



Full wwPDB EM Validation Report ⓘ

Sep 10, 2026 – 07:56 pm BST

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.dev133
Mogul : 1.8.4, CSD as541be (2020)
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) : 2.50

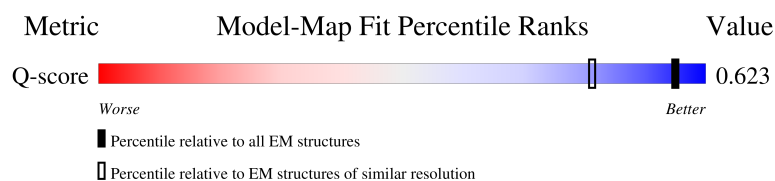
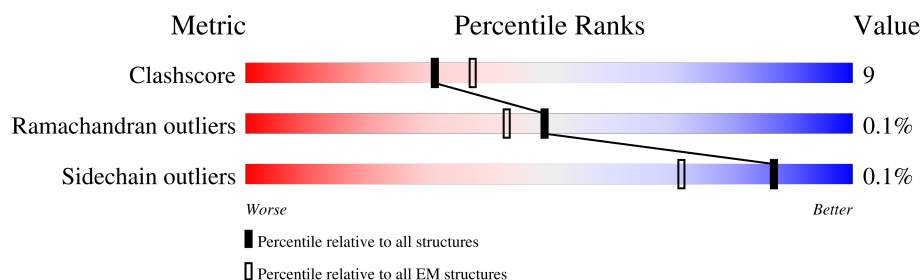
1 Overall quality at a glance

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.



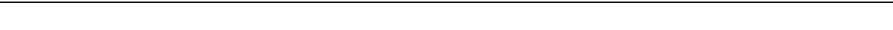
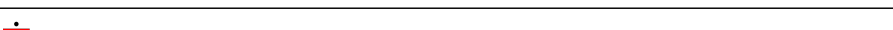
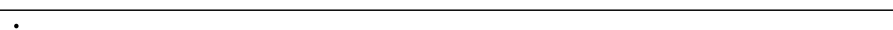
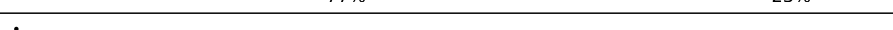
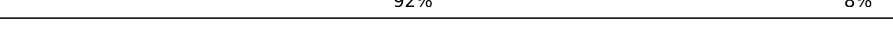
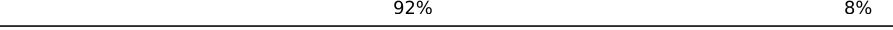
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5787 (1.94 - 2.93)

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%

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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%

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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	D	404	X	-	-	-
34	C7Z	B	519	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	C7Z	b	519	X	-	-	-
45	RRX	H	101	X	-	-	-
45	RRX	h	101	X	-	-	-
46	CHL	G	601	X	-	-	-
46	CHL	G	607	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	609	X	-	-	-
46	CHL	S	309	X	-	-	-
46	CHL	Y	302	X	-	-	-
46	CHL	Y	307	X	-	-	-
46	CHL	Y	308	X	-	-	-
46	CHL	Y	310	X	-	-	-
46	CHL	g	601	X	-	-	-
46	CHL	g	607	X	-	-	-
46	CHL	g	609	X	-	-	-
46	CHL	n	601	X	-	-	-
46	CHL	n	605	X	-	-	-
46	CHL	n	606	X	-	-	-
46	CHL	n	608	X	-	-	-
46	CHL	s	309	X	-	-	-
46	CHL	y	301	X	-	-	-
46	CHL	y	303	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	S	0	0
			266	183	40	43			

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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		

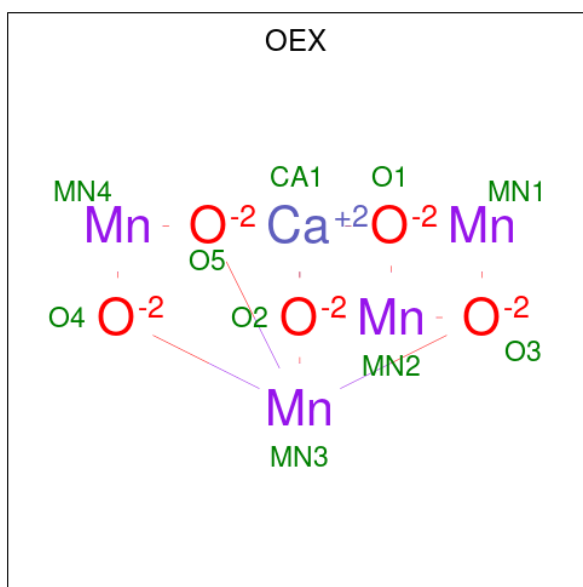
- Molecule 24 is a protein called Chlorophyll a-b binding protein of LHCII type 1, chloroplastic.

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	

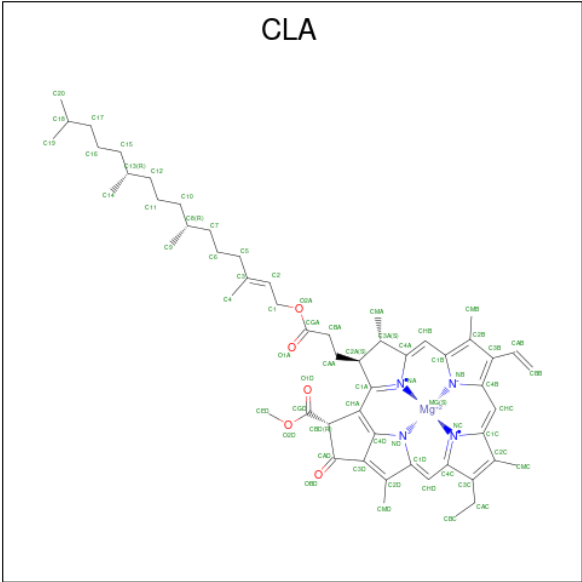
- Molecule 27 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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	

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

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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

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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

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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

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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

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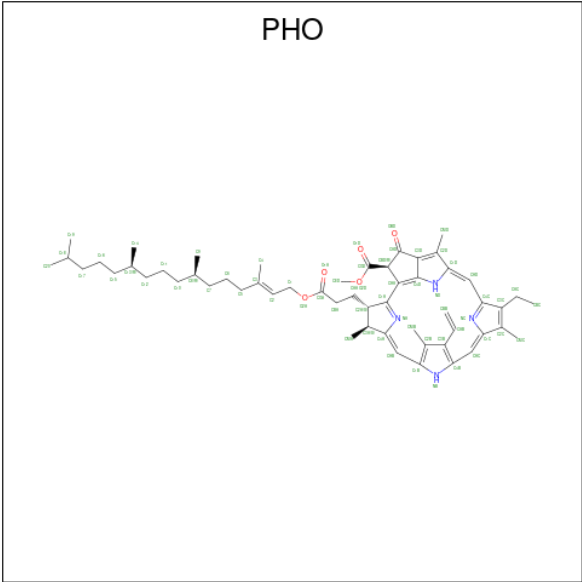
Mol	Chain	Residues	Atoms					AltConf
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 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

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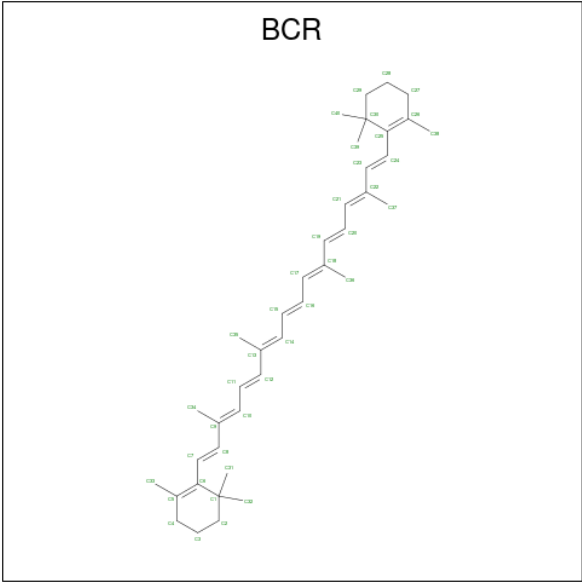
Mol	Chain	Residues	Atoms					AltConf
29	s	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			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: $C_{40}H_{56}$).



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

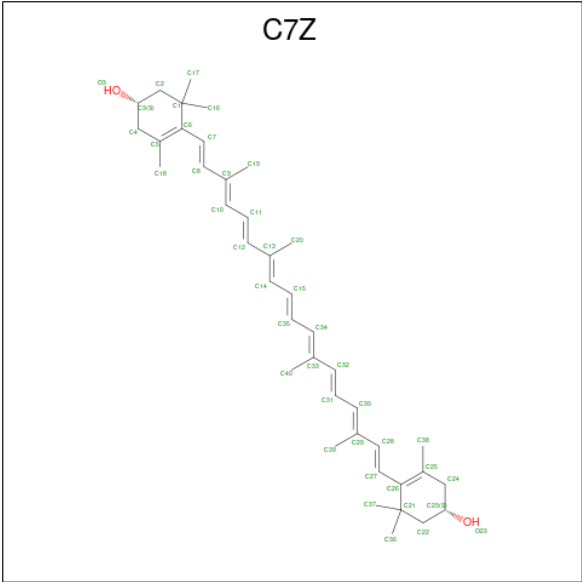
- Molecule 32 is SODIUM ION (CCD ID: NA) (formula: Na).

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).

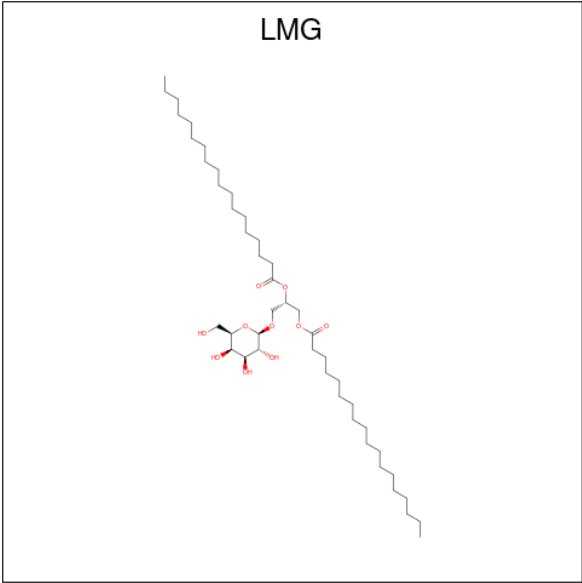


- Molecule 34 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: $C_{40}H_{56}O_2$).



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).



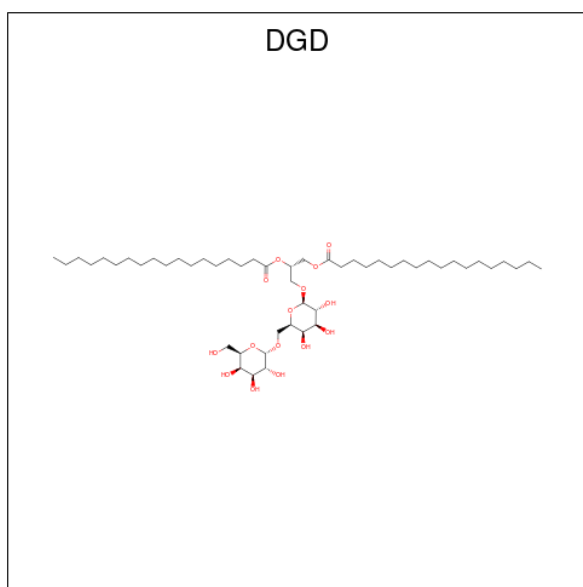
Mol	Chain	Residues	Atoms			AltConf
35	B	1	Total	C	O	0
			44	34	10	

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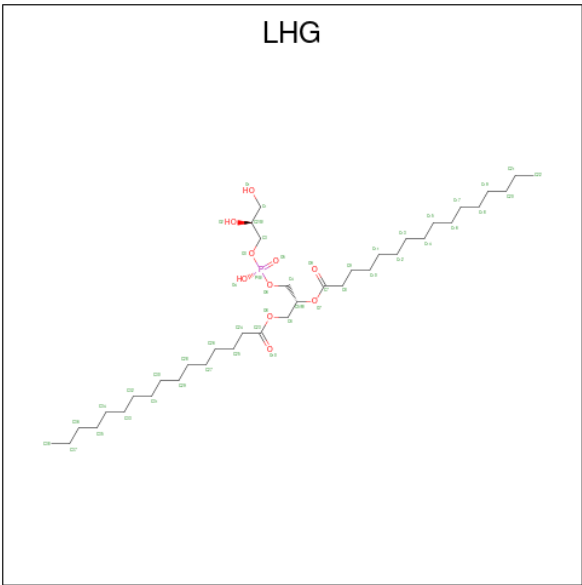
Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			47	37	10	
35	C	1	Total	C	O	0
			55	45	10	
35	C	1	Total	C	O	0
			42	32	10	
35	D	1	Total	C	O	0
			42	32	10	
35	D	1	Total	C	O	0
			48	38	10	
35	W	1	Total	C	O	0
			40	30	10	
35	W	1	Total	C	O	0
			39	29	10	
35	b	1	Total	C	O	0
			44	34	10	
35	c	1	Total	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: $C_{38}H_{75}O_{10}P$).



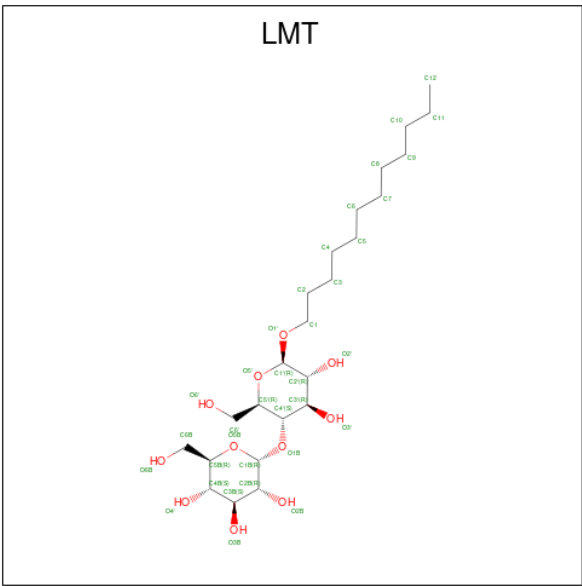
Mol	Chain	Residues	Atoms				AltConf
37	B	1	Total	C	O	P	0
			44	33	10	1	
37	D	1	Total	C	O	P	0
			49	38	10	1	
37	D	1	Total	C	O	P	0
			39	28	10	1	
37	L	1	Total	C	O	P	0
			49	38	10	1	
37	N	1	Total	C	O	P	0
			49	38	10	1	
37	G	1	Total	C	O	P	0
			49	38	10	1	
37	S	1	Total	C	O	P	0
			35	24	10	1	
37	S	1	Total	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	

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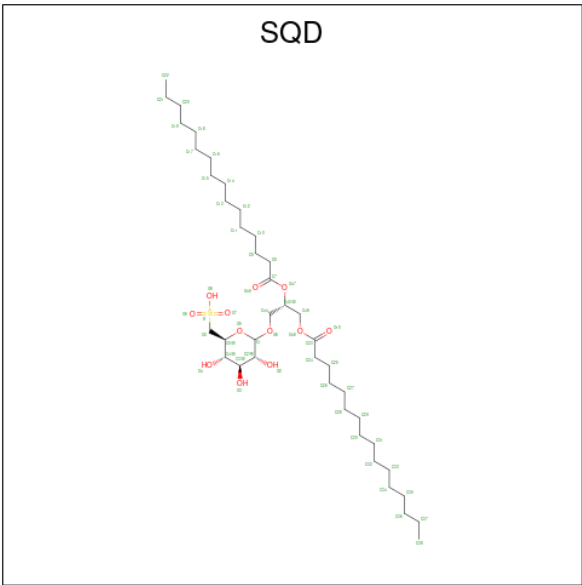
Mol	Chain	Residues	Atoms				AltConf
37	n	1	Total	C	O	P	0
			42	31	10	1	
37	g	1	Total	C	O	P	0
			49	38	10	1	
37	s	1	Total	C	O	P	0
			38	27	10	1	
37	s	1	Total	C	O	P	0
			45	34	10	1	
37	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 38 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



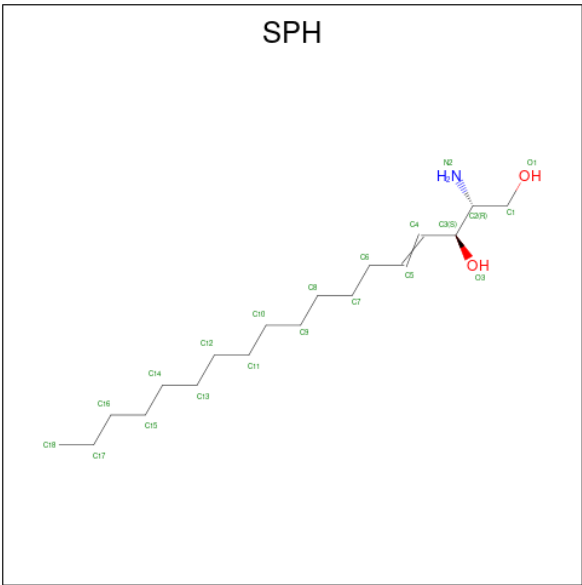
Mol	Chain	Residues	Atoms			AltConf
38	B	1	Total	C	O	0
			35	24	11	
38	b	1	Total	C	O	0
			35	24	11	

- Molecule 39 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



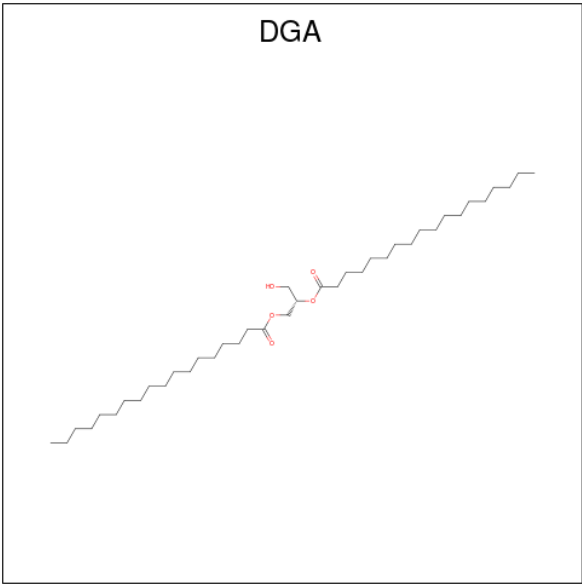
Mol	Chain	Residues	Atoms				AltConf
39	C	1	Total	C	O	S	0
			42	29	12	1	
39	C	1	Total	C	O	S	0
			36	23	12	1	
39	L	1	Total	C	O	S	0
			42	29	12	1	
39	M	1	Total	C	O	S	0
			42	29	12	1	
39	a	1	Total	C	O	S	0
			51	38	12	1	
39	b	1	Total	C	O	S	0
			54	41	12	1	
39	c	1	Total	C	O	S	0
			54	41	12	1	
39	l	1	Total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



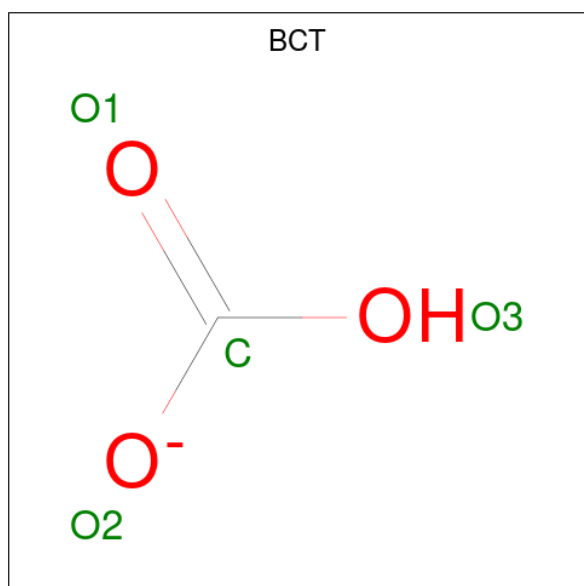
Mol	Chain	Residues	Atoms				AltConf
40	C	1	Total	C	N	O	0
			21	18	1	2	
40	I	1	Total	C	N	O	0
			21	18	1	2	
40	c	1	Total	C	N	O	0
			21	18	1	2	
40	i	1	Total	C	N	O	0
			21	18	1	2	

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



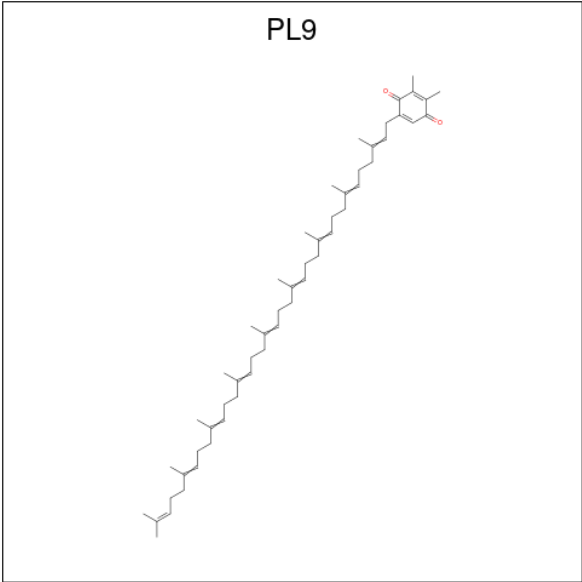
Mol	Chain	Residues	Atoms			AltConf
41	D	1	Total	C	O	0
			37	32	5	
41	J	1	Total	C	O	0
			29	24	5	
41	W	1	Total	C	O	0
			44	39	5	
41	b	1	Total	C	O	0
			44	39	5	
41	j	1	Total	C	O	0
			29	24	5	
41	w	1	Total	C	O	0
			44	39	5	

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



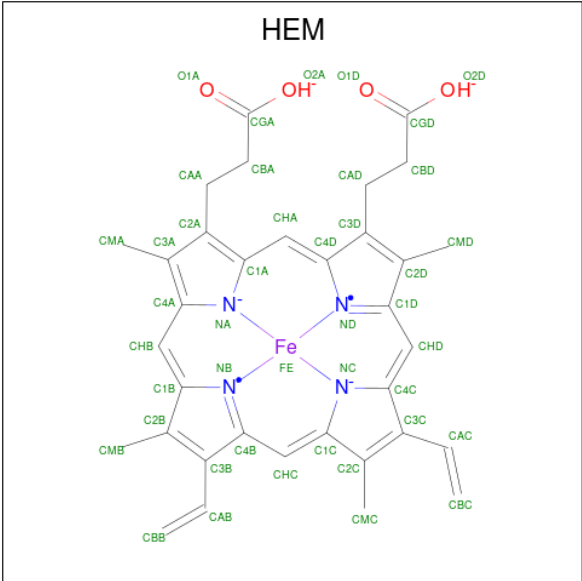
Mol	Chain	Residues	Atoms			AltConf
42	D	1	Total	C	O	0
			4	1	3	
42	a	1	Total	C	O	0
			4	1	3	

- 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: $C_{34}H_{32}FeN_4O_4$).



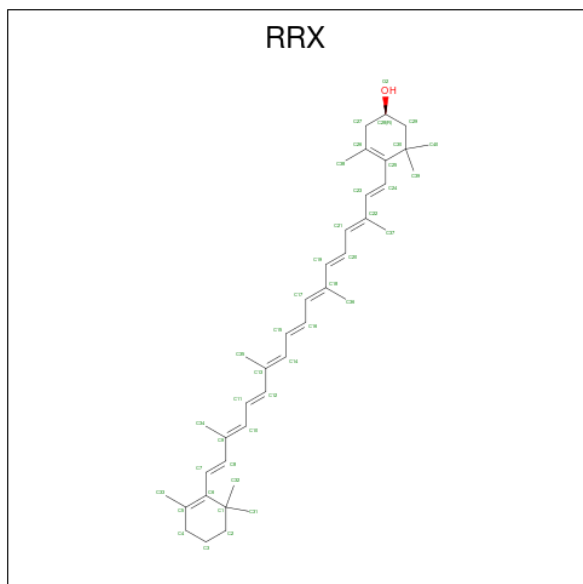
Mol	Chain	Residues	Atoms					AltConf
44	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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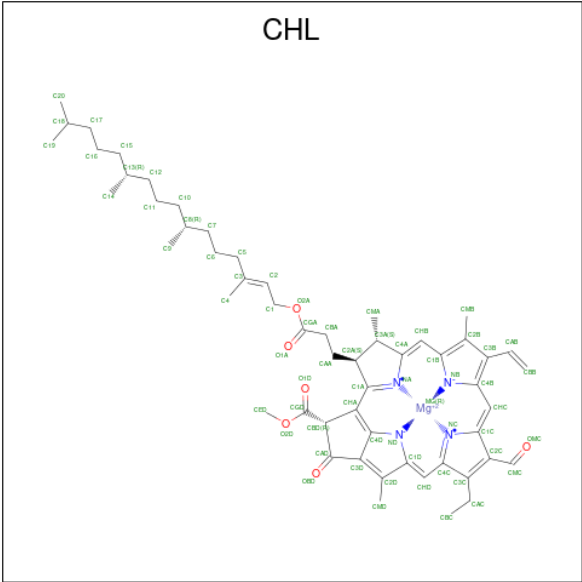
Mol	Chain	Residues	Atoms					AltConf
44	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- 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	C	Mg	N	O		0
			66	55	1	4	6		
46	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
46	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
46	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
46	N	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
46	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
46	G	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
46	G	1	Total	C	Mg	N	O		0
			48	37	1	4	6		
46	G	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
46	G	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
46	G	1	Total	C	Mg	N	O		0
			44	35	1	4	4		
46	G	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
46	R	1	Total	C	Mg	N	O		0
			44	35	1	4	4		
46	R	1	Total	C	Mg	N	O		0
			50	39	1	4	6		

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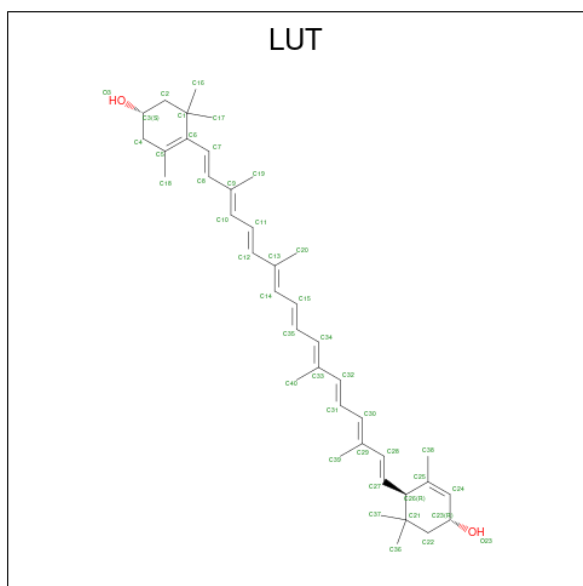
Mol	Chain	Residues	Atoms					AltConf
46	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
46	S	1	Total 44	C 35	Mg 1	N 4	O 4	0
46	S	1	Total 43	C 34	Mg 1	N 4	O 4	0
46	S	1	Total 61	C 50	Mg 1	N 4	O 6	0
46	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
46	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	Y	1	Total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

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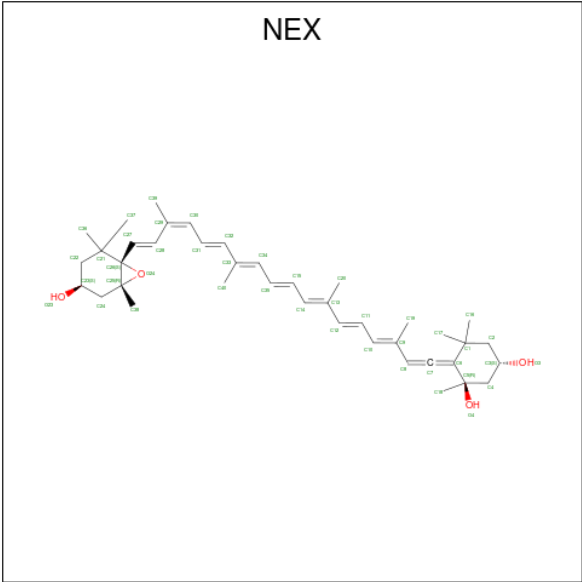
Mol	Chain	Residues	Atoms					AltConf
46	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
46	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
46	s	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
46	s	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
46	s	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
46	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	y	1	Total	C	Mg	N	O	0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



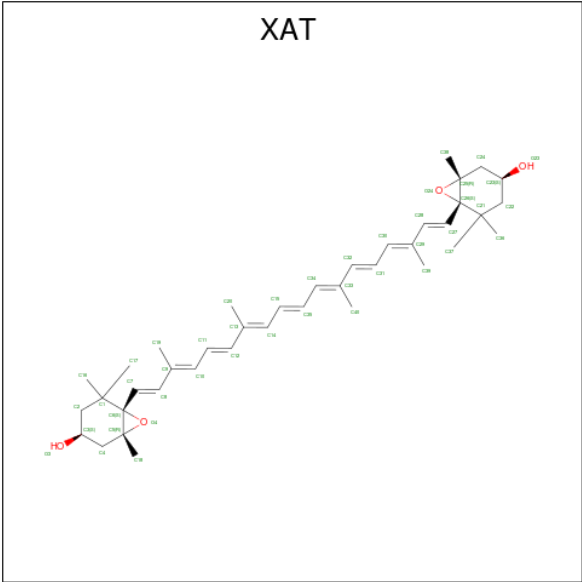
Mol	Chain	Residues	Atoms			AltConf
47	N	1	Total	C	O	0
			42	40	2	
47	N	1	Total	C	O	0
			42	40	2	
47	G	1	Total	C	O	0
			42	40	2	
47	G	1	Total	C	O	0
			42	40	2	
47	R	1	Total	C	O	0
			42	40	2	
47	S	1	Total	C	O	0
			42	40	2	
47	S	1	Total	C	O	0
			42	40	2	
47	Y	1	Total	C	O	0
			42	40	2	
47	Y	1	Total	C	O	0
			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).



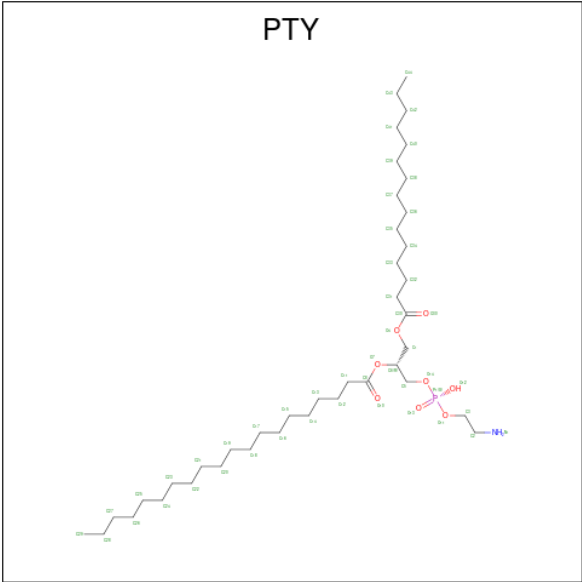
Mol	Chain	Residues	Atoms			AltConf
48	N	1	Total	C	O	0
			44	40	4	
48	G	1	Total	C	O	0
			44	40	4	
48	R	1	Total	C	O	0
			27	25	2	
48	S	1	Total	C	O	0
			44	40	4	
48	Y	1	Total	C	O	0
			44	40	4	
48	n	1	Total	C	O	0
			44	40	4	
48	g	1	Total	C	O	0
			44	40	4	
48	r	1	Total	C	O	0
			27	25	2	
48	s	1	Total	C	O	0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



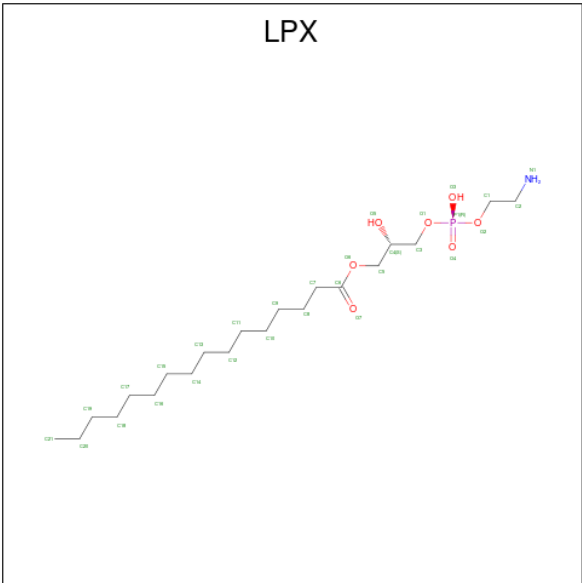
Mol	Chain	Residues	Atoms			AltConf
49	N	1	Total	C	O	0
			44	40	4	
49	G	1	Total	C	O	0
			44	40	4	
49	R	1	Total	C	O	0
			44	40	4	
49	Y	1	Total	C	O	0
			44	40	4	
49	n	1	Total	C	O	0
			44	40	4	
49	g	1	Total	C	O	0
			44	40	4	
49	r	1	Total	C	O	0
			44	40	4	
49	y	1	Total	C	O	0
			44	40	4	

- 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	

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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

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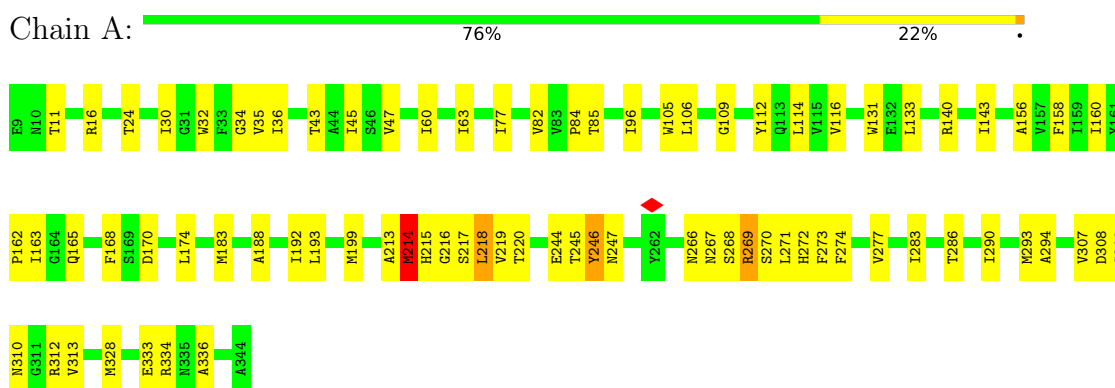
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Mol	Chain	Residues	Atoms		AltConf
52	p	64	Total 64	O 64	0
52	t	2	Total 2	O 2	0
52	w	12	Total 12	O 12	0
52	x	9	Total 9	O 9	0
52	z	6	Total 6	O 6	0
52	n	36	Total 36	O 36	0
52	g	33	Total 33	O 33	0
52	r	33	Total 33	O 33	0
52	s	40	Total 40	O 40	0
52	y	61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

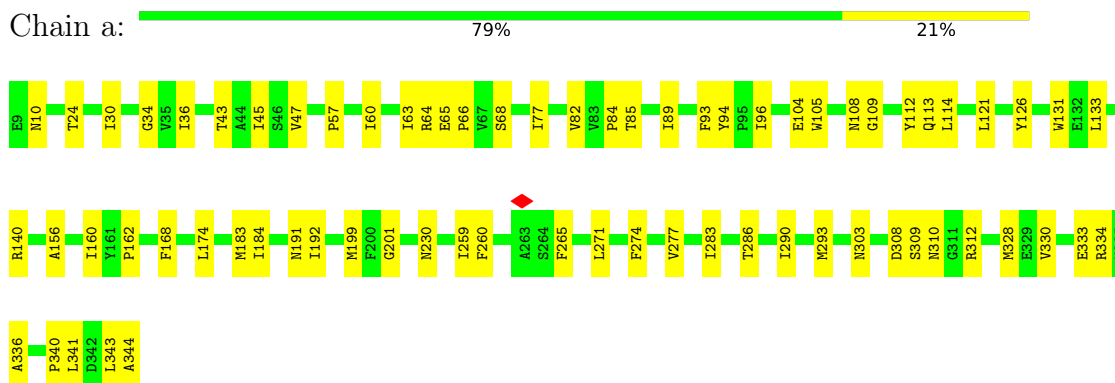
3 Residue-property plots

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.

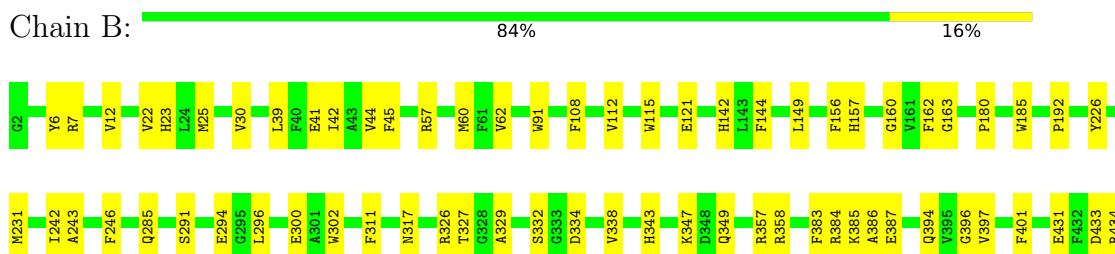
• Molecule 1: Photosystem II protein D1



• Molecule 1: Photosystem II protein D1



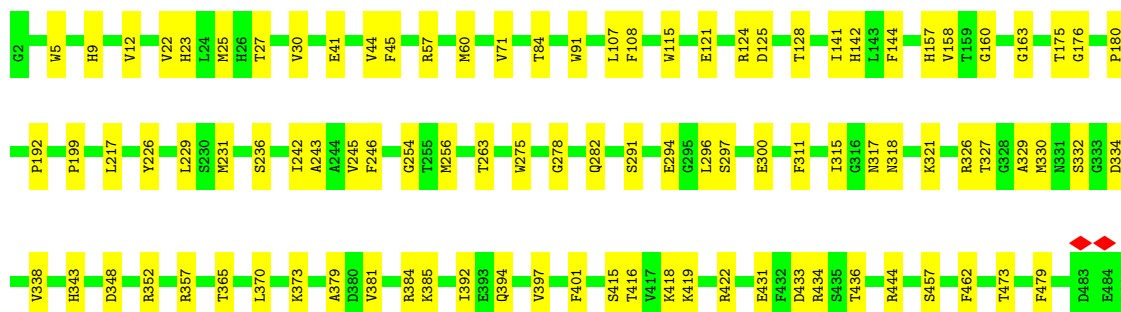
• Molecule 2: Photosystem II CP47 reaction center protein





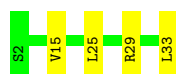
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 80% 20%



- Molecule 3: Photosystem II reaction center protein Ycf12

Chain V: 88% 12%



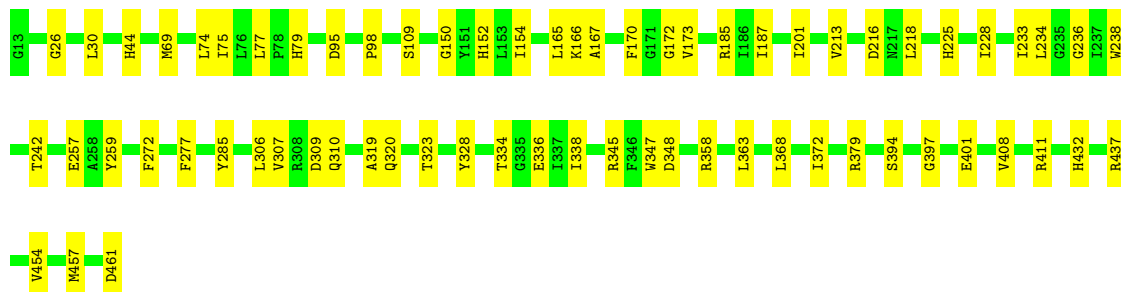
- Molecule 3: Photosystem II reaction center protein Ycf12

Chain v: 88% 12%



- Molecule 4: Photosystem II CP43 reaction center protein

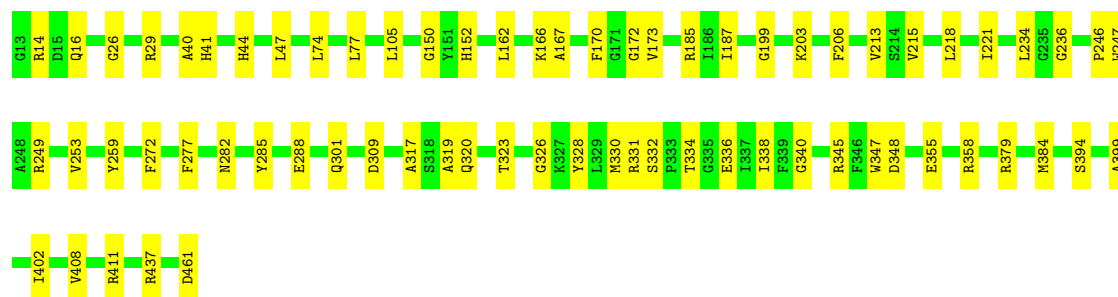
Chain C: 85% 15%



- Molecule 4: Photosystem II CP43 reaction center protein

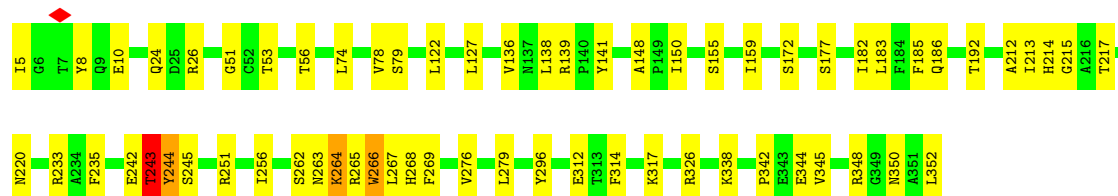
Chain c: 85% 15%





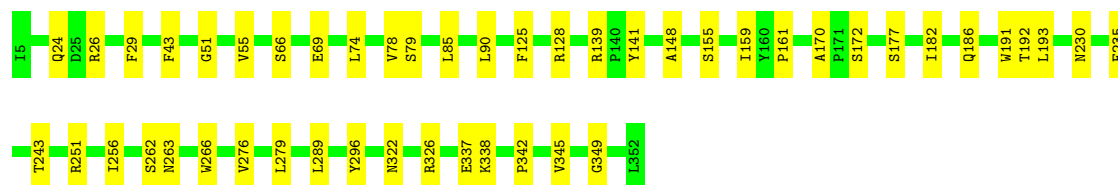
• Molecule 5: Photosystem II D2 protein

Chain D: 82% 17%



• Molecule 5: Photosystem II D2 protein

Chain d: 86% 14%



• Molecule 6: Cytochrome b559 subunit alpha

Chain E: 82% 18%



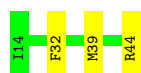
• Molecule 6: Cytochrome b559 subunit alpha

Chain e: 83% 17%



• Molecule 7: Cytochrome b559 subunit beta

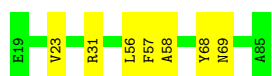
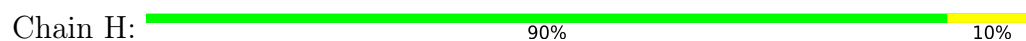
Chain F: 90% 10%



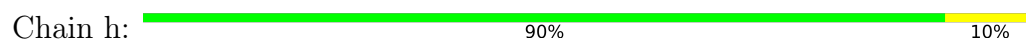
- Molecule 7: Cytochrome b559 subunit beta



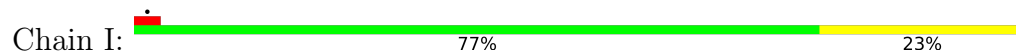
- Molecule 8: Photosystem II reaction center protein H



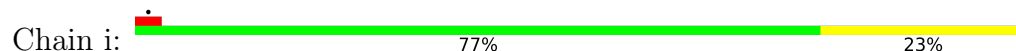
- Molecule 8: Photosystem II reaction center protein H



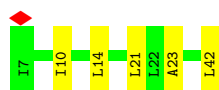
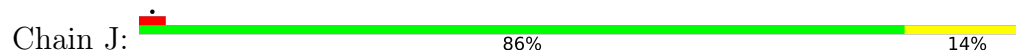
- Molecule 9: Photosystem II reaction center protein I



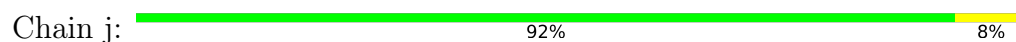
- Molecule 9: Photosystem II reaction center protein I



- 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%



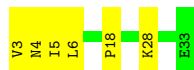
- Molecule 12: Photosystem II reaction center protein L

Chain l: 87% 13%



- Molecule 13: Photosystem II reaction center protein M

Chain M: 81% 19%



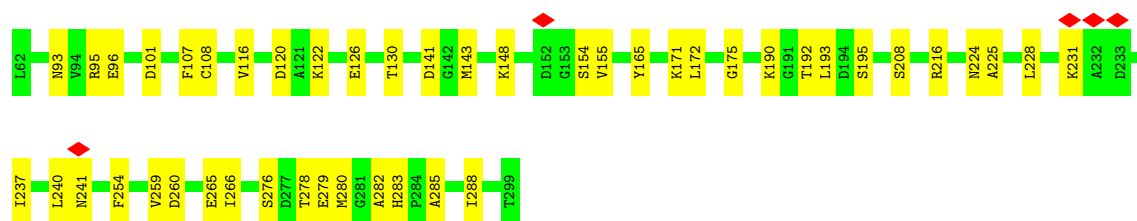
- Molecule 13: Photosystem II reaction center protein M

Chain m: 77% 23%



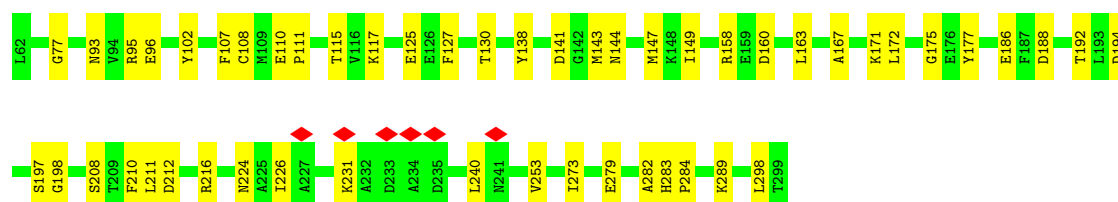
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain O: 81% 19%



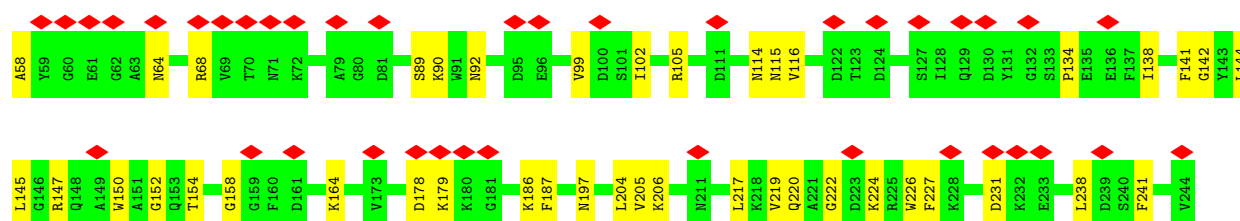
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain o: 79% 21%



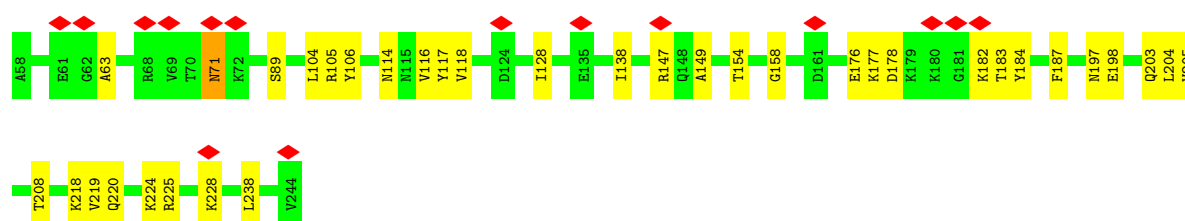
- Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

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%



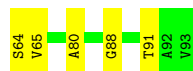
- Molecule 17: PSII 6.1 kDa protein

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

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

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

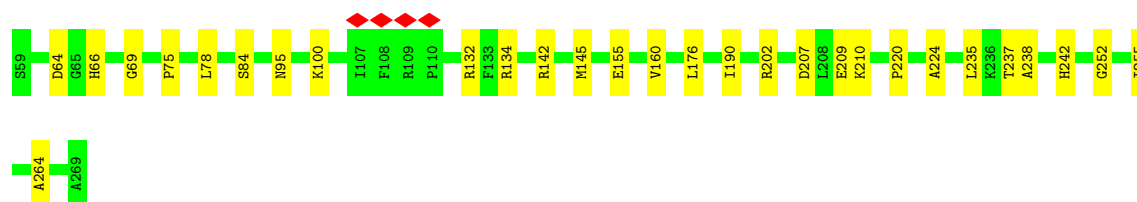
- Molecule 21: Chlorophyll a-b binding protein of LHCII type 2, chloroplastic

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

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



WORLD WIDE
PDB
PROTEIN DATA BANK



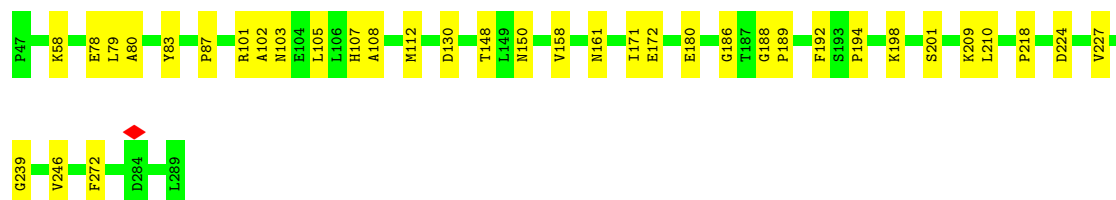
- Molecule 23: Chlorophyll a-b binding protein, chloroplastic, CP26

Chain S: 88% 12%



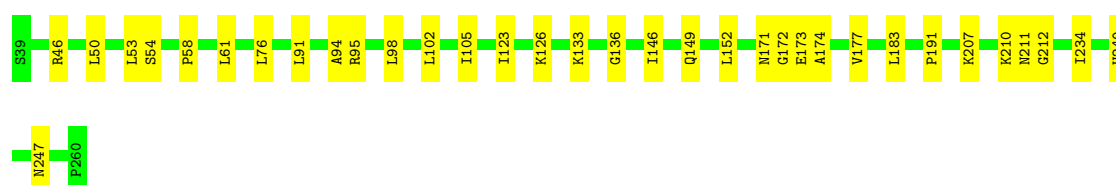
- Molecule 23: Chlorophyll a-b binding protein, chloroplastic, CP26

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

Satisfaction Level	Percentage
Very satisfied	63%
Satisfied	37%



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: LMT, DGD, DGA, CLA, C7Z, PL9, XAT, SQD, CL, CHL, OEX, LUT, NEX, FE2, BCR, PHO, SEP, 3PH, LPX, RRX, NA, BCT, LMG, HEM, CSD, SPH, PTY, LHG

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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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:H142	29:Y:315:CLA:H112	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:315:CLA:H61	29:Y:315:CLA:H41	1.79	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

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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

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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

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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

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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

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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	3,7,8	0.88	0	1,8,10	0.59	0
22	SEP	R	84	22	8,9,10	1.50	1 (12%)	8,12,14	1.64	2 (25%)
22	SEP	r	84	22	8,9,10	1.52	1 (12%)	8,12,14	1.53	2 (25%)
2	CSD	B	218	2	3,7,8	0.83	0	1,8,10	0.58	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	-	1/5/8/10	-
22	SEP	r	84	22	-	4/5/8/10	-
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	3.35	1.61	1.50
22	r	84	SEP	P-O1P	3.33	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	84	SEP	P-OG-CB	-3.02	109.98	118.30
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
22	r	84	SEP	P-OG-CB	-2.25	112.11	118.30

