CHD-C1D-ND	-2.33	121.53	124.80
47	Y	316	LUT	C11-C10-C9	-2.33	124.02	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	515	BCR	C39-C30-C25	-2.32	106.60	110.24
31	c	515	BCR	C36-C18-C17	-2.32	119.05	122.82
47	r	311	LUT	C37-C21-C22	-2.32	105.08	109.41
29	B	514	CLA	C1-C2-C3	-2.32	122.40	126.20
29	y	310	CLA	CHA-C1A-NA	-2.32	121.14	126.39
29	N	602	CLA	CHD-C1D-ND	-2.32	121.54	124.80
31	c	514	BCR	C31-C1-C6	-2.32	106.61	110.24
46	N	601	CHL	C4C-CHD-C1D	2.31	124.35	116.07
29	N	611	CLA	CMB-C2B-C1B	2.31	128.94	125.42
46	N	609	CHL	C4C-CHD-C1D	2.31	124.35	116.07
29	b	509	CLA	C1-C2-C3	-2.31	122.41	126.20
45	H	101	RRX	C15-C16-C17	-2.31	118.79	123.52
29	B	501	CLA	CHA-C1A-NA	-2.31	121.15	126.39
49	n	618	XAT	C19-C9-C10	-2.31	119.07	122.82
37	s	320	LHG	C5-O7-C7	-2.31	112.26	117.80
29	B	516	CLA	C3B-C2B-C1B	-2.31	104.44	107.17
29	n	603	CLA	CHA-C1A-NA	-2.31	121.16	126.39
29	Y	313	CLA	C3B-C2B-C1B	-2.31	104.45	107.17
29	B	510	CLA	C3B-C4B-NB	-2.31	108.47	110.53
29	Y	305	CLA	CHA-C1A-NA	-2.31	121.16	126.39
43	D	406	PL9	O2-C1-C6	2.31	124.15	120.48
29	y	306	CLA	CHA-C1A-NA	-2.31	121.17	126.39
29	B	513	CLA	CHD-C1D-ND	-2.31	121.56	124.80
47	N	615	LUT	C30-C31-C32	-2.31	116.52	123.20
29	Y	315	CLA	CHD-C1D-ND	-2.31	121.56	124.80
46	G	606	CHL	CMA-C3A-C4A	2.31	119.58	114.61
29	S	304	CLA	C1-C2-C3	-2.31	122.42	126.20
48	y	319	NEX	O24-C25-C38	-2.31	112.47	115.05
29	s	314	CLA	O2A-CGA-O1A	-2.30	117.86	123.63
29	S	313	CLA	CHD-C1D-ND	-2.30	121.56	124.80
29	y	314	CLA	CHD-C1D-ND	-2.30	121.56	124.80
30	a	407	PHO	C1-C2-C3	-2.30	122.43	126.20
47	n	614	LUT	C19-C9-C8	2.30	121.60	118.09
49	g	619	XAT	C18-C5-C6	-2.30	118.52	122.30
48	n	616	NEX	O24-C25-C38	-2.30	112.48	115.05
29	B	502	CLA	C3B-C2B-C1B	-2.30	104.46	107.17
29	y	304	CLA	CHD-C1D-ND	-2.30	121.57	124.80
29	b	511	CLA	C3B-C4B-NB	-2.30	108.48	110.53
46	G	605	CHL	C1-O2A-CGA	2.30	123.20	116.67
29	S	312	CLA	CHD-C1D-ND	-2.30	121.57	124.80
29	g	603	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
29	N	610	CLA	CHD-C1D-ND	-2.30	121.57	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	N	619	XAT	O4-C6-C7	-2.30	110.30	116.88
29	R	309	CLA	C3B-C2B-C1B	-2.30	104.46	107.17
29	S	304	CLA	CHA-C1A-NA	-2.30	121.19	126.39
31	K	101	BCR	C37-C22-C23	2.29	121.59	118.09
29	c	507	CLA	CHA-C1A-NA	-2.29	121.20	126.39
29	B	507	CLA	CHA-C1A-NA	-2.29	121.20	126.39
46	n	605	CHL	C1-C2-C3	-2.29	122.44	126.20
39	C	523	SQD	O3-C3-C2	-2.29	104.97	110.38
29	B	508	CLA	C3B-C2B-C1B	-2.29	104.47	107.17
47	n	614	LUT	C26-C27-C28	-2.29	121.01	124.58
29	b	511	CLA	C3C-C4C-NC	-2.29	107.49	110.43
47	y	317	LUT	C39-C29-C28	2.29	121.59	118.09
49	N	619	XAT	O24-C26-C27	-2.29	110.31	116.88
46	y	311	CHL	C1-C2-C3	-2.29	122.44	126.20
31	c	514	BCR	C34-C9-C8	2.29	121.59	118.09
29	c	513	CLA	CHD-C1D-ND	-2.29	121.58	124.80
46	Y	308	CHL	C4C-CHD-C1D	2.29	124.26	116.07
48	R	312	NEX	C20-C13-C12	2.29	119.86	114.59
29	g	610	CLA	CHD-C1D-ND	-2.29	121.58	124.80
29	r	308	CLA	CHA-C1A-NA	-2.29	121.21	126.39
48	S	319	NEX	C20-C13-C14	-2.29	119.11	122.82
29	Y	309	CLA	C3B-C4B-NB	-2.29	108.49	110.53
39	b	523	SQD	O3-C3-C2	-2.29	104.98	110.38
47	n	614	LUT	C38-C25-C24	-2.29	117.95	123.36
46	G	608	CHL	CMA-C3A-C4A	2.29	119.54	114.61
29	c	506	CLA	CHD-C1D-ND	-2.29	121.59	124.80
29	b	515	CLA	CMB-C2B-C1B	2.29	128.90	125.42
31	z	101	BCR	C35-C13-C12	2.28	121.58	118.09
29	b	515	CLA	CHD-C1D-ND	-2.28	121.59	124.80
29	y	306	CLA	CHD-C1D-ND	-2.28	121.59	124.80
36	c	517	DGD	O1G-C1A-O1A	-2.28	117.92	123.63
47	Y	316	LUT	C15-C35-C34	-2.28	118.85	123.52
31	v	101	BCR	C34-C9-C10	-2.28	119.12	122.82
47	s	317	LUT	C38-C25-C24	-2.28	117.96	123.36
46	S	308	CHL	C4C-CHD-C1D	2.28	124.23	116.07
47	g	615	LUT	C22-C23-C24	-2.28	107.80	111.18
48	n	616	NEX	C40-C33-C34	-2.28	119.12	122.82
31	K	101	BCR	C34-C9-C10	-2.28	119.12	122.82
46	g	601	CHL	C4C-CHD-C1D	2.28	124.22	116.07
29	G	612	CLA	CHD-C1D-ND	-2.28	121.59	124.80
46	y	301	CHL	C4C-CHD-C1D	2.28	124.22	116.07
29	G	610	CLA	C3B-C4B-NB	-2.28	108.50	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	n	608	CHL	C4C-CHD-C1D	2.28	124.22	116.07
29	c	507	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
29	b	514	CLA	C3B-C2B-C1B	-2.28	104.48	107.17
46	G	608	CHL	C4C-CHD-C1D	2.28	124.22	116.07
29	C	503	CLA	CHD-C1D-ND	-2.28	121.60	124.80
29	Y	315	CLA	C1-C2-C3	-2.28	122.47	126.20
29	B	509	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
46	R	304	CHL	C4C-CHD-C1D	2.28	124.22	116.07
47	r	311	LUT	C18-C5-C6	-2.28	122.00	124.48
47	R	310	LUT	C30-C31-C32	-2.28	116.61	123.20
29	b	510	CLA	C3B-C4B-NB	-2.28	108.50	110.53
31	b	518	BCR	C33-C5-C4	2.27	118.45	113.60
29	D	404	CLA	C17-C16-C15	-2.27	103.09	113.28
29	B	501	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
29	r	307	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
46	g	606	CHL	C4C-CHD-C1D	2.27	124.20	116.07
49	g	619	XAT	C19-C9-C10	-2.27	119.13	122.82
29	N	614	CLA	C3B-C2B-C1B	-2.27	104.49	107.17
49	G	619	XAT	O24-C25-C38	-2.27	112.51	115.05
29	n	604	CLA	CHD-C1D-ND	-2.27	121.60	124.80
31	K	101	BCR	C12-C13-C14	-2.27	115.44	119.01
29	Y	309	CLA	CHA-C1A-NA	-2.27	121.25	126.39
29	C	513	CLA	C1-C2-C3	-2.27	122.48	126.20
46	S	309	CHL	CMA-C3A-C4A	2.27	119.50	114.61
46	Y	308	CHL	CMA-C3A-C4A	2.27	119.50	114.61
29	B	514	CLA	C3B-C2B-C1B	-2.27	104.49	107.17
48	Y	318	NEX	O24-C25-C38	-2.27	112.51	115.05
47	N	615	LUT	C19-C9-C8	2.27	121.55	118.09
46	y	311	CHL	C1C-C2C-CMC	2.27	130.89	126.80
39	L	102	SQD	O3-C3-C2	-2.27	105.04	110.38
29	N	612	CLA	CHD-C1D-ND	-2.26	121.61	124.80
29	s	316	CLA	C2A-C1A-CHA	2.26	127.80	123.87
46	y	311	CHL	CMA-C3A-C4A	2.26	119.49	114.61
35	c	519	LMG	C8-O7-C10	-2.26	112.38	117.80
47	s	317	LUT	C22-C23-C24	-2.26	107.82	111.18
29	B	504	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
31	v	101	BCR	C33-C5-C4	2.26	118.42	113.60
46	s	302	CHL	CMA-C3A-C4A	2.26	119.48	114.61
29	c	508	CLA	C3C-C4C-NC	-2.26	107.54	110.43
29	D	404	CLA	CHA-C4D-ND	-2.26	127.89	132.55
29	Y	304	CLA	C1-C2-C3	-2.26	122.50	126.20
48	N	617	NEX	O24-C25-C38	-2.26	112.53	115.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	f	101	BCR	C38-C26-C25	-2.26	122.02	124.48
46	s	309	CHL	CMA-C3A-C4A	2.26	119.47	114.61
29	c	510	CLA	C1-C2-C3	-2.26	122.50	126.20
29	a	405	CLA	C4A-NA-C1A	2.26	107.71	106.68
31	F	101	BCR	C36-C18-C17	-2.26	119.16	122.82
29	s	306	CLA	CHD-C1D-ND	-2.26	121.63	124.80
47	Y	317	LUT	C35-C15-C14	-2.25	118.91	123.52
29	y	312	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
29	s	306	CLA	C3C-C4C-NC	-2.25	107.54	110.43
45	h	101	RRX	C11-C12-C13	-2.25	120.19	126.36
46	S	309	CHL	C3D-C4D-ND	-2.25	109.33	112.94
29	S	303	CLA	C1-C2-C3	-2.25	122.51	126.20
29	n	603	CLA	CHD-C1D-ND	-2.25	121.64	124.80
29	b	509	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
46	N	601	CHL	CMA-C3A-C4A	2.25	119.46	114.61
46	Y	306	CHL	C4C-CHD-C1D	2.25	124.12	116.07
46	r	305	CHL	C4C-CHD-C1D	2.25	124.12	116.07
29	B	511	CLA	CHD-C1D-ND	-2.25	121.64	124.80
29	N	602	CLA	C1-C2-C3	-2.25	122.51	126.20
29	b	512	CLA	C3B-C4B-NB	-2.25	108.53	110.53
29	b	505	CLA	C1-C2-C3	-2.25	122.52	126.20
35	C	524	LMG	O1-C1-C2	2.25	111.68	108.27
29	B	503	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
43	d	405	PL9	C37-C38-C39	-2.24	122.49	127.62
29	y	310	CLA	C3B-C2B-C1B	-2.24	104.52	107.17
29	N	614	CLA	CHA-C1A-NA	-2.24	121.31	126.39
29	S	311	CLA	C3B-C2B-C1B	-2.24	104.53	107.17
46	y	309	CHL	C4C-CHD-C1D	2.24	124.09	116.07
29	R	301	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
47	g	615	LUT	C39-C29-C28	2.24	121.51	118.09
45	h	101	RRX	C35-C13-C14	-2.24	119.19	122.82
46	n	605	CHL	C4C-CHD-C1D	2.24	124.08	116.07
29	B	514	CLA	C3B-C4B-NB	-2.24	108.53	110.53
47	n	615	LUT	C31-C30-C29	-2.24	124.14	127.28
48	S	319	NEX	C16-C1-C6	-2.24	108.47	110.47
29	S	314	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
29	a	405	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
29	c	502	CLA	C1-C2-C3	-2.24	122.53	126.20
29	Y	312	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
45	h	101	RRX	C7-C8-C9	-2.23	122.93	126.23
46	y	307	CHL	C4C-CHD-C1D	2.23	124.05	116.07
29	r	303	CLA	O2A-CGA-O1A	-2.23	118.05	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s	316	CLA	C1-C2-C3	-2.23	123.15	126.76
29	b	506	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
39	c	522	SQD	O3-C3-C2	-2.23	105.12	110.38
29	S	311	CLA	C3B-C4B-NB	-2.23	108.54	110.53
48	r	313	NEX	C20-C13-C12	2.23	119.71	114.59
29	n	610	CLA	CHA-C1A-NA	-2.23	121.35	126.39
46	y	303	CHL	CMA-C3A-C4A	2.22	119.40	114.61
29	y	304	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
31	K	101	BCR	C29-C28-C27	2.22	116.16	111.28
39	o	301	SQD	O3-C3-C2	-2.22	105.14	110.38
29	R	307	CLA	C3B-C4B-NB	-2.22	108.55	110.53
47	S	318	LUT	C22-C23-C24	-2.22	107.88	111.18
47	g	616	LUT	C35-C15-C14	-2.22	118.97	123.52
29	S	304	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
46	g	605	CHL	CMA-C3A-C4A	2.22	119.40	114.61
47	y	317	LUT	C11-C10-C9	-2.22	124.16	127.28
29	r	302	CLA	CHA-C1A-NA	-2.22	121.36	126.39
47	Y	317	LUT	C27-C28-C29	-2.22	121.56	126.32
43	d	405	PL9	O2-C1-C6	2.22	124.01	120.48
29	b	509	CLA	C3B-C4B-NB	-2.22	108.55	110.53
29	S	304	CLA	C2D-C1D-ND	-2.22	107.93	110.13
29	D	405	CLA	C1C-C2C-C3C	-2.22	104.65	106.98
46	r	306	CHL	CMA-C3A-C4A	2.22	119.39	114.61
29	Y	314	CLA	CHD-C1D-ND	-2.22	121.68	124.80
29	C	509	CLA	C3B-C4B-NB	-2.22	108.55	110.53
49	G	619	XAT	C18-C5-C6	-2.22	118.66	122.30
39	M	101	SQD	O3-C3-C2	-2.21	105.16	110.38
31	B	517	BCR	C23-C22-C21	-2.21	115.53	119.01
45	h	101	RRX	C30-C29-C28	-2.21	108.74	113.59
29	r	309	CLA	C3C-C4C-NC	-2.21	107.60	110.43
46	s	308	CHL	CMA-C3A-C4A	2.21	119.38	114.61
29	g	603	CLA	CHD-C1D-ND	-2.21	121.69	124.80
46	s	302	CHL	C4C-CHD-C1D	2.21	123.98	116.07
29	Y	312	CLA	CHA-C1A-NA	-2.21	121.39	126.39
46	n	601	CHL	CMA-C3A-C4A	2.21	119.37	114.61
46	g	609	CHL	CMA-C3A-C4A	2.21	119.37	114.61
39	a	410	SQD	O3-C3-C2	-2.21	105.17	110.38
29	C	502	CLA	CHD-C1D-ND	-2.21	121.70	124.80
37	D	407	LHG	O8-C23-C24	2.21	118.56	111.83
46	S	302	CHL	C1C-C2C-CMC	2.21	130.78	126.80
47	g	615	LUT	C38-C25-C24	-2.21	118.14	123.36
29	S	310	CLA	C3B-C4B-NB	-2.21	108.56	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	517	BCR	C37-C22-C23	2.21	121.46	118.09
29	B	513	CLA	C3B-C4B-NB	-2.20	108.56	110.53
47	n	615	LUT	C35-C15-C14	-2.20	119.01	123.52
29	s	315	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
37	S	320	LHG	C5-O7-C7	-2.20	112.52	117.80
37	n	617	LHG	C6-C5-C4	-2.20	106.65	111.78
48	S	319	NEX	C19-C9-C10	-2.20	119.25	122.82
29	Y	303	CLA	C3B-C4B-NB	-2.20	108.56	110.53
29	b	508	CLA	C3B-C2B-C1B	-2.20	104.57	107.17
46	N	607	CHL	C4C-CHD-C1D	2.20	123.94	116.07
43	d	405	PL9	C20-C19-C21	2.20	119.05	115.23
29	s	311	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
49	n	618	XAT	C18-C5-C6	-2.20	118.68	122.30
29	n	602	CLA	CHA-C1A-NA	-2.20	121.41	126.39
29	y	314	CLA	C3B-C2B-C1B	-2.20	104.58	107.17
37	G	618	LHG	C5-O7-C7	-2.20	112.53	117.80
29	s	312	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
46	Y	306	CHL	CMA-C3A-C4A	2.20	119.35	114.61
47	s	318	LUT	C38-C25-C24	-2.20	118.16	123.36
29	b	501	CLA	CHA-C1A-NA	-2.20	121.42	126.39
29	n	604	CLA	C1-C2-C3	-2.20	122.60	126.20
29	s	312	CLA	CHA-C1A-NA	-2.20	121.42	126.39
39	C	501	SQD	O3-C3-C2	-2.19	105.20	110.38
43	D	406	PL9	C37-C38-C39	-2.19	122.61	127.62
35	W	201	LMG	O7-C10-O9	-2.19	118.58	123.70
49	r	312	XAT	O24-C25-C24	2.19	115.54	113.49
34	b	519	C7Z	C30-C31-C32	-2.19	116.85	123.20
37	N	618	LHG	C6-C5-C4	-2.19	106.68	111.78
46	Y	307	CHL	C4C-CHD-C1D	2.19	123.90	116.07
29	G	602	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
46	G	605	CHL	C1A-CHA-C4D	2.19	122.63	118.98
29	a	408	CLA	CHA-C1A-NA	-2.19	121.44	126.39
29	s	310	CLA	CHA-C1A-NA	-2.19	121.44	126.39
29	b	506	CLA	CHD-C1D-ND	-2.19	121.73	124.80
29	c	501	CLA	CHD-C1D-ND	-2.19	121.73	124.80
29	B	506	CLA	C1-C2-C3	-2.19	122.62	126.20
45	h	101	RRX	C15-C16-C17	-2.19	119.05	123.52
49	G	619	XAT	C26-C27-C28	-2.19	121.37	125.99
29	B	509	CLA	C3B-C4B-NB	-2.18	108.58	110.53
29	B	506	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
46	y	311	CHL	C4C-CHD-C1D	2.18	123.88	116.07
29	C	503	CLA	C3B-C2B-C1B	-2.18	104.60	107.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y	313	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
29	a	405	CLA	CHA-C1A-NA	-2.18	121.45	126.39
46	G	607	CHL	C4C-CHD-C1D	2.18	123.87	116.07
46	S	307	CHL	C4C-CHD-C1D	2.18	123.87	116.07
29	N	604	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
29	r	307	CLA	CHA-C1A-NA	-2.18	121.45	126.39
46	s	307	CHL	C4C-CHD-C1D	2.18	123.86	116.07
31	z	101	BCR	C19-C18-C17	2.18	122.44	119.01
29	y	313	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
29	C	512	CLA	C1-C2-C3	-2.18	122.63	126.20
45	H	101	RRX	C35-C13-C14	-2.18	119.29	122.82
29	g	614	CLA	CHA-C1A-NA	-2.18	121.46	126.39
49	Y	301	XAT	C26-C27-C28	-2.18	121.39	125.99
48	S	319	NEX	C4-C3-C2	2.18	114.86	110.79
29	s	303	CLA	C3B-C4B-NB	-2.18	108.59	110.53
48	n	616	NEX	C19-C9-C10	-2.17	119.29	122.82
31	C	516	BCR	C37-C22-C23	2.17	121.41	118.09
39	m	101	SQD	O3-C3-C2	-2.17	105.25	110.38
47	Y	316	LUT	C19-C9-C8	2.17	121.41	118.09
29	S	306	CLA	C3B-C4B-NB	-2.17	108.59	110.53
47	N	616	LUT	C26-C27-C28	-2.17	121.20	124.58
31	B	517	BCR	C34-C9-C8	2.17	121.40	118.09
29	N	613	CLA	CMB-C2B-C1B	2.17	128.72	125.42
47	S	318	LUT	C39-C29-C28	2.17	121.40	118.09
49	g	619	XAT	C26-C27-C28	-2.17	121.41	125.99
29	n	602	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
49	Y	301	XAT	O24-C25-C24	2.16	115.52	113.49
50	y	321	PTY	C6-O7-C8	-2.16	114.02	117.85
29	b	503	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
29	g	613	CLA	C3B-C4B-NB	-2.16	108.60	110.53
46	N	606	CHL	CMD-C2D-C3D	2.16	129.00	124.68
29	N	610	CLA	C3B-C4B-NB	-2.16	108.60	110.53
47	R	310	LUT	C1-C6-C7	2.16	121.51	115.65
29	N	604	CLA	CHA-C1A-NA	-2.16	121.50	126.39
29	c	505	CLA	C3B-C2B-C1B	-2.16	104.62	107.17
29	n	609	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
47	g	615	LUT	C15-C35-C34	-2.16	119.10	123.52
29	B	516	CLA	CHD-C1D-ND	-2.16	121.77	124.80
29	B	510	CLA	C2B-C1B-NB	-2.16	108.09	110.33
47	S	317	LUT	C40-C33-C32	2.16	121.38	118.09
47	y	317	LUT	C15-C35-C34	-2.16	119.11	123.52
29	C	506	CLA	C3B-C2B-C1B	-2.16	104.63	107.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	404	CLA	CHB-C1B-C2B	-2.15	121.17	127.43
47	r	311	LUT	C38-C25-C24	-2.15	118.26	123.36
29	S	312	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
29	G	612	CLA	CHA-C1A-NA	-2.15	121.52	126.39
29	n	611	CLA	CHA-C1A-NA	-2.15	121.52	126.39
29	D	404	CLA	C4-C3-C5	2.15	118.96	115.23
29	R	301	CLA	CHD-C1D-ND	-2.15	121.78	124.80
29	C	509	CLA	C3C-C4C-NC	-2.15	107.67	110.43
47	g	616	LUT	C38-C25-C24	-2.15	118.27	123.36
29	B	504	CLA	CAA-C2A-C3A	-2.15	107.20	113.00
29	A	407	CLA	C3B-C2B-C1B	-2.15	104.64	107.17
29	y	312	CLA	C3B-C4B-NB	-2.15	108.61	110.53
29	b	506	CLA	C1-C2-C3	-2.15	122.68	126.20
29	G	603	CLA	CHD-C1D-ND	-2.15	121.78	124.80
29	b	501	CLA	C3B-C4B-NB	-2.15	108.61	110.53
29	g	611	CLA	C2B-C1B-NB	-2.14	108.10	110.33
29	S	315	CLA	C3B-C4B-NB	-2.14	108.62	110.53
48	S	319	NEX	C26-C27-C28	-2.14	121.46	125.99
39	l	101	SQD	O6-C1-C2	-2.14	105.02	108.27
29	R	301	CLA	CHA-C1A-NA	-2.14	121.54	126.39
36	r	301	DGD	O2G-C1B-O1B	-2.14	118.70	123.70
29	C	508	CLA	CHA-C1A-NA	-2.14	121.54	126.39
46	g	605	CHL	C1-O2A-CGA	2.14	122.75	116.67
29	s	304	CLA	C1-C2-C3	-2.14	122.69	126.20
46	S	307	CHL	CMD-C2D-C3D	2.14	128.96	124.68
46	n	607	CHL	C3D-C4D-ND	-2.14	109.51	112.94
29	S	303	CLA	C3B-C2B-C1B	-2.14	104.65	107.17
29	b	504	CLA	CBA-CAA-C2A	2.14	120.16	113.79
29	b	515	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
49	R	311	XAT	C27-C28-C29	2.14	128.85	125.53
43	D	406	PL9	C40-C39-C41	2.14	118.94	115.23
48	s	319	NEX	C20-C13-C14	-2.14	119.35	122.82
29	B	504	CLA	CMB-C2B-C1B	2.14	128.67	125.42
29	s	311	CLA	CHA-C1A-NA	-2.14	121.56	126.39
29	S	314	CLA	C3B-C4B-NB	-2.14	108.62	110.53
29	s	304	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
29	R	307	CLA	CHD-C1D-C2D	2.13	129.92	125.49
29	d	404	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
47	G	615	LUT	C39-C29-C28	2.13	121.34	118.09
29	G	604	CLA	C3B-C2B-C1B	-2.13	104.66	107.17
46	G	601	CHL	CMA-C3A-C4A	2.13	119.20	114.61
46	G	606	CHL	CMD-C2D-C3D	2.13	128.94	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	517	BCR	C33-C5-C4	2.13	118.14	113.60
29	y	304	CLA	C3B-C4B-NB	-2.13	108.63	110.53
35	W	203	LMG	O7-C10-O9	-2.13	118.73	123.70
29	D	405	CLA	C1-C2-C3	-2.13	122.71	126.20
46	N	609	CHL	C3D-C4D-ND	-2.13	109.52	112.94
34	B	519	C7Z	C21-C26-C25	-2.13	119.73	122.64
31	C	517	BCR	C36-C18-C17	-2.13	119.37	122.82
29	c	511	CLA	C3B-C2B-C1B	-2.13	104.66	107.17
29	c	508	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
48	Y	318	NEX	C20-C13-C14	-2.13	119.37	122.82
29	c	506	CLA	C2D-C1D-ND	-2.13	108.02	110.13
49	R	311	XAT	O4-C5-C18	-2.13	112.67	115.05
29	g	602	CLA	C3B-C4B-NB	-2.13	108.63	110.53
29	G	611	CLA	CHA-C1A-NA	-2.13	121.58	126.39
47	S	318	LUT	C16-C1-C6	-2.13	106.91	110.24
29	B	504	CLA	C4-C3-C5	2.12	118.92	115.23
29	y	314	CLA	C1-C2-C3	-2.12	122.72	126.20
46	S	308	CHL	CMD-C2D-C3D	2.12	128.93	124.68
48	N	617	NEX	C19-C9-C10	-2.12	119.38	122.82
46	G	609	CHL	C4C-CHD-C1D	2.12	123.66	116.07
48	g	617	NEX	C20-C13-C14	-2.12	119.38	122.82
36	B	521	DGD	O2G-C1B-O1B	-2.12	118.74	123.70
29	D	404	CLA	C6-C7-C8	2.12	123.02	115.97
29	g	614	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
46	Y	310	CHL	C4C-CHD-C1D	2.12	123.65	116.07
46	s	308	CHL	C1C-C2C-CMC	2.12	130.62	126.80
29	b	503	CLA	C1-C2-C3	-2.12	122.73	126.20
29	c	501	CLA	C3B-C4B-NB	-2.12	108.64	110.53
34	b	519	C7Z	C4-C5-C6	-2.12	116.41	120.76
47	G	615	LUT	C31-C30-C29	-2.12	124.31	127.28
48	R	312	NEX	C38-C25-C26	-2.12	118.82	122.30
47	Y	316	LUT	C39-C29-C28	2.12	121.32	118.09
46	y	307	CHL	CMA-C3A-C4A	2.11	119.17	114.61
29	S	315	CLA	C1-C2-C3	-2.11	123.34	126.76
29	d	404	CLA	C1C-C2C-C3C	-2.11	104.76	106.98
47	Y	316	LUT	C20-C13-C12	2.11	121.32	118.09
29	R	307	CLA	C2D-C1D-ND	-2.11	108.03	110.13
29	c	510	CLA	C2D-C1D-ND	-2.11	108.03	110.13
46	y	309	CHL	C3D-C4D-ND	-2.11	109.55	112.94
29	r	302	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
46	g	601	CHL	C1-O2A-CGA	2.11	121.76	116.65
46	n	606	CHL	CMA-C3A-C4A	2.11	119.16	114.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	h	101	RRX	C34-C9-C10	-2.11	119.39	122.82
46	n	607	CHL	CMD-C2D-C3D	2.11	128.90	124.68
29	A	407	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
29	c	506	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
46	Y	308	CHL	CMD-C2D-C3D	2.11	128.90	124.68
29	b	516	CLA	CHD-C1D-ND	-2.11	121.83	124.80
46	R	305	CHL	CMD-C2D-C3D	2.11	128.90	124.68
34	b	519	C7Z	C21-C26-C25	-2.11	119.75	122.64
29	R	302	CLA	C1-C2-C3	-2.11	122.74	126.20
29	d	404	CLA	CHA-C1A-NA	-2.11	121.61	126.39
45	h	101	RRX	C23-C22-C21	2.11	122.33	119.01
29	g	603	CLA	CHA-C1A-NA	-2.11	121.62	126.39
29	n	610	CLA	C3B-C4B-NB	-2.11	108.65	110.53
29	S	315	CLA	C3B-C2B-C1B	-2.11	104.69	107.17
29	N	611	CLA	CHA-C1A-NA	-2.11	121.62	126.39
46	s	309	CHL	CMD-C2D-C3D	2.11	128.89	124.68
29	b	516	CLA	CHA-C1A-NA	-2.11	121.62	126.39
46	N	606	CHL	C1-O2A-CGA	2.11	121.75	116.65
29	y	315	CLA	CMB-C2B-C1B	2.11	128.62	125.42
46	g	609	CHL	C4C-CHD-C1D	2.11	123.60	116.07
47	s	317	LUT	C40-C33-C32	2.11	121.30	118.09
47	y	317	LUT	C30-C31-C32	-2.10	117.10	123.20
29	Y	312	CLA	C1-C2-C3	-2.10	122.75	126.20
49	R	311	XAT	C24-C23-C22	-2.10	106.85	110.79
29	N	602	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
34	B	519	C7Z	C36-C21-C26	-2.10	106.94	110.24
46	s	307	CHL	CMD-C2D-C3D	2.10	128.89	124.68
29	Y	305	CLA	CHD-C1D-ND	-2.10	121.84	124.80
34	B	519	C7Z	C15-C35-C34	-2.10	119.22	123.52
46	s	308	CHL	CMD-C2D-C3D	2.10	128.88	124.68
29	Y	311	CLA	C1-C2-C3	-2.10	122.75	126.20
29	S	316	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
29	c	501	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
48	N	617	NEX	C40-C33-C34	-2.10	119.41	122.82
29	B	515	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
29	N	614	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
46	g	608	CHL	CMD-C2D-C3D	2.10	128.88	124.68
30	d	402	PHO	O2A-CGA-O1A	-2.10	118.38	123.63
29	y	313	CLA	CHA-C1A-NA	-2.10	121.64	126.39
47	n	614	LUT	C22-C23-C24	-2.10	108.07	111.18
36	C	519	DGD	O1G-C1A-O1A	-2.10	118.38	123.63
29	b	502	CLA	O2A-CGA-O1A	-2.10	118.39	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	512	CLA	C3B-C4B-NB	-2.10	108.66	110.53
46	y	309	CHL	CMD-C2D-C3D	2.10	128.87	124.68
43	D	406	PL9	O2-C1-C2	-2.09	117.07	121.83
46	y	308	CHL	CMD-C2D-C3D	2.09	128.87	124.68
46	g	605	CHL	C1A-CHA-C4D	2.09	122.48	118.98
29	n	609	CLA	C2A-C1A-CHA	2.09	127.50	123.87
29	N	602	CLA	C3B-C2B-C1B	-2.09	104.70	107.17
46	g	607	CHL	CMD-C2D-C3D	2.09	128.87	124.68
46	s	302	CHL	C1C-C2C-CMC	2.09	130.57	126.80
46	G	608	CHL	CMD-C2D-C3D	2.09	128.86	124.68
29	N	612	CLA	CHA-C1A-NA	-2.09	121.66	126.39
29	G	614	CLA	C3B-C4B-NB	-2.09	108.66	110.53
29	Y	315	CLA	C3B-C2B-C1B	-2.09	104.70	107.17
29	A	406	CLA	C3B-C4B-NB	-2.09	108.66	110.53
47	s	318	LUT	C39-C29-C28	2.09	121.28	118.09
29	G	613	CLA	CHD-C1D-ND	-2.09	121.86	124.80
46	G	608	CHL	C3D-C4D-ND	-2.09	109.59	112.94
29	d	404	CLA	C1-C2-C3	-2.09	122.77	126.20
29	R	301	CLA	C3B-C4B-NB	-2.09	108.67	110.53
29	c	508	CLA	C3B-C4B-NB	-2.09	108.67	110.53
34	b	519	C7Z	C36-C21-C26	-2.09	106.97	110.24
29	c	502	CLA	C3B-C2B-C1B	-2.09	104.71	107.17
35	B	520	LMG	O7-C8-C9	2.09	115.84	108.34
29	A	407	CLA	C3B-C4B-NB	-2.09	108.67	110.53
29	Y	312	CLA	C1C-C2C-C3C	-2.09	104.79	106.98
47	y	318	LUT	C36-C21-C26	-2.09	106.39	109.55
47	s	317	LUT	C28-C29-C30	-2.09	115.73	119.01
29	b	511	CLA	CHD-C1D-ND	-2.09	121.87	124.80
29	c	512	CLA	CHD-C1D-ND	-2.09	121.87	124.80
31	c	515	BCR	C34-C9-C10	-2.09	119.44	122.82
46	R	304	CHL	CMD-C2D-C3D	2.08	128.85	124.68
29	y	316	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
29	b	509	CLA	C3B-C2B-C1B	-2.08	104.71	107.17
29	b	507	CLA	C3B-C4B-NB	-2.08	108.67	110.53
36	B	521	DGD	O6E-C5E-C4E	2.08	113.45	109.70
46	S	309	CHL	C4C-CHD-C1D	2.08	123.52	116.07
38	B	524	LMT	C1'-O5'-C5'	-2.08	109.65	113.72
29	b	513	CLA	C3B-C4B-NB	-2.08	108.67	110.53
29	s	313	CLA	C3B-C4B-NB	-2.08	108.67	110.53
29	y	315	CLA	CHD-C1D-ND	-2.08	121.87	124.80
35	C	521	LMG	O7-C10-O9	-2.08	118.84	123.70
29	A	405	CLA	CHD-C1D-ND	-2.08	121.87	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G	602	CLA	C3B-C4B-NB	-2.08	108.67	110.53
29	C	507	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
29	C	502	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
29	A	407	CLA	CHA-C1A-NA	-2.08	121.68	126.39
46	n	606	CHL	CMD-C2D-C3D	2.08	128.84	124.68
37	g	618	LHG	C6-C5-C4	-2.08	106.94	111.78
46	y	307	CHL	CMD-C2D-C3D	2.08	128.84	124.68
49	r	312	XAT	O4-C5-C18	-2.08	112.73	115.05
29	R	307	CLA	C3B-C2B-C1B	-2.08	104.72	107.17
48	y	319	NEX	C20-C13-C14	-2.08	119.45	122.82
46	y	308	CHL	C3D-C4D-ND	-2.08	109.61	112.94
31	v	101	BCR	C38-C26-C25	-2.08	122.22	124.48
29	c	501	CLA	CMB-C2B-C1B	2.08	128.58	125.42
29	y	305	CLA	C1C-C2C-C3C	-2.08	104.80	106.98
46	y	311	CHL	CMD-C2D-C3D	2.08	128.83	124.68
29	n	602	CLA	C3B-C2B-C1B	-2.08	104.72	107.17
46	N	608	CHL	CMD-C2D-C3D	2.08	128.83	124.68
29	S	313	CLA	C3B-C4B-NB	-2.08	108.68	110.53
43	d	405	PL9	O2-C1-C2	-2.08	117.11	121.83
44	e	101	HEM	C1B-NB-C4B	2.08	107.67	105.21
29	b	510	CLA	CMB-C2B-C1B	2.07	128.58	125.42
29	b	501	CLA	C1-C2-C3	-2.07	122.80	126.20
29	S	313	CLA	O2A-CGA-O1A	-2.07	118.00	123.33
47	N	615	LUT	C39-C29-C28	2.07	121.26	118.09
29	a	406	CLA	C3B-C4B-NB	-2.07	108.68	110.53
29	N	613	CLA	CHD-C1D-ND	-2.07	121.89	124.80
29	c	510	CLA	CHA-C1A-NA	-2.07	121.70	126.39
29	g	612	CLA	C3B-C4B-NB	-2.07	108.68	110.53
30	A	408	PHO	C3B-C4B-NB	-2.07	106.11	107.46
29	C	509	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
47	N	615	LUT	C20-C13-C12	2.07	121.25	118.09
46	N	609	CHL	CMD-C2D-C3D	2.07	128.82	124.68
46	s	302	CHL	CMD-C2D-C3D	2.07	128.82	124.68
29	C	511	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
46	r	305	CHL	CMD-C2D-C3D	2.07	128.82	124.68
29	C	502	CLA	C3B-C4B-NB	-2.07	108.68	110.53
29	r	310	CLA	C3B-C4B-NB	-2.07	108.69	110.53
29	y	313	CLA	C3B-C4B-NB	-2.07	108.69	110.53
29	a	404	CLA	CHD-C1D-ND	-2.07	121.89	124.80
29	R	309	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
29	c	503	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
29	c	513	CLA	O2A-CGA-O1A	-2.07	118.46	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	G	617	NEX	C40-C33-C34	-2.07	119.47	122.82
29	b	504	CLA	C3B-C4B-NB	-2.07	108.69	110.53
31	C	516	BCR	C34-C9-C10	-2.07	119.47	122.82
46	Y	306	CHL	CMD-C2D-C3D	2.07	128.81	124.68
46	G	605	CHL	CMD-C2D-C3D	2.06	128.81	124.68
46	g	606	CHL	C3D-C4D-ND	-2.06	109.63	112.94
46	g	605	CHL	CMD-C2D-C3D	2.06	128.81	124.68
47	G	616	LUT	C22-C23-C24	-2.06	108.12	111.18
31	c	514	BCR	C37-C22-C23	2.06	121.24	118.09
29	n	610	CLA	C4A-NA-C1A	2.06	107.62	106.68
29	G	602	CLA	C3B-C2B-C1B	-2.06	104.74	107.17
29	N	603	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
29	R	302	CLA	CHD-C1D-ND	-2.06	121.90	124.80
46	n	605	CHL	CMD-C2D-C3D	2.06	128.80	124.68
46	N	608	CHL	C3D-C4D-ND	-2.06	109.63	112.94
43	d	405	PL9	C12-C13-C14	-2.06	122.91	127.62
46	Y	302	CHL	CMD-C2D-C3D	2.06	128.80	124.68
47	n	614	LUT	C30-C31-C32	-2.06	117.23	123.20
46	G	607	CHL	CMD-C2D-C3D	2.06	128.79	124.68
31	c	515	BCR	C12-C13-C14	-2.06	115.77	119.01
29	g	613	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
29	Y	304	CLA	C3B-C2B-C1B	-2.06	104.75	107.17
46	N	607	CHL	CMA-C3A-C2A	2.06	122.07	114.13
46	G	605	CHL	C1C-C2C-CMC	2.05	130.50	126.80
46	Y	310	CHL	CMD-C2D-C3D	2.05	128.78	124.68
29	r	303	CLA	C1D-ND-C4D	-2.05	104.87	106.31
31	v	101	BCR	C12-C13-C14	-2.05	115.78	119.01
46	g	606	CHL	CMD-C2D-C3D	2.05	128.78	124.68
46	r	306	CHL	CMD-C2D-C3D	2.05	128.78	124.68
29	D	404	CLA	CHD-C1D-ND	-2.05	121.92	124.80
29	N	614	CLA	C3B-C4B-NB	-2.05	108.70	110.53
47	g	615	LUT	C20-C13-C12	2.05	121.22	118.09
29	G	604	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
49	y	302	XAT	C19-C9-C10	-2.05	119.50	122.82
47	n	614	LUT	C20-C13-C12	2.05	121.22	118.09
29	s	306	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
47	g	615	LUT	C30-C31-C32	-2.05	117.27	123.20
48	R	312	NEX	O24-C25-C38	-2.05	112.76	115.05
47	g	615	LUT	C35-C15-C14	-2.05	119.33	123.52
29	B	508	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
29	C	504	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
31	f	101	BCR	C30-C25-C24	2.05	121.20	115.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	G	601	CHL	C1-O2A-CGA	2.05	121.61	116.65
34	b	519	C7Z	C31-C32-C33	-2.05	120.75	126.36
29	y	314	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
46	S	302	CHL	CMD-C2D-C3D	2.05	128.77	124.68
29	S	310	CLA	CHA-C1A-NA	-2.05	121.76	126.39
29	S	313	CLA	CHA-C1A-NA	-2.05	121.76	126.39
29	b	501	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
29	c	504	CLA	C1-C2-C3	-2.05	122.85	126.20
29	B	516	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
48	n	616	NEX	C20-C13-C14	-2.04	119.50	122.82
47	r	311	LUT	C22-C23-C24	-2.04	108.15	111.18
29	S	304	CLA	CMD-C2D-C1D	-2.04	121.13	124.73
48	y	319	NEX	C11-C10-C9	2.04	130.14	127.28
31	f	101	BCR	C38-C26-C27	2.04	117.95	113.60
29	D	405	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
29	y	305	CLA	CMB-C2B-C1B	2.04	128.53	125.42
47	N	616	LUT	C31-C30-C29	-2.04	124.41	127.28
47	S	317	LUT	C20-C13-C12	2.04	121.20	118.09
46	S	302	CHL	CMA-C3A-C4A	2.04	119.00	114.61
34	b	519	C7Z	C15-C35-C34	-2.04	119.35	123.52
47	Y	316	LUT	C22-C23-C24	-2.04	108.16	111.18
31	A	410	BCR	C31-C1-C6	-2.04	107.05	110.24
29	B	510	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
47	n	614	LUT	C15-C35-C34	-2.04	119.35	123.52
46	N	601	CHL	CMD-C2D-C3D	2.04	128.75	124.68
29	s	316	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
29	c	502	CLA	CHA-C1A-NA	-2.04	121.78	126.39
29	b	516	CLA	C4D-C3D-CAD	-2.04	105.89	108.11
29	a	406	CLA	C3B-C2B-C1B	-2.04	104.77	107.17
46	r	305	CHL	C3D-C4D-ND	-2.04	109.67	112.94
46	N	605	CHL	CMD-C2D-C3D	2.03	128.75	124.68
29	C	509	CLA	CHA-C1A-NA	-2.03	121.78	126.39
31	c	515	BCR	C33-C5-C4	2.03	117.93	113.60
46	R	304	CHL	C3D-C4D-ND	-2.03	109.67	112.94
46	s	307	CHL	C3D-C4D-ND	-2.03	109.68	112.94
31	c	514	BCR	C34-C9-C10	-2.03	119.52	122.82
29	r	308	CLA	C3B-C2B-C1B	-2.03	104.77	107.17
29	s	313	CLA	O2A-CGA-O1A	-2.03	118.11	123.33
46	n	607	CHL	C4C-CHD-C1D	2.03	123.33	116.07
29	g	611	CLA	C1-C2-C3	-2.03	122.87	126.20
46	N	608	CHL	C4C-CHD-C1D	2.03	123.33	116.07
47	Y	316	LUT	C30-C31-C32	-2.03	117.32	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	507	CLA	C1D-ND-C4D	-2.03	104.89	106.31
29	b	514	CLA	CHA-C1A-NA	-2.03	121.80	126.39
31	f	101	BCR	C37-C22-C21	-2.03	119.53	122.82
29	y	316	CLA	CHA-C1A-NA	-2.03	121.80	126.39
29	Y	304	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
29	c	504	CLA	CHA-C1A-NA	-2.03	121.80	126.39
29	G	603	CLA	C1-C2-C3	-2.03	122.88	126.20
47	y	317	LUT	C19-C9-C8	2.03	121.18	118.09
29	s	306	CLA	CHA-C1A-NA	-2.03	121.81	126.39
29	N	604	CLA	C1-C2-C3	-2.02	122.88	126.20
49	N	619	XAT	C39-C29-C30	-2.02	119.54	122.82
46	y	301	CHL	CMA-C3A-C4A	2.02	118.97	114.61
47	S	317	LUT	C39-C29-C28	2.02	121.18	118.09
47	R	310	LUT	C35-C15-C14	-2.02	119.38	123.52
29	S	316	CLA	C1-C2-C3	-2.02	123.49	126.76
37	s	301	LHG	O7-C7-O9	-2.02	118.98	123.70
29	S	304	CLA	C1D-ND-C4D	2.02	107.73	106.31
48	g	617	NEX	C19-C9-C10	-2.02	119.54	122.82
47	y	317	LUT	C20-C13-C12	2.02	121.17	118.09
29	S	306	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
29	c	503	CLA	CMB-C2B-C1B	2.02	128.49	125.42
29	N	611	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
46	G	609	CHL	C3D-C4D-ND	-2.02	109.70	112.94
29	G	613	CLA	C1-C2-C3	-2.02	122.89	126.20
31	B	517	BCR	C36-C18-C17	-2.02	119.55	122.82
31	C	515	BCR	C37-C22-C23	2.02	121.17	118.09
37	g	618	LHG	C5-O7-C7	-2.02	112.97	117.80
29	r	303	CLA	C4D-C3D-CAD	-2.02	105.92	108.11
29	s	303	CLA	C3B-C2B-C1B	-2.01	104.79	107.17
48	G	617	NEX	C20-C13-C14	-2.01	119.55	122.82
29	n	604	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
29	A	409	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
29	B	502	CLA	C1-C2-C3	-2.01	122.90	126.20
29	D	404	CLA	C11-C12-C13	-2.01	109.28	115.97
29	b	508	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
46	g	607	CHL	C4C-CHD-C1D	2.01	123.26	116.07
37	N	618	LHG	O7-C7-O9	-2.01	119.01	123.70
29	C	513	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
46	n	601	CHL	CMD-C2D-C3D	2.01	128.69	124.68
30	D	401	PHO	C3B-C4B-NB	-2.01	106.16	107.46
34	B	519	C7Z	C31-C32-C33	-2.01	120.86	126.36
46	n	608	CHL	CMD-C2D-C3D	2.00	128.69	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	406	CLA	C1C-C2C-C3C	-2.00	104.87	106.98
46	g	609	CHL	CMD-C2D-C3D	2.00	128.69	124.68
29	Y	315	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
43	D	406	PL9	C20-C19-C21	2.00	118.71	115.23
29	b	512	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
46	G	609	CHL	CMD-C2D-C3D	2.00	128.69	124.68
47	r	311	LUT	C26-C27-C28	-2.00	121.46	124.58
46	y	303	CHL	CMD-C2D-C3D	2.00	128.69	124.68
31	B	518	BCR	C33-C5-C4	2.00	117.86	113.60
46	y	301	CHL	CMD-C2D-C3D	2.00	128.68	124.68
29	B	509	CLA	CHA-C1A-NA	-2.00	121.86	126.39
29	c	512	CLA	CHA-C1A-NA	-2.00	121.86	126.39
47	S	318	LUT	C20-C13-C12	2.00	121.14	118.09
29	S	314	CLA	CMB-C2B-C1B	2.00	128.47	125.42
37	D	408	LHG	C5-O7-C7	-2.00	113.01	117.80
48	G	617	NEX	C28-C29-C30	2.00	122.16	119.01
46	y	301	CHL	C1C-C2C-CMC	2.00	130.41	126.80

All (311) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	A	405	CLA	ND
29	A	406	CLA	ND
29	A	407	CLA	ND
29	B	501	CLA	ND
29	B	502	CLA	ND
29	B	503	CLA	ND
29	B	504	CLA	ND
29	B	505	CLA	ND
29	B	506	CLA	ND
29	B	507	CLA	ND
29	B	508	CLA	ND
29	B	509	CLA	ND
29	B	510	CLA	ND
29	B	512	CLA	ND
29	B	513	CLA	ND
29	B	514	CLA	ND
29	B	515	CLA	ND
29	B	516	CLA	ND
29	C	503	CLA	ND
29	C	505	CLA	ND
29	C	506	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
29	C	508	CLA	ND
29	C	509	CLA	ND
29	C	510	CLA	ND
29	C	511	CLA	ND
29	C	512	CLA	ND
29	C	513	CLA	ND
29	D	404	CLA	C8
29	D	405	CLA	ND
29	N	602	CLA	ND
29	N	603	CLA	ND
29	N	604	CLA	ND
29	N	610	CLA	ND
29	N	611	CLA	ND
29	N	612	CLA	ND
29	N	613	CLA	ND
29	N	614	CLA	ND
29	G	602	CLA	ND
29	G	603	CLA	ND
29	G	604	CLA	ND
29	G	610	CLA	ND
29	G	611	CLA	ND
29	G	612	CLA	ND
29	G	613	CLA	ND
29	G	614	CLA	ND
29	R	301	CLA	ND
29	R	303	CLA	ND
29	R	306	CLA	ND
29	R	307	CLA	ND
29	R	308	CLA	ND
29	R	309	CLA	ND
29	S	303	CLA	ND
29	S	304	CLA	ND
29	S	305	CLA	ND
29	S	306	CLA	ND
29	S	310	CLA	ND
29	S	311	CLA	ND
29	S	312	CLA	ND
29	S	313	CLA	ND
29	S	314	CLA	ND
29	S	315	CLA	ND
29	S	316	CLA	ND
29	Y	303	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
29	Y	304	CLA	ND
29	Y	305	CLA	ND
29	Y	309	CLA	ND
29	Y	311	CLA	ND
29	Y	312	CLA	ND
29	Y	313	CLA	ND
29	Y	314	CLA	ND
29	Y	315	CLA	ND
29	a	404	CLA	ND
29	a	405	CLA	ND
29	b	501	CLA	ND
29	b	502	CLA	ND
29	b	503	CLA	ND
29	b	504	CLA	ND
29	b	505	CLA	ND
29	b	506	CLA	ND
29	b	507	CLA	ND
29	b	509	CLA	ND
29	b	510	CLA	ND
29	b	512	CLA	ND
29	b	513	CLA	ND
29	b	514	CLA	ND
29	b	515	CLA	ND
29	b	516	CLA	ND
29	c	502	CLA	ND
29	c	504	CLA	ND
29	c	505	CLA	ND
29	c	507	CLA	ND
29	c	508	CLA	ND
29	c	509	CLA	ND
29	c	510	CLA	ND
29	c	512	CLA	ND
29	d	403	CLA	ND
29	d	404	CLA	ND
29	n	602	CLA	ND
29	n	603	CLA	ND
29	n	604	CLA	ND
29	n	609	CLA	ND
29	n	610	CLA	ND
29	n	611	CLA	ND
29	n	613	CLA	ND
29	g	602	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
29	g	603	CLA	ND
29	g	604	CLA	ND
29	g	610	CLA	ND
29	g	611	CLA	ND
29	g	614	CLA	ND
29	r	302	CLA	ND
29	r	304	CLA	ND
29	r	307	CLA	ND
29	r	308	CLA	ND
29	r	309	CLA	ND
29	r	310	CLA	ND
29	s	303	CLA	ND
29	s	305	CLA	ND
29	s	310	CLA	ND
29	s	311	CLA	ND
29	s	312	CLA	ND
29	s	313	CLA	ND
29	s	314	CLA	ND
29	s	315	CLA	ND
29	s	316	CLA	ND
29	y	304	CLA	ND
29	y	305	CLA	ND
29	y	306	CLA	ND
29	y	310	CLA	ND
29	y	312	CLA	ND
29	y	313	CLA	ND
29	y	314	CLA	ND
29	y	316	CLA	ND
34	B	519	C7Z	C3
34	b	519	C7Z	C3
45	H	101	RRX	C28
45	h	101	RRX	C28
46	N	601	CHL	C8
46	N	601	CHL	NC
46	N	601	CHL	NA
46	N	601	CHL	ND
46	N	605	CHL	C8
46	N	605	CHL	NC
46	N	605	CHL	NA
46	N	605	CHL	ND
46	N	606	CHL	C8
46	N	606	CHL	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
46	N	606	CHL	NA
46	N	606	CHL	ND
46	N	607	CHL	C8
46	N	607	CHL	NC
46	N	607	CHL	NA
46	N	607	CHL	ND
46	N	608	CHL	NC
46	N	608	CHL	NA
46	N	608	CHL	ND
46	N	609	CHL	C8
46	N	609	CHL	NC
46	N	609	CHL	NA
46	N	609	CHL	ND
46	G	601	CHL	C8
46	G	601	CHL	NC
46	G	601	CHL	NA
46	G	601	CHL	ND
46	G	605	CHL	NC
46	G	605	CHL	NA
46	G	605	CHL	ND
46	G	606	CHL	NC
46	G	606	CHL	NA
46	G	606	CHL	ND
46	G	607	CHL	C8
46	G	607	CHL	NC
46	G	607	CHL	NA
46	G	607	CHL	ND
46	G	608	CHL	NC
46	G	608	CHL	NA
46	G	608	CHL	ND
46	G	609	CHL	C8
46	G	609	CHL	NC
46	G	609	CHL	NA
46	G	609	CHL	ND
46	R	304	CHL	NC
46	R	304	CHL	NA
46	R	304	CHL	ND
46	R	305	CHL	NC
46	R	305	CHL	NA
46	R	305	CHL	ND
46	S	302	CHL	NC
46	S	302	CHL	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
46	S	302	CHL	ND
46	S	307	CHL	NC
46	S	307	CHL	NA
46	S	307	CHL	ND
46	S	308	CHL	NC
46	S	308	CHL	NA
46	S	308	CHL	ND
46	S	309	CHL	C8
46	S	309	CHL	NC
46	S	309	CHL	NA
46	S	309	CHL	ND
46	Y	302	CHL	C8
46	Y	302	CHL	NC
46	Y	302	CHL	NA
46	Y	302	CHL	ND
46	Y	306	CHL	NC
46	Y	306	CHL	NA
46	Y	306	CHL	ND
46	Y	307	CHL	C8
46	Y	307	CHL	NC
46	Y	307	CHL	NA
46	Y	307	CHL	ND
46	Y	308	CHL	C8
46	Y	308	CHL	NC
46	Y	308	CHL	NA
46	Y	308	CHL	ND
46	Y	310	CHL	C8
46	Y	310	CHL	NC
46	Y	310	CHL	NA
46	Y	310	CHL	ND
46	n	601	CHL	C8
46	n	601	CHL	NC
46	n	601	CHL	NA
46	n	601	CHL	ND
46	n	605	CHL	C8
46	n	605	CHL	NC
46	n	605	CHL	NA
46	n	605	CHL	ND
46	n	606	CHL	C8
46	n	606	CHL	NC
46	n	606	CHL	NA
46	n	606	CHL	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
46	n	607	CHL	NC
46	n	607	CHL	NA
46	n	607	CHL	ND
46	n	608	CHL	C8
46	n	608	CHL	NC
46	n	608	CHL	NA
46	n	608	CHL	ND
46	g	601	CHL	C8
46	g	601	CHL	NC
46	g	601	CHL	NA
46	g	601	CHL	ND
46	g	605	CHL	NC
46	g	605	CHL	NA
46	g	605	CHL	ND
46	g	606	CHL	NC
46	g	606	CHL	NA
46	g	606	CHL	ND
46	g	607	CHL	C8
46	g	607	CHL	NC
46	g	607	CHL	NA
46	g	607	CHL	ND
46	g	608	CHL	NC
46	g	608	CHL	NA
46	g	608	CHL	ND
46	g	609	CHL	C8
46	g	609	CHL	NC
46	g	609	CHL	NA
46	g	609	CHL	ND
46	r	305	CHL	NC
46	r	305	CHL	NA
46	r	305	CHL	ND
46	r	306	CHL	NC
46	r	306	CHL	NA
46	r	306	CHL	ND
46	s	302	CHL	NC
46	s	302	CHL	NA
46	s	302	CHL	ND
46	s	307	CHL	NC
46	s	307	CHL	NA
46	s	307	CHL	ND
46	s	308	CHL	NC
46	s	308	CHL	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
46	s	308	CHL	ND
46	s	309	CHL	C8
46	s	309	CHL	NC
46	s	309	CHL	NA
46	s	309	CHL	ND
46	y	301	CHL	C8
46	y	301	CHL	NC
46	y	301	CHL	NA
46	y	301	CHL	ND
46	y	303	CHL	C8
46	y	303	CHL	NC
46	y	303	CHL	NA
46	y	303	CHL	ND
46	y	307	CHL	NC
46	y	307	CHL	NA
46	y	307	CHL	ND
46	y	308	CHL	NC
46	y	308	CHL	NA
46	y	308	CHL	ND
46	y	309	CHL	C8
46	y	309	CHL	NC
46	y	309	CHL	NA
46	y	309	CHL	ND
46	y	311	CHL	C8
46	y	311	CHL	NC
46	y	311	CHL	NA
46	y	311	CHL	ND
49	N	619	XAT	C6
49	N	619	XAT	C26
49	G	619	XAT	C6
49	R	311	XAT	C6
49	R	311	XAT	C26
49	Y	301	XAT	C6
49	n	618	XAT	C6
49	n	618	XAT	C26
49	g	619	XAT	C6
49	r	312	XAT	C6
49	y	302	XAT	C6