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	R	84	SEP	N-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	Y	304	24	69,73,73	1.09	5 (7%)	83,113,113	1.02	5 (6%)
37	LHG	S	320	29	44,44,48	0.41	0	47,50,54	1.04	3 (6%)
46	CHL	S	308	-	47,51,74	0.95	2 (4%)	52,86,114	1.46	10 (19%)
46	CHL	Y	310	24	70,74,74	0.80	2 (2%)	80,114,114	1.27	12 (15%)
39	SQD	b	523	-	53,54,54	0.80	0	62,65,65	0.90	2 (3%)
31	BCR	c	515	-	41,41,41	1.83	4 (9%)	56,56,56	4.25	20 (35%)
29	CLA	g	613	21	69,73,73	1.10	5 (7%)	83,113,113	1.02	3 (3%)
47	LUT	G	616	-	42,43,43	2.34	1 (2%)	51,60,60	1.93	11 (21%)
29	CLA	y	314	24	69,73,73	1.09	5 (7%)	83,113,113	1.07	5 (6%)
35	LMG	W	201	-	40,40,55	0.76	2 (5%)	48,48,63	1.15	4 (8%)
49	XAT	Y	301	-	39,47,47	0.71	1 (2%)	54,74,74	2.00	14 (25%)
49	XAT	R	311	-	39,47,47	0.67	1 (2%)	54,74,74	1.87	13 (24%)
29	CLA	s	304	23	69,73,73	1.15	8 (11%)	83,113,113	1.27	7 (8%)
35	LMG	c	520	-	55,55,55	1.13	6 (10%)	63,63,63	1.02	2 (3%)
43	PL9	D	406	-	55,55,55	1.34	6 (10%)	68,69,69	1.47	11 (16%)
29	CLA	C	514	-	69,73,73	1.08	5 (7%)	83,113,113	1.03	2 (2%)
36	DGD	C	520	-	54,54,67	0.93	4 (7%)	68,68,81	0.90	2 (2%)
29	CLA	N	610	-	69,73,73	1.09	6 (8%)	83,113,113	1.14	4 (4%)
29	CLA	c	510	-	69,73,73	1.08	5 (7%)	83,113,113	1.03	6 (7%)
29	CLA	B	516	2	59,63,73	1.21	7 (11%)	71,101,113	1.14	6 (8%)
49	XAT	G	619	-	39,47,47	0.68	1 (2%)	54,74,74	3.75	20 (37%)
36	DGD	c	516	-	56,56,67	0.98	4 (7%)	70,70,81	0.94	2 (2%)
34	C7Z	b	519	-	43,43,43	5.29	27 (62%)	58,60,60	2.41	24 (41%)
46	CHL	y	307	24	50,54,74	0.97	2 (4%)	56,90,114	1.36	9 (16%)
29	CLA	A	406	52	69,73,73	1.09	5 (7%)	83,113,113	1.13	4 (4%)
46	CHL	g	608	-	48,52,74	1.01	2 (4%)	53,87,114	1.45	11 (20%)
46	CHL	r	305	-	48,52,74	0.98	2 (4%)	53,87,114	1.37	9 (16%)
29	CLA	r	302	22	64,68,73	1.12	5 (7%)	77,107,113	1.14	5 (6%)
46	CHL	N	609	20	70,74,74	0.82	2 (2%)	80,114,114	1.25	12 (15%)
29	CLA	c	503	-	69,73,73	1.11	5 (7%)	83,113,113	1.11	9 (10%)
37	LHG	n	617	-	41,41,48	0.41	0	44,47,54	1.15	4 (9%)
41	DGA	W	202	-	43,43,43	1.12	3 (6%)	45,45,45	1.49	3 (6%)
46	CHL	n	605	20	70,74,74	0.88	3 (4%)	80,114,114	1.26	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	B	505	2	69,73,73	1.10	5 (7%)	83,113,113	1.20	5 (6%)
46	CHL	G	605	21	52,56,74	0.89	1 (1%)	58,92,114	1.40	10 (17%)
34	C7Z	B	519	-	43,43,43	5.30	27 (62%)	58,60,60	2.46	23 (39%)
29	CLA	b	501	-	69,73,73	1.08	5 (7%)	83,113,113	1.03	5 (6%)
46	CHL	R	305	-	54,58,74	0.92	2 (3%)	59,94,114	1.42	10 (16%)
46	CHL	g	605	21	52,56,74	0.95	2 (3%)	58,92,114	1.34	11 (18%)
46	CHL	y	311	24	70,74,74	0.82	2 (2%)	80,114,114	1.35	13 (16%)
29	CLA	C	509	4	69,73,73	1.08	4 (5%)	83,113,113	1.10	7 (8%)
29	CLA	B	513	2	69,73,73	1.10	6 (8%)	83,113,113	0.98	3 (3%)
46	CHL	g	607	-	70,74,74	0.83	2 (2%)	80,114,114	1.30	14 (17%)
48	NEX	n	616	-	38,46,46	3.36	9 (23%)	50,70,70	1.60	10 (20%)
29	CLA	c	501	4	69,73,73	1.08	5 (7%)	83,113,113	1.09	8 (9%)
30	PHO	A	408	-	58,69,69	1.99	10 (17%)	56,99,99	1.54	7 (12%)
37	LHG	D	407	-	48,48,48	0.40	0	51,54,54	1.00	3 (5%)
46	CHL	N	607	-	70,74,74	0.83	2 (2%)	80,114,114	1.25	12 (15%)
29	CLA	B	514	2	69,73,73	1.11	5 (7%)	83,113,113	1.13	6 (7%)
26	OEX	A	401	52,4,1	0,14,14	-	-	-	-	-
43	PL9	d	405	-	55,55,55	1.28	5 (9%)	68,69,69	1.51	11 (16%)
29	CLA	r	308	22	64,68,73	1.17	4 (6%)	77,107,113	1.07	4 (5%)
39	SQD	o	301	-	53,54,54	0.80	0	62,65,65	0.92	2 (3%)
48	NEX	s	319	-	38,46,46	3.36	9 (23%)	50,70,70	1.67	10 (20%)
29	CLA	B	509	-	69,73,73	1.11	7 (10%)	83,113,113	1.09	5 (6%)
41	DGA	D	402	-	36,36,43	1.19	2 (5%)	38,38,45	1.30	3 (7%)
46	CHL	y	301	-	70,74,74	0.83	2 (2%)	80,114,114	1.21	12 (15%)
29	CLA	B	511	2	69,73,73	1.09	6 (8%)	83,113,113	1.11	5 (6%)
35	LMG	C	524	-	42,42,55	0.78	2 (4%)	50,50,63	1.17	4 (8%)
29	CLA	c	512	-	69,73,73	1.09	5 (7%)	83,113,113	1.02	4 (4%)
46	CHL	S	307	-	48,52,74	0.97	2 (4%)	53,87,114	1.36	8 (15%)
46	CHL	s	307	-	48,52,74	0.97	2 (4%)	53,87,114	1.36	8 (15%)
29	CLA	G	613	21	69,73,73	1.08	4 (5%)	83,113,113	0.99	2 (2%)
31	BCR	b	517	-	41,41,41	1.85	4 (9%)	56,56,56	4.22	15 (26%)
29	CLA	C	503	4	69,73,73	1.09	5 (7%)	83,113,113	1.10	4 (4%)
29	CLA	R	308	22	64,68,73	1.13	5 (7%)	77,107,113	1.12	6 (7%)
47	LUT	g	615	-	42,43,43	2.33	1 (2%)	51,60,60	1.96	13 (25%)
31	BCR	v	101	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	BCR	A	410	-	41,41,41	1.84	5 (12%)	56,56,56	4.27	15 (26%)
31	BCR	B	517	-	41,41,41	1.86	5 (12%)	56,56,56	4.22	19 (33%)
29	CLA	G	602	21	69,73,73	1.10	5 (7%)	83,113,113	1.01	4 (4%)
46	CHL	n	607	-	54,58,74	0.94	2 (3%)	59,94,114	1.36	11 (18%)
29	CLA	A	409	1	64,68,73	1.13	7 (10%)	77,107,113	1.16	6 (7%)
46	CHL	Y	307	-	70,74,74	0.87	2 (2%)	80,114,114	1.19	10 (12%)
35	LMG	b	520	-	44,44,55	0.86	2 (4%)	52,52,63	1.07	2 (3%)
41	DGA	b	522	-	43,43,43	1.11	2 (4%)	45,45,45	1.52	3 (6%)
47	LUT	S	317	-	42,43,43	2.25	1 (2%)	51,60,60	1.85	10 (19%)
39	SQD	c	522	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
46	CHL	g	609	21	70,74,74	0.86	2 (2%)	80,114,114	1.21	12 (15%)
51	LPX	s	321	-	18,18,29	1.23	2 (11%)	20,22,33	1.03	1 (5%)
29	CLA	c	504	-	69,73,73	1.08	5 (7%)	83,113,113	1.07	3 (3%)
29	CLA	S	312	37	69,73,73	1.10	5 (7%)	83,113,113	1.09	4 (4%)
29	CLA	s	306	23	54,58,73	1.22	6 (11%)	65,95,113	1.26	8 (12%)
29	CLA	S	304	23	69,73,73	1.13	7 (10%)	83,113,113	1.25	9 (10%)
37	LHG	N	618	29	48,48,48	0.39	0	51,54,54	1.05	4 (7%)
29	CLA	Y	313	24	69,73,73	1.09	5 (7%)	83,113,113	1.02	4 (4%)
35	LMG	B	520	-	44,44,55	0.86	3 (6%)	52,52,63	1.08	3 (5%)
46	CHL	G	609	21	70,74,74	0.82	2 (2%)	80,114,114	1.23	13 (16%)
29	CLA	B	504	2	69,73,73	1.09	4 (5%)	83,113,113	1.24	7 (8%)
36	DGD	c	518	-	60,60,67	1.06	6 (10%)	74,74,81	0.95	2 (2%)
40	SPH	i	102	-	19,20,20	0.65	0	18,21,21	1.08	1 (5%)
29	CLA	N	614	-	53,57,73	1.24	5 (9%)	62,93,113	1.11	5 (8%)
29	CLA	b	515	2	69,73,73	1.08	5 (7%)	83,113,113	0.99	4 (4%)
29	CLA	s	314	23	59,63,73	1.19	6 (10%)	71,101,113	1.17	5 (7%)
29	CLA	D	405	-	64,68,73	1.14	5 (7%)	77,107,113	1.17	6 (7%)
29	CLA	r	307	-	64,68,73	1.14	6 (9%)	77,107,113	1.13	4 (5%)
35	LMG	C	521	-	47,47,55	0.96	4 (8%)	55,55,63	1.12	4 (7%)
49	XAT	y	302	-	39,47,47	0.73	1 (2%)	54,74,74	2.03	13 (24%)
29	CLA	B	512	2	69,73,73	1.09	5 (7%)	83,113,113	1.05	2 (2%)
46	CHL	n	606	-	70,74,74	0.90	2 (2%)	80,114,114	1.17	10 (12%)
29	CLA	B	507	52	69,73,73	1.09	5 (7%)	83,113,113	1.03	3 (3%)
50	PTY	N	620	-	49,49,49	0.87	4 (8%)	52,54,54	1.05	2 (3%)
29	CLA	y	306	52	69,73,73	1.08	6 (8%)	83,113,113	1.11	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	XAT	r	312	-	39,47,47	0.67	1 (2%)	54,74,74	1.89	11 (20%)
29	CLA	R	307	22	50,54,73	1.28	5 (10%)	60,90,113	1.22	6 (10%)
29	CLA	n	611	20	49,53,73	1.30	5 (10%)	59,89,113	1.20	6 (10%)
36	DGD	C	519	-	54,54,67	1.00	4 (7%)	68,68,81	0.91	3 (4%)
29	CLA	B	501	-	69,73,73	1.09	5 (7%)	83,113,113	1.05	5 (6%)
29	CLA	r	310	22	55,59,73	1.26	5 (9%)	66,96,113	1.28	7 (10%)
29	CLA	N	611	37	53,57,73	1.26	6 (11%)	62,93,113	1.17	6 (9%)
37	LHG	S	301	-	34,34,48	0.44	0	37,40,54	1.17	2 (5%)
33	3PH	s	322	-	47,47,47	0.86	4 (8%)	51,52,52	1.10	2 (3%)
29	CLA	N	602	20	69,73,73	1.10	6 (8%)	83,113,113	1.02	7 (8%)
29	CLA	s	311	23	69,73,73	1.11	8 (11%)	83,113,113	1.12	6 (7%)
39	SQD	M	101	-	41,42,54	0.88	0	50,53,65	0.96	3 (6%)
29	CLA	N	603	20	69,73,73	1.10	5 (7%)	83,113,113	0.97	4 (4%)
29	CLA	y	316	24	69,73,73	1.10	5 (7%)	83,113,113	1.07	5 (6%)
46	CHL	G	608	-	48,52,74	0.99	2 (4%)	53,87,114	1.42	9 (16%)
29	CLA	b	506	2	61,65,73	1.15	6 (9%)	73,103,113	1.15	5 (6%)
29	CLA	y	305	24	69,73,73	1.09	5 (7%)	83,113,113	1.04	4 (4%)
29	CLA	Y	303	24	69,73,73	1.10	5 (7%)	83,113,113	1.09	6 (7%)
46	CHL	y	309	-	70,74,74	0.83	2 (2%)	80,114,114	1.22	11 (13%)
39	SQD	C	523	-	35,36,54	0.94	0	44,47,65	1.04	2 (4%)
29	CLA	S	303	23	64,68,73	1.14	5 (7%)	77,107,113	1.02	5 (6%)
29	CLA	S	316	23	54,58,73	1.27	6 (11%)	65,95,113	1.38	10 (15%)
41	DGA	J	101	-	28,28,43	1.29	3 (10%)	30,30,45	1.24	2 (6%)
29	CLA	S	305	-	59,63,73	1.18	6 (10%)	71,101,113	1.08	2 (2%)
39	SQD	m	101	-	41,42,54	0.89	0	50,53,65	0.96	3 (6%)
46	CHL	N	605	20	70,74,74	0.79	2 (2%)	80,114,114	1.23	9 (11%)
46	CHL	G	607	-	70,74,74	0.79	2 (2%)	80,114,114	1.22	10 (12%)
29	CLA	R	306	-	64,68,73	1.15	7 (10%)	77,107,113	1.07	4 (5%)
45	RRX	H	101	-	42,42,42	4.88	24 (57%)	57,58,58	2.58	22 (38%)
31	BCR	a	409	-	41,41,41	1.83	5 (12%)	56,56,56	4.25	15 (26%)
46	CHL	r	306	-	54,58,74	0.94	2 (3%)	59,94,114	1.45	10 (16%)
31	BCR	f	101	-	41,41,41	1.82	4 (9%)	56,56,56	4.27	17 (30%)
46	CHL	g	606	-	54,58,74	0.98	3 (5%)	59,94,114	1.40	11 (18%)
29	CLA	N	604	-	69,73,73	1.09	6 (8%)	83,113,113	1.05	4 (4%)
37	LHG	B	523	-	43,43,48	0.41	0	46,49,54	1.02	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	LHG	d	406	-	48,48,48	0.39	0	51,54,54	1.00	3 (5%)
29	CLA	n	604	-	69,73,73	1.09	6 (8%)	83,113,113	0.99	4 (4%)
48	NEX	Y	318	-	38,46,46	3.31	9 (23%)	50,70,70	1.84	11 (22%)
37	LHG	L	101	-	48,48,48	0.38	0	51,54,54	1.23	3 (5%)
29	CLA	g	610	21	69,73,73	1.10	7 (10%)	83,113,113	1.27	6 (7%)
40	SPH	C	525	-	19,20,20	0.63	0	18,21,21	1.08	1 (5%)
31	BCR	F	101	-	41,41,41	1.84	4 (9%)	56,56,56	4.13	14 (25%)
35	LMG	d	408	-	48,48,55	0.99	4 (8%)	56,56,63	1.11	2 (3%)
29	CLA	b	507	52	69,73,73	1.09	6 (8%)	83,113,113	1.11	2 (2%)
35	LMG	c	519	-	51,51,55	1.06	6 (11%)	59,59,63	1.11	3 (5%)
39	SQD	L	102	-	41,42,54	0.87	0	50,53,65	0.96	3 (6%)
29	CLA	y	312	24	69,73,73	1.10	7 (10%)	83,113,113	1.11	5 (6%)
35	LMG	C	522	-	55,55,55	1.12	6 (10%)	63,63,63	1.04	2 (3%)
29	CLA	n	610	-	53,57,73	1.25	6 (11%)	62,93,113	1.10	4 (6%)
40	SPH	I	101	-	19,20,20	0.64	0	18,21,21	1.07	1 (5%)
26	OEX	a	401	52,4,1	0,14,14	-	-	-	-	-
46	CHL	Y	302	24	70,74,74	0.81	2 (2%)	80,114,114	1.18	10 (12%)
38	LMT	B	524	-	36,36,36	1.22	5 (13%)	47,47,47	1.18	5 (10%)
46	CHL	y	303	24	70,74,74	0.84	2 (2%)	80,114,114	1.22	12 (15%)
48	NEX	G	617	-	38,46,46	3.31	9 (23%)	50,70,70	1.83	15 (30%)
47	LUT	y	318	-	42,43,43	2.36	1 (2%)	51,60,60	2.01	13 (25%)
37	LHG	Y	319	29	48,48,48	0.40	0	51,54,54	0.99	2 (3%)
35	LMG	W	203	-	39,39,55	0.85	2 (5%)	47,47,63	1.16	3 (6%)
29	CLA	D	404	5	69,73,73	3.35	29 (42%)	83,113,113	3.76	34 (40%)
29	CLA	b	516	2	69,73,73	1.11	7 (10%)	83,113,113	1.05	5 (6%)
29	CLA	b	503	2	69,73,73	1.09	6 (8%)	83,113,113	1.16	4 (4%)
29	CLA	b	510	52	69,73,73	1.09	4 (5%)	83,113,113	1.01	4 (4%)
39	SQD	l	101	-	41,42,54	0.88	0	50,53,65	1.00	3 (6%)
35	LMG	D	410	-	48,48,55	0.99	4 (8%)	56,56,63	1.08	2 (3%)
46	CHL	G	606	-	54,58,74	0.93	2 (3%)	59,94,114	1.43	11 (18%)
37	LHG	g	618	29	48,48,48	0.39	0	51,54,54	1.03	3 (5%)
47	LUT	n	614	-	42,43,43	2.36	1 (2%)	51,60,60	1.89	12 (23%)
31	BCR	C	517	-	41,41,41	1.83	4 (9%)	56,56,56	4.24	18 (32%)
29	CLA	G	610	21	69,73,73	1.10	6 (8%)	83,113,113	1.23	6 (7%)
30	PHO	a	407	-	58,69,69	1.95	9 (15%)	56,99,99	1.52	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	c	508	4	69,73,73	1.08	5 (7%)	83,113,113	1.08	4 (4%)
29	CLA	b	502	-	69,73,73	1.08	5 (7%)	83,113,113	1.06	6 (7%)
46	CHL	S	309	-	65,69,74	0.85	2 (3%)	74,108,114	1.37	13 (17%)
29	CLA	b	511	-	69,73,73	1.09	5 (7%)	83,113,113	1.14	6 (7%)
29	CLA	g	604	-	53,57,73	1.23	6 (11%)	62,93,113	1.13	4 (6%)
29	CLA	r	309	22	64,68,73	1.14	5 (7%)	77,107,113	1.21	7 (9%)
49	XAT	n	618	-	39,47,47	0.73	1 (2%)	54,74,74	1.99	13 (24%)
29	CLA	c	513	-	69,73,73	1.07	5 (7%)	83,113,113	1.08	3 (3%)
29	CLA	s	316	23	54,58,73	1.25	6 (11%)	65,95,113	1.26	8 (12%)
29	CLA	s	305	-	59,63,73	1.17	5 (8%)	71,101,113	1.24	4 (5%)
46	CHL	R	304	-	48,52,74	0.98	2 (4%)	53,87,114	1.37	9 (16%)
48	NEX	r	313	-	24,28,46	3.23	6 (25%)	32,42,70	1.83	7 (21%)
29	CLA	c	502	4	69,73,73	1.10	5 (7%)	83,113,113	1.12	5 (6%)
29	CLA	b	513	2	69,73,73	1.10	6 (8%)	83,113,113	1.01	2 (2%)
29	CLA	d	404	-	69,73,73	1.10	5 (7%)	83,113,113	1.13	6 (7%)
31	BCR	z	101	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	13 (23%)
44	HEM	e	101	6,7	50,50,50	1.37	7 (14%)	66,82,82	1.14	4 (6%)
31	BCR	C	515	-	41,41,41	1.82	4 (9%)	56,56,56	4.21	14 (25%)
29	CLA	s	315	-	59,63,73	1.20	6 (10%)	71,101,113	1.09	4 (5%)
33	3PH	B	522	-	47,47,47	0.86	4 (8%)	51,52,52	1.11	2 (3%)
41	DGA	j	101	-	28,28,43	1.28	3 (10%)	30,30,45	1.28	2 (6%)
29	CLA	g	612	21	47,51,73	1.29	6 (12%)	56,86,113	1.17	2 (3%)
29	CLA	C	502	4	69,73,73	1.08	5 (7%)	83,113,113	1.05	4 (4%)
29	CLA	N	612	20	49,53,73	1.29	5 (10%)	59,89,113	1.12	5 (8%)
29	CLA	b	508	2	69,73,73	1.10	6 (8%)	83,113,113	1.06	4 (4%)
29	CLA	g	603	21	69,73,73	1.11	6 (8%)	83,113,113	1.07	5 (6%)
37	LHG	a	414	-	38,38,48	0.41	0	41,44,54	1.09	2 (4%)
37	LHG	y	320	29	48,48,48	0.38	0	51,54,54	1.11	4 (7%)
29	CLA	C	510	4	69,73,73	1.10	5 (7%)	83,113,113	1.06	4 (4%)
37	LHG	G	618	-	48,48,48	0.38	0	51,54,54	1.07	3 (5%)
46	CHL	N	601	20	70,74,74	0.79	2 (2%)	80,114,114	1.25	12 (15%)
48	NEX	R	312	-	24,28,46	3.24	6 (25%)	32,42,70	1.76	7 (21%)
31	BCR	b	518	-	41,41,41	1.85	5 (12%)	56,56,56	4.12	15 (26%)
50	PTY	y	321	-	18,18,49	1.30	3 (16%)	21,23,54	1.42	2 (9%)
29	CLA	c	507	52	69,73,73	1.10	6 (8%)	83,113,113	1.09	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	y	313	37	69,73,73	1.09	5 (7%)	83,113,113	1.02	5 (6%)
29	CLA	s	312	37	69,73,73	1.10	6 (8%)	83,113,113	1.14	5 (6%)
45	RRX	h	101	-	42,42,42	4.88	24 (57%)	57,58,58	2.50	23 (40%)
47	LUT	g	616	-	42,43,43	2.37	1 (2%)	51,60,60	2.08	12 (23%)
36	DGD	C	518	-	52,52,67	1.02	4 (7%)	66,66,81	0.93	2 (3%)
47	LUT	s	318	-	42,43,43	2.29	1 (2%)	51,60,60	1.92	12 (23%)
36	DGD	B	521	-	44,44,67	0.86	1 (2%)	58,58,81	1.15	5 (8%)
49	XAT	g	619	-	39,47,47	0.70	1 (2%)	54,74,74	3.73	17 (31%)
29	CLA	n	609	20	69,73,73	1.11	7 (10%)	83,113,113	1.20	8 (9%)
31	BCR	B	518	-	41,41,41	1.85	5 (12%)	56,56,56	4.12	15 (26%)
47	LUT	y	317	-	42,43,43	2.38	1 (2%)	51,60,60	1.87	13 (25%)
29	CLA	b	509	-	69,73,73	1.10	6 (8%)	83,113,113	1.12	7 (8%)
29	CLA	S	313	23	49,53,73	1.29	5 (10%)	59,89,113	1.08	4 (6%)
29	CLA	n	612	20	69,73,73	1.10	5 (7%)	83,113,113	1.05	5 (6%)
38	LMT	b	524	-	36,36,36	1.24	6 (16%)	47,47,47	1.16	4 (8%)
35	LMG	D	409	-	42,42,55	0.76	2 (4%)	50,50,63	0.97	2 (4%)
33	3PH	A	412	-	47,47,47	0.84	3 (6%)	51,52,52	1.12	2 (3%)
29	CLA	r	304	-	53,57,73	1.23	5 (9%)	62,93,113	1.08	2 (3%)
46	CHL	s	309	-	65,69,74	0.81	2 (3%)	74,108,114	1.27	11 (14%)
37	LHG	D	408	-	38,38,48	0.42	0	41,44,54	1.04	2 (4%)
48	NEX	g	617	-	38,46,46	3.29	9 (23%)	50,70,70	1.87	13 (26%)
29	CLA	a	404	-	69,73,73	1.11	4 (5%)	83,113,113	1.15	5 (6%)
29	CLA	A	407	-	54,58,73	1.22	5 (9%)	65,95,113	1.15	5 (7%)
29	CLA	R	309	-	54,58,73	1.26	6 (11%)	65,95,113	1.21	8 (12%)
30	PHO	d	402	-	58,69,69	2.00	10 (17%)	56,99,99	1.65	8 (14%)
31	BCR	c	514	-	41,41,41	1.82	5 (12%)	56,56,56	4.17	19 (33%)
29	CLA	G	612	21	47,51,73	1.29	5 (10%)	56,86,113	1.11	3 (5%)
29	CLA	B	502	-	69,73,73	1.08	5 (7%)	83,113,113	1.10	4 (4%)
37	LHG	l	102	-	48,48,48	0.40	0	51,54,54	1.00	2 (3%)
35	LMG	w	202	-	39,39,55	0.86	2 (5%)	47,47,63	1.05	2 (4%)
37	LHG	c	521	-	46,46,48	0.40	0	49,52,54	1.03	2 (4%)
29	CLA	C	506	4	64,68,73	1.16	7 (10%)	77,107,113	1.12	5 (6%)
29	CLA	s	310	-	64,68,73	1.13	5 (7%)	77,107,113	1.08	3 (3%)
29	CLA	N	613	20	69,73,73	1.11	6 (8%)	83,113,113	1.06	5 (6%)
29	CLA	S	306	23	54,58,73	1.24	6 (11%)	65,95,113	1.35	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	SPH	c	523	-	19,20,20	0.65	0	18,21,21	1.10	1 (5%)
46	CHL	G	601	21	70,74,74	0.79	2 (2%)	80,114,114	1.27	11 (13%)
39	SQD	C	501	-	41,42,54	0.87	0	50,53,65	0.99	2 (4%)
50	PTY	n	619	-	49,49,49	0.88	4 (8%)	52,54,54	1.05	2 (3%)
29	CLA	b	514	2	69,73,73	1.11	5 (7%)	83,113,113	1.10	7 (8%)
29	CLA	R	303	-	53,57,73	1.23	5 (9%)	62,93,113	1.06	1 (1%)
29	CLA	C	511	-	69,73,73	1.07	5 (7%)	83,113,113	1.01	4 (4%)
29	CLA	B	503	2	69,73,73	1.09	6 (8%)	83,113,113	1.15	6 (7%)
47	LUT	r	311	-	42,43,43	2.42	2 (4%)	51,60,60	1.94	14 (27%)
29	CLA	R	302	22	64,68,73	1.16	6 (9%)	77,107,113	1.16	7 (9%)
30	PHO	D	401	-	58,69,69	2.02	10 (17%)	56,99,99	1.58	7 (12%)
46	CHL	Y	306	24	50,54,74	0.95	2 (4%)	56,90,114	1.36	10 (17%)
29	CLA	b	505	2	69,73,73	1.10	5 (7%)	83,113,113	1.18	6 (7%)
36	DGD	c	517	-	63,63,67	1.11	7 (11%)	77,77,81	0.94	3 (3%)
48	NEX	S	319	-	38,46,46	3.33	9 (23%)	50,70,70	1.80	13 (26%)
29	CLA	s	303	23	64,68,73	1.13	5 (7%)	77,107,113	1.19	4 (5%)
29	CLA	b	504	2	69,73,73	1.10	6 (8%)	83,113,113	1.25	5 (6%)
29	CLA	n	603	20	69,73,73	1.10	5 (7%)	83,113,113	1.05	5 (6%)
35	LMG	d	407	-	46,46,55	0.91	3 (6%)	54,54,63	1.05	2 (3%)
29	CLA	C	507	4	69,73,73	1.08	4 (5%)	83,113,113	1.04	6 (7%)
29	CLA	n	613	-	53,57,73	1.24	5 (9%)	62,93,113	1.21	3 (4%)
46	CHL	S	302	23	50,54,74	0.95	2 (4%)	56,90,114	1.42	7 (12%)
29	CLA	a	406	52	53,57,73	1.23	6 (11%)	62,93,113	1.22	4 (6%)
37	LHG	s	301	-	37,37,48	0.44	0	40,43,54	1.16	3 (7%)
47	LUT	N	616	-	42,43,43	2.34	1 (2%)	51,60,60	1.92	12 (23%)
47	LUT	R	310	-	42,43,43	2.38	1 (2%)	51,60,60	2.01	14 (27%)
29	CLA	g	611	37	69,73,73	1.11	6 (8%)	83,113,113	1.13	5 (6%)
47	LUT	Y	317	-	42,43,43	2.36	1 (2%)	51,60,60	2.00	13 (25%)
29	CLA	n	602	20	69,73,73	1.10	5 (7%)	83,113,113	1.11	7 (8%)
47	LUT	N	615	-	42,43,43	2.36	1 (2%)	51,60,60	1.88	13 (25%)
29	CLA	Y	309	52	54,58,73	1.23	6 (11%)	65,95,113	1.16	4 (6%)
29	CLA	Y	315	24	69,73,73	1.09	5 (7%)	83,113,113	1.12	7 (8%)
29	CLA	b	512	2	69,73,73	1.09	6 (8%)	83,113,113	1.03	3 (3%)
29	CLA	G	614	-	53,57,73	1.24	5 (9%)	62,93,113	1.12	3 (4%)
29	CLA	a	408	1	64,68,73	1.13	7 (10%)	77,107,113	1.15	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	LUT	S	318	-	42,43,43	2.31	1 (2%)	51,60,60	1.94	12 (23%)
33	3PH	a	415	-	47,47,47	0.85	4 (8%)	51,52,52	1.18	2 (3%)
47	LUT	s	317	-	42,43,43	2.36	1 (2%)	51,60,60	1.99	15 (29%)
46	CHL	y	308	52	55,59,74	0.97	3 (5%)	62,96,114	1.34	11 (17%)
29	CLA	G	603	21	69,73,73	1.10	5 (7%)	83,113,113	1.02	4 (4%)
29	CLA	Y	314	24	69,73,73	1.09	5 (7%)	83,113,113	0.98	3 (3%)
29	CLA	B	506	2	69,73,73	1.10	5 (7%)	83,113,113	1.12	6 (7%)
47	LUT	Y	316	-	42,43,43	2.37	1 (2%)	51,60,60	1.92	15 (29%)
46	CHL	s	302	23	50,54,74	0.94	2 (4%)	56,90,114	1.41	9 (16%)
51	LPX	S	321	-	19,19,29	1.20	2 (10%)	21,23,33	1.04	1 (4%)
29	CLA	Y	312	37	69,73,73	1.08	5 (7%)	83,113,113	1.05	6 (7%)
44	HEM	E	101	6,7	50,50,50	1.39	5 (10%)	66,82,82	1.16	4 (6%)
47	LUT	n	615	-	42,43,43	2.32	1 (2%)	51,60,60	1.81	12 (23%)
41	DGA	w	201	-	43,43,43	1.12	3 (6%)	45,45,45	1.50	3 (6%)
36	DGD	r	301	-	44,44,67	0.86	1 (2%)	58,58,81	1.19	5 (8%)
29	CLA	B	510	52	69,73,73	1.09	4 (5%)	83,113,113	1.05	5 (6%)
29	CLA	G	611	-	69,73,73	1.11	6 (8%)	83,113,113	1.13	5 (6%)
29	CLA	y	315	24	69,73,73	1.08	5 (7%)	83,113,113	0.98	3 (3%)
29	CLA	C	508	52	69,73,73	1.09	5 (7%)	83,113,113	1.10	3 (3%)
29	CLA	s	313	23	49,53,73	1.30	5 (10%)	59,89,113	1.17	4 (6%)
29	CLA	d	403	5	69,73,73	1.10	6 (8%)	83,113,113	1.09	3 (3%)
29	CLA	y	304	24	69,73,73	1.10	5 (7%)	83,113,113	1.13	6 (7%)
29	CLA	c	511	4	69,73,73	1.10	5 (7%)	83,113,113	1.13	4 (4%)
37	LHG	s	320	29	44,44,48	0.41	0	47,50,54	1.03	3 (6%)
37	LHG	a	413	-	43,43,48	0.41	0	46,49,54	1.05	2 (4%)
33	3PH	b	521	-	38,38,47	0.96	4 (10%)	42,43,52	1.17	2 (4%)
29	CLA	Y	311	24	69,73,73	1.09	6 (8%)	83,113,113	1.12	4 (4%)
29	CLA	S	311	23	69,73,73	1.09	5 (7%)	83,113,113	1.09	6 (7%)
29	CLA	A	405	-	69,73,73	1.09	5 (7%)	83,113,113	1.04	4 (4%)
47	LUT	G	615	-	42,43,43	2.37	1 (2%)	51,60,60	1.92	13 (25%)
49	XAT	N	619	-	39,47,47	0.70	1 (2%)	54,74,74	1.97	12 (22%)
46	CHL	N	608	-	54,58,74	0.90	2 (3%)	59,94,114	1.36	10 (16%)
29	CLA	c	505	4	69,73,73	1.11	6 (8%)	83,113,113	1.13	6 (7%)
29	CLA	C	513	-	69,73,73	1.10	5 (7%)	83,113,113	0.95	3 (3%)
46	CHL	Y	308	-	70,74,74	0.78	2 (2%)	80,114,114	1.18	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LMG	i	101	-	48,48,55	0.99	5 (10%)	56,56,63	1.07	3 (5%)
29	CLA	c	509	4	69,73,73	1.10	5 (7%)	83,113,113	1.10	4 (4%)
39	SQD	a	410	-	50,51,54	0.81	0	59,62,65	0.93	2 (3%)
29	CLA	g	602	21	69,73,73	1.08	5 (7%)	83,113,113	1.04	4 (4%)
29	CLA	y	310	-	54,58,73	1.24	6 (11%)	65,95,113	1.15	6 (9%)
50	PTY	Y	320	-	18,18,49	1.29	3 (16%)	21,23,54	1.45	2 (9%)
29	CLA	C	505	52	59,63,73	1.16	5 (8%)	71,101,113	1.12	2 (2%)
29	CLA	a	405	52	69,73,73	1.10	5 (7%)	83,113,113	1.09	6 (7%)
29	CLA	S	314	23	59,63,73	1.19	5 (8%)	71,101,113	1.21	7 (9%)
48	NEX	N	617	-	38,46,46	3.33	9 (23%)	50,70,70	1.61	11 (22%)
29	CLA	c	506	-	64,68,73	1.12	4 (6%)	77,107,113	1.17	8 (10%)
29	CLA	G	604	-	53,57,73	1.26	5 (9%)	62,93,113	1.09	5 (8%)
29	CLA	R	301	22	64,68,73	1.12	5 (7%)	77,107,113	1.12	4 (5%)
31	BCR	K	101	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	15 (26%)
29	CLA	C	504	-	69,73,73	1.11	5 (7%)	83,113,113	1.05	7 (8%)
29	CLA	B	515	2	69,73,73	1.08	5 (7%)	83,113,113	0.98	4 (4%)
29	CLA	r	303	22	64,68,73	1.16	6 (9%)	77,107,113	1.19	10 (12%)
29	CLA	S	315	23	54,58,73	1.25	5 (9%)	65,95,113	1.14	5 (7%)
31	BCR	C	516	-	41,41,41	1.82	4 (9%)	56,56,56	4.23	14 (25%)
46	CHL	n	608	20	70,74,74	0.85	2 (2%)	80,114,114	1.26	11 (13%)
29	CLA	B	508	2	69,73,73	1.11	7 (10%)	83,113,113	1.04	5 (6%)
46	CHL	s	308	-	47,51,74	1.00	2 (4%)	52,86,114	1.45	9 (17%)
46	CHL	N	606	-	70,74,74	0.85	2 (2%)	80,114,114	1.20	11 (13%)
29	CLA	Y	305	52	69,73,73	1.08	5 (7%)	83,113,113	1.01	5 (6%)
42	BCT	D	403	27	2,3,3	1.29	0	2,3,3	1.23	0
33	3PH	S	322	-	29,29,47	1.09	4 (13%)	33,34,52	1.24	2 (6%)
46	CHL	n	601	20	70,74,74	0.81	2 (2%)	80,114,114	1.26	11 (13%)
48	NEX	y	319	-	38,46,46	3.31	11 (28%)	50,70,70	1.82	13 (26%)
42	BCT	a	412	27	2,3,3	0.31	0	2,3,3	5.05	2 (100%)
29	CLA	C	512	4	69,73,73	1.10	5 (7%)	83,113,113	1.04	5 (6%)
29	CLA	S	310	23	64,68,73	1.14	5 (7%)	77,107,113	1.14	5 (6%)
29	CLA	g	614	-	53,57,73	1.24	5 (9%)	62,93,113	1.14	4 (6%)
46	CHL	g	601	21	70,74,74	0.79	2 (2%)	80,114,114	1.25	12 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	Y	304	24	-	15/39/115/115	-
37	LHG	S	320	29	-	15/49/49/53	-
46	CHL	S	308	-	-	0/14/90/117	-
46	CHL	Y	310	24	1/1/15/21	6/41/117/117	-
39	SQD	b	523	-	-	19/49/69/69	0/1/1/1
31	BCR	c	515	-	-	10/29/63/63	0/2/2/2
29	CLA	g	613	21	-	22/39/115/115	-
47	LUT	G	616	-	-	2/29/67/67	0/2/2/2
49	XAT	Y	301	-	1/1/12/26	0/31/93/93	0/4/4/4
29	CLA	y	314	24	-	13/39/115/115	-
35	LMG	W	201	-	-	10/35/55/70	0/1/1/1
49	XAT	R	311	-	2/2/12/26	0/31/93/93	0/4/4/4
29	CLA	s	304	23	-	15/39/115/115	-
35	LMG	c	520	-	-	13/50/70/70	0/1/1/1
43	PL9	D	406	-	-	10/53/73/73	0/1/1/1
29	CLA	C	514	-	-	13/39/115/115	-
36	DGD	C	520	-	-	5/42/82/95	0/2/2/2
29	CLA	N	610	-	-	13/39/115/115	-
29	CLA	c	510	-	-	9/39/115/115	-
29	CLA	B	516	2	-	11/27/103/115	-
49	XAT	G	619	-	1/1/12/26	0/31/93/93	0/4/4/4
36	DGD	c	516	-	-	10/44/84/95	0/2/2/2
34	C7Z	b	519	-	1/1/12/26	7/29/67/67	0/2/2/2
46	CHL	y	307	24	-	4/17/93/117	-
29	CLA	A	406	52	-	17/39/115/115	-
46	CHL	g	608	-	-	0/15/91/117	-
46	CHL	r	305	-	-	4/15/91/117	-
29	CLA	r	302	22	-	8/33/109/115	-
46	CHL	N	609	20	1/1/15/21	6/41/117/117	-
29	CLA	c	503	-	-	15/39/115/115	-
37	LHG	n	617	-	-	30/46/46/53	-
41	DGA	W	202	-	-	23/45/45/45	-
46	CHL	n	605	20	1/1/15/21	11/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	505	2	-	8/39/115/115	-
46	CHL	G	605	21	-	6/20/96/117	-
34	C7Z	B	519	-	1/1/12/26	9/29/67/67	0/2/2/2
29	CLA	b	501	-	-	23/39/115/115	-
46	CHL	R	305	-	-	6/22/98/117	-
46	CHL	y	311	24	1/1/15/21	6/41/117/117	-
46	CHL	g	605	21	-	4/20/96/117	-
29	CLA	C	509	4	-	7/39/115/115	-
29	CLA	B	513	2	-	11/39/115/115	-
46	CHL	g	607	-	1/1/15/21	11/41/117/117	-
48	NEX	n	616	-	-	2/27/83/83	1/3/3/3
29	CLA	c	501	4	-	15/39/115/115	-
30	PHO	A	408	-	-	8/37/103/103	0/5/6/6
37	LHG	D	407	-	-	18/53/53/53	-
46	CHL	N	607	-	1/1/15/21	12/41/117/117	-
29	CLA	B	514	2	-	11/39/115/115	-
43	PL9	d	405	-	-	11/53/73/73	0/1/1/1
29	CLA	r	308	22	-	13/33/109/115	-
39	SQD	o	301	-	-	14/49/69/69	0/1/1/1
48	NEX	s	319	-	-	2/27/83/83	0/3/3/3
29	CLA	B	509	-	-	13/39/115/115	-
41	DGA	D	402	-	-	19/38/38/45	-
46	CHL	y	301	-	1/1/15/21	12/41/117/117	-
29	CLA	B	511	2	-	11/39/115/115	-
35	LMG	C	524	-	-	19/37/57/70	0/1/1/1
29	CLA	c	512	-	-	16/39/115/115	-
46	CHL	S	307	-	-	1/15/91/117	-
46	CHL	s	307	-	-	1/15/91/117	-
29	CLA	G	613	21	-	11/39/115/115	-
31	BCR	b	517	-	-	11/29/63/63	0/2/2/2
29	CLA	C	503	4	-	11/39/115/115	-
29	CLA	R	308	22	-	12/33/109/115	-
47	LUT	g	615	-	-	2/29/67/67	0/2/2/2
31	BCR	v	101	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	A	410	-	-	9/29/63/63	0/2/2/2
31	BCR	B	517	-	-	8/29/63/63	0/2/2/2
29	CLA	G	602	21	-	15/39/115/115	-
46	CHL	n	607	-	-	4/22/98/117	-
29	CLA	A	409	1	-	9/33/109/115	-
46	CHL	Y	307	-	1/1/15/21	16/41/117/117	-
35	LMG	b	520	-	-	12/39/59/70	0/1/1/1
41	DGA	b	522	-	-	19/45/45/45	-
47	LUT	S	317	-	-	3/29/67/67	0/2/2/2
39	SQD	c	522	-	-	15/49/69/69	0/1/1/1
46	CHL	g	609	21	1/1/15/21	8/41/117/117	-
51	LPX	s	321	-	-	10/20/20/31	-
29	CLA	c	504	-	-	13/39/115/115	-
29	CLA	S	312	37	-	18/39/115/115	-
29	CLA	s	306	23	-	6/21/97/115	-
29	CLA	S	304	23	-	18/39/115/115	-
37	LHG	N	618	29	-	30/53/53/53	-
29	CLA	Y	313	24	-	15/39/115/115	-
35	LMG	B	520	-	-	13/39/59/70	0/1/1/1
46	CHL	G	609	21	1/1/15/21	11/41/117/117	-
29	CLA	B	504	2	-	18/39/115/115	-
36	DGD	c	518	-	-	8/48/88/95	0/2/2/2
40	SPH	i	102	-	-	11/21/21/21	-
29	CLA	N	614	-	-	9/20/96/115	-
29	CLA	b	515	2	-	13/39/115/115	-
29	CLA	s	314	23	-	12/27/103/115	-
29	CLA	D	405	-	-	11/33/109/115	-
29	CLA	r	307	-	-	14/33/109/115	-
35	LMG	C	521	-	-	9/42/62/70	0/1/1/1
49	XAT	y	302	-	1/1/12/26	0/31/93/93	0/4/4/4
29	CLA	B	512	2	-	9/39/115/115	-
46	CHL	n	606	-	1/1/15/21	9/41/117/117	-
29	CLA	B	507	52	-	23/39/115/115	-
50	PTY	N	620	-	-	18/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	y	306	52	-	16/39/115/115	-
49	XAT	r	312	-	1/1/12/26	0/31/93/93	0/4/4/4
29	CLA	R	307	22	-	8/17/93/115	-
29	CLA	n	611	20	-	7/15/91/115	-
36	DGD	C	519	-	-	11/42/82/95	0/2/2/2
29	CLA	B	501	-	-	19/39/115/115	-
29	CLA	r	310	22	-	9/23/99/115	-
29	CLA	N	611	37	-	5/20/96/115	-
37	LHG	S	301	-	-	23/39/39/53	-
33	3PH	s	322	-	-	23/49/49/49	-
29	CLA	N	602	20	-	15/39/115/115	-
29	CLA	s	311	23	-	11/39/115/115	-
39	SQD	M	101	-	-	21/37/57/69	0/1/1/1
29	CLA	N	603	20	-	22/39/115/115	-
29	CLA	y	316	24	-	15/39/115/115	-
46	CHL	G	608	-	-	1/15/91/117	-
29	CLA	b	506	2	-	13/30/106/115	-
29	CLA	y	305	24	-	16/39/115/115	-
29	CLA	Y	303	24	-	13/39/115/115	-
46	CHL	y	309	-	1/1/15/21	12/41/117/117	-
39	SQD	C	523	-	-	12/31/51/69	0/1/1/1
29	CLA	S	303	23	-	10/33/109/115	-
29	CLA	S	316	23	-	6/21/97/115	-
41	DGA	J	101	-	-	14/30/30/45	-
29	CLA	S	305	-	-	8/27/103/115	-
39	SQD	m	101	-	-	20/37/57/69	0/1/1/1
46	CHL	N	605	20	1/1/15/21	15/41/117/117	-
46	CHL	G	607	-	1/1/15/21	14/41/117/117	-
29	CLA	R	306	-	-	12/33/109/115	-
45	RRX	H	101	-	1/1/11/25	8/29/65/65	0/2/2/2
31	BCR	a	409	-	-	9/29/63/63	0/2/2/2
46	CHL	r	306	-	-	5/22/98/117	-
31	BCR	f	101	-	-	11/29/63/63	0/2/2/2
46	CHL	g	606	-	-	3/22/98/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	N	604	-	-	8/39/115/115	-
37	LHG	B	523	-	-	16/48/48/53	-
37	LHG	d	406	-	-	22/53/53/53	-
29	CLA	n	604	-	-	14/39/115/115	-
48	NEX	Y	318	-	-	8/27/83/83	0/3/3/3
37	LHG	L	101	-	-	33/53/53/53	-
29	CLA	g	610	21	-	7/39/115/115	-
40	SPH	C	525	-	-	11/21/21/21	-
31	BCR	F	101	-	-	12/29/63/63	0/2/2/2
35	LMG	d	408	-	-	13/43/63/70	0/1/1/1
29	CLA	b	507	52	-	7/39/115/115	-
35	LMG	c	519	-	-	21/46/66/70	0/1/1/1
39	SQD	L	102	-	-	13/37/57/69	0/1/1/1
29	CLA	y	312	24	-	6/39/115/115	-
35	LMG	C	522	-	-	21/50/70/70	0/1/1/1
29	CLA	n	610	-	-	6/20/96/115	-
40	SPH	I	101	-	-	10/21/21/21	-
46	CHL	Y	302	24	1/1/15/21	6/41/117/117	-
38	LMT	B	524	-	-	2/21/61/61	0/2/2/2
46	CHL	y	303	24	1/1/15/21	8/41/117/117	-
48	NEX	G	617	-	-	4/27/83/83	0/3/3/3
47	LUT	y	318	-	-	1/29/67/67	0/2/2/2
37	LHG	Y	319	29	-	28/53/53/53	-
35	LMG	W	203	-	-	16/34/54/70	0/1/1/1
29	CLA	D	404	5	1/1/15/20	11/39/115/115	-
29	CLA	b	516	2	-	15/39/115/115	-
29	CLA	b	503	2	-	10/39/115/115	-
29	CLA	b	510	52	-	7/39/115/115	-
39	SQD	l	101	-	-	14/37/57/69	0/1/1/1
35	LMG	D	410	-	-	17/43/63/70	0/1/1/1
46	CHL	G	606	-	-	5/22/98/117	-
37	LHG	g	618	29	-	30/53/53/53	-
47	LUT	n	614	-	-	4/29/67/67	0/2/2/2
31	BCR	C	517	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	G	610	21	-	6/39/115/115	-
30	PHO	a	407	-	-	7/37/103/103	0/5/6/6
29	CLA	c	508	4	-	7/39/115/115	-
29	CLA	b	502	-	-	9/39/115/115	-
46	CHL	S	309	-	1/1/14/21	7/35/111/117	-
29	CLA	b	511	-	-	13/39/115/115	-
29	CLA	g	604	-	-	10/20/96/115	-
29	CLA	r	309	22	-	7/33/109/115	-
49	XAT	n	618	-	2/2/12/26	1/31/93/93	0/4/4/4
29	CLA	c	513	-	-	12/39/115/115	-
29	CLA	s	316	23	-	5/21/97/115	-
29	CLA	s	305	-	-	13/27/103/115	-
46	CHL	R	304	-	-	4/15/91/117	-
48	NEX	r	313	-	-	5/19/50/83	0/2/2/3
29	CLA	c	502	4	-	12/39/115/115	-
29	CLA	b	513	2	-	12/39/115/115	-
29	CLA	d	404	-	-	11/39/115/115	-
31	BCR	z	101	-	-	13/29/63/63	0/2/2/2
44	HEM	e	101	6,7	-	1/14/54/54	-
31	BCR	C	515	-	-	13/29/63/63	0/2/2/2
29	CLA	s	315	-	-	8/27/103/115	-
33	3PH	B	522	-	-	20/49/49/49	-
41	DGA	j	101	-	-	16/30/30/45	-
29	CLA	g	612	21	-	3/13/89/115	-
29	CLA	C	502	4	-	14/39/115/115	-
29	CLA	N	612	20	-	5/15/91/115	-
29	CLA	b	508	2	-	4/39/115/115	-
29	CLA	g	603	21	-	21/39/115/115	-
37	LHG	a	414	-	-	21/43/43/53	-
37	LHG	y	320	29	-	28/53/53/53	-
29	CLA	C	510	4	-	16/39/115/115	-
37	LHG	G	618	-	-	29/53/53/53	-
46	CHL	N	601	20	1/1/15/21	9/41/117/117	-
48	NEX	R	312	-	-	9/19/50/83	0/2/2/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	b	518	-	-	12/29/63/63	0/2/2/2
50	PTY	y	321	-	-	14/20/20/53	-
29	CLA	c	507	52	-	13/39/115/115	-
29	CLA	y	313	37	-	7/39/115/115	-
29	CLA	s	312	37	-	15/39/115/115	-
45	RRX	h	101	-	1/1/11/25	13/29/65/65	0/2/2/2
47	LUT	g	616	-	-	1/29/67/67	0/2/2/2
36	DGD	C	518	-	-	8/40/80/95	0/2/2/2
47	LUT	s	318	-	-	1/29/67/67	0/2/2/2
36	DGD	B	521	-	-	13/32/72/95	0/2/2/2
49	XAT	g	619	-	1/1/12/26	1/31/93/93	0/4/4/4
29	CLA	n	609	20	-	12/39/115/115	-
31	BCR	B	518	-	-	13/29/63/63	0/2/2/2
47	LUT	y	317	-	-	2/29/67/67	0/2/2/2
29	CLA	b	509	-	-	7/39/115/115	-
29	CLA	S	313	23	-	3/15/91/115	-
29	CLA	n	612	20	-	15/39/115/115	-
38	LMT	b	524	-	-	13/21/61/61	0/2/2/2
35	LMG	D	409	-	-	3/37/57/70	0/1/1/1
33	3PH	A	412	-	-	27/49/49/49	-
29	CLA	r	304	-	-	11/20/96/115	-
46	CHL	s	309	-	1/1/14/21	5/35/111/117	-
37	LHG	D	408	-	-	18/43/43/53	-
48	NEX	g	617	-	-	5/27/83/83	0/3/3/3
29	CLA	a	404	-	-	12/39/115/115	-
29	CLA	A	407	-	-	10/21/97/115	-
29	CLA	R	309	-	-	9/21/97/115	-
30	PHO	d	402	-	-	6/37/103/103	0/5/6/6
31	BCR	c	514	-	-	13/29/63/63	0/2/2/2
29	CLA	G	612	21	-	4/13/89/115	-
29	CLA	B	502	-	-	5/39/115/115	-
37	LHG	l	102	-	-	31/53/53/53	-
35	LMG	w	202	-	-	17/34/54/70	0/1/1/1
37	LHG	c	521	-	-	30/51/51/53	-
29	CLA	C	506	4	-	14/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	s	310	-	-	17/33/109/115	-
29	CLA	N	613	20	-	15/39/115/115	-
29	CLA	S	306	23	-	8/21/97/115	-
46	CHL	G	601	21	1/1/15/21	11/41/117/117	-
40	SPH	c	523	-	-	3/21/21/21	-
39	SQD	C	501	-	-	9/37/57/69	0/1/1/1
50	PTY	n	619	-	-	28/53/53/53	-
29	CLA	b	514	2	-	14/39/115/115	-
29	CLA	R	303	-	-	8/20/96/115	-
29	CLA	C	511	-	-	15/39/115/115	-
29	CLA	B	503	2	-	11/39/115/115	-
47	LUT	r	311	-	-	5/29/67/67	0/2/2/2
29	CLA	R	302	22	-	13/33/109/115	-
30	PHO	D	401	-	-	4/37/103/103	0/5/6/6
46	CHL	Y	306	24	-	5/17/93/117	-
29	CLA	b	505	2	-	9/39/115/115	-
36	DGD	c	517	-	-	17/51/91/95	0/2/2/2
48	NEX	S	319	-	-	2/27/83/83	0/3/3/3
29	CLA	s	303	23	-	8/33/109/115	-
29	CLA	b	504	2	-	13/39/115/115	-
29	CLA	n	603	20	-	13/39/115/115	-
35	LMG	d	407	-	-	7/41/61/70	0/1/1/1
29	CLA	C	507	4	-	8/39/115/115	-
29	CLA	n	613	-	-	3/20/96/115	-
46	CHL	S	302	23	-	3/17/93/117	-
29	CLA	a	406	52	-	6/20/96/115	-
37	LHG	s	301	-	-	19/42/42/53	-
47	LUT	N	616	-	-	3/29/67/67	0/2/2/2
47	LUT	R	310	-	-	5/29/67/67	0/2/2/2
29	CLA	g	611	37	-	9/39/115/115	-
47	LUT	Y	317	-	-	2/29/67/67	0/2/2/2
29	CLA	n	602	20	-	12/39/115/115	-
47	LUT	N	615	-	-	3/29/67/67	0/2/2/2
29	CLA	Y	309	52	-	10/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	Y	315	24	-	15/39/115/115	-
29	CLA	b	512	2	-	10/39/115/115	-
29	CLA	G	614	-	-	9/20/96/115	-
29	CLA	a	408	1	-	8/33/109/115	-
47	LUT	S	318	-	-	3/29/67/67	0/2/2/2
33	3PH	a	415	-	-	25/49/49/49	-
47	LUT	s	317	-	-	4/29/67/67	0/2/2/2
46	CHL	y	308	52	-	3/23/99/117	-
29	CLA	G	603	21	-	11/39/115/115	-
29	CLA	Y	314	24	-	20/39/115/115	-
29	CLA	B	506	2	-	16/39/115/115	-
47	LUT	Y	316	-	-	2/29/67/67	0/2/2/2
46	CHL	s	302	23	-	4/17/93/117	-
51	LPX	S	321	-	-	7/21/21/31	-
29	CLA	Y	312	37	-	10/39/115/115	-
44	HEM	E	101	6,7	-	1/14/54/54	-
47	LUT	n	615	-	-	2/29/67/67	0/2/2/2
41	DGA	w	201	-	-	27/45/45/45	-
36	DGD	r	301	-	-	8/32/72/95	0/2/2/2
29	CLA	B	510	52	-	8/39/115/115	-
29	CLA	G	611	-	-	13/39/115/115	-
29	CLA	y	315	24	-	10/39/115/115	-
29	CLA	C	508	52	-	12/39/115/115	-
29	CLA	s	313	23	-	2/15/91/115	-
29	CLA	d	403	5	-	7/39/115/115	-
29	CLA	y	304	24	-	6/39/115/115	-
29	CLA	c	511	4	-	13/39/115/115	-
37	LHG	s	320	29	-	22/49/49/53	-
37	LHG	a	413	-	-	22/48/48/53	-
33	3PH	b	521	-	-	28/40/40/49	-
29	CLA	Y	311	24	-	5/39/115/115	-
29	CLA	S	311	23	-	10/39/115/115	-
29	CLA	A	405	-	-	12/39/115/115	-
47	LUT	G	615	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	XAT	N	619	-	2/2/12/26	1/31/93/93	0/4/4/4
46	CHL	N	608	-	-	6/22/98/117	-
29	CLA	c	505	4	-	18/39/115/115	-
46	CHL	Y	308	-	1/1/15/21	12/41/117/117	-
29	CLA	C	513	-	-	17/39/115/115	-
35	LMG	i	101	-	-	18/43/63/70	0/1/1/1
29	CLA	c	509	4	-	15/39/115/115	-
39	SQD	a	410	-	-	17/46/66/69	0/1/1/1
29	CLA	g	602	21	-	17/39/115/115	-
29	CLA	y	310	-	-	9/21/97/115	-
50	PTY	Y	320	-	-	12/20/20/53	-
29	CLA	C	505	52	-	10/27/103/115	-
29	CLA	a	405	52	-	16/39/115/115	-
29	CLA	S	314	23	-	13/27/103/115	-
48	NEX	N	617	-	-	2/27/83/83	1/3/3/3
29	CLA	c	506	-	-	9/33/109/115	-
29	CLA	G	604	-	-	10/20/96/115	-
29	CLA	R	301	22	-	7/33/109/115	-
31	BCR	K	101	-	-	11/29/63/63	0/2/2/2
29	CLA	C	504	-	-	12/39/115/115	-
29	CLA	B	515	2	-	10/39/115/115	-
29	CLA	r	303	22	-	14/33/109/115	-
29	CLA	S	315	23	-	9/21/97/115	-
31	BCR	C	516	-	-	10/29/63/63	0/2/2/2
46	CHL	n	608	20	1/1/15/21	7/41/117/117	-
29	CLA	B	508	2	-	7/39/115/115	-
46	CHL	s	308	-	-	0/14/90/117	-
46	CHL	N	606	-	1/1/15/21	9/41/117/117	-
29	CLA	Y	305	52	-	16/39/115/115	-
33	3PH	S	322	-	-	7/31/31/49	-
46	CHL	n	601	20	1/1/15/21	12/41/117/117	-
48	NEX	y	319	-	-	8/27/83/83	0/3/3/3
29	CLA	C	512	4	-	7/39/115/115	-
29	CLA	S	310	23	-	10/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	g	614	-	-	10/20/96/115	-
46	CHL	g	601	21	1/1/15/21	10/41/117/117	-