All (3521) torsion outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	A	405	CLA	CBD-CGD-O2D-CED
29	A	406	CLA	C1A-C2A-CAA-CBA
29	A	406	CLA	C3A-C2A-CAA-CBA
29	A	406	CLA	C2-C1-O2A-CGA
29	A	407	CLA	C1A-C2A-CAA-CBA
29	A	407	CLA	C3A-C2A-CAA-CBA
29	B	501	CLA	C1A-C2A-CAA-CBA
29	B	501	CLA	CAD-CBD-CGD-O1D
29	B	501	CLA	CAD-CBD-CGD-O2D
29	B	506	CLA	C2B-C3B-CAB-CBB
29	B	507	CLA	C1A-C2A-CAA-CBA
29	B	507	CLA	C3A-C2A-CAA-CBA
29	C	502	CLA	CBD-CGD-O2D-CED
29	C	503	CLA	CAD-CBD-CGD-O1D
29	C	503	CLA	CAD-CBD-CGD-O2D
29	C	505	CLA	C4B-C3B-CAB-CBB
29	C	511	CLA	CBD-CGD-O2D-CED
29	C	514	CLA	C1A-C2A-CAA-CBA
29	C	514	CLA	C3A-C2A-CAA-CBA
29	D	404	CLA	C14-C13-C15-C16
29	N	610	CLA	C1A-C2A-CAA-CBA
29	N	610	CLA	C3A-C2A-CAA-CBA
29	N	612	CLA	C4B-C3B-CAB-CBB
29	N	612	CLA	CHA-CBD-CGD-O1D
29	N	612	CLA	CHA-CBD-CGD-O2D
29	N	613	CLA	C4B-C3B-CAB-CBB
29	N	613	CLA	CBD-CGD-O2D-CED
29	N	614	CLA	C1A-C2A-CAA-CBA
29	G	602	CLA	C3A-C2A-CAA-CBA
29	G	603	CLA	C1A-C2A-CAA-CBA
29	G	603	CLA	C3A-C2A-CAA-CBA
29	G	603	CLA	C4B-C3B-CAB-CBB
29	G	612	CLA	C4B-C3B-CAB-CBB
29	G	612	CLA	CBD-CGD-O2D-CED
29	G	614	CLA	C1A-C2A-CAA-CBA
29	G	614	CLA	C4B-C3B-CAB-CBB
29	R	302	CLA	C1A-C2A-CAA-CBA
29	R	302	CLA	C3A-C2A-CAA-CBA
29	R	302	CLA	CBA-CGA-O2A-C1
29	R	302	CLA	C4B-C3B-CAB-CBB
29	R	302	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	R	302	CLA	O1D-CGD-O2D-CED
29	R	303	CLA	C4B-C3B-CAB-CBB
29	R	306	CLA	C1A-C2A-CAA-CBA
29	R	306	CLA	C3A-C2A-CAA-CBA
29	R	309	CLA	CBD-CGD-O2D-CED
29	S	303	CLA	C1A-C2A-CAA-CBA
29	S	303	CLA	CHA-CBD-CGD-O1D
29	S	303	CLA	CHA-CBD-CGD-O2D
29	S	304	CLA	C1A-C2A-CAA-CBA
29	S	304	CLA	C3A-C2A-CAA-CBA
29	S	304	CLA	C11-C12-C13-C14
29	S	306	CLA	C1A-C2A-CAA-CBA
29	S	310	CLA	C11-C10-C8-C9
29	S	311	CLA	C1A-C2A-CAA-CBA
29	S	311	CLA	C3A-C2A-CAA-CBA
29	S	311	CLA	C6-C7-C8-C10
29	S	312	CLA	C1A-C2A-CAA-CBA
29	S	312	CLA	C3A-C2A-CAA-CBA
29	S	314	CLA	C4B-C3B-CAB-CBB
29	S	314	CLA	CBD-CGD-O2D-CED
29	Y	304	CLA	C1A-C2A-CAA-CBA
29	Y	304	CLA	C3A-C2A-CAA-CBA
29	Y	309	CLA	C1A-C2A-CAA-CBA
29	Y	312	CLA	O1A-CGA-O2A-C1
29	Y	314	CLA	C4B-C3B-CAB-CBB
29	Y	315	CLA	C4B-C3B-CAB-CBB
29	a	404	CLA	CBD-CGD-O2D-CED
29	a	405	CLA	C1A-C2A-CAA-CBA
29	a	405	CLA	C3A-C2A-CAA-CBA
29	a	405	CLA	C2-C1-O2A-CGA
29	b	501	CLA	C4B-C3B-CAB-CBB
29	b	501	CLA	C11-C12-C13-C14
29	b	504	CLA	C1A-C2A-CAA-CBA
29	b	506	CLA	C2B-C3B-CAB-CBB
29	c	501	CLA	C4B-C3B-CAB-CBB
29	c	502	CLA	CAD-CBD-CGD-O1D
29	c	502	CLA	CAD-CBD-CGD-O2D
29	c	504	CLA	C6-C7-C8-C9
29	c	505	CLA	C11-C10-C8-C9
29	c	507	CLA	CHA-CBD-CGD-O2D
29	c	509	CLA	C2-C1-O2A-CGA
29	c	509	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	c	513	CLA	C1A-C2A-CAA-CBA
29	d	403	CLA	C4B-C3B-CAB-CBB
29	n	603	CLA	C1A-C2A-CAA-CBA
29	n	603	CLA	C3A-C2A-CAA-CBA
29	n	609	CLA	C1A-C2A-CAA-CBA
29	n	609	CLA	C3A-C2A-CAA-CBA
29	n	610	CLA	C4B-C3B-CAB-CBB
29	n	611	CLA	C4B-C3B-CAB-CBB
29	n	611	CLA	CHA-CBD-CGD-O1D
29	n	611	CLA	CHA-CBD-CGD-O2D
29	n	612	CLA	C1A-C2A-CAA-CBA
29	g	602	CLA	C1A-C2A-CAA-CBA
29	g	602	CLA	C3A-C2A-CAA-CBA
29	g	604	CLA	C1A-C2A-CAA-CBA
29	g	612	CLA	C4B-C3B-CAB-CBB
29	r	303	CLA	C1A-C2A-CAA-CBA
29	r	303	CLA	C3A-C2A-CAA-CBA
29	r	303	CLA	C2B-C3B-CAB-CBB
29	r	303	CLA	C4B-C3B-CAB-CBB
29	r	303	CLA	CBD-CGD-O2D-CED
29	r	304	CLA	C4B-C3B-CAB-CBB
29	r	308	CLA	C1A-C2A-CAA-CBA
29	r	308	CLA	CBD-CGD-O2D-CED
29	r	310	CLA	CBA-CGA-O2A-C1
29	r	310	CLA	O1A-CGA-O2A-C1
29	s	304	CLA	C1A-C2A-CAA-CBA
29	s	304	CLA	C3A-C2A-CAA-CBA
29	s	306	CLA	C1A-C2A-CAA-CBA
29	s	310	CLA	C1A-C2A-CAA-CBA
29	s	310	CLA	C3A-C2A-CAA-CBA
29	s	311	CLA	C3A-C2A-CAA-CBA
29	s	313	CLA	CHA-CBD-CGD-O1D
29	s	313	CLA	CHA-CBD-CGD-O2D
29	y	305	CLA	C4B-C3B-CAB-CBB
29	y	306	CLA	CBD-CGD-O2D-CED
29	y	306	CLA	C6-C7-C8-C9
29	y	310	CLA	C1A-C2A-CAA-CBA
29	y	310	CLA	CBD-CGD-O2D-CED
29	y	315	CLA	C4B-C3B-CAB-CBB
29	y	316	CLA	C4B-C3B-CAB-CBB
30	D	401	PHO	C3A-C2A-CAA-CBA
31	B	517	BCR	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	517	BCR	C7-C8-C9-C34
31	B	517	BCR	C21-C22-C23-C24
31	B	518	BCR	C7-C8-C9-C10
31	B	518	BCR	C7-C8-C9-C34
31	B	518	BCR	C11-C10-C9-C8
31	B	518	BCR	C11-C10-C9-C34
31	B	518	BCR	C10-C11-C12-C13
31	C	515	BCR	C11-C10-C9-C8
31	C	515	BCR	C11-C10-C9-C34
31	C	515	BCR	C10-C11-C12-C13
31	C	515	BCR	C11-C12-C13-C14
31	C	515	BCR	C11-C12-C13-C35
31	C	515	BCR	C17-C18-C19-C20
31	C	516	BCR	C7-C8-C9-C10
31	C	516	BCR	C17-C18-C19-C20
31	C	516	BCR	C36-C18-C19-C20
31	C	517	BCR	C11-C10-C9-C8
31	C	517	BCR	C11-C10-C9-C34
31	C	517	BCR	C10-C11-C12-C13
31	C	517	BCR	C17-C18-C19-C20
31	C	517	BCR	C36-C18-C19-C20
31	F	101	BCR	C11-C10-C9-C8
31	F	101	BCR	C11-C10-C9-C34
31	K	101	BCR	C5-C6-C7-C8
31	K	101	BCR	C7-C8-C9-C10
31	K	101	BCR	C7-C8-C9-C34
31	K	101	BCR	C11-C10-C9-C8
31	K	101	BCR	C11-C10-C9-C34
31	a	409	BCR	C17-C18-C19-C20
31	b	517	BCR	C11-C10-C9-C8
31	b	517	BCR	C11-C10-C9-C34
31	b	517	BCR	C10-C11-C12-C13
31	b	517	BCR	C17-C18-C19-C20
31	b	518	BCR	C7-C8-C9-C10
31	b	518	BCR	C11-C10-C9-C8
31	b	518	BCR	C11-C10-C9-C34
31	b	518	BCR	C10-C11-C12-C13
31	v	101	BCR	C5-C6-C7-C8
31	v	101	BCR	C7-C8-C9-C10
31	v	101	BCR	C7-C8-C9-C34
31	v	101	BCR	C11-C10-C9-C8
31	v	101	BCR	C11-C10-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	c	514	BCR	C11-C10-C9-C8
31	c	514	BCR	C11-C10-C9-C34
31	c	514	BCR	C10-C11-C12-C13
31	c	514	BCR	C11-C12-C13-C14
31	c	514	BCR	C11-C12-C13-C35
31	c	514	BCR	C17-C18-C19-C20
31	c	515	BCR	C11-C10-C9-C8
31	c	515	BCR	C11-C10-C9-C34
31	c	515	BCR	C10-C11-C12-C13
31	c	515	BCR	C17-C18-C19-C20
31	c	515	BCR	C36-C18-C19-C20
31	f	101	BCR	C11-C10-C9-C8
31	f	101	BCR	C11-C10-C9-C34
31	f	101	BCR	C10-C11-C12-C13
31	f	101	BCR	C21-C22-C23-C24
31	f	101	BCR	C37-C22-C23-C24
31	f	101	BCR	C23-C24-C25-C26
31	f	101	BCR	C23-C24-C25-C30
31	z	101	BCR	C7-C8-C9-C10
31	z	101	BCR	C11-C10-C9-C8
31	z	101	BCR	C11-C10-C9-C34
31	z	101	BCR	C10-C11-C12-C13
33	A	412	3PH	C1-O11-P-O13
33	A	412	3PH	C1-O11-P-O14
33	S	322	3PH	O22-C21-O21-C2
33	a	415	3PH	C1-O11-P-O13
33	a	415	3PH	C1-O11-P-O14
33	a	415	3PH	O22-C21-O21-C2
33	b	521	3PH	C1-O11-P-O13
33	b	521	3PH	C1-O11-P-O14
33	b	521	3PH	O11-C1-C2-O21
33	b	521	3PH	O22-C21-O21-C2
33	s	322	3PH	C22-C21-O21-C2
34	B	519	C7Z	C5-C6-C7-C8
34	b	519	C7Z	C1-C6-C7-C8
35	B	520	LMG	O6-C1-O1-C7
35	C	524	LMG	O9-C10-O7-C8
35	C	524	LMG	C11-C10-O7-C8
35	W	201	LMG	O6-C1-O1-C7
35	W	203	LMG	O6-C1-O1-C7
35	W	203	LMG	C7-C8-O7-C10
35	W	203	LMG	C11-C10-O7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	b	520	LMG	O6-C1-O1-C7
35	i	101	LMG	O1-C7-C8-O7
35	w	202	LMG	O6-C1-O1-C7
36	B	521	DGD	C2B-C1B-O2G-C2G
36	r	301	DGD	C2A-C1A-O1G-C1G
36	r	301	DGD	O1A-C1A-O1G-C1G
36	r	301	DGD	O1B-C1B-O2G-C2G
37	B	523	LHG	C4-O6-P-O3
37	B	523	LHG	C4-O6-P-O5
37	D	407	LHG	C4-O6-P-O3
37	D	407	LHG	C4-O6-P-O4
37	D	407	LHG	C4-O6-P-O5
37	D	408	LHG	C3-O3-P-O5
37	D	408	LHG	C4-O6-P-O5
37	D	408	LHG	O7-C5-C6-O8
37	L	101	LHG	O1-C1-C2-C3
37	L	101	LHG	C1-C2-C3-O3
37	L	101	LHG	C4-O6-P-O3
37	L	101	LHG	O9-C7-O7-C5
37	L	101	LHG	C8-C7-O7-C5
37	N	618	LHG	C3-O3-P-O5
37	N	618	LHG	C4-O6-P-O3
37	N	618	LHG	C4-O6-P-O4
37	N	618	LHG	C4-O6-P-O5
37	N	618	LHG	O7-C5-C6-O8
37	G	618	LHG	O1-C1-C2-O2
37	G	618	LHG	C4-O6-P-O3
37	G	618	LHG	C4-O6-P-O4
37	G	618	LHG	O7-C5-C6-O8
37	S	301	LHG	O1-C1-C2-C3
37	S	301	LHG	C1-C2-C3-O3
37	S	301	LHG	C3-O3-P-O4
37	S	301	LHG	C4-O6-P-O3
37	S	301	LHG	C4-O6-P-O5
37	Y	319	LHG	C1-C2-C3-O3
37	Y	319	LHG	C3-O3-P-O5
37	Y	319	LHG	C4-O6-P-O3
37	Y	319	LHG	C4-O6-P-O4
37	Y	319	LHG	C4-O6-P-O5
37	a	413	LHG	O1-C1-C2-C3
37	a	413	LHG	C1-C2-C3-O3
37	a	413	LHG	C3-O3-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	a	413	LHG	C3-O3-P-O6
37	a	413	LHG	C4-O6-P-O5
37	a	414	LHG	C3-O3-P-O5
37	a	414	LHG	C4-O6-P-O5
37	a	414	LHG	O7-C5-C6-O8
37	c	521	LHG	C1-C2-C3-O3
37	c	521	LHG	C4-O6-P-O3
37	c	521	LHG	C4-O6-P-O4
37	d	406	LHG	C1-C2-C3-O3
37	d	406	LHG	C4-O6-P-O3
37	d	406	LHG	C4-O6-P-O5
37	l	102	LHG	O1-C1-C2-C3
37	l	102	LHG	C3-O3-P-O4
37	l	102	LHG	C3-O3-P-O5
37	l	102	LHG	C3-O3-P-O6
37	l	102	LHG	C4-O6-P-O3
37	l	102	LHG	C4-O6-P-O5
37	n	617	LHG	C3-O3-P-O5
37	n	617	LHG	C4-O6-P-O3
37	n	617	LHG	C4-O6-P-O4
37	n	617	LHG	C4-O6-P-O5
37	n	617	LHG	O7-C5-C6-O8
37	g	618	LHG	C4-O6-P-O3
37	g	618	LHG	C4-O6-P-O4
37	g	618	LHG	O7-C5-C6-O8
37	s	301	LHG	C3-O3-P-O4
37	s	301	LHG	C3-O3-P-O5
37	s	301	LHG	C3-O3-P-O6
37	s	301	LHG	O9-C7-O7-C5
37	s	301	LHG	C8-C7-O7-C5
37	s	320	LHG	O1-C1-C2-C3
37	s	320	LHG	C4-O6-P-O3
37	s	320	LHG	C4-O6-P-O4
37	y	320	LHG	O2-C2-C3-O3
37	y	320	LHG	C3-O3-P-O4
37	y	320	LHG	C3-O3-P-O5
37	y	320	LHG	C3-O3-P-O6
37	y	320	LHG	C4-O6-P-O3
37	y	320	LHG	C4-O6-P-O5
38	b	524	LMT	O5'-C1'-O1'-C1
39	C	523	SQD	C5-C6-S-O7
39	C	523	SQD	C5-C6-S-O9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	L	102	SQD	O5-C1-O6-C44
39	M	101	SQD	O5-C5-C6-S
39	M	101	SQD	C5-C6-S-O7
39	M	101	SQD	C5-C6-S-O8
39	M	101	SQD	C5-C6-S-O9
39	a	410	SQD	O5-C5-C6-S
39	b	523	SQD	O5-C1-O6-C44
39	c	522	SQD	O10-C23-O48-C46
39	c	522	SQD	O5-C5-C6-S
39	l	101	SQD	O5-C1-O6-C44
39	l	101	SQD	O5-C5-C6-S
39	m	101	SQD	C5-C6-S-O7
39	m	101	SQD	C5-C6-S-O8
39	m	101	SQD	C5-C6-S-O9
39	o	301	SQD	C2-C1-O6-C44
39	o	301	SQD	O5-C1-O6-C44
39	o	301	SQD	C8-C7-O47-C45
39	o	301	SQD	C5-C6-S-O7
39	o	301	SQD	C5-C6-S-O8
39	o	301	SQD	C5-C6-S-O9
40	C	525	SPH	O1-C1-C2-C3
40	C	525	SPH	C2-C3-C4-C5
40	C	525	SPH	O3-C3-C4-C5
40	I	101	SPH	O1-C1-C2-C3
40	I	101	SPH	C1-C2-C3-O3
40	I	101	SPH	N2-C2-C3-C4
40	i	102	SPH	C1-C2-C3-O3
40	i	102	SPH	C1-C2-C3-C4
40	i	102	SPH	N2-C2-C3-O3
40	i	102	SPH	N2-C2-C3-C4
41	D	402	DGA	OB1-CB1-OG2-CG2
41	W	202	DGA	OG2-CG2-CG3-OXT
41	b	522	DGA	CG1-CG2-CG3-OXT
41	b	522	DGA	OG2-CG2-CG3-OXT
41	j	101	DGA	OG2-CG2-CG3-OXT
41	w	201	DGA	OG2-CG2-CG3-OXT
43	D	406	PL9	C37-C38-C39-C40
43	D	406	PL9	C37-C38-C39-C41
43	d	405	PL9	C37-C38-C39-C40
43	d	405	PL9	C37-C38-C39-C41
45	H	101	RRX	C37-C22-C23-C24
45	H	101	RRX	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	h	101	RRX	C37-C22-C23-C24
45	h	101	RRX	C21-C22-C23-C24
45	h	101	RRX	C36-C18-C19-C20
45	h	101	RRX	C17-C18-C19-C20
46	G	606	CHL	C1A-C2A-CAA-CBA
46	G	607	CHL	CHA-CBD-CGD-O1D
46	G	607	CHL	CHA-CBD-CGD-O2D
46	n	605	CHL	C14-C13-C15-C16
46	n	606	CHL	C14-C13-C15-C16
46	g	601	CHL	C3A-C2A-CAA-CBA
46	g	605	CHL	C1A-C2A-CAA-CBA
46	g	607	CHL	C1A-C2A-CAA-CBA
46	g	607	CHL	C3A-C2A-CAA-CBA
46	y	311	CHL	C11-C12-C13-C14
47	N	616	LUT	C21-C26-C27-C28
47	R	310	LUT	C25-C26-C27-C28
47	S	317	LUT	C21-C26-C27-C28
47	Y	317	LUT	C21-C26-C27-C28
47	n	615	LUT	C21-C26-C27-C28
47	s	317	LUT	C21-C26-C27-C28
48	R	312	NEX	C12-C13-C14-C15
48	R	312	NEX	C32-C33-C34-C35
48	R	312	NEX	C40-C33-C34-C35
48	Y	318	NEX	C7-C8-C9-C10
48	Y	318	NEX	C10-C11-C12-C13
48	r	313	NEX	C12-C13-C14-C15
48	y	319	NEX	C7-C8-C9-C10
50	N	620	PTY	O4-C1-C6-O7
50	N	620	PTY	N1-C2-C3-O11
50	N	620	PTY	C3-O11-P1-O13
50	N	620	PTY	C3-O11-P1-O14
50	N	620	PTY	C5-O14-P1-O11
50	N	620	PTY	C5-O14-P1-O12
50	Y	320	PTY	C11-C8-O7-C6
50	Y	320	PTY	C3-O11-P1-O12
50	Y	320	PTY	C3-O11-P1-O13
50	Y	320	PTY	C3-O11-P1-O14
50	n	619	PTY	N1-C2-C3-O11
50	n	619	PTY	C3-O11-P1-O12
50	n	619	PTY	C3-O11-P1-O14
50	y	321	PTY	N1-C2-C3-O11
50	y	321	PTY	C3-O11-P1-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	y	321	PTY	C3-O11-P1-O14
51	S	321	LPX	C3-C4-C5-O6
51	S	321	LPX	C1-O2-P1-O1
51	S	321	LPX	C1-O2-P1-O3
51	s	321	LPX	C3-C4-C5-O6
51	s	321	LPX	C3-O1-P1-O3
51	s	321	LPX	C1-O2-P1-O4
29	r	308	CLA	O1D-CGD-O2D-CED
29	s	314	CLA	O1D-CGD-O2D-CED
50	y	321	PTY	C11-C8-O7-C6
29	a	404	CLA	O1D-CGD-O2D-CED
29	r	303	CLA	O1D-CGD-O2D-CED
29	C	504	CLA	CBD-CGD-O2D-CED
29	R	307	CLA	CBD-CGD-O2D-CED
29	S	304	CLA	CBD-CGD-O2D-CED
29	S	316	CLA	CBD-CGD-O2D-CED
29	Y	309	CLA	CBD-CGD-O2D-CED
29	b	505	CLA	CBD-CGD-O2D-CED
29	b	514	CLA	CBD-CGD-O2D-CED
29	c	502	CLA	CBD-CGD-O2D-CED
29	c	503	CLA	CBD-CGD-O2D-CED
29	n	604	CLA	CBD-CGD-O2D-CED
29	s	314	CLA	CBD-CGD-O2D-CED
29	B	501	CLA	O1A-CGA-O2A-C1
29	C	510	CLA	O1A-CGA-O2A-C1
29	R	302	CLA	O1A-CGA-O2A-C1
29	S	315	CLA	O1A-CGA-O2A-C1
29	n	610	CLA	O1A-CGA-O2A-C1
29	g	614	CLA	O1A-CGA-O2A-C1
29	r	307	CLA	O1A-CGA-O2A-C1
35	C	521	LMG	O10-C28-O8-C9
29	A	405	CLA	O1D-CGD-O2D-CED
29	S	314	CLA	O1D-CGD-O2D-CED
37	L	101	LHG	C5-C6-O8-C23
29	C	504	CLA	O1D-CGD-O2D-CED
29	S	304	CLA	O1D-CGD-O2D-CED
29	Y	309	CLA	O1D-CGD-O2D-CED
29	b	505	CLA	O1D-CGD-O2D-CED
29	S	315	CLA	CBA-CGA-O2A-C1
29	Y	305	CLA	CBA-CGA-O2A-C1
29	n	610	CLA	CBA-CGA-O2A-C1
29	g	614	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	r	307	CLA	CBA-CGA-O2A-C1
29	s	312	CLA	CBA-CGA-O2A-C1
50	Y	320	PTY	O10-C8-O7-C6
29	A	406	CLA	O1A-CGA-O2A-C1
29	C	514	CLA	O1A-CGA-O2A-C1
29	N	603	CLA	O1A-CGA-O2A-C1
29	N	611	CLA	O1A-CGA-O2A-C1
29	G	604	CLA	O1A-CGA-O2A-C1
29	G	611	CLA	O1A-CGA-O2A-C1
29	S	306	CLA	O1A-CGA-O2A-C1
29	S	314	CLA	O1A-CGA-O2A-C1
29	Y	305	CLA	O1A-CGA-O2A-C1
29	Y	309	CLA	O1A-CGA-O2A-C1
29	c	509	CLA	O1A-CGA-O2A-C1
29	g	604	CLA	O1A-CGA-O2A-C1
29	g	611	CLA	O1A-CGA-O2A-C1
29	r	303	CLA	O1A-CGA-O2A-C1
29	s	312	CLA	O1A-CGA-O2A-C1
29	s	314	CLA	O1A-CGA-O2A-C1
29	s	315	CLA	O1A-CGA-O2A-C1
29	y	306	CLA	O1A-CGA-O2A-C1
29	y	313	CLA	O1A-CGA-O2A-C1
33	A	412	3PH	O32-C31-O31-C3
35	C	522	LMG	O10-C28-O8-C9
35	C	524	LMG	O10-C28-O8-C9
35	W	203	LMG	O10-C28-O8-C9
35	c	520	LMG	O10-C28-O8-C9
50	n	619	PTY	O30-C30-O4-C1
29	C	502	CLA	O1D-CGD-O2D-CED
29	C	511	CLA	O1D-CGD-O2D-CED
29	N	613	CLA	O1D-CGD-O2D-CED
29	R	309	CLA	O1D-CGD-O2D-CED
29	y	306	CLA	O1D-CGD-O2D-CED
50	y	321	PTY	O10-C8-O7-C6
29	y	305	CLA	O1A-CGA-O2A-C1
33	A	412	3PH	O22-C21-O21-C2
33	s	322	3PH	O22-C21-O21-C2
35	B	520	LMG	O9-C10-O7-C8
35	W	203	LMG	O9-C10-O7-C8
35	b	520	LMG	O9-C10-O7-C8
36	B	521	DGD	O1B-C1B-O2G-C2G
39	o	301	SQD	O49-C7-O47-C45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
41	b	522	DGA	OB1-CB1-OG2-CG2
29	A	409	CLA	C3-C5-C6-C7
29	B	507	CLA	C3-C5-C6-C7
29	B	516	CLA	C3-C5-C6-C7
29	N	610	CLA	C3-C5-C6-C7
29	G	613	CLA	C3-C5-C6-C7
29	R	301	CLA	C3-C5-C6-C7
29	S	314	CLA	C3-C5-C6-C7
29	a	408	CLA	C3-C5-C6-C7
29	y	315	CLA	C3-C5-C6-C7
30	D	401	PHO	C3-C5-C6-C7
29	A	406	CLA	CBA-CGA-O2A-C1
29	B	501	CLA	CBA-CGA-O2A-C1
29	C	510	CLA	CBA-CGA-O2A-C1
29	C	513	CLA	CBA-CGA-O2A-C1
29	N	603	CLA	CBA-CGA-O2A-C1
29	N	611	CLA	CBA-CGA-O2A-C1
29	N	614	CLA	CBA-CGA-O2A-C1
29	G	611	CLA	CBA-CGA-O2A-C1
29	S	306	CLA	CBA-CGA-O2A-C1
29	Y	312	CLA	CBA-CGA-O2A-C1
29	a	404	CLA	CBA-CGA-O2A-C1
29	d	404	CLA	CBA-CGA-O2A-C1
29	g	602	CLA	CBA-CGA-O2A-C1
29	g	611	CLA	CBA-CGA-O2A-C1
29	g	613	CLA	CBA-CGA-O2A-C1
29	r	303	CLA	CBA-CGA-O2A-C1
29	s	314	CLA	CBA-CGA-O2A-C1
29	y	306	CLA	CBA-CGA-O2A-C1
29	y	310	CLA	CBA-CGA-O2A-C1
35	C	521	LMG	C29-C28-O8-C9
35	C	522	LMG	C29-C28-O8-C9
35	W	203	LMG	C29-C28-O8-C9
35	c	520	LMG	C29-C28-O8-C9
39	c	522	SQD	C24-C23-O48-C46
50	Y	320	PTY	O30-C30-O4-C1
29	B	509	CLA	CBD-CGD-O2D-CED
29	B	514	CLA	CBD-CGD-O2D-CED
29	C	503	CLA	CBD-CGD-O2D-CED
29	D	405	CLA	CBD-CGD-O2D-CED
29	N	604	CLA	CBD-CGD-O2D-CED
29	G	610	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	G	613	CLA	CBD-CGD-O2D-CED
29	Y	305	CLA	CBD-CGD-O2D-CED
29	c	510	CLA	CBD-CGD-O2D-CED
29	c	511	CLA	CBD-CGD-O2D-CED
33	A	412	3PH	C22-C21-O21-C2
33	S	322	3PH	C22-C21-O21-C2
33	a	415	3PH	C22-C21-O21-C2
33	b	521	3PH	C22-C21-O21-C2
35	B	520	LMG	C11-C10-O7-C8
35	b	520	LMG	C11-C10-O7-C8
36	r	301	DGD	C2B-C1B-O2G-C2G
41	D	402	DGA	CB2-CB1-OG2-CG2
29	G	612	CLA	O1D-CGD-O2D-CED
29	y	310	CLA	O1D-CGD-O2D-CED
29	A	407	CLA	O1A-CGA-O2A-C1
29	n	603	CLA	O1A-CGA-O2A-C1
29	B	504	CLA	C4-C3-C5-C6
29	B	507	CLA	C4-C3-C5-C6
29	C	505	CLA	C4-C3-C5-C6
29	b	502	CLA	C4-C3-C5-C6
29	r	307	CLA	C4-C3-C5-C6
46	N	606	CHL	C4-C3-C5-C6
46	n	601	CHL	C4-C3-C5-C6
46	g	609	CHL	C4-C3-C5-C6
29	B	507	CLA	C2-C3-C5-C6
29	C	505	CLA	C2-C3-C5-C6
29	b	502	CLA	C2-C3-C5-C6
29	r	307	CLA	C2-C3-C5-C6
46	n	601	CHL	C2-C3-C5-C6
46	g	609	CHL	C2-C3-C5-C6
29	R	307	CLA	CBA-CGA-O2A-C1
29	y	305	CLA	CBD-CGD-O2D-CED
29	S	316	CLA	O1D-CGD-O2D-CED
29	c	503	CLA	O1D-CGD-O2D-CED
29	Y	309	CLA	C2A-CAA-CBA-CGA
29	a	404	CLA	C2A-CAA-CBA-CGA
29	D	405	CLA	O1A-CGA-O2A-C1
29	b	504	CLA	C3-C5-C6-C7
29	b	509	CLA	C3-C5-C6-C7
29	g	613	CLA	C3-C5-C6-C7
29	s	310	CLA	C3-C5-C6-C7
29	A	405	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	C	514	CLA	CBA-CGA-O2A-C1
29	D	405	CLA	CBA-CGA-O2A-C1
29	G	604	CLA	CBA-CGA-O2A-C1
29	R	303	CLA	CBA-CGA-O2A-C1
29	R	306	CLA	CBA-CGA-O2A-C1
29	S	310	CLA	CBA-CGA-O2A-C1
29	S	314	CLA	CBA-CGA-O2A-C1
29	S	316	CLA	CBA-CGA-O2A-C1
29	Y	309	CLA	CBA-CGA-O2A-C1
29	c	509	CLA	CBA-CGA-O2A-C1
29	g	604	CLA	CBA-CGA-O2A-C1
29	s	315	CLA	CBA-CGA-O2A-C1
29	y	305	CLA	CBA-CGA-O2A-C1
29	y	313	CLA	CBA-CGA-O2A-C1
33	A	412	3PH	C32-C31-O31-C3
35	C	524	LMG	C29-C28-O8-C9
35	c	519	LMG	C29-C28-O8-C9
50	n	619	PTY	C31-C30-O4-C1
35	C	522	LMG	C41-C42-C43-C44
35	W	201	LMG	C17-C18-C19-C20
35	b	520	LMG	C17-C18-C19-C20
35	c	519	LMG	C35-C36-C37-C38
35	w	202	LMG	C35-C36-C37-C38
36	c	516	DGD	C8B-C9B-CAB-CBB
36	c	518	DGD	CBB-CCB-CDB-CEB
50	Y	320	PTY	C31-C30-O4-C1
50	y	321	PTY	C31-C30-O4-C1
35	D	410	LMG	C35-C36-C37-C38
35	c	520	LMG	C23-C24-C25-C26
35	D	409	LMG	C17-C18-C19-C20
35	d	408	LMG	C35-C36-C37-C38
36	C	518	DGD	C8B-C9B-CAB-CBB
29	A	405	CLA	O1A-CGA-O2A-C1
29	B	507	CLA	O1A-CGA-O2A-C1
29	R	303	CLA	O1A-CGA-O2A-C1
29	R	306	CLA	O1A-CGA-O2A-C1
29	S	304	CLA	O1A-CGA-O2A-C1
29	Y	304	CLA	O1A-CGA-O2A-C1
29	a	404	CLA	O1A-CGA-O2A-C1
29	a	405	CLA	O1A-CGA-O2A-C1
29	c	513	CLA	O1A-CGA-O2A-C1
29	d	404	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	y	310	CLA	O1A-CGA-O2A-C1
35	c	519	LMG	O10-C28-O8-C9
37	L	101	LHG	O10-C23-O8-C6
37	l	102	LHG	O10-C23-O8-C6
35	C	522	LMG	C17-C18-C19-C20
29	R	307	CLA	O1A-CGA-O2A-C1
35	B	520	LMG	C17-C18-C19-C20
35	C	521	LMG	C35-C36-C37-C38
35	D	410	LMG	C38-C39-C40-C41
35	W	203	LMG	C35-C36-C37-C38
35	W	203	LMG	C38-C39-C40-C41
35	c	519	LMG	C17-C18-C19-C20
35	c	519	LMG	C20-C21-C22-C23
35	c	520	LMG	C17-C18-C19-C20
35	c	520	LMG	C41-C42-C43-C44
35	d	407	LMG	C17-C18-C19-C20
35	d	407	LMG	C20-C21-C22-C23
35	d	408	LMG	C38-C39-C40-C41
35	i	101	LMG	C17-C18-C19-C20
35	i	101	LMG	C35-C36-C37-C38
35	i	101	LMG	C38-C39-C40-C41
35	w	202	LMG	C38-C39-C40-C41
36	C	519	DGD	CBB-CCB-CDB-CEB
36	c	517	DGD	C8A-C9A-CAA-CBA
36	c	517	DGD	CBB-CCB-CDB-CEB
29	c	502	CLA	O1D-CGD-O2D-CED
29	C	507	CLA	C3-C5-C6-C7
46	N	606	CHL	C3-C5-C6-C7
29	N	614	CLA	CBD-CGD-O2D-CED
29	c	501	CLA	CBD-CGD-O2D-CED
29	s	316	CLA	CBD-CGD-O2D-CED
35	c	520	LMG	C20-C21-C22-C23
37	B	523	LHG	O2-C2-C3-O3
37	L	101	LHG	O2-C2-C3-O3
37	N	618	LHG	O2-C2-C3-O3
37	S	301	LHG	O2-C2-C3-O3
37	Y	319	LHG	O2-C2-C3-O3
37	d	406	LHG	O2-C2-C3-O3
37	l	102	LHG	O2-C2-C3-O3
29	R	307	CLA	O1D-CGD-O2D-CED
29	A	407	CLA	CBA-CGA-O2A-C1
29	B	507	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	N	610	CLA	CBA-CGA-O2A-C1
29	G	602	CLA	CBA-CGA-O2A-C1
29	c	507	CLA	CBA-CGA-O2A-C1
29	n	612	CLA	CBA-CGA-O2A-C1
29	s	316	CLA	CBA-CGA-O2A-C1
33	a	415	3PH	C32-C31-O31-C3
37	l	102	LHG	C24-C23-O8-C6
29	C	513	CLA	O1A-CGA-O2A-C1
29	N	614	CLA	O1A-CGA-O2A-C1
29	g	602	CLA	O1A-CGA-O2A-C1
29	g	613	CLA	O1A-CGA-O2A-C1
29	s	316	CLA	O1A-CGA-O2A-C1
51	s	321	LPX	O5-C4-C5-O6
29	Y	315	CLA	CBD-CGD-O2D-CED
29	b	501	CLA	CBD-CGD-O2D-CED
37	n	617	LHG	C8-C7-O7-C5
41	b	522	DGA	CB2-CB1-OG2-CG2
33	a	415	3PH	O32-C31-O31-C3
36	c	516	DGD	O6E-C5E-C6E-O5E
29	B	504	CLA	C3-C5-C6-C7
29	S	311	CLA	C3-C5-C6-C7
29	n	612	CLA	C3-C5-C6-C7
46	g	601	CHL	C3-C5-C6-C7
29	N	603	CLA	CBD-CGD-O2D-CED
29	d	404	CLA	CBD-CGD-O2D-CED
29	b	514	CLA	O1D-CGD-O2D-CED
29	B	516	CLA	CBA-CGA-O2A-C1
29	S	304	CLA	CBA-CGA-O2A-C1
29	Y	304	CLA	CBA-CGA-O2A-C1
29	a	405	CLA	CBA-CGA-O2A-C1
29	c	513	CLA	CBA-CGA-O2A-C1
29	n	603	CLA	CBA-CGA-O2A-C1
37	L	101	LHG	C24-C23-O8-C6
29	B	509	CLA	C4-C3-C5-C6
29	C	508	CLA	C4-C3-C5-C6
29	R	308	CLA	C4-C3-C5-C6
29	a	408	CLA	C4-C3-C5-C6
29	B	509	CLA	C2-C3-C5-C6
46	N	606	CHL	C2-C3-C5-C6
29	G	602	CLA	O1A-CGA-O2A-C1
29	n	612	CLA	O1A-CGA-O2A-C1
43	D	406	PL9	C39-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
43	d	405	PL9	C39-C41-C42-C43
46	s	302	CHL	C2A-CAA-CBA-CGA
29	B	516	CLA	O1A-CGA-O2A-C1
29	N	610	CLA	O1A-CGA-O2A-C1
29	S	310	CLA	O1A-CGA-O2A-C1
29	S	316	CLA	O1A-CGA-O2A-C1
29	c	507	CLA	O1A-CGA-O2A-C1
35	C	524	LMG	O6-C1-O1-C7
35	i	101	LMG	O6-C1-O1-C7
39	M	101	SQD	O5-C1-O6-C44
29	n	604	CLA	O1D-CGD-O2D-CED
29	C	512	CLA	CBD-CGD-O2D-CED
29	N	612	CLA	CBD-CGD-O2D-CED
29	S	312	CLA	CBD-CGD-O2D-CED
29	b	515	CLA	CBD-CGD-O2D-CED
29	g	613	CLA	CBD-CGD-O2D-CED
29	r	304	CLA	CBD-CGD-O2D-CED
29	s	304	CLA	CBD-CGD-O2D-CED
29	s	305	CLA	CBD-CGD-O2D-CED
38	b	524	LMT	O5B-C5B-C6B-O6B
31	C	515	BCR	C9-C10-C11-C12
33	b	521	3PH	O32-C31-O31-C3
37	l	102	LHG	C1-C2-C3-O3
37	g	618	LHG	C1-C2-C3-O3
37	y	320	LHG	C1-C2-C3-O3
29	G	603	CLA	CBA-CGA-O2A-C1
29	R	309	CLA	CBA-CGA-O2A-C1
29	S	311	CLA	CBA-CGA-O2A-C1
29	g	603	CLA	CBA-CGA-O2A-C1
29	r	304	CLA	CBA-CGA-O2A-C1
29	s	306	CLA	CBA-CGA-O2A-C1
29	y	316	CLA	CBA-CGA-O2A-C1
33	b	521	3PH	C32-C31-O31-C3
36	C	520	DGD	C2A-C1A-O1G-C1G
37	D	408	LHG	C24-C23-O8-C6
39	M	101	SQD	C24-C23-O48-C46
39	m	101	SQD	C24-C23-O48-C46
51	S	321	LPX	C7-C6-O6-C5
29	B	513	CLA	CBD-CGD-O2D-CED
29	B	516	CLA	CBD-CGD-O2D-CED
37	N	618	LHG	C11-C12-C13-C14
37	N	618	LHG	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	B	504	CLA	C2-C3-C5-C6
29	R	308	CLA	C2-C3-C5-C6
29	g	602	CLA	CBD-CGD-O2D-CED
29	A	409	CLA	C6-C7-C8-C9
29	B	502	CLA	C14-C13-C15-C16
29	B	504	CLA	C6-C7-C8-C9
29	B	509	CLA	C6-C7-C8-C9
29	B	513	CLA	C11-C12-C13-C14
29	B	515	CLA	C11-C10-C8-C9
29	C	502	CLA	C11-C12-C13-C14
29	C	507	CLA	C6-C7-C8-C9
29	C	510	CLA	C6-C7-C8-C9
29	C	514	CLA	C11-C10-C8-C9
29	D	404	CLA	C6-C7-C8-C9
29	N	604	CLA	C11-C12-C13-C14
29	G	611	CLA	C14-C13-C15-C16
29	R	301	CLA	C6-C7-C8-C9
29	R	308	CLA	C6-C7-C8-C9
29	S	303	CLA	C11-C10-C8-C9
29	S	312	CLA	C6-C7-C8-C9
29	Y	304	CLA	C6-C7-C8-C9
29	Y	305	CLA	C11-C10-C8-C9
29	Y	314	CLA	C6-C7-C8-C9
29	b	514	CLA	C11-C12-C13-C14
29	b	515	CLA	C11-C10-C8-C9
29	b	516	CLA	C14-C13-C15-C16
29	c	501	CLA	C11-C12-C13-C14
29	c	504	CLA	C11-C12-C13-C14
29	c	506	CLA	C6-C7-C8-C9
29	c	513	CLA	C11-C10-C8-C9
29	n	604	CLA	C14-C13-C15-C16
29	r	302	CLA	C6-C7-C8-C9
29	s	311	CLA	C6-C7-C8-C9
29	y	305	CLA	C6-C7-C8-C9
46	N	605	CHL	C14-C13-C15-C16
46	N	607	CHL	C14-C13-C15-C16
46	G	609	CHL	C14-C13-C15-C16
46	Y	308	CHL	C6-C7-C8-C9
46	Y	308	CHL	C14-C13-C15-C16
46	Y	310	CHL	C11-C12-C13-C14
46	n	601	CHL	C11-C10-C8-C9
46	n	608	CHL	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	g	601	CHL	C14-C13-C15-C16
46	g	609	CHL	C14-C13-C15-C16
46	y	309	CHL	C6-C7-C8-C9
46	y	309	CHL	C14-C13-C15-C16
29	B	509	CLA	O1D-CGD-O2D-CED
29	B	514	CLA	O1D-CGD-O2D-CED
29	N	604	CLA	O1D-CGD-O2D-CED
29	G	613	CLA	O1D-CGD-O2D-CED
35	C	524	LMG	C2-C1-O1-C7
39	L	102	SQD	C2-C1-O6-C44
39	M	101	SQD	C2-C1-O6-C44
39	b	523	SQD	C2-C1-O6-C44
39	l	101	SQD	C2-C1-O6-C44
33	s	322	3PH	C31-C32-C33-C34
37	L	101	LHG	C7-C8-C9-C10
29	C	503	CLA	O1D-CGD-O2D-CED
29	G	610	CLA	O1D-CGD-O2D-CED
29	g	603	CLA	O1A-CGA-O2A-C1
29	s	306	CLA	O1A-CGA-O2A-C1
29	b	516	CLA	CBD-CGD-O2D-CED
29	Y	305	CLA	O1D-CGD-O2D-CED
31	A	410	BCR	C36-C18-C19-C20
31	B	517	BCR	C36-C18-C19-C20
31	B	517	BCR	C37-C22-C23-C24
31	B	518	BCR	C11-C12-C13-C35
31	C	515	BCR	C36-C18-C19-C20
31	C	516	BCR	C7-C8-C9-C34
31	F	101	BCR	C11-C12-C13-C35
31	a	409	BCR	C36-C18-C19-C20
31	b	517	BCR	C36-C18-C19-C20
31	b	517	BCR	C37-C22-C23-C24
31	b	518	BCR	C7-C8-C9-C34
31	c	514	BCR	C36-C18-C19-C20
31	z	101	BCR	C7-C8-C9-C34
31	z	101	BCR	C36-C18-C19-C20
45	h	101	RRX	C11-C12-C13-C35
45	h	101	RRX	C7-C8-C9-C34
31	v	101	BCR	C21-C22-C23-C24
45	h	101	RRX	C7-C8-C9-C10
41	j	101	DGA	CB1-CB2-CB3-CB4
29	G	603	CLA	O1A-CGA-O2A-C1
29	R	309	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	y	316	CLA	O1A-CGA-O2A-C1
37	D	408	LHG	O10-C23-O8-C6
51	S	321	LPX	O7-C6-O6-C5
29	A	405	CLA	C4C-C3C-CAC-CBC
37	n	617	LHG	O9-C7-O7-C5
37	N	618	LHG	C8-C7-O7-C5
41	W	202	DGA	CB2-CB1-OG2-CG2
29	Y	313	CLA	CBA-CGA-O2A-C1
37	S	301	LHG	C23-C24-C25-C26
29	C	510	CLA	C2-C1-O2A-CGA
50	y	321	PTY	O30-C30-O4-C1
29	D	405	CLA	O1D-CGD-O2D-CED
29	c	511	CLA	O1D-CGD-O2D-CED
30	A	408	PHO	CBD-CGD-O2D-CED
29	B	509	CLA	C5-C6-C7-C8
29	B	515	CLA	C13-C15-C16-C17
29	c	504	CLA	C13-C15-C16-C17
29	c	510	CLA	C8-C10-C11-C12
29	y	312	CLA	C13-C15-C16-C17
46	G	609	CHL	C8-C10-C11-C12
43	d	405	PL9	C47-C48-C49-C51
29	c	510	CLA	O1D-CGD-O2D-CED
37	L	101	LHG	O1-C1-C2-O2
37	g	618	LHG	O1-C1-C2-O2
37	n	617	LHG	C23-C24-C25-C26
29	C	510	CLA	C15-C16-C17-C18
46	G	607	CHL	C10-C11-C12-C13
29	G	614	CLA	CBD-CGD-O2D-CED
29	b	506	CLA	CBD-CGD-O2D-CED
29	y	316	CLA	CBD-CGD-O2D-CED
29	b	513	CLA	C11-C10-C8-C7
29	r	308	CLA	C6-C7-C8-C10
29	y	316	CLA	C6-C7-C8-C10
46	Y	307	CHL	C12-C13-C15-C16
46	y	303	CHL	C12-C13-C15-C16
29	s	310	CLA	CBA-CGA-O2A-C1
29	n	609	CLA	C4-C3-C5-C6
29	B	513	CLA	C10-C11-C12-C13
29	N	613	CLA	C5-C6-C7-C8
29	c	508	CLA	C5-C6-C7-C8
35	b	520	LMG	C28-C29-C30-C31
37	l	102	LHG	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	c	514	BCR	C19-C20-C21-C22
45	h	101	RRX	C19-C20-C21-C22
47	N	616	LUT	C29-C30-C31-C32
47	n	615	LUT	C29-C30-C31-C32
33	s	322	3PH	C34-C35-C36-C37
38	b	524	LMT	C4B-C5B-C6B-O6B
46	G	608	CHL	C2A-CAA-CBA-CGA
29	C	505	CLA	C5-C6-C7-C8
29	Y	303	CLA	C13-C15-C16-C17
46	G	607	CHL	C13-C15-C16-C17
35	c	519	LMG	C28-C29-C30-C31
37	N	618	LHG	C7-C8-C9-C10
37	a	413	LHG	C7-C8-C9-C10
41	J	101	DGA	CB1-CB2-CB3-CB4
41	W	202	DGA	CB1-CB2-CB3-CB4
50	n	619	PTY	C8-C11-C12-C13
29	S	311	CLA	O1A-CGA-O2A-C1
29	r	304	CLA	O1A-CGA-O2A-C1
36	C	520	DGD	O1A-C1A-O1G-C1G
39	M	101	SQD	O10-C23-O48-C46
29	B	507	CLA	C8-C10-C11-C12
29	C	514	CLA	C8-C10-C11-C12
29	G	602	CLA	C13-C15-C16-C17
29	S	312	CLA	C15-C16-C17-C18
29	Y	314	CLA	C15-C16-C17-C18
29	b	503	CLA	C8-C10-C11-C12
29	d	404	CLA	C8-C10-C11-C12
29	n	604	CLA	C8-C10-C11-C12
29	y	306	CLA	C13-C15-C16-C17
29	y	315	CLA	C15-C16-C17-C18
29	y	316	CLA	C8-C10-C11-C12
46	N	607	CHL	C8-C10-C11-C12
46	Y	307	CHL	C5-C6-C7-C8
44	E	101	HEM	C3D-CAD-CBD-CGD
29	A	405	CLA	C2A-CAA-CBA-CGA
29	B	512	CLA	C2A-CAA-CBA-CGA
29	R	309	CLA	C2A-CAA-CBA-CGA
29	s	304	CLA	C2A-CAA-CBA-CGA
29	s	316	CLA	C2A-CAA-CBA-CGA
46	N	605	CHL	C2A-CAA-CBA-CGA
46	N	606	CHL	C2A-CAA-CBA-CGA
46	N	608	CHL	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	Y	306	CHL	C2A-CAA-CBA-CGA
46	Y	308	CHL	C2A-CAA-CBA-CGA
31	K	101	BCR	C10-C11-C12-C13
31	v	101	BCR	C10-C11-C12-C13
48	y	319	NEX	C10-C11-C12-C13
29	C	507	CLA	C5-C6-C7-C8
29	C	509	CLA	C5-C6-C7-C8
29	G	603	CLA	C5-C6-C7-C8
29	b	501	CLA	C10-C11-C12-C13
29	b	507	CLA	C10-C11-C12-C13
29	c	503	CLA	C15-C16-C17-C18
29	s	310	CLA	C10-C11-C12-C13
29	s	312	CLA	C15-C16-C17-C18
35	D	410	LMG	C28-C29-C30-C31
36	C	518	DGD	C1B-C2B-C3B-C4B
37	D	407	LHG	C7-C8-C9-C10
37	D	408	LHG	C23-C24-C25-C26
37	S	320	LHG	C23-C24-C25-C26
37	a	414	LHG	C23-C24-C25-C26
37	d	406	LHG	C7-C8-C9-C10
39	M	101	SQD	C7-C8-C9-C10
39	m	101	SQD	C7-C8-C9-C10
41	W	202	DGA	CA1-CA2-CA3-CA4
39	m	101	SQD	O10-C23-O48-C46
36	B	521	DGD	O6D-C1D-O3G-C3G
39	m	101	SQD	O5-C1-O6-C44
33	s	322	3PH	C32-C33-C34-C35
37	B	523	LHG	C31-C32-C33-C34
29	C	504	CLA	C15-C16-C17-C18
29	C	508	CLA	C15-C16-C17-C18
29	G	611	CLA	C10-C11-C12-C13
29	R	308	CLA	C5-C6-C7-C8
29	S	314	CLA	C5-C6-C7-C8
29	Y	312	CLA	C5-C6-C7-C8
29	Y	315	CLA	C8-C10-C11-C12
29	b	507	CLA	C13-C15-C16-C17
29	d	404	CLA	C10-C11-C12-C13
29	g	611	CLA	C10-C11-C12-C13
46	G	607	CHL	C15-C16-C17-C18
46	S	309	CHL	C5-C6-C7-C8
37	a	413	LHG	O2-C2-C3-O3
37	c	521	LHG	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	g	618	LHG	O2-C2-C3-O3
29	b	516	CLA	CBA-CGA-O2A-C1
36	c	518	DGD	C2A-C1A-O1G-C1G
46	S	307	CHL	C2A-CAA-CBA-CGA
37	D	407	LHG	C23-C24-C25-C26
37	N	618	LHG	C23-C24-C25-C26
37	a	414	LHG	C7-C8-C9-C10
37	n	617	LHG	C7-C8-C9-C10
29	B	507	CLA	C5-C6-C7-C8
29	C	504	CLA	C5-C6-C7-C8
29	Y	303	CLA	C15-C16-C17-C18
29	y	305	CLA	O1D-CGD-O2D-CED
29	B	503	CLA	C15-C16-C17-C18
29	N	613	CLA	C8-C10-C11-C12
29	G	611	CLA	C13-C15-C16-C17
29	Y	315	CLA	C5-C6-C7-C8
29	b	516	CLA	C13-C15-C16-C17
29	g	602	CLA	C8-C10-C11-C12
29	g	602	CLA	C13-C15-C16-C17
29	Y	313	CLA	O1A-CGA-O2A-C1
29	a	408	CLA	C2-C3-C5-C6
37	l	102	LHG	C5-C6-O8-C23
29	N	614	CLA	O1D-CGD-O2D-CED
29	B	505	CLA	C5-C6-C7-C8
29	C	509	CLA	C15-C16-C17-C18
29	D	404	CLA	C8-C10-C11-C12
29	G	602	CLA	C8-C10-C11-C12
29	Y	311	CLA	C5-C6-C7-C8
29	b	509	CLA	C15-C16-C17-C18
29	c	503	CLA	C5-C6-C7-C8
29	r	307	CLA	C10-C11-C12-C13
37	a	414	LHG	C24-C23-O8-C6
39	l	101	SQD	C24-C23-O48-C46
29	r	307	CLA	CBD-CGD-O2D-CED
39	L	102	SQD	C8-C7-O47-C45
39	M	101	SQD	C8-C7-O47-C45
33	S	322	3PH	C32-C33-C34-C35
29	c	501	CLA	O1D-CGD-O2D-CED
29	s	316	CLA	O1D-CGD-O2D-CED
33	s	322	3PH	C21-C22-C23-C24
29	B	507	CLA	C13-C15-C16-C17
29	b	509	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	r	302	CLA	C3-C5-C6-C7
29	n	611	CLA	CBD-CGD-O2D-CED
31	b	517	BCR	C9-C10-C11-C12
47	Y	317	LUT	C29-C30-C31-C32
47	y	318	LUT	C29-C30-C31-C32
29	y	314	CLA	C13-C15-C16-C17
46	Y	307	CHL	C15-C16-C17-C18
36	c	516	DGD	C1B-C2B-C3B-C4B
37	N	618	LHG	O9-C7-O7-C5
39	L	102	SQD	O49-C7-O47-C45
39	M	101	SQD	O49-C7-O47-C45
41	W	202	DGA	OB1-CB1-OG2-CG2
29	C	508	CLA	C2A-CAA-CBA-CGA
29	r	308	CLA	C2A-CAA-CBA-CGA
46	n	607	CHL	C2A-CAA-CBA-CGA
46	y	307	CHL	C2A-CAA-CBA-CGA
29	b	501	CLA	CBA-CGA-O2A-C1
29	s	304	CLA	CBA-CGA-O2A-C1
29	s	311	CLA	CBA-CGA-O2A-C1
33	S	322	3PH	C32-C31-O31-C3
36	B	521	DGD	C2A-C1A-O1G-C1G
29	S	312	CLA	C8-C10-C11-C12
29	Y	313	CLA	C15-C16-C17-C18
29	b	511	CLA	C13-C15-C16-C17
29	c	510	CLA	C15-C16-C17-C18
29	g	613	CLA	C13-C15-C16-C17
29	s	312	CLA	C8-C10-C11-C12
29	s	312	CLA	C10-C11-C12-C13
46	N	601	CHL	C13-C15-C16-C17
46	G	607	CHL	C5-C6-C7-C8
46	Y	308	CHL	C5-C6-C7-C8
29	G	611	CLA	CBD-CGD-O2D-CED
29	c	507	CLA	CBD-CGD-O2D-CED
37	S	320	LHG	C30-C31-C32-C33
29	Y	315	CLA	O1D-CGD-O2D-CED
29	b	501	CLA	O1D-CGD-O2D-CED
35	B	520	LMG	C28-C29-C30-C31
29	B	511	CLA	C13-C15-C16-C17
29	C	511	CLA	C15-C16-C17-C18
29	S	312	CLA	C5-C6-C7-C8
29	Y	314	CLA	C5-C6-C7-C8
29	Y	314	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	b	501	CLA	C13-C15-C16-C17
29	c	512	CLA	C5-C6-C7-C8
29	g	603	CLA	C5-C6-C7-C8
46	y	301	CHL	C15-C16-C17-C18
36	C	518	DGD	O6E-C5E-C6E-O5E
29	B	501	CLA	C13-C15-C16-C17
29	C	508	CLA	C13-C15-C16-C17
29	Y	313	CLA	C13-C15-C16-C17
29	b	505	CLA	C5-C6-C7-C8
29	b	515	CLA	C13-C15-C16-C17
29	c	509	CLA	C15-C16-C17-C18
29	y	314	CLA	C8-C10-C11-C12
46	g	607	CHL	C5-C6-C7-C8
46	s	309	CHL	C8-C10-C11-C12
29	B	512	CLA	CBA-CGA-O2A-C1
29	B	516	CLA	C4-C3-C5-C6
29	b	503	CLA	C4-C3-C5-C6
29	s	311	CLA	C4-C3-C5-C6
46	G	609	CHL	C4-C3-C5-C6
29	C	508	CLA	C2-C3-C5-C6
29	N	603	CLA	C8-C10-C11-C12
29	b	516	CLA	C5-C6-C7-C8
29	c	504	CLA	C10-C11-C12-C13
46	N	605	CHL	C13-C15-C16-C17
46	y	309	CHL	C5-C6-C7-C8
39	b	523	SQD	C8-C7-O47-C45
50	n	619	PTY	C11-C8-O7-C6
29	b	503	CLA	C11-C10-C8-C9
39	b	523	SQD	O49-C7-O47-C45
39	m	101	SQD	O49-C7-O47-C45
36	B	521	DGD	C2D-C1D-O3G-C3G
36	r	301	DGD	C2D-C1D-O3G-C3G
39	m	101	SQD	C2-C1-O6-C44
29	Y	313	CLA	C8-C10-C11-C12
29	N	603	CLA	O1D-CGD-O2D-CED
29	a	405	CLA	C2C-C3C-CAC-CBC
29	b	514	CLA	CBA-CGA-O2A-C1
29	C	502	CLA	C16-C17-C18-C19
29	Y	314	CLA	C16-C17-C18-C20
29	b	502	CLA	C13-C15-C16-C17
31	C	516	BCR	C11-C10-C9-C34
48	N	617	NEX	C39-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	R	312	NEX	C39-C29-C30-C31
48	Y	318	NEX	C11-C10-C9-C19
48	Y	318	NEX	C39-C29-C30-C31
48	n	616	NEX	C39-C29-C30-C31
48	g	617	NEX	C11-C10-C9-C19
48	y	319	NEX	C11-C10-C9-C19
37	a	413	LHG	C23-C24-C25-C26
29	C	508	CLA	CBD-CGD-O2D-CED
29	c	511	CLA	C8-C10-C11-C12
31	K	101	BCR	C37-C22-C23-C24
31	b	518	BCR	C36-C18-C19-C20
31	v	101	BCR	C37-C22-C23-C24
34	b	519	C7Z	C7-C8-C9-C19
45	H	101	RRX	C11-C12-C13-C35
45	H	101	RRX	C7-C8-C9-C34
47	R	310	LUT	C7-C8-C9-C19
47	r	311	LUT	C7-C8-C9-C19
31	A	410	BCR	C17-C18-C19-C20
31	B	518	BCR	C11-C12-C13-C14
31	F	101	BCR	C11-C12-C13-C14
31	K	101	BCR	C21-C22-C23-C24
34	b	519	C7Z	C7-C8-C9-C10
45	H	101	RRX	C7-C8-C9-C10
45	h	101	RRX	C11-C12-C13-C14
47	r	311	LUT	C7-C8-C9-C10
44	e	101	HEM	C3D-CAD-CBD-CGD
29	b	501	CLA	O1A-CGA-O2A-C1
29	s	310	CLA	O1A-CGA-O2A-C1
36	B	521	DGD	O1A-C1A-O1G-C1G
29	r	304	CLA	C2A-CAA-CBA-CGA
29	s	305	CLA	C2A-CAA-CBA-CGA
46	S	309	CHL	C2A-CAA-CBA-CGA
46	Y	307	CHL	C2A-CAA-CBA-CGA
46	y	308	CHL	C2A-CAA-CBA-CGA
29	n	604	CLA	C13-C15-C16-C17
37	B	523	LHG	O1-C1-C2-C3
37	D	407	LHG	O1-C1-C2-C3
37	G	618	LHG	O1-C1-C2-C3
37	S	320	LHG	O1-C1-C2-C3
37	Y	319	LHG	O1-C1-C2-C3
37	a	414	LHG	O1-C1-C2-C3
37	c	521	LHG	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	d	406	LHG	O1-C1-C2-C3
37	g	618	LHG	O1-C1-C2-C3
37	y	320	LHG	O1-C1-C2-C3
36	c	518	DGD	C1A-C2A-C3A-C4A
29	A	405	CLA	O2A-C1-C2-C3
29	a	404	CLA	O2A-C1-C2-C3
35	B	520	LMG	C9-C8-O7-C10
29	D	404	CLA	C16-C17-C18-C20
29	R	306	CLA	C11-C12-C13-C15
29	Y	315	CLA	C16-C17-C18-C19
29	c	501	CLA	C16-C17-C18-C19
29	c	501	CLA	C16-C17-C18-C20
29	d	403	CLA	C16-C17-C18-C20
29	g	602	CLA	C16-C17-C18-C20
29	r	309	CLA	C11-C12-C13-C15
29	y	316	CLA	C16-C17-C18-C19
29	d	404	CLA	O1D-CGD-O2D-CED
29	C	513	CLA	C3-C5-C6-C7
46	S	309	CHL	C3-C5-C6-C7
31	C	516	BCR	C11-C10-C9-C8
48	N	617	NEX	C28-C29-C30-C31
48	R	312	NEX	C28-C29-C30-C31
48	Y	318	NEX	C11-C10-C9-C8
48	Y	318	NEX	C28-C29-C30-C31
48	n	616	NEX	C28-C29-C30-C31
48	g	617	NEX	C11-C10-C9-C8
48	r	313	NEX	C28-C29-C30-C31
48	y	319	NEX	C11-C10-C9-C8
50	n	619	PTY	O10-C8-O7-C6
36	r	301	DGD	O6D-C1D-O3G-C3G
35	W	201	LMG	C11-C10-O7-C8
35	c	519	LMG	C11-C10-O7-C8
39	m	101	SQD	C8-C7-O47-C45
39	a	410	SQD	O47-C45-C46-O48
36	c	516	DGD	C4E-C5E-C6E-O5E
39	L	102	SQD	C24-C23-O48-C46
29	N	603	CLA	C2-C1-O2A-CGA
29	Y	309	CLA	C2-C1-O2A-CGA
29	b	501	CLA	C2-C1-O2A-CGA
29	s	312	CLA	C2-C1-O2A-CGA
29	B	512	CLA	C16-C17-C18-C20
29	Y	315	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	c	512	CLA	C16-C17-C18-C20
29	d	403	CLA	C16-C17-C18-C19
29	s	305	CLA	C6-C7-C8-C9
29	s	305	CLA	C6-C7-C8-C10
33	S	322	3PH	O32-C31-O31-C3
29	S	314	CLA	C4C-C3C-CAC-CBC
33	a	415	3PH	C39-C3A-C3B-C3C
35	c	520	LMG	C29-C30-C31-C32
37	L	101	LHG	C9-C10-C11-C12
37	L	101	LHG	C33-C34-C35-C36
37	y	320	LHG	C28-C29-C30-C31
48	R	312	NEX	C14-C15-C35-C34
33	B	522	3PH	C24-C25-C26-C27
33	s	322	3PH	C24-C25-C26-C27
39	o	301	SQD	C12-C13-C14-C15
41	W	202	DGA	CCA-CDA-CEA-CFA
29	r	304	CLA	O1D-CGD-O2D-CED
29	b	508	CLA	C13-C15-C16-C17
29	c	505	CLA	C13-C15-C16-C17
29	s	304	CLA	C15-C16-C17-C18
33	a	415	3PH	C32-C33-C34-C35
37	S	301	LHG	C25-C26-C27-C28
37	a	413	LHG	C25-C26-C27-C28
37	l	102	LHG	C28-C29-C30-C31
29	b	516	CLA	O1A-CGA-O2A-C1
36	c	518	DGD	O1A-C1A-O1G-C1G
29	B	514	CLA	CBA-CGA-O2A-C1
38	b	524	LMT	C1-C2-C3-C4
33	B	522	3PH	C26-C27-C28-C29
33	b	521	3PH	C24-C25-C26-C27
37	Y	319	LHG	C26-C27-C28-C29
39	c	522	SQD	C17-C18-C19-C20
40	C	525	SPH	C14-C15-C16-C17
35	W	201	LMG	O9-C10-O7-C8
37	D	407	LHG	O1-C1-C2-O2
37	S	301	LHG	O1-C1-C2-O2
37	a	413	LHG	O1-C1-C2-O2
37	a	414	LHG	O1-C1-C2-O2
37	l	102	LHG	O1-C1-C2-O2
37	y	320	LHG	O1-C1-C2-O2
38	b	524	LMT	C2-C1-O1'-C1'
37	N	618	LHG	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	y	320	LHG	C13-C14-C15-C16
29	N	612	CLA	O1D-CGD-O2D-CED
29	a	404	CLA	C4C-C3C-CAC-CBC
29	A	407	CLA	C4B-C3B-CAB-CBB
29	B	501	CLA	C4B-C3B-CAB-CBB
29	N	611	CLA	C4B-C3B-CAB-CBB
29	N	614	CLA	C4B-C3B-CAB-CBB
29	G	611	CLA	C4B-C3B-CAB-CBB
29	R	306	CLA	C4B-C3B-CAB-CBB
29	S	306	CLA	C4B-C3B-CAB-CBB
29	S	310	CLA	C4B-C3B-CAB-CBB
29	Y	304	CLA	C4B-C3B-CAB-CBB
29	b	509	CLA	C4B-C3B-CAB-CBB
29	b	510	CLA	C4B-C3B-CAB-CBB
37	L	101	LHG	C11-C12-C13-C14
37	s	320	LHG	C12-C13-C14-C15
41	j	101	DGA	CB6-CB7-CB8-CB9
29	C	502	CLA	C16-C17-C18-C20
29	C	510	CLA	C16-C17-C18-C19
29	C	510	CLA	C16-C17-C18-C20
29	D	404	CLA	C16-C17-C18-C19
29	R	306	CLA	C11-C12-C13-C14
29	a	408	CLA	C11-C12-C13-C14
29	a	408	CLA	C11-C12-C13-C15
29	c	509	CLA	C16-C17-C18-C19
29	c	509	CLA	C16-C17-C18-C20
29	c	512	CLA	C16-C17-C18-C19
29	g	613	CLA	C16-C17-C18-C20
29	y	316	CLA	C16-C17-C18-C20
30	a	407	PHO	C16-C17-C18-C20
39	l	101	SQD	O10-C23-O48-C46
33	b	521	3PH	C37-C38-C39-C3A
37	c	521	LHG	C13-C14-C15-C16
37	n	617	LHG	C24-C25-C26-C27
46	s	307	CHL	C2A-CAA-CBA-CGA
29	B	511	CLA	C15-C16-C17-C18
29	C	513	CLA	C5-C6-C7-C8
29	R	306	CLA	C5-C6-C7-C8
37	S	320	LHG	C8-C7-O7-C5
37	Y	319	LHG	C8-C7-O7-C5
37	y	320	LHG	C8-C7-O7-C5
33	s	322	3PH	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	c	517	DGD	C5A-C6A-C7A-C8A
37	D	408	LHG	C9-C10-C11-C12
29	B	501	CLA	C11-C10-C8-C7
29	N	613	CLA	C11-C12-C13-C15
29	n	609	CLA	C12-C13-C15-C16
36	C	519	DGD	C4B-C5B-C6B-C7B
37	Y	319	LHG	C33-C34-C35-C36
37	L	101	LHG	C23-C24-C25-C26
29	s	305	CLA	O1D-CGD-O2D-CED
29	Y	314	CLA	C10-C11-C12-C13
33	A	412	3PH	C38-C39-C3A-C3B
33	B	522	3PH	C3C-C3D-C3E-C3F
33	s	322	3PH	C2A-C2B-C2C-C2D
37	g	618	LHG	C11-C12-C13-C14
37	y	320	LHG	C11-C12-C13-C14
29	s	311	CLA	O1A-CGA-O2A-C1
29	A	406	CLA	C3-C5-C6-C7
46	G	601	CHL	C3-C5-C6-C7
29	N	603	CLA	C3A-C2A-CAA-CBA
29	G	614	CLA	C3A-C2A-CAA-CBA
29	R	309	CLA	C3A-C2A-CAA-CBA
29	S	306	CLA	C3A-C2A-CAA-CBA
29	S	315	CLA	C3A-C2A-CAA-CBA
29	Y	309	CLA	C3A-C2A-CAA-CBA
29	b	504	CLA	C3A-C2A-CAA-CBA
29	c	504	CLA	C4-C3-C5-C6
29	c	513	CLA	C3A-C2A-CAA-CBA
29	n	612	CLA	C3A-C2A-CAA-CBA
29	g	603	CLA	C3A-C2A-CAA-CBA
29	r	308	CLA	C3A-C2A-CAA-CBA
29	r	310	CLA	C3A-C2A-CAA-CBA
29	s	306	CLA	C3A-C2A-CAA-CBA
29	y	305	CLA	C3A-C2A-CAA-CBA
30	a	407	PHO	C3A-C2A-CAA-CBA
46	G	606	CHL	C3A-C2A-CAA-CBA
46	g	605	CHL	C3A-C2A-CAA-CBA
46	y	303	CHL	C3A-C2A-CAA-CBA
29	g	613	CLA	O1D-CGD-O2D-CED
37	n	617	LHG	C11-C12-C13-C14
37	n	617	LHG	C14-C15-C16-C17
29	s	310	CLA	CBD-CGD-O2D-CED
33	B	522	3PH	C29-C2A-C2B-C2C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	c	521	LHG	C11-C12-C13-C14
29	B	503	CLA	C10-C11-C12-C13
29	b	503	CLA	C15-C16-C17-C18
35	C	524	LMG	C8-C9-O8-C28
29	S	312	CLA	O1D-CGD-O2D-CED
37	D	407	LHG	C13-C14-C15-C16
31	C	517	BCR	C9-C10-C11-C12
31	c	514	BCR	C9-C10-C11-C12
47	g	616	LUT	C29-C30-C31-C32
29	b	501	CLA	C16-C17-C18-C20
29	g	602	CLA	C16-C17-C18-C19
29	g	613	CLA	C16-C17-C18-C19
29	r	309	CLA	C11-C12-C13-C14
46	Y	307	CHL	C16-C17-C18-C19
29	s	304	CLA	O1A-CGA-O2A-C1
41	D	402	DGA	CB5-CB6-CB7-CB8
35	c	520	LMG	O1-C7-C8-C9
37	G	618	LHG	C13-C14-C15-C16
37	Y	319	LHG	C11-C10-C9-C8
37	y	320	LHG	C29-C30-C31-C32
40	C	525	SPH	C11-C10-C9-C8
50	n	619	PTY	C31-C32-C33-C34
29	d	404	CLA	C3-C5-C6-C7
29	r	303	CLA	C3-C5-C6-C7
35	d	408	LMG	C28-C29-C30-C31
41	D	402	DGA	CB1-CB2-CB3-CB4
29	c	510	CLA	C13-C15-C16-C17
29	y	305	CLA	C15-C16-C17-C18
46	r	306	CHL	C2C-C3C-CAC-CBC
29	C	512	CLA	O1D-CGD-O2D-CED
33	B	522	3PH	C2B-C2C-C2D-C2E
35	C	524	LMG	C14-C15-C16-C17
35	d	408	LMG	C12-C13-C14-C15
35	i	101	LMG	C39-C40-C41-C42
36	c	517	DGD	C4B-C5B-C6B-C7B
37	N	618	LHG	C25-C26-C27-C28
37	Y	319	LHG	C13-C14-C15-C16
37	g	618	LHG	C11-C10-C9-C8
37	g	618	LHG	C9-C10-C11-C12
37	g	618	LHG	C13-C14-C15-C16
37	s	320	LHG	C13-C14-C15-C16
41	W	202	DGA	CA8-CA9-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
41	w	201	DGA	CB4-CB5-CB6-CB7
50	N	620	PTY	C36-C37-C38-C39
29	B	512	CLA	O1A-CGA-O2A-C1
29	b	514	CLA	O1A-CGA-O2A-C1
37	a	414	LHG	O10-C23-O8-C6
37	B	523	LHG	C28-C29-C30-C31
37	a	413	LHG	C11-C12-C13-C14
41	D	402	DGA	CA4-CA5-CA6-CA7
35	D	410	LMG	C13-C14-C15-C16
37	d	406	LHG	C34-C35-C36-C37
37	n	617	LHG	C13-C14-C15-C16
37	s	320	LHG	C30-C31-C32-C33
29	D	405	CLA	C11-C12-C13-C15
29	b	511	CLA	C16-C17-C18-C20
29	B	504	CLA	C2B-C3B-CAB-CBB
29	C	505	CLA	C2B-C3B-CAB-CBB
29	Y	309	CLA	C2B-C3B-CAB-CBB
29	Y	315	CLA	C2B-C3B-CAB-CBB
29	b	504	CLA	C2B-C3B-CAB-CBB
29	d	403	CLA	C2B-C3B-CAB-CBB
31	A	410	BCR	C23-C24-C25-C30
31	C	515	BCR	C1-C6-C7-C8
31	C	515	BCR	C5-C6-C7-C8
31	K	101	BCR	C1-C6-C7-C8
31	b	517	BCR	C1-C6-C7-C8
31	b	517	BCR	C5-C6-C7-C8
31	v	101	BCR	C1-C6-C7-C8
31	f	101	BCR	C1-C6-C7-C8
31	f	101	BCR	C5-C6-C7-C8
31	z	101	BCR	C1-C6-C7-C8
31	z	101	BCR	C5-C6-C7-C8
34	B	519	C7Z	C1-C6-C7-C8
34	b	519	C7Z	C5-C6-C7-C8
37	D	407	LHG	C10-C11-C12-C13
41	J	101	DGA	CA2-CA1-OG1-CG1
46	n	601	CHL	C15-C16-C17-C18
35	B	520	LMG	C15-C16-C17-C18
37	c	521	LHG	C33-C34-C35-C36
50	N	620	PTY	C40-C41-C42-C43
29	s	304	CLA	O1D-CGD-O2D-CED
37	l	102	LHG	C26-C27-C28-C29
39	L	102	SQD	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	N	620	PTY	C15-C16-C17-C18
29	R	306	CLA	C2A-CAA-CBA-CGA
29	S	303	CLA	C2A-CAA-CBA-CGA
29	S	315	CLA	C2A-CAA-CBA-CGA
29	g	613	CLA	C2A-CAA-CBA-CGA
29	s	314	CLA	C2A-CAA-CBA-CGA
46	n	605	CHL	C2A-CAA-CBA-CGA
35	C	522	LMG	C10-C11-C12-C13
29	B	514	CLA	O1A-CGA-O2A-C1
39	L	102	SQD	O10-C23-O48-C46
35	B	520	LMG	C11-C12-C13-C14
41	W	202	DGA	CA5-CA6-CA7-CA8
50	N	620	PTY	C39-C40-C41-C42
35	c	519	LMG	O9-C10-O7-C8
37	Y	319	LHG	O9-C7-O7-C5
37	y	320	LHG	O9-C7-O7-C5
29	A	409	CLA	C4-C3-C5-C6
37	d	406	LHG	C11-C12-C13-C14
38	b	524	LMT	C11-C10-C9-C8
41	D	402	DGA	CB3-CB4-CB5-CB6
41	J	101	DGA	CB3-CB4-CB5-CB6
29	B	516	CLA	C2-C3-C5-C6
29	b	503	CLA	C2-C3-C5-C6
29	c	504	CLA	C2-C3-C5-C6
29	n	609	CLA	C2-C3-C5-C6
29	s	311	CLA	C2-C3-C5-C6
46	G	609	CHL	C2-C3-C5-C6
29	B	501	CLA	C16-C17-C18-C20
33	a	415	3PH	C2A-C2B-C2C-C2D
33	s	322	3PH	C25-C26-C27-C28
35	C	522	LMG	C18-C19-C20-C21
35	c	519	LMG	C29-C30-C31-C32
38	b	524	LMT	C3-C4-C5-C6
37	D	408	LHG	C7-C8-C9-C10
39	C	501	SQD	C7-C8-C9-C10
39	c	522	SQD	C23-C24-C25-C26
29	c	506	CLA	CBA-CGA-O2A-C1
33	B	522	3PH	C32-C31-O31-C3
29	n	612	CLA	C14-C13-C15-C16
36	c	517	DGD	C7A-C8A-C9A-CAA
39	M	101	SQD	C11-C10-C9-C8
29	C	513	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	g	603	CLA	C15-C16-C17-C18
33	a	415	3PH	C38-C39-C3A-C3B
37	G	618	LHG	C24-C25-C26-C27
37	d	406	LHG	C25-C26-C27-C28
37	y	320	LHG	C11-C10-C9-C8
40	i	102	SPH	C6-C7-C8-C9
50	n	619	PTY	C24-C25-C26-C27
39	a	410	SQD	O5-C1-O6-C44
37	y	320	LHG	C16-C17-C18-C19
37	y	320	LHG	C31-C32-C33-C34
35	B	520	LMG	C2-C1-O1-C7
39	a	410	SQD	C2-C1-O6-C44
29	B	510	CLA	CBD-CGD-O2D-CED
29	B	515	CLA	C8-C10-C11-C12
29	D	404	CLA	C10-C11-C12-C13
33	A	412	3PH	C22-C23-C24-C25
37	d	406	LHG	C13-C14-C15-C16
37	l	102	LHG	C34-C35-C36-C37
39	l	101	SQD	C24-C25-C26-C27
39	o	301	SQD	C30-C31-C32-C33
41	J	101	DGA	CA6-CA7-CA8-CA9
37	n	617	LHG	O2-C2-C3-O3
33	a	415	3PH	C22-C23-C24-C25
29	C	511	CLA	C13-C15-C16-C17
45	h	101	RRX	C15-C16-C17-C18
47	G	616	LUT	C29-C30-C31-C32
29	G	602	CLA	C16-C17-C18-C20
29	Y	314	CLA	C16-C17-C18-C19
33	B	522	3PH	C22-C21-O21-C2
35	C	521	LMG	C11-C10-O7-C8
35	C	522	LMG	C11-C10-O7-C8
35	i	101	LMG	C11-C10-O7-C8
37	G	618	LHG	C8-C7-O7-C5
37	S	301	LHG	C8-C7-O7-C5
37	g	618	LHG	C8-C7-O7-C5
37	s	320	LHG	C8-C7-O7-C5
39	C	501	SQD	C8-C7-O47-C45
39	c	522	SQD	C8-C7-O47-C45
39	l	101	SQD	C8-C7-O47-C45
37	G	618	LHG	C23-C24-C25-C26
37	g	618	LHG	C7-C8-C9-C10
37	g	618	LHG	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	B	522	3PH	O22-C21-O21-C2
37	g	618	LHG	O9-C7-O7-C5
39	l	101	SQD	O49-C7-O47-C45
36	c	516	DGD	C2B-C3B-C4B-C5B
37	y	320	LHG	C9-C10-C11-C12
37	G	618	LHG	C31-C32-C33-C34
31	A	410	BCR	C37-C22-C23-C24
31	F	101	BCR	C36-C18-C19-C20
41	J	101	DGA	CB5-CB6-CB7-CB8
50	n	619	PTY	C19-C20-C21-C22
29	s	304	CLA	C2C-C3C-CAC-CBC
31	z	101	BCR	C17-C18-C19-C20
36	C	519	DGD	C2G-C3G-O3G-C1D
37	D	407	LHG	C11-C12-C13-C14
41	W	202	DGA	CA6-CA7-CA8-CA9
29	s	310	CLA	C2A-CAA-CBA-CGA
29	C	504	CLA	C16-C17-C18-C20
29	D	405	CLA	C11-C12-C13-C14
29	S	310	CLA	C11-C12-C13-C15
29	b	510	CLA	C16-C17-C18-C19
29	b	510	CLA	C16-C17-C18-C20
29	b	511	CLA	C16-C17-C18-C19
29	s	303	CLA	C11-C12-C13-C14
29	s	303	CLA	C11-C12-C13-C15
29	s	314	CLA	C6-C7-C8-C9
30	A	408	PHO	C16-C17-C18-C20
33	a	415	3PH	C36-C37-C38-C39
35	b	520	LMG	C11-C12-C13-C14
37	s	320	LHG	C31-C32-C33-C34
29	C	513	CLA	C4-C3-C5-C6
29	N	603	CLA	C4-C3-C5-C6
29	G	613	CLA	C4-C3-C5-C6
46	N	601	CHL	C4-C3-C5-C6
33	a	415	3PH	C2E-C2F-C2G-C2H
37	B	523	LHG	C24-C25-C26-C27
29	b	515	CLA	O1D-CGD-O2D-CED
29	g	603	CLA	C13-C15-C16-C17
29	C	514	CLA	C15-C16-C17-C18
29	S	312	CLA	C10-C11-C12-C13
29	b	511	CLA	C15-C16-C17-C18
39	a	410	SQD	C10-C11-C12-C13
29	C	503	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	d	406	LHG	C23-C24-C25-C26
33	A	412	3PH	C2E-C2F-C2G-C2H
40	I	101	SPH	C6-C7-C8-C9
35	C	521	LMG	O9-C10-O7-C8
35	C	522	LMG	O9-C10-O7-C8
37	S	301	LHG	O9-C7-O7-C5
36	c	517	DGD	O6E-C5E-C6E-O5E
37	c	521	LHG	C27-C28-C29-C30
41	D	402	DGA	CB9-CAB-CBB-CCB
46	y	301	CHL	C8-C10-C11-C12
29	B	512	CLA	C16-C17-C18-C19
29	b	501	CLA	C16-C17-C18-C19
37	L	101	LHG	C17-C18-C19-C20
36	r	301	DGD	O6E-C5E-C6E-O5E
37	S	320	LHG	C26-C27-C28-C29
37	l	102	LHG	C14-C15-C16-C17
41	w	201	DGA	CB2-CB3-CB4-CB5
37	s	301	LHG	C7-C8-C9-C10
29	b	511	CLA	C10-C11-C12-C13
29	c	505	CLA	C10-C11-C12-C13
29	s	310	CLA	C8-C10-C11-C12
29	B	513	CLA	O1D-CGD-O2D-CED
33	s	322	3PH	C2D-C2E-C2F-C2G
36	r	301	DGD	C3A-C4A-C5A-C6A
37	a	413	LHG	C28-C29-C30-C31
35	C	524	LMG	O6-C5-C6-O5
35	D	410	LMG	O6-C5-C6-O5
37	s	301	LHG	O7-C5-C6-O8
33	A	412	3PH	C28-C29-C2A-C2B
37	n	617	LHG	C25-C26-C27-C28
39	m	101	SQD	C10-C11-C12-C13
41	J	101	DGA	OA1-CA1-OG1-CG1
41	j	101	DGA	CA4-CA5-CA6-CA7
35	c	519	LMG	O6-C5-C6-O5
35	d	407	LMG	C30-C31-C32-C33
29	S	310	CLA	CBD-CGD-O2D-CED
37	a	413	LHG	C13-C14-C15-C16
29	N	611	CLA	C2-C1-O2A-CGA
29	Y	305	CLA	C2-C1-O2A-CGA
35	C	521	LMG	O6-C5-C6-O5
35	D	409	LMG	O6-C5-C6-O5
38	B	524	LMT	O5'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	b	524	LMT	O5'-C5'-C6'-O6'
29	B	501	CLA	C16-C17-C18-C19
29	B	510	CLA	C16-C17-C18-C20
33	A	412	3PH	C37-C38-C39-C3A
37	g	618	LHG	C31-C32-C33-C34
41	w	201	DGA	CCB-CDB-CEB-CFB
33	a	415	3PH	C23-C24-C25-C26
29	N	603	CLA	C2-C3-C5-C6
29	G	613	CLA	C2-C3-C5-C6
37	G	618	LHG	O9-C7-O7-C5
37	S	320	LHG	O9-C7-O7-C5
29	b	510	CLA	C15-C16-C17-C18
33	B	522	3PH	C25-C26-C27-C28
37	a	413	LHG	C24-C25-C26-C27
37	c	521	LHG	C34-C35-C36-C37
37	g	618	LHG	C24-C25-C26-C27
29	N	613	CLA	C2A-CAA-CBA-CGA
29	S	314	CLA	C2A-CAA-CBA-CGA
46	R	305	CHL	C2A-CAA-CBA-CGA
46	r	306	CHL	C2A-CAA-CBA-CGA
46	y	309	CHL	C2A-CAA-CBA-CGA
29	R	308	CLA	CBD-CGD-O2D-CED
29	c	502	CLA	CBA-CGA-O2A-C1
36	C	518	DGD	C2A-C1A-O1G-C1G
35	W	201	LMG	C16-C17-C18-C19
29	B	516	CLA	O1D-CGD-O2D-CED
29	c	512	CLA	C13-C15-C16-C17
37	G	618	LHG	C7-C8-C9-C10
37	Y	319	LHG	C7-C8-C9-C10
33	A	412	3PH	C2D-C2E-C2F-C2G
41	D	402	DGA	CA3-CA4-CA5-CA6
29	G	602	CLA	C16-C17-C18-C19
37	s	320	LHG	O1-C1-C2-O2
37	s	320	LHG	C28-C29-C30-C31
38	b	524	LMT	C4-C5-C6-C7
29	A	409	CLA	C1A-C2A-CAA-CBA
29	B	506	CLA	C1A-C2A-CAA-CBA
29	C	507	CLA	C1A-C2A-CAA-CBA
29	N	603	CLA	C1A-C2A-CAA-CBA
29	G	602	CLA	C1A-C2A-CAA-CBA
29	G	604	CLA	C1A-C2A-CAA-CBA
29	G	610	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	G	611	CLA	C1A-C2A-CAA-CBA
29	R	307	CLA	C1A-C2A-CAA-CBA
29	R	308	CLA	C1A-C2A-CAA-CBA
29	R	309	CLA	C1A-C2A-CAA-CBA
29	Y	303	CLA	C1A-C2A-CAA-CBA
29	Y	305	CLA	C1A-C2A-CAA-CBA
29	a	408	CLA	C1A-C2A-CAA-CBA
29	b	501	CLA	C1A-C2A-CAA-CBA
29	b	506	CLA	C1A-C2A-CAA-CBA
29	b	511	CLA	C1A-C2A-CAA-CBA
29	c	501	CLA	C1A-C2A-CAA-CBA
29	c	506	CLA	C1A-C2A-CAA-CBA
29	n	602	CLA	C1A-C2A-CAA-CBA
29	n	613	CLA	C1A-C2A-CAA-CBA
29	g	603	CLA	C1A-C2A-CAA-CBA
29	g	610	CLA	C1A-C2A-CAA-CBA
29	g	611	CLA	C1A-C2A-CAA-CBA
29	g	614	CLA	C1A-C2A-CAA-CBA
29	r	309	CLA	C1A-C2A-CAA-CBA
29	r	310	CLA	C1A-C2A-CAA-CBA
29	s	311	CLA	C1A-C2A-CAA-CBA
29	s	315	CLA	C1A-C2A-CAA-CBA
29	y	304	CLA	C1A-C2A-CAA-CBA
29	y	305	CLA	C1A-C2A-CAA-CBA
29	y	306	CLA	C1A-C2A-CAA-CBA
46	Y	307	CHL	C10-C11-C12-C13
41	w	201	DGA	CAB-CBB-CCB-CDB
46	G	601	CHL	C15-C16-C17-C18
33	b	521	3PH	O11-C1-C2-C3
37	G	618	LHG	O6-C4-C5-C6
51	S	321	LPX	O5-C4-C5-O6
35	i	101	LMG	O9-C10-O7-C8
39	c	522	SQD	O49-C7-O47-C45
33	b	521	3PH	C28-C29-C2A-C2B
38	b	524	LMT	C5-C6-C7-C8
29	A	409	CLA	C6-C7-C8-C10
29	A	409	CLA	C11-C10-C8-C7
29	B	503	CLA	C11-C12-C13-C15
29	B	509	CLA	C6-C7-C8-C10
29	B	515	CLA	C11-C12-C13-C15
29	C	502	CLA	C12-C13-C15-C16
29	C	510	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	C	511	CLA	C6-C7-C8-C10
29	C	511	CLA	C12-C13-C15-C16
29	C	514	CLA	C11-C12-C13-C15
29	D	404	CLA	C12-C13-C15-C16
29	D	405	CLA	C11-C10-C8-C7
29	N	610	CLA	C11-C12-C13-C15
29	G	602	CLA	C6-C7-C8-C10
29	R	308	CLA	C6-C7-C8-C10
29	R	308	CLA	C11-C10-C8-C7
29	S	310	CLA	C11-C10-C8-C7
29	Y	314	CLA	C11-C12-C13-C15
29	Y	314	CLA	C12-C13-C15-C16
29	b	506	CLA	C11-C10-C8-C7
29	b	516	CLA	C12-C13-C15-C16
29	c	501	CLA	C12-C13-C15-C16
29	c	503	CLA	C12-C13-C15-C16
29	c	504	CLA	C11-C10-C8-C7
29	c	507	CLA	C12-C13-C15-C16
29	c	509	CLA	C12-C13-C15-C16
29	c	513	CLA	C6-C7-C8-C10
29	c	513	CLA	C11-C10-C8-C7
29	d	403	CLA	C11-C12-C13-C15
29	y	305	CLA	C6-C7-C8-C10
29	y	315	CLA	C11-C10-C8-C7
46	N	605	CHL	C11-C12-C13-C15
46	N	607	CHL	C11-C12-C13-C15
46	G	601	CHL	C11-C12-C13-C15
46	G	609	CHL	C12-C13-C15-C16
46	Y	308	CHL	C12-C13-C15-C16
46	Y	310	CHL	C11-C12-C13-C15
46	Y	310	CHL	C12-C13-C15-C16
46	n	605	CHL	C11-C10-C8-C7
46	y	309	CHL	C6-C7-C8-C10
46	y	309	CHL	C12-C13-C15-C16
29	c	506	CLA	O1A-CGA-O2A-C1
36	c	517	DGD	C9A-CAA-CBA-CCA
29	B	510	CLA	C15-C16-C17-C18
29	b	507	CLA	C15-C16-C17-C18
29	y	316	CLA	C13-C15-C16-C17
40	C	525	SPH	C6-C7-C8-C9
33	B	522	3PH	O32-C31-O31-C3
36	B	521	DGD	O6E-C5E-C6E-O5E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	a	415	3PH	C29-C2A-C2B-C2C
35	c	520	LMG	C21-C22-C23-C24
35	d	408	LMG	C11-C10-O7-C8
29	A	407	CLA	C2A-CAA-CBA-CGA
29	B	514	CLA	C2A-CAA-CBA-CGA
30	D	401	PHO	C2A-CAA-CBA-CGA
46	N	607	CHL	C2A-CAA-CBA-CGA
46	y	301	CHL	C2A-CAA-CBA-CGA
29	A	405	CLA	C14-C13-C15-C16
29	B	507	CLA	C11-C12-C13-C14
29	B	511	CLA	C14-C13-C15-C16
29	B	514	CLA	C6-C7-C8-C9
29	C	502	CLA	C14-C13-C15-C16
29	C	511	CLA	C14-C13-C15-C16
29	N	603	CLA	C6-C7-C8-C9
29	N	610	CLA	C11-C12-C13-C14
29	G	610	CLA	C11-C10-C8-C9
29	S	304	CLA	C11-C10-C8-C9
29	Y	314	CLA	C14-C13-C15-C16
29	b	501	CLA	C11-C10-C8-C9
29	b	514	CLA	C6-C7-C8-C9
29	c	501	CLA	C14-C13-C15-C16
29	c	509	CLA	C14-C13-C15-C16
29	n	603	CLA	C11-C10-C8-C9
29	n	604	CLA	C6-C7-C8-C9
29	g	602	CLA	C6-C7-C8-C9
29	g	610	CLA	C11-C10-C8-C9
29	r	303	CLA	C11-C10-C8-C9
29	r	309	CLA	C11-C10-C8-C9
29	y	315	CLA	C11-C10-C8-C9
46	N	607	CHL	C11-C12-C13-C14
39	m	101	SQD	C12-C13-C14-C15
39	m	101	SQD	C27-C28-C29-C30
41	b	522	DGA	CBB-CCB-CDB-CEB
35	d	408	LMG	O6-C5-C6-O5
35	c	520	LMG	C10-C11-C12-C13
31	B	518	BCR	C19-C20-C21-C22
31	b	518	BCR	C19-C20-C21-C22
46	N	605	CHL	C16-C17-C18-C19
36	c	517	DGD	CCB-CDB-CEB-CFB
37	c	521	LHG	C15-C16-C17-C18
29	b	512	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	w	202	LMG	C29-C28-O8-C9
36	C	519	DGD	O6E-C5E-C6E-O5E
29	g	602	CLA	O1D-CGD-O2D-CED
37	l	102	LHG	C13-C14-C15-C16
40	i	102	SPH	C12-C13-C14-C15
33	A	412	3PH	C1-C2-C3-O31
33	B	522	3PH	C1-C2-C3-O31
33	s	322	3PH	C1-C2-C3-O31
35	C	522	LMG	C7-C8-C9-O8
35	D	410	LMG	C7-C8-C9-O8
35	W	201	LMG	O1-C7-C8-C9
37	D	408	LHG	C4-C5-C6-O8
37	G	618	LHG	C4-C5-C6-O8
37	S	301	LHG	C4-C5-C6-O8
37	c	521	LHG	C4-C5-C6-O8
37	l	102	LHG	C4-C5-C6-O8
39	m	101	SQD	C44-C45-C46-O48
41	W	202	DGA	OG1-CG1-CG2-CG3
50	Y	320	PTY	O4-C1-C6-C5
33	a	415	3PH	C2D-C2E-C2F-C2G
33	s	322	3PH	C29-C2A-C2B-C2C
39	M	101	SQD	C26-C27-C28-C29
33	B	522	3PH	C2A-C2B-C2C-C2D
29	C	510	CLA	C10-C11-C12-C13
29	b	515	CLA	C8-C10-C11-C12
35	d	408	LMG	C36-C37-C38-C39
29	S	305	CLA	CBA-CGA-O2A-C1
33	s	322	3PH	C32-C31-O31-C3
35	D	410	LMG	C10-C11-C12-C13
35	d	407	LMG	O6-C5-C6-O5
29	B	510	CLA	C16-C17-C18-C19
29	C	505	CLA	C6-C7-C8-C10
30	a	407	PHO	C16-C17-C18-C19
33	a	415	3PH	C37-C38-C39-C3A
37	Y	319	LHG	C29-C30-C31-C32
39	a	410	SQD	C11-C12-C13-C14
41	b	522	DGA	CBB-CAB-CB9-CB8
29	c	505	CLA	C5-C6-C7-C8
29	C	503	CLA	O1A-CGA-O2A-C1
35	C	521	LMG	C29-C30-C31-C32
37	g	618	LHG	C16-C17-C18-C19
29	G	614	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	b	516	CLA	O1D-CGD-O2D-CED
46	s	309	CHL	CHA-CBD-CGD-O1D
48	r	313	NEX	C39-C29-C30-C31
29	b	505	CLA	C15-C16-C17-C18
35	w	202	LMG	C36-C37-C38-C39
36	c	517	DGD	C1B-C2B-C3B-C4B
50	n	619	PTY	C30-C31-C32-C33
29	c	502	CLA	O1A-CGA-O2A-C1
36	C	518	DGD	O1A-C1A-O1G-C1G
33	a	415	3PH	C27-C28-C29-C2A
37	a	414	LHG	C33-C34-C35-C36
29	c	505	CLA	C2-C3-C5-C6
37	G	618	LHG	C11-C12-C13-C14
29	C	502	CLA	C10-C11-C12-C13
29	N	603	CLA	C13-C15-C16-C17
29	n	603	CLA	C5-C6-C7-C8
29	s	312	CLA	C5-C6-C7-C8
31	B	518	BCR	C36-C18-C19-C20
34	B	519	C7Z	C7-C8-C9-C19
37	l	102	LHG	C33-C34-C35-C36
36	C	519	DGD	C1B-C2B-C3B-C4B
31	b	518	BCR	C17-C18-C19-C20
34	B	519	C7Z	C7-C8-C9-C10
29	s	311	CLA	C8-C10-C11-C12
29	y	304	CLA	C8-C10-C11-C12
29	G	604	CLA	CBD-CGD-O2D-CED
33	A	412	3PH	C1-O11-P-O12
33	a	415	3PH	C1-O11-P-O12
33	b	521	3PH	C1-O11-P-O12
39	b	523	SQD	C10-C11-C12-C13
41	b	522	DGA	CB3-CB4-CB5-CB6
29	n	602	CLA	C2A-CAA-CBA-CGA
35	C	522	LMG	C16-C17-C18-C19
29	y	316	CLA	O1D-CGD-O2D-CED
29	c	511	CLA	CBA-CGA-O2A-C1
29	r	310	CLA	O2A-C1-C2-C3
35	b	520	LMG	C9-C8-O7-C10
41	D	402	DGA	CG1-CG2-OG2-CB1
41	b	522	DGA	CG1-CG2-OG2-CB1
29	Y	313	CLA	C10-C11-C12-C13
29	b	514	CLA	C10-C11-C12-C13
29	g	603	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	A	410	BCR	C19-C20-C21-C22
31	a	409	BCR	C19-C20-C21-C22
31	c	515	BCR	C9-C10-C11-C12
45	h	101	RRX	C9-C10-C11-C12
29	S	305	CLA	C6-C7-C8-C9
33	A	412	3PH	C3A-C3B-C3C-C3D
37	g	618	LHG	C28-C29-C30-C31
37	s	301	LHG	C28-C29-C30-C31
33	A	412	3PH	C31-C32-C33-C34
30	A	408	PHO	O1D-CGD-O2D-CED
30	d	402	PHO	C3-C5-C6-C7
37	g	618	LHG	C26-C27-C28-C29
36	C	519	DGD	CCB-CDB-CEB-CFB
37	B	523	LHG	C1-C2-C3-O3
37	L	101	LHG	O6-C4-C5-O7
37	a	414	LHG	O6-C4-C5-O7
29	N	602	CLA	C10-C11-C12-C13
29	B	505	CLA	CBA-CGA-O2A-C1
37	S	301	LHG	C24-C23-O8-C6
29	b	506	CLA	O1D-CGD-O2D-CED
39	l	101	SQD	C25-C26-C27-C28
39	l	101	SQD	C26-C27-C28-C29
40	i	102	SPH	C7-C8-C9-C10
41	D	402	DGA	CA6-CA7-CA8-CA9
29	s	310	CLA	C4-C3-C5-C6
29	s	312	CLA	C4-C3-C5-C6
29	Y	305	CLA	C2-C3-C5-C6
37	S	320	LHG	C9-C10-C11-C12
29	b	512	CLA	C16-C17-C18-C20
29	g	603	CLA	CBD-CGD-O2D-CED
35	c	520	LMG	C18-C19-C20-C21
37	s	320	LHG	C34-C35-C36-C37
33	B	522	3PH	C21-C22-C23-C24
35	D	410	LMG	C36-C37-C38-C39
39	M	101	SQD	C27-C28-C29-C30
35	W	201	LMG	O1-C7-C8-O7
37	y	320	LHG	O7-C5-C6-O8
39	M	101	SQD	O47-C45-C46-O48
37	G	618	LHG	C16-C17-C18-C19
37	l	102	LHG	C31-C32-C33-C34
33	B	522	3PH	C2C-C2D-C2E-C2F
37	S	301	LHG	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	l	102	LHG	C35-C36-C37-C38
29	b	501	CLA	CAA-CBA-CGA-O2A
37	G	618	LHG	C9-C10-C11-C12
37	G	618	LHG	C35-C36-C37-C38
50	n	619	PTY	C41-C42-C43-C44
29	b	512	CLA	O1A-CGA-O2A-C1
35	i	101	LMG	C30-C31-C32-C33
29	c	505	CLA	CBA-CGA-O2A-C1
37	c	521	LHG	C8-C7-O7-C5
36	c	518	DGD	CCB-CDB-CEB-CFB
37	L	101	LHG	C13-C14-C15-C16
29	C	506	CLA	C5-C6-C7-C8
29	n	612	CLA	C13-C15-C16-C17
29	r	307	CLA	C3-C5-C6-C7
33	S	322	3PH	C21-C22-C23-C24
46	R	305	CHL	C2C-C3C-CAC-CBC
29	a	406	CLA	C2C-C3C-CAC-CBC
35	C	522	LMG	C42-C43-C44-C45
37	g	618	LHG	C35-C36-C37-C38
29	C	509	CLA	C13-C15-C16-C17
29	c	513	CLA	C10-C11-C12-C13
46	N	605	CHL	C8-C10-C11-C12
29	r	307	CLA	O1D-CGD-O2D-CED
46	s	309	CHL	C11-C12-C13-C15
29	c	505	CLA	C4-C3-C5-C6
29	y	316	CLA	C4-C3-C5-C6
29	y	306	CLA	C2-C3-C5-C6
29	Y	315	CLA	CBA-CGA-O2A-C1
29	y	314	CLA	C10-C11-C12-C13
35	i	101	LMG	C15-C16-C17-C18
37	s	320	LHG	O9-C7-O7-C5
39	C	501	SQD	O49-C7-O47-C45
37	B	523	LHG	O1-C1-C2-O2
37	Y	319	LHG	O1-C1-C2-O2
29	B	501	CLA	C6-C7-C8-C9
29	B	503	CLA	C11-C12-C13-C14
29	B	515	CLA	C11-C12-C13-C14
29	C	510	CLA	C14-C13-C15-C16
29	C	511	CLA	C6-C7-C8-C9
29	C	513	CLA	C14-C13-C15-C16
29	C	514	CLA	C11-C12-C13-C14
29	D	404	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	D	405	CLA	C11-C10-C8-C9
29	N	613	CLA	C11-C12-C13-C14
29	R	308	CLA	C11-C10-C8-C9
29	S	304	CLA	C14-C13-C15-C16
29	Y	313	CLA	C11-C10-C8-C9
29	Y	314	CLA	C11-C12-C13-C14
29	a	404	CLA	C14-C13-C15-C16
29	b	506	CLA	C11-C10-C8-C9
29	b	515	CLA	C11-C12-C13-C14
29	c	503	CLA	C11-C12-C13-C14
29	c	503	CLA	C14-C13-C15-C16
29	c	504	CLA	C11-C10-C8-C9
29	c	505	CLA	C14-C13-C15-C16
29	c	507	CLA	C14-C13-C15-C16
29	c	513	CLA	C6-C7-C8-C9
29	d	403	CLA	C11-C12-C13-C14
29	n	609	CLA	C14-C13-C15-C16
46	N	601	CHL	C11-C10-C8-C9
46	G	601	CHL	C11-C12-C13-C14
46	Y	307	CHL	C14-C13-C15-C16
46	n	605	CHL	C11-C10-C8-C9
46	n	605	CHL	C11-C12-C13-C14
46	y	311	CHL	C14-C13-C15-C16
37	N	618	LHG	C9-C10-C11-C12
29	B	507	CLA	C15-C16-C17-C18
29	B	513	CLA	C5-C6-C7-C8
29	Y	305	CLA	C8-C10-C11-C12
29	c	509	CLA	C10-C11-C12-C13
29	s	312	CLA	C13-C15-C16-C17
29	B	506	CLA	C4B-C3B-CAB-CBB
29	B	510	CLA	C4B-C3B-CAB-CBB
29	B	515	CLA	C4B-C3B-CAB-CBB
29	C	504	CLA	C4B-C3B-CAB-CBB
29	D	405	CLA	C4B-C3B-CAB-CBB
29	N	603	CLA	C4B-C3B-CAB-CBB
29	S	304	CLA	C4B-C3B-CAB-CBB
29	S	305	CLA	C4B-C3B-CAB-CBB
29	S	315	CLA	C4B-C3B-CAB-CBB
29	Y	309	CLA	C4B-C3B-CAB-CBB
29	Y	313	CLA	C4B-C3B-CAB-CBB
29	a	406	CLA	C4B-C3B-CAB-CBB
29	b	506	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	c	503	CLA	C4B-C3B-CAB-CBB
29	n	603	CLA	C4B-C3B-CAB-CBB
29	g	613	CLA	C4B-C3B-CAB-CBB
29	r	307	CLA	C4B-C3B-CAB-CBB
29	s	303	CLA	C4B-C3B-CAB-CBB
29	s	304	CLA	C4B-C3B-CAB-CBB
29	s	305	CLA	C4B-C3B-CAB-CBB
29	y	310	CLA	C4B-C3B-CAB-CBB
29	y	313	CLA	C4B-C3B-CAB-CBB
37	Y	319	LHG	C34-C35-C36-C37
40	C	525	SPH	C11-C12-C13-C14
50	N	620	PTY	C19-C20-C21-C22
35	w	202	LMG	O7-C10-C11-C12
33	s	322	3PH	C35-C36-C37-C38
46	N	606	CHL	C8-C10-C11-C12
29	Y	304	CLA	C16-C17-C18-C20
36	c	517	DGD	C2E-C1E-O5D-C6D
39	c	522	SQD	C2-C1-O6-C44
37	Y	319	LHG	C16-C17-C18-C19
37	s	320	LHG	C33-C34-C35-C36
41	J	101	DGA	CB6-CB7-CB8-CB9
37	Y	319	LHG	C35-C36-C37-C38
33	B	522	3PH	O11-C1-C2-C3
37	D	407	LHG	O6-C4-C5-C6
37	D	408	LHG	O6-C4-C5-C6
37	L	101	LHG	O6-C4-C5-C6
37	a	414	LHG	O6-C4-C5-C6
37	c	521	LHG	O6-C4-C5-C6
37	l	102	LHG	O6-C4-C5-C6
37	g	618	LHG	O6-C4-C5-C6
50	Y	320	PTY	O14-C5-C6-C1
50	y	321	PTY	O14-C5-C6-C1
29	n	611	CLA	O1D-CGD-O2D-CED
41	j	101	DGA	CBB-CAB-CB9-CB8
35	D	410	LMG	O7-C10-C11-C12
29	A	405	CLA	C12-C13-C15-C16
29	B	506	CLA	C11-C10-C8-C7
29	B	507	CLA	C11-C12-C13-C15
29	B	511	CLA	C12-C13-C15-C16
29	B	514	CLA	C6-C7-C8-C10
29	B	515	CLA	C11-C10-C8-C7
29	C	506	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	C	507	CLA	C6-C7-C8-C10
29	C	510	CLA	C6-C7-C8-C10
29	C	513	CLA	C12-C13-C15-C16
29	D	404	CLA	C6-C7-C8-C10
29	N	602	CLA	C11-C12-C13-C15
29	N	603	CLA	C6-C7-C8-C10
29	N	604	CLA	C11-C12-C13-C15
29	G	602	CLA	C12-C13-C15-C16
29	G	610	CLA	C11-C10-C8-C7
29	G	613	CLA	C12-C13-C15-C16
29	R	301	CLA	C6-C7-C8-C10
29	S	304	CLA	C11-C10-C8-C7
29	S	304	CLA	C12-C13-C15-C16
29	Y	303	CLA	C6-C7-C8-C10
29	Y	313	CLA	C11-C10-C8-C7
29	a	404	CLA	C12-C13-C15-C16
29	b	501	CLA	C11-C10-C8-C7
29	b	501	CLA	C11-C12-C13-C15
29	b	514	CLA	C6-C7-C8-C10
29	b	515	CLA	C11-C12-C13-C15
29	c	503	CLA	C11-C12-C13-C15
29	c	504	CLA	C6-C7-C8-C10
29	c	505	CLA	C12-C13-C15-C16
29	c	509	CLA	C6-C7-C8-C10
29	c	513	CLA	C11-C12-C13-C15
29	n	603	CLA	C11-C10-C8-C7
29	n	604	CLA	C6-C7-C8-C10
29	g	602	CLA	C6-C7-C8-C10
29	g	602	CLA	C12-C13-C15-C16
29	g	610	CLA	C11-C10-C8-C7
29	r	303	CLA	C11-C10-C8-C7
29	r	309	CLA	C11-C10-C8-C7
29	y	305	CLA	C12-C13-C15-C16
29	y	314	CLA	C11-C10-C8-C7
46	N	607	CHL	C12-C13-C15-C16
46	Y	307	CHL	C6-C7-C8-C10
46	n	601	CHL	C11-C10-C8-C7
46	n	601	CHL	C11-C12-C13-C15
46	n	605	CHL	C12-C13-C15-C16
46	n	606	CHL	C11-C12-C13-C15
46	n	606	CHL	C12-C13-C15-C16
46	g	601	CHL	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	g	609	CHL	C11-C12-C13-C15
46	y	301	CHL	C11-C10-C8-C7
46	y	311	CHL	C12-C13-C15-C16
41	W	202	DGA	CB6-CB7-CB8-CB9
51	s	321	LPX	O1-C3-C4-O5
43	d	405	PL9	C47-C48-C49-C50
36	B	521	DGD	C1A-C2A-C3A-C4A
33	b	521	3PH	C22-C23-C24-C25
36	c	516	DGD	C5B-C6B-C7B-C8B
37	c	521	LHG	C30-C31-C32-C33
33	s	322	3PH	O32-C31-O31-C3
35	w	202	LMG	O10-C28-O8-C9
29	c	512	CLA	C4-C3-C5-C6
29	s	305	CLA	C4-C3-C5-C6
30	d	402	PHO	C3A-C2A-CAA-CBA
43	d	405	PL9	C15-C14-C16-C17
43	d	405	PL9	C40-C39-C41-C42
46	N	601	CHL	C3A-C2A-CAA-CBA
46	G	601	CHL	C3A-C2A-CAA-CBA
46	G	607	CHL	C4-C3-C5-C6
46	Y	302	CHL	C3A-C2A-CAA-CBA
46	n	601	CHL	C3A-C2A-CAA-CBA
29	B	505	CLA	C15-C16-C17-C18
29	c	505	CLA	C8-C10-C11-C12
36	c	517	DGD	O6E-C1E-O5D-C6D
29	S	305	CLA	O1A-CGA-O2A-C1
46	n	601	CHL	C8-C10-C11-C12
29	s	305	CLA	CBA-CGA-O2A-C1
41	w	201	DGA	CDA-CEA-CFA-CGA
31	C	516	BCR	C19-C20-C21-C22
31	f	101	BCR	C19-C20-C21-C22
31	z	101	BCR	C9-C10-C11-C12
47	S	318	LUT	C29-C30-C31-C32
47	r	311	LUT	C9-C10-C11-C12
47	s	318	LUT	C29-C30-C31-C32
48	R	312	NEX	C33-C34-C35-C15
29	b	504	CLA	C4C-C3C-CAC-CBC
31	b	517	BCR	C21-C22-C23-C24
37	N	618	LHG	C30-C31-C32-C33
37	d	406	LHG	C26-C27-C28-C29
39	a	410	SQD	C28-C29-C30-C31
41	D	402	DGA	CB4-CB5-CB6-CB7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	S	302	CHL	C2A-CAA-CBA-CGA
33	s	322	3PH	C3B-C3C-C3D-C3E
35	c	520	LMG	C13-C14-C15-C16
35	w	202	LMG	O1-C7-C8-C9
37	N	618	LHG	C4-C5-C6-O8
37	n	617	LHG	C4-C5-C6-O8
37	g	618	LHG	C4-C5-C6-O8
37	s	301	LHG	C4-C5-C6-O8
37	y	320	LHG	C4-C5-C6-O8
39	M	101	SQD	C44-C45-C46-O48
39	a	410	SQD	C44-C45-C46-O48
50	N	620	PTY	O4-C1-C6-C5
50	n	619	PTY	O4-C1-C6-C5
50	y	321	PTY	O4-C1-C6-C5
35	d	407	LMG	C18-C19-C20-C21
29	G	602	CLA	C15-C16-C17-C18
46	Y	307	CHL	C13-C15-C16-C17
29	c	511	CLA	O1A-CGA-O2A-C1
29	R	306	CLA	CBD-CGD-O2D-CED
30	a	407	PHO	C1A-C2A-CAA-CBA
41	j	101	DGA	CG1-CG2-CG3-OXT
41	w	201	DGA	CG1-CG2-CG3-OXT
46	Y	306	CHL	C1A-C2A-CAA-CBA
46	g	601	CHL	C1A-C2A-CAA-CBA
46	y	303	CHL	C1A-C2A-CAA-CBA
39	b	523	SQD	C27-C28-C29-C30
29	Y	305	CLA	C4-C3-C5-C6
29	y	306	CLA	C4-C3-C5-C6
46	y	309	CHL	C4-C3-C5-C6
37	y	320	LHG	C30-C31-C32-C33
41	w	201	DGA	CB7-CB8-CB9-CAB
29	g	603	CLA	C3-C5-C6-C7
29	s	305	CLA	C3-C5-C6-C7
29	b	501	CLA	C15-C16-C17-C18
29	C	508	CLA	O1D-CGD-O2D-CED
29	c	507	CLA	O1D-CGD-O2D-CED
41	J	101	DGA	CA4-CA5-CA6-CA7
37	Y	319	LHG	C11-C12-C13-C14
29	N	602	CLA	C16-C17-C18-C20
29	b	512	CLA	C16-C17-C18-C19
29	g	611	CLA	C16-C17-C18-C20
37	c	521	LHG	O9-C7-O7-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	c	521	LHG	O6-C4-C5-O7
37	s	301	LHG	O6-C4-C5-O7
50	Y	320	PTY	O14-C5-C6-O7
33	S	322	3PH	C24-C25-C26-C27
37	L	101	LHG	C34-C35-C36-C37
29	G	611	CLA	O1D-CGD-O2D-CED
31	C	516	BCR	C23-C24-C25-C30
31	F	101	BCR	C1-C6-C7-C8
31	F	101	BCR	C23-C24-C25-C30
31	a	409	BCR	C23-C24-C25-C30
31	c	514	BCR	C1-C6-C7-C8
31	c	514	BCR	C23-C24-C25-C30
34	B	519	C7Z	C21-C26-C27-C28
35	D	410	LMG	C11-C10-O7-C8
33	A	412	3PH	C2-C1-O11-P
37	D	408	LHG	C2-C3-O3-P
37	B	523	LHG	C7-C8-C9-C10
33	b	521	3PH	C36-C37-C38-C39
40	C	525	SPH	O1-C1-C2-N2
40	I	101	SPH	O1-C1-C2-N2
41	w	201	DGA	CA5-CA6-CA7-CA8
29	B	506	CLA	CBD-CGD-O2D-CED
46	Y	307	CHL	C16-C17-C18-C20
29	S	311	CLA	C13-C15-C16-C17
35	C	524	LMG	O1-C7-C8-O7
35	D	410	LMG	O7-C8-C9-O8
35	c	520	LMG	O1-C7-C8-O7
35	w	202	LMG	O7-C8-C9-O8
37	S	301	LHG	O7-C5-C6-O8
37	Y	319	LHG	O7-C5-C6-O8
39	C	523	SQD	O6-C44-C45-O47
41	W	202	DGA	OG1-CG1-CG2-OG2
29	S	304	CLA	C2C-C3C-CAC-CBC
43	D	406	PL9	C40-C39-C41-C42
37	S	320	LHG	C31-C32-C33-C34
29	A	409	CLA	C2-C3-C5-C6
29	s	305	CLA	C2-C3-C5-C6
43	d	405	PL9	C13-C14-C16-C17
46	G	607	CHL	C2-C3-C5-C6
46	y	309	CHL	C2-C3-C5-C6
43	D	406	PL9	C47-C48-C49-C51
29	s	310	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	N	607	CHL	C16-C17-C18-C20
37	N	618	LHG	C16-C17-C18-C19
29	A	406	CLA	C5-C6-C7-C8
29	c	503	CLA	C13-C15-C16-C17
37	n	617	LHG	C9-C10-C11-C12
29	B	506	CLA	C11-C10-C8-C9
29	N	602	CLA	C11-C12-C13-C14
29	N	604	CLA	C14-C13-C15-C16
29	G	602	CLA	C6-C7-C8-C9
29	b	502	CLA	C14-C13-C15-C16
29	b	511	CLA	C14-C13-C15-C16
29	b	513	CLA	C11-C10-C8-C9
29	c	513	CLA	C11-C12-C13-C14
29	g	602	CLA	C14-C13-C15-C16
29	r	307	CLA	C11-C10-C8-C9
29	y	314	CLA	C11-C10-C8-C9
46	N	605	CHL	C11-C12-C13-C14
46	G	601	CHL	C6-C7-C8-C9
46	Y	310	CHL	C14-C13-C15-C16
37	N	618	LHG	C28-C29-C30-C31
37	c	521	LHG	C11-C10-C9-C8
37	Y	319	LHG	C9-C10-C11-C12
36	C	519	DGD	O6E-C1E-O5D-C6D
37	s	301	LHG	C25-C26-C27-C28
37	n	617	LHG	C28-C29-C30-C31
33	A	412	3PH	C24-C25-C26-C27
37	l	102	LHG	C29-C30-C31-C32
29	G	604	CLA	O2A-C1-C2-C3
29	n	613	CLA	O2A-C1-C2-C3
29	g	604	CLA	O2A-C1-C2-C3
33	a	415	3PH	C25-C26-C27-C28
37	L	101	LHG	C28-C29-C30-C31
29	B	501	CLA	C15-C16-C17-C18
29	Y	314	CLA	CBA-CGA-O2A-C1
48	r	313	NEX	C13-C14-C15-C35
35	c	519	LMG	O7-C10-C11-C12
38	b	524	LMT	C9-C10-C11-C12
29	y	316	CLA	C2-C3-C5-C6
46	N	605	CHL	C16-C17-C18-C20
37	B	523	LHG	C25-C26-C27-C28
29	N	610	CLA	C13-C15-C16-C17
40	c	523	SPH	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	Y	315	CLA	C13-C15-C16-C17
29	b	513	CLA	C5-C6-C7-C8
37	N	618	LHG	C1-C2-C3-O3
37	a	413	LHG	C26-C27-C28-C29
46	y	303	CHL	C3-C5-C6-C7
29	A	407	CLA	C2C-C3C-CAC-CBC
29	S	310	CLA	C10-C11-C12-C13
35	d	407	LMG	C19-C20-C21-C22
39	L	102	SQD	C11-C10-C9-C8
41	j	101	DGA	CB5-CB6-CB7-CB8
29	B	510	CLA	O1D-CGD-O2D-CED
29	C	504	CLA	C16-C17-C18-C19
29	C	505	CLA	C6-C7-C8-C9
29	S	305	CLA	C6-C7-C8-C10
33	A	412	3PH	C26-C27-C28-C29
35	W	203	LMG	C29-C30-C31-C32
37	s	320	LHG	C11-C12-C13-C14
29	B	501	CLA	C12-C13-C15-C16
29	B	504	CLA	C12-C13-C15-C16
29	D	404	CLA	C11-C12-C13-C15
29	N	602	CLA	C6-C7-C8-C10
29	N	603	CLA	C12-C13-C15-C16
29	N	613	CLA	C12-C13-C15-C16
29	S	303	CLA	C11-C10-C8-C7
29	a	405	CLA	C6-C7-C8-C10
29	b	504	CLA	C11-C12-C13-C15
29	b	511	CLA	C12-C13-C15-C16
29	b	515	CLA	C11-C10-C8-C7
29	c	502	CLA	C11-C12-C13-C15
29	c	504	CLA	C11-C12-C13-C15
29	n	603	CLA	C12-C13-C15-C16
29	g	603	CLA	C12-C13-C15-C16
29	y	304	CLA	C6-C7-C8-C10
29	y	306	CLA	C6-C7-C8-C10
29	y	306	CLA	C11-C10-C8-C7
46	N	605	CHL	C11-C10-C8-C7
46	N	606	CHL	C12-C13-C15-C16
46	G	601	CHL	C6-C7-C8-C10
46	G	607	CHL	C11-C12-C13-C15
46	G	609	CHL	C11-C12-C13-C15
46	g	601	CHL	C6-C7-C8-C10
46	y	311	CHL	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	A	412	3PH	C36-C37-C38-C39
29	Y	304	CLA	C13-C15-C16-C17
31	B	517	BCR	C17-C18-C19-C20
31	B	518	BCR	C17-C18-C19-C20
31	F	101	BCR	C17-C18-C19-C20
47	R	310	LUT	C7-C8-C9-C10
39	C	501	SQD	C24-C23-O48-C46
29	B	505	CLA	O1A-CGA-O2A-C1
29	c	505	CLA	O1A-CGA-O2A-C1
35	W	203	LMG	C8-C7-O1-C1
35	w	202	LMG	C8-C7-O1-C1
36	C	519	DGD	C5D-C6D-O5D-C1E
36	c	517	DGD	C2G-C3G-O3G-C1D
36	c	517	DGD	C5D-C6D-O5D-C1E
39	C	501	SQD	C45-C44-O6-C1
39	C	523	SQD	C5-C6-S-O8
48	R	312	NEX	C20-C13-C14-C15
41	D	402	DGA	CA1-CA2-CA3-CA4
29	D	405	CLA	C8-C10-C11-C12
29	Y	303	CLA	C8-C10-C11-C12
29	c	503	CLA	C10-C11-C12-C13
29	s	310	CLA	C5-C6-C7-C8
46	n	608	CHL	C8-C10-C11-C12
46	y	301	CHL	C10-C11-C12-C13
29	R	303	CLA	C2A-CAA-CBA-CGA
29	S	305	CLA	C2A-CAA-CBA-CGA
29	b	514	CLA	C2A-CAA-CBA-CGA
29	r	307	CLA	C2A-CAA-CBA-CGA
33	A	412	3PH	C2B-C2C-C2D-C2E
33	s	322	3PH	C37-C38-C39-C3A
37	L	101	LHG	C30-C31-C32-C33
29	s	314	CLA	C6-C7-C8-C10
30	A	408	PHO	C16-C17-C18-C19
35	d	408	LMG	O9-C10-O7-C8
41	W	202	DGA	CB9-CAB-CBB-CCB
43	D	406	PL9	C15-C14-C16-C17
29	Y	315	CLA	O1A-CGA-O2A-C1
37	S	301	LHG	O10-C23-O8-C6
37	N	618	LHG	C31-C32-C33-C34
29	B	504	CLA	C15-C16-C17-C18
39	L	102	SQD	C46-C45-O47-C7
39	m	101	SQD	C46-C45-O47-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	s	305	CLA	O1A-CGA-O2A-C1
35	b	520	LMG	C12-C13-C14-C15
29	S	310	CLA	C11-C12-C13-C14
35	C	522	LMG	C12-C13-C14-C15
29	Y	314	CLA	O1A-CGA-O2A-C1
29	G	603	CLA	C10-C11-C12-C13
35	D	410	LMG	O9-C10-O7-C8
33	B	522	3PH	O11-C1-C2-O21
37	D	407	LHG	O6-C4-C5-O7
37	n	617	LHG	O6-C4-C5-O7
37	g	618	LHG	O6-C4-C5-O7
50	y	321	PTY	O14-C5-C6-O7
35	i	101	LMG	O1-C7-C8-C9
37	Y	319	LHG	C4-C5-C6-O8
37	a	414	LHG	C4-C5-C6-O8
41	w	201	DGA	OG1-CG1-CG2-CG3
29	g	613	CLA	C5-C6-C7-C8
30	A	408	PHO	C15-C16-C17-C18
29	g	611	CLA	C16-C17-C18-C19
37	s	320	LHG	C24-C25-C26-C27
29	y	314	CLA	C3-C5-C6-C7
37	d	406	LHG	C10-C11-C12-C13
41	W	202	DGA	CA4-CA5-CA6-CA7
46	r	305	CHL	C2A-CAA-CBA-CGA
38	b	524	LMT	O1'-C1-C2-C3
35	D	410	LMG	C12-C13-C14-C15
29	C	513	CLA	C2-C3-C5-C6
46	N	601	CHL	C2-C3-C5-C6
41	W	202	DGA	CA3-CA4-CA5-CA6
40	I	101	SPH	C1-C2-C3-C4
48	Y	318	NEX	C7-C8-C9-C19
48	y	319	NEX	C7-C8-C9-C19
50	n	619	PTY	C2-C3-O11-P1
50	y	321	PTY	C2-C3-O11-P1
46	n	606	CHL	C13-C15-C16-C17
39	l	101	SQD	C11-C10-C9-C8
33	B	522	3PH	O21-C2-C3-O31
35	C	522	LMG	O1-C7-C8-O7
35	w	202	LMG	O1-C7-C8-O7
37	l	102	LHG	O7-C5-C6-O8
39	C	501	SQD	O6-C44-C45-O47
39	C	523	SQD	O47-C45-C46-O48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	a	410	SQD	O6-C44-C45-O47
39	m	101	SQD	O47-C45-C46-O48
41	w	201	DGA	OG1-CG1-CG2-OG2
50	n	619	PTY	O4-C1-C6-O7
50	y	321	PTY	O4-C1-C6-O7
29	b	516	CLA	C8-C10-C11-C12
29	S	311	CLA	C6-C7-C8-C9
29	a	405	CLA	C6-C7-C8-C9
29	b	510	CLA	C11-C12-C13-C14
29	c	507	CLA	C11-C10-C8-C9
29	c	510	CLA	C14-C13-C15-C16
29	y	304	CLA	C6-C7-C8-C9
46	G	609	CHL	C11-C10-C8-C9
46	g	601	CHL	C6-C7-C8-C9
36	C	520	DGD	C3A-C4A-C5A-C6A
37	a	414	LHG	C25-C26-C27-C28
39	b	523	SQD	C30-C31-C32-C33
33	a	415	3PH	C24-C25-C26-C27
37	s	320	LHG	C14-C15-C16-C17
37	s	320	LHG	C29-C30-C31-C32
40	i	102	SPH	C13-C14-C15-C16
29	B	504	CLA	C13-C15-C16-C17
29	n	609	CLA	C5-C6-C7-C8
29	r	308	CLA	C10-C11-C12-C13
46	g	609	CHL	C13-C15-C16-C17
37	N	618	LHG	C35-C36-C37-C38
46	Y	302	CHL	C3-C5-C6-C7
37	D	408	LHG	C8-C7-O7-C5
29	n	603	CLA	C2-C1-O2A-CGA
46	g	607	CHL	C2-C1-O2A-CGA
36	C	519	DGD	C2E-C1E-O5D-C6D
29	Y	304	CLA	C16-C17-C18-C19
41	w	201	DGA	CEA-CFA-CGA-CHA
39	o	301	SQD	C24-C25-C26-C27
50	n	619	PTY	C37-C38-C39-C40
29	c	507	CLA	C13-C15-C16-C17
46	N	605	CHL	C4-C3-C5-C6
29	S	310	CLA	O1D-CGD-O2D-CED
29	c	501	CLA	C2A-CAA-CBA-CGA
29	C	506	CLA	CBA-CGA-O2A-C1
46	N	607	CHL	C16-C17-C18-C19
29	g	610	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	B	520	LMG	C31-C32-C33-C34
41	j	101	DGA	CA1-CA2-CA3-CA4
33	b	521	3PH	C26-C27-C28-C29
35	c	519	LMG	C33-C34-C35-C36
37	S	320	LHG	C24-C25-C26-C27
37	y	320	LHG	C26-C27-C28-C29
37	l	102	LHG	C15-C16-C17-C18
39	M	101	SQD	C4-C5-C6-S
39	a	410	SQD	C4-C5-C6-S
33	b	521	3PH	C32-C33-C34-C35
37	B	523	LHG	C23-C24-C25-C26
33	A	412	3PH	C3B-C3C-C3D-C3E
37	y	320	LHG	C35-C36-C37-C38
29	N	602	CLA	C16-C17-C18-C19
35	C	524	LMG	C15-C16-C17-C18
29	R	306	CLA	C3-C5-C6-C7
37	L	101	LHG	C10-C11-C12-C13
29	B	505	CLA	C1A-C2A-CAA-CBA
29	N	602	CLA	C1A-C2A-CAA-CBA
29	N	604	CLA	C1A-C2A-CAA-CBA
29	S	312	CLA	C4B-C3B-CAB-CBB
29	S	315	CLA	C1A-C2A-CAA-CBA
29	Y	311	CLA	C1A-C2A-CAA-CBA
29	a	406	CLA	C1A-C2A-CAA-CBA
29	b	515	CLA	C4B-C3B-CAB-CBB
29	c	512	CLA	C1A-C2A-CAA-CBA
29	n	602	CLA	C4B-C3B-CAB-CBB
29	g	603	CLA	C4B-C3B-CAB-CBB
29	s	312	CLA	C4B-C3B-CAB-CBB
29	n	602	CLA	CBA-CGA-O2A-C1
43	d	405	PL9	C45-C44-C46-C47
35	d	408	LMG	O7-C10-C11-C12
37	N	618	LHG	O8-C23-C24-C25
39	c	522	SQD	C32-C33-C34-C35
41	w	201	DGA	CDB-CEB-CFB-CGB
31	A	410	BCR	C21-C22-C23-C24
45	H	101	RRX	C11-C12-C13-C14
40	c	523	SPH	C11-C10-C9-C8
33	B	522	3PH	C3B-C3C-C3D-C3E
37	a	413	LHG	C11-C10-C9-C8
29	N	603	CLA	C15-C16-C17-C18
29	g	613	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	N	618	LHG	O6-C4-C5-C6
37	s	301	LHG	O6-C4-C5-C6
50	n	619	PTY	O14-C5-C6-C1
29	B	504	CLA	CBD-CGD-O2D-CED
39	C	501	SQD	O10-C23-O48-C46
29	r	310	CLA	C2-C3-C5-C6
37	G	618	LHG	C30-C31-C32-C33
41	W	202	DGA	CB7-CB8-CB9-CAB
29	C	502	CLA	C11-C12-C13-C15
29	C	503	CLA	C11-C12-C13-C15
29	C	506	CLA	C6-C7-C8-C10
29	C	510	CLA	C11-C10-C8-C7
29	C	513	CLA	C11-C10-C8-C7
29	N	602	CLA	C12-C13-C15-C16
29	N	603	CLA	C11-C10-C8-C7
29	N	604	CLA	C6-C7-C8-C10
29	Y	304	CLA	C11-C10-C8-C7
29	Y	312	CLA	C6-C7-C8-C10
29	b	501	CLA	C12-C13-C15-C16
29	b	507	CLA	C12-C13-C15-C16
29	c	501	CLA	C11-C12-C13-C15
29	c	505	CLA	C6-C7-C8-C10
29	g	603	CLA	C11-C10-C8-C7
29	g	613	CLA	C11-C12-C13-C15
29	r	302	CLA	C6-C7-C8-C10
29	s	312	CLA	C11-C10-C8-C7
46	N	605	CHL	C12-C13-C15-C16
46	Y	308	CHL	C11-C12-C13-C15
46	n	606	CHL	C11-C10-C8-C7
46	y	309	CHL	C11-C12-C13-C15
33	b	521	3PH	C27-C28-C29-C2A
29	G	604	CLA	O1D-CGD-O2D-CED
29	g	603	CLA	O1D-CGD-O2D-CED
29	C	506	CLA	CBD-CGD-O2D-CED
41	w	201	DGA	CA8-CA9-CAA-CBA
37	D	407	LHG	C24-C23-O8-C6
29	n	602	CLA	C15-C16-C17-C18
35	C	524	LMG	C32-C33-C34-C35
29	g	602	CLA	C15-C16-C17-C18
46	Y	307	CHL	C8-C10-C11-C12
37	c	521	LHG	C7-C8-C9-C10
33	b	521	3PH	C2-C1-O11-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	s	301	LHG	C2-C3-O3-P
37	L	101	LHG	C11-C10-C9-C8
37	a	414	LHG	C11-C10-C9-C8
29	B	512	CLA	C3A-C2A-CAA-CBA
29	N	614	CLA	C3A-C2A-CAA-CBA
46	Y	307	CHL	C4-C3-C5-C6
37	S	320	LHG	C29-C30-C31-C32
37	n	617	LHG	C26-C27-C28-C29
40	C	525	SPH	C10-C11-C12-C13
41	w	201	DGA	CA6-CA7-CA8-CA9
37	D	408	LHG	O6-C4-C5-O7
37	N	618	LHG	O6-C4-C5-O7
37	l	102	LHG	O6-C4-C5-O7
50	n	619	PTY	O14-C5-C6-O7
41	b	522	DGA	CB1-CB2-CB3-CB4
41	w	201	DGA	CB2-CB1-OG2-CG2
29	R	308	CLA	O1D-CGD-O2D-CED
29	G	613	CLA	C2A-CAA-CBA-CGA
29	Y	314	CLA	C2A-CAA-CBA-CGA
29	B	501	CLA	C14-C13-C15-C16
29	B	504	CLA	C14-C13-C15-C16
29	N	603	CLA	C14-C13-C15-C16
29	N	613	CLA	C14-C13-C15-C16
29	G	613	CLA	C14-C13-C15-C16
29	b	504	CLA	C11-C12-C13-C14
29	c	502	CLA	C11-C12-C13-C14
29	n	603	CLA	C14-C13-C15-C16
29	g	603	CLA	C14-C13-C15-C16
29	y	306	CLA	C11-C10-C8-C9
46	Y	307	CHL	C6-C7-C8-C9
29	D	405	CLA	C10-C11-C12-C13
35	W	203	LMG	C36-C37-C38-C39
45	H	101	RRX	C9-C10-C11-C12
47	n	614	LUT	C29-C30-C31-C32
47	s	317	LUT	C29-C30-C31-C32
48	g	617	NEX	C9-C10-C11-C12
29	C	506	CLA	C11-C12-C13-C14
36	c	518	DGD	O6D-C5D-C6D-O5D
35	C	524	LMG	C30-C31-C32-C33
29	N	611	CLA	C1-C2-C3-C4
29	G	604	CLA	C1-C2-C3-C4
29	G	614	CLA	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	n	610	CLA	C1-C2-C3-C4
29	g	604	CLA	C1-C2-C3-C4
29	g	614	CLA	C1-C2-C3-C4
39	L	102	SQD	O5-C5-C6-S
46	N	608	CHL	C1-C2-C3-C4
46	G	606	CHL	C1-C2-C3-C4
46	R	305	CHL	C1-C2-C3-C4
46	n	607	CHL	C1-C2-C3-C4
46	g	606	CHL	C1-C2-C3-C4
46	r	306	CHL	C1-C2-C3-C4
35	c	519	LMG	C18-C19-C20-C21
41	b	522	DGA	CDB-CEB-CFB-CGB
41	w	201	DGA	CEB-CFB-CGB-CHB
37	S	320	LHG	C15-C16-C17-C18
37	s	301	LHG	C11-C12-C13-C14
33	b	521	3PH	C2B-C2C-C2D-C2E
29	C	506	CLA	O1A-CGA-O2A-C1
33	s	322	3PH	O21-C2-C3-O31
35	C	522	LMG	O7-C8-C9-O8
37	L	101	LHG	O7-C5-C6-O8
37	c	521	LHG	O7-C5-C6-O8
39	b	523	SQD	O6-C44-C45-O47
29	B	511	CLA	C4C-C3C-CAC-CBC
35	C	522	LMG	O1-C7-C8-C9
35	C	524	LMG	O1-C7-C8-C9
35	i	101	LMG	C7-C8-C9-O8
39	C	501	SQD	O6-C44-C45-C46
39	a	410	SQD	O6-C44-C45-C46
41	J	101	DGA	OG1-CG1-CG2-CG3
46	N	609	CHL	C4-C3-C5-C6
46	S	309	CHL	C4-C3-C5-C6
37	a	414	LHG	C34-C35-C36-C37
29	Y	312	CLA	C3-C5-C6-C7
29	R	306	CLA	O1D-CGD-O2D-CED
36	C	520	DGD	O6D-C5D-C6D-O5D
29	B	507	CLA	CAD-CBD-CGD-O2D
29	n	604	CLA	CAD-CBD-CGD-O2D
29	r	310	CLA	CAD-CBD-CGD-O2D
29	s	303	CLA	CAD-CBD-CGD-O2D
46	N	609	CHL	CAD-CBD-CGD-O2D
46	R	304	CHL	CAD-CBD-CGD-O2D
46	r	305	CHL	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	B	520	LMG	C18-C19-C20-C21
30	a	407	PHO	C15-C16-C17-C18
29	G	611	CLA	C16-C17-C18-C20
29	R	302	CLA	C2C-C3C-CAC-CBC
29	Y	303	CLA	C2A-CAA-CBA-CGA
33	b	521	3PH	C35-C36-C37-C38
29	n	602	CLA	O1A-CGA-O2A-C1
35	c	519	LMG	C32-C33-C34-C35
39	o	301	SQD	C25-C26-C27-C28
29	B	507	CLA	CAD-CBD-CGD-O1D
29	C	505	CLA	CAD-CBD-CGD-O1D
29	C	508	CLA	CHA-CBD-CGD-O1D
29	C	508	CLA	CHA-CBD-CGD-O2D
29	N	603	CLA	CHA-CBD-CGD-O1D
29	N	603	CLA	CHA-CBD-CGD-O2D
29	Y	303	CLA	CHA-CBD-CGD-O1D
29	Y	303	CLA	CHA-CBD-CGD-O2D
29	c	507	CLA	CHA-CBD-CGD-O1D
29	c	509	CLA	CHA-CBD-CGD-O1D
29	c	509	CLA	CHA-CBD-CGD-O2D
29	n	602	CLA	CHA-CBD-CGD-O1D
29	n	602	CLA	CHA-CBD-CGD-O2D
29	n	604	CLA	CAD-CBD-CGD-O1D
29	r	310	CLA	CAD-CBD-CGD-O1D
29	s	303	CLA	CAD-CBD-CGD-O1D
29	s	304	CLA	CHA-CBD-CGD-O1D
29	s	304	CLA	CHA-CBD-CGD-O2D
29	s	305	CLA	CHA-CBD-CGD-O1D
29	s	305	CLA	CHA-CBD-CGD-O2D
29	y	304	CLA	CHA-CBD-CGD-O1D
29	y	304	CLA	CHA-CBD-CGD-O2D
30	d	402	PHO	CHA-CBD-CGD-O2D
31	B	518	BCR	C9-C10-C11-C12
31	F	101	BCR	C13-C14-C15-C16
31	F	101	BCR	C19-C20-C21-C22
31	f	101	BCR	C9-C10-C11-C12
31	z	101	BCR	C13-C14-C15-C16
31	z	101	BCR	C19-C20-C21-C22
37	B	523	LHG	C4-O6-P-O4
37	L	101	LHG	C4-O6-P-O4
37	L	101	LHG	C4-O6-P-O5
37	S	301	LHG	C3-O3-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	S	301	LHG	C3-O3-P-O6
37	S	301	LHG	C4-O6-P-O4
37	S	320	LHG	C3-O3-P-O5
37	a	413	LHG	C4-O6-P-O3
37	a	414	LHG	C3-O3-P-O4
37	a	414	LHG	C3-O3-P-O6
37	d	406	LHG	C4-O6-P-O4
37	s	320	LHG	C4-O6-P-O5
37	y	320	LHG	C4-O6-P-O4
46	N	609	CHL	CAD-CBD-CGD-O1D
46	G	608	CHL	CHA-CBD-CGD-O2D
46	R	304	CHL	CAD-CBD-CGD-O1D
46	S	308	CHL	CHA-CBD-CGD-O2D
46	Y	308	CHL	CHA-CBD-CGD-O1D
46	Y	308	CHL	CHA-CBD-CGD-O2D
46	n	606	CHL	CHA-CBD-CGD-O1D
46	n	606	CHL	CHA-CBD-CGD-O2D
46	n	607	CHL	CHA-CBD-CGD-O1D
46	n	607	CHL	CHA-CBD-CGD-O2D
46	g	607	CHL	CHA-CBD-CGD-O2D
46	r	305	CHL	CAD-CBD-CGD-O1D
46	s	309	CHL	CHA-CBD-CGD-O2D
46	y	309	CHL	CHA-CBD-CGD-O2D
47	S	318	LUT	C25-C26-C27-C28
48	R	312	NEX	C13-C14-C15-C35
50	n	619	PTY	C5-O14-P1-O13
50	y	321	PTY	C3-O11-P1-O13
51	s	321	LPX	C3-O1-P1-O2
51	s	321	LPX	C3-O1-P1-O4
33	s	322	3PH	C3E-C3F-C3G-C3H
29	C	514	CLA	C16-C17-C18-C20
37	a	414	LHG	C24-C25-C26-C27
29	r	308	CLA	C8-C10-C11-C12
29	B	503	CLA	C4-C3-C5-C6
29	A	406	CLA	C2B-C3B-CAB-CBB
29	N	613	CLA	C2B-C3B-CAB-CBB
29	G	611	CLA	C2B-C3B-CAB-CBB
29	G	613	CLA	C2B-C3B-CAB-CBB
29	G	614	CLA	C2B-C3B-CAB-CBB
29	R	302	CLA	C2B-C3B-CAB-CBB
29	Y	305	CLA	C2B-C3B-CAB-CBB
29	Y	312	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	b	503	CLA	C2B-C3B-CAB-CBB
29	c	503	CLA	C2B-C3B-CAB-CBB
29	r	304	CLA	C2B-C3B-CAB-CBB
29	y	306	CLA	C2B-C3B-CAB-CBB
31	A	410	BCR	C23-C24-C25-C26
31	a	409	BCR	C37-C22-C23-C24
37	a	414	LHG	C2-C3-O3-P
37	c	521	LHG	C2-C3-O3-P
37	l	102	LHG	C2-C3-O3-P
41	w	201	DGA	OB1-CB1-OG2-CG2
29	B	515	CLA	C16-C17-C18-C20
35	c	519	LMG	C15-C16-C17-C18
35	C	522	LMG	C36-C37-C38-C39
37	s	320	LHG	C9-C10-C11-C12
38	B	524	LMT	C6-C7-C8-C9
39	c	522	SQD	C28-C29-C30-C31
37	d	406	LHG	O1-C1-C2-O2
37	s	320	LHG	C23-C24-C25-C26
35	d	408	LMG	C13-C14-C15-C16
41	W	202	DGA	CBB-CAB-CB9-CB8
33	A	412	3PH	C3-C2-O21-C21
33	a	415	3PH	C3-C2-O21-C21
35	C	524	LMG	C7-C8-O7-C10
39	M	101	SQD	C46-C45-O47-C7
39	l	101	SQD	C46-C45-O47-C7
29	y	315	CLA	C4-C3-C5-C6
37	G	618	LHG	C28-C29-C30-C31
37	G	618	LHG	C33-C34-C35-C36
37	G	618	LHG	O8-C23-C24-C25
29	s	312	CLA	C2-C3-C5-C6
46	N	605	CHL	C2-C3-C5-C6
46	Y	307	CHL	C2-C3-C5-C6
37	y	320	LHG	C23-C24-C25-C26
35	i	101	LMG	C11-C12-C13-C14
37	d	406	LHG	C11-C10-C9-C8
29	B	511	CLA	C16-C17-C18-C20
29	S	314	CLA	C6-C7-C8-C9
29	Y	312	CLA	C13-C15-C16-C17
29	c	503	CLA	C8-C10-C11-C12
37	a	413	LHG	C35-C36-C37-C38
29	N	602	CLA	C3-C5-C6-C7
29	Y	313	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	B	507	CLA	C6-C7-C8-C9
29	B	509	CLA	C11-C12-C13-C14
29	B	510	CLA	C11-C12-C13-C14
29	B	514	CLA	C11-C10-C8-C9
29	C	512	CLA	C6-C7-C8-C9
29	N	604	CLA	C6-C7-C8-C9
29	G	602	CLA	C14-C13-C15-C16
29	Y	303	CLA	C6-C7-C8-C9
29	y	305	CLA	C14-C13-C15-C16
29	y	313	CLA	C14-C13-C15-C16
29	y	316	CLA	C6-C7-C8-C9
46	N	606	CHL	C14-C13-C15-C16
46	n	606	CHL	C11-C12-C13-C14
46	g	609	CHL	C11-C12-C13-C14
46	y	301	CHL	C11-C10-C8-C9
29	C	512	CLA	C6-C7-C8-C10
29	b	516	CLA	C6-C7-C8-C10
29	c	510	CLA	C12-C13-C15-C16
29	y	313	CLA	C12-C13-C15-C16
46	n	608	CHL	C12-C13-C15-C16
48	S	319	NEX	C28-C29-C30-C31
37	G	618	LHG	O6-C4-C5-O7
40	i	102	SPH	C9-C10-C11-C12
41	w	201	DGA	CB3-CB4-CB5-CB6
29	R	307	CLA	C2A-CAA-CBA-CGA
29	S	316	CLA	C2A-CAA-CBA-CGA
29	C	506	CLA	C11-C12-C13-C15
29	N	603	CLA	C16-C17-C18-C19
29	N	603	CLA	C16-C17-C18-C20
46	y	309	CHL	C10-C11-C12-C13
37	l	102	LHG	C30-C31-C32-C33
40	I	101	SPH	C10-C11-C12-C13
41	w	201	DGA	CB9-CAB-CBB-CCB
29	B	507	CLA	C10-C11-C12-C13
29	B	506	CLA	O1D-CGD-O2D-CED
43	D	406	PL9	C45-C44-C46-C47
41	w	201	DGA	CAA-CBA-CCA-CDA
29	s	310	CLA	C2-C3-C5-C6
41	w	201	DGA	CA3-CA4-CA5-CA6
40	C	525	SPH	C15-C16-C17-C18
35	c	519	LMG	C19-C20-C21-C22
36	c	517	DGD	C6B-C7B-C8B-C9B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	Y	320	PTY	O4-C1-C6-O7
29	S	314	CLA	C6-C7-C8-C10
37	D	407	LHG	C31-C32-C33-C34
29	S	311	CLA	C8-C10-C11-C12
29	c	501	CLA	C10-C11-C12-C13
39	l	101	SQD	O47-C7-C8-C9
37	S	301	LHG	C29-C30-C31-C32
37	D	408	LHG	O9-C7-O7-C5
29	A	405	CLA	C2-C1-O2A-CGA
29	G	604	CLA	C2-C1-O2A-CGA
29	Y	315	CLA	C4-C3-C5-C6
46	n	608	CHL	C4-C3-C5-C6
37	c	521	LHG	C26-C27-C28-C29
29	N	614	CLA	O2A-C1-C2-C3
39	M	101	SQD	O47-C7-C8-C9
46	S	309	CHL	CAA-CBA-CGA-O2A
29	c	512	CLA	C2-C3-C5-C6
33	A	412	3PH	C3F-C3G-C3H-C3I
39	C	523	SQD	O6-C44-C45-C46
46	N	607	CHL	CAA-CBA-CGA-O2A
35	D	410	LMG	C29-C30-C31-C32
37	g	618	LHG	C29-C30-C31-C32
37	S	320	LHG	C35-C36-C37-C38
36	B	521	DGD	C2G-C3G-O3G-C1D
35	b	520	LMG	C19-C20-C21-C22
29	S	306	CLA	C2A-CAA-CBA-CGA
29	c	511	CLA	C2A-CAA-CBA-CGA
46	G	605	CHL	C2A-CAA-CBA-CGA
46	G	607	CHL	C2A-CAA-CBA-CGA
31	C	515	BCR	C15-C16-C17-C18
31	C	515	BCR	C19-C20-C21-C22
29	N	610	CLA	C16-C17-C18-C20
35	w	202	LMG	C28-C29-C30-C31
37	n	617	LHG	C16-C17-C18-C19
29	B	505	CLA	C4-C3-C5-C6
39	C	523	SQD	C24-C23-O48-C46
35	w	202	LMG	C29-C30-C31-C32
39	a	410	SQD	C11-C10-C9-C8
41	b	522	DGA	CAB-CBB-CCB-CDB
50	N	620	PTY	C35-C36-C37-C38
29	B	504	CLA	C4C-C3C-CAC-CBC
29	C	511	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	n	602	CLA	C16-C17-C18-C20
29	s	310	CLA	C11-C12-C13-C14
29	y	312	CLA	C16-C17-C18-C20
35	C	524	LMG	C13-C14-C15-C16
29	C	503	CLA	C11-C12-C13-C14
29	C	506	CLA	C6-C7-C8-C9
29	C	513	CLA	C6-C7-C8-C9
29	C	513	CLA	C11-C10-C8-C9
29	N	603	CLA	C11-C10-C8-C9
29	b	507	CLA	C14-C13-C15-C16
29	d	404	CLA	C11-C12-C13-C14
29	g	613	CLA	C11-C12-C13-C14
29	s	304	CLA	C11-C10-C8-C9
29	s	312	CLA	C11-C10-C8-C9
46	G	609	CHL	C11-C12-C13-C14
37	a	413	LHG	C29-C30-C31-C32
29	C	508	CLA	CBA-CGA-O2A-C1
29	r	302	CLA	CBA-CGA-O2A-C1
29	c	512	CLA	C4B-C3B-CAB-CBB
29	d	404	CLA	C4B-C3B-CAB-CBB
29	n	612	CLA	C4B-C3B-CAB-CBB
29	g	602	CLA	C4B-C3B-CAB-CBB
29	r	302	CLA	C4B-C3B-CAB-CBB
29	y	314	CLA	C4B-C3B-CAB-CBB
37	Y	319	LHG	C17-C18-C19-C20
29	N	610	CLA	C5-C6-C7-C8
35	W	203	LMG	C37-C38-C39-C40
41	W	202	DGA	CA9-CAA-CBA-CCA
29	c	512	CLA	CBA-CGA-O2A-C1
29	B	516	CLA	C5-C6-C7-C8
29	C	502	CLA	C15-C16-C17-C18
29	N	602	CLA	C15-C16-C17-C18
29	c	512	CLA	C10-C11-C12-C13
29	b	512	CLA	C2A-CAA-CBA-CGA
29	Y	304	CLA	C4-C3-C5-C6
29	y	305	CLA	C4-C3-C5-C6
46	Y	310	CHL	C4-C3-C5-C6
46	g	607	CHL	C4-C3-C5-C6
46	y	311	CHL	C4-C3-C5-C6
46	s	309	CHL	CAA-CBA-CGA-O2A
43	d	405	PL9	C43-C44-C46-C47
46	N	609	CHL	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	n	617	LHG	O6-C4-C5-C6
33	b	521	3PH	C23-C24-C25-C26
39	C	523	SQD	O10-C23-O48-C46
31	K	101	BCR	C9-C10-C11-C12
31	v	101	BCR	C9-C10-C11-C12
37	a	413	LHG	C33-C34-C35-C36
41	w	201	DGA	CBB-CCB-CDB-CEB
37	n	617	LHG	O8-C23-C24-C25
29	C	504	CLA	C12-C13-C15-C16
29	Y	305	CLA	C11-C12-C13-C15
29	Y	313	CLA	C6-C7-C8-C10
29	b	507	CLA	C11-C12-C13-C15
29	n	602	CLA	C12-C13-C15-C16
29	n	609	CLA	C6-C7-C8-C10
46	g	609	CHL	C12-C13-C15-C16
29	c	506	CLA	C5-C6-C7-C8
29	C	508	CLA	O1A-CGA-O2A-C1
29	c	512	CLA	O1A-CGA-O2A-C1
29	a	406	CLA	CBA-CGA-O2A-C1
29	n	603	CLA	C8-C10-C11-C12
37	g	618	LHG	C15-C16-C17-C18
50	N	620	PTY	C37-C38-C39-C40
29	C	514	CLA	C16-C17-C18-C19
29	G	611	CLA	C16-C17-C18-C19
29	R	308	CLA	C11-C12-C13-C14
46	s	309	CHL	C11-C12-C13-C14
29	n	604	CLA	C15-C16-C17-C18
29	r	302	CLA	O1A-CGA-O2A-C1
33	A	412	3PH	O21-C2-C3-O31
35	d	408	LMG	O7-C8-C9-O8
39	b	523	SQD	C28-C29-C30-C31
41	W	202	DGA	CCB-CDB-CEB-CFB
29	S	303	CLA	C3A-C2A-CAA-CBA
29	c	512	CLA	C3A-C2A-CAA-CBA
46	Y	306	CHL	C3A-C2A-CAA-CBA
46	Y	308	CHL	C4-C3-C5-C6
37	s	301	LHG	C24-C25-C26-C27
37	c	521	LHG	C9-C10-C11-C12
48	G	617	NEX	C39-C29-C30-C31
48	S	319	NEX	C39-C29-C30-C31
48	g	617	NEX	C39-C29-C30-C31
48	s	319	NEX	C39-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	y	319	NEX	C39-C29-C30-C31
29	b	501	CLA	CAA-CBA-CGA-O1A
29	Y	313	CLA	C5-C6-C7-C8
29	b	502	CLA	C5-C6-C7-C8
37	S	301	LHG	C28-C29-C30-C31
36	c	517	DGD	C2B-C3B-C4B-C5B
31	C	516	BCR	C13-C14-C15-C16
47	g	615	LUT	C29-C30-C31-C32
29	r	310	CLA	C4-C3-C5-C6
33	A	412	3PH	C3D-C3E-C3F-C3G
37	B	523	LHG	C30-C31-C32-C33
37	y	320	LHG	C34-C35-C36-C37
41	j	101	DGA	CB3-CB4-CB5-CB6
36	c	516	DGD	C2A-C3A-C4A-C5A
29	b	513	CLA	C4-C3-C5-C6
29	c	511	CLA	C4-C3-C5-C6
36	B	521	DGD	C1B-C2B-C3B-C4B
46	S	309	CHL	C2-C3-C5-C6
29	g	614	CLA	O2A-C1-C2-C3
46	N	608	CHL	O2A-C1-C2-C3
35	w	202	LMG	C37-C38-C39-C40
29	b	505	CLA	C2A-CAA-CBA-CGA
29	b	511	CLA	CBD-CGD-O2D-CED
29	R	307	CLA	C4C-C3C-CAC-CBC
37	L	101	LHG	C4-C5-C6-O8
39	C	523	SQD	C44-C45-C46-O48
35	i	101	LMG	C31-C32-C33-C34
29	C	513	CLA	C15-C16-C17-C18
29	b	501	CLA	C8-C10-C11-C12
35	C	522	LMG	C34-C35-C36-C37
46	R	304	CHL	C2A-CAA-CBA-CGA
29	C	504	CLA	C11-C10-C8-C9
29	b	504	CLA	C6-C7-C8-C9
29	n	602	CLA	C14-C13-C15-C16
29	n	609	CLA	C6-C7-C8-C9
29	n	609	CLA	C11-C12-C13-C14
29	g	603	CLA	C6-C7-C8-C9
29	r	307	CLA	C6-C7-C8-C9
29	s	310	CLA	C11-C10-C8-C9
29	y	314	CLA	C11-C12-C13-C14
30	d	402	PHO	C6-C7-C8-C9
46	N	606	CHL	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	N	609	CHL	C11-C12-C13-C14
46	n	608	CHL	C11-C10-C8-C9
29	b	504	CLA	C16-C17-C18-C20
29	y	314	CLA	CBA-CGA-O2A-C1
36	c	518	DGD	C4A-C5A-C6A-C7A
40	I	101	SPH	C11-C10-C9-C8
29	r	307	CLA	C5-C6-C7-C8
41	w	201	DGA	CCA-CDA-CEA-CFA
41	D	402	DGA	CG1-CG2-CG3-OXT
41	W	202	DGA	CG1-CG2-CG3-OXT
46	N	601	CHL	C1A-C2A-CAA-CBA
46	G	607	CHL	C1A-C2A-CAA-CBA
46	n	601	CHL	C1A-C2A-CAA-CBA
46	g	609	CHL	C1A-C2A-CAA-CBA
29	S	303	CLA	C4-C3-C5-C6
46	y	301	CHL	CAA-CBA-CGA-O2A
29	Y	304	CLA	C2-C3-C5-C6
29	c	511	CLA	C2-C3-C5-C6
46	n	608	CHL	C2-C3-C5-C6
50	n	619	PTY	C23-C24-C25-C26
37	c	521	LHG	O1-C1-C2-O2
39	a	410	SQD	C15-C16-C17-C18
35	W	203	LMG	C2-C1-O1-C7
41	w	201	DGA	CFA-CGA-CHA-CIA
29	C	502	CLA	C2A-CAA-CBA-CGA
29	y	304	CLA	C2A-CAA-CBA-CGA
29	y	312	CLA	C2A-CAA-CBA-CGA
29	y	315	CLA	C2A-CAA-CBA-CGA
35	w	202	LMG	O9-C10-C11-C12
29	B	511	CLA	C1A-C2A-CAA-CBA
29	B	512	CLA	C1A-C2A-CAA-CBA
29	C	502	CLA	C1A-C2A-CAA-CBA
29	b	516	CLA	C1A-C2A-CAA-CBA
29	d	404	CLA	C1A-C2A-CAA-CBA
29	s	314	CLA	C1A-C2A-CAA-CBA
48	G	617	NEX	C28-C29-C30-C31
48	g	617	NEX	C28-C29-C30-C31
48	s	319	NEX	C28-C29-C30-C31
48	y	319	NEX	C28-C29-C30-C31
29	s	310	CLA	C11-C12-C13-C15
36	C	518	DGD	O6D-C5D-C6D-O5D
37	l	102	LHG	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	a	410	SQD	C29-C30-C31-C32
29	C	510	CLA	C13-C15-C16-C17
29	B	502	CLA	C2B-C3B-CAB-CBB
29	B	509	CLA	C2B-C3B-CAB-CBB
29	C	512	CLA	C2B-C3B-CAB-CBB
29	G	604	CLA	C2B-C3B-CAB-CBB
29	R	303	CLA	C2B-C3B-CAB-CBB
29	S	314	CLA	C2B-C3B-CAB-CBB
29	Y	314	CLA	C2B-C3B-CAB-CBB
29	b	502	CLA	C2B-C3B-CAB-CBB
29	b	509	CLA	C2B-C3B-CAB-CBB
29	b	511	CLA	C2B-C3B-CAB-CBB
29	c	501	CLA	C2B-C3B-CAB-CBB
29	c	504	CLA	C2B-C3B-CAB-CBB
29	g	604	CLA	C2B-C3B-CAB-CBB
29	g	610	CLA	C2B-C3B-CAB-CBB
29	g	611	CLA	C2B-C3B-CAB-CBB
29	s	303	CLA	C2B-C3B-CAB-CBB
29	s	315	CLA	C2B-C3B-CAB-CBB
31	B	518	BCR	C23-C24-C25-C30
31	C	516	BCR	C23-C24-C25-C26
31	C	517	BCR	C1-C6-C7-C8
31	F	101	BCR	C5-C6-C7-C8
31	F	101	BCR	C23-C24-C25-C26
31	a	409	BCR	C23-C24-C25-C26
31	c	514	BCR	C23-C24-C25-C26
34	B	519	C7Z	C25-C26-C27-C28
34	b	519	C7Z	C21-C26-C27-C28
34	b	519	C7Z	C25-C26-C27-C28
45	H	101	RRX	C5-C6-C7-C8
47	N	615	LUT	C1-C6-C7-C8
29	b	505	CLA	CBA-CGA-O2A-C1
29	a	406	CLA	O1A-CGA-O2A-C1
37	D	407	LHG	C2-C3-O3-P
37	D	407	LHG	C29-C30-C31-C32
37	G	618	LHG	C26-C27-C28-C29
37	c	521	LHG	C25-C26-C27-C28
46	S	302	CHL	CAA-CBA-CGA-O1A
29	g	612	CLA	C4C-C3C-CAC-CBC
29	b	514	CLA	C4-C3-C5-C6
29	y	315	CLA	C2-C3-C5-C6
43	D	406	PL9	C43-C44-C46-C47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
43	d	405	PL9	C38-C39-C41-C42
46	y	311	CHL	C2-C3-C5-C6
37	D	408	LHG	C30-C31-C32-C33
46	G	606	CHL	O2A-C1-C2-C3
46	n	607	CHL	O2A-C1-C2-C3
29	n	611	CLA	CAA-CBA-CGA-O2A
46	S	302	CHL	CAA-CBA-CGA-O2A
46	s	302	CHL	CAA-CBA-CGA-O1A
29	b	513	CLA	O1D-CGD-O2D-CED
29	A	406	CLA	C11-C10-C8-C7
29	B	508	CLA	C6-C7-C8-C10
29	B	509	CLA	C11-C12-C13-C15
29	B	513	CLA	C11-C10-C8-C7
29	C	507	CLA	C11-C10-C8-C7
29	S	312	CLA	C6-C7-C8-C10
29	b	502	CLA	C11-C10-C8-C7
29	c	509	CLA	C11-C10-C8-C7
29	d	404	CLA	C11-C12-C13-C15
29	n	609	CLA	C11-C12-C13-C15
29	n	612	CLA	C11-C10-C8-C7
29	g	603	CLA	C6-C7-C8-C10
29	s	304	CLA	C11-C10-C8-C7
29	s	312	CLA	C11-C12-C13-C15
29	y	312	CLA	C12-C13-C15-C16
46	Y	307	CHL	C11-C12-C13-C15
46	Y	308	CHL	C6-C7-C8-C10
46	g	607	CHL	C11-C10-C8-C7
29	B	506	CLA	C2A-CAA-CBA-CGA
29	y	310	CLA	C2A-CAA-CBA-CGA
35	C	522	LMG	C15-C16-C17-C18
37	c	521	LHG	C31-C32-C33-C34
41	J	101	DGA	OG1-CG1-CG2-OG2
37	D	408	LHG	C32-C33-C34-C35
39	b	523	SQD	C12-C13-C14-C15
50	n	619	PTY	C17-C18-C19-C20
29	r	309	CLA	CBD-CGD-O2D-CED
31	C	517	BCR	C7-C8-C9-C34
34	B	519	C7Z	C27-C28-C29-C39
47	r	311	LUT	C11-C12-C13-C20
29	y	314	CLA	O1A-CGA-O2A-C1
29	B	502	CLA	C4-C3-C5-C6
29	b	513	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	y	305	CLA	C2-C3-C5-C6
46	Y	310	CHL	C2-C3-C5-C6
46	g	607	CHL	C2-C3-C5-C6
29	B	504	CLA	O1D-CGD-O2D-CED
37	D	407	LHG	O10-C23-O8-C6
29	B	513	CLA	C2-C1-O2A-CGA
40	I	101	SPH	O3-C3-C4-C5
29	B	503	CLA	C13-C15-C16-C17
29	b	504	CLA	C13-C15-C16-C17
29	C	506	CLA	O1D-CGD-O2D-CED
29	b	506	CLA	C2A-CAA-CBA-CGA
29	B	503	CLA	C14-C13-C15-C16
29	a	404	CLA	C11-C12-C13-C14
29	B	509	CLA	C15-C16-C17-C18
29	y	313	CLA	C13-C15-C16-C17
47	N	615	LUT	C29-C30-C31-C32
29	Y	314	CLA	C13-C15-C16-C17
29	b	503	CLA	C13-C15-C16-C17
29	s	311	CLA	C10-C11-C12-C13
29	n	611	CLA	CAA-CBA-CGA-O1A
35	W	201	LMG	C11-C12-C13-C14
36	c	517	DGD	C3A-C4A-C5A-C6A
39	b	523	SQD	C11-C10-C9-C8
46	G	601	CHL	C4-C3-C5-C6
37	S	301	LHG	C24-C25-C26-C27
37	n	617	LHG	C18-C19-C20-C21
41	b	522	DGA	CBA-CCA-CDA-CEA
29	b	511	CLA	C4C-C3C-CAC-CBC
43	D	406	PL9	C38-C39-C41-C42
29	C	510	CLA	CBD-CGD-O2D-CED
29	b	505	CLA	O1A-CGA-O2A-C1
39	b	523	SQD	C11-C12-C13-C14
29	S	312	CLA	C16-C17-C18-C19
29	R	301	CLA	C10-C11-C12-C13
29	A	406	CLA	C4C-C3C-CAC-CBC
35	W	201	LMG	C7-C8-C9-O8
35	d	408	LMG	C7-C8-C9-O8
39	b	523	SQD	O6-C44-C45-C46
41	b	522	DGA	CB7-CB8-CB9-CAB
29	D	404	CLA	O1D-CGD-O2D-CED
29	C	506	CLA	C2A-CAA-CBA-CGA
29	N	602	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	c	502	CLA	C13-C15-C16-C17
37	s	301	LHG	C26-C27-C28-C29
46	y	307	CHL	CAA-CBA-CGA-O2A
29	b	511	CLA	O1D-CGD-O2D-CED
29	c	512	CLA	C15-C16-C17-C18
29	B	513	CLA	C4-C3-C5-C6
39	C	523	SQD	C7-C8-C9-C10
36	C	520	DGD	C9A-CAA-CBA-CCA
29	N	610	CLA	C16-C17-C18-C19
37	s	301	LHG	C30-C31-C32-C33
29	B	504	CLA	C4B-C3B-CAB-CBB
29	N	602	CLA	C4B-C3B-CAB-CBB
29	Y	303	CLA	C4B-C3B-CAB-CBB
29	g	610	CLA	C4B-C3B-CAB-CBB
29	g	614	CLA	C4B-C3B-CAB-CBB
29	c	501	CLA	C15-C16-C17-C18
41	j	101	DGA	OA1-CA1-OG1-CG1
35	W	201	LMG	O7-C10-C11-C12
37	g	618	LHG	O8-C23-C24-C25
33	s	322	3PH	C33-C34-C35-C36
29	Y	304	CLA	C2C-C3C-CAC-CBC
29	B	511	CLA	C16-C17-C18-C19
29	S	303	CLA	C11-C12-C13-C14
29	S	312	CLA	C16-C17-C18-C20
29	y	312	CLA	C16-C17-C18-C19
46	N	607	CHL	C13-C15-C16-C17
30	D	401	PHO	CHA-CBD-CGD-O2D
30	d	402	PHO	CHA-CBD-CGD-O1D
46	S	307	CHL	CHA-CBD-CGD-O1D
46	S	307	CHL	CHA-CBD-CGD-O2D
46	S	308	CHL	CHA-CBD-CGD-O1D
46	Y	310	CHL	CHA-CBD-CGD-O1D
46	Y	310	CHL	CHA-CBD-CGD-O2D
46	g	607	CHL	CHA-CBD-CGD-O1D
46	g	609	CHL	CHA-CBD-CGD-O1D
46	g	609	CHL	CHA-CBD-CGD-O2D
46	r	306	CHL	CHA-CBD-CGD-O2D
46	s	302	CHL	CHA-CBD-CGD-O1D
46	s	302	CHL	CHA-CBD-CGD-O2D
46	s	307	CHL	CHA-CBD-CGD-O1D
46	s	307	CHL	CHA-CBD-CGD-O2D
46	y	311	CHL	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	y	311	CHL	CHA-CBD-CGD-O2D
29	S	304	CLA	C13-C15-C16-C17
29	y	315	CLA	C5-C6-C7-C8
46	N	607	CHL	C15-C16-C17-C18
29	S	313	CLA	CAA-CBA-CGA-O2A
46	s	302	CHL	CAA-CBA-CGA-O2A
39	b	523	SQD	C9-C10-C11-C12
29	s	314	CLA	C4C-C3C-CAC-CBC
46	S	309	CHL	C11-C12-C13-C15
36	B	521	DGD	O2G-C2G-C3G-O3G
35	D	410	LMG	O9-C10-C11-C12
35	D	410	LMG	C34-C35-C36-C37
37	d	406	LHG	C31-C32-C33-C34
29	C	510	CLA	O1D-CGD-O2D-CED
29	S	304	CLA	C11-C12-C13-C15
29	Y	304	CLA	C6-C7-C8-C10
46	n	605	CHL	C11-C12-C13-C15
33	a	415	3PH	C2B-C2C-C2D-C2E
41	W	202	DGA	CAA-CBA-CCA-CDA
36	C	519	DGD	C3B-C4B-C5B-C6B
37	d	406	LHG	C12-C13-C14-C15
37	g	618	LHG	C30-C31-C32-C33
31	C	515	BCR	C13-C14-C15-C16
31	b	518	BCR	C9-C10-C11-C12
49	n	618	XAT	C29-C30-C31-C32
39	L	102	SQD	O47-C7-C8-C9
35	C	522	LMG	C11-C12-C13-C14
41	D	402	DGA	CA9-CAA-CBA-CCA
29	r	308	CLA	C4C-C3C-CAC-CBC
33	b	521	3PH	C21-C22-C23-C24
46	y	307	CHL	CAA-CBA-CGA-O1A
29	A	406	CLA	C6-C7-C8-C9
29	B	501	CLA	C11-C12-C13-C14
29	B	504	CLA	C11-C12-C13-C14
29	B	508	CLA	C11-C12-C13-C14
29	N	602	CLA	C14-C13-C15-C16
29	N	610	CLA	C6-C7-C8-C9
29	c	507	CLA	C6-C7-C8-C9
46	N	605	CHL	C11-C10-C8-C9
46	g	607	CHL	C14-C13-C15-C16
39	o	301	SQD	C10-C11-C12-C13
50	n	619	PTY	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	B	511	CLA	CBD-CGD-O2D-CED
35	C	524	LMG	C8-C7-O1-C1
36	r	301	DGD	C2G-C3G-O3G-C1D
48	r	313	NEX	C20-C13-C14-C15
29	s	306	CLA	C2A-CAA-CBA-CGA
29	b	508	CLA	C2-C1-O2A-CGA
46	y	301	CHL	C2-C1-O2A-CGA
29	R	302	CLA	C11-C12-C13-C15
29	n	602	CLA	C16-C17-C18-C19
29	n	602	CLA	C13-C15-C16-C17
41	j	101	DGA	CA2-CA1-OG1-CG1
29	b	516	CLA	C3A-C2A-CAA-CBA
29	g	604	CLA	C3A-C2A-CAA-CBA
46	N	608	CHL	C3A-C2A-CAA-CBA
29	B	503	CLA	C2-C3-C5-C6
50	N	620	PTY	C22-C23-C24-C25
46	G	609	CHL	C3-C5-C6-C7
35	c	519	LMG	C21-C22-C23-C24
39	L	102	SQD	C24-C25-C26-C27
29	B	507	CLA	C16-C17-C18-C20
29	C	513	CLA	C16-C17-C18-C20
35	C	521	LMG	O7-C10-C11-C12
41	j	101	DGA	CA7-CA8-CA9-CAA
37	G	618	LHG	C34-C35-C36-C37
37	c	521	LHG	C16-C17-C18-C19
33	A	412	3PH	C33-C34-C35-C36
37	l	102	LHG	C11-C12-C13-C14
29	R	307	CLA	CAA-CBA-CGA-O2A
46	N	605	CHL	CAA-CBA-CGA-O2A
29	B	507	CLA	C16-C17-C18-C19
29	b	504	CLA	C16-C17-C18-C19
41	b	522	DGA	CA2-CA3-CA4-CA5
43	D	406	PL9	C13-C14-C16-C17
37	L	101	LHG	C29-C30-C31-C32
49	g	619	XAT	O24-C26-C27-C28
37	s	320	LHG	C2-C3-O3-P
29	R	303	CLA	O2A-C1-C2-C3
29	r	304	CLA	O2A-C1-C2-C3
29	B	511	CLA	O1D-CGD-O2D-CED
36	C	519	DGD	C2B-C3B-C4B-C5B
35	w	202	LMG	C7-C8-C9-O8
39	L	102	SQD	O6-C44-C45-C46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	B	506	CLA	C13-C15-C16-C17
29	r	308	CLA	C5-C6-C7-C8
29	C	511	CLA	C16-C17-C18-C19
35	c	519	LMG	C14-C15-C16-C17
37	n	617	LHG	O1-C1-C2-O2
37	s	301	LHG	O1-C1-C2-O2
46	Y	308	CHL	C10-C11-C12-C13
37	D	407	LHG	C28-C29-C30-C31
37	G	618	LHG	C11-C10-C9-C8
40	C	525	SPH	C12-C13-C14-C15
29	a	406	CLA	C2A-CAA-CBA-CGA
29	c	503	CLA	C2A-CAA-CBA-CGA
31	z	101	BCR	C15-C16-C17-C18
40	I	101	SPH	N2-C2-C3-O3
40	c	523	SPH	C1-C2-C3-O3
37	d	406	LHG	C30-C31-C32-C33
37	D	408	LHG	C25-C26-C27-C28
29	S	306	CLA	CBD-CGD-O2D-CED
37	d	406	LHG	C35-C36-C37-C38
35	d	408	LMG	C31-C32-C33-C34
29	a	405	CLA	CAA-CBA-CGA-O2A
29	b	513	CLA	CAA-CBA-CGA-O2A
35	C	522	LMG	O7-C10-C11-C12
50	N	620	PTY	O4-C30-C31-C32
51	s	321	LPX	O6-C6-C7-C8
41	w	201	DGA	CFB-CGB-CHB-CIB
41	w	201	DGA	CB5-CB6-CB7-CB8
49	N	619	XAT	C14-C15-C35-C34
29	B	504	CLA	C11-C10-C8-C9
29	B	506	CLA	C14-C13-C15-C16
29	N	602	CLA	C6-C7-C8-C9
29	R	302	CLA	C6-C7-C8-C9
29	b	501	CLA	C14-C13-C15-C16
29	b	513	CLA	C14-C13-C15-C16
29	b	516	CLA	C11-C10-C8-C9
29	g	603	CLA	C11-C10-C8-C9
29	g	611	CLA	C14-C13-C15-C16
29	r	308	CLA	C6-C7-C8-C9
46	n	601	CHL	C11-C12-C13-C14
46	n	606	CHL	C11-C10-C8-C9
46	g	607	CHL	C11-C10-C8-C9
46	y	303	CHL	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	i	101	LMG	C18-C19-C20-C21
29	g	614	CLA	CAA-CBA-CGA-O2A
41	j	101	DGA	OG1-CA1-CA2-CA3
46	n	605	CHL	CAA-CBA-CGA-O2A
37	D	408	LHG	C24-C25-C26-C27
29	S	313	CLA	CAA-CBA-CGA-O1A
31	a	409	BCR	C21-C22-C23-C24
36	c	518	DGD	C2A-C3A-C4A-C5A
29	b	509	CLA	C4-C3-C5-C6
37	S	320	LHG	C12-C13-C14-C15
29	B	507	CLA	CAA-CBA-CGA-O2A
29	n	604	CLA	C2A-CAA-CBA-CGA
29	n	610	CLA	C2A-CAA-CBA-CGA
29	B	502	CLA	C12-C13-C15-C16
29	B	506	CLA	C11-C12-C13-C15
29	B	508	CLA	C11-C12-C13-C15
29	B	513	CLA	C11-C12-C13-C15
29	N	610	CLA	C6-C7-C8-C10
29	S	312	CLA	C11-C10-C8-C7
29	Y	305	CLA	C11-C10-C8-C7
29	Y	311	CLA	C12-C13-C15-C16
29	Y	312	CLA	C11-C10-C8-C7
29	Y	314	CLA	C6-C7-C8-C10
29	b	514	CLA	C11-C12-C13-C15
29	c	505	CLA	C11-C10-C8-C7
29	c	507	CLA	C6-C7-C8-C10
29	n	604	CLA	C12-C13-C15-C16
29	y	314	CLA	C6-C7-C8-C10
29	B	511	CLA	C10-C11-C12-C13
29	C	504	CLA	C10-C11-C12-C13
29	A	407	CLA	C2B-C3B-CAB-CBB
29	B	503	CLA	C2B-C3B-CAB-CBB
29	C	502	CLA	C2B-C3B-CAB-CBB
29	C	511	CLA	C2B-C3B-CAB-CBB
29	G	610	CLA	C2B-C3B-CAB-CBB
29	R	308	CLA	C2B-C3B-CAB-CBB
29	Y	311	CLA	C2B-C3B-CAB-CBB
29	a	405	CLA	C2B-C3B-CAB-CBB
29	c	508	CLA	C2B-C3B-CAB-CBB
29	c	511	CLA	C2B-C3B-CAB-CBB
29	n	604	CLA	C2B-C3B-CAB-CBB
29	n	609	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	s	305	CLA	C2B-C3B-CAB-CBB
29	y	315	CLA	C2B-C3B-CAB-CBB
31	B	518	BCR	C23-C24-C25-C26
31	C	517	BCR	C5-C6-C7-C8
31	c	514	BCR	C5-C6-C7-C8
31	c	515	BCR	C5-C6-C7-C8
45	h	101	RRX	C23-C24-C25-C26
45	h	101	RRX	C5-C6-C7-C8
47	N	615	LUT	C5-C6-C7-C8
47	S	317	LUT	C1-C6-C7-C8
47	S	317	LUT	C5-C6-C7-C8
47	Y	316	LUT	C1-C6-C7-C8
47	Y	316	LUT	C5-C6-C7-C8
37	n	617	LHG	O7-C7-C8-C9
40	i	102	SPH	C4-C5-C6-C7
50	n	619	PTY	C38-C39-C40-C41
29	S	311	CLA	C2-C1-O2A-CGA
29	b	504	CLA	C2-C1-O2A-CGA
29	b	513	CLA	C2-C1-O2A-CGA
29	d	403	CLA	C2-C1-O2A-CGA
29	n	610	CLA	C2-C1-O2A-CGA
29	n	612	CLA	C2-C1-O2A-CGA
46	N	607	CHL	C2-C1-O2A-CGA
46	G	607	CHL	C2-C1-O2A-CGA
37	N	618	LHG	C19-C20-C21-C22
35	b	520	LMG	C22-C23-C24-C25
29	B	513	CLA	CAA-CBA-CGA-O2A
29	b	506	CLA	CAA-CBA-CGA-O2A
37	G	618	LHG	O7-C7-C8-C9
35	D	409	LMG	C10-C11-C12-C13
37	d	406	LHG	C33-C34-C35-C36
29	B	515	CLA	CBA-CGA-O2A-C1
29	R	309	CLA	CAA-CBA-CGA-O2A
29	y	314	CLA	CAA-CBA-CGA-O2A
39	a	410	SQD	O48-C23-C24-C25
39	m	101	SQD	O47-C7-C8-C9
41	D	402	DGA	OG2-CB1-CB2-CB3
29	Y	315	CLA	C2-C3-C5-C6
29	b	509	CLA	C2-C3-C5-C6
46	Y	308	CHL	C2-C3-C5-C6
39	M	101	SQD	C11-C12-C13-C14
29	S	312	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	Y	311	CLA	C2A-CAA-CBA-CGA
29	c	505	CLA	C2A-CAA-CBA-CGA
29	s	311	CLA	C2A-CAA-CBA-CGA
29	c	506	CLA	C10-C11-C12-C13
29	R	303	CLA	CAA-CBA-CGA-O2A
33	a	415	3PH	O31-C31-C32-C33
39	c	522	SQD	O47-C7-C8-C9
35	d	407	LMG	C15-C16-C17-C18
37	L	101	LHG	C31-C32-C33-C34
29	c	507	CLA	CAA-CBA-CGA-O2A
29	s	304	CLA	CAA-CBA-CGA-O2A
36	c	516	DGD	O2G-C1B-C2B-C3B
35	c	519	LMG	O9-C10-C11-C12
39	C	523	SQD	C4-C5-C6-S
39	b	523	SQD	C4-C5-C6-S
39	c	522	SQD	C4-C5-C6-S
37	n	617	LHG	C19-C20-C21-C22
50	n	619	PTY	C13-C14-C15-C16
29	S	304	CLA	CAA-CBA-CGA-O2A
29	S	312	CLA	CAA-CBA-CGA-O2A
29	B	505	CLA	C2-C3-C5-C6
29	b	513	CLA	C2-C3-C5-C6
37	N	618	LHG	C18-C19-C20-C21
46	G	606	CHL	C2A-CAA-CBA-CGA
35	C	524	LMG	C11-C12-C13-C14
29	N	613	CLA	CAA-CBA-CGA-O2A
29	B	508	CLA	C6-C7-C8-C9
29	C	510	CLA	C11-C10-C8-C9
29	Y	312	CLA	C6-C7-C8-C9
29	b	503	CLA	C14-C13-C15-C16
29	g	611	CLA	C11-C12-C13-C14
29	y	312	CLA	C14-C13-C15-C16
46	y	309	CHL	C11-C12-C13-C14
29	A	406	CLA	C2C-C3C-CAC-CBC
39	l	101	SQD	C23-C24-C25-C26
29	B	514	CLA	CAA-CBA-CGA-O2A
29	c	512	CLA	CAA-CBA-CGA-O2A
37	N	618	LHG	O7-C7-C8-C9
41	D	402	DGA	OG1-CA1-CA2-CA3
29	B	515	CLA	O1A-CGA-O2A-C1
29	S	306	CLA	O1D-CGD-O2D-CED
29	b	511	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	g	610	CLA	C8-C10-C11-C12
46	N	601	CHL	C8-C10-C11-C12
29	G	602	CLA	C4B-C3B-CAB-CBB
29	R	301	CLA	C4B-C3B-CAB-CBB
29	b	514	CLA	C4B-C3B-CAB-CBB
29	s	314	CLA	C4B-C3B-CAB-CBB
29	y	313	CLA	C1A-C2A-CAA-CBA
29	g	613	CLA	C4-C3-C5-C6
46	g	601	CHL	C4-C3-C5-C6
29	B	506	CLA	C8-C10-C11-C12
39	c	522	SQD	O5-C1-O6-C44
29	A	405	CLA	CAA-CBA-CGA-O2A
29	B	516	CLA	CAA-CBA-CGA-O2A
29	C	511	CLA	CAA-CBA-CGA-O2A
29	G	603	CLA	CAA-CBA-CGA-O2A
29	S	315	CLA	CAA-CBA-CGA-O2A
29	r	304	CLA	CAA-CBA-CGA-O2A
36	B	521	DGD	O1G-C1A-C2A-C3A
29	b	514	CLA	C2-C3-C5-C6
35	W	203	LMG	C32-C33-C34-C35
34	B	519	C7Z	C27-C28-C29-C30
47	R	310	LUT	C27-C28-C29-C30
48	G	617	NEX	C9-C10-C11-C12
48	G	617	NEX	C13-C14-C15-C35
29	s	304	CLA	C8-C10-C11-C12
41	D	402	DGA	CA2-CA3-CA4-CA5
29	Y	312	CLA	C16-C17-C18-C19
46	Y	306	CHL	CAA-CBA-CGA-O2A
29	b	512	CLA	CAA-CBA-CGA-O2A
35	c	519	LMG	O8-C28-C29-C30
35	i	101	LMG	O7-C10-C11-C12
37	Y	319	LHG	O8-C23-C24-C25
41	b	522	DGA	OG2-CB1-CB2-CB3
46	G	605	CHL	CAA-CBA-CGA-O2A
46	n	606	CHL	CAA-CBA-CGA-O2A
39	m	101	SQD	C11-C10-C9-C8
36	C	518	DGD	CCB-CDB-CEB-CFB
37	Y	319	LHG	C32-C33-C34-C35
35	C	524	LMG	O8-C28-C29-C30
37	c	521	LHG	O7-C7-C8-C9
50	n	619	PTY	O4-C30-C31-C32
37	g	618	LHG	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	a	414	LHG	C29-C30-C31-C32
46	y	303	CHL	C13-C15-C16-C17
29	r	309	CLA	O1D-CGD-O2D-CED
29	B	508	CLA	C2-C1-O2A-CGA
29	C	513	CLA	C2-C1-O2A-CGA
29	r	304	CLA	C2-C1-O2A-CGA
29	r	310	CLA	C2-C1-O2A-CGA
46	Y	307	CHL	C2-C1-O2A-CGA
46	y	308	CHL	C2-C1-O2A-CGA
29	A	406	CLA	CAA-CBA-CGA-O2A
33	s	322	3PH	O21-C21-C22-C23
35	b	520	LMG	O7-C10-C11-C12
37	L	101	LHG	O7-C7-C8-C9
29	B	504	CLA	C6-C7-C8-C10
29	B	504	CLA	C11-C12-C13-C15
29	Y	315	CLA	C11-C10-C8-C7
29	b	504	CLA	C12-C13-C15-C16
29	b	512	CLA	C11-C10-C8-C7
29	c	505	CLA	C11-C12-C13-C15
29	c	508	CLA	C6-C7-C8-C10
29	n	612	CLA	C12-C13-C15-C16
29	s	311	CLA	C11-C10-C8-C7
46	g	607	CHL	C12-C13-C15-C16
29	Y	303	CLA	CBA-CGA-O2A-C1
35	w	202	LMG	C30-C31-C32-C33
33	b	521	3PH	C3-C2-O21-C21
29	B	501	CLA	C5-C6-C7-C8
29	a	405	CLA	C15-C16-C17-C18
37	a	413	LHG	C30-C31-C32-C33
39	o	301	SQD	C11-C12-C13-C14
41	j	101	DGA	CB7-CB8-CB9-CAB
39	b	523	SQD	O10-C23-O48-C46
29	c	510	CLA	CAA-CBA-CGA-O2A
35	W	203	LMG	O8-C28-C29-C30
33	B	522	3PH	C2E-C2F-C2G-C2H
29	B	508	CLA	C2A-CAA-CBA-CGA
29	b	503	CLA	C2A-CAA-CBA-CGA
29	r	302	CLA	C2A-CAA-CBA-CGA
29	s	303	CLA	C2A-CAA-CBA-CGA
29	S	304	CLA	C16-C17-C18-C19
29	b	515	CLA	C16-C17-C18-C20
41	j	101	DGA	CB4-CB5-CB6-CB7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	B	514	CLA	C5-C6-C7-C8
36	c	517	DGD	C1A-C2A-C3A-C4A
37	S	301	LHG	C2-C3-O3-P
39	o	301	SQD	C19-C20-C21-C22
36	c	516	DGD	C4A-C5A-C6A-C7A
39	c	522	SQD	C27-C28-C29-C30
29	B	501	CLA	C3A-C2A-CAA-CBA
29	b	502	CLA	C3A-C2A-CAA-CBA
29	n	604	CLA	C4-C3-C5-C6
29	y	310	CLA	C3A-C2A-CAA-CBA
46	G	605	CHL	C3A-C2A-CAA-CBA
46	G	607	CHL	C3A-C2A-CAA-CBA
35	C	522	LMG	O9-C10-C11-C12
39	a	410	SQD	O10-C23-C24-C25
29	C	513	CLA	CAA-CBA-CGA-O2A
41	b	522	DGA	OG1-CA1-CA2-CA3
29	S	303	CLA	C2-C3-C5-C6
35	i	101	LMG	C13-C14-C15-C16
29	R	303	CLA	CAA-CBA-CGA-O1A
29	R	309	CLA	CAA-CBA-CGA-O1A
29	c	510	CLA	CAA-CBA-CGA-O1A
50	N	620	PTY	O30-C30-C31-C32
35	D	410	LMG	C37-C38-C39-C40
39	b	523	SQD	C24-C23-O48-C46
41	J	101	DGA	OG1-CA1-CA2-CA3
29	Y	303	CLA	O1A-CGA-O2A-C1
29	y	314	CLA	CAA-CBA-CGA-O1A
37	N	618	LHG	O9-C7-C8-C9
37	n	617	LHG	O9-C7-C8-C9
33	b	521	3PH	C2C-C2D-C2E-C2F
29	c	509	CLA	C13-C15-C16-C17
29	G	602	CLA	C2A-CAA-CBA-CGA
29	R	301	CLA	C2A-CAA-CBA-CGA
29	A	406	CLA	C11-C10-C8-C9
29	A	409	CLA	C11-C10-C8-C9
29	C	503	CLA	C6-C7-C8-C9
29	C	507	CLA	C11-C10-C8-C9
29	Y	304	CLA	C11-C10-C8-C9
29	a	408	CLA	C11-C10-C8-C9
29	b	502	CLA	C11-C10-C8-C9
29	b	516	CLA	C6-C7-C8-C9
29	c	505	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	c	511	CLA	C11-C12-C13-C14
29	n	612	CLA	C11-C10-C8-C9
29	s	312	CLA	C11-C12-C13-C14
46	G	607	CHL	C11-C12-C13-C14
33	s	322	3PH	O22-C21-C22-C23
51	s	321	LPX	O7-C6-C7-C8
29	B	506	CLA	C10-C11-C12-C13
29	B	507	CLA	CAA-CBA-CGA-O1A
46	n	605	CHL	CAA-CBA-CGA-O1A
46	G	607	CHL	CAA-CBA-CGA-O2A
39	C	523	SQD	O5-C5-C6-S
39	b	523	SQD	O5-C5-C6-S
39	m	101	SQD	O5-C5-C6-S
47	G	615	LUT	C21-C26-C27-C28
47	G	616	LUT	C21-C26-C27-C28
47	g	615	LUT	C21-C26-C27-C28
47	g	616	LUT	C21-C26-C27-C28
47	y	318	LUT	C21-C26-C27-C28
29	B	514	CLA	CAA-CBA-CGA-O1A
29	a	405	CLA	CAA-CBA-CGA-O1A
29	g	614	CLA	CAA-CBA-CGA-O1A
36	c	516	DGD	O1B-C1B-C2B-C3B
29	S	314	CLA	C2C-C3C-CAC-CBC
29	B	506	CLA	CAA-CBA-CGA-O2A
29	Y	303	CLA	C10-C11-C12-C13
31	C	517	BCR	C7-C8-C9-C10
31	K	101	BCR	C17-C18-C19-C20
34	b	519	C7Z	C27-C28-C29-C30
29	A	406	CLA	CAA-CBA-CGA-O1A
29	b	506	CLA	CAA-CBA-CGA-O1A
33	a	415	3PH	O32-C31-C32-C33
37	G	618	LHG	O9-C7-C8-C9
41	D	402	DGA	OA1-CA1-CA2-CA3
29	B	509	CLA	C8-C10-C11-C12
35	D	409	LMG	C8-C7-O1-C1
36	C	518	DGD	C5D-C6D-O5D-C1E
39	C	523	SQD	C45-C44-O6-C1
46	Y	306	CHL	CAA-CBA-CGA-O1A
29	B	513	CLA	CAA-CBA-CGA-O1A
29	S	304	CLA	CAA-CBA-CGA-O1A
39	c	522	SQD	O49-C7-C8-C9
50	n	619	PTY	O30-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	L	101	LHG	C27-C28-C29-C30
41	b	522	DGA	OA1-CA1-OG1-CG1
40	c	523	SPH	C10-C11-C12-C13
29	b	512	CLA	CAA-CBA-CGA-O1A
29	b	513	CLA	CAA-CBA-CGA-O1A
36	B	521	DGD	O1A-C1A-C2A-C3A
41	D	402	DGA	OB1-CB1-CB2-CB3
41	b	522	DGA	OB1-CB1-CB2-CB3
41	j	101	DGA	OA1-CA1-CA2-CA3
38	b	524	LMT	C2-C3-C4-C5
29	y	305	CLA	C5-C6-C7-C8
29	y	316	CLA	C5-C6-C7-C8
46	y	301	CHL	C5-C6-C7-C8
33	B	522	3PH	C2-C1-O11-P
29	b	506	CLA	C3-C5-C6-C7
29	c	507	CLA	CAA-CBA-CGA-O1A
35	W	203	LMG	O10-C28-C29-C30
46	G	605	CHL	CAA-CBA-CGA-O1A
29	S	303	CLA	C11-C12-C13-C15
29	B	508	CLA	CAD-CBD-CGD-O2D
29	C	505	CLA	CAD-CBD-CGD-O2D
29	C	507	CLA	CAD-CBD-CGD-O2D
29	r	302	CLA	CAD-CBD-CGD-O2D
29	y	305	CLA	CAD-CBD-CGD-O2D
29	y	316	CLA	CAD-CBD-CGD-O2D
46	N	601	CHL	CAD-CBD-CGD-O2D
46	n	605	CHL	CAD-CBD-CGD-O2D
29	Y	303	CLA	C5-C6-C7-C8
29	a	404	CLA	CAA-CBA-CGA-O2A
35	B	520	LMG	O7-C10-C11-C12
46	g	606	CHL	CAA-CBA-CGA-O2A
29	N	613	CLA	CAA-CBA-CGA-O1A
29	r	304	CLA	CAA-CBA-CGA-O1A
29	N	602	CLA	C13-C15-C16-C17
46	N	605	CHL	C15-C16-C17-C18
36	C	518	DGD	C4D-C5D-C6D-O5D
36	c	517	DGD	O6D-C5D-C6D-O5D
37	B	523	LHG	C27-C28-C29-C30
39	m	101	SQD	C26-C27-C28-C29
29	a	404	CLA	C2-C1-O2A-CGA
29	B	516	CLA	CAA-CBA-CGA-O1A
29	C	511	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	s	304	CLA	CAA-CBA-CGA-O1A
29	n	612	CLA	CAA-CBA-CGA-O2A
46	G	601	CHL	C1A-C2A-CAA-CBA
46	Y	302	CHL	C1A-C2A-CAA-CBA
33	b	521	3PH	C29-C2A-C2B-C2C
40	i	102	SPH	C15-C16-C17-C18
39	b	523	SQD	C13-C14-C15-C16
29	S	312	CLA	CAA-CBA-CGA-O1A
29	c	512	CLA	CAA-CBA-CGA-O1A
37	L	101	LHG	O9-C7-C8-C9
46	n	606	CHL	CAA-CBA-CGA-O1A
29	C	512	CLA	C8-C10-C11-C12
29	a	408	CLA	C8-C10-C11-C12
29	B	512	CLA	CAA-CBA-CGA-O2A
29	C	502	CLA	CAA-CBA-CGA-O2A
29	g	603	CLA	CAA-CBA-CGA-O2A
33	b	521	3PH	O21-C21-C22-C23
39	C	501	SQD	O47-C7-C8-C9
41	W	202	DGA	OG1-CA1-CA2-CA3
35	i	101	LMG	C14-C15-C16-C17
29	G	603	CLA	CAA-CBA-CGA-O1A
35	C	524	LMG	O10-C28-C29-C30
41	b	522	DGA	OA1-CA1-CA2-CA3
29	R	302	CLA	C5-C6-C7-C8
35	C	521	LMG	C12-C13-C14-C15
37	n	617	LHG	C27-C28-C29-C30
29	S	303	CLA	CAA-CBA-CGA-O2A
41	J	101	DGA	OG2-CB1-CB2-CB3
29	g	612	CLA	C2A-CAA-CBA-CGA
29	A	405	CLA	CAA-CBA-CGA-O1A
29	B	506	CLA	CAA-CBA-CGA-O1A
29	S	315	CLA	CAA-CBA-CGA-O1A
35	c	519	LMG	O10-C28-C29-C30
35	i	101	LMG	O9-C10-C11-C12
37	Y	319	LHG	O10-C23-C24-C25
29	S	305	CLA	O1D-CGD-O2D-CED

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
48	n	616	NEX	C1-C2-C3-C4-C5-C6
48	N	617	NEX	C1-C2-C3-C4-C5-C6

329 monomers are involved in 756 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B	515	CLA	4	0
39	l	101	SQD	3	0
29	B	511	CLA	1	0
29	y	313	CLA	4	0
46	y	307	CHL	1	0
29	c	511	CLA	3	0
51	S	321	LPX	3	0
29	C	508	CLA	4	0
30	a	407	PHO	4	0
41	D	402	DGA	3	0
36	c	516	DGD	5	0
37	a	414	LHG	3	0
33	B	522	3PH	3	0
29	s	310	CLA	3	0
29	c	510	CLA	3	0
30	d	402	PHO	2	0
35	C	521	LMG	1	0
31	C	515	BCR	8	0
29	s	313	CLA	2	0
29	s	305	CLA	2	0
48	G	617	NEX	3	0
29	a	404	CLA	5	0
29	C	512	CLA	3	0
29	r	304	CLA	3	0
39	c	522	SQD	3	0
29	S	306	CLA	1	0
31	f	101	BCR	2	0
29	a	408	CLA	5	0
29	R	303	CLA	2	0
46	G	609	CHL	3	0
48	s	319	NEX	3	0
29	b	501	CLA	2	0
29	b	515	CLA	7	0
31	c	514	BCR	5	0
31	K	101	BCR	4	0
29	d	403	CLA	4	0
29	R	307	CLA	1	0
47	n	615	LUT	4	0
29	s	304	CLA	5	0
29	G	604	CLA	3	0
46	S	302	CHL	1	0
29	Y	304	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	W	202	DGA	4	0
46	R	305	CHL	1	0
29	Y	315	CLA	4	0
29	C	502	CLA	2	0
29	G	603	CLA	6	0
29	c	501	CLA	1	0
29	B	505	CLA	4	0
29	G	612	CLA	2	0
37	B	523	LHG	3	0
47	g	616	LUT	4	0
38	B	524	LMT	2	0
49	N	619	XAT	5	0
29	b	507	CLA	4	0
43	D	406	PL9	2	0
35	C	522	LMG	2	0
29	c	504	CLA	2	0
49	y	302	XAT	4	0
46	S	308	CHL	3	0
31	C	516	BCR	1	0
39	a	410	SQD	1	0
37	D	407	LHG	7	0
40	c	523	SPH	4	0
29	S	313	CLA	4	0
36	c	517	DGD	5	0
29	g	604	CLA	2	0
48	g	617	NEX	2	0
29	b	509	CLA	5	0
46	Y	302	CHL	2	0
46	N	608	CHL	1	0
29	N	604	CLA	3	0
35	c	520	LMG	9	0
29	g	603	CLA	3	0
29	c	502	CLA	2	0
46	Y	306	CHL	1	0
29	y	316	CLA	3	0
49	G	619	XAT	3	0
29	g	610	CLA	2	0
29	N	612	CLA	1	0
46	N	601	CHL	2	0
47	S	317	LUT	5	0
29	c	505	CLA	5	0
29	S	315	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	Y	303	CLA	2	0
31	v	101	BCR	3	0
29	R	306	CLA	4	0
29	B	512	CLA	4	0
29	b	506	CLA	3	0
29	y	306	CLA	2	0
29	C	504	CLA	2	0
29	s	303	CLA	3	0
29	G	613	CLA	3	0
29	g	613	CLA	1	0
46	g	605	CHL	1	0
37	y	320	LHG	3	0
29	n	611	CLA	1	0
46	s	309	CHL	4	0
29	C	513	CLA	2	0
29	A	405	CLA	9	0
29	b	511	CLA	1	0
29	c	512	CLA	4	0
46	n	601	CHL	4	0
29	g	602	CLA	4	0
37	n	617	LHG	5	0
29	s	315	CLA	1	0
29	a	405	CLA	4	0
29	d	404	CLA	3	0
42	D	403	BCT	1	0
46	G	601	CHL	2	0
29	N	614	CLA	1	0
35	i	101	LMG	2	0
29	S	304	CLA	4	0
37	Y	319	LHG	8	0
31	B	517	BCR	6	0
36	C	519	DGD	2	0
46	s	308	CHL	2	0
48	r	313	NEX	1	0
47	Y	316	LUT	3	0
37	D	408	LHG	2	0
46	G	607	CHL	5	0
46	g	609	CHL	1	0
49	r	312	XAT	4	0
29	R	302	CLA	2	0
46	n	605	CHL	4	0
46	g	608	CHL	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	y	303	CHL	1	0
37	S	320	LHG	3	0
46	y	301	CHL	5	0
29	y	304	CLA	6	0
29	c	506	CLA	4	0
30	A	408	PHO	5	0
47	r	311	LUT	3	0
39	L	102	SQD	5	0
35	d	407	LMG	2	0
29	n	610	CLA	2	0
29	G	614	CLA	1	0
29	r	309	CLA	5	0
41	J	101	DGA	2	0
29	A	407	CLA	1	0
29	S	312	CLA	7	0
37	l	102	LHG	3	0
46	y	309	CHL	6	0
29	B	504	CLA	4	0
29	B	514	CLA	4	0
37	d	406	LHG	5	0
29	y	305	CLA	5	0
46	y	308	CHL	1	0
29	C	510	CLA	1	0
47	S	318	LUT	3	0
46	Y	307	CHL	3	0
29	C	506	CLA	2	0
31	z	101	BCR	5	0
29	g	614	CLA	1	0
47	Y	317	LUT	3	0
37	G	618	LHG	1	0
35	d	408	LMG	2	0
37	N	618	LHG	4	0
47	N	615	LUT	2	0
47	g	615	LUT	2	0
29	Y	305	CLA	2	0
48	y	319	NEX	3	0
41	j	101	DGA	3	0
47	n	614	LUT	3	0
39	m	101	SQD	1	0
29	C	503	CLA	1	0
49	R	311	XAT	1	0
47	s	318	LUT	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	y	314	CLA	4	0
36	C	520	DGD	3	0
35	W	203	LMG	3	0
29	C	505	CLA	3	0
29	B	508	CLA	2	0
50	N	620	PTY	8	0
29	s	311	CLA	3	0
46	r	305	CHL	3	0
35	W	201	LMG	1	0
30	D	401	PHO	3	0
29	C	511	CLA	1	0
29	B	509	CLA	3	0
29	D	405	CLA	3	0
45	h	101	RRX	2	0
29	B	506	CLA	1	0
44	E	101	HEM	1	0
35	D	409	LMG	2	0
47	R	310	LUT	4	0
29	n	603	CLA	6	0
48	n	616	NEX	1	0
47	N	616	LUT	4	0
29	s	306	CLA	2	0
29	N	610	CLA	3	0
29	b	508	CLA	3	0
37	L	101	LHG	3	0
47	G	615	LUT	2	0
35	B	520	LMG	3	0
31	B	518	BCR	1	0
41	w	201	DGA	6	0
35	D	410	LMG	3	0
46	G	608	CHL	1	0
46	R	304	CHL	2	0
26	a	401	OEX	1	0
36	c	518	DGD	1	0
46	Y	308	CHL	4	0
29	N	611	CLA	2	0
29	s	312	CLA	6	0
29	b	512	CLA	3	0
29	C	507	CLA	4	0
46	s	307	CHL	2	0
29	Y	312	CLA	3	0
44	e	101	HEM	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	n	618	XAT	4	0
46	g	601	CHL	3	0
29	c	508	CLA	4	0
39	o	301	SQD	1	0
31	F	101	BCR	2	0
29	S	303	CLA	3	0
39	M	101	SQD	2	0
29	y	315	CLA	2	0
46	y	311	CHL	5	0
46	g	607	CHL	3	0
37	c	521	LHG	7	0
29	n	613	CLA	1	0
47	y	318	LUT	3	0
31	c	515	BCR	3	0
29	A	406	CLA	6	0
48	N	617	NEX	3	0
29	g	611	CLA	3	0
29	G	611	CLA	1	0
29	a	406	CLA	1	0
29	B	502	CLA	2	0
29	N	602	CLA	2	0
38	b	524	LMT	4	0
29	b	502	CLA	3	0
46	r	306	CHL	1	0
48	Y	318	NEX	3	0
36	B	521	DGD	1	0
46	Y	310	CHL	4	0
29	b	513	CLA	4	0
29	y	310	CLA	1	0
40	i	102	SPH	1	0
47	s	317	LUT	3	0
37	a	413	LHG	2	0
48	R	312	NEX	3	0
29	c	509	CLA	2	0
29	B	501	CLA	2	0
47	y	317	LUT	1	0
31	A	410	BCR	3	0
50	n	619	PTY	5	0
31	b	517	BCR	10	0
36	r	301	DGD	1	0
46	N	607	CHL	4	0
29	R	308	CLA	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	N	609	CHL	5	0
29	n	612	CLA	2	0
46	S	307	CHL	3	0
29	Y	311	CLA	1	0
49	Y	301	XAT	3	0
49	g	619	XAT	2	0
29	r	303	CLA	5	0
29	c	507	CLA	2	0
29	G	602	CLA	5	0
33	s	322	3PH	3	0
37	g	618	LHG	4	0
29	b	514	CLA	3	0
29	B	516	CLA	4	0
37	s	320	LHG	4	0
39	b	523	SQD	4	0
46	N	606	CHL	2	0
33	a	415	3PH	3	0
31	C	517	BCR	2	0
46	n	606	CHL	5	0
43	d	405	PL9	2	0
31	a	409	BCR	2	0
29	n	609	CLA	6	0
37	S	301	LHG	3	0
29	b	504	CLA	2	0
41	b	522	DGA	2	0
29	r	310	CLA	1	0
29	Y	309	CLA	1	0
35	b	520	LMG	4	0
35	w	202	LMG	2	0
29	c	503	CLA	1	0
29	B	513	CLA	3	0
29	S	310	CLA	1	0
35	c	519	LMG	1	0
45	H	101	RRX	3	0
37	s	301	LHG	2	0
29	D	404	CLA	6	0
33	A	412	3PH	1	0
29	r	308	CLA	3	0
46	g	606	CHL	3	0
29	s	316	CLA	1	0
26	A	401	OEX	1	0
46	S	309	CHL	6	0

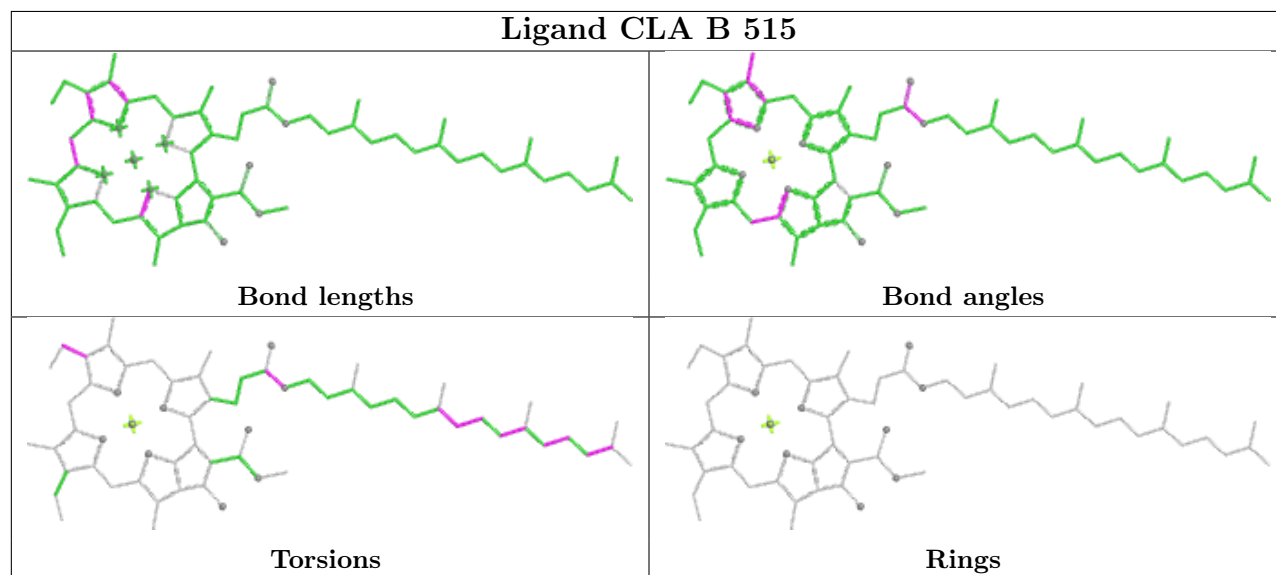
Continued on next page...

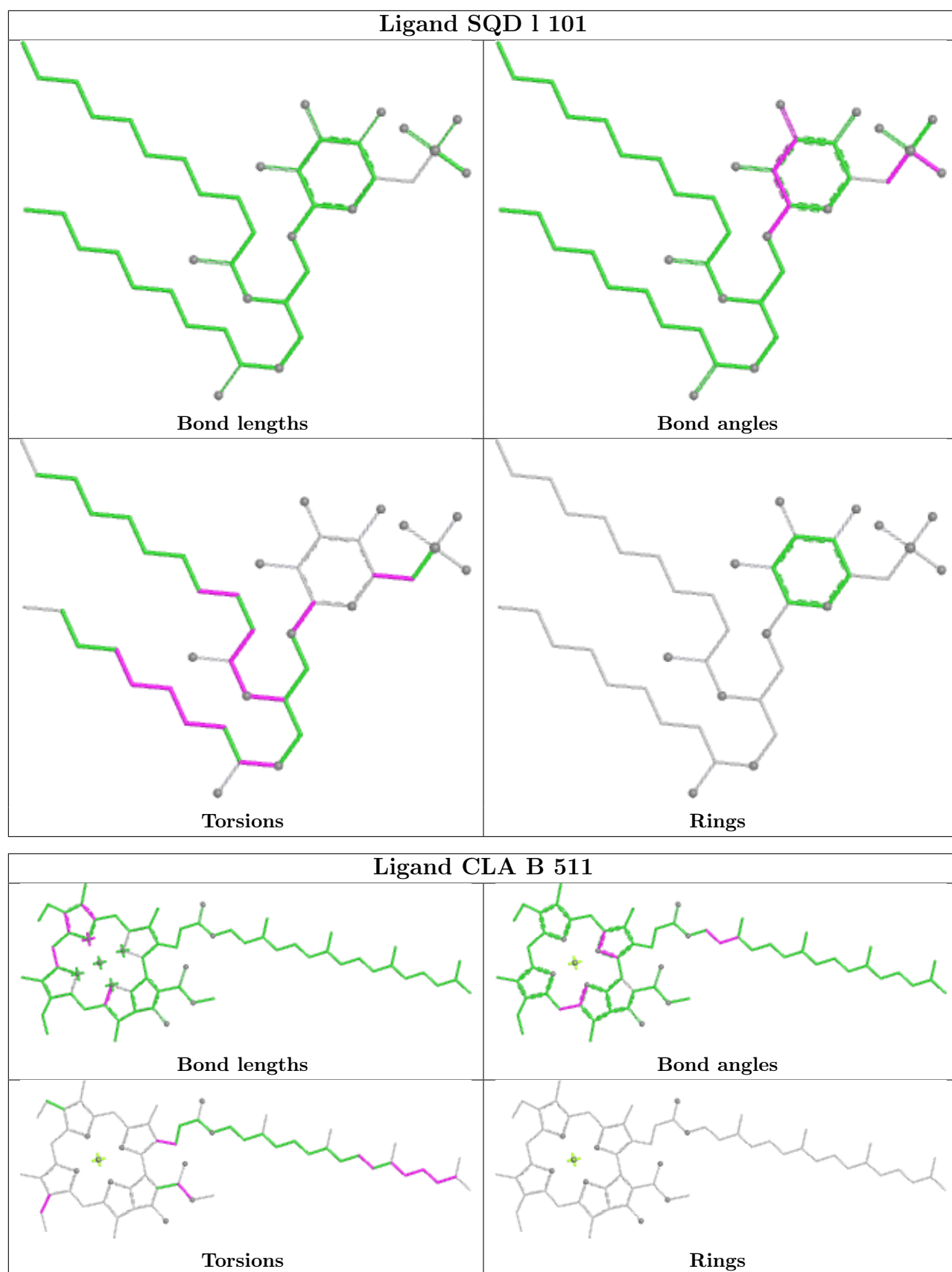
Continued from previous page...

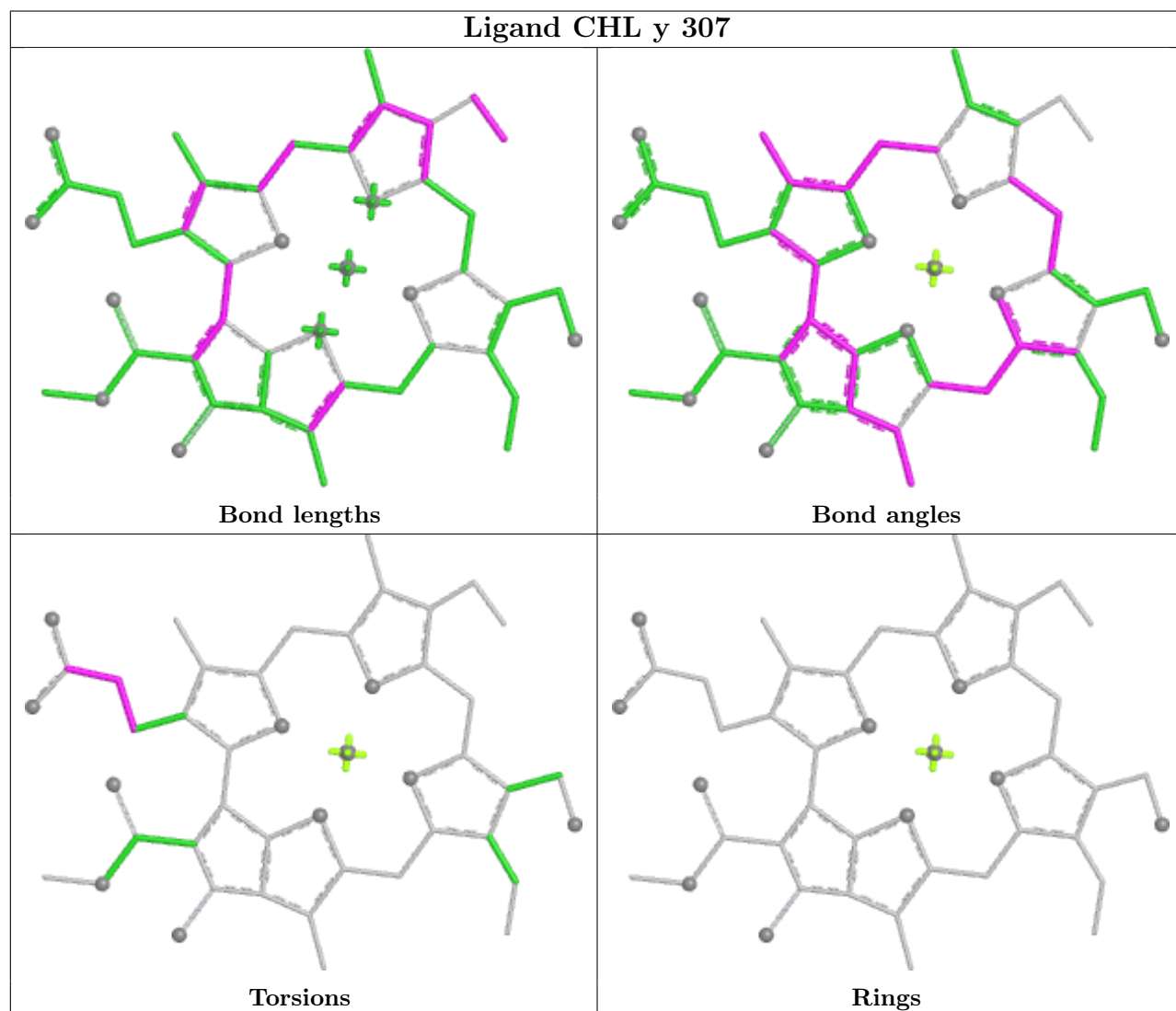
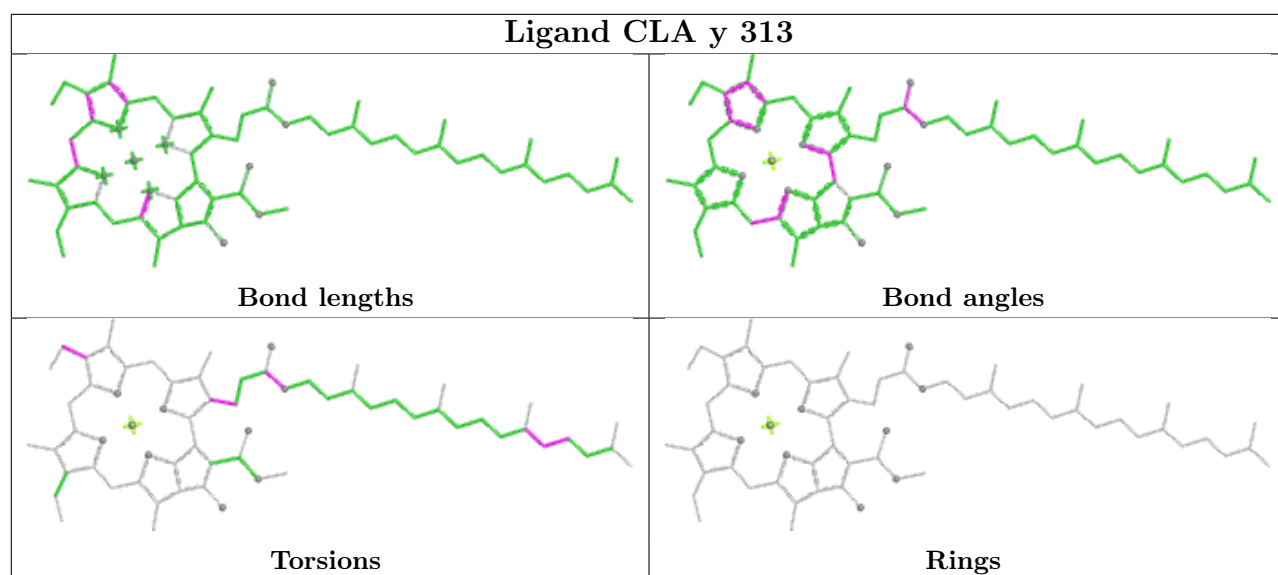
Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	C	525	SPH	1	0
29	n	604	CLA	2	0
29	S	314	CLA	3	0
29	S	305	CLA	1	0
29	Y	313	CLA	2	0
29	b	505	CLA	3	0
46	s	302	CHL	1	0
29	A	409	CLA	5	0
29	B	507	CLA	4	0
47	G	616	LUT	4	0
46	N	605	CHL	7	0
46	n	608	CHL	2	0
29	r	307	CLA	3	0
29	c	513	CLA	6	0
29	n	602	CLA	4	0
29	B	503	CLA	1	0
33	S	322	3PH	2	0
46	G	606	CHL	2	0
29	Y	314	CLA	6	0
29	N	603	CLA	3	0
46	n	607	CHL	1	0
36	C	518	DGD	4	0
29	S	311	CLA	6	0
46	G	605	CHL	1	0
35	C	524	LMG	2	0
39	C	501	SQD	2	0
48	S	319	NEX	4	0
40	I	101	SPH	3	0
29	B	510	CLA	3	0
29	G	610	CLA	2	0
29	C	514	CLA	6	0
29	b	510	CLA	2	0
29	S	316	CLA	3	0
33	b	521	3PH	4	0
29	N	613	CLA	3	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

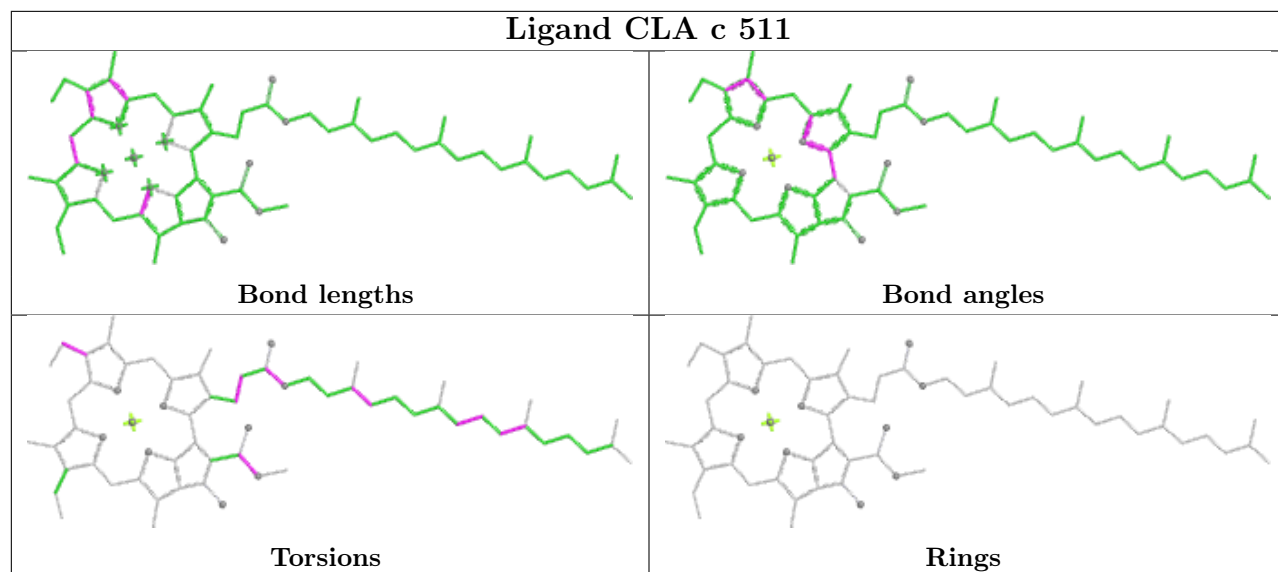
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



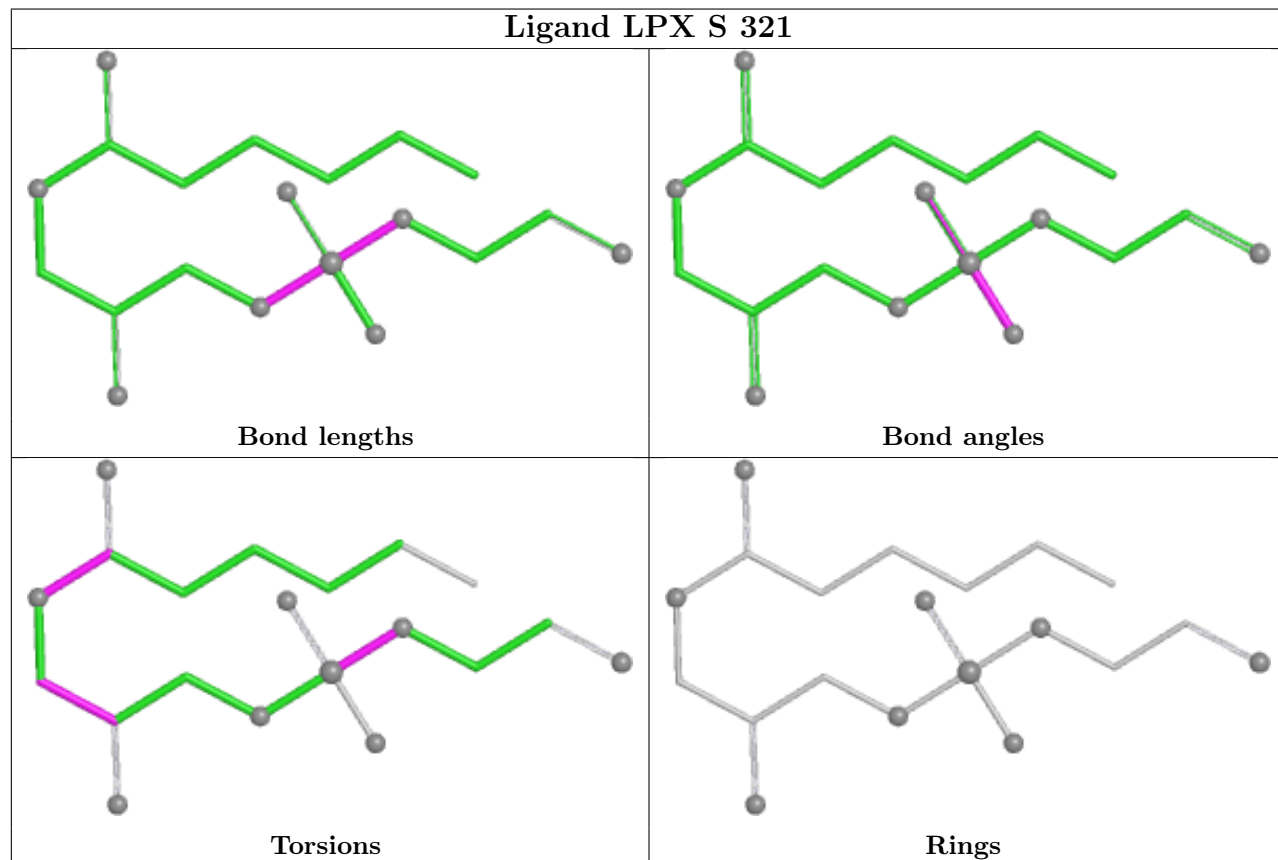


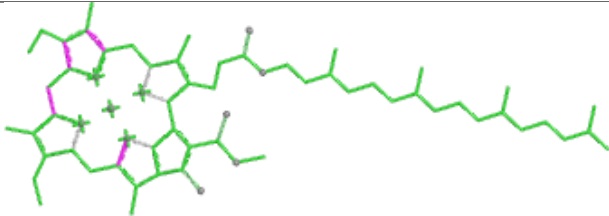
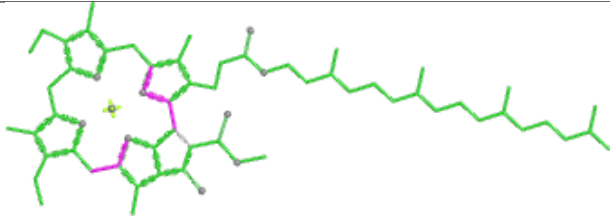
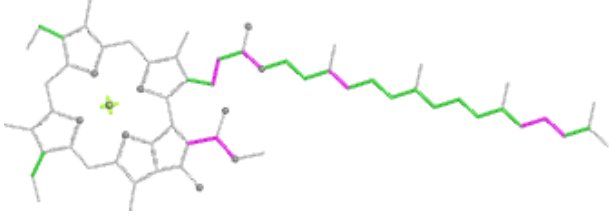
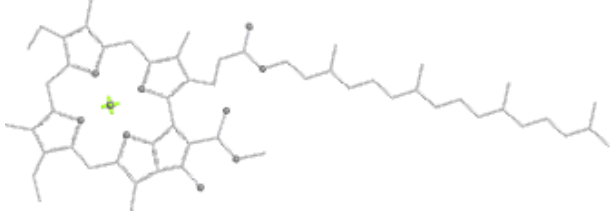


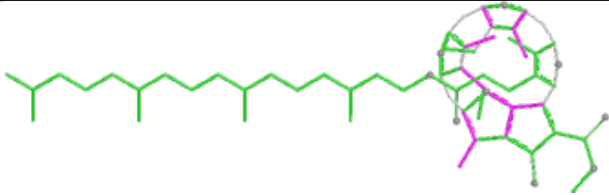
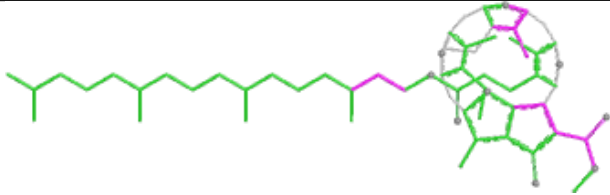
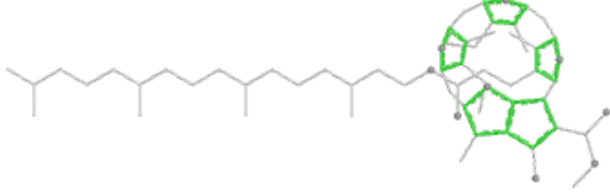
Ligand CLA c 511

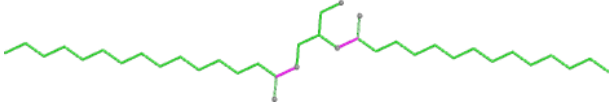
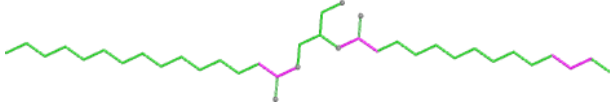
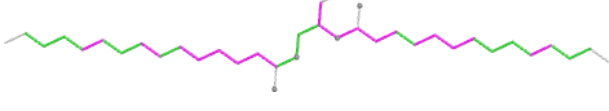
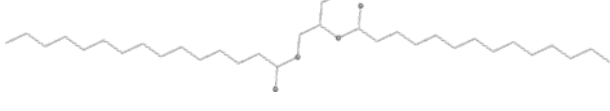


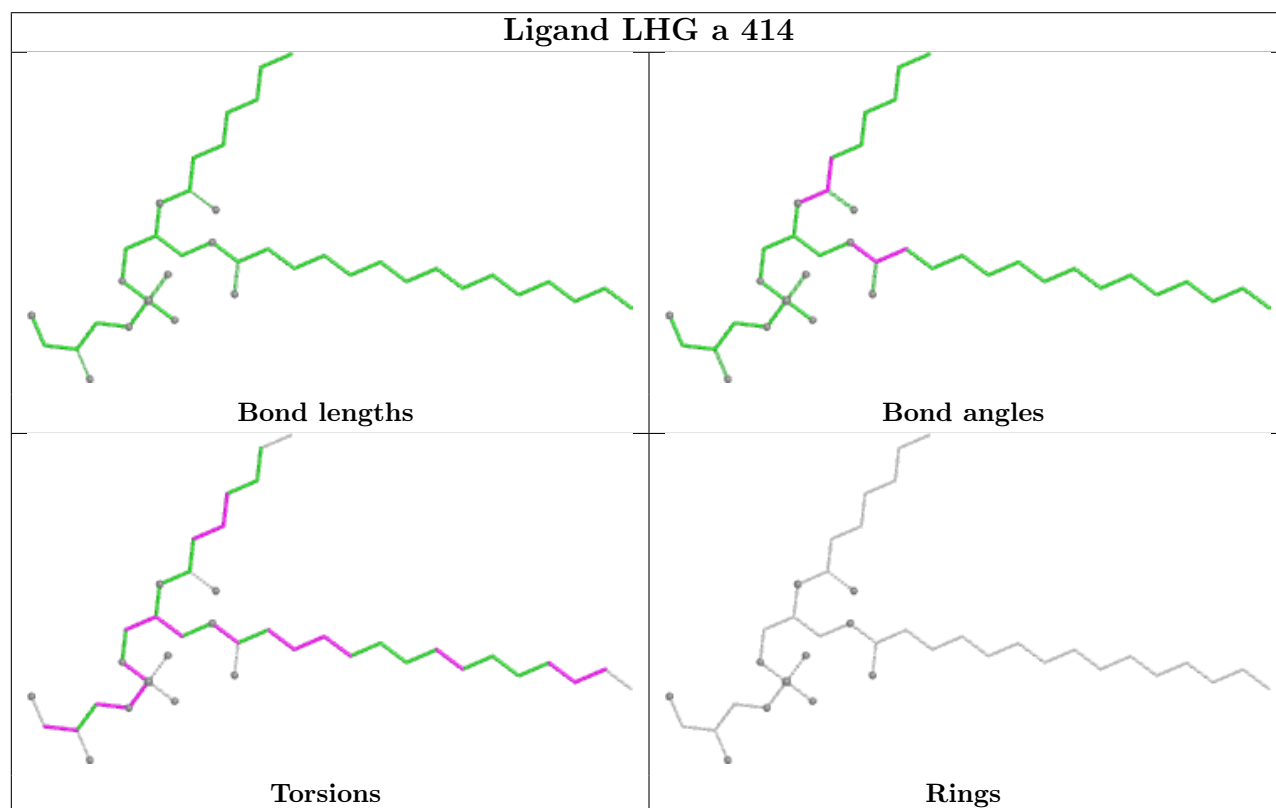
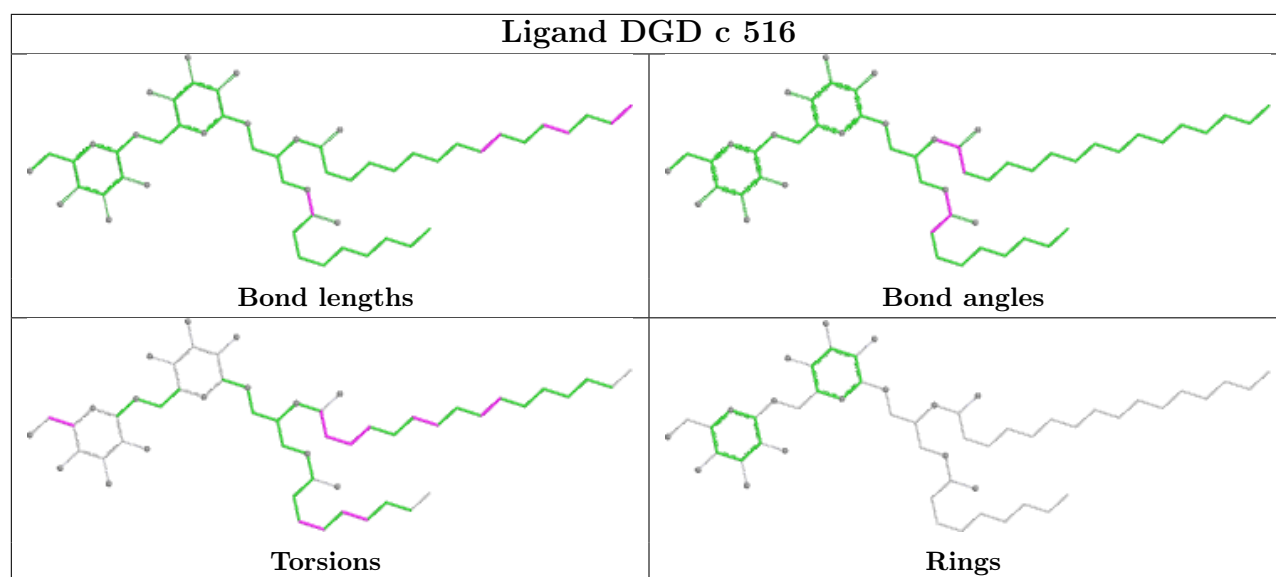
Ligand LPX S 321

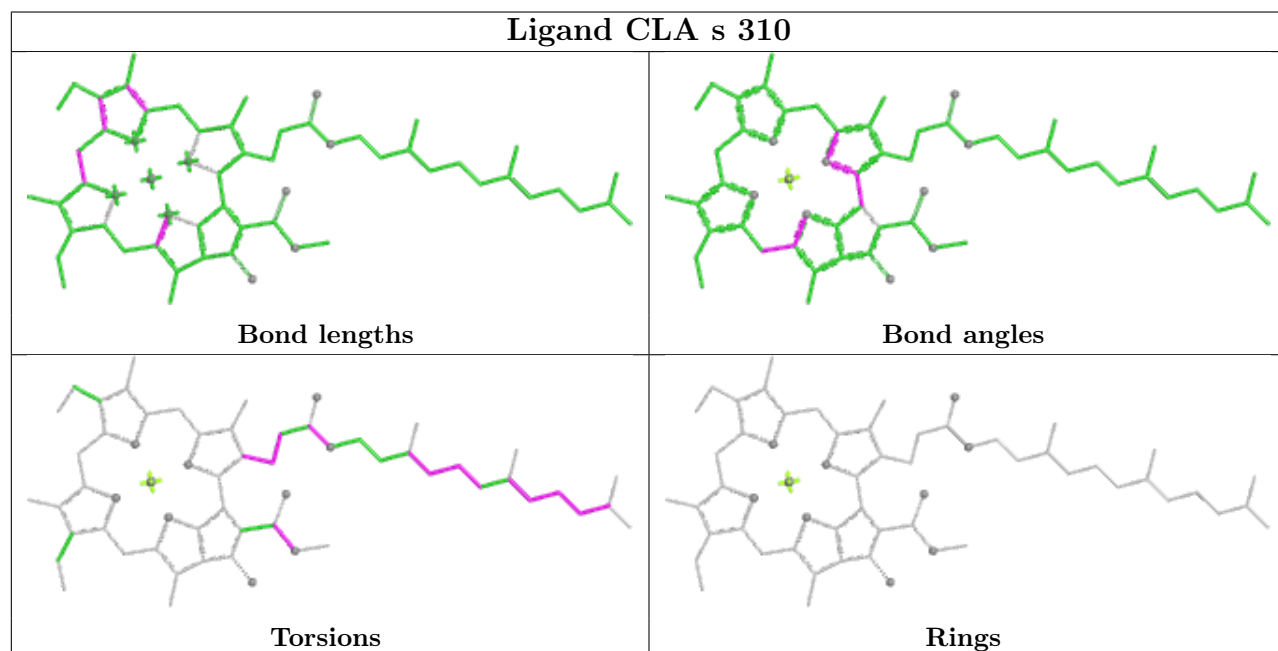
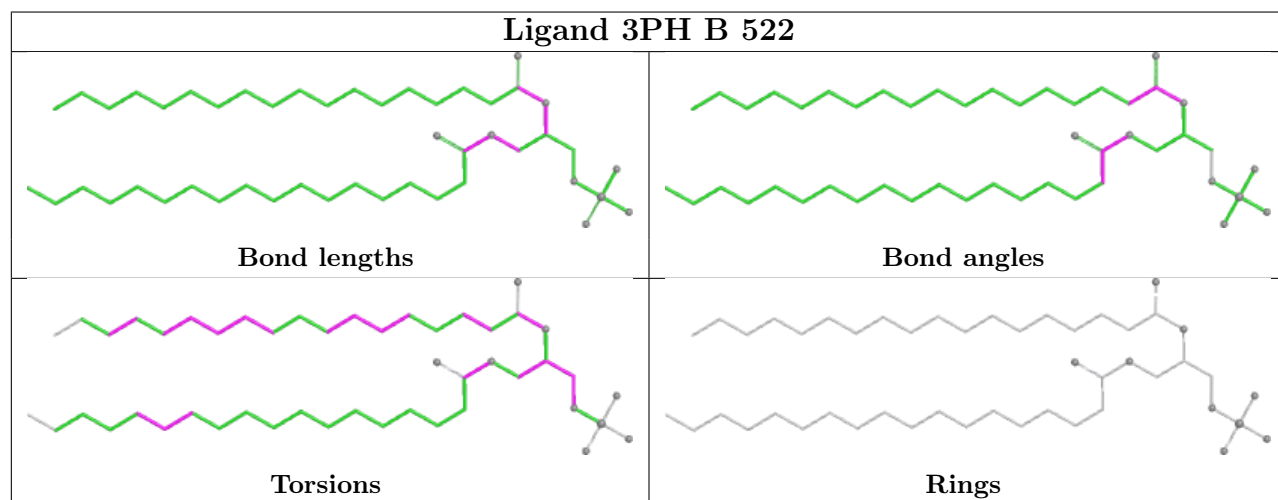
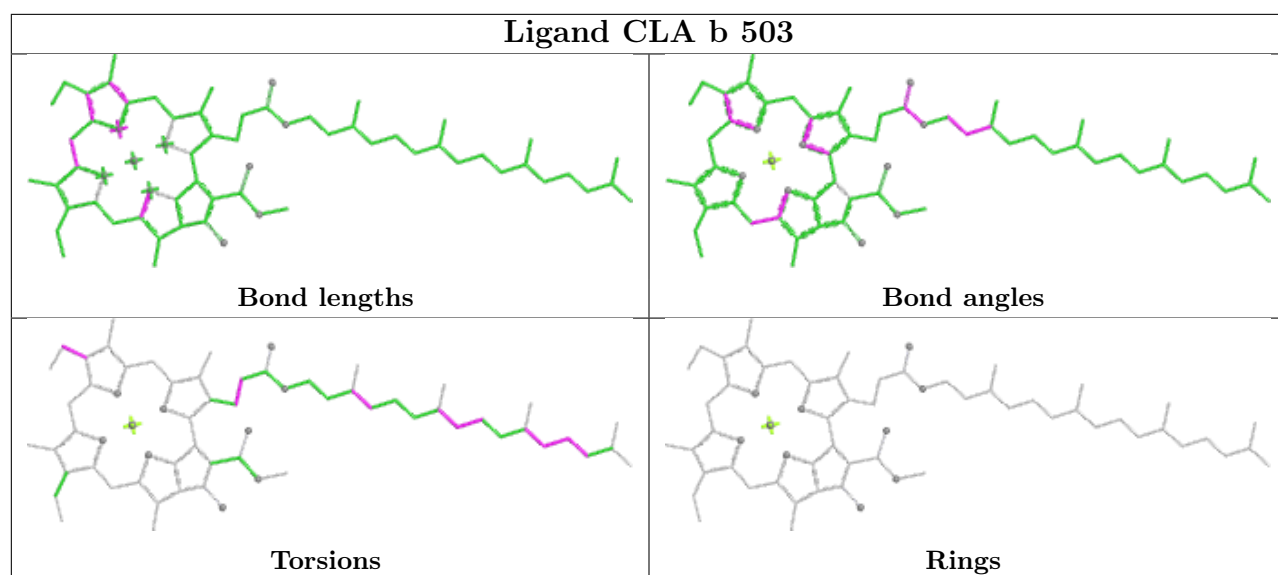


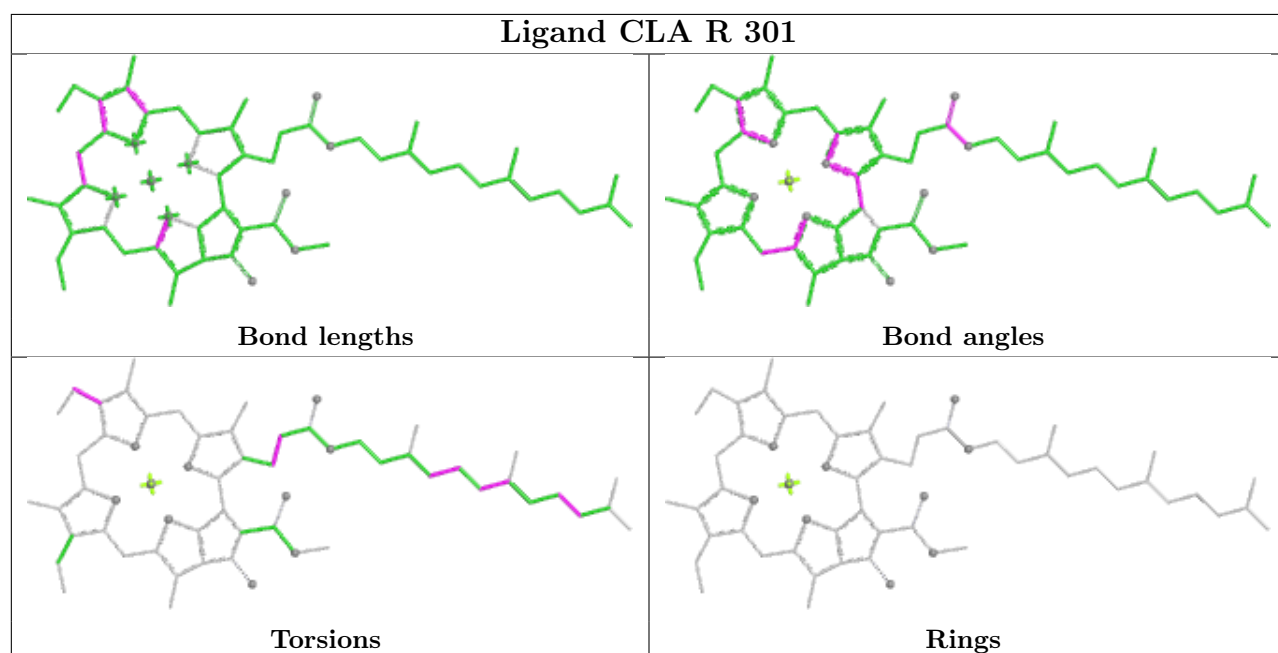
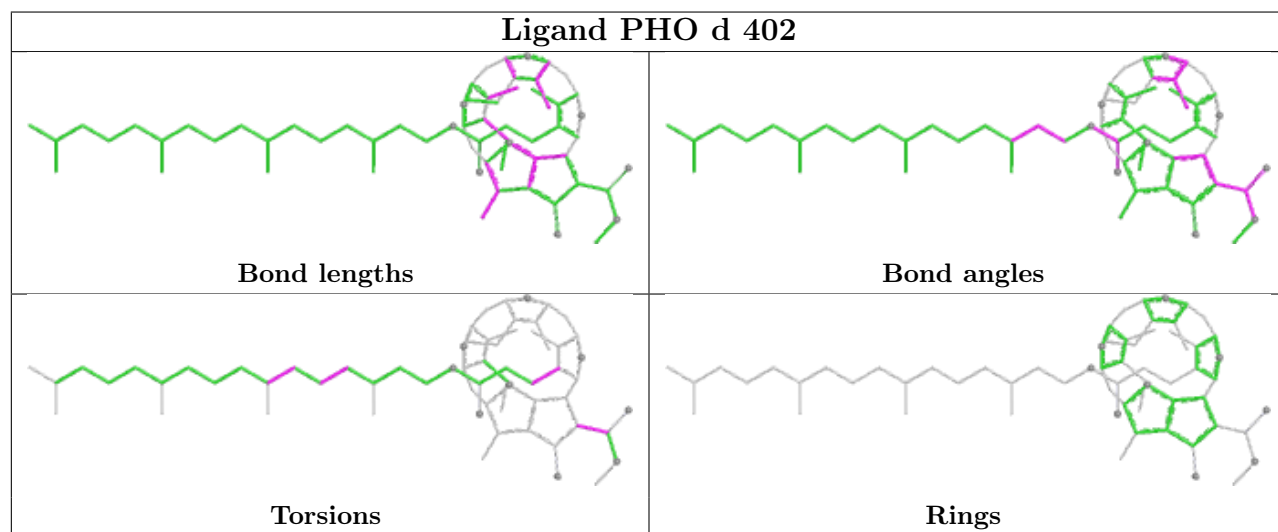
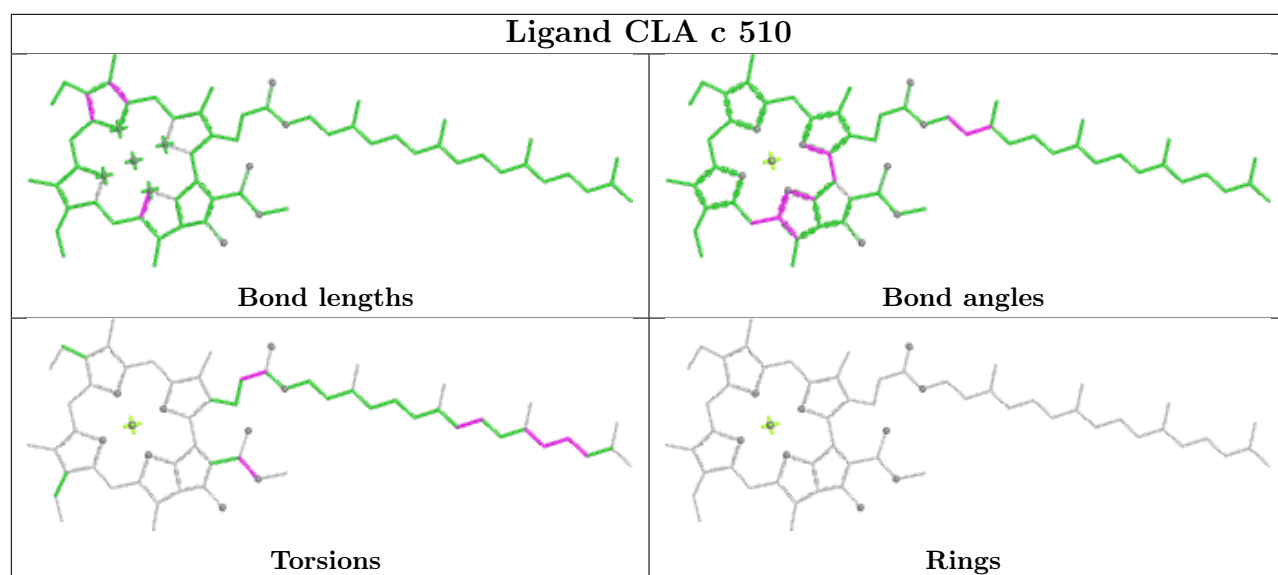
Ligand CLA C 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

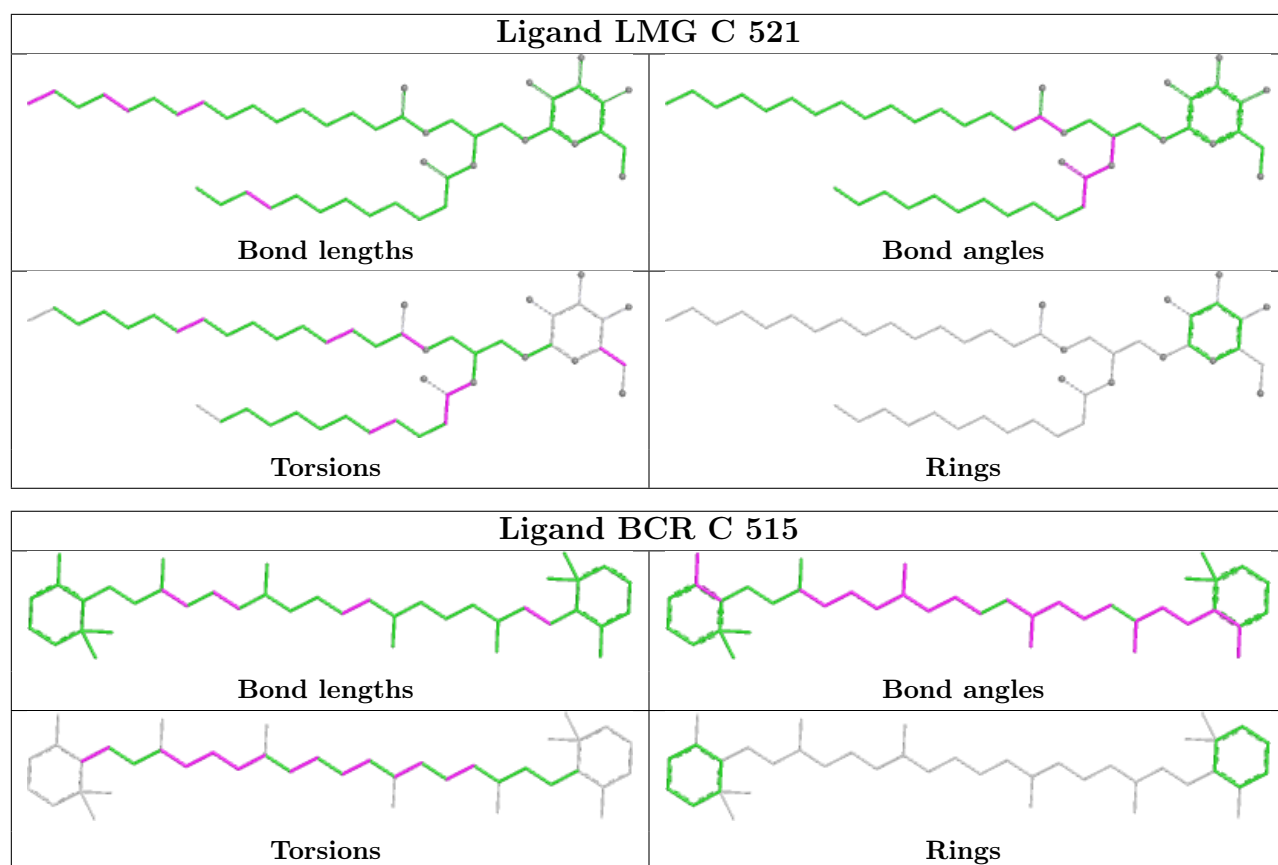
Ligand PHO a 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGA D 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

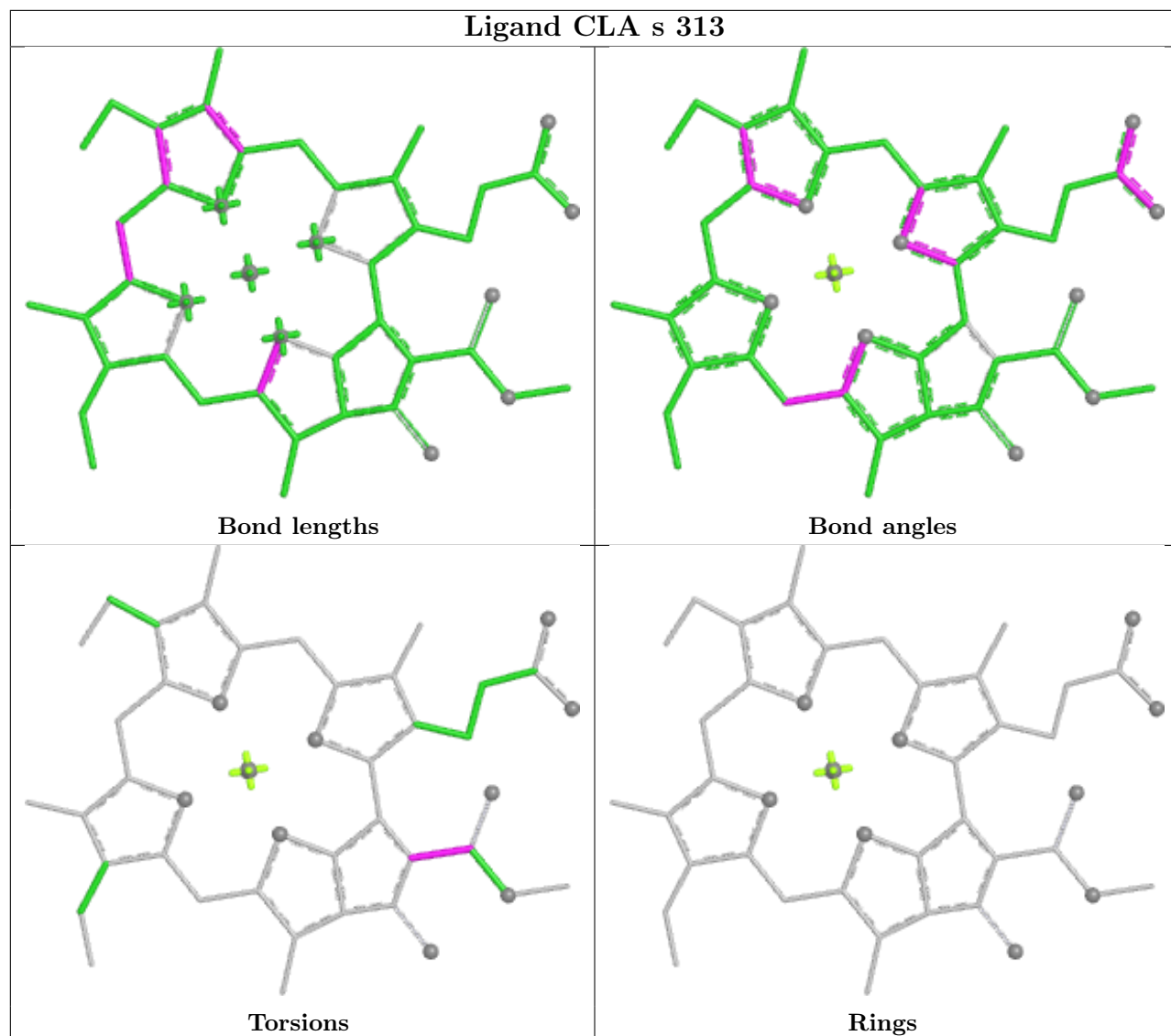




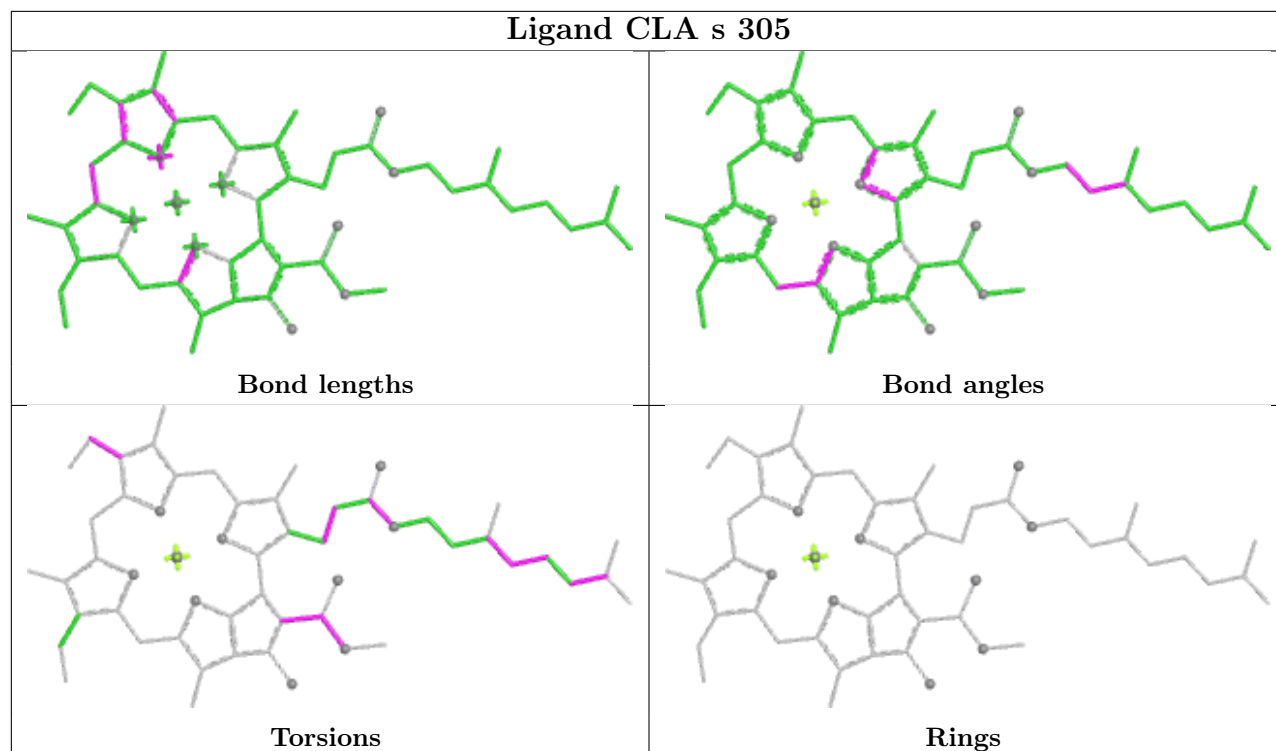




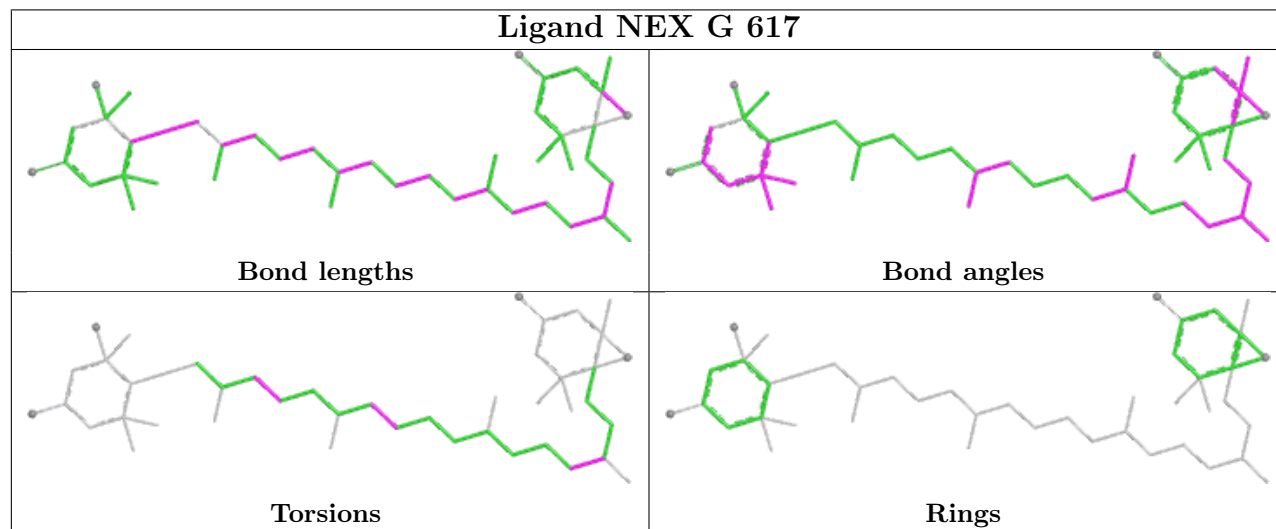
Ligand CLA s 313

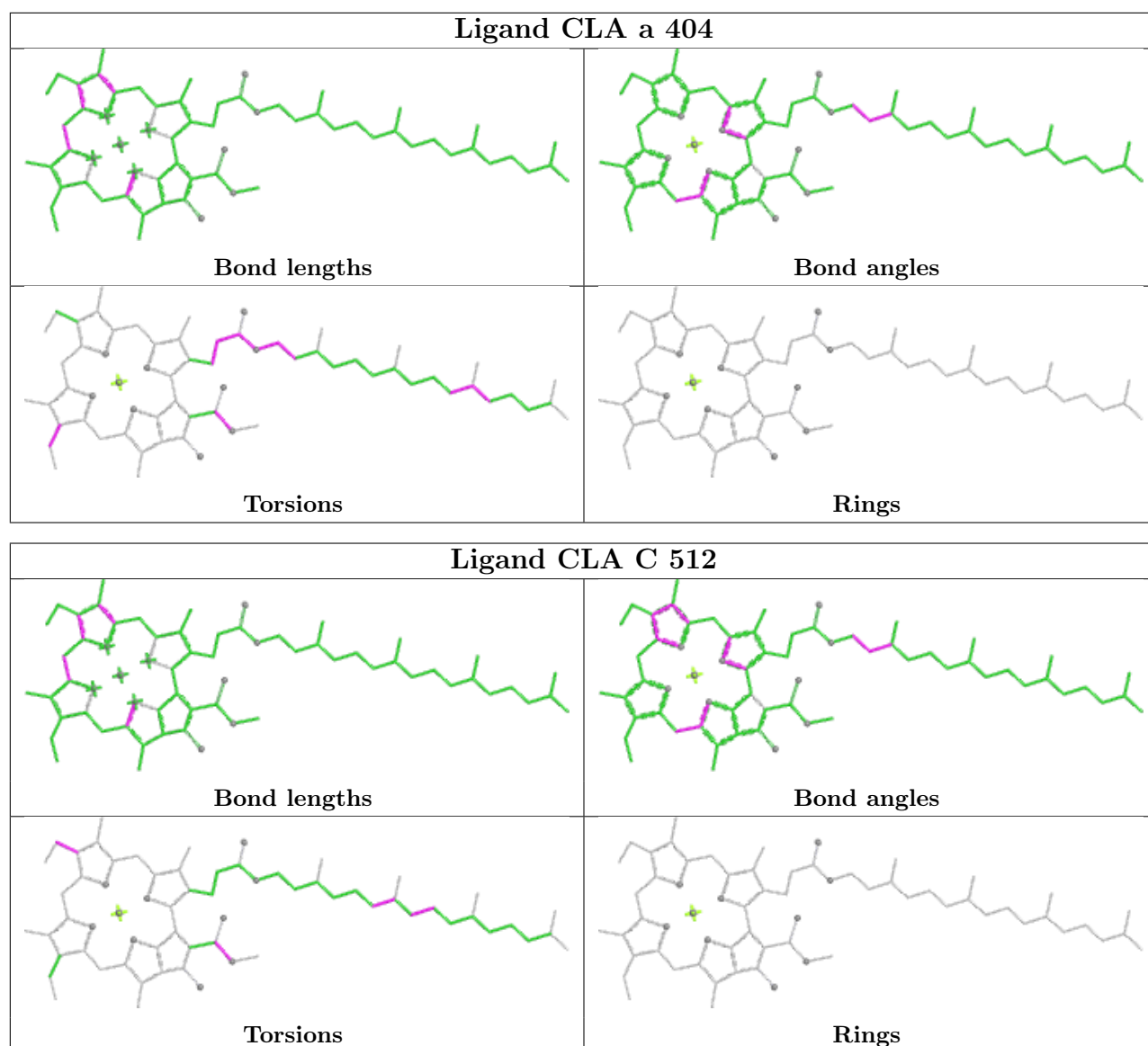


Ligand CLA s 305

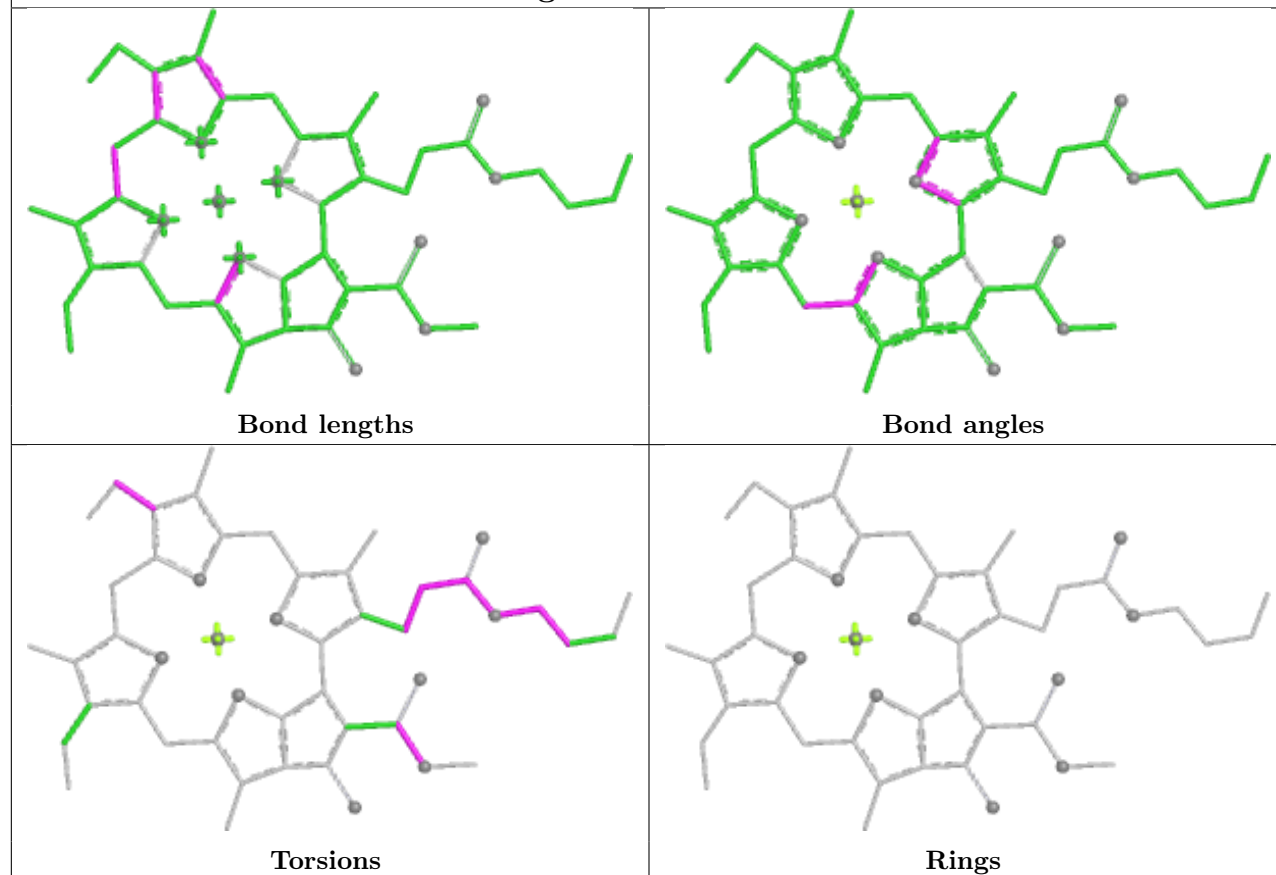


Ligand NEX G 617

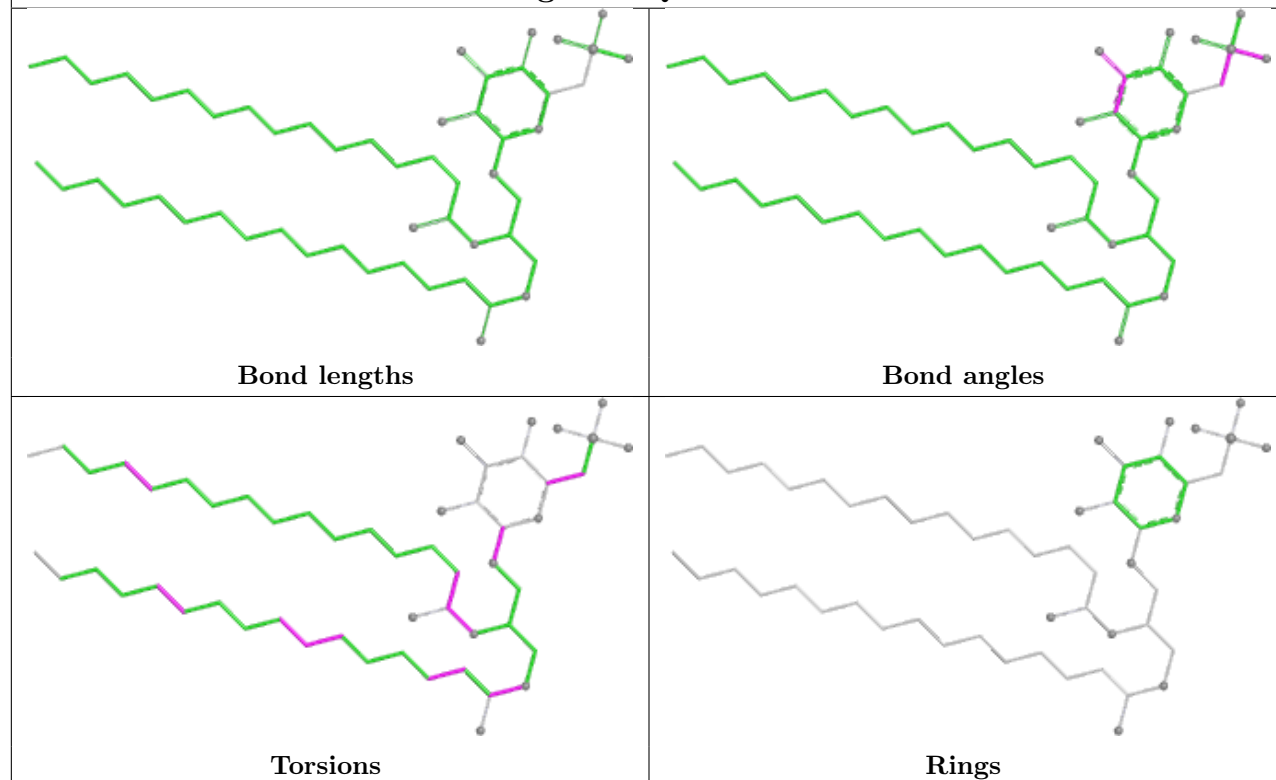




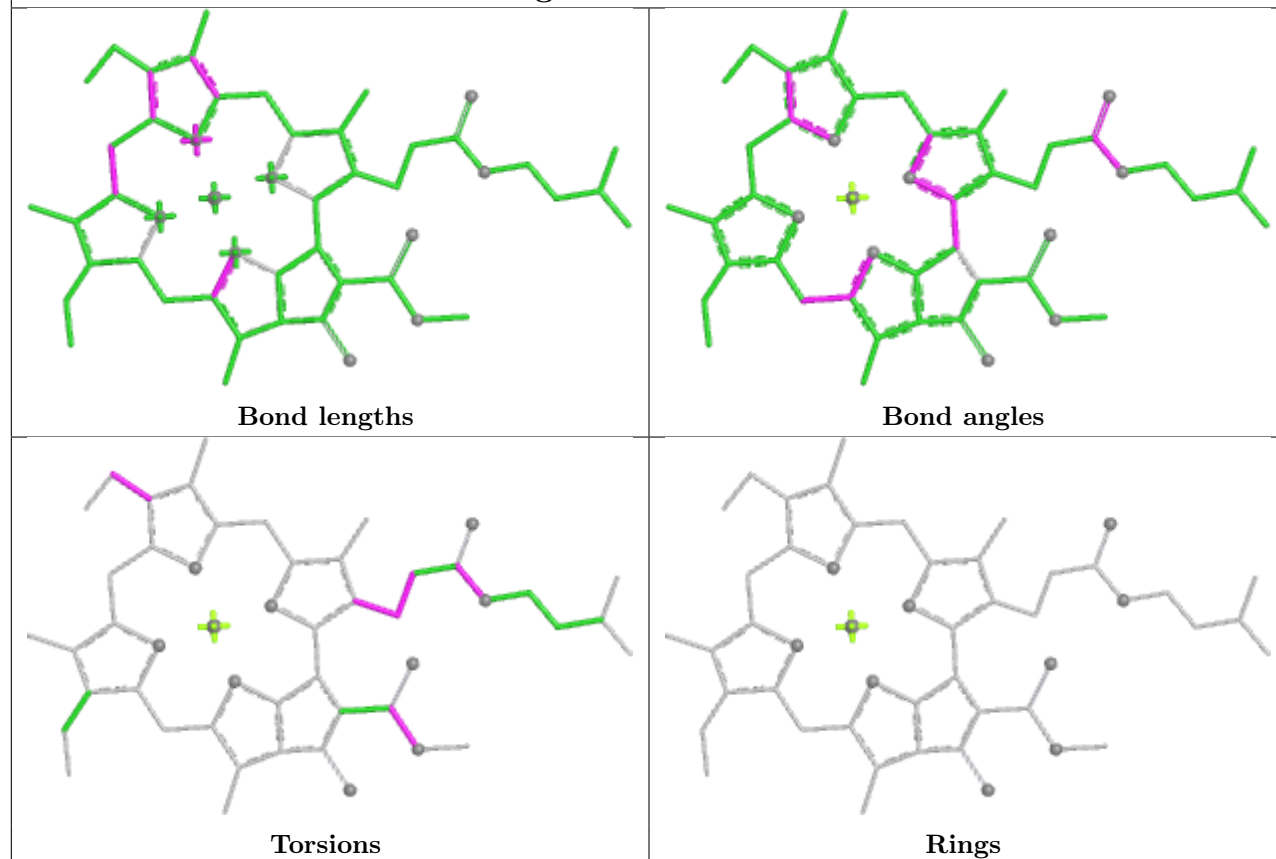
Ligand CLA r 304



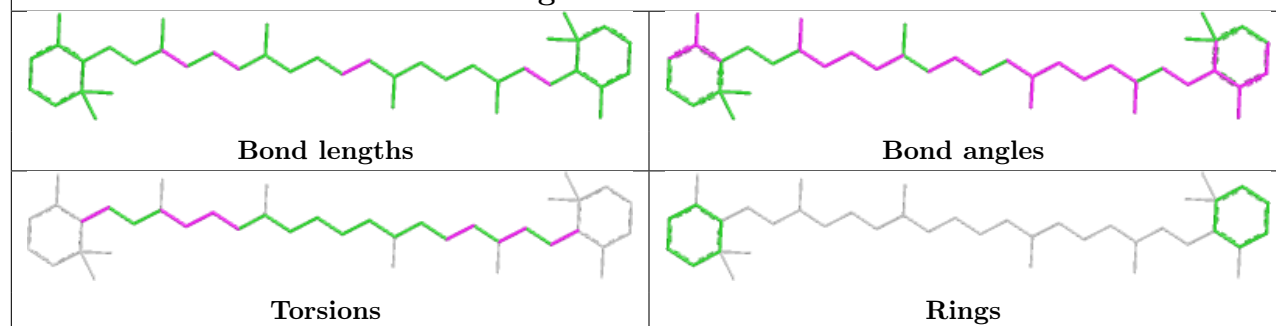
Ligand SQD c 522



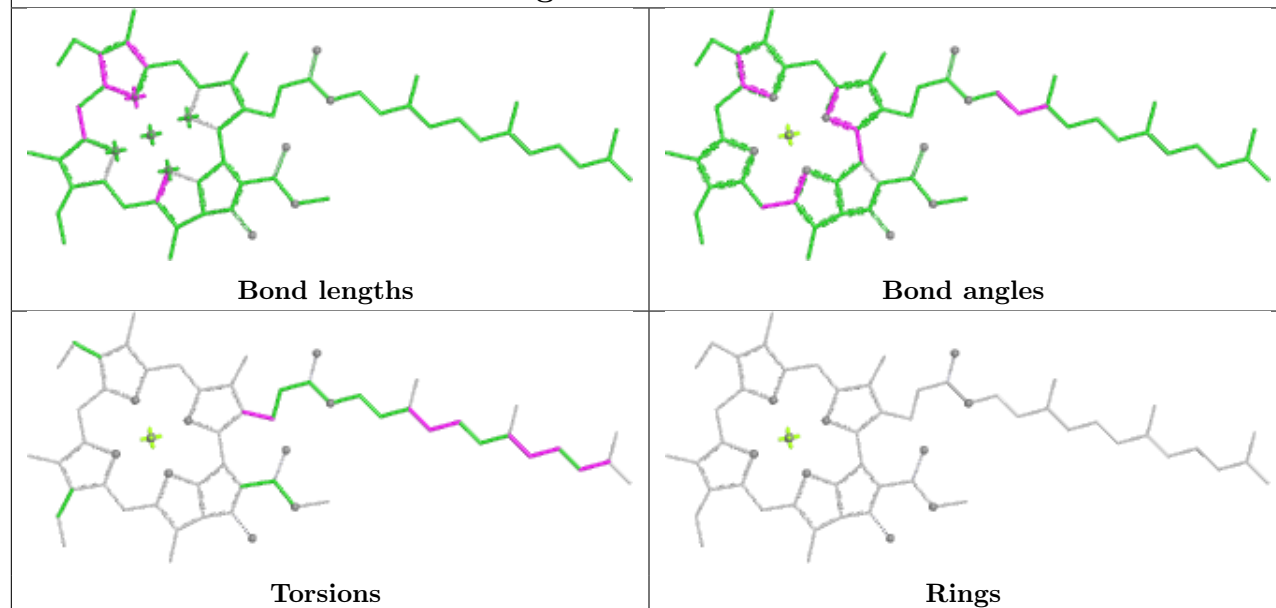
Ligand CLA S 306



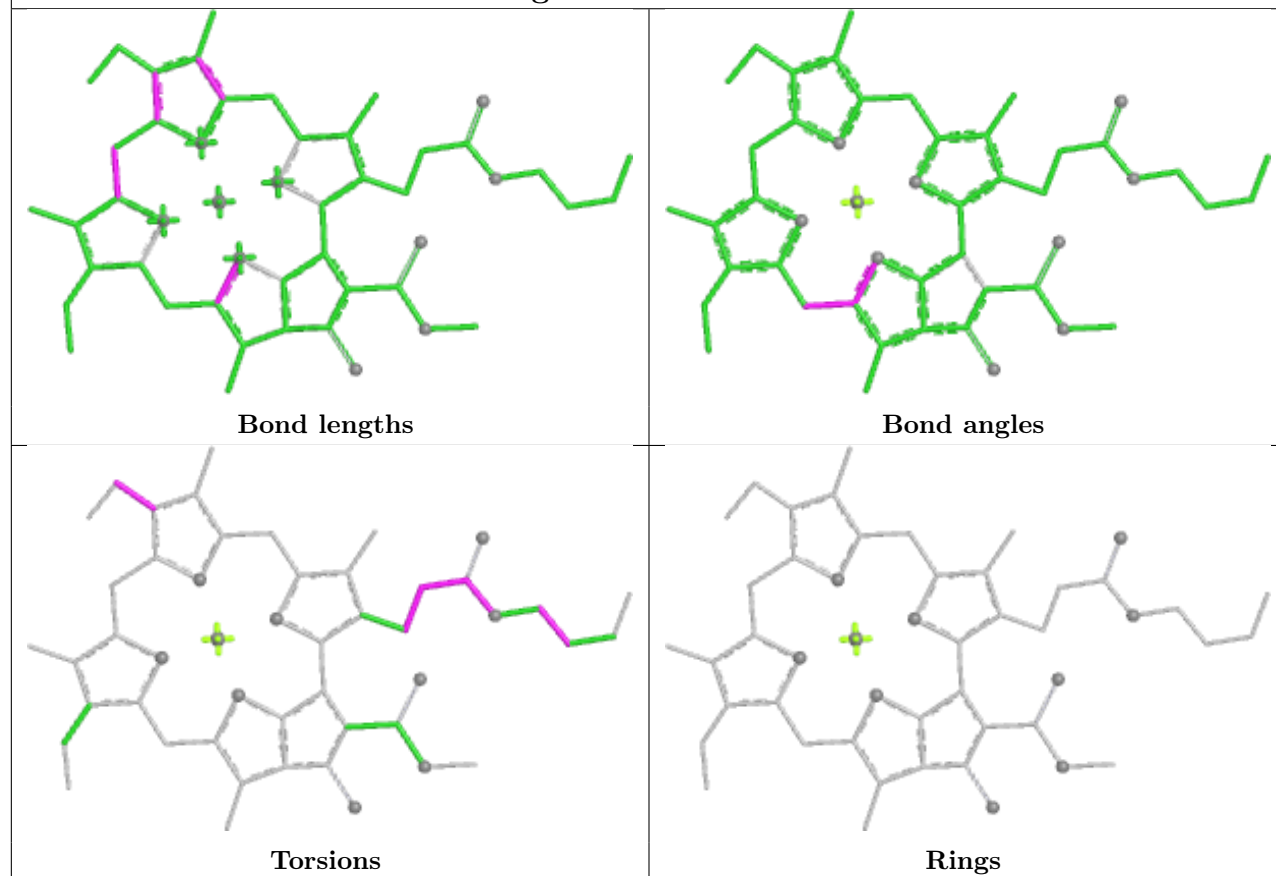
Ligand BCR f 101

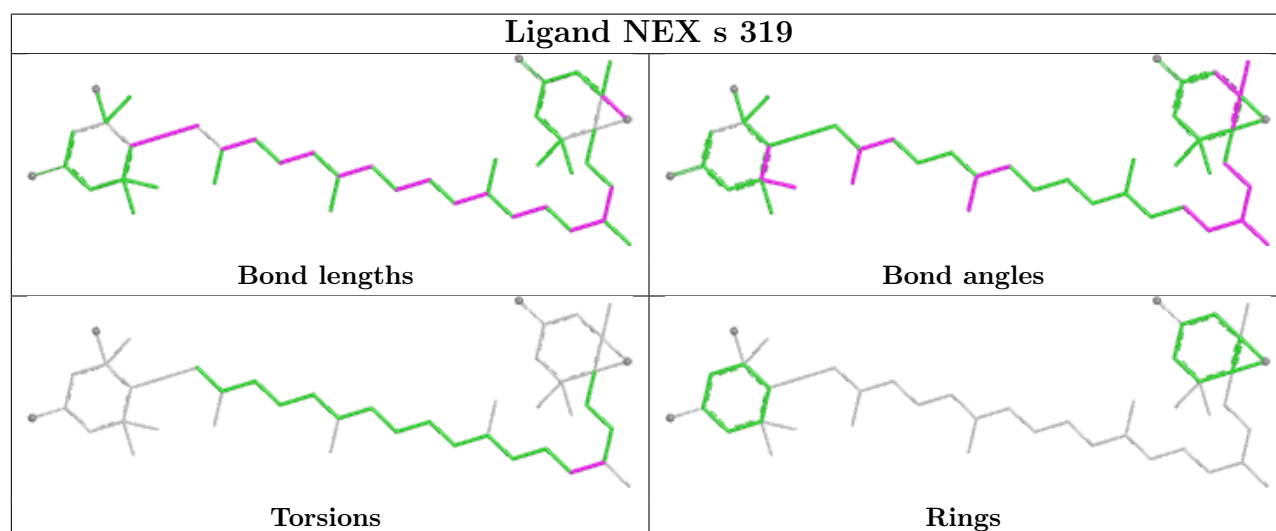
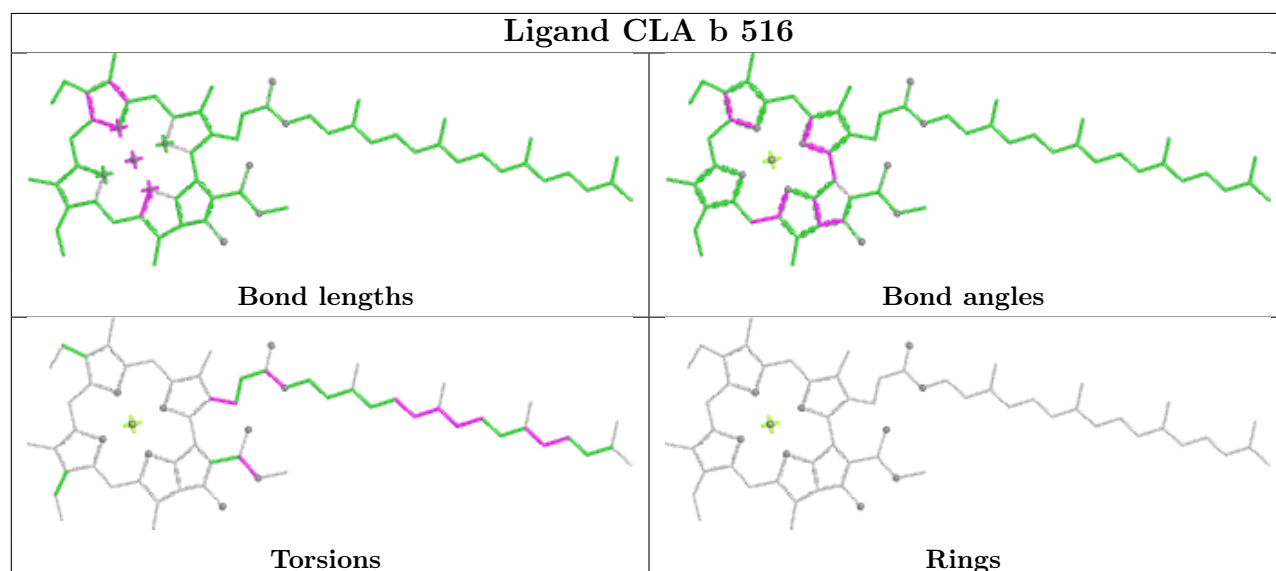
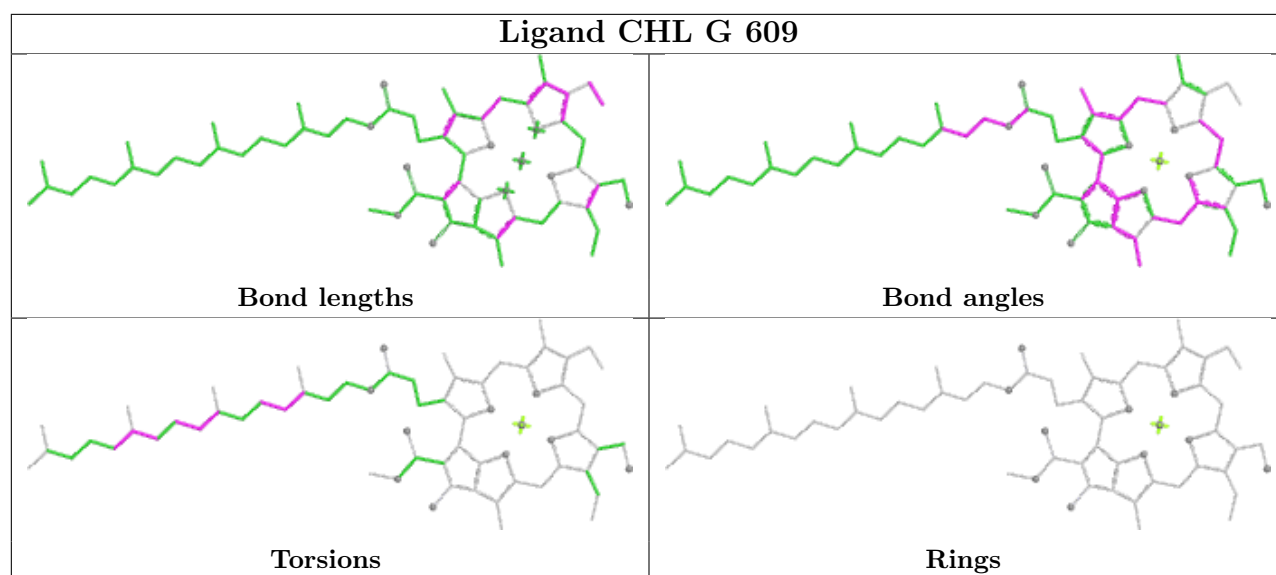


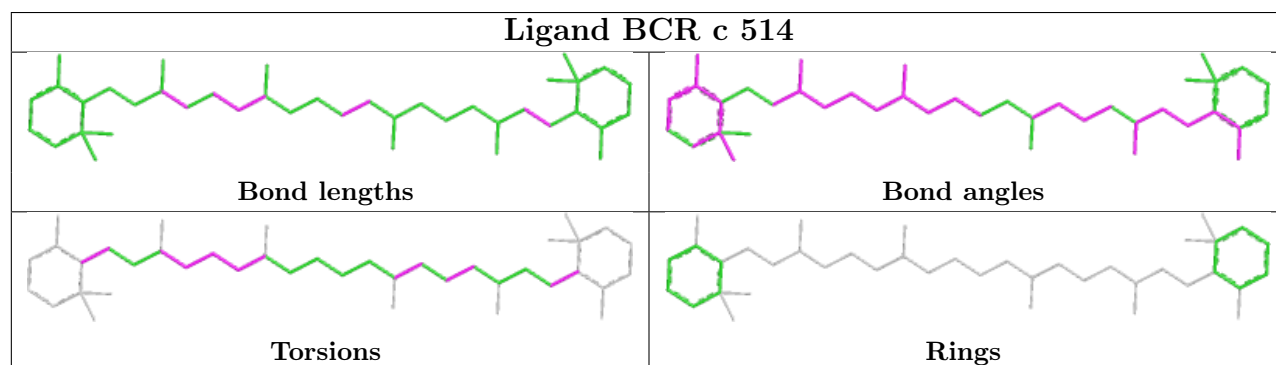
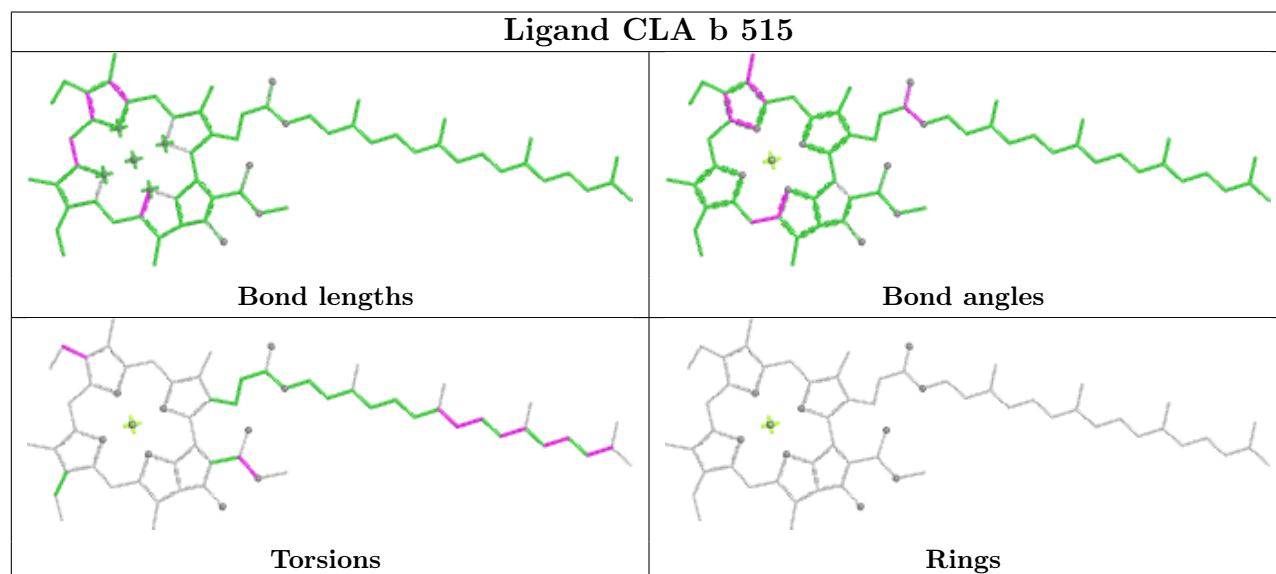
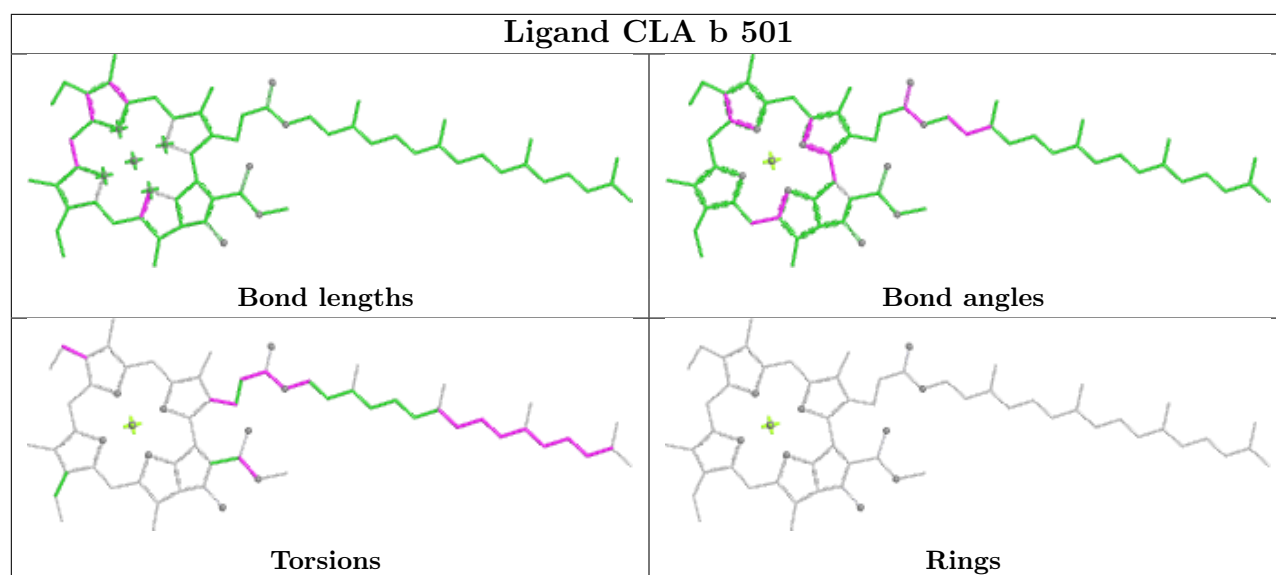
Ligand CLA a 408

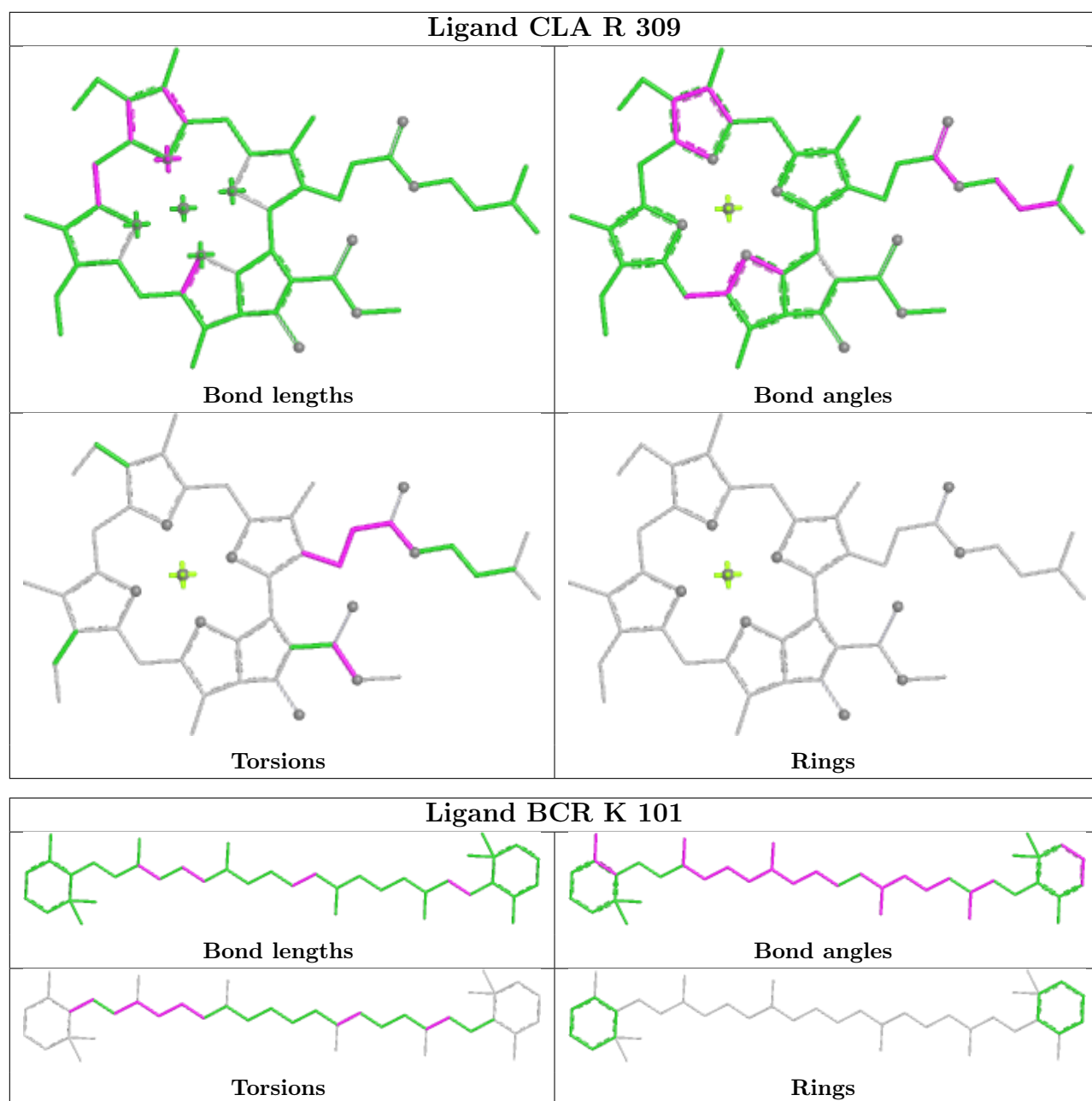


Ligand CLA R 303

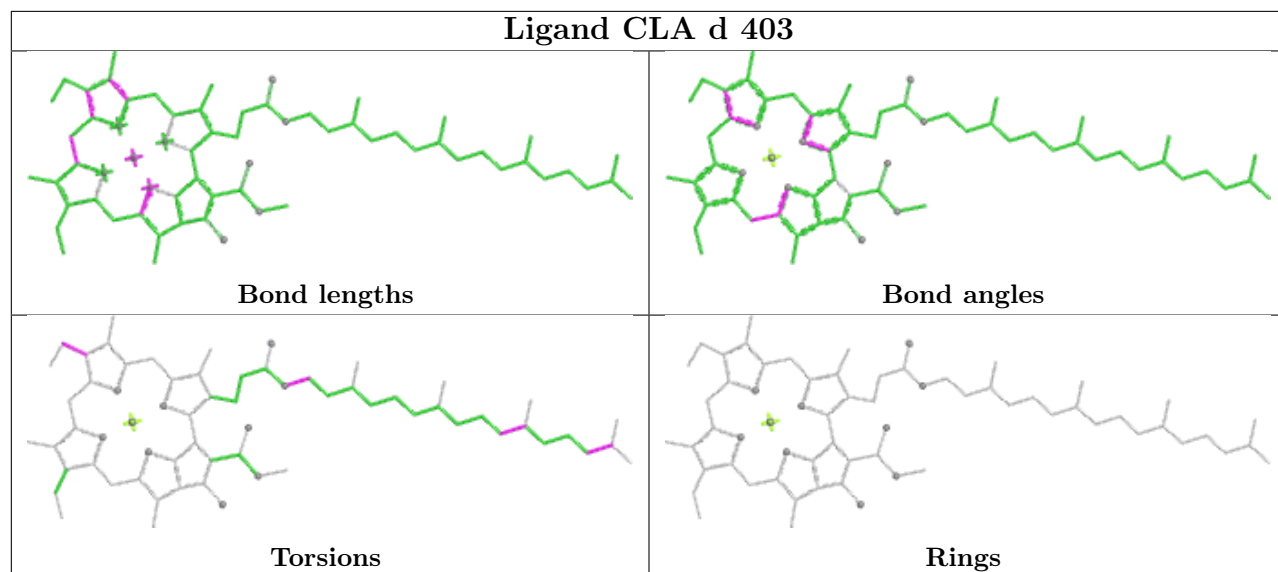




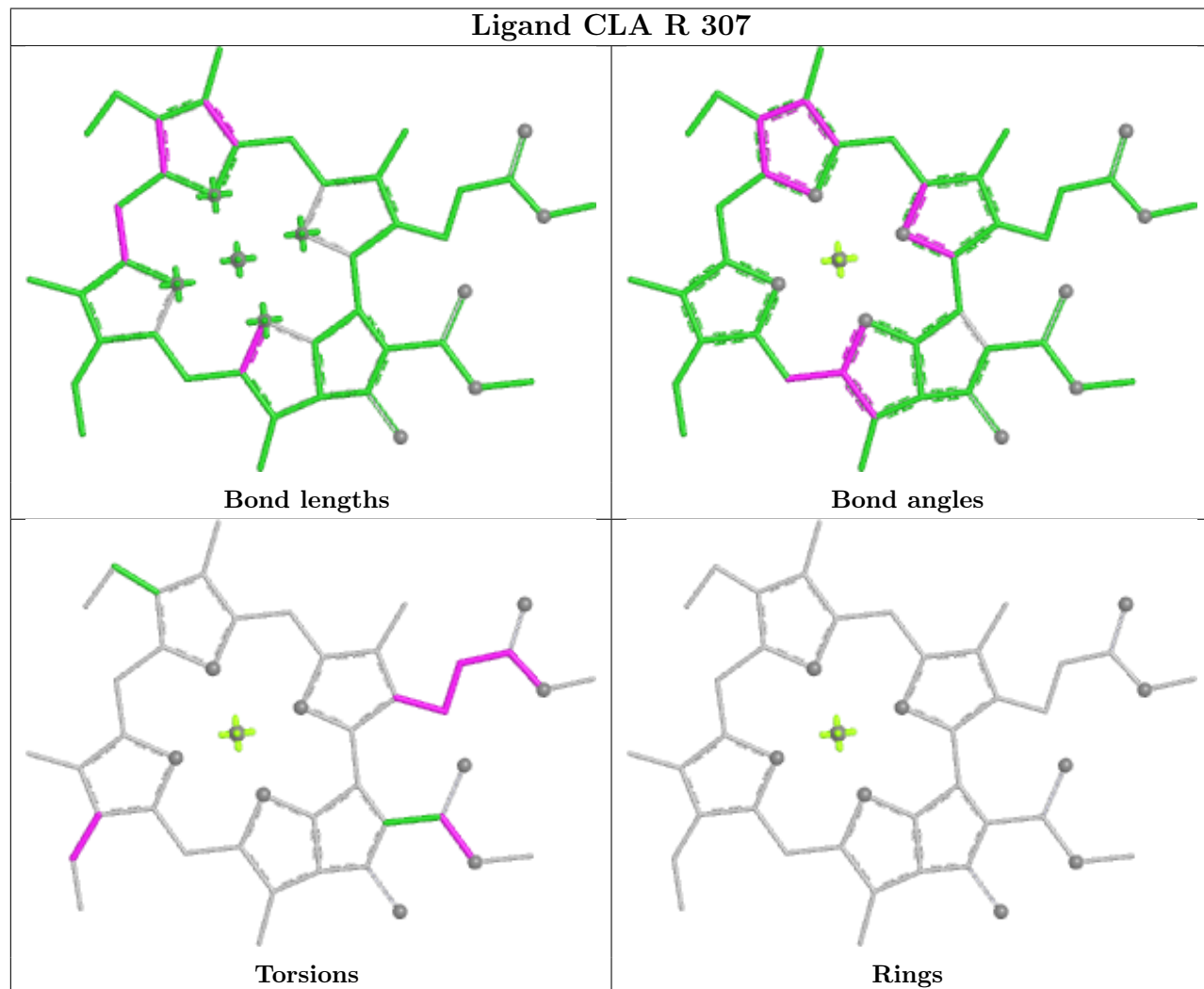


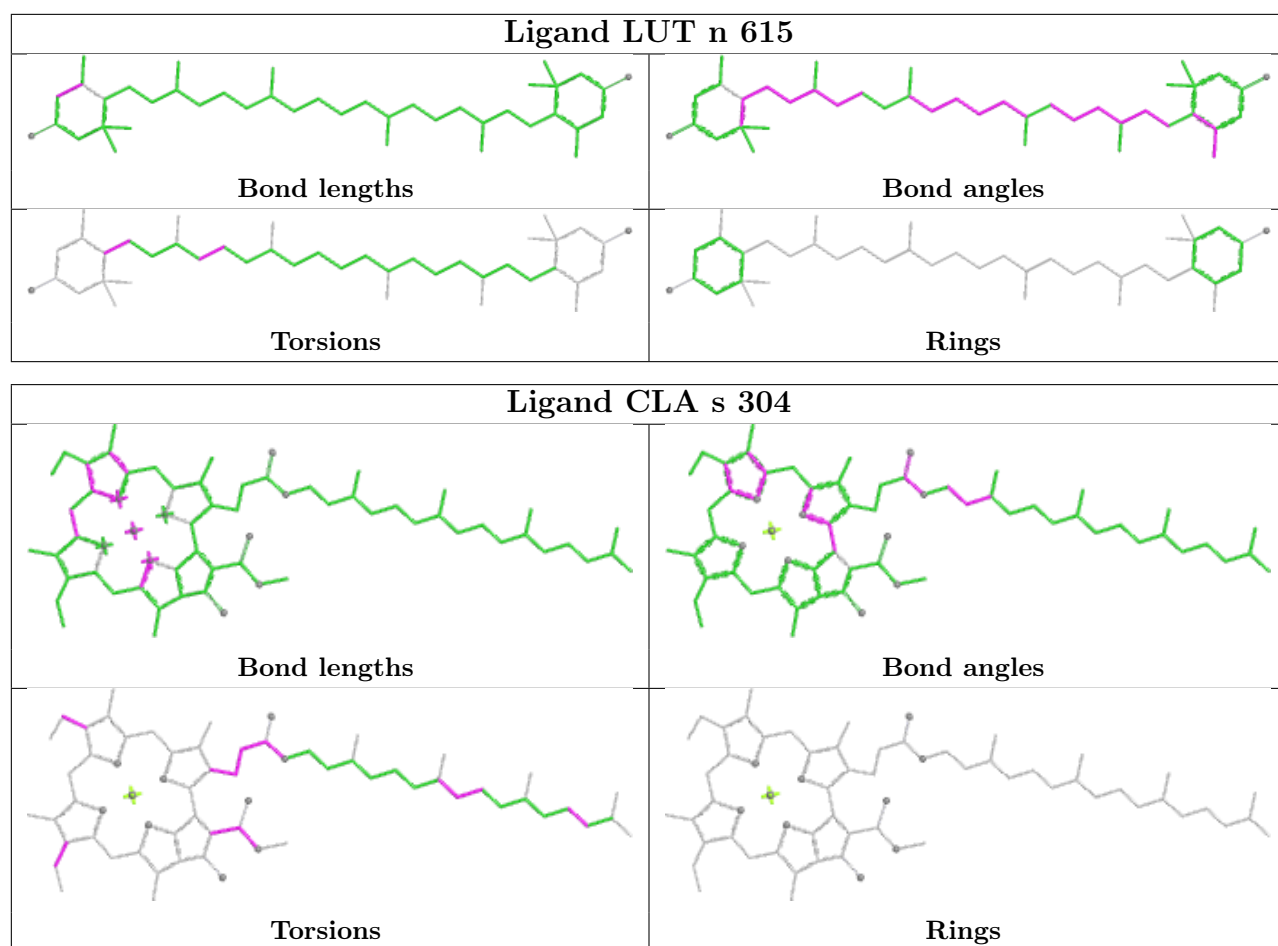


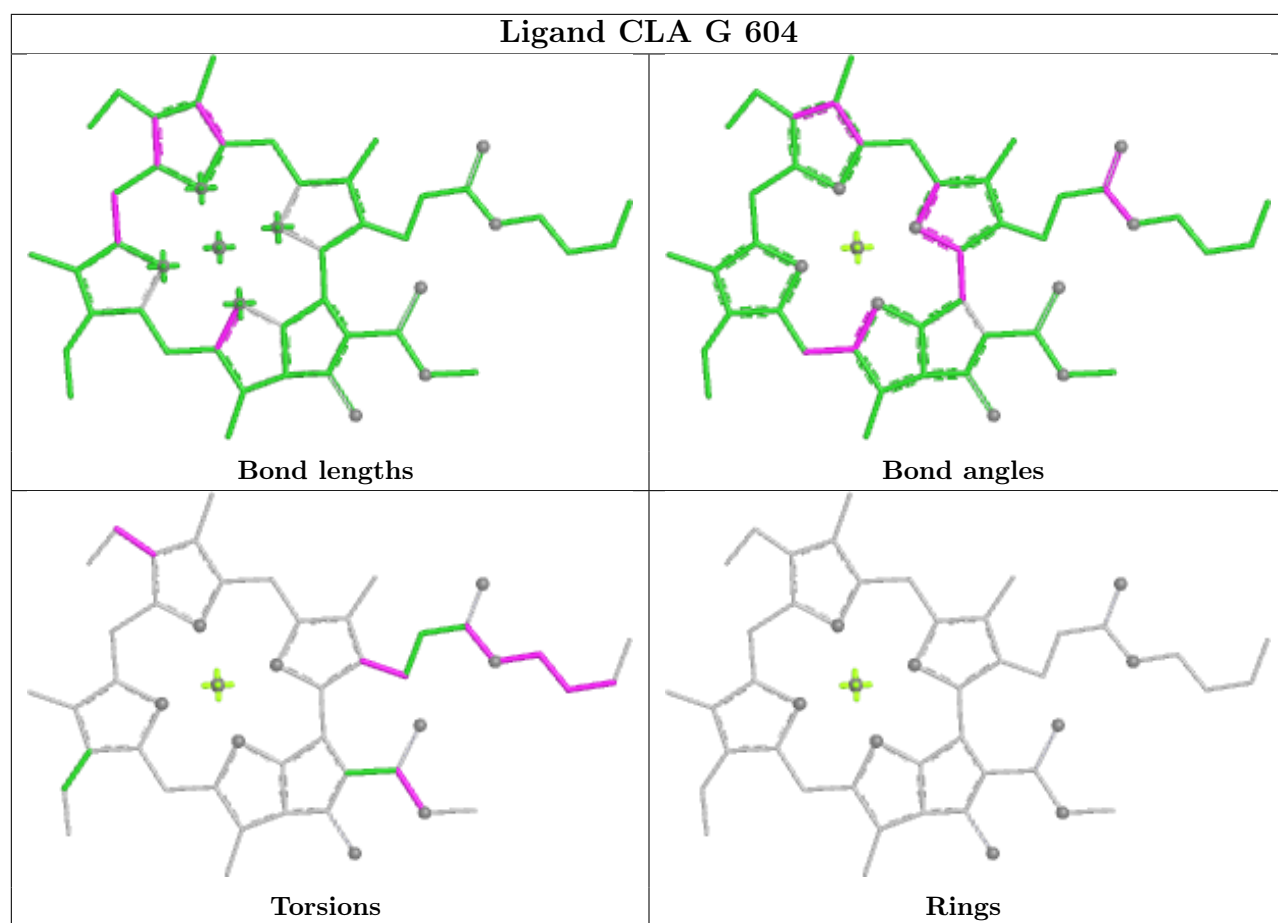
Ligand CLA d 403



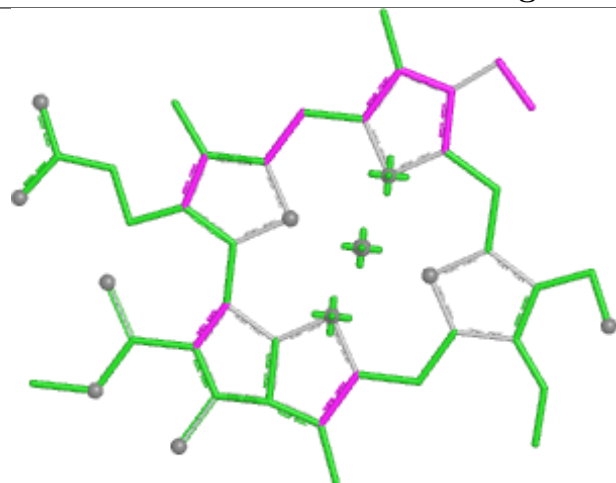
Ligand CLA R 307



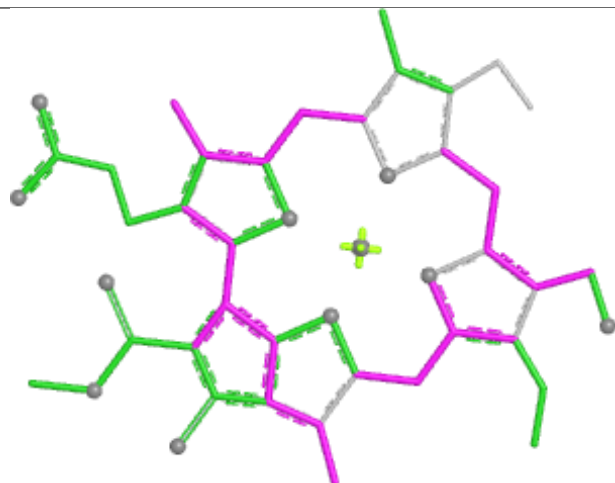




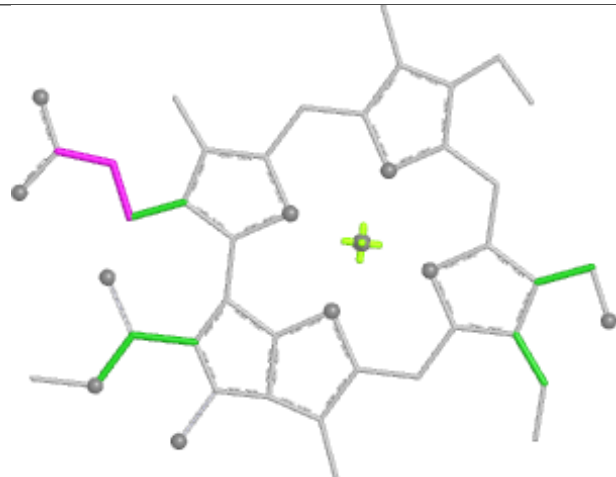
Ligand CHL S 302



Bond lengths



Bond angles

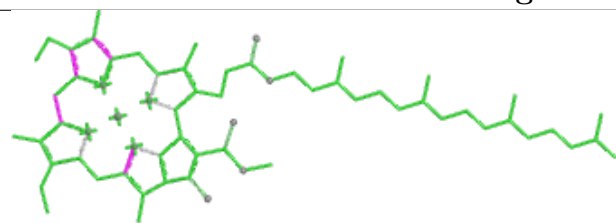


Torsions

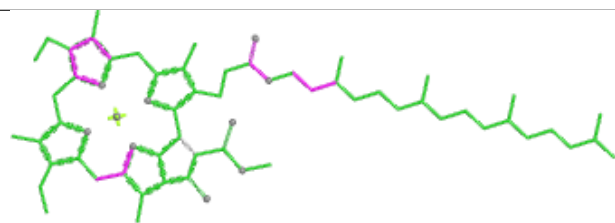


Rings

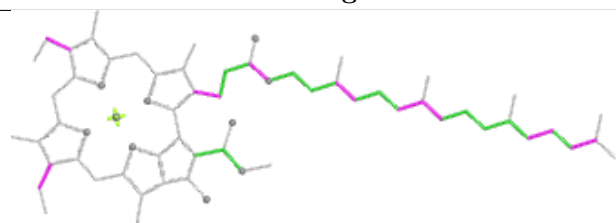
Ligand CLA Y 304



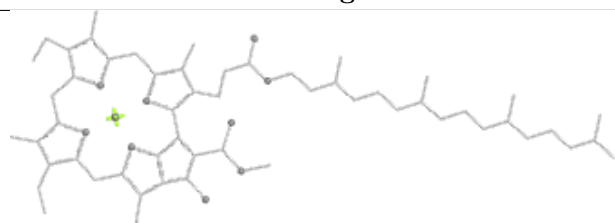
Bond lengths



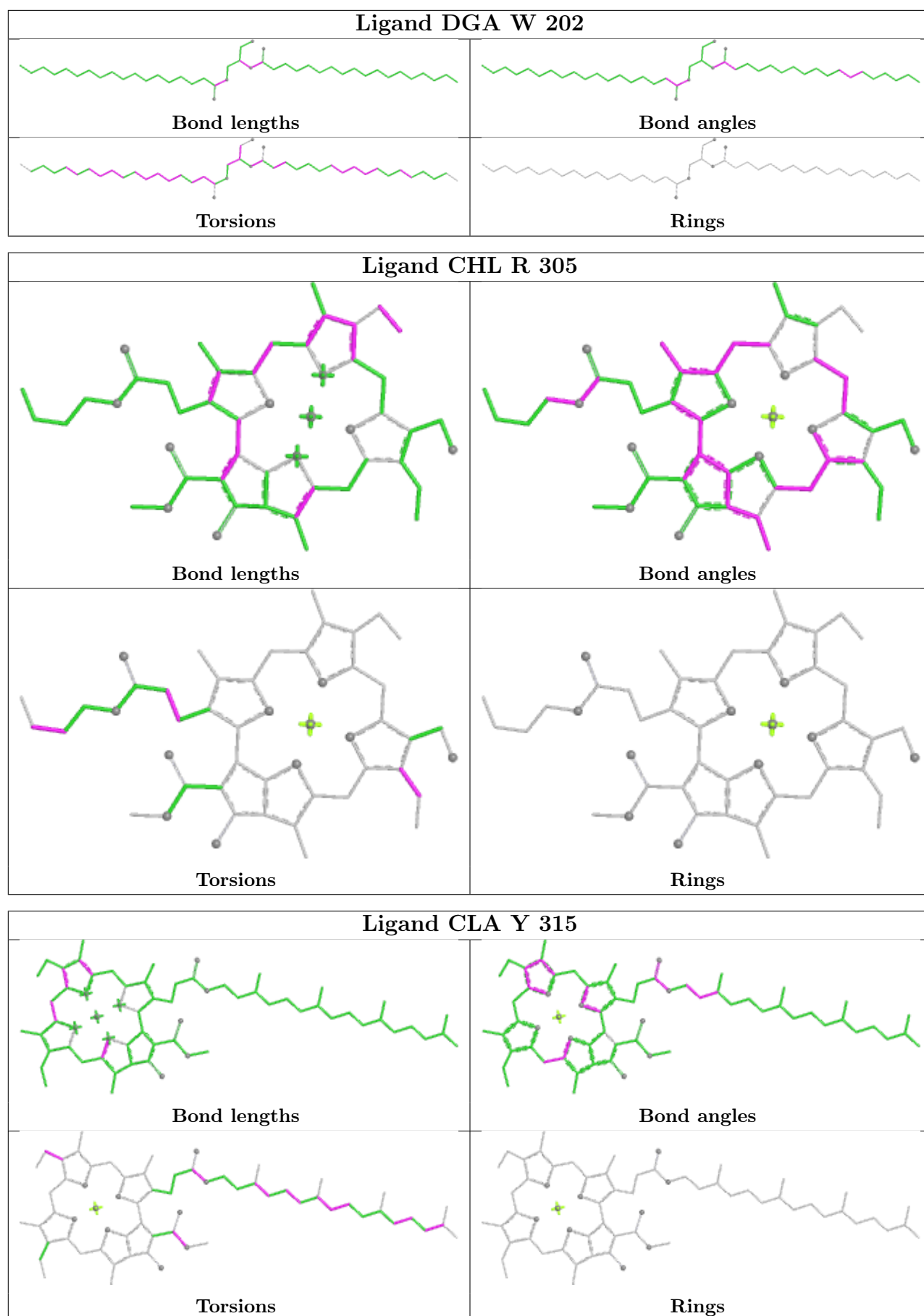
Bond angles

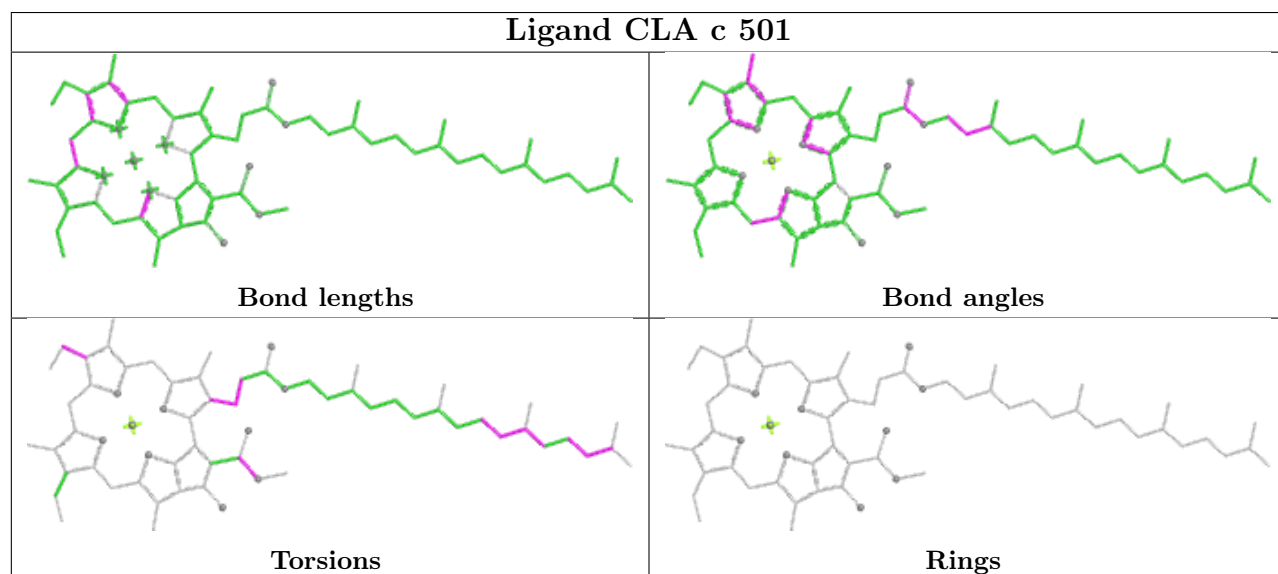
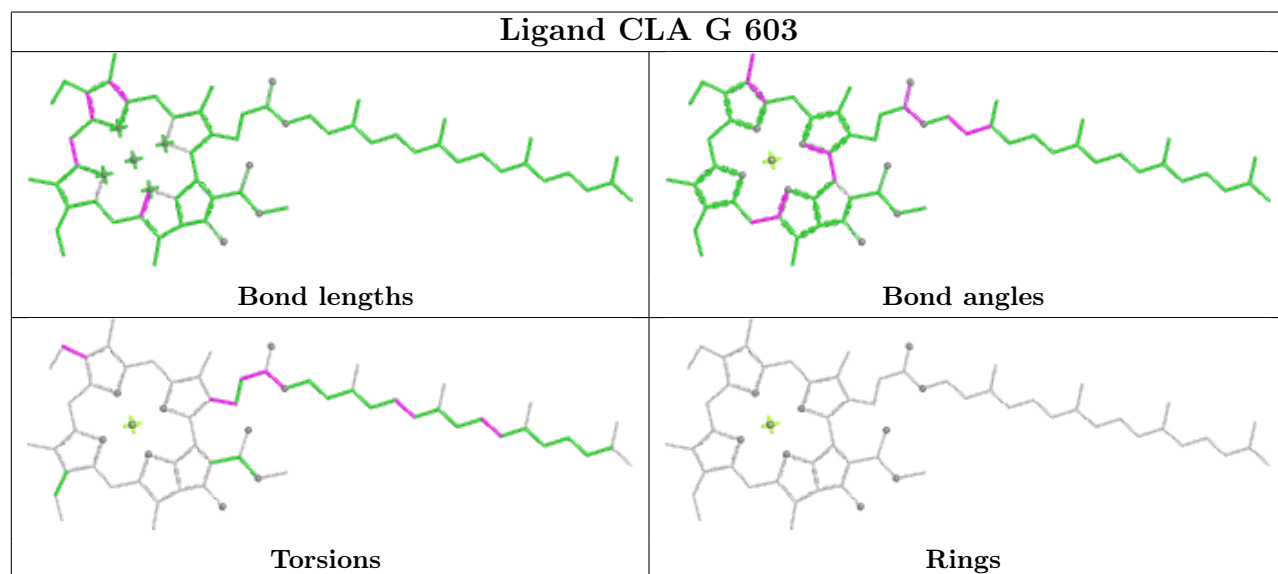
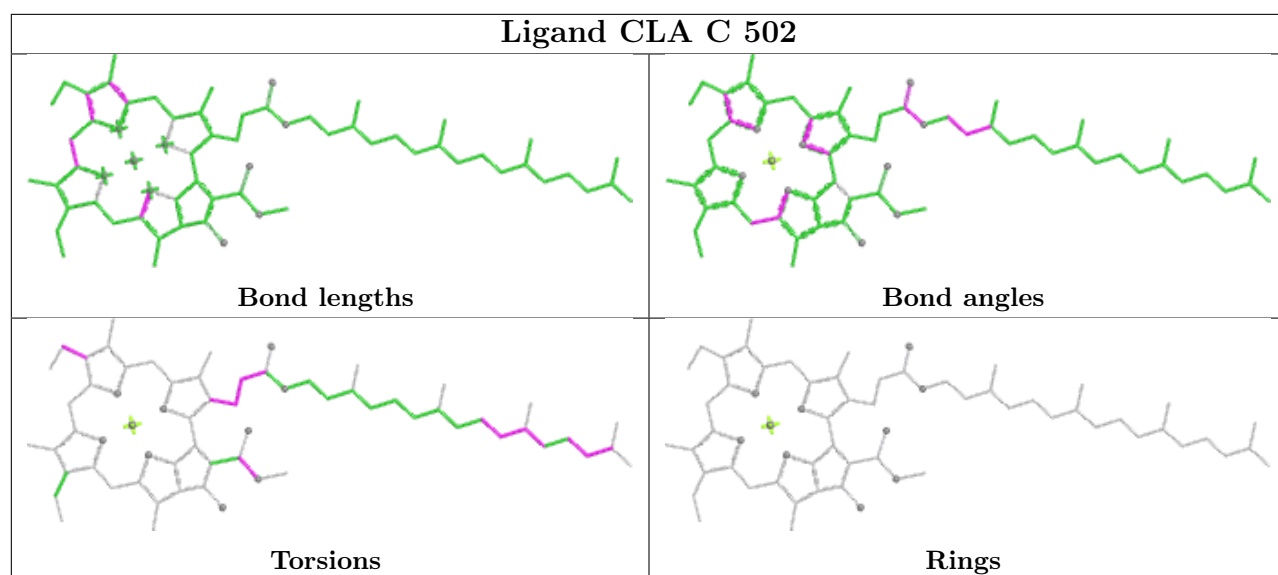


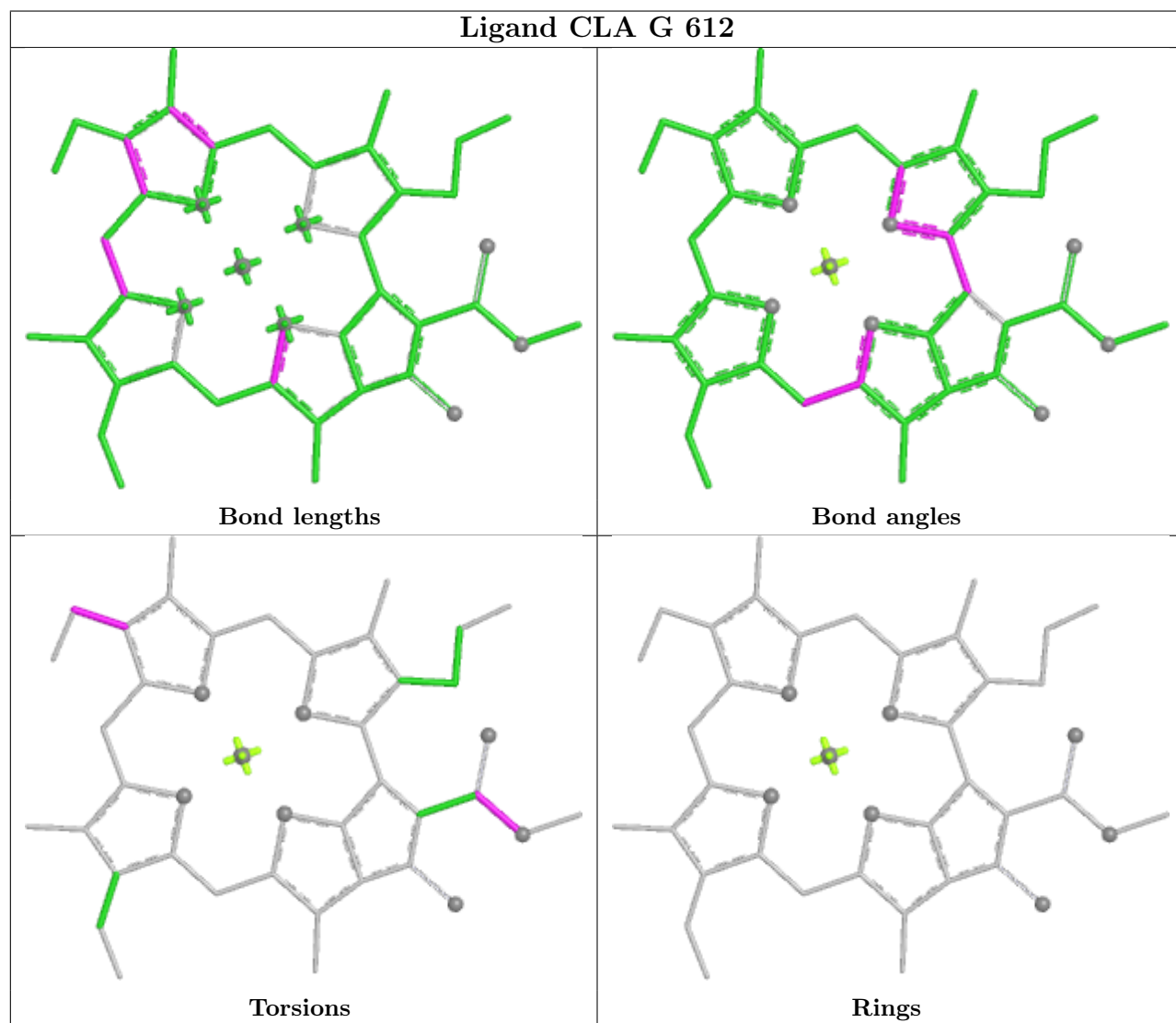
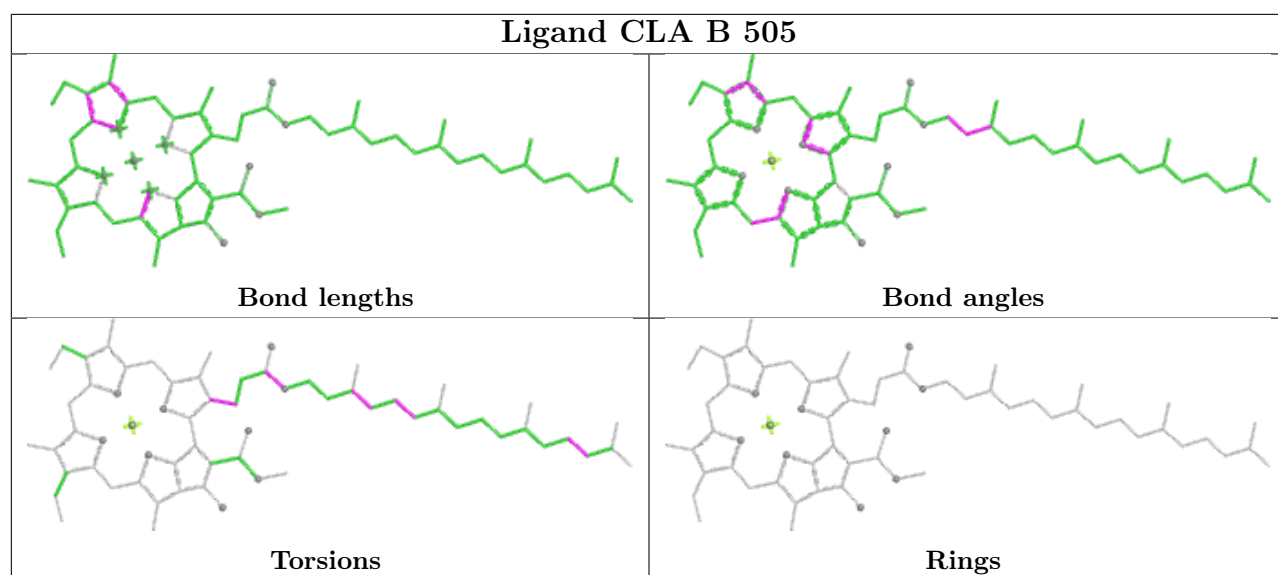
Torsions