All (1462) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	H	101	RRX	C26-C25	15.61	1.61	1.34
45	h	101	RRX	C26-C25	15.51	1.61	1.34
34	B	519	C7Z	C25-C26	15.39	1.61	1.34
34	b	519	C7Z	C25-C26	15.36	1.61	1.34
34	B	519	C7Z	C5-C6	14.83	1.60	1.34
34	b	519	C7Z	C5-C6	14.79	1.60	1.34
45	h	101	RRX	C5-C6	14.78	1.60	1.34
45	H	101	RRX	C5-C6	14.77	1.60	1.34
47	r	311	LUT	C24-C25	14.73	1.51	1.33
47	G	615	LUT	C24-C25	14.58	1.51	1.33
47	y	317	LUT	C24-C25	14.55	1.51	1.33
47	Y	316	LUT	C24-C25	14.55	1.51	1.33
47	N	615	LUT	C24-C25	14.52	1.51	1.33
47	g	616	LUT	C24-C25	14.51	1.51	1.33
47	Y	317	LUT	C24-C25	14.48	1.51	1.33
47	s	317	LUT	C24-C25	14.45	1.51	1.33
47	R	310	LUT	C24-C25	14.45	1.51	1.33
47	y	318	LUT	C24-C25	14.41	1.51	1.33
47	N	616	LUT	C24-C25	14.41	1.51	1.33
47	G	616	LUT	C24-C25	14.41	1.51	1.33
47	n	614	LUT	C24-C25	14.36	1.51	1.33
47	n	615	LUT	C24-C25	14.25	1.50	1.33
47	g	615	LUT	C24-C25	14.19	1.50	1.33
47	S	318	LUT	C24-C25	14.12	1.50	1.33
47	s	318	LUT	C24-C25	14.02	1.50	1.33
47	S	317	LUT	C24-C25	13.79	1.50	1.33
29	D	404	CLA	C4B-NB	-11.69	1.23	1.37
34	B	519	C7Z	C24-C23	11.53	1.72	1.52
34	b	519	C7Z	C24-C23	11.41	1.72	1.52
29	D	404	CLA	C3D-C4D	-11.02	1.19	1.44
34	B	519	C7Z	C2-C3	-10.64	1.37	1.52
34	b	519	C7Z	C22-C23	-10.60	1.37	1.52
34	B	519	C7Z	C22-C23	-10.50	1.37	1.52
45	H	101	RRX	C29-C28	-10.47	1.37	1.52
45	h	101	RRX	C29-C28	-10.40	1.37	1.52
34	b	519	C7Z	C2-C3	-10.38	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	404	CLA	C1B-NB	-9.66	1.25	1.37
30	d	402	PHO	C1B-C2B	9.11	1.49	1.39
30	D	401	PHO	C1B-C2B	9.08	1.49	1.39
30	A	408	PHO	C1B-C2B	9.00	1.49	1.39
30	a	407	PHO	C1B-C2B	8.66	1.49	1.39
34	b	519	C7Z	C4-C3	8.32	1.66	1.52
34	B	519	C7Z	C4-C3	8.27	1.66	1.52
45	h	101	RRX	C27-C28	7.93	1.66	1.52
45	H	101	RRX	C27-C28	7.91	1.66	1.52
30	D	401	PHO	C3B-C4B	7.74	1.50	1.41
48	R	312	NEX	C30-C29	-7.63	1.25	1.35
48	g	617	NEX	C10-C9	-7.62	1.25	1.35
48	n	616	NEX	C34-C33	-7.58	1.25	1.35
48	n	616	NEX	C14-C13	-7.58	1.25	1.35
48	s	319	NEX	C14-C13	-7.56	1.25	1.35
30	A	408	PHO	C3B-C4B	7.52	1.50	1.41
30	d	402	PHO	C3B-C4B	7.51	1.50	1.41
48	n	616	NEX	C10-C9	-7.50	1.25	1.35
48	Y	318	NEX	C30-C29	-7.47	1.25	1.35
48	s	319	NEX	C34-C33	-7.47	1.25	1.35
48	N	617	NEX	C14-C13	-7.47	1.25	1.35
48	r	313	NEX	C34-C33	-7.47	1.25	1.35
48	r	313	NEX	C30-C29	-7.46	1.25	1.35
48	S	319	NEX	C14-C13	-7.46	1.25	1.35
48	N	617	NEX	C34-C33	-7.45	1.25	1.35
48	g	617	NEX	C14-C13	-7.44	1.25	1.35
48	n	616	NEX	C30-C29	-7.43	1.25	1.35
48	R	312	NEX	C34-C33	-7.42	1.25	1.35
48	N	617	NEX	C30-C29	-7.41	1.26	1.35
48	s	319	NEX	C30-C29	-7.40	1.26	1.35
48	s	319	NEX	C10-C9	-7.39	1.26	1.35
48	G	617	NEX	C34-C33	-7.38	1.26	1.35
48	Y	318	NEX	C34-C33	-7.37	1.26	1.35
48	S	319	NEX	C30-C29	-7.36	1.26	1.35
48	g	617	NEX	C30-C29	-7.36	1.26	1.35
48	G	617	NEX	C14-C13	-7.35	1.26	1.35
48	S	319	NEX	C34-C33	-7.35	1.26	1.35
48	Y	318	NEX	C14-C13	-7.34	1.26	1.35
48	G	617	NEX	C10-C9	-7.34	1.26	1.35
29	D	404	CLA	O1D-CGD	-7.32	1.02	1.21
48	y	319	NEX	C14-C13	-7.32	1.26	1.35
48	y	319	NEX	C34-C33	-7.32	1.26	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	y	319	NEX	C30-C29	-7.32	1.26	1.35
48	S	319	NEX	C10-C9	-7.31	1.26	1.35
48	N	617	NEX	C10-C9	-7.31	1.26	1.35
30	a	407	PHO	C3B-C4B	7.31	1.49	1.41
48	G	617	NEX	C30-C29	-7.30	1.26	1.35
48	y	319	NEX	C10-C9	-7.28	1.26	1.35
48	Y	318	NEX	C10-C9	-7.22	1.26	1.35
48	g	617	NEX	C34-C33	-7.21	1.26	1.35
31	v	101	BCR	C10-C9	7.08	1.45	1.35
31	K	101	BCR	C10-C9	7.07	1.45	1.35
31	F	101	BCR	C10-C9	7.00	1.45	1.35
31	z	101	BCR	C10-C9	6.91	1.44	1.35
48	n	616	NEX	C35-C15	-6.85	1.18	1.36
31	f	101	BCR	C10-C9	6.83	1.44	1.35
48	s	319	NEX	C35-C15	-6.80	1.18	1.36
48	R	312	NEX	C35-C15	-6.79	1.18	1.36
48	N	617	NEX	C35-C15	-6.78	1.18	1.36
48	r	313	NEX	C35-C15	-6.76	1.18	1.36
48	S	319	NEX	C35-C15	-6.75	1.18	1.36
48	g	617	NEX	C35-C15	-6.73	1.18	1.36
31	b	517	BCR	C10-C9	6.73	1.44	1.35
48	Y	318	NEX	C35-C15	-6.71	1.18	1.36
48	G	617	NEX	C35-C15	-6.71	1.18	1.36
48	y	319	NEX	C35-C15	-6.71	1.18	1.36
31	C	517	BCR	C10-C9	6.70	1.44	1.35
31	c	515	BCR	C10-C9	6.66	1.44	1.35
31	C	515	BCR	C10-C9	6.56	1.44	1.35
31	C	516	BCR	C10-C9	6.54	1.44	1.35
31	B	517	BCR	C10-C9	6.52	1.44	1.35
45	H	101	RRX	C2-C3	-6.50	1.36	1.52
45	h	101	RRX	C2-C3	-6.47	1.36	1.52
31	A	410	BCR	C10-C9	6.43	1.44	1.35
31	B	518	BCR	C10-C9	6.42	1.44	1.35
31	b	518	BCR	C10-C9	6.41	1.44	1.35
31	c	514	BCR	C10-C9	6.33	1.44	1.35
48	n	616	NEX	C11-C12	-6.32	1.18	1.34
48	s	319	NEX	C11-C12	-6.32	1.18	1.34
48	s	319	NEX	C31-C32	-6.31	1.18	1.34
48	n	616	NEX	C31-C32	-6.29	1.18	1.34
48	S	319	NEX	C31-C32	-6.29	1.18	1.34
48	R	312	NEX	C31-C32	-6.28	1.18	1.34
31	a	409	BCR	C10-C9	6.27	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	G	617	NEX	C11-C12	-6.24	1.18	1.34
48	Y	318	NEX	C31-C32	-6.23	1.18	1.34
48	y	319	NEX	C31-C32	-6.23	1.18	1.34
48	r	313	NEX	C31-C32	-6.22	1.18	1.34
48	y	319	NEX	C11-C12	-6.22	1.18	1.34
29	D	404	CLA	C1C-C2C	-6.21	1.32	1.44
48	g	617	NEX	C31-C32	-6.21	1.18	1.34
48	g	617	NEX	C11-C12	-6.21	1.18	1.34
48	N	617	NEX	C11-C12	-6.21	1.18	1.34
48	N	617	NEX	C31-C32	-6.20	1.18	1.34
48	S	319	NEX	C11-C12	-6.19	1.18	1.34
48	Y	318	NEX	C11-C12	-6.19	1.18	1.34
48	G	617	NEX	C31-C32	-6.13	1.18	1.34
29	D	404	CLA	C1C-NC	-6.05	1.28	1.37
45	H	101	RRX	C1-C6	-5.95	1.45	1.53
45	h	101	RRX	C1-C6	-5.90	1.45	1.53
31	F	101	BCR	C24-C23	5.73	1.50	1.33
31	v	101	BCR	C24-C23	5.72	1.50	1.33
31	K	101	BCR	C24-C23	5.69	1.50	1.33
31	b	518	BCR	C24-C23	5.67	1.50	1.33
31	f	101	BCR	C24-C23	5.67	1.50	1.33
31	B	518	BCR	C24-C23	5.66	1.50	1.33
48	s	319	NEX	C7-C8	5.61	1.41	1.32
31	c	515	BCR	C24-C23	5.59	1.50	1.33
31	C	517	BCR	C24-C23	5.57	1.49	1.33
31	b	518	BCR	C11-C12	-5.56	1.20	1.34
31	B	518	BCR	C11-C12	-5.56	1.20	1.34
31	a	409	BCR	C11-C12	-5.54	1.20	1.34
31	C	515	BCR	C24-C23	5.54	1.49	1.33
31	z	101	BCR	C24-C23	5.53	1.49	1.33
34	b	519	C7Z	C12-C13	5.53	1.57	1.45
31	c	514	BCR	C11-C12	-5.51	1.20	1.34
31	A	410	BCR	C24-C23	5.50	1.49	1.33
31	a	409	BCR	C24-C23	5.48	1.49	1.33
31	C	516	BCR	C24-C23	5.47	1.49	1.33
31	A	410	BCR	C11-C12	-5.47	1.20	1.34
48	S	319	NEX	C7-C8	5.47	1.41	1.32
48	N	617	NEX	C7-C8	5.47	1.41	1.32
34	B	519	C7Z	C12-C13	5.46	1.57	1.45
31	B	517	BCR	C11-C12	-5.45	1.20	1.34
29	D	404	CLA	C4D-ND	-5.45	1.30	1.37
48	Y	318	NEX	C7-C8	5.45	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	y	319	NEX	C7-C8	5.44	1.41	1.32
31	c	515	BCR	C11-C12	-5.41	1.20	1.34
31	C	517	BCR	C11-C12	-5.41	1.20	1.34
45	H	101	RRX	C30-C25	-5.39	1.46	1.53
31	b	517	BCR	C11-C12	-5.38	1.20	1.34
31	C	515	BCR	C11-C12	-5.38	1.20	1.34
31	c	514	BCR	C24-C23	5.37	1.49	1.33
48	G	617	NEX	C7-C8	5.36	1.40	1.32
31	B	517	BCR	C24-C23	5.34	1.49	1.33
34	b	519	C7Z	C24-C25	-5.33	1.42	1.51
48	S	319	NEX	C28-C29	-5.33	1.34	1.45
45	h	101	RRX	C30-C25	-5.33	1.46	1.53
31	C	516	BCR	C11-C12	-5.30	1.20	1.34
48	n	616	NEX	C7-C8	5.29	1.40	1.32
31	z	101	BCR	C11-C12	-5.29	1.21	1.34
31	b	517	BCR	C24-C23	5.28	1.49	1.33
34	B	519	C7Z	C24-C25	-5.27	1.42	1.51
48	s	319	NEX	C28-C29	-5.27	1.34	1.45
48	r	313	NEX	C28-C29	-5.27	1.34	1.45
48	R	312	NEX	C28-C29	-5.26	1.34	1.45
34	b	519	C7Z	C1-C6	-5.26	1.46	1.53
31	f	101	BCR	C11-C12	-5.24	1.21	1.34
48	g	617	NEX	C28-C29	-5.23	1.34	1.45
48	Y	318	NEX	C28-C29	-5.23	1.34	1.45
31	F	101	BCR	C11-C12	-5.20	1.21	1.34
48	n	616	NEX	C28-C29	-5.18	1.34	1.45
31	K	101	BCR	C11-C12	-5.16	1.21	1.34
48	G	617	NEX	C28-C29	-5.16	1.34	1.45
45	h	101	RRX	C2-C1	5.15	1.66	1.54
48	y	319	NEX	C28-C29	-5.15	1.34	1.45
31	v	101	BCR	C11-C12	-5.14	1.21	1.34
48	N	617	NEX	C28-C29	-5.10	1.35	1.45
45	H	101	RRX	C2-C1	5.10	1.65	1.54
29	D	404	CLA	C2A-C1A	-5.05	1.40	1.52
45	h	101	RRX	C19-C18	5.05	1.56	1.45
34	B	519	C7Z	C1-C6	-5.05	1.46	1.53
29	D	404	CLA	C4C-C3C	-5.01	1.36	1.45
45	H	101	RRX	C19-C18	4.97	1.56	1.45
48	g	617	NEX	C7-C8	4.88	1.40	1.32
43	D	406	PL9	C7-C3	-4.73	1.46	1.51
45	h	101	RRX	C8-C9	4.72	1.56	1.45
34	b	519	C7Z	C28-C29	4.70	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	409	BCR	C16-C17	-4.65	1.29	1.43
34	B	519	C7Z	C28-C29	4.65	1.55	1.45
45	H	101	RRX	C8-C9	4.63	1.55	1.45
31	A	410	BCR	C16-C17	-4.63	1.29	1.43
31	c	514	BCR	C16-C17	-4.63	1.29	1.43
31	B	517	BCR	C16-C17	-4.57	1.29	1.43
31	B	518	BCR	C16-C17	-4.56	1.29	1.43
29	D	404	CLA	CHB-C4A	-4.56	1.27	1.37
31	b	518	BCR	C16-C17	-4.54	1.29	1.43
31	C	517	BCR	C16-C17	-4.50	1.29	1.43
31	c	515	BCR	C16-C17	-4.50	1.29	1.43
31	C	516	BCR	C16-C17	-4.50	1.29	1.43
34	b	519	C7Z	C32-C33	4.50	1.55	1.45
31	b	517	BCR	C16-C17	-4.49	1.29	1.43
29	D	404	CLA	O2D-CED	-4.48	1.34	1.45
34	B	519	C7Z	C4-C5	-4.48	1.44	1.51
34	B	519	C7Z	C32-C33	4.47	1.55	1.45
29	D	404	CLA	OBD-CAD	-4.45	1.14	1.22
34	b	519	C7Z	C4-C5	-4.45	1.44	1.51
45	h	101	RRX	C12-C13	4.44	1.55	1.45
31	C	515	BCR	C16-C17	-4.43	1.29	1.43
31	F	101	BCR	C16-C17	-4.41	1.29	1.43
31	z	101	BCR	C16-C17	-4.40	1.29	1.43
45	h	101	RRX	C27-C26	-4.36	1.44	1.51
31	v	101	BCR	C16-C17	-4.36	1.29	1.43
46	G	607	CHL	CBB-CAB	4.32	1.51	1.30
46	Y	302	CHL	CBB-CAB	4.30	1.51	1.30
31	K	101	BCR	C16-C17	-4.30	1.30	1.43
45	H	101	RRX	C12-C13	4.30	1.55	1.45
46	G	605	CHL	CBB-CAB	4.30	1.51	1.30
46	n	608	CHL	CBB-CAB	4.30	1.51	1.30
45	H	101	RRX	C27-C26	-4.29	1.44	1.51
46	g	605	CHL	CBB-CAB	4.28	1.51	1.30
36	B	521	DGD	O1G-C1A	4.28	1.45	1.33
46	N	608	CHL	CBB-CAB	4.27	1.51	1.30
46	g	607	CHL	CBB-CAB	4.26	1.51	1.30
46	g	608	CHL	CBB-CAB	4.26	1.51	1.30
36	C	518	DGD	O1G-C1A	4.25	1.45	1.33
31	f	101	BCR	C16-C17	-4.25	1.30	1.43
46	y	303	CHL	CBB-CAB	4.25	1.51	1.30
46	Y	306	CHL	CBB-CAB	4.24	1.51	1.30
36	c	516	DGD	O1G-C1A	4.24	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	y	307	CHL	CBB-CAB	4.24	1.51	1.30
36	r	301	DGD	O1G-C1A	4.24	1.45	1.33
46	n	601	CHL	CBB-CAB	4.24	1.51	1.30
46	N	609	CHL	CBB-CAB	4.24	1.51	1.30
46	s	307	CHL	CBB-CAB	4.23	1.51	1.30
46	y	311	CHL	CBB-CAB	4.23	1.51	1.30
46	N	601	CHL	CBB-CAB	4.23	1.51	1.30
46	g	601	CHL	CBB-CAB	4.23	1.51	1.30
46	Y	310	CHL	CBB-CAB	4.23	1.51	1.30
46	n	607	CHL	CBB-CAB	4.23	1.51	1.30
45	H	101	RRX	C3-C4	4.23	1.65	1.52
46	G	601	CHL	CBB-CAB	4.23	1.51	1.30
45	h	101	RRX	C3-C4	4.22	1.65	1.52
46	G	609	CHL	CBB-CAB	4.22	1.51	1.30
46	g	609	CHL	CBB-CAB	4.21	1.51	1.30
46	S	308	CHL	CBB-CAB	4.21	1.51	1.30
46	N	605	CHL	CBB-CAB	4.20	1.51	1.30
36	C	520	DGD	O1G-C1A	4.19	1.45	1.33
46	n	605	CHL	CBB-CAB	4.17	1.50	1.30
46	S	309	CHL	CBB-CAB	4.16	1.50	1.30
46	Y	308	CHL	CBB-CAB	4.16	1.50	1.30
34	b	519	C7Z	C31-C30	4.16	1.56	1.43
36	C	519	DGD	O1G-C1A	4.14	1.45	1.33
46	s	309	CHL	CBB-CAB	4.13	1.50	1.30
46	y	301	CHL	CBB-CAB	4.12	1.50	1.30
46	R	304	CHL	CBB-CAB	4.10	1.50	1.30
46	y	309	CHL	CBB-CAB	4.10	1.50	1.30
34	B	519	C7Z	C31-C30	4.10	1.56	1.43
36	c	518	DGD	O1G-C1A	4.10	1.45	1.33
34	b	519	C7Z	C11-C10	4.10	1.56	1.43
46	R	305	CHL	CBB-CAB	4.08	1.50	1.30
46	S	307	CHL	CBB-CAB	4.08	1.50	1.30
30	D	401	PHO	C1D-C2D	4.07	1.44	1.39
34	b	519	C7Z	C8-C9	4.07	1.54	1.45
36	c	517	DGD	O1G-C1A	4.06	1.45	1.33
46	r	305	CHL	CBB-CAB	4.06	1.50	1.30
46	G	608	CHL	CBB-CAB	4.06	1.50	1.30
46	s	308	CHL	CBB-CAB	4.05	1.50	1.30
46	r	306	CHL	CBB-CAB	4.05	1.50	1.30
46	g	606	CHL	CBB-CAB	4.04	1.50	1.30
34	B	519	C7Z	C11-C10	4.03	1.55	1.43
34	B	519	C7Z	C8-C9	4.03	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	h	101	RRX	C20-C21	4.01	1.55	1.43
46	n	606	CHL	CBB-CAB	4.00	1.50	1.30
46	N	607	CHL	CBB-CAB	3.99	1.50	1.30
46	G	606	CHL	CBB-CAB	3.97	1.50	1.30
46	s	302	CHL	CBB-CAB	3.96	1.49	1.30
46	Y	307	CHL	CBB-CAB	3.95	1.49	1.30
46	N	606	CHL	CBB-CAB	3.94	1.49	1.30
43	d	405	PL9	C7-C3	-3.91	1.47	1.51
45	H	101	RRX	C20-C21	3.91	1.55	1.43
30	d	402	PHO	C1D-C2D	3.91	1.43	1.39
46	S	302	CHL	CBB-CAB	3.90	1.49	1.30
30	A	408	PHO	C1D-C2D	3.88	1.43	1.39
43	D	406	PL9	C3-C4	-3.88	1.43	1.49
34	b	519	C7Z	C22-C21	3.87	1.67	1.54
29	G	603	CLA	C1D-ND	3.87	1.42	1.37
29	N	614	CLA	C1D-ND	3.85	1.42	1.37
46	y	308	CHL	CBB-CAB	3.85	1.49	1.30
34	B	519	C7Z	C22-C21	3.84	1.66	1.54
29	N	603	CLA	C1D-ND	3.80	1.42	1.37
45	h	101	RRX	C15-C14	3.80	1.55	1.43
29	C	506	CLA	C4D-ND	-3.79	1.32	1.37
29	C	514	CLA	C1D-ND	3.77	1.42	1.37
29	d	403	CLA	C4D-ND	-3.76	1.32	1.37
48	r	313	NEX	C14-C13	-3.76	1.26	1.35
48	R	312	NEX	C14-C13	-3.75	1.26	1.35
29	N	611	CLA	C1D-ND	3.75	1.42	1.37
45	H	101	RRX	C15-C14	3.75	1.55	1.43
29	r	308	CLA	C4D-ND	-3.74	1.32	1.37
45	h	101	RRX	C23-C22	3.74	1.54	1.45
29	s	316	CLA	C1D-ND	3.74	1.42	1.37
29	S	316	CLA	C1D-ND	3.73	1.42	1.37
29	S	315	CLA	C4D-ND	-3.73	1.32	1.37
29	a	406	CLA	C4D-ND	-3.73	1.32	1.37
29	B	509	CLA	C4D-ND	-3.73	1.32	1.37
29	G	604	CLA	C1D-ND	3.71	1.42	1.37
29	y	313	CLA	C1D-ND	3.70	1.42	1.37
29	a	404	CLA	C4D-ND	-3.70	1.32	1.37
29	g	614	CLA	C1D-ND	3.69	1.42	1.37
29	g	611	CLA	C1D-ND	3.69	1.42	1.37
29	B	513	CLA	C4D-ND	-3.69	1.32	1.37
29	S	314	CLA	C1D-ND	3.68	1.42	1.37
29	r	304	CLA	C1D-ND	3.68	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	404	CLA	O2A-C1	-3.67	1.35	1.46
29	G	612	CLA	C1D-ND	3.67	1.42	1.37
29	B	516	CLA	C4D-ND	-3.66	1.32	1.37
29	C	512	CLA	C1D-ND	3.66	1.42	1.37
44	E	101	HEM	FE-NA	3.66	2.07	1.95
29	R	306	CLA	C4D-ND	-3.66	1.32	1.37
29	b	516	CLA	C4D-ND	-3.66	1.32	1.37
29	C	502	CLA	C1D-ND	3.66	1.42	1.37
29	Y	309	CLA	C4D-ND	-3.65	1.32	1.37
29	G	611	CLA	C1D-ND	3.65	1.42	1.37
29	s	310	CLA	C1D-ND	3.65	1.42	1.37
29	r	310	CLA	C1D-ND	3.65	1.42	1.37
29	R	307	CLA	C4D-ND	-3.65	1.32	1.37
29	y	304	CLA	C1D-ND	3.65	1.42	1.37
29	b	513	CLA	C4D-ND	-3.65	1.32	1.37
29	c	503	CLA	C4D-ND	-3.64	1.32	1.37
29	B	514	CLA	C4D-ND	-3.64	1.32	1.37
45	H	101	RRX	C23-C22	3.64	1.53	1.45
29	Y	304	CLA	C1D-ND	3.64	1.42	1.37
29	s	312	CLA	C1D-ND	3.63	1.42	1.37
29	y	316	CLA	C4D-ND	-3.62	1.32	1.37
29	n	603	CLA	C1D-ND	3.62	1.42	1.37
29	y	315	CLA	C1D-ND	3.62	1.42	1.37
29	S	312	CLA	C1D-ND	3.62	1.42	1.37
29	S	305	CLA	C1D-ND	3.62	1.42	1.37
29	a	405	CLA	C4D-ND	-3.61	1.32	1.37
29	n	613	CLA	C4D-ND	-3.61	1.32	1.37
29	s	314	CLA	C1D-ND	3.61	1.42	1.37
29	c	505	CLA	C4D-ND	-3.61	1.32	1.37
30	a	407	PHO	C1D-C2D	3.60	1.43	1.39
29	R	309	CLA	C1D-ND	3.60	1.42	1.37
29	b	514	CLA	C1D-ND	3.60	1.42	1.37
29	B	514	CLA	C1D-ND	3.59	1.42	1.37
29	Y	312	CLA	C1D-ND	3.59	1.42	1.37
29	n	612	CLA	C1D-ND	3.59	1.42	1.37
29	B	508	CLA	C1D-ND	3.59	1.42	1.37
29	C	504	CLA	C1D-ND	3.59	1.42	1.37
29	Y	314	CLA	C1D-ND	3.59	1.42	1.37
41	D	402	DGA	OG2-CB1	3.59	1.44	1.34
29	y	310	CLA	C4D-ND	-3.58	1.32	1.37
29	c	513	CLA	C1D-ND	3.58	1.42	1.37
29	r	307	CLA	C4D-ND	-3.58	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	n	610	CLA	C1D-ND	3.58	1.42	1.37
29	b	514	CLA	C4D-ND	-3.58	1.32	1.37
29	c	502	CLA	C4D-ND	-3.57	1.32	1.37
29	b	505	CLA	C4D-ND	-3.57	1.32	1.37
29	N	613	CLA	C1D-ND	3.57	1.42	1.37
29	b	515	CLA	C1D-ND	3.57	1.42	1.37
29	C	509	CLA	C4D-ND	-3.57	1.32	1.37
29	g	613	CLA	C1D-ND	3.57	1.42	1.37
29	D	405	CLA	C1D-ND	3.57	1.42	1.37
29	b	502	CLA	C4D-ND	-3.57	1.32	1.37
29	c	511	CLA	C1D-ND	3.56	1.42	1.37
34	b	519	C7Z	C15-C14	3.56	1.54	1.43
29	c	507	CLA	C4D-ND	-3.56	1.32	1.37
41	b	522	DGA	OG2-CB1	3.56	1.44	1.34
29	Y	303	CLA	C1D-ND	3.56	1.42	1.37
29	n	602	CLA	C1D-ND	3.56	1.42	1.37
44	E	101	HEM	FE-NB	3.55	2.05	1.94
29	G	602	CLA	C1D-ND	3.55	1.42	1.37
29	N	602	CLA	C4D-ND	-3.55	1.32	1.37
29	G	602	CLA	C4D-ND	-3.55	1.32	1.37
29	b	509	CLA	C4D-ND	-3.55	1.32	1.37
29	C	505	CLA	C1D-ND	3.55	1.42	1.37
29	B	511	CLA	C4D-ND	-3.55	1.32	1.37
29	G	610	CLA	C1D-ND	3.55	1.42	1.37
29	B	506	CLA	C1D-ND	3.54	1.42	1.37
29	R	302	CLA	C1D-ND	3.54	1.42	1.37
43	d	405	PL9	C3-C4	-3.54	1.43	1.49
29	c	510	CLA	C4D-ND	-3.54	1.32	1.37
29	g	603	CLA	C1D-ND	3.54	1.42	1.37
29	S	306	CLA	C1D-ND	3.54	1.42	1.37
29	B	504	CLA	C1D-ND	3.54	1.42	1.37
29	d	404	CLA	C1D-ND	3.54	1.42	1.37
29	B	515	CLA	C1D-ND	3.54	1.42	1.37
29	S	313	CLA	C1D-ND	3.53	1.42	1.37
29	r	303	CLA	C1D-ND	3.53	1.42	1.37
29	n	611	CLA	C1D-ND	3.53	1.42	1.37
29	A	406	CLA	C1D-ND	3.53	1.42	1.37
29	g	602	CLA	C1D-ND	3.53	1.42	1.37
29	y	305	CLA	C1D-ND	3.52	1.42	1.37
29	S	310	CLA	C1D-ND	3.52	1.42	1.37
34	B	519	C7Z	C7-C6	3.52	1.57	1.45
34	b	519	C7Z	C2-C1	3.51	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	R	301	CLA	C1D-ND	3.51	1.42	1.37
29	C	510	CLA	C1D-ND	3.51	1.42	1.37
29	b	511	CLA	C4D-ND	-3.51	1.32	1.37
29	s	306	CLA	C1D-ND	3.51	1.42	1.37
29	S	311	CLA	C1D-ND	3.51	1.42	1.37
29	B	507	CLA	C4D-ND	-3.50	1.32	1.37
29	g	612	CLA	C1D-ND	3.50	1.42	1.37
29	B	505	CLA	C4D-ND	-3.50	1.32	1.37
29	C	504	CLA	C4D-ND	-3.50	1.32	1.37
29	b	508	CLA	C1D-ND	3.50	1.42	1.37
29	S	303	CLA	C4D-ND	-3.50	1.32	1.37
29	c	506	CLA	C4D-ND	-3.50	1.32	1.37
29	G	614	CLA	C1D-ND	3.50	1.42	1.37
29	c	501	CLA	C1D-ND	3.50	1.42	1.37
29	b	507	CLA	C4D-ND	-3.50	1.32	1.37
29	B	512	CLA	C4D-ND	-3.50	1.32	1.37
29	r	308	CLA	C1D-ND	3.50	1.42	1.37
29	S	316	CLA	C4D-ND	-3.49	1.32	1.37
29	n	602	CLA	C4D-ND	-3.49	1.32	1.37
29	n	609	CLA	C4D-ND	-3.49	1.32	1.37
29	y	310	CLA	C1D-ND	3.49	1.42	1.37
41	J	101	DGA	OG2-CB1	3.49	1.44	1.34
29	c	504	CLA	C4D-ND	-3.49	1.32	1.37
29	c	508	CLA	C4D-ND	-3.49	1.32	1.37
29	N	612	CLA	C1D-ND	3.49	1.42	1.37
29	A	405	CLA	C4D-ND	-3.48	1.32	1.37
29	g	603	CLA	C4D-ND	-3.48	1.32	1.37
29	r	302	CLA	C4D-ND	-3.48	1.32	1.37
29	N	610	CLA	C1D-ND	3.48	1.42	1.37
29	b	510	CLA	C1D-ND	3.48	1.42	1.37
29	n	604	CLA	C1D-ND	3.48	1.42	1.37
29	a	408	CLA	C4D-ND	-3.48	1.32	1.37
29	C	510	CLA	C4D-ND	-3.47	1.32	1.37
29	B	501	CLA	C1D-ND	3.47	1.42	1.37
45	h	101	RRX	C11-C10	3.47	1.54	1.43
29	r	303	CLA	C4D-ND	-3.47	1.32	1.37
29	C	503	CLA	C1D-ND	3.47	1.42	1.37
29	C	508	CLA	C4D-ND	-3.47	1.32	1.37
34	B	519	C7Z	C15-C14	3.47	1.54	1.43
29	Y	315	CLA	C4D-ND	-3.47	1.32	1.37
29	c	509	CLA	C1D-ND	3.47	1.42	1.37
29	s	315	CLA	C1D-ND	3.47	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	n	603	CLA	C4D-ND	-3.47	1.32	1.37
29	D	405	CLA	C4D-ND	-3.47	1.32	1.37
34	B	519	C7Z	C2-C1	3.47	1.65	1.54
29	c	503	CLA	C1D-ND	3.46	1.42	1.37
29	s	313	CLA	C1D-ND	3.46	1.42	1.37
29	G	613	CLA	C1D-ND	3.46	1.42	1.37
29	s	311	CLA	C1D-ND	3.46	1.42	1.37
29	b	512	CLA	C4D-ND	-3.46	1.32	1.37
29	c	505	CLA	C1D-ND	3.46	1.42	1.37
29	B	502	CLA	C4D-ND	-3.45	1.32	1.37
29	r	309	CLA	C1D-ND	3.45	1.42	1.37
29	c	509	CLA	C4D-ND	-3.45	1.33	1.37
29	S	303	CLA	C1D-ND	3.45	1.42	1.37
34	b	519	C7Z	C7-C6	3.45	1.57	1.45
29	s	303	CLA	C1D-ND	3.44	1.42	1.37
29	A	409	CLA	C4D-ND	-3.44	1.33	1.37
29	B	510	CLA	C1D-ND	3.44	1.42	1.37
29	Y	305	CLA	C1D-ND	3.44	1.42	1.37
29	b	511	CLA	C1D-ND	3.44	1.42	1.37
29	A	407	CLA	C1D-ND	3.44	1.42	1.37
29	s	303	CLA	C4D-ND	-3.44	1.33	1.37
29	y	314	CLA	C4D-ND	-3.44	1.33	1.37
29	N	604	CLA	C1D-ND	3.43	1.42	1.37
29	R	309	CLA	C4D-ND	-3.43	1.33	1.37
29	s	315	CLA	C4D-ND	-3.43	1.33	1.37
29	G	604	CLA	C4D-ND	-3.43	1.33	1.37
29	Y	313	CLA	C1D-ND	3.43	1.42	1.37
29	b	503	CLA	C4D-ND	-3.43	1.33	1.37
29	b	506	CLA	C4D-ND	-3.43	1.33	1.37
29	Y	313	CLA	C4D-ND	-3.43	1.33	1.37
29	C	507	CLA	C1D-ND	3.43	1.42	1.37
29	r	302	CLA	C1D-ND	3.43	1.42	1.37
29	g	602	CLA	C4D-ND	-3.43	1.33	1.37
29	C	503	CLA	C4D-ND	-3.43	1.33	1.37
45	H	101	RRX	C11-C10	3.43	1.54	1.43
29	c	508	CLA	C1D-ND	3.42	1.42	1.37
29	S	304	CLA	C4D-ND	-3.42	1.33	1.37
41	j	101	DGA	OG2-CB1	3.42	1.43	1.34
29	A	407	CLA	C4D-ND	-3.42	1.33	1.37
29	n	611	CLA	C4D-ND	-3.42	1.33	1.37
29	C	508	CLA	C1D-ND	3.42	1.42	1.37
29	d	404	CLA	C4D-ND	-3.41	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	501	CLA	C1D-ND	3.41	1.42	1.37
34	b	519	C7Z	C27-C26	3.41	1.57	1.45
29	G	614	CLA	C4D-ND	-3.41	1.33	1.37
29	s	311	CLA	C4D-ND	-3.41	1.33	1.37
29	S	314	CLA	C4D-ND	-3.40	1.33	1.37
29	C	513	CLA	C1D-ND	3.40	1.42	1.37
29	R	307	CLA	C1D-ND	3.40	1.42	1.37
29	Y	315	CLA	C1D-ND	3.40	1.42	1.37
29	c	506	CLA	C1D-ND	3.40	1.42	1.37
29	B	503	CLA	C4D-ND	-3.40	1.33	1.37
34	B	519	C7Z	C27-C26	3.40	1.57	1.45
29	c	512	CLA	C4D-ND	-3.40	1.33	1.37
29	y	306	CLA	C1D-ND	3.39	1.42	1.37
34	b	519	C7Z	C35-C34	3.39	1.54	1.43
29	N	604	CLA	C4D-ND	-3.39	1.33	1.37
29	R	306	CLA	C1D-ND	3.39	1.42	1.37
29	g	604	CLA	C4D-ND	-3.39	1.33	1.37
29	y	312	CLA	C4D-ND	-3.39	1.33	1.37
29	c	507	CLA	C1D-ND	3.39	1.42	1.37
29	R	303	CLA	C4D-ND	-3.39	1.33	1.37
29	R	308	CLA	C4D-ND	-3.39	1.33	1.37
29	r	309	CLA	C4D-ND	-3.39	1.33	1.37
29	y	316	CLA	C1D-ND	3.39	1.41	1.37
29	g	610	CLA	C4D-ND	-3.38	1.33	1.37
29	y	313	CLA	C4D-ND	-3.38	1.33	1.37
29	R	308	CLA	C1D-ND	3.38	1.41	1.37
44	e	101	HEM	FE-ND	3.38	2.05	1.94
41	W	202	DGA	OG2-CB1	3.38	1.43	1.34
29	r	310	CLA	C4D-ND	-3.38	1.33	1.37
41	w	201	DGA	OG2-CB1	3.38	1.43	1.34
29	r	307	CLA	C1D-ND	3.38	1.41	1.37
29	n	609	CLA	C1D-ND	3.38	1.41	1.37
29	s	313	CLA	C4D-ND	-3.38	1.33	1.37
29	C	513	CLA	C4D-ND	-3.38	1.33	1.37
29	n	613	CLA	C1D-ND	3.38	1.41	1.37
29	b	510	CLA	C4D-ND	-3.38	1.33	1.37
29	N	602	CLA	C1D-ND	3.38	1.41	1.37
29	D	404	CLA	CAA-CBA	-3.37	1.42	1.52
29	A	409	CLA	C1D-ND	3.37	1.41	1.37
29	C	511	CLA	C1D-ND	3.37	1.41	1.37
29	s	304	CLA	C1D-ND	3.37	1.41	1.37
29	g	610	CLA	C1D-ND	3.37	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	y	305	CLA	C4D-ND	-3.37	1.33	1.37
29	g	604	CLA	C1D-ND	3.37	1.41	1.37
29	R	302	CLA	C4D-ND	-3.37	1.33	1.37
29	s	312	CLA	C4D-ND	-3.37	1.33	1.37
29	g	611	CLA	C4D-ND	-3.36	1.33	1.37
29	s	305	CLA	C4D-ND	-3.36	1.33	1.37
29	C	509	CLA	C1D-ND	3.35	1.41	1.37
29	B	510	CLA	C4D-ND	-3.35	1.33	1.37
29	a	405	CLA	C1D-ND	3.35	1.41	1.37
29	c	501	CLA	C4D-ND	-3.35	1.33	1.37
29	s	305	CLA	C1D-ND	3.35	1.41	1.37
29	D	404	CLA	C3B-C4B	-3.35	1.35	1.42
29	C	507	CLA	C4D-ND	-3.35	1.33	1.37
29	Y	311	CLA	C4D-ND	-3.35	1.33	1.37
35	b	520	LMG	C22-C21	-3.35	1.32	1.51
29	B	502	CLA	C1D-ND	3.34	1.41	1.37
29	Y	304	CLA	C4D-ND	-3.34	1.33	1.37
29	C	502	CLA	C4D-ND	-3.34	1.33	1.37
29	b	508	CLA	C4D-ND	-3.34	1.33	1.37
29	Y	309	CLA	C1D-ND	3.34	1.41	1.37
41	w	201	DGA	OG1-CA1	3.34	1.43	1.33
29	A	406	CLA	C4D-ND	-3.34	1.33	1.37
29	N	613	CLA	C4D-ND	-3.33	1.33	1.37
29	C	505	CLA	C4D-ND	-3.33	1.33	1.37
29	S	312	CLA	C4D-ND	-3.33	1.33	1.37
29	a	408	CLA	C1D-ND	3.33	1.41	1.37
34	B	519	C7Z	C35-C34	3.33	1.53	1.43
44	e	101	HEM	FE-NA	3.33	2.06	1.95
29	c	502	CLA	C1D-ND	3.33	1.41	1.37
29	S	311	CLA	C4D-ND	-3.33	1.33	1.37
29	c	512	CLA	C1D-ND	3.32	1.41	1.37
29	b	505	CLA	C1D-ND	3.32	1.41	1.37
29	B	506	CLA	C4D-ND	-3.32	1.33	1.37
29	R	301	CLA	C4D-ND	-3.32	1.33	1.37
29	G	612	CLA	C4D-ND	-3.32	1.33	1.37
29	Y	314	CLA	C4D-ND	-3.31	1.33	1.37
29	B	511	CLA	C1D-ND	3.31	1.41	1.37
29	Y	311	CLA	C1D-ND	3.31	1.41	1.37
29	S	306	CLA	C4D-ND	-3.31	1.33	1.37
29	B	516	CLA	C1D-ND	3.30	1.41	1.37
29	S	315	CLA	C1D-ND	3.30	1.41	1.37
29	g	612	CLA	C4D-ND	-3.30	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	518	DGD	CAB-C9B	-3.30	1.33	1.51
29	n	612	CLA	C4D-ND	-3.30	1.33	1.37
29	C	506	CLA	C1D-ND	3.30	1.41	1.37
29	y	312	CLA	C1D-ND	3.30	1.41	1.37
45	h	101	RRX	C16-C17	3.30	1.53	1.43
29	Y	312	CLA	C4D-ND	-3.30	1.33	1.37
29	B	508	CLA	C4D-ND	-3.29	1.33	1.37
29	S	305	CLA	C4D-ND	-3.29	1.33	1.37
29	Y	305	CLA	C4D-ND	-3.29	1.33	1.37
29	c	504	CLA	C1D-ND	3.29	1.41	1.37
41	J	101	DGA	OG1-CA1	3.29	1.42	1.33
29	S	310	CLA	C4D-ND	-3.29	1.33	1.37
35	B	520	LMG	C22-C21	-3.29	1.33	1.51
41	W	202	DGA	OG1-CA1	3.28	1.42	1.33
41	D	402	DGA	OG1-CA1	3.28	1.42	1.33
29	s	306	CLA	C4D-ND	-3.28	1.33	1.37
29	R	303	CLA	C1D-ND	3.28	1.41	1.37
29	B	509	CLA	C1D-ND	3.28	1.41	1.37
36	c	517	DGD	CAB-C9B	-3.28	1.33	1.51
41	j	101	DGA	OG1-CA1	3.27	1.42	1.33
35	c	520	LMG	C40-C39	-3.27	1.33	1.51
29	b	504	CLA	C1D-ND	3.27	1.41	1.37
29	y	314	CLA	C1D-ND	3.27	1.41	1.37
29	C	511	CLA	C4D-ND	-3.27	1.33	1.37
35	b	520	LMG	C19-C18	-3.27	1.33	1.51
29	b	509	CLA	C1D-ND	3.26	1.41	1.37
35	B	520	LMG	C19-C18	-3.26	1.33	1.51
35	c	519	LMG	C40-C39	-3.26	1.33	1.51
35	C	521	LMG	C40-C39	-3.26	1.33	1.51
29	S	313	CLA	C4D-ND	-3.26	1.33	1.37
29	b	516	CLA	C1D-ND	3.26	1.41	1.37
36	c	517	DGD	CDA-CCA	-3.26	1.33	1.51
29	a	406	CLA	C1D-ND	3.26	1.41	1.37
35	D	410	LMG	C19-C18	-3.26	1.33	1.51
29	b	502	CLA	C1D-ND	3.26	1.41	1.37
35	d	408	LMG	C19-C18	-3.25	1.33	1.51
30	d	402	PHO	C4D-CHA	3.25	1.44	1.39
29	Y	303	CLA	C4D-ND	-3.25	1.33	1.37
29	N	610	CLA	C4D-ND	-3.25	1.33	1.37
29	y	306	CLA	C4D-ND	-3.25	1.33	1.37
29	s	314	CLA	C4D-ND	-3.25	1.33	1.37
35	c	519	LMG	C22-C21	-3.24	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	521	LMG	C19-C18	-3.24	1.33	1.51
36	C	518	DGD	CDB-CCB	-3.24	1.33	1.51
35	c	519	LMG	C37-C36	-3.24	1.33	1.51
36	C	519	DGD	CAB-C9B	-3.24	1.33	1.51
29	G	611	CLA	C4D-ND	-3.23	1.33	1.37
35	c	520	LMG	C37-C36	-3.23	1.33	1.51
29	n	604	CLA	C4D-ND	-3.23	1.33	1.37
35	c	519	LMG	C19-C18	-3.23	1.33	1.51
35	D	409	LMG	C19-C18	-3.23	1.33	1.51
41	b	522	DGA	OG1-CA1	3.23	1.42	1.33
35	C	521	LMG	C37-C36	-3.23	1.33	1.51
35	C	522	LMG	C25-C24	-3.23	1.33	1.51
36	C	520	DGD	CAA-C9A	-3.23	1.33	1.51
29	B	503	CLA	C1D-ND	3.23	1.41	1.37
29	B	507	CLA	C1D-ND	3.23	1.41	1.37
29	b	512	CLA	C1D-ND	3.23	1.41	1.37
36	c	516	DGD	CDB-CCB	-3.23	1.33	1.51
30	D	401	PHO	C4D-CHA	3.22	1.44	1.39
34	B	519	C7Z	C21-C26	-3.22	1.49	1.53
36	c	518	DGD	CAA-C9A	-3.22	1.33	1.51
35	C	522	LMG	C22-C21	-3.22	1.33	1.51
29	c	510	CLA	C1D-ND	3.22	1.41	1.37
36	c	516	DGD	CAB-C9B	-3.22	1.33	1.51
36	c	517	DGD	CDB-CCB	-3.22	1.33	1.51
29	B	505	CLA	C1D-ND	3.22	1.41	1.37
29	N	611	CLA	C4D-ND	-3.22	1.33	1.37
29	G	610	CLA	C4D-ND	-3.22	1.33	1.37
35	C	524	LMG	C37-C36	-3.22	1.33	1.51
29	b	504	CLA	C4D-ND	-3.22	1.33	1.37
45	H	101	RRX	C16-C17	3.21	1.53	1.43
35	c	520	LMG	C43-C42	-3.21	1.33	1.51
35	c	520	LMG	C19-C18	-3.21	1.33	1.51
35	i	101	LMG	C37-C36	-3.21	1.33	1.51
35	C	522	LMG	C40-C39	-3.21	1.33	1.51
35	C	522	LMG	C37-C36	-3.21	1.33	1.51
36	C	519	DGD	CDB-CCB	-3.21	1.33	1.51
35	c	520	LMG	C22-C21	-3.21	1.33	1.51
29	b	506	CLA	C1D-ND	3.21	1.41	1.37
30	A	408	PHO	C4D-CHA	3.21	1.44	1.39
35	d	407	LMG	C19-C18	-3.20	1.33	1.51
36	C	518	DGD	CAB-C9B	-3.20	1.33	1.51
29	b	503	CLA	C1D-ND	3.20	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	s	304	CLA	C4D-ND	-3.20	1.33	1.37
34	B	519	C7Z	C38-C25	3.20	1.56	1.50
35	c	520	LMG	C25-C24	-3.20	1.33	1.51
35	i	101	LMG	C40-C39	-3.20	1.33	1.51
36	c	517	DGD	CAA-C9A	-3.20	1.33	1.51
35	w	202	LMG	C37-C36	-3.20	1.33	1.51
29	B	515	CLA	C3B-C4B	3.20	1.50	1.42
35	W	203	LMG	C37-C36	-3.20	1.33	1.51
29	g	613	CLA	C4D-ND	-3.19	1.33	1.37
29	y	315	CLA	C4D-ND	-3.19	1.33	1.37
29	g	614	CLA	C4D-ND	-3.19	1.33	1.37
35	i	101	LMG	C19-C18	-3.19	1.33	1.51
35	C	522	LMG	C43-C42	-3.19	1.33	1.51
35	D	410	LMG	C40-C39	-3.18	1.33	1.51
29	s	316	CLA	C4D-ND	-3.18	1.33	1.37
29	C	512	CLA	C4D-ND	-3.18	1.33	1.37
29	b	513	CLA	C1D-ND	3.18	1.41	1.37
35	D	410	LMG	C37-C36	-3.18	1.33	1.51
36	c	518	DGD	CDB-CCB	-3.18	1.33	1.51
29	N	612	CLA	C4D-ND	-3.18	1.33	1.37
29	A	405	CLA	C1D-ND	3.18	1.41	1.37
29	B	501	CLA	C4D-ND	-3.18	1.33	1.37
29	b	507	CLA	C1D-ND	3.18	1.41	1.37
29	G	613	CLA	C4D-ND	-3.17	1.33	1.37
35	d	408	LMG	C37-C36	-3.17	1.33	1.51
35	W	201	LMG	C19-C18	-3.17	1.33	1.51
29	y	304	CLA	C4D-ND	-3.17	1.33	1.37
29	D	404	CLA	O2A-CGA	3.17	1.42	1.33
29	b	501	CLA	C4D-ND	-3.17	1.33	1.37
35	d	408	LMG	C40-C39	-3.16	1.33	1.51
29	r	304	CLA	C4D-ND	-3.16	1.33	1.37
45	h	101	RRX	C24-C25	3.16	1.56	1.45
29	D	404	CLA	CAA-C2A	-3.16	1.48	1.54
29	n	610	CLA	C4D-ND	-3.15	1.33	1.37
35	d	407	LMG	C22-C21	-3.15	1.33	1.51
34	b	519	C7Z	C38-C25	3.15	1.56	1.50
45	H	101	RRX	C4-C5	-3.15	1.44	1.51
29	N	603	CLA	C4D-ND	-3.15	1.33	1.37
44	E	101	HEM	CAC-C3C	3.15	1.56	1.47
29	G	603	CLA	C4D-ND	-3.15	1.33	1.37
29	c	513	CLA	C4D-ND	-3.15	1.33	1.37
35	W	203	LMG	C40-C39	-3.14	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	512	CLA	C1D-ND	3.14	1.41	1.37
35	w	202	LMG	C40-C39	-3.14	1.33	1.51
29	s	310	CLA	C4D-ND	-3.14	1.33	1.37
35	C	522	LMG	C19-C18	-3.14	1.34	1.51
29	B	513	CLA	C1D-ND	3.13	1.41	1.37
29	C	514	CLA	C4D-ND	-3.12	1.33	1.37
29	c	511	CLA	C4D-ND	-3.12	1.33	1.37
46	y	309	CHL	C1B-NB	-3.12	1.33	1.37
29	B	504	CLA	C4D-ND	-3.12	1.33	1.37
46	n	608	CHL	C1B-NB	-3.12	1.34	1.37
29	b	515	CLA	C3B-C4B	3.11	1.50	1.42
29	b	515	CLA	C4D-ND	-3.09	1.33	1.37
45	H	101	RRX	C24-C25	3.09	1.56	1.45
45	h	101	RRX	C4-C5	-3.09	1.44	1.51
29	a	404	CLA	C1D-ND	3.08	1.41	1.37
44	e	101	HEM	CAC-C3C	3.08	1.55	1.47
34	b	519	C7Z	C21-C26	-3.08	1.49	1.53
46	y	301	CHL	C1B-NB	-3.06	1.34	1.37
29	S	310	CLA	C3B-C4B	3.06	1.49	1.42
44	E	101	HEM	CAB-C3B	3.06	1.55	1.47
45	h	101	RRX	C29-C30	3.05	1.64	1.54
29	r	307	CLA	C3B-C4B	3.05	1.49	1.42
29	B	515	CLA	C4D-ND	-3.05	1.33	1.37
44	e	101	HEM	CAB-C3B	3.05	1.55	1.47
29	N	614	CLA	C4D-ND	-3.03	1.33	1.37
29	B	501	CLA	C3B-C4B	3.03	1.49	1.42
29	N	612	CLA	C3B-C4B	3.02	1.49	1.42
29	r	309	CLA	C3B-C4B	3.02	1.49	1.42
46	n	606	CHL	C1B-NB	-3.02	1.34	1.37
29	G	603	CLA	C3B-C4B	3.01	1.49	1.42
30	a	407	PHO	C4D-CHA	3.01	1.44	1.39
29	s	312	CLA	C3B-C4B	3.00	1.49	1.42
29	G	610	CLA	C3B-C4B	3.00	1.49	1.42
29	Y	303	CLA	C3B-C4B	3.00	1.49	1.42
29	n	610	CLA	C3B-C4B	2.99	1.49	1.42
29	N	611	CLA	C3B-C4B	2.98	1.49	1.42
29	S	311	CLA	C3B-C4B	2.98	1.49	1.42
29	B	510	CLA	C3B-C4B	2.97	1.49	1.42
29	G	604	CLA	C3B-C4B	2.97	1.49	1.42
29	S	312	CLA	C3B-C4B	2.97	1.49	1.42
45	H	101	RRX	C29-C30	2.97	1.64	1.54
29	n	603	CLA	C3B-C4B	2.97	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	R	308	CLA	C3B-C4B	2.96	1.49	1.42
29	n	609	CLA	C3B-C4B	2.96	1.49	1.42
29	G	611	CLA	C3B-C4B	2.96	1.49	1.42
29	S	306	CLA	C3B-C4B	2.96	1.49	1.42
29	n	611	CLA	C3B-C4B	2.96	1.49	1.42
29	y	304	CLA	C3B-C4B	2.96	1.49	1.42
45	h	101	RRX	C7-C6	2.96	1.55	1.45
29	g	611	CLA	C3B-C4B	2.96	1.49	1.42
29	d	403	CLA	C3B-C4B	2.96	1.49	1.42
29	C	505	CLA	C3B-C4B	2.95	1.49	1.42
29	N	602	CLA	C3B-C4B	2.95	1.49	1.42
29	Y	304	CLA	C3B-C4B	2.95	1.49	1.42
29	C	514	CLA	C3B-C4B	2.95	1.49	1.42
29	s	304	CLA	C3B-C4B	2.95	1.49	1.42
29	n	602	CLA	C3B-C4B	2.95	1.49	1.42
29	G	614	CLA	C3B-C4B	2.94	1.49	1.42
29	y	316	CLA	C3B-C4B	2.94	1.49	1.42
46	y	308	CHL	C1B-NB	-2.94	1.34	1.37
29	g	614	CLA	C3B-C4B	2.93	1.49	1.42
45	H	101	RRX	C7-C6	2.93	1.55	1.45
29	g	603	CLA	C3B-C4B	2.93	1.49	1.42
29	N	614	CLA	C3B-C4B	2.93	1.49	1.42
29	S	304	CLA	C1D-ND	2.92	1.41	1.37
43	d	405	PL9	C6-C1	-2.92	1.43	1.48
29	b	501	CLA	C3B-C4B	2.92	1.49	1.42
29	D	405	CLA	C3B-C4B	2.92	1.49	1.42
29	C	503	CLA	C3B-C4B	2.92	1.49	1.42
29	B	503	CLA	C3B-C4B	2.92	1.49	1.42
29	G	612	CLA	C3B-C4B	2.91	1.49	1.42
29	n	613	CLA	C3B-C4B	2.91	1.49	1.42
29	B	512	CLA	C3B-C4B	2.91	1.49	1.42
29	s	311	CLA	C3B-C4B	2.91	1.49	1.42
29	s	310	CLA	C3B-C4B	2.91	1.49	1.42
29	R	306	CLA	C3B-C4B	2.91	1.49	1.42
29	b	508	CLA	C3B-C4B	2.91	1.49	1.42
29	b	512	CLA	C3B-C4B	2.91	1.49	1.42
29	Y	311	CLA	C3B-C4B	2.90	1.49	1.42
29	c	501	CLA	C3B-C4B	2.90	1.49	1.42
29	N	603	CLA	C3B-C4B	2.89	1.49	1.42
29	S	315	CLA	C3B-C4B	2.89	1.49	1.42
29	g	610	CLA	C3B-C4B	2.89	1.49	1.42
29	r	310	CLA	C3B-C4B	2.89	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	513	CLA	C3B-C4B	2.88	1.49	1.42
29	b	510	CLA	C3B-C4B	2.87	1.49	1.42
29	N	610	CLA	C3B-C4B	2.87	1.49	1.42
29	g	602	CLA	C3B-C4B	2.87	1.49	1.42
29	g	612	CLA	C3B-C4B	2.87	1.49	1.42
29	S	304	CLA	C3B-C4B	2.87	1.49	1.42
29	c	507	CLA	C3B-C4B	2.87	1.49	1.42
43	D	406	PL9	C6-C1	-2.87	1.43	1.48
29	G	602	CLA	C3B-C4B	2.86	1.49	1.42
38	b	524	LMT	O3'-C3'	-2.86	1.36	1.43
29	g	604	CLA	C3B-C4B	2.86	1.49	1.42
29	b	503	CLA	C3B-C4B	2.86	1.49	1.42
29	y	315	CLA	C3B-C4B	2.86	1.49	1.42
29	Y	314	CLA	C3B-C4B	2.86	1.49	1.42
29	B	513	CLA	C3B-C4B	2.85	1.49	1.42
29	B	506	CLA	C3B-C4B	2.85	1.49	1.42
29	y	305	CLA	C3B-C4B	2.85	1.49	1.42
29	C	502	CLA	C3B-C4B	2.85	1.49	1.42
29	d	404	CLA	C3B-C4B	2.85	1.49	1.42
29	S	305	CLA	C3B-C4B	2.85	1.49	1.42
29	A	407	CLA	C3B-C4B	2.85	1.49	1.42
29	b	502	CLA	C3B-C4B	2.85	1.49	1.42
29	S	313	CLA	C3B-C4B	2.84	1.49	1.42
29	D	404	CLA	CMC-C2C	-2.84	1.44	1.50
29	C	512	CLA	C3B-C4B	2.84	1.49	1.42
29	s	303	CLA	C3B-C4B	2.84	1.49	1.42
29	D	404	CLA	CHB-C1B	2.84	1.45	1.39
29	y	312	CLA	C3B-C4B	2.84	1.49	1.42
46	g	607	CHL	C1B-NB	-2.83	1.34	1.37
29	R	307	CLA	C3B-C4B	2.83	1.49	1.42
29	B	502	CLA	C3B-C4B	2.83	1.49	1.42
29	S	303	CLA	C3B-C4B	2.83	1.49	1.42
29	Y	305	CLA	C3B-C4B	2.83	1.49	1.42
29	n	604	CLA	C3B-C4B	2.83	1.49	1.42
29	b	506	CLA	C3B-C4B	2.83	1.49	1.42
29	b	513	CLA	C3B-C4B	2.83	1.49	1.42
29	s	315	CLA	C3B-C4B	2.83	1.49	1.42
29	S	316	CLA	C3B-C4B	2.82	1.49	1.42
29	R	302	CLA	C3B-C4B	2.82	1.49	1.42
29	N	604	CLA	C3B-C4B	2.82	1.49	1.42
29	A	406	CLA	C3B-C4B	2.82	1.49	1.42
29	B	508	CLA	C3B-C4B	2.82	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	s	321	LPX	P1-O1	2.82	1.70	1.59
29	a	404	CLA	C3B-C4B	2.81	1.49	1.42
29	C	510	CLA	C3B-C4B	2.81	1.49	1.42
29	a	406	CLA	C3B-C4B	2.81	1.49	1.42
29	G	613	CLA	C3B-C4B	2.81	1.49	1.42
29	c	504	CLA	C3B-C4B	2.81	1.49	1.42
29	c	512	CLA	C3B-C4B	2.81	1.49	1.42
29	C	504	CLA	C3B-C4B	2.80	1.49	1.42
29	Y	309	CLA	C3B-C4B	2.80	1.49	1.42
29	R	309	CLA	C3B-C4B	2.80	1.49	1.42
29	a	405	CLA	C3B-C4B	2.80	1.49	1.42
29	C	513	CLA	C3B-C4B	2.80	1.49	1.42
29	C	506	CLA	C3B-C4B	2.79	1.49	1.42
29	c	509	CLA	C3B-C4B	2.79	1.49	1.42
46	Y	302	CHL	C1B-NB	-2.79	1.34	1.37
29	Y	312	CLA	C3B-C4B	2.79	1.49	1.42
29	c	511	CLA	C3B-C4B	2.79	1.49	1.42
29	R	301	CLA	C3B-C4B	2.79	1.49	1.42
30	a	407	PHO	C4D-ND	-2.79	1.34	1.38
29	y	313	CLA	C3B-C4B	2.79	1.49	1.42
38	B	524	LMT	O3'-C3'	-2.79	1.36	1.43
29	C	509	CLA	C3B-C4B	2.79	1.49	1.42
29	a	408	CLA	C3B-C4B	2.78	1.49	1.42
29	R	303	CLA	C3B-C4B	2.78	1.49	1.42
29	s	316	CLA	C3B-C4B	2.78	1.49	1.42
29	c	505	CLA	C3B-C4B	2.78	1.49	1.42
29	C	508	CLA	C3B-C4B	2.77	1.49	1.42
29	Y	315	CLA	C3B-C4B	2.77	1.49	1.42
29	r	304	CLA	C3B-C4B	2.76	1.49	1.42
29	s	306	CLA	C3B-C4B	2.76	1.49	1.42
29	N	613	CLA	C3B-C4B	2.76	1.49	1.42
29	Y	313	CLA	C3B-C4B	2.76	1.49	1.42
46	N	607	CHL	C1B-NB	-2.76	1.34	1.37
29	g	613	CLA	C3B-C4B	2.76	1.49	1.42
29	b	505	CLA	C3B-C4B	2.76	1.49	1.42
46	n	607	CHL	C1B-NB	-2.75	1.34	1.37
29	b	509	CLA	C3B-C4B	2.75	1.49	1.42
29	y	310	CLA	C3B-C4B	2.75	1.49	1.42
46	N	609	CHL	C1B-NB	-2.74	1.34	1.37
29	A	409	CLA	C3B-C4B	2.74	1.49	1.42
29	r	302	CLA	C3B-C4B	2.73	1.49	1.42
29	B	505	CLA	C3B-C4B	2.73	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	s	314	CLA	C3B-C4B	2.72	1.49	1.42
29	s	313	CLA	C3B-C4B	2.72	1.49	1.42
29	c	502	CLA	C3B-C4B	2.72	1.49	1.42
29	s	305	CLA	C3B-C4B	2.71	1.49	1.42
29	b	511	CLA	C3B-C4B	2.71	1.49	1.42
29	r	303	CLA	C3B-C4B	2.71	1.49	1.42
29	c	503	CLA	C3B-C4B	2.70	1.49	1.42
29	B	511	CLA	C3B-C4B	2.70	1.49	1.42
29	C	507	CLA	C3B-C4B	2.70	1.49	1.42
30	a	407	PHO	CMC-C2C	-2.70	1.46	1.50
45	H	101	RRX	C32-C1	2.70	1.59	1.53
46	Y	308	CHL	C1B-NB	-2.70	1.34	1.37
29	B	509	CLA	C3B-C4B	2.70	1.49	1.42
46	r	306	CHL	C1B-NB	-2.69	1.34	1.37
29	r	308	CLA	C3B-C4B	2.69	1.49	1.42
29	n	612	CLA	C3B-C4B	2.69	1.49	1.42
29	S	314	CLA	C3B-C4B	2.68	1.49	1.42
51	S	321	LPX	P1-O1	2.68	1.70	1.59
46	y	303	CHL	C1B-NB	-2.68	1.34	1.37
29	b	514	CLA	C3B-C4B	2.67	1.49	1.42
29	S	316	CLA	C1B-C2B	2.67	1.49	1.43
45	h	101	RRX	C32-C1	2.67	1.59	1.53
29	y	306	CLA	C3B-C4B	2.66	1.49	1.42
29	C	511	CLA	C3B-C4B	2.66	1.49	1.42
29	c	508	CLA	C3B-C4B	2.65	1.49	1.42
29	A	405	CLA	C3B-C4B	2.65	1.49	1.42
30	d	402	PHO	CMC-C2C	-2.65	1.46	1.50
29	N	613	CLA	C1B-C2B	2.65	1.49	1.43
46	g	609	CHL	C1B-NB	-2.65	1.34	1.37
46	s	307	CHL	C1B-NB	-2.64	1.34	1.37
29	y	314	CLA	C3B-C4B	2.64	1.48	1.42
29	d	403	CLA	C1D-ND	2.64	1.41	1.37
29	s	316	CLA	C1B-C2B	2.64	1.49	1.43
29	B	514	CLA	C3B-C4B	2.64	1.48	1.42
29	r	310	CLA	C1B-C2B	2.64	1.49	1.43
29	B	507	CLA	C3B-C4B	2.63	1.48	1.42
29	b	516	CLA	C3B-C4B	2.63	1.48	1.42
29	B	516	CLA	C3B-C4B	2.63	1.48	1.42
29	n	612	CLA	C1B-C2B	2.62	1.49	1.43
44	E	101	HEM	FE-ND	2.61	2.02	1.94
46	n	605	CHL	C1B-NB	-2.60	1.34	1.37
29	c	506	CLA	C3B-C4B	2.60	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	s	315	CLA	C1B-C2B	2.60	1.49	1.43
29	b	507	CLA	C3B-C4B	2.59	1.48	1.42
35	C	524	LMG	C40-C39	-2.59	1.33	1.51
30	D	401	PHO	CMC-C2C	-2.58	1.46	1.50
46	n	605	CHL	C3A-C2A	-2.58	1.47	1.54
29	B	505	CLA	C1B-C2B	2.58	1.49	1.43
29	N	614	CLA	C1B-C2B	2.57	1.49	1.43
35	d	407	LMG	C37-C36	-2.57	1.33	1.51
46	G	607	CHL	C1B-NB	-2.56	1.34	1.37
29	R	309	CLA	C1B-C2B	2.56	1.49	1.43
29	S	314	CLA	C1B-C2B	2.56	1.49	1.43
46	g	608	CHL	C1B-NB	-2.56	1.34	1.37
35	D	409	LMG	C37-C36	-2.55	1.33	1.51
29	s	304	CLA	MG-NB	-2.55	2.00	2.05
29	s	314	CLA	C1B-C2B	2.55	1.49	1.43
29	g	613	CLA	C1B-C2B	2.55	1.49	1.43
38	b	524	LMT	O2'-C2'	-2.55	1.37	1.43
30	A	408	PHO	C4D-ND	-2.54	1.35	1.38
29	c	510	CLA	C3B-C4B	2.53	1.48	1.42
29	B	504	CLA	C3B-C4B	2.53	1.48	1.42
46	R	304	CHL	C1B-NB	-2.53	1.34	1.37
29	s	306	CLA	C1B-C2B	2.53	1.49	1.43
29	b	505	CLA	C1B-C2B	2.53	1.49	1.43
38	B	524	LMT	O2'-C2'	-2.52	1.37	1.43
29	S	303	CLA	C1B-C2B	2.52	1.49	1.43
30	A	408	PHO	CMC-C2C	-2.52	1.46	1.50
46	y	311	CHL	C1B-NB	-2.52	1.34	1.37
46	r	305	CHL	C1B-NB	-2.52	1.34	1.37
29	r	302	CLA	C1B-C2B	2.51	1.49	1.43
33	B	522	3PH	O21-C2	-2.51	1.40	1.46
29	S	306	CLA	C1B-C2B	2.51	1.49	1.43
29	y	310	CLA	C1B-C2B	2.51	1.49	1.43
29	n	613	CLA	C1B-C2B	2.51	1.49	1.43
29	g	614	CLA	C1B-C2B	2.51	1.49	1.43
46	s	308	CHL	C1B-NB	-2.51	1.34	1.37
50	y	321	PTY	O7-C6	-2.50	1.40	1.46
29	G	614	CLA	C1B-C2B	2.50	1.49	1.43
50	n	619	PTY	O7-C6	-2.50	1.40	1.46
29	G	612	CLA	C1B-C2B	2.49	1.49	1.43
29	N	611	CLA	C1B-C2B	2.49	1.49	1.43
33	b	521	3PH	O21-C2	-2.49	1.40	1.46
29	b	504	CLA	C3B-C4B	2.49	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	407	PHO	CMD-C2D	-2.49	1.46	1.51
43	D	406	PL9	C52-C5	-2.49	1.45	1.50
29	C	508	CLA	C1B-C2B	2.49	1.49	1.43
30	d	402	PHO	C4D-ND	-2.48	1.35	1.38
29	N	612	CLA	C1B-C2B	2.48	1.49	1.43
29	c	511	CLA	C1B-C2B	2.48	1.49	1.43
33	b	521	3PH	O31-C31	2.47	1.40	1.33
46	n	601	CHL	C1B-NB	-2.47	1.34	1.37
29	r	308	CLA	C1B-C2B	2.47	1.49	1.43
29	G	613	CLA	C1B-C2B	2.47	1.49	1.43
29	S	304	CLA	C1B-C2B	2.46	1.49	1.43
29	Y	314	CLA	C1B-C2B	2.46	1.49	1.43
29	s	303	CLA	C1B-C2B	2.46	1.49	1.43
29	S	315	CLA	C1B-C2B	2.46	1.49	1.43
50	Y	320	PTY	O7-C6	-2.46	1.40	1.46
29	C	511	CLA	C1B-C2B	2.46	1.49	1.43
46	g	606	CHL	C1B-NB	-2.46	1.34	1.37
29	b	501	CLA	C1B-C2B	2.46	1.49	1.43
29	s	304	CLA	C1B-C2B	2.46	1.49	1.43
29	g	611	CLA	C1B-C2B	2.46	1.49	1.43
29	C	513	CLA	C1B-C2B	2.45	1.49	1.43
29	n	610	CLA	C1B-C2B	2.45	1.49	1.43
29	C	512	CLA	C1B-C2B	2.45	1.49	1.43
30	A	408	PHO	CMD-C2D	-2.45	1.46	1.51
29	c	506	CLA	C1B-C2B	2.44	1.49	1.43
50	N	620	PTY	O7-C6	-2.44	1.40	1.46
29	D	404	CLA	C1D-C2D	-2.44	1.40	1.45
29	G	611	CLA	C1B-C2B	2.44	1.49	1.43
29	R	307	CLA	C1B-C2B	2.44	1.49	1.43
30	D	401	PHO	C4D-ND	-2.44	1.35	1.38
29	Y	312	CLA	C1B-C2B	2.44	1.49	1.43
29	A	407	CLA	C1B-C2B	2.43	1.49	1.43
29	S	313	CLA	C1B-C2B	2.43	1.49	1.43
33	S	322	3PH	O21-C2	-2.43	1.40	1.46
29	y	305	CLA	C1B-C2B	2.43	1.49	1.43
29	R	301	CLA	C1B-C2B	2.43	1.49	1.43
29	B	509	CLA	C1B-C2B	2.43	1.49	1.43
29	c	507	CLA	C1B-C2B	2.43	1.49	1.43
29	y	313	CLA	C1B-C2B	2.43	1.49	1.43
29	b	509	CLA	C1B-C2B	2.43	1.49	1.43
29	g	603	CLA	C1B-C2B	2.43	1.49	1.43
33	B	522	3PH	O31-C31	2.43	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S	312	CLA	C1B-C2B	2.43	1.49	1.43
29	Y	315	CLA	C1B-C2B	2.43	1.49	1.43
45	H	101	RRX	C35-C13	2.42	1.55	1.50
29	B	502	CLA	C1B-C2B	2.42	1.49	1.43
38	b	524	LMT	O2B-C2B	-2.42	1.37	1.43
38	B	524	LMT	O2B-C2B	-2.42	1.37	1.43
29	b	502	CLA	C1B-C2B	2.42	1.49	1.43
29	B	506	CLA	C1B-C2B	2.42	1.49	1.43
34	B	519	C7Z	C20-C13	2.42	1.55	1.50
29	Y	304	CLA	C1B-C2B	2.42	1.48	1.43
29	d	404	CLA	C1B-C2B	2.42	1.48	1.43
29	D	405	CLA	C1B-C2B	2.42	1.48	1.43
29	s	313	CLA	C1B-C2B	2.42	1.48	1.43
29	s	312	CLA	C1B-C2B	2.42	1.48	1.43
44	e	101	HEM	FE-NB	2.42	2.02	1.94
33	S	322	3PH	O31-C31	2.41	1.40	1.33
29	B	504	CLA	C1B-C2B	2.41	1.48	1.43
46	N	601	CHL	C1B-NB	-2.41	1.34	1.37
29	n	602	CLA	C1B-C2B	2.41	1.48	1.43
29	c	505	CLA	C1B-C2B	2.41	1.48	1.43
29	c	512	CLA	C1B-C2B	2.41	1.48	1.43
29	D	404	CLA	O1A-CGA	-2.41	1.15	1.22
30	d	402	PHO	CMD-C2D	-2.41	1.46	1.51
50	N	620	PTY	O4-C30	2.41	1.40	1.33
45	h	101	RRX	C35-C13	2.41	1.55	1.50
33	s	322	3PH	O31-C31	2.40	1.40	1.33
29	A	405	CLA	C1B-C2B	2.40	1.48	1.43
50	n	619	PTY	O4-C30	2.40	1.40	1.33
30	D	401	PHO	CMD-C2D	-2.40	1.46	1.51
29	G	603	CLA	C1B-C2B	2.40	1.48	1.43
29	C	514	CLA	C1B-C2B	2.39	1.48	1.43
46	N	606	CHL	C1B-NB	-2.39	1.34	1.37
29	C	506	CLA	C1B-C2B	2.39	1.48	1.43
29	N	603	CLA	C1B-C2B	2.39	1.48	1.43
29	r	309	CLA	CHC-C1C	2.39	1.43	1.38
29	S	304	CLA	MG-NB	-2.39	2.01	2.05
29	g	612	CLA	C1B-C2B	2.39	1.48	1.43
46	S	309	CHL	C1B-NB	-2.38	1.34	1.37
34	b	519	C7Z	C20-C13	2.38	1.55	1.50
46	g	605	CHL	C1B-NB	-2.38	1.34	1.37
29	B	508	CLA	C1B-C2B	2.38	1.48	1.43
33	s	322	3PH	O21-C2	-2.38	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	502	CLA	C1B-C2B	2.38	1.48	1.43
46	G	609	CHL	C1B-NB	-2.38	1.34	1.37
46	Y	310	CHL	C1B-NB	-2.38	1.34	1.37
34	B	519	C7Z	C10-C9	-2.38	1.32	1.35
30	a	407	PHO	CMB-C2B	-2.37	1.46	1.51
29	D	404	CLA	CHC-C1C	2.37	1.43	1.38
29	n	604	CLA	C1B-C2B	2.37	1.48	1.43
29	r	304	CLA	C1B-C2B	2.37	1.48	1.43
29	S	304	CLA	MG-ND	-2.37	2.01	2.05
29	C	504	CLA	C1B-C2B	2.37	1.48	1.43
29	y	316	CLA	C1B-C2B	2.37	1.48	1.43
29	y	315	CLA	C1B-C2B	2.37	1.48	1.43
29	Y	313	CLA	C1B-C2B	2.37	1.48	1.43
29	C	507	CLA	C1B-C2B	2.36	1.48	1.43
33	A	412	3PH	O31-C31	2.36	1.40	1.33
30	A	408	PHO	CMB-C2B	-2.36	1.46	1.51
50	y	321	PTY	O7-C8	2.36	1.40	1.35
29	Y	309	CLA	C1B-C2B	2.36	1.48	1.43
29	c	510	CLA	C1B-C2B	2.36	1.48	1.43
29	n	611	CLA	C1B-C2B	2.35	1.48	1.43
29	S	310	CLA	C1B-C2B	2.35	1.48	1.43
29	B	501	CLA	C1B-C2B	2.35	1.48	1.43
29	g	610	CLA	CHC-C1C	2.35	1.43	1.38
29	R	308	CLA	CHC-C1C	2.35	1.43	1.38
29	N	604	CLA	C1B-C2B	2.35	1.48	1.43
33	a	415	3PH	O31-C31	2.35	1.40	1.33
33	A	412	3PH	O21-C21	2.35	1.40	1.34
29	C	510	CLA	C1B-C2B	2.34	1.48	1.43
29	b	508	CLA	C1B-C2B	2.34	1.48	1.43
46	R	305	CHL	C1B-NB	-2.34	1.34	1.37
29	b	513	CLA	C1B-C2B	2.34	1.48	1.43
46	y	307	CHL	C1B-NB	-2.34	1.34	1.37
29	g	610	CLA	C1B-C2B	2.34	1.48	1.43
29	G	602	CLA	C1B-C2B	2.34	1.48	1.43
29	R	303	CLA	C1B-C2B	2.34	1.48	1.43
29	n	609	CLA	CHC-C1C	2.34	1.43	1.38
29	c	501	CLA	C1B-C2B	2.34	1.48	1.43
29	R	306	CLA	C1B-C2B	2.34	1.48	1.43
29	s	310	CLA	C1B-C2B	2.34	1.48	1.43
50	Y	320	PTY	O7-C8	2.33	1.40	1.35
29	s	311	CLA	CHC-C1C	2.33	1.43	1.38
29	b	504	CLA	C1B-C2B	2.33	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	G	610	CLA	CHC-C1C	2.33	1.43	1.38
29	N	610	CLA	C1B-C2B	2.33	1.48	1.43
29	Y	305	CLA	C1B-C2B	2.33	1.48	1.43
29	S	305	CLA	C1B-C2B	2.33	1.48	1.43
29	C	503	CLA	C1B-C2B	2.33	1.48	1.43
29	y	304	CLA	C1B-C2B	2.33	1.48	1.43
29	c	513	CLA	C1B-C2B	2.33	1.48	1.43
29	b	506	CLA	C1B-C2B	2.33	1.48	1.43
46	Y	307	CHL	C1B-NB	-2.33	1.34	1.37
46	N	608	CHL	C1B-NB	-2.33	1.34	1.37
49	n	618	XAT	O24-C25	-2.33	1.42	1.46
29	d	403	CLA	CHC-C1C	2.32	1.43	1.38
29	N	611	CLA	CHC-C1C	2.32	1.43	1.38
29	g	602	CLA	CHC-C1C	2.32	1.43	1.38
29	c	502	CLA	C1B-C2B	2.32	1.48	1.43
29	Y	303	CLA	CHC-C1C	2.31	1.43	1.38
29	b	507	CLA	C1B-C2B	2.31	1.48	1.43
29	B	513	CLA	C1B-C2B	2.31	1.48	1.43
29	B	507	CLA	C1B-C2B	2.31	1.48	1.43
29	n	603	CLA	C1B-C2B	2.31	1.48	1.43
29	G	604	CLA	C1B-C2B	2.31	1.48	1.43
29	G	610	CLA	C1B-C2B	2.31	1.48	1.43
33	S	322	3PH	O21-C21	2.31	1.40	1.34
29	B	503	CLA	C1B-C2B	2.31	1.48	1.43
29	c	503	CLA	C1B-C2B	2.31	1.48	1.43
29	b	516	CLA	C1B-C2B	2.31	1.48	1.43
29	a	406	CLA	C1B-C2B	2.30	1.48	1.43
29	g	602	CLA	C1B-C2B	2.30	1.48	1.43
29	r	307	CLA	C1B-C2B	2.30	1.48	1.43
29	y	314	CLA	C1B-C2B	2.30	1.48	1.43
29	r	309	CLA	C1B-C2B	2.30	1.48	1.43
29	A	406	CLA	C1B-C2B	2.30	1.48	1.43
29	b	515	CLA	C1B-C2B	2.30	1.48	1.43
49	y	302	XAT	O24-C25	-2.30	1.42	1.46
29	G	602	CLA	CHC-C1C	2.30	1.43	1.38
29	G	611	CLA	CHC-C1C	2.29	1.43	1.38
29	s	311	CLA	C1B-C2B	2.29	1.48	1.43
29	b	503	CLA	C1B-C2B	2.29	1.48	1.43
29	A	409	CLA	C1B-C2B	2.29	1.48	1.43
29	S	316	CLA	CHC-C1C	2.29	1.43	1.38
33	s	322	3PH	O21-C21	2.29	1.40	1.34
29	S	311	CLA	C1B-C2B	2.29	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	505	CLA	C1B-C2B	2.28	1.48	1.43
29	c	509	CLA	C1B-C2B	2.28	1.48	1.43
33	a	415	3PH	O21-C2	-2.28	1.40	1.46
29	B	516	CLA	C1B-C2B	2.28	1.48	1.43
29	B	510	CLA	C1B-C2B	2.28	1.48	1.43
51	s	321	LPX	P1-O2	2.28	1.68	1.59
51	S	321	LPX	P1-O2	2.28	1.68	1.59
49	g	619	XAT	O24-C25	-2.28	1.43	1.46
29	R	308	CLA	C1B-C2B	2.27	1.48	1.43
33	a	415	3PH	O21-C21	2.27	1.40	1.34
29	B	516	CLA	C4B-NB	-2.27	1.35	1.37
29	N	610	CLA	CHC-C1C	2.27	1.43	1.38
38	b	524	LMT	O3B-C3B	-2.27	1.37	1.43
29	n	609	CLA	C1B-C2B	2.27	1.48	1.43
46	G	608	CHL	C1B-NB	-2.27	1.35	1.37
29	b	510	CLA	C1B-C2B	2.27	1.48	1.43
34	b	519	C7Z	C18-C5	2.27	1.54	1.50
29	y	304	CLA	CHC-C1C	2.26	1.43	1.38
29	c	513	CLA	CHC-C1C	2.26	1.43	1.38
29	b	514	CLA	C1B-C2B	2.26	1.48	1.43
29	s	311	CLA	MG-NB	-2.26	2.01	2.05
29	b	503	CLA	CHC-C1C	2.26	1.43	1.38
29	B	512	CLA	C1B-C2B	2.26	1.48	1.43
29	B	515	CLA	C1B-C2B	2.26	1.48	1.43
29	B	503	CLA	CHC-C1C	2.26	1.43	1.38
29	s	305	CLA	C1B-C2B	2.26	1.48	1.43
29	G	604	CLA	CHC-C1C	2.26	1.43	1.38
30	d	402	PHO	CMB-C2B	-2.26	1.46	1.51
29	S	311	CLA	CHC-C1C	2.26	1.43	1.38
49	N	619	XAT	O24-C25	-2.26	1.43	1.46
29	y	306	CLA	C1B-C2B	2.26	1.48	1.43
29	r	303	CLA	MG-ND	-2.26	2.01	2.05
29	g	604	CLA	C1B-C2B	2.25	1.48	1.43
29	S	312	CLA	CHC-C1C	2.25	1.43	1.38
29	B	514	CLA	C1B-C2B	2.25	1.48	1.43
29	C	514	CLA	CHC-C1C	2.25	1.43	1.38
49	G	619	XAT	O24-C25	-2.25	1.43	1.46
49	R	311	XAT	O24-C25	-2.25	1.43	1.46
29	n	610	CLA	CHC-C1C	2.25	1.43	1.38
29	b	512	CLA	C1B-C2B	2.24	1.48	1.43
29	g	611	CLA	CHC-C1C	2.24	1.43	1.38
29	N	612	CLA	CHC-C1C	2.24	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	y	312	CLA	C1B-C2B	2.24	1.48	1.43
46	N	605	CHL	C1B-NB	-2.24	1.35	1.37
29	N	602	CLA	CHC-C1C	2.24	1.43	1.38
29	Y	303	CLA	C1B-C2B	2.23	1.48	1.43
29	N	602	CLA	C1B-C2B	2.23	1.48	1.43
29	a	404	CLA	C1B-C2B	2.23	1.48	1.43
29	s	312	CLA	CHC-C1C	2.23	1.43	1.38
29	a	408	CLA	C1B-C2B	2.23	1.48	1.43
29	D	404	CLA	CMD-C2D	-2.23	1.46	1.50
29	B	506	CLA	CHC-C1C	2.22	1.43	1.38
29	c	504	CLA	C1B-C2B	2.22	1.48	1.43
49	Y	301	XAT	O24-C25	-2.22	1.43	1.46
49	r	312	XAT	O24-C25	-2.21	1.43	1.46
29	b	512	CLA	CHC-C1C	2.21	1.43	1.38
34	B	519	C7Z	C18-C5	2.21	1.54	1.50
29	Y	311	CLA	C1B-C2B	2.21	1.48	1.43
38	B	524	LMT	O3B-C3B	-2.21	1.37	1.43
29	y	312	CLA	MG-NB	-2.21	2.01	2.05
29	B	501	CLA	CHC-C1C	2.21	1.43	1.38
29	B	515	CLA	CHC-C1C	2.21	1.43	1.38
29	D	404	CLA	C1B-C2B	-2.20	1.38	1.43
34	b	519	C7Z	C10-C9	-2.20	1.32	1.35
30	D	401	PHO	CMB-C2B	-2.20	1.47	1.51
30	a	407	PHO	CAC-C3C	-2.20	1.47	1.51
29	s	316	CLA	CHC-C1C	2.20	1.43	1.38
29	A	409	CLA	C4B-NB	-2.20	1.35	1.37
29	a	408	CLA	C4B-NB	-2.20	1.35	1.37
41	w	201	DGA	OG2-CG2	-2.20	1.41	1.46
29	g	610	CLA	MG-NB	-2.20	2.01	2.05
29	b	504	CLA	MG-ND	-2.20	2.01	2.05
29	s	303	CLA	CHC-C1C	2.19	1.43	1.38
38	B	524	LMT	O4'-C4B	-2.19	1.37	1.43
29	c	507	CLA	CHC-C1C	2.19	1.43	1.38
29	A	407	CLA	CHC-C1C	2.19	1.43	1.38
29	C	506	CLA	CHC-C1C	2.19	1.43	1.38
43	d	405	PL9	C52-C5	-2.19	1.46	1.50
29	D	405	CLA	CHC-C1C	2.19	1.43	1.38
30	D	401	PHO	CAC-C3C	-2.18	1.47	1.51
29	d	403	CLA	C1B-C2B	2.18	1.48	1.43
29	b	502	CLA	CHC-C1C	2.18	1.43	1.38
29	G	614	CLA	CHC-C1C	2.18	1.43	1.38
29	s	304	CLA	C4B-NB	-2.18	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	j	101	DGA	OG2-CG2	-2.18	1.41	1.46
46	s	302	CHL	C1B-NB	-2.18	1.35	1.37
29	r	303	CLA	MG-NB	-2.18	2.01	2.05
29	c	505	CLA	CHC-C1C	2.18	1.42	1.38
46	S	308	CHL	C1B-NB	-2.18	1.35	1.37
29	c	512	CLA	CHC-C1C	2.18	1.42	1.38
29	d	404	CLA	CHC-C1C	2.18	1.42	1.38
29	R	309	CLA	CHC-C1C	2.17	1.42	1.38
50	N	620	PTY	O7-C8	2.17	1.40	1.34
29	n	611	CLA	CHC-C1C	2.17	1.42	1.38
29	S	313	CLA	CHC-C1C	2.17	1.42	1.38
41	W	202	DGA	OG2-CG2	-2.17	1.41	1.46
29	b	503	CLA	MG-NB	-2.17	2.01	2.05
29	n	602	CLA	CHC-C1C	2.17	1.42	1.38
46	Y	306	CHL	C1B-NB	-2.17	1.35	1.37
29	B	512	CLA	CHC-C1C	2.17	1.42	1.38
33	S	322	3PH	O31-C3	-2.17	1.40	1.45
29	B	513	CLA	CHC-C1C	2.17	1.42	1.38
38	b	524	LMT	O4'-C4B	-2.16	1.37	1.43
29	S	310	CLA	CHC-C1C	2.16	1.42	1.38
29	R	301	CLA	CHC-C1C	2.16	1.42	1.38
33	B	522	3PH	O31-C3	-2.16	1.40	1.45
30	d	402	PHO	CAC-C3C	-2.16	1.47	1.51
29	c	509	CLA	CHC-C1C	2.16	1.42	1.38
29	b	501	CLA	CHC-C1C	2.16	1.42	1.38
50	n	619	PTY	O7-C8	2.16	1.40	1.34
29	D	404	CLA	C3A-C4A	-2.16	1.44	1.51
29	C	513	CLA	CHC-C1C	2.15	1.42	1.38
29	D	404	CLA	C3D-CAD	-2.15	1.37	1.45
29	N	604	CLA	CHC-C1C	2.15	1.42	1.38
29	n	613	CLA	CHC-C1C	2.15	1.42	1.38
30	A	408	PHO	CAC-C3C	-2.15	1.47	1.51
29	B	503	CLA	MG-NB	-2.15	2.01	2.05
29	S	306	CLA	CHC-C1C	2.15	1.42	1.38
46	g	601	CHL	C1B-NB	-2.15	1.35	1.37
29	C	505	CLA	CHC-C1C	2.15	1.42	1.38
43	d	405	PL9	C53-C6	-2.15	1.46	1.50
50	n	619	PTY	O4-C1	-2.15	1.40	1.45
29	y	312	CLA	CHC-C1C	2.15	1.42	1.38
29	D	404	CLA	C3A-C2A	-2.15	1.48	1.54
29	G	612	CLA	CHC-C1C	2.15	1.42	1.38
29	Y	314	CLA	CHC-C1C	2.15	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	s	315	CLA	CHC-C1C	2.14	1.42	1.38
46	G	606	CHL	C1B-NB	-2.14	1.35	1.37
29	S	315	CLA	CHC-C1C	2.14	1.42	1.38
29	a	405	CLA	C1B-C2B	2.14	1.48	1.43
29	Y	311	CLA	CHC-C1C	2.14	1.42	1.38
31	B	518	BCR	C12-C13	-2.14	1.41	1.45
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	R	302	CLA	MG-NB	-2.14	2.01	2.05
29	R	302	CLA	C1B-C2B	2.13	1.48	1.43
46	G	601	CHL	C1B-NB	-2.13	1.35	1.37
29	n	609	CLA	MG-NB	-2.13	2.01	2.05
29	b	515	CLA	CHC-C1C	2.13	1.42	1.38
29	n	604	CLA	CHC-C1C	2.13	1.42	1.38
29	r	304	CLA	CHC-C1C	2.13	1.42	1.38
33	b	521	3PH	O21-C21	2.13	1.40	1.34
29	b	508	CLA	CHC-C1C	2.13	1.42	1.38
29	B	502	CLA	CHC-C1C	2.13	1.42	1.38
29	c	508	CLA	MG-NB	-2.13	2.01	2.05
29	C	502	CLA	CHC-C1C	2.13	1.42	1.38
29	g	614	CLA	CHC-C1C	2.13	1.42	1.38
29	B	508	CLA	CHC-C1C	2.13	1.42	1.38
29	A	409	CLA	CHC-C1C	2.13	1.42	1.38
29	y	306	CLA	MG-NB	-2.13	2.01	2.05
29	b	505	CLA	C4B-NB	-2.13	1.35	1.37
29	C	503	CLA	CHC-C1C	2.12	1.42	1.38
29	B	505	CLA	C4B-NB	-2.12	1.35	1.37
29	G	610	CLA	MG-NB	-2.12	2.01	2.05
29	b	514	CLA	CHC-C1C	2.12	1.42	1.38
29	b	506	CLA	CHC-C1C	2.12	1.42	1.38
33	s	322	3PH	O31-C3	-2.12	1.40	1.45
29	s	314	CLA	CHC-C1C	2.12	1.42	1.38
29	s	315	CLA	MG-NB	-2.12	2.01	2.05
29	g	612	CLA	MG-NB	-2.12	2.01	2.05
29	G	611	CLA	MG-NB	-2.12	2.01	2.05
29	y	315	CLA	CHC-C1C	2.12	1.42	1.38
29	g	603	CLA	CHC-C1C	2.11	1.42	1.38
29	y	316	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
34	b	519	C7Z	C40-C33	2.11	1.55	1.50
29	C	504	CLA	CHC-C1C	2.11	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	509	CLA	CHC-C1C	2.11	1.42	1.38
29	Y	315	CLA	CHC-C1C	2.11	1.42	1.38
29	Y	305	CLA	CHC-C1C	2.11	1.42	1.38
29	C	508	CLA	CHC-C1C	2.11	1.42	1.38
29	a	406	CLA	CHC-C1C	2.11	1.42	1.38
29	g	604	CLA	CHC-C1C	2.11	1.42	1.38
31	c	514	BCR	C12-C13	-2.11	1.41	1.45
29	c	501	CLA	CHC-C1C	2.11	1.42	1.38
29	S	303	CLA	CHC-C1C	2.11	1.42	1.38
46	g	606	CHL	C3A-C2A	-2.11	1.48	1.54
47	r	311	LUT	C22-C21	-2.11	1.52	1.54
29	S	304	CLA	CHC-C1C	2.11	1.42	1.38
33	A	412	3PH	O31-C3	-2.10	1.40	1.45
46	y	308	CHL	C3A-C2A	-2.10	1.48	1.54
31	b	518	BCR	C12-C13	-2.10	1.41	1.45
29	Y	312	CLA	CHC-C1C	2.10	1.42	1.38
29	C	509	CLA	MG-NB	-2.10	2.01	2.05
29	C	510	CLA	CHC-C1C	2.10	1.42	1.38
29	r	303	CLA	C1B-C2B	2.10	1.48	1.43
29	b	509	CLA	MG-NB	-2.10	2.01	2.05
29	N	611	CLA	MG-NB	-2.10	2.01	2.05
29	n	609	CLA	MG-ND	-2.10	2.01	2.05
29	y	313	CLA	CHC-C1C	2.09	1.42	1.38
29	B	513	CLA	MG-NB	-2.09	2.01	2.05
43	D	406	PL9	C53-C6	-2.09	1.46	1.50
43	D	406	PL9	C7-C8	-2.09	1.47	1.50
29	B	514	CLA	CHC-C1C	2.09	1.42	1.38
29	C	512	CLA	CHC-C1C	2.09	1.42	1.38
29	a	408	CLA	CHC-C1C	2.09	1.42	1.38
29	G	603	CLA	CHC-C1C	2.09	1.42	1.38
29	S	314	CLA	CHC-C1C	2.09	1.42	1.38
29	N	613	CLA	CHC-C1C	2.09	1.42	1.38
29	R	306	CLA	CHC-C1C	2.09	1.42	1.38
29	c	511	CLA	CHC-C1C	2.09	1.42	1.38
29	C	506	CLA	MG-NB	-2.09	2.01	2.05
29	b	513	CLA	CHC-C1C	2.09	1.42	1.38
29	S	316	CLA	MG-NB	-2.09	2.01	2.05
29	R	307	CLA	CHC-C1C	2.09	1.42	1.38
33	B	522	3PH	O21-C21	2.09	1.40	1.34
46	s	309	CHL	C1B-NB	-2.09	1.35	1.37
29	B	516	CLA	MG-NB	-2.09	2.01	2.05
29	N	610	CLA	MG-NB	-2.09	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	N	614	CLA	CHC-C1C	2.08	1.42	1.38
29	R	303	CLA	CHC-C1C	2.08	1.42	1.38
29	s	313	CLA	CHC-C1C	2.08	1.42	1.38
29	b	511	CLA	C1B-C2B	2.08	1.48	1.43
29	A	409	CLA	MG-NB	-2.08	2.01	2.05
29	b	516	CLA	MG-NB	-2.08	2.01	2.05
29	g	604	CLA	MG-NB	-2.08	2.01	2.05
33	b	521	3PH	O31-C3	-2.08	1.40	1.45
29	S	306	CLA	MG-NB	-2.08	2.01	2.05
29	B	509	CLA	CHC-C1C	2.08	1.42	1.38
29	b	516	CLA	C4B-NB	-2.08	1.35	1.37
46	S	307	CHL	C1B-NB	-2.08	1.35	1.37
50	Y	320	PTY	O4-C1	-2.08	1.40	1.45
29	R	306	CLA	MG-ND	-2.08	2.01	2.05
34	B	519	C7Z	C40-C33	2.07	1.55	1.50
29	n	604	CLA	MG-NB	-2.07	2.01	2.05
29	b	507	CLA	C4B-NB	-2.07	1.35	1.37
29	B	508	CLA	C4B-NB	-2.07	1.35	1.37
29	Y	304	CLA	CHC-C1C	2.07	1.42	1.38
29	Y	309	CLA	MG-NB	-2.07	2.01	2.05
33	a	415	3PH	O31-C3	-2.07	1.40	1.45
29	s	306	CLA	CHC-C1C	2.07	1.42	1.38
30	A	408	PHO	C3D-C4D	2.07	1.44	1.41
29	g	612	CLA	CHC-C1C	2.07	1.42	1.38
29	N	602	CLA	MG-NB	-2.07	2.01	2.05
31	B	517	BCR	C12-C13	-2.06	1.41	1.45
30	D	401	PHO	C3D-C4D	2.06	1.44	1.41
29	N	613	CLA	MG-NB	-2.06	2.01	2.05
30	d	402	PHO	C3D-C4D	2.06	1.44	1.41
29	y	314	CLA	MG-NB	-2.06	2.01	2.05
29	A	406	CLA	CHC-C1C	2.06	1.42	1.38
48	y	319	NEX	C1-C6	-2.06	1.51	1.54
29	R	306	CLA	MG-NB	-2.06	2.01	2.05
29	b	507	CLA	MG-NB	-2.06	2.01	2.05
29	Y	309	CLA	CHC-C1C	2.06	1.42	1.38
29	r	302	CLA	CHC-C1C	2.06	1.42	1.38
29	n	610	CLA	MG-NB	-2.06	2.01	2.05
29	s	310	CLA	CHC-C1C	2.05	1.42	1.38
46	S	302	CHL	C1B-NB	-2.05	1.35	1.37
29	B	509	CLA	MG-ND	-2.05	2.01	2.05
29	y	312	CLA	MG-ND	-2.05	2.01	2.05
38	b	524	LMT	O1'-C1'	-2.05	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	506	CLA	MG-NB	-2.05	2.01	2.05
41	J	101	DGA	OG2-CG2	-2.05	1.41	1.46
29	a	405	CLA	MG-NB	-2.05	2.01	2.05
50	y	321	PTY	O4-C1	-2.05	1.40	1.45
29	a	408	CLA	MG-NB	-2.04	2.01	2.05
29	C	506	CLA	MG-ND	-2.04	2.01	2.05
29	r	310	CLA	CHC-C1C	2.04	1.42	1.38
29	g	610	CLA	MG-ND	-2.04	2.01	2.05
29	B	516	CLA	MG-ND	-2.04	2.01	2.05
35	D	410	LMG	C22-C21	-2.04	1.33	1.49
29	B	509	CLA	MG-NB	-2.04	2.01	2.05
29	N	603	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	r	307	CLA	CHC-C1C	2.04	1.42	1.38
29	n	603	CLA	CHC-C1C	2.04	1.42	1.38
35	d	408	LMG	C22-C21	-2.03	1.33	1.49
31	a	409	BCR	C12-C13	-2.03	1.41	1.45
29	c	508	CLA	C1B-C2B	2.03	1.48	1.43
29	s	306	CLA	MG-NB	-2.03	2.01	2.05
29	N	604	CLA	MG-NB	-2.03	2.01	2.05
29	s	311	CLA	MG-ND	-2.03	2.01	2.05
44	e	101	HEM	CMB-C2B	2.03	1.55	1.50
29	B	507	CLA	MG-NB	-2.03	2.01	2.05
29	c	503	CLA	MG-NB	-2.03	2.01	2.05
36	C	519	DGD	CGB-CFB	-2.03	1.33	1.49
36	c	516	DGD	CGB-CFB	-2.03	1.33	1.49
29	g	613	CLA	CHC-C1C	2.03	1.42	1.38
35	c	519	LMG	C43-C42	-2.03	1.33	1.49
29	B	511	CLA	CHC-C1C	2.03	1.42	1.38
29	s	312	CLA	MG-NB	-2.03	2.01	2.05
29	D	404	CLA	CMB-C2B	-2.03	1.46	1.50
29	c	504	CLA	MG-NB	-2.03	2.01	2.05
29	Y	313	CLA	CHC-C1C	2.03	1.42	1.38
29	g	611	CLA	MG-NB	-2.03	2.01	2.05
29	B	511	CLA	MG-NB	-2.02	2.01	2.05
29	r	307	CLA	MG-ND	-2.02	2.01	2.05
36	c	518	DGD	CDA-CCA	-2.02	1.33	1.49
29	b	516	CLA	MG-ND	-2.02	2.01	2.05
29	R	309	CLA	MG-NB	-2.02	2.01	2.05
36	C	520	DGD	CAB-C9B	-2.02	1.33	1.49
29	s	311	CLA	C4B-NB	-2.02	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	y	310	CLA	MG-NB	-2.02	2.01	2.05
31	A	410	BCR	C12-C13	-2.02	1.41	1.45
29	C	511	CLA	CHC-C1C	2.02	1.42	1.38
29	d	403	CLA	MG-ND	-2.02	2.01	2.05
36	c	517	DGD	CGB-CFB	-2.02	1.33	1.49
29	y	306	CLA	CHC-C1C	2.02	1.42	1.38
29	b	512	CLA	MG-NB	-2.02	2.01	2.05
29	s	304	CLA	CHC-C1C	2.02	1.42	1.38
35	c	519	LMG	C25-C24	-2.02	1.33	1.49
29	y	305	CLA	CHC-C1C	2.02	1.42	1.38
48	y	319	NEX	O24-C25	-2.01	1.43	1.46
29	A	405	CLA	CHC-C1C	2.01	1.42	1.38
36	C	518	DGD	CGB-CFB	-2.01	1.33	1.49
29	B	511	CLA	C1B-C2B	2.01	1.48	1.43
29	b	513	CLA	MG-NB	-2.01	2.01	2.05
35	C	521	LMG	C43-C42	-2.01	1.33	1.49
35	B	520	LMG	C25-C24	-2.01	1.33	1.49
44	e	101	HEM	FE-NC	2.01	2.01	1.95
29	g	603	CLA	MG-NB	-2.01	2.01	2.05
36	c	518	DGD	CGB-CFB	-2.01	1.33	1.49
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
50	N	620	PTY	O4-C1	-2.01	1.40	1.45
29	y	310	CLA	CHC-C1C	2.01	1.42	1.38
35	i	101	LMG	C22-C21	-2.01	1.33	1.49
29	D	404	CLA	C4-C3	-2.01	1.45	1.50
29	s	316	CLA	MG-NB	-2.01	2.01	2.05
36	C	520	DGD	CDA-CCA	-2.00	1.33	1.49
29	S	305	CLA	MG-NB	-2.00	2.01	2.05
29	b	511	CLA	MG-NB	-2.00	2.01	2.05
35	i	101	LMG	C43-C42	-2.00	1.33	1.49
29	b	504	CLA	MG-NB	-2.00	2.01	2.05
35	W	201	LMG	C22-C21	-2.00	1.33	1.49
36	c	517	DGD	CGA-CFA	-2.00	1.33	1.49
29	c	510	CLA	C4B-NB	-2.00	1.35	1.37
29	n	612	CLA	MG-NB	-2.00	2.01	2.05
29	S	305	CLA	CHC-C1C	2.00	1.42	1.38
29	B	508	CLA	MG-NB	-2.00	2.01	2.05