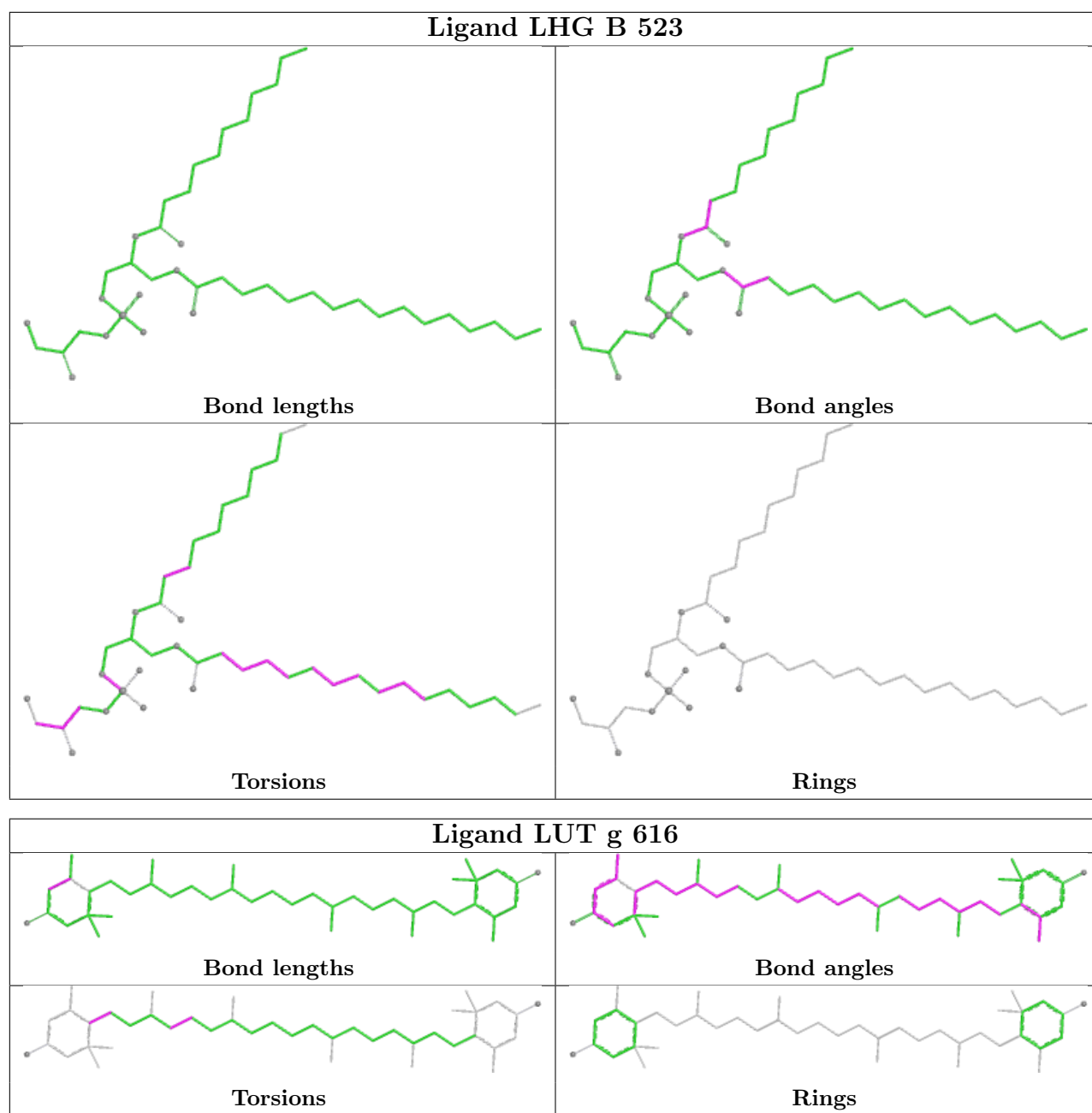


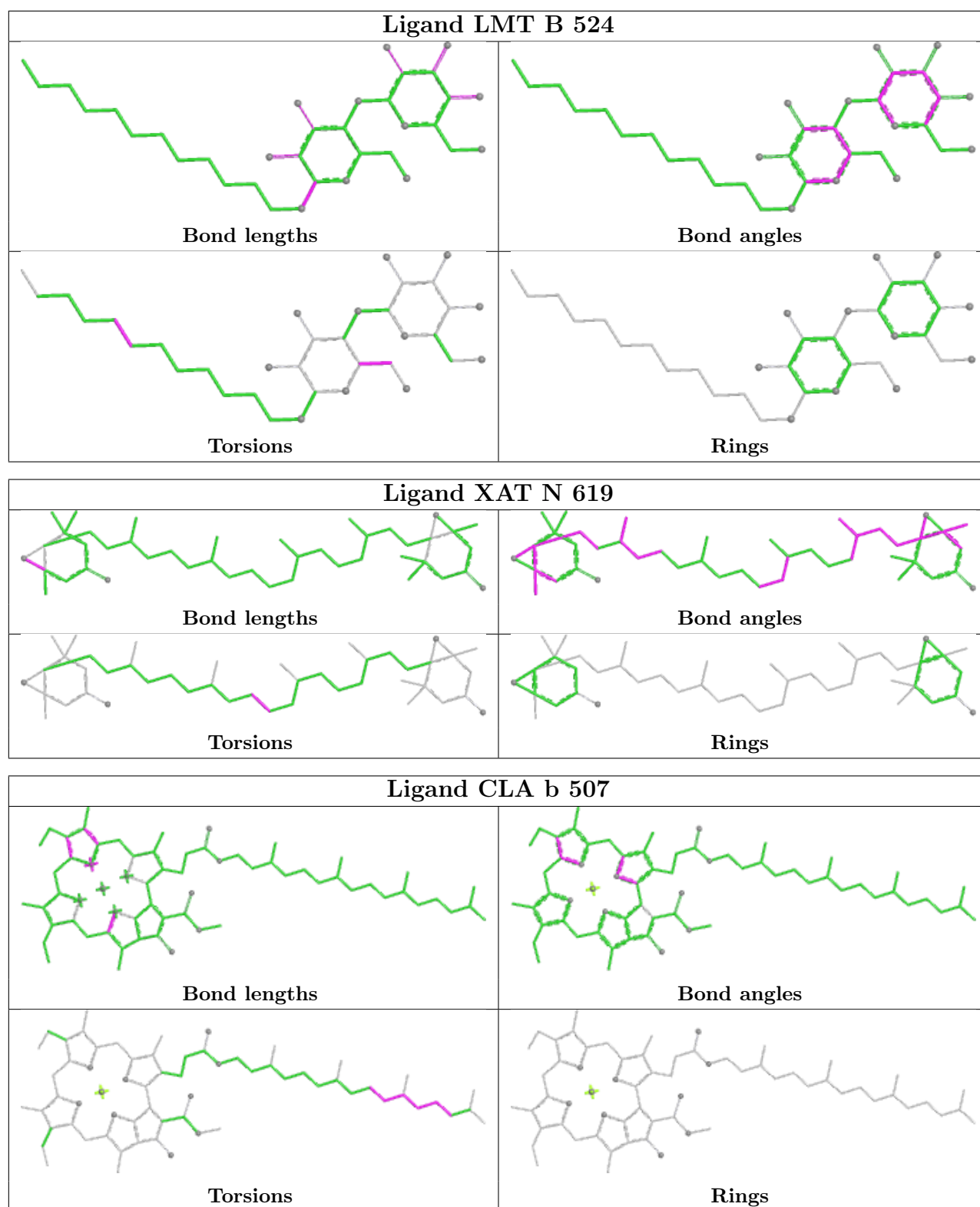
Rings

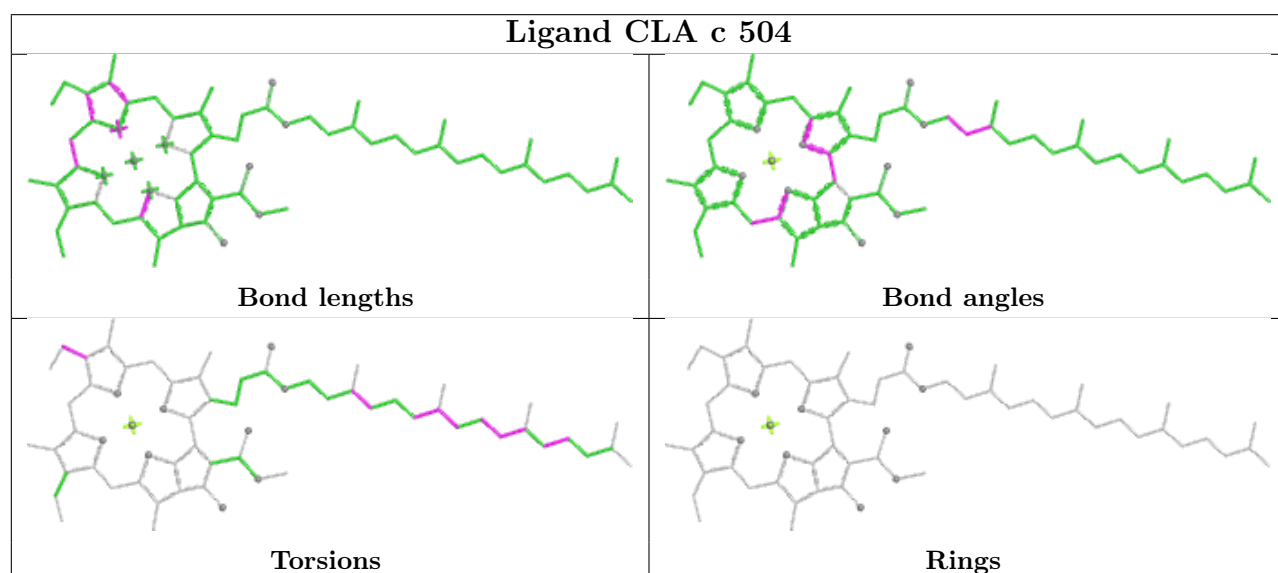
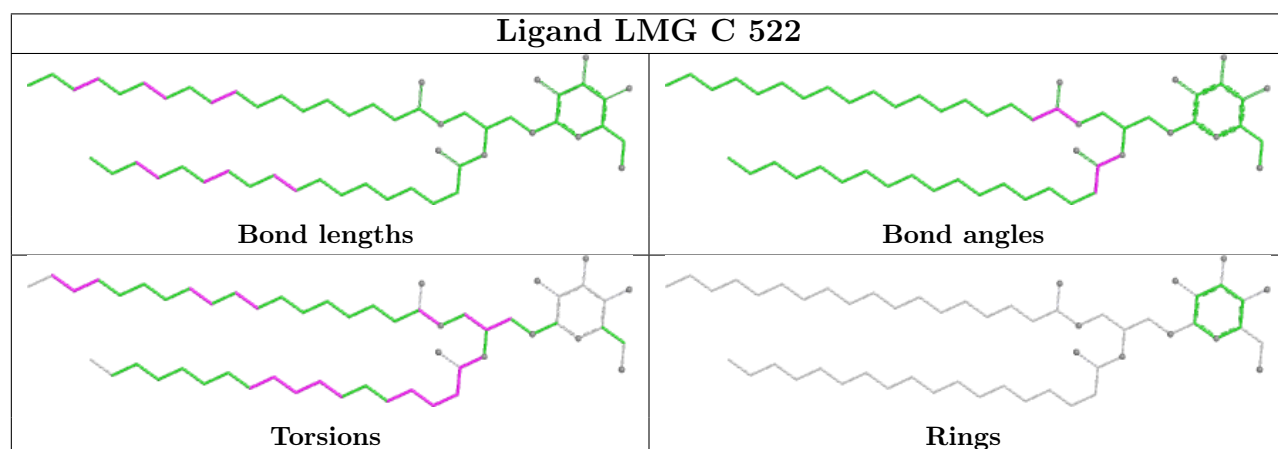
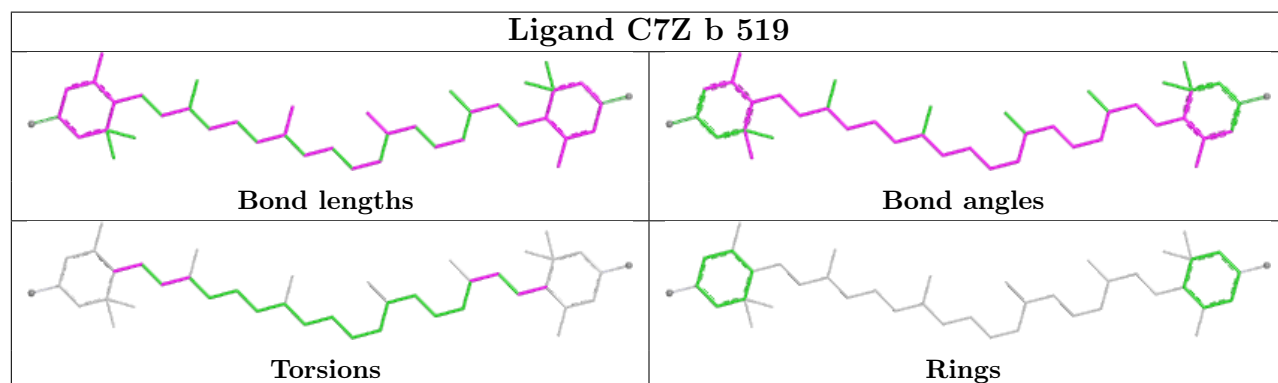
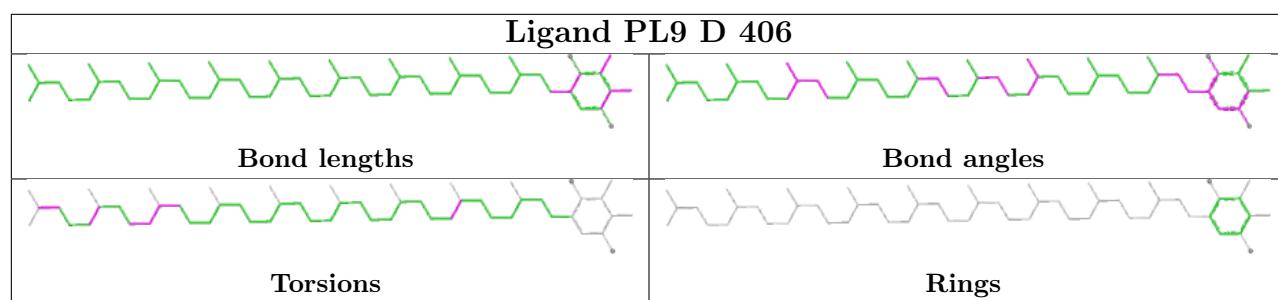




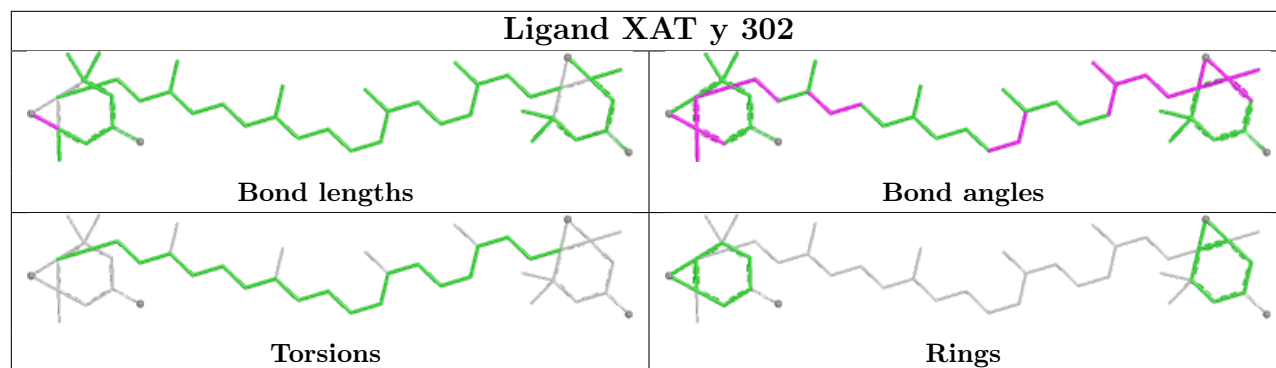




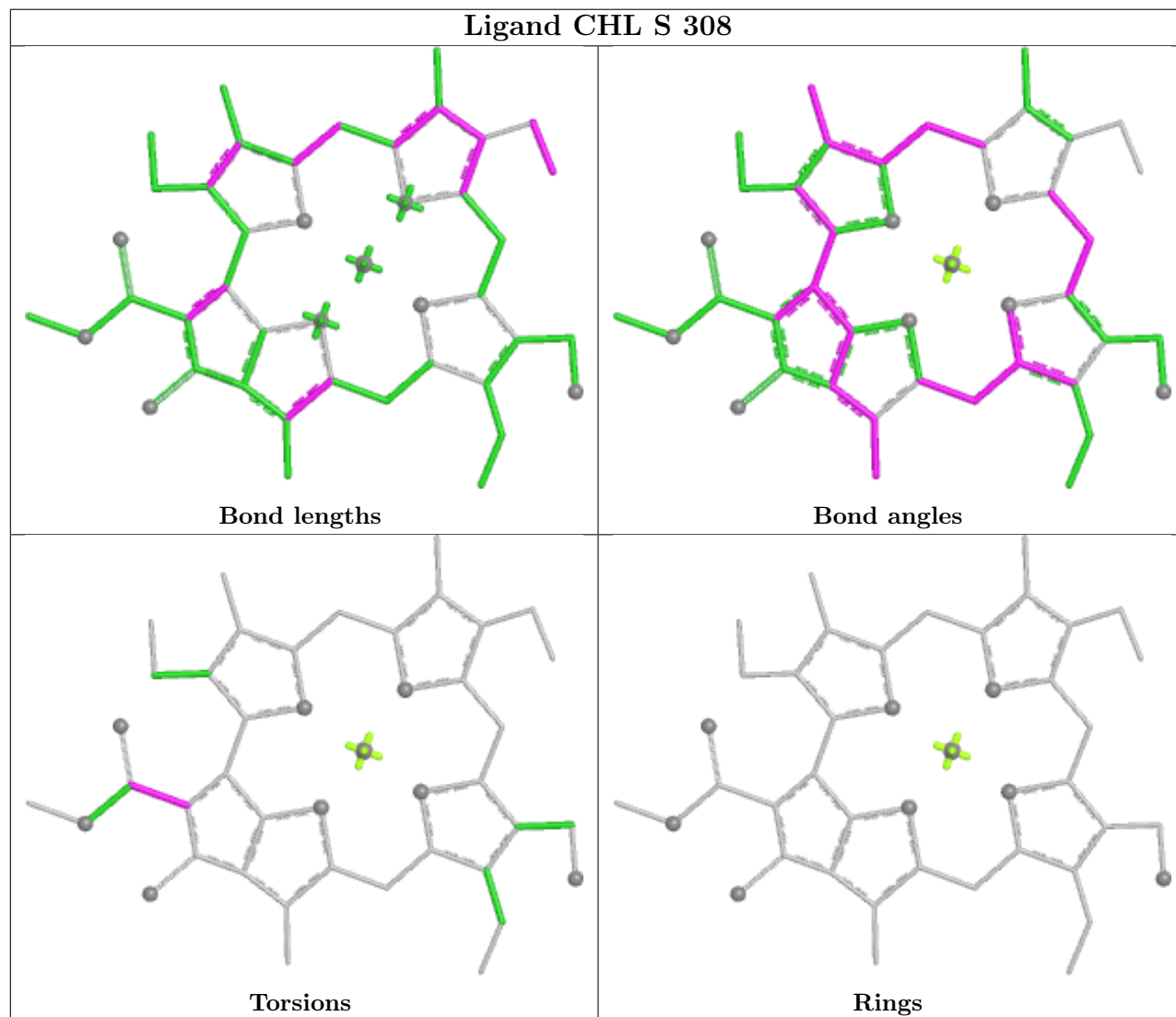


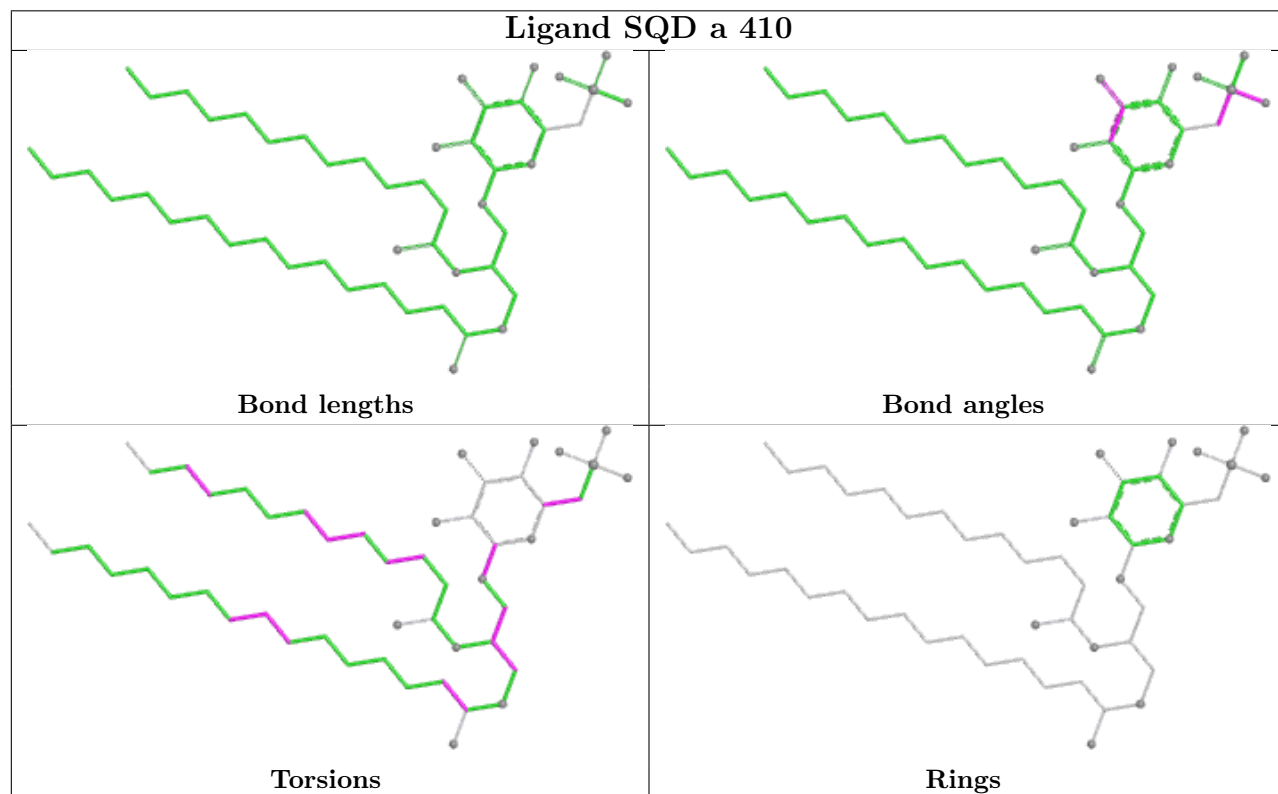
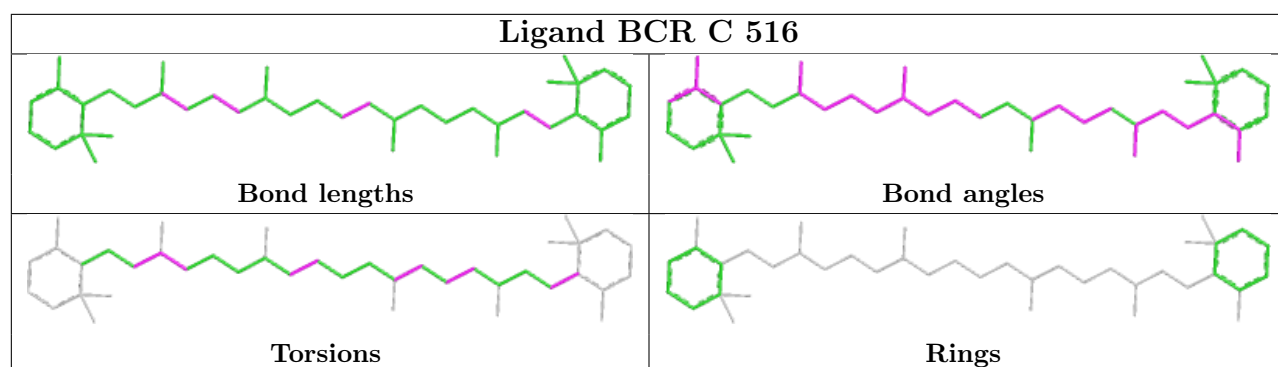


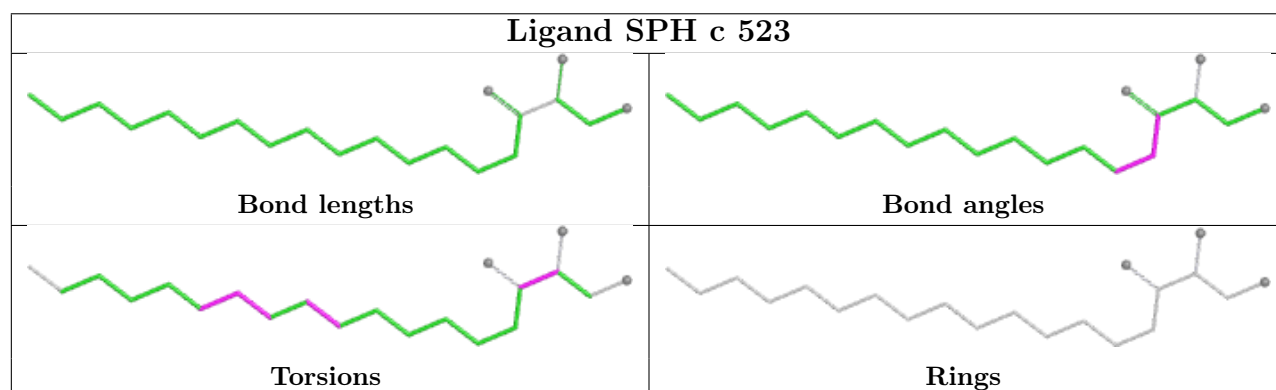
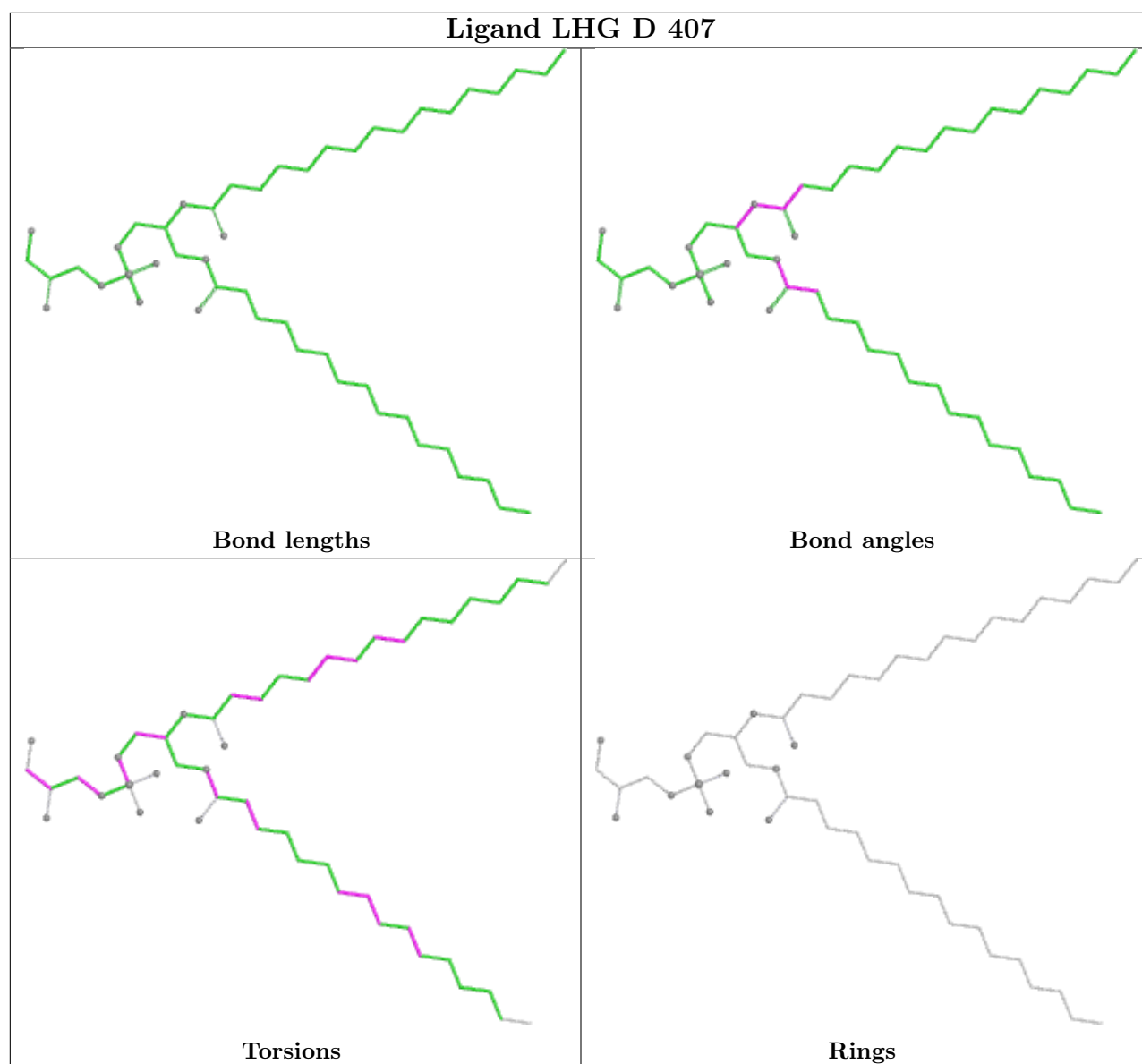
Ligand XAT y 302



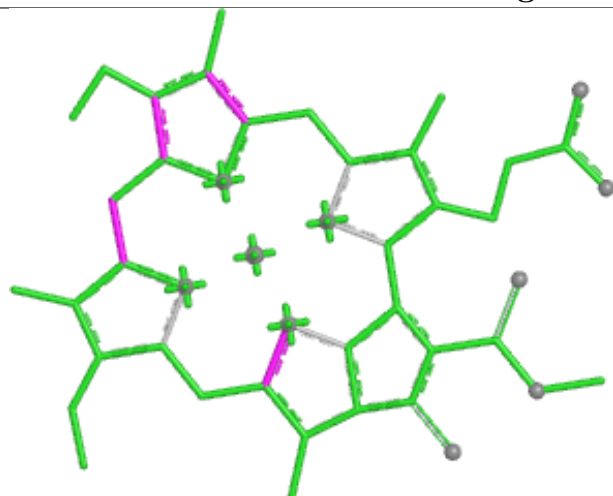
Ligand CHL S 308



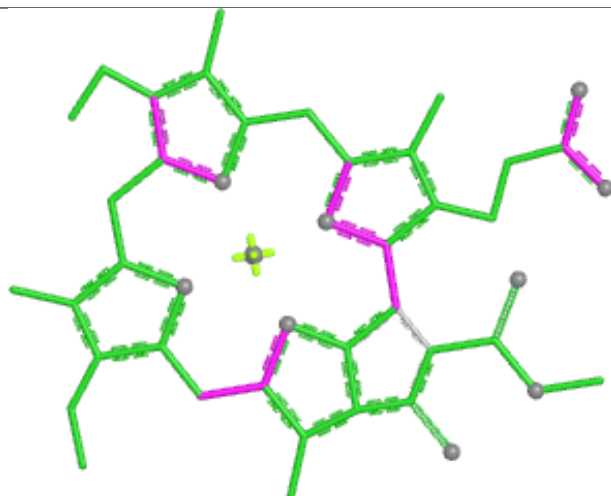




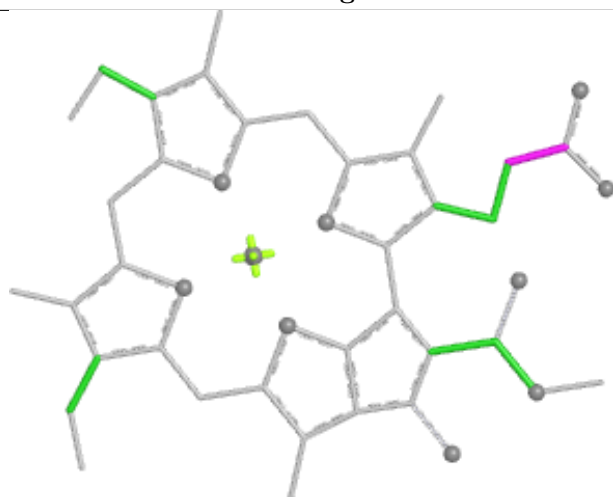
Ligand CLA S 313



Bond lengths



Bond angles

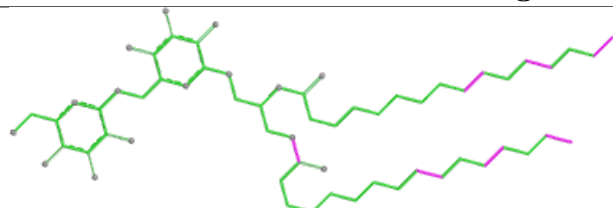


Torsions

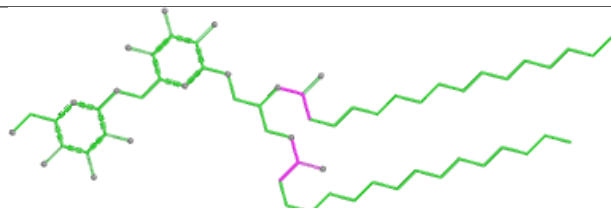


Rings

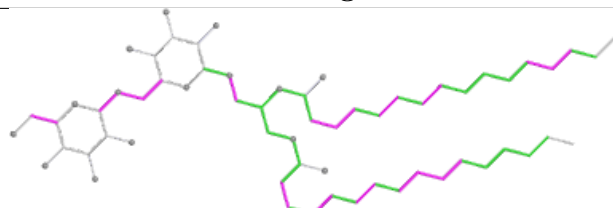
Ligand DGD c 517



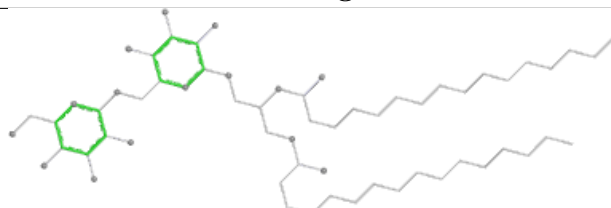
Bond lengths



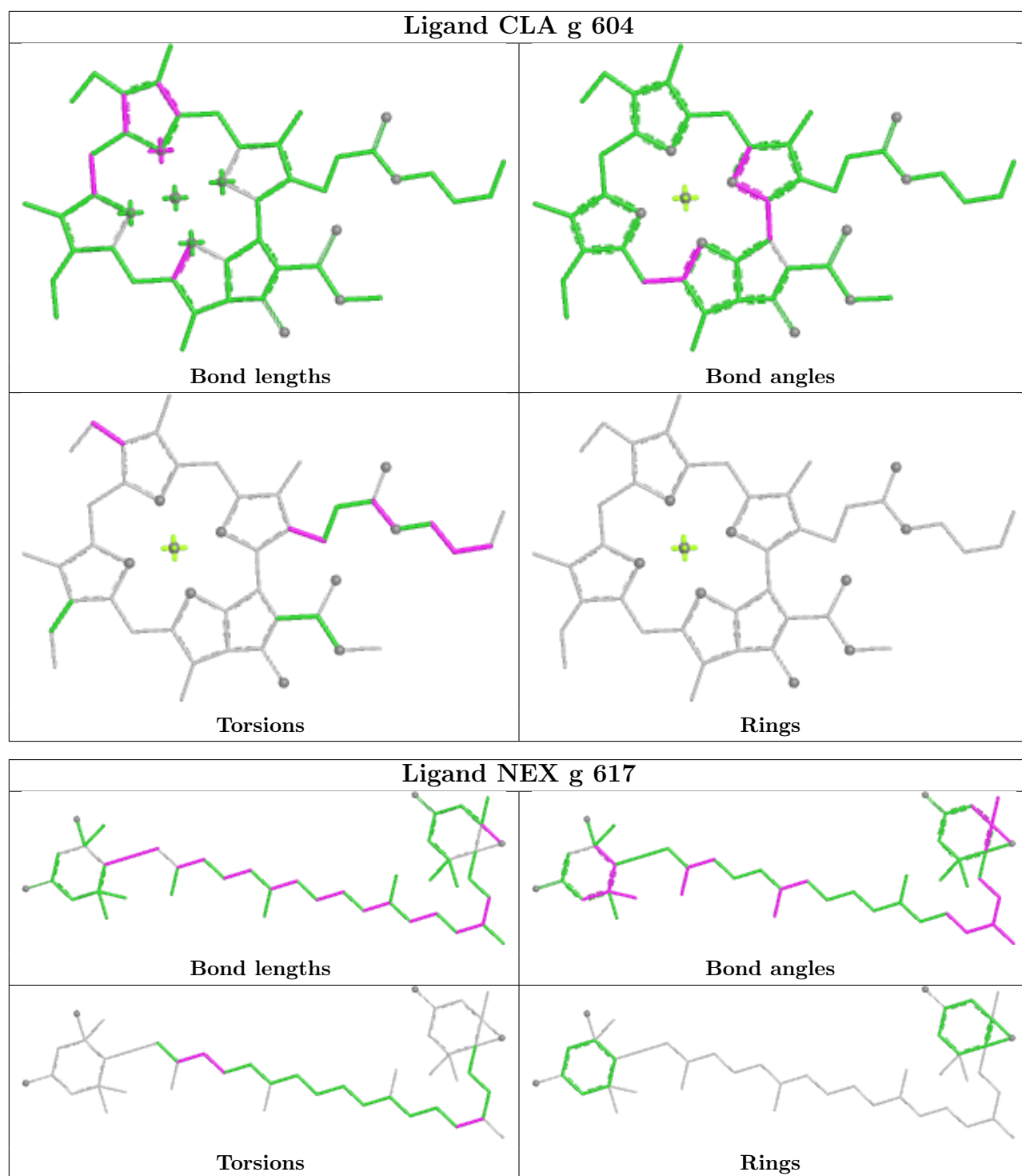
Bond angles

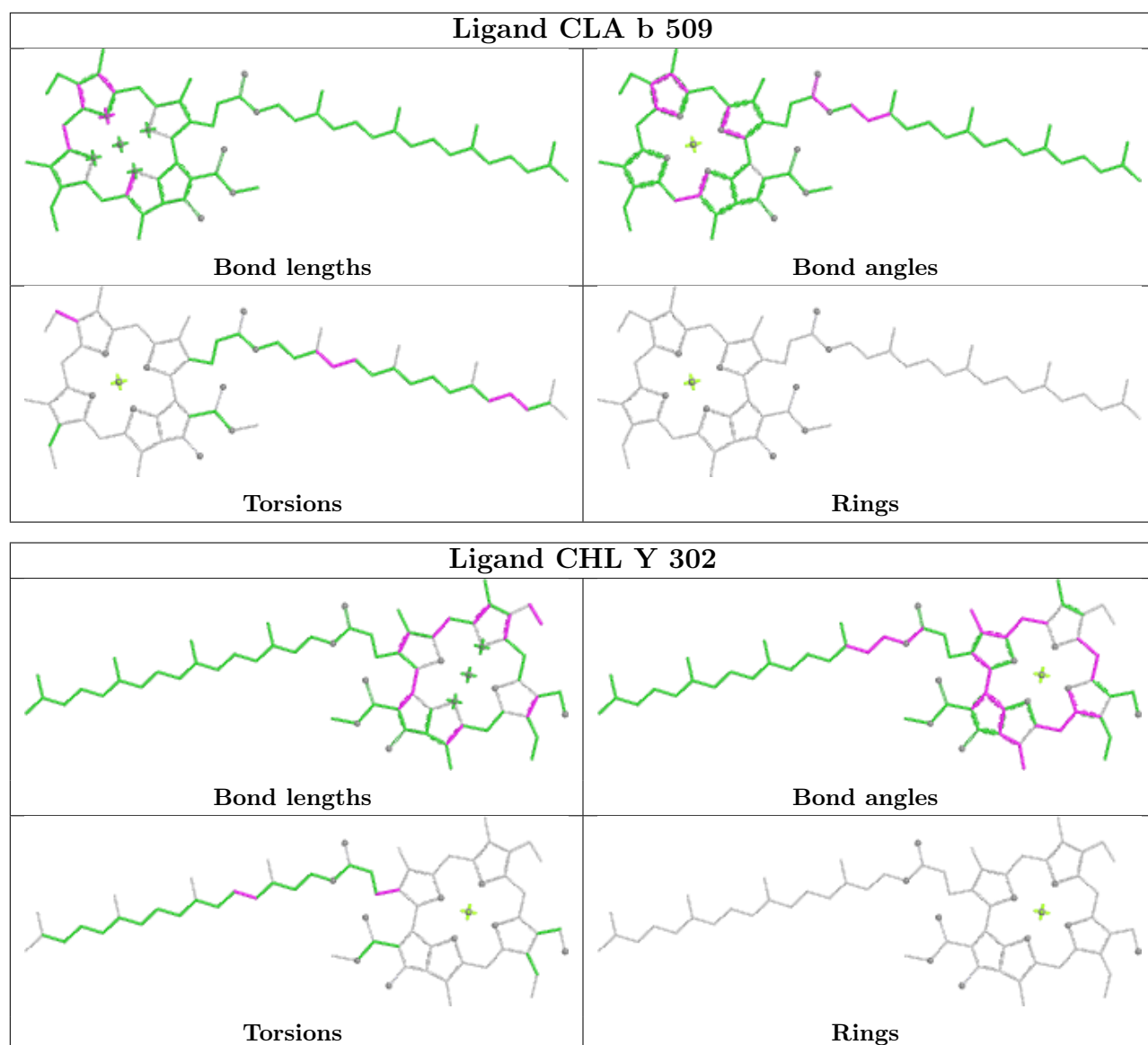


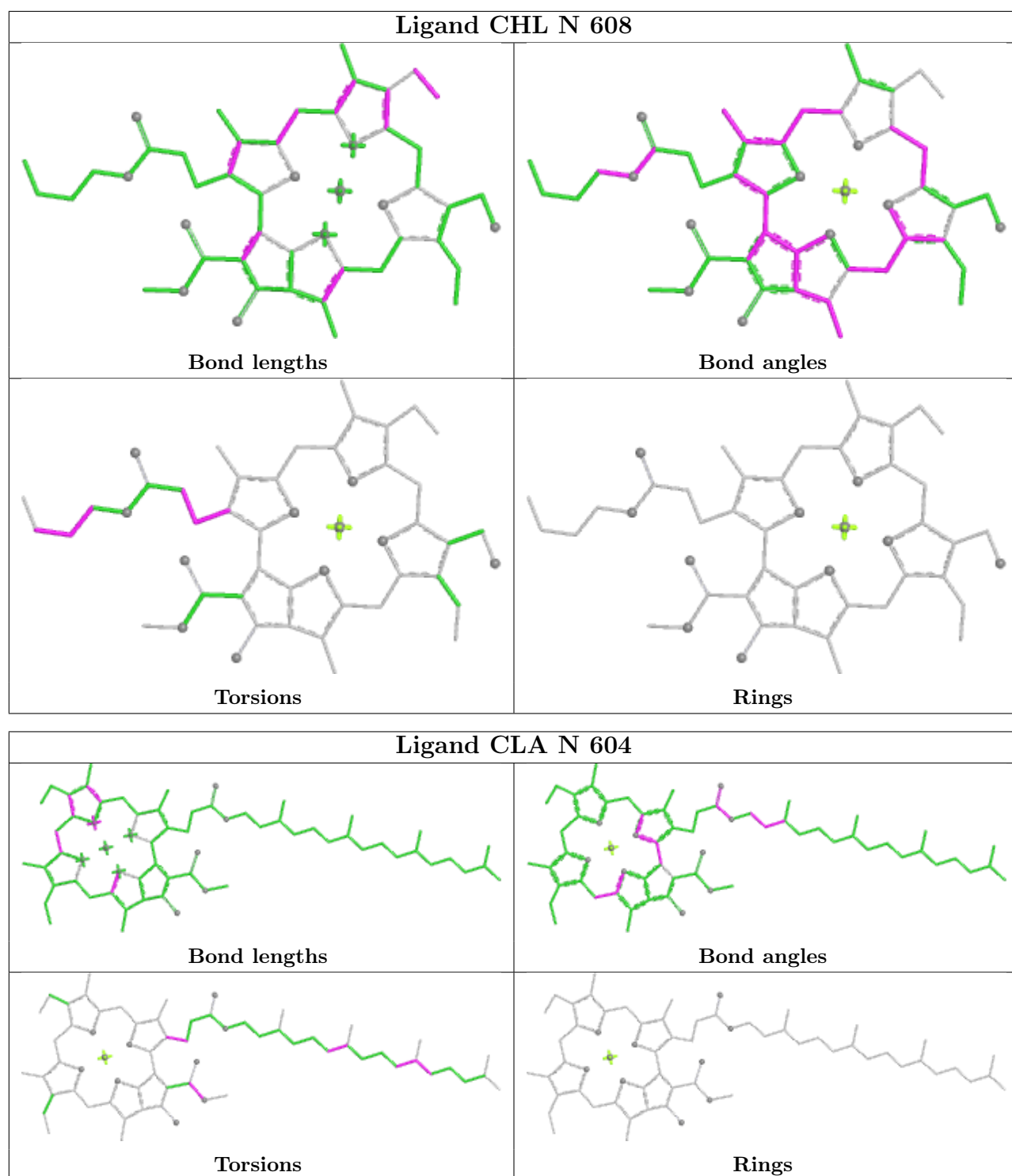
Torsions

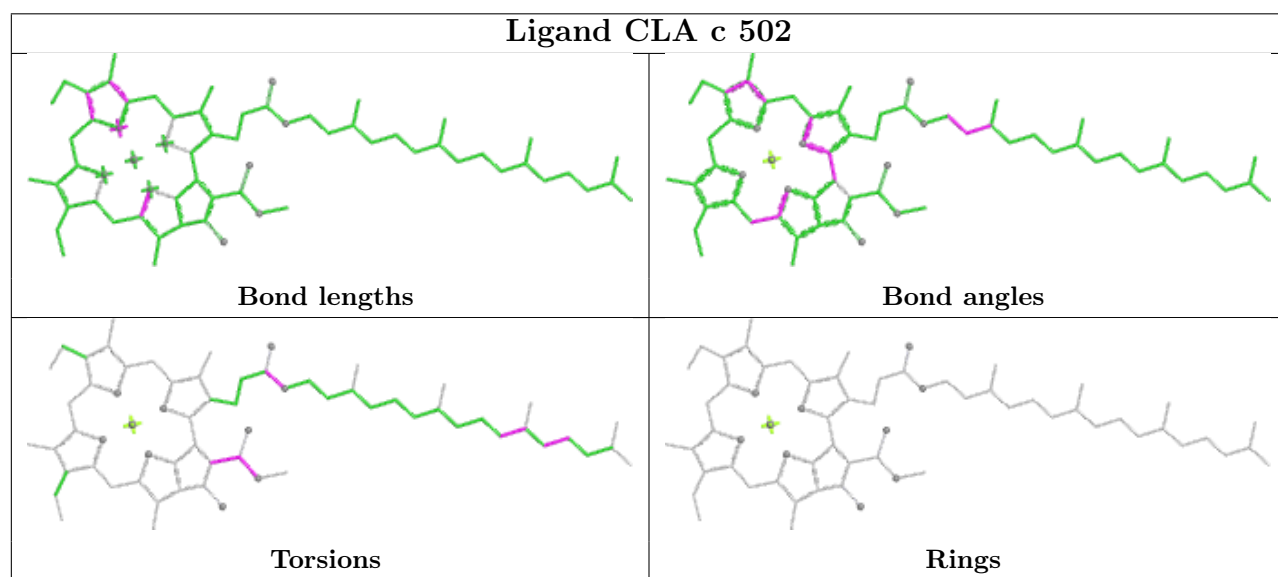
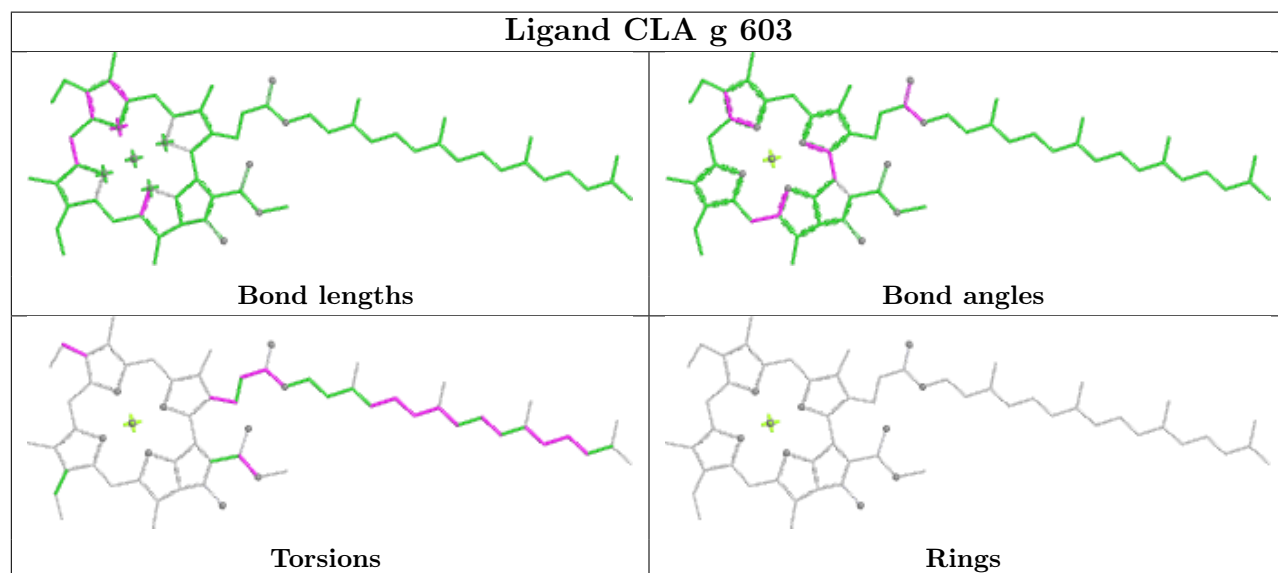
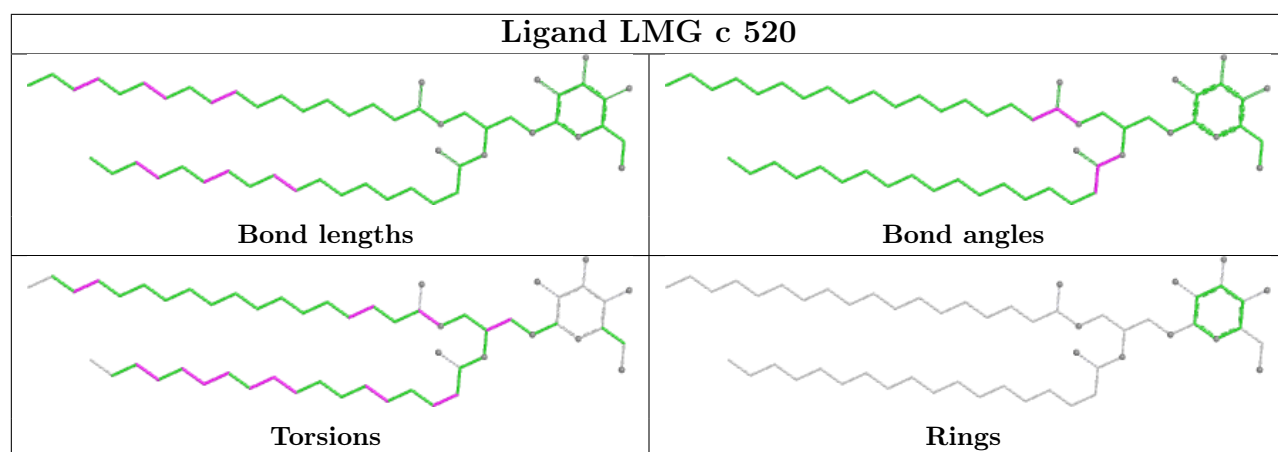


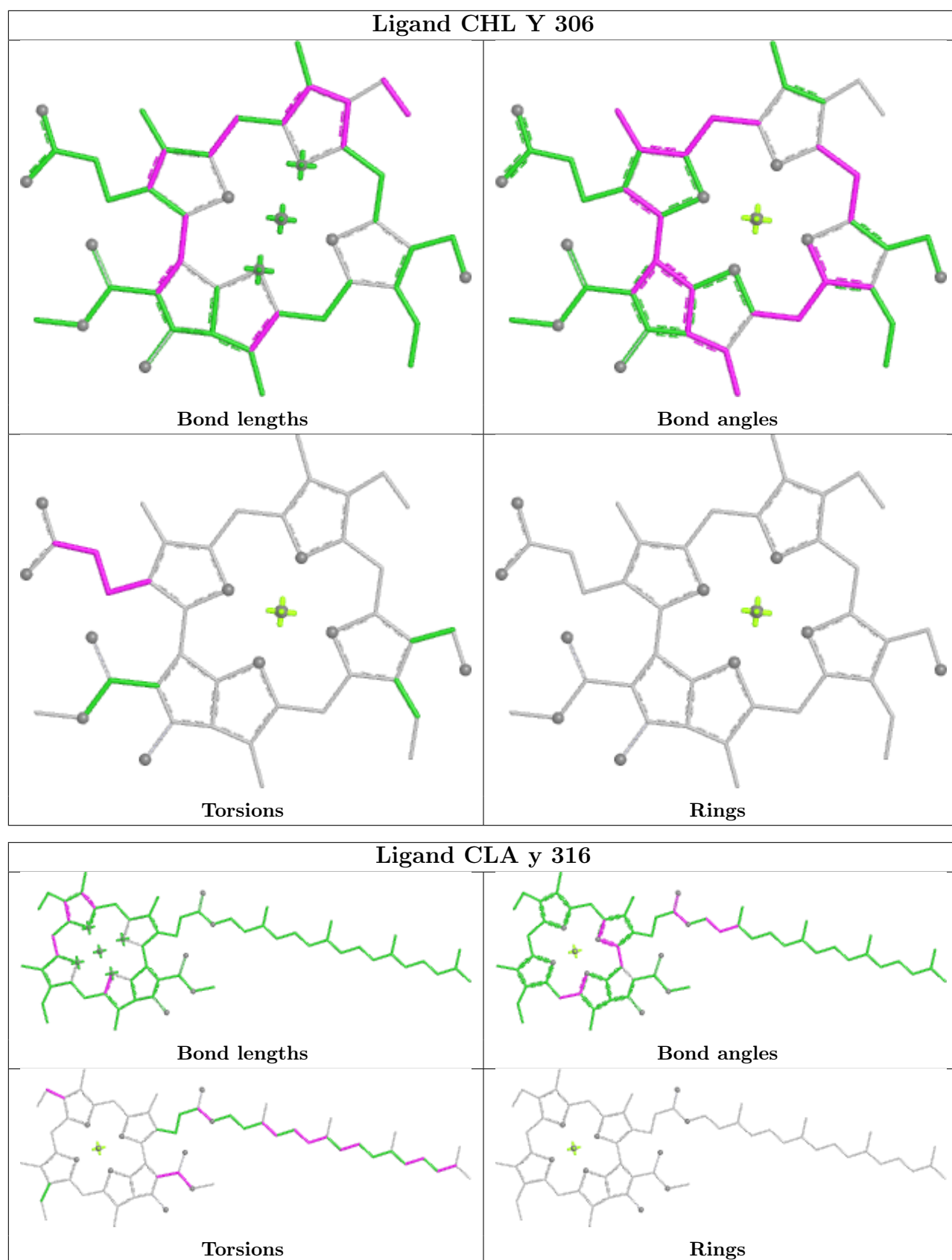
Rings

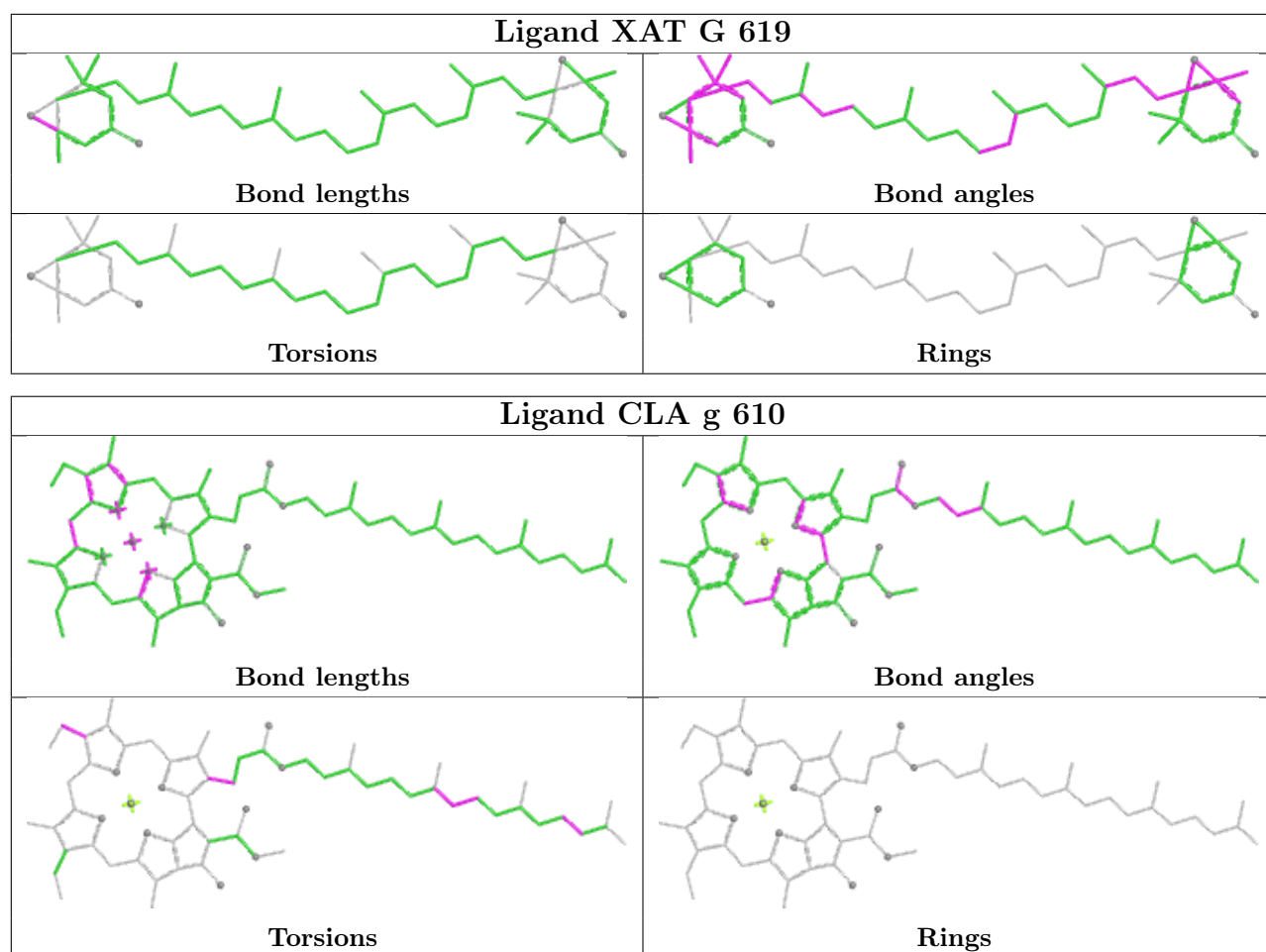


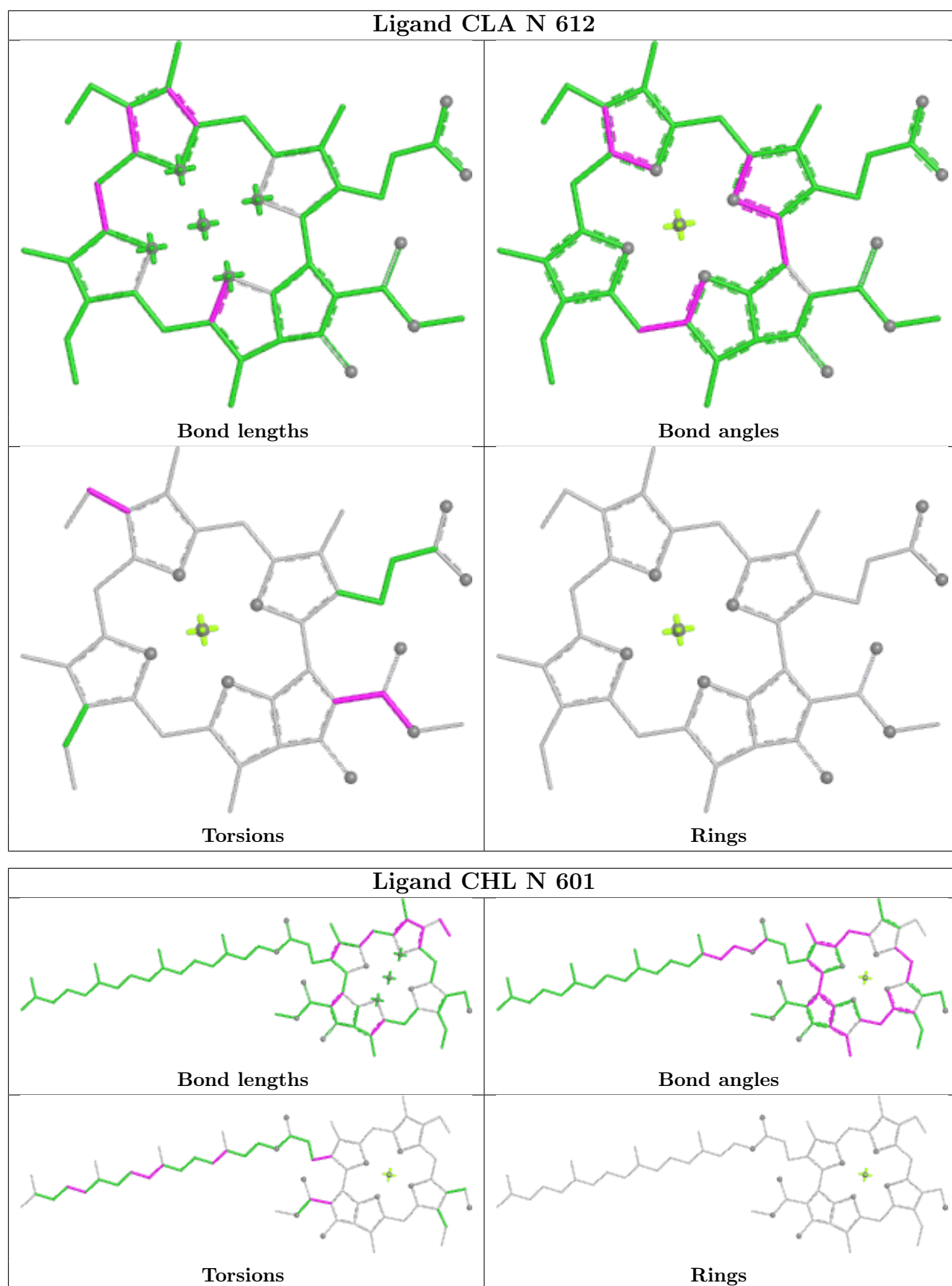


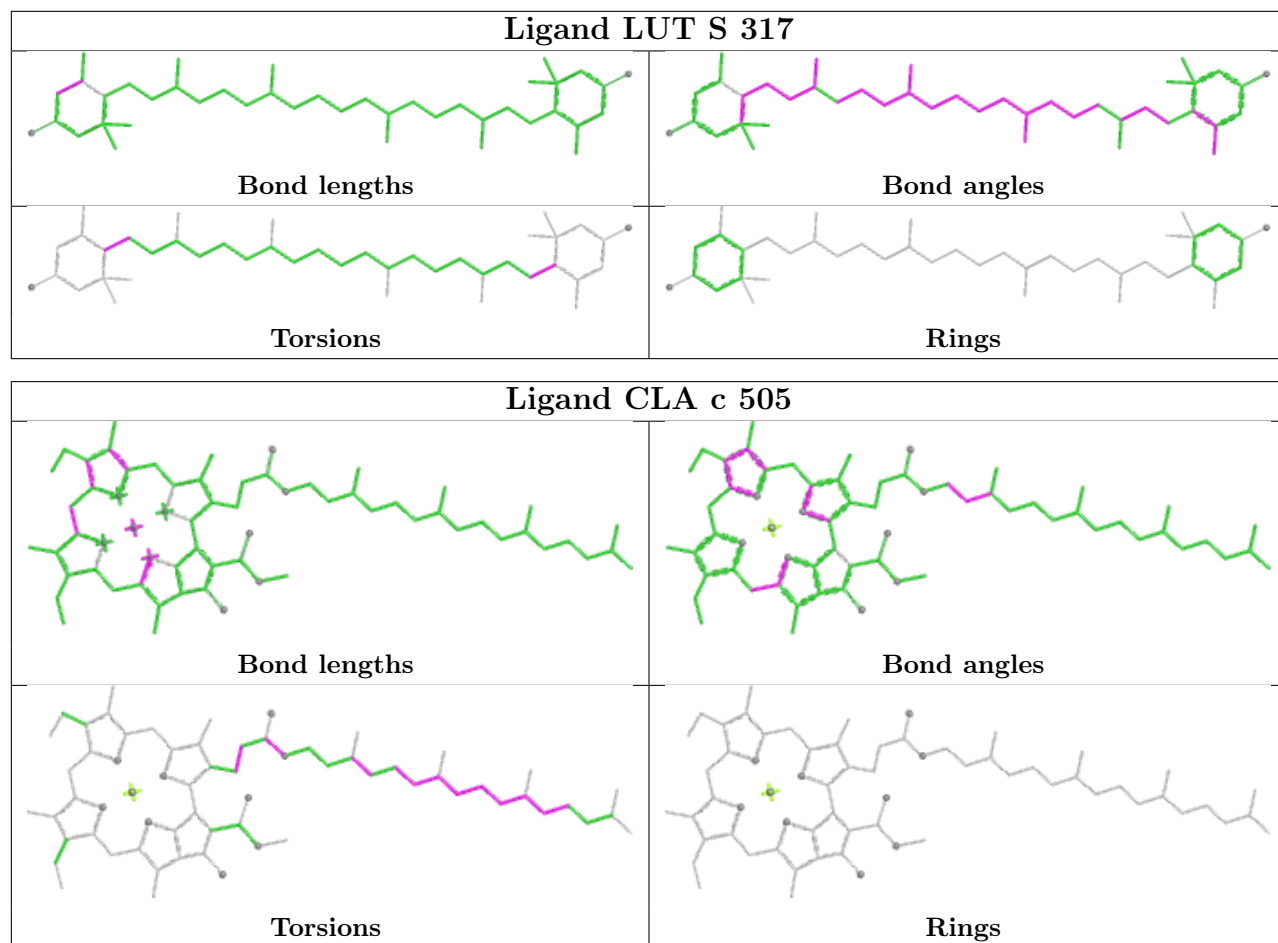




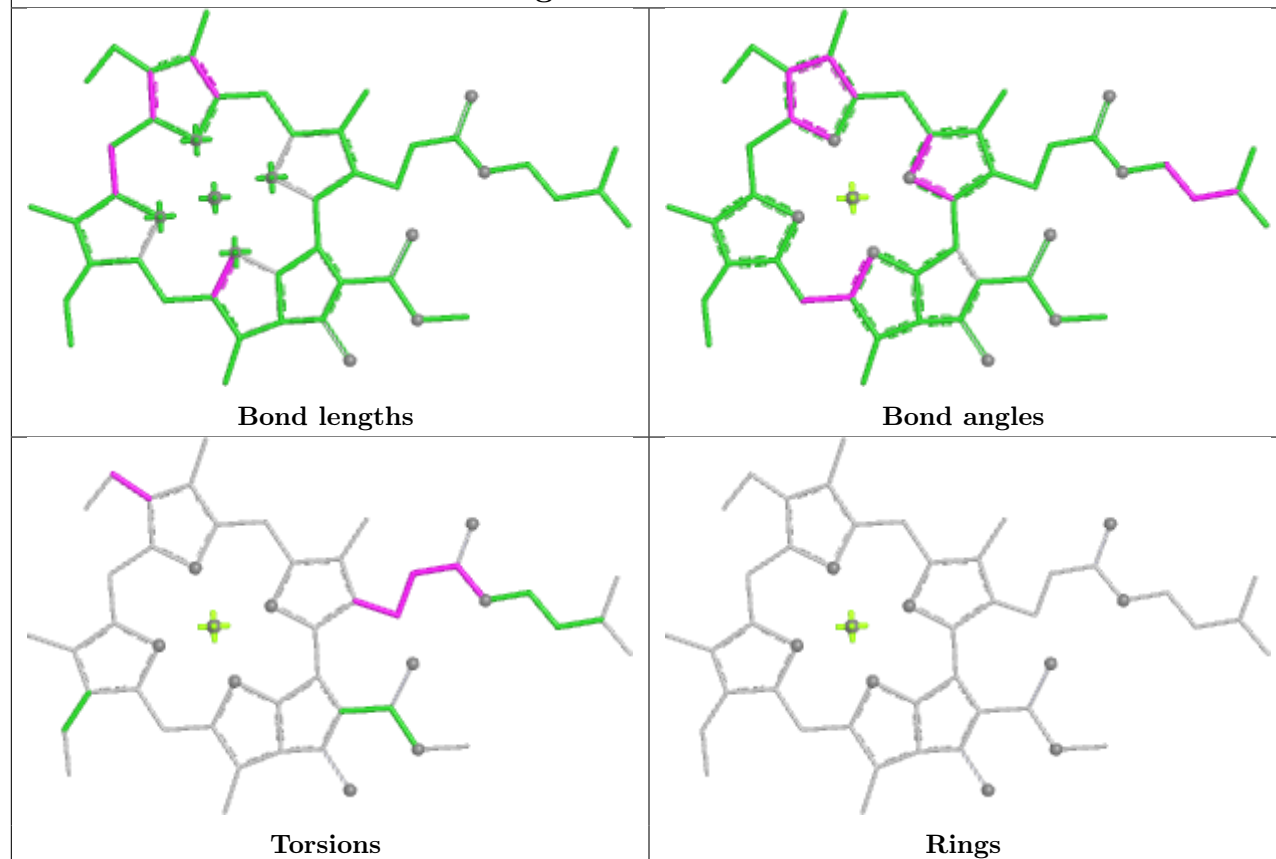




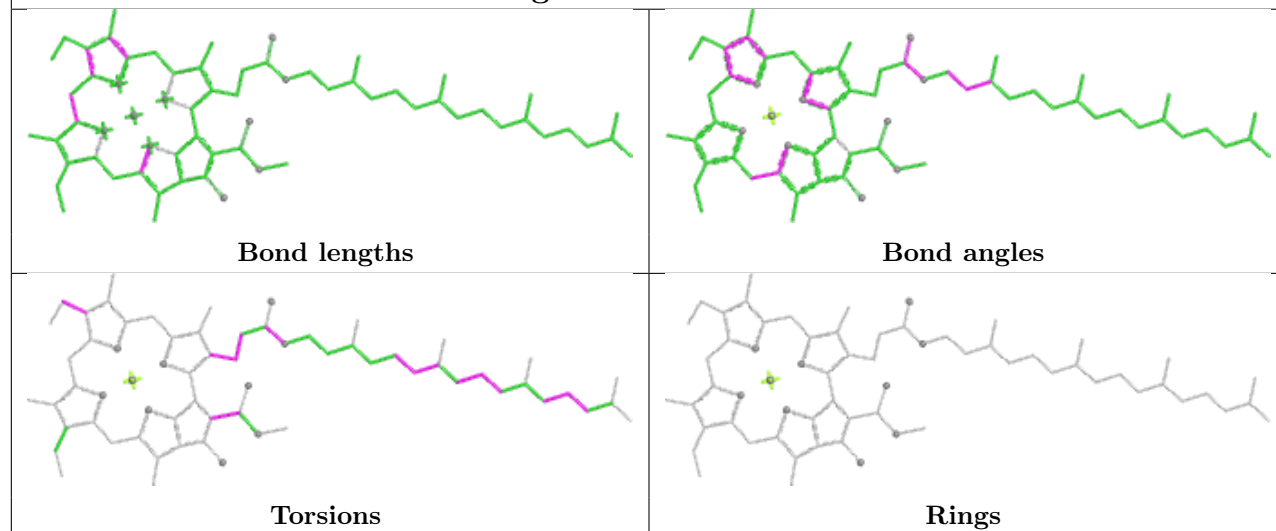


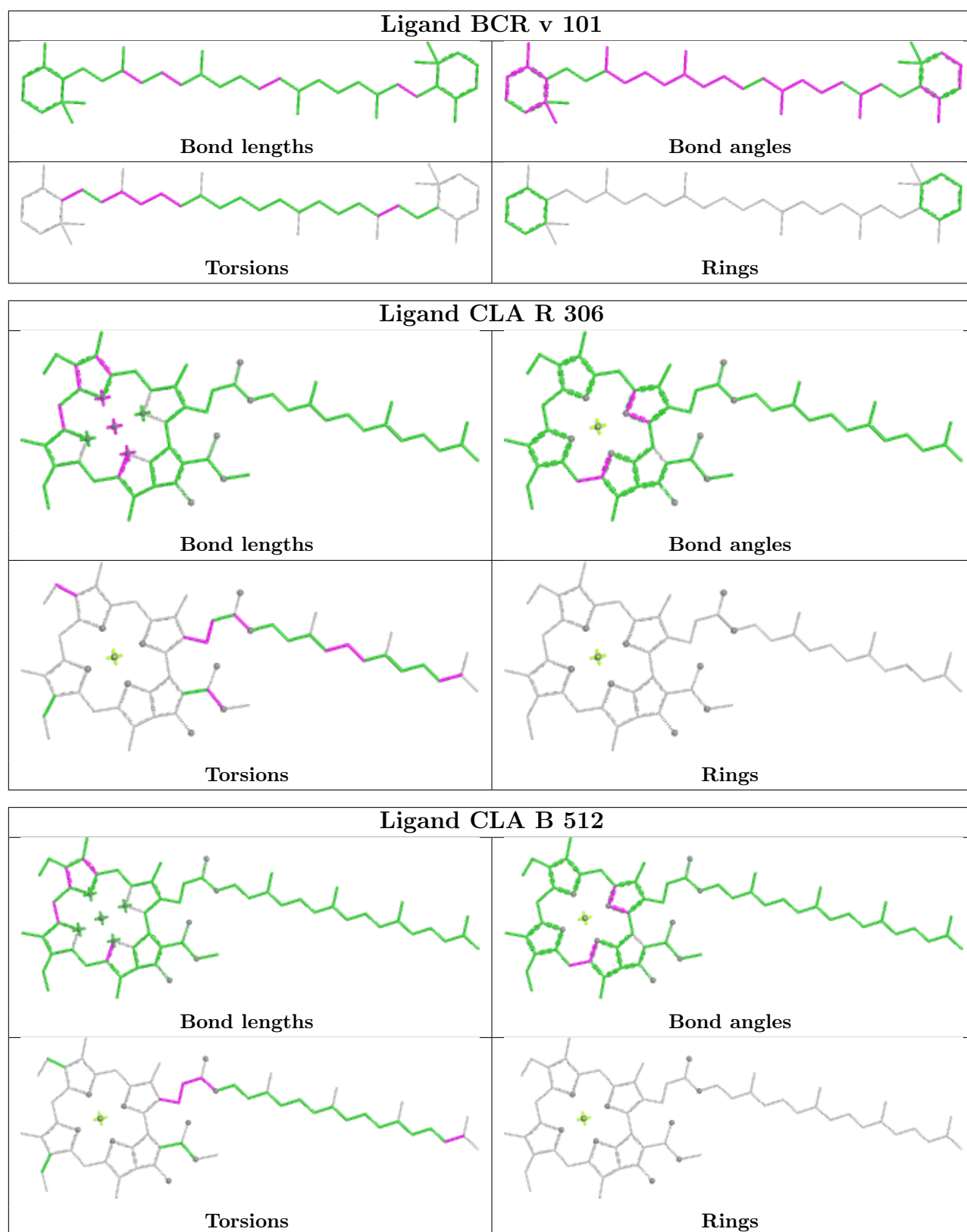


Ligand CLA S 315

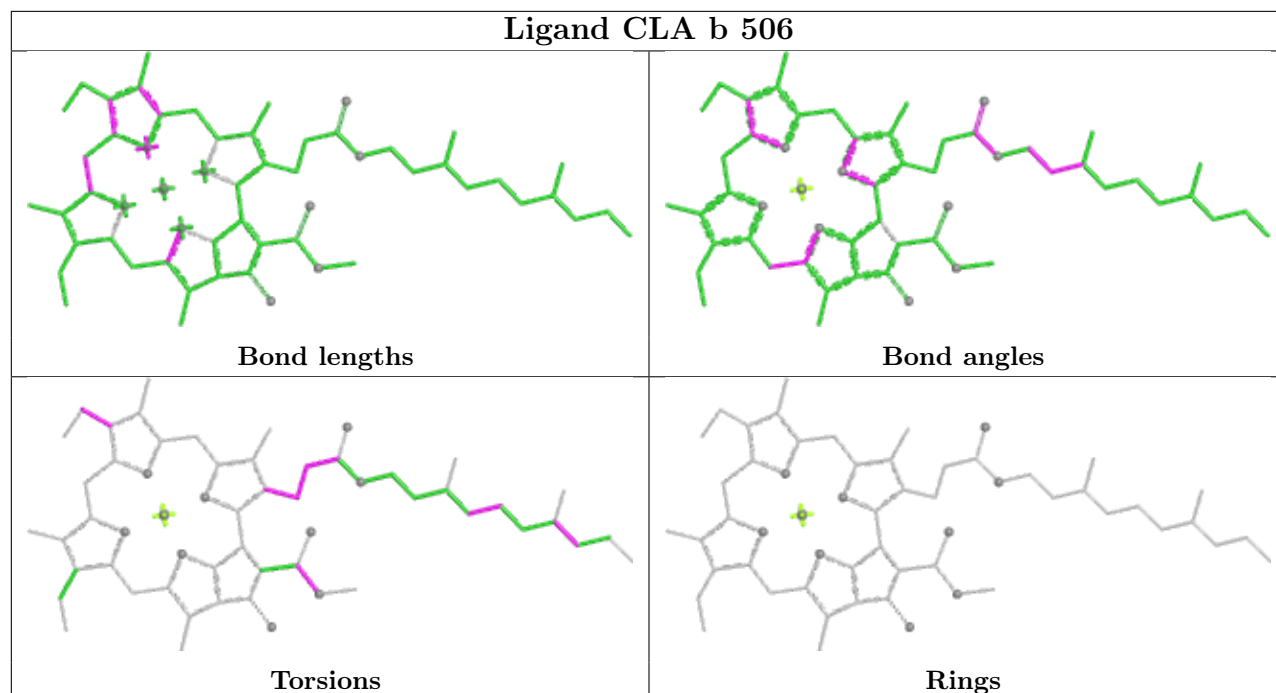


Ligand CLA Y 303

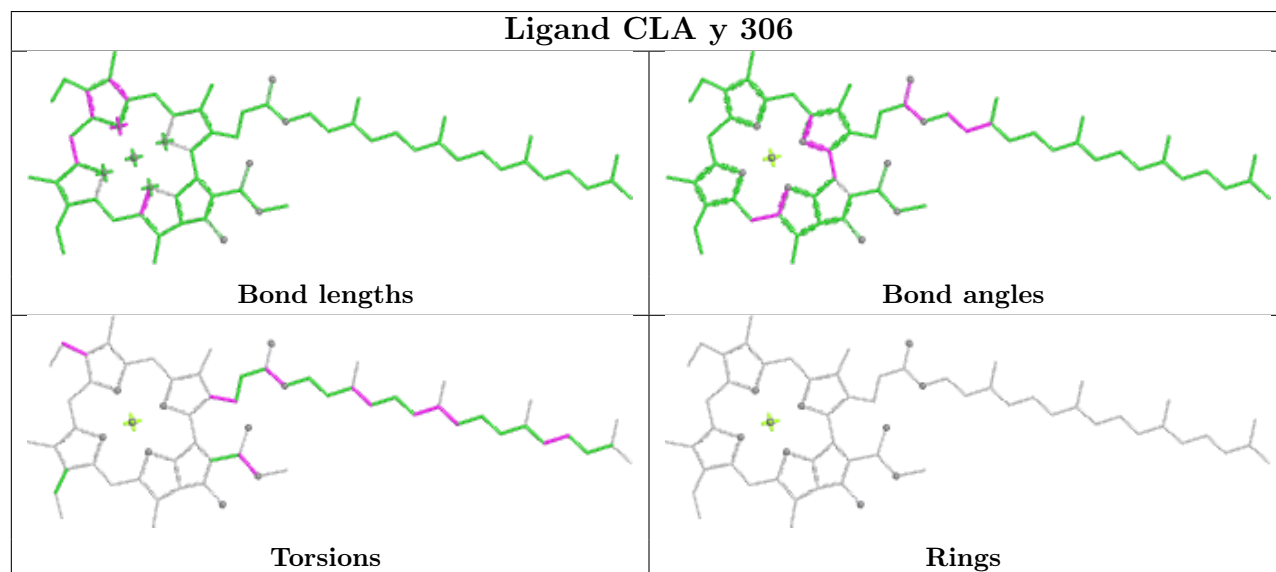


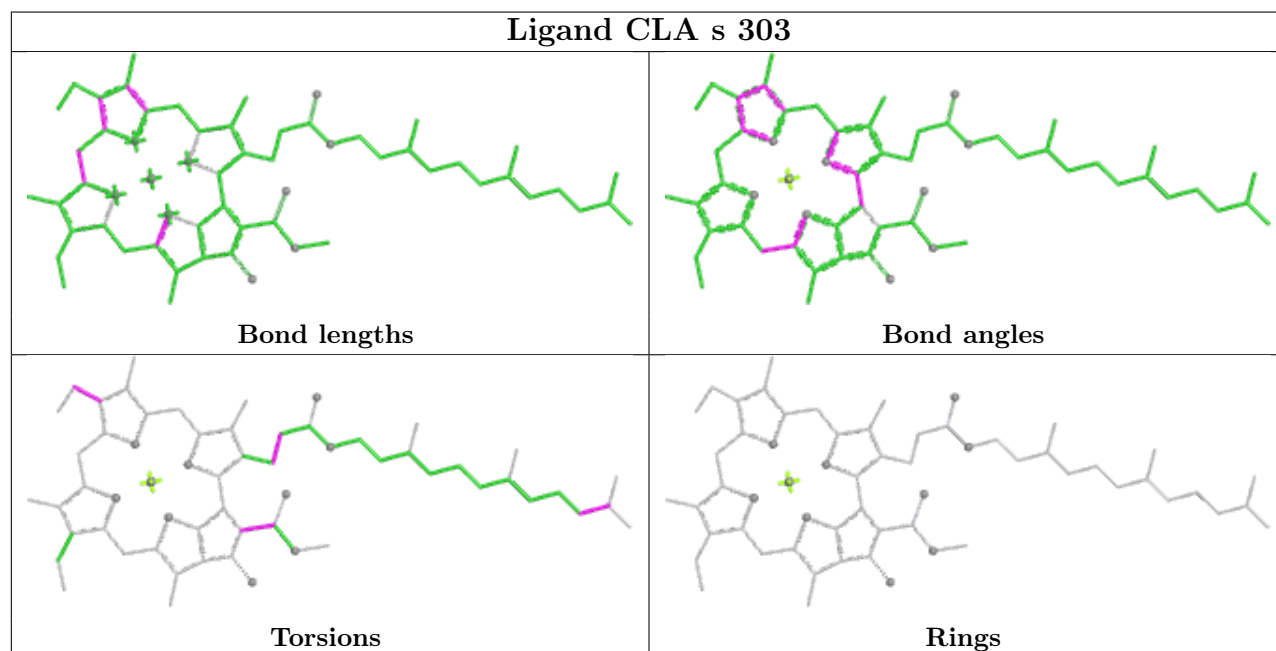
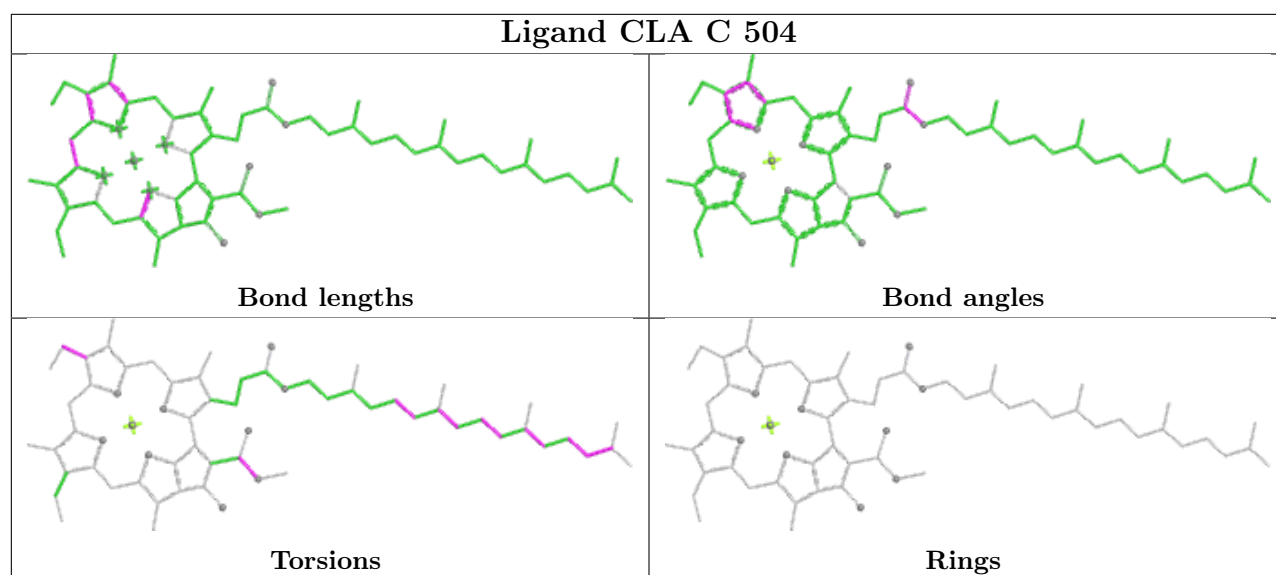


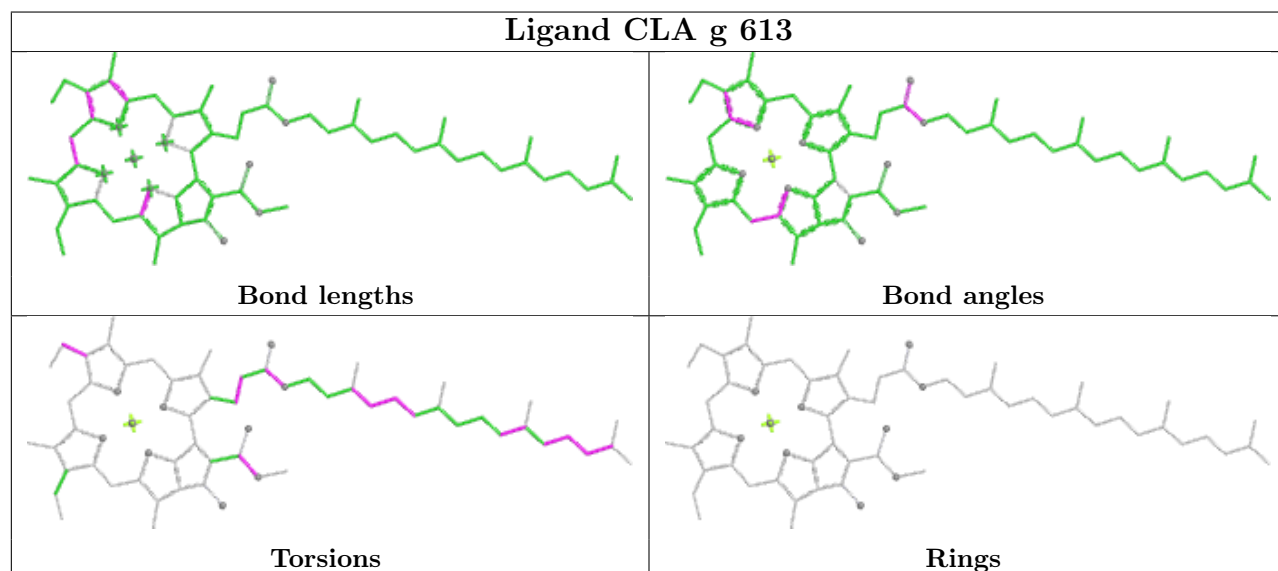
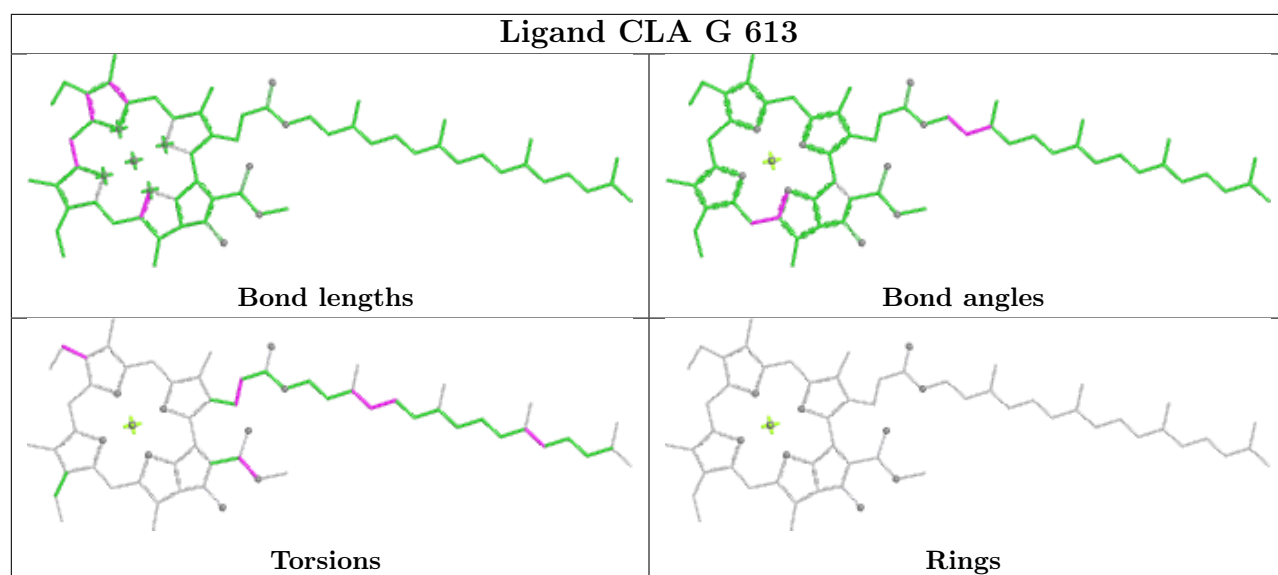
Ligand CLA b 506

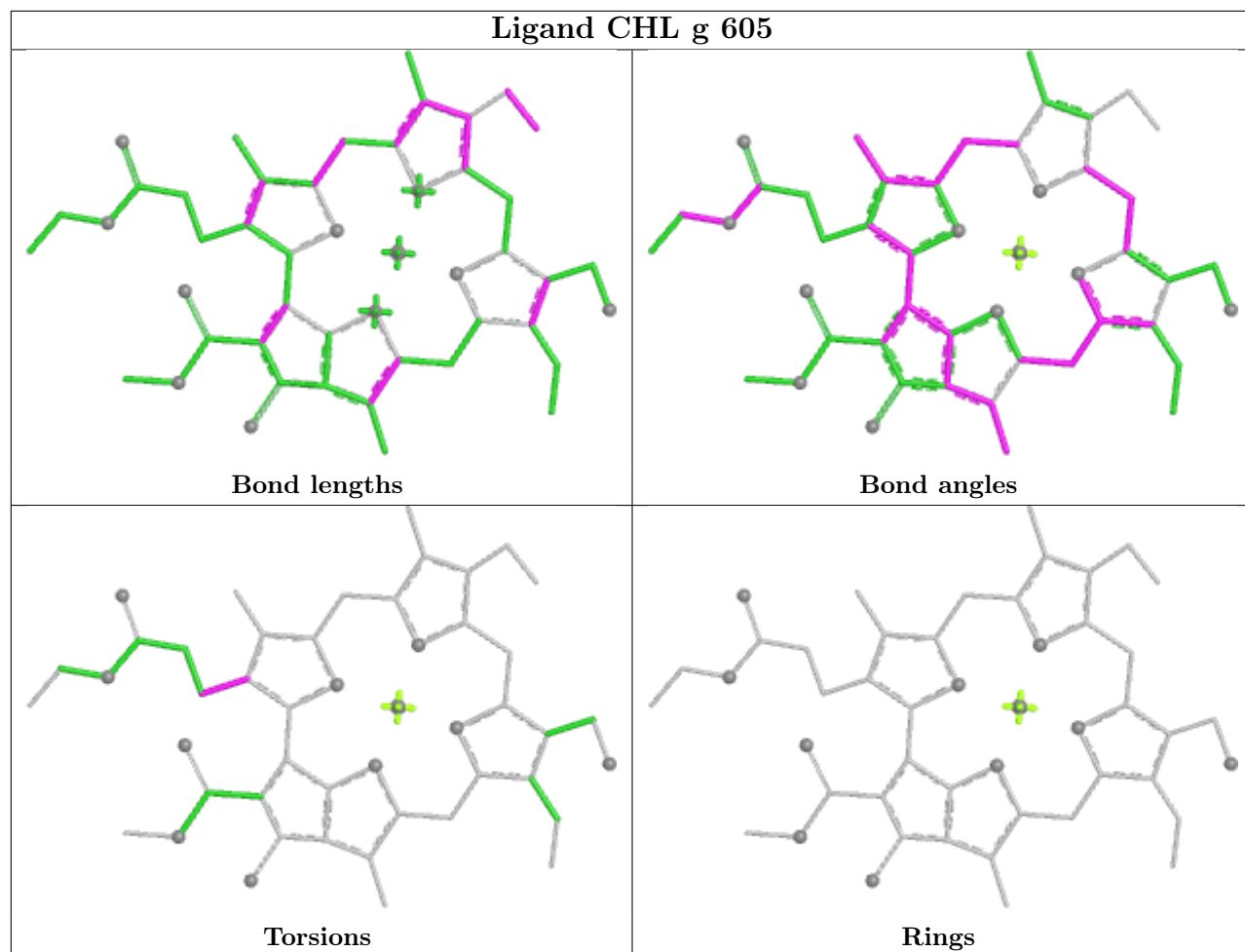


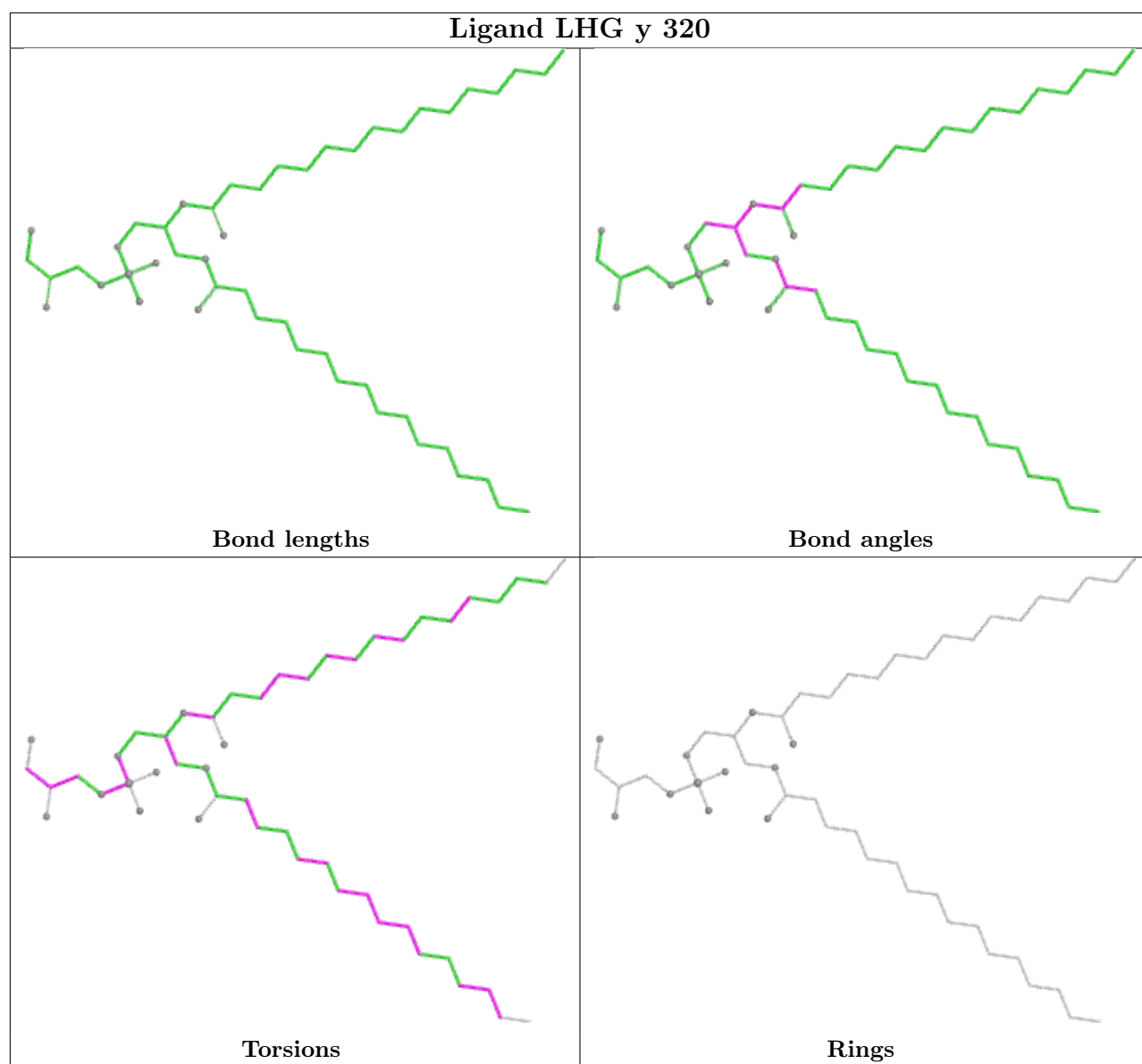
Ligand CLA y 306



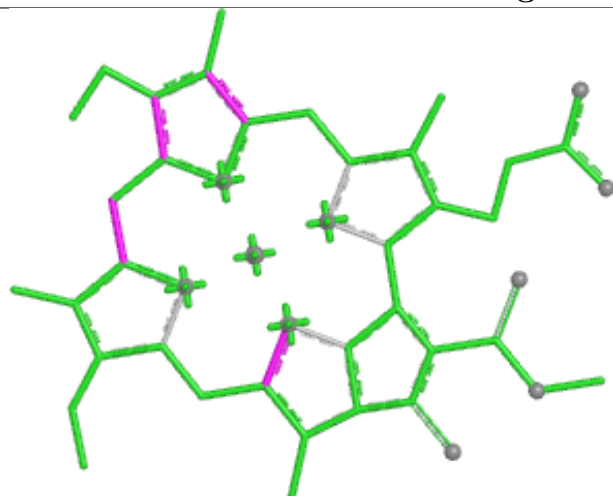




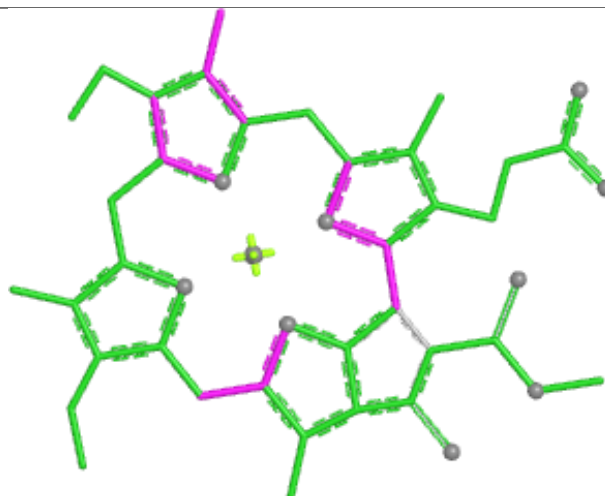




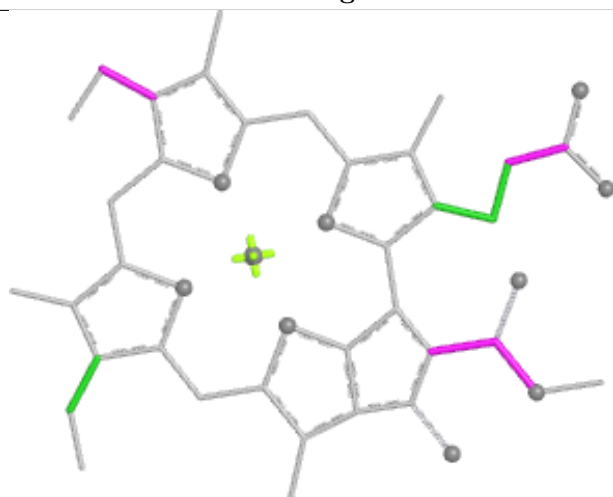
Ligand CLA n 611



Bond lengths



Bond angles

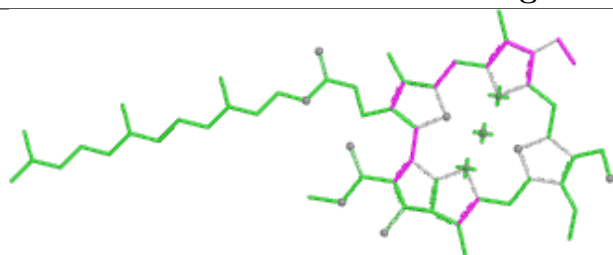


Torsions

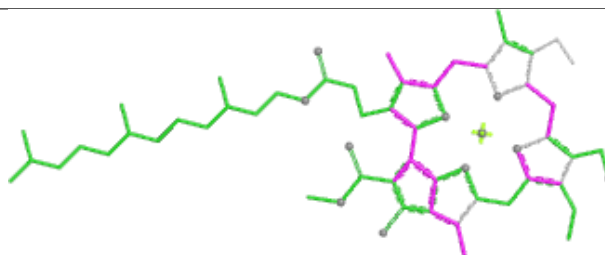


Rings

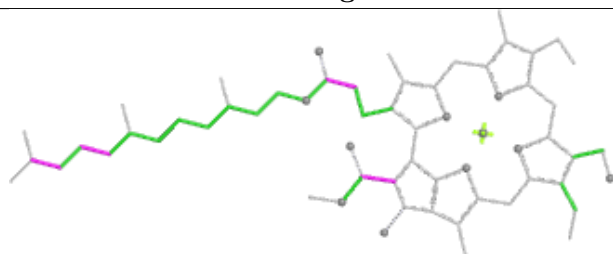
Ligand CHL s 309



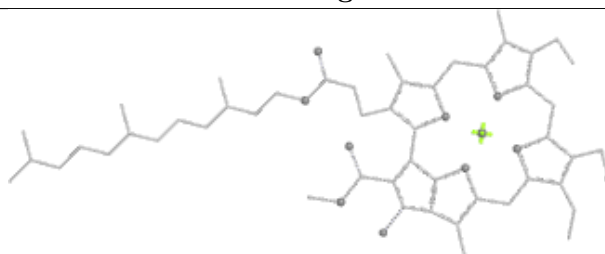
Bond lengths



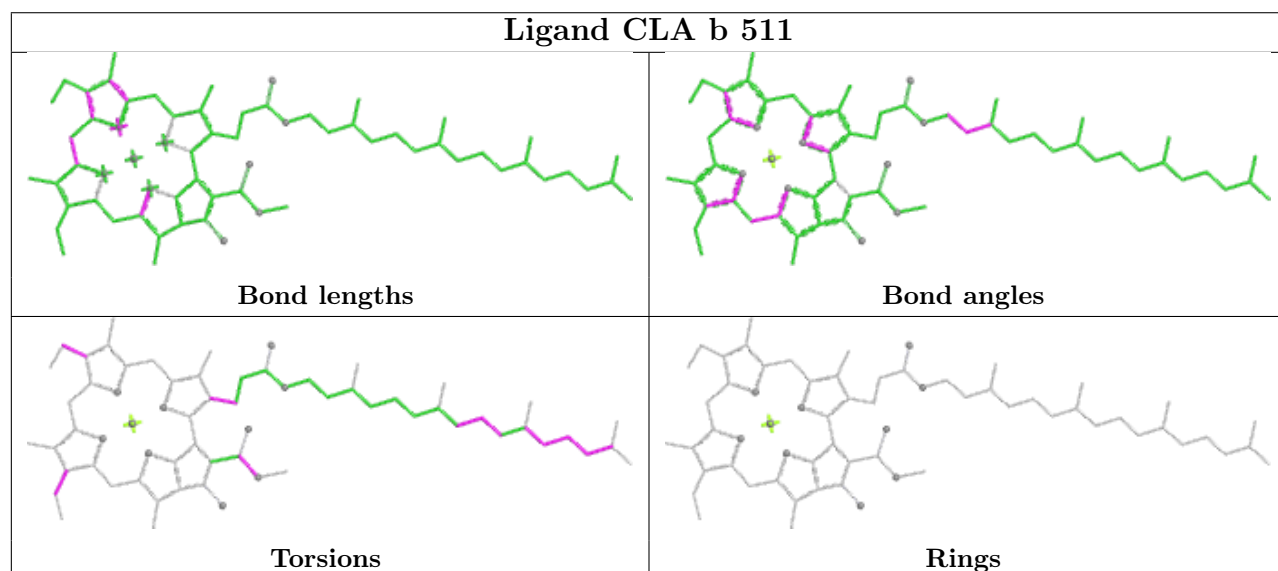
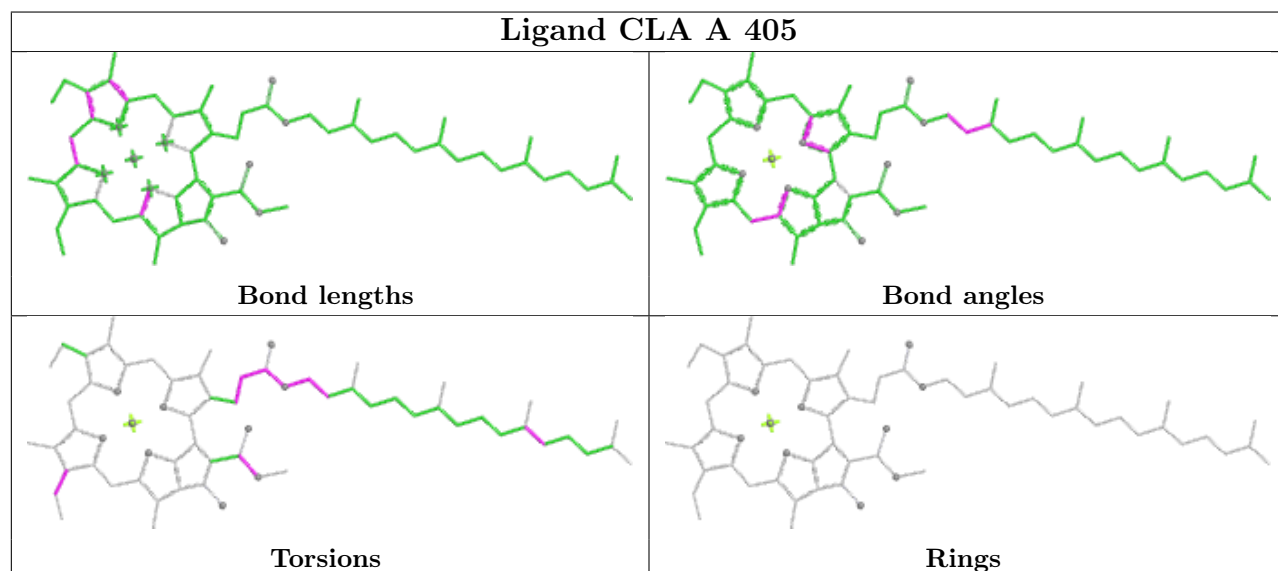
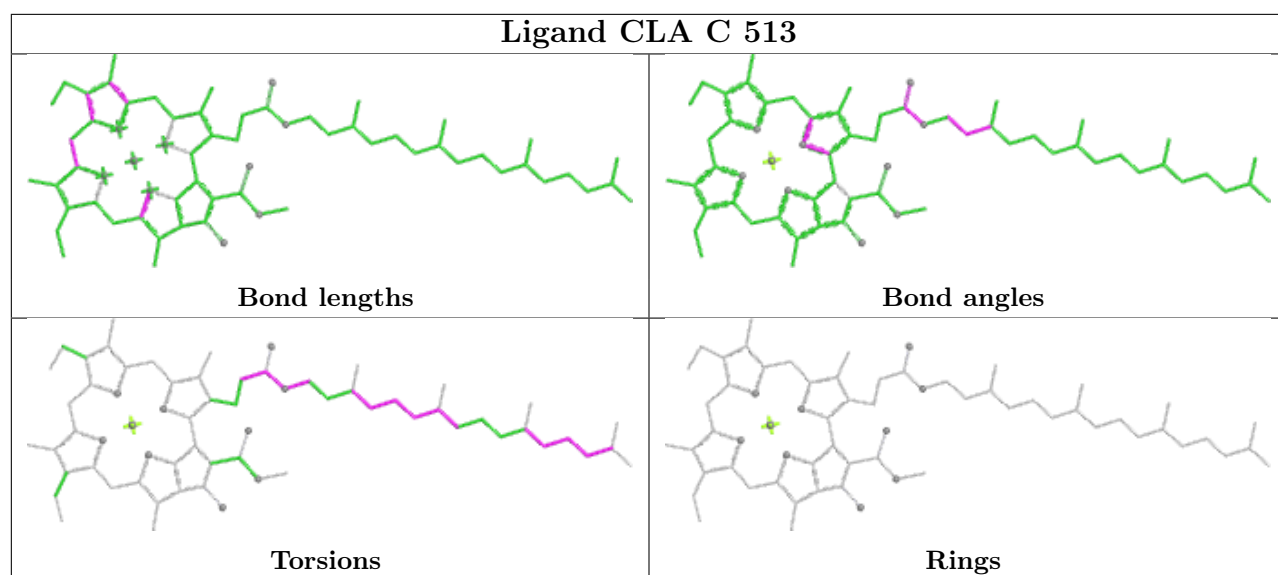
Bond angles

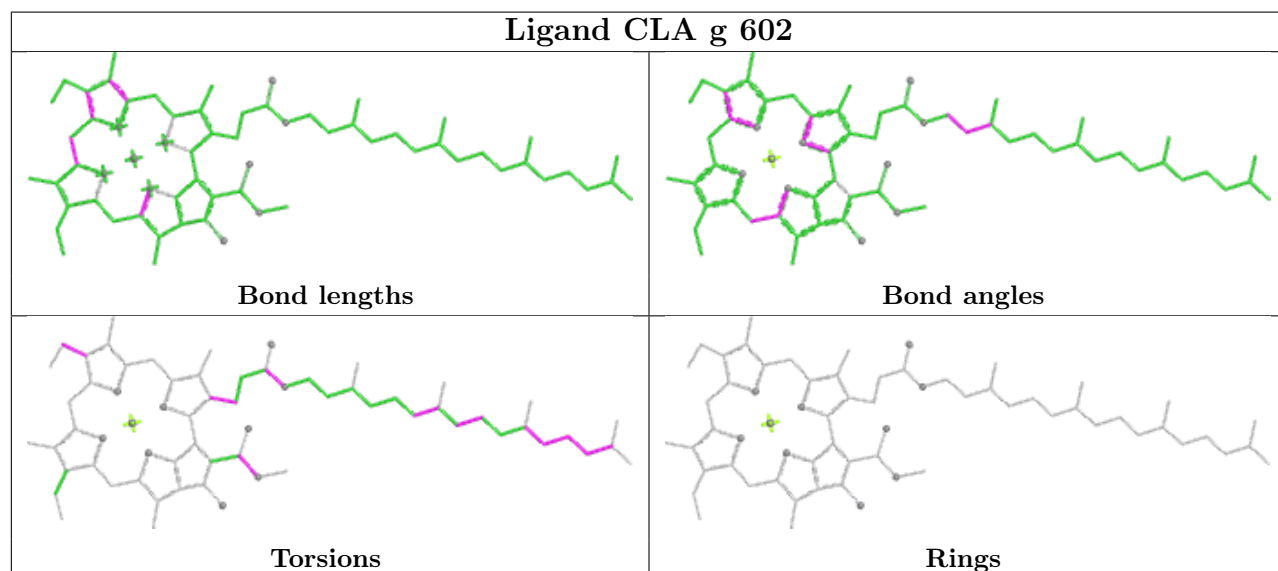
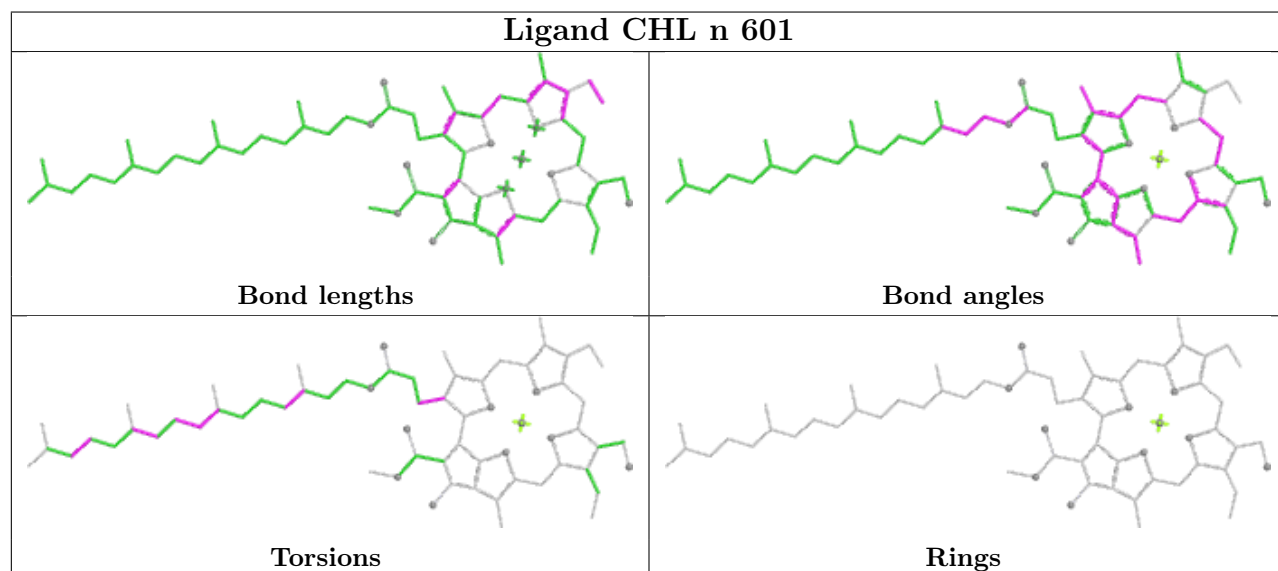
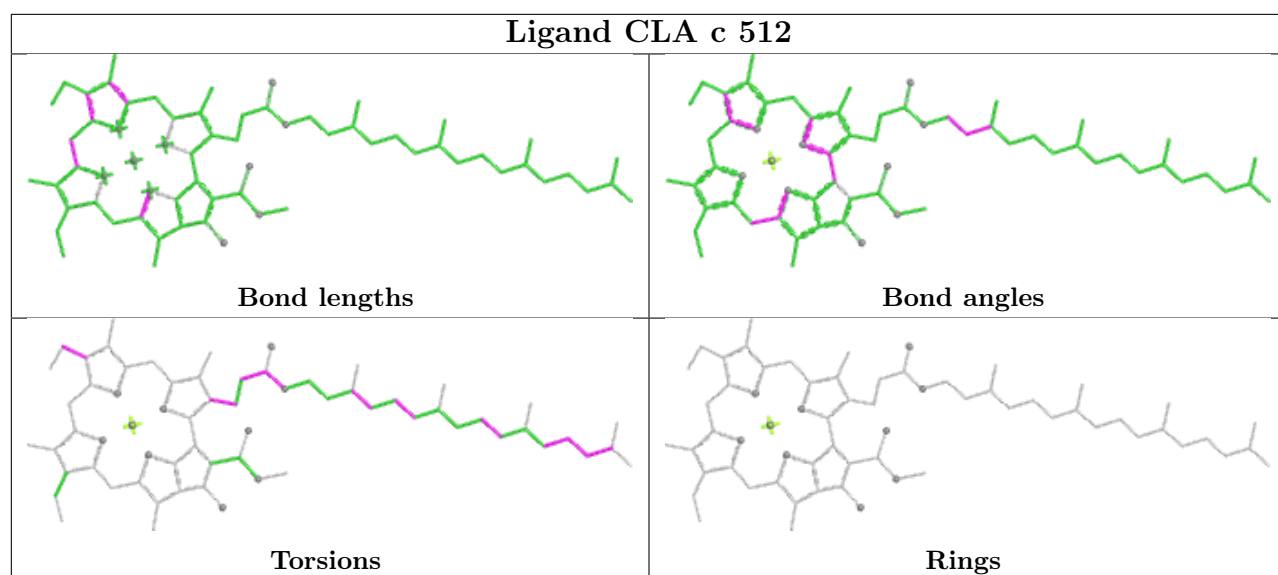


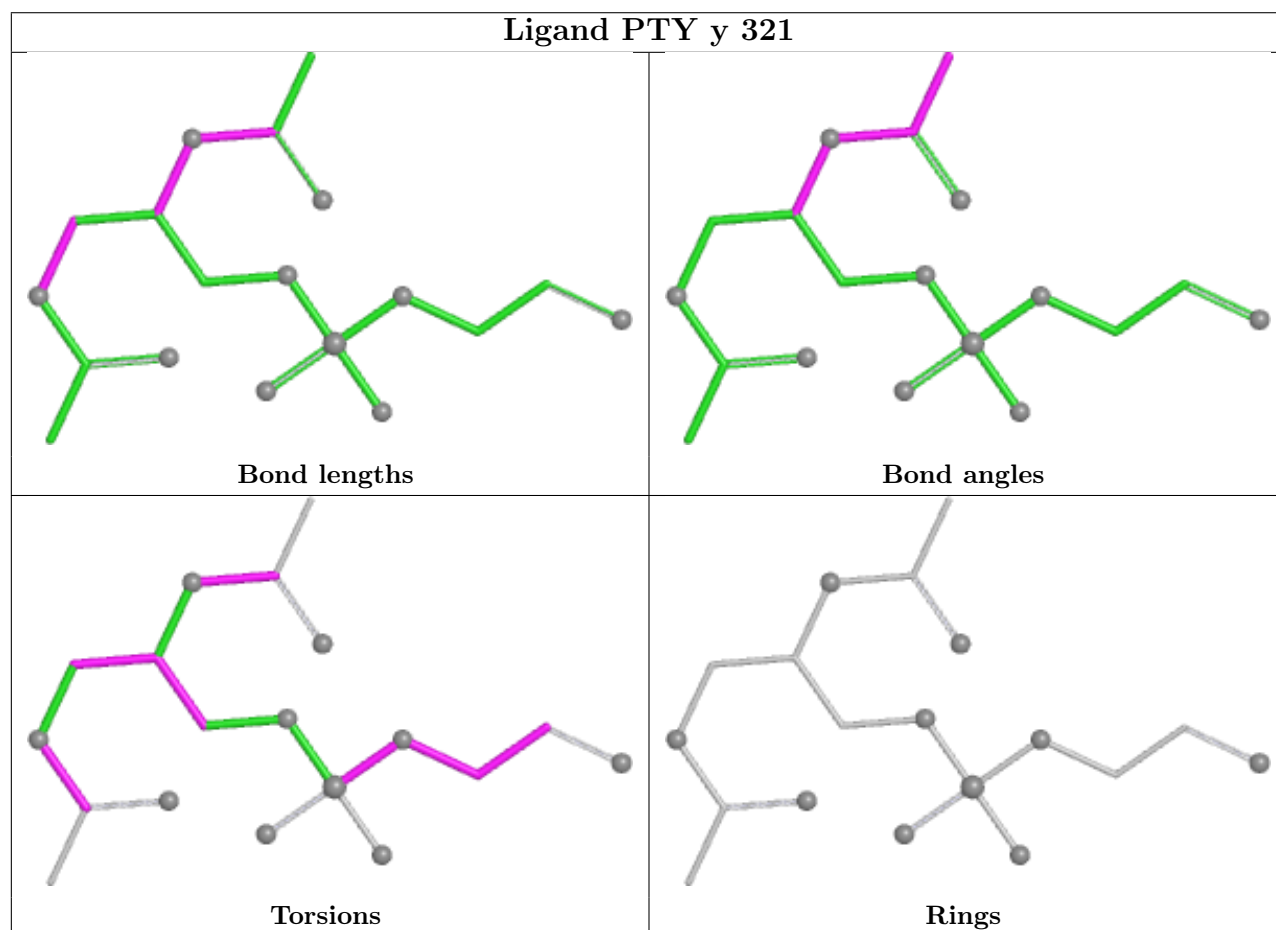
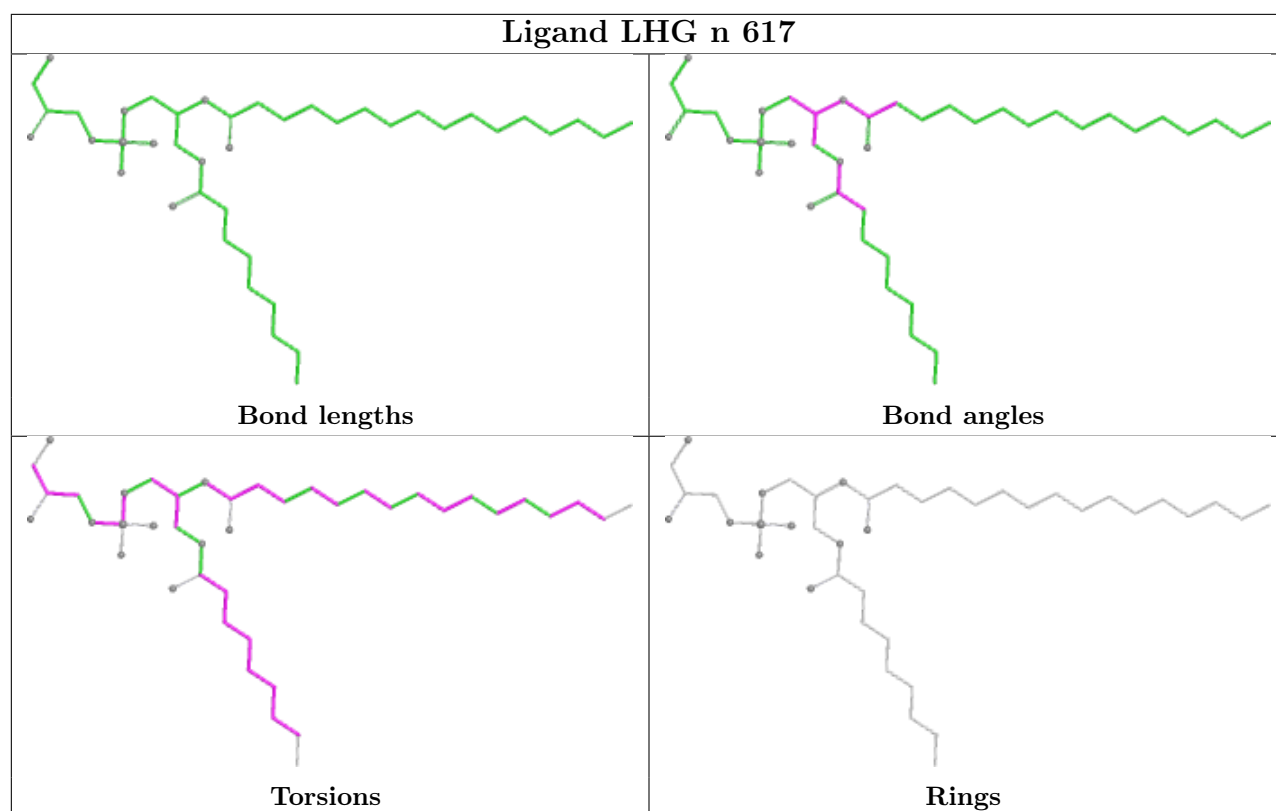
Torsions



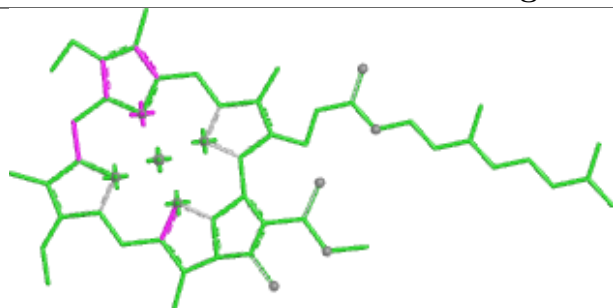
Rings



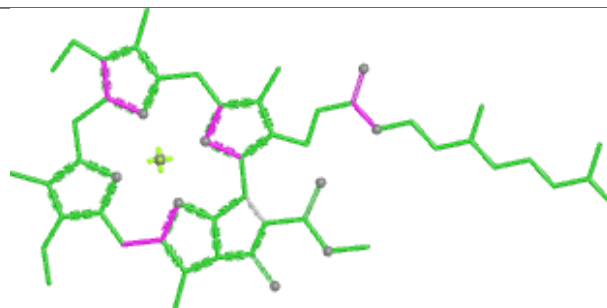




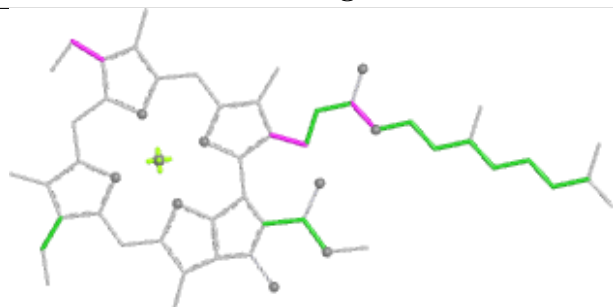
Ligand CLA s 315



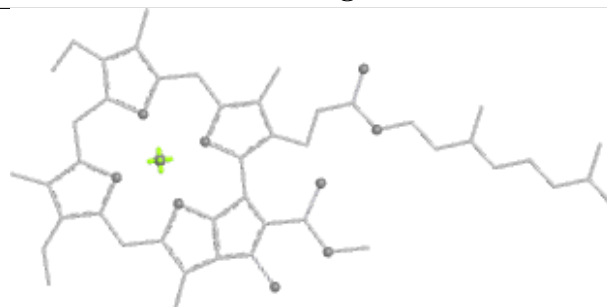
Bond lengths



Bond angles

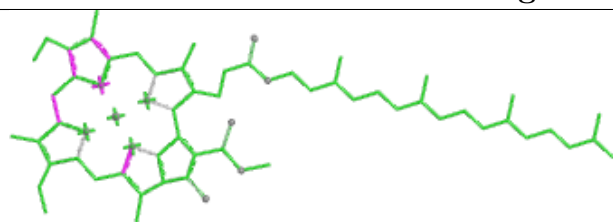


Torsions

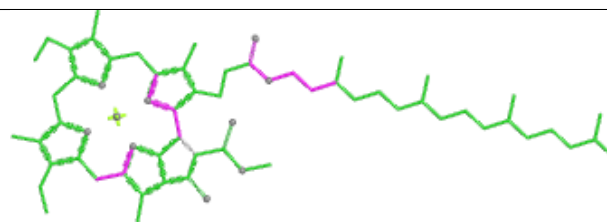


Rings

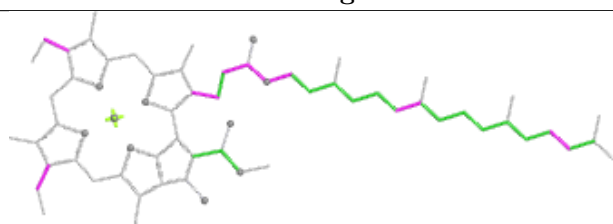
Ligand CLA a 405



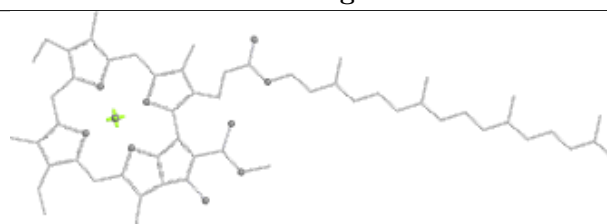
Bond lengths



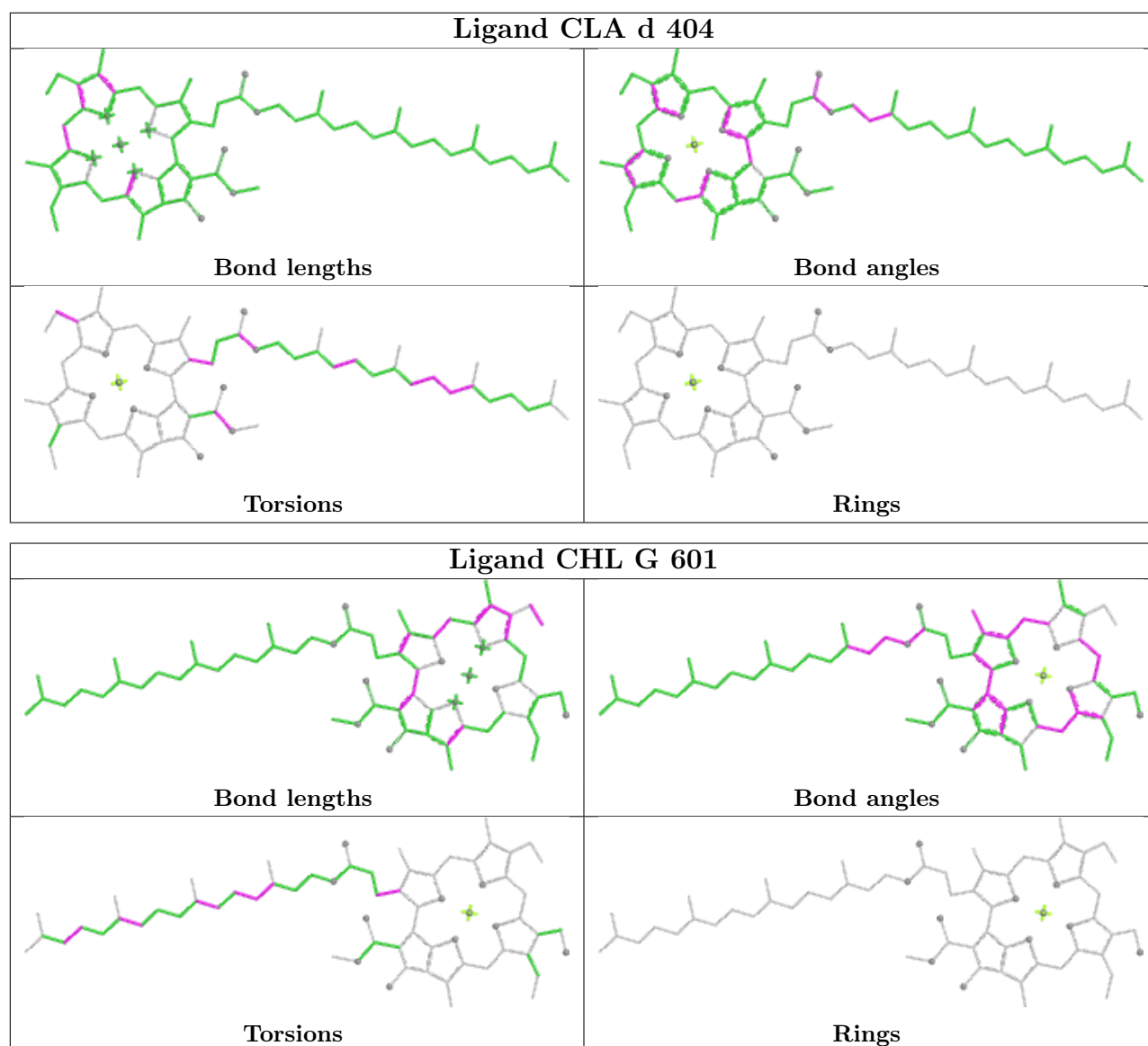
Bond angles

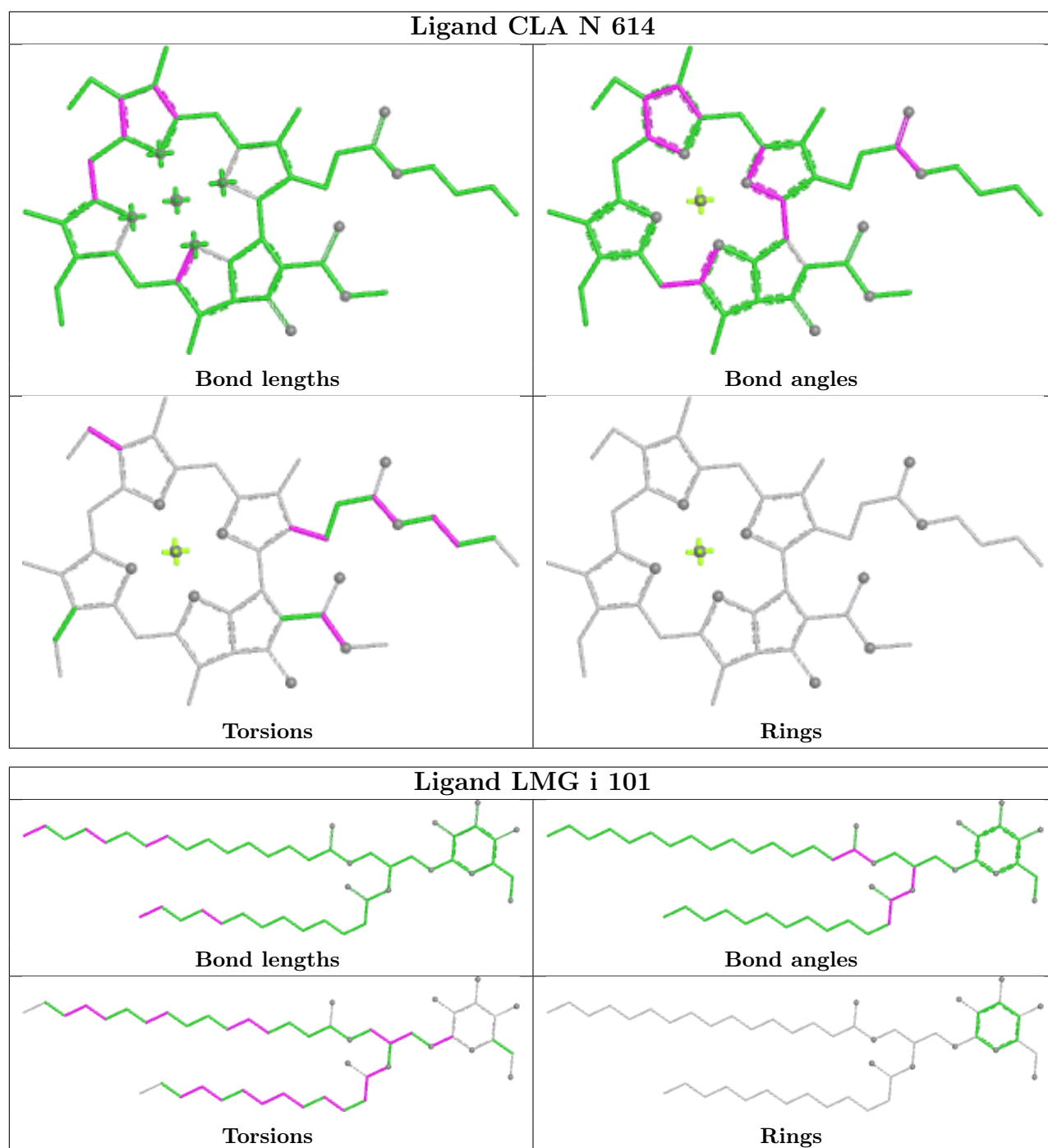


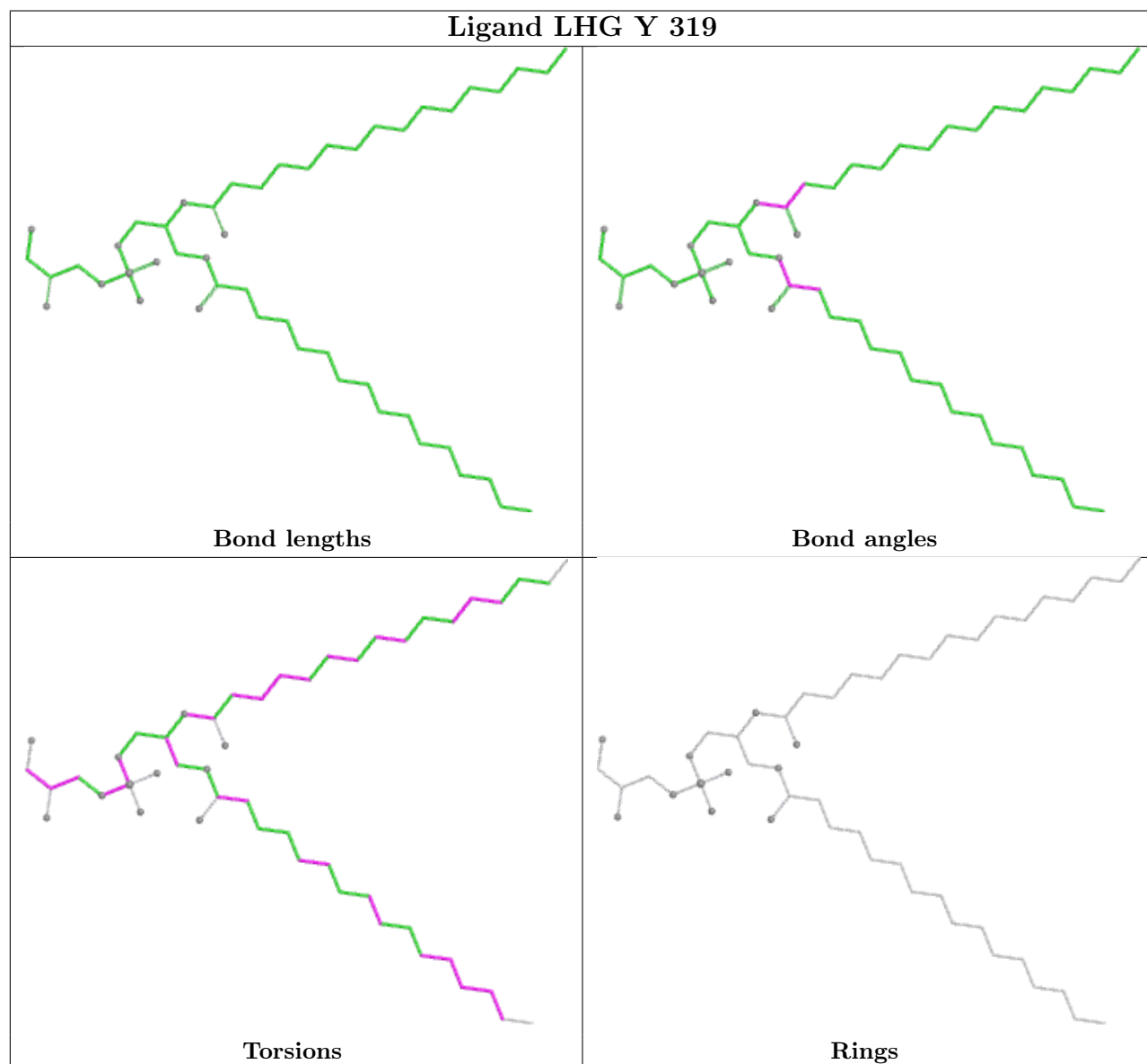
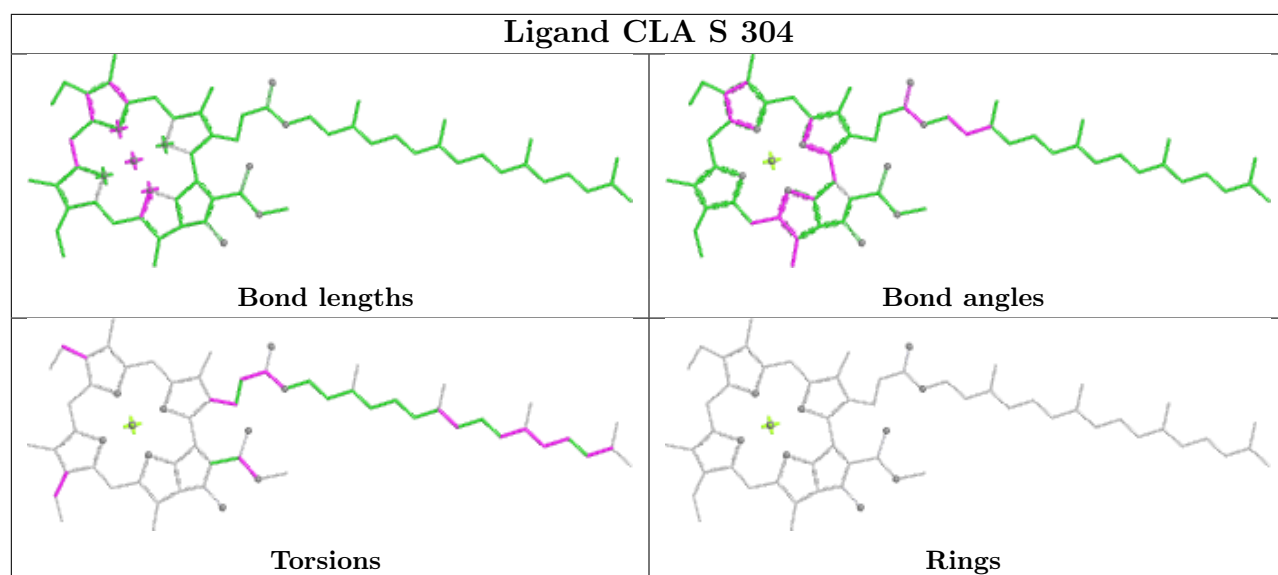
Torsions