All (2337) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	f	101	BCR	C10-C11-C12	17.66	178.32	123.22
31	C	517	BCR	C10-C11-C12	17.51	177.86	123.22
31	c	515	BCR	C10-C11-C12	17.44	177.64	123.22
31	b	517	BCR	C10-C11-C12	17.38	177.47	123.22
31	b	518	BCR	C10-C11-C12	17.35	177.38	123.22
31	B	518	BCR	C10-C11-C12	17.21	176.91	123.22
31	F	101	BCR	C10-C11-C12	17.20	176.89	123.22
31	v	101	BCR	C10-C11-C12	17.11	176.63	123.22
29	D	404	CLA	O2D-CGD-O1D	-17.07	90.46	123.84
31	K	101	BCR	C10-C11-C12	16.95	176.10	123.22
31	C	515	BCR	C10-C11-C12	16.93	176.05	123.22
31	c	514	BCR	C10-C11-C12	16.90	175.95	123.22
31	z	101	BCR	C10-C11-C12	16.90	175.95	123.22
49	G	619	XAT	C37-C21-C36	-16.82	82.56	107.37
31	C	516	BCR	C10-C11-C12	16.71	175.35	123.22
49	g	619	XAT	C37-C21-C36	-16.67	82.78	107.37
31	B	517	BCR	C10-C11-C12	16.64	175.15	123.22
31	a	409	BCR	C10-C11-C12	16.54	174.83	123.22
31	A	410	BCR	C10-C11-C12	16.48	174.65	123.22
31	z	101	BCR	C11-C10-C9	14.43	147.90	127.31
31	v	101	BCR	C11-C10-C9	13.59	146.70	127.31
31	K	101	BCR	C11-C10-C9	13.59	146.70	127.31
29	D	404	CLA	O2D-CGD-CBD	13.30	134.91	111.27
31	a	409	BCR	C11-C10-C9	13.23	146.19	127.31
31	A	410	BCR	C11-C10-C9	13.22	146.17	127.31
31	C	515	BCR	C11-C10-C9	13.16	146.09	127.31
31	f	101	BCR	C21-C20-C19	13.14	164.21	123.22
31	b	517	BCR	C11-C10-C9	13.04	145.91	127.31
31	B	517	BCR	C11-C10-C9	12.51	145.17	127.31
49	g	619	XAT	C37-C21-C22	-12.49	87.28	108.98
31	A	410	BCR	C11-C12-C13	12.28	160.91	126.42
49	G	619	XAT	C37-C21-C22	-12.26	87.67	108.98
31	a	409	BCR	C11-C12-C13	12.24	160.81	126.42
31	A	410	BCR	C21-C20-C19	12.15	161.13	123.22
31	C	516	BCR	C11-C10-C9	12.15	144.65	127.31
31	B	517	BCR	C11-C12-C13	12.14	160.51	126.42
31	c	515	BCR	C11-C10-C9	12.12	144.61	127.31
31	C	516	BCR	C11-C12-C13	12.11	160.44	126.42
31	C	515	BCR	C16-C15-C14	12.06	148.18	123.47
31	a	409	BCR	C21-C20-C19	12.05	160.82	123.22
31	c	515	BCR	C21-C20-C19	12.04	160.78	123.22
31	C	517	BCR	C21-C20-C19	12.03	160.75	123.22
31	C	517	BCR	C11-C10-C9	11.92	144.33	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	z	101	BCR	C16-C15-C14	11.78	147.60	123.47
31	c	514	BCR	C11-C10-C9	11.71	144.03	127.31
31	B	518	BCR	C11-C10-C9	11.69	143.99	127.31
31	C	516	BCR	C16-C15-C14	11.69	147.41	123.47
31	f	101	BCR	C16-C15-C14	11.67	147.38	123.47
31	F	101	BCR	C11-C12-C13	11.63	159.08	126.42
31	b	518	BCR	C11-C10-C9	11.43	143.62	127.31
31	K	101	BCR	C11-C12-C13	11.43	158.51	126.42
31	F	101	BCR	C11-C10-C9	11.41	143.60	127.31
31	v	101	BCR	C21-C20-C19	11.35	158.65	123.22
31	c	515	BCR	C16-C15-C14	11.34	146.71	123.47
31	c	514	BCR	C16-C15-C14	11.24	146.51	123.47
31	f	101	BCR	C11-C10-C9	11.22	143.32	127.31
31	v	101	BCR	C11-C12-C13	11.20	157.87	126.42
31	z	101	BCR	C21-C20-C19	11.18	158.10	123.22
31	b	517	BCR	C16-C15-C14	11.17	146.36	123.47
31	b	518	BCR	C21-C20-C19	11.17	158.08	123.22
31	C	517	BCR	C16-C15-C14	11.15	146.31	123.47
31	b	518	BCR	C16-C15-C14	11.11	146.22	123.47
31	F	101	BCR	C21-C20-C19	11.10	157.85	123.22
31	K	101	BCR	C21-C20-C19	11.05	157.72	123.22
31	z	101	BCR	C11-C12-C13	10.97	157.24	126.42
31	C	515	BCR	C21-C20-C19	10.92	157.28	123.22
31	b	518	BCR	C11-C12-C13	10.86	156.93	126.42
31	B	518	BCR	C11-C12-C13	10.83	156.84	126.42
31	B	518	BCR	C21-C20-C19	10.79	156.89	123.22
31	c	515	BCR	C11-C12-C13	10.78	156.69	126.42
31	B	518	BCR	C16-C15-C14	10.77	145.53	123.47
31	b	517	BCR	C21-C20-C19	10.76	156.80	123.22
31	C	517	BCR	C11-C12-C13	10.75	156.61	126.42
31	f	101	BCR	C11-C12-C13	10.69	156.44	126.42
31	c	514	BCR	C11-C12-C13	10.66	156.35	126.42
31	A	410	BCR	C16-C15-C14	10.55	145.09	123.47
31	B	517	BCR	C21-C20-C19	10.52	156.05	123.22
31	K	101	BCR	C16-C15-C14	10.47	144.91	123.47
31	v	101	BCR	C16-C15-C14	10.46	144.90	123.47
31	b	517	BCR	C11-C12-C13	10.39	155.60	126.42
31	a	409	BCR	C16-C15-C14	10.34	144.66	123.47
31	F	101	BCR	C16-C15-C14	10.31	144.60	123.47
31	C	516	BCR	C21-C20-C19	10.28	155.30	123.22
31	C	515	BCR	C11-C12-C13	10.01	154.54	126.42
31	c	514	BCR	C21-C20-C19	10.00	154.42	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	517	BCR	C16-C15-C14	9.66	143.25	123.47
31	c	514	BCR	C20-C19-C18	9.57	153.29	126.42
31	C	516	BCR	C20-C19-C18	9.24	152.37	126.42
29	D	404	CLA	CED-O2D-CGD	8.81	135.86	115.94
31	B	517	BCR	C20-C19-C18	8.58	150.52	126.42
31	C	515	BCR	C20-C19-C18	8.49	150.28	126.42
31	b	517	BCR	C20-C19-C18	8.37	149.93	126.42
31	B	518	BCR	C20-C19-C18	8.30	149.74	126.42
31	z	101	BCR	C20-C19-C18	8.20	149.45	126.42
31	v	101	BCR	C20-C19-C18	8.11	149.20	126.42
31	K	101	BCR	C20-C19-C18	8.09	149.15	126.42
31	F	101	BCR	C20-C19-C18	8.05	149.04	126.42
31	b	518	BCR	C20-C19-C18	8.00	148.88	126.42
45	H	101	RRX	C20-C21-C22	-7.63	116.41	127.31
31	c	515	BCR	C20-C19-C18	7.62	147.84	126.42
29	D	404	CLA	C3D-C2D-C1D	-7.61	95.44	105.83
31	C	517	BCR	C20-C19-C18	7.59	147.74	126.42
30	d	402	PHO	C4D-CHA-CBD	-7.51	105.12	108.52
49	G	619	XAT	C36-C21-C22	7.46	121.94	108.98
29	D	404	CLA	C3B-C2B-C1B	-7.43	98.20	107.16
31	A	410	BCR	C20-C19-C18	7.41	147.24	126.42
31	a	409	BCR	C20-C19-C18	7.40	147.19	126.42
29	D	404	CLA	C1D-ND-C4D	-7.32	101.13	106.33
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
49	g	619	XAT	C36-C21-C22	7.20	121.50	108.98
30	D	401	PHO	C4D-CHA-CBD	-7.03	105.34	108.52
45	h	101	RRX	C11-C10-C9	-7.02	117.30	127.31
45	h	101	RRX	C20-C21-C22	-6.92	117.44	127.31
45	H	101	RRX	C11-C10-C9	-6.85	117.53	127.31
41	b	522	DGA	CDB-CCB-CBB	-6.82	79.81	114.42
34	B	519	C7Z	C11-C10-C9	-6.77	117.64	127.31
29	D	404	CLA	O2A-CGA-O1A	-6.77	106.51	123.59
29	g	610	CLA	C4A-NA-C1A	6.68	109.71	106.71
41	W	202	DGA	CDB-CCB-CBB	-6.62	80.82	114.42
41	w	201	DGA	CDB-CCB-CBB	-6.62	80.83	114.42
45	H	101	RRX	C15-C14-C13	-6.59	117.91	127.31
30	A	408	PHO	C4D-CHA-CBD	-6.58	105.54	108.52
29	D	404	CLA	C2B-C1B-NB	6.51	114.59	110.23
49	Y	301	XAT	C31-C30-C29	-6.47	118.08	127.31
30	a	407	PHO	C4D-CHA-CBD	-6.33	105.66	108.52
45	h	101	RRX	C16-C17-C18	-6.32	118.30	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	f	101	BCR	C20-C19-C18	6.31	144.14	126.42
34	b	519	C7Z	C11-C10-C9	-6.23	118.41	127.31
29	G	610	CLA	C4A-NA-C1A	6.17	109.48	106.71
49	g	619	XAT	C31-C30-C29	-6.10	118.60	127.31
49	n	618	XAT	C15-C14-C13	-6.07	118.65	127.31
49	N	619	XAT	C31-C30-C29	-6.04	118.69	127.31
29	b	504	CLA	C4A-NA-C1A	6.04	109.42	106.71
45	h	101	RRX	C15-C14-C13	-6.03	118.70	127.31
47	g	615	LUT	C21-C26-C25	6.01	122.19	111.42
49	G	619	XAT	C31-C30-C29	-6.00	118.75	127.31
29	D	404	CLA	CAC-C3C-C4C	5.98	132.57	124.81
45	H	101	RRX	C24-C23-C22	-5.98	117.20	126.23
29	S	306	CLA	C4A-NA-C1A	5.85	109.34	106.71
47	Y	316	LUT	C21-C26-C25	5.83	121.86	111.42
49	n	618	XAT	C31-C30-C29	-5.83	118.99	127.31
47	g	616	LUT	C21-C26-C25	5.81	121.82	111.42
47	s	317	LUT	C21-C26-C25	5.78	121.78	111.42
47	G	616	LUT	C21-C26-C25	5.78	121.77	111.42
47	G	615	LUT	C21-C26-C25	5.72	121.67	111.42
29	s	304	CLA	C4A-NA-C1A	5.71	109.27	106.71
47	N	615	LUT	C21-C26-C25	5.70	121.63	111.42
47	N	616	LUT	C21-C26-C25	5.68	121.59	111.42
49	y	302	XAT	C31-C30-C29	-5.63	119.27	127.31
47	y	317	LUT	C21-C26-C25	5.62	121.49	111.42
37	L	101	LHG	O7-C7-C8	5.58	123.53	111.50
34	B	519	C7Z	C18-C5-C6	-5.58	118.26	124.53
29	C	508	CLA	C4A-NA-C1A	5.54	109.20	106.71
34	b	519	C7Z	C18-C5-C6	-5.51	118.34	124.53
29	N	610	CLA	C4A-NA-C1A	5.51	109.19	106.71
47	Y	317	LUT	C21-C26-C25	5.49	121.26	111.42
29	D	404	CLA	O2A-CGA-CBA	5.47	129.08	111.91
29	b	507	CLA	C4A-NA-C1A	5.45	109.16	106.71
34	B	519	C7Z	C35-C34-C33	-5.45	119.54	127.31
49	N	619	XAT	C15-C14-C13	-5.41	119.58	127.31
45	H	101	RRX	C16-C17-C18	-5.39	119.62	127.31
47	n	615	LUT	C21-C26-C25	5.38	121.05	111.42
42	a	412	BCT	O2-C-O1	5.38	133.49	119.55
47	S	318	LUT	C21-C26-C25	5.35	121.00	111.42
47	y	318	LUT	C21-C26-C25	5.33	120.97	111.42
49	G	619	XAT	C15-C14-C13	-5.32	119.72	127.31
47	s	318	LUT	C21-C26-C25	5.29	120.89	111.42
49	y	302	XAT	C15-C14-C13	-5.24	119.83	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	404	CLA	CMD-C2D-C1D	5.22	133.91	124.71
49	r	312	XAT	C31-C30-C29	-5.22	119.86	127.31
47	n	614	LUT	C21-C26-C25	5.19	120.72	111.42
29	y	312	CLA	C4A-NA-C1A	5.18	109.04	106.71
49	Y	301	XAT	C15-C14-C13	-5.15	119.96	127.31
34	b	519	C7Z	C35-C34-C33	-5.11	120.02	127.31
29	s	305	CLA	C4A-NA-C1A	5.11	109.00	106.71
29	B	504	CLA	C4A-NA-C1A	5.09	109.00	106.71
49	g	619	XAT	C15-C14-C13	-5.07	120.07	127.31
48	S	319	NEX	C2-C1-C6	5.06	114.13	109.21
49	R	311	XAT	C31-C30-C29	-5.03	120.13	127.31
47	S	317	LUT	C21-C26-C25	5.02	120.42	111.42
47	S	317	LUT	C21-C26-C27	5.00	119.02	112.70
29	r	302	CLA	C4A-NA-C1A	5.00	108.95	106.71
29	B	505	CLA	C4A-NA-C1A	4.98	108.94	106.71
29	c	507	CLA	C4A-NA-C1A	4.98	108.94	106.71
29	b	505	CLA	C4A-NA-C1A	4.98	108.94	106.71
43	d	405	PL9	C7-C3-C4	4.97	120.92	116.88
50	Y	320	PTY	O7-C8-C11	4.97	120.23	111.09
29	D	404	CLA	C1-O2A-CGA	4.96	129.46	116.44
50	y	321	PTY	O7-C8-C11	4.96	120.22	111.09
29	R	301	CLA	C4A-NA-C1A	4.93	108.92	106.71
29	r	307	CLA	C4A-NA-C1A	4.91	108.91	106.71
47	r	311	LUT	C21-C26-C25	4.90	120.20	111.42
29	D	404	CLA	O1D-CGD-CBD	4.89	134.48	124.48
48	Y	318	NEX	C2-C1-C6	4.88	113.96	109.21
29	c	502	CLA	C4A-NA-C1A	4.87	108.89	106.71
29	Y	311	CLA	C4A-NA-C1A	4.83	108.88	106.71
34	B	519	C7Z	C38-C25-C26	-4.83	119.11	124.53
47	R	310	LUT	C21-C26-C25	4.82	120.05	111.42
29	d	404	CLA	C4A-NA-C1A	4.82	108.87	106.71
34	b	519	C7Z	C1-C6-C5	-4.81	115.84	122.61
29	B	507	CLA	C4A-NA-C1A	4.80	108.86	106.71
29	b	503	CLA	C4A-NA-C1A	4.80	108.86	106.71
29	B	503	CLA	C4A-NA-C1A	4.80	108.86	106.71
29	c	511	CLA	C4A-NA-C1A	4.79	108.86	106.71
36	r	301	DGD	O2G-C1B-C2B	4.77	121.79	111.50
29	G	611	CLA	C4A-NA-C1A	4.76	108.85	106.71
29	C	503	CLA	C4A-NA-C1A	4.76	108.84	106.71
29	D	405	CLA	C4A-NA-C1A	4.73	108.83	106.71
48	r	313	NEX	C38-C25-C24	4.72	119.59	114.28
42	a	412	BCT	O3-C-O1	-4.71	107.32	119.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	y	302	XAT	C38-C25-C24	4.71	119.58	114.28
43	D	406	PL9	C7-C3-C4	4.69	120.69	116.88
34	b	519	C7Z	C38-C25-C26	-4.69	119.26	124.53
29	D	404	CLA	C2C-C1C-NC	4.69	114.36	109.97
47	y	318	LUT	C22-C23-C24	-4.68	106.41	111.74
29	s	316	CLA	C4A-NA-C1A	4.68	108.81	106.71
49	y	302	XAT	C18-C5-C4	4.68	119.54	114.28
48	S	319	NEX	C38-C25-C24	4.67	119.53	114.28
47	n	615	LUT	C21-C26-C27	4.65	118.58	112.70
29	n	609	CLA	C4A-NA-C1A	4.65	108.80	106.71
29	s	303	CLA	C4A-NA-C1A	4.64	108.79	106.71
47	n	614	LUT	C21-C26-C27	4.64	118.57	112.70
49	G	619	XAT	C18-C5-C4	4.64	119.50	114.28
29	c	505	CLA	C4A-NA-C1A	4.63	108.79	106.71
48	Y	318	NEX	C38-C25-C24	4.63	119.49	114.28
48	y	319	NEX	C38-C25-C24	4.62	119.48	114.28
35	W	201	LMG	O7-C10-C11	4.62	121.46	111.50
47	r	311	LUT	C21-C26-C27	4.62	118.54	112.70
29	S	314	CLA	C4A-NA-C1A	4.62	108.78	106.71
29	s	311	CLA	C4A-NA-C1A	4.61	108.78	106.71
29	y	304	CLA	C4A-NA-C1A	4.60	108.78	106.71
47	y	318	LUT	C21-C26-C27	4.60	118.52	112.70
48	s	319	NEX	C38-C25-C24	4.60	119.45	114.28
29	g	612	CLA	C4A-NA-C1A	4.59	108.77	106.71
48	R	312	NEX	C38-C25-C24	4.59	119.44	114.28
35	W	203	LMG	O7-C10-C11	4.58	121.38	111.50
47	N	616	LUT	C21-C26-C27	4.58	118.48	112.70
48	g	617	NEX	C27-C28-C29	-4.57	118.44	125.53
49	G	619	XAT	C38-C25-C24	4.55	119.40	114.28
48	n	616	NEX	C27-C28-C29	-4.55	118.47	125.53
48	G	617	NEX	C38-C25-C24	4.54	119.39	114.28
29	s	306	CLA	C4A-NA-C1A	4.54	108.75	106.71
29	y	306	CLA	C4A-NA-C1A	4.54	108.75	106.71
33	a	415	3PH	O21-C21-C22	4.53	121.26	111.50
48	G	617	NEX	C27-C28-C29	-4.53	118.50	125.53
29	s	310	CLA	C4A-NA-C1A	4.52	108.74	106.71
49	Y	301	XAT	C18-C5-C4	4.52	119.36	114.28
49	Y	301	XAT	C38-C25-C24	4.52	119.36	114.28
29	B	506	CLA	C4A-NA-C1A	4.52	108.74	106.71
34	B	519	C7Z	C7-C8-C9	-4.50	119.44	126.23
29	B	516	CLA	C4A-NA-C1A	4.49	108.72	106.71
34	B	519	C7Z	C1-C6-C5	-4.48	116.31	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	N	619	XAT	C18-C5-C4	4.46	119.30	114.28
47	g	616	LUT	C21-C26-C27	4.46	118.33	112.70
48	r	313	NEX	C27-C28-C29	-4.45	118.62	125.53
29	S	311	CLA	C4A-NA-C1A	4.44	108.70	106.71
33	S	322	3PH	O21-C21-C22	4.44	121.06	111.50
34	b	519	C7Z	C15-C14-C13	-4.43	120.99	127.31
31	K	101	BCR	C33-C5-C6	-4.43	119.55	124.53
47	R	310	LUT	C21-C26-C27	4.41	118.28	112.70
48	N	617	NEX	C38-C25-C24	4.41	119.25	114.28
29	a	404	CLA	C4A-NA-C1A	4.41	108.69	106.71
29	b	509	CLA	C4A-NA-C1A	4.41	108.69	106.71
49	n	618	XAT	C7-C8-C9	-4.41	118.69	125.53
29	Y	315	CLA	C4A-NA-C1A	4.40	108.68	106.71
29	d	403	CLA	CHD-C1D-ND	-4.39	120.42	124.45
49	N	619	XAT	C7-C8-C9	-4.38	118.73	125.53
36	B	521	DGD	O2G-C1B-C2B	4.38	120.95	111.50
29	S	316	CLA	C4A-NA-C1A	4.38	108.68	106.71
49	n	618	XAT	C18-C5-C4	4.37	119.20	114.28
48	g	617	NEX	C38-C25-C24	4.37	119.19	114.28
29	D	404	CLA	C4A-NA-C1A	4.36	108.67	106.71
48	n	616	NEX	C38-C25-C24	4.36	119.18	114.28
49	R	311	XAT	C38-C25-C24	4.35	119.18	114.28
29	r	309	CLA	C4A-NA-C1A	4.34	108.66	106.71
29	b	506	CLA	C4A-NA-C1A	4.34	108.66	106.71
49	g	619	XAT	C18-C5-C4	4.33	119.15	114.28
46	y	311	CHL	C2C-C3C-C4C	4.33	109.58	106.49
35	C	524	LMG	O7-C10-C11	4.32	120.82	111.50
47	s	317	LUT	C21-C26-C27	4.32	118.16	112.70
34	B	519	C7Z	C15-C14-C13	-4.31	121.16	127.31
29	n	613	CLA	C4A-NA-C1A	4.30	108.64	106.71
29	c	504	CLA	C4A-NA-C1A	4.30	108.64	106.71
48	y	319	NEX	C27-C28-C29	-4.30	118.86	125.53
37	N	618	LHG	O7-C7-C8	4.29	120.74	111.50
49	g	619	XAT	C7-C8-C9	-4.27	118.90	125.53
33	b	521	3PH	O21-C21-C22	4.27	120.71	111.50
47	S	318	LUT	C35-C34-C33	-4.27	121.21	127.31
48	Y	318	NEX	C27-C28-C29	-4.27	118.90	125.53
49	r	312	XAT	C18-C5-C4	4.27	119.08	114.28
29	g	611	CLA	C4A-NA-C1A	4.26	108.62	106.71
37	n	617	LHG	O7-C7-C8	4.26	120.69	111.50
37	S	301	LHG	O7-C7-C8	4.26	120.68	111.50
29	s	314	CLA	C4A-NA-C1A	4.26	108.62	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	g	614	CLA	C4A-NA-C1A	4.24	108.61	106.71
48	N	617	NEX	C27-C28-C29	-4.23	118.96	125.53
47	Y	317	LUT	C22-C23-C24	-4.23	106.93	111.74
48	R	312	NEX	C27-C28-C29	-4.23	118.97	125.53
49	g	619	XAT	C38-C25-C24	4.22	119.03	114.28
34	b	519	C7Z	C7-C8-C9	-4.21	119.88	126.23
29	R	303	CLA	CHD-C1D-ND	-4.21	120.59	124.45
47	Y	317	LUT	C21-C26-C27	4.19	117.99	112.70
29	n	613	CLA	CHD-C1D-ND	-4.19	120.61	124.45
45	h	101	RRX	C24-C23-C22	-4.18	119.91	126.23
29	S	312	CLA	C4A-NA-C1A	4.17	108.58	106.71
46	S	309	CHL	CHD-C1D-ND	-4.17	120.62	124.45
35	C	521	LMG	O7-C10-C11	4.16	120.46	111.50
47	g	616	LUT	C15-C14-C13	-4.15	121.38	127.31
29	S	304	CLA	C4A-NA-C1A	4.15	108.57	106.71
29	S	304	CLA	CHD-C1D-ND	-4.14	120.65	124.45
46	g	601	CHL	CHD-C1D-ND	-4.14	120.65	124.45
47	g	616	LUT	C35-C34-C33	-4.14	121.41	127.31
47	N	615	LUT	C21-C26-C27	4.13	117.93	112.70
47	g	615	LUT	C35-C34-C33	-4.13	121.42	127.31
47	Y	316	LUT	C15-C14-C13	-4.12	121.43	127.31
46	n	608	CHL	CHD-C1D-ND	-4.12	120.67	124.45
49	r	312	XAT	C38-C25-C24	4.11	118.90	114.28
48	g	617	NEX	C17-C1-C6	-4.11	106.80	110.47
37	s	301	LHG	O7-C7-C8	4.10	120.34	111.50
29	B	509	CLA	C4A-NA-C1A	4.10	108.55	106.71
37	c	521	LHG	O7-C7-C8	4.09	120.33	111.50
37	S	320	LHG	O7-C7-C8	4.09	120.32	111.50
37	y	320	LHG	O7-C7-C8	4.09	120.32	111.50
46	y	311	CHL	CHD-C1D-ND	-4.09	120.70	124.45
46	Y	310	CHL	CHD-C1D-ND	-4.08	120.70	124.45
34	b	519	C7Z	C27-C28-C29	-4.08	120.07	126.23
33	s	322	3PH	O21-C21-C22	4.07	120.28	111.50
35	i	101	LMG	O7-C10-C11	4.07	120.27	111.50
47	r	311	LUT	C1-C6-C5	-4.07	116.89	122.61
49	g	619	XAT	C36-C21-C26	4.06	121.00	110.05
37	G	618	LHG	O7-C7-C8	4.05	120.24	111.50
47	R	310	LUT	C15-C14-C13	-4.04	121.54	127.31
29	B	502	CLA	C4A-NA-C1A	4.04	108.52	106.71
29	R	306	CLA	C4A-NA-C1A	4.04	108.52	106.71
47	s	318	LUT	C35-C34-C33	-4.04	121.55	127.31
29	S	316	CLA	CHD-C1D-ND	-4.03	120.75	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S	310	CLA	C4A-NA-C1A	4.03	108.52	106.71
29	B	512	CLA	C4A-NA-C1A	4.02	108.51	106.71
29	A	406	CLA	C4A-NA-C1A	4.01	108.51	106.71
47	R	310	LUT	C18-C5-C6	-4.01	120.03	124.53
47	G	616	LUT	C15-C14-C13	-4.01	121.59	127.31
47	G	615	LUT	C22-C23-C24	-4.00	107.19	111.74
46	G	601	CHL	CHD-C1D-ND	-4.00	120.78	124.45
47	R	310	LUT	C11-C10-C9	-4.00	121.60	127.31
30	A	408	PHO	C2B-C1B-NB	-3.99	106.77	109.53
29	n	602	CLA	C4A-NA-C1A	3.99	108.50	106.71
46	n	605	CHL	CHD-C1D-ND	-3.99	120.79	124.45
33	A	412	3PH	O21-C21-C22	3.98	120.07	111.50
33	B	522	3PH	O21-C21-C22	3.98	120.07	111.50
35	d	408	LMG	O7-C10-C11	3.97	120.06	111.50
37	g	618	LHG	O7-C7-C8	3.97	120.06	111.50
29	c	513	CLA	C4A-NA-C1A	3.97	108.49	106.71
37	a	414	LHG	O7-C7-C8	3.97	120.05	111.50
48	S	319	NEX	C17-C1-C6	-3.96	106.93	110.47
37	s	320	LHG	O7-C7-C8	3.96	120.03	111.50
49	G	619	XAT	C36-C21-C26	3.96	120.73	110.05
47	N	616	LUT	C22-C23-C24	-3.95	107.24	111.74
29	a	406	CLA	CHD-C1D-ND	-3.95	120.82	124.45
46	N	605	CHL	CHD-C1D-ND	-3.95	120.82	124.45
47	G	615	LUT	C21-C26-C27	3.95	117.70	112.70
49	r	312	XAT	C15-C14-C13	-3.95	121.68	127.31
46	y	311	CHL	C3C-C4C-NC	-3.95	106.14	110.57
29	C	509	CLA	CHD-C1D-ND	-3.94	120.83	124.45
48	S	319	NEX	C27-C28-C29	-3.94	119.42	125.53
47	g	616	LUT	C22-C23-C24	-3.93	107.26	111.74
41	J	101	DGA	OG2-CB1-CB2	3.93	119.97	111.50
29	N	614	CLA	C4A-NA-C1A	3.92	108.47	106.71
49	R	311	XAT	C18-C5-C4	3.92	118.69	114.28
47	Y	317	LUT	C15-C14-C13	-3.92	121.72	127.31
47	s	318	LUT	C21-C26-C27	3.91	117.64	112.70
34	b	519	C7Z	C31-C30-C29	-3.90	121.74	127.31
46	Y	307	CHL	CHD-C1D-ND	-3.90	120.87	124.45
34	B	519	C7Z	C27-C28-C29	-3.90	120.34	126.23
41	w	201	DGA	OG2-CB1-CB2	3.90	119.91	111.50
34	B	519	C7Z	C31-C30-C29	-3.90	121.75	127.31
29	C	505	CLA	C4A-NA-C1A	3.90	108.46	106.71
45	h	101	RRX	C38-C26-C25	-3.90	120.15	124.53
30	D	401	PHO	C2B-C1B-NB	-3.90	106.84	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	522	LMG	O7-C10-C11	3.89	119.89	111.50
46	N	606	CHL	C3B-C4B-NB	-3.89	106.91	110.52
37	D	408	LHG	O7-C7-C8	3.89	119.89	111.50
29	g	602	CLA	C4A-NA-C1A	3.88	108.45	106.71
48	s	319	NEX	C27-C28-C29	-3.87	119.52	125.53
46	G	609	CHL	CHD-C1D-ND	-3.87	120.89	124.45
41	D	402	DGA	OG2-CB1-CB2	3.87	119.85	111.50
41	b	522	DGA	OG2-CB1-CB2	3.87	119.84	111.50
48	G	617	NEX	C31-C30-C29	3.87	132.83	127.31
35	b	520	LMG	O7-C10-C11	3.86	119.83	111.50
46	Y	306	CHL	CHD-C1D-ND	-3.86	120.90	124.45
47	Y	317	LUT	C7-C8-C9	-3.86	120.40	126.23
29	G	612	CLA	C4A-NA-C1A	3.86	108.44	106.71
29	r	310	CLA	CHD-C1D-ND	-3.86	120.91	124.45
50	n	619	PTY	O7-C8-C11	3.86	119.81	111.50
49	r	312	XAT	O4-C5-C4	-3.86	110.49	113.38
50	N	620	PTY	O7-C8-C11	3.85	119.81	111.50
49	R	311	XAT	C15-C14-C13	-3.85	121.81	127.31
47	y	318	LUT	C15-C14-C13	-3.85	121.82	127.31
47	S	318	LUT	C21-C26-C27	3.85	117.56	112.70
29	R	307	CLA	CHD-C1D-ND	-3.84	120.92	124.45
29	s	304	CLA	C3B-C4B-NB	-3.84	106.95	110.52
35	c	519	LMG	O7-C10-C11	3.84	119.78	111.50
47	y	318	LUT	C35-C34-C33	-3.84	121.83	127.31
47	Y	317	LUT	C35-C34-C33	-3.84	121.83	127.31
41	W	202	DGA	OG2-CB1-CB2	3.83	119.77	111.50
41	j	101	DGA	OG2-CB1-CB2	3.83	119.76	111.50
29	S	314	CLA	CHD-C1D-ND	-3.83	120.94	124.45
47	G	616	LUT	C21-C26-C27	3.83	117.54	112.70
29	b	514	CLA	C4A-NA-C1A	3.81	108.42	106.71
30	d	402	PHO	C2B-C1B-NB	-3.81	106.89	109.53
47	g	616	LUT	C7-C8-C9	-3.81	120.48	126.23
46	g	609	CHL	CHD-C1D-ND	-3.80	120.96	124.45
29	B	514	CLA	C4A-NA-C1A	3.80	108.41	106.71
29	y	314	CLA	C4A-NA-C1A	3.80	108.41	106.71
36	c	516	DGD	O2G-C1B-C2B	3.80	119.69	111.50
29	S	303	CLA	CHD-C1D-ND	-3.80	120.96	124.45
47	G	616	LUT	C35-C34-C33	-3.79	121.89	127.31
36	C	520	DGD	O2G-C1B-C2B	3.79	119.67	111.50
47	n	615	LUT	C35-C34-C33	-3.79	121.90	127.31
35	D	410	LMG	O7-C10-C11	3.79	119.66	111.50
49	G	619	XAT	C7-C8-C9	-3.79	119.66	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S	315	CLA	CHD-C1D-ND	-3.78	120.98	124.45
29	B	514	CLA	CHD-C1D-ND	-3.78	120.98	124.45
29	C	510	CLA	CHD-C1D-ND	-3.78	120.98	124.45
47	s	317	LUT	C35-C34-C33	-3.78	121.91	127.31
37	a	413	LHG	O7-C7-C8	3.78	119.65	111.50
29	S	305	CLA	C4A-NA-C1A	3.78	108.41	106.71
29	R	308	CLA	C4A-NA-C1A	3.77	108.40	106.71
47	y	317	LUT	C15-C14-C13	-3.77	121.94	127.31
46	y	307	CHL	CHD-C1D-ND	-3.77	120.99	124.45
29	s	303	CLA	CHD-C1D-ND	-3.76	121.00	124.45
37	Y	319	LHG	O7-C7-C8	3.76	119.61	111.50
46	s	309	CHL	CHD-C1D-ND	-3.76	121.00	124.45
49	n	618	XAT	C38-C25-C24	3.76	118.51	114.28
41	D	402	DGA	CDB-CCB-CBB	-3.76	80.40	115.30
31	B	517	BCR	C33-C5-C4	3.76	120.84	113.62
36	c	518	DGD	O2G-C1B-C2B	3.76	119.60	111.50
31	A	410	BCR	C12-C13-C14	-3.76	113.18	118.94
29	a	405	CLA	CHD-C1D-ND	-3.76	121.00	124.45
47	N	616	LUT	C35-C34-C33	-3.75	121.95	127.31
29	s	312	CLA	C4A-NA-C1A	3.75	108.39	106.71
46	s	302	CHL	CHD-C1D-ND	-3.74	121.01	124.45
29	A	407	CLA	CHD-C1D-ND	-3.74	121.01	124.45
46	r	306	CHL	CHD-C1D-ND	-3.74	121.02	124.45
29	y	305	CLA	CHD-C1D-ND	-3.74	121.02	124.45
37	B	523	LHG	O7-C7-C8	3.74	119.56	111.50
46	g	606	CHL	CHD-C1D-ND	-3.73	121.02	124.45
29	C	511	CLA	CHD-C1D-ND	-3.73	121.03	124.45
29	Y	312	CLA	CHD-C1D-ND	-3.73	121.03	124.45
49	r	312	XAT	C6-C7-C8	-3.73	118.11	125.99
47	R	310	LUT	C35-C34-C33	-3.73	121.99	127.31
29	s	312	CLA	CHD-C1D-ND	-3.72	121.03	124.45
29	D	404	CLA	CBC-CAC-C3C	-3.72	102.18	112.43
29	B	512	CLA	CHD-C1D-ND	-3.72	121.04	124.45
49	N	619	XAT	C38-C25-C24	3.72	118.46	114.28
29	R	307	CLA	C4A-NA-C1A	3.71	108.37	106.71
29	b	514	CLA	CHD-C1D-ND	-3.71	121.05	124.45
47	S	317	LUT	C15-C14-C13	-3.71	122.02	127.31
47	g	615	LUT	C15-C14-C13	-3.71	122.02	127.31
46	r	306	CHL	C3C-C4C-NC	-3.70	106.42	110.57
35	B	520	LMG	O7-C10-C11	3.70	119.48	111.50
46	N	608	CHL	CHD-C1D-ND	-3.70	121.05	124.45
46	S	308	CHL	CHD-C1D-ND	-3.70	121.06	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y	303	CLA	C4A-NA-C1A	3.69	108.37	106.71
45	h	101	RRX	C33-C5-C6	-3.69	120.38	124.53
39	a	410	SQD	O7-S-C6	-3.69	102.55	106.94
31	a	409	BCR	C12-C13-C14	-3.69	113.28	118.94
31	B	517	BCR	C33-C5-C6	-3.69	120.38	124.53
46	R	305	CHL	CHD-C1D-ND	-3.69	121.07	124.45
46	S	302	CHL	CHD-C1D-ND	-3.68	121.08	124.45
47	Y	316	LUT	C21-C26-C27	3.68	117.35	112.70
46	Y	307	CHL	C3B-C4B-NB	-3.67	107.11	110.52
46	S	307	CHL	CHD-C1D-ND	-3.67	121.08	124.45
29	c	509	CLA	CHD-C1D-ND	-3.67	121.08	124.45
29	b	513	CLA	C4A-NA-C1A	3.67	108.36	106.71
46	N	607	CHL	CHD-C1D-ND	-3.67	121.08	124.45
29	G	602	CLA	CHD-C1D-ND	-3.67	121.08	124.45
29	d	403	CLA	C4A-NA-C1A	3.66	108.35	106.71
39	o	301	SQD	O7-S-C6	-3.66	102.59	106.94
35	d	407	LMG	O7-C10-C11	3.66	119.39	111.50
46	s	307	CHL	CHD-C1D-ND	-3.66	121.09	124.45
30	d	402	PHO	CMB-C2B-C3B	3.65	131.52	124.68
48	g	617	NEX	C31-C30-C29	3.65	132.53	127.31
39	C	501	SQD	O7-S-C6	-3.65	102.60	106.94
29	s	313	CLA	C4A-NA-C1A	3.65	108.35	106.71
46	n	601	CHL	CHD-C1D-ND	-3.65	121.10	124.45
31	b	517	BCR	C23-C24-C25	-3.65	116.95	127.20
46	y	303	CHL	CHD-C1D-ND	-3.65	121.10	124.45
48	g	617	NEX	C2-C1-C6	3.65	112.76	109.21
29	s	311	CLA	CHD-C1D-ND	-3.65	121.10	124.45
31	K	101	BCR	C36-C18-C17	-3.65	117.81	122.92
49	R	311	XAT	O4-C5-C4	-3.65	110.64	113.38
29	c	508	CLA	CHD-C1D-ND	-3.65	121.10	124.45
46	G	601	CHL	C3C-C4C-NC	-3.64	106.48	110.57
29	R	306	CLA	CHD-C1D-ND	-3.64	121.11	124.45
46	G	605	CHL	C2C-C3C-C4C	3.64	109.08	106.49
29	c	509	CLA	C4A-NA-C1A	3.63	108.34	106.71
30	D	401	PHO	CMB-C2B-C3B	3.63	131.47	124.68
29	s	314	CLA	CHD-C1D-ND	-3.63	121.12	124.45
46	n	607	CHL	CHD-C1D-ND	-3.63	121.12	124.45
46	G	606	CHL	C3B-C4B-NB	-3.62	107.15	110.52
35	c	520	LMG	O7-C10-C11	3.62	119.30	111.50
47	y	318	LUT	C7-C8-C9	-3.62	120.77	126.23
29	s	304	CLA	C2B-C1B-NB	-3.62	107.81	110.23
47	r	311	LUT	C11-C10-C9	-3.61	122.16	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	s	319	NEX	C5-C4-C3	3.61	116.02	111.75
46	s	308	CHL	CHD-C1D-ND	-3.61	121.14	124.45
39	c	522	SQD	O7-S-C6	-3.61	102.65	106.94
31	A	410	BCR	C33-C5-C6	-3.60	120.48	124.53
29	y	313	CLA	CHD-C1D-ND	-3.60	121.14	124.45
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
29	n	611	CLA	CHD-C1D-ND	-3.60	121.15	124.45
47	N	615	LUT	C22-C23-C24	-3.60	107.65	111.74
29	B	509	CLA	CHD-C1D-ND	-3.60	121.15	124.45
45	H	101	RRX	C33-C5-C6	-3.60	120.49	124.53
29	N	611	CLA	CHD-C1D-ND	-3.59	121.15	124.45
47	s	318	LUT	C15-C14-C13	-3.59	122.18	127.31
34	B	519	C7Z	C1-C6-C7	3.59	125.93	115.78
37	d	406	LHG	O7-C7-C8	3.59	119.24	111.50
47	R	310	LUT	C7-C8-C9	-3.59	120.81	126.23
49	y	302	XAT	C6-C7-C8	-3.59	118.41	125.99
46	y	301	CHL	CHD-C1D-ND	-3.59	121.16	124.45
49	y	302	XAT	O4-C5-C4	-3.58	110.69	113.38
47	G	615	LUT	C35-C34-C33	-3.58	122.19	127.31
46	n	608	CHL	C3C-C4C-NC	-3.58	106.55	110.57
49	y	302	XAT	C7-C8-C9	-3.58	119.97	125.53
46	S	302	CHL	C3B-C4B-NB	-3.58	107.19	110.52
39	M	101	SQD	O7-S-C6	-3.58	102.68	106.94
47	g	616	LUT	C11-C10-C9	-3.58	122.20	127.31
46	g	607	CHL	C1-O2A-CGA	3.58	125.84	116.44
29	s	315	CLA	CHD-C1D-ND	-3.58	121.17	124.45
31	C	517	BCR	C28-C27-C26	-3.58	107.69	114.08
29	Y	309	CLA	C4A-NA-C1A	3.58	108.31	106.71
29	S	306	CLA	CHD-C1D-ND	-3.58	121.17	124.45
47	N	615	LUT	C35-C34-C33	-3.57	122.21	127.31
29	C	510	CLA	C4A-NA-C1A	3.57	108.31	106.71
46	n	601	CHL	C3C-C4C-NC	-3.57	106.57	110.57
29	Y	309	CLA	CHD-C1D-ND	-3.57	121.17	124.45
29	Y	305	CLA	C4A-NA-C1A	3.57	108.31	106.71
49	Y	301	XAT	C6-C7-C8	-3.57	118.45	125.99
31	B	517	BCR	C12-C13-C14	-3.56	113.47	118.94
30	a	407	PHO	C2B-C1B-NB	-3.56	107.07	109.53
29	B	513	CLA	C4A-NA-C1A	3.56	108.31	106.71
47	y	317	LUT	C21-C26-C27	3.56	117.20	112.70
46	n	605	CHL	C3C-C4C-NC	-3.56	106.58	110.57
29	b	508	CLA	CHD-C1D-ND	-3.56	121.18	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s	313	CLA	CHD-C1D-ND	-3.56	121.19	124.45
47	S	318	LUT	C18-C5-C6	-3.56	120.53	124.53
48	G	617	NEX	C39-C29-C30	-3.56	117.94	122.92
46	G	608	CHL	CHD-C1D-ND	-3.55	121.19	124.45
29	y	316	CLA	CHD-C1D-ND	-3.55	121.19	124.45
29	n	612	CLA	C4A-NA-C1A	3.55	108.30	106.71
39	m	101	SQD	O7-S-C6	-3.55	102.72	106.94
29	B	511	CLA	C4A-NA-C1A	3.55	108.30	106.71
35	w	202	LMG	O7-C10-C11	3.55	119.14	111.50
48	Y	318	NEX	C17-C1-C6	-3.55	107.30	110.47
31	C	516	BCR	C23-C24-C25	-3.54	117.25	127.20
29	g	604	CLA	CHD-C1D-ND	-3.54	121.20	124.45
29	r	308	CLA	C4A-NA-C1A	3.53	108.30	106.71
29	s	312	CLA	C3B-C4B-NB	-3.53	107.24	110.52
29	S	310	CLA	CHD-C1D-ND	-3.53	121.21	124.45
46	g	606	CHL	C3B-C4B-NB	-3.53	107.24	110.52
29	Y	303	CLA	CHD-C1D-ND	-3.53	121.21	124.45
46	g	608	CHL	CHD-C1D-ND	-3.52	121.22	124.45
47	G	615	LUT	C15-C14-C13	-3.52	122.28	127.31
48	y	319	NEX	C39-C29-C30	-3.52	117.99	122.92
29	c	507	CLA	CHD-C1D-ND	-3.52	121.22	124.45
29	b	502	CLA	CHD-C1D-ND	-3.52	121.22	124.45
29	n	602	CLA	CHD-C1D-ND	-3.52	121.22	124.45
31	a	409	BCR	C33-C5-C6	-3.52	120.58	124.53
29	B	505	CLA	CHD-C1D-ND	-3.51	121.22	124.45
48	g	617	NEX	C39-C29-C30	-3.51	118.00	122.92
39	b	523	SQD	O7-S-C6	-3.51	102.77	106.94
29	c	501	CLA	C4A-NA-C1A	3.51	108.28	106.71
31	v	101	BCR	C36-C18-C17	-3.50	118.02	122.92
30	A	408	PHO	CMB-C2B-C3B	3.50	131.23	124.68
31	c	514	BCR	C23-C24-C25	-3.50	117.38	127.20
29	a	408	CLA	C4A-NA-C1A	3.50	108.28	106.71
29	r	308	CLA	CHD-C1D-ND	-3.50	121.24	124.45
29	s	316	CLA	CHD-C1D-ND	-3.49	121.24	124.45
46	G	601	CHL	C2C-C3C-C4C	3.49	108.98	106.49
46	g	607	CHL	CHD-C1D-ND	-3.49	121.24	124.45
48	r	313	NEX	C31-C30-C29	3.49	132.29	127.31
29	C	506	CLA	CHD-C1D-ND	-3.49	121.25	124.45
46	S	302	CHL	C3C-C4C-NC	-3.49	106.66	110.57
46	g	607	CHL	C1-C2-C3	-3.49	120.01	126.04
31	a	409	BCR	C23-C24-C25	-3.49	117.41	127.20
46	s	302	CHL	C3B-C4B-NB	-3.48	107.28	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	Y	302	CHL	CHD-C1D-ND	-3.48	121.25	124.45
46	g	601	CHL	C3C-C4C-NC	-3.48	106.66	110.57
47	s	318	LUT	C7-C8-C9	-3.48	120.97	126.23
29	y	312	CLA	CHD-C1D-ND	-3.48	121.26	124.45
36	C	519	DGD	O2G-C1B-C2B	3.48	119.00	111.50
39	C	523	SQD	O7-S-C6	-3.48	102.80	106.94
31	f	101	BCR	C19-C18-C17	3.48	124.28	118.94
36	C	518	DGD	O2G-C1B-C2B	3.48	118.99	111.50
29	y	310	CLA	CHD-C1D-ND	-3.47	121.26	124.45
29	C	506	CLA	C4A-NA-C1A	3.47	108.27	106.71
29	y	310	CLA	C4A-NA-C1A	3.47	108.27	106.71
46	G	606	CHL	C2C-C3C-C4C	3.47	108.97	106.49
31	v	101	BCR	C33-C5-C6	-3.47	120.63	124.53
47	g	615	LUT	C22-C23-C24	-3.47	107.80	111.74
46	y	309	CHL	C4A-NA-C1A	3.46	108.26	106.71
47	s	317	LUT	C7-C8-C9	-3.46	121.00	126.23
29	n	609	CLA	CHD-C1D-ND	-3.46	121.27	124.45
47	g	615	LUT	C7-C8-C9	-3.46	121.01	126.23
46	G	606	CHL	CHD-C1D-ND	-3.46	121.28	124.45
29	s	305	CLA	CHD-C1D-ND	-3.45	121.28	124.45
35	D	409	LMG	O7-C10-C11	3.45	118.94	111.50
49	y	302	XAT	O24-C25-C24	3.45	115.97	113.38
47	g	615	LUT	C21-C26-C27	3.45	117.06	112.70
46	N	609	CHL	C3C-C4C-NC	-3.45	106.70	110.57
29	B	503	CLA	CHD-C1D-ND	-3.44	121.29	124.45
29	B	502	CLA	CHD-C1D-ND	-3.44	121.29	124.45
47	n	614	LUT	C15-C14-C13	-3.44	122.40	127.31
47	s	317	LUT	C22-C23-C24	-3.44	107.82	111.74
39	l	101	SQD	O7-S-C6	-3.44	102.85	106.94
29	r	309	CLA	CHD-C1D-ND	-3.44	121.29	124.45
48	y	319	NEX	C31-C30-C29	3.44	132.22	127.31
30	a	407	PHO	CMB-C2B-C3B	3.44	131.11	124.68
29	Y	304	CLA	CHD-C1D-ND	-3.43	121.30	124.45
29	C	514	CLA	C4A-NA-C1A	3.43	108.25	106.71
29	b	512	CLA	CHD-C1D-ND	-3.43	121.30	124.45
46	N	601	CHL	CHD-C1D-ND	-3.43	121.30	124.45
49	R	311	XAT	C6-C7-C8	-3.43	118.74	125.99
46	G	605	CHL	C3C-C4C-NC	-3.43	106.73	110.57
29	b	505	CLA	CHD-C1D-ND	-3.43	121.31	124.45
29	b	503	CLA	CHD-C1D-ND	-3.42	121.31	124.45
46	r	305	CHL	CHD-C1D-ND	-3.42	121.31	124.45
47	G	616	LUT	C7-C8-C9	-3.42	121.06	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	511	CLA	C4A-NA-C1A	3.42	108.25	106.71
47	S	317	LUT	C35-C34-C33	-3.42	122.42	127.31
29	g	611	CLA	CHD-C1D-ND	-3.42	121.31	124.45
46	n	606	CHL	C3B-C4B-NB	-3.42	107.35	110.52
46	y	308	CHL	CHD-C1D-ND	-3.41	121.32	124.45
39	L	102	SQD	O7-S-C6	-3.41	102.88	106.94
29	S	316	CLA	C3B-C4B-NB	-3.41	107.35	110.52
29	b	501	CLA	C4A-NA-C1A	3.41	108.24	106.71
48	R	312	NEX	C39-C29-C30	-3.40	118.16	122.92
29	G	604	CLA	CHD-C1D-ND	-3.40	121.33	124.45
46	G	608	CHL	C3B-C4B-NB	-3.40	107.36	110.52
46	R	304	CHL	CHD-C1D-ND	-3.40	121.33	124.45
48	N	617	NEX	C39-C29-C30	-3.39	118.17	122.92
49	N	619	XAT	C38-C25-C26	-3.39	116.58	122.26
31	A	410	BCR	C23-C24-C25	-3.39	117.67	127.20
34	B	519	C7Z	C28-C27-C26	-3.39	117.68	127.20
49	Y	301	XAT	O4-C5-C4	-3.39	110.83	113.38
47	S	318	LUT	C15-C14-C13	-3.39	122.47	127.31
47	S	318	LUT	C22-C23-C24	-3.39	107.88	111.74
47	N	616	LUT	C7-C8-C9	-3.39	121.11	126.23
47	n	615	LUT	C7-C8-C9	-3.39	121.12	126.23
48	G	617	NEX	C17-C1-C6	-3.38	107.44	110.47
47	n	615	LUT	C15-C14-C13	-3.38	122.48	127.31
46	N	609	CHL	CHD-C1D-ND	-3.38	121.35	124.45
49	n	618	XAT	C38-C25-C26	-3.38	116.59	122.26
29	d	404	CLA	CHD-C1D-ND	-3.38	121.35	124.45
48	r	313	NEX	C39-C29-C30	-3.38	118.19	122.92
29	A	409	CLA	CHD-C1D-ND	-3.38	121.35	124.45
29	D	405	CLA	CHD-C1D-ND	-3.38	121.35	124.45
29	c	502	CLA	CHD-C1D-ND	-3.38	121.35	124.45
29	D	404	CLA	C2A-C1A-CHA	-3.38	117.95	123.86
37	l	102	LHG	O7-C7-C8	3.37	118.77	111.50
31	B	517	BCR	C23-C24-C25	-3.37	117.72	127.20
29	b	513	CLA	CHD-C1D-ND	-3.37	121.35	124.45
46	N	605	CHL	C3C-C4C-NC	-3.37	106.79	110.57
29	r	307	CLA	CHD-C1D-ND	-3.37	121.36	124.45
35	C	524	LMG	O8-C28-C29	3.37	122.49	111.91
46	R	305	CHL	C3C-C4C-NC	-3.37	106.79	110.57
29	y	316	CLA	C4A-NA-C1A	3.37	108.22	106.71
45	H	101	RRX	C38-C26-C25	-3.37	120.75	124.53
47	N	615	LUT	C15-C14-C13	-3.36	122.52	127.31
29	A	406	CLA	CHD-C1D-ND	-3.36	121.37	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	R	309	CLA	C3B-C4B-NB	-3.36	107.40	110.52
46	y	301	CHL	C3C-C4C-NC	-3.36	106.81	110.57
29	Y	311	CLA	CHD-C1D-ND	-3.36	121.37	124.45
29	b	510	CLA	CHD-C1D-ND	-3.35	121.37	124.45
47	n	614	LUT	C35-C34-C33	-3.35	122.53	127.31
46	N	605	CHL	C2C-C3C-C4C	3.35	108.88	106.49
46	G	605	CHL	CHD-C1D-ND	-3.35	121.38	124.45
46	s	302	CHL	C3C-C4C-NC	-3.35	106.82	110.57
47	y	317	LUT	C35-C34-C33	-3.35	122.53	127.31
29	S	316	CLA	C2D-C1D-ND	-3.35	107.64	110.10
46	S	307	CHL	C3B-C4B-NB	-3.34	107.41	110.52
46	n	601	CHL	C2C-C3C-C4C	3.34	108.87	106.49
46	Y	310	CHL	C3C-C4C-NC	-3.34	106.82	110.57
29	G	610	CLA	CHD-C1D-ND	-3.34	121.38	124.45
29	N	604	CLA	C4A-NA-C1A	3.34	108.21	106.71
47	s	317	LUT	C15-C14-C13	-3.34	122.55	127.31
31	c	514	BCR	C12-C13-C14	-3.34	113.82	118.94
36	c	517	DGD	O2G-C1B-C2B	3.33	118.69	111.50
29	G	614	CLA	CHD-C1D-ND	-3.33	121.39	124.45
48	n	616	NEX	C39-C29-C30	-3.33	118.26	122.92
29	N	611	CLA	C4A-NA-C1A	3.33	108.20	106.71
29	g	613	CLA	CHD-C1D-ND	-3.33	121.40	124.45
29	B	510	CLA	CHD-C1D-ND	-3.33	121.40	124.45
46	S	309	CHL	C2C-C3C-C4C	3.32	108.86	106.49
47	G	616	LUT	C31-C30-C29	-3.32	122.57	127.31
48	Y	318	NEX	C39-C29-C30	-3.32	118.27	122.92
29	c	504	CLA	CHD-C1D-ND	-3.32	121.40	124.45
47	s	317	LUT	C35-C15-C14	-3.32	116.68	123.47
29	S	304	CLA	C3B-C4B-NB	-3.32	107.44	110.52
29	g	612	CLA	CHD-C1D-ND	-3.31	121.41	124.45
29	Y	313	CLA	C4A-NA-C1A	3.31	108.19	106.71
47	r	311	LUT	C15-C14-C13	-3.31	122.59	127.31
49	Y	301	XAT	C7-C8-C9	-3.31	120.40	125.53
46	s	308	CHL	C2C-C3C-C4C	3.31	108.84	106.49
31	f	101	BCR	C36-C18-C17	-3.30	118.30	122.92
46	S	309	CHL	C3C-C4C-NC	-3.30	106.87	110.57
47	Y	316	LUT	C35-C34-C33	-3.30	122.60	127.31
46	s	308	CHL	C3B-C4B-NB	-3.30	107.45	110.52
31	c	514	BCR	C2-C1-C6	3.30	115.56	110.48
29	Y	313	CLA	CHD-C1D-ND	-3.30	121.42	124.45
47	g	616	LUT	C18-C5-C6	-3.30	120.83	124.53
46	S	308	CHL	C3C-C4C-NC	-3.30	106.88	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	N	601	CHL	C3C-C4C-NC	-3.29	106.88	110.57
29	c	510	CLA	CHD-C1D-ND	-3.29	121.43	124.45
29	C	509	CLA	C4A-NA-C1A	3.29	108.19	106.71
29	N	613	CLA	C4A-NA-C1A	3.29	108.19	106.71
46	s	309	CHL	C4B-CHC-C1C	3.29	134.14	126.34
29	a	408	CLA	CHD-C1D-ND	-3.29	121.43	124.45
48	y	319	NEX	C5-C4-C3	3.28	115.63	111.75
31	a	409	BCR	C35-C13-C12	3.28	123.25	118.08
31	A	410	BCR	C35-C13-C12	3.28	123.25	118.08
46	s	308	CHL	C3C-C4C-NC	-3.28	106.89	110.57
29	g	614	CLA	CHD-C1D-ND	-3.28	121.44	124.45
29	S	311	CLA	CHD-C1D-ND	-3.28	121.44	124.45
29	n	610	CLA	CHD-C1D-ND	-3.28	121.44	124.45
31	F	101	BCR	C33-C5-C6	-3.28	120.84	124.53
31	C	516	BCR	C33-C5-C6	-3.28	120.84	124.53
29	g	602	CLA	CHD-C1D-ND	-3.28	121.44	124.45
46	S	302	CHL	C2C-C3C-C4C	3.28	108.83	106.49
29	r	302	CLA	CHD-C1D-ND	-3.28	121.44	124.45
48	s	319	NEX	C19-C9-C10	-3.28	118.33	122.92
29	s	310	CLA	CHD-C1D-ND	-3.27	121.45	124.45
48	N	617	NEX	C31-C30-C29	3.27	131.98	127.31
29	D	404	CLA	C4D-CHA-C1A	-3.27	117.27	121.25
31	K	101	BCR	C19-C18-C17	3.26	123.94	118.94
31	B	517	BCR	C35-C13-C12	3.26	123.21	118.08
46	y	307	CHL	C3C-C4C-NC	-3.26	106.92	110.57
29	G	611	CLA	CHD-C1D-ND	-3.25	121.46	124.45
29	A	409	CLA	C4A-NA-C1A	3.25	108.17	106.71
34	b	519	C7Z	C28-C27-C26	-3.25	118.07	127.20
29	B	506	CLA	CHD-C1D-ND	-3.25	121.47	124.45
29	C	505	CLA	CHD-C1D-ND	-3.25	121.47	124.45
46	g	607	CHL	C3C-C4C-NC	-3.25	106.93	110.57
29	B	501	CLA	CHD-C1D-ND	-3.24	121.47	124.45
29	R	309	CLA	CHD-C1D-ND	-3.24	121.48	124.45
29	c	505	CLA	CHD-C1D-ND	-3.24	121.48	124.45
46	R	305	CHL	C3B-C4B-NB	-3.24	107.51	110.52
29	r	304	CLA	CHD-C1D-ND	-3.24	121.48	124.45
29	S	313	CLA	C4A-NA-C1A	3.24	108.16	106.71
29	b	512	CLA	C4A-NA-C1A	3.24	108.16	106.71
31	b	518	BCR	C33-C5-C6	-3.24	120.89	124.53
47	s	317	LUT	C18-C5-C6	-3.23	120.90	124.53
46	r	306	CHL	C2C-C3C-C4C	3.23	108.79	106.49
46	g	601	CHL	C2C-C3C-C4C	3.23	108.79	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	508	CLA	CHD-C1D-ND	-3.23	121.49	124.45
47	n	614	LUT	C22-C23-C24	-3.23	108.07	111.74
29	C	514	CLA	CHD-C1D-ND	-3.22	121.49	124.45
46	S	309	CHL	C3B-C4B-NB	-3.22	107.53	110.52
43	d	405	PL9	C7-C3-C2	-3.22	119.07	123.30
43	D	406	PL9	C7-C3-C2	-3.22	119.07	123.30
29	r	310	CLA	C4A-NA-C1A	3.21	108.15	106.71
29	b	509	CLA	CHD-C1D-ND	-3.21	121.50	124.45
29	N	614	CLA	CHD-C1D-ND	-3.21	121.50	124.45
37	D	407	LHG	O7-C7-C8	3.21	118.42	111.50
29	S	305	CLA	CHD-C1D-ND	-3.21	121.50	124.45
47	G	616	LUT	C11-C10-C9	-3.21	122.73	127.31
29	C	508	CLA	CHD-C1D-ND	-3.21	121.51	124.45
46	G	607	CHL	CHD-C1D-ND	-3.21	121.51	124.45
31	f	101	BCR	C34-C9-C10	-3.20	118.44	122.92
46	y	308	CHL	C4B-CHC-C1C	3.20	133.93	126.34
46	S	308	CHL	C2C-C3C-C4C	3.20	108.77	106.49
46	G	608	CHL	C3C-C4C-NC	-3.20	106.98	110.57
48	y	319	NEX	C17-C1-C6	-3.20	107.61	110.47
29	B	510	CLA	C2B-C1B-NB	-3.20	108.09	110.23
29	B	515	CLA	CHD-C1D-ND	-3.19	121.52	124.45
29	C	512	CLA	CHD-C1D-ND	-3.19	121.52	124.45
46	G	606	CHL	C3C-C4C-NC	-3.19	107.00	110.57
31	b	517	BCR	C33-C5-C4	3.18	119.73	113.62
45	h	101	RRX	C4-C5-C6	-3.18	118.11	122.73
46	Y	302	CHL	C4A-NA-C1A	3.18	108.14	106.71
29	N	604	CLA	CHD-C1D-ND	-3.18	121.53	124.45
29	R	308	CLA	CHD-C1D-ND	-3.18	121.53	124.45
29	b	501	CLA	CHD-C1D-ND	-3.18	121.53	124.45
45	H	101	RRX	C4-C5-C6	-3.18	118.11	122.73
47	G	616	LUT	C22-C23-C24	-3.18	108.12	111.74
46	g	605	CHL	CHD-C1D-ND	-3.18	121.53	124.45
47	S	318	LUT	C7-C8-C9	-3.18	121.43	126.23
46	G	608	CHL	C2C-C3C-C4C	3.18	108.76	106.49
46	n	605	CHL	C3B-C4B-NB	-3.18	107.57	110.52
29	g	611	CLA	C2B-C1B-NB	-3.18	108.10	110.23
47	S	317	LUT	C7-C8-C9	-3.17	121.44	126.23
29	B	501	CLA	C4A-NA-C1A	3.17	108.13	106.71
29	N	602	CLA	CHD-C1D-ND	-3.17	121.54	124.45
46	r	306	CHL	C3B-C4B-NB	-3.16	107.58	110.52
31	C	515	BCR	C23-C24-C25	-3.16	118.32	127.20
47	g	616	LUT	C31-C30-C29	-3.16	122.80	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	n	606	CHL	CHD-C1D-ND	-3.16	121.55	124.45
46	r	305	CHL	C3B-C4B-NB	-3.16	107.59	110.52
47	r	311	LUT	C22-C23-C24	-3.16	108.15	111.74
46	y	309	CHL	C3C-C4C-NC	-3.16	107.03	110.57
34	b	519	C7Z	C1-C6-C7	3.15	124.70	115.78
29	B	513	CLA	CHD-C1D-ND	-3.15	121.56	124.45
46	y	308	CHL	CMA-C3A-C4A	3.15	120.25	111.77
29	Y	315	CLA	CHD-C1D-ND	-3.15	121.56	124.45
31	B	518	BCR	C12-C13-C14	-3.15	114.11	118.94
46	y	308	CHL	C4D-CHA-C1A	3.15	125.08	121.25
29	D	404	CLA	CMC-C2C-C1C	3.15	129.84	125.04
49	y	302	XAT	C38-C25-C26	-3.15	116.98	122.26
47	Y	316	LUT	C22-C23-C24	-3.15	108.16	111.74
46	N	607	CHL	CHB-C4A-NA	3.15	128.87	124.51
29	S	313	CLA	CHD-C1D-ND	-3.15	121.56	124.45
29	y	314	CLA	CHD-C1D-ND	-3.15	121.56	124.45
49	Y	301	XAT	C38-C25-C26	-3.15	116.99	122.26
29	y	304	CLA	CHD-C1D-ND	-3.14	121.57	124.45
29	S	312	CLA	CHD-C1D-ND	-3.14	121.57	124.45
29	N	610	CLA	CHD-C1D-ND	-3.14	121.57	124.45
45	h	101	RRX	C1-C6-C5	-3.14	118.20	122.61
46	Y	306	CHL	C3C-C4C-NC	-3.13	107.06	110.57
46	N	601	CHL	C2C-C3C-C4C	3.13	108.72	106.49
46	Y	308	CHL	CHD-C1D-ND	-3.13	121.58	124.45
29	c	513	CLA	CHD-C1D-ND	-3.13	121.58	124.45
31	c	515	BCR	C28-C27-C26	-3.13	108.49	114.08
29	g	610	CLA	CHD-C1D-ND	-3.13	121.58	124.45
29	c	506	CLA	CHD-C1D-ND	-3.12	121.59	124.45
46	S	309	CHL	C1-O2A-CGA	3.12	124.63	116.44
46	Y	307	CHL	CMA-C3A-C4A	3.12	120.16	111.77
31	B	518	BCR	C23-C24-C25	-3.12	118.44	127.20
31	F	101	BCR	C34-C9-C10	-3.12	118.55	122.92
47	N	616	LUT	C15-C14-C13	-3.12	122.86	127.31
29	b	515	CLA	CHD-C1D-ND	-3.12	121.59	124.45
29	y	306	CLA	CHD-C1D-ND	-3.12	121.59	124.45
31	B	518	BCR	C33-C5-C6	-3.12	121.03	124.53
46	N	609	CHL	CMA-C3A-C4A	3.11	120.14	111.77
46	S	307	CHL	CMA-C3A-C4A	3.11	120.14	111.77
29	G	612	CLA	CHD-C1D-ND	-3.11	121.59	124.45
46	y	309	CHL	CHB-C4A-NA	3.11	128.81	124.51
29	C	503	CLA	CHD-C1D-ND	-3.11	121.60	124.45
45	H	101	RRX	C1-C6-C5	-3.11	118.24	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	518	BCR	C23-C22-C21	-3.11	114.17	118.94
46	Y	310	CHL	C4B-CHC-C1C	3.10	133.70	126.34
46	s	302	CHL	C2C-C3C-C4C	3.10	108.70	106.49
29	g	603	CLA	C3B-C4B-NB	-3.10	107.64	110.52
31	C	516	BCR	C12-C13-C14	-3.10	114.18	118.94
29	n	604	CLA	CHD-C1D-ND	-3.10	121.60	124.45
45	H	101	RRX	C33-C5-C4	3.09	119.56	113.62
29	b	508	CLA	C3B-C4B-NB	-3.09	107.64	110.52
47	r	311	LUT	C35-C34-C33	-3.09	122.90	127.31
47	n	615	LUT	C11-C10-C9	-3.09	122.90	127.31
48	y	319	NEX	C2-C1-C6	3.09	112.21	109.21
29	N	612	CLA	CHD-C1D-ND	-3.09	121.61	124.45
49	R	311	XAT	C38-C25-C26	-3.09	117.08	122.26
47	G	615	LUT	C7-C8-C9	-3.08	121.57	126.23
29	n	609	CLA	CHA-C1A-NA	-3.08	119.34	126.40
46	G	607	CHL	C4A-NA-C1A	3.08	108.09	106.71
31	v	101	BCR	C19-C18-C17	3.08	123.67	118.94
47	S	317	LUT	C35-C15-C14	-3.08	117.17	123.47
46	S	309	CHL	C4B-CHC-C1C	3.08	133.63	126.34
46	N	608	CHL	C3C-C4C-NC	-3.08	107.12	110.57
46	y	301	CHL	C2C-C3C-C4C	3.08	108.68	106.49
46	Y	302	CHL	CHB-C4A-NA	3.07	128.76	124.51
47	y	317	LUT	C22-C23-C24	-3.07	108.24	111.74
29	s	306	CLA	CHD-C1D-ND	-3.07	121.63	124.45
47	n	614	LUT	C10-C11-C12	-3.07	113.63	123.22
46	n	605	CHL	C2C-C3C-C4C	3.07	108.68	106.49
38	b	524	LMT	O5B-C1B-C2B	3.07	116.85	110.35
29	B	508	CLA	C3B-C4B-NB	-3.07	107.67	110.52
29	n	603	CLA	CHD-C1D-ND	-3.07	121.64	124.45
46	s	307	CHL	C3C-C4C-NC	-3.07	107.13	110.57
38	B	524	LMT	O5B-C1B-C2B	3.07	116.84	110.35
46	s	309	CHL	C3B-C4B-NB	-3.07	107.67	110.52
46	n	607	CHL	C3C-C4C-NC	-3.07	107.13	110.57
29	B	511	CLA	CHD-C1D-ND	-3.07	121.64	124.45
46	R	305	CHL	CMA-C3A-C4A	3.06	120.01	111.77
46	y	303	CHL	CHB-C4A-NA	3.06	128.75	124.51
29	n	611	CLA	C4A-NA-C1A	3.06	108.08	106.71
49	R	311	XAT	C26-C27-C28	-3.06	119.53	125.99
46	g	608	CHL	C4B-CHC-C1C	3.06	133.59	126.34
46	Y	310	CHL	C2C-C3C-C4C	3.05	108.67	106.49
46	G	605	CHL	CMA-C3A-C4A	3.05	119.97	111.77
47	R	310	LUT	C18-C5-C4	3.05	120.00	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	518	BCR	C37-C22-C23	3.04	122.87	118.08
48	N	617	NEX	C5-C4-C3	3.04	115.35	111.75
46	Y	308	CHL	C3C-C4C-NC	-3.04	107.16	110.57
46	N	606	CHL	CHD-C1D-ND	-3.04	121.66	124.45
29	B	504	CLA	C1-C2-C3	-3.04	120.79	126.04
48	g	617	NEX	C5-C4-C3	-3.03	108.15	111.75
46	N	606	CHL	CMA-C3A-C4A	3.03	119.92	111.77
46	G	609	CHL	CMA-C3A-C4A	3.03	119.92	111.77
46	N	608	CHL	C2C-C3C-C4C	3.03	108.65	106.49
49	G	619	XAT	O4-C5-C4	-3.03	111.11	113.38
31	C	515	BCR	C33-C5-C6	-3.03	121.13	124.53
46	N	609	CHL	C2C-C3C-C4C	3.02	108.64	106.49
46	r	306	CHL	CHD-C4C-C3C	3.02	129.28	124.84
48	s	319	NEX	C39-C29-C30	-3.02	118.69	122.92
46	N	608	CHL	CMA-C3A-C4A	3.02	119.89	111.77
45	h	101	RRX	C23-C24-C25	-3.02	118.72	127.20
29	Y	314	CLA	CHD-C1D-ND	-3.01	121.68	124.45
29	r	309	CLA	C1-C2-C3	-3.01	120.84	126.04
31	b	518	BCR	C23-C24-C25	-3.01	118.75	127.20
46	G	607	CHL	C3C-C4C-NC	-3.01	107.20	110.57
29	g	603	CLA	CHD-C1D-ND	-3.01	121.69	124.45
46	Y	302	CHL	C3C-C4C-NC	-3.00	107.20	110.57
46	R	304	CHL	C3B-C4B-NB	-3.00	107.73	110.52
48	s	319	NEX	C17-C1-C6	-3.00	107.78	110.47
45	H	101	RRX	C20-C19-C18	-3.00	117.98	126.42
46	S	308	CHL	CMA-C3A-C4A	3.00	119.84	111.77
47	s	318	LUT	C18-C5-C6	-3.00	121.16	124.53
29	C	502	CLA	CHD-C1D-ND	-3.00	121.70	124.45
46	Y	306	CHL	C3B-C4B-NB	-3.00	107.73	110.52
31	C	516	BCR	C35-C13-C12	3.00	122.80	118.08
46	s	309	CHL	C3C-C4C-NC	-2.99	107.22	110.57
29	A	406	CLA	C1-C2-C3	-2.99	120.88	126.04
46	g	608	CHL	C3C-C4C-NC	-2.98	107.22	110.57
43	d	405	PL9	C7-C8-C9	-2.98	121.83	126.79
29	G	614	CLA	C4A-NA-C1A	2.98	108.05	106.71
46	g	608	CHL	CMA-C3A-C4A	2.98	119.78	111.77
46	n	608	CHL	CMA-C3A-C4A	2.98	119.78	111.77
46	g	606	CHL	CMA-C3A-C4A	2.98	119.78	111.77
49	r	312	XAT	C26-C27-C28	-2.98	119.70	125.99
46	Y	310	CHL	CMA-C3A-C4A	2.98	119.77	111.77
29	c	506	CLA	C1D-ND-C4D	-2.97	104.22	106.33
46	g	607	CHL	CMA-C3A-C4A	2.97	119.77	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	Y	302	CHL	CMA-C3A-C4A	2.97	119.76	111.77
46	g	607	CHL	C4B-CHC-C1C	2.97	133.39	126.34
46	g	609	CHL	C4B-CHC-C1C	2.97	133.38	126.34
46	R	304	CHL	CMA-C3A-C4A	2.97	119.75	111.77
29	b	506	CLA	CHD-C1D-ND	-2.97	121.73	124.45
29	c	501	CLA	CHD-C1D-ND	-2.97	121.73	124.45
29	D	404	CLA	CMB-C2B-C3B	2.97	133.78	126.59
30	d	402	PHO	O2D-CGD-O1D	-2.97	118.04	123.84
46	G	609	CHL	C4B-CHC-C1C	2.97	133.37	126.34
47	r	311	LUT	C18-C5-C4	2.96	119.85	114.36
46	n	607	CHL	CMA-C3A-C4A	2.96	119.74	111.77
46	g	601	CHL	CMA-C3A-C4A	2.96	119.74	111.77
45	h	101	RRX	C33-C5-C4	2.96	119.31	113.62
46	s	307	CHL	CMA-C3A-C4A	2.96	119.73	111.77
47	G	616	LUT	C18-C5-C6	-2.96	121.20	124.53
46	n	607	CHL	C2C-C3C-C4C	2.96	108.60	106.49
29	S	303	CLA	C4A-NA-C1A	2.96	108.04	106.71
45	h	101	RRX	C8-C7-C6	-2.96	118.90	127.20
46	S	309	CHL	C1-C2-C3	-2.96	120.93	126.04
29	c	508	CLA	C4A-NA-C1A	2.96	108.03	106.71
29	r	304	CLA	C4A-NA-C1A	2.96	108.03	106.71
29	R	308	CLA	C1-C2-C3	-2.96	120.93	126.04
31	z	101	BCR	C36-C18-C17	-2.95	118.79	122.92
46	s	307	CHL	C2C-C3C-C4C	2.95	108.59	106.49
37	B	523	LHG	O8-C23-C24	2.95	121.16	111.91
46	S	307	CHL	C4B-CHC-C1C	2.95	133.33	126.34
29	S	304	CLA	C2D-C1D-ND	-2.95	107.93	110.10
47	Y	317	LUT	C11-C10-C9	-2.95	123.10	127.31
31	A	410	BCR	C38-C26-C25	-2.94	121.22	124.53
46	g	606	CHL	C1-O2A-CGA	2.94	124.17	116.44
47	y	318	LUT	C38-C25-C24	-2.94	117.26	123.56
46	n	605	CHL	C4B-CHC-C1C	2.94	133.31	126.34
46	y	301	CHL	CHB-C4A-NA	2.94	128.58	124.51
46	g	609	CHL	C1-O2A-CGA	2.94	124.15	116.44
46	g	605	CHL	CHB-C4A-NA	2.94	128.57	124.51
29	c	506	CLA	C4A-NA-C1A	2.94	108.03	106.71
45	H	101	RRX	C8-C7-C6	-2.93	118.96	127.20
29	n	603	CLA	C4A-NA-C1A	-2.93	105.39	106.71
48	n	616	NEX	C5-C4-C3	2.93	115.22	111.75
47	S	318	LUT	C35-C15-C14	-2.93	117.47	123.47
31	B	517	BCR	C8-C7-C6	-2.93	118.97	127.20
46	G	607	CHL	CMA-C3A-C4A	2.93	119.64	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	n	618	XAT	C26-C27-C28	-2.93	119.81	125.99
29	B	516	CLA	CHD-C1D-ND	-2.92	121.77	124.45
31	A	410	BCR	C37-C22-C23	2.92	122.68	118.08
46	r	305	CHL	CMA-C3A-C4A	2.92	119.62	111.77
34	b	519	C7Z	C11-C12-C13	-2.92	118.21	126.42
31	c	514	BCR	C35-C13-C12	2.92	122.68	118.08
29	D	404	CLA	C4D-C3D-CAD	-2.92	104.66	108.10
46	N	607	CHL	C3C-C4C-NC	-2.92	107.30	110.57
46	R	305	CHL	C2C-C3C-C4C	2.92	108.57	106.49
48	R	312	NEX	C31-C30-C29	2.92	131.47	127.31
47	s	318	LUT	C22-C23-C24	-2.91	108.42	111.74
29	R	301	CLA	CHD-C1D-ND	-2.91	121.78	124.45
48	Y	318	NEX	C31-C30-C29	2.91	131.47	127.31
29	S	312	CLA	C3B-C4B-NB	-2.91	107.82	110.52
45	H	101	RRX	C7-C8-C9	-2.91	121.84	126.23
29	G	603	CLA	CHD-C1D-ND	-2.91	121.78	124.45
31	a	409	BCR	C37-C22-C23	2.91	122.66	118.08
46	G	606	CHL	CMA-C3A-C4A	2.90	119.58	111.77
29	S	316	CLA	C2B-C1B-NB	-2.90	108.28	110.23
49	g	619	XAT	C6-C7-C8	-2.90	119.85	125.99
46	y	308	CHL	C1-C2-C3	-2.90	122.06	126.75
46	N	606	CHL	C3C-C4C-NC	-2.90	107.32	110.57
35	C	521	LMG	O8-C28-C29	2.90	121.01	111.91
47	N	615	LUT	C38-C25-C24	-2.90	117.36	123.56
47	n	614	LUT	C18-C5-C6	-2.90	121.27	124.53
43	D	406	PL9	C7-C8-C9	-2.90	121.97	126.79
45	h	101	RRX	C38-C26-C27	2.90	119.72	114.36
47	n	614	LUT	C7-C8-C9	-2.90	121.86	126.23
30	a	407	PHO	O2D-CGD-O1D	-2.90	118.18	123.84
29	D	404	CLA	C1C-C2C-C3C	-2.90	103.91	106.96
29	b	504	CLA	CHA-C1A-NA	-2.89	119.77	126.40
35	C	522	LMG	O8-C28-C29	2.89	120.98	111.91
31	C	515	BCR	C36-C18-C17	-2.89	118.87	122.92
29	A	409	CLA	C3B-C4B-NB	-2.89	107.83	110.52
46	G	608	CHL	CMA-C3A-C4A	2.89	119.54	111.77
47	n	614	LUT	C31-C30-C29	-2.89	123.19	127.31
46	N	607	CHL	CHC-C1C-NC	2.89	128.58	124.20
46	n	605	CHL	C1-O2A-CGA	2.89	124.02	116.44
46	g	605	CHL	C3C-C4C-NC	-2.88	107.34	110.57
46	y	311	CHL	C4A-NA-C1A	2.88	108.00	106.71
46	y	307	CHL	C3B-C4B-NB	-2.88	107.84	110.52
47	s	318	LUT	C35-C15-C14	-2.88	117.57	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	r	312	XAT	O24-C25-C24	2.88	115.54	113.38
46	n	606	CHL	C1-C2-C3	-2.88	121.07	126.04
46	S	309	CHL	CMA-C3A-C4A	2.88	119.50	111.77
46	Y	308	CHL	CMA-C3A-C4A	2.88	119.50	111.77
48	n	616	NEX	C31-C30-C29	2.87	131.41	127.31
37	a	413	LHG	O8-C23-C24	2.87	120.93	111.91
46	y	311	CHL	CMA-C3A-C4A	2.87	119.49	111.77
46	N	607	CHL	C4B-CHC-C1C	2.87	133.14	126.34
29	B	511	CLA	C1-C2-C3	-2.87	121.08	126.04
46	s	302	CHL	CMA-C3A-C4A	2.87	119.48	111.77
31	F	101	BCR	C35-C13-C12	2.87	122.59	118.08
46	s	309	CHL	CMA-C3A-C4A	2.87	119.47	111.77
46	N	601	CHL	C1-C2-C3	-2.86	121.09	126.04
46	n	608	CHL	C2C-C3C-C4C	2.86	108.53	106.49
47	N	616	LUT	C11-C10-C9	-2.86	123.23	127.31
46	N	601	CHL	CMA-C3A-C4A	2.86	119.46	111.77
29	r	303	CLA	C2B-C1B-NB	-2.86	108.32	110.23
46	n	601	CHL	C1-C2-C3	-2.86	121.10	126.04
46	y	307	CHL	C4B-CHC-C1C	2.86	133.11	126.34
49	G	619	XAT	C6-C7-C8	-2.86	119.96	125.99
30	D	401	PHO	O1D-CGD-CBD	2.85	129.49	124.74
31	K	101	BCR	C35-C13-C12	2.85	122.57	118.08
31	C	516	BCR	C33-C5-C4	2.85	119.10	113.62
29	b	516	CLA	CHD-C1D-ND	-2.85	121.83	124.45
47	Y	317	LUT	C38-C25-C24	-2.85	117.46	123.56
46	n	607	CHL	C4B-CHC-C1C	2.85	133.10	126.34
46	y	303	CHL	C3C-C4C-NC	-2.85	107.37	110.57
31	z	101	BCR	C33-C5-C6	-2.85	121.33	124.53
46	S	308	CHL	C3B-C4B-NB	-2.85	107.87	110.52
46	N	609	CHL	CHB-C4A-NA	2.85	128.45	124.51
49	N	619	XAT	C19-C9-C10	-2.85	118.93	122.92
29	a	406	CLA	C4A-NA-C1A	2.85	107.99	106.71
46	N	608	CHL	C4B-CHC-C1C	2.85	133.09	126.34
29	C	506	CLA	C3B-C4B-NB	-2.85	107.87	110.52
29	r	303	CLA	C4A-NA-C1A	2.85	107.99	106.71
49	g	619	XAT	C38-C25-C26	-2.85	117.49	122.26
49	Y	301	XAT	O24-C25-C24	2.85	115.52	113.38
46	Y	306	CHL	C4B-CHC-C1C	2.85	133.09	126.34
46	r	305	CHL	C4B-CHC-C1C	2.84	133.08	126.34
29	Y	305	CLA	CHD-C1D-ND	-2.84	121.84	124.45
47	y	318	LUT	C10-C11-C12	-2.84	114.35	123.22
46	Y	307	CHL	C1-O2A-CGA	2.84	123.90	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	y	303	CHL	CMA-C3A-C4A	2.84	119.40	111.77
47	g	615	LUT	C11-C10-C9	-2.84	123.26	127.31
48	S	319	NEX	C39-C29-C30	-2.84	118.95	122.92
46	g	605	CHL	CMA-C3A-C4A	2.84	119.40	111.77
34	B	519	C7Z	C11-C12-C13	-2.84	118.45	126.42
47	y	317	LUT	C10-C11-C12	-2.84	114.37	123.22
29	B	516	CLA	C3B-C4B-NB	-2.83	107.89	110.52
29	Y	315	CLA	C3B-C4B-NB	-2.83	107.89	110.52
47	N	615	LUT	C10-C11-C12	-2.83	114.38	123.22
46	r	306	CHL	CMA-C3A-C4A	2.83	119.39	111.77
29	A	409	CLA	C1-C2-C3	-2.83	121.15	126.04
46	Y	308	CHL	C2C-C3C-C4C	2.83	108.51	106.49
29	g	604	CLA	C4A-NA-C1A	2.83	107.98	106.71
49	G	619	XAT	C38-C25-C26	-2.83	117.52	122.26
46	s	308	CHL	CMA-C3A-C4A	2.83	119.38	111.77
47	S	317	LUT	C10-C11-C12	-2.83	114.39	123.22
29	c	506	CLA	C2D-C1D-ND	-2.83	108.02	110.10
46	n	601	CHL	CMA-C3A-C4A	2.83	119.37	111.77
46	g	609	CHL	CMA-C3A-C4A	2.83	119.37	111.77
46	g	608	CHL	C3B-C4B-NB	-2.82	107.89	110.52
46	s	309	CHL	C4D-CHA-C1A	2.82	124.68	121.25
34	b	519	C7Z	C24-C25-C26	-2.82	114.56	120.85
46	y	311	CHL	C1-O2A-CGA	2.82	123.84	116.44
29	G	613	CLA	CHD-C1D-ND	-2.82	121.86	124.45
46	Y	307	CHL	C4B-CHC-C1C	2.82	133.03	126.34
47	y	318	LUT	C11-C10-C9	-2.82	123.29	127.31
44	E	101	HEM	C4D-ND-C1D	2.82	107.98	105.07
30	A	408	PHO	O2D-CGD-O1D	-2.82	118.33	123.84
46	g	609	CHL	C3C-C4C-NC	-2.82	107.41	110.57
46	Y	306	CHL	CMA-C3A-C4A	2.82	119.35	111.77
47	g	615	LUT	C18-C5-C6	-2.81	121.37	124.53
29	b	511	CLA	CHD-C1D-ND	-2.81	121.87	124.45
29	c	512	CLA	CHD-C1D-ND	-2.81	121.87	124.45
46	Y	310	CHL	C3B-C4B-NB	-2.81	107.91	110.52
48	s	319	NEX	C38-C25-C26	-2.81	117.55	122.26
29	y	315	CLA	CHD-C1D-ND	-2.81	121.87	124.45
29	A	405	CLA	CHD-C1D-ND	-2.81	121.87	124.45
29	Y	303	CLA	C1-C2-C3	-2.81	121.19	126.04
29	R	307	CLA	C2D-C1D-ND	-2.81	108.03	110.10
29	c	510	CLA	C2D-C1D-ND	-2.81	108.03	110.10
47	N	616	LUT	C38-C25-C24	-2.81	117.55	123.56
47	Y	316	LUT	C10-C11-C12	-2.81	114.46	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	y	317	LUT	C18-C5-C6	-2.81	121.38	124.53
41	j	101	DGA	OG1-CA1-CA2	2.81	120.71	111.91
46	g	601	CHL	C3B-C4B-NB	-2.80	107.92	110.52
46	Y	310	CHL	C1-O2A-CGA	2.80	123.79	116.44
30	D	401	PHO	O2D-CGD-O1D	-2.80	118.36	123.84
46	n	608	CHL	CHB-C4A-NA	2.80	128.38	124.51
29	C	504	CLA	C3B-C2B-C1B	-2.80	103.78	107.16
51	s	321	LPX	O3-P1-O4	2.80	126.08	112.24
46	r	306	CHL	CHB-C4A-NA	2.80	128.38	124.51
47	s	318	LUT	C11-C10-C9	-2.80	123.32	127.31
46	g	608	CHL	C4D-CHA-C1A	2.80	124.65	121.25
47	y	317	LUT	C38-C25-C24	-2.80	117.58	123.56
29	c	503	CLA	C3B-C4B-NB	-2.80	107.92	110.52
29	N	613	CLA	CHD-C1D-ND	-2.79	121.89	124.45
46	Y	308	CHL	C4A-NA-C1A	2.79	107.96	106.71
46	G	607	CHL	CHB-C4A-NA	2.79	128.37	124.51
31	C	517	BCR	C27-C26-C25	-2.79	118.68	122.73
37	S	301	LHG	O8-C23-C24	2.79	120.67	111.91
46	s	307	CHL	C4D-CHA-C1A	2.79	124.65	121.25
35	d	408	LMG	O8-C28-C29	2.79	120.65	111.91
29	a	404	CLA	CHD-C1D-ND	-2.79	121.89	124.45
47	s	317	LUT	C39-C29-C28	2.78	122.47	118.08
47	S	318	LUT	C38-C25-C24	-2.78	117.60	123.56
37	L	101	LHG	O8-C23-C24	2.78	120.64	111.91
37	l	102	LHG	O8-C23-C24	2.78	120.64	111.91
47	S	317	LUT	C18-C5-C6	-2.78	121.41	124.53
29	R	302	CLA	CHD-C1D-ND	-2.78	121.90	124.45
45	H	101	RRX	C38-C26-C27	2.77	119.50	114.36
29	a	405	CLA	C1-C2-C3	-2.77	121.24	126.04
46	G	609	CHL	C3C-C4C-NC	-2.77	107.46	110.57
46	R	304	CHL	C4B-CHC-C1C	2.77	132.92	126.34
34	B	519	C7Z	C24-C25-C26	-2.77	114.67	120.85
46	G	601	CHL	CHB-C4A-NA	2.77	128.34	124.51
31	b	517	BCR	C33-C5-C6	-2.77	121.42	124.53
46	g	607	CHL	CHB-C4A-NA	2.77	128.34	124.51
46	G	601	CHL	CMA-C3A-C4A	2.76	119.20	111.77
29	y	304	CLA	C1-C2-C3	-2.76	121.26	126.04
35	W	203	LMG	O8-C28-C29	2.76	120.58	111.91
47	Y	317	LUT	C31-C30-C29	-2.76	123.37	127.31
46	g	601	CHL	C4B-CHC-C1C	2.76	132.89	126.34
31	c	515	BCR	C36-C18-C17	-2.76	119.05	122.92
29	D	404	CLA	CHD-C1D-ND	-2.76	121.92	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	g	615	LUT	C10-C11-C12	-2.76	114.60	123.22
46	n	607	CHL	C1-O2A-CGA	2.76	123.68	116.44
29	D	404	CLA	CHC-C1C-C2C	-2.76	119.07	126.73
30	d	402	PHO	O1D-CGD-CBD	2.75	129.33	124.74
46	n	601	CHL	CHB-C4A-NA	2.75	128.32	124.51
46	y	307	CHL	CMA-C3A-C4A	2.75	119.17	111.77
49	n	618	XAT	C19-C9-C10	-2.75	119.07	122.92
51	S	321	LPX	O3-P1-O4	2.75	125.83	112.24
46	N	608	CHL	C1-O2A-CGA	2.75	123.66	116.44
46	y	311	CHL	C4B-CHC-C1C	2.75	132.86	126.34
46	n	606	CHL	CMA-C3A-C4A	2.75	119.16	111.77
36	c	517	DGD	O1G-C1A-C2A	2.75	120.53	111.91
47	G	615	LUT	C11-C10-C9	-2.75	123.39	127.31
36	C	519	DGD	O1G-C1A-C2A	2.74	120.52	111.91
37	s	301	LHG	O8-C23-C24	2.74	120.52	111.91
46	N	606	CHL	C2C-C3C-C4C	2.74	108.44	106.49
29	b	511	CLA	C3C-C4C-NC	-2.74	107.49	110.57
46	Y	310	CHL	C4D-CHA-C1A	2.74	124.59	121.25
46	y	303	CHL	C1-C2-C3	-2.74	121.31	126.04
31	F	101	BCR	C12-C13-C14	-2.74	114.74	118.94
46	G	609	CHL	C1-O2A-CGA	2.74	123.62	116.44
38	B	524	LMT	C1B-C2B-C3B	2.74	115.69	110.00
46	N	608	CHL	C4D-CHA-C1A	2.74	124.58	121.25
46	y	309	CHL	C2C-C3C-C4C	2.73	108.44	106.49
46	n	608	CHL	C4B-CHC-C1C	2.73	132.82	126.34
36	C	518	DGD	O1G-C1A-C2A	2.73	120.48	111.91
46	G	607	CHL	C1-C2-C3	-2.73	121.32	126.04
46	y	309	CHL	CHD-C1D-ND	-2.73	121.95	124.45
48	S	319	NEX	C38-C25-C26	-2.73	117.69	122.26
33	b	521	3PH	O31-C31-C32	2.73	120.46	111.91
47	R	310	LUT	C8-C7-C6	-2.72	119.55	127.20
48	S	319	NEX	C20-C13-C14	-2.72	119.11	122.92
31	B	517	BCR	C4-C5-C6	-2.72	118.78	122.73
35	B	520	LMG	O8-C28-C29	2.72	120.45	111.91
29	B	505	CLA	C3B-C2B-C1B	-2.72	103.88	107.16
46	G	605	CHL	C3B-C4B-NB	-2.72	107.99	110.52
49	r	312	XAT	C38-C25-C26	-2.72	117.70	122.26
29	S	304	CLA	C2B-C1B-NB	-2.72	108.41	110.23
31	z	101	BCR	C23-C24-C25	-2.72	119.57	127.20
47	y	317	LUT	C7-C8-C9	-2.72	122.13	126.23
46	G	605	CHL	CHB-C4A-NA	2.72	128.27	124.51
50	N	620	PTY	O4-C30-C31	2.72	120.44	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	b	519	C7Z	C18-C5-C4	2.72	119.39	114.36
29	a	404	CLA	C1-C2-C3	2.72	130.74	126.04
31	v	101	BCR	C34-C9-C10	-2.72	119.12	122.92
46	G	601	CHL	C1-C2-C3	-2.72	121.35	126.04
46	N	601	CHL	C4B-CHC-C1C	2.72	132.78	126.34
46	G	606	CHL	C1-O2A-CGA	2.71	123.57	116.44
48	n	616	NEX	C40-C33-C34	-2.71	119.12	122.92
31	B	517	BCR	C1-C6-C5	-2.71	118.79	122.61