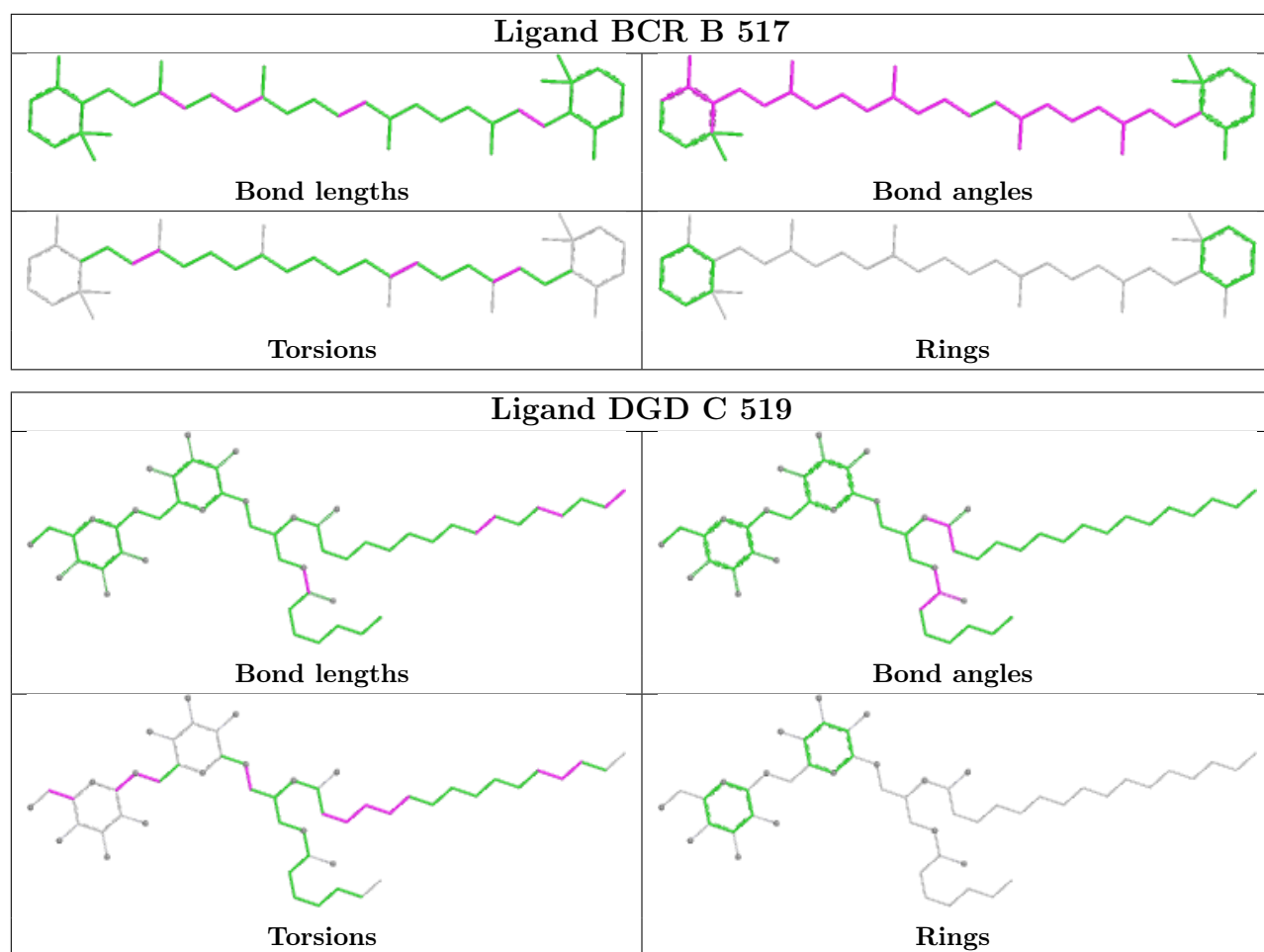


Rings

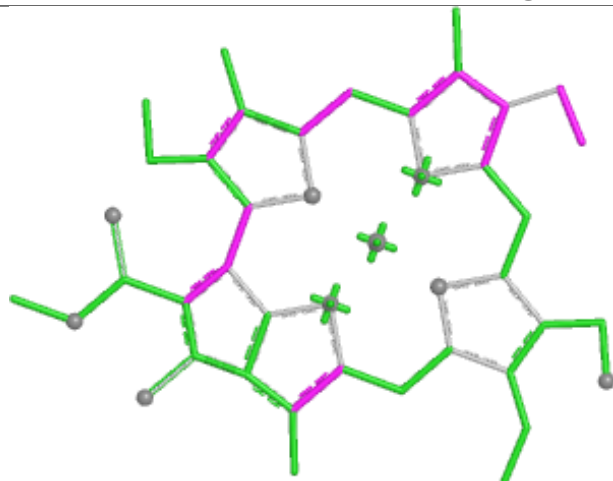




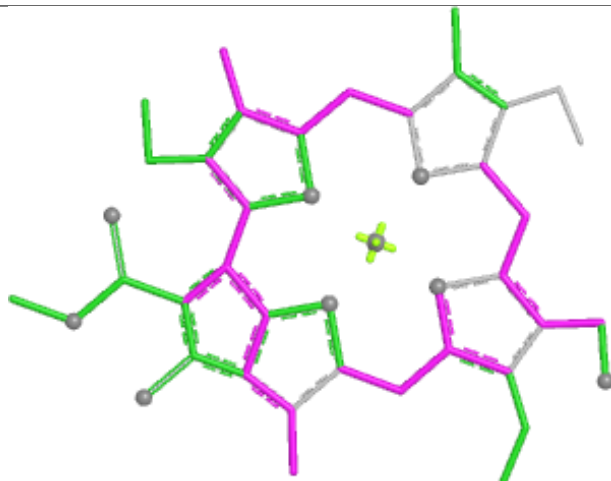




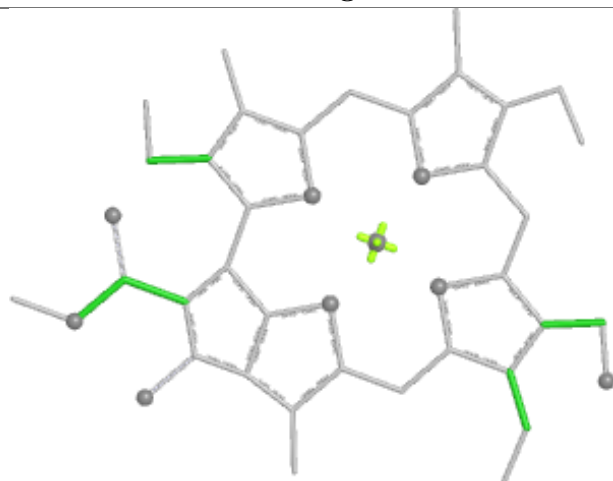
Ligand CHL s 308



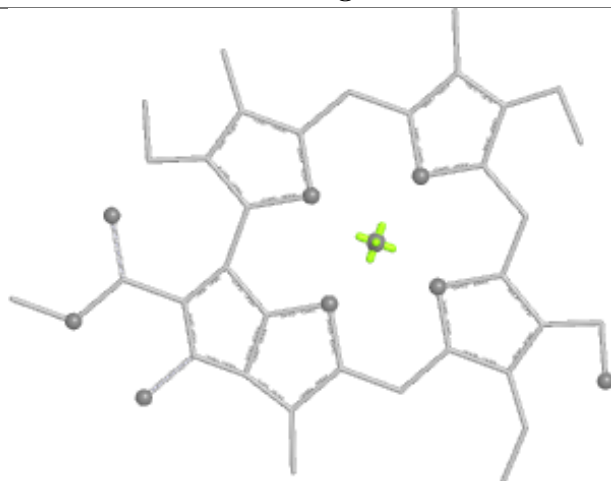
Bond lengths



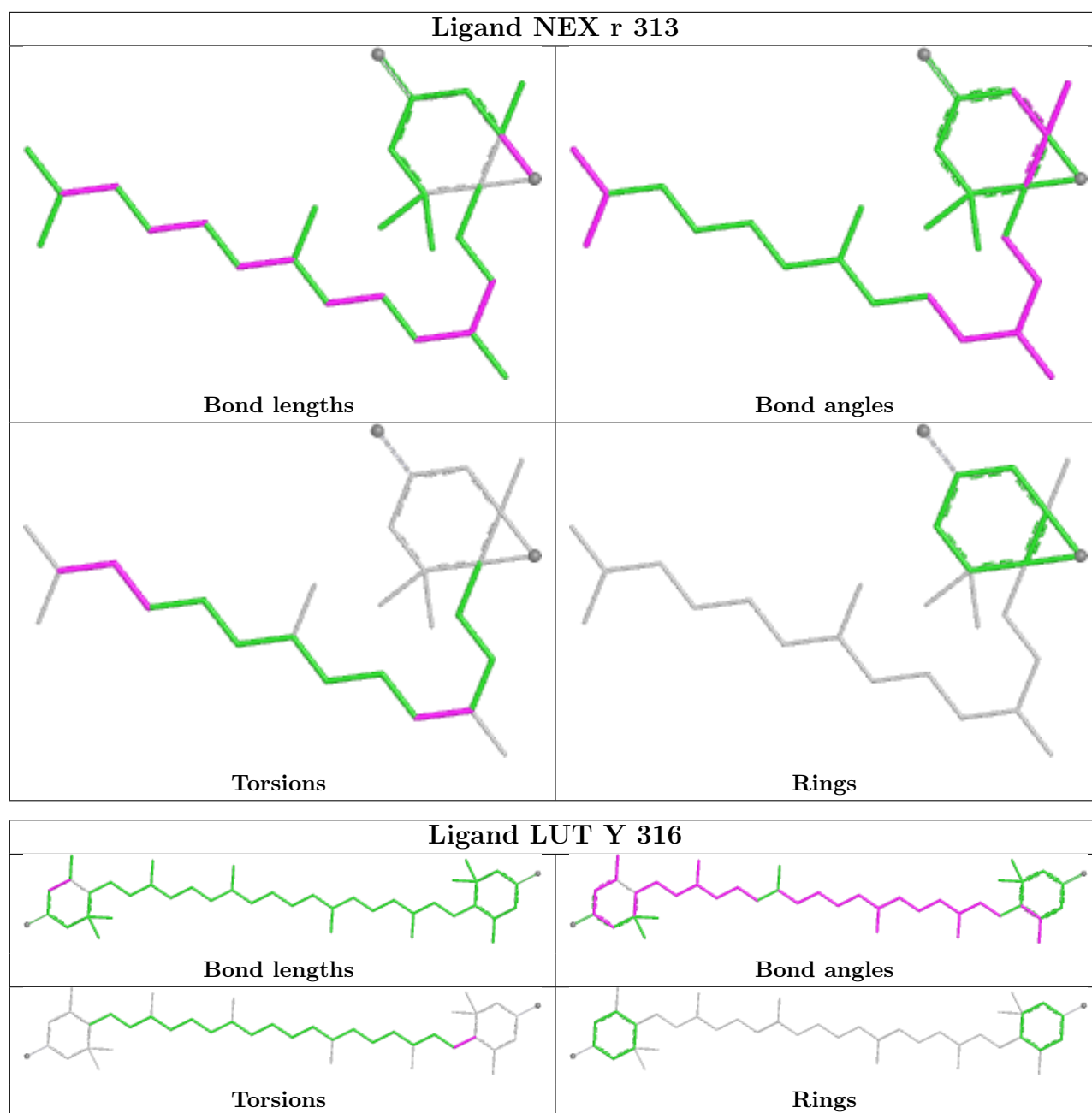
Bond angles

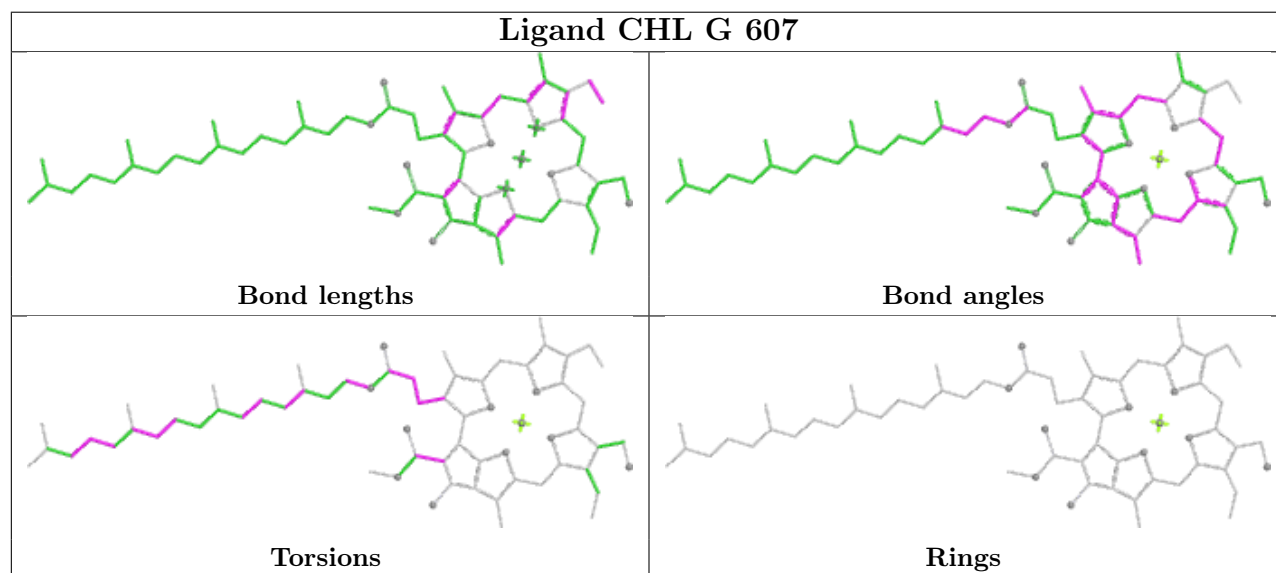
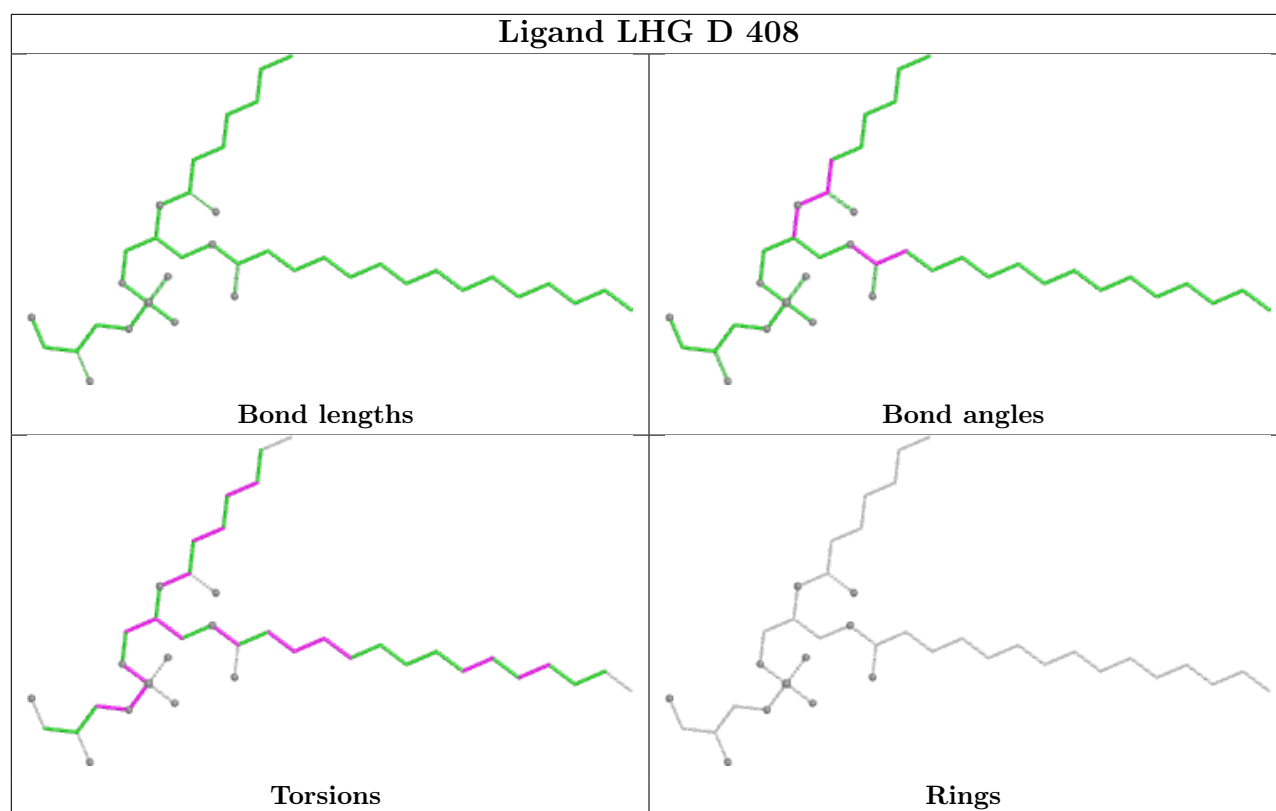


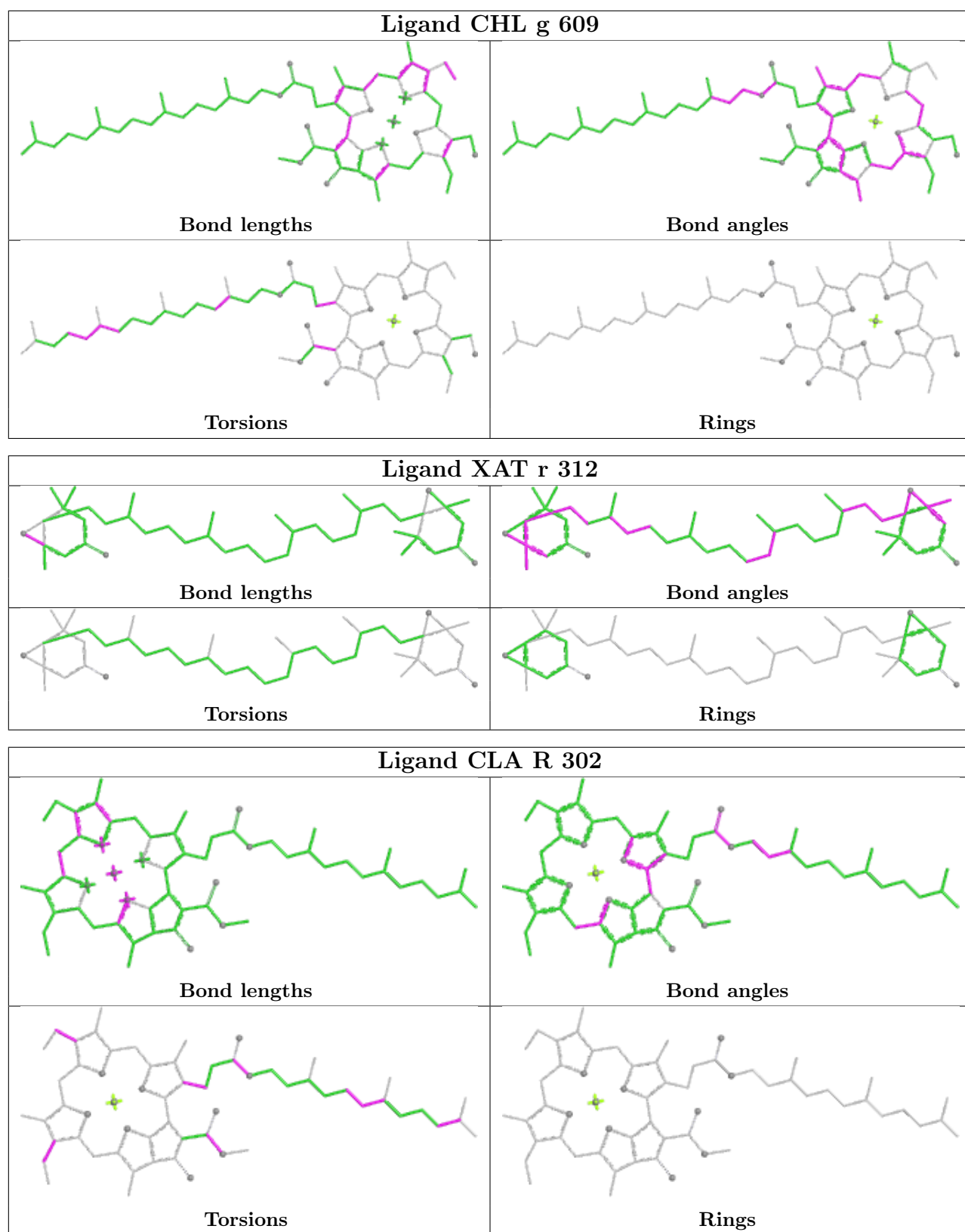
Torsions



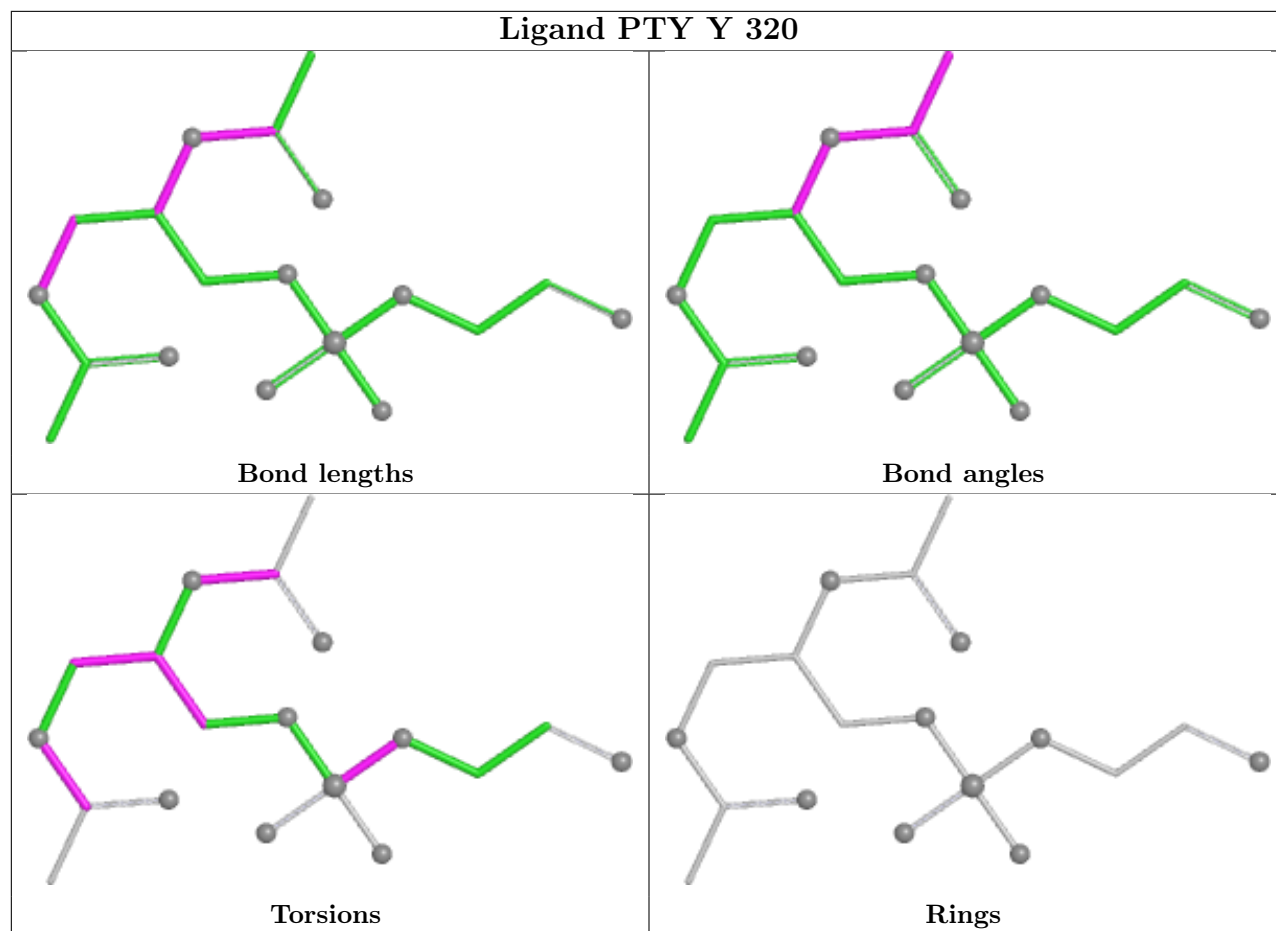
Rings



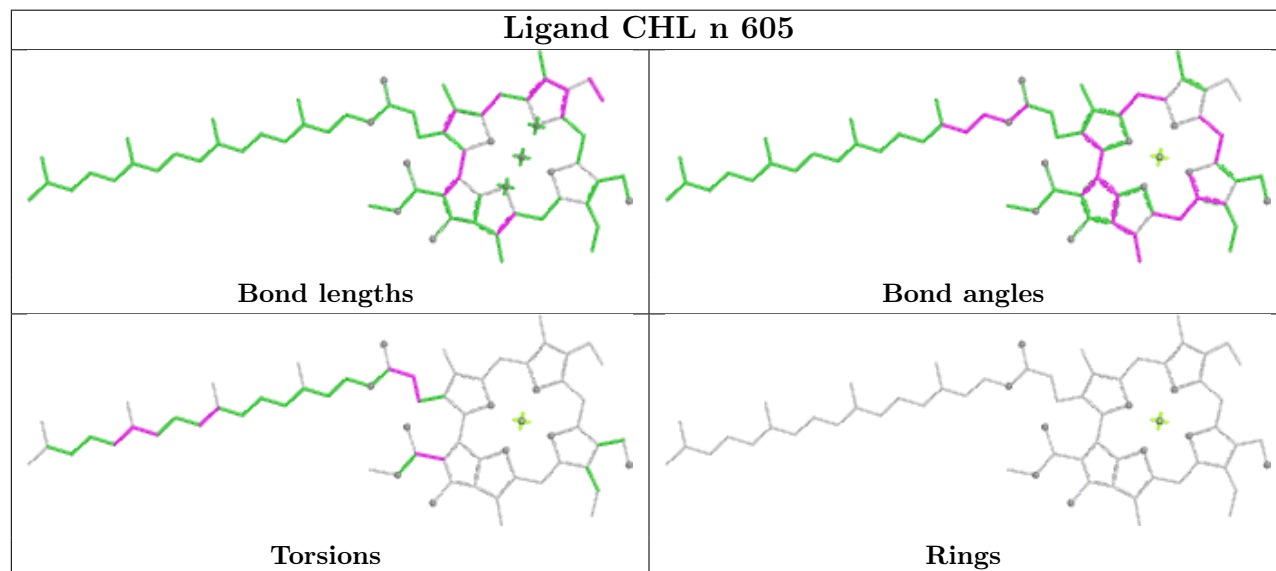


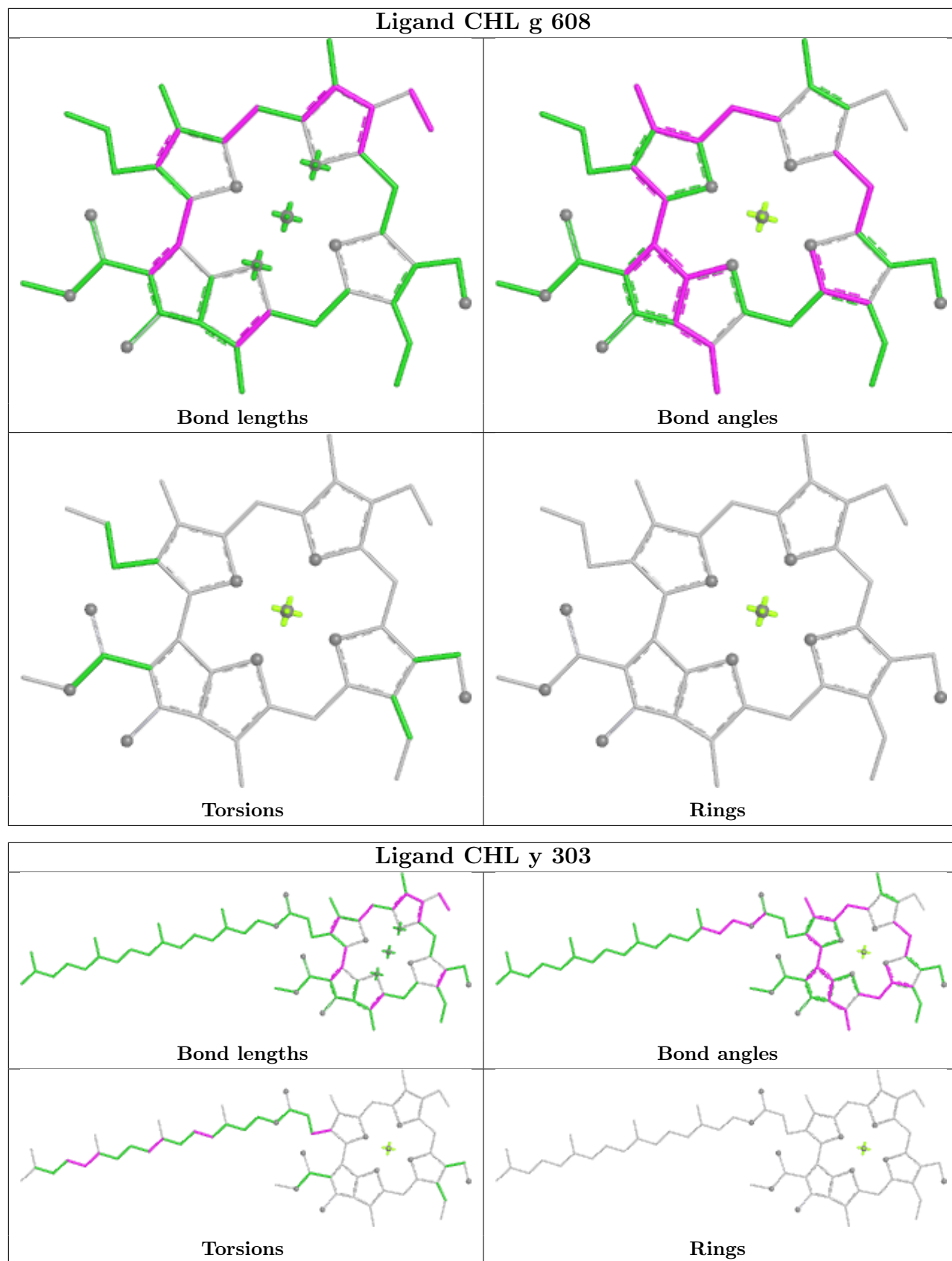


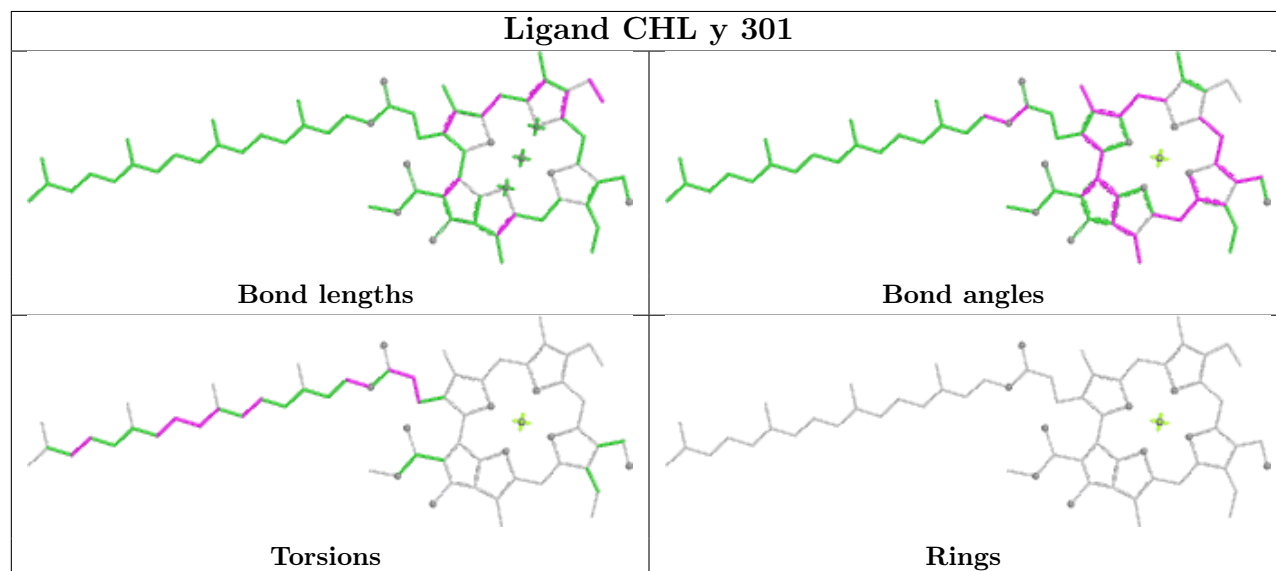
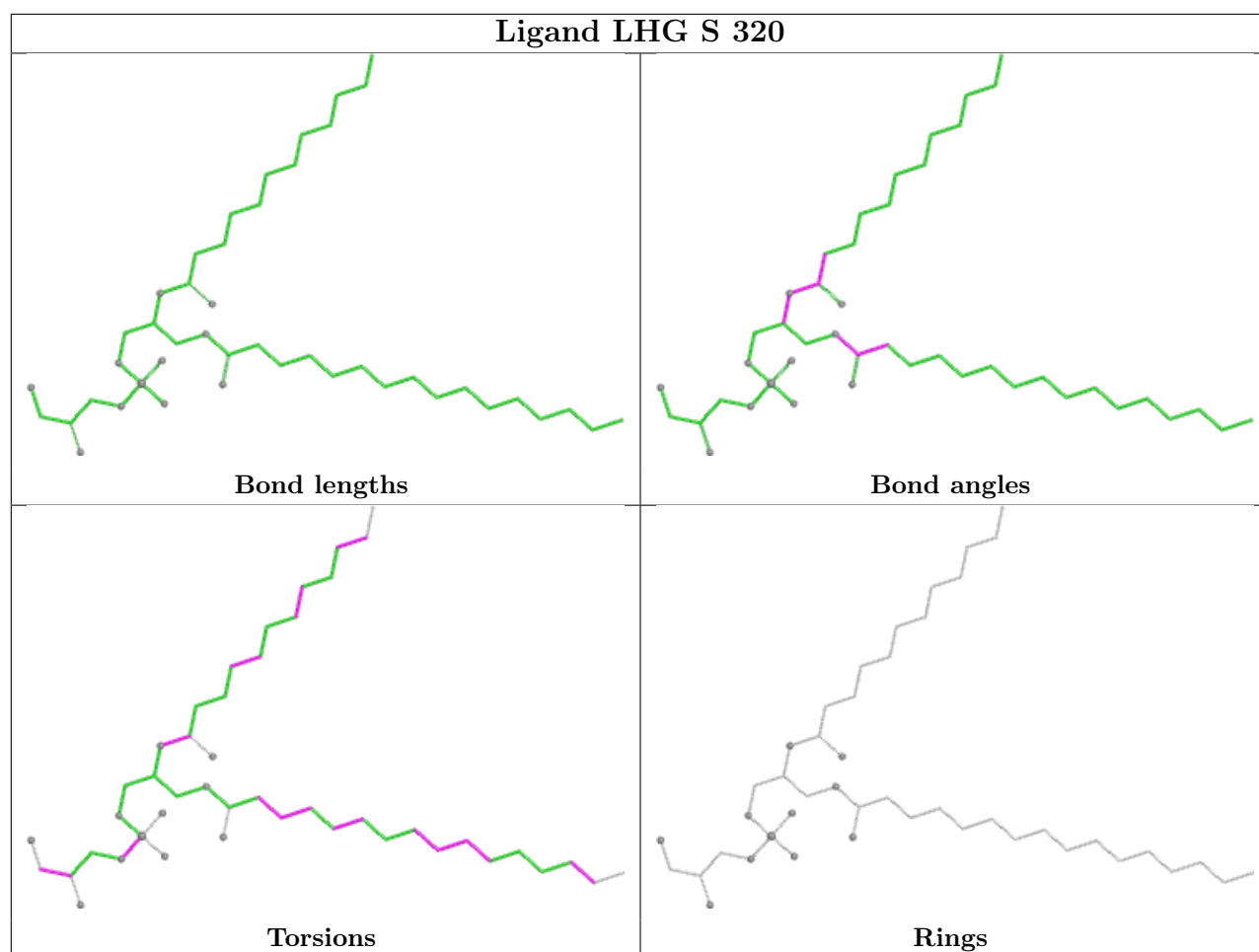
Ligand PTY Y 320

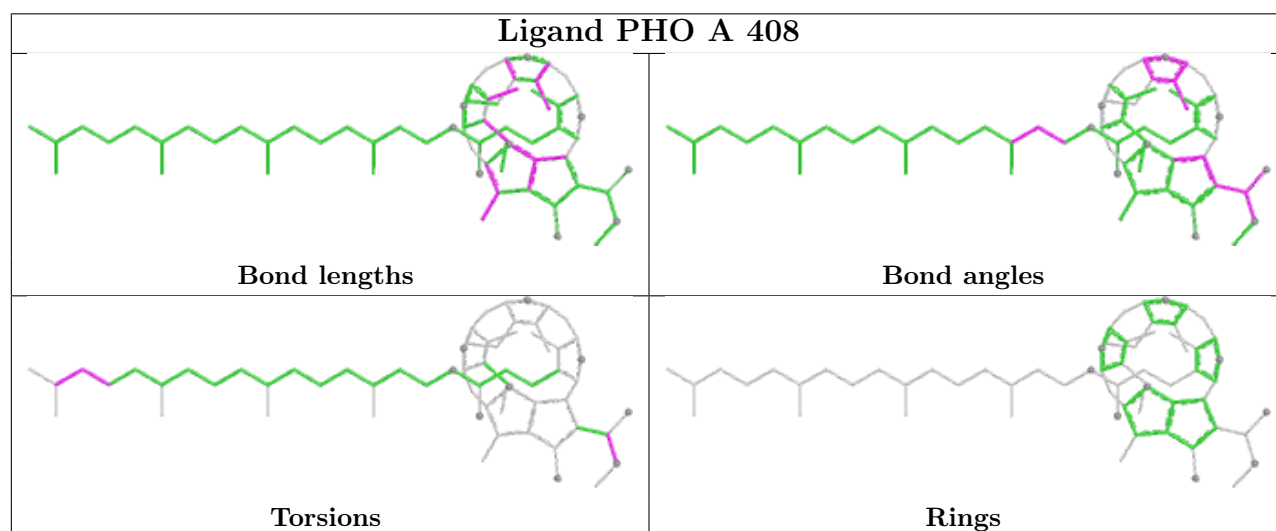
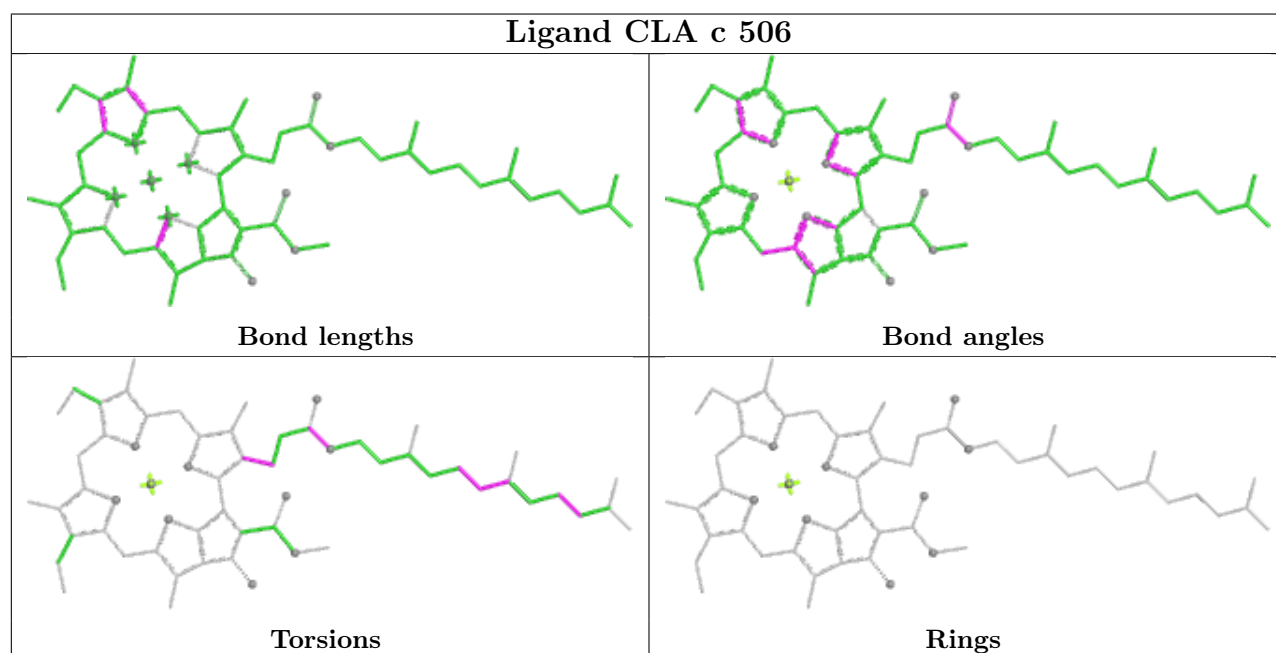
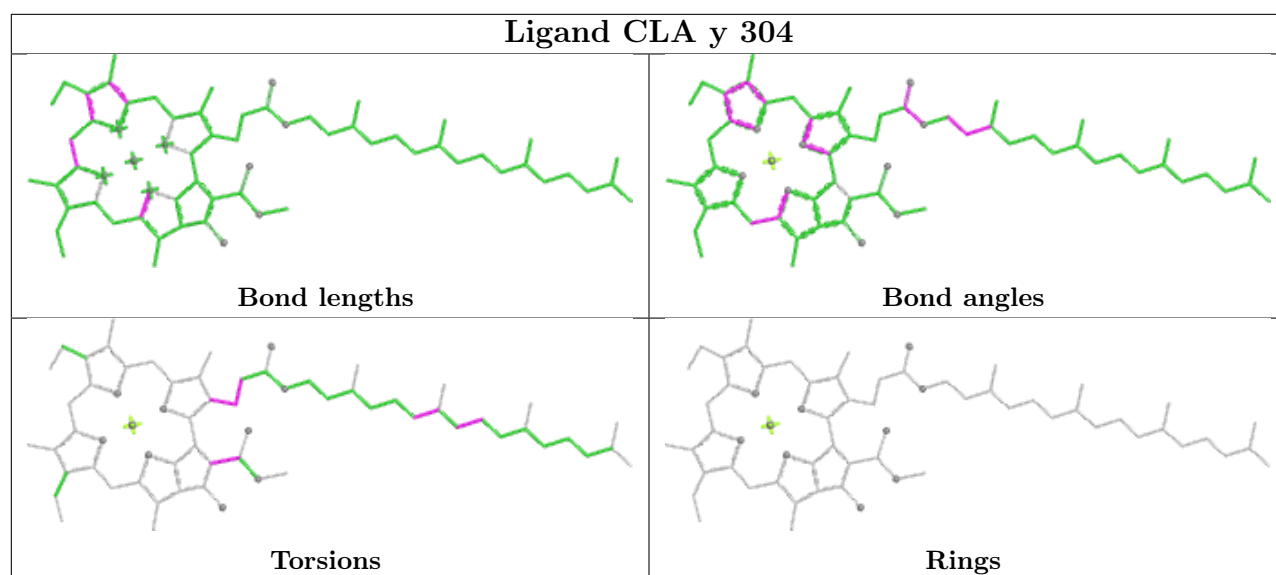


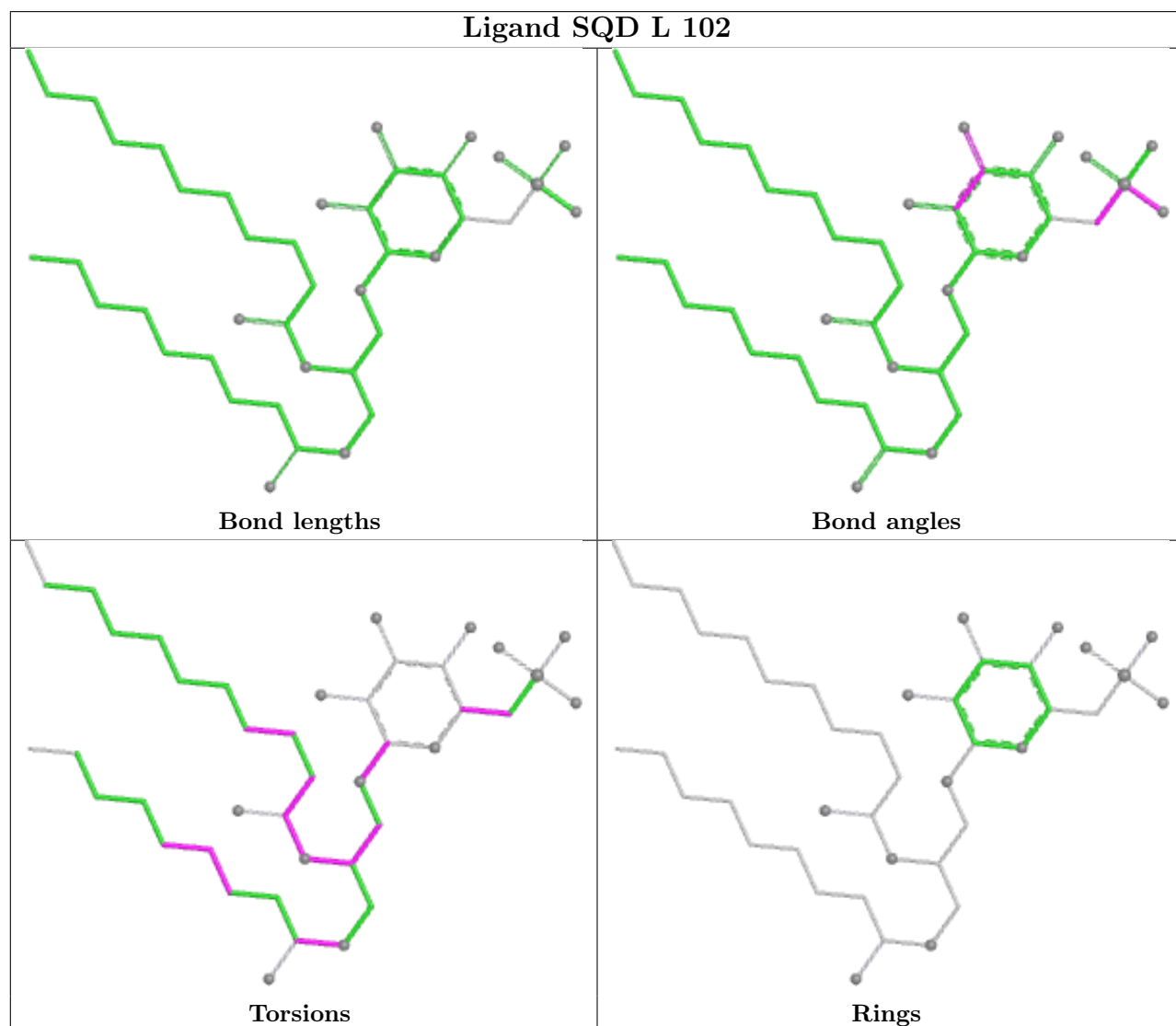
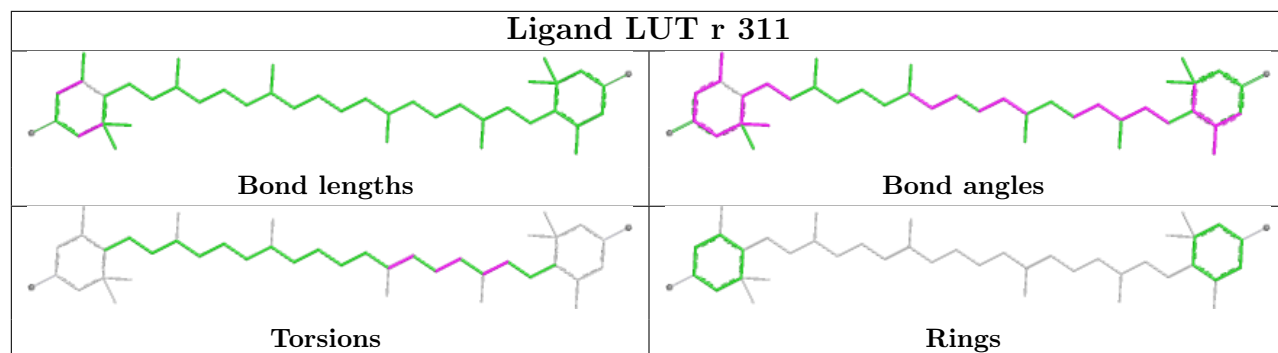
Ligand CHL n 605

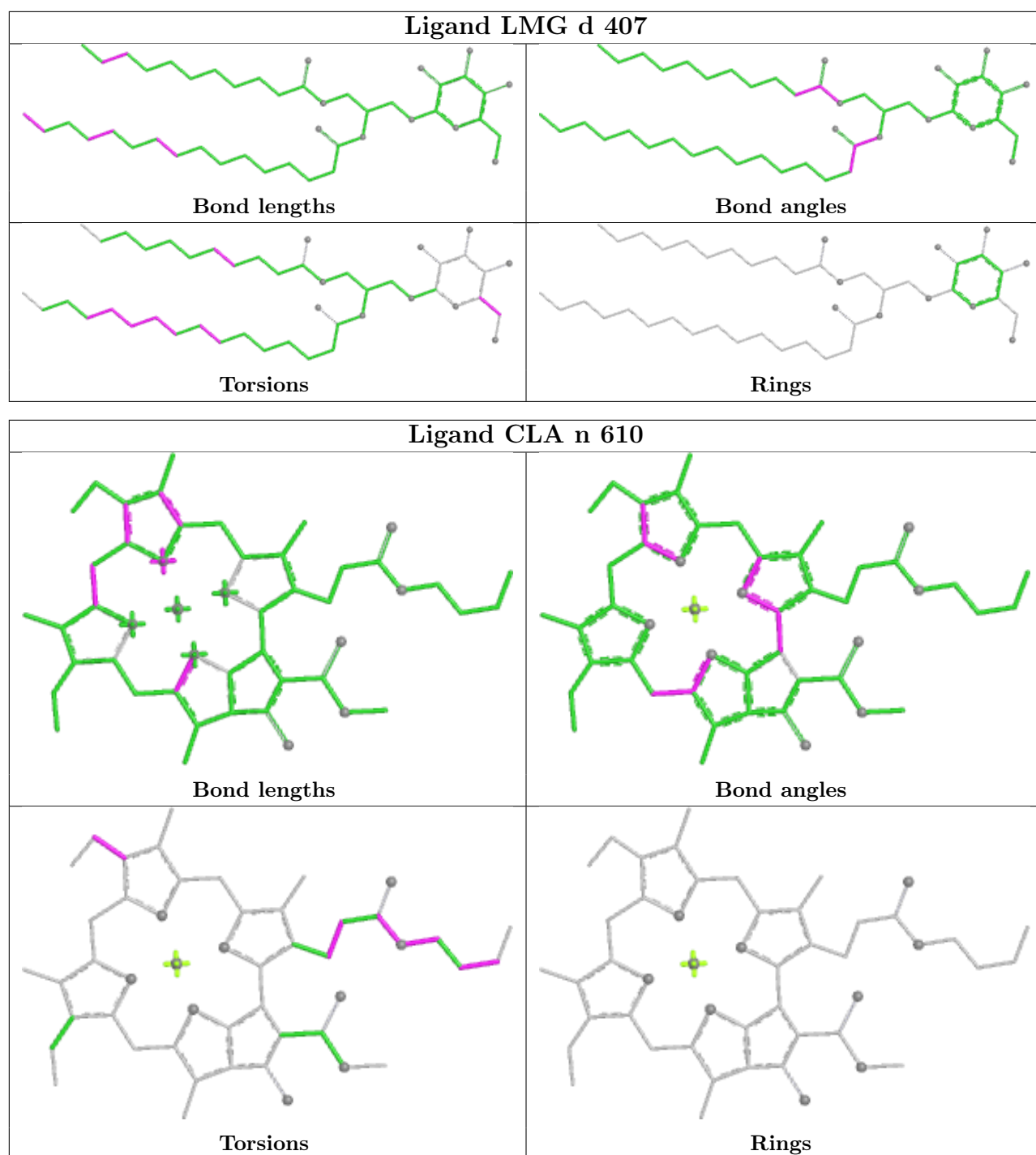




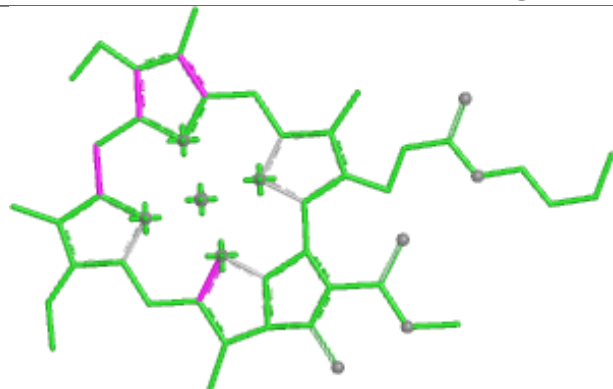




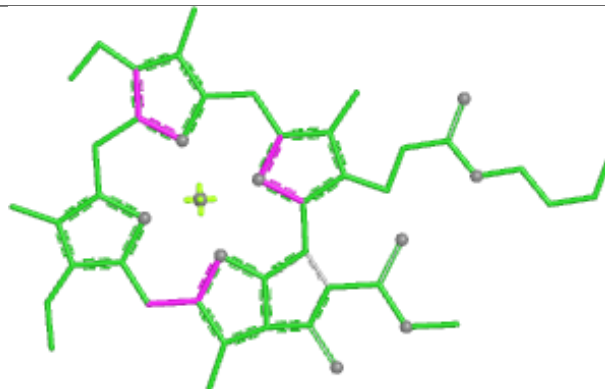




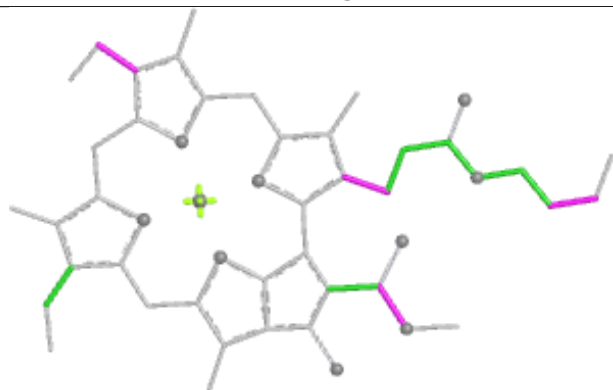
Ligand CLA G 614



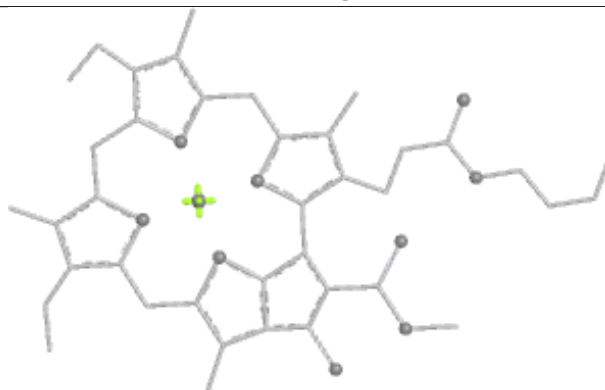
Bond lengths



Bond angles

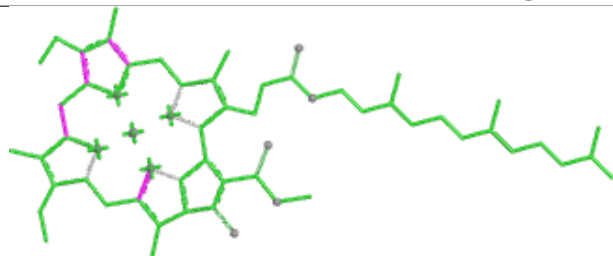


Torsions

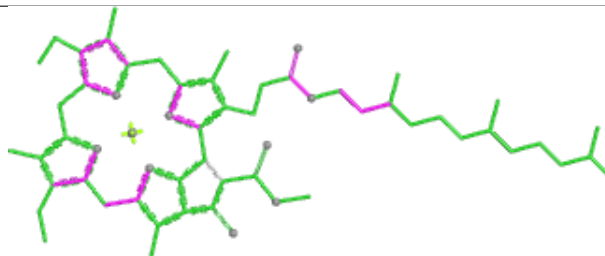


Rings

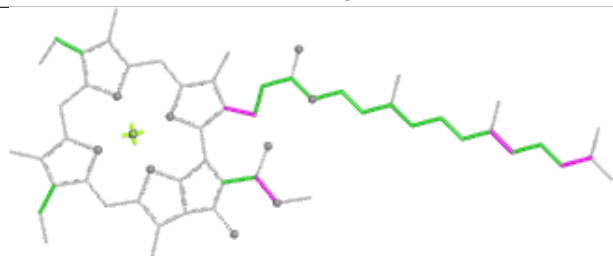
Ligand CLA r 309



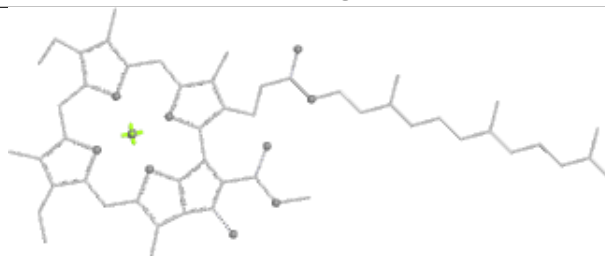
Bond lengths



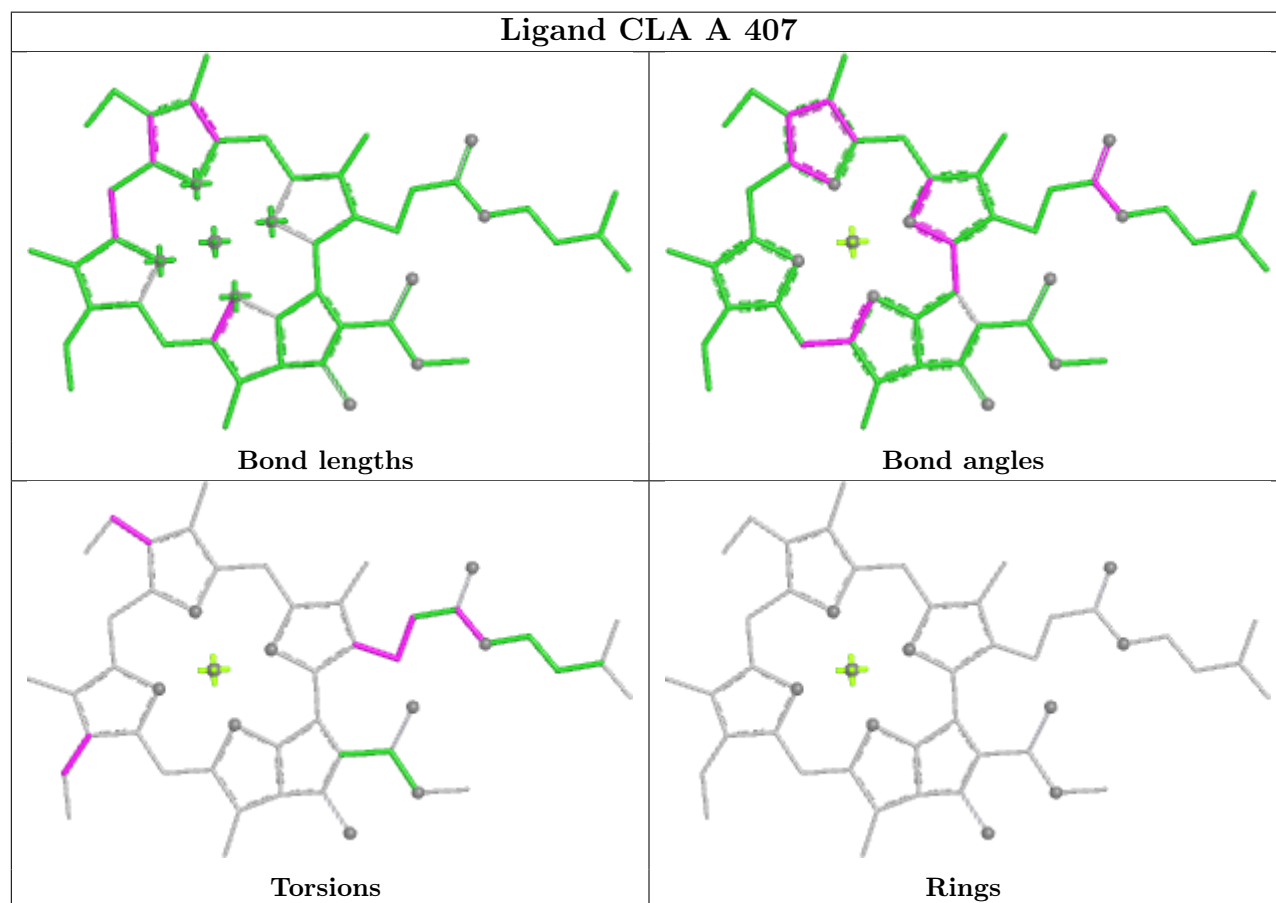
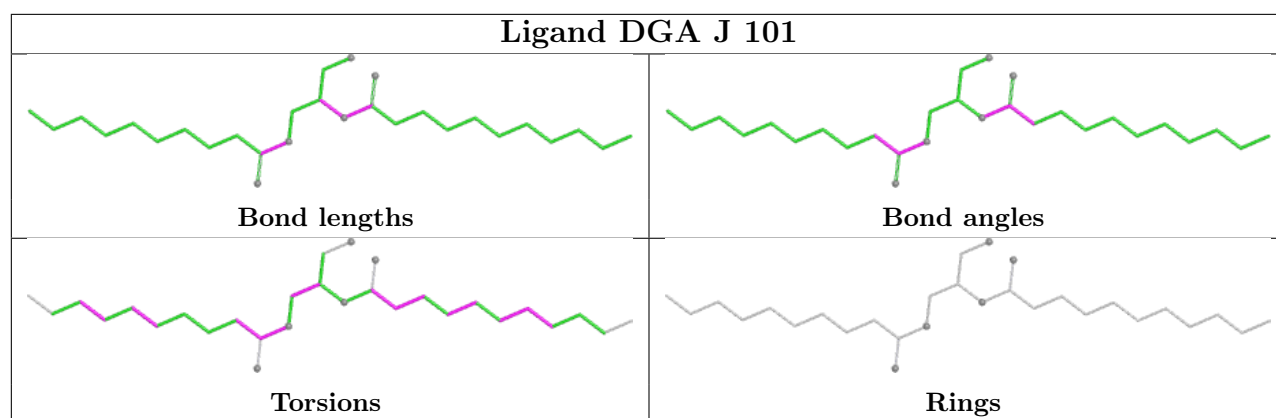
Bond angles

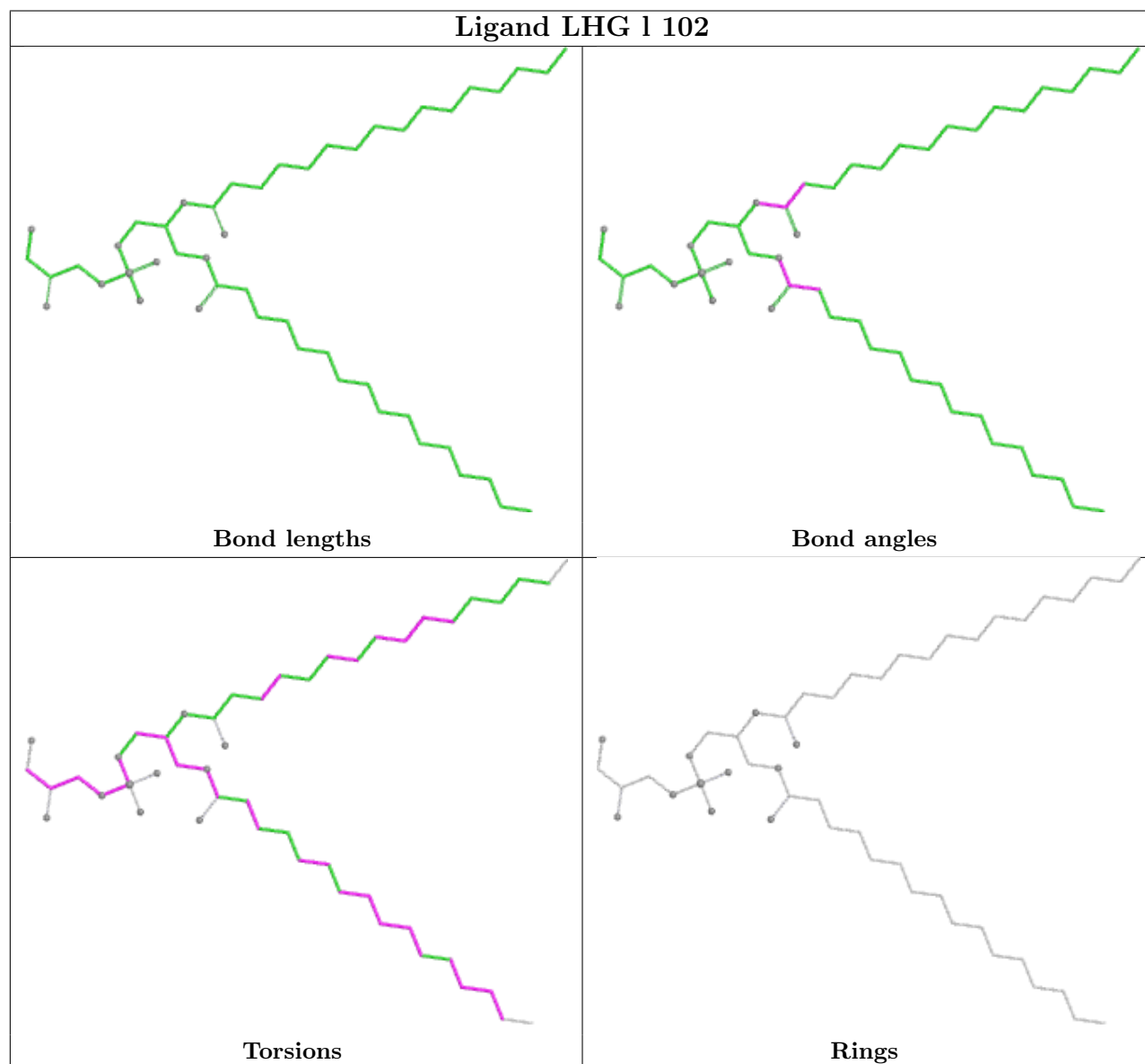
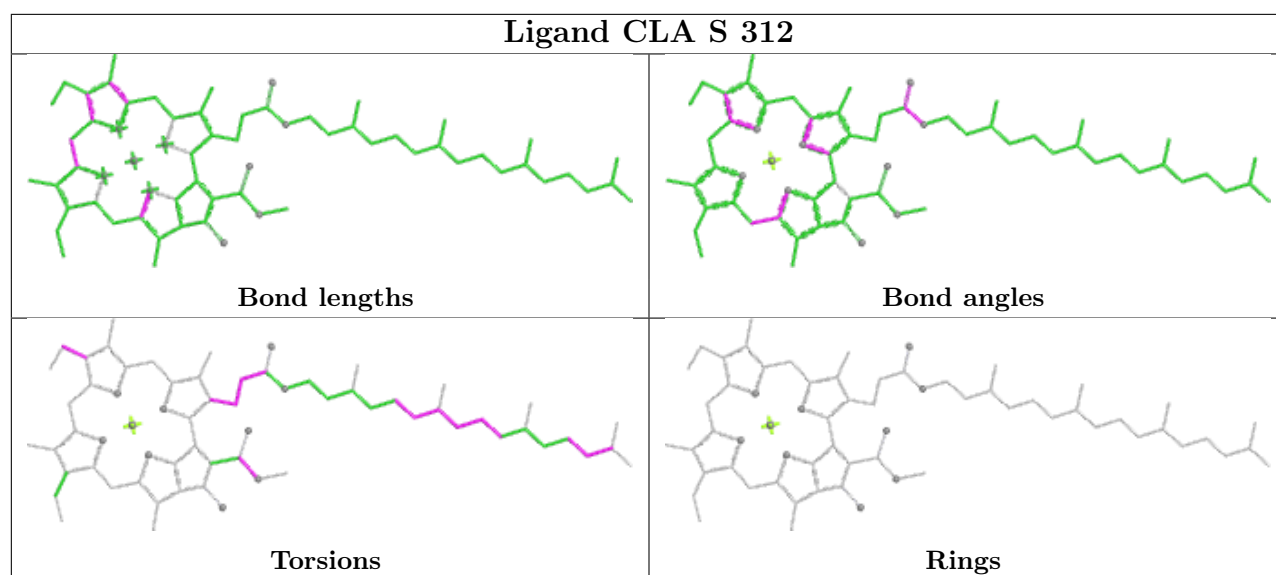


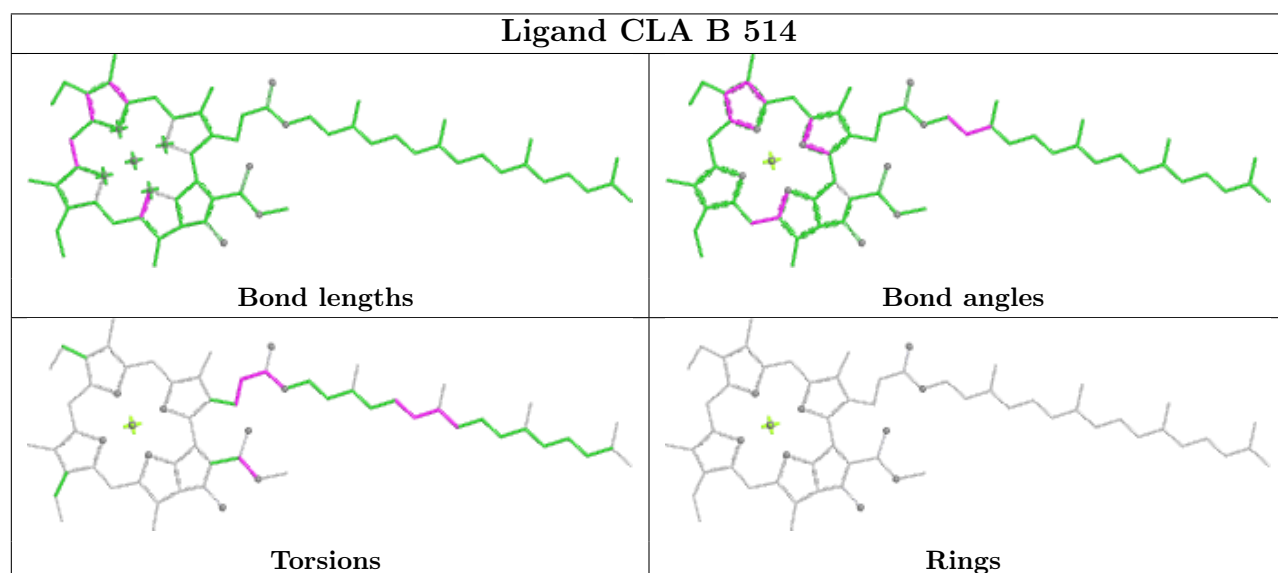
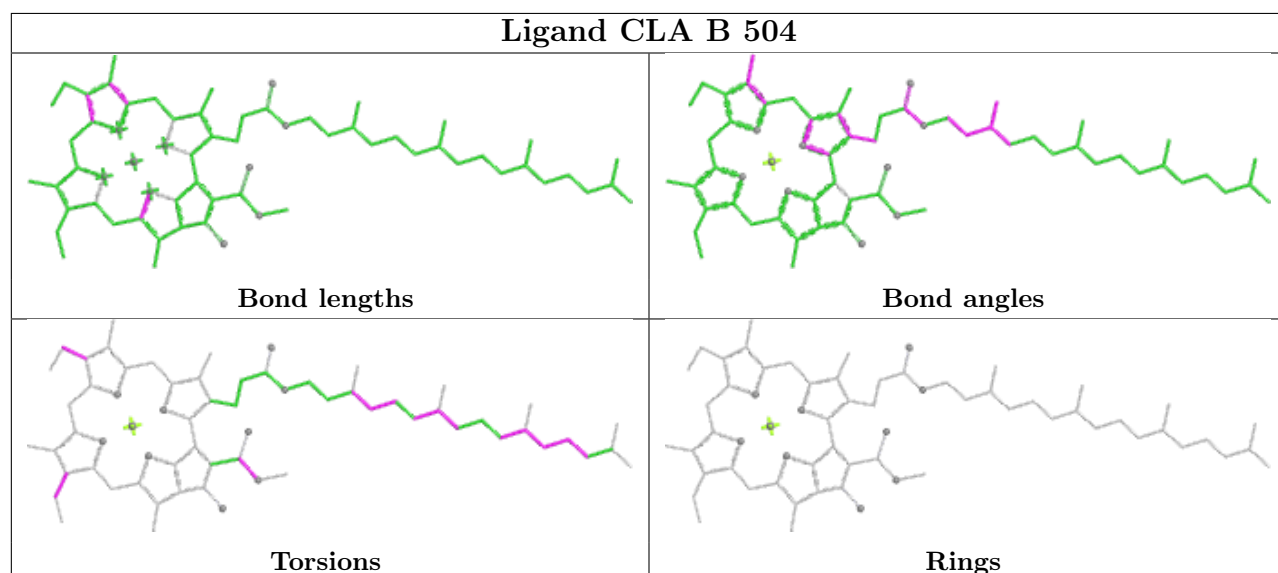
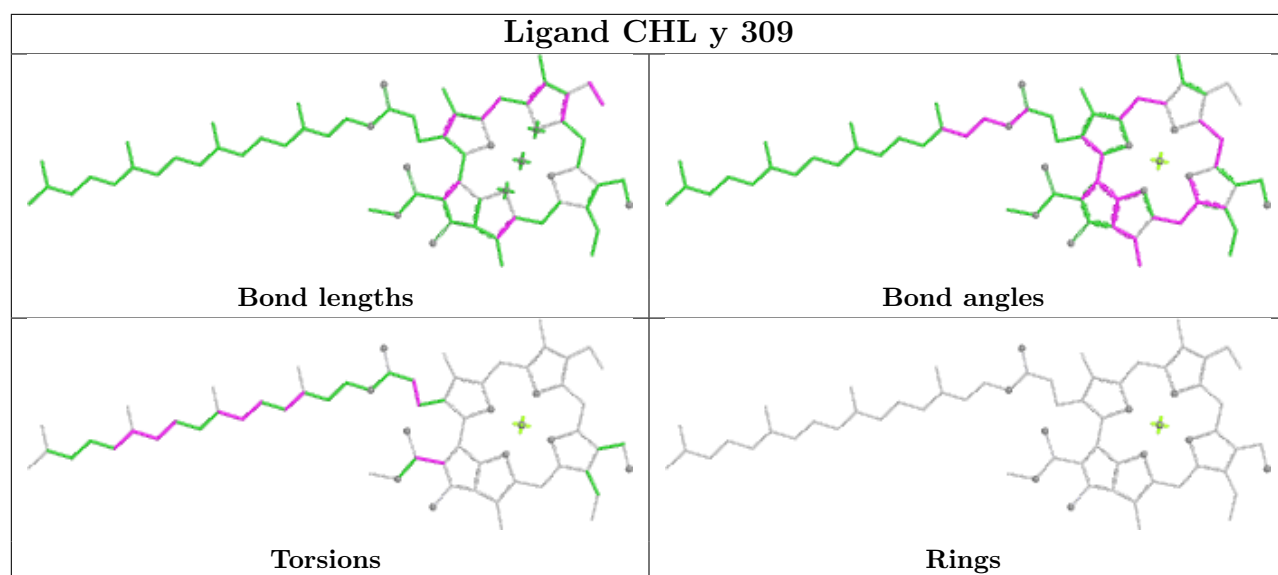
Torsions

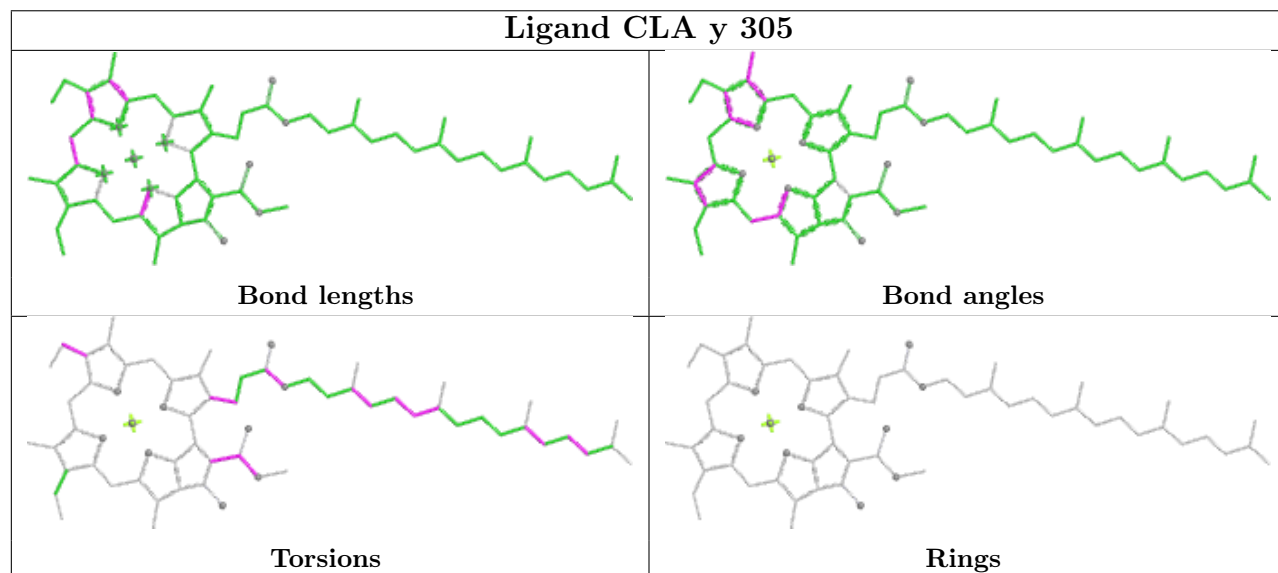
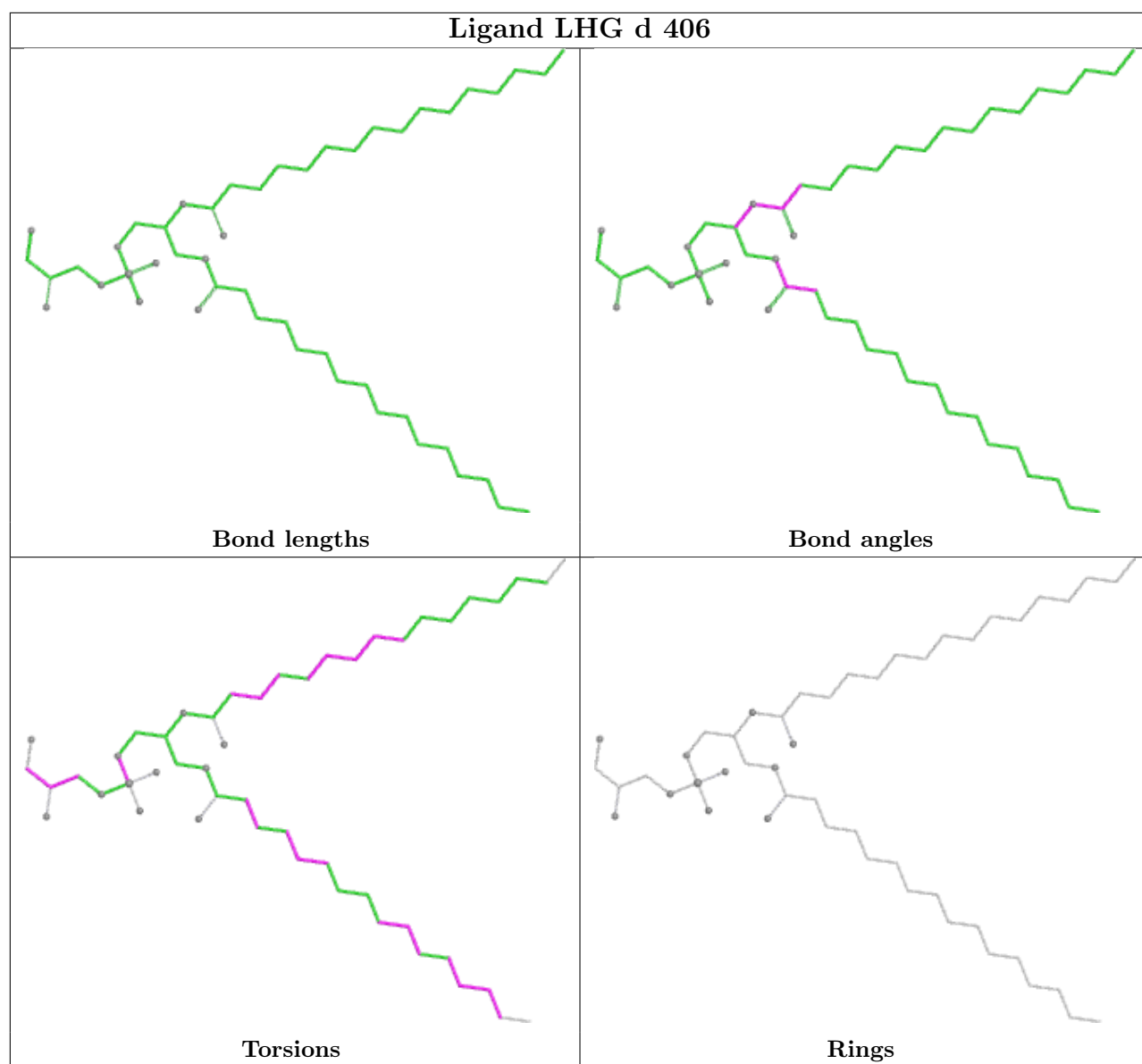


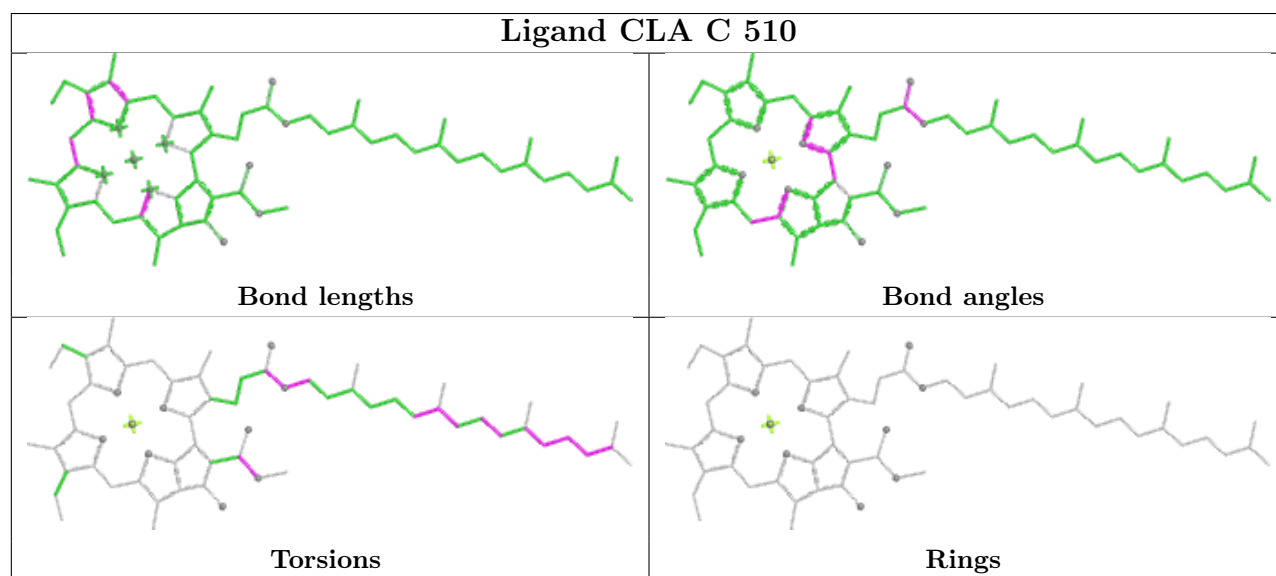
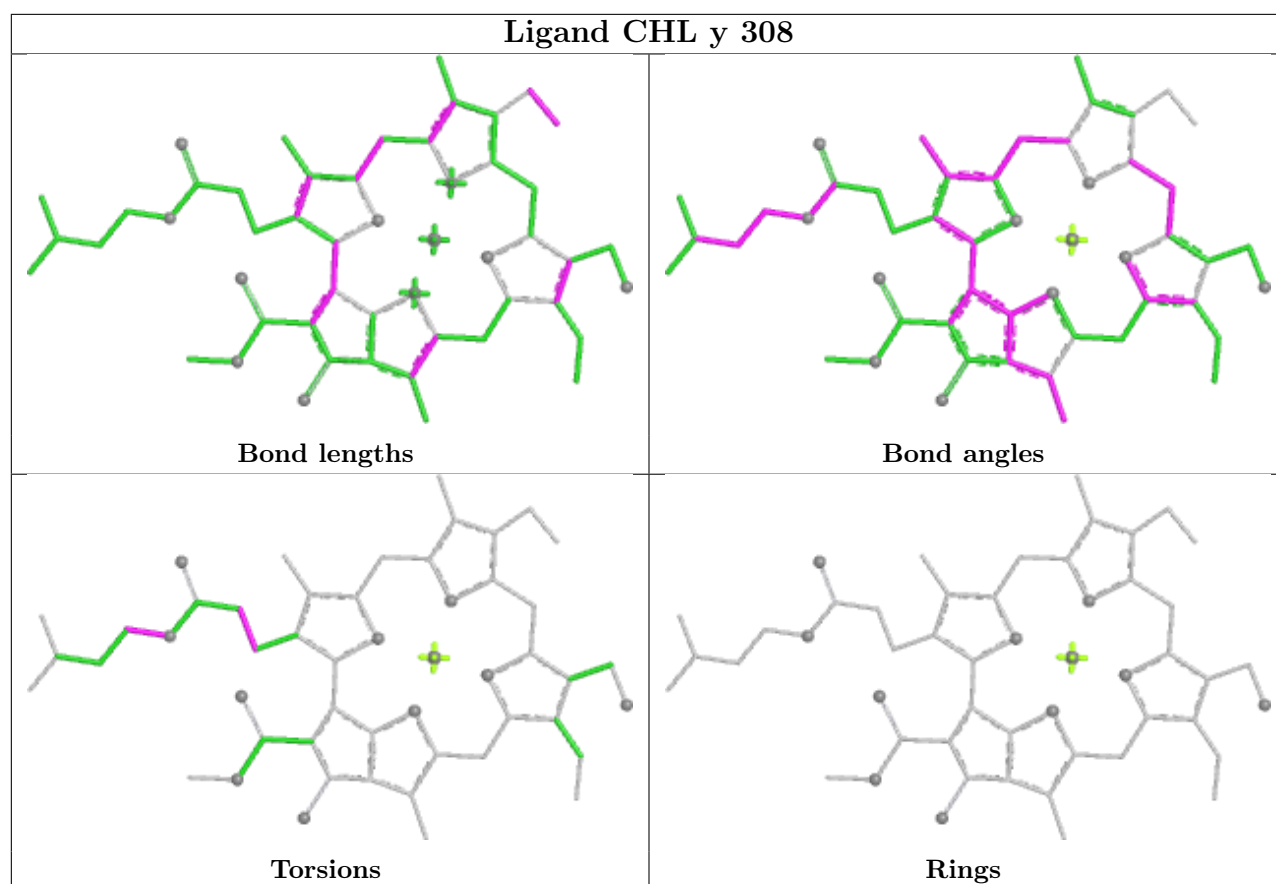
Rings

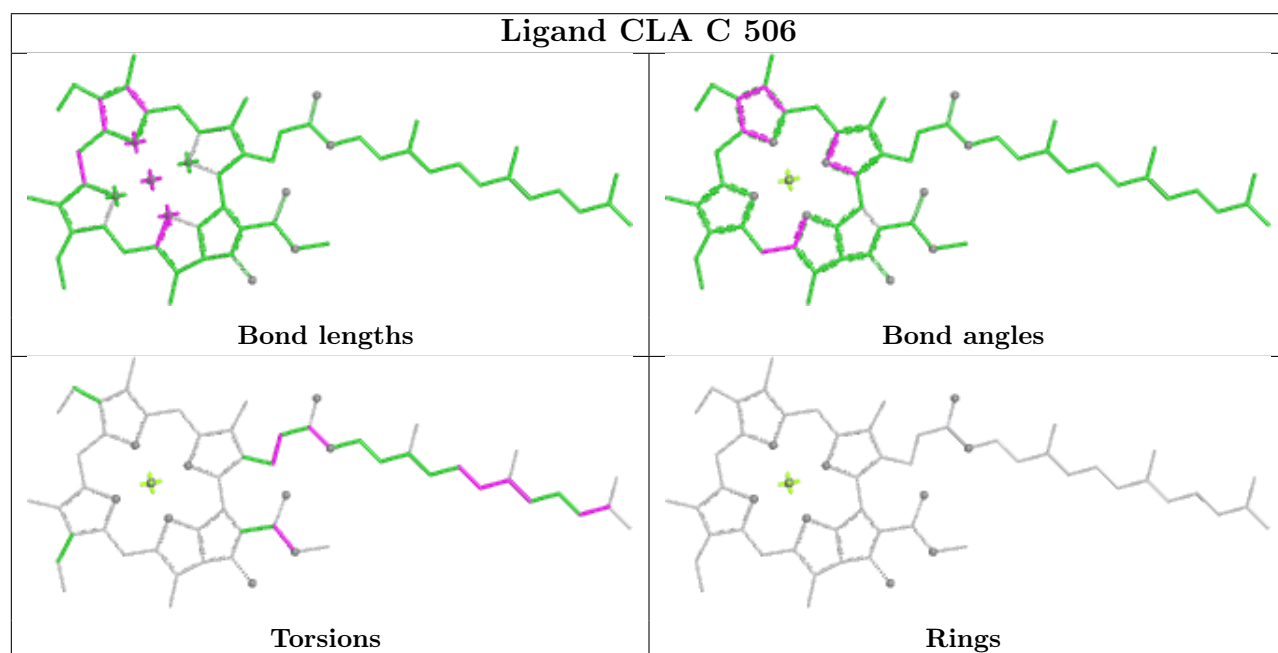
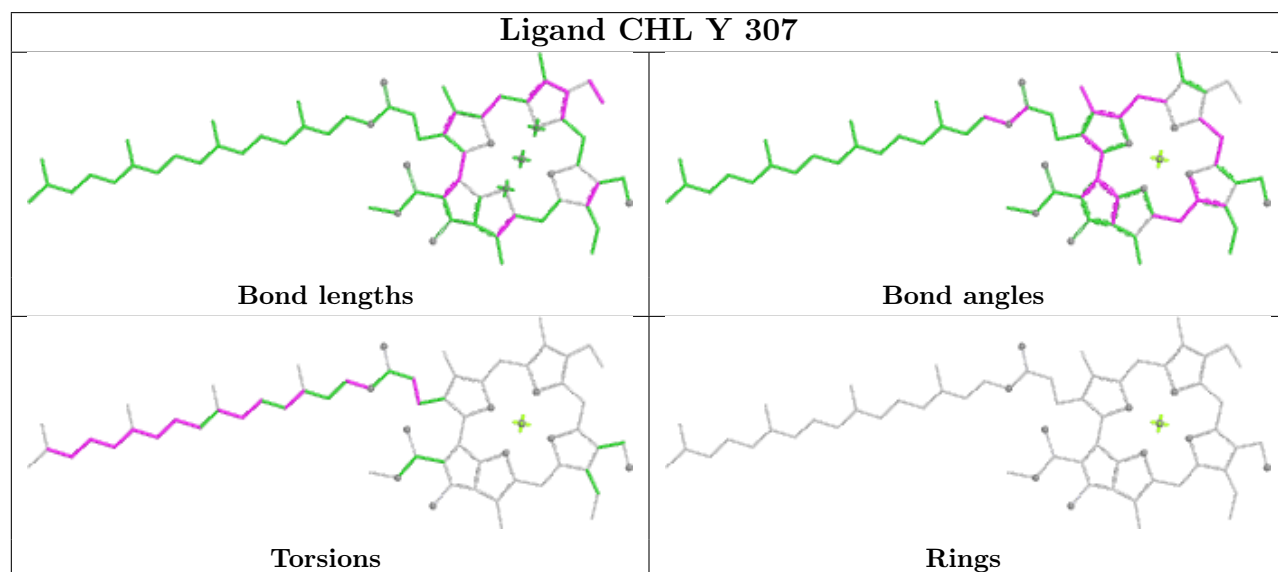
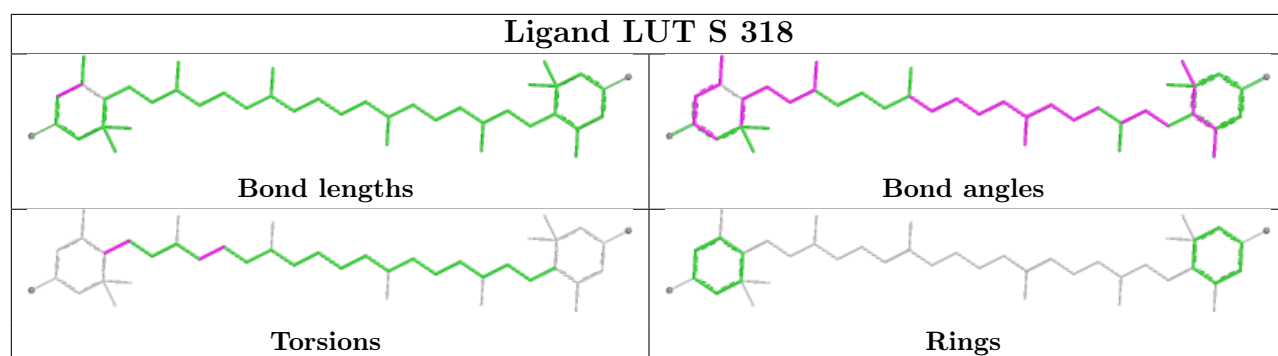


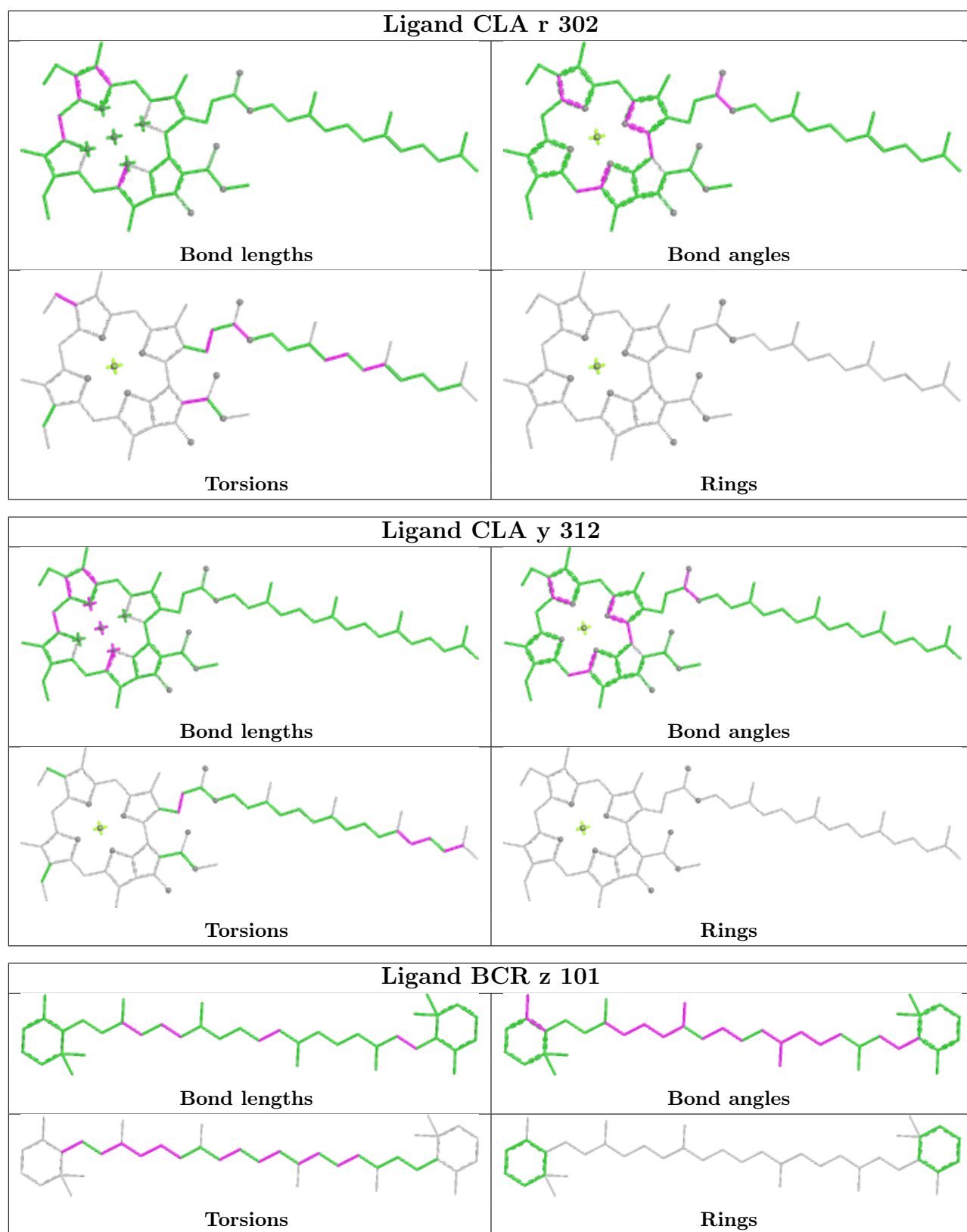




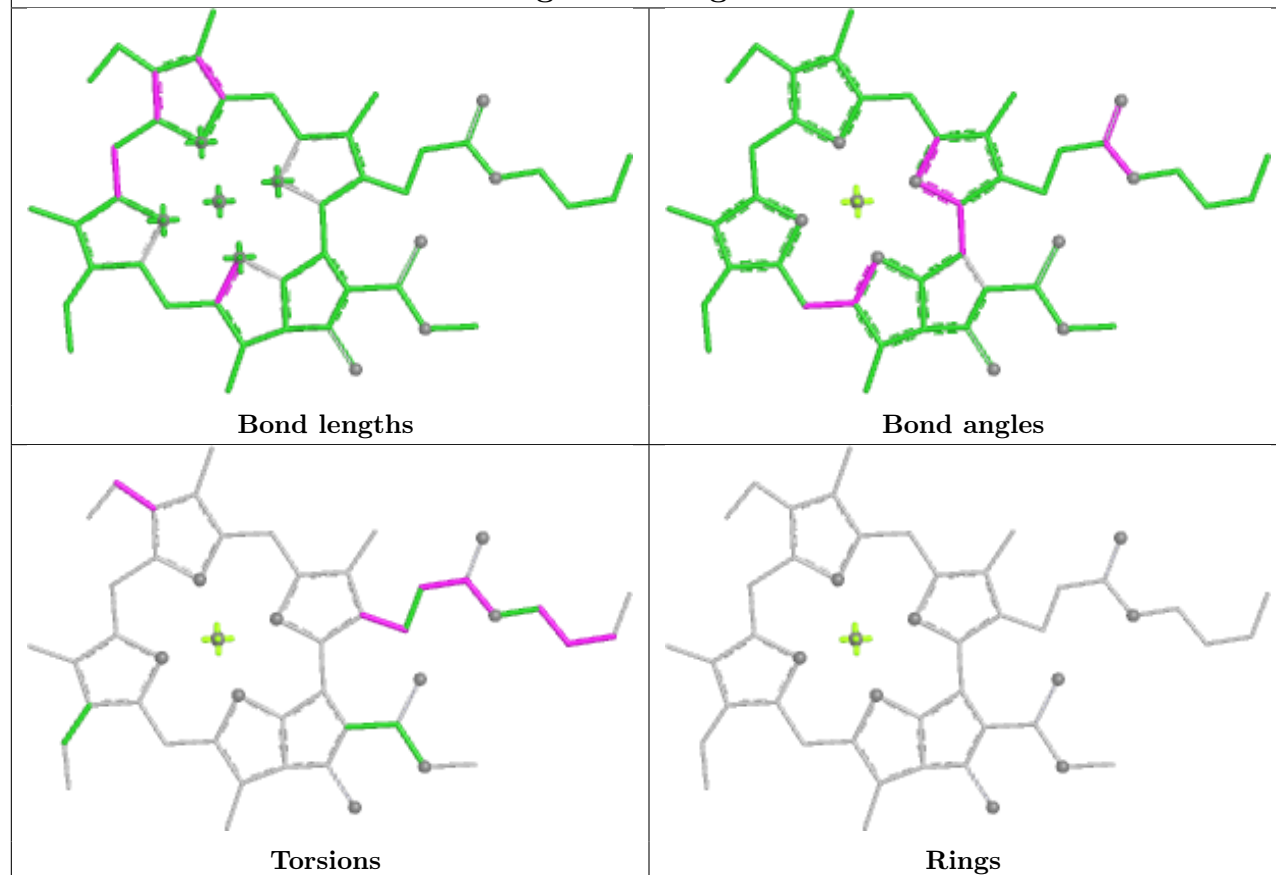




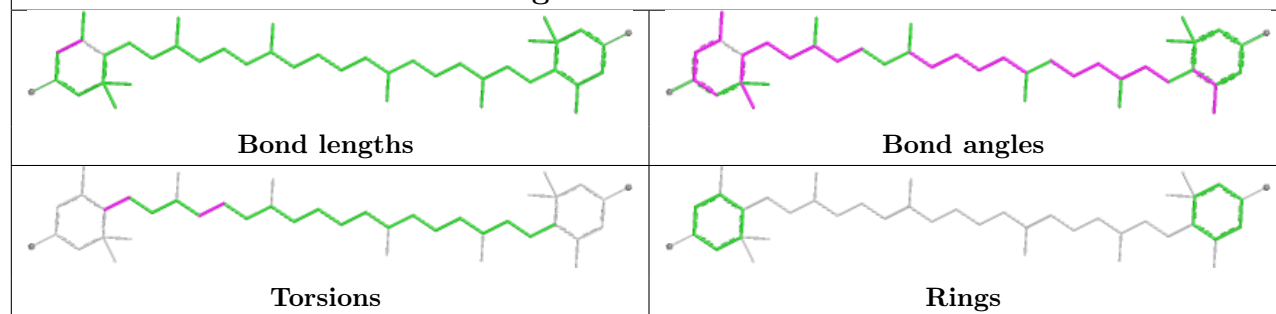


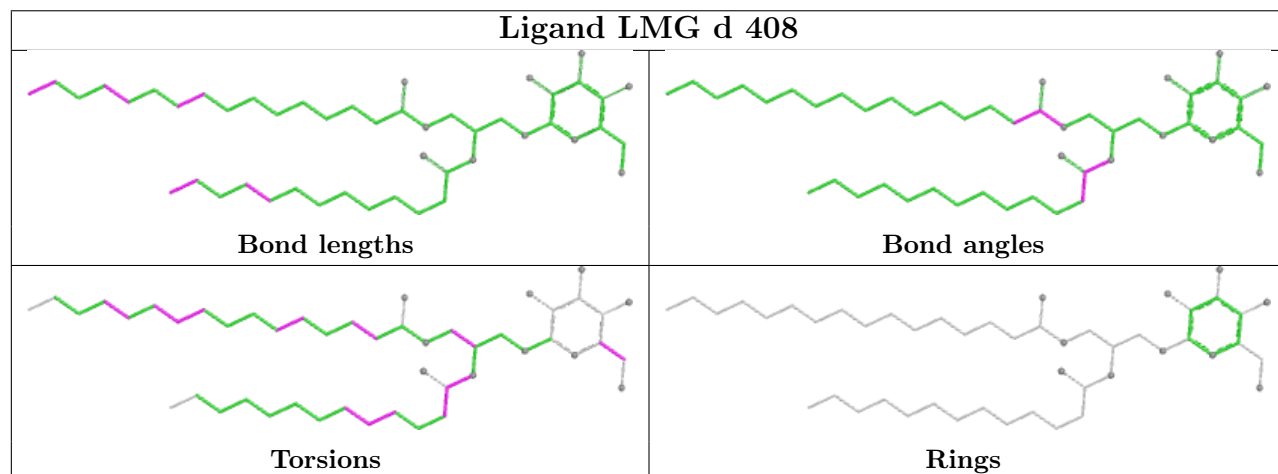
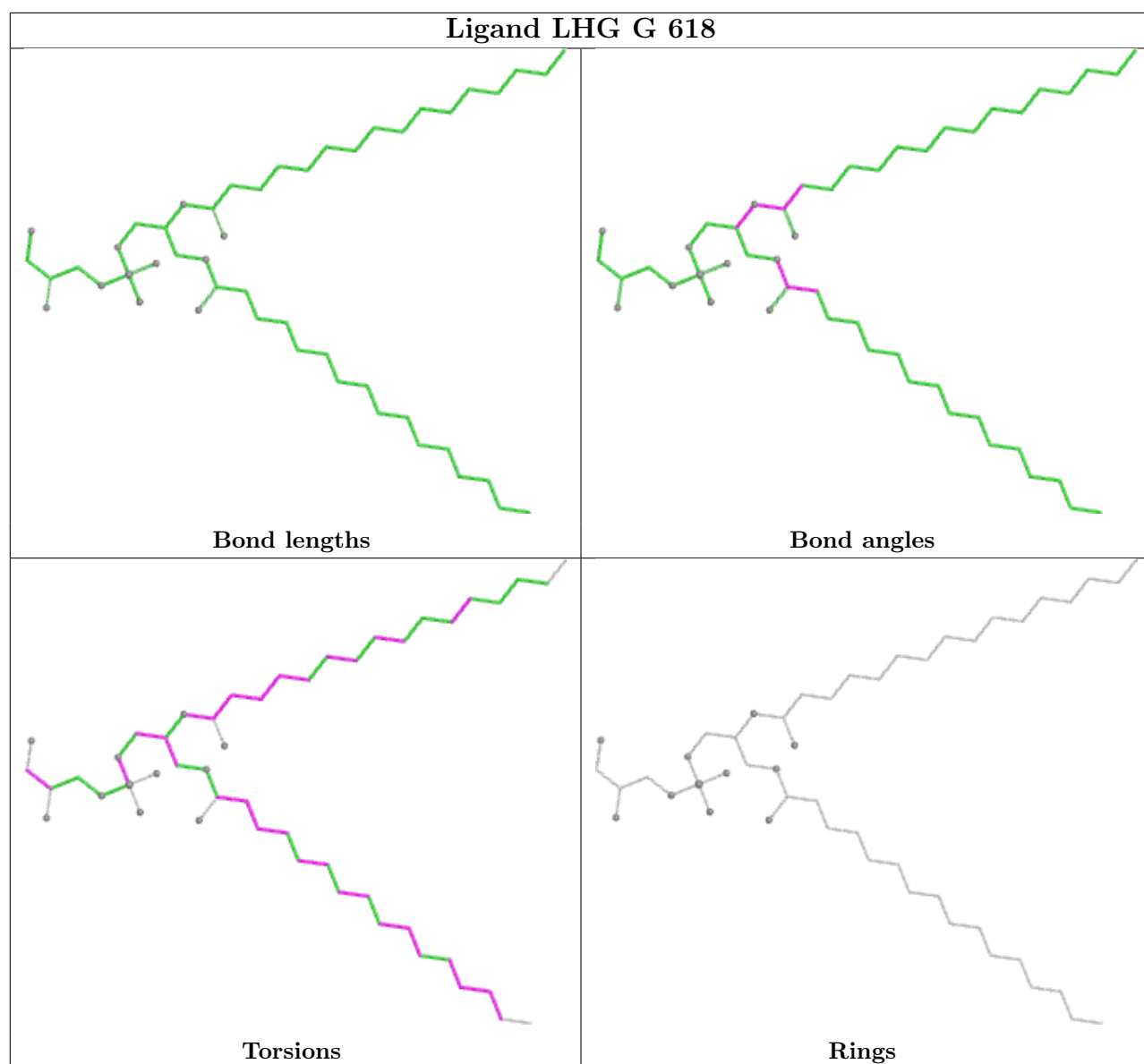


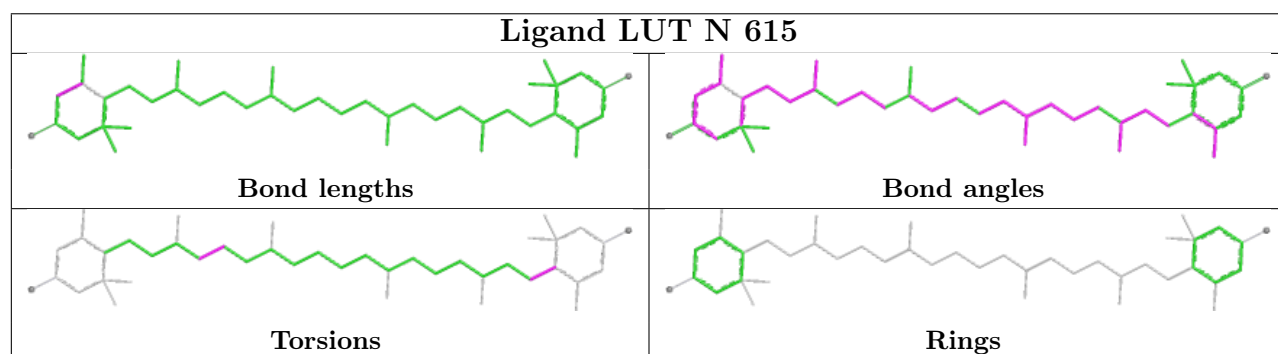
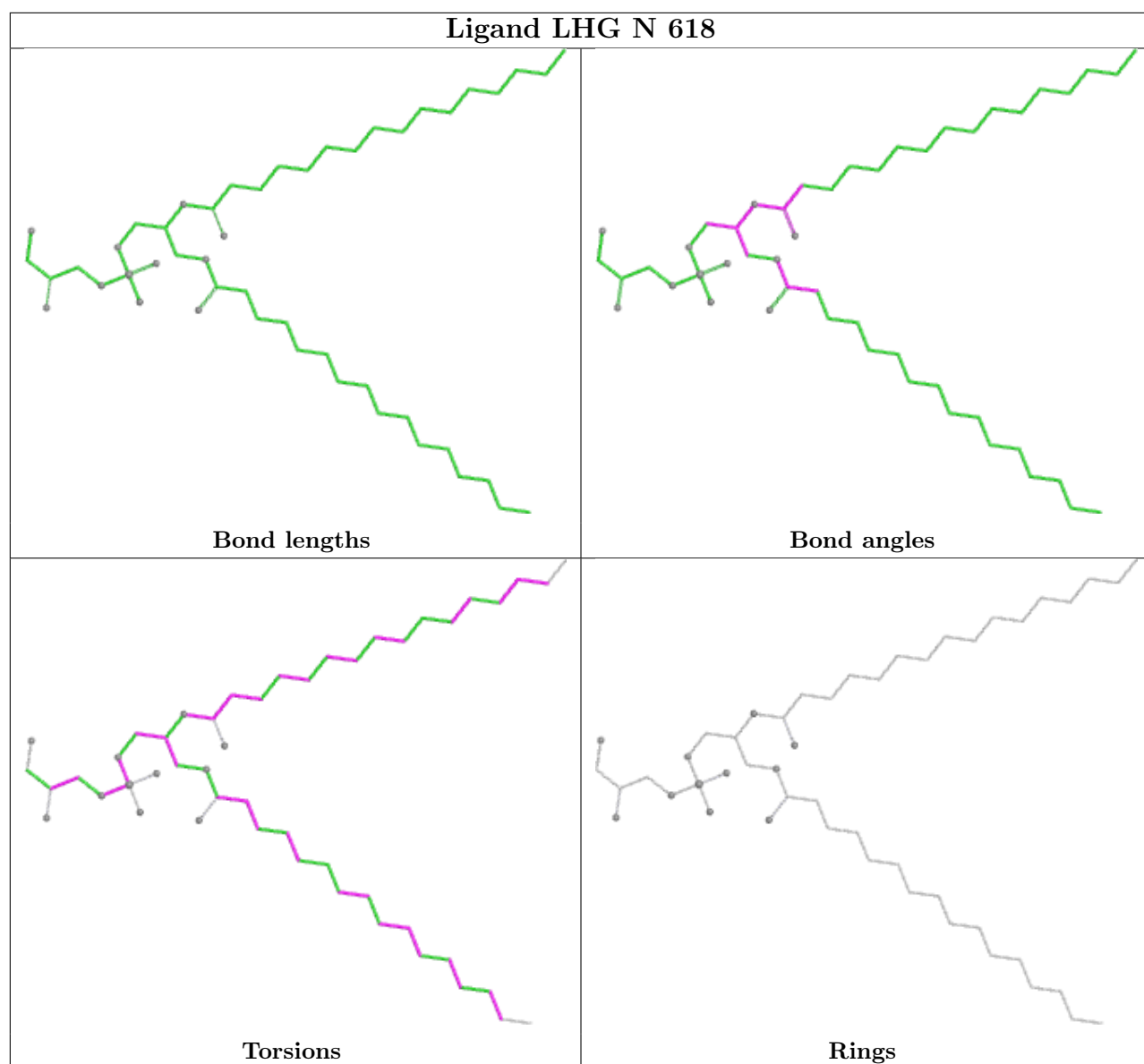
Ligand CLA g 614



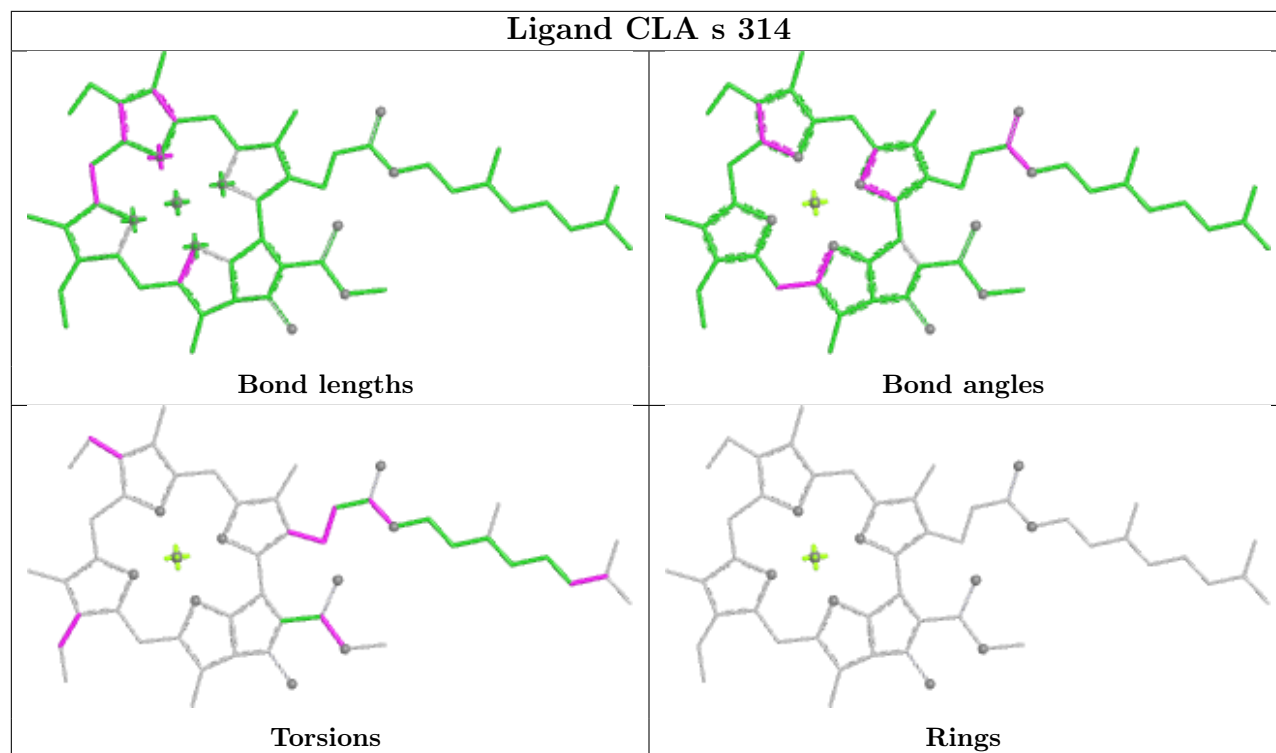
Ligand LUT Y 317



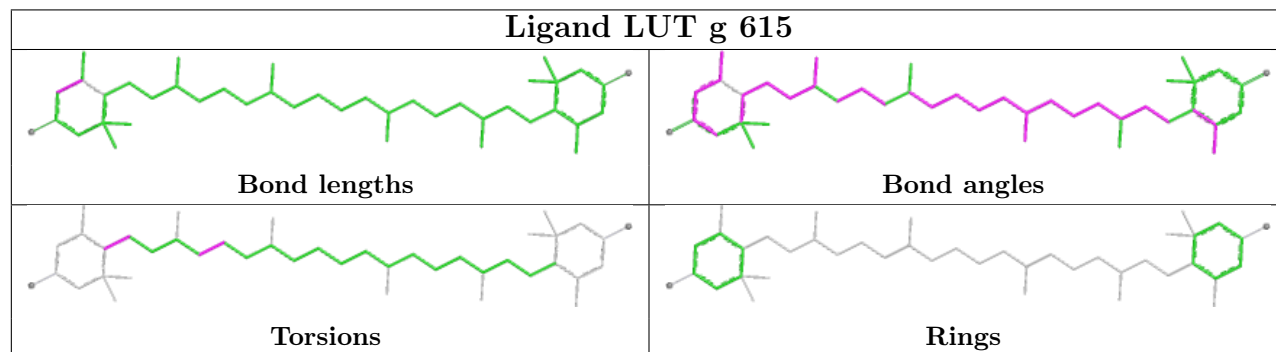




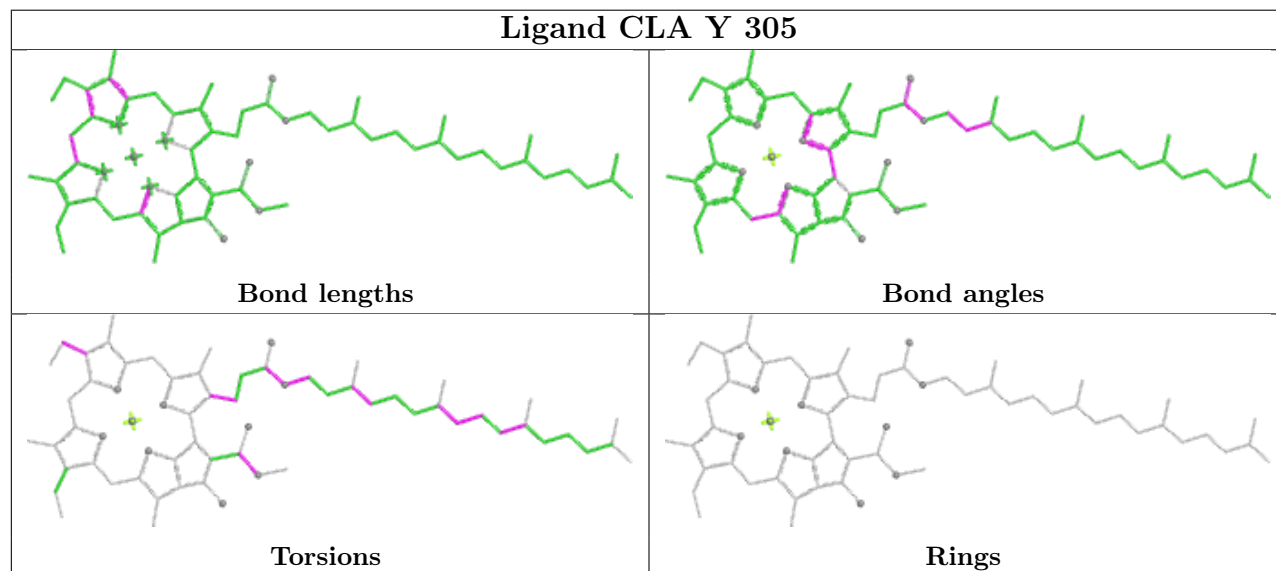
Ligand CLA s 314

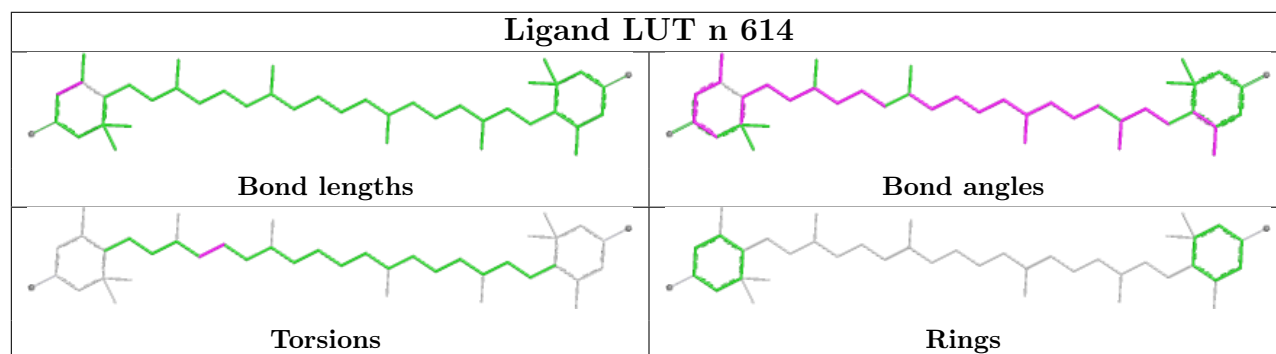
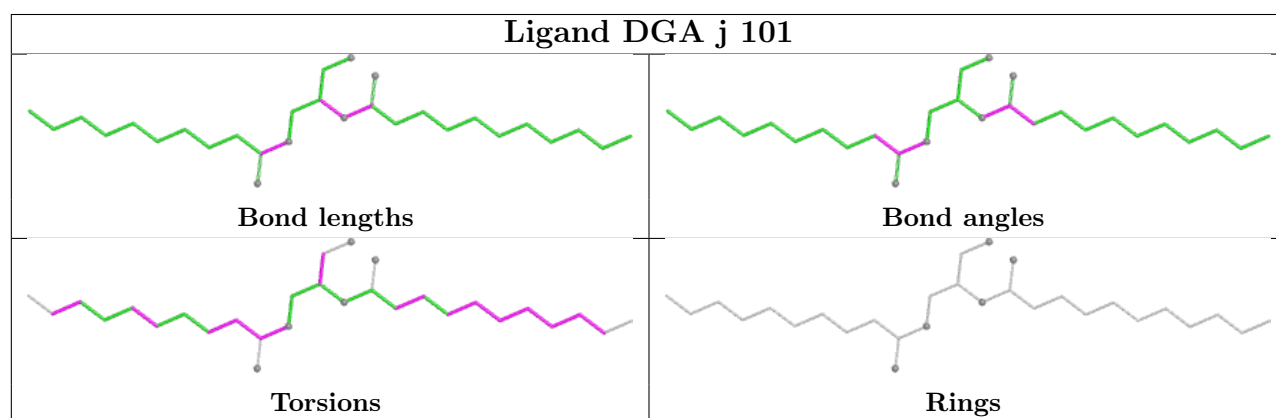
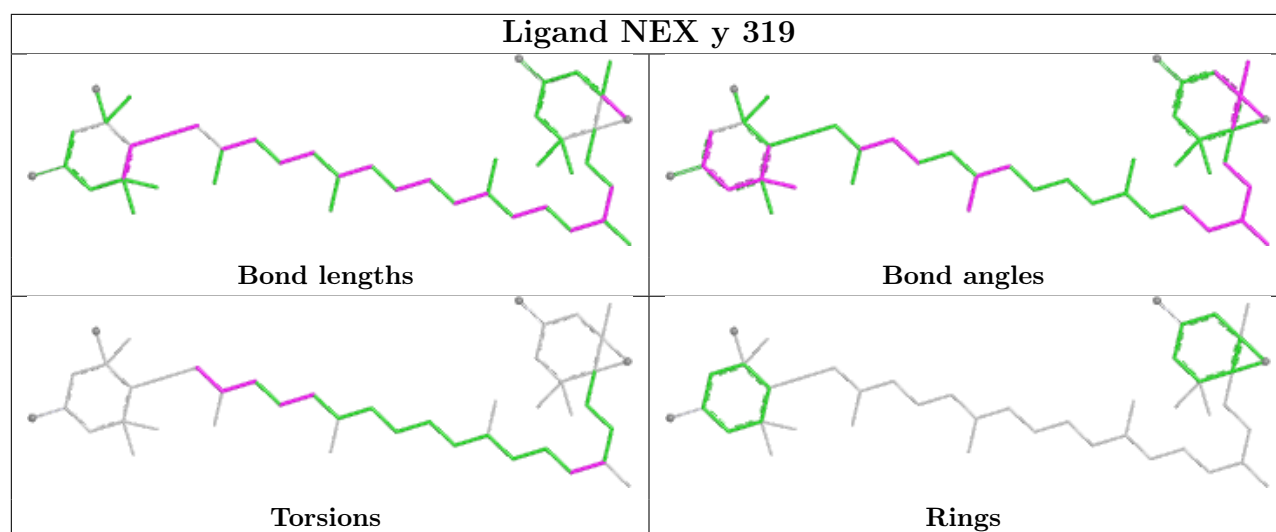