31	K	101	BCR	C34-C9-C10	-2.71	119.12	122.92
46	g	606	CHL	C4B-CHC-C1C	2.71	132.77	126.34
46	n	601	CHL	C3B-C4B-NB	-2.71	108.00	110.52
46	y	307	CHL	C2C-C3C-C4C	2.71	108.42	106.49
47	n	615	LUT	C18-C5-C6	-2.71	121.48	124.53
46	N	609	CHL	C1-O2A-CGA	2.71	123.56	116.44
29	g	611	CLA	C3B-C2B-C1B	-2.71	103.89	107.16
29	g	610	CLA	C1-C2-C3	-2.71	121.36	126.04
47	r	311	LUT	C7-C8-C9	-2.71	122.14	126.23
46	N	601	CHL	CHB-C4A-NA	2.71	128.26	124.51
29	c	503	CLA	C3B-C2B-C1B	-2.71	103.89	107.16
46	G	607	CHL	C1-O2A-CGA	2.71	123.55	116.44
31	b	518	BCR	C12-C13-C14	-2.71	114.79	118.94
31	F	101	BCR	C23-C24-C25	-2.71	119.60	127.20
49	g	619	XAT	C19-C9-C10	-2.71	119.13	122.92
29	c	508	CLA	C3C-C4C-NC	-2.71	107.54	110.57
47	Y	316	LUT	C38-C25-C24	-2.71	117.77	123.56
36	r	301	DGD	O6E-C5E-C4E	2.70	114.60	109.69
46	R	305	CHL	CHD-C4C-C3C	2.70	128.81	124.84
46	R	304	CHL	C4A-NA-C1A	2.70	107.92	106.71
46	n	608	CHL	C1-O2A-CGA	2.70	123.53	116.44
29	s	306	CLA	C3C-C4C-NC	-2.70	107.54	110.57
46	R	305	CHL	C4B-CHC-C1C	2.70	132.74	126.34
29	c	512	CLA	C4A-NA-C1A	2.70	107.92	106.71
35	c	519	LMG	O8-C28-C29	2.69	120.36	111.91
29	R	309	CLA	C2B-C1B-NB	-2.69	108.43	110.23
47	Y	316	LUT	C18-C5-C6	-2.69	121.50	124.53
46	N	605	CHL	C3B-C4B-NB	-2.69	108.02	110.52
46	G	601	CHL	C3B-C4B-NB	-2.69	108.02	110.52
46	S	302	CHL	CMA-C3A-C4A	2.69	119.00	111.77
29	c	503	CLA	C2B-C1B-NB	-2.69	108.43	110.23
33	S	322	3PH	O31-C31-C32	2.69	120.34	111.91
47	N	616	LUT	C18-C5-C6	-2.68	121.51	124.53
31	F	101	BCR	C36-C18-C17	-2.68	119.16	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s	315	CLA	C4A-NA-C1A	2.68	107.91	106.71
31	a	409	BCR	C38-C26-C25	-2.68	121.51	124.53
31	b	518	BCR	C37-C22-C23	2.68	122.31	118.08
46	y	303	CHL	C1-O2A-CGA	2.68	123.48	116.44
29	A	405	CLA	C4A-NA-C1A	2.68	107.91	106.71
29	R	302	CLA	C4A-NA-C1A	2.68	107.91	106.71
31	B	518	BCR	C35-C13-C12	2.68	122.30	118.08
37	c	521	LHG	O8-C23-C24	2.68	120.31	111.91
29	C	502	CLA	C4A-NA-C1A	2.68	107.91	106.71
47	G	615	LUT	C38-C25-C24	-2.68	117.83	123.56
46	y	301	CHL	CMA-C3A-C4A	2.68	118.97	111.77
30	A	408	PHO	O1D-CGD-CBD	2.68	129.20	124.74
31	b	517	BCR	C4-C5-C6	-2.68	118.84	122.73
33	B	522	3PH	O31-C31-C32	2.68	120.31	111.91
49	N	619	XAT	C26-C27-C28	-2.68	120.33	125.99
47	G	615	LUT	C18-C5-C6	-2.68	121.52	124.53
46	S	302	CHL	CHB-C4A-NA	2.67	128.21	124.51
47	Y	317	LUT	C10-C11-C12	-2.67	114.87	123.22
29	s	305	CLA	C1-C2-C3	-2.67	121.42	126.04
38	B	524	LMT	C3B-C4B-C5B	-2.67	105.47	110.24
47	N	615	LUT	C18-C5-C6	-2.67	121.53	124.53
46	n	607	CHL	C4D-CHA-C1A	2.67	124.50	121.25
46	g	609	CHL	C3B-C4B-NB	-2.67	108.04	110.52
46	G	607	CHL	C4B-CHC-C1C	2.67	132.67	126.34
29	a	408	CLA	C1-C2-C3	-2.67	121.43	126.04
45	h	101	RRX	C35-C13-C14	-2.67	119.19	122.92
46	g	607	CHL	C4A-NA-C1A	2.66	107.90	106.71
29	a	406	CLA	CHA-C1A-NA	-2.66	120.30	126.40
35	b	520	LMG	O8-C28-C29	2.66	120.27	111.91
36	c	518	DGD	O1G-C1A-C2A	2.66	120.26	111.91
37	d	406	LHG	O8-C23-C24	2.66	120.26	111.91
29	s	316	CLA	CHA-C1A-NA	-2.66	120.30	126.40
46	s	307	CHL	C4B-CHC-C1C	2.66	132.65	126.34
37	g	618	LHG	O8-C23-C24	2.66	120.25	111.91
45	H	101	RRX	C11-C12-C13	-2.66	118.95	126.42
46	g	605	CHL	C3B-C4B-NB	-2.66	108.05	110.52
29	N	603	CLA	CHD-C1D-ND	-2.66	122.01	124.45
34	B	519	C7Z	C35-C15-C14	-2.66	118.03	123.47
31	c	514	BCR	C3-C4-C5	-2.66	109.34	114.08
50	n	619	PTY	O4-C30-C31	2.66	120.24	111.91
46	n	605	CHL	CMA-C3A-C4A	2.65	118.91	111.77
29	r	309	CLA	C3C-C4C-NC	-2.65	107.60	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	511	CLA	C1-C2-C3	-2.65	121.46	126.04
29	Y	305	CLA	C1-C2-C3	-2.65	121.46	126.04
47	Y	317	LUT	C18-C5-C6	-2.65	121.55	124.53
29	r	310	CLA	CHA-C1A-NA	-2.65	120.33	126.40
31	v	101	BCR	C35-C13-C12	2.65	122.25	118.08
46	N	605	CHL	CHB-C4A-NA	2.65	128.18	124.51
29	S	315	CLA	C4A-NA-C1A	2.65	107.90	106.71
46	r	305	CHL	C4A-NA-C1A	2.64	107.89	106.71
29	G	610	CLA	CHA-C1A-NA	-2.64	120.35	126.40
33	a	415	3PH	O31-C31-C32	2.64	120.20	111.91
29	s	315	CLA	C3B-C4B-NB	-2.64	108.06	110.52
46	g	608	CHL	C2C-C3C-C4C	2.64	108.37	106.49
29	D	404	CLA	CAC-C3C-C2C	-2.64	123.02	127.53
29	c	503	CLA	CHD-C1D-ND	-2.64	122.03	124.45
31	c	514	BCR	C33-C5-C4	2.64	118.68	113.62
46	N	609	CHL	C4B-CHC-C1C	2.64	132.59	126.34
46	s	308	CHL	CHB-C4A-NA	2.64	128.16	124.51
38	b	524	LMT	C1B-C2B-C3B	2.63	115.48	110.00
46	G	601	CHL	C4B-CHC-C1C	2.63	132.59	126.34
31	f	101	BCR	C33-C5-C4	2.63	118.67	113.62
35	W	201	LMG	C8-O7-C10	-2.63	111.31	117.79
37	G	618	LHG	O8-C23-C24	2.63	120.17	111.91
46	N	601	CHL	C3B-C4B-NB	-2.63	108.07	110.52
46	y	303	CHL	C2B-C1B-NB	-2.63	108.47	110.23
46	S	307	CHL	C4D-CHA-C1A	2.63	124.45	121.25
41	w	201	DGA	OG1-CA1-CA2	2.63	120.15	111.91
46	n	606	CHL	CHB-C4A-NA	2.63	128.14	124.51
36	C	520	DGD	O1G-C1A-C2A	2.62	120.14	111.91
31	C	517	BCR	C23-C24-C25	-2.62	119.83	127.20
29	b	503	CLA	C3B-C4B-NB	-2.62	108.08	110.52
48	S	319	NEX	C19-C9-C10	-2.62	119.25	122.92
46	n	601	CHL	C4B-CHC-C1C	2.62	132.56	126.34
47	n	614	LUT	C38-C25-C24	-2.62	117.95	123.56
47	G	615	LUT	C10-C11-C12	-2.62	115.04	123.22
46	Y	308	CHL	CHB-C4A-NA	2.62	128.13	124.51
46	y	309	CHL	C1-C2-C3	-2.62	121.51	126.04
47	s	317	LUT	C38-C25-C24	-2.62	117.96	123.56
47	y	318	LUT	C18-C5-C6	-2.62	121.59	124.53
29	C	504	CLA	CHD-C1D-ND	-2.62	122.05	124.45
30	a	407	PHO	O1D-CGD-CBD	2.62	129.09	124.74
29	R	302	CLA	CHA-C1A-NA	-2.61	120.41	126.40
46	N	607	CHL	C4A-NA-C1A	2.61	107.88	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	i	101	LMG	O8-C28-C29	2.61	120.10	111.91
29	b	502	CLA	C3B-C4B-NB	-2.61	108.09	110.52
46	G	607	CHL	C2C-C3C-C4C	2.61	108.35	106.49
47	R	310	LUT	C22-C23-C24	-2.61	108.77	111.74
46	s	309	CHL	C2C-C3C-C4C	2.61	108.35	106.49
29	r	303	CLA	CHA-C1A-NA	-2.61	120.43	126.40
29	s	316	CLA	C3B-C4B-NB	-2.61	108.10	110.52
46	Y	302	CHL	C1-O2A-CGA	2.60	123.28	116.44
46	y	301	CHL	C4B-CHC-C1C	2.60	132.52	126.34
47	s	317	LUT	C30-C31-C32	-2.60	115.09	123.22
46	Y	306	CHL	C2C-C3C-C4C	2.60	108.34	106.49
29	b	505	CLA	C3B-C2B-C1B	-2.60	104.02	107.16
46	g	601	CHL	CHB-C4A-NA	2.60	128.11	124.51
46	g	605	CHL	C2B-C1B-NB	-2.60	108.49	110.23
49	N	619	XAT	C18-C5-C6	-2.60	117.91	122.26
46	r	305	CHL	CHB-C4A-NA	2.60	128.10	124.51
47	s	317	LUT	C10-C11-C12	-2.60	115.11	123.22
29	R	302	CLA	C2A-C1A-CHA	2.60	128.40	123.86
45	H	101	RRX	C35-C13-C14	-2.59	119.29	122.92
29	b	507	CLA	CHD-C1D-ND	-2.59	122.07	124.45
48	n	616	NEX	C19-C9-C10	-2.59	119.29	122.92
35	c	520	LMG	O8-C28-C29	2.59	120.04	111.91
46	Y	308	CHL	C1-C2-C3	-2.59	121.57	126.04
31	c	515	BCR	C31-C1-C6	-2.59	106.10	110.30
31	c	515	BCR	C23-C24-C25	-2.59	119.94	127.20
47	R	310	LUT	C1-C6-C5	-2.59	118.97	122.61
34	b	519	C7Z	C38-C25-C24	2.58	119.14	114.36
31	C	517	BCR	C2-C1-C6	2.58	114.46	110.48
29	Y	312	CLA	C4A-NA-C1A	2.58	107.87	106.71
46	S	308	CHL	C4B-CHC-C1C	2.58	132.46	126.34
29	C	509	CLA	C3C-C4C-NC	-2.58	107.67	110.57
46	N	605	CHL	C1-C2-C3	-2.58	121.58	126.04
46	y	307	CHL	C2B-C1B-NB	-2.58	108.50	110.23
31	C	515	BCR	C35-C13-C12	2.58	122.14	118.08
46	N	607	CHL	C3B-C4B-NB	-2.58	108.12	110.52
33	A	412	3PH	O31-C31-C32	2.58	120.00	111.91
37	D	407	LHG	C5-O7-C7	-2.58	111.45	117.79
29	g	610	CLA	C3B-C4B-NB	-2.58	108.12	110.52
46	G	609	CHL	C4D-CHA-C1A	2.58	124.38	121.25
46	G	609	CHL	C3B-C4B-NB	-2.58	108.13	110.52
46	r	306	CHL	C1-O2A-CGA	2.57	123.20	116.44
46	y	303	CHL	C3B-C4B-NB	-2.57	108.13	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	B	521	DGD	C1E-O6E-C5E	2.57	118.74	113.69
29	G	604	CLA	C4A-NA-C1A	2.57	107.86	106.71
29	s	304	CLA	CHD-C1D-ND	-2.57	122.09	124.45
46	N	606	CHL	C1-C2-C3	-2.57	121.60	126.04
46	R	304	CHL	CHB-C4A-NA	2.57	128.06	124.51
46	y	309	CHL	CMA-C3A-C4A	2.57	118.68	111.77
46	s	302	CHL	C4B-CHC-C1C	2.57	132.43	126.34
29	N	612	CLA	C3B-C4B-NB	-2.57	108.13	110.52
29	b	504	CLA	CAA-C2A-C1A	2.57	120.39	111.97
31	C	515	BCR	C12-C13-C14	-2.57	115.00	118.94
29	c	511	CLA	CHD-C1D-ND	-2.56	122.10	124.45
46	N	609	CHL	C4A-NA-C1A	2.56	107.86	106.71
46	y	311	CHL	C3B-C4B-NB	-2.56	108.14	110.52
29	C	513	CLA	CHD-C1D-ND	-2.56	122.10	124.45
46	G	609	CHL	CHC-C1C-NC	2.56	128.09	124.20
29	c	512	CLA	C3B-C4B-NB	-2.56	108.14	110.52
49	n	618	XAT	C6-C7-C8	-2.56	120.58	125.99
35	W	201	LMG	O8-C28-C29	2.56	119.95	111.91
46	G	606	CHL	CHB-C4A-NA	2.56	128.05	124.51
48	Y	318	NEX	C1-C2-C3	2.55	119.41	113.64
29	D	404	CLA	CMA-C3A-C4A	2.55	118.64	111.77
29	c	501	CLA	C1-C2-C3	-2.55	121.63	126.04
47	s	317	LUT	C11-C10-C9	-2.55	123.67	127.31
46	r	306	CHL	C4B-CHC-C1C	2.55	132.38	126.34
29	N	603	CLA	C3B-C4B-NB	-2.55	108.15	110.52
48	s	319	NEX	C20-C13-C14	-2.55	119.35	122.92
41	J	101	DGA	OG1-CA1-CA2	2.55	119.90	111.91
29	B	507	CLA	CHD-C1D-ND	-2.55	122.11	124.45
29	B	506	CLA	C3B-C4B-NB	-2.55	108.15	110.52
29	y	310	CLA	C3B-C4B-NB	-2.54	108.15	110.52
46	y	301	CHL	C4A-NA-C1A	2.54	107.85	106.71
33	s	322	3PH	O31-C31-C32	2.54	119.89	111.91
46	g	601	CHL	C1-C2-C3	-2.54	121.64	126.04
31	C	517	BCR	C36-C18-C17	-2.54	119.37	122.92
37	L	101	LHG	O7-C7-O9	-2.54	117.57	123.70
34	B	519	C7Z	C38-C25-C24	2.54	119.06	114.36
48	Y	318	NEX	C20-C13-C14	-2.54	119.37	122.92
48	G	617	NEX	C16-C1-C6	-2.54	108.20	110.47
29	c	509	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
29	g	604	CLA	CHA-C1A-NA	-2.53	120.59	126.40
35	w	202	LMG	O8-C28-C29	2.53	119.86	111.91
47	Y	316	LUT	C7-C8-C9	-2.53	122.41	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	g	615	LUT	C38-C25-C24	-2.53	118.14	123.56
37	a	414	LHG	O8-C23-C24	2.53	119.86	111.91
46	g	607	CHL	C2C-C3C-C4C	2.53	108.29	106.49
29	b	504	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
48	N	617	NEX	C19-C9-C10	-2.53	119.38	122.92
49	y	302	XAT	C26-C27-C28	-2.53	120.64	125.99
48	g	617	NEX	C20-C13-C14	-2.53	119.38	122.92
46	R	305	CHL	C1-O2A-CGA	2.53	123.08	116.44
38	b	524	LMT	C3B-C4B-C5B	-2.53	105.73	110.24
37	s	320	LHG	O8-C23-C24	2.53	119.84	111.91
29	C	510	CLA	CHA-C1A-NA	-2.53	120.61	126.40
29	Y	303	CLA	C3B-C2B-C1B	-2.53	104.11	107.16
37	N	618	LHG	O8-C23-C24	2.53	119.83	111.91
31	v	101	BCR	C2-C1-C6	2.52	114.37	110.48
35	C	521	LMG	C8-O7-C10	-2.52	111.58	117.79
29	c	503	CLA	CHC-C4B-NB	2.52	126.93	124.26
47	s	318	LUT	C38-C25-C24	-2.52	118.16	123.56
29	C	502	CLA	C1-C2-C3	-2.52	121.68	126.04
29	y	315	CLA	C3B-C4B-NB	-2.52	108.17	110.52
46	y	311	CHL	C4D-CHA-C1A	2.52	124.32	121.25
46	N	607	CHL	CMA-C3A-C4A	2.52	118.55	111.77
45	h	101	RRX	C34-C9-C10	-2.52	119.39	122.92
46	N	605	CHL	CMA-C3A-C4A	2.52	118.54	111.77
29	r	303	CLA	CHC-C4B-NB	2.52	126.92	124.26
29	y	306	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
29	n	603	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
46	y	303	CHL	C4B-CHC-C1C	2.52	132.31	126.34
29	g	611	CLA	C3B-C4B-NB	-2.51	108.18	110.52
31	b	518	BCR	C33-C5-C4	2.51	118.45	113.62
29	d	404	CLA	C3B-C4B-NB	-2.51	108.19	110.52
29	R	309	CLA	C1D-ND-C4D	-2.51	104.55	106.33
46	R	305	CHL	CHB-C4A-NA	2.51	127.98	124.51
44	e	101	HEM	C1B-NB-C4B	2.51	107.67	105.07
47	Y	316	LUT	C31-C30-C29	-2.51	123.73	127.31
48	S	319	NEX	C31-C30-C29	2.51	130.89	127.31
46	g	608	CHL	C4A-NA-C1A	2.51	107.83	106.71
29	Y	304	CLA	C3B-C4B-NB	-2.51	108.19	110.52
47	y	318	LUT	C35-C15-C14	-2.51	118.34	123.47
31	c	515	BCR	C33-C5-C6	-2.51	121.71	124.53
29	C	507	CLA	CHD-C1D-ND	-2.51	122.15	124.45
48	N	617	NEX	C40-C33-C34	-2.50	119.41	122.92
46	N	609	CHL	C3B-C4B-NB	-2.50	108.19	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	W	202	DGA	OG1-CA1-CA2	2.50	119.76	111.91
37	s	301	LHG	C5-O7-C7	-2.50	111.63	117.79
46	Y	308	CHL	C4B-CHC-C1C	2.50	132.27	126.34
29	s	304	CLA	CHA-C1A-NA	-2.50	120.67	126.40
29	c	509	CLA	CHA-C1A-NA	-2.50	120.67	126.40
31	v	101	BCR	C33-C5-C4	2.50	118.42	113.62
35	D	409	LMG	O8-C28-C29	2.50	119.75	111.91
29	R	302	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
29	C	507	CLA	C3B-C4B-NB	-2.49	108.20	110.52
37	n	617	LHG	C5-O7-C7	-2.49	111.65	117.79
46	y	309	CHL	C4B-CHC-C1C	2.49	132.25	126.34
29	r	309	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
31	c	515	BCR	C35-C13-C12	2.49	122.00	118.08
29	D	404	CLA	CHD-C4C-NC	-2.49	120.28	124.20
31	v	101	BCR	C3-C4-C5	-2.49	109.63	114.08
37	S	320	LHG	O8-C23-C24	2.49	119.72	111.91
46	Y	306	CHL	C2B-C1B-NB	-2.49	108.56	110.23
31	c	515	BCR	C34-C9-C10	-2.49	119.44	122.92
43	d	405	PL9	C22-C23-C24	-2.49	121.67	127.66
46	g	609	CHL	C4D-CHA-C1A	2.49	124.28	121.25
31	v	101	BCR	C31-C1-C6	-2.48	106.27	110.30
29	n	604	CLA	C4A-NA-C1A	2.48	107.82	106.71
46	Y	308	CHL	C1-O2A-CGA	2.48	122.96	116.44
41	D	402	DGA	OG1-CA1-CA2	2.48	119.69	111.91
46	g	609	CHL	CHC-C1C-NC	2.48	127.97	124.20
29	y	306	CLA	C1-C2-C3	-2.48	121.76	126.04
48	y	319	NEX	C20-C13-C14	-2.48	119.45	122.92
46	r	305	CHL	C2B-C1B-NB	-2.48	108.57	110.23
47	r	311	LUT	C38-C25-C24	-2.48	118.26	123.56
37	n	617	LHG	O8-C23-C24	2.48	119.67	111.91
46	G	605	CHL	C4A-NA-C1A	2.47	107.82	106.71
46	y	311	CHL	CHB-C4A-NA	2.47	127.93	124.51
47	g	616	LUT	C38-C25-C24	-2.47	118.27	123.56
37	y	320	LHG	O8-C23-C24	2.47	119.66	111.91
46	G	608	CHL	C4B-CHC-C1C	2.47	132.20	126.34
46	N	607	CHL	C4D-CHA-C1A	2.47	124.25	121.25
44	E	101	HEM	C4C-NC-C1C	2.47	107.77	105.35
45	H	101	RRX	C23-C22-C21	2.47	122.73	118.94
48	G	617	NEX	C40-C33-C34	-2.47	119.47	122.92
49	R	311	XAT	C7-C8-C9	-2.47	121.70	125.53
31	C	516	BCR	C34-C9-C10	-2.47	119.47	122.92
46	S	308	CHL	CHB-C4A-NA	2.46	127.92	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	n	605	CHL	CHB-C4A-NA	2.46	127.92	124.51
46	R	305	CHL	C2B-C1B-NB	-2.46	108.58	110.23
31	b	518	BCR	C35-C13-C12	2.46	121.96	118.08
36	B	521	DGD	O1G-C1A-C2A	2.46	119.64	111.91
38	b	524	LMT	C3'-C4'-C5'	-2.46	105.28	110.93
29	r	303	CLA	C2A-C1A-CHA	2.46	128.16	123.86
47	Y	317	LUT	C36-C21-C26	-2.46	105.82	109.55
46	R	304	CHL	C2B-C1B-NB	-2.46	108.58	110.23
29	D	405	CLA	C3B-C4B-NB	-2.46	108.23	110.52
29	N	611	CLA	C3B-C4B-NB	-2.46	108.23	110.52
37	Y	319	LHG	O8-C23-C24	2.46	119.63	111.91
36	r	301	DGD	O1G-C1A-C2A	2.46	119.63	111.91
46	g	606	CHL	C4D-CHA-C1A	2.46	124.24	121.25
46	g	605	CHL	C4B-CHC-C1C	2.46	132.17	126.34
29	s	306	CLA	C2A-C1A-CHA	2.46	128.16	123.86
29	b	516	CLA	C4A-NA-C1A	2.46	107.81	106.71
29	C	510	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
48	g	617	NEX	C38-C25-C26	-2.45	118.15	122.26
29	d	403	CLA	C3B-C4B-NB	-2.45	108.24	110.52
29	R	302	CLA	C2B-C1B-NB	-2.45	108.59	110.23
29	s	311	CLA	C3B-C4B-NB	-2.45	108.24	110.52
29	C	504	CLA	C2B-C1B-NB	-2.45	108.59	110.23
46	N	605	CHL	C4B-CHC-C1C	2.45	132.15	126.34
46	s	302	CHL	CHB-C4A-NA	2.45	127.90	124.51
36	c	516	DGD	O1G-C1A-C2A	2.45	119.59	111.91
46	N	607	CHL	CHD-C4C-C3C	2.45	128.44	124.84
29	r	310	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
48	G	617	NEX	O24-C25-C38	-2.45	112.12	115.06
49	y	302	XAT	C19-C9-C10	-2.45	119.50	122.92
34	b	519	C7Z	C35-C15-C14	-2.45	118.46	123.47
46	N	601	CHL	C1-O2A-CGA	2.45	122.86	116.44
29	B	502	CLA	C3B-C4B-NB	-2.44	108.25	110.52
46	N	606	CHL	C2B-C1B-NB	-2.44	108.59	110.23
29	N	612	CLA	C4A-NA-C1A	2.44	107.80	106.71
48	n	616	NEX	C20-C13-C14	-2.44	119.50	122.92
29	G	603	CLA	CMB-C2B-C1B	2.44	129.09	125.37
29	G	611	CLA	C3B-C4B-NB	-2.44	108.25	110.52
46	Y	302	CHL	C1-C2-C3	-2.44	121.83	126.04
46	g	607	CHL	C4D-CHA-C1A	2.44	124.22	121.25
46	g	609	CHL	CHB-C4A-NA	2.44	127.88	124.51
37	y	320	LHG	C5-O7-C7	-2.44	111.79	117.79
29	n	611	CLA	CMB-C2B-C1B	2.44	129.08	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	v	101	BCR	C37-C22-C23	2.44	121.92	118.08
48	N	617	NEX	C38-C25-C26	-2.43	118.18	122.26
29	Y	311	CLA	CHA-C1A-NA	-2.43	120.83	126.40
48	n	616	NEX	C38-C25-C26	-2.43	118.19	122.26
46	S	302	CHL	C4B-CHC-C1C	2.43	132.10	126.34
44	e	101	HEM	C4A-NA-C1A	2.43	107.73	105.35
38	B	524	LMT	C3'-C4'-C5'	-2.43	105.36	110.93
29	C	512	CLA	C4A-NA-C1A	2.43	107.80	106.71
49	Y	301	XAT	C18-C5-C6	-2.43	118.19	122.26
31	c	514	BCR	C34-C9-C10	-2.43	119.52	122.92
29	G	604	CLA	CHA-C1A-NA	-2.43	120.84	126.40
29	c	505	CLA	C3B-C4B-NB	-2.43	108.26	110.52
45	H	101	RRX	C30-C29-C28	-2.43	108.16	113.64
29	N	603	CLA	CHA-C1A-NA	-2.43	120.84	126.40
29	r	309	CLA	C3B-C2B-C1B	-2.43	104.23	107.16
29	c	506	CLA	CHC-C4B-NB	2.42	126.82	124.26
46	G	608	CHL	CHB-C4A-NA	2.42	127.86	124.51
34	B	519	C7Z	C18-C5-C4	2.42	118.84	114.36
29	A	407	CLA	C4A-NA-C1A	2.42	107.80	106.71
46	N	601	CHL	C4A-NA-C1A	2.42	107.80	106.71
31	f	101	BCR	C37-C22-C21	-2.42	119.53	122.92
31	C	517	BCR	C33-C5-C6	-2.42	121.81	124.53
46	g	606	CHL	C3C-C4C-NC	-2.42	107.86	110.57
29	a	408	CLA	C3B-C4B-NB	-2.42	108.27	110.52
45	H	101	RRX	C23-C24-C25	-2.42	120.41	127.20
46	G	605	CHL	C2B-C1B-NB	-2.42	108.61	110.23
49	N	619	XAT	C6-C7-C8	-2.42	120.88	125.99
49	N	619	XAT	C39-C29-C30	-2.42	119.54	122.92
29	c	510	CLA	C1D-ND-C4D	-2.42	104.62	106.33
29	R	309	CLA	C1-C2-C3	-2.42	122.84	126.75
31	C	516	BCR	C38-C26-C25	-2.42	121.82	124.53
46	S	309	CHL	CHB-C4A-NA	2.41	127.85	124.51
48	g	617	NEX	C19-C9-C10	-2.41	119.54	122.92
46	y	303	CHL	C4A-NA-C1A	2.41	107.79	106.71
29	A	406	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
29	N	610	CLA	CHA-C1A-NA	-2.41	120.88	126.40
31	B	517	BCR	C36-C18-C17	-2.41	119.55	122.92
29	B	511	CLA	C3C-C4C-NC	-2.41	107.87	110.57
46	n	601	CHL	C1-O2A-CGA	2.41	122.77	116.44
40	I	101	SPH	C3-C4-C5	-2.41	119.42	124.79
29	B	515	CLA	CMB-C2B-C1B	2.41	129.04	125.37
29	n	609	CLA	C3B-C4B-NB	-2.41	108.28	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	f	101	BCR	C33-C5-C6	-2.41	121.82	124.53
48	S	319	NEX	C1-C2-C3	2.41	119.08	113.64
31	B	517	BCR	C37-C22-C23	2.41	121.87	118.08
48	G	617	NEX	C20-C13-C14	-2.41	119.55	122.92
43	D	406	PL9	C27-C28-C29	-2.40	121.87	127.66
46	Y	307	CHL	C2B-C1B-NB	-2.40	108.62	110.23
40	c	523	SPH	C3-C4-C5	-2.40	119.43	124.79
46	Y	302	CHL	C4B-CHC-C1C	2.40	132.04	126.34
48	G	617	NEX	C38-C25-C26	-2.40	118.23	122.26
35	d	407	LMG	O8-C28-C29	2.40	119.45	111.91
29	n	612	CLA	CHD-C1D-ND	-2.40	122.25	124.45
35	D	410	LMG	O8-C28-C29	2.40	119.44	111.91
44	E	101	HEM	C4A-NA-C1A	2.40	107.70	105.35
46	G	608	CHL	C2B-C1B-NB	-2.40	108.62	110.23
29	g	610	CLA	CHA-C1A-NA	-2.40	120.91	126.40
47	y	318	LUT	C31-C30-C29	-2.40	123.89	127.31
36	r	301	DGD	C1E-O6E-C5E	2.40	118.39	113.69
43	d	405	PL9	C40-C39-C41	2.40	119.30	115.27
46	s	308	CHL	C4B-CHC-C1C	2.39	132.02	126.34
35	C	524	LMG	O8-C28-O10	-2.39	117.55	123.59
29	Y	314	CLA	CMB-C2B-C1B	2.39	129.01	125.37
29	G	602	CLA	C1-C2-C3	-2.39	121.90	126.04
29	C	513	CLA	C4A-NA-C1A	2.39	107.78	106.71
29	B	506	CLA	C2D-C1D-ND	-2.39	108.34	110.10
29	b	516	CLA	C3B-C4B-NB	-2.39	108.30	110.52
29	A	405	CLA	C1-C2-C3	2.39	130.18	126.04
46	y	308	CHL	C3C-C4C-NC	-2.39	107.89	110.57
48	y	319	NEX	C38-C25-C26	-2.39	118.26	122.26
31	b	518	BCR	C23-C22-C21	-2.39	115.28	118.94
46	N	606	CHL	C4B-CHC-C1C	2.39	132.00	126.34
47	N	616	LUT	C10-C11-C12	-2.39	115.77	123.22
41	b	522	DGA	OG1-CA1-CA2	2.39	119.39	111.91
39	l	101	SQD	O3-C3-C2	-2.39	104.83	110.35
29	Y	305	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
46	y	309	CHL	C1-O2A-CGA	2.38	122.69	116.44
46	s	307	CHL	C3B-C4B-NB	-2.38	108.31	110.52
40	i	102	SPH	C3-C4-C5	-2.38	119.48	124.79
46	g	608	CHL	C2B-C1B-NB	-2.38	108.64	110.23
31	f	101	BCR	C28-C27-C26	-2.38	109.83	114.08
48	R	312	NEX	C20-C13-C12	2.38	119.86	114.60
46	n	606	CHL	C3C-C4C-NC	-2.38	107.90	110.57
29	G	603	CLA	O2A-CGA-O1A	-2.38	117.59	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	503	CLA	C2D-C1D-ND	-2.38	108.35	110.10
29	B	510	CLA	CMB-C2B-C1B	2.37	128.99	125.37
29	c	511	CLA	CHA-C1A-NA	-2.37	120.96	126.40
47	n	615	LUT	C10-C11-C12	-2.37	115.81	123.22
35	i	101	LMG	C8-O7-C10	-2.37	111.95	117.79
37	y	320	LHG	C6-C5-C4	-2.37	106.18	111.79
29	b	502	CLA	C4A-NA-C1A	2.37	107.77	106.71
29	g	610	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
47	N	615	LUT	C7-C8-C9	-2.37	122.65	126.23
29	G	611	CLA	C3B-C2B-C1B	-2.37	104.30	107.16
46	y	307	CHL	CHB-C4A-NA	2.37	127.79	124.51
47	y	317	LUT	C31-C30-C29	-2.37	123.93	127.31
46	g	606	CHL	CHB-C4A-NA	2.37	127.78	124.51
47	g	616	LUT	C10-C11-C12	-2.37	115.83	123.22
46	g	607	CHL	C3A-C2A-C1A	2.37	104.88	101.34
49	Y	301	XAT	C39-C29-C30	-2.37	119.61	122.92
46	g	609	CHL	C2B-C1B-NB	-2.37	108.65	110.23
46	n	607	CHL	CHB-C4A-NA	2.37	127.78	124.51
31	c	514	BCR	C33-C5-C6	-2.37	121.87	124.53
30	A	408	PHO	C1C-C2C-C3C	-2.36	106.64	108.61
29	N	602	CLA	C4A-NA-C1A	2.36	107.77	106.71
29	G	610	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
31	c	515	BCR	C2-C1-C6	2.36	114.12	110.48
29	n	613	CLA	CHA-C1A-NA	-2.36	120.99	126.40
29	y	305	CLA	C3B-C4B-NB	-2.36	108.32	110.52
31	A	410	BCR	C23-C22-C21	-2.36	115.32	118.94
48	G	617	NEX	C19-C9-C10	-2.36	119.62	122.92
29	Y	314	CLA	C3B-C4B-NB	-2.36	108.33	110.52
43	d	405	PL9	C27-C28-C29	-2.36	121.98	127.66
29	R	308	CLA	C3B-C2B-C1B	-2.36	104.31	107.16
29	r	309	CLA	C3B-C4B-NB	-2.36	108.33	110.52
29	s	306	CLA	C3B-C2B-C1B	-2.36	104.31	107.16
46	n	608	CHL	C4A-NA-C1A	2.36	107.77	106.71
29	B	503	CLA	C3B-C4B-NB	-2.36	108.33	110.52
31	b	518	BCR	C36-C18-C17	-2.36	119.62	122.92
46	S	309	CHL	C2B-C1B-NB	-2.36	108.65	110.23
46	g	606	CHL	C2B-C1B-NB	-2.36	108.65	110.23
43	D	406	PL9	C22-C23-C24	-2.36	121.99	127.66
29	n	611	CLA	C3B-C4B-NB	-2.36	108.33	110.52
31	C	517	BCR	C33-C5-C4	2.35	118.14	113.62
46	y	308	CHL	C1-O2A-CGA	2.35	122.62	116.44
29	y	312	CLA	CHA-C1A-NA	-2.35	121.01	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	y	311	CHL	C2B-C1B-NB	-2.35	108.66	110.23
31	C	517	BCR	C34-C9-C10	-2.35	119.63	122.92
48	Y	318	NEX	C16-C1-C6	-2.35	108.37	110.47
46	S	307	CHL	C2B-C1B-NB	-2.35	108.66	110.23
45	H	101	RRX	C2-C1-C6	2.35	114.10	110.48
46	g	605	CHL	C4A-NA-C1A	2.35	107.76	106.71
49	r	312	XAT	C7-C8-C9	-2.35	121.89	125.53
40	C	525	SPH	C3-C4-C5	-2.35	119.55	124.79
47	S	317	LUT	C30-C31-C32	-2.35	115.89	123.22
29	a	404	CLA	C3C-C4C-NC	-2.35	107.94	110.57
46	Y	307	CHL	C3C-C4C-NC	-2.35	107.94	110.57
29	N	611	CLA	CMB-C2B-C1B	2.35	128.94	125.37
31	c	515	BCR	C3-C4-C5	-2.35	109.89	114.08
48	N	617	NEX	C17-C1-C6	-2.35	108.37	110.47
29	B	503	CLA	C2D-C1D-ND	-2.35	108.38	110.10
29	n	602	CLA	C1-C2-C3	-2.35	121.99	126.04
47	n	615	LUT	C22-C23-C24	-2.34	109.07	111.74
46	s	309	CHL	C2B-C1B-NB	-2.34	108.66	110.23
29	r	310	CLA	O2A-CGA-O1A	-2.34	117.67	123.59
46	n	607	CHL	C4A-NA-C1A	2.34	107.76	106.71
29	B	508	CLA	C2B-C1B-NB	-2.34	108.66	110.23
29	g	602	CLA	C1-C2-C3	-2.34	121.99	126.04
47	G	616	LUT	C10-C11-C12	-2.34	115.91	123.22
31	C	517	BCR	C3-C4-C5	-2.34	109.89	114.08
29	n	603	CLA	C3B-C4B-NB	-2.34	108.34	110.52
31	a	409	BCR	C23-C22-C21	-2.34	115.35	118.94
29	y	304	CLA	C3B-C2B-C1B	-2.34	104.34	107.16
30	d	402	PHO	C1-C2-C3	-2.34	122.00	126.04
30	a	407	PHO	C1C-C2C-C3C	-2.34	106.66	108.61
31	c	514	BCR	C38-C26-C25	-2.34	121.90	124.53
49	N	619	XAT	C40-C33-C34	-2.34	119.65	122.92
29	R	308	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
47	r	311	LUT	C37-C21-C26	2.34	113.08	109.55
31	C	517	BCR	C31-C1-C6	-2.34	106.51	110.30
29	s	314	CLA	C3B-C4B-NB	-2.33	108.35	110.52
46	Y	307	CHL	C4D-CHA-C1A	2.33	124.09	121.25
46	N	608	CHL	C4A-NA-C1A	2.33	107.75	106.71
29	n	604	CLA	CHA-C1A-NA	-2.33	121.06	126.40
31	C	517	BCR	C35-C13-C12	2.33	121.75	118.08
46	Y	310	CHL	C1-C2-C3	-2.33	122.01	126.04
31	C	515	BCR	C38-C26-C25	-2.33	121.91	124.53
29	b	508	CLA	C2B-C1B-NB	-2.33	108.67	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	G	609	CHL	CHB-C4A-NA	2.33	127.73	124.51
48	Y	318	NEX	C38-C25-C26	-2.33	118.36	122.26
39	C	523	SQD	O3-C3-C2	-2.33	104.97	110.35
29	D	404	CLA	C6-C5-C3	-2.33	107.36	113.45
29	c	505	CLA	C1-C2-C3	-2.32	122.02	126.04
46	g	608	CHL	CHB-C4A-NA	2.32	127.72	124.51
46	N	607	CHL	C1-O2A-CGA	2.32	122.54	116.44
37	d	406	LHG	C5-O7-C7	-2.32	112.07	117.79
29	B	515	CLA	C3B-C4B-NB	-2.32	108.36	110.52
39	b	523	SQD	O3-C3-C2	-2.32	104.98	110.35
29	C	511	CLA	C2D-C1D-ND	-2.32	108.39	110.10
47	N	616	LUT	C35-C15-C14	-2.32	118.72	123.47
46	G	605	CHL	C4B-CHC-C1C	2.32	131.84	126.34
29	b	502	CLA	C3B-C2B-C1B	-2.32	104.36	107.16
29	b	515	CLA	CMB-C2B-C1B	2.32	128.90	125.37
49	G	619	XAT	C19-C9-C10	-2.32	119.68	122.92
49	y	302	XAT	C18-C5-C6	-2.32	118.38	122.26
48	r	313	NEX	C20-C13-C12	2.31	119.71	114.60
29	N	602	CLA	CHA-C1A-NA	-2.31	121.11	126.40
29	C	504	CLA	C3B-C4B-NB	-2.31	108.37	110.52
29	s	303	CLA	CHA-C1A-NA	-2.31	121.11	126.40
29	C	507	CLA	C2B-C1B-NB	-2.31	108.68	110.23
29	b	516	CLA	C2B-C1B-NB	-2.31	108.68	110.23
29	G	603	CLA	CHA-C1A-NA	-2.31	121.11	126.40
45	H	101	RRX	C34-C9-C10	-2.31	119.69	122.92
47	Y	316	LUT	C11-C10-C9	-2.31	124.02	127.31
29	Y	303	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
29	y	313	CLA	C3B-C2B-C1B	-2.31	104.38	107.16
29	N	613	CLA	CHC-C4B-NB	2.31	126.70	124.26
31	b	517	BCR	C1-C6-C5	-2.31	119.36	122.61
29	B	514	CLA	CHC-C4B-NB	2.31	126.70	124.26
29	S	306	CLA	CHA-C1A-NA	-2.30	121.12	126.40
46	s	307	CHL	CHB-C4A-NA	2.30	127.70	124.51
34	b	519	C7Z	C7-C6-C5	-2.30	115.89	121.46
46	n	608	CHL	C1-C2-C3	-2.30	122.06	126.04
29	Y	311	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
29	s	306	CLA	C3B-C4B-NB	-2.30	108.38	110.52
47	r	311	LUT	C37-C21-C22	-2.30	105.08	109.44
46	n	608	CHL	C4D-CHA-C1A	2.30	124.05	121.25
46	y	301	CHL	C1-O2A-CGA	2.30	122.48	116.44
29	N	613	CLA	C3B-C4B-NB	-2.30	108.38	110.52
48	y	319	NEX	C4-C3-C2	2.30	115.21	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S	316	CLA	C3B-C2B-C1B	-2.30	104.39	107.16
31	C	517	BCR	C29-C30-C25	2.30	114.02	110.48
39	L	102	SQD	O3-C3-C2	-2.30	105.04	110.35
31	c	515	BCR	C27-C26-C25	-2.30	119.39	122.73
46	S	308	CHL	C4A-NA-C1A	2.30	107.74	106.71
29	S	310	CLA	C3B-C2B-C1B	-2.30	104.39	107.16
29	S	303	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
46	G	606	CHL	C4B-CHC-C1C	2.30	131.78	126.34
29	y	310	CLA	CHA-C1A-NA	-2.30	121.14	126.40
46	s	302	CHL	C4D-CHA-C1A	2.30	124.04	121.25
29	C	503	CLA	C1-C2-C3	-2.29	122.08	126.04
31	f	101	BCR	C23-C24-C25	-2.29	120.76	127.20
29	r	303	CLA	C3B-C4B-NB	-2.29	108.39	110.52
48	g	617	NEX	O24-C25-C38	-2.29	112.31	115.06
29	C	511	CLA	CHC-C4B-NB	2.29	126.68	124.26
29	c	506	CLA	C3B-C4B-NB	-2.29	108.39	110.52
46	Y	306	CHL	CHB-C4A-NA	2.29	127.68	124.51
29	B	501	CLA	CHA-C1A-NA	-2.29	121.15	126.40
49	R	311	XAT	O24-C25-C24	2.29	115.10	113.38
45	H	101	RRX	C15-C16-C17	-2.29	118.79	123.47
46	y	308	CHL	C3B-C4B-NB	-2.29	108.39	110.52
46	n	606	CHL	C2B-C1B-NB	-2.29	108.70	110.23
29	n	603	CLA	CHA-C1A-NA	-2.29	121.16	126.40
46	Y	306	CHL	C4D-CHA-C1A	2.29	124.03	121.25
43	d	405	PL9	O1-C4-C3	-2.29	118.20	120.72
34	B	519	C7Z	C7-C6-C5	-2.29	115.92	121.46
46	N	609	CHL	C2B-C1B-NB	-2.29	108.70	110.23
46	S	309	CHL	CHD-C4C-C3C	2.29	128.20	124.84
49	R	311	XAT	C40-C33-C34	-2.29	119.72	122.92
49	n	618	XAT	C40-C33-C34	-2.29	119.72	122.92
48	s	319	NEX	C31-C30-C29	2.29	130.57	127.31
29	Y	305	CLA	CHA-C1A-NA	-2.29	121.16	126.40
31	K	101	BCR	C12-C13-C14	-2.28	115.44	118.94
29	y	306	CLA	CHA-C1A-NA	-2.28	121.17	126.40
46	G	609	CHL	CHD-C4C-C3C	2.28	128.20	124.84
29	R	308	CLA	C3B-C4B-NB	-2.28	108.40	110.52
29	C	512	CLA	C3B-C2B-C1B	-2.28	104.41	107.16
48	r	313	NEX	C38-C25-C26	-2.28	118.43	122.26
29	b	510	CLA	C2B-C1B-NB	-2.28	108.70	110.23
29	b	506	CLA	C3B-C4B-NB	-2.28	108.40	110.52
31	c	515	BCR	C39-C30-C25	-2.28	106.60	110.30
37	N	618	LHG	C5-O7-C7	-2.28	112.18	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	v	101	BCR	C29-C28-C27	2.28	116.47	111.38
31	c	514	BCR	C4-C5-C6	-2.28	119.42	122.73
29	b	514	CLA	C3B-C4B-NB	-2.28	108.40	110.52
31	z	101	BCR	C19-C18-C17	2.28	122.44	118.94
48	G	617	NEX	C4-C3-C2	2.28	115.17	110.77
31	F	101	BCR	C37-C22-C23	2.28	121.67	118.08
29	C	507	CLA	CHC-C4B-NB	2.28	126.67	124.26
29	b	515	CLA	C3B-C4B-NB	-2.28	108.40	110.52
31	b	517	BCR	C35-C13-C12	2.28	121.66	118.08
45	h	101	RRX	C36-C18-C17	-2.28	119.74	122.92
37	D	408	LHG	O8-C23-C24	2.28	119.05	111.91
31	c	514	BCR	C31-C1-C6	-2.27	106.61	110.30
29	S	304	CLA	CHA-C1A-NA	-2.27	121.19	126.40
49	n	618	XAT	O24-C25-C24	2.27	115.09	113.38
29	G	610	CLA	C1-C2-C3	-2.27	122.11	126.04
31	B	518	BCR	C36-C18-C17	-2.27	119.74	122.92
29	c	507	CLA	CHA-C1A-NA	-2.27	121.20	126.40
45	h	101	RRX	C2-C1-C6	2.27	113.98	110.48
29	B	507	CLA	CHA-C1A-NA	-2.27	121.20	126.40
29	s	314	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
46	Y	310	CHL	CHD-C4C-C3C	2.27	128.18	124.84
46	G	609	CHL	C1-C2-C3	-2.27	122.12	126.04
29	r	308	CLA	CHA-C1A-NA	-2.27	121.21	126.40
46	g	606	CHL	CAA-C2A-C3A	-2.27	106.57	112.78
46	R	304	CHL	C3C-C4C-NC	-2.26	108.03	110.57
50	Y	320	PTY	C6-O7-C8	-2.26	113.68	117.90
29	g	603	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
46	r	305	CHL	C3C-C4C-NC	-2.26	108.03	110.57
39	c	522	SQD	O3-C3-C2	-2.26	105.12	110.35
29	r	302	CLA	C3B-C4B-NB	-2.26	108.42	110.52
46	r	306	CHL	C2B-C1B-NB	-2.26	108.72	110.23
47	G	616	LUT	C38-C25-C24	-2.26	118.73	123.56
47	Y	316	LUT	C15-C35-C34	-2.26	118.85	123.47
46	S	308	CHL	C4D-CHA-C1A	2.26	124.00	121.25
46	n	608	CHL	CHD-C4C-C3C	2.26	128.16	124.84
48	N	617	NEX	C20-C13-C14	-2.26	119.76	122.92
31	f	101	BCR	C38-C26-C27	2.26	117.95	113.62
30	D	401	PHO	C1-C2-C3	-2.26	122.14	126.04
29	B	501	CLA	C3B-C4B-NB	-2.26	108.42	110.52
29	y	314	CLA	C3B-C4B-NB	-2.26	108.42	110.52
39	o	301	SQD	O3-C3-C2	-2.25	105.14	110.35
29	s	316	CLA	C2A-C1A-CHA	2.25	127.80	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	r	311	LUT	C18-C5-C6	-2.25	122.00	124.53
29	B	516	CLA	C3B-C2B-C1B	-2.25	104.44	107.16
47	s	318	LUT	C10-C11-C12	-2.25	116.19	123.22
29	Y	309	CLA	CHA-C1A-NA	-2.25	121.25	126.40
29	Y	313	CLA	C3B-C2B-C1B	-2.25	104.45	107.16
29	s	311	CLA	C1-C2-C3	-2.25	122.15	126.04
36	c	517	DGD	O1G-C1A-O1A	-2.25	117.92	123.59
49	Y	301	XAT	C19-C9-C10	-2.25	119.77	122.92
31	c	515	BCR	C33-C5-C4	2.25	117.93	113.62
46	Y	310	CHL	CHB-C4A-NA	2.25	127.62	124.51
39	M	101	SQD	O3-C3-C2	-2.25	105.16	110.35
29	b	511	CLA	C2B-C1B-NB	-2.25	108.73	110.23
29	B	505	CLA	CHC-C4B-NB	2.25	126.64	124.26
37	s	320	LHG	C5-O7-C7	-2.25	112.26	117.79
43	d	405	PL9	C20-C19-C21	2.25	119.05	115.27
49	r	312	XAT	C40-C33-C34	-2.24	119.78	122.92
29	c	507	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
29	N	602	CLA	C3B-C4B-NB	-2.24	108.43	110.52
29	B	509	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
29	n	602	CLA	C3B-C4B-NB	-2.24	108.44	110.52
46	s	308	CHL	C2B-C1B-NB	-2.24	108.73	110.23
46	r	305	CHL	C4D-CHA-C1A	2.24	123.98	121.25
39	a	410	SQD	O3-C3-C2	-2.24	105.17	110.35
29	n	612	CLA	C3B-C4B-NB	-2.24	108.44	110.52
29	B	502	CLA	C3B-C2B-C1B	-2.24	104.46	107.16
29	B	501	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
29	r	307	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
48	S	319	NEX	C16-C1-C6	-2.24	108.47	110.47
47	n	614	LUT	C19-C9-C8	2.24	121.60	118.08
29	R	309	CLA	C3B-C2B-C1B	-2.24	104.46	107.16
44	e	101	HEM	C4D-ND-C1D	2.24	107.38	105.07
49	g	619	XAT	C18-C5-C6	-2.23	118.52	122.26
46	S	307	CHL	C3C-C4C-NC	-2.23	108.07	110.57
31	f	101	BCR	C38-C26-C25	-2.23	122.02	124.53
29	B	508	CLA	C3B-C2B-C1B	-2.23	104.47	107.16
48	G	617	NEX	C5-C4-C3	2.23	114.39	111.75
46	s	309	CHL	CHB-C4A-NA	2.23	127.60	124.51
31	K	101	BCR	C37-C22-C23	2.23	121.59	118.08
29	c	506	CLA	C2B-C1B-NB	-2.23	108.74	110.23
47	Y	317	LUT	C35-C15-C14	-2.23	118.91	123.47
47	S	318	LUT	C10-C11-C12	-2.23	116.26	123.22
47	y	317	LUT	C39-C29-C28	2.23	121.59	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	405	CLA	C4A-NA-C1A	2.23	107.71	106.71
31	c	514	BCR	C34-C9-C8	2.23	121.59	118.08
46	G	605	CHL	C1-O2A-CGA	2.23	123.20	116.73
29	a	405	CLA	C1-O2A-CGA	2.23	122.29	116.44
39	C	501	SQD	O3-C3-C2	-2.23	105.20	110.35
29	B	504	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
43	D	406	PL9	O1-C4-C3	-2.23	118.27	120.72
31	B	517	BCR	C23-C22-C21	-2.22	115.53	118.94
29	s	316	CLA	C1-C2-C3	-2.22	123.15	126.75
47	R	310	LUT	C38-C25-C24	-2.22	118.80	123.56
29	s	313	CLA	CHC-C4B-NB	2.22	126.61	124.26
31	f	101	BCR	C4-C5-C6	-2.22	119.50	122.73
47	n	615	LUT	C31-C30-C29	-2.22	124.14	127.31
31	z	101	BCR	C35-C13-C12	2.22	121.58	118.08
44	E	101	HEM	C1B-NB-C4B	2.22	107.37	105.07
29	N	614	CLA	CHA-C1A-NA	-2.22	121.31	126.40
29	y	312	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
29	b	514	CLA	C3B-C2B-C1B	-2.22	104.48	107.16
45	h	101	RRX	C11-C12-C13	-2.22	120.19	126.42
29	b	509	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
46	G	606	CHL	C4D-CHA-C1A	2.22	123.95	121.25
29	N	614	CLA	C3B-C2B-C1B	-2.21	104.49	107.16
46	n	606	CHL	C4B-CHC-C1C	2.21	131.59	126.34
48	r	313	NEX	C40-C33-C34	-2.21	119.82	122.92
29	B	503	CLA	C1-C2-C3	-2.21	122.22	126.04
31	B	518	BCR	C33-C5-C4	2.21	117.86	113.62
29	B	503	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
29	B	514	CLA	C3B-C2B-C1B	-2.21	104.49	107.16
29	D	404	CLA	C17-C16-C15	-2.21	103.09	113.24
46	g	609	CHL	CHD-C4C-C3C	2.21	128.09	124.84
47	N	615	LUT	C19-C9-C8	2.21	121.55	118.08
29	R	301	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
45	h	101	RRX	C23-C22-C21	2.21	122.33	118.94
29	B	510	CLA	C3B-C4B-NB	-2.21	108.47	110.52
47	y	317	LUT	C11-C10-C9	-2.21	124.16	127.31
44	e	101	HEM	C4C-NC-C1C	2.20	107.51	105.35
29	n	610	CLA	CHA-C1A-NA	-2.20	121.35	126.40
46	S	307	CHL	CHB-C4A-NA	2.20	127.56	124.51
39	m	101	SQD	O3-C3-C2	-2.20	105.25	110.35
29	D	404	CLA	CHA-C4D-ND	-2.20	127.89	132.50
29	S	314	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
29	a	405	CLA	O2A-CGA-O1A	-2.20	118.03	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	N	613	CLA	CMB-C2B-C1B	2.20	128.72	125.37
30	D	401	PHO	C1C-C2C-C3C	-2.20	106.78	108.61
31	b	517	BCR	C34-C9-C10	-2.20	119.84	122.92
31	B	517	BCR	C1-C6-C7	2.20	122.00	115.78
29	Y	312	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
29	r	302	CLA	CHA-C1A-NA	-2.20	121.36	126.40
30	A	408	PHO	C1-C2-C3	-2.20	122.24	126.04
35	c	519	LMG	C8-O7-C10	-2.20	112.38	117.79
31	c	515	BCR	C29-C30-C25	2.20	113.86	110.48
47	g	616	LUT	C35-C15-C14	-2.20	118.97	123.47
46	N	605	CHL	C2B-C1B-NB	-2.20	108.76	110.23
29	r	303	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
29	b	511	CLA	C3B-C4B-NB	-2.20	108.48	110.52
49	G	619	XAT	C39-C29-C30	-2.20	119.85	122.92
29	b	506	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
29	D	404	CLA	C4-C3-C5	2.20	118.96	115.27
29	D	404	CLA	C6-C7-C8	2.20	123.02	115.92
29	D	405	CLA	C1C-C2C-C3C	-2.19	104.65	106.96
29	c	501	CLA	C3C-C4C-NC	-2.19	108.11	110.57
29	y	304	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
29	Y	312	CLA	CHA-C1A-NA	-2.19	121.39	126.40
29	S	304	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
46	G	607	CHL	C4D-CHA-C1A	2.19	123.91	121.25
31	C	515	BCR	C33-C5-C4	2.19	117.82	113.62
46	N	608	CHL	CHB-C4A-NA	2.19	127.53	124.51
45	h	101	RRX	C7-C8-C9	-2.19	122.93	126.23
49	G	619	XAT	C20-C13-C14	-2.19	119.86	122.92
29	y	310	CLA	C3B-C2B-C1B	-2.19	104.52	107.16
49	G	619	XAT	C26-C27-C28	-2.19	121.37	125.99
29	Y	309	CLA	C3B-C4B-NB	-2.18	108.49	110.52
29	S	311	CLA	C3B-C2B-C1B	-2.18	104.53	107.16
46	R	304	CHL	C4D-CHA-C1A	2.18	123.91	121.25
29	b	514	CLA	C1-C2-C3	-2.18	122.27	126.04
43	D	406	PL9	C40-C39-C41	2.18	118.94	115.27
47	n	615	LUT	C35-C15-C14	-2.18	119.01	123.47
47	g	615	LUT	C39-C29-C28	2.18	121.51	118.08
39	M	101	SQD	O8-S-C6	-2.18	102.27	105.74
34	b	519	C7Z	C2-C3-C4	2.18	113.28	110.30
29	n	602	CLA	CHA-C1A-NA	-2.18	121.41	126.40
29	R	302	CLA	CHC-C4B-NB	2.18	126.56	124.26
29	Y	304	CLA	CHC-C4B-NB	2.18	126.56	124.26
29	G	610	CLA	C3B-C4B-NB	-2.18	108.50	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	Y	301	XAT	C26-C27-C28	-2.18	121.39	125.99
29	B	504	CLA	CHD-C1D-ND	-2.18	122.45	124.45
29	b	501	CLA	CHA-C1A-NA	-2.17	121.42	126.40
29	s	312	CLA	CHA-C1A-NA	-2.17	121.42	126.40
29	b	510	CLA	C3B-C4B-NB	-2.17	108.50	110.52
37	n	617	LHG	C6-C5-C4	-2.17	106.65	111.79
29	C	512	CLA	CHC-C4B-NB	2.17	126.56	124.26
29	c	510	CLA	CHC-C4B-NB	2.17	126.56	124.26
45	h	101	RRX	C30-C29-C28	-2.17	108.74	113.64
29	A	405	CLA	C3C-C4C-NC	-2.17	108.14	110.57
29	s	315	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
46	g	601	CHL	C2B-C1B-NB	-2.17	108.78	110.23
49	n	618	XAT	C39-C29-C30	-2.17	119.89	122.92
29	B	504	CLA	CMB-C2B-C1B	2.17	128.67	125.37
46	g	609	CHL	C1-C2-C3	-2.17	122.29	126.04
49	g	619	XAT	C26-C27-C28	-2.17	121.41	125.99
34	B	519	C7Z	C30-C31-C32	-2.17	116.45	123.22
29	B	504	CLA	C4-C3-C5	2.17	118.92	115.27
31	b	517	BCR	C36-C18-C17	-2.17	119.89	122.92
29	s	311	CLA	O2A-CGA-O1A	-2.17	118.13	123.59
29	a	408	CLA	CHA-C1A-NA	-2.17	121.44	126.40
29	s	310	CLA	CHA-C1A-NA	-2.16	121.44	126.40
35	C	524	LMG	O1-C1-C2	2.16	111.68	108.30
29	s	312	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
48	s	319	NEX	C40-C33-C34	-2.16	119.89	122.92
46	g	607	CHL	CHD-C4C-C3C	2.16	128.02	124.84
29	b	514	CLA	CHC-C4B-NB	2.16	126.55	124.26
29	S	311	CLA	C1-C2-C3	-2.16	122.31	126.04
45	h	101	RRX	C15-C16-C17	-2.16	119.05	123.47
29	a	405	CLA	CHA-C1A-NA	-2.16	121.45	126.40
37	N	618	LHG	C6-C5-C4	-2.16	106.68	111.79
46	N	609	CHL	C1-C2-C3	-2.16	122.31	126.04
29	r	307	CLA	CHA-C1A-NA	-2.16	121.45	126.40
29	y	316	CLA	C1-C2-C3	-2.16	122.31	126.04
29	b	505	CLA	C2D-C1D-ND	-2.16	108.51	110.10
29	G	613	CLA	CHC-C4B-NB	2.16	126.54	124.26
48	y	319	NEX	O24-C25-C38	-2.16	112.47	115.06
29	g	614	CLA	CHA-C1A-NA	-2.15	121.46	126.40
31	A	410	BCR	C33-C5-C4	2.15	117.75	113.62
29	G	602	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
48	n	616	NEX	O24-C25-C38	-2.15	112.48	115.06
49	G	619	XAT	C18-C5-C6	-2.15	118.66	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G	614	CLA	CHC-C4B-NB	2.15	126.53	124.26
29	B	506	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
43	d	405	PL9	C37-C38-C39	-2.15	122.49	127.66
29	D	404	CLA	CHB-C1B-C2B	-2.15	121.17	127.24
29	Y	313	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
47	n	615	LUT	C38-C25-C24	-2.15	118.96	123.56
47	N	615	LUT	C30-C31-C32	-2.15	116.52	123.22
46	y	301	CHL	C3B-C4B-NB	-2.15	108.52	110.52
29	N	604	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
46	y	309	CHL	C4D-CHA-C1A	2.15	123.86	121.25
29	a	404	CLA	C2D-C1D-ND	-2.15	108.52	110.10
31	b	517	BCR	C37-C22-C23	2.15	121.46	118.08
29	b	512	CLA	C3B-C4B-NB	-2.15	108.53	110.52
29	y	313	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
46	Y	302	CHL	CHD-C4C-C3C	2.14	127.99	124.84
48	S	319	NEX	C26-C27-C28	-2.14	121.46	125.99
29	b	508	CLA	C3B-C2B-C1B	-2.14	104.57	107.16
46	G	601	CHL	C2B-C1B-NB	-2.14	108.80	110.23
46	y	301	CHL	C4D-CHA-C1A	2.14	123.86	121.25
31	K	101	BCR	C29-C28-C27	2.14	116.16	111.38
29	y	314	CLA	C3B-C2B-C1B	-2.14	104.58	107.16
46	N	606	CHL	CHB-C4A-NA	2.14	127.47	124.51
37	S	320	LHG	C5-O7-C7	-2.14	112.52	117.79
29	N	604	CLA	CHA-C1A-NA	-2.14	121.50	126.40
29	B	514	CLA	C3B-C4B-NB	-2.14	108.53	110.52
29	y	315	CLA	CMB-C2B-C1B	2.14	128.62	125.37
49	R	311	XAT	C27-C28-C29	2.14	128.85	125.53
46	y	308	CHL	C3A-C2A-C1A	2.14	104.54	101.34
49	n	618	XAT	C18-C5-C6	-2.14	118.68	122.26
29	c	512	CLA	C1-C2-C3	-2.14	122.35	126.04
37	G	618	LHG	C5-O7-C7	-2.13	112.53	117.79
47	g	615	LUT	C15-C35-C34	-2.13	119.10	123.47
29	n	602	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
47	y	317	LUT	C15-C35-C34	-2.13	119.11	123.47
29	b	504	CLA	CBA-CAA-C2A	2.13	120.16	113.86
29	r	308	CLA	C2D-C1D-ND	-2.13	108.53	110.10
29	G	612	CLA	CHA-C1A-NA	-2.13	121.52	126.40
29	n	611	CLA	CHA-C1A-NA	-2.13	121.52	126.40
29	b	503	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
29	S	314	CLA	CHC-C4B-NB	2.13	126.51	124.26
29	S	311	CLA	C3B-C4B-NB	-2.13	108.54	110.52
46	n	605	CHL	C4D-CHA-C1A	2.13	123.84	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S	313	CLA	O2A-CGA-O1A	-2.13	118.00	123.30
49	G	619	XAT	O24-C25-C38	-2.13	112.51	115.06
29	S	314	CLA	C2B-C1B-NB	-2.13	108.81	110.23
46	n	601	CHL	C2B-C1B-NB	-2.13	108.81	110.23
29	n	609	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
34	B	519	C7Z	C19-C9-C10	-2.13	119.95	122.92
29	C	503	CLA	C3B-C2B-C1B	-2.12	104.60	107.16
47	G	615	LUT	C2-C3-C4	-2.12	107.40	110.30
46	S	309	CHL	CHD-C1D-C2D	2.12	129.94	125.48
46	G	601	CHL	CHD-C4C-C3C	2.12	127.96	124.84
48	Y	318	NEX	O24-C25-C38	-2.12	112.51	115.06
29	n	612	CLA	C2B-C1B-NB	-2.12	108.81	110.23
29	R	307	CLA	C3B-C4B-NB	-2.12	108.55	110.52
29	R	301	CLA	CHA-C1A-NA	-2.12	121.54	126.40
29	C	508	CLA	CHA-C1A-NA	-2.12	121.54	126.40
29	B	505	CLA	C1-C2-C3	-2.12	122.38	126.04
37	D	407	LHG	O8-C23-C24	2.12	118.56	111.91
29	S	312	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
29	R	307	CLA	CHD-C1D-C2D	2.12	129.92	125.48
29	n	612	CLA	CHC-C4B-NB	2.12	126.50	124.26
31	a	409	BCR	C33-C5-C4	2.12	117.69	113.62
35	W	201	LMG	O7-C10-O9	-2.12	118.58	123.70
47	R	310	LUT	C30-C31-C32	-2.12	116.61	123.22
30	d	402	PHO	C1C-C2C-C3C	-2.12	106.85	108.61
29	b	509	CLA	C3B-C4B-NB	-2.12	108.55	110.52
29	C	509	CLA	C3B-C4B-NB	-2.12	108.55	110.52
49	G	619	XAT	C40-C33-C34	-2.12	119.96	122.92
46	n	605	CHL	CHD-C4C-C3C	2.12	127.95	124.84
48	S	319	NEX	C4-C3-C2	2.12	114.86	110.77
29	n	609	CLA	C2B-C1B-NB	-2.12	108.81	110.23
31	C	516	BCR	C37-C22-C23	2.11	121.41	118.08
29	s	311	CLA	CHA-C1A-NA	-2.11	121.56	126.40
46	N	601	CHL	C2B-C1B-NB	-2.11	108.81	110.23
46	n	607	CHL	C3B-C4B-NB	-2.11	108.56	110.52
48	N	617	NEX	O24-C25-C38	-2.11	112.53	115.06
47	Y	316	LUT	C19-C9-C8	2.11	121.41	118.08
34	B	519	C7Z	C2-C3-C4	2.11	113.19	110.30
31	B	517	BCR	C34-C9-C8	2.11	121.40	118.08
29	C	504	CLA	CHC-C4B-NB	2.11	126.49	124.26
29	r	303	CLA	CHD-C1D-ND	-2.11	122.52	124.45
47	S	318	LUT	C39-C29-C28	2.11	121.40	118.08
46	N	606	CHL	C4D-CHA-C1A	2.11	123.82	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	g	601	CHL	C4D-CHA-C1A	2.11	123.82	121.25
29	c	501	CLA	CMB-C2B-C1B	2.11	128.58	125.37
29	B	511	CLA	CHB-C1B-NB	2.11	126.49	124.26
29	S	315	CLA	C1-C2-C3	-2.11	123.34	126.75
29	b	510	CLA	CMB-C2B-C1B	2.11	128.58	125.37
29	B	514	CLA	C1-C2-C3	-2.11	122.40	126.04
29	b	506	CLA	CHC-C4B-NB	2.11	126.49	124.26
29	S	310	CLA	C3B-C4B-NB	-2.11	108.56	110.52
46	n	601	CHL	CHD-C4C-C3C	2.11	127.94	124.84
29	B	513	CLA	C3B-C4B-NB	-2.11	108.56	110.52
29	b	515	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
29	G	611	CLA	CHA-C1A-NA	-2.11	121.58	126.40
39	l	101	SQD	O6-C1-C2	-2.10	105.02	108.30
48	R	312	NEX	C40-C33-C34	-2.10	119.98	122.92
29	c	501	CLA	CHC-C4B-NB	2.10	126.48	124.26
29	Y	303	CLA	C3B-C4B-NB	-2.10	108.56	110.52
47	G	615	LUT	C31-C30-C29	-2.10	124.31	127.31
46	y	307	CHL	C4D-CHA-C1A	2.10	123.81	121.25
29	b	509	CLA	C1-C2-C3	-2.10	122.41	126.04
29	c	505	CLA	C3B-C2B-C1B	-2.10	104.62	107.16
29	s	304	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
46	s	308	CHL	C4D-CHA-C1A	2.10	123.81	121.25
46	G	609	CHL	C2B-C1B-NB	-2.10	108.82	110.23
46	s	309	CHL	C4A-NA-C1A	2.10	107.65	106.71
43	D	406	PL9	C37-C38-C39	-2.10	122.61	127.66
29	d	404	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
29	C	506	CLA	C3B-C2B-C1B	-2.10	104.63	107.16
46	Y	308	CHL	C4D-CHA-C1A	2.10	123.80	121.25
47	S	317	LUT	C40-C33-C32	2.10	121.38	118.08
46	s	309	CHL	CHD-C4C-C3C	2.10	127.92	124.84
29	s	305	CLA	CHC-C4B-NB	2.10	126.48	124.26
29	c	508	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
29	s	314	CLA	CHC-C4B-NB	2.10	126.47	124.26
29	S	304	CLA	C1-C2-C3	-2.09	122.42	126.04
48	G	617	NEX	C28-C29-C30	2.09	122.16	118.94
46	g	601	CHL	CHD-C4C-C3C	2.09	127.92	124.84
46	g	607	CHL	CHC-C1C-NC	2.09	127.38	124.20
47	s	317	LUT	C28-C29-C30	-2.09	115.73	118.94
49	y	302	XAT	C39-C29-C30	-2.09	119.99	122.92
29	d	404	CLA	C1C-C2C-C3C	-2.09	104.76	106.96
46	g	608	CHL	CHC-C1C-NC	2.09	127.38	124.20
29	r	303	CLA	C2D-C1D-ND	-2.09	108.56	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	407	PHO	C1-C2-C3	-2.09	122.43	126.04
29	g	603	CLA	C2B-C1B-NB	-2.09	108.83	110.23
31	K	101	BCR	C33-C5-C4	2.09	117.63	113.62
46	Y	307	CHL	CHB-C4A-NA	2.09	127.40	124.51
29	B	516	CLA	C2B-C1B-NB	-2.09	108.83	110.23
29	A	407	CLA	C3B-C2B-C1B	-2.09	104.64	107.16
47	S	318	LUT	C16-C1-C6	-2.09	106.91	110.30
29	d	404	CLA	CHA-C1A-NA	-2.09	121.61	126.40
29	g	603	CLA	CHA-C1A-NA	-2.09	121.62	126.40
29	N	611	CLA	CHA-C1A-NA	-2.09	121.62	126.40
29	g	614	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
29	B	509	CLA	C3B-C4B-NB	-2.09	108.58	110.52
29	b	516	CLA	CHA-C1A-NA	-2.09	121.62	126.40
47	y	318	LUT	C36-C21-C26	-2.09	106.39	109.55
45	h	101	RRX	C8-C9-C10	2.08	122.14	118.94
29	s	313	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
46	n	605	CHL	C1-C2-C3	-2.08	122.44	126.04
29	n	609	CLA	C2A-C1A-CHA	2.08	127.50	123.86
29	S	303	CLA	C3B-C2B-C1B	-2.08	104.65	107.16
46	n	606	CHL	C3A-C2A-C1A	2.08	104.46	101.34
46	y	311	CHL	C1-C2-C3	-2.08	122.44	126.04
29	r	302	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
34	B	519	C7Z	C15-C35-C34	-2.08	119.22	123.47
29	y	310	CLA	CHC-C4B-NB	2.08	126.46	124.26
46	y	308	CHL	CHC-C1C-NC	2.08	127.36	124.20
48	y	319	NEX	C40-C33-C34	-2.08	120.01	122.92
46	N	608	CHL	C3B-C4B-NB	-2.08	108.59	110.52
29	A	407	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
29	c	506	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
50	y	321	PTY	C6-O7-C8	-2.08	114.02	117.90
29	y	313	CLA	CHA-C1A-NA	-2.08	121.64	126.40
29	s	303	CLA	C3B-C4B-NB	-2.08	108.59	110.52
46	S	309	CHL	CHA-C4D-ND	2.08	136.84	132.50
46	Y	302	CHL	CHC-C1C-NC	2.08	127.35	124.20
31	C	515	BCR	C38-C26-C27	2.08	117.60	113.62
29	G	604	CLA	C3B-C2B-C1B	-2.08	104.66	107.16
46	g	605	CHL	CHD-C4C-C3C	2.08	127.89	124.84
29	b	502	CLA	CHC-C4B-NB	2.08	126.45	124.26
29	b	505	CLA	CHC-C4B-NB	2.08	126.45	124.26
46	G	609	CHL	C4A-NA-C1A	2.08	107.64	106.71
29	a	406	CLA	C3C-C4C-NC	-2.07	108.24	110.57
29	y	305	CLA	CMB-C2B-C1B	2.07	128.53	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	G	615	LUT	C39-C29-C28	2.07	121.34	118.08
46	g	605	CHL	C1-O2A-CGA	2.07	122.75	116.73
29	S	316	CLA	C3C-C4C-NC	-2.07	108.25	110.57
29	S	306	CLA	C3B-C4B-NB	-2.07	108.59	110.52
47	r	311	LUT	C3-C4-C5	-2.07	107.72	111.85
29	c	511	CLA	C3B-C2B-C1B	-2.07	104.66	107.16
29	s	316	CLA	C2B-C1B-NB	-2.07	108.84	110.23
29	N	602	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
36	r	301	DGD	O2G-C1B-O1B	-2.07	118.70	123.70
29	N	612	CLA	CHA-C1A-NA	-2.07	121.66	126.40
36	B	521	DGD	O6E-C5E-C4E	2.07	113.45	109.69
34	B	519	C7Z	C36-C21-C26	-2.07	106.94	110.30
29	S	316	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
29	c	501	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
29	Y	315	CLA	C1-C2-C3	-2.07	122.47	126.04
29	B	515	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
29	N	614	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
30	d	402	PHO	O2A-CGA-O1A	-2.07	118.38	123.59
29	g	613	CLA	C3B-C4B-NB	-2.07	108.60	110.52
46	y	303	CHL	CHC-C1C-NC	2.07	127.34	124.20
31	c	515	BCR	C12-C13-C14	-2.06	115.77	118.94
29	Y	312	CLA	C1C-C2C-C3C	-2.06	104.79	106.96
36	C	519	DGD	O1G-C1A-O1A	-2.06	118.38	123.59
29	b	502	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
29	N	610	CLA	C3B-C4B-NB	-2.06	108.60	110.52
39	L	102	SQD	O8-S-C6	-2.06	102.45	105.74
29	C	513	CLA	C1-C2-C3	-2.06	122.48	126.04
29	C	506	CLA	C2B-C1B-NB	-2.06	108.85	110.23
29	A	407	CLA	CHA-C1A-NA	-2.06	121.68	126.40
46	y	301	CHL	CHD-C4C-C3C	2.06	127.87	124.84
29	c	503	CLA	C3C-C4C-NC	-2.06	108.26	110.57
29	r	303	CLA	C1D-ND-C4D	-2.06	104.87	106.33
31	v	101	BCR	C12-C13-C14	-2.06	115.78	118.94
46	n	606	CHL	CHC-C4B-NB	-2.06	122.08	124.26
35	W	203	LMG	O7-C10-O9	-2.06	118.73	123.70
47	Y	316	LUT	C39-C29-C28	2.06	121.32	118.08
43	D	406	PL9	O2-C1-C2	-2.06	117.07	121.78
29	B	506	CLA	CHC-C4B-NB	2.06	126.44	124.26
31	v	101	BCR	C38-C26-C25	-2.06	122.22	124.53
46	Y	310	CHL	C2B-C1B-NB	-2.06	108.85	110.23
43	D	406	PL9	O2-C1-C6	2.06	124.15	120.59
31	a	409	BCR	C36-C18-C17	-2.06	120.04	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	Y	316	LUT	C20-C13-C12	2.06	121.32	118.08
38	B	524	LMT	C1'-O5'-C5'	-2.06	109.65	113.69
29	B	509	CLA	CHC-C4B-NB	2.06	126.43	124.26
29	C	504	CLA	C3C-C4C-NC	-2.06	108.27	110.57
29	y	305	CLA	C1C-C2C-C3C	-2.05	104.80	106.96
46	Y	308	CHL	C3B-C4B-NB	-2.05	108.61	110.52
29	g	604	CLA	CHB-C1B-NB	2.05	126.43	124.26
34	b	519	C7Z	C36-C21-C26	-2.05	106.97	110.30
29	D	404	CLA	C11-C12-C13	-2.05	109.28	115.92
48	R	312	NEX	C38-C25-C26	-2.05	118.82	122.26
35	B	520	LMG	O7-C8-C9	2.05	115.84	108.40
46	s	302	CHL	CHC-C1C-NC	2.05	127.32	124.20
29	c	503	CLA	CMB-C2B-C1B	2.05	128.49	125.37
46	y	308	CHL	CHD-C4C-C3C	2.05	127.86	124.84
29	c	510	CLA	CHA-C1A-NA	-2.05	121.70	126.40
29	S	315	CLA	C3B-C2B-C1B	-2.05	104.69	107.16
36	B	521	DGD	O2G-C1B-O1B	-2.05	118.74	123.70
29	y	316	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
49	g	619	XAT	C39-C29-C30	-2.05	120.05	122.92
37	g	618	LHG	C6-C5-C4	-2.05	106.94	111.79
34	B	519	C7Z	C21-C26-C25	-2.05	119.73	122.61
46	g	606	CHL	CHA-C1A-NA	-2.05	121.70	126.40
29	Y	304	CLA	C1-C2-C3	-2.05	122.50	126.04
29	y	312	CLA	C3B-C4B-NB	-2.05	108.61	110.52
29	a	408	CLA	C3C-C4C-NC	-2.05	108.27	110.57
29	C	507	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
47	s	317	LUT	C40-C33-C32	2.05	121.30	118.08
29	C	502	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
29	b	501	CLA	C3B-C4B-NB	-2.05	108.61	110.52
29	c	510	CLA	C1-C2-C3	-2.05	122.50	126.04
29	S	316	CLA	CHC-C4B-NB	2.05	126.42	124.26
31	b	518	BCR	C34-C9-C10	-2.05	120.06	122.92
29	S	315	CLA	C3B-C4B-NB	-2.05	108.62	110.52
46	S	308	CHL	C2B-C1B-NB	-2.05	108.86	110.23
48	g	617	NEX	C28-C29-C30	2.05	122.08	118.94
49	g	619	XAT	C40-C33-C34	-2.04	120.06	122.92
48	y	319	NEX	C28-C29-C30	2.04	122.08	118.94
29	S	303	CLA	C1-C2-C3	-2.04	122.51	126.04
46	N	609	CHL	CHD-C4C-C3C	2.04	127.84	124.84
46	N	607	CHL	CMA-C3A-C2A	2.04	122.07	113.83
43	D	406	PL9	C20-C19-C21	2.04	118.71	115.27
29	N	602	CLA	C1-C2-C3	-2.04	122.51	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	b	519	C7Z	C30-C31-C32	-2.04	116.85	123.22
34	b	519	C7Z	C19-C9-C10	-2.04	120.07	122.92
43	d	405	PL9	O2-C1-C2	-2.04	117.11	121.78
29	N	602	CLA	C3B-C2B-C1B	-2.04	104.70	107.16
29	S	314	CLA	C3B-C4B-NB	-2.04	108.62	110.52
29	B	504	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
29	C	509	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
29	b	505	CLA	C1-C2-C3	-2.04	122.52	126.04
29	A	409	CLA	C3C-C4C-NC	-2.04	108.29	110.57
29	C	511	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
29	C	507	CLA	C1D-ND-C4D	-2.04	104.89	106.33
29	Y	315	CLA	C3B-C2B-C1B	-2.04	104.70	107.16
29	R	309	CLA	CHC-C4B-NB	2.03	126.41	124.26
29	S	304	CLA	CMD-C2D-C1D	-2.03	121.13	124.71
29	y	304	CLA	C3B-C4B-NB	-2.03	108.63	110.52
46	g	607	CHL	C3B-C4B-NB	-2.03	108.63	110.52
29	R	309	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
29	c	503	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
47	s	318	LUT	C39-C29-C28	2.03	121.28	118.08
29	c	502	CLA	C3B-C2B-C1B	-2.03	104.71	107.16
29	c	513	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
29	n	610	CLA	C4A-NA-C1A	2.03	107.62	106.71
29	S	314	CLA	CMB-C2B-C1B	2.03	128.47	125.37
29	b	509	CLA	CHC-C4B-NB	2.03	126.41	124.26
34	b	519	C7Z	C21-C26-C25	-2.03	119.75	122.61
31	z	101	BCR	C33-C5-C4	2.03	117.52	113.62
46	G	606	CHL	C2B-C1B-NB	-2.03	108.87	110.23
29	s	304	CLA	C2D-C1D-ND	-2.03	108.61	110.10
29	g	602	CLA	C3B-C4B-NB	-2.03	108.63	110.52
29	c	502	CLA	C1-C2-C3	-2.03	122.53	126.04
49	R	311	XAT	C24-C23-C22	-2.03	106.85	110.77
47	N	616	LUT	C31-C30-C29	-2.03	124.41	127.31
29	N	603	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
29	b	509	CLA	C3B-C2B-C1B	-2.03	104.71	107.16
29	Y	315	CLA	CMB-C2B-C1B	2.03	128.46	125.37
39	m	101	SQD	O8-S-C6	-2.03	102.51	105.74
31	z	101	BCR	C34-C9-C10	-2.03	120.08	122.92
46	g	601	CHL	C1-O2A-CGA	2.03	121.76	116.44
47	R	310	LUT	C1-C6-C7	2.03	121.51	115.78
46	n	605	CHL	C3A-C2A-C1A	2.03	104.37	101.34
29	S	310	CLA	CHA-C1A-NA	-2.03	121.76	126.40
29	S	313	CLA	CHA-C1A-NA	-2.03	121.76	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n	611	CLA	O2A-CGA-O1A	-2.02	118.25	123.30
46	G	606	CHL	CHA-C1A-NA	-2.02	121.76	126.40
29	g	613	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
49	Y	301	XAT	C40-C33-C34	-2.02	120.09	122.92
43	d	405	PL9	C31-C32-C33	-2.02	105.23	111.88
47	g	615	LUT	C35-C15-C14	-2.02	119.33	123.47
29	R	307	CLA	C3B-C2B-C1B	-2.02	104.72	107.16
29	r	310	CLA	CMB-C2B-C1B	2.02	128.45	125.37
46	N	606	CHL	C1-O2A-CGA	2.02	121.75	116.44
29	c	501	CLA	C3B-C4B-NB	-2.02	108.64	110.52
29	n	602	CLA	C3B-C2B-C1B	-2.02	104.72	107.16
29	Y	315	CLA	CHC-C4B-NB	2.02	126.39	124.26
29	R	306	CLA	C2D-C1D-ND	-2.02	108.62	110.10
47	N	615	LUT	C39-C29-C28	2.02	121.26	118.08
46	y	303	CHL	CHD-C4C-C3C	2.02	127.81	124.84
29	c	502	CLA	CHA-C1A-NA	-2.02	121.78	126.40
29	G	604	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
34	b	519	C7Z	C31-C32-C33	-2.02	120.75	126.42
46	y	301	CHL	C3A-C2A-C1A	2.02	104.36	101.34
29	c	505	CLA	CHC-C4B-NB	2.02	126.39	124.26
29	s	306	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
29	B	508	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
29	S	316	CLA	C1-C2-C3	-2.01	123.49	126.75
29	C	509	CLA	CHA-C1A-NA	-2.01	121.78	126.40
34	b	519	C7Z	C15-C35-C34	-2.01	119.35	123.47
46	g	605	CHL	C2C-C3C-C4C	2.01	107.92	106.49
29	C	504	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
29	y	314	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
46	G	608	CHL	C4D-CHA-C1A	2.01	123.70	121.25
47	N	615	LUT	C20-C13-C12	2.01	121.25	118.08
29	b	501	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
47	n	614	LUT	C15-C35-C34	-2.01	119.35	123.47
46	n	607	CHL	CHD-C4C-C3C	2.01	127.80	124.84
35	C	521	LMG	O7-C10-O9	-2.01	118.84	123.70
29	C	509	CLA	CHB-C1B-NB	2.01	126.39	124.26
29	n	610	CLA	C3B-C4B-NB	-2.01	108.65	110.52
29	N	612	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
29	B	516	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
29	y	313	CLA	CHC-C4B-NB	2.01	126.39	124.26
46	y	309	CHL	CHD-C4C-C3C	2.01	127.80	124.84
29	D	405	CLA	CHC-C4B-NB	2.01	126.39	124.26
46	Y	307	CHL	C3A-C2A-C1A	2.01	104.35	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	405	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
29	b	514	CLA	CHA-C1A-NA	-2.01	121.80	126.40
29	G	602	CLA	C3B-C2B-C1B	-2.01	104.74	107.16
29	N	611	CLA	C2B-C1B-NB	-2.01	108.89	110.23
29	y	316	CLA	CHA-C1A-NA	-2.01	121.80	126.40
31	F	101	BCR	C19-C18-C17	2.01	122.02	118.94
46	Y	306	CHL	CHD-C4C-C3C	2.01	127.79	124.84
31	c	514	BCR	C37-C22-C23	2.01	121.24	118.08
29	c	504	CLA	CHA-C1A-NA	-2.01	121.80	126.40
29	r	310	CLA	C2B-C1B-NB	-2.01	108.89	110.23
29	s	306	CLA	CHA-C1A-NA	-2.01	121.81	126.40
29	S	311	CLA	CHB-C1B-NB	2.01	126.38	124.26
29	n	604	CLA	CHC-C4B-NB	2.01	126.38	124.26
29	B	510	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
31	A	410	BCR	C31-C1-C6	-2.00	107.05	110.30
46	y	311	CHL	CHD-C4C-C3C	2.00	127.79	124.84
29	s	316	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
29	Y	312	CLA	C3C-C4C-NC	-2.00	108.32	110.57
46	G	601	CHL	CHC-C1C-NC	2.00	127.24	124.20
29	Y	304	CLA	C3B-C2B-C1B	-2.00	104.75	107.16
29	R	306	CLA	CMB-C2B-C1B	2.00	128.42	125.37
29	n	609	CLA	C3C-C4C-NC	-2.00	108.33	110.57
29	A	409	CLA	CHB-C1B-C2B	-2.00	121.59	127.24
29	C	512	CLA	C3B-C4B-NB	-2.00	108.66	110.52
31	B	518	BCR	C34-C9-C10	-2.00	120.12	122.92
46	N	601	CHL	CHD-C4C-C3C	2.00	127.78	124.84