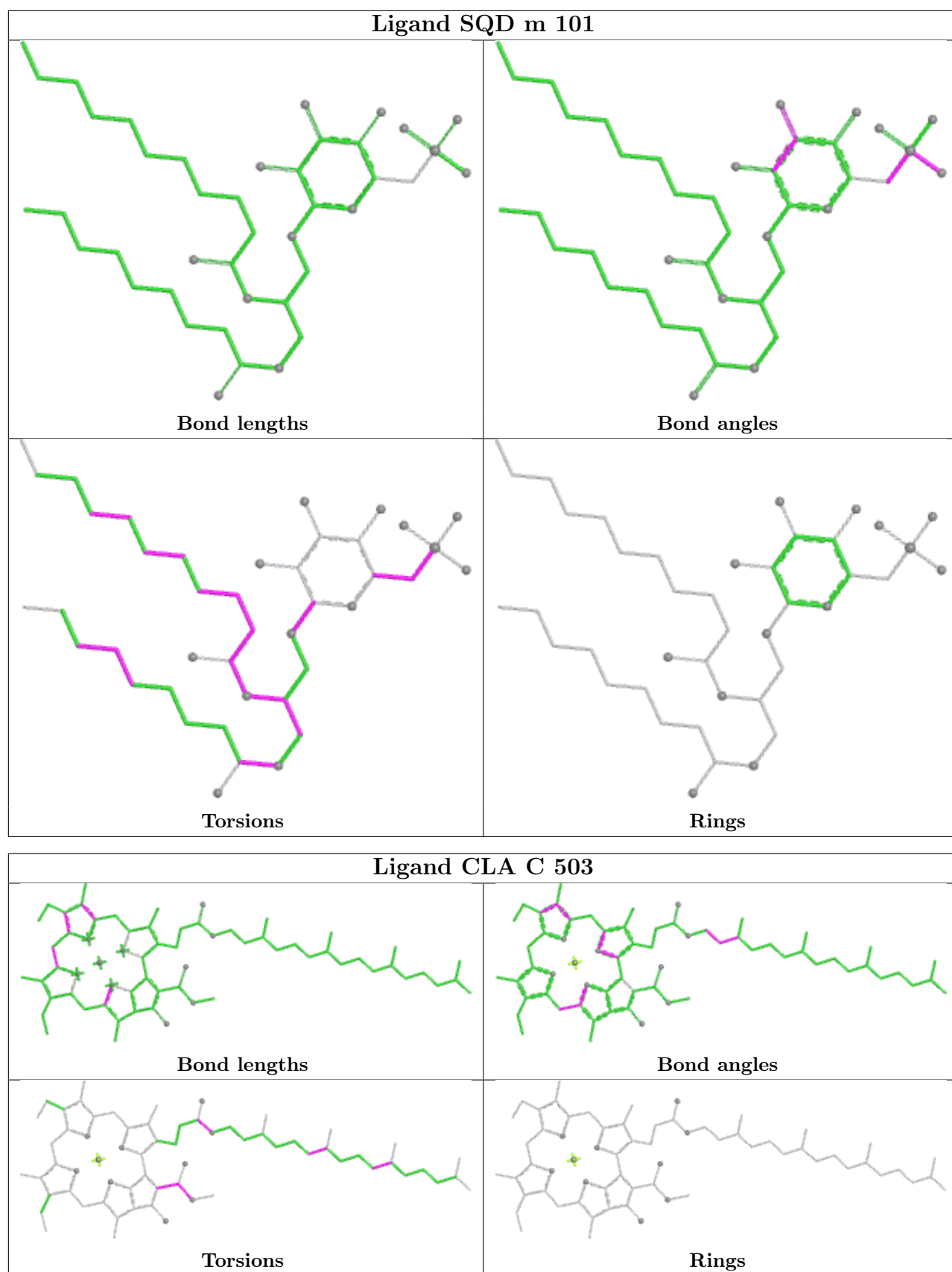
Ligand LUT g 615

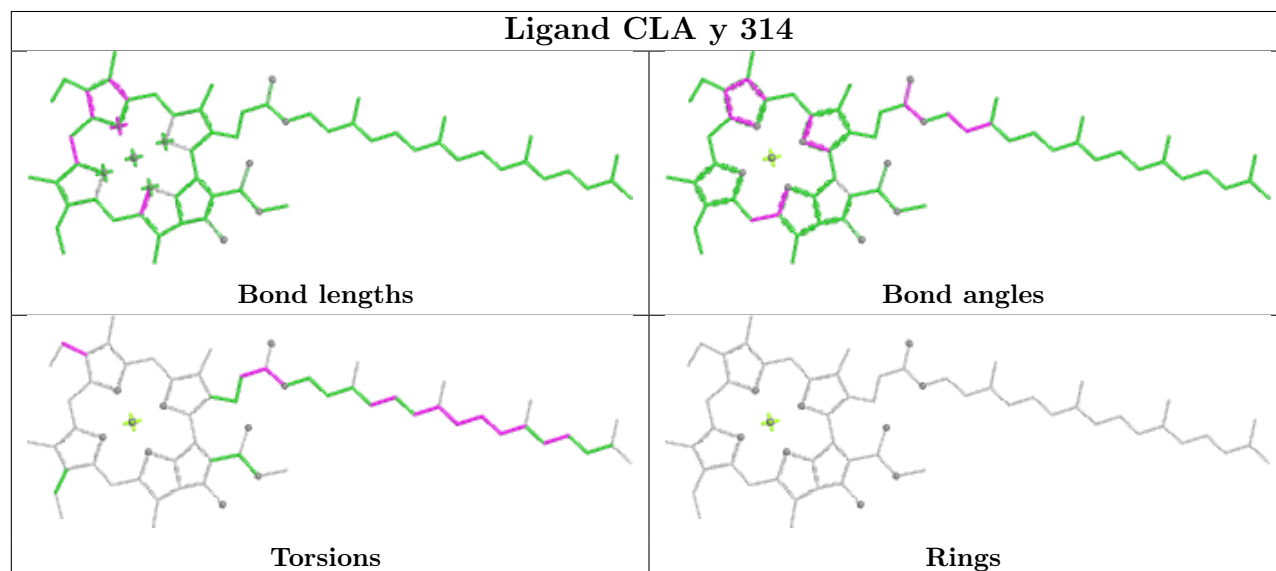
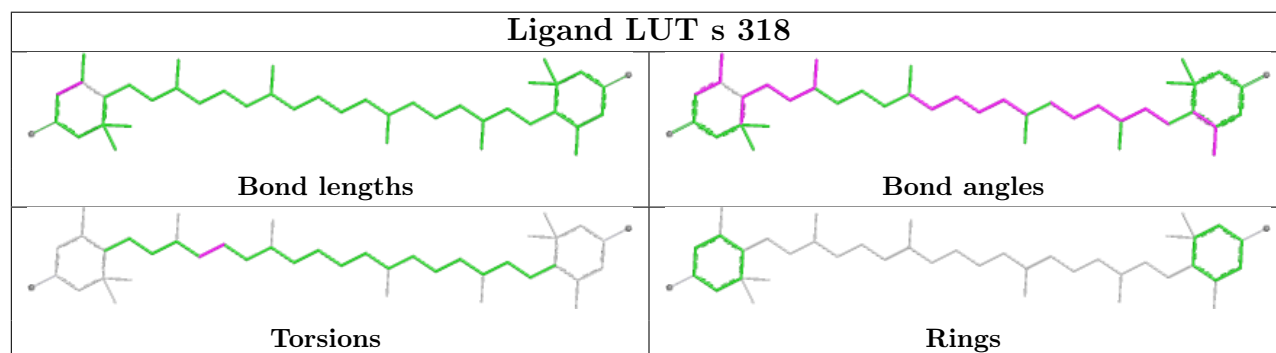
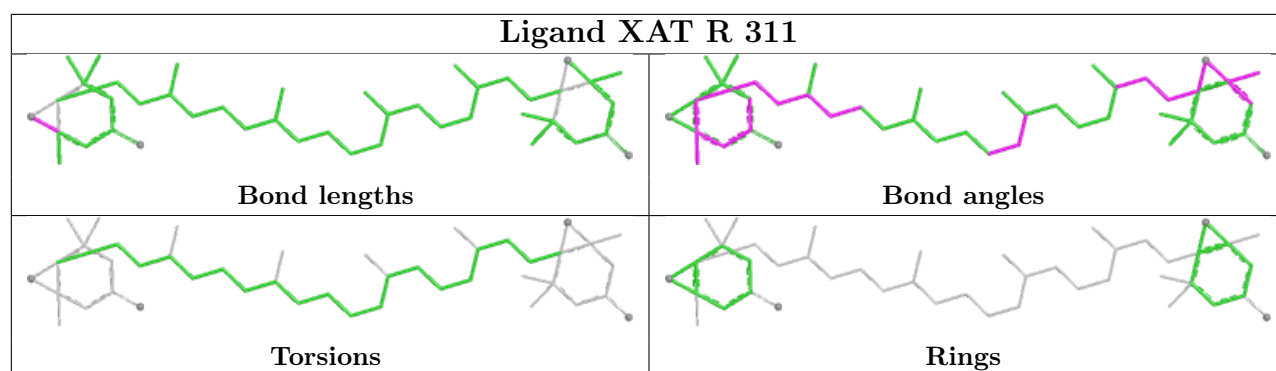


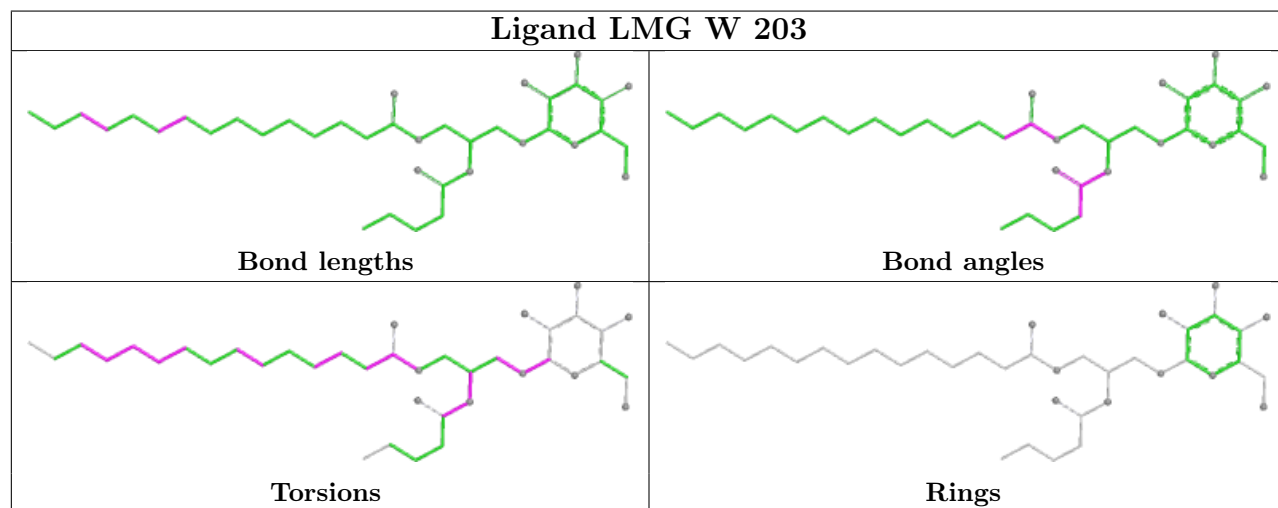
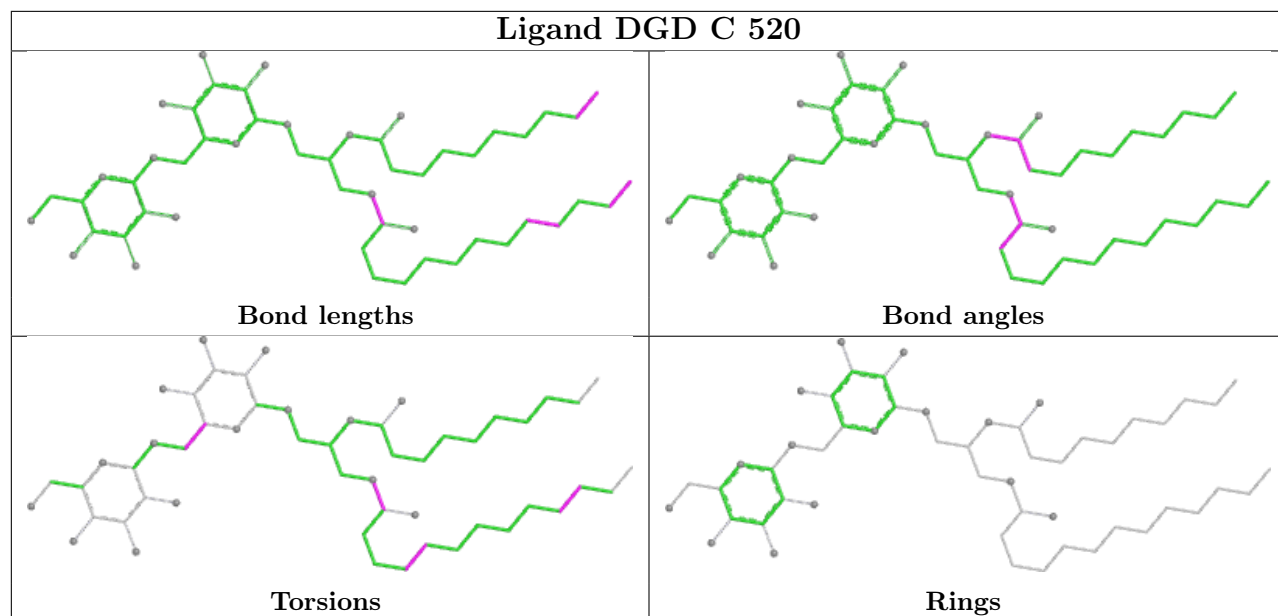
Ligand CLA Y 305

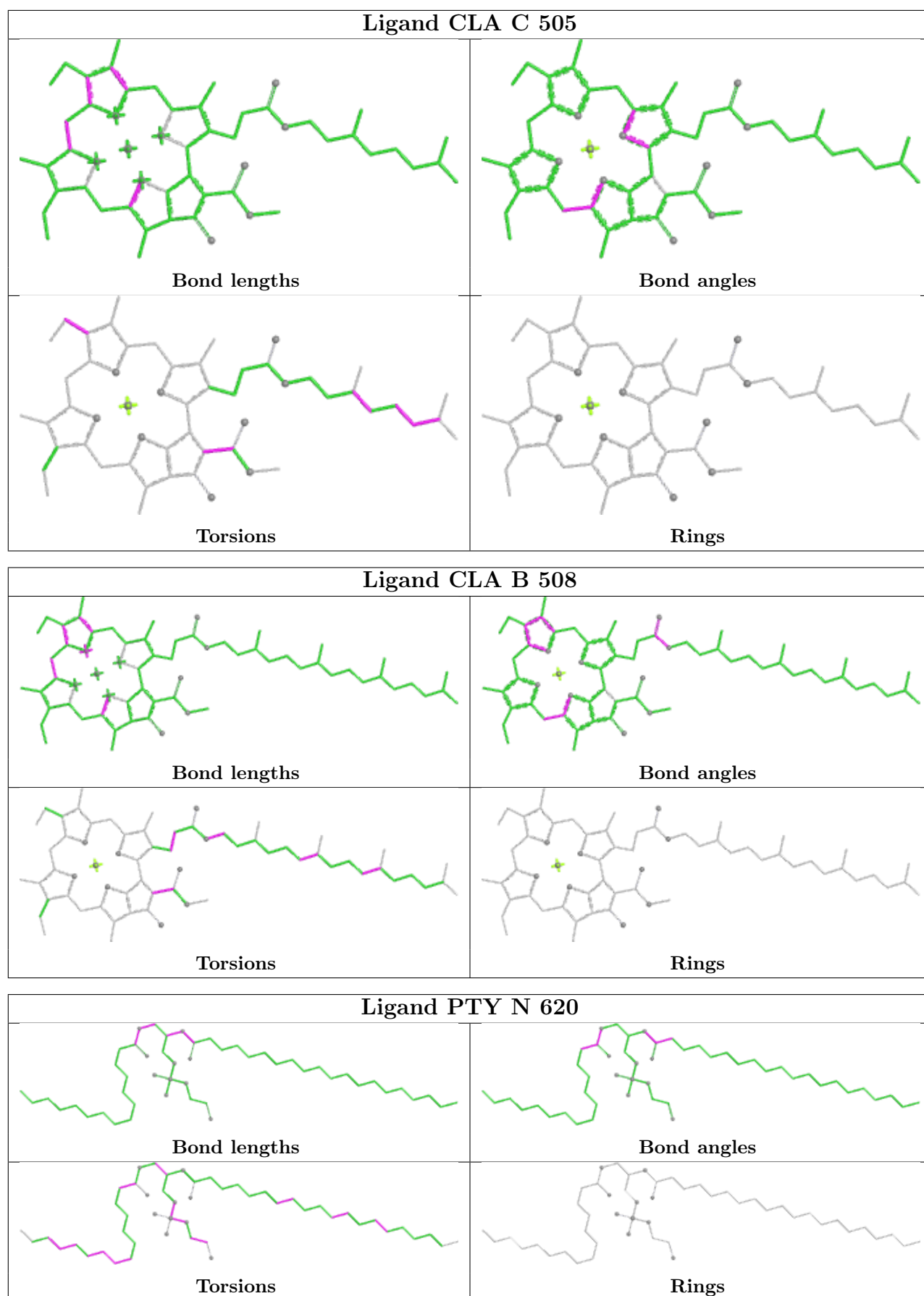




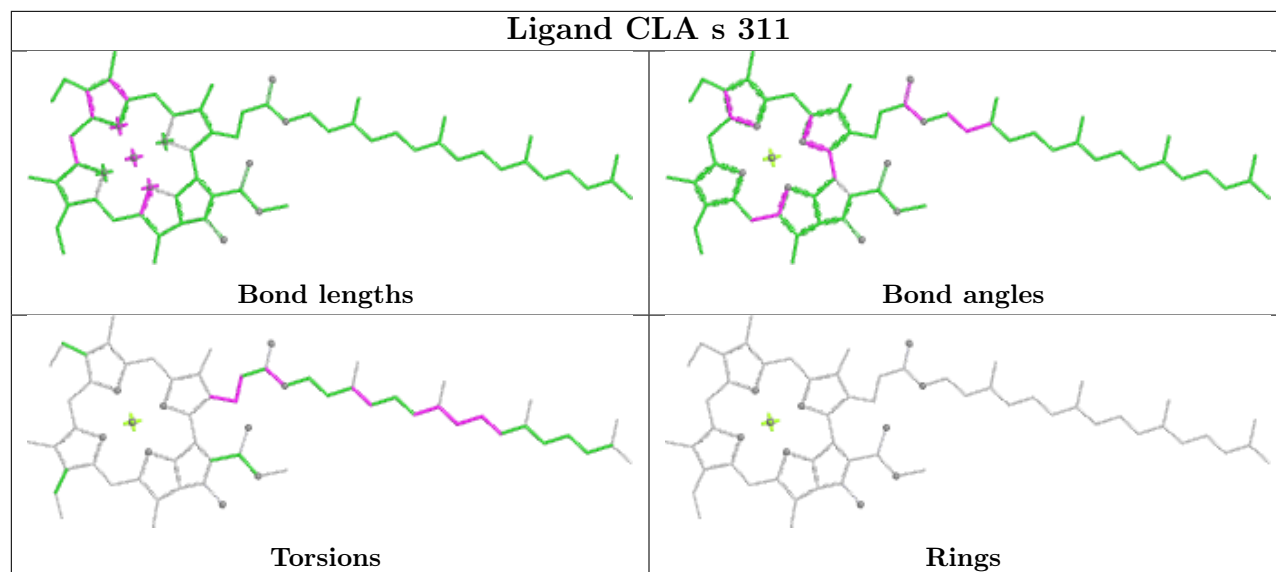




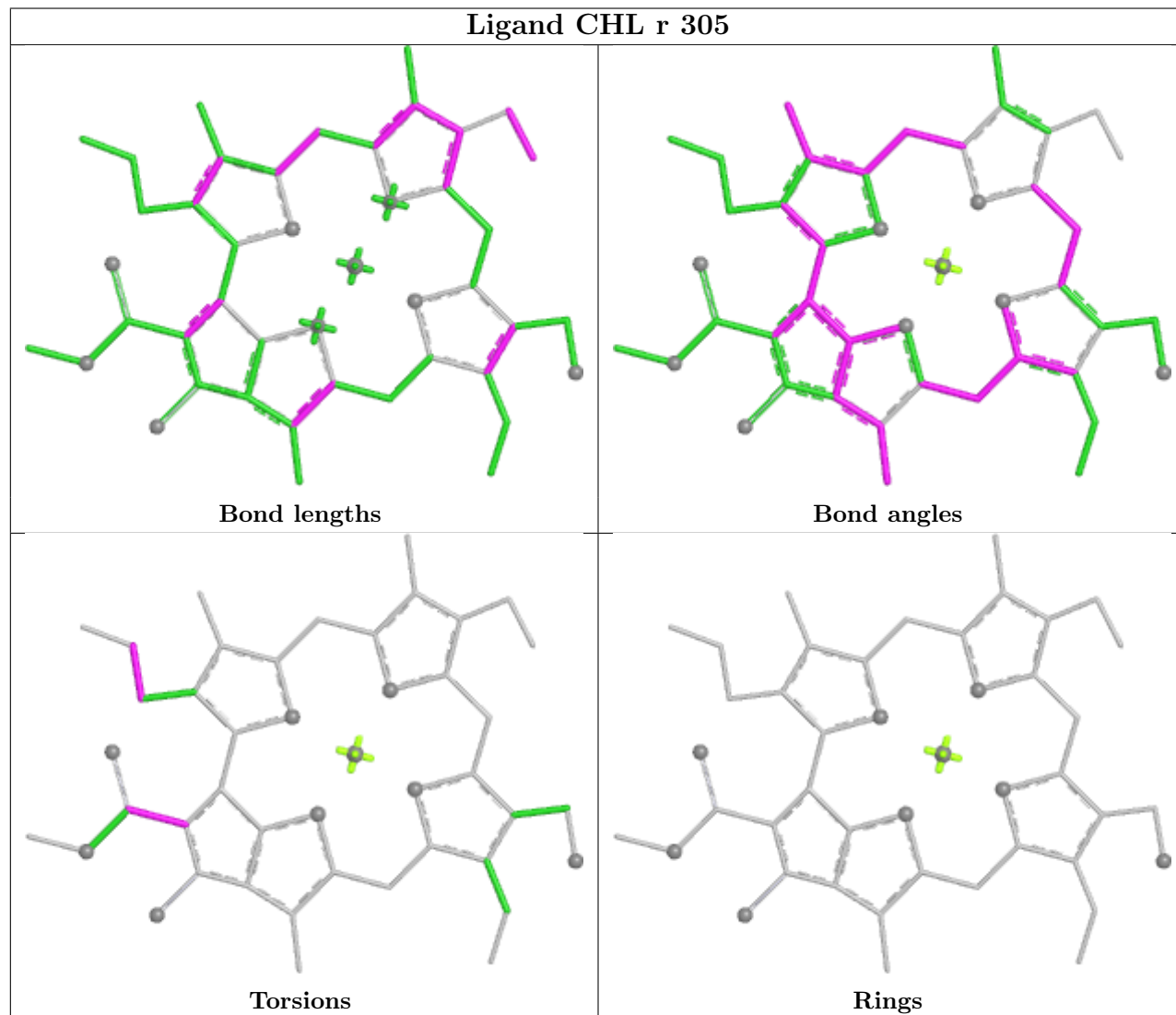


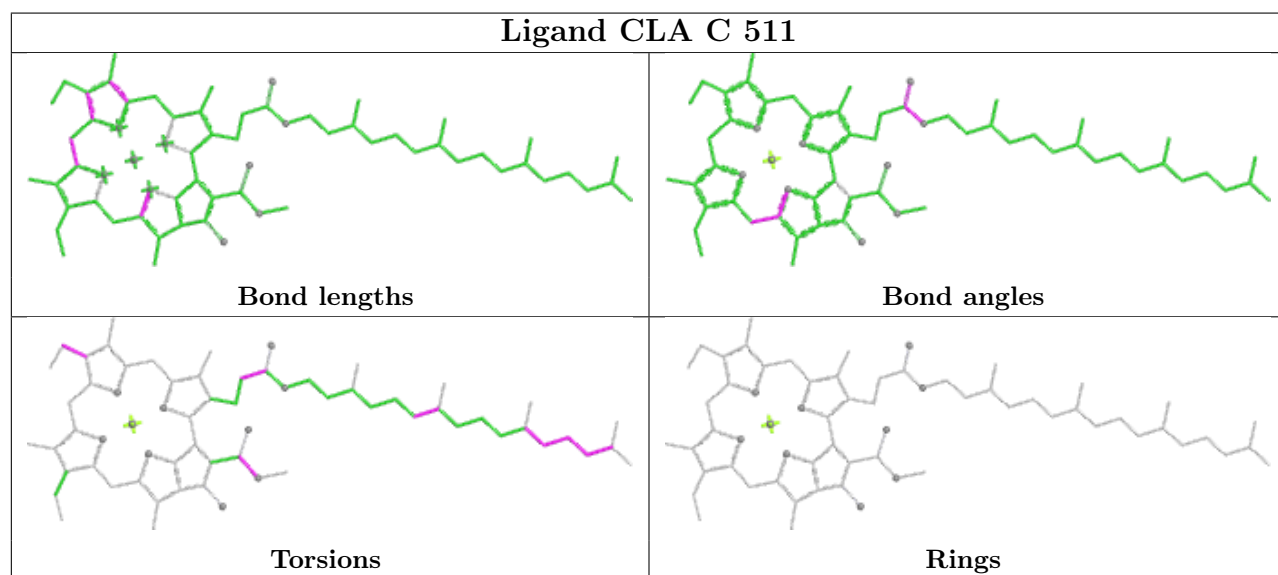
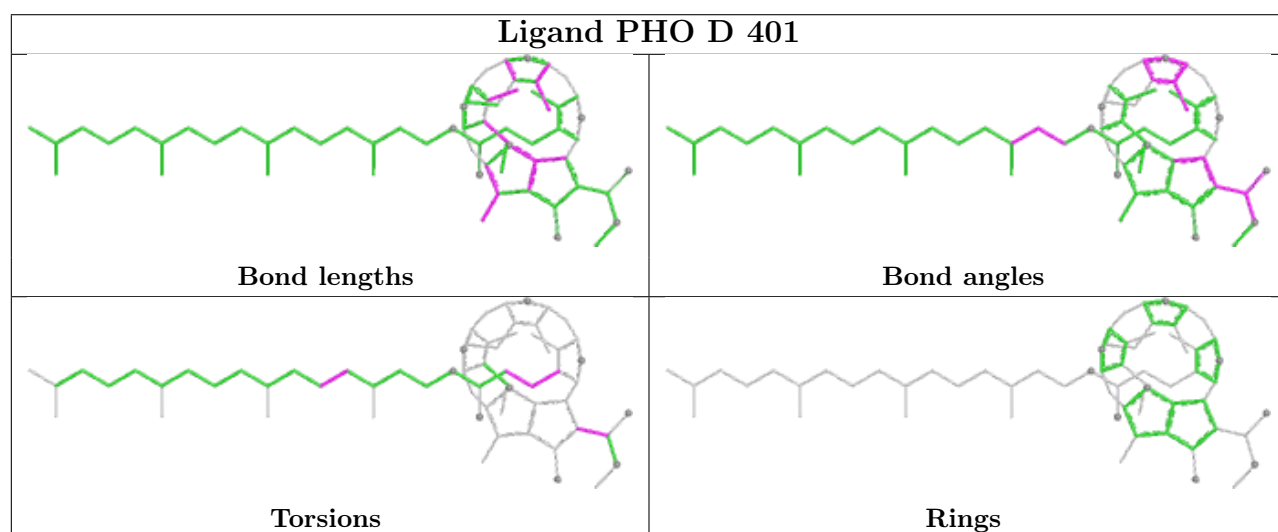
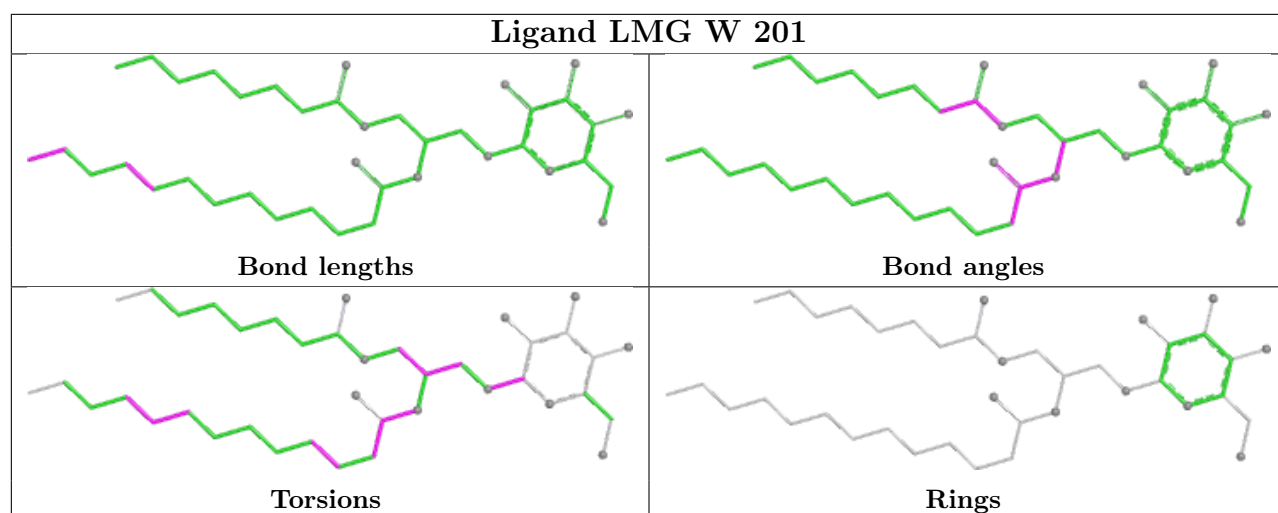


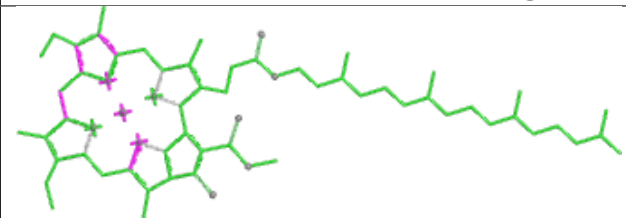
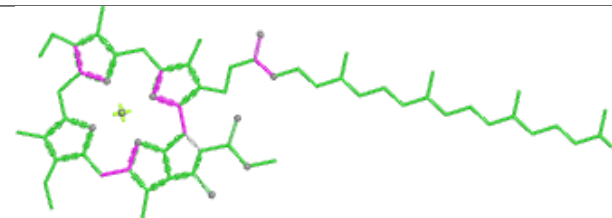
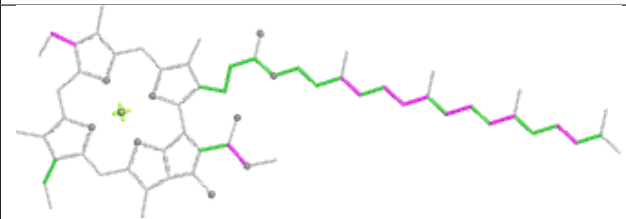
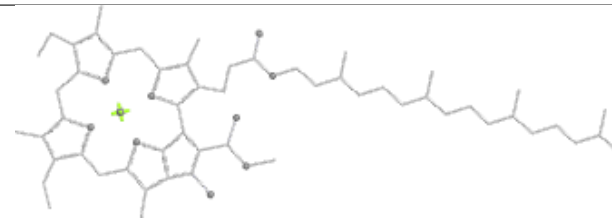
Ligand CLA s 311

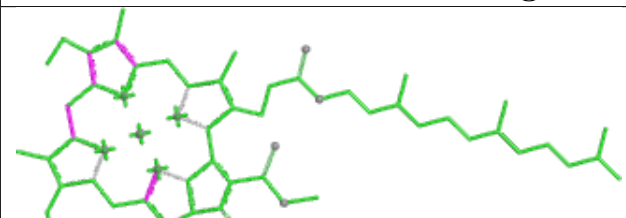
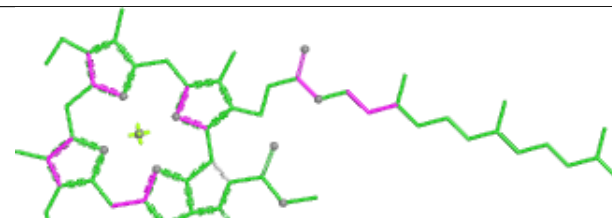
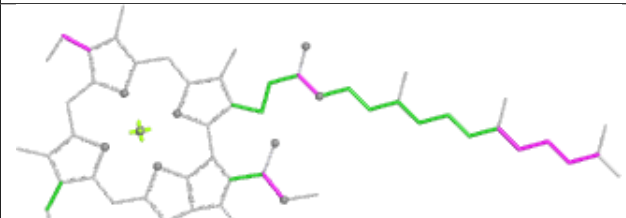
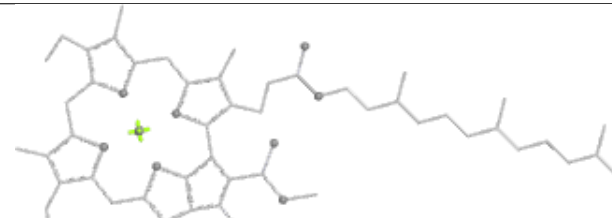


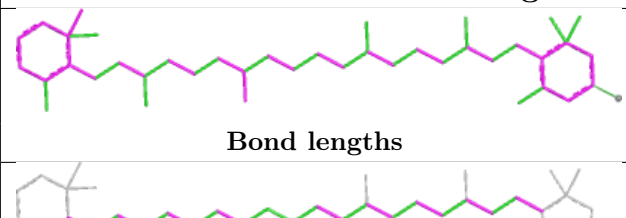
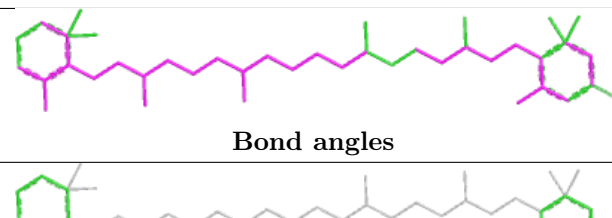
Ligand CHL r 305

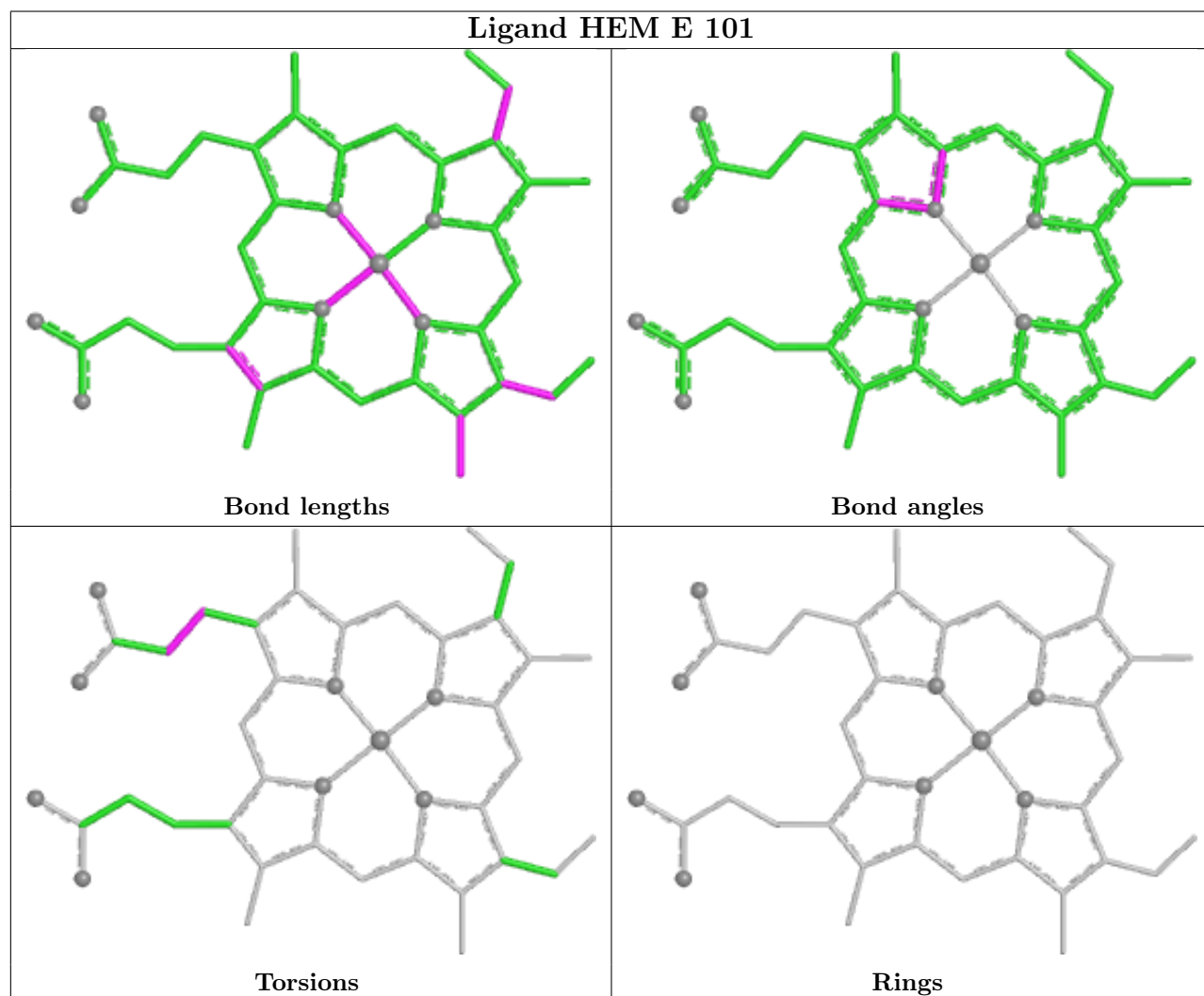
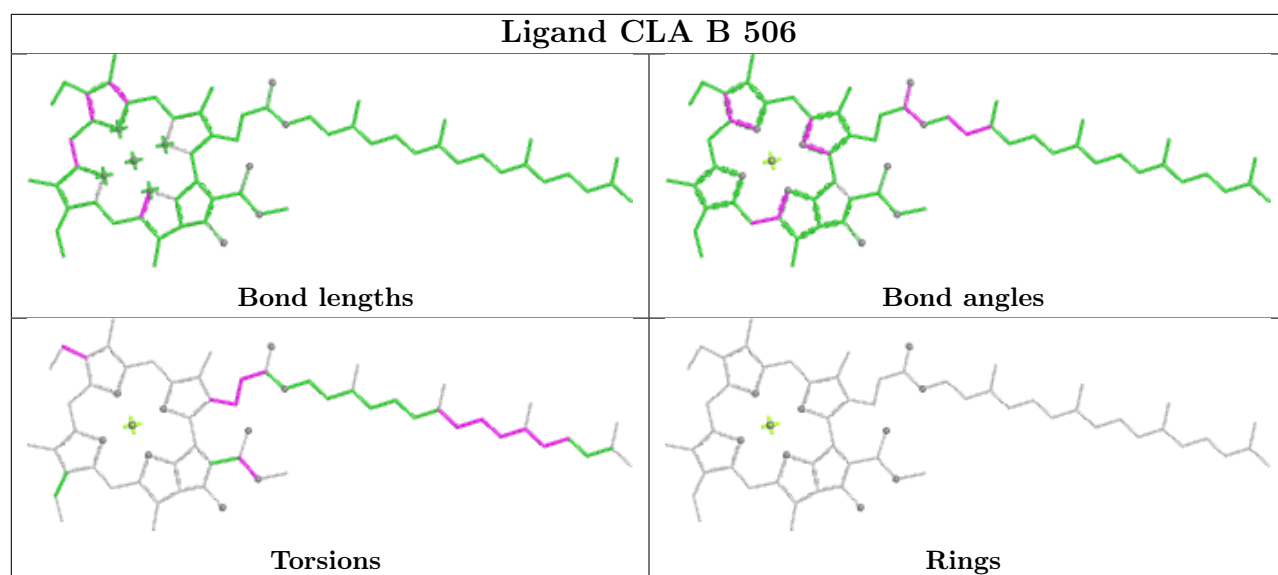


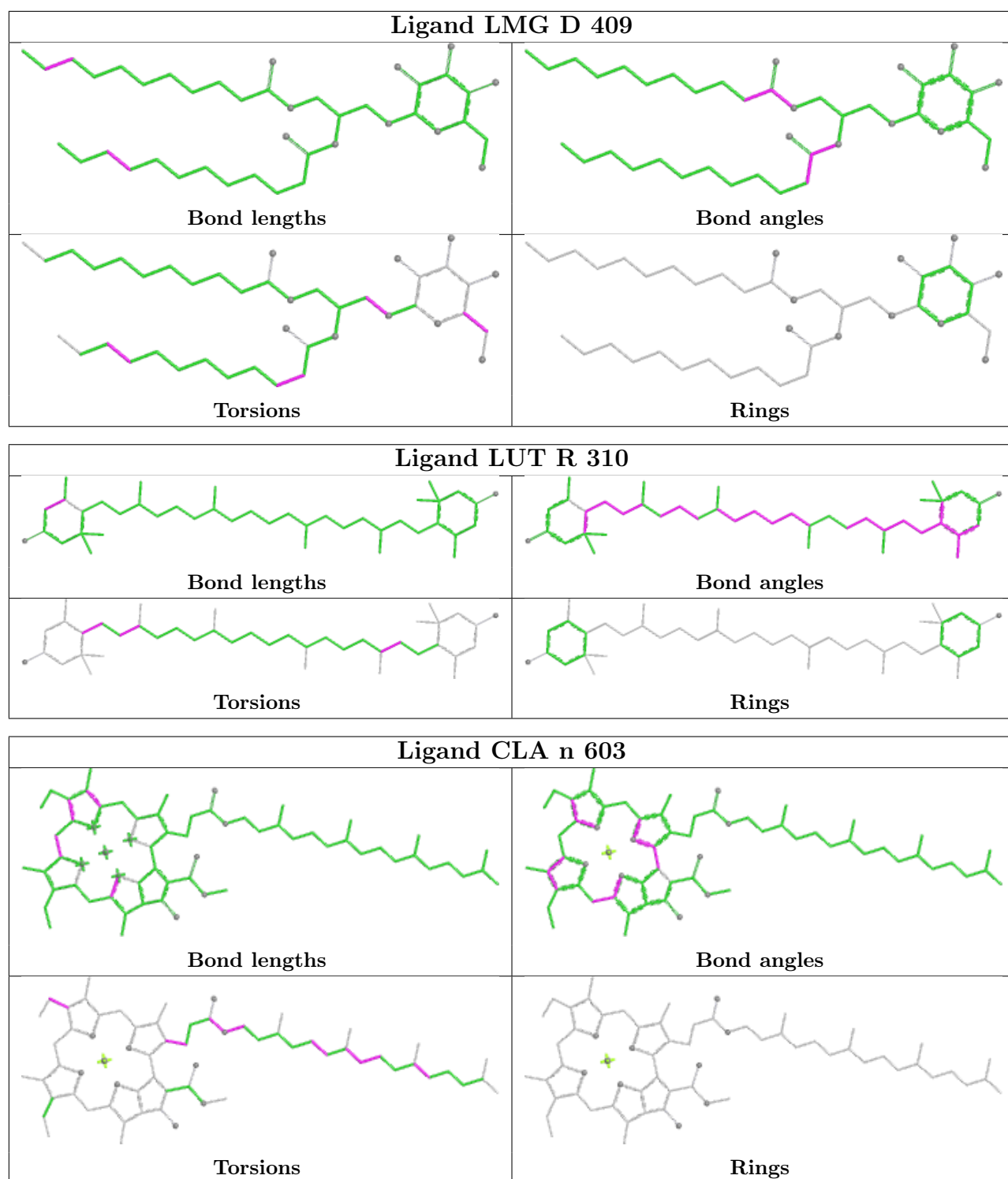


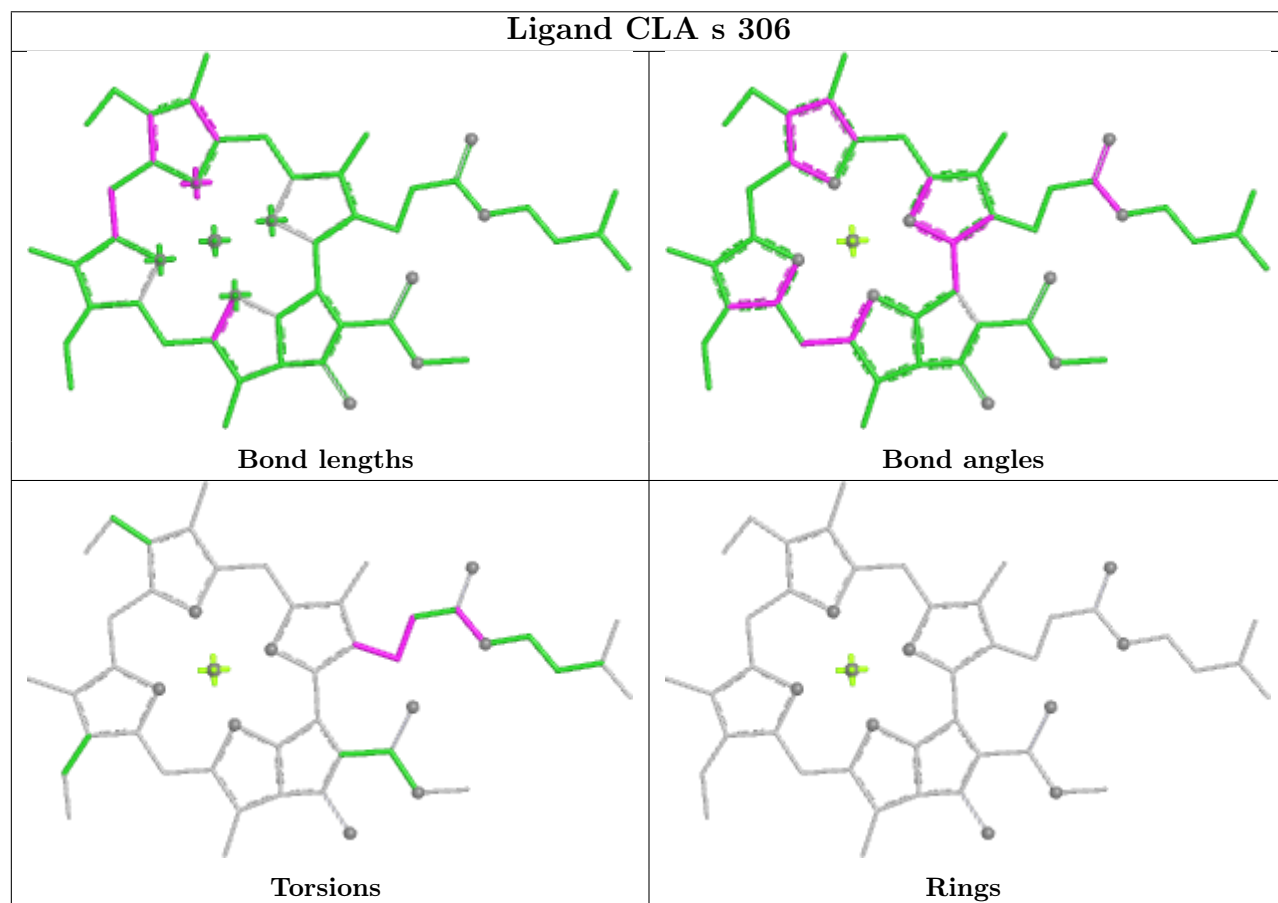
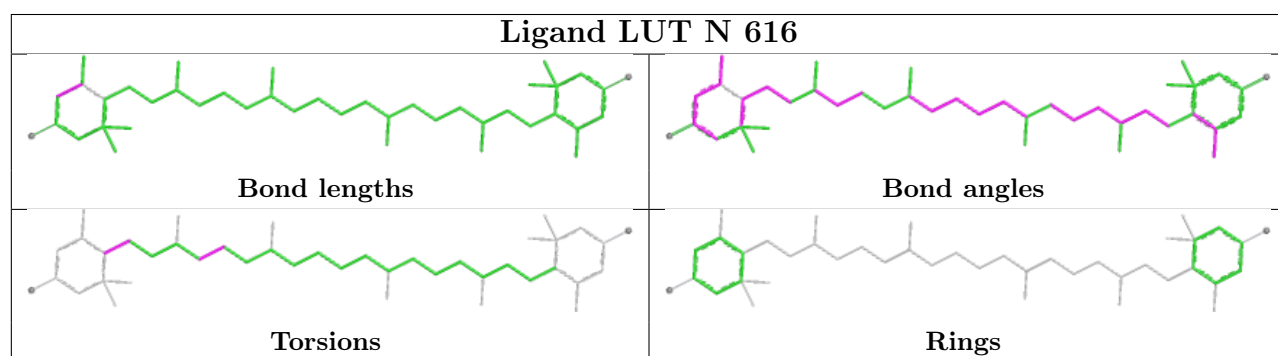
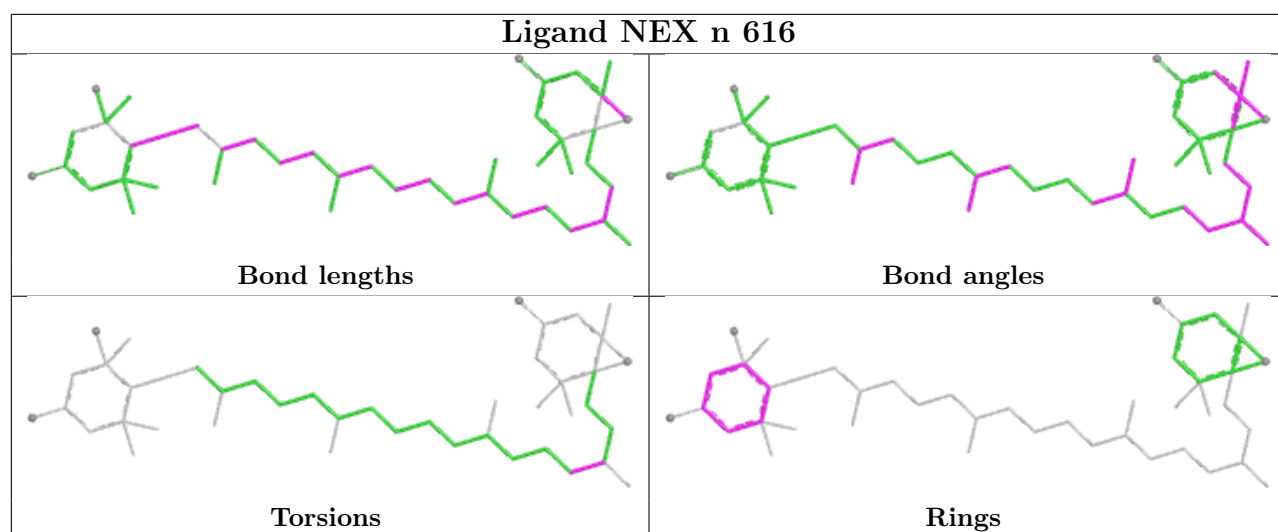
Ligand CLA B 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

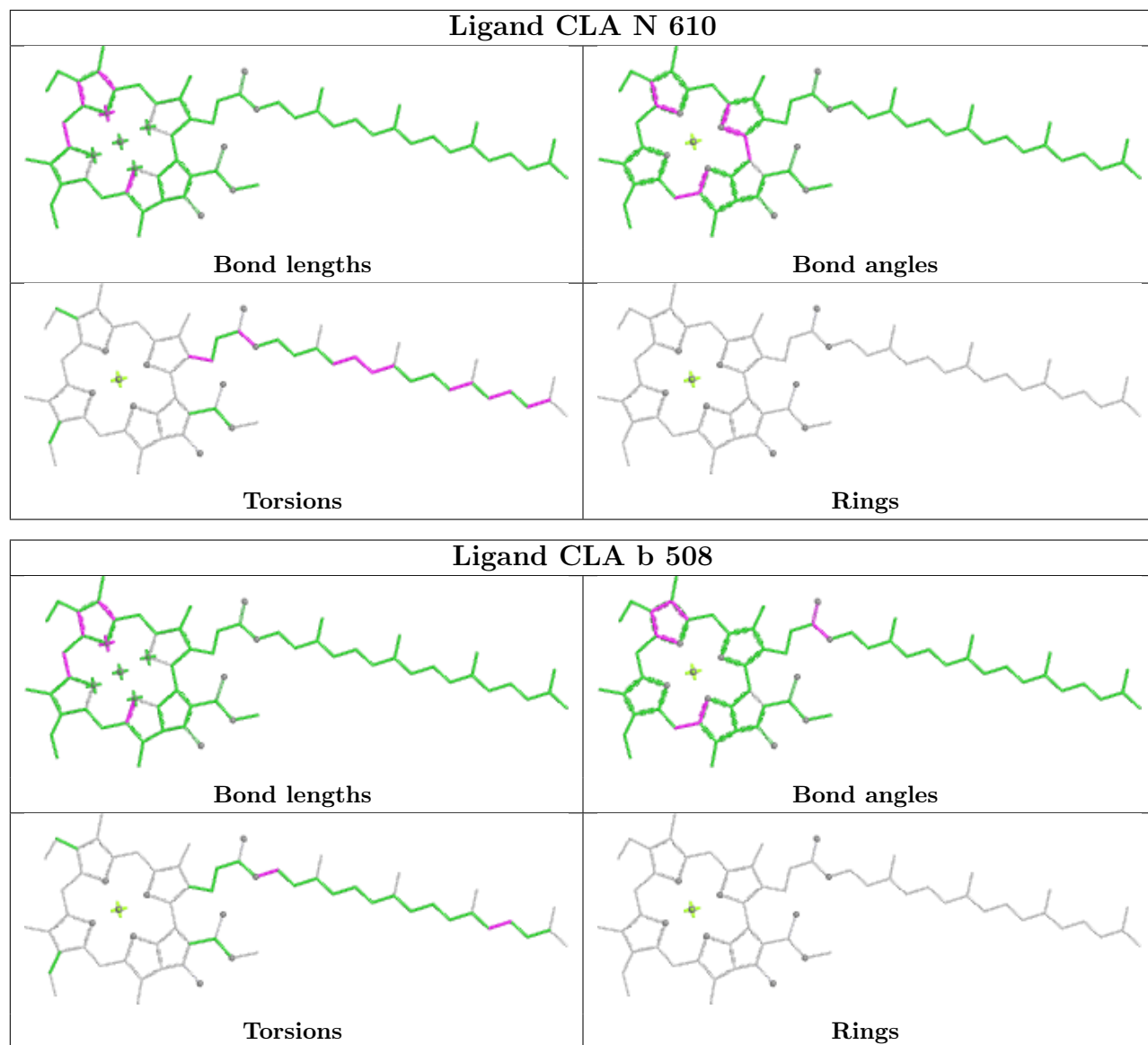
Ligand CLA D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

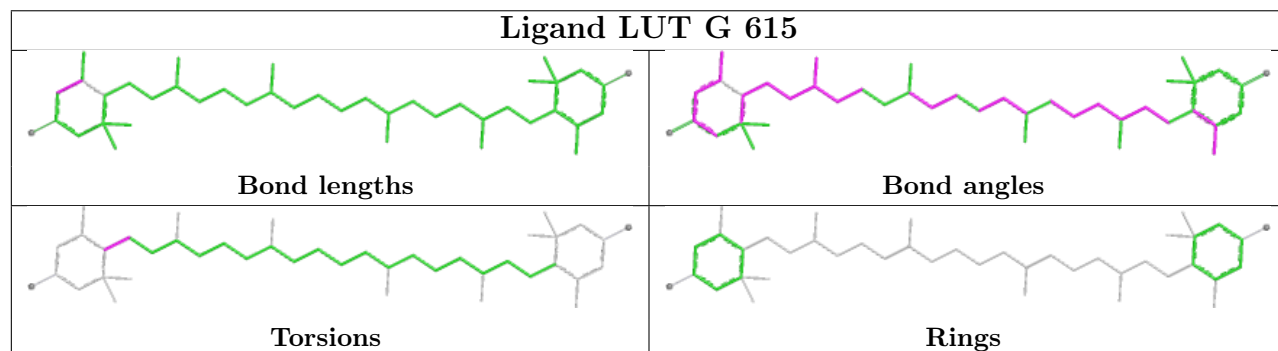
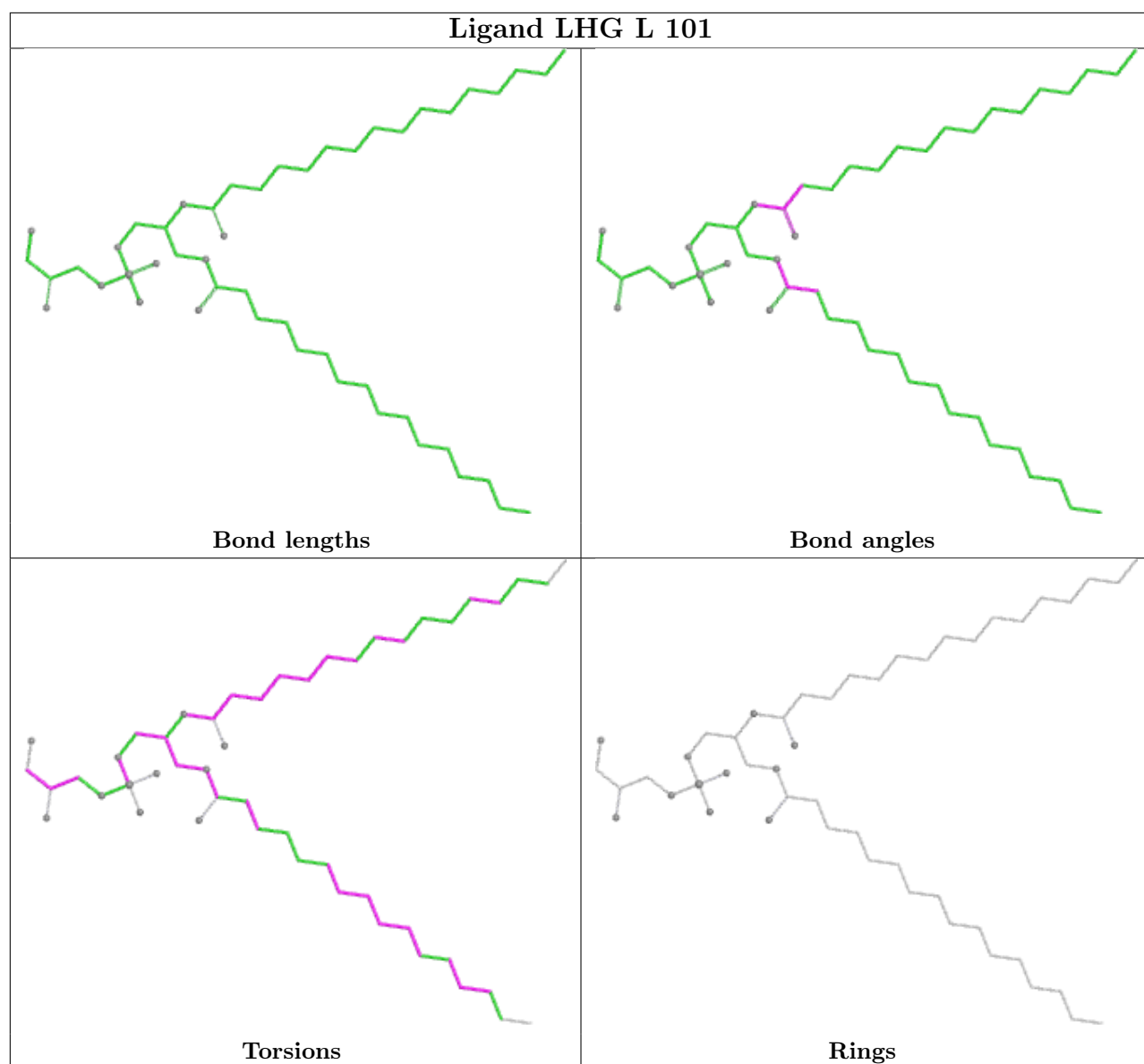
Ligand RRX h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

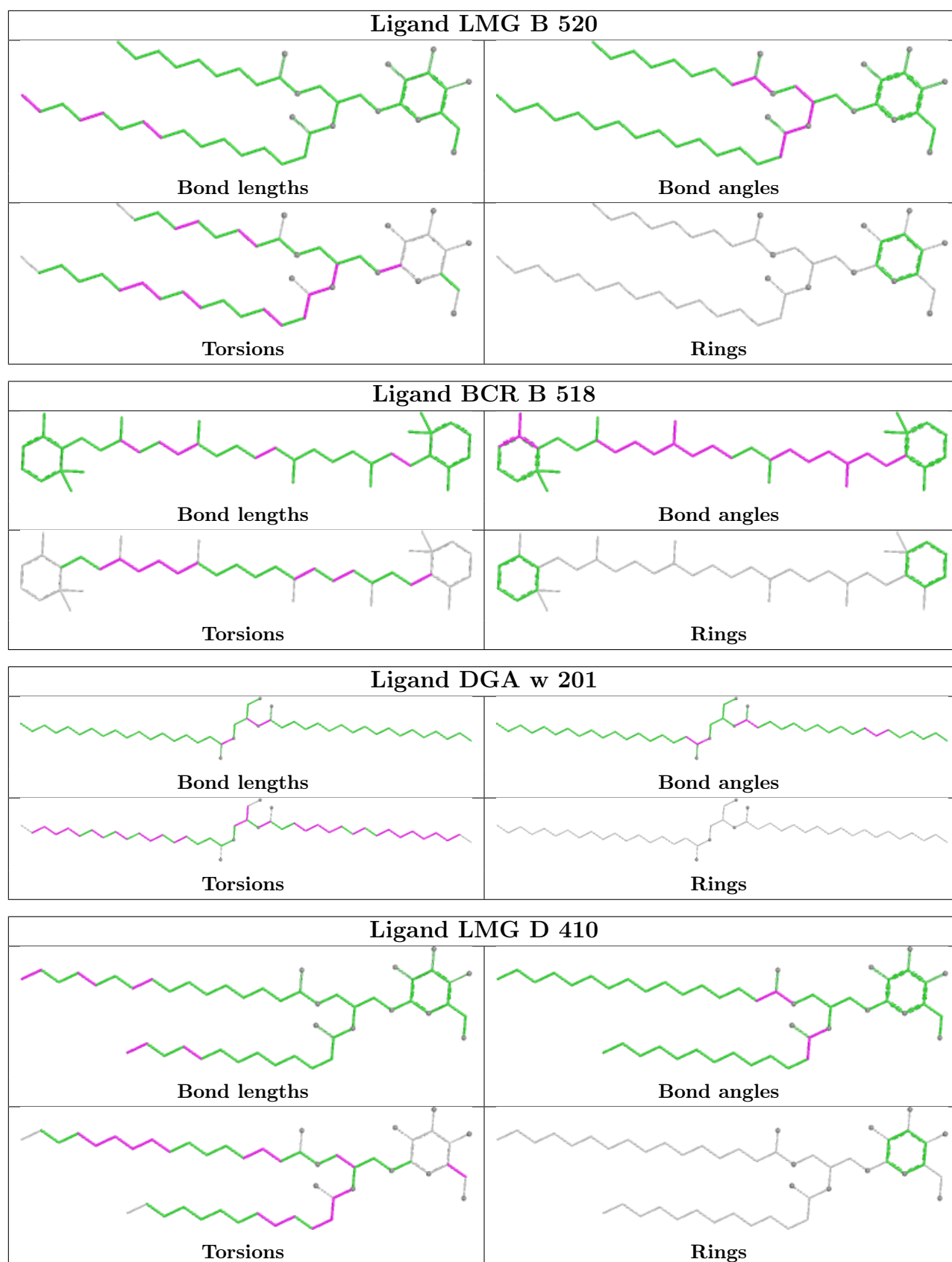


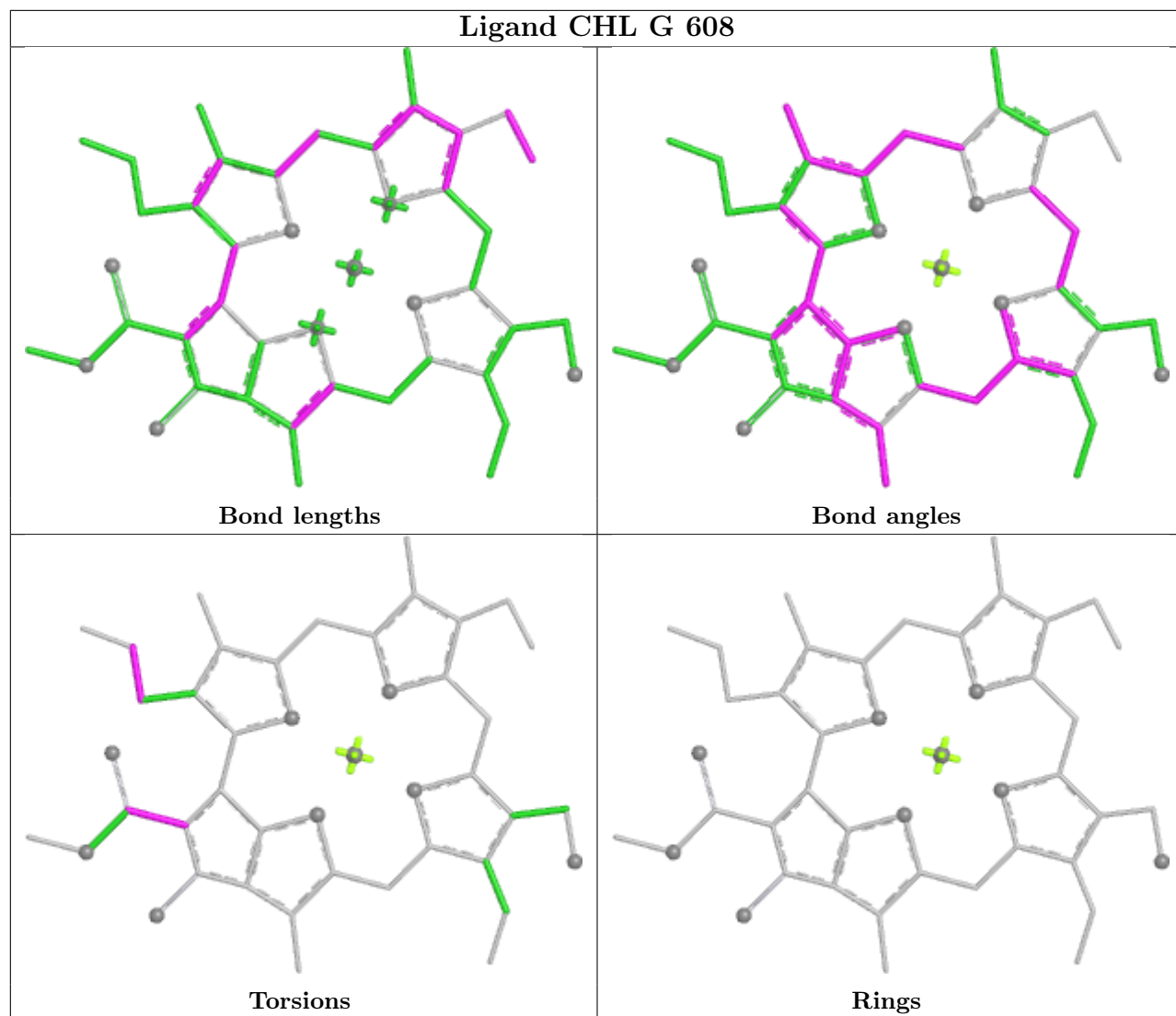




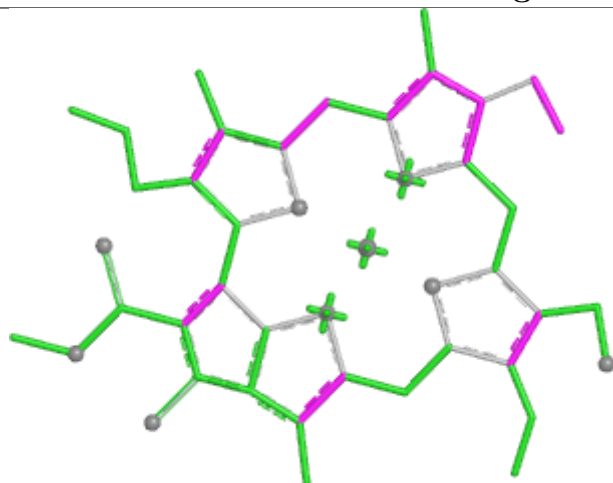




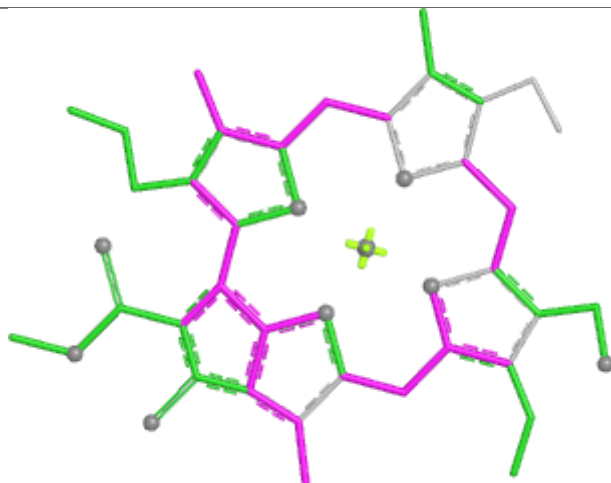




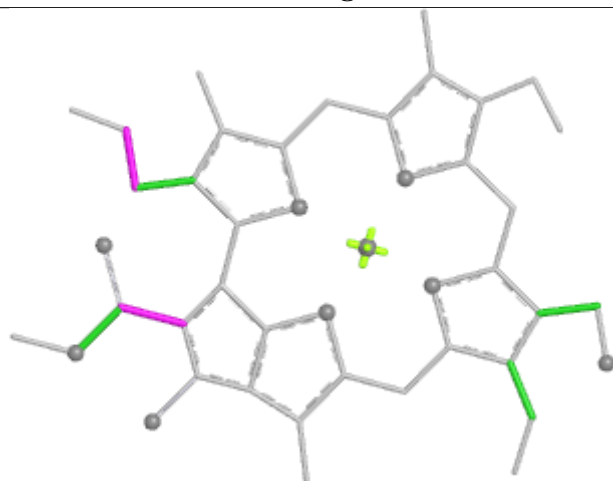
Ligand CHL R 304



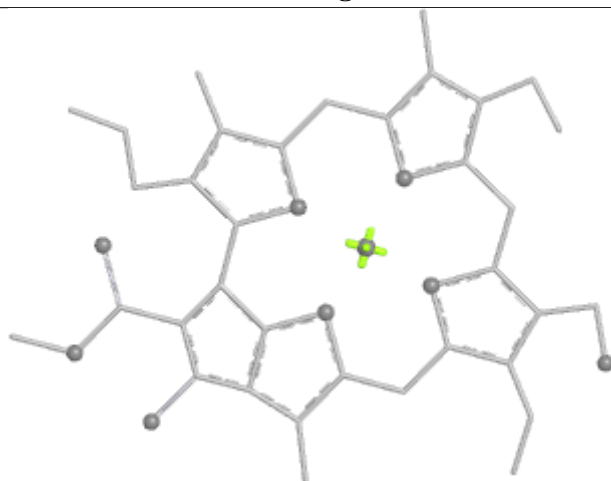
Bond lengths



Bond angles

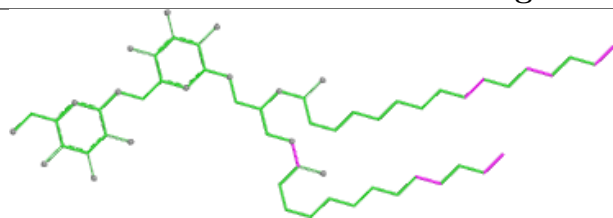


Torsions

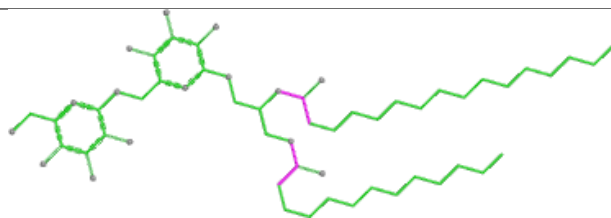


Rings

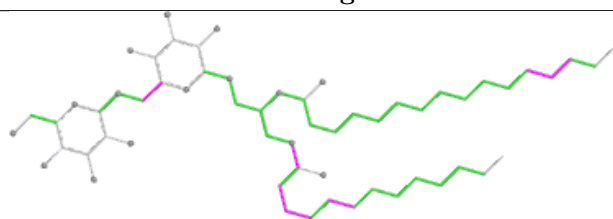
Ligand DGD c 518



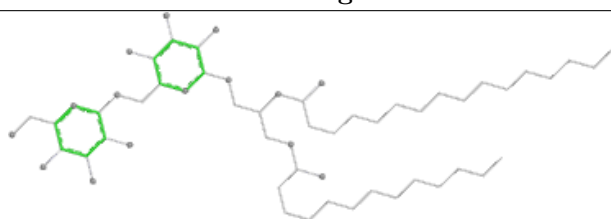
Bond lengths



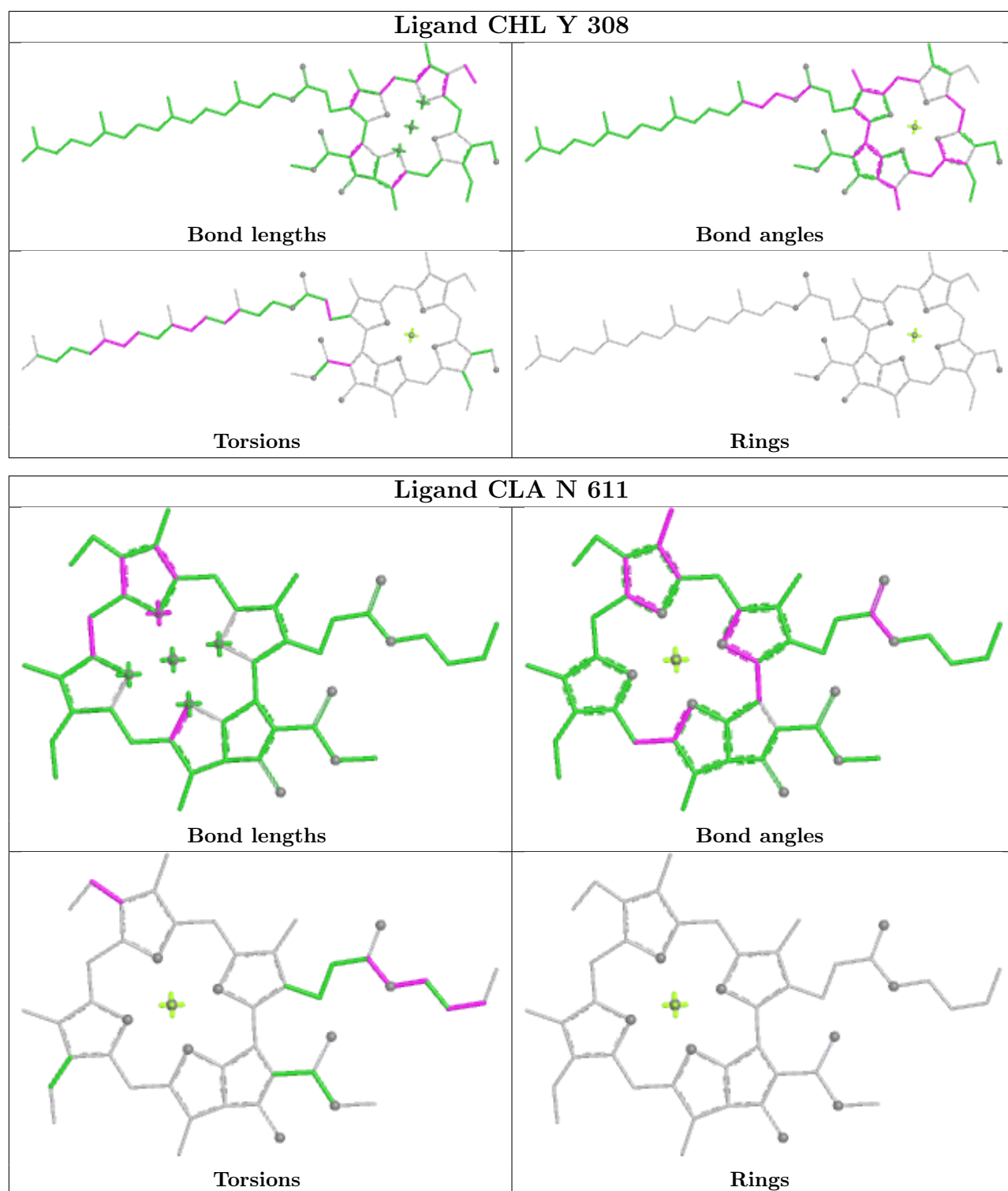
Bond angles

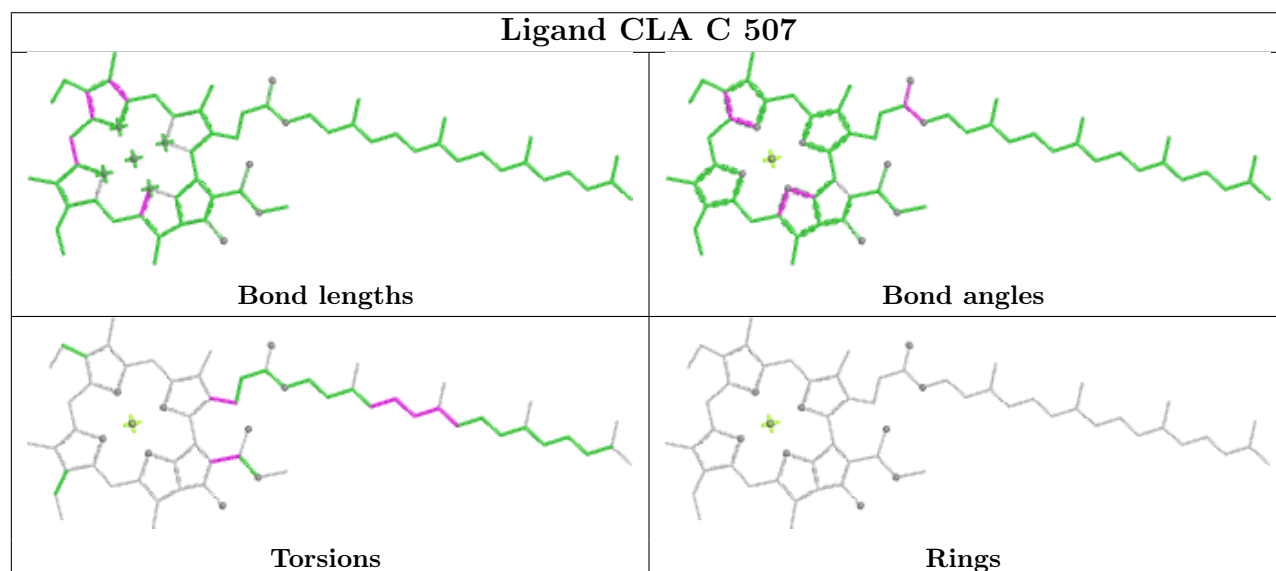
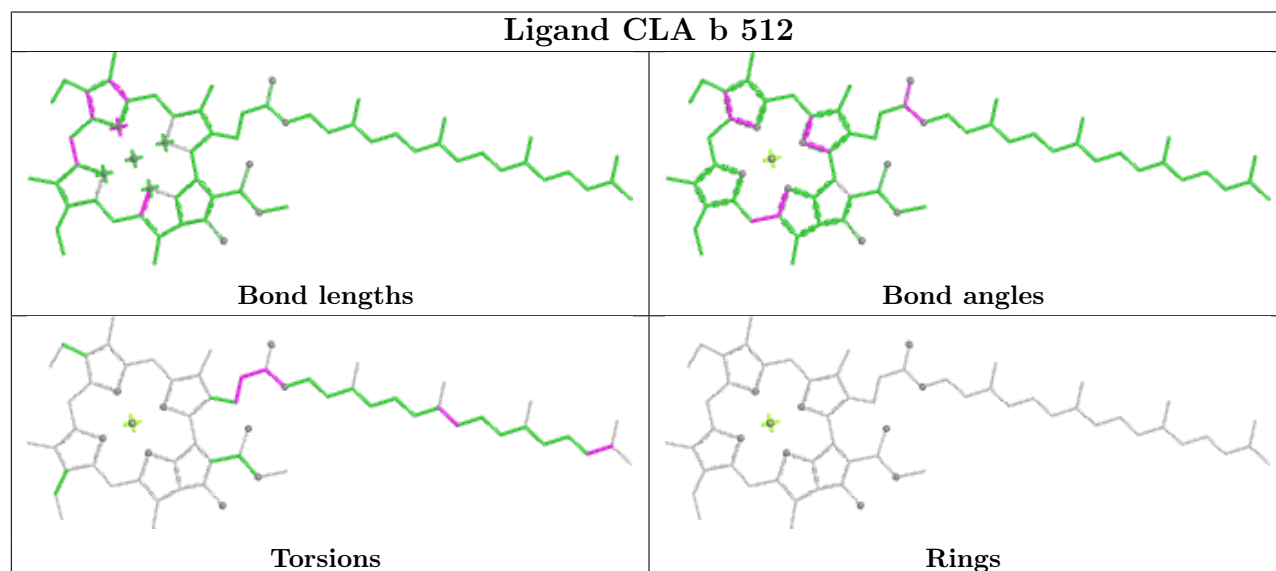
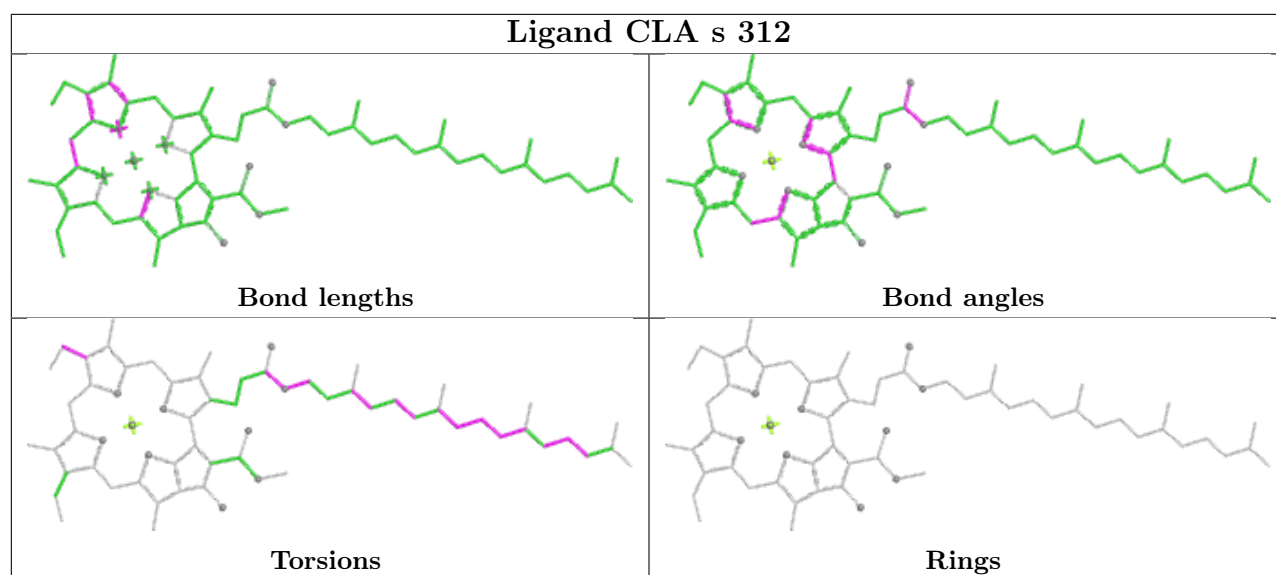


Torsions

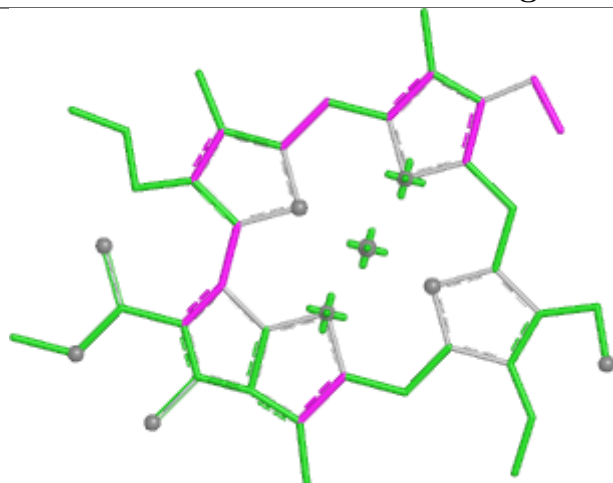


Rings

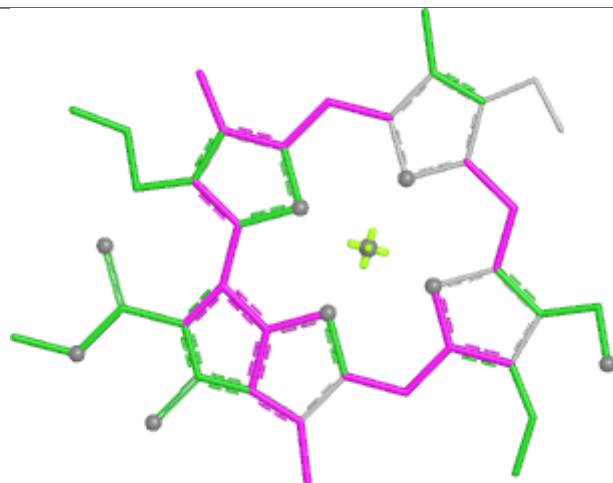




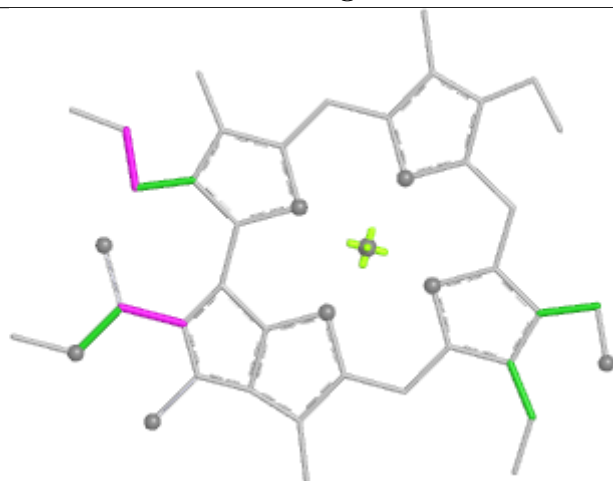
Ligand CHL s 307



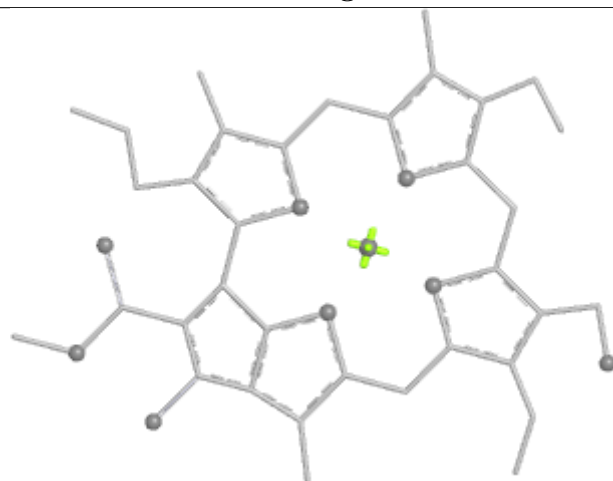
Bond lengths



Bond angles

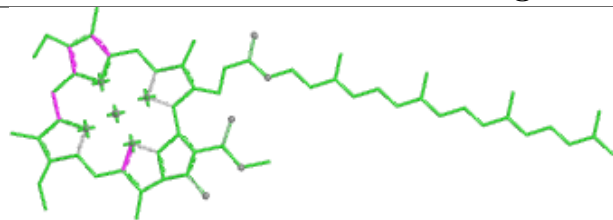


Torsions

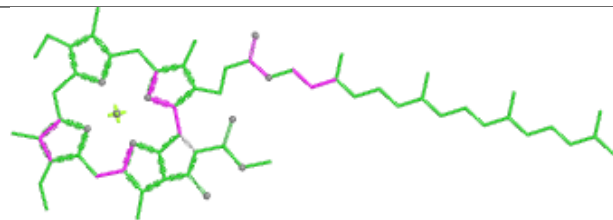


Rings

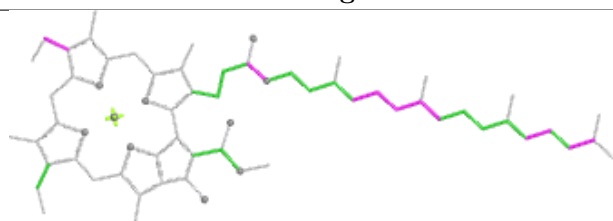
Ligand CLA Y 312



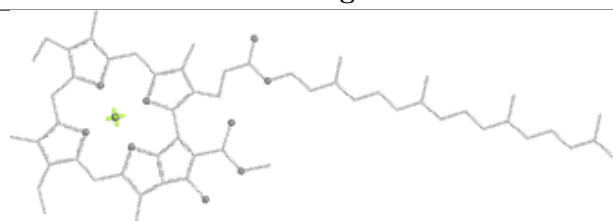
Bond lengths



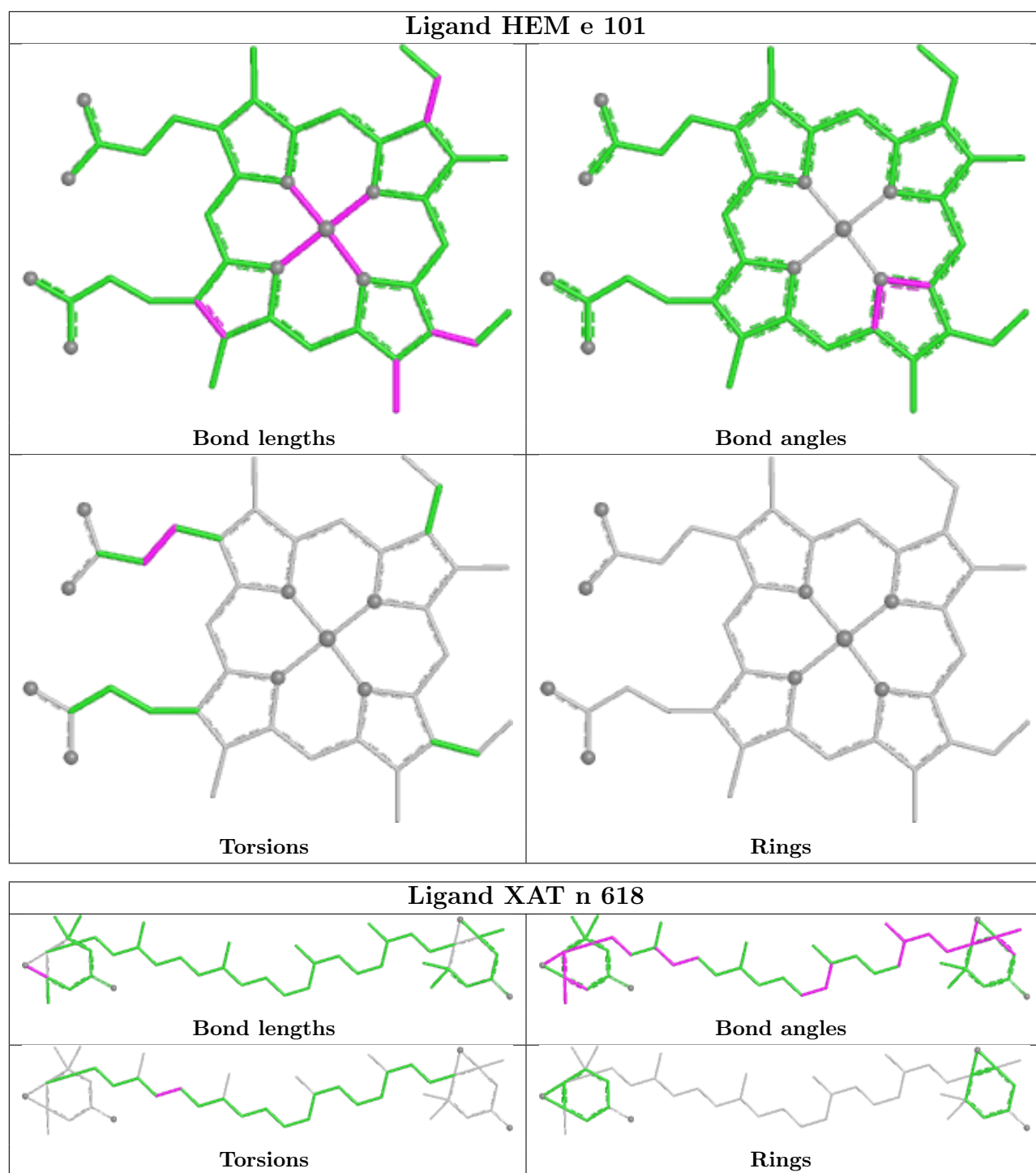
Bond angles

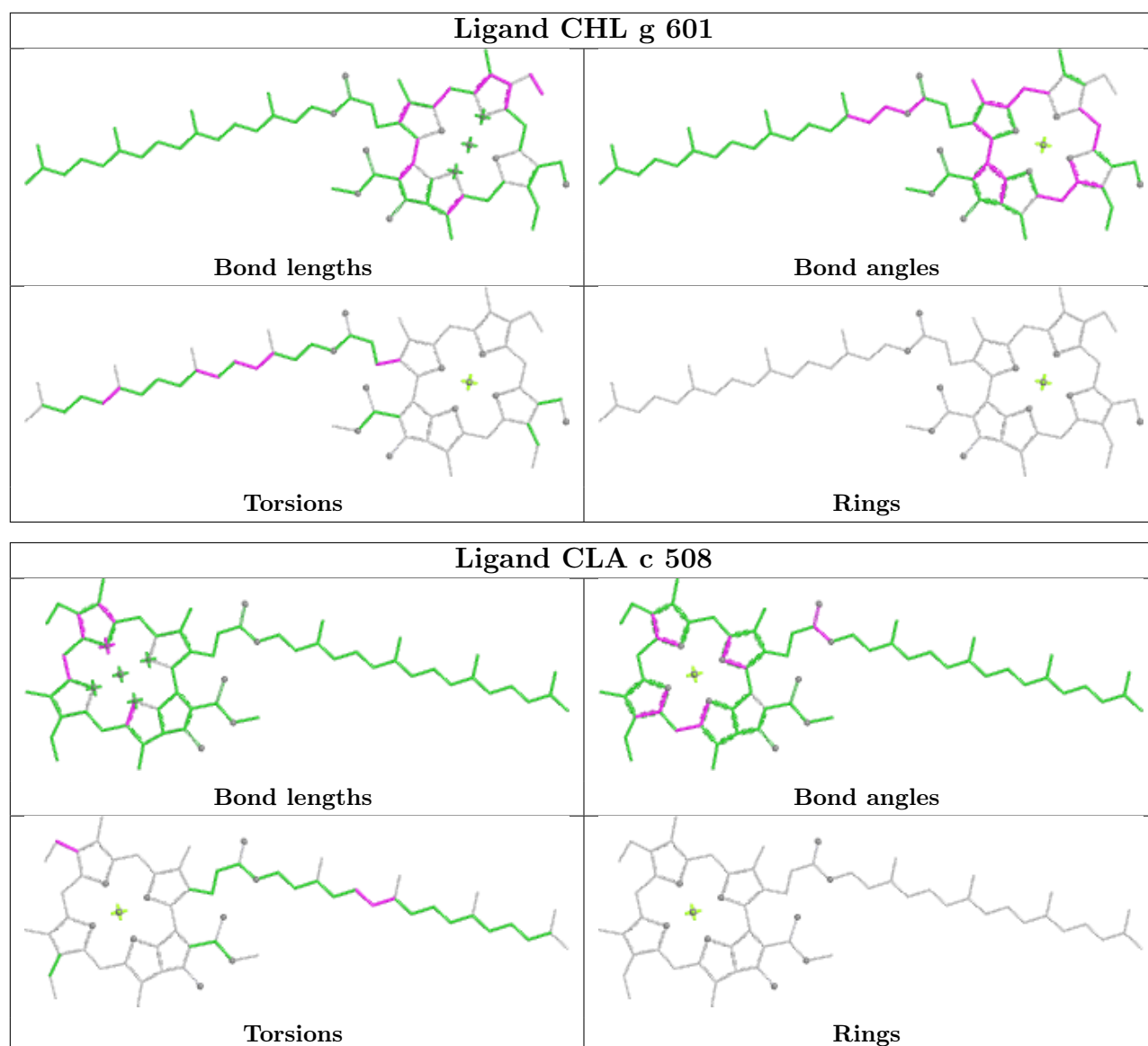


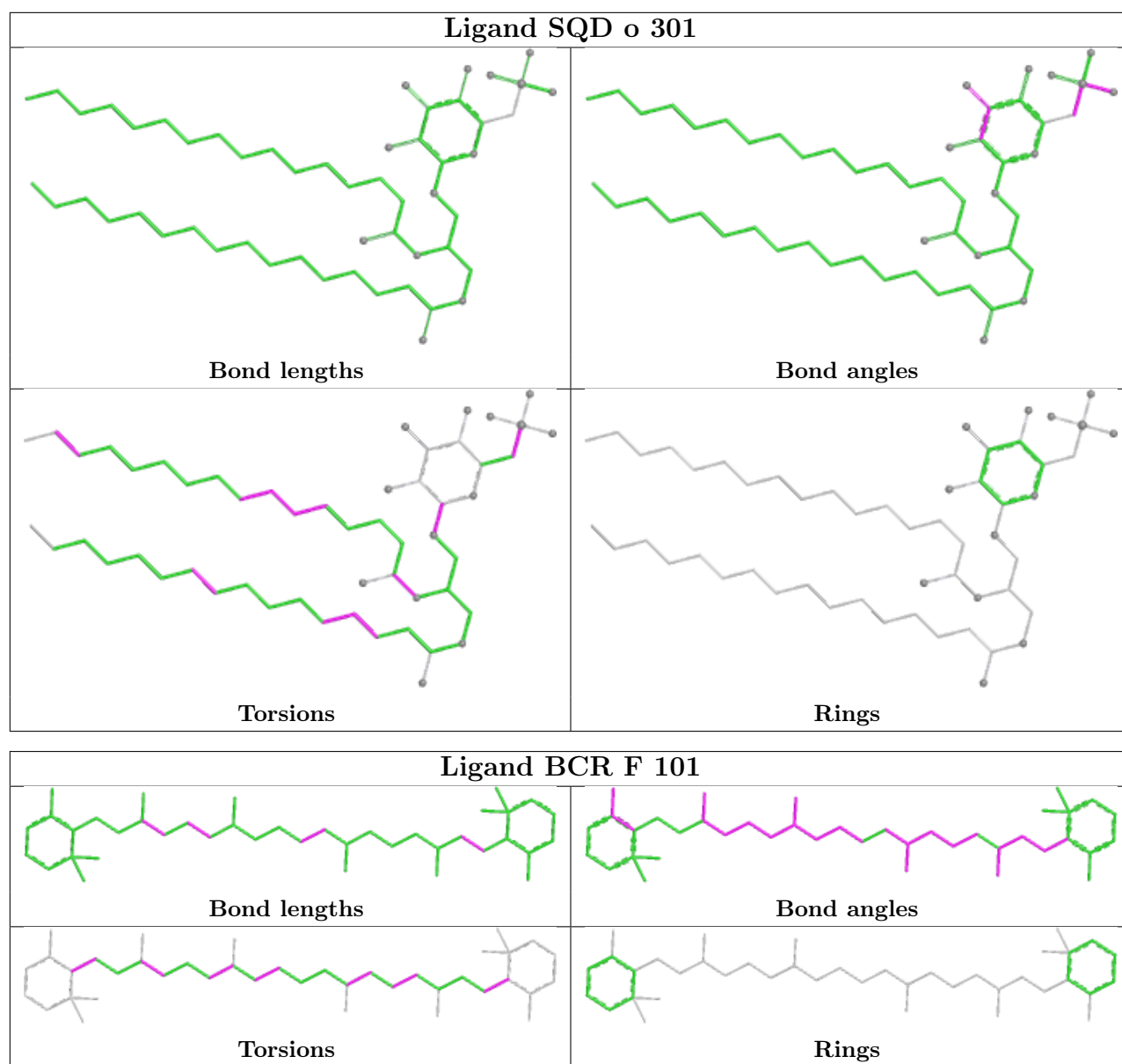
Torsions

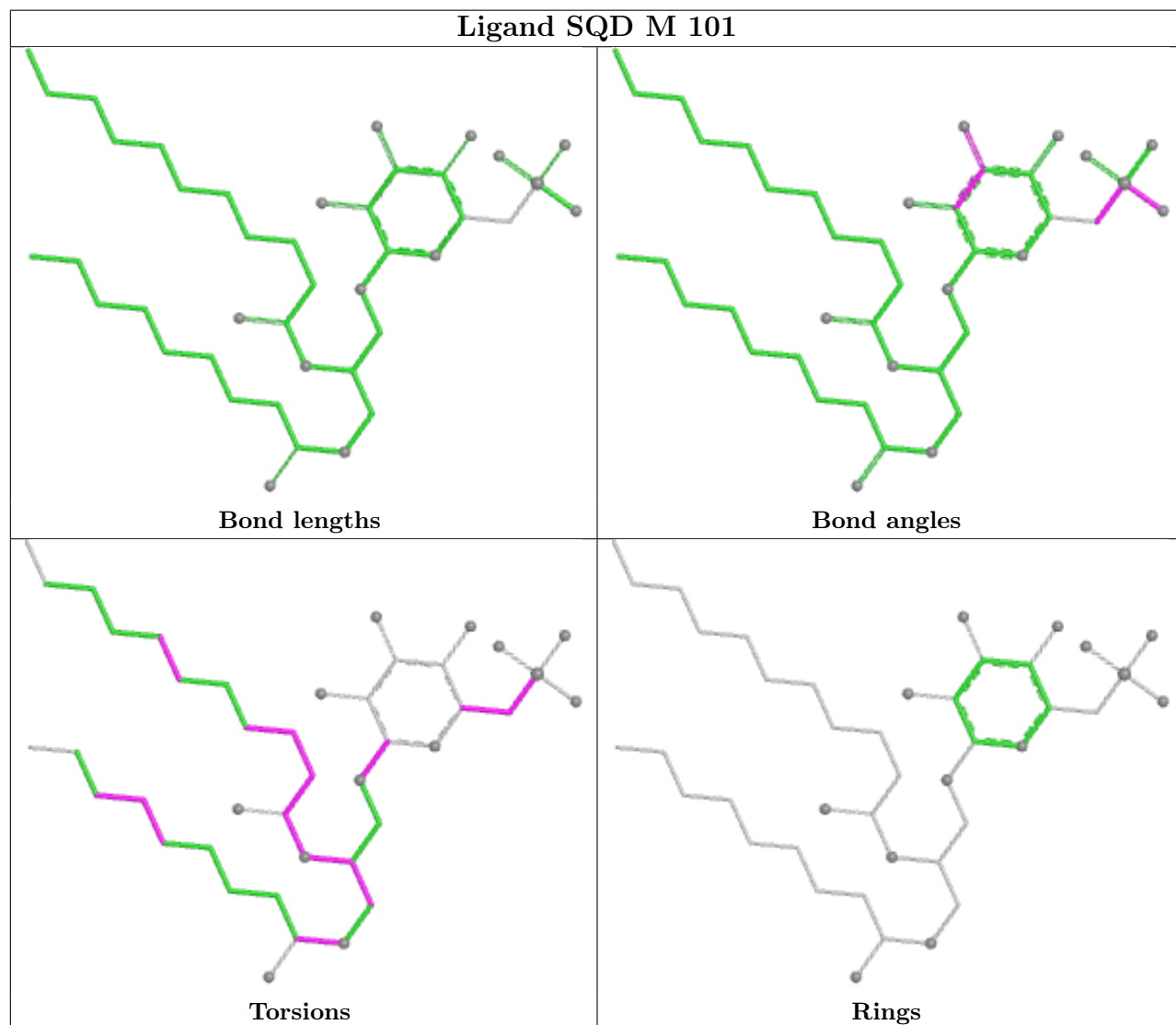
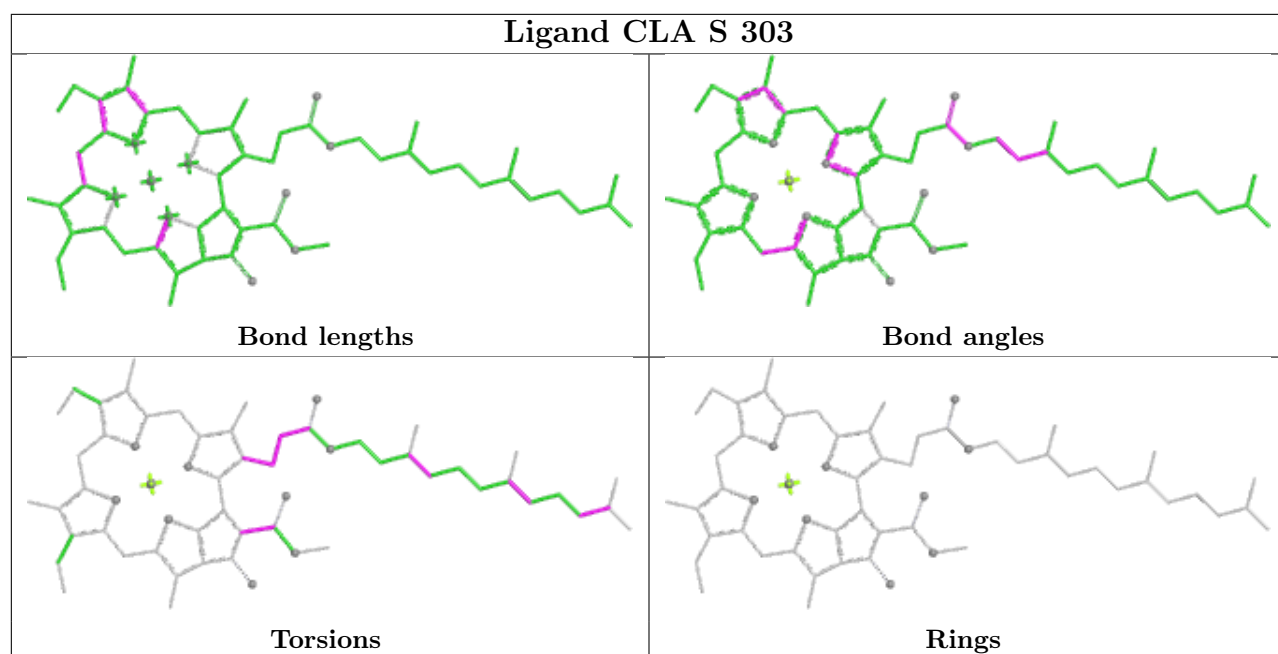


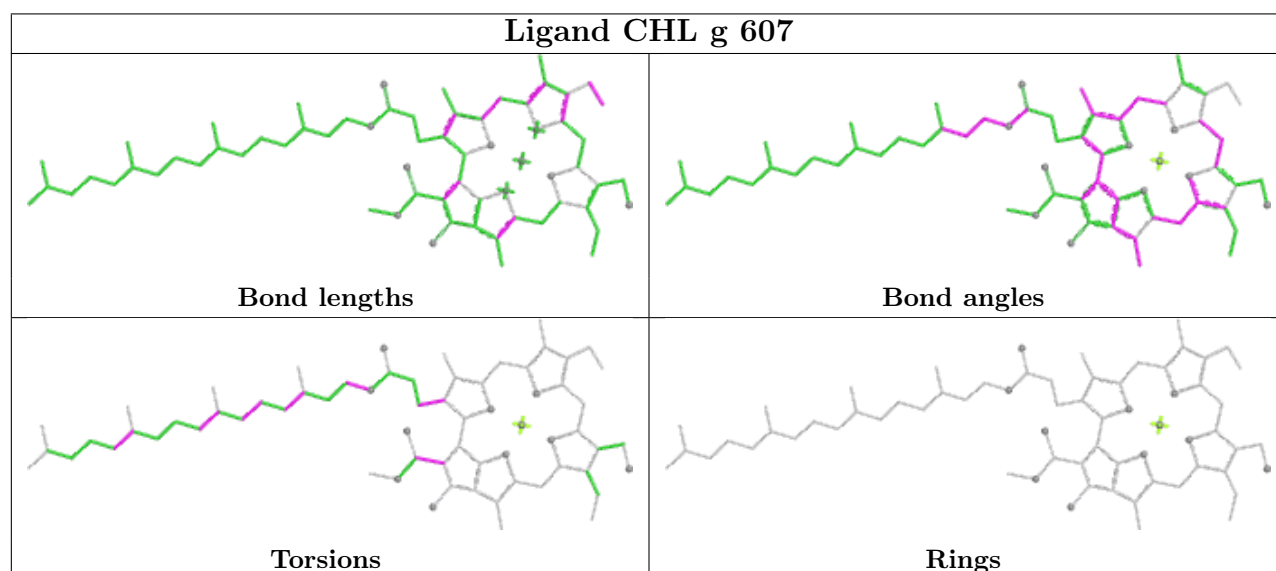
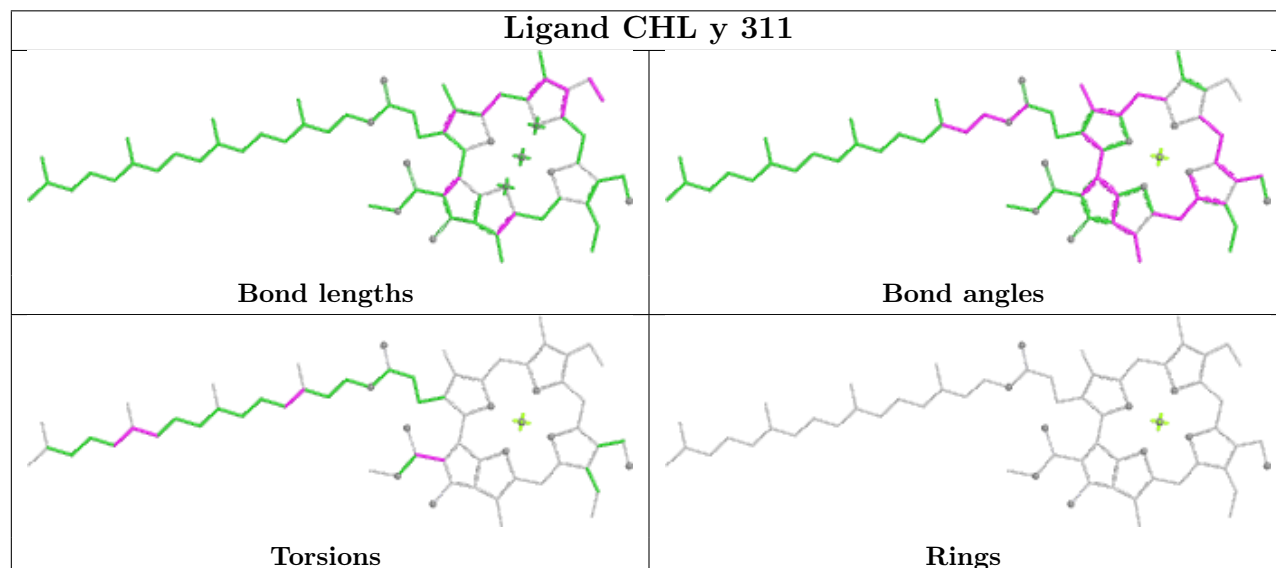
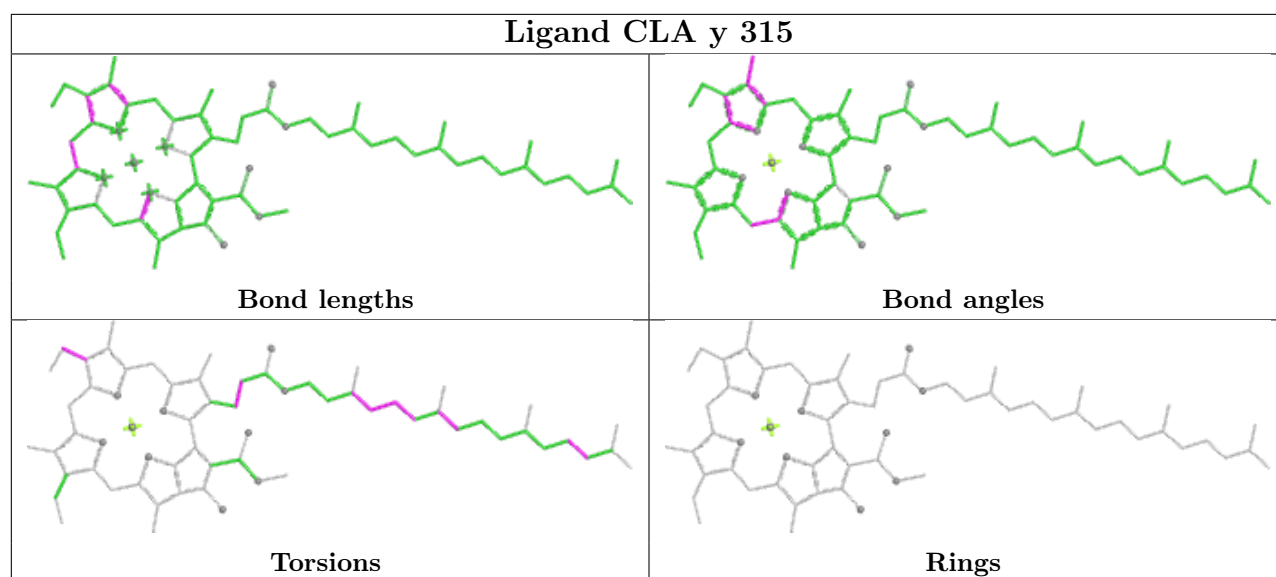
Rings

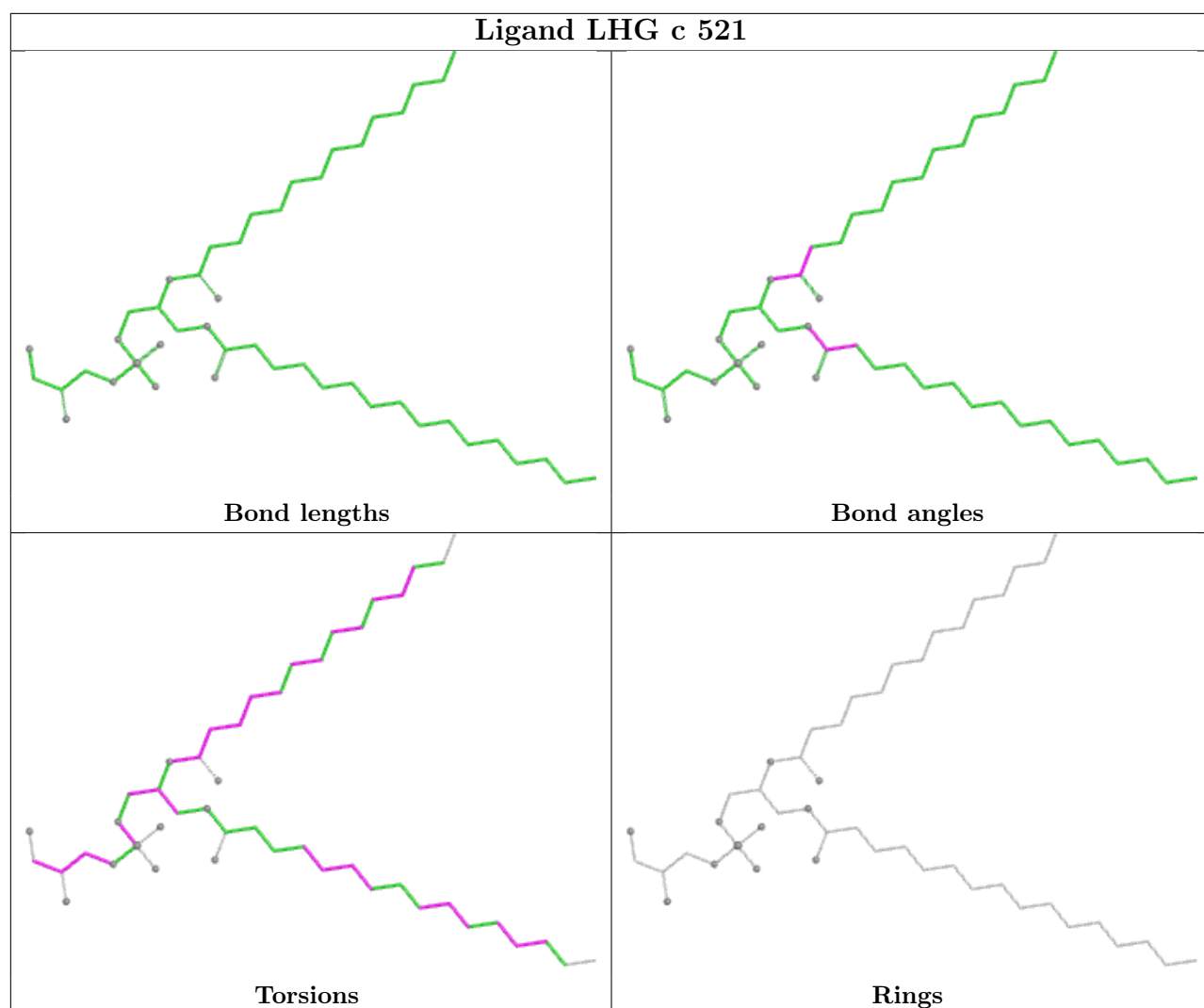


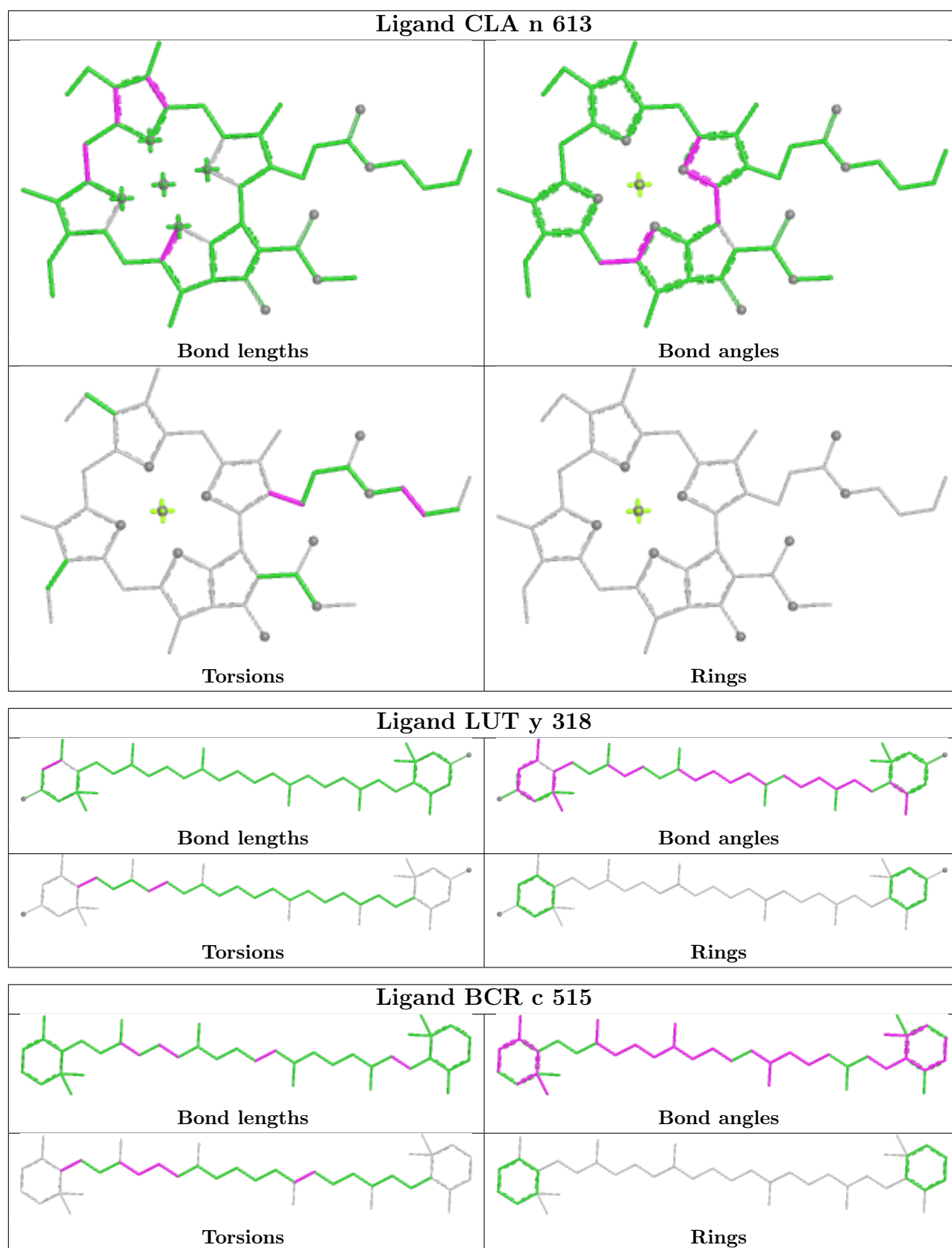


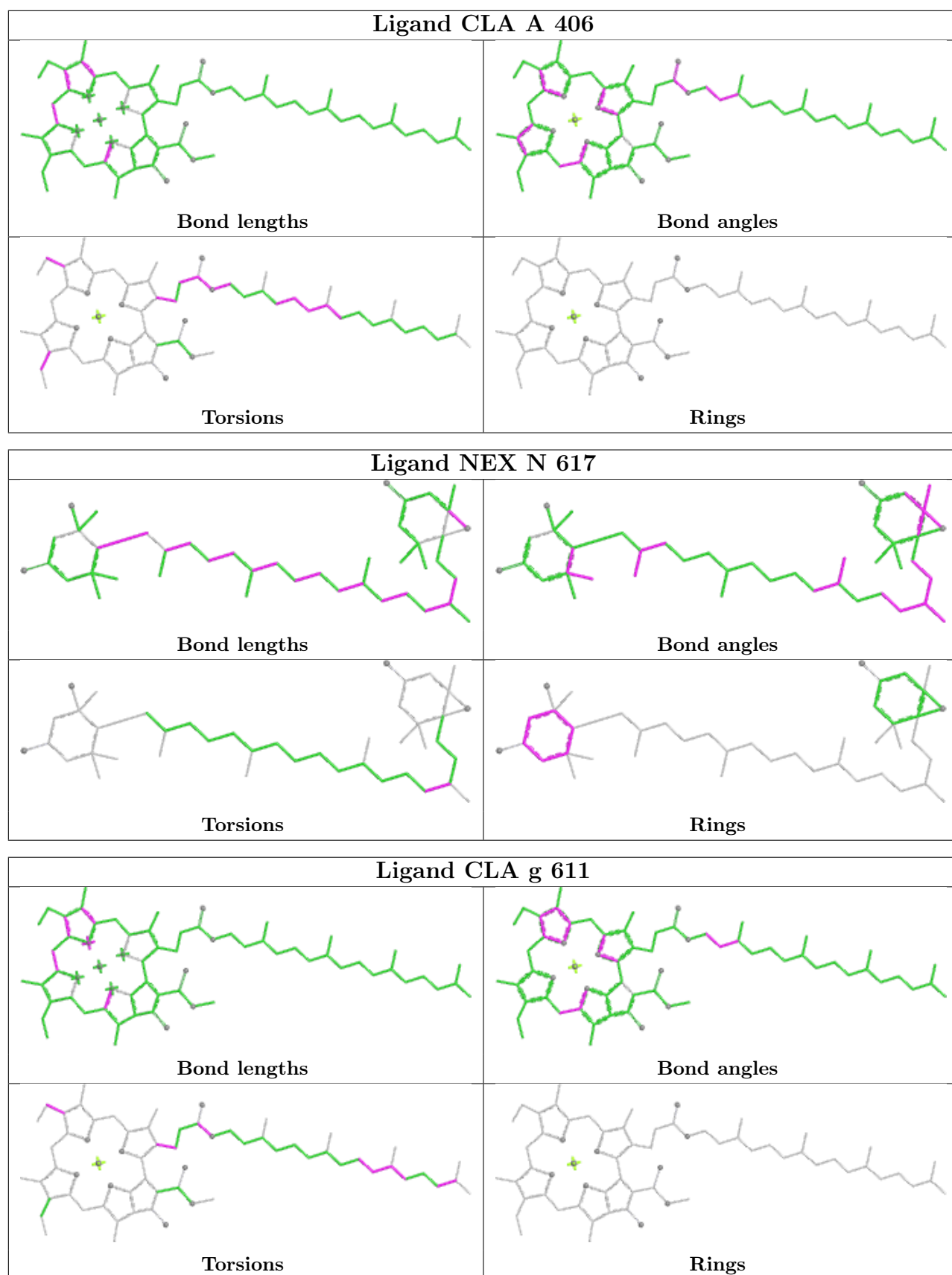


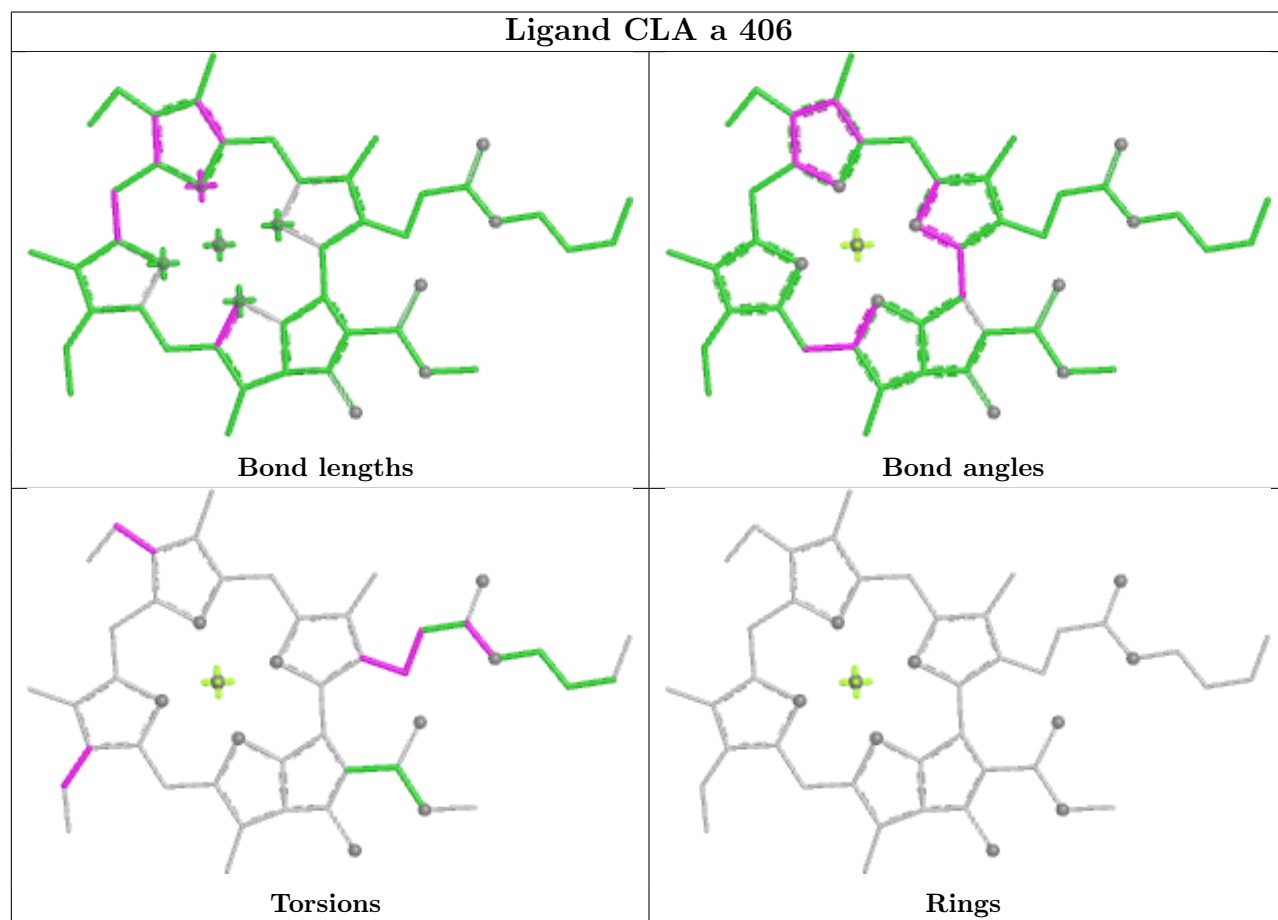
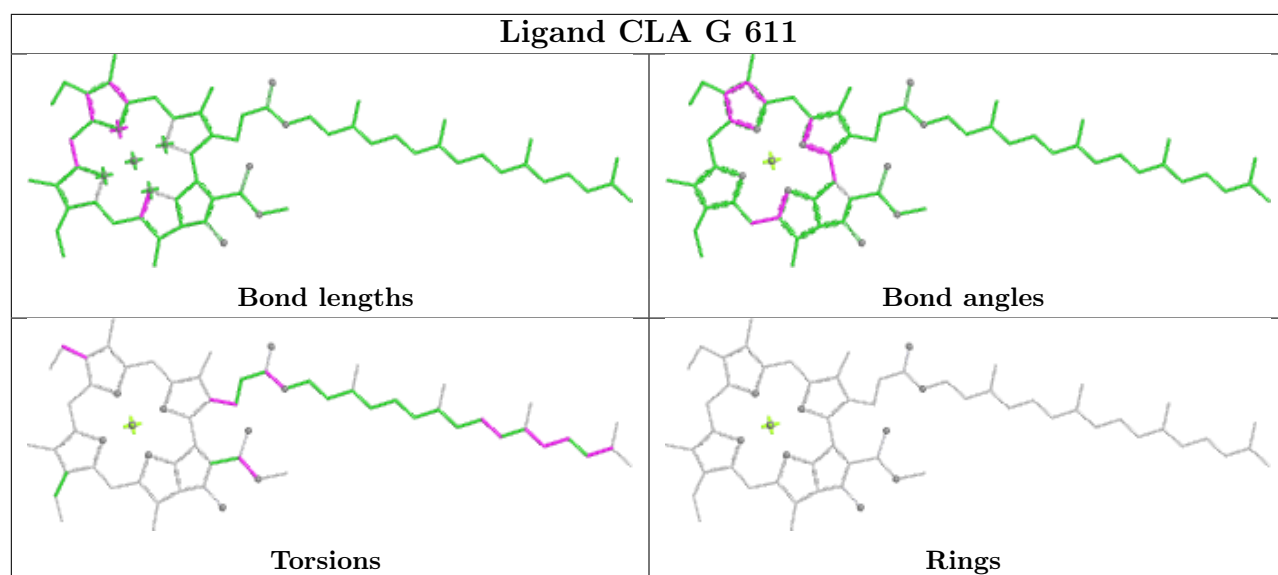


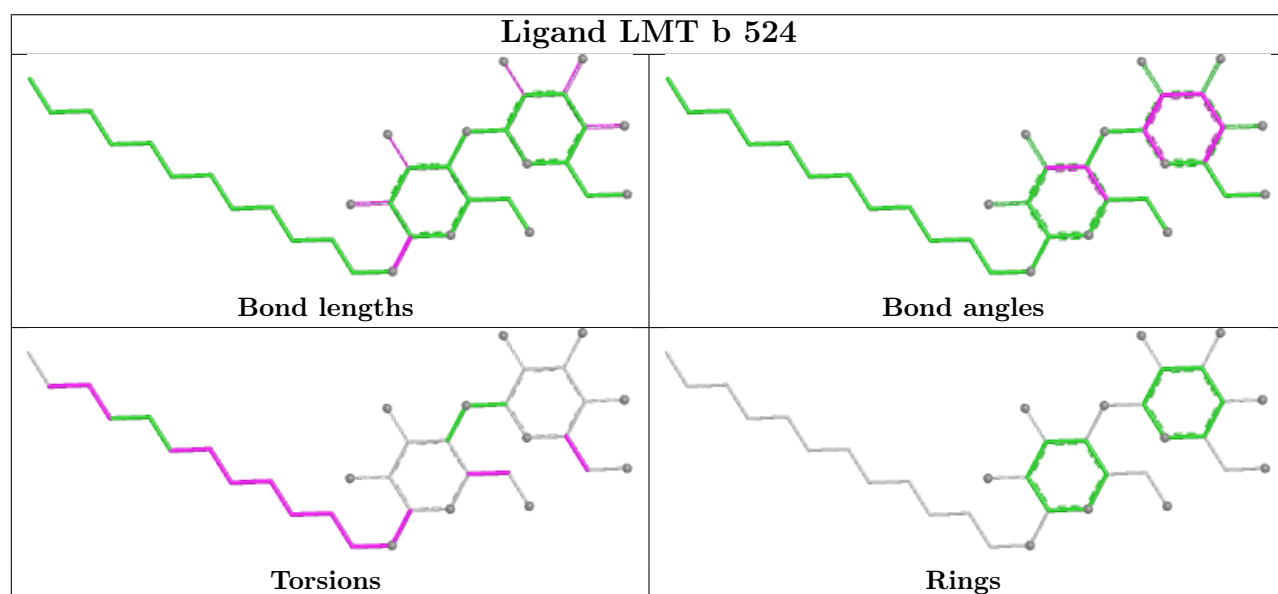
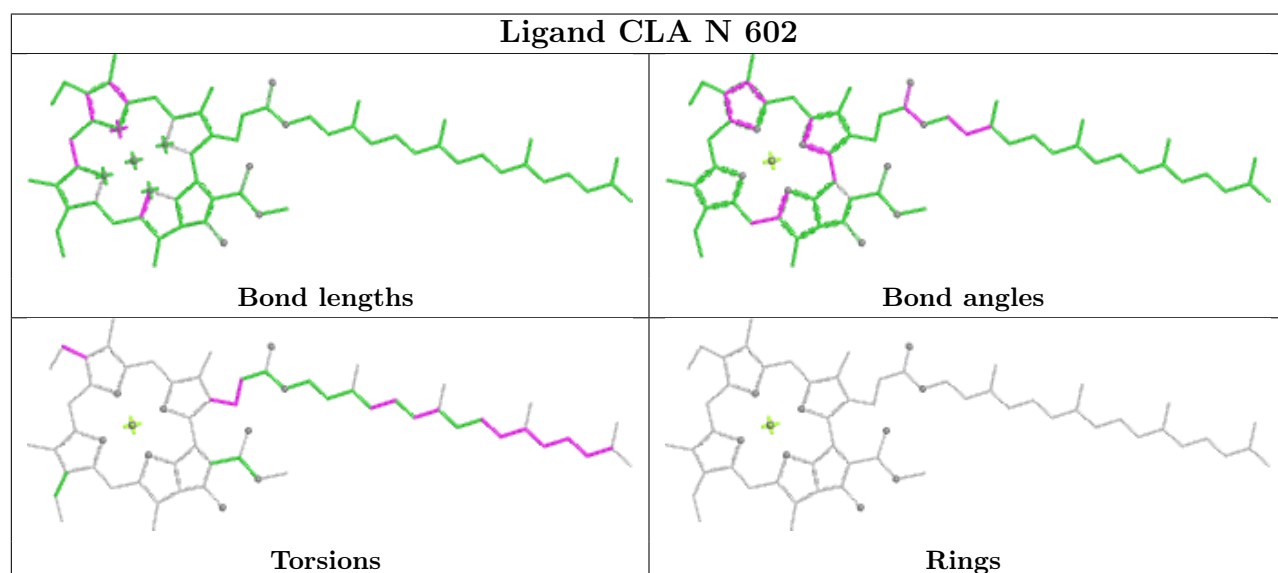
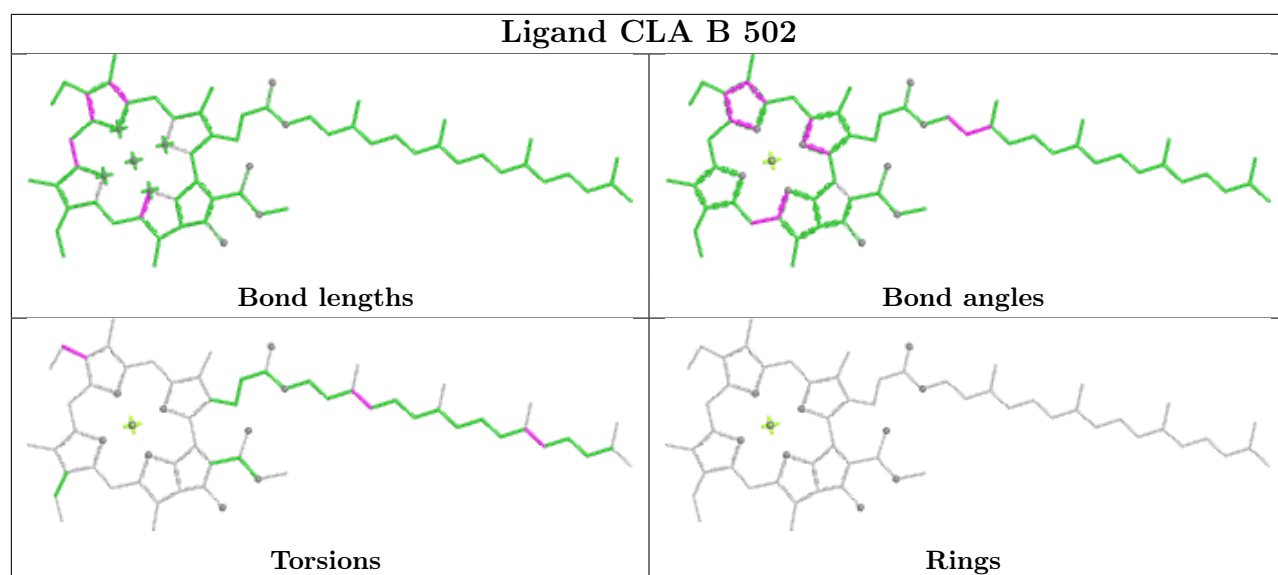


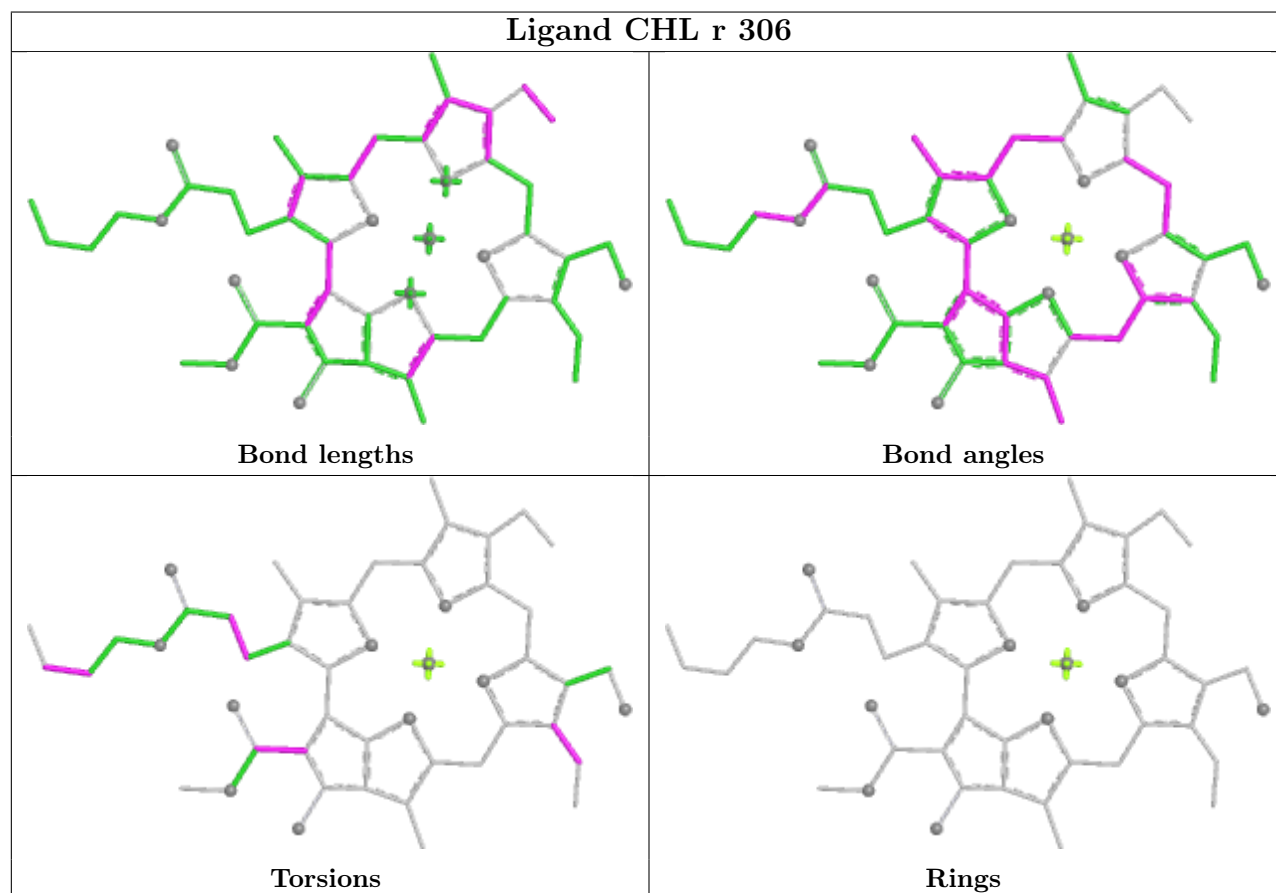
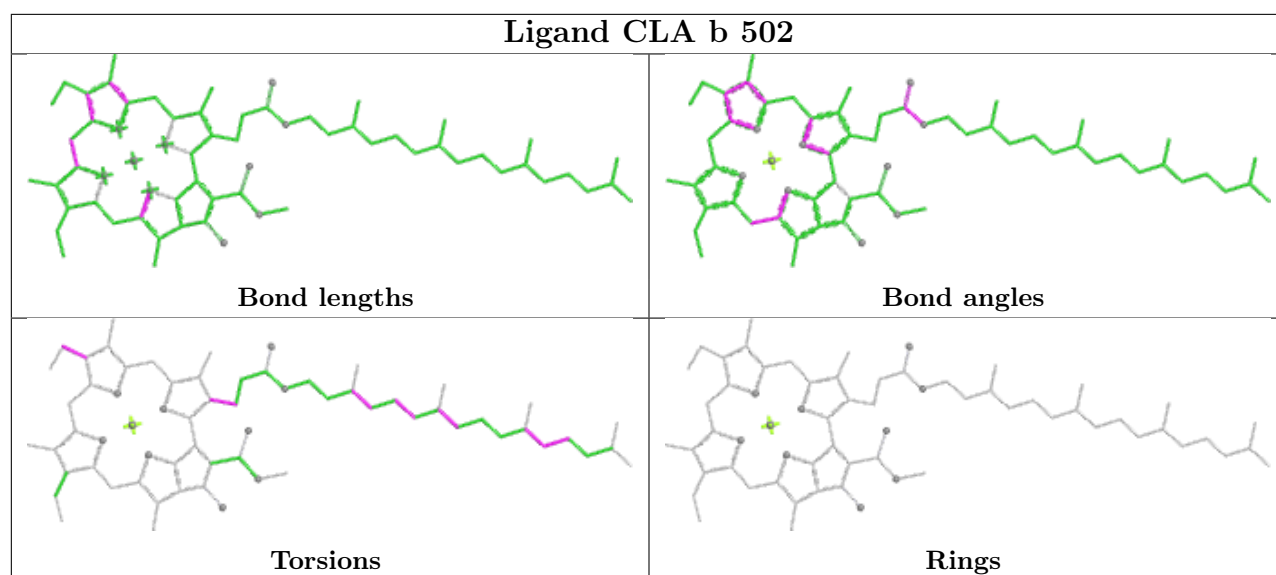


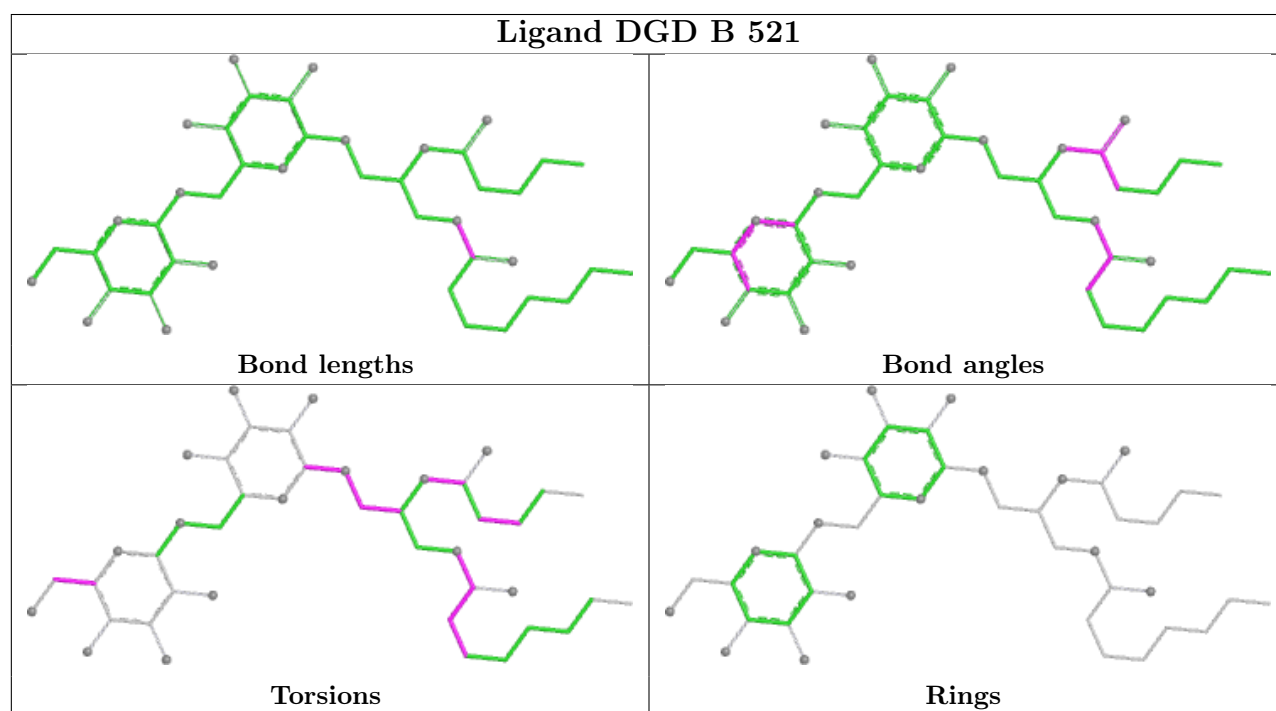
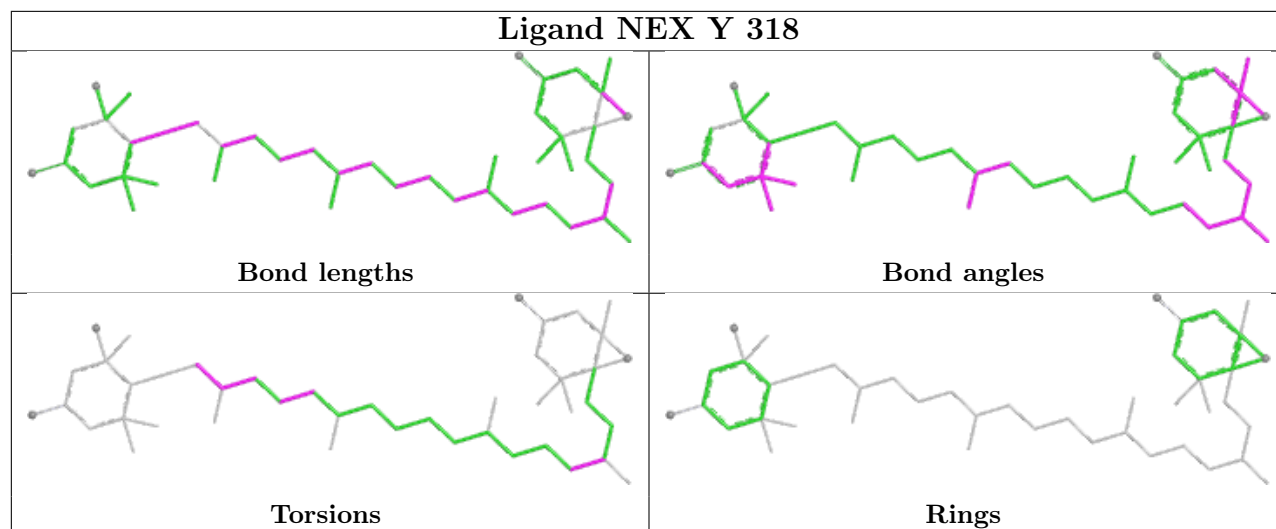


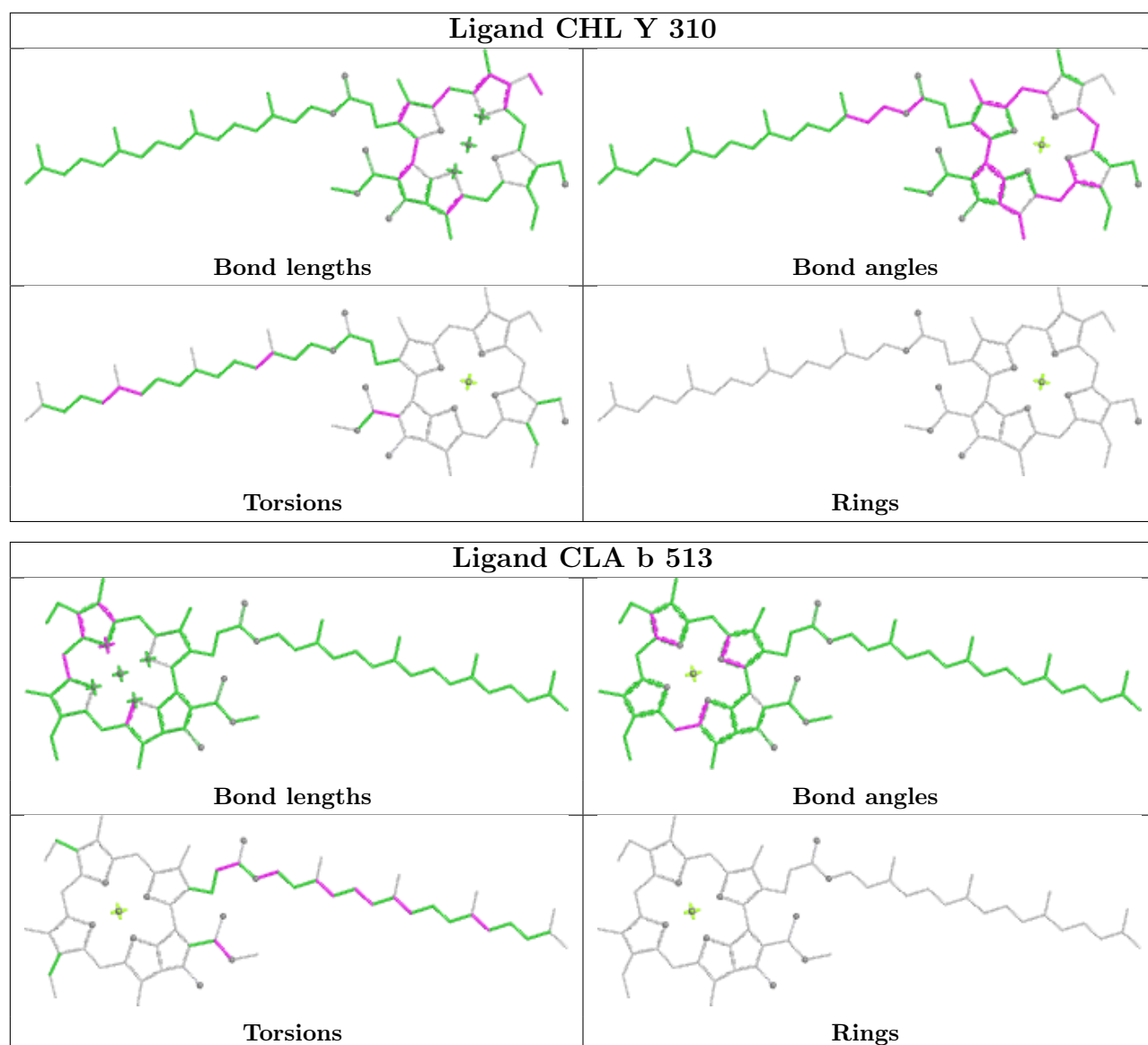


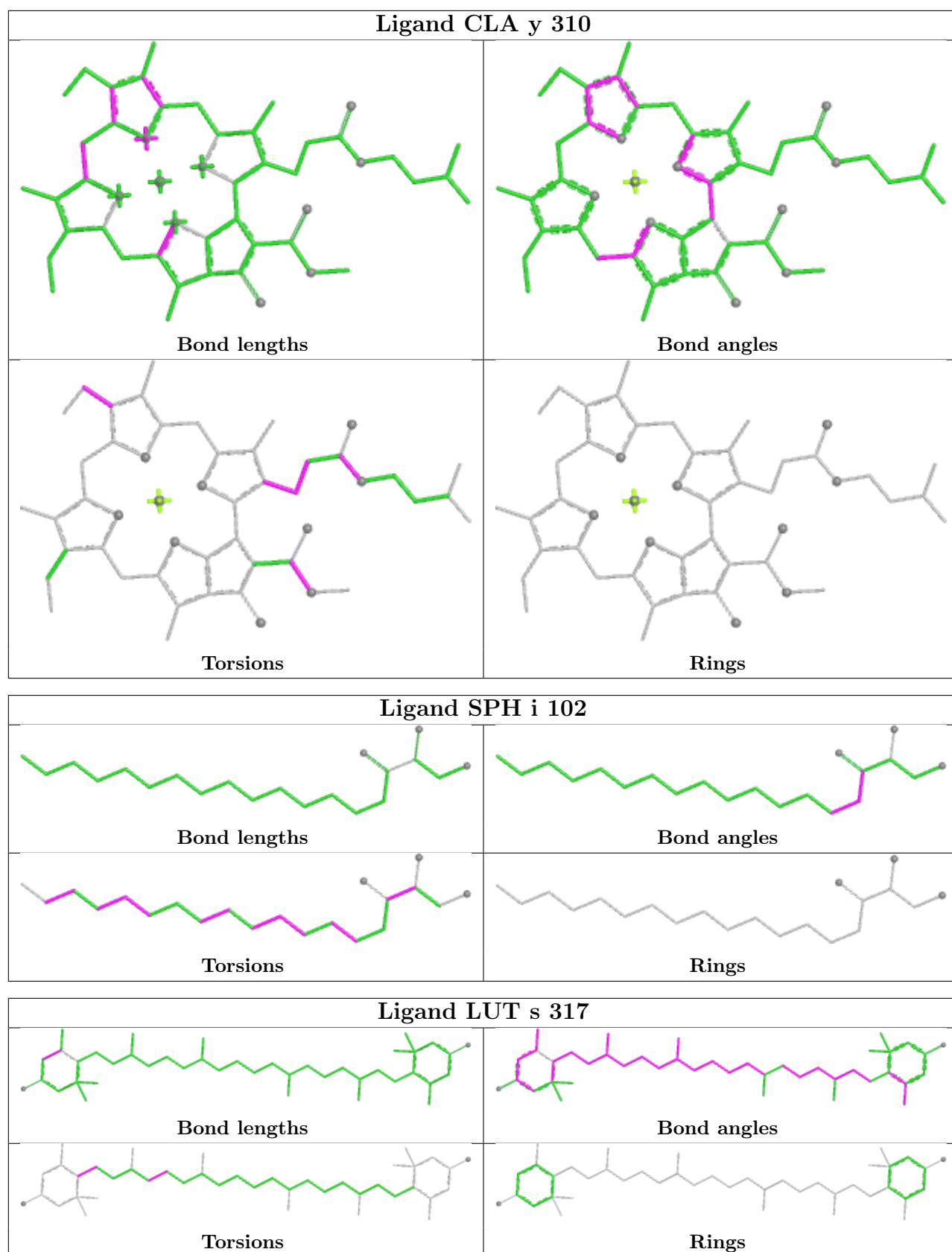


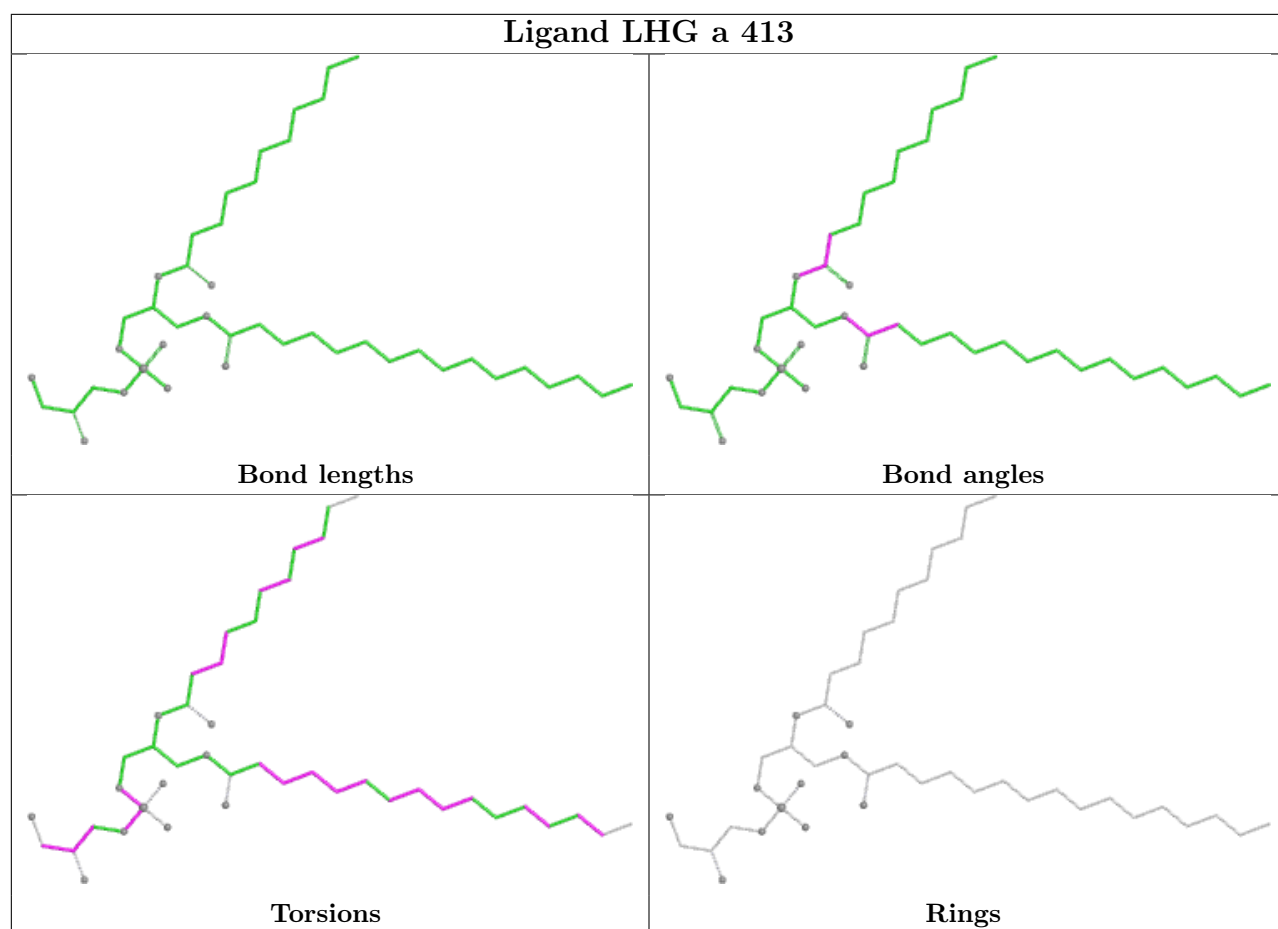


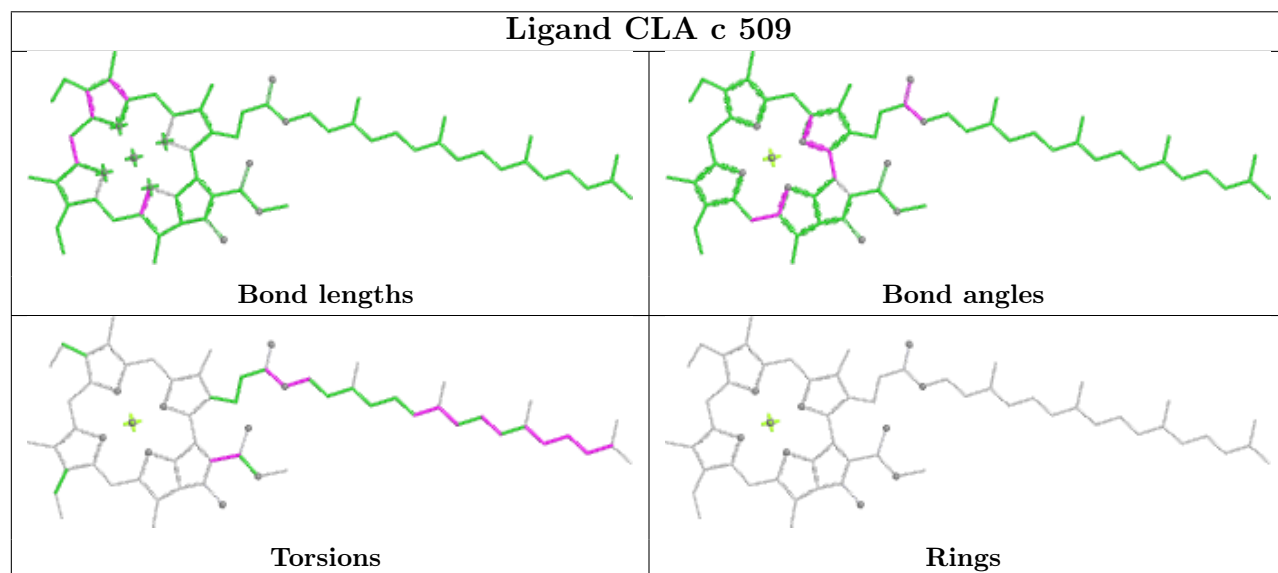
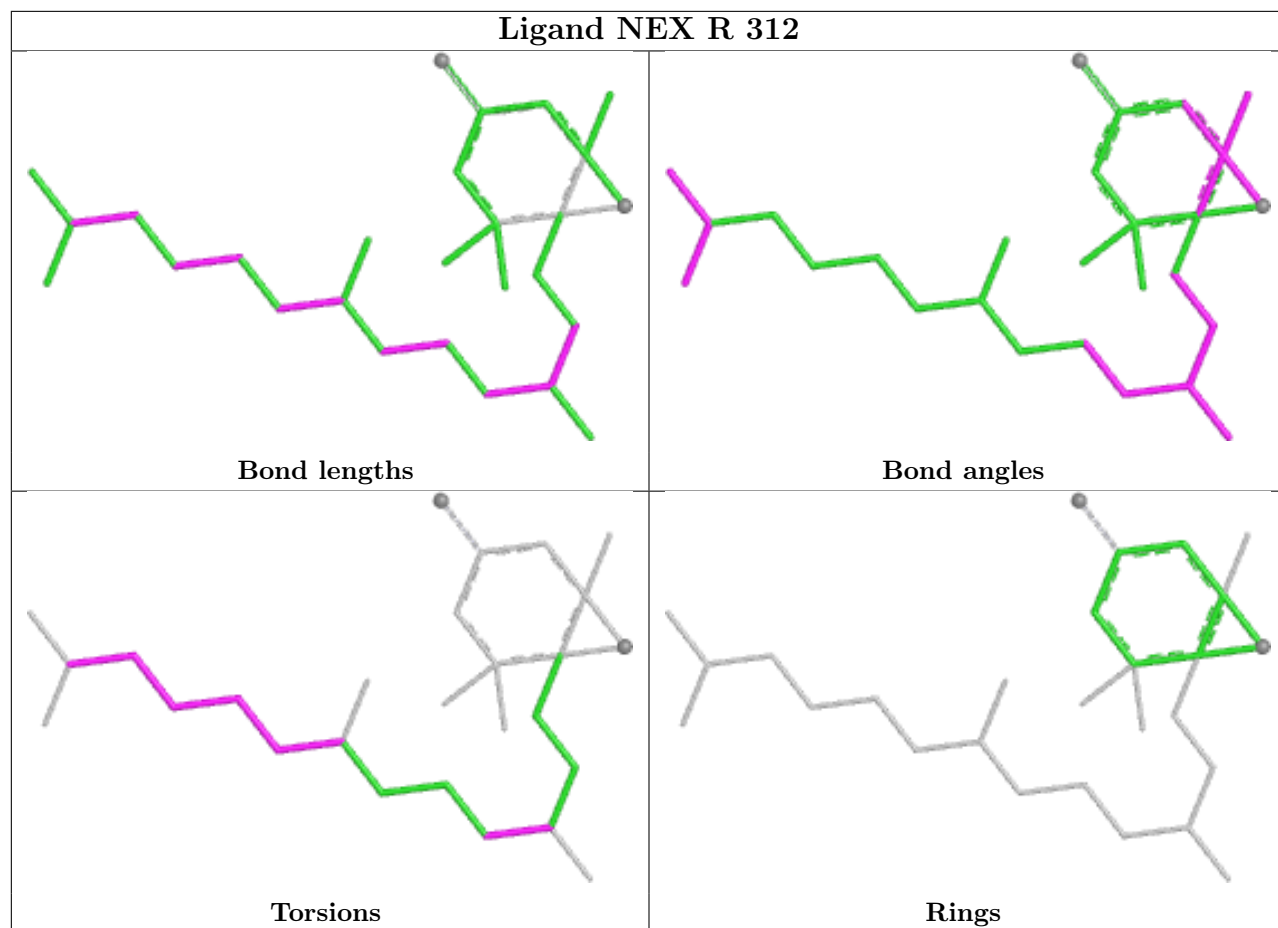


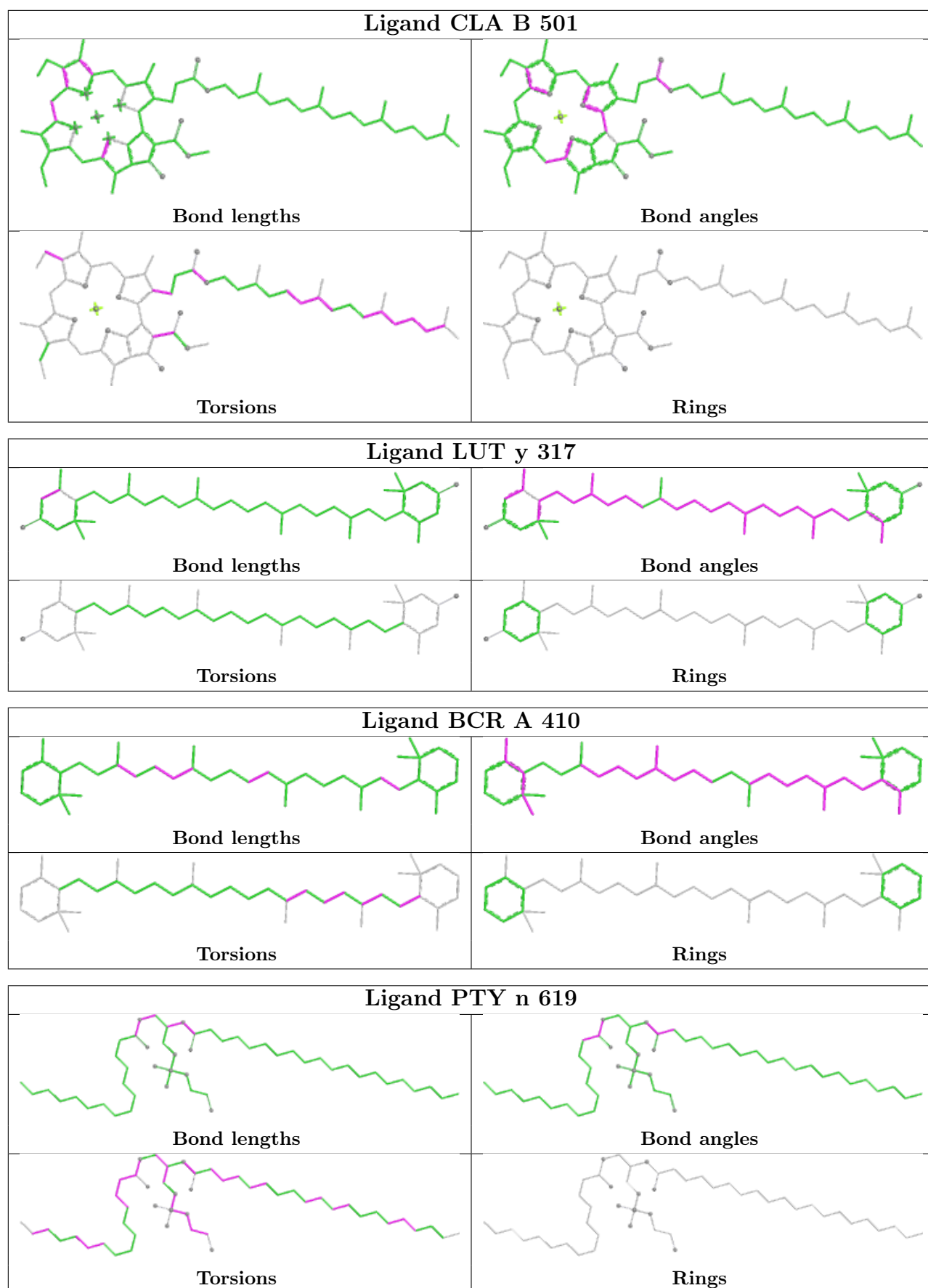


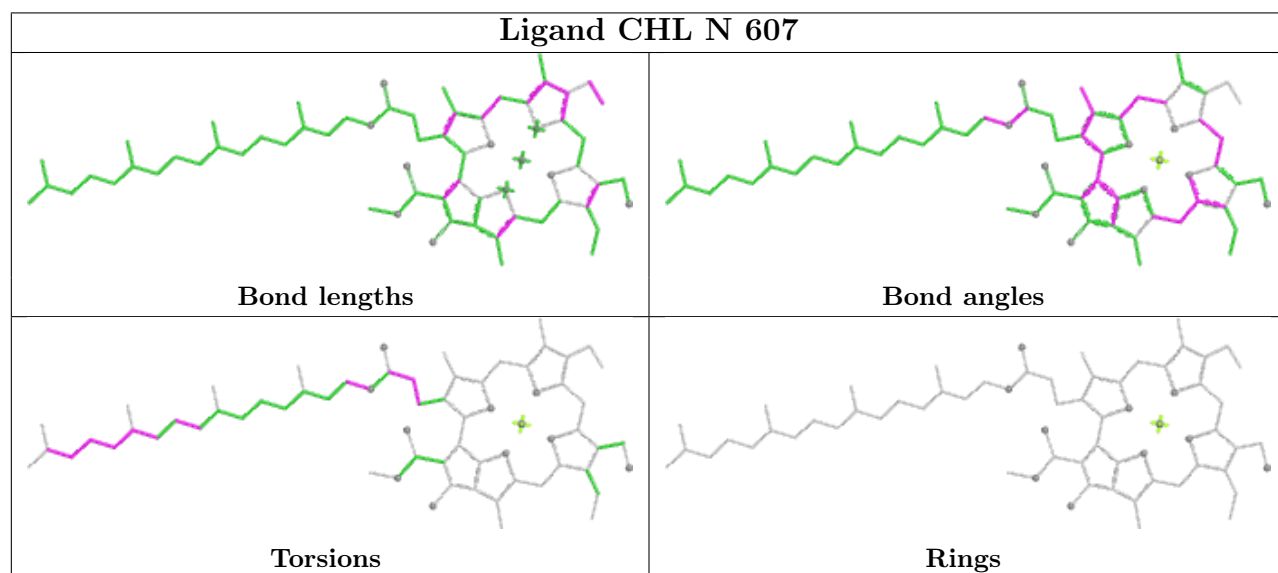
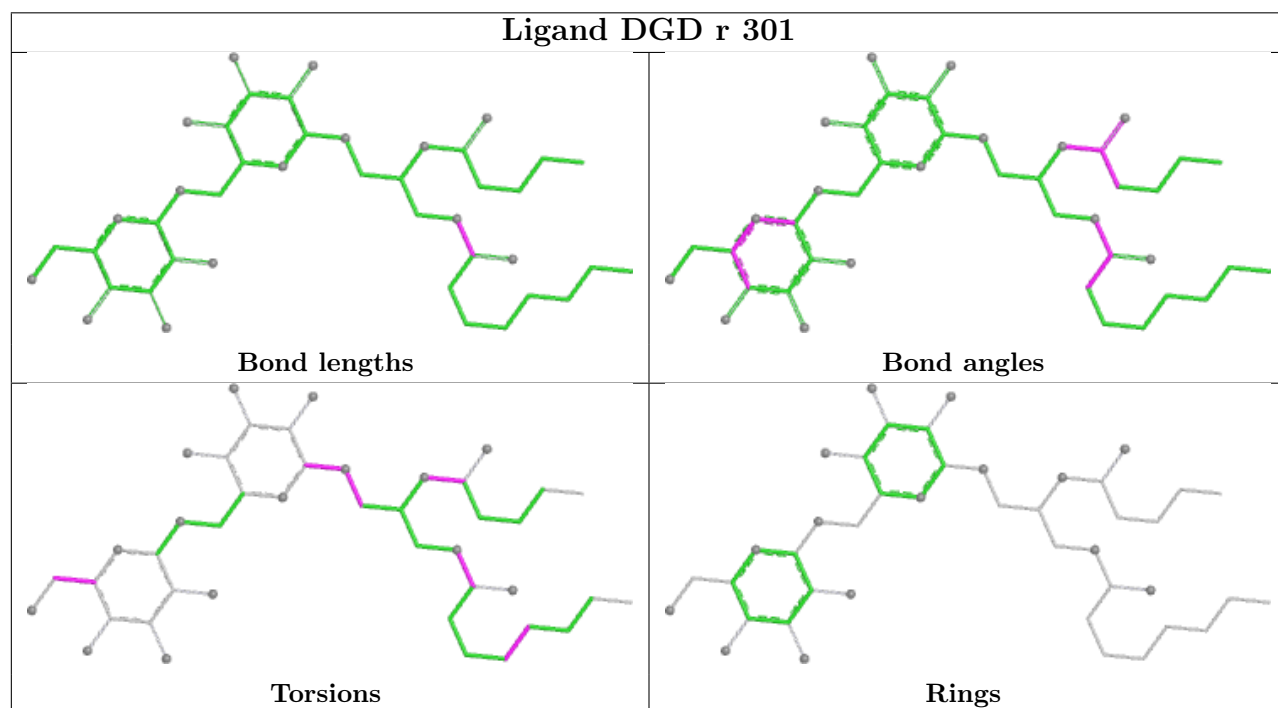
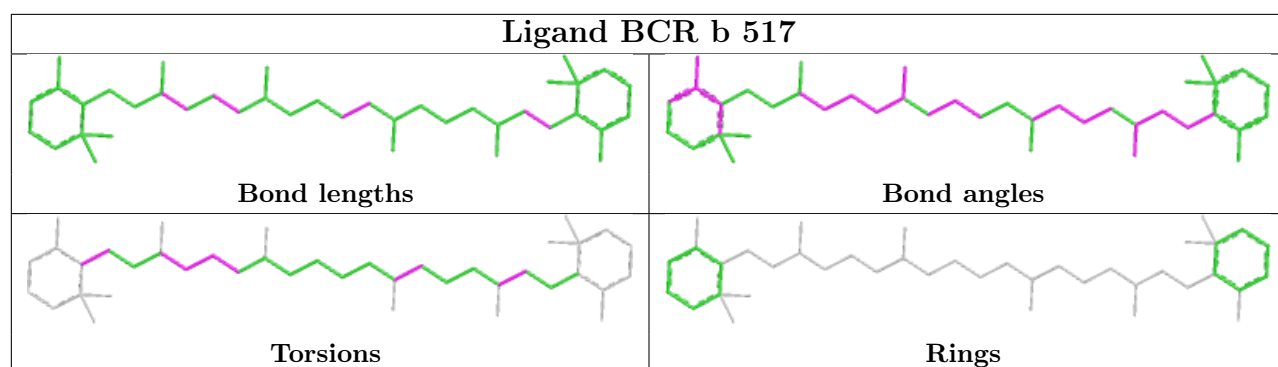


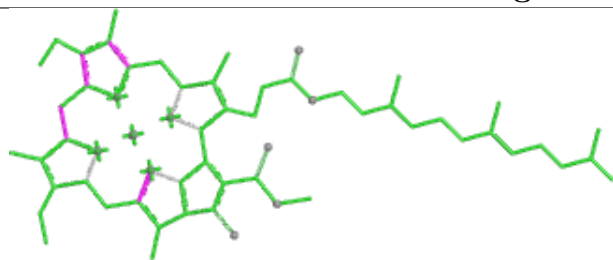
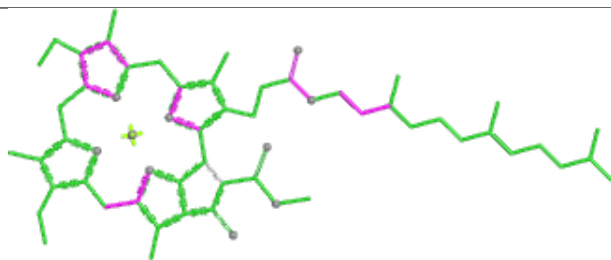
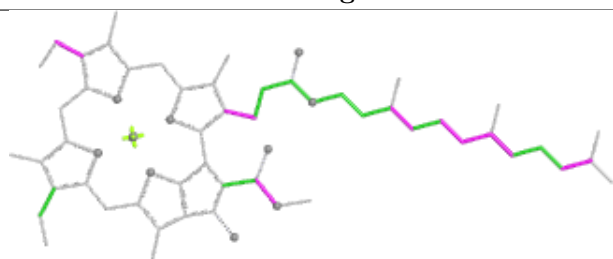
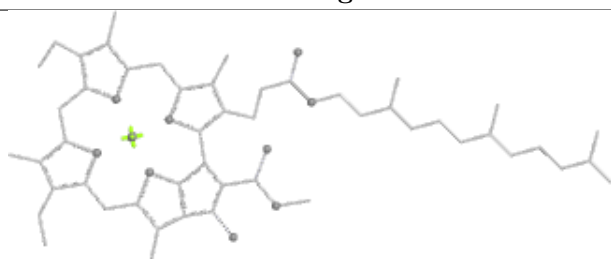
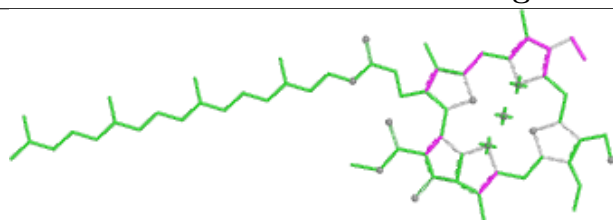
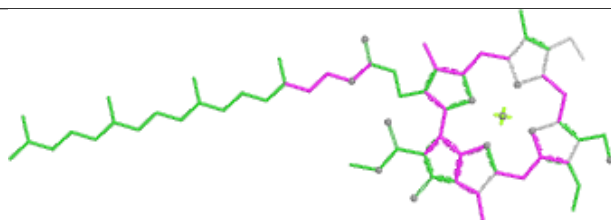
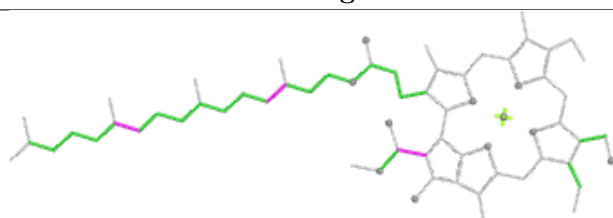
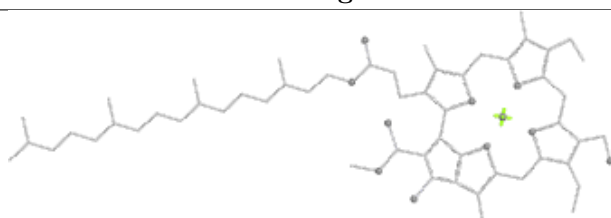


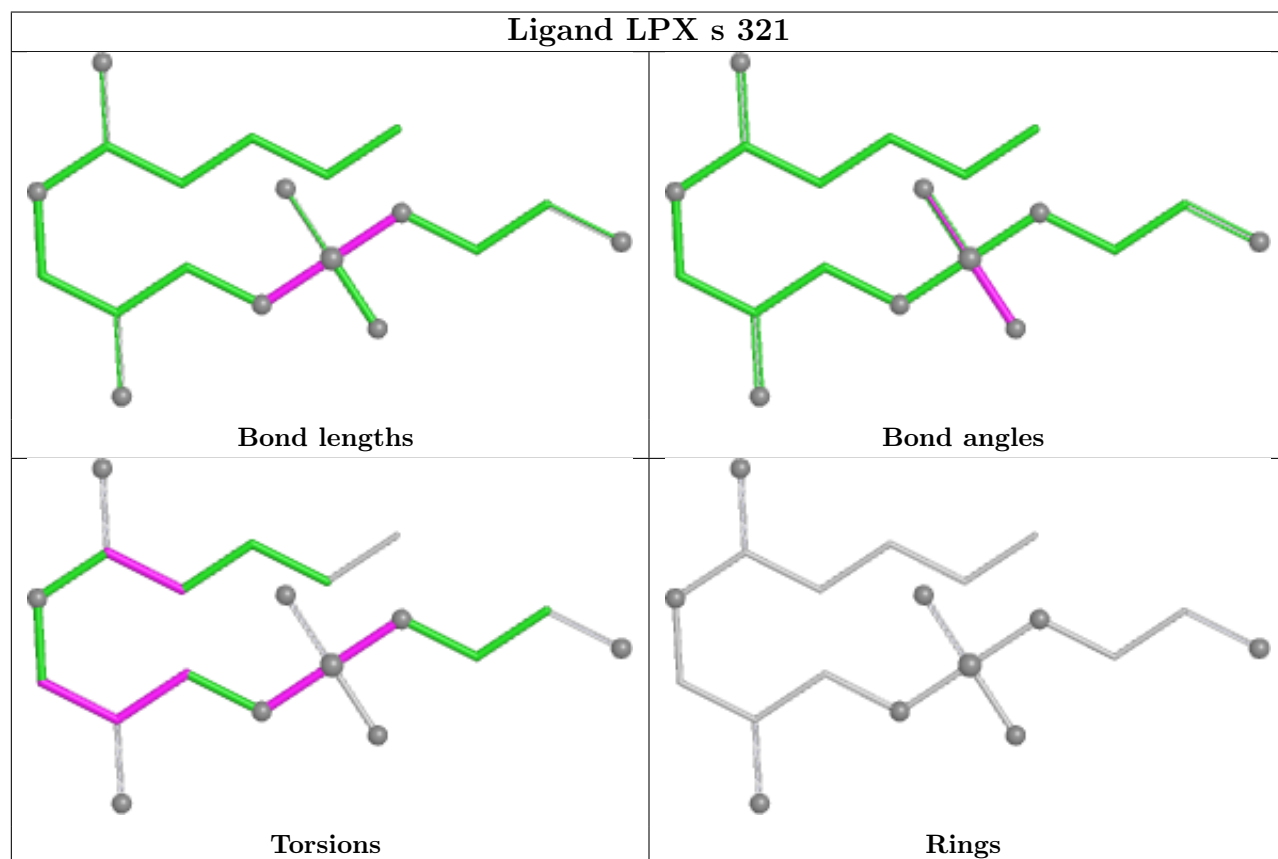
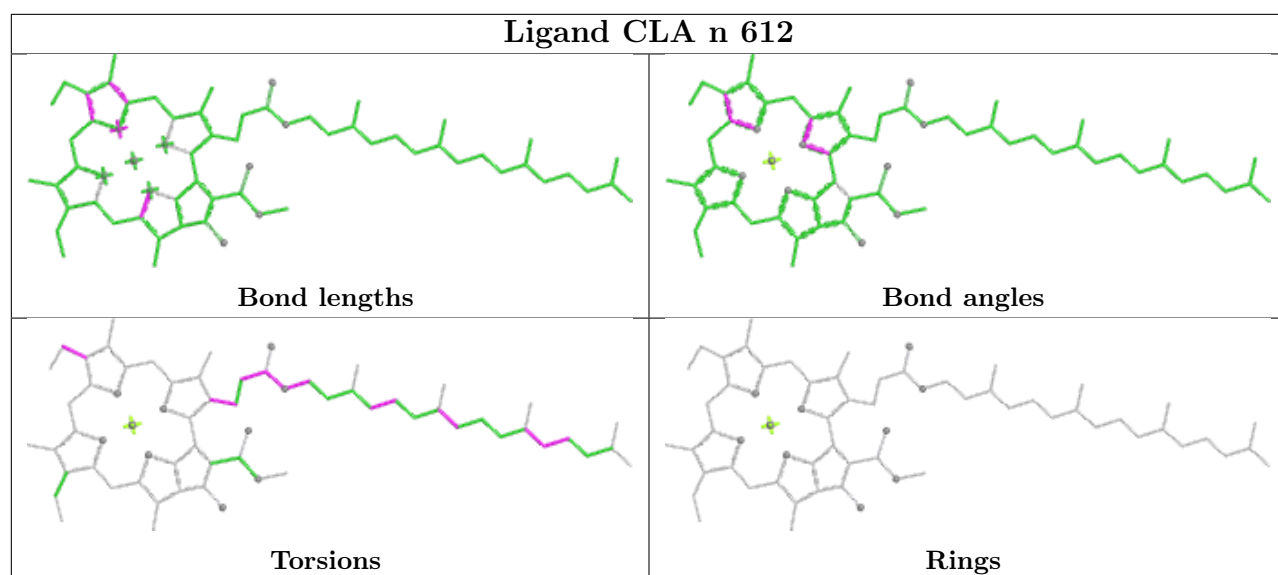




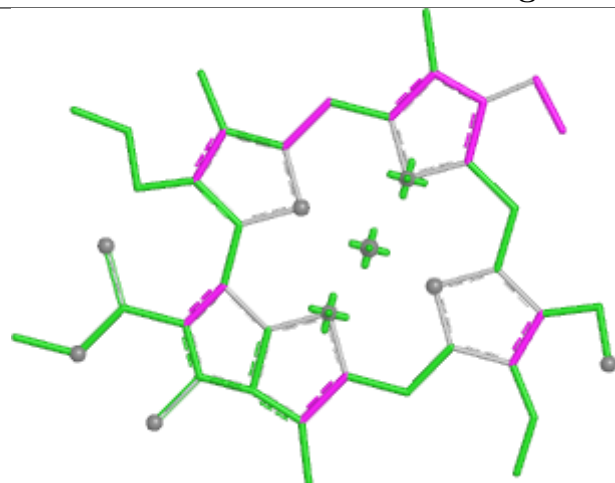




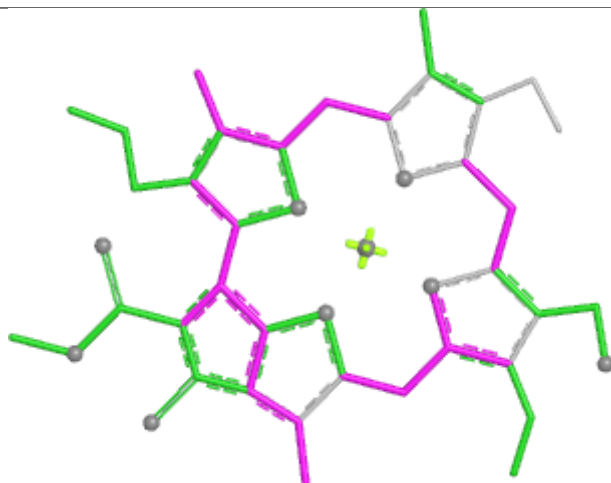
Ligand CLA R 308**Bond lengths****Bond angles****Torsions****Rings****Ligand CHL N 609****Bond lengths****Bond angles****Torsions****Rings**



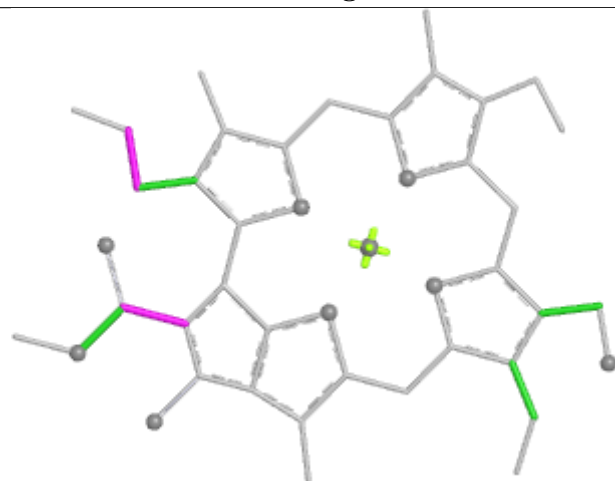
Ligand CHL S 307



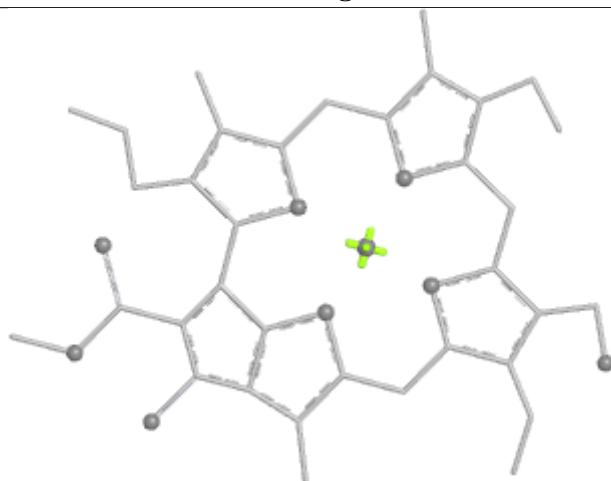
Bond lengths



Bond angles

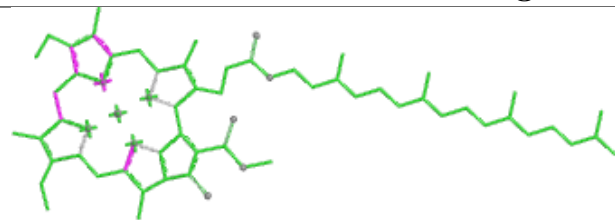


Torsions

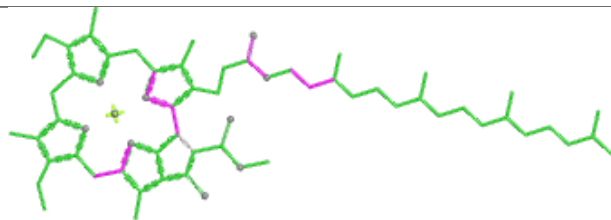


Rings

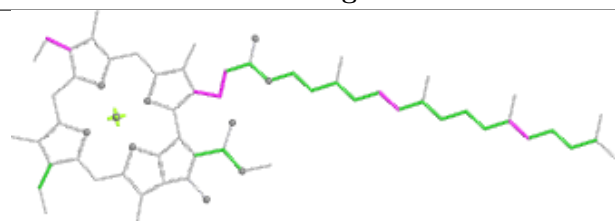
Ligand CLA Y 311



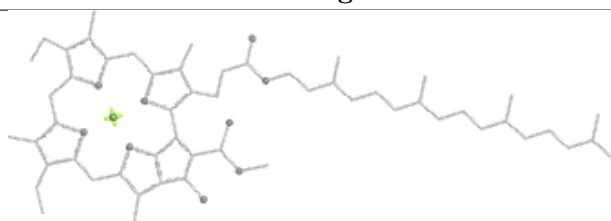
Bond lengths



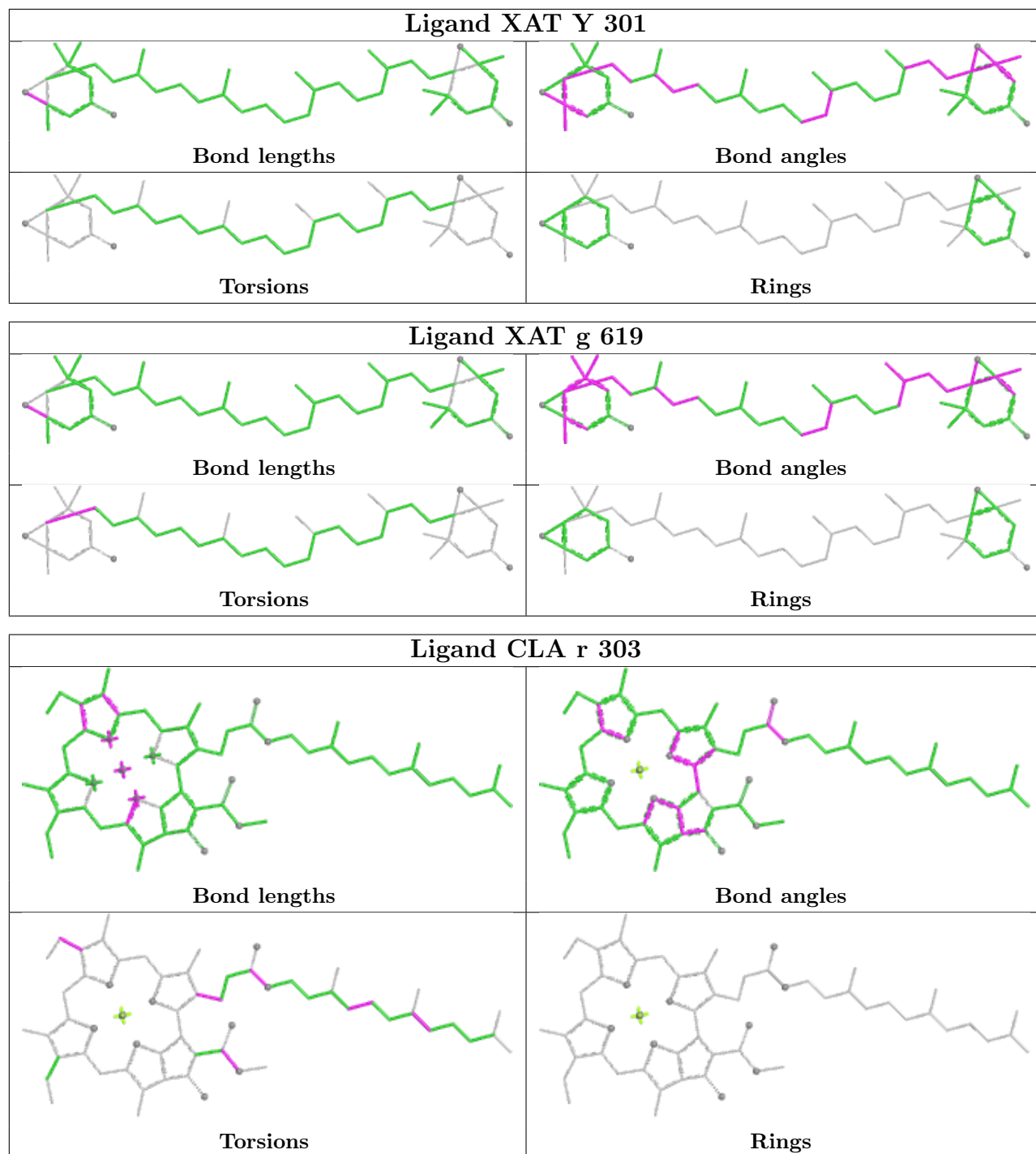
Bond angles

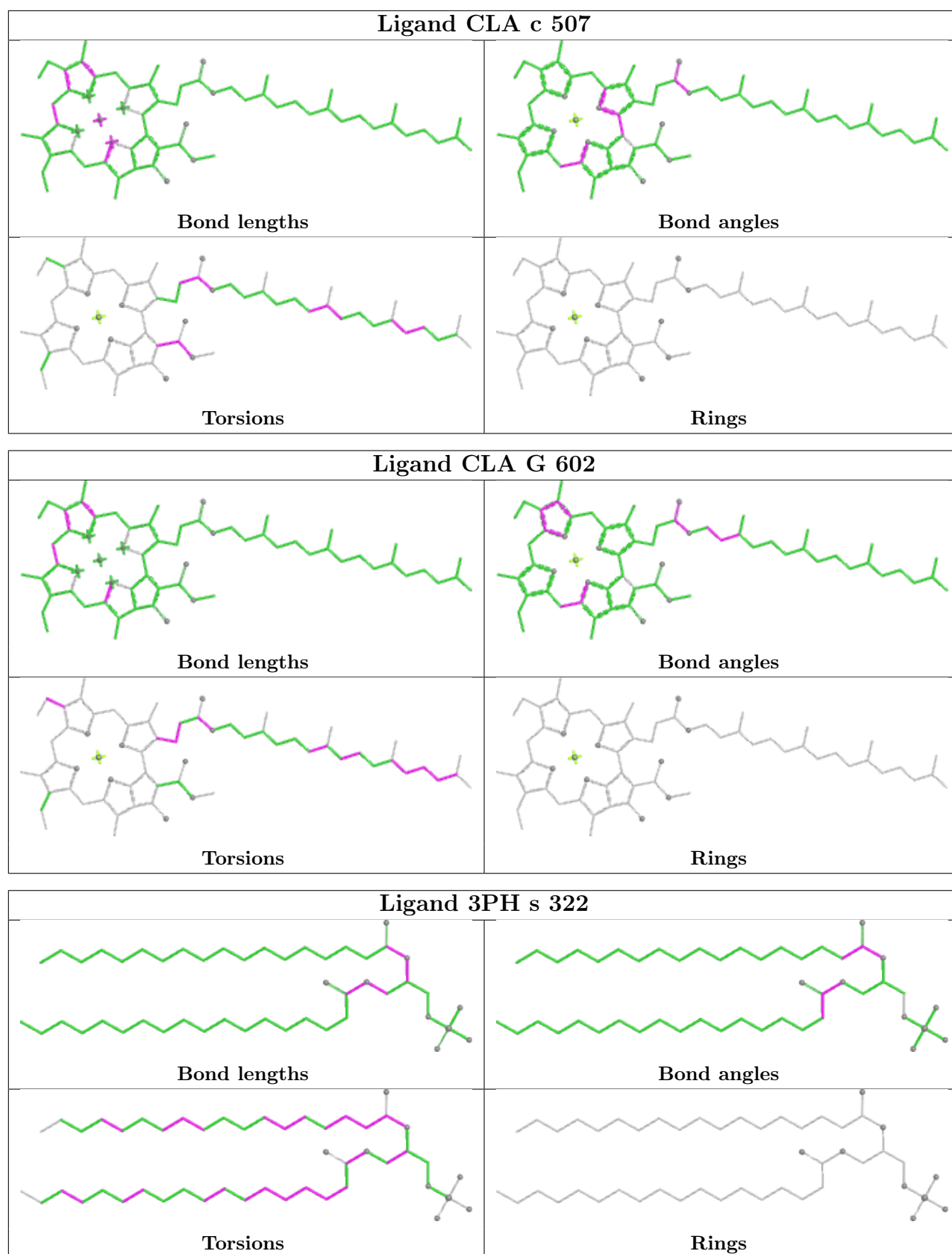


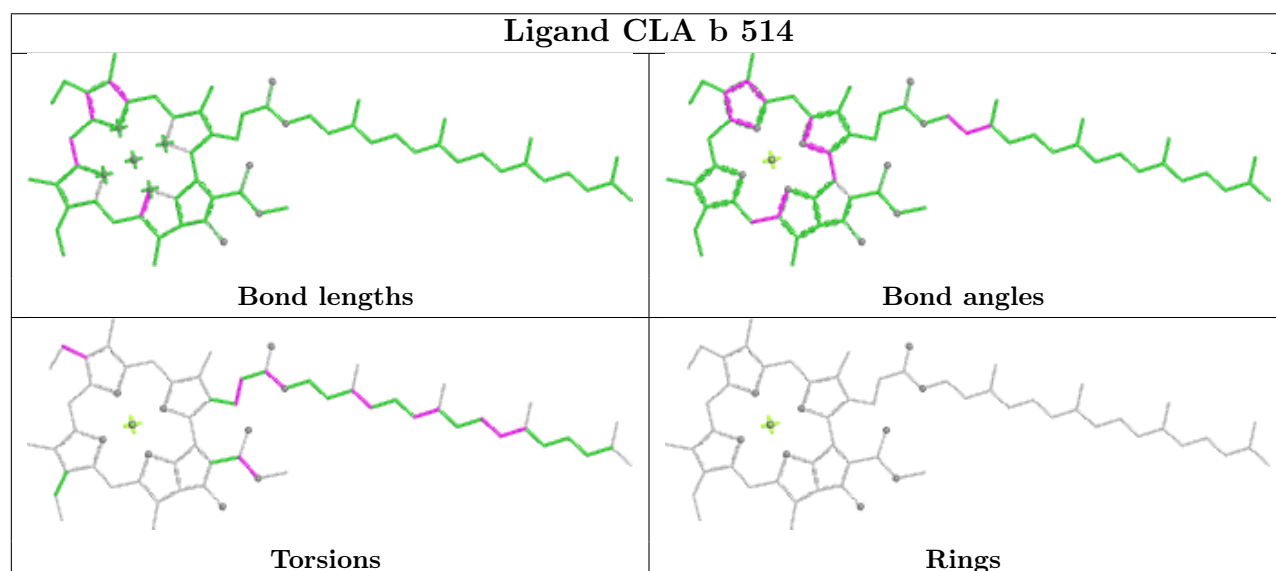
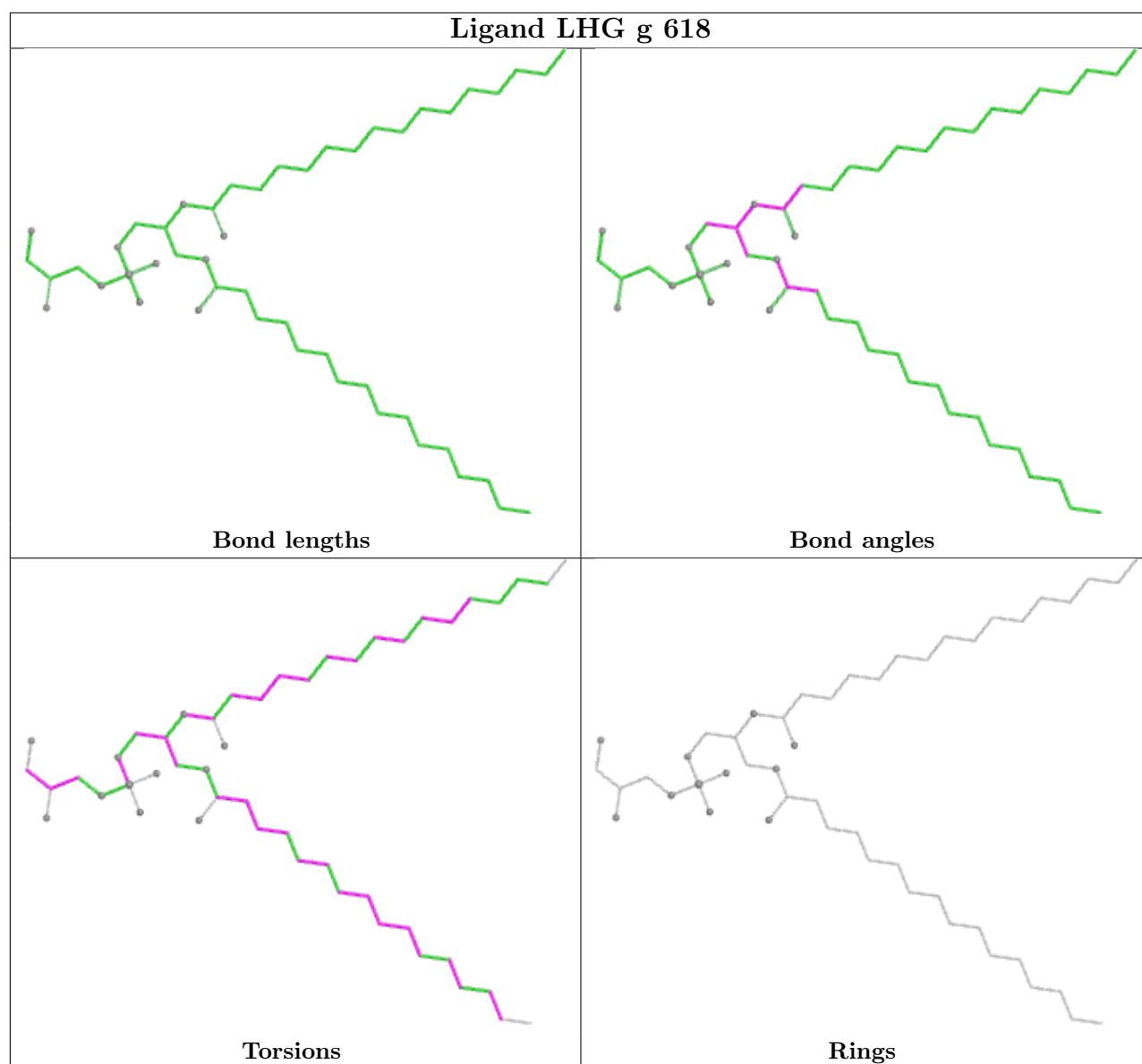
Torsions

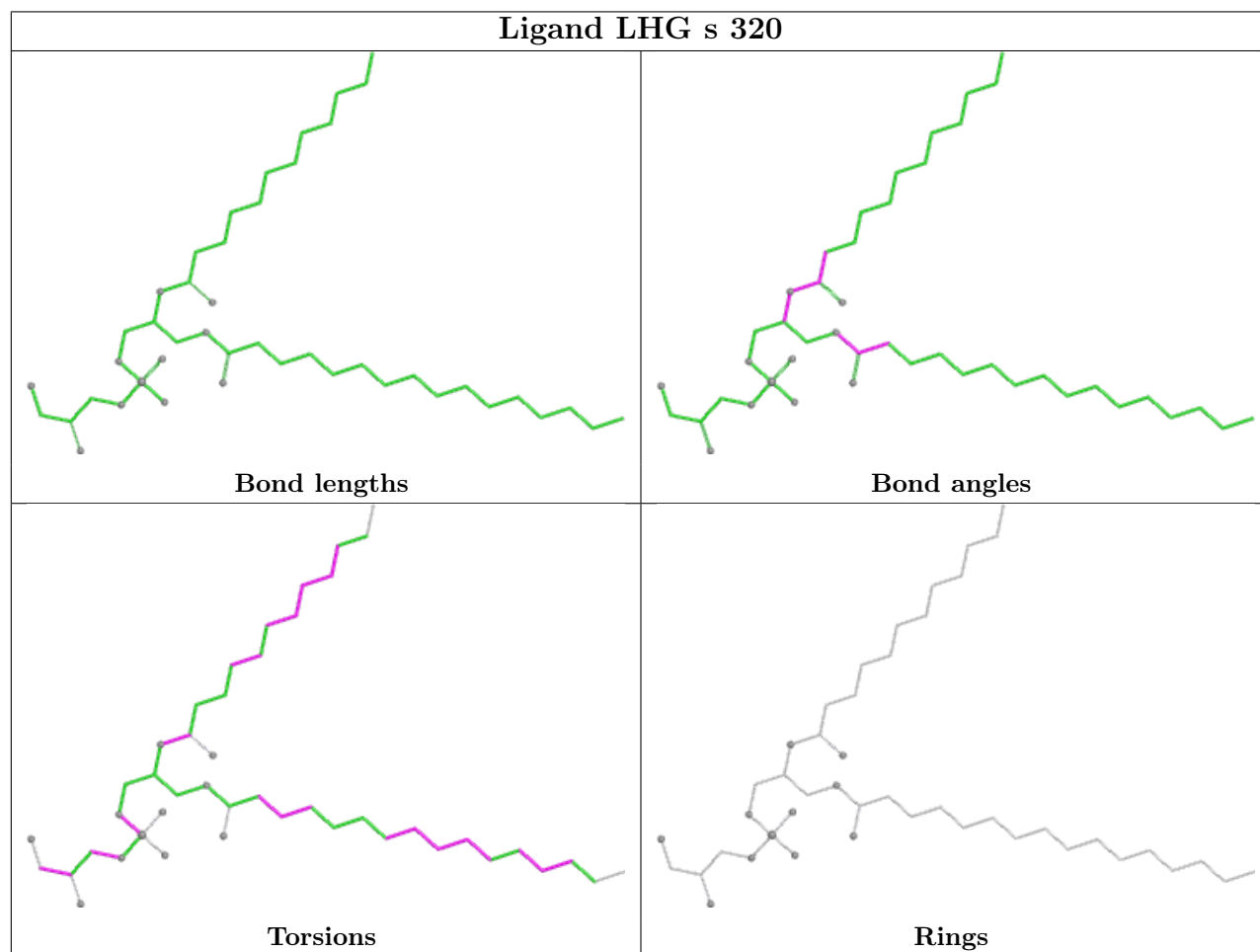
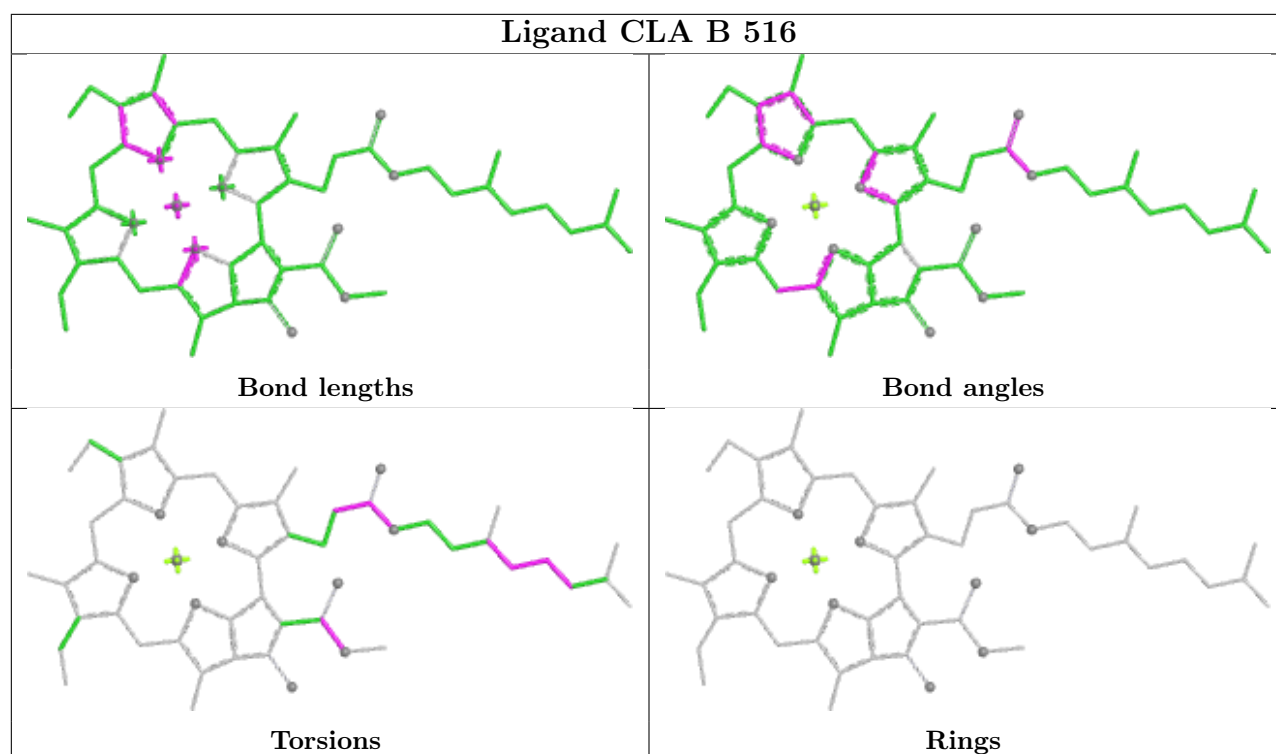


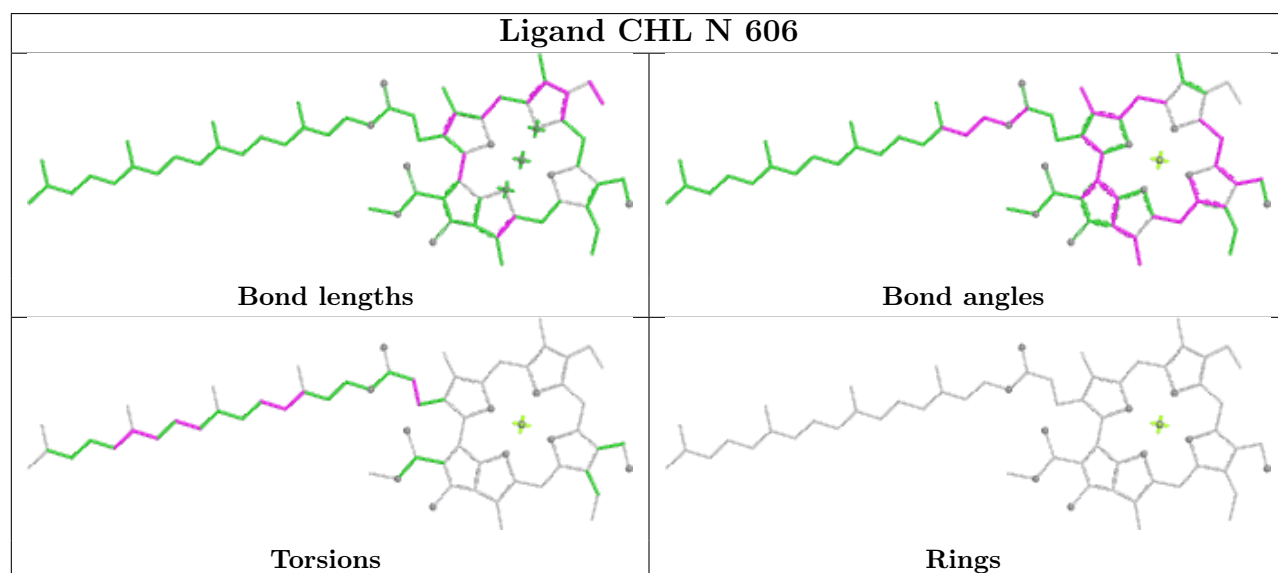
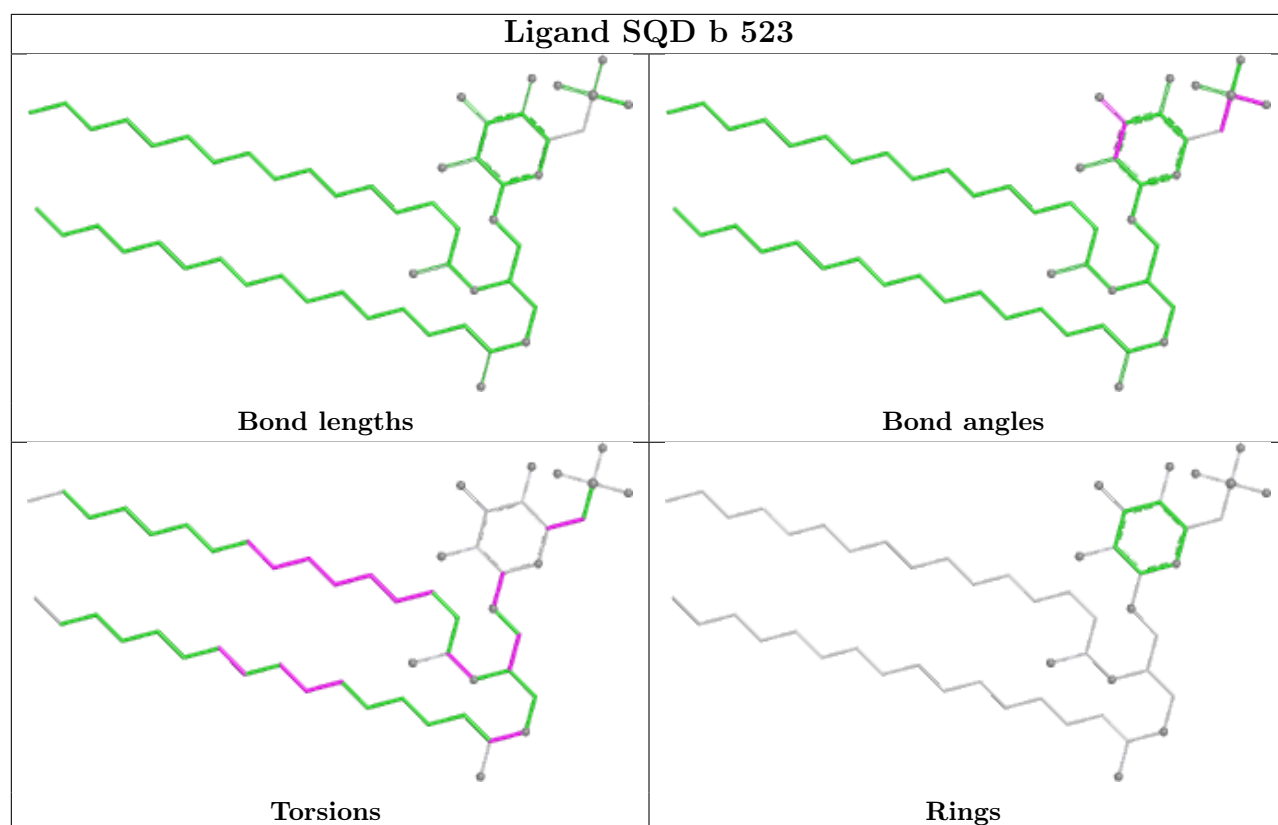
Rings

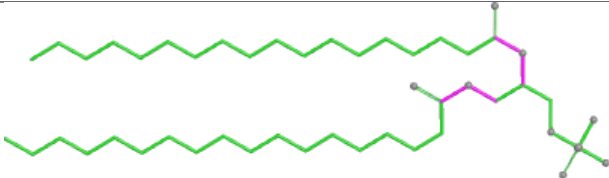
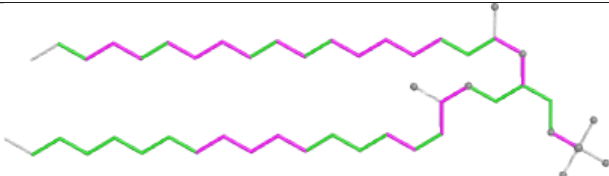
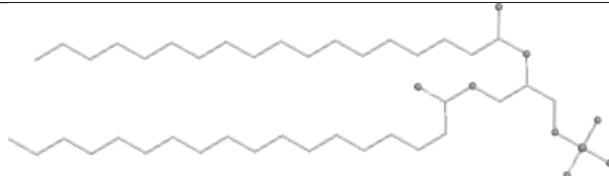
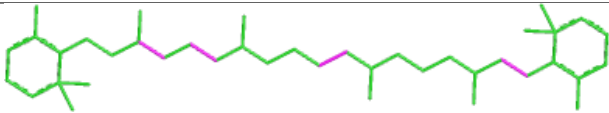
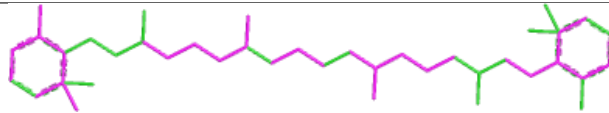
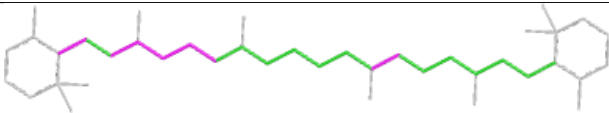
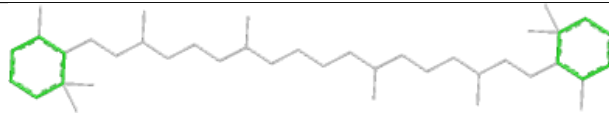
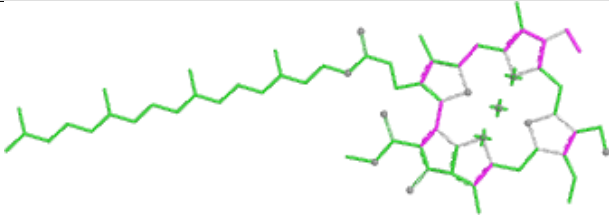
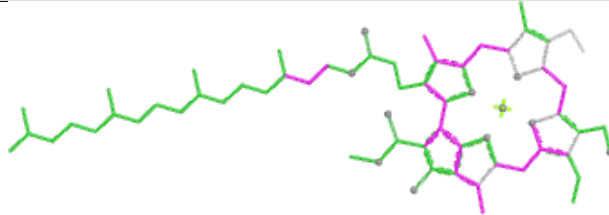
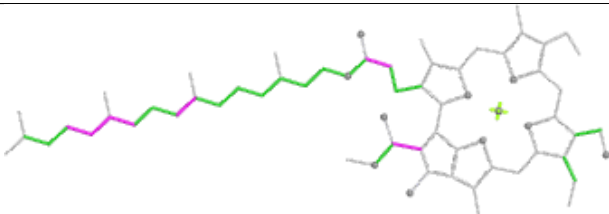
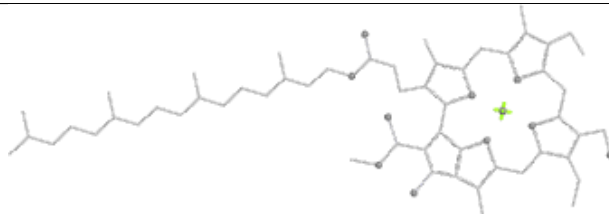
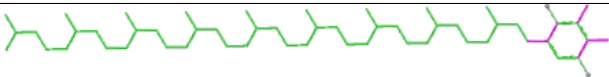
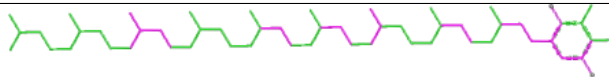
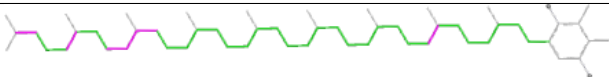
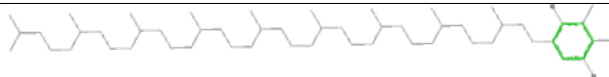


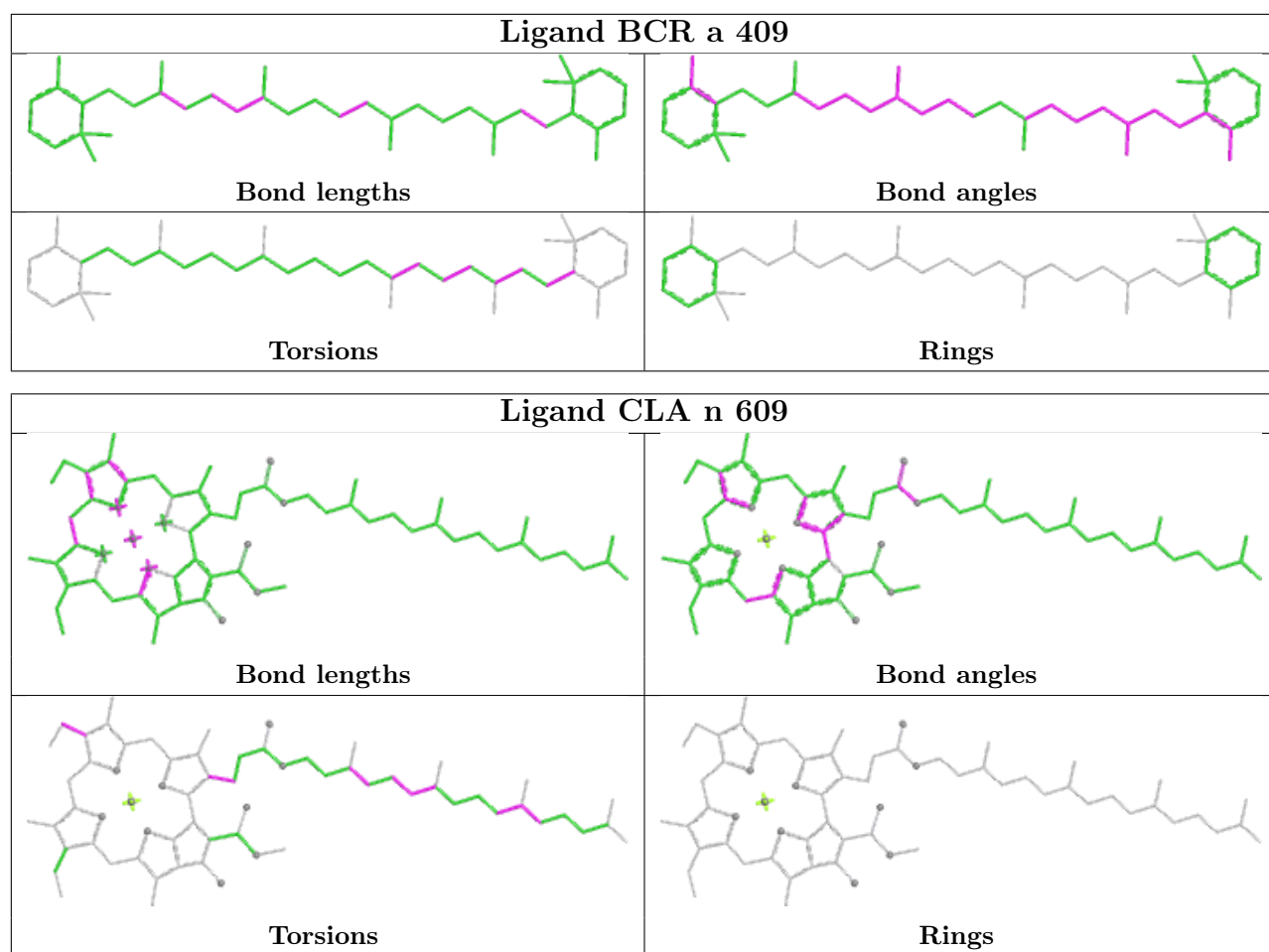


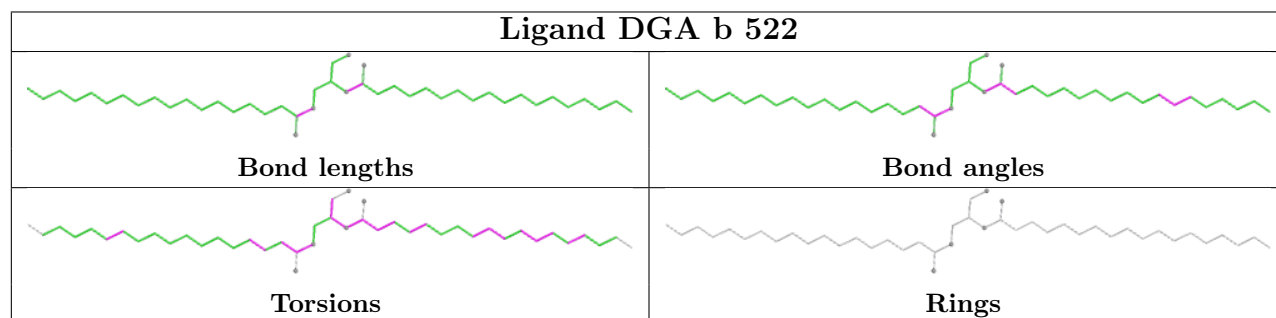
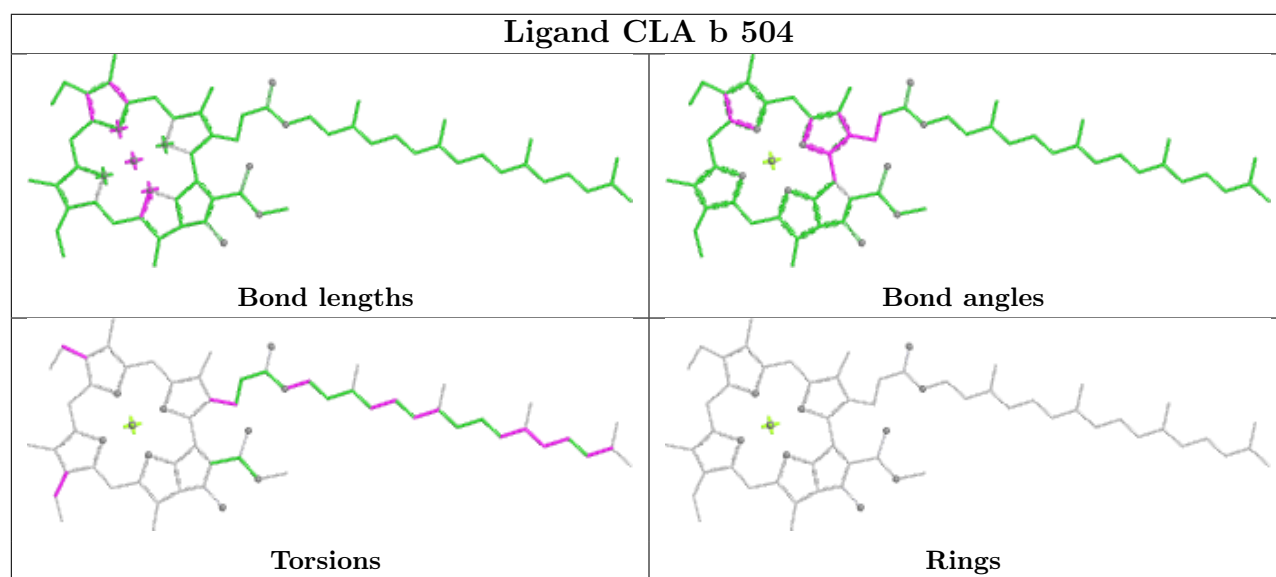
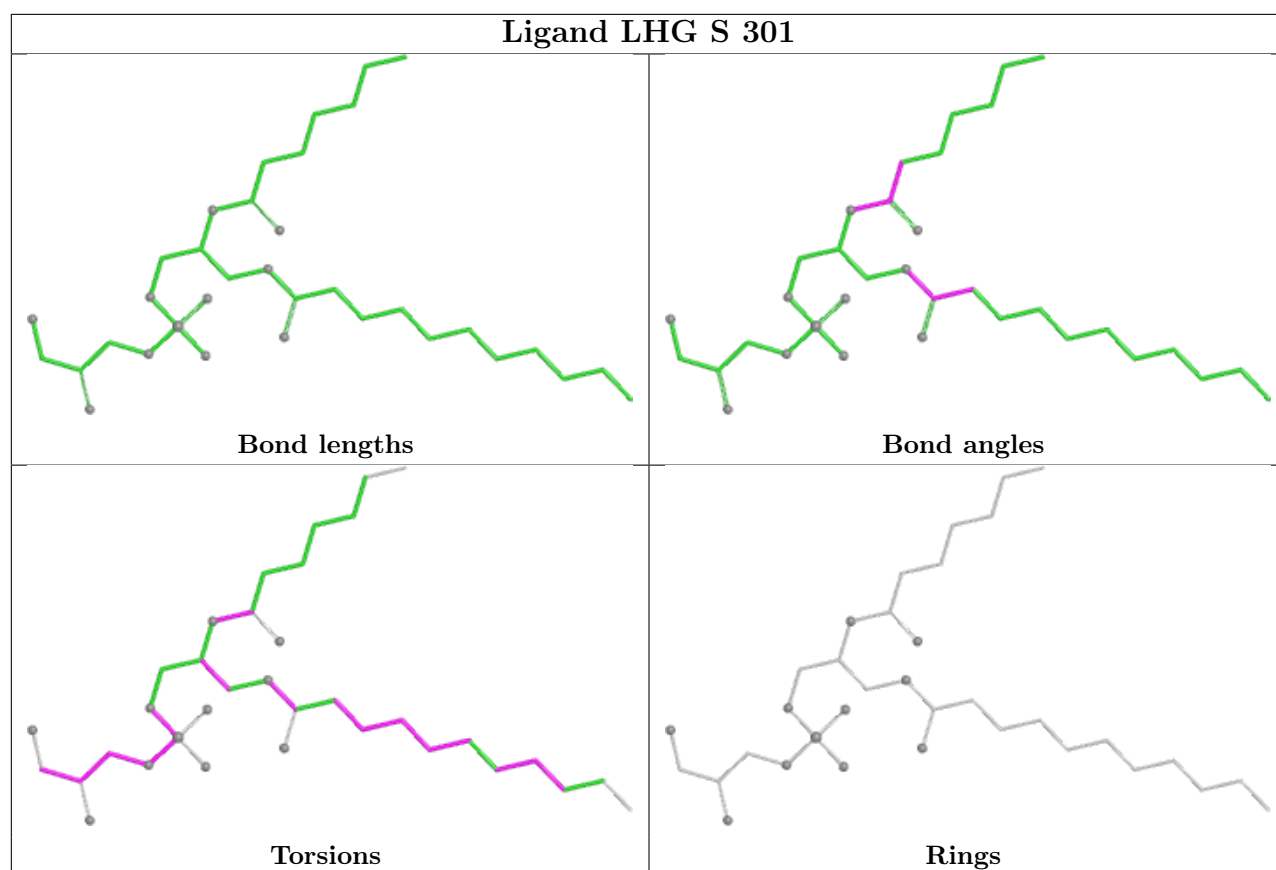




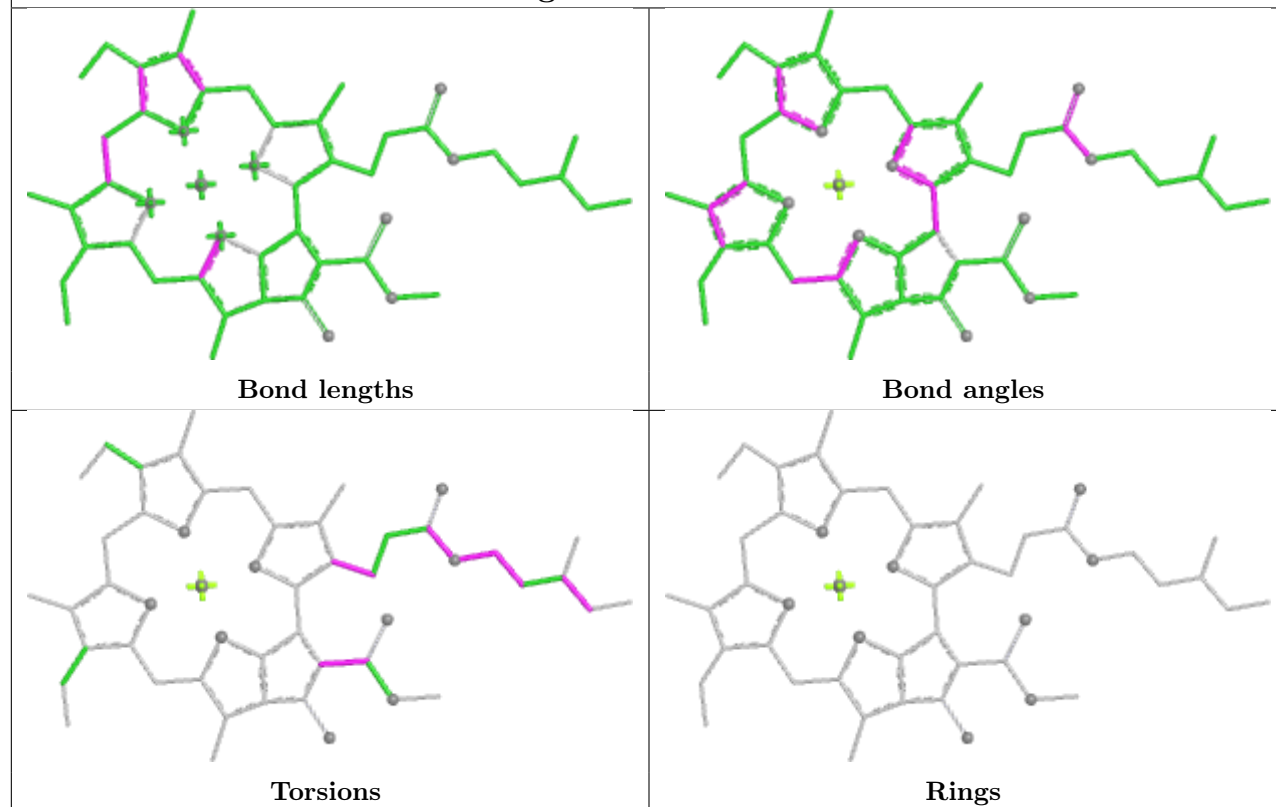


Ligand 3PH a 415	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 517	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CHL n 606	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

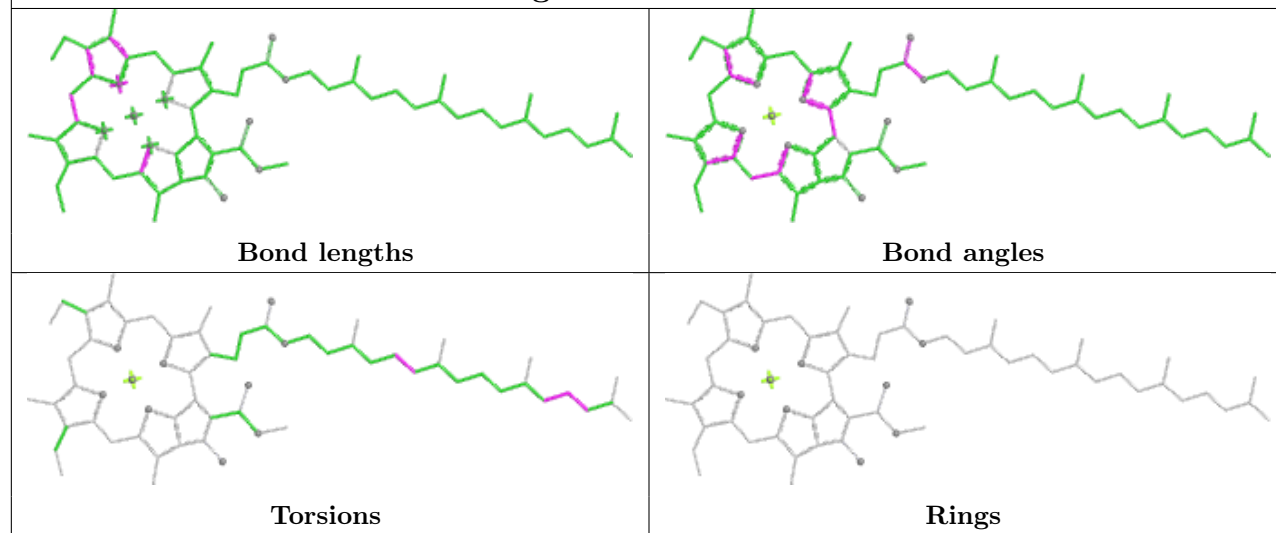




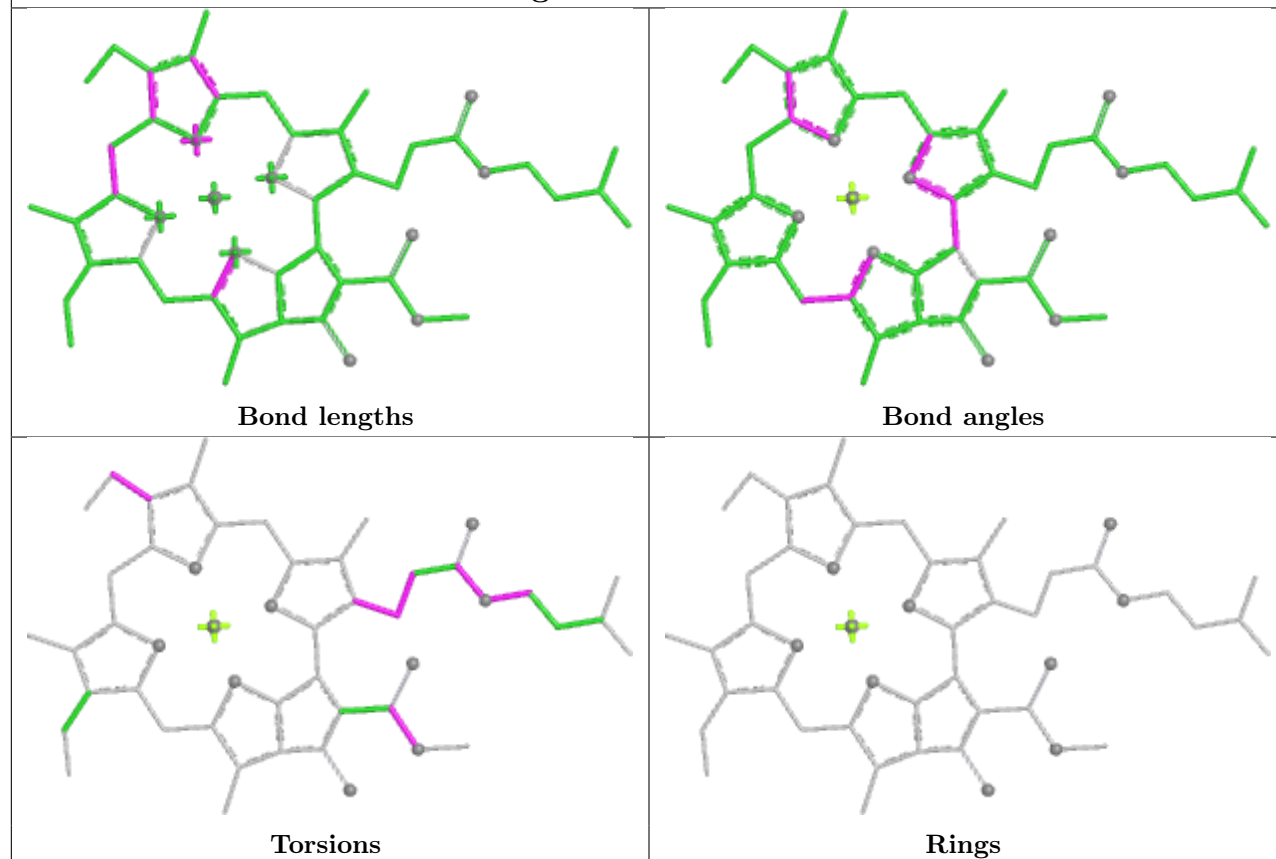
Ligand CLA r 310



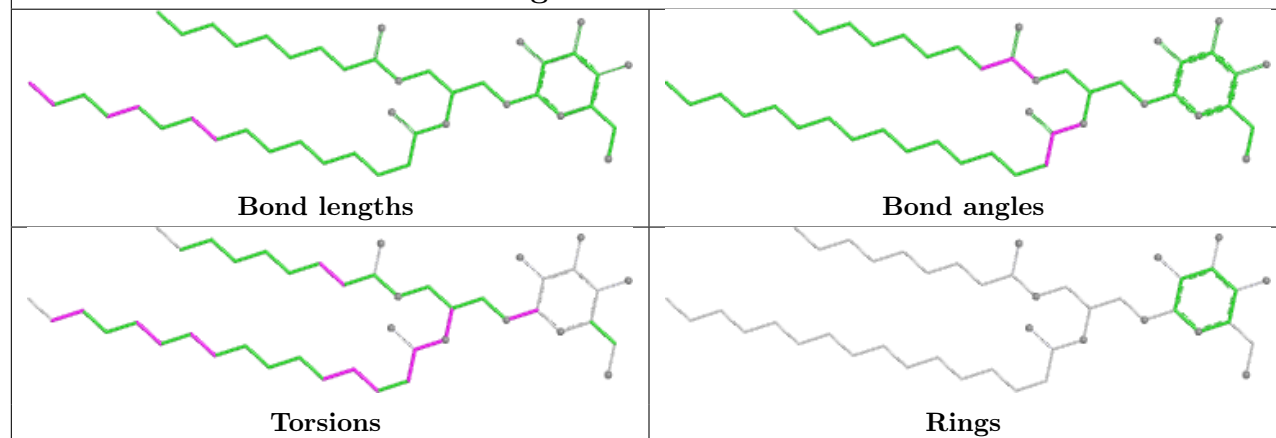
Ligand CLA C 509



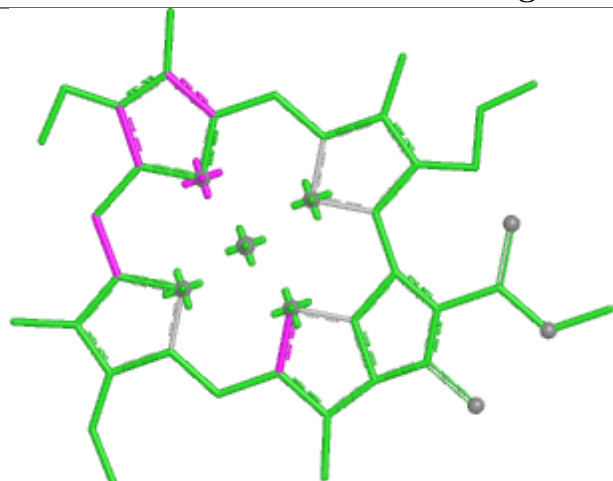
Ligand CLA Y 309



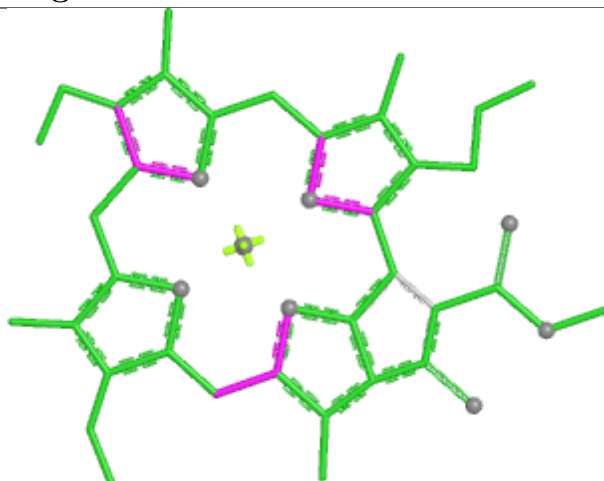
Ligand LMG b 520



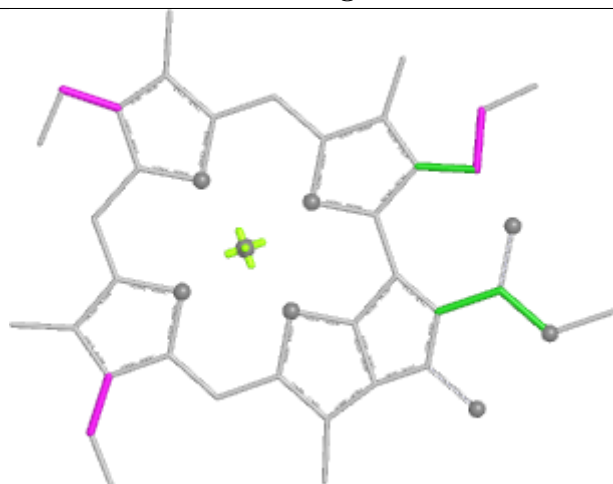
Ligand CLA g 612



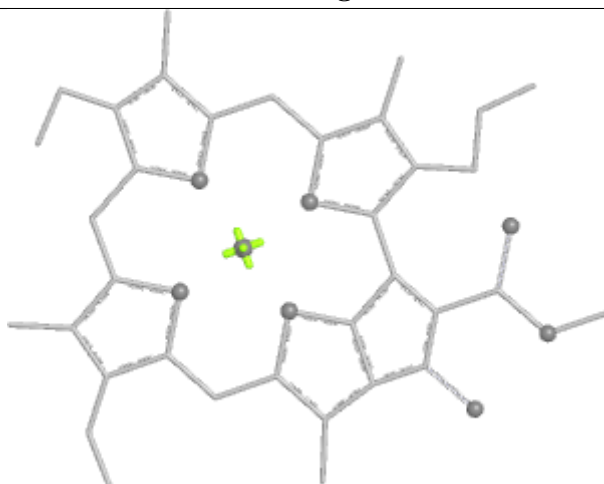
Bond lengths



Bond angles

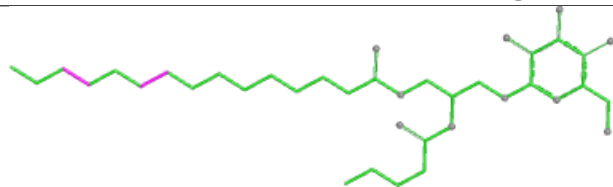


Torsions

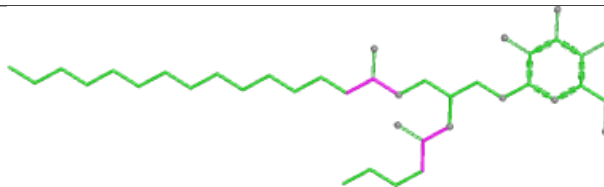


Rings

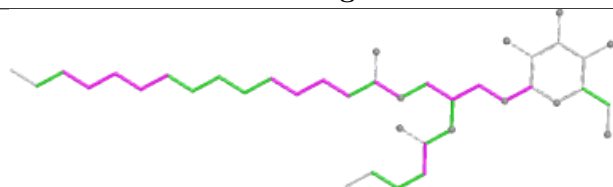
Ligand LMG w 202



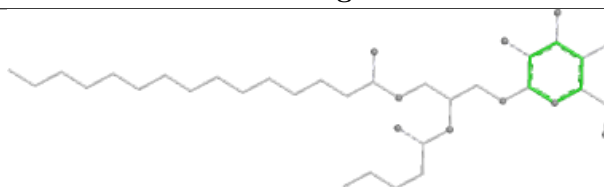
Bond lengths



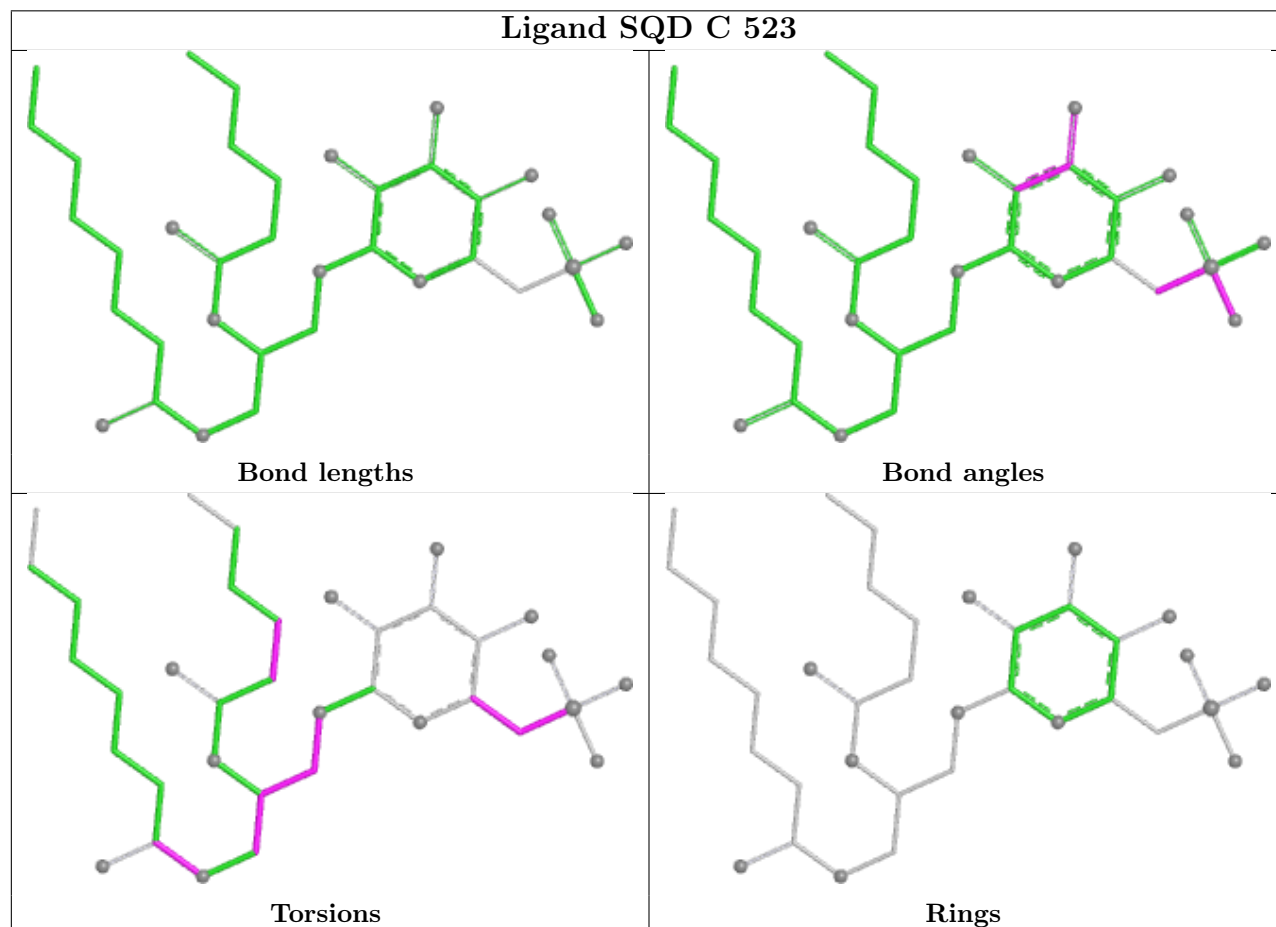
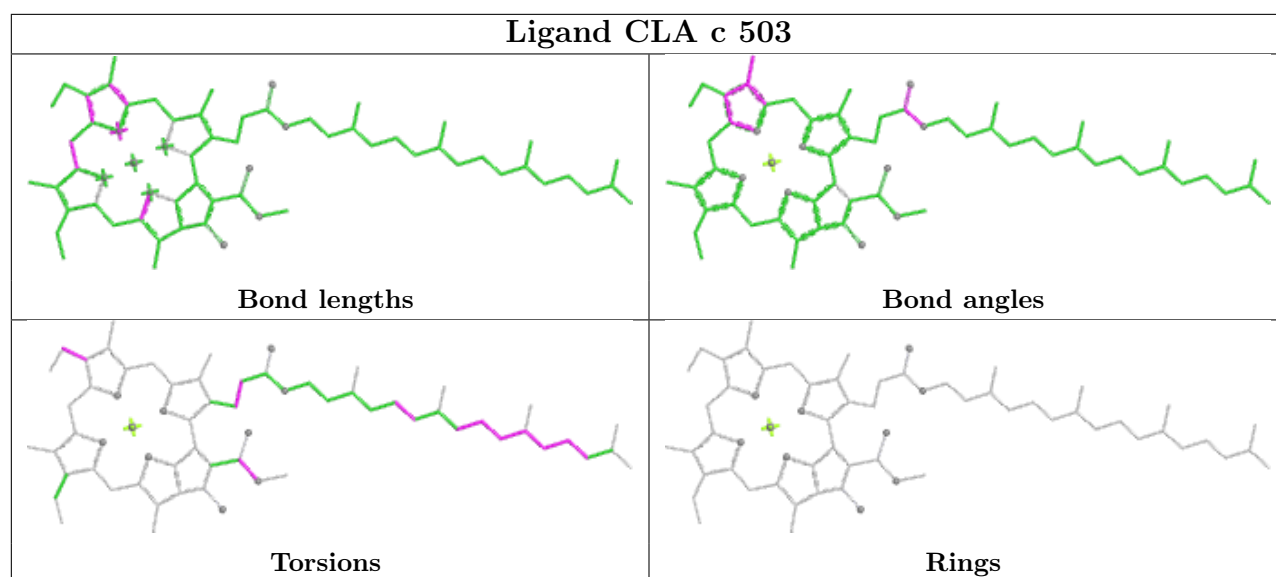
Bond angles