All (41) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	D	404	CLA	C8
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	605	CHL	C8
46	N	606	CHL	C8
46	N	607	CHL	C8
46	N	609	CHL	C8
46	G	601	CHL	C8
46	G	607	CHL	C8

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Mol	Chain	Res	Type	Atom
46	G	609	CHL	C8
46	S	309	CHL	C8
46	Y	302	CHL	C8
46	Y	307	CHL	C8
46	Y	308	CHL	C8
46	Y	310	CHL	C8
46	n	601	CHL	C8
46	n	605	CHL	C8
46	n	606	CHL	C8
46	n	608	CHL	C8
46	g	601	CHL	C8
46	g	607	CHL	C8
46	g	609	CHL	C8
46	s	309	CHL	C8
46	y	301	CHL	C8
46	y	303	CHL	C8
46	y	309	CHL	C8
46	y	311	CHL	C8
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 (3728) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	A	405	CLA	CBD-CGD-O2D-CED
29	A	405	CLA	O2A-C1-C2-C3
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	406	CLA	CHA-CBD-CGD-O1D
29	A	406	CLA	CHA-CBD-CGD-O2D
29	A	407	CLA	C1A-C2A-CAA-CBA
29	A	407	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	A	407	CLA	CHA-CBD-CGD-O1D
29	A	407	CLA	CHA-CBD-CGD-O2D
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	504	CLA	C2B-C3B-CAB-CBB
29	B	504	CLA	C4-C3-C5-C6
29	B	506	CLA	C2B-C3B-CAB-CBB
29	B	506	CLA	CHA-CBD-CGD-O1D
29	B	507	CLA	C1A-C2A-CAA-CBA
29	B	507	CLA	C3A-C2A-CAA-CBA
29	B	507	CLA	C2-C3-C5-C6
29	B	507	CLA	C4-C3-C5-C6
29	C	502	CLA	CBD-CGD-O2D-CED
29	C	503	CLA	CHA-CBD-CGD-O1D
29	C	503	CLA	CHA-CBD-CGD-O2D
29	C	503	CLA	CAD-CBD-CGD-O1D
29	C	505	CLA	C4B-C3B-CAB-CBB
29	C	505	CLA	C2-C3-C5-C6
29	C	505	CLA	C4-C3-C5-C6
29	C	509	CLA	CHA-CBD-CGD-O1D
29	C	509	CLA	CHA-CBD-CGD-O2D
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	613	CLA	C4B-C3B-CAB-CBB
29	N	613	CLA	CHA-CBD-CGD-O1D
29	N	613	CLA	CHA-CBD-CGD-O2D
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	613	CLA	CHA-CBD-CGD-O1D
29	G	613	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
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	CHA-CBD-CGD-O1D
29	R	302	CLA	CHA-CBD-CGD-O2D
29	R	302	CLA	CBD-CGD-O2D-CED
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-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	309	CLA	C2A-CAA-CBA-CGA
29	Y	309	CLA	C2B-C3B-CAB-CBB
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	C2A-CAA-CBA-CGA
29	a	404	CLA	CBD-CGD-O2D-CED
29	a	404	CLA	O2A-C1-C2-C3
29	a	405	CLA	C1A-C2A-CAA-CBA
29	a	405	CLA	C3A-C2A-CAA-CBA
29	a	405	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
29	a	405	CLA	CHA-CBD-CGD-O1D
29	a	405	CLA	CHA-CBD-CGD-O2D
29	b	501	CLA	C4B-C3B-CAB-CBB
29	b	501	CLA	C11-C12-C13-C14
29	b	502	CLA	C2-C3-C5-C6
29	b	502	CLA	C4-C3-C5-C6
29	b	504	CLA	C1A-C2A-CAA-CBA
29	b	504	CLA	C2B-C3B-CAB-CBB
29	b	506	CLA	C2B-C3B-CAB-CBB
29	c	501	CLA	C4B-C3B-CAB-CBB
29	c	502	CLA	CHA-CBD-CGD-O1D
29	c	502	CLA	CHA-CBD-CGD-O2D
29	c	502	CLA	CAD-CBD-CGD-O1D
29	c	504	CLA	C6-C7-C8-C9
29	c	505	CLA	C11-C10-C8-C9
29	c	508	CLA	CHA-CBD-CGD-O1D
29	c	508	CLA	CHA-CBD-CGD-O2D
29	c	509	CLA	C2-C1-O2A-CGA
29	c	509	CLA	C6-C7-C8-C9
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	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	g	613	CLA	CHA-CBD-CGD-O1D
29	g	613	CLA	CHA-CBD-CGD-O2D
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	CHA-CBD-CGD-O1D
29	r	303	CLA	CHA-CBD-CGD-O2D
29	r	303	CLA	CBD-CGD-O2D-CED
29	r	304	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	r	307	CLA	C2-C3-C5-C6
29	r	307	CLA	C4-C3-C5-C6
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	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	A	410	BCR	C36-C18-C19-C20
31	B	517	BCR	C7-C8-C9-C10
31	B	517	BCR	C7-C8-C9-C34
31	B	517	BCR	C36-C18-C19-C20
31	B	517	BCR	C21-C22-C23-C24
31	B	517	BCR	C37-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	B	518	BCR	C11-C12-C13-C35
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	515	BCR	C36-C18-C19-C20
31	C	516	BCR	C7-C8-C9-C10
31	C	516	BCR	C7-C8-C9-C34
31	C	516	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
31	C	516	BCR	C36-C18-C19-C20
31	C	516	BCR	C23-C24-C25-C30
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	C1-C6-C7-C8
31	F	101	BCR	C11-C10-C9-C8
31	F	101	BCR	C11-C10-C9-C34
31	F	101	BCR	C11-C12-C13-C35
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	a	409	BCR	C36-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	517	BCR	C36-C18-C19-C20
31	b	517	BCR	C37-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	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
31	c	514	BCR	C1-C6-C7-C8
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	514	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
31	c	514	BCR	C23-C24-C25-C30
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	C7-C8-C9-C34
31	z	101	BCR	C11-C10-C9-C8
31	z	101	BCR	C11-C10-C9-C34
31	z	101	BCR	C10-C11-C12-C13
31	z	101	BCR	C36-C18-C19-C20
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	C21-C26-C27-C28
34	b	519	C7Z	C1-C6-C7-C8
35	B	520	LMG	O6-C1-O1-C7
35	C	524	LMG	C2-C1-O1-C7
35	C	524	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

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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-O5
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	O7-C5-C6-O8
37	L	101	LHG	O1-C1-C2-C3
37	L	101	LHG	C1-C2-C3-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-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-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
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

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Mol	Chain	Res	Type	Atoms
37	c	521	LHG	C4-O6-P-O4
37	d	406	LHG	C1-C2-C3-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	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-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-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-O5
38	b	524	LMT	O5'-C1'-O1'-C1
38	b	524	LMT	C2-C1-O1'-C1'
39	C	523	SQD	C5-C6-S-O9
39	L	102	SQD	C2-C1-O6-C44
39	L	102	SQD	O5-C1-O6-C44
39	M	101	SQD	C2-C1-O6-C44
39	M	101	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	C2-C1-O6-C44
39	b	523	SQD	O5-C1-O6-C44
39	c	522	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
39	c	522	SQD	O5-C5-C6-S
39	l	101	SQD	C2-C1-O6-C44
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	C1-C2-C3-C4
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
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
45	h	101	RRX	C11-C12-C13-C35
46	N	609	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
46	N	609	CHL	CHA-CBD-CGD-O2D
46	G	601	CHL	CHA-CBD-CGD-O1D
46	G	601	CHL	CHA-CBD-CGD-O2D
46	G	605	CHL	CHA-CBD-CGD-O1D
46	G	605	CHL	CHA-CBD-CGD-O2D
46	G	609	CHL	CHA-CBD-CGD-O1D
46	G	609	CHL	CHA-CBD-CGD-O2D
46	Y	302	CHL	CHA-CBD-CGD-O1D
46	Y	302	CHL	CHA-CBD-CGD-O2D
46	n	601	CHL	C2-C3-C5-C6
46	n	601	CHL	C4-C3-C5-C6
46	n	605	CHL	C14-C13-C15-C16
46	n	606	CHL	C14-C13-C15-C16
46	g	601	CHL	C1A-C2A-CAA-CBA
46	g	601	CHL	C3A-C2A-CAA-CBA
46	g	601	CHL	CHA-CBD-CGD-O1D
46	g	601	CHL	CHA-CBD-CGD-O2D
46	g	607	CHL	C1A-C2A-CAA-CBA
46	g	607	CHL	C3A-C2A-CAA-CBA
46	g	609	CHL	C2-C3-C5-C6
46	g	609	CHL	C4-C3-C5-C6
46	y	303	CHL	CHA-CBD-CGD-O1D
46	y	303	CHL	CHA-CBD-CGD-O2D
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	Y	320	PTY	C3-O11-P1-O12

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Mol	Chain	Res	Type	Atoms
50	Y	320	PTY	C3-O11-P1-O13
50	n	619	PTY	N1-C2-C3-O11
50	y	321	PTY	N1-C2-C3-O11
50	y	321	PTY	C3-O11-P1-O12
51	S	321	LPX	C3-C4-C5-O6
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
50	Y	320	PTY	C11-C8-O7-C6
50	y	321	PTY	C11-C8-O7-C6
29	r	308	CLA	O1D-CGD-O2D-CED
29	s	314	CLA	O1D-CGD-O2D-CED
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	C	504	CLA	O1D-CGD-O2D-CED
29	S	304	CLA	O1D-CGD-O2D-CED
29	S	314	CLA	O1D-CGD-O2D-CED
29	Y	309	CLA	O1D-CGD-O2D-CED
29	b	505	CLA	O1D-CGD-O2D-CED
37	L	101	LHG	C5-C6-O8-C23
29	C	502	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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	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
29	r	307	CLA	CBA-CGA-O2A-C1
29	s	312	CLA	CBA-CGA-O2A-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
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
29	y	305	CLA	CBD-CGD-O2D-CED
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

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Mol	Chain	Res	Type	Atoms
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	y	306	CLA	O1D-CGD-O2D-CED
50	y	321	PTY	O10-C8-O7-C6
29	G	612	CLA	O1D-CGD-O2D-CED
29	y	310	CLA	O1D-CGD-O2D-CED
50	Y	320	PTY	O30-C30-O4-C1
29	N	614	CLA	CBD-CGD-O2D-CED
29	c	501	CLA	CBD-CGD-O2D-CED
29	s	316	CLA	CBD-CGD-O2D-CED
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
41	b	522	DGA	OB1-CB1-OG2-CG2
29	y	305	CLA	O1A-CGA-O2A-C1
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

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Mol	Chain	Res	Type	Atoms
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
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	S	316	CLA	O1D-CGD-O2D-CED
29	c	503	CLA	O1D-CGD-O2D-CED
29	Y	315	CLA	CBD-CGD-O2D-CED
29	b	501	CLA	CBD-CGD-O2D-CED
29	A	407	CLA	O1A-CGA-O2A-C1
29	n	603	CLA	O1A-CGA-O2A-C1
50	y	321	PTY	C31-C30-O4-C1
29	R	307	CLA	CBA-CGA-O2A-C1
29	C	508	CLA	C4-C3-C5-C6
29	R	308	CLA	C4-C3-C5-C6
29	a	408	CLA	C4-C3-C5-C6
46	N	606	CHL	C4-C3-C5-C6
29	N	603	CLA	CBD-CGD-O2D-CED
29	d	404	CLA	CBD-CGD-O2D-CED
29	A	405	CLA	C2A-CAA-CBA-CGA
29	R	309	CLA	C2A-CAA-CBA-CGA
29	s	316	CLA	C2A-CAA-CBA-CGA
46	N	606	CHL	C2A-CAA-CBA-CGA
46	N	608	CHL	C2A-CAA-CBA-CGA
46	Y	306	CHL	C2A-CAA-CBA-CGA
46	Y	308	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
46	s	302	CHL	C2A-CAA-CBA-CGA
29	D	405	CLA	O1A-CGA-O2A-C1
35	B	520	LMG	C17-C18-C19-C20
35	C	521	LMG	C35-C36-C37-C38
35	C	522	LMG	C17-C18-C19-C20
35	C	522	LMG	C41-C42-C43-C44
35	D	409	LMG	C17-C18-C19-C20
35	D	410	LMG	C35-C36-C37-C38
35	D	410	LMG	C38-C39-C40-C41
35	W	201	LMG	C17-C18-C19-C20
35	W	203	LMG	C35-C36-C37-C38
35	W	203	LMG	C38-C39-C40-C41
35	b	520	LMG	C17-C18-C19-C20
35	c	519	LMG	C17-C18-C19-C20
35	c	519	LMG	C20-C21-C22-C23
35	c	519	LMG	C35-C36-C37-C38
35	c	520	LMG	C17-C18-C19-C20
35	c	520	LMG	C20-C21-C22-C23
35	c	520	LMG	C23-C24-C25-C26
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	C35-C36-C37-C38
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	C35-C36-C37-C38
35	w	202	LMG	C38-C39-C40-C41
36	C	518	DGD	C8B-C9B-CAB-CBB
36	C	519	DGD	CBB-CCB-CDB-CEB
36	c	516	DGD	C8B-C9B-CAB-CBB
36	c	517	DGD	C8A-C9A-CAA-CBA
36	c	517	DGD	CBB-CCB-CDB-CEB
36	c	518	DGD	CBB-CCB-CDB-CEB
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
29	C	514	CLA	CBA-CGA-O2A-C1
29	D	405	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
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
50	Y	320	PTY	C31-C30-O4-C1
29	c	502	CLA	O1D-CGD-O2D-CED
29	R	307	CLA	O1D-CGD-O2D-CED
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
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
29	R	307	CLA	O1A-CGA-O2A-C1
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

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Mol	Chain	Res	Type	Atoms
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	C	507	CLA	C3-C5-C6-C7
46	N	606	CHL	C3-C5-C6-C7
29	A	407	CLA	CBA-CGA-O2A-C1
29	B	507	CLA	CBA-CGA-O2A-C1
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
29	b	514	CLA	O1D-CGD-O2D-CED
51	s	321	LPX	O5-C4-C5-O6
37	n	617	LHG	C8-C7-O7-C5
41	b	522	DGA	CB2-CB1-OG2-CG2
29	B	513	CLA	CBD-CGD-O2D-CED
29	B	516	CLA	CBD-CGD-O2D-CED
36	c	516	DGD	O6E-C5E-C6E-O5E
33	a	415	3PH	O32-C31-O31-C3
37	N	618	LHG	C11-C12-C13-C14
29	g	602	CLA	CBD-CGD-O2D-CED
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	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

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Mol	Chain	Res	Type	Atoms
29	n	603	CLA	CBA-CGA-O2A-C1
37	L	101	LHG	C24-C23-O8-C6
29	n	604	CLA	O1D-CGD-O2D-CED
37	N	618	LHG	C13-C14-C15-C16
29	G	602	CLA	O1A-CGA-O2A-C1
29	n	612	CLA	O1A-CGA-O2A-C1
43	d	405	PL9	C47-C48-C49-C51
29	B	509	CLA	C4-C3-C5-C6
29	B	504	CLA	C2-C3-C5-C6
29	B	509	CLA	C2-C3-C5-C6
46	N	606	CHL	C2-C3-C5-C6
29	b	516	CLA	CBD-CGD-O2D-CED
37	L	101	LHG	C7-C8-C9-C10
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	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	i	101	LMG	O6-C1-O1-C7
43	D	406	PL9	C39-C41-C42-C43
43	d	405	PL9	C39-C41-C42-C43
38	b	524	LMT	O5B-C5B-C6B-O6B
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	610	CLA	O1D-CGD-O2D-CED
29	G	613	CLA	O1D-CGD-O2D-CED
30	A	408	PHO	CBD-CGD-O2D-CED
29	C	503	CLA	O1D-CGD-O2D-CED
37	l	102	LHG	C1-C2-C3-O3
37	g	618	LHG	C1-C2-C3-O3
37	y	320	LHG	C1-C2-C3-O3
33	b	521	3PH	O32-C31-O31-C3
29	Y	305	CLA	O1D-CGD-O2D-CED
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

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Mol	Chain	Res	Type	Atoms
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	G	614	CLA	CBD-CGD-O2D-CED
29	b	506	CLA	CBD-CGD-O2D-CED
29	y	316	CLA	CBD-CGD-O2D-CED
31	C	515	BCR	C9-C10-C11-C12
33	s	322	3PH	C31-C32-C33-C34
46	G	607	CHL	C10-C11-C12-C13
33	s	322	3PH	C34-C35-C36-C37
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
41	j	101	DGA	CB1-CB2-CB3-CB4
39	a	410	SQD	C2-C1-O6-C44
33	s	322	3PH	C32-C33-C34-C35
50	y	321	PTY	O30-C30-O4-C1
29	g	603	CLA	O1A-CGA-O2A-C1
29	s	306	CLA	O1A-CGA-O2A-C1
29	n	609	CLA	C4-C3-C5-C6
29	R	308	CLA	C2-C3-C5-C6
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