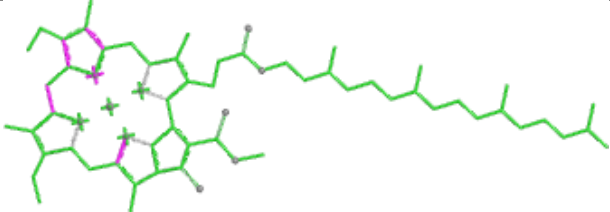
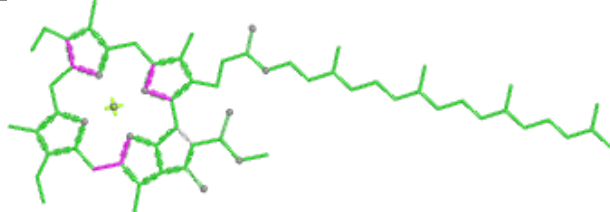
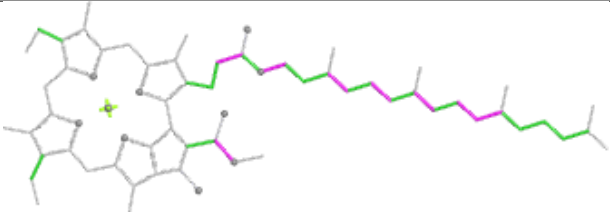
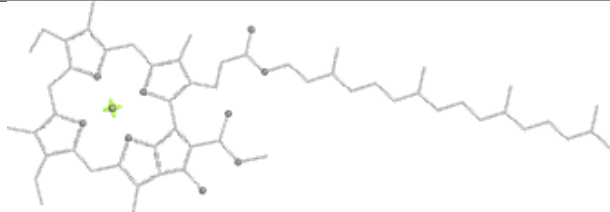
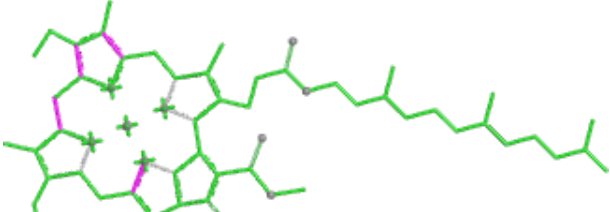
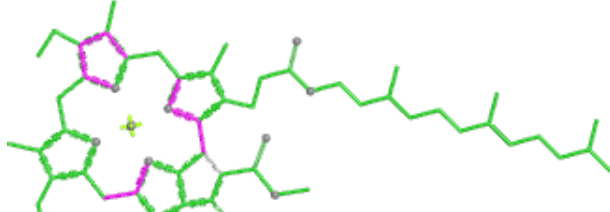
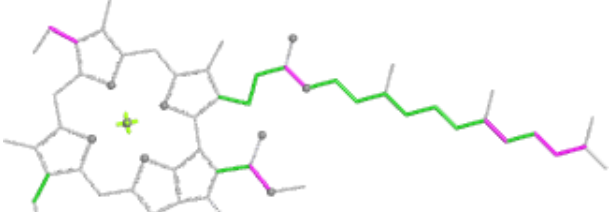
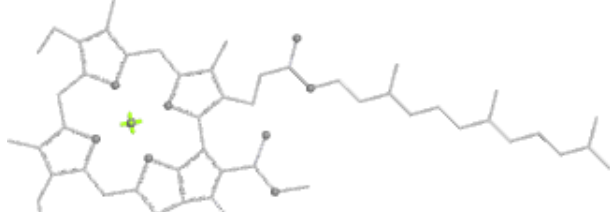
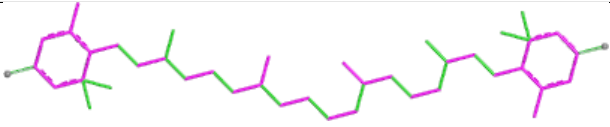
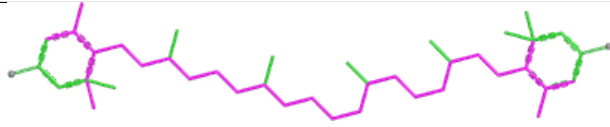
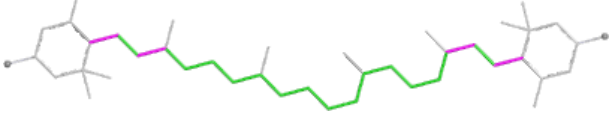
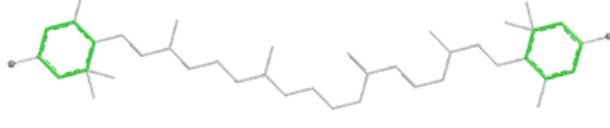


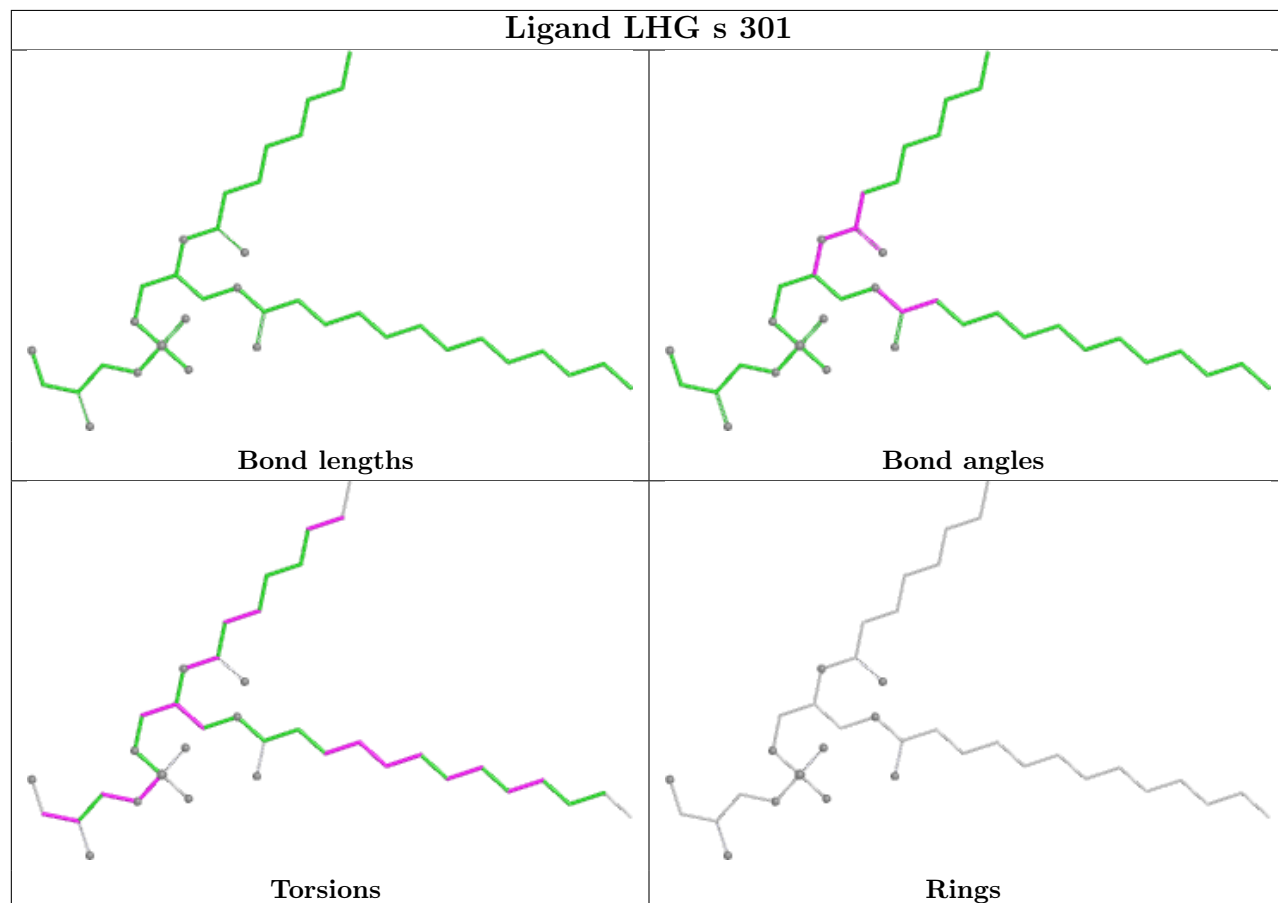
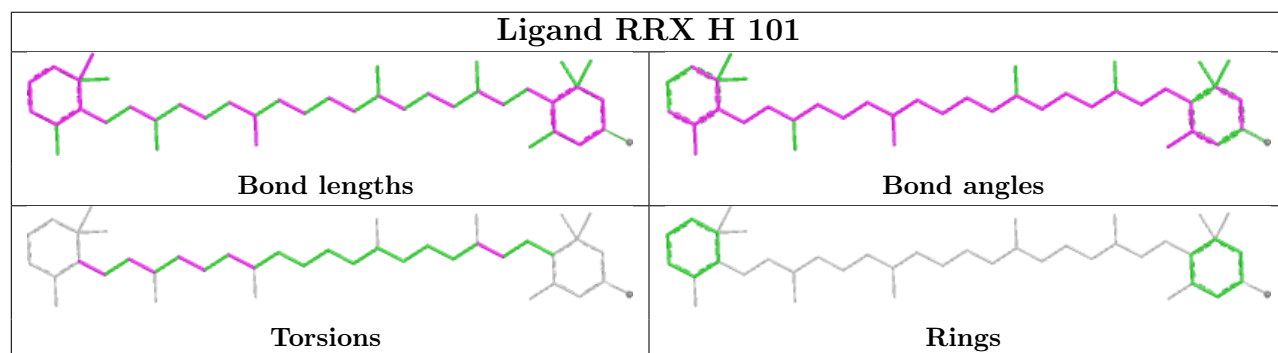
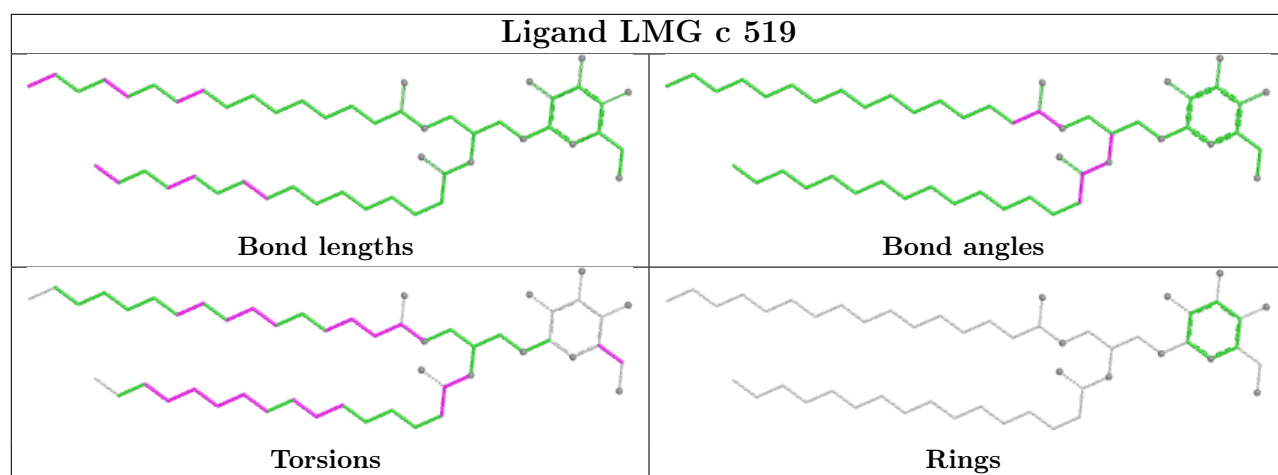
Torsions

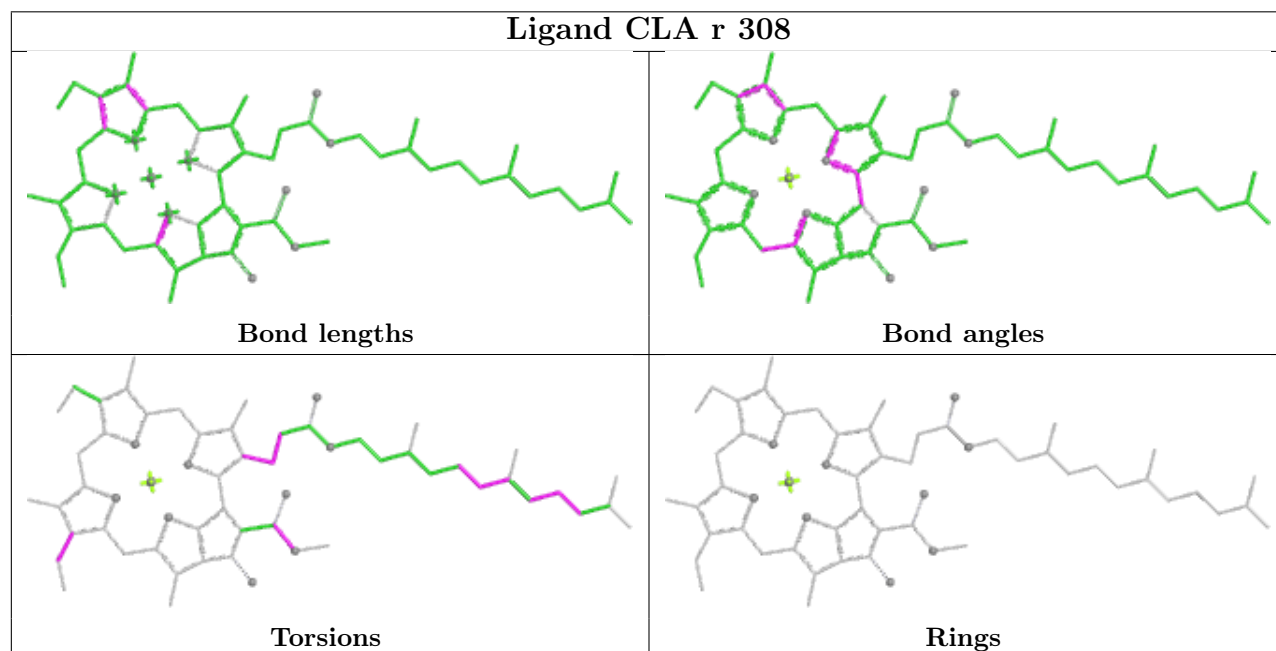
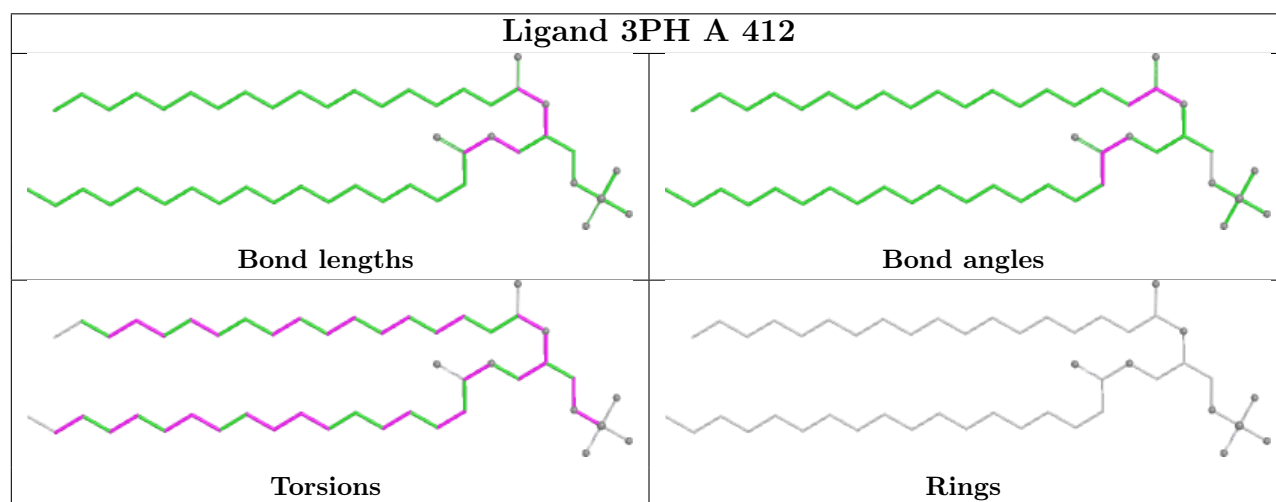
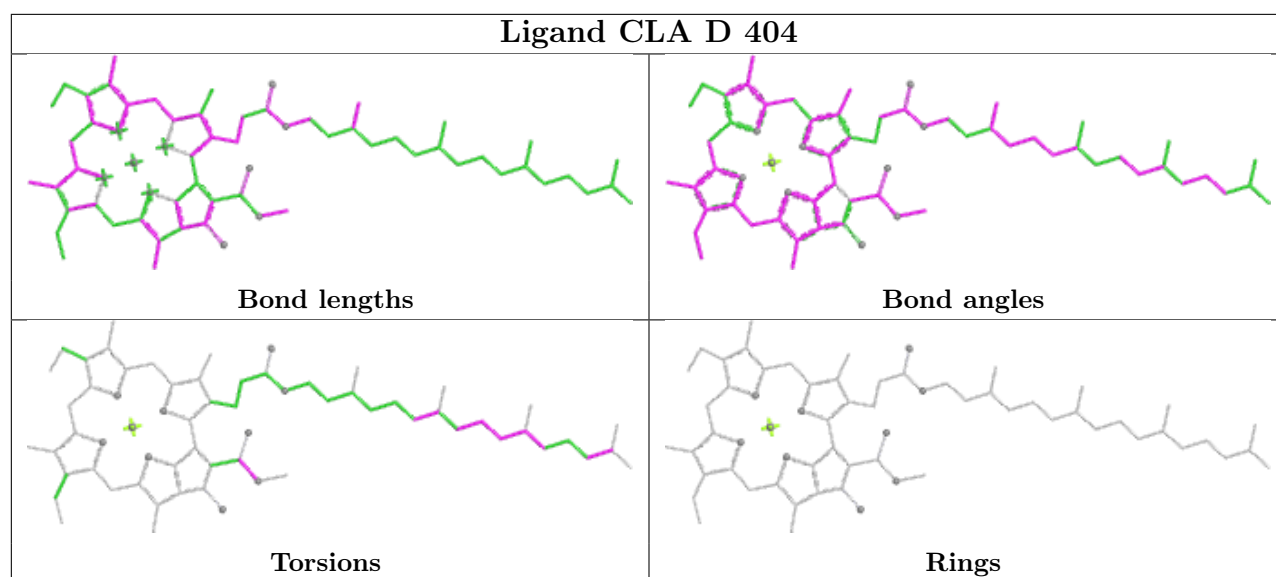


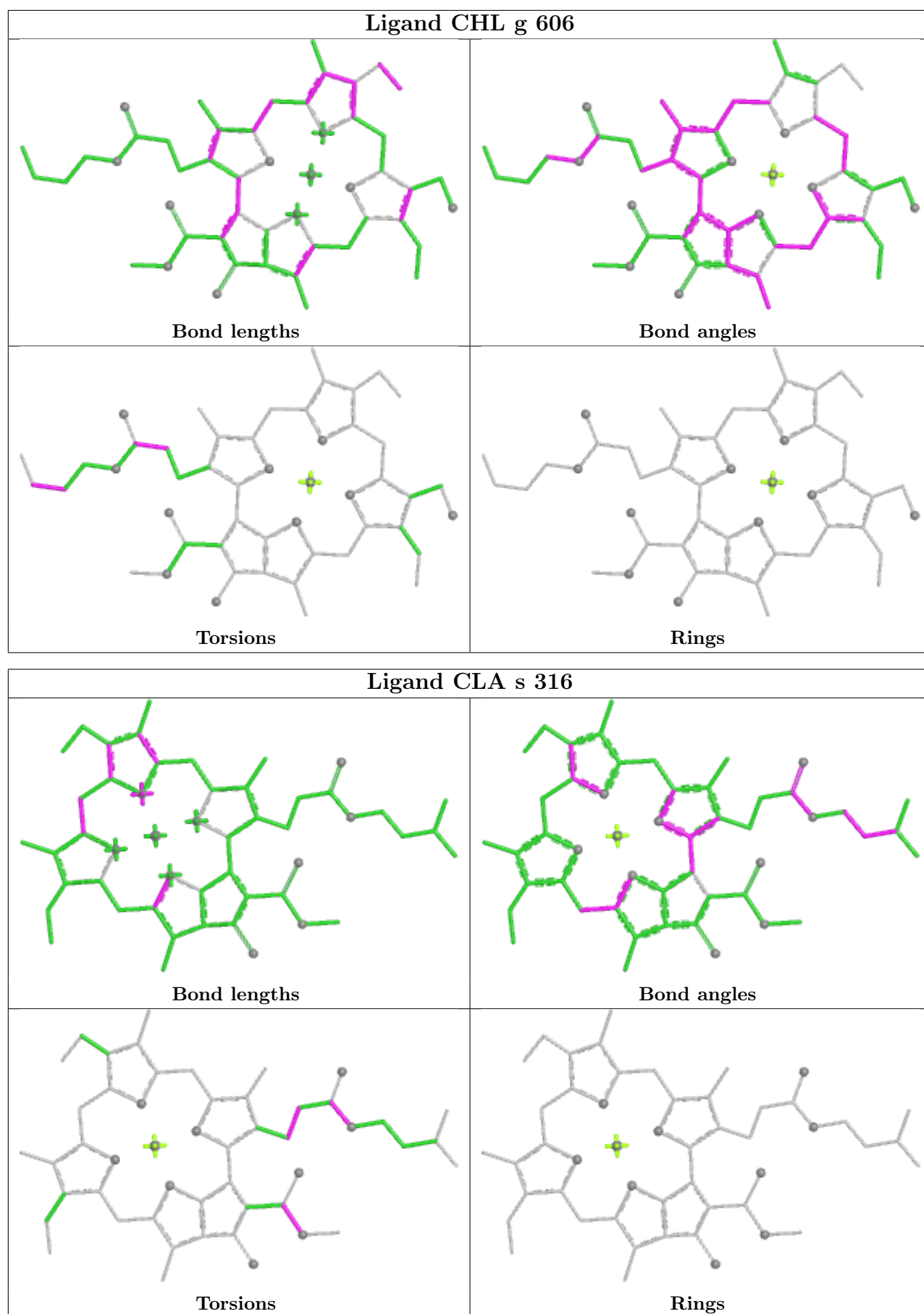
Rings

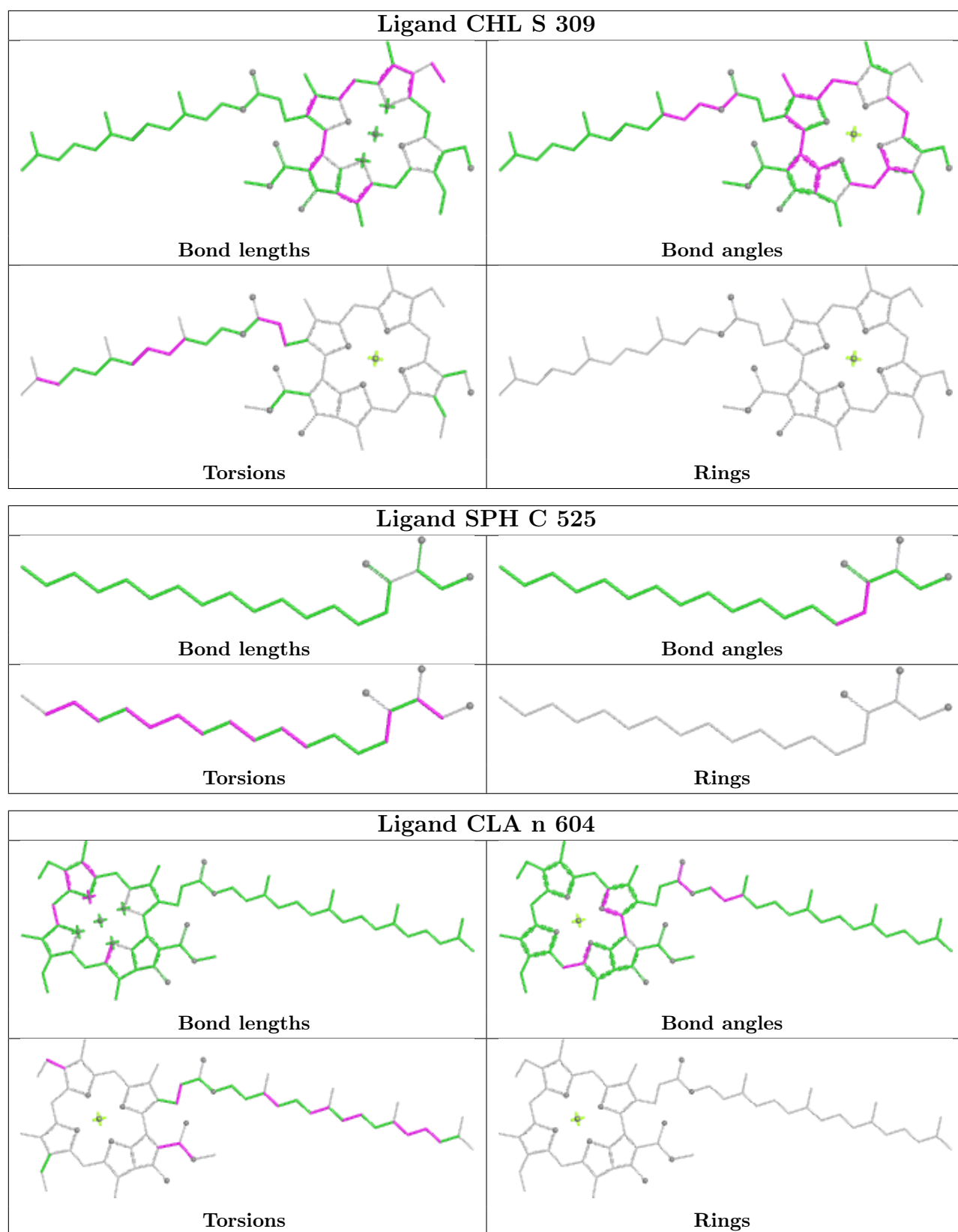


Ligand CLA B 513	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA S 310	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand C7Z B 519	
 Bond lengths	 Bond angles
 Torsions	 Rings

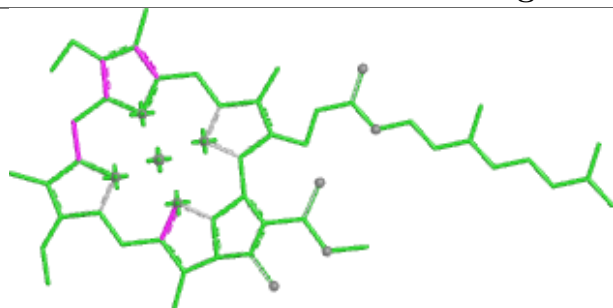




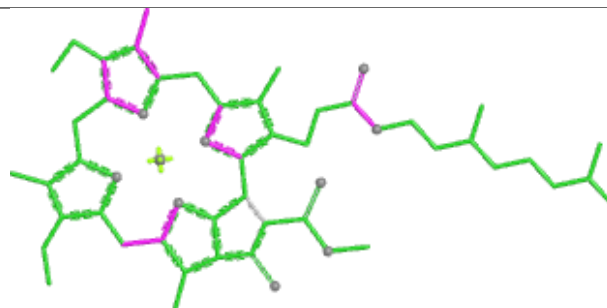




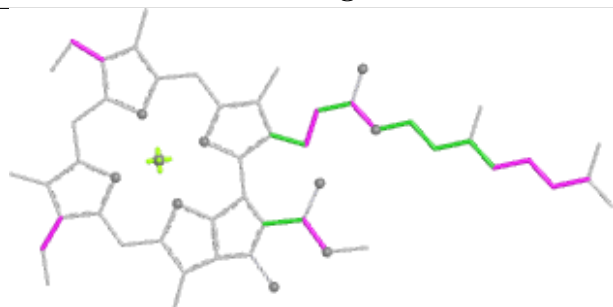
Ligand CLA S 314



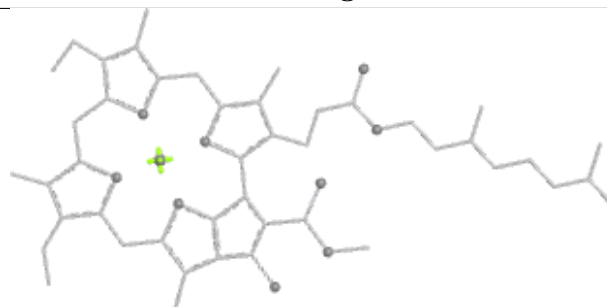
Bond lengths



Bond angles

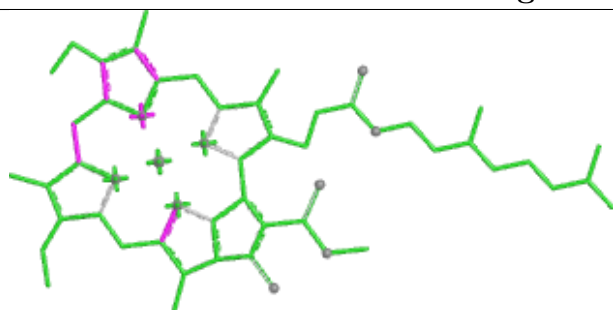


Torsions

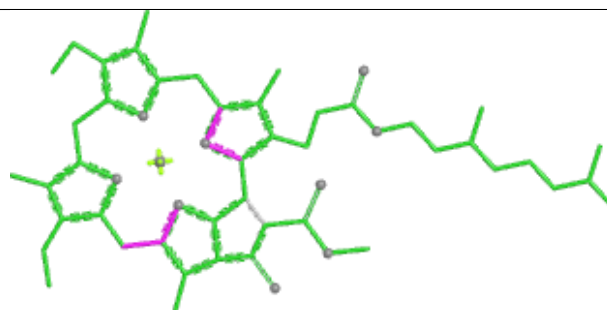


Rings

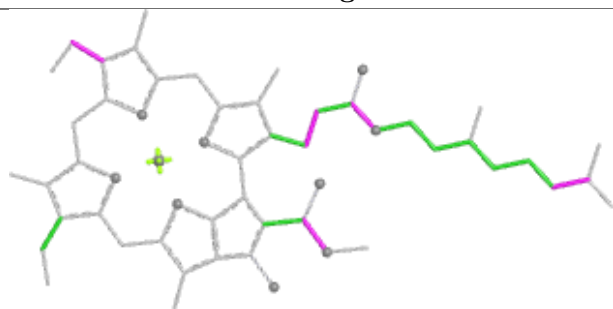
Ligand CLA S 305



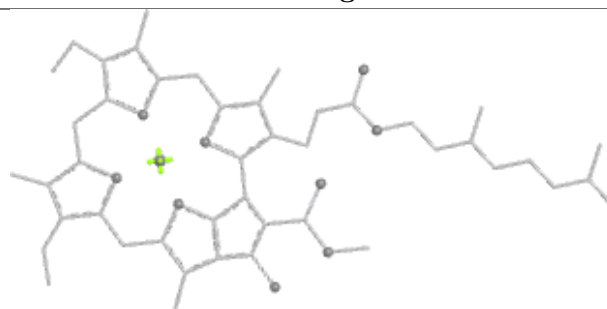
Bond lengths



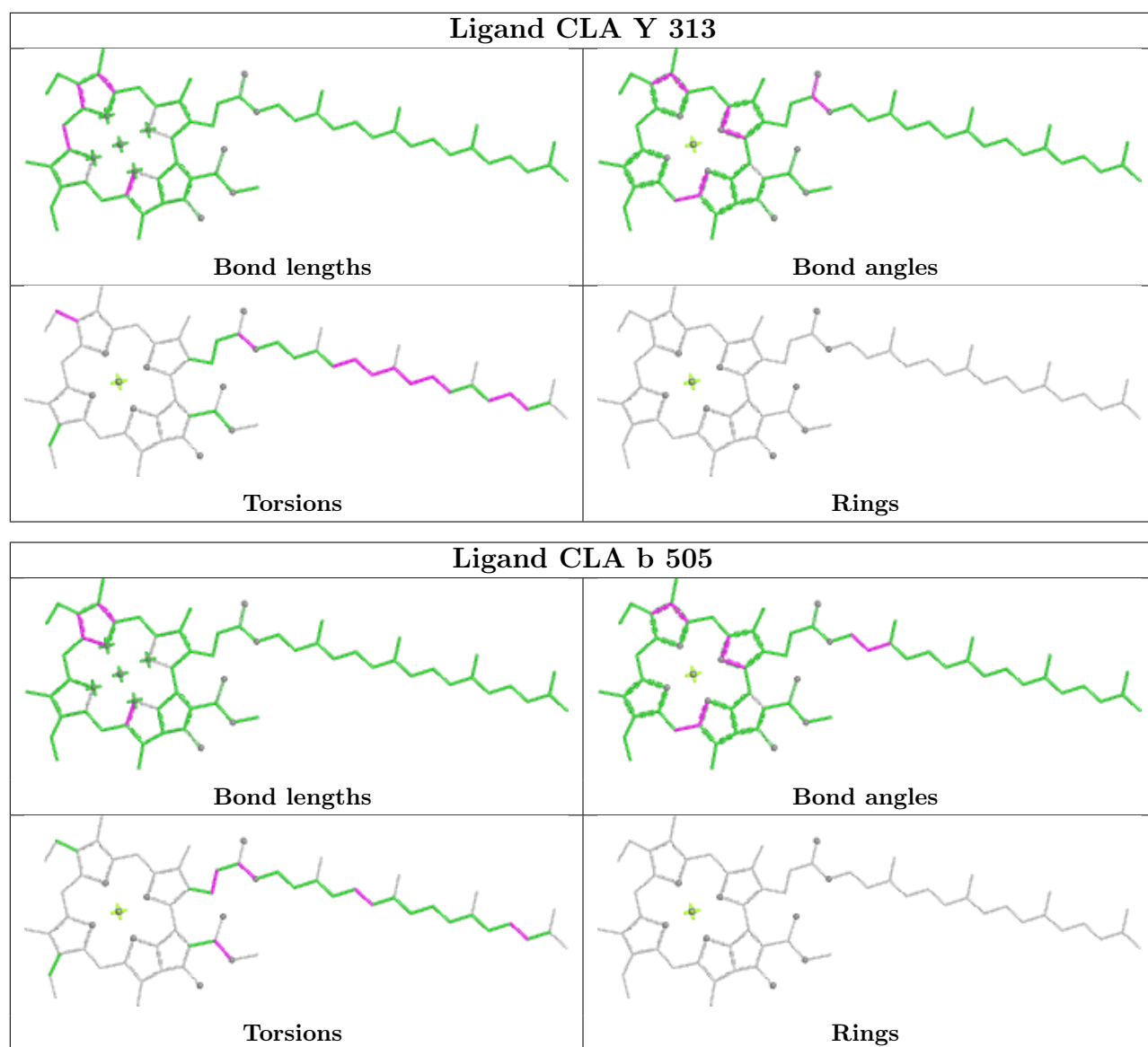
Bond angles



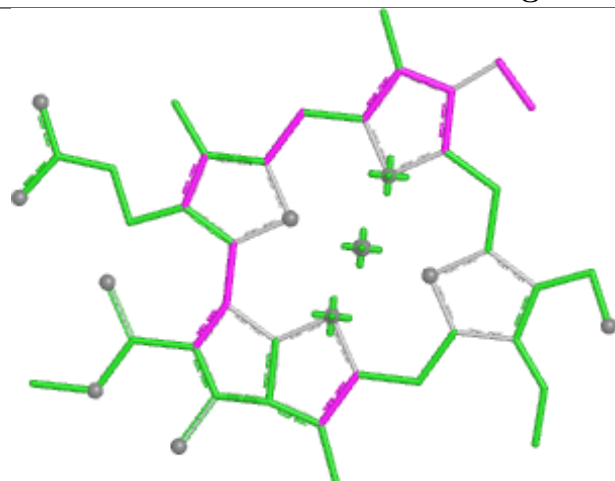
Torsions



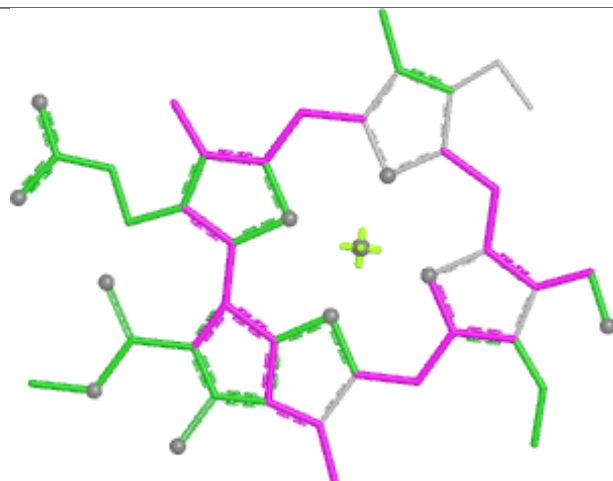
Rings



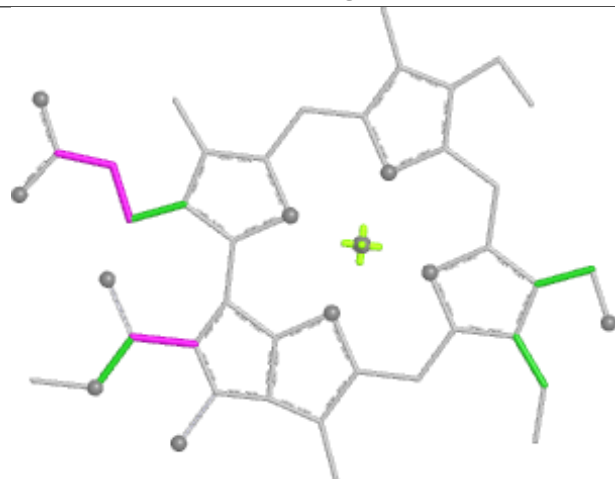
Ligand CHL s 302



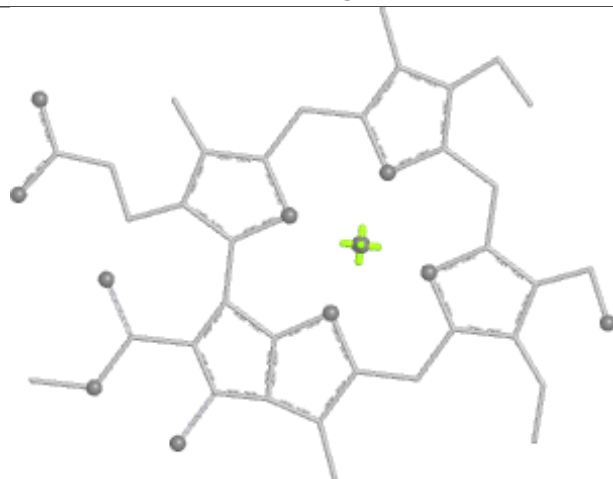
Bond lengths



Bond angles

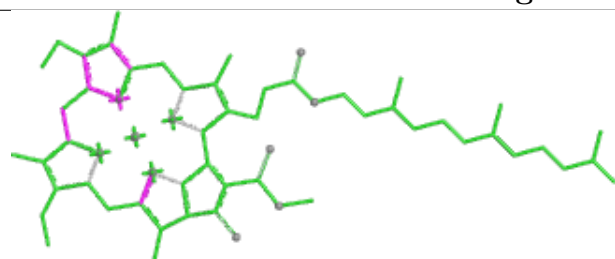


Torsions

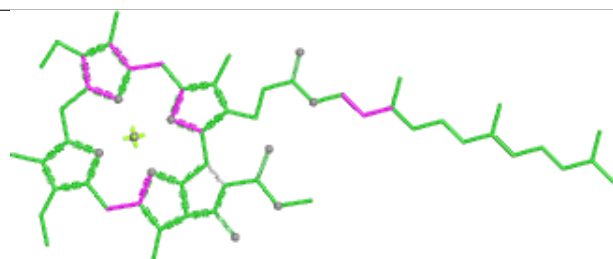


Rings

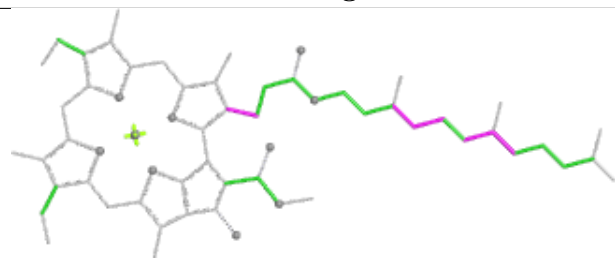
Ligand CLA A 409



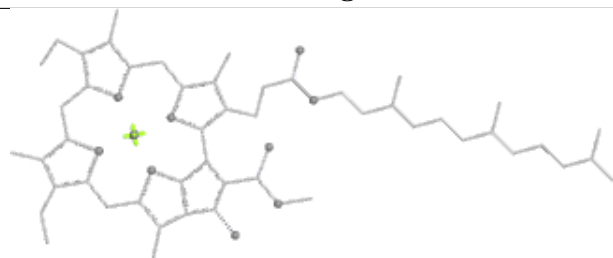
Bond lengths



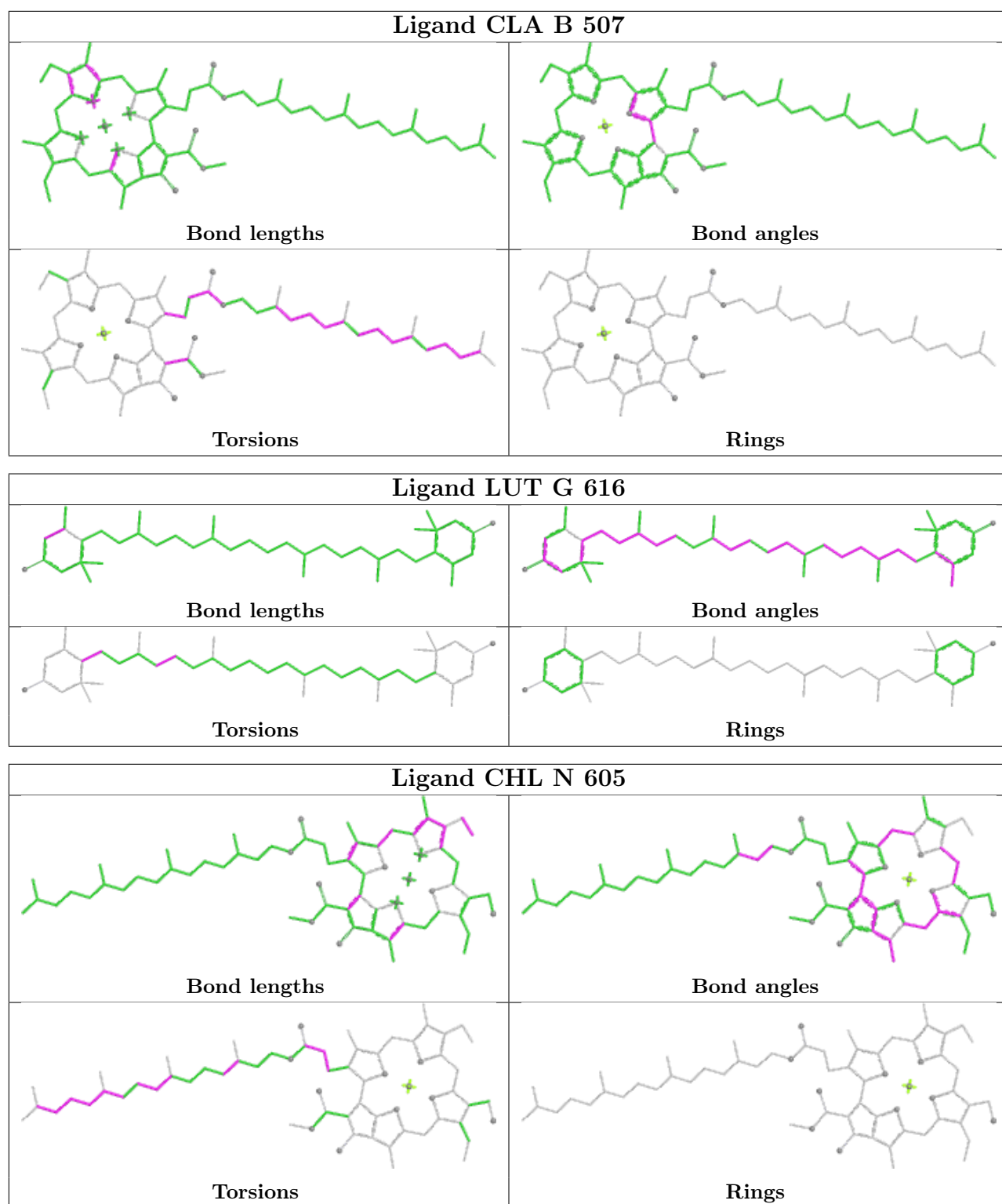
Bond angles

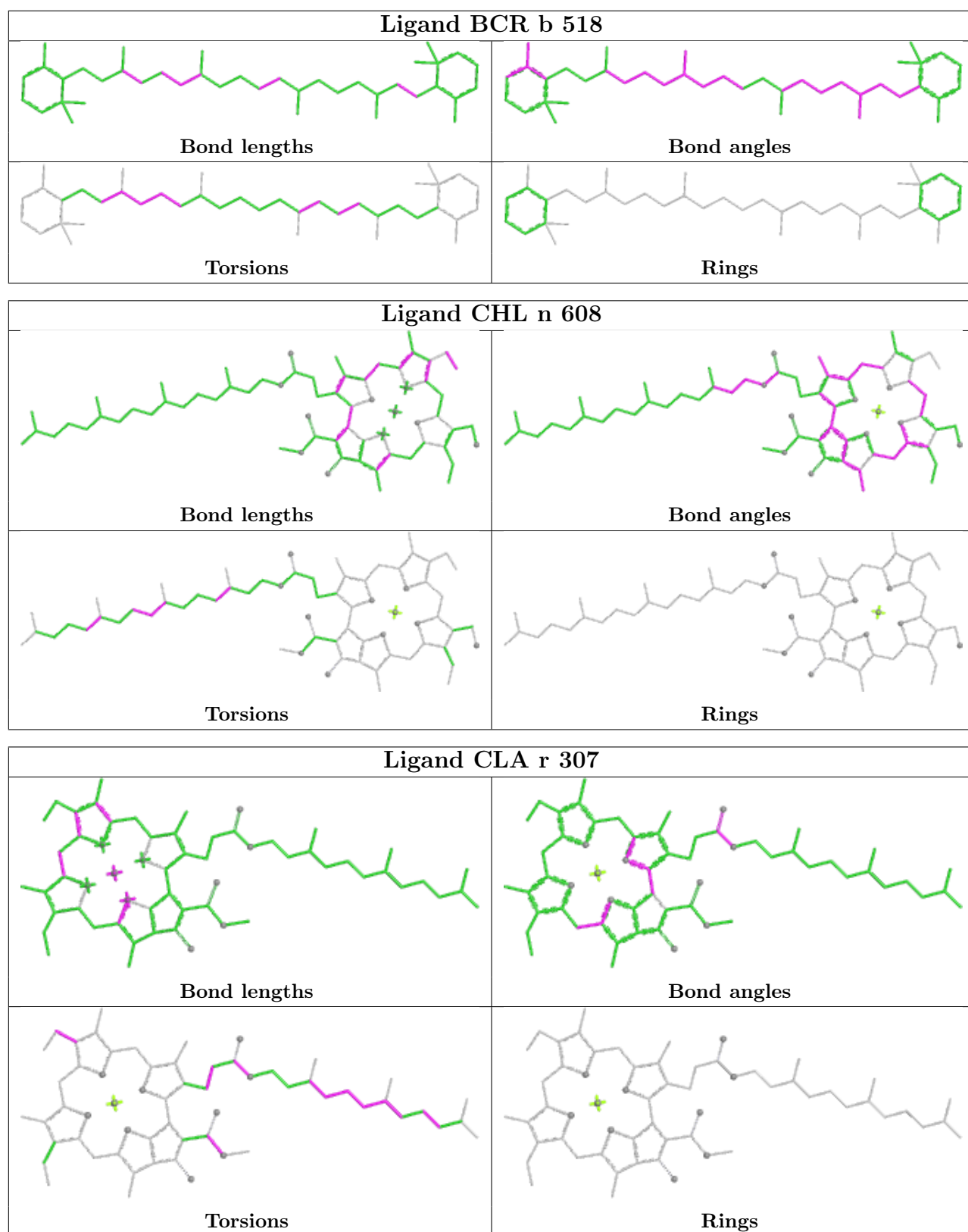


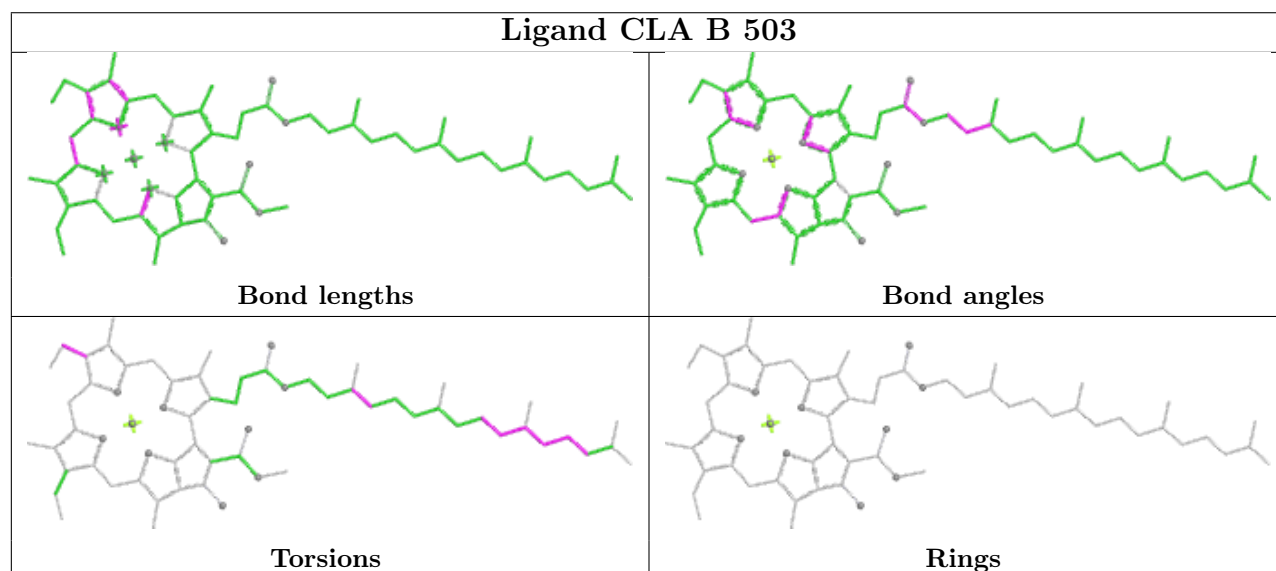
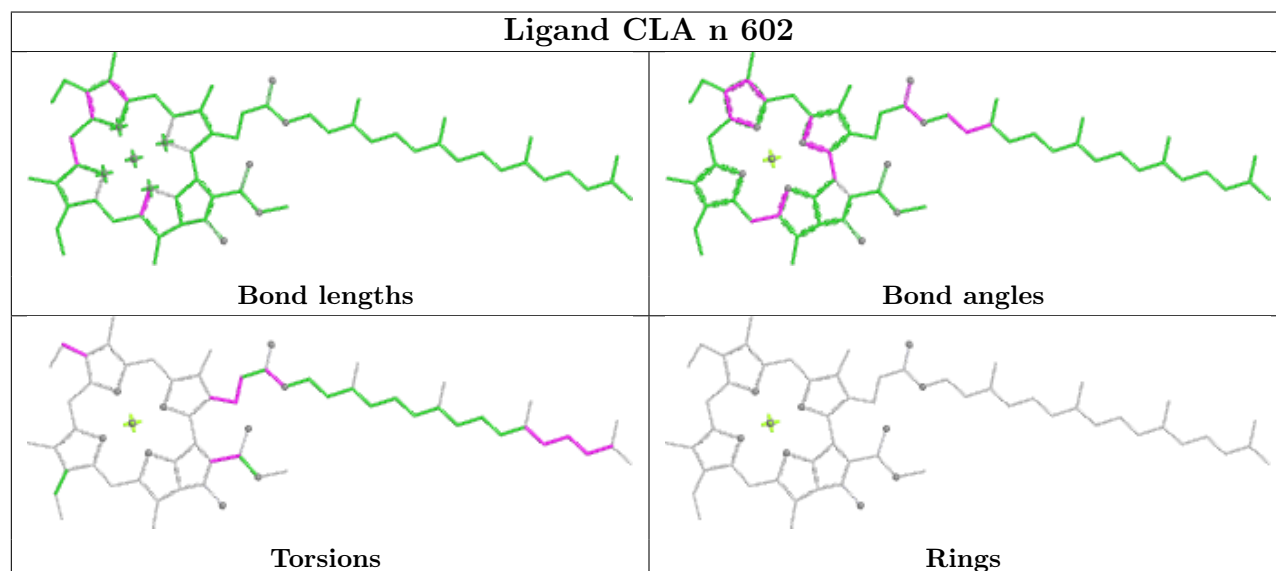
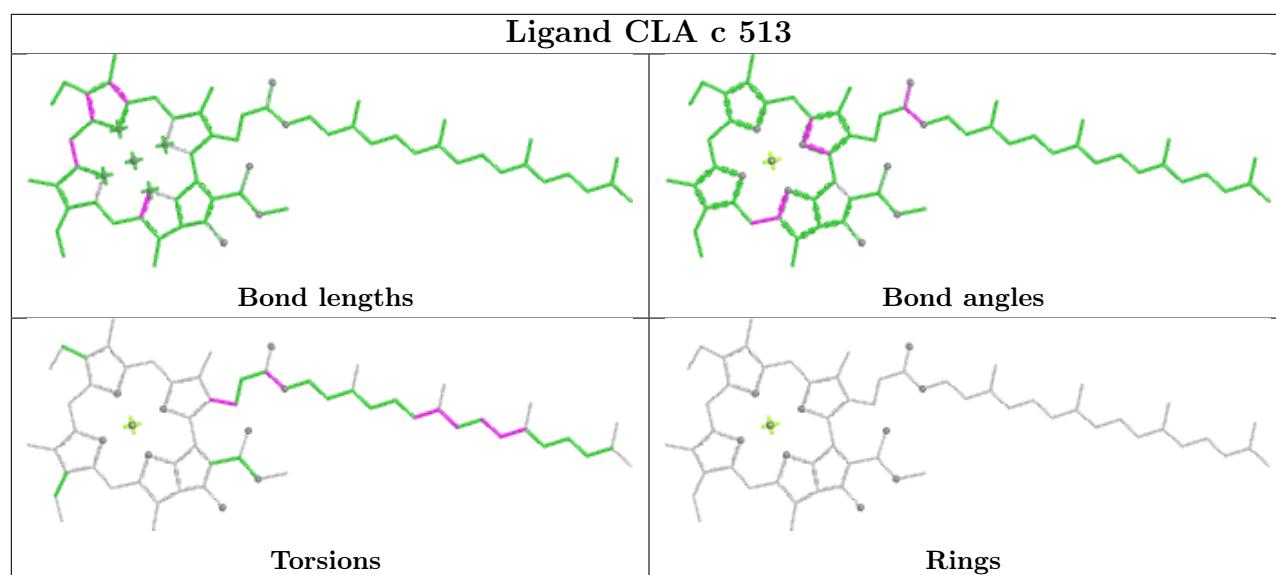
Torsions

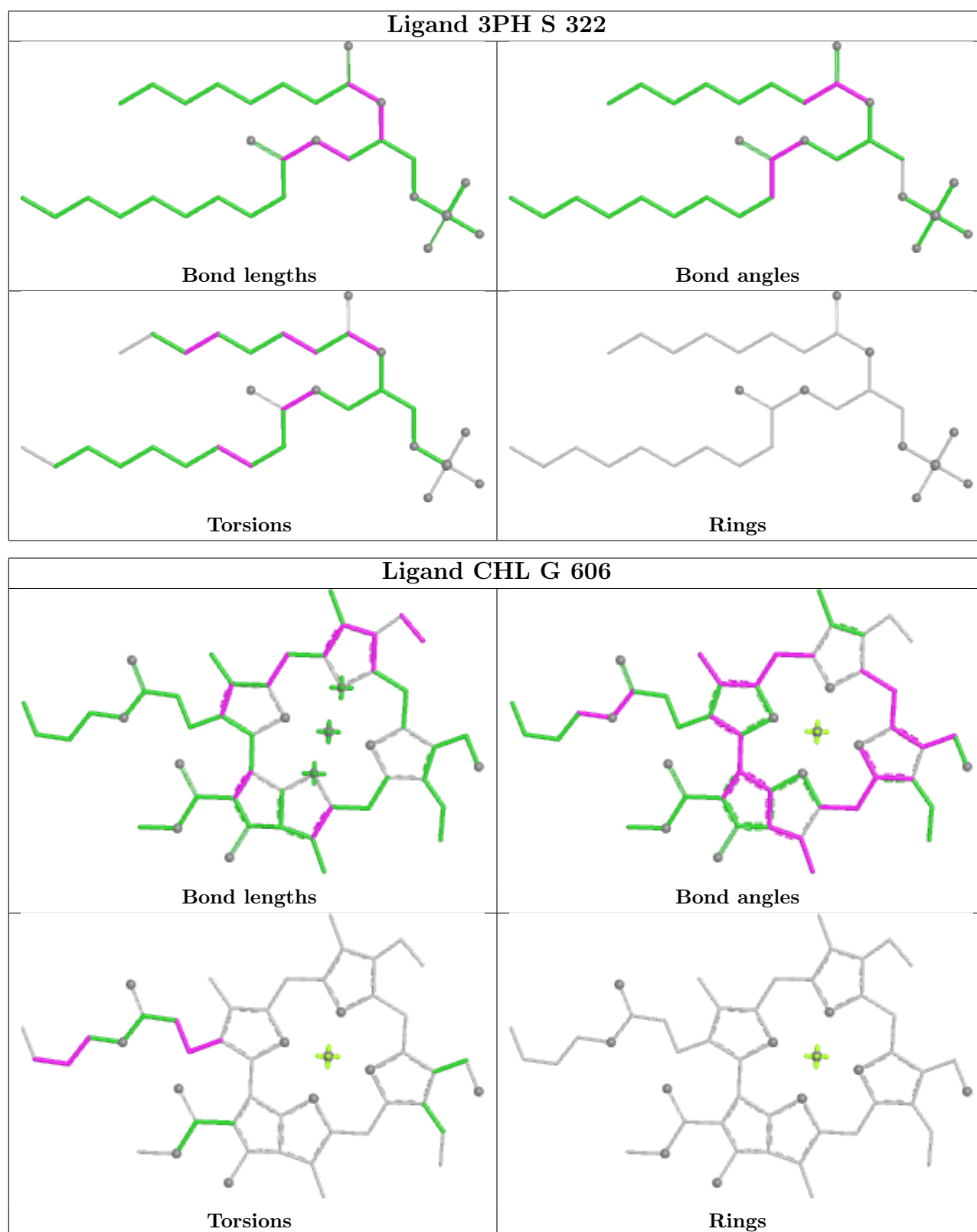


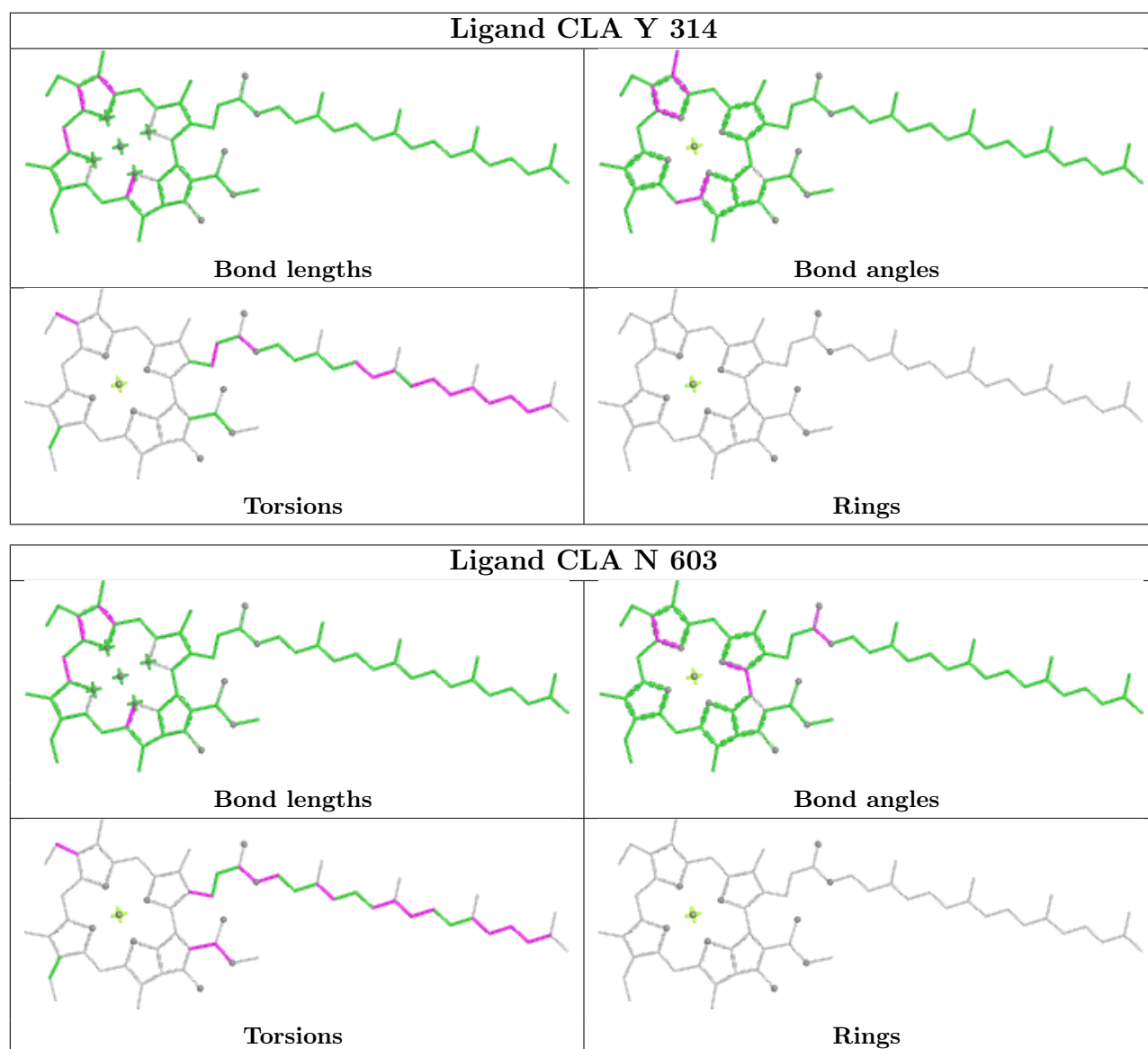
Rings

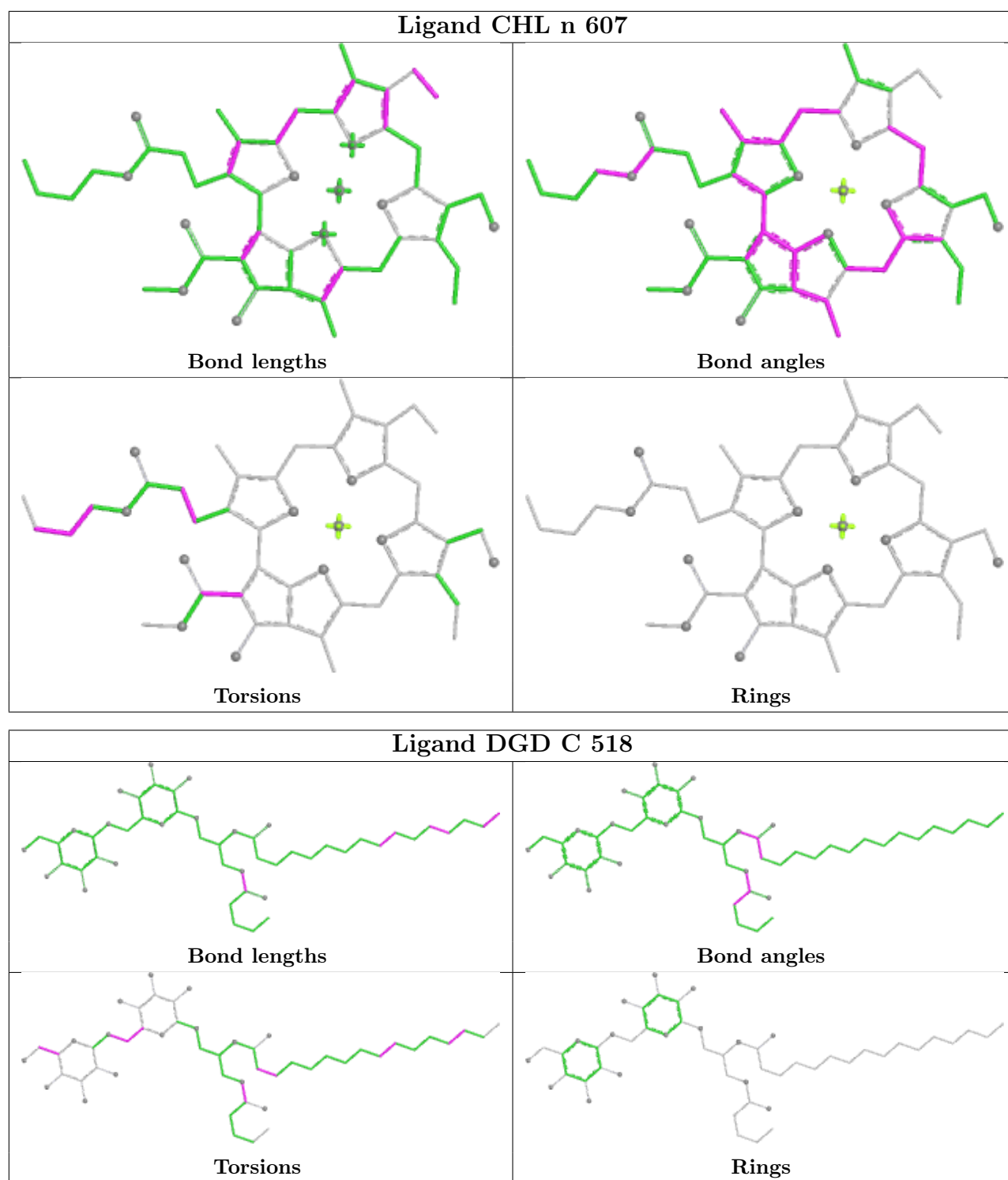


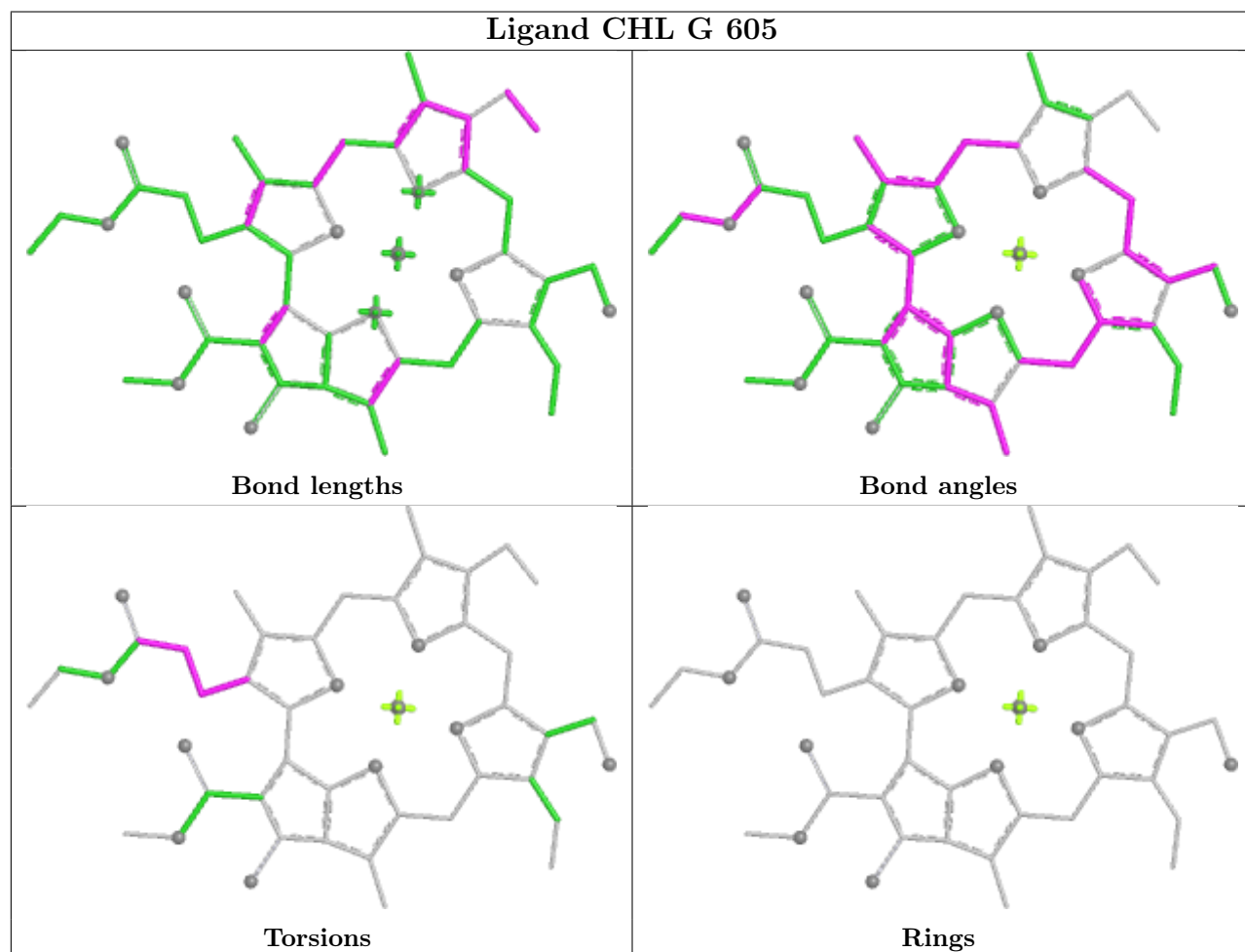
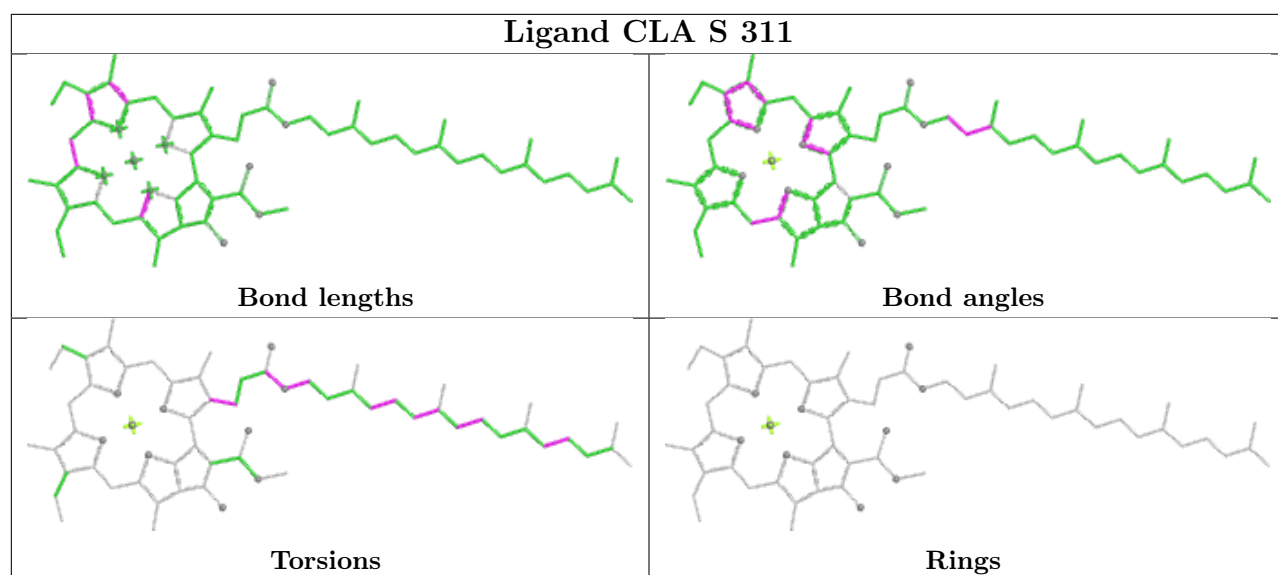


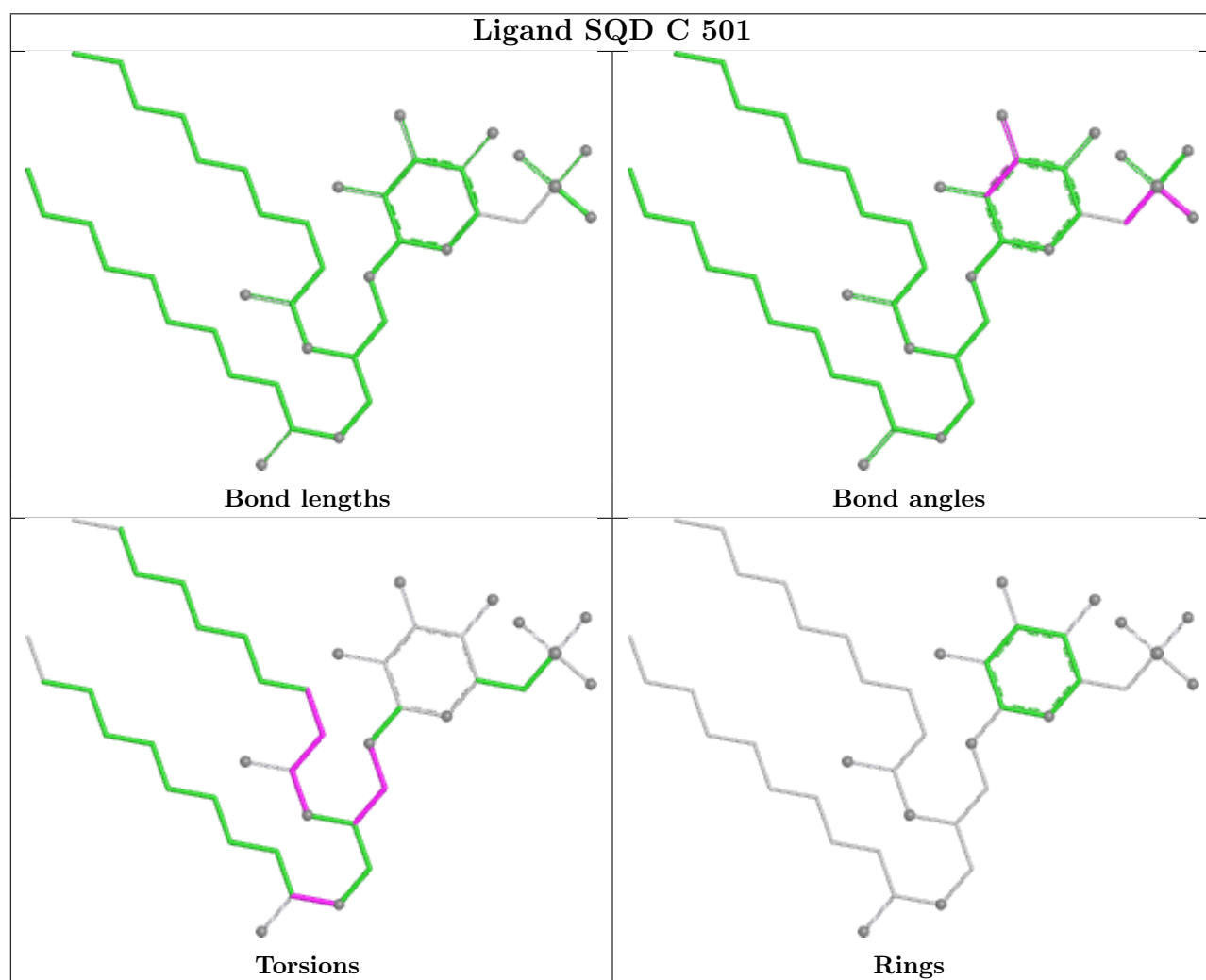
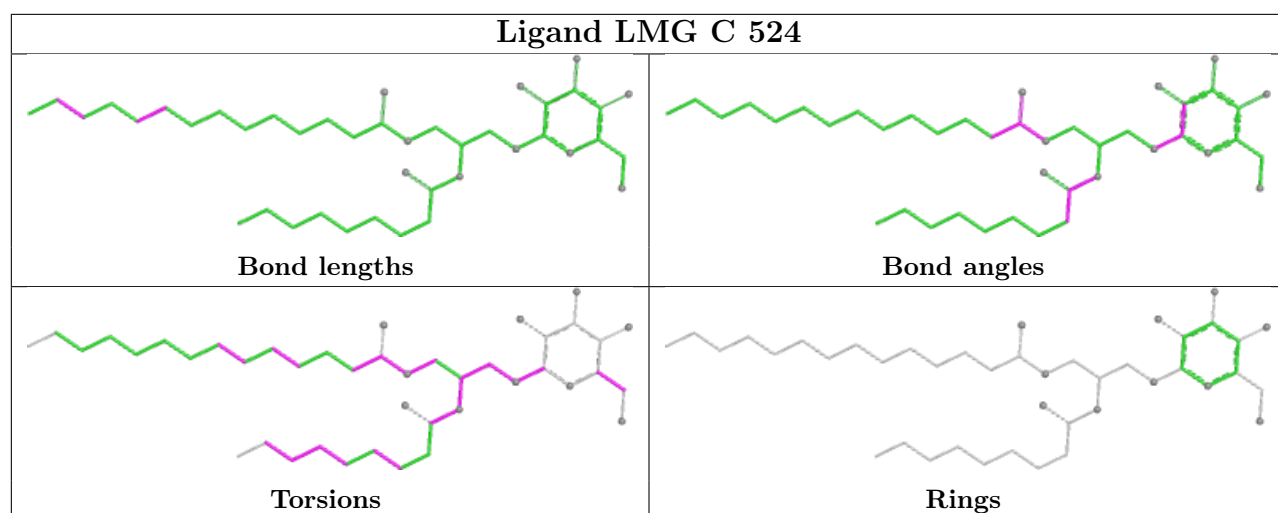


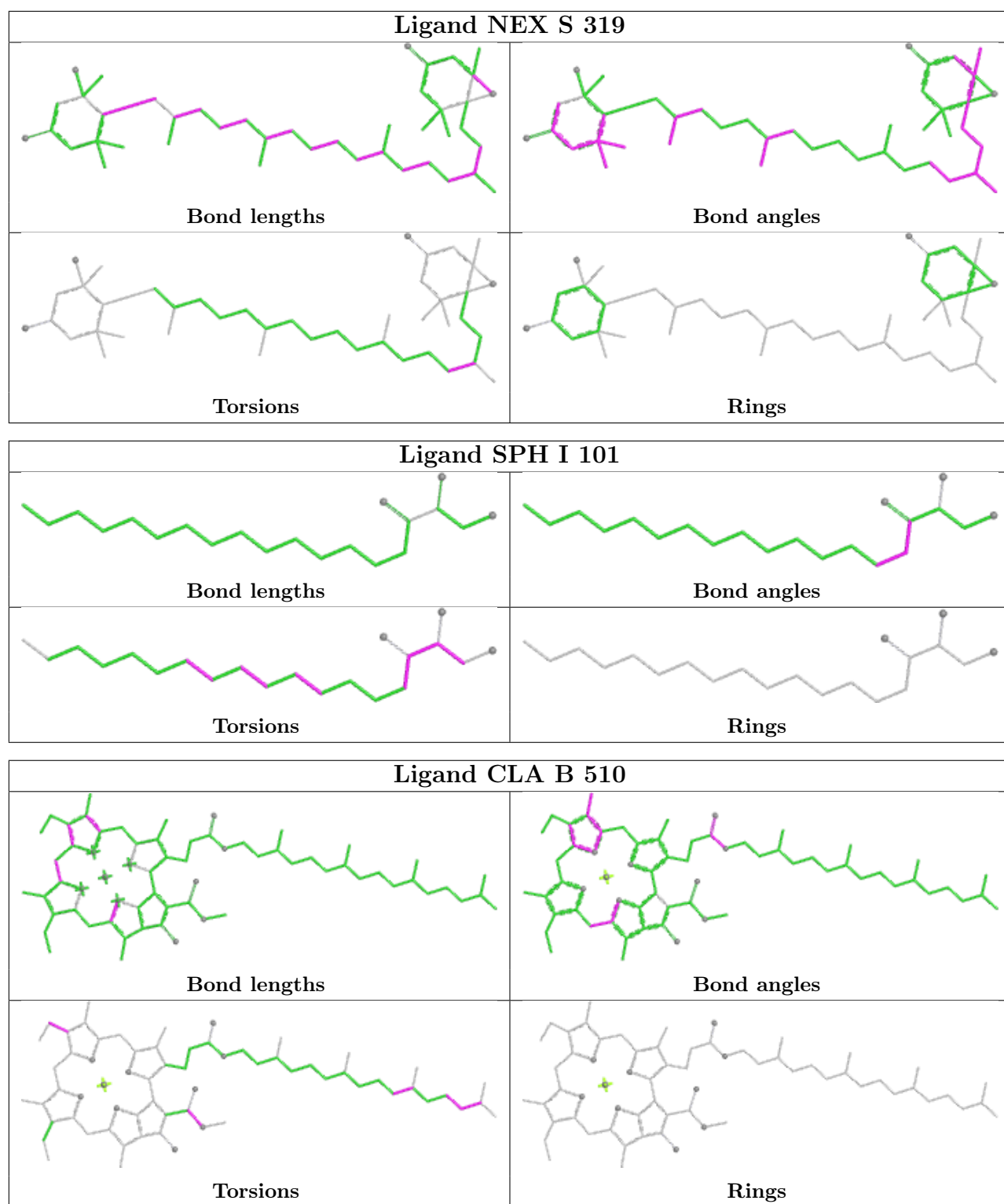


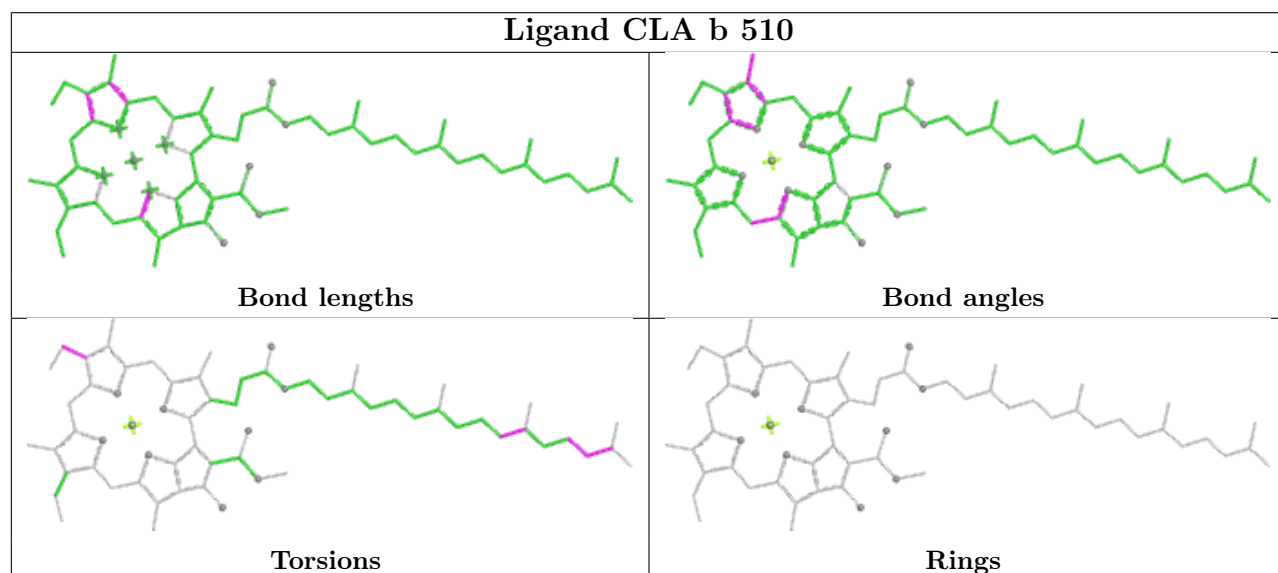
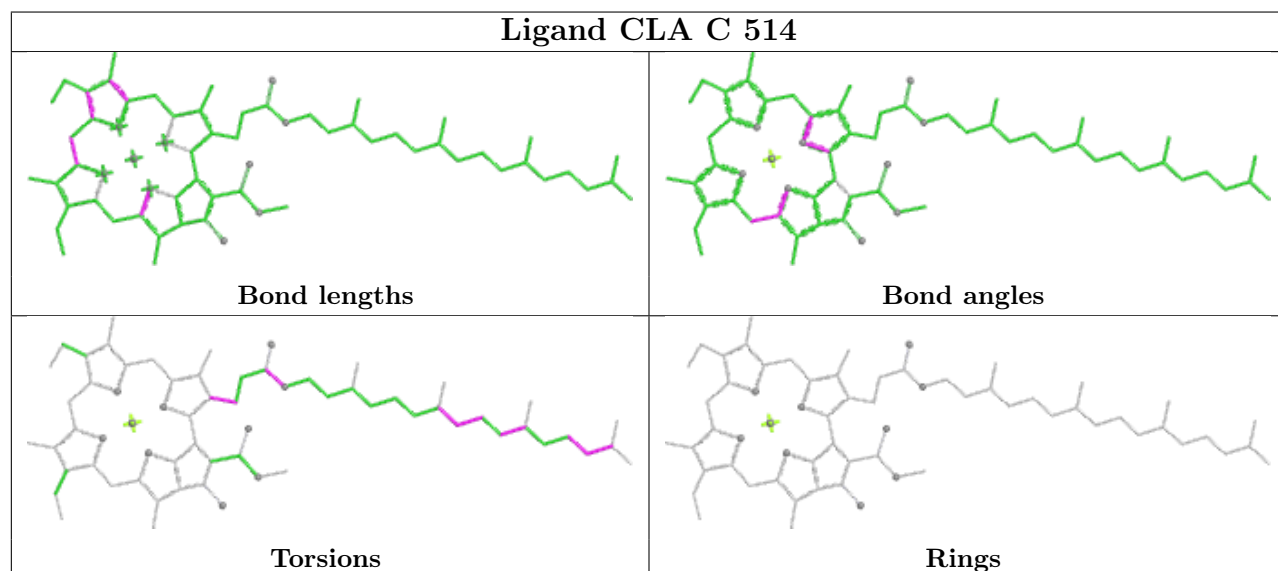
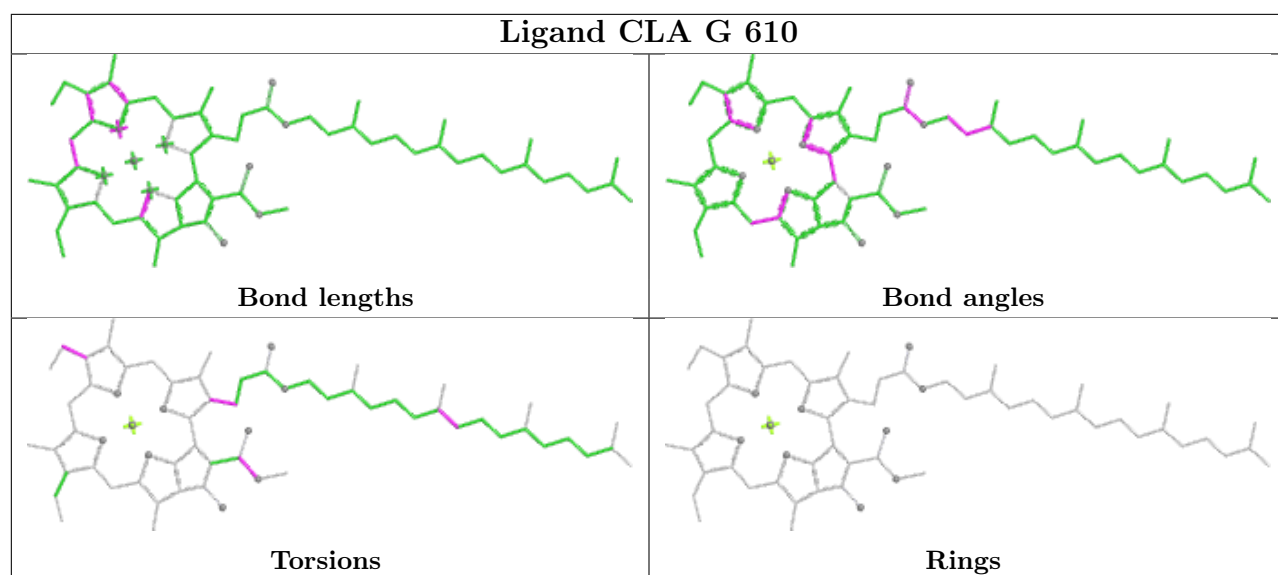




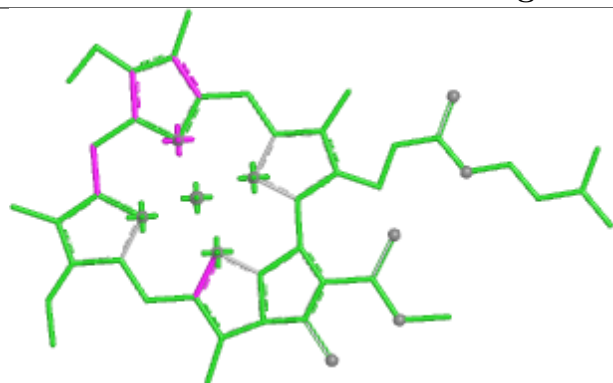




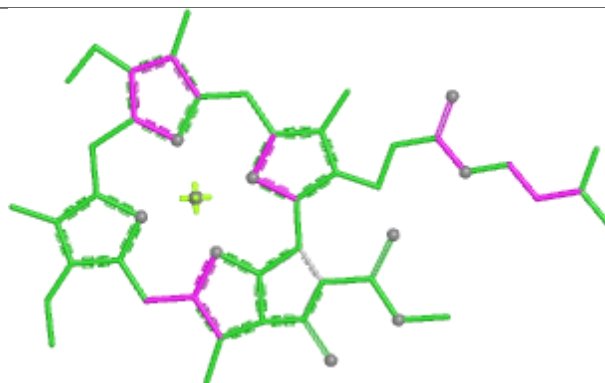




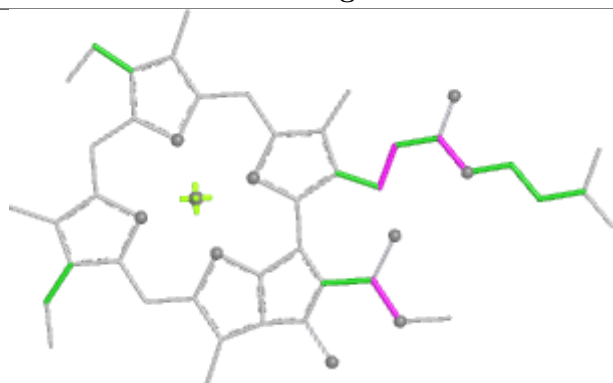
Ligand CLA S 316



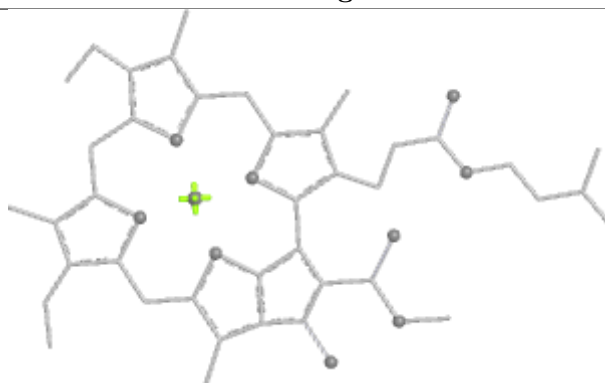
Bond lengths



Bond angles

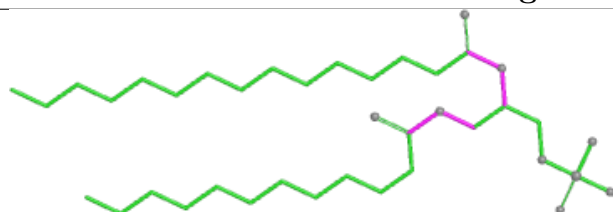


Torsions

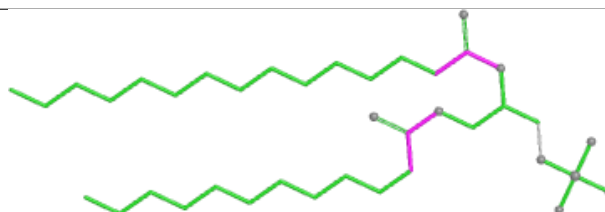


Rings

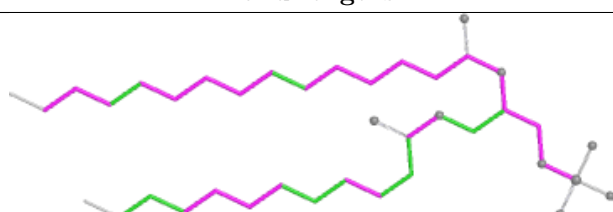
Ligand 3PH b 521



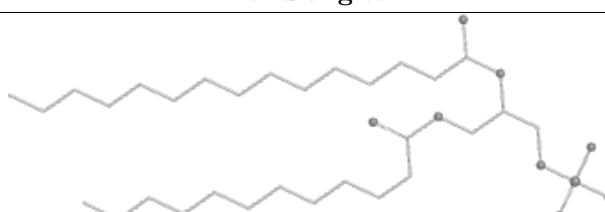
Bond lengths



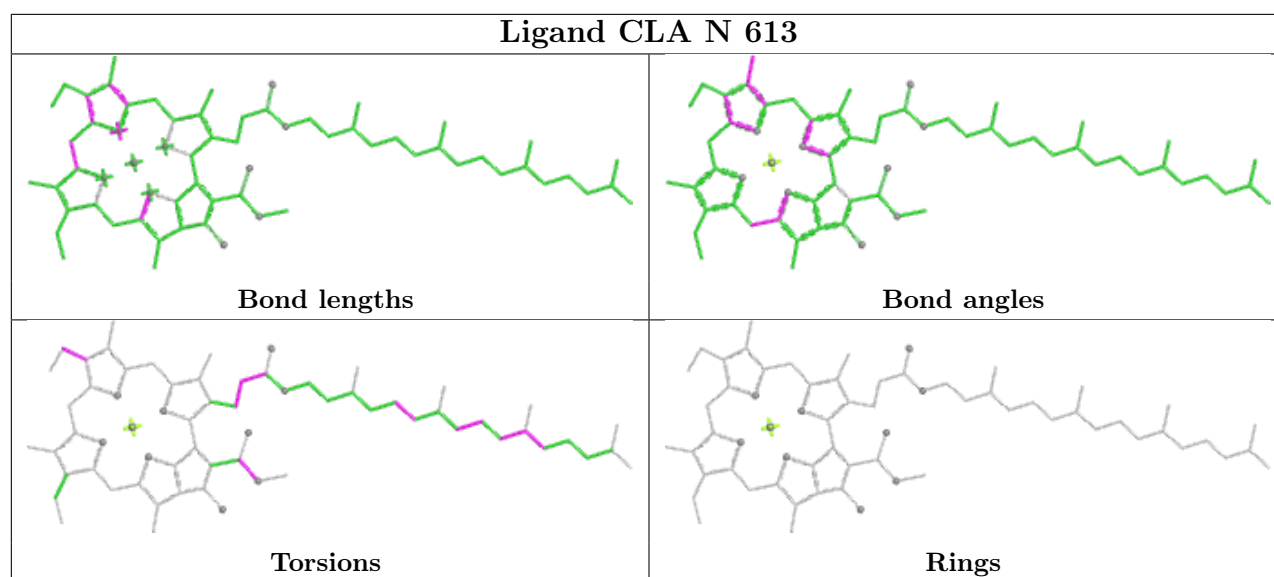
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	D	6
1	A	3
22	r	1
22	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	110:PRO	C	126:GLU	N	13.60
1	R	110:PRO	C	126:GLU	N	12.92
1	A	269:ARG	C	270:SER	N	1.20
1	D	243:THR	C	244:TYR	N	1.20
1	D	213:ILE	C	214:HIS	N	1.19
1	D	266:TRP	C	267:LEU	N	1.19
1	D	214:HIS	C	215:GLY	N	1.18
1	A	218:LEU	C	219:VAL	N	1.17
1	D	262:SER	C	263:ASN	N	1.17
1	D	265:ARG	C	266:TRP	N	1.16
1	A	215:HIS	C	216:GLY	N	1.15

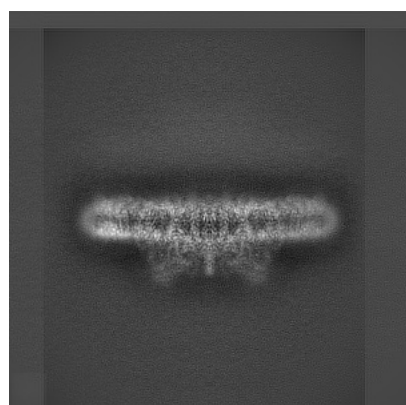
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13429. These allow visual inspection of the internal detail of the map and identification of artifacts.

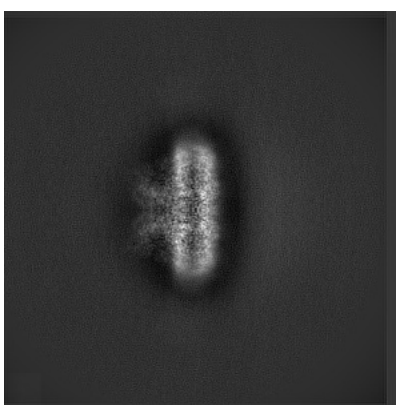
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

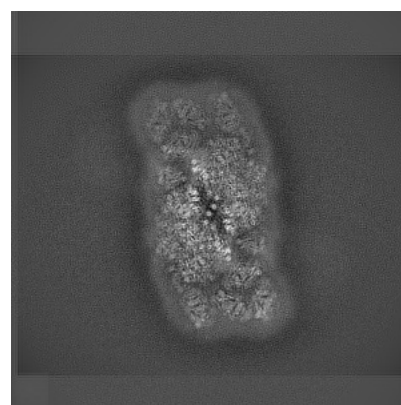
6.1.1 Primary map



X



Y

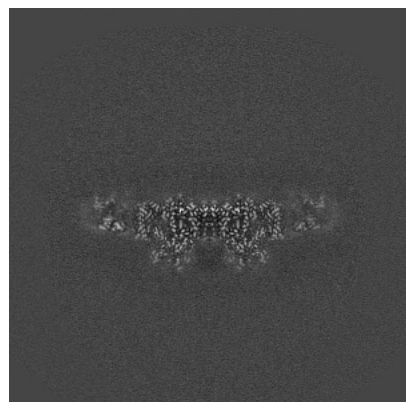


Z

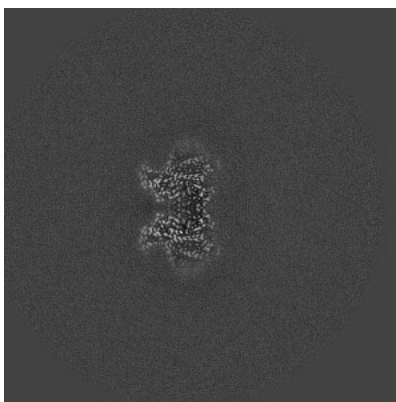
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

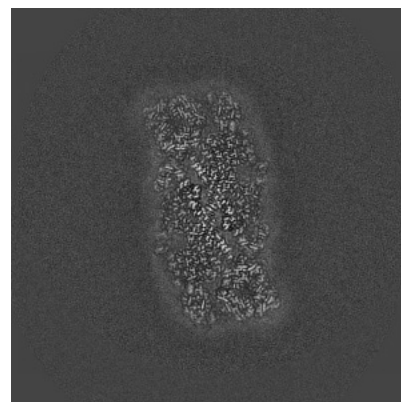
6.2.1 Primary map



X Index: 250



Y Index: 250

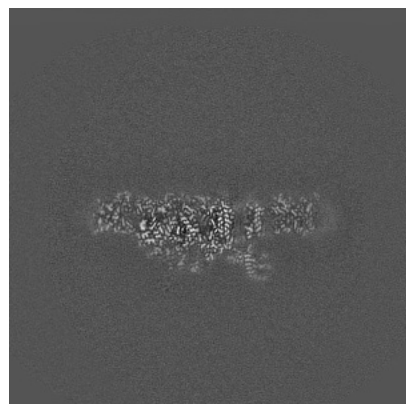


Z Index: 250

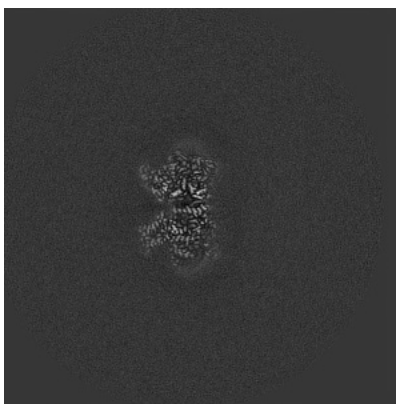
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

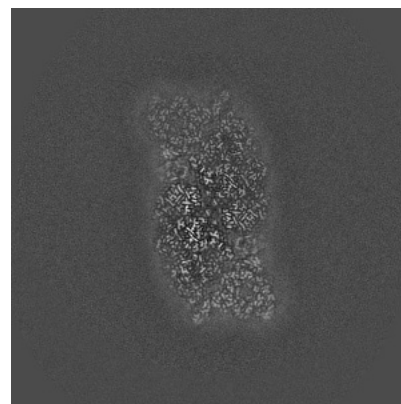
6.3.1 Primary map



X Index: 229



Y Index: 247

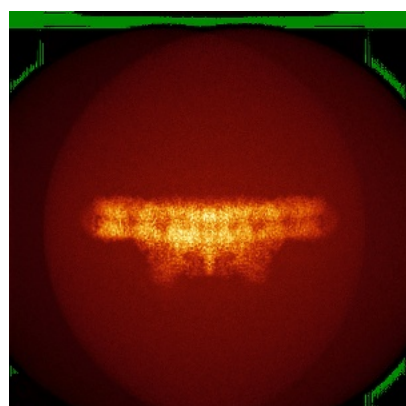


Z Index: 221

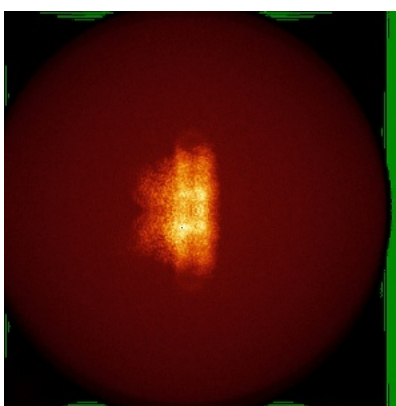
The images above show the largest variance slices of the map in three orthogonal directions.

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

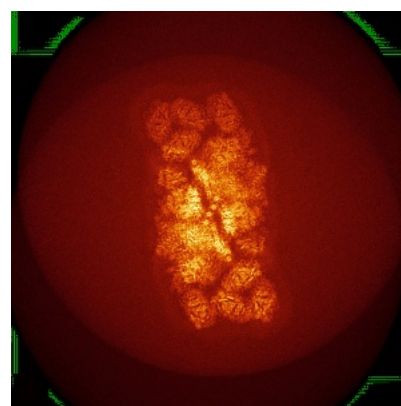
6.4.1 Primary map



X



Y

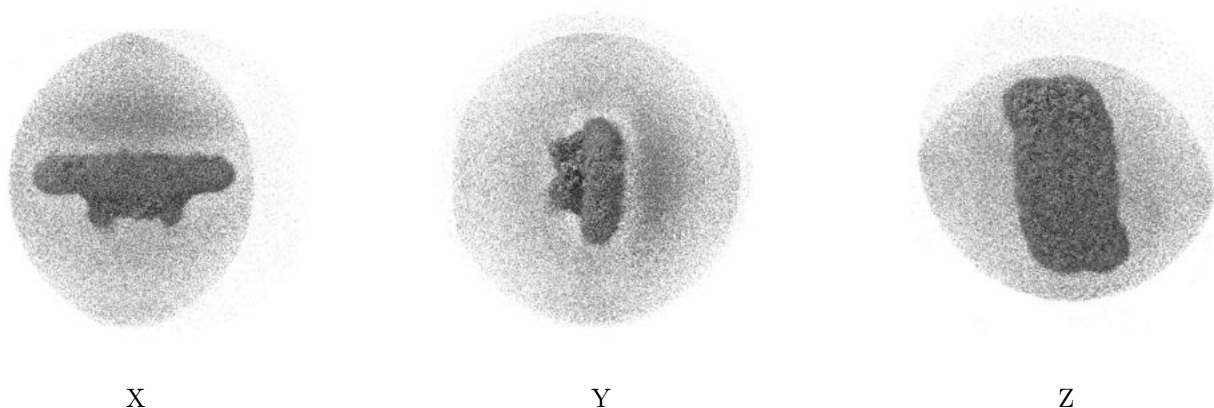


Z

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

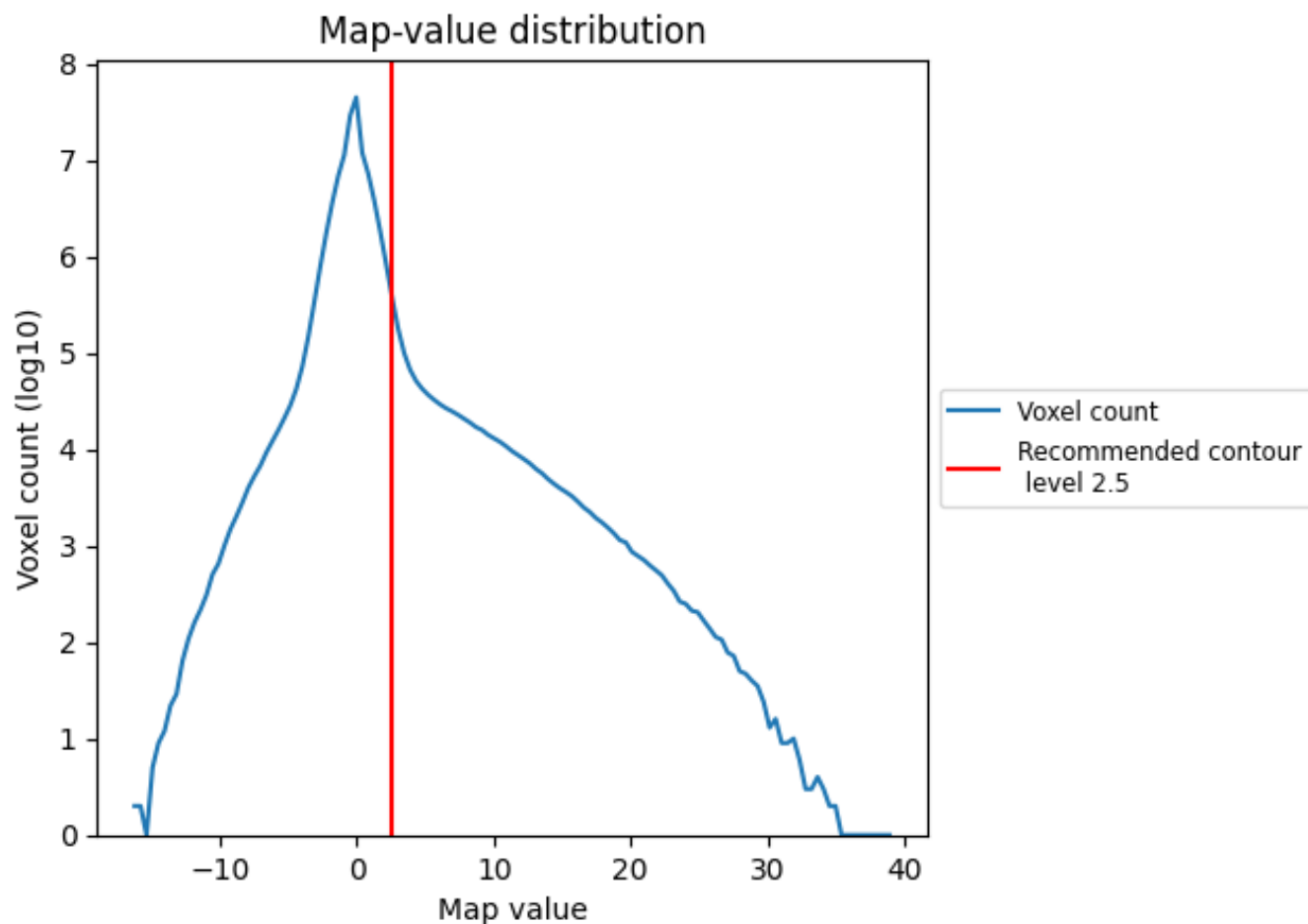
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

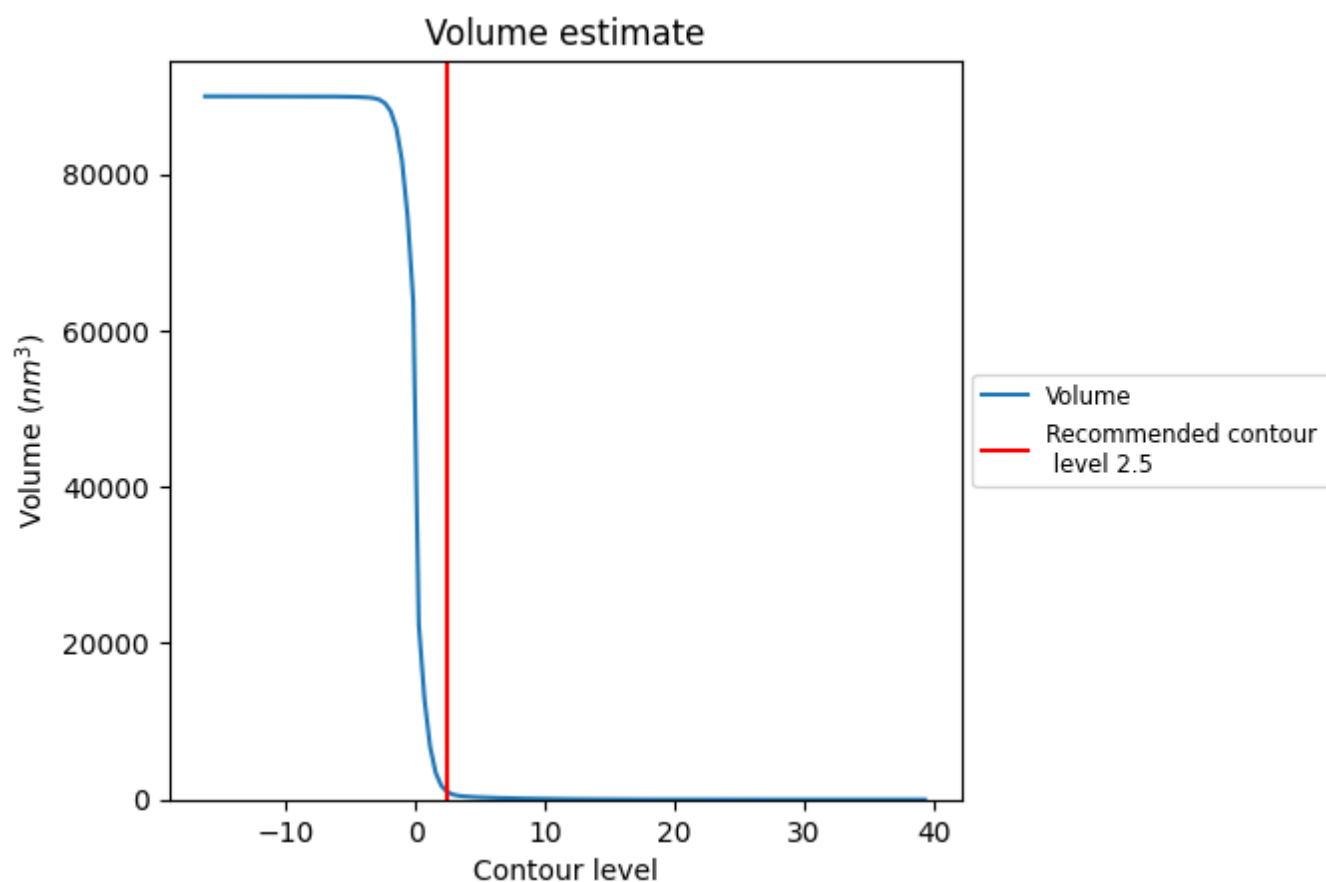
This section contains the results of statistical analysis of the map.

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.

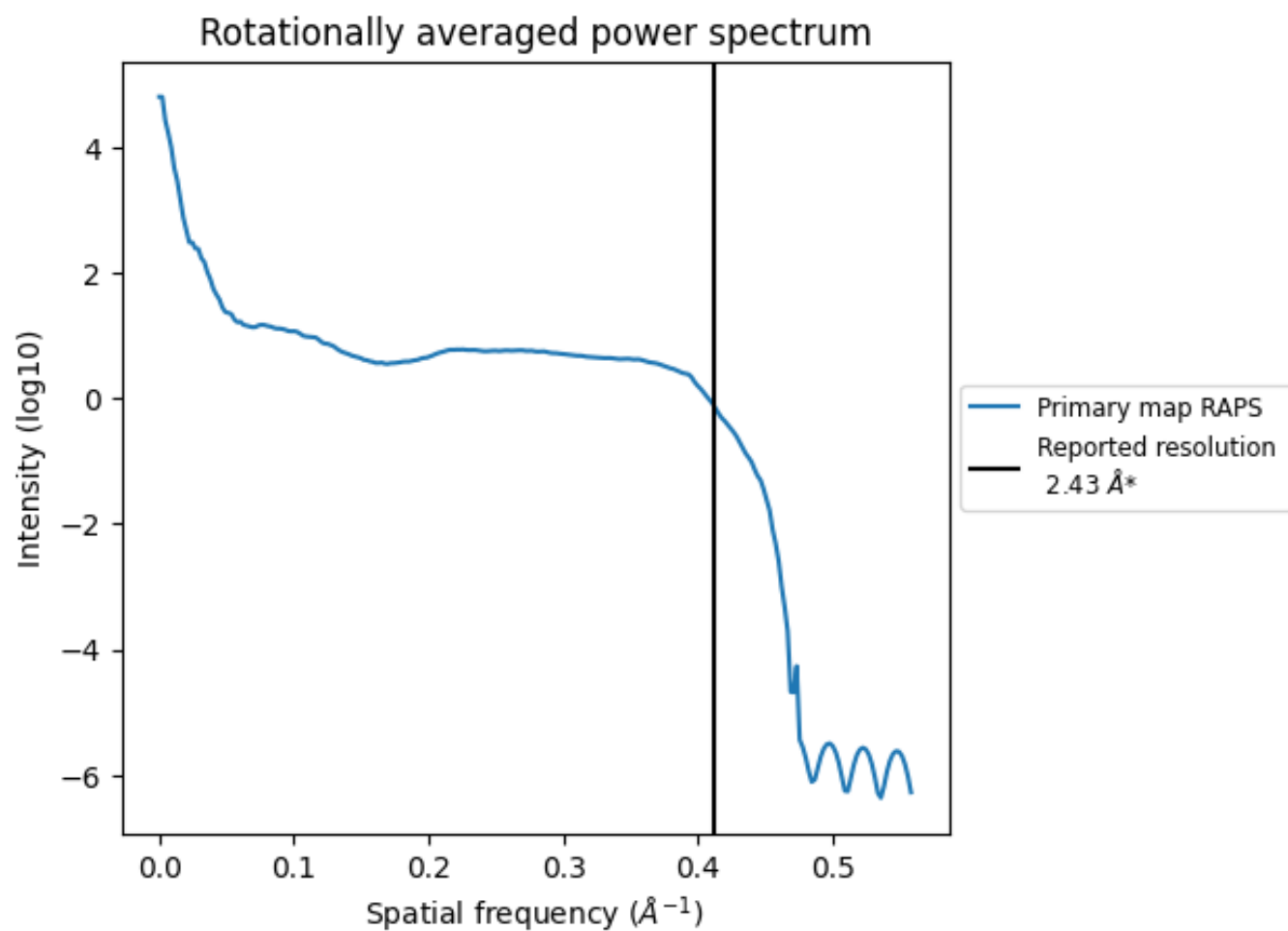
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 948 nm^3 ; this corresponds to an approximate mass of 856 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 ⓘ

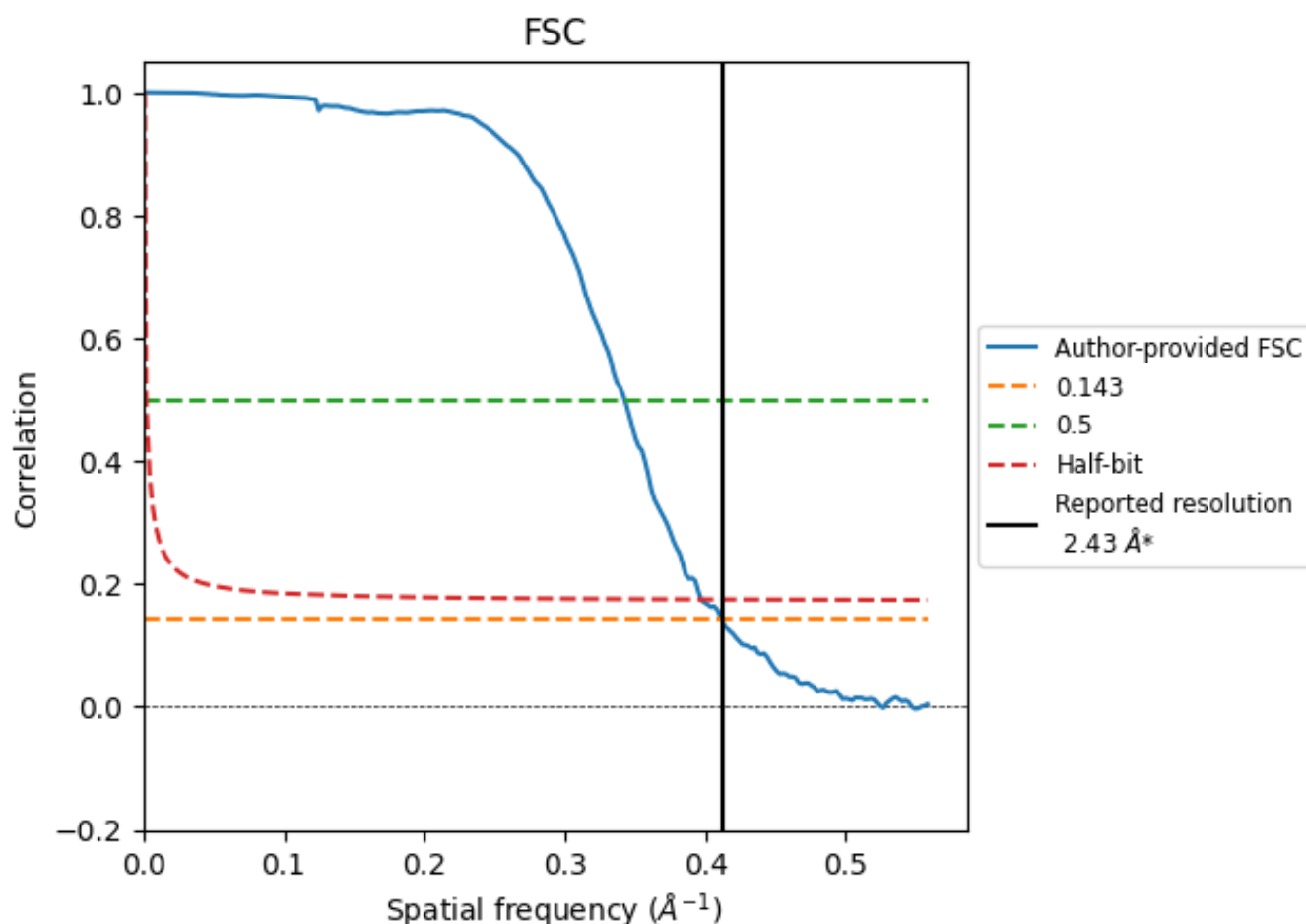


*Reported resolution corresponds to spatial frequency of 0.412 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.412 Å⁻¹

8.2 Resolution estimates [i](#)

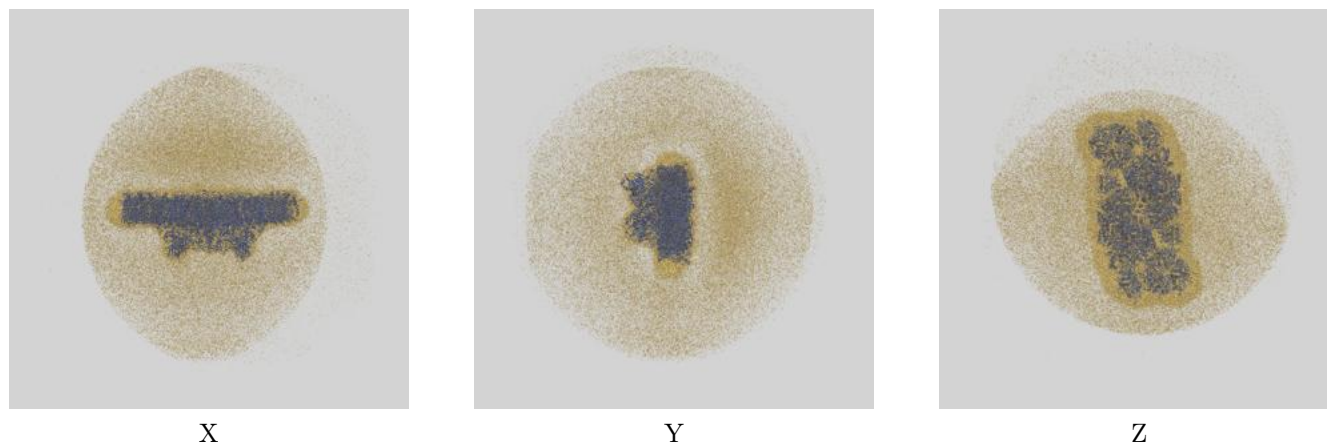
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.43	-	-
Author-provided FSC curve	2.43	2.92	2.52
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

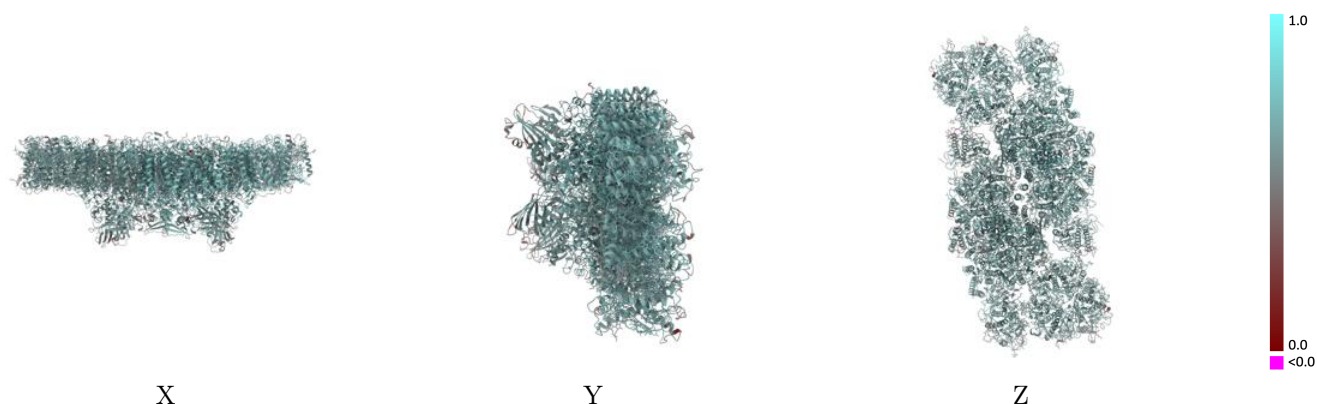
This section contains information regarding the fit between EMDB map EMD-13429 and PDB model 7PI0. Per-residue inclusion information can be found in section 3 on page 47.

9.1 Map-model overlay [i](#)



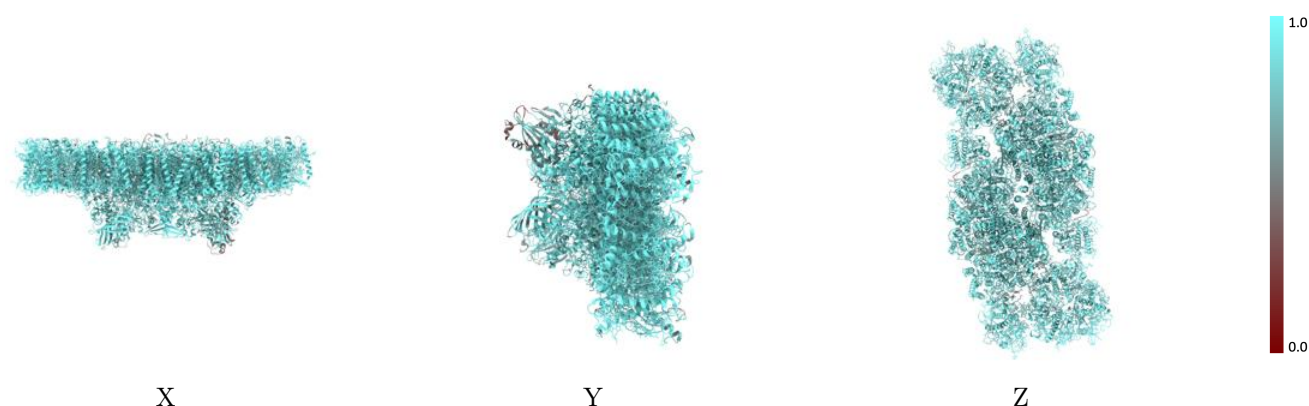
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



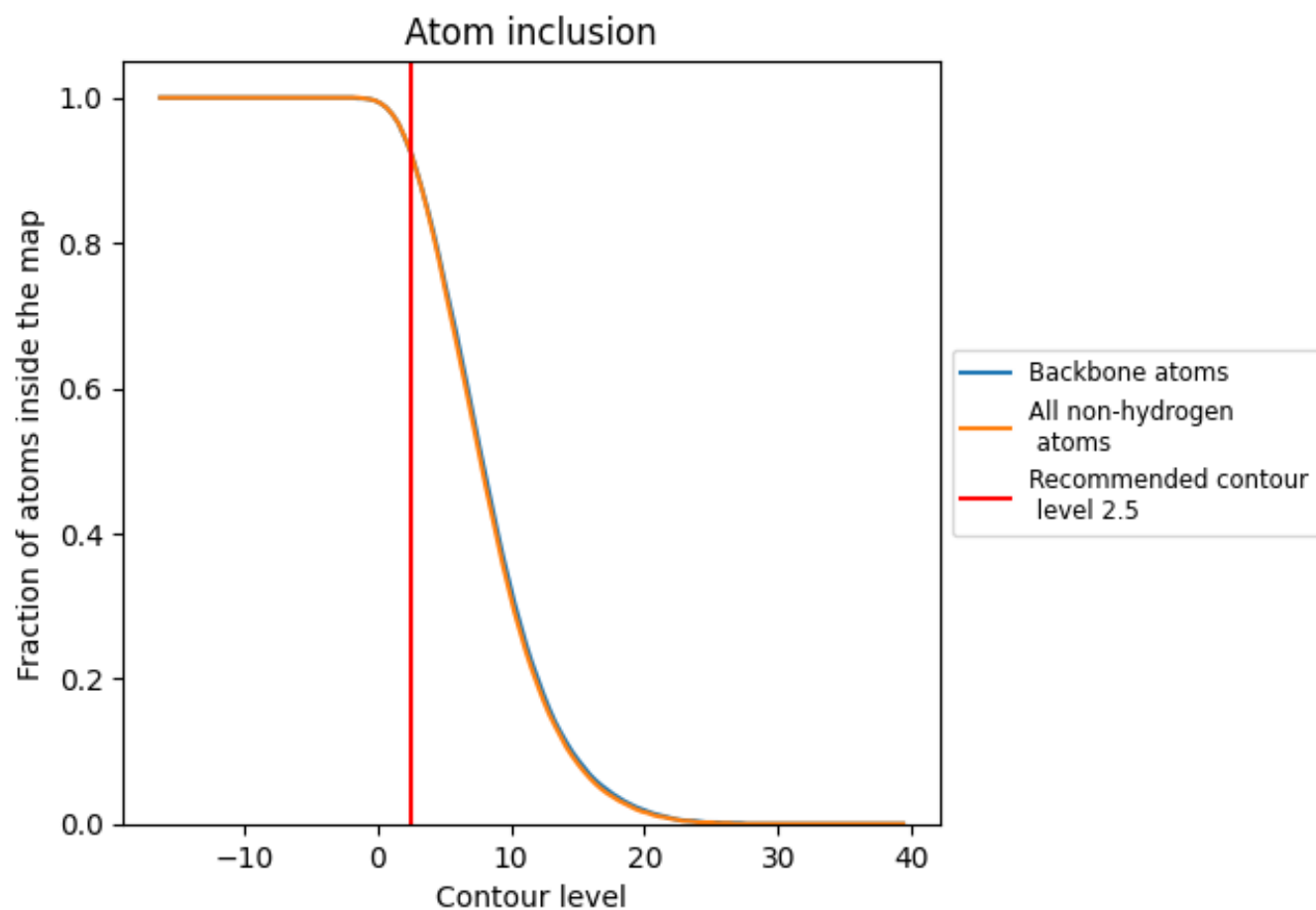
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9250	 0.6230
A	 0.9700	 0.6740
B	 0.9620	 0.6610
C	 0.9500	 0.6650
D	 0.9640	 0.6760
E	 0.9400	 0.6310
F	 0.9510	 0.6330
G	 0.9000	 0.6040
H	 0.9590	 0.6480
I	 0.9530	 0.6540
J	 0.9210	 0.6230
K	 0.9490	 0.6590
L	 0.9470	 0.6280
M	 0.9380	 0.6120
N	 0.9070	 0.6180
O	 0.8920	 0.5830
P	 0.6080	 0.5280
R	 0.8970	 0.5670
S	 0.9130	 0.6180
T	 0.9340	 0.6320
U	 0.8300	 0.5380
V	 0.9290	 0.6250
W	 0.8820	 0.5940
X	 0.8950	 0.5910
Y	 0.9250	 0.6340
Z	 0.9580	 0.6380
a	 0.9590	 0.6550
b	 0.9560	 0.6450
c	 0.9430	 0.6440
d	 0.9590	 0.6520
e	 0.9330	 0.5960
f	 0.9160	 0.6000
g	 0.9360	 0.5770
h	 0.9610	 0.6250
i	 0.9360	 0.6510



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
j	 0.9070	 0.6080
k	 0.9560	 0.6300
l	 0.9570	 0.6330
m	 0.9490	 0.6100
n	 0.9410	 0.6030
o	 0.8940	 0.5620
p	 0.7120	 0.5100
r	 0.9090	 0.5520
s	 0.9200	 0.5880
t	 0.9300	 0.6340
u	 0.7940	 0.5130
v	 0.9170	 0.6030
w	 0.8730	 0.5780
x	 0.8860	 0.5720
y	 0.9390	 0.6210
z	 0.9540	 0.6120