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Mol	Chain	Res	Type	Atoms
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	503	CLA	C11-C10-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
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	D	405	CLA	O1D-CGD-O2D-CED
29	c	511	CLA	O1D-CGD-O2D-CED
29	A	405	CLA	C4C-C3C-CAC-CBC
29	B	513	CLA	C10-C11-C12-C13
29	C	510	CLA	C15-C16-C17-C18
29	N	613	CLA	C5-C6-C7-C8
46	S	309	CHL	C2A-CAA-CBA-CGA
31	A	410	BCR	C37-C22-C23-C24
31	F	101	BCR	C36-C18-C19-C20
31	b	518	BCR	C36-C18-C19-C20
45	H	101	RRX	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
45	h	101	RRX	C7-C8-C9-C34
47	R	310	LUT	C7-C8-C9-C19
31	v	101	BCR	C21-C22-C23-C24
45	h	101	RRX	C7-C8-C9-C10
29	c	510	CLA	O1D-CGD-O2D-CED
37	n	617	LHG	O9-C7-O7-C5
37	N	618	LHG	C8-C7-O7-C5
41	W	202	DGA	CB2-CB1-OG2-CG2
37	B	523	LHG	C31-C32-C33-C34
38	b	524	LMT	C4B-C5B-C6B-O6B
37	S	301	LHG	C23-C24-C25-C26
37	n	617	LHG	C23-C24-C25-C26
41	W	202	DGA	CA1-CA2-CA3-CA4
29	G	603	CLA	O1A-CGA-O2A-C1
29	R	309	CLA	O1A-CGA-O2A-C1
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	C	505	CLA	C5-C6-C7-C8
29	C	514	CLA	C8-C10-C11-C12
29	G	602	CLA	C13-C15-C16-C17
29	Y	303	CLA	C13-C15-C16-C17
29	Y	314	CLA	C15-C16-C17-C18
29	b	503	CLA	C8-C10-C11-C12
29	y	306	CLA	C13-C15-C16-C17
46	G	607	CHL	C13-C15-C16-C17
46	Y	307	CHL	C5-C6-C7-C8
46	G	608	CHL	C2A-CAA-CBA-CGA
29	Y	313	CLA	CBA-CGA-O2A-C1
29	B	507	CLA	C8-C10-C11-C12
29	C	507	CLA	C5-C6-C7-C8
29	S	312	CLA	C15-C16-C17-C18
29	b	501	CLA	C10-C11-C12-C13
29	c	503	CLA	C15-C16-C17-C18
29	c	508	CLA	C5-C6-C7-C8
29	d	404	CLA	C8-C10-C11-C12
29	n	604	CLA	C8-C10-C11-C12
29	y	315	CLA	C15-C16-C17-C18
29	y	316	CLA	C8-C10-C11-C12
46	N	607	CHL	C8-C10-C11-C12
35	b	520	LMG	C28-C29-C30-C31
37	D	407	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
37	l	102	LHG	C23-C24-C25-C26
41	J	101	DGA	CB1-CB2-CB3-CB4
41	W	202	DGA	CB1-CB2-CB3-CB4
33	S	322	3PH	C32-C33-C34-C35
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	b	507	CLA	C10-C11-C12-C13
29	b	507	CLA	C13-C15-C16-C17
29	g	611	CLA	C10-C11-C12-C13
29	s	310	CLA	C10-C11-C12-C13
46	G	607	CHL	C15-C16-C17-C18
37	L	101	LHG	O1-C1-C2-O2
37	g	618	LHG	O1-C1-C2-O2
35	D	410	LMG	C28-C29-C30-C31
35	c	519	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	N	618	LHG	C7-C8-C9-C10
37	a	413	LHG	C7-C8-C9-C10
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
50	n	619	PTY	C8-C11-C12-C13
29	C	509	CLA	C5-C6-C7-C8
29	G	603	CLA	C5-C6-C7-C8
29	Y	312	CLA	C5-C6-C7-C8
29	Y	315	CLA	C8-C10-C11-C12
29	s	312	CLA	C15-C16-C17-C18
46	S	309	CHL	C5-C6-C7-C8
29	s	310	CLA	CBA-CGA-O2A-C1
29	C	510	CLA	C2-C1-O2A-CGA
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	d	404	CLA	C10-C11-C12-C13
37	N	618	LHG	C23-C24-C25-C26
37	S	320	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
37	a	414	LHG	C7-C8-C9-C10
37	n	617	LHG	C7-C8-C9-C10
29	r	307	CLA	CBD-CGD-O2D-CED
46	S	307	CHL	C2A-CAA-CBA-CGA
37	S	320	LHG	C30-C31-C32-C33
44	E	101	HEM	C3D-CAD-CBD-CGD
29	B	503	CLA	C15-C16-C17-C18
29	B	505	CLA	C5-C6-C7-C8
29	N	613	CLA	C8-C10-C11-C12
29	Y	315	CLA	C5-C6-C7-C8
29	g	602	CLA	C13-C15-C16-C17
29	S	304	CLA	C11-C12-C13-C15
29	Y	304	CLA	C6-C7-C8-C10
29	b	513	CLA	C11-C10-C8-C7
29	n	602	CLA	C12-C13-C15-C16
29	n	609	CLA	C6-C7-C8-C10
29	n	609	CLA	C11-C12-C13-C15
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	n	605	CHL	C11-C12-C13-C15
46	g	609	CHL	C12-C13-C15-C16
46	y	303	CHL	C12-C13-C15-C16
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
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
29	n	611	CLA	CBD-CGD-O2D-CED
29	B	512	CLA	C2A-CAA-CBA-CGA
29	s	304	CLA	C2A-CAA-CBA-CGA
46	N	605	CHL	C2A-CAA-CBA-CGA
29	N	614	CLA	O1D-CGD-O2D-CED
29	y	305	CLA	O1D-CGD-O2D-CED
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	G	611	CLA	C13-C15-C16-C17
29	Y	311	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	b	509	CLA	C13-C15-C16-C17
29	b	509	CLA	C15-C16-C17-C18
29	b	516	CLA	C13-C15-C16-C17
29	c	503	CLA	C5-C6-C7-C8
29	g	602	CLA	C8-C10-C11-C12
29	r	307	CLA	C10-C11-C12-C13
39	m	101	SQD	O10-C23-O48-C46
29	G	611	CLA	CBD-CGD-O2D-CED
29	c	507	CLA	CBD-CGD-O2D-CED
36	B	521	DGD	O6D-C1D-O3G-C3G
39	m	101	SQD	O5-C1-O6-C44
29	B	507	CLA	C13-C15-C16-C17
29	y	314	CLA	C13-C15-C16-C17
46	Y	307	CHL	C15-C16-C17-C18
29	c	501	CLA	O1D-CGD-O2D-CED
29	s	316	CLA	O1D-CGD-O2D-CED
35	B	520	LMG	C28-C29-C30-C31
31	K	101	BCR	C10-C11-C12-C13
31	v	101	BCR	C10-C11-C12-C13
48	y	319	NEX	C10-C11-C12-C13
37	a	413	LHG	O2-C2-C3-O3
37	c	521	LHG	O2-C2-C3-O3
37	g	618	LHG	O2-C2-C3-O3
37	l	102	LHG	C5-C6-O8-C23
29	s	312	CLA	C10-C11-C12-C13
46	N	601	CHL	C13-C15-C16-C17
46	Y	308	CHL	C5-C6-C7-C8
29	b	516	CLA	CBA-CGA-O2A-C1
36	c	518	DGD	C2A-C1A-O1G-C1G
29	Y	313	CLA	O1A-CGA-O2A-C1
33	s	322	3PH	C21-C22-C23-C24
36	c	516	DGD	C1B-C2B-C3B-C4B
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	S	312	CLA	C8-C10-C11-C12
29	Y	313	CLA	C15-C16-C17-C18
29	Y	314	CLA	C5-C6-C7-C8
29	b	501	CLA	C13-C15-C16-C17
29	b	511	CLA	C13-C15-C16-C17
29	c	510	CLA	C15-C16-C17-C18
29	c	512	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	g	613	CLA	C13-C15-C16-C17
29	s	312	CLA	C8-C10-C11-C12
46	G	607	CHL	C5-C6-C7-C8
46	y	301	CHL	C15-C16-C17-C18
29	Y	315	CLA	O1D-CGD-O2D-CED
29	b	501	CLA	O1D-CGD-O2D-CED
39	L	102	SQD	C8-C7-O47-C45
39	M	101	SQD	C8-C7-O47-C45
29	B	501	CLA	C13-C15-C16-C17
29	Y	313	CLA	C13-C15-C16-C17
29	Y	314	CLA	C8-C10-C11-C12
29	b	505	CLA	C5-C6-C7-C8
29	b	515	CLA	C13-C15-C16-C17
29	b	516	CLA	C5-C6-C7-C8
29	c	504	CLA	C10-C11-C12-C13
29	c	509	CLA	C15-C16-C17-C18
29	g	603	CLA	C5-C6-C7-C8
29	y	314	CLA	C8-C10-C11-C12
46	s	309	CHL	C8-C10-C11-C12
46	y	309	CHL	C5-C6-C7-C8
37	D	407	LHG	C4-O6-P-O3
37	L	101	LHG	C4-O6-P-O3
37	G	618	LHG	C4-O6-P-O3
37	S	301	LHG	C4-O6-P-O3
37	c	521	LHG	C4-O6-P-O3
37	d	406	LHG	C4-O6-P-O3
37	l	102	LHG	C3-O3-P-O6
37	g	618	LHG	C4-O6-P-O3
37	s	320	LHG	C4-O6-P-O3
37	y	320	LHG	C4-O6-P-O3
50	N	620	PTY	C5-O14-P1-O11
50	Y	320	PTY	C3-O11-P1-O14
50	n	619	PTY	C3-O11-P1-O14
37	a	413	LHG	C23-C24-C25-C26
29	r	302	CLA	C3-C5-C6-C7
37	a	414	LHG	C24-C23-O8-C6
39	l	101	SQD	C24-C23-O48-C46
29	C	508	CLA	CBD-CGD-O2D-CED
29	C	508	CLA	C13-C15-C16-C17
29	N	603	CLA	C8-C10-C11-C12
29	b	502	CLA	C13-C15-C16-C17
46	N	605	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
46	g	607	CHL	C5-C6-C7-C8
36	c	518	DGD	C1A-C2A-C3A-C4A
36	C	518	DGD	O6E-C5E-C6E-O5E
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	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	a	408	CLA	C2-C3-C5-C6
29	Y	313	CLA	C8-C10-C11-C12
29	c	511	CLA	C8-C10-C11-C12
29	n	604	CLA	C13-C15-C16-C17
29	N	603	CLA	O1D-CGD-O2D-CED
29	C	508	CLA	C2A-CAA-CBA-CGA
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	r	304	CLA	C2A-CAA-CBA-CGA
29	s	314	CLA	C2A-CAA-CBA-CGA
46	Y	307	CHL	C2A-CAA-CBA-CGA
46	y	308	CHL	C2A-CAA-CBA-CGA
29	C	502	CLA	C16-C17-C18-C19
29	Y	314	CLA	C16-C17-C18-C20
36	c	516	DGD	C4E-C5E-C6E-O5E
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
31	b	517	BCR	C9-C10-C11-C12
47	Y	317	LUT	C29-C30-C31-C32
47	y	318	LUT	C29-C30-C31-C32
33	a	415	3PH	C39-C3A-C3B-C3C
37	L	101	LHG	C9-C10-C11-C12
37	L	101	LHG	C33-C34-C35-C36
39	b	523	SQD	C8-C7-O47-C45
50	n	619	PTY	C11-C8-O7-C6
31	C	516	BCR	C11-C10-C9-C34
48	N	617	NEX	C39-C29-C30-C31

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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
33	s	322	3PH	C24-C25-C26-C27
35	c	520	LMG	C29-C30-C31-C32
37	a	413	LHG	C25-C26-C27-C28
37	y	320	LHG	C28-C29-C30-C31
39	o	301	SQD	C12-C13-C14-C15
41	W	202	DGA	CCA-CDA-CEA-CFA
29	d	404	CLA	O1D-CGD-O2D-CED
29	D	404	CLA	C16-C17-C18-C20
29	Y	315	CLA	C16-C17-C18-C19
29	c	501	CLA	C16-C17-C18-C19
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	B	512	CLA	CBA-CGA-O2A-C1
33	a	415	3PH	C32-C33-C34-C35
33	b	521	3PH	C37-C38-C39-C3A
37	L	101	LHG	C11-C12-C13-C14
37	Y	319	LHG	C26-C27-C28-C29
37	c	521	LHG	C13-C14-C15-C16
37	l	102	LHG	C28-C29-C30-C31
37	n	617	LHG	C24-C25-C26-C27
37	s	320	LHG	C12-C13-C14-C15
39	c	522	SQD	C17-C18-C19-C20
40	C	525	SPH	C14-C15-C16-C17
35	B	520	LMG	C9-C8-O7-C10
39	b	523	SQD	O49-C7-O47-C45
39	m	101	SQD	O49-C7-O47-C45
50	n	619	PTY	O10-C8-O7-C6
29	a	405	CLA	C2C-C3C-CAC-CBC
33	s	322	3PH	C2A-C2B-C2C-C2D
36	C	519	DGD	C4B-C5B-C6B-C7B
37	y	320	LHG	C13-C14-C15-C16
41	j	101	DGA	CB6-CB7-CB8-CB9
33	A	412	3PH	C38-C39-C3A-C3B
33	B	522	3PH	C24-C25-C26-C27
33	B	522	3PH	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
33	b	521	3PH	C24-C25-C26-C27
36	c	517	DGD	C5A-C6A-C7A-C8A
37	S	301	LHG	C25-C26-C27-C28
37	c	521	LHG	C11-C12-C13-C14
37	n	617	LHG	C11-C12-C13-C14
37	g	618	LHG	C11-C12-C13-C14
29	b	508	CLA	C13-C15-C16-C17
29	c	505	CLA	C13-C15-C16-C17
29	s	304	CLA	C15-C16-C17-C18
44	e	101	HEM	C3D-CAD-CBD-CGD
37	D	407	LHG	C13-C14-C15-C16
37	N	618	LHG	C33-C34-C35-C36
37	s	320	LHG	C13-C14-C15-C16
41	D	402	DGA	CB5-CB6-CB7-CB8
46	S	309	CHL	C3-C5-C6-C7
37	L	101	LHG	C23-C24-C25-C26
29	r	304	CLA	O1D-CGD-O2D-CED
31	C	516	BCR	C11-C10-C9-C8
36	B	521	DGD	C2D-C1D-O3G-C3G
36	r	301	DGD	C2D-C1D-O3G-C3G
39	m	101	SQD	C2-C1-O6-C44
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
39	a	410	SQD	O47-C45-C46-O48
29	b	514	CLA	CBA-CGA-O2A-C1
33	s	322	3PH	C22-C23-C24-C25
37	D	408	LHG	C9-C10-C11-C12
37	Y	319	LHG	C33-C34-C35-C36
37	g	618	LHG	C9-C10-C11-C12
37	g	618	LHG	C13-C14-C15-C16
41	w	201	DGA	CB4-CB5-CB6-CB7
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	B	512	CLA	C16-C17-C18-C20
29	R	306	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
29	c	501	CLA	C16-C17-C18-C20
29	s	305	CLA	C6-C7-C8-C9
29	y	316	CLA	C16-C17-C18-C19
29	N	612	CLA	O1D-CGD-O2D-CED
29	N	603	CLA	C4-C3-C5-C6
29	G	613	CLA	C4-C3-C5-C6
33	B	522	3PH	C29-C2A-C2B-C2C
33	B	522	3PH	C3C-C3D-C3E-C3F
35	d	408	LMG	C12-C13-C14-C15
36	c	517	DGD	C4B-C5B-C6B-C7B
37	Y	319	LHG	C11-C10-C9-C8
37	a	413	LHG	C11-C12-C13-C14
37	n	617	LHG	C14-C15-C16-C17
37	y	320	LHG	C11-C12-C13-C14
40	C	525	SPH	C11-C10-C9-C8
29	C	508	CLA	C2-C3-C5-C6
29	B	504	CLA	C11-C10-C8-C9
29	B	504	CLA	C11-C12-C13-C14
29	N	610	CLA	C6-C7-C8-C9
29	c	507	CLA	C6-C7-C8-C9
29	n	612	CLA	C14-C13-C15-C16
29	r	308	CLA	C6-C7-C8-C9
46	s	307	CHL	C2A-CAA-CBA-CGA
35	B	520	LMG	C15-C16-C17-C18
35	i	101	LMG	C39-C40-C41-C42
37	l	102	LHG	C26-C27-C28-C29
39	L	102	SQD	C25-C26-C27-C28
41	W	202	DGA	CA5-CA6-CA7-CA8
41	W	202	DGA	CA8-CA9-CAA-CBA
50	N	620	PTY	C39-C40-C41-C42
29	R	306	CLA	C5-C6-C7-C8
29	g	613	CLA	C2A-CAA-CBA-CGA
29	s	305	CLA	C2A-CAA-CBA-CGA
46	n	605	CHL	C2A-CAA-CBA-CGA
31	B	518	BCR	C36-C18-C19-C20
31	K	101	BCR	C37-C22-C23-C24
31	v	101	BCR	C37-C22-C23-C24
34	b	519	C7Z	C7-C8-C9-C19
45	H	101	RRX	C7-C8-C9-C34
47	r	311	LUT	C7-C8-C9-C19
29	S	314	CLA	C4C-C3C-CAC-CBC
33	a	415	3PH	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
50	N	620	PTY	C40-C41-C42-C43
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
37	d	406	LHG	O1-C1-C2-C3
37	g	618	LHG	O1-C1-C2-C3
37	y	320	LHG	O1-C1-C2-C3
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
29	C	513	CLA	C3-C5-C6-C7
29	s	305	CLA	O1D-CGD-O2D-CED
35	W	201	LMG	O9-C10-O7-C8
35	W	201	LMG	C11-C10-O7-C8
35	c	519	LMG	C11-C10-O7-C8
39	m	101	SQD	C8-C7-O47-C45
35	B	520	LMG	C11-C12-C13-C14
35	C	522	LMG	C18-C19-C20-C21
36	c	517	DGD	C7A-C8A-C9A-CAA
37	y	320	LHG	C29-C30-C31-C32
38	b	524	LMT	C11-C10-C9-C8
41	J	101	DGA	CB3-CB4-CB5-CB6
50	n	619	PTY	C31-C32-C33-C34
29	s	310	CLA	CBD-CGD-O2D-CED
35	d	408	LMG	C28-C29-C30-C31
41	D	402	DGA	CB1-CB2-CB3-CB4
29	g	613	CLA	O1D-CGD-O2D-CED
33	A	412	3PH	C22-C23-C24-C25
37	G	618	LHG	C24-C25-C26-C27
37	Y	319	LHG	C13-C14-C15-C16
37	y	320	LHG	C16-C17-C18-C19
37	y	320	LHG	C31-C32-C33-C34
41	J	101	DGA	CA6-CA7-CA8-CA9

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Mol	Chain	Res	Type	Atoms
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
29	C	510	CLA	C16-C17-C18-C19
29	C	510	CLA	C16-C17-C18-C20
29	R	306	CLA	C11-C12-C13-C14
29	Y	315	CLA	C16-C17-C18-C20
29	a	408	CLA	C11-C12-C13-C14
29	a	408	CLA	C11-C12-C13-C15
29	b	501	CLA	C16-C17-C18-C20
29	c	509	CLA	C16-C17-C18-C19
29	c	509	CLA	C16-C17-C18-C20
29	c	512	CLA	C16-C17-C18-C20
29	d	403	CLA	C16-C17-C18-C19
29	g	613	CLA	C16-C17-C18-C20
29	s	305	CLA	C6-C7-C8-C10
30	a	407	PHO	C16-C17-C18-C20
36	r	301	DGD	O6D-C1D-O3G-C3G
39	a	410	SQD	O5-C1-O6-C44
29	B	511	CLA	C15-C16-C17-C18
29	C	513	CLA	C5-C6-C7-C8
29	a	404	CLA	C4C-C3C-CAC-CBC
33	B	522	3PH	C2B-C2C-C2D-C2E
33	a	415	3PH	C22-C23-C24-C25
33	a	415	3PH	C38-C39-C3A-C3B
37	B	523	LHG	C28-C29-C30-C31
37	N	618	LHG	C25-C26-C27-C28
37	G	618	LHG	C13-C14-C15-C16
37	c	521	LHG	C33-C34-C35-C36
37	d	406	LHG	C13-C14-C15-C16
37	l	102	LHG	C34-C35-C36-C37
37	g	618	LHG	C11-C10-C9-C8
39	l	101	SQD	C24-C25-C26-C27
39	o	301	SQD	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
50	N	620	PTY	C36-C37-C38-C39
29	S	312	CLA	O1D-CGD-O2D-CED
33	a	415	3PH	C36-C37-C38-C39
35	b	520	LMG	C11-C12-C13-C14
37	s	320	LHG	C31-C32-C33-C34
41	D	402	DGA	CA4-CA5-CA6-CA7
41	J	101	DGA	CB5-CB6-CB7-CB8
41	W	202	DGA	CA6-CA7-CA8-CA9
35	C	522	LMG	C10-C11-C12-C13
29	Y	314	CLA	C10-C11-C12-C13
33	S	322	3PH	O32-C31-O31-C3
37	B	523	LHG	C24-C25-C26-C27
39	a	410	SQD	C10-C11-C12-C13
41	D	402	DGA	CB9-CAB-CBB-CCB
29	C	512	CLA	O1D-CGD-O2D-CED
29	d	404	CLA	C3-C5-C6-C7
29	r	303	CLA	C3-C5-C6-C7
39	L	102	SQD	C24-C23-O48-C46
37	d	406	LHG	C34-C35-C36-C37
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	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	B	503	CLA	C10-C11-C12-C13
29	b	503	CLA	C15-C16-C17-C18
33	s	322	3PH	C2D-C2E-C2F-C2G
35	C	524	LMG	C14-C15-C16-C17
35	D	410	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
36	r	301	DGD	C3A-C4A-C5A-C6A
37	D	407	LHG	C10-C11-C12-C13
37	c	521	LHG	C27-C28-C29-C30
37	l	102	LHG	C14-C15-C16-C17
37	n	617	LHG	C13-C14-C15-C16
37	s	320	LHG	C30-C31-C32-C33
41	w	201	DGA	CB2-CB3-CB4-CB5
29	b	516	CLA	O1A-CGA-O2A-C1
36	c	518	DGD	O1A-C1A-O1G-C1G
29	C	502	CLA	C16-C17-C18-C20
29	D	405	CLA	C11-C12-C13-C15
29	c	512	CLA	C16-C17-C18-C19
29	g	613	CLA	C16-C17-C18-C19
33	A	412	3PH	C28-C29-C2A-C2B
39	M	101	SQD	C11-C10-C9-C8
41	D	402	DGA	CB3-CB4-CB5-CB6
29	s	304	CLA	O1D-CGD-O2D-CED
35	c	520	LMG	O1-C7-C8-C9
35	d	407	LMG	C30-C31-C32-C33
37	d	406	LHG	C11-C12-C13-C14
41	j	101	DGA	CA4-CA5-CA6-CA7
50	N	620	PTY	C15-C16-C17-C18
29	r	310	CLA	O2A-C1-C2-C3
48	R	312	NEX	C14-C15-C35-C34
29	A	406	CLA	C3-C5-C6-C7
46	G	601	CHL	C3-C5-C6-C7
38	b	524	LMT	C1-C2-C3-C4
46	r	306	CHL	C2C-C3C-CAC-CBC
39	l	101	SQD	O10-C23-O48-C46
29	c	510	CLA	C13-C15-C16-C17
29	y	305	CLA	C15-C16-C17-C18
29	c	504	CLA	C4-C3-C5-C6
29	B	514	CLA	CBA-CGA-O2A-C1
29	N	603	CLA	C2-C3-C5-C6
29	G	613	CLA	C2-C3-C5-C6
29	Y	305	CLA	C2-C3-C5-C6
43	d	405	PL9	C13-C14-C16-C17
46	y	309	CHL	C2-C3-C5-C6
37	S	320	LHG	C8-C7-O7-C5
37	Y	319	LHG	C8-C7-O7-C5
37	y	320	LHG	C8-C7-O7-C5
35	C	524	LMG	C8-C9-O8-C28

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Mol	Chain	Res	Type	Atoms
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
33	s	322	3PH	C25-C26-C27-C28
35	c	519	LMG	C29-C30-C31-C32
37	a	413	LHG	C13-C14-C15-C16
38	b	524	LMT	C3-C4-C5-C6
29	s	311	CLA	O1A-CGA-O2A-C1
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	D	404	CLA	C16-C17-C18-C19
29	b	511	CLA	C16-C17-C18-C20
29	g	602	CLA	C16-C17-C18-C19
29	y	316	CLA	C16-C17-C18-C20
46	Y	307	CHL	C16-C17-C18-C19
40	i	102	SPH	C6-C7-C8-C9
29	A	406	CLA	C2B-C3B-CAB-CBB
29	C	505	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
29	Y	315	CLA	C2B-C3B-CAB-CBB
29	b	503	CLA	C2B-C3B-CAB-CBB
29	c	503	CLA	C2B-C3B-CAB-CBB
29	d	403	CLA	C2B-C3B-CAB-CBB
29	r	304	CLA	C2B-C3B-CAB-CBB
29	y	306	CLA	C2B-C3B-CAB-CBB
37	n	617	LHG	O2-C2-C3-O3
46	n	601	CHL	C15-C16-C17-C18
33	B	522	3PH	C25-C26-C27-C28
33	a	415	3PH	C23-C24-C25-C26
37	d	406	LHG	C25-C26-C27-C28
37	g	618	LHG	C24-C25-C26-C27
37	y	320	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
41	w	201	DGA	CCB-CDB-CEB-CFB
50	n	619	PTY	C24-C25-C26-C27
29	s	304	CLA	O1A-CGA-O2A-C1
37	G	618	LHG	C23-C24-C25-C26
37	g	618	LHG	C23-C24-C25-C26
29	B	510	CLA	CBD-CGD-O2D-CED
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	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
33	A	412	3PH	C2D-C2E-C2F-C2G
36	c	516	DGD	C2B-C3B-C4B-C5B
37	G	618	LHG	C31-C32-C33-C34
37	y	320	LHG	C9-C10-C11-C12
29	C	513	CLA	C13-C15-C16-C17
29	g	603	CLA	C15-C16-C17-C18
29	B	512	CLA	O1A-CGA-O2A-C1
29	b	514	CLA	O1A-CGA-O2A-C1
37	a	414	LHG	O10-C23-O8-C6
29	B	501	CLA	C16-C17-C18-C20
29	r	309	CLA	C11-C12-C13-C14
31	A	410	BCR	C23-C24-C25-C26
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	C	516	BCR	C23-C24-C25-C26
31	F	101	BCR	C5-C6-C7-C8
31	F	101	BCR	C23-C24-C25-C26
31	F	101	BCR	C23-C24-C25-C30
31	K	101	BCR	C1-C6-C7-C8
31	a	409	BCR	C23-C24-C25-C26
31	a	409	BCR	C23-C24-C25-C30
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	c	514	BCR	C23-C24-C25-C26
31	f	101	BCR	C1-C6-C7-C8
31	f	101	BCR	C5-C6-C7-C8
31	z	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	z	101	BCR	C5-C6-C7-C8
34	B	519	C7Z	C1-C6-C7-C8
34	B	519	C7Z	C25-C26-C27-C28
34	b	519	C7Z	C5-C6-C7-C8
34	b	519	C7Z	C25-C26-C27-C28
45	H	101	RRX	C5-C6-C7-C8
37	D	407	LHG	C11-C12-C13-C14
50	n	619	PTY	C19-C20-C21-C22
29	b	515	CLA	O1D-CGD-O2D-CED
29	B	515	CLA	C8-C10-C11-C12
29	D	404	CLA	C10-C11-C12-C13
33	a	415	3PH	C2E-C2F-C2G-C2H
37	d	406	LHG	C23-C24-C25-C26
37	g	618	LHG	C7-C8-C9-C10
37	S	320	LHG	C26-C27-C28-C29
29	C	511	CLA	C13-C15-C16-C17
29	C	514	CLA	C15-C16-C17-C18
38	b	524	LMT	C5-C6-C7-C8
29	A	409	CLA	C4-C3-C5-C6
29	y	306	CLA	C4-C3-C5-C6
43	D	406	PL9	C15-C14-C16-C17
46	y	309	CHL	C4-C3-C5-C6
29	B	513	CLA	O1D-CGD-O2D-CED
29	B	501	CLA	C11-C10-C8-C7
29	B	502	CLA	C12-C13-C15-C16
29	B	504	CLA	C6-C7-C8-C10
29	B	504	CLA	C11-C12-C13-C15
29	B	508	CLA	C11-C12-C13-C15
29	B	509	CLA	C11-C12-C13-C15
29	B	513	CLA	C11-C12-C13-C15
29	C	512	CLA	C6-C7-C8-C10
29	N	610	CLA	C6-C7-C8-C10
29	N	613	CLA	C11-C12-C13-C15
29	Y	305	CLA	C11-C10-C8-C7
29	Y	314	CLA	C6-C7-C8-C10
29	c	505	CLA	C2-C3-C5-C6
29	c	507	CLA	C6-C7-C8-C10
29	c	510	CLA	C12-C13-C15-C16
29	d	404	CLA	C11-C12-C13-C15
29	n	604	CLA	C12-C13-C15-C16
29	n	609	CLA	C12-C13-C15-C16
29	n	612	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	g	603	CLA	C6-C7-C8-C10
29	s	304	CLA	C11-C10-C8-C7
29	y	306	CLA	C2-C3-C5-C6
29	y	313	CLA	C12-C13-C15-C16
46	Y	308	CHL	C6-C7-C8-C10
46	n	608	CHL	C12-C13-C15-C16
46	g	607	CHL	C12-C13-C15-C16
46	y	311	CHL	C11-C12-C13-C15
29	B	514	CLA	O1A-CGA-O2A-C1
39	L	102	SQD	O10-C23-O48-C46
29	s	304	CLA	C2C-C3C-CAC-CBC
33	A	412	3PH	C2E-C2F-C2G-C2H
33	b	521	3PH	C28-C29-C2A-C2B
29	S	312	CLA	C10-C11-C12-C13
46	y	301	CHL	C8-C10-C11-C12
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	G	602	CLA	C16-C17-C18-C20
33	B	522	3PH	O22-C21-O21-C2
37	g	618	LHG	O9-C7-O7-C5
39	l	101	SQD	O49-C7-O47-C45
29	c	506	CLA	CBA-CGA-O2A-C1
33	B	522	3PH	C32-C31-O31-C3
41	J	101	DGA	CA2-CA1-OG1-CG1
40	I	101	SPH	C6-C7-C8-C9
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	b	511	CLA	C10-C11-C12-C13
29	c	505	CLA	C10-C11-C12-C13
29	s	310	CLA	C8-C10-C11-C12
37	L	101	LHG	C17-C18-C19-C20
40	C	525	SPH	C6-C7-C8-C9
37	a	413	LHG	C28-C29-C30-C31
37	s	301	LHG	C7-C8-C9-C10
29	B	516	CLA	O1D-CGD-O2D-CED
33	a	415	3PH	C2D-C2E-C2F-C2G
37	n	617	LHG	C25-C26-C27-C28
39	m	101	SQD	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
39	m	101	SQD	C27-C28-C29-C30
40	i	102	SPH	C12-C13-C14-C15
41	b	522	DGA	CBB-CCB-CDB-CEB
33	A	412	3PH	C37-C38-C39-C3A
37	l	102	LHG	C13-C14-C15-C16
37	g	618	LHG	C31-C32-C33-C34
36	c	517	DGD	O6E-C5E-C6E-O5E
29	S	310	CLA	CBD-CGD-O2D-CED
29	C	504	CLA	C16-C17-C18-C20
29	b	510	CLA	C16-C17-C18-C20
29	s	303	CLA	C11-C12-C13-C14
29	g	603	CLA	C13-C15-C16-C17
33	a	415	3PH	C37-C38-C39-C3A
37	a	413	LHG	C24-C25-C26-C27
37	c	521	LHG	C34-C35-C36-C37
39	a	410	SQD	C11-C12-C13-C14
41	b	522	DGA	CBB-CAB-CB9-CB8
35	c	520	LMG	C10-C11-C12-C13
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
35	W	201	LMG	C16-C17-C18-C19
29	b	511	CLA	C15-C16-C17-C18
29	c	512	CLA	C13-C15-C16-C17
29	R	308	CLA	CBD-CGD-O2D-CED
33	a	415	3PH	C27-C28-C29-C2A
35	w	202	LMG	C36-C37-C38-C39
37	a	414	LHG	C33-C34-C35-C36
51	s	321	LPX	O1-C3-C4-O5
35	C	521	LMG	O9-C10-O7-C8
35	C	522	LMG	O9-C10-O7-C8
35	i	101	LMG	O9-C10-O7-C8
37	G	618	LHG	O9-C7-O7-C5
37	S	301	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
37	G	618	LHG	C7-C8-C9-C10
37	Y	319	LHG	C7-C8-C9-C10
37	l	102	LHG	C33-C34-C35-C36
38	b	524	LMT	C4-C5-C6-C7
41	D	402	DGA	CA3-CA4-CA5-CA6
35	B	520	LMG	C2-C1-O1-C7
39	c	522	SQD	C2-C1-O6-C44
37	s	301	LHG	O7-C5-C6-O8
37	s	320	LHG	C28-C29-C30-C31
29	B	512	CLA	C16-C17-C18-C19
29	Y	314	CLA	C16-C17-C18-C19
39	b	523	SQD	C10-C11-C12-C13
39	m	101	SQD	C12-C13-C14-C15
35	D	409	LMG	O6-C5-C6-O5
38	B	524	LMT	O5'-C5'-C6'-O6'
38	b	524	LMT	O5'-C5'-C6'-O6'
46	Y	307	CHL	C10-C11-C12-C13
29	C	513	CLA	C4-C3-C5-C6
29	Y	305	CLA	C4-C3-C5-C6
43	d	405	PL9	C15-C14-C16-C17
46	N	601	CHL	C4-C3-C5-C6
36	c	517	DGD	C1B-C2B-C3B-C4B
50	n	619	PTY	C30-C31-C32-C33
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	508	CLA	C11-C12-C13-C14
29	B	509	CLA	C11-C12-C13-C14
29	C	511	CLA	C14-C13-C15-C16
29	C	512	CLA	C6-C7-C8-C9
29	C	514	CLA	C11-C12-C13-C14
29	N	604	CLA	C6-C7-C8-C9
29	G	602	CLA	C6-C7-C8-C9
29	Y	314	CLA	C14-C13-C15-C16
29	c	509	CLA	C14-C13-C15-C16
29	c	510	CLA	C14-C13-C15-C16
29	d	404	CLA	C11-C12-C13-C14
29	n	602	CLA	C14-C13-C15-C16
29	n	609	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	n	609	CLA	C11-C12-C13-C14
29	g	603	CLA	C6-C7-C8-C9
29	s	304	CLA	C11-C10-C8-C9
29	y	313	CLA	C14-C13-C15-C16
29	y	315	CLA	C11-C10-C8-C9
46	g	607	CHL	C14-C13-C15-C16
46	y	301	CHL	C11-C10-C8-C9
36	r	301	DGD	O6E-C5E-C6E-O5E
41	w	201	DGA	CAB-CBB-CCB-CDB
29	A	407	CLA	C2A-CAA-CBA-CGA
29	B	514	CLA	C2A-CAA-CBA-CGA
29	s	310	CLA	C2A-CAA-CBA-CGA
46	N	607	CHL	C2A-CAA-CBA-CGA
46	y	301	CHL	C2A-CAA-CBA-CGA
35	C	524	LMG	O6-C5-C6-O5
35	D	410	LMG	O6-C5-C6-O5
29	C	503	CLA	CBA-CGA-O2A-C1
36	C	519	DGD	C1B-C2B-C3B-C4B
29	g	602	CLA	O1D-CGD-O2D-CED
33	A	412	3PH	C3A-C3B-C3C-C3D
36	c	517	DGD	C9A-CAA-CBA-CCA
37	g	618	LHG	C28-C29-C30-C31
37	s	301	LHG	C28-C29-C30-C31
31	z	101	BCR	C17-C18-C19-C20
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
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

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Mol	Chain	Res	Type	Atoms
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
35	c	519	LMG	O6-C5-C6-O5
46	G	606	CHL	C1A-C2A-CAA-CBA
46	Y	306	CHL	C1A-C2A-CAA-CBA
46	g	605	CHL	C1A-C2A-CAA-CBA
46	y	303	CHL	C1A-C2A-CAA-CBA
29	B	510	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	511	CLA	C16-C17-C18-C19
29	s	303	CLA	C11-C12-C13-C15
29	s	314	CLA	C6-C7-C8-C9
30	A	408	PHO	C16-C17-C18-C20
37	S	320	LHG	O9-C7-O7-C5
39	c	522	SQD	O49-C7-O47-C45
33	a	415	3PH	C29-C2A-C2B-C2C
35	c	520	LMG	C21-C22-C23-C24
45	h	101	RRX	C15-C16-C17-C18
47	G	616	LUT	C29-C30-C31-C32
29	b	507	CLA	C15-C16-C17-C18
29	b	510	CLA	C15-C16-C17-C18
29	y	316	CLA	C13-C15-C16-C17
37	a	414	LHG	C3-O3-P-O6
37	n	617	LHG	C3-O3-P-O6
51	S	321	LPX	C1-O2-P1-O1
33	A	412	3PH	C31-C32-C33-C34
35	C	521	LMG	O6-C5-C6-O5
37	g	618	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
41	J	101	DGA	OA1-CA1-OG1-CG1
46	G	601	CHL	C15-C16-C17-C18
33	b	521	3PH	O11-C1-C2-C3
37	G	618	LHG	O6-C4-C5-C6
36	c	517	DGD	CCB-CDB-CEB-CFB
37	c	521	LHG	C15-C16-C17-C18
29	b	516	CLA	O1D-CGD-O2D-CED
39	l	101	SQD	C26-C27-C28-C29
40	i	102	SPH	C7-C8-C9-C10
29	B	510	CLA	C15-C16-C17-C18
29	b	501	CLA	C16-C17-C18-C19
41	D	402	DGA	CA6-CA7-CA8-CA9
29	G	614	CLA	O1D-CGD-O2D-CED
33	s	322	3PH	C29-C2A-C2B-C2C
39	M	101	SQD	C26-C27-C28-C29
33	B	522	3PH	C21-C22-C23-C24
35	D	410	LMG	C10-C11-C12-C13
33	B	522	3PH	C2A-C2B-C2C-C2D
35	c	520	LMG	C18-C19-C20-C21
39	M	101	SQD	C27-C28-C29-C30
29	c	502	CLA	CBA-CGA-O2A-C1
36	C	518	DGD	C2A-C1A-O1G-C1G
29	c	505	CLA	C4-C3-C5-C6
29	C	510	CLA	C10-C11-C12-C13
29	b	515	CLA	C8-C10-C11-C12
29	G	604	CLA	CBD-CGD-O2D-CED
35	d	408	LMG	C36-C37-C38-C39
37	s	320	LHG	C34-C35-C36-C37
33	S	322	3PH	C21-C22-C23-C24
29	n	602	CLA	C2A-CAA-CBA-CGA
30	D	401	PHO	C2A-CAA-CBA-CGA
29	B	501	CLA	C16-C17-C18-C19
29	y	316	CLA	O1D-CGD-O2D-CED
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	521	LMG	C29-C30-C31-C32
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

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Mol	Chain	Res	Type	Atoms
37	S	301	LHG	C4-C5-C6-O8
37	Y	319	LHG	C29-C30-C31-C32
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
29	b	505	CLA	C15-C16-C17-C18
33	B	522	3PH	C2C-C2D-C2E-C2F
37	S	301	LHG	C26-C27-C28-C29
37	l	102	LHG	C31-C32-C33-C34
37	g	618	LHG	C16-C17-C18-C19
35	W	203	LMG	C8-C7-O1-C1
35	w	202	LMG	C8-C7-O1-C1
36	C	519	DGD	C2G-C3G-O3G-C1D
36	C	519	DGD	C5D-C6D-O5D-C1E
36	c	517	DGD	C2G-C3G-O3G-C1D
36	c	517	DGD	C5D-C6D-O5D-C1E
30	A	408	PHO	O1D-CGD-O2D-CED
37	G	618	LHG	C9-C10-C11-C12
37	G	618	LHG	C11-C12-C13-C14
29	C	502	CLA	C10-C11-C12-C13
29	c	505	CLA	C5-C6-C7-C8
29	n	603	CLA	C5-C6-C7-C8
29	s	312	CLA	C5-C6-C7-C8
29	b	501	CLA	CAA-CBA-CGA-O2A
29	b	506	CLA	O1D-CGD-O2D-CED
36	B	521	DGD	O6E-C5E-C6E-O5E
29	c	506	CLA	O1A-CGA-O2A-C1
37	S	320	LHG	C9-C10-C11-C12
41	b	522	DGA	CB3-CB4-CB5-CB6
29	G	602	CLA	C16-C17-C18-C19
35	C	522	LMG	C16-C17-C18-C19
29	g	603	CLA	CBD-CGD-O2D-CED
35	d	408	LMG	O6-C5-C6-O5
36	C	519	DGD	O6E-C5E-C6E-O5E
37	s	320	LHG	O1-C1-C2-O2
36	C	519	DGD	CCB-CDB-CEB-CFB
50	n	619	PTY	C41-C42-C43-C44
29	N	603	CLA	C13-C15-C16-C17
33	B	522	3PH	O32-C31-O31-C3
35	i	101	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
51	S	321	LPX	O5-C4-C5-O6
35	d	408	LMG	C11-C10-O7-C8
37	L	101	LHG	C13-C14-C15-C16
29	y	304	CLA	C8-C10-C11-C12
35	d	407	LMG	O6-C5-C6-O5
48	r	313	NEX	C39-C29-C30-C31
29	s	305	CLA	C4-C3-C5-C6
29	y	316	CLA	C4-C3-C5-C6
46	G	607	CHL	C4-C3-C5-C6
30	a	407	PHO	C16-C17-C18-C19
46	N	605	CHL	C16-C17-C18-C19
29	b	512	CLA	CBA-CGA-O2A-C1
35	w	202	LMG	C29-C28-O8-C9
39	l	101	SQD	C25-C26-C27-C28
29	s	311	CLA	C8-C10-C11-C12
35	i	101	LMG	C15-C16-C17-C18
37	l	102	LHG	C35-C36-C37-C38
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	B	513	CLA	C2-C1-O2A-CGA
29	N	611	CLA	C2-C1-O2A-CGA
29	Y	305	CLA	C2-C1-O2A-CGA
29	n	603	CLA	C2-C1-O2A-CGA
46	g	607	CHL	C2-C1-O2A-CGA
37	N	618	LHG	C9-C10-C11-C12
30	d	402	PHO	C3-C5-C6-C7
37	G	618	LHG	C35-C36-C37-C38
40	C	525	SPH	C11-C12-C13-C14
29	r	307	CLA	O1D-CGD-O2D-CED
46	N	605	CHL	C8-C10-C11-C12
33	A	412	3PH	C1-O11-P-O12
33	a	415	3PH	C1-O11-P-O12
33	b	521	3PH	C1-O11-P-O12
35	D	410	LMG	C36-C37-C38-C39
37	G	618	LHG	C16-C17-C18-C19
29	S	305	CLA	CBA-CGA-O2A-C1
33	s	322	3PH	C32-C31-O31-C3
29	C	503	CLA	O1A-CGA-O2A-C1
37	L	101	LHG	O6-C4-C5-O7
37	a	414	LHG	O6-C4-C5-O7
35	w	202	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	B	510	CLA	C16-C17-C18-C19
29	C	505	CLA	C6-C7-C8-C10
37	g	618	LHG	C35-C36-C37-C38
41	J	101	DGA	CB6-CB7-CB8-CB9
29	Y	313	CLA	C10-C11-C12-C13
29	b	514	CLA	C10-C11-C12-C13
29	g	603	CLA	C10-C11-C12-C13
35	C	522	LMG	C42-C43-C44-C45
37	Y	319	LHG	C16-C17-C18-C19
29	c	502	CLA	O1A-CGA-O2A-C1
36	C	518	DGD	O1A-C1A-O1G-C1G
36	B	521	DGD	C1A-C2A-C3A-C4A
29	B	507	CLA	C15-C16-C17-C18
29	B	513	CLA	C5-C6-C7-C8
29	c	509	CLA	C10-C11-C12-C13
29	s	312	CLA	C13-C15-C16-C17
36	c	517	DGD	C2E-C1E-O5D-C6D
37	Y	319	LHG	C34-C35-C36-C37
37	s	320	LHG	C33-C34-C35-C36
41	j	101	DGA	CBB-CAB-CB9-CB8
35	D	410	LMG	O7-C10-C11-C12
35	W	201	LMG	O1-C7-C8-O7
37	y	320	LHG	O7-C5-C6-O8
39	M	101	SQD	O47-C45-C46-O48
36	c	518	DGD	CCB-CDB-CEB-CFB
37	s	320	LHG	O9-C7-O7-C5
39	C	501	SQD	O49-C7-O47-C45
29	N	602	CLA	C10-C11-C12-C13
29	n	611	CLA	O1D-CGD-O2D-CED
33	b	521	3PH	C22-C23-C24-C25
36	c	516	DGD	C5B-C6B-C7B-C8B
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	C6-C7-C8-C10
29	C	510	CLA	C12-C13-C15-C16
29	C	511	CLA	C6-C7-C8-C10
29	C	511	CLA	C12-C13-C15-C16
29	C	514	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
29	D	404	CLA	C12-C13-C15-C16
29	D	405	CLA	C11-C10-C8-C7
29	N	604	CLA	C6-C7-C8-C10
29	N	604	CLA	C11-C12-C13-C15
29	N	610	CLA	C11-C12-C13-C15
29	G	602	CLA	C6-C7-C8-C10
29	G	602	CLA	C12-C13-C15-C16
29	G	613	CLA	C12-C13-C15-C16
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	303	CLA	C6-C7-C8-C10
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	506	CLA	C6-C7-C8-C10
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	s	305	CLA	C2-C3-C5-C6
29	y	305	CLA	C6-C7-C8-C10
29	y	305	CLA	C12-C13-C15-C16
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	607	CHL	C2-C3-C5-C6
46	G	609	CHL	C12-C13-C15-C16
46	Y	307	CHL	C6-C7-C8-C10
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	601	CHL	C11-C10-C8-C7
46	n	601	CHL	C11-C12-C13-C15
46	n	605	CHL	C11-C10-C8-C7
46	y	301	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
46	y	309	CHL	C6-C7-C8-C10
46	y	309	CHL	C12-C13-C15-C16
46	y	311	CHL	C12-C13-C15-C16
29	r	307	CLA	C3-C5-C6-C7
29	A	405	CLA	C14-C13-C15-C16
29	B	501	CLA	C6-C7-C8-C9
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	B	515	CLA	C11-C12-C13-C14
29	C	502	CLA	C14-C13-C15-C16
29	C	510	CLA	C14-C13-C15-C16
29	C	511	CLA	C6-C7-C8-C9
29	D	405	CLA	C11-C10-C8-C9
29	N	603	CLA	C6-C7-C8-C9
29	N	610	CLA	C11-C12-C13-C14
29	N	613	CLA	C11-C12-C13-C14
29	G	610	CLA	C11-C10-C8-C9
29	S	304	CLA	C11-C10-C8-C9
29	a	404	CLA	C14-C13-C15-C16
29	a	408	CLA	C11-C10-C8-C9
29	b	501	CLA	C11-C10-C8-C9
29	b	506	CLA	C11-C10-C8-C9
29	b	514	CLA	C6-C7-C8-C9
29	b	515	CLA	C11-C12-C13-C14
29	c	501	CLA	C14-C13-C15-C16
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	511	CLA	C11-C12-C13-C14
29	c	513	CLA	C6-C7-C8-C9
29	d	403	CLA	C11-C12-C13-C14
29	n	603	CLA	C11-C10-C8-C9
29	n	604	CLA	C6-C7-C8-C9
29	n	609	CLA	C14-C13-C15-C16
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
46	N	601	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
46	N	607	CHL	C11-C12-C13-C14
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
31	B	518	BCR	C19-C20-C21-C22
31	b	518	BCR	C19-C20-C21-C22
29	R	306	CLA	CBD-CGD-O2D-CED
41	w	201	DGA	CDA-CEA-CFA-CGA
29	c	511	CLA	CBA-CGA-O2A-C1
43	d	405	PL9	C47-C48-C49-C50
34	B	519	C7Z	C7-C8-C9-C19
29	S	305	CLA	C6-C7-C8-C9
29	b	512	CLA	C16-C17-C18-C20
29	a	406	CLA	C2C-C3C-CAC-CBC
46	R	305	CHL	C2C-C3C-CAC-CBC
50	N	620	PTY	C19-C20-C21-C22
31	b	517	BCR	C21-C22-C23-C24
31	b	518	BCR	C17-C18-C19-C20
34	B	519	C7Z	C7-C8-C9-C10
33	s	322	3PH	C35-C36-C37-C38
37	Y	319	LHG	C35-C36-C37-C38
37	d	406	LHG	C26-C27-C28-C29
37	B	523	LHG	C1-C2-C3-O3
29	B	505	CLA	C15-C16-C17-C18
37	c	521	LHG	C8-C7-O7-C5
37	N	618	LHG	C30-C31-C32-C33
41	D	402	DGA	CB4-CB5-CB6-CB7
29	B	505	CLA	CBA-CGA-O2A-C1
37	S	301	LHG	C24-C23-O8-C6
37	c	521	LHG	C30-C31-C32-C33
41	W	202	DGA	CB6-CB7-CB8-CB9
29	C	506	CLA	C5-C6-C7-C8
29	C	509	CLA	C13-C15-C16-C17
29	c	513	CLA	C10-C11-C12-C13
29	n	612	CLA	C13-C15-C16-C17
29	b	504	CLA	C4C-C3C-CAC-CBC
33	s	322	3PH	C3B-C3C-C3D-C3E
35	c	520	LMG	C13-C14-C15-C16
35	d	407	LMG	C18-C19-C20-C21
29	B	506	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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
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
36	c	517	DGD	O6E-C1E-O5D-C6D
29	y	314	CLA	C10-C11-C12-C13
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
39	a	410	SQD	C28-C29-C30-C31
37	B	523	LHG	C7-C8-C9-C10
29	Y	305	CLA	C8-C10-C11-C12
46	N	606	CHL	C8-C10-C11-C12
46	Y	307	CHL	C13-C15-C16-C17
29	C	508	CLA	O1D-CGD-O2D-CED
29	c	507	CLA	O1D-CGD-O2D-CED
29	s	310	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	s	312	CLA	C4-C3-C5-C6
29	y	315	CLA	C4-C3-C5-C6
43	d	405	PL9	C40-C39-C41-C42
29	y	316	CLA	C2-C3-C5-C6
37	c	521	LHG	O9-C7-O7-C5
29	b	512	CLA	O1A-CGA-O2A-C1
29	G	611	CLA	O1D-CGD-O2D-CED
46	s	309	CHL	C11-C12-C13-C15
33	S	322	3PH	C24-C25-C26-C27
37	L	101	LHG	C34-C35-C36-C37
37	Y	319	LHG	C11-C12-C13-C14
41	J	101	DGA	CA4-CA5-CA6-CA7
29	c	505	CLA	CBA-CGA-O2A-C1
33	b	521	3PH	C36-C37-C38-C39
37	y	320	LHG	C30-C31-C32-C33
41	w	201	DGA	CB7-CB8-CB9-CAB
30	d	402	PHO	C3A-C2A-CAA-CBA
46	N	601	CHL	C3A-C2A-CAA-CBA
46	G	601	CHL	C3A-C2A-CAA-CBA
46	Y	302	CHL	C3A-C2A-CAA-CBA
46	n	601	CHL	C3A-C2A-CAA-CBA
39	b	523	SQD	C27-C28-C29-C30
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	c	505	CLA	C8-C10-C11-C12
29	Y	315	CLA	CBA-CGA-O2A-C1
46	n	601	CHL	C8-C10-C11-C12
35	w	202	LMG	O1-C7-C8-C9
37	N	618	LHG	C4-C5-C6-O8
37	Y	319	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
37	S	320	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
43	D	406	PL9	C47-C48-C49-C51
29	s	310	CLA	O1D-CGD-O2D-CED
41	w	201	DGA	CA5-CA6-CA7-CA8
29	c	512	CLA	C4-C3-C5-C6
29	Y	304	CLA	C16-C17-C18-C20
37	n	617	LHG	C9-C10-C11-C12
37	n	617	LHG	C28-C29-C30-C31
37	B	523	LHG	C4-O6-P-O3
50	y	321	PTY	C3-O11-P1-O14
33	s	322	3PH	O32-C31-O31-C3
35	w	202	LMG	O10-C28-O8-C9
29	g	603	CLA	C3-C5-C6-C7
29	s	305	CLA	C3-C5-C6-C7
46	S	302	CHL	C2A-CAA-CBA-CGA
37	B	523	LHG	O1-C1-C2-O2
37	Y	319	LHG	O1-C1-C2-O2
29	A	406	CLA	C5-C6-C7-C8
29	G	602	CLA	C15-C16-C17-C18
29	c	503	CLA	C13-C15-C16-C17
37	N	618	LHG	C28-C29-C30-C31
37	Y	319	LHG	C9-C10-C11-C12
37	c	521	LHG	C11-C10-C9-C8
37	s	301	LHG	C25-C26-C27-C28
37	c	521	LHG	O6-C4-C5-O7
37	s	301	LHG	O6-C4-C5-O7
50	Y	320	PTY	O14-C5-C6-O7
29	s	305	CLA	CBA-CGA-O2A-C1
37	N	618	LHG	C16-C17-C18-C19
29	S	305	CLA	O1A-CGA-O2A-C1
29	b	512	CLA	C16-C17-C18-C19
46	N	605	CHL	C16-C17-C18-C20
46	N	607	CHL	C16-C17-C18-C20
46	Y	307	CHL	C16-C17-C18-C20
29	b	501	CLA	C15-C16-C17-C18
35	c	519	LMG	O7-C10-C11-C12
29	B	502	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	g	610	CLA	C2B-C3B-CAB-CBB
29	g	611	CLA	C2B-C3B-CAB-CBB
29	s	303	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	s	315	CLA	C2B-C3B-CAB-CBB
33	a	415	3PH	C25-C26-C27-C28
37	l	102	LHG	C29-C30-C31-C32
29	S	304	CLA	C2C-C3C-CAC-CBC
37	L	101	LHG	C28-C29-C30-C31
33	A	412	3PH	C24-C25-C26-C27
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
35	D	410	LMG	C11-C10-O7-C8
29	C	505	CLA	C6-C7-C8-C9
29	S	305	CLA	C6-C7-C8-C10
40	c	523	SPH	C11-C12-C13-C14
36	C	519	DGD	O6E-C1E-O5D-C6D
29	B	501	CLA	C15-C16-C17-C18
29	S	311	CLA	C13-C15-C16-C17
37	N	618	LHG	C1-C2-C3-O3
41	j	101	DGA	CG1-CG2-CG3-OXT
41	w	201	DGA	CG1-CG2-CG3-OXT
37	a	413	LHG	C26-C27-C28-C29
35	d	408	LMG	O9-C10-O7-C8
29	b	504	CLA	C2-C1-O2A-CGA
29	B	510	CLA	O1D-CGD-O2D-CED
37	B	523	LHG	C25-C26-C27-C28
29	c	511	CLA	O1A-CGA-O2A-C1
29	B	503	CLA	C11-C12-C13-C14
29	C	513	CLA	C14-C13-C15-C16
29	D	404	CLA	C11-C12-C13-C14
29	N	604	CLA	C14-C13-C15-C16
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	b	502	CLA	C14-C13-C15-C16
29	b	510	CLA	C11-C12-C13-C14
29	c	507	CLA	C11-C10-C8-C9
29	r	307	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
46	G	609	CHL	C11-C10-C8-C9
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	Y	315	CLA	C13-C15-C16-C17
29	b	513	CLA	C5-C6-C7-C8
30	a	407	PHO	C1A-C2A-CAA-CBA
33	A	412	3PH	C2-C1-O11-P
33	b	521	3PH	C2-C1-O11-P
37	D	408	LHG	C2-C3-O3-P
37	l	102	LHG	C2-C3-O3-P
33	A	412	3PH	C36-C37-C38-C39
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	R	303	CLA	C2A-CAA-CBA-CGA
29	b	514	CLA	C2A-CAA-CBA-CGA
29	r	307	CLA	C2A-CAA-CBA-CGA
29	N	602	CLA	C16-C17-C18-C20
29	g	611	CLA	C16-C17-C18-C20
29	s	314	CLA	C6-C7-C8-C10
30	A	408	PHO	C16-C17-C18-C19
31	B	518	BCR	C23-C24-C25-C26
31	B	518	BCR	C23-C24-C25-C30
31	C	517	BCR	C1-C6-C7-C8
31	C	517	BCR	C5-C6-C7-C8
31	c	514	BCR	C5-C6-C7-C8
31	c	515	BCR	C5-C6-C7-C8
34	b	519	C7Z	C21-C26-C27-C28
45	h	101	RRX	C23-C24-C25-C26
45	h	101	RRX	C5-C6-C7-C8
47	N	615	LUT	C1-C6-C7-C8
47	N	615	LUT	C5-C6-C7-C8
47	S	317	LUT	C5-C6-C7-C8
47	Y	316	LUT	C5-C6-C7-C8
33	A	412	3PH	C2B-C2C-C2D-C2E
33	s	322	3PH	C37-C38-C39-C3A
37	L	101	LHG	C30-C31-C32-C33
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

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Mol	Chain	Res	Type	Atoms
48	R	312	NEX	C20-C13-C14-C15
48	r	313	NEX	C20-C13-C14-C15
29	Y	304	CLA	C13-C15-C16-C17
35	D	410	LMG	O9-C10-O7-C8
41	W	202	DGA	CB9-CAB-CBB-CCB
29	S	310	CLA	C11-C12-C13-C14
37	N	618	LHG	C31-C32-C33-C34
29	A	407	CLA	C2C-C3C-CAC-CBC
35	b	520	LMG	C12-C13-C14-C15
43	D	406	PL9	C40-C39-C41-C42
35	C	522	LMG	C12-C13-C14-C15
38	b	524	LMT	C9-C10-C11-C12
29	A	405	CLA	C12-C13-C15-C16
29	A	409	CLA	C2-C3-C5-C6
29	B	501	CLA	C12-C13-C15-C16
29	B	504	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
29	C	507	CLA	C6-C7-C8-C10
29	C	513	CLA	C12-C13-C15-C16
29	D	404	CLA	C6-C7-C8-C10
29	D	404	CLA	C11-C12-C13-C15
29	N	602	CLA	C6-C7-C8-C10
29	N	602	CLA	C11-C12-C13-C15
29	N	603	CLA	C6-C7-C8-C10
29	N	603	CLA	C12-C13-C15-C16
29	N	613	CLA	C12-C13-C15-C16
29	G	610	CLA	C11-C10-C8-C7
29	R	301	CLA	C6-C7-C8-C10
29	S	303	CLA	C11-C10-C8-C7
29	S	304	CLA	C11-C10-C8-C7
29	S	304	CLA	C12-C13-C15-C16
29	Y	313	CLA	C11-C10-C8-C7
29	a	404	CLA	C12-C13-C15-C16
29	a	405	CLA	C6-C7-C8-C10
29	b	501	CLA	C11-C10-C8-C7
29	b	501	CLA	C11-C12-C13-C15
29	b	504	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
29	b	514	CLA	C6-C7-C8-C10
29	b	515	CLA	C11-C12-C13-C15
29	c	502	CLA	C11-C12-C13-C15
29	c	503	CLA	C11-C12-C13-C15
29	c	504	CLA	C6-C7-C8-C10
29	c	504	CLA	C11-C12-C13-C15
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	603	CLA	C12-C13-C15-C16
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	603	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	304	CLA	C6-C7-C8-C10
29	y	306	CLA	C11-C10-C8-C7
29	y	314	CLA	C11-C10-C8-C7
46	N	605	CHL	C11-C10-C8-C7
46	N	607	CHL	C12-C13-C15-C16
46	G	607	CHL	C11-C12-C13-C15
46	G	609	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	C6-C7-C8-C10
46	g	601	CHL	C12-C13-C15-C16
46	g	609	CHL	C11-C12-C13-C15
29	N	610	CLA	C13-C15-C16-C17
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	C	504	CLA	C16-C17-C18-C19
41	D	402	DGA	CA1-CA2-CA3-CA4
41	W	202	DGA	CA4-CA5-CA6-CA7

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Mol	Chain	Res	Type	Atoms
29	G	603	CLA	C10-C11-C12-C13
30	A	408	PHO	C15-C16-C17-C18
29	S	305	CLA	C2A-CAA-CBA-CGA
29	S	310	CLA	C10-C11-C12-C13
41	j	101	DGA	CA1-CA2-CA3-CA4
29	b	516	CLA	C8-C10-C11-C12
29	c	503	CLA	C10-C11-C12-C13
46	n	606	CHL	C13-C15-C16-C17
46	y	301	CHL	C10-C11-C12-C13
29	Y	314	CLA	CBA-CGA-O2A-C1
37	d	406	LHG	C10-C11-C12-C13
37	s	320	LHG	C24-C25-C26-C27
41	W	202	DGA	CA3-CA4-CA5-CA6
37	B	523	LHG	C23-C24-C25-C26
33	a	415	3PH	C24-C25-C26-C27
37	s	320	LHG	C14-C15-C16-C17
39	l	101	SQD	C11-C10-C9-C8
40	i	102	SPH	C13-C14-C15-C16
29	B	504	CLA	C13-C15-C16-C17
29	B	505	CLA	CAD-CBD-CGD-O2D
29	B	508	CLA	CAD-CBD-CGD-O2D
29	B	510	CLA	CAD-CBD-CGD-O2D
29	C	503	CLA	CAD-CBD-CGD-O2D
29	C	506	CLA	CAD-CBD-CGD-O2D
29	C	514	CLA	CAD-CBD-CGD-O2D
29	N	614	CLA	CAD-CBD-CGD-O2D
29	G	611	CLA	CAD-CBD-CGD-O2D
29	S	315	CLA	CAD-CBD-CGD-O2D
29	b	510	CLA	CAD-CBD-CGD-O2D
29	c	502	CLA	CAD-CBD-CGD-O2D
29	c	513	CLA	CAD-CBD-CGD-O2D
29	g	602	CLA	CAD-CBD-CGD-O2D
29	r	302	CLA	CAD-CBD-CGD-O2D
29	r	308	CLA	CAD-CBD-CGD-O2D
29	s	310	CLA	CAD-CBD-CGD-O2D
29	y	305	CLA	CAD-CBD-CGD-O2D
29	y	316	CLA	CAD-CBD-CGD-O2D
30	a	407	PHO	CAD-CBD-CGD-O2D
39	L	102	SQD	C46-C45-O47-C7
39	m	101	SQD	C46-C45-O47-C7
46	n	605	CHL	CAD-CBD-CGD-O2D
48	Y	318	NEX	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
48	y	319	NEX	C7-C8-C9-C19
46	y	303	CHL	C3-C5-C6-C7
35	D	410	LMG	C12-C13-C14-C15
39	b	523	SQD	C30-C31-C32-C33
46	g	609	CHL	C13-C15-C16-C17
37	a	414	LHG	C25-C26-C27-C28
37	s	320	LHG	C29-C30-C31-C32
39	C	501	SQD	C24-C23-O48-C46
29	Y	304	CLA	C16-C17-C18-C19
36	C	520	DGD	C3A-C4A-C5A-C6A
29	D	405	CLA	C8-C10-C11-C12
29	Y	303	CLA	C8-C10-C11-C12
29	s	310	CLA	C5-C6-C7-C8
46	n	608	CHL	C8-C10-C11-C12
29	S	310	CLA	O1D-CGD-O2D-CED
35	i	101	LMG	O1-C7-C8-C9
35	i	101	LMG	C7-C8-C9-O8
37	a	414	LHG	C4-C5-C6-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
41	w	201	DGA	OG1-CG1-CG2-CG3
29	B	504	CLA	CBD-CGD-O2D-CED
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	d	408	LMG	O7-C10-C11-C12
37	N	618	LHG	O8-C23-C24-C25
29	G	604	CLA	O2A-C1-C2-C3
29	n	613	CLA	O2A-C1-C2-C3
29	g	604	CLA	O2A-C1-C2-C3
29	c	501	CLA	C2A-CAA-CBA-CGA
29	B	504	CLA	C15-C16-C17-C18
29	g	610	CLA	C15-C16-C17-C18
29	C	506	CLA	CBD-CGD-O2D-CED
38	b	524	LMT	O1'-C1-C2-C3
41	w	201	DGA	CEA-CFA-CGA-CHA
29	B	506	CLA	CHA-CBD-CGD-O2D
29	B	507	CLA	CHA-CBD-CGD-O1D
29	B	507	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	C	505	CLA	CHA-CBD-CGD-O1D
29	S	303	CLA	CHA-CBD-CGD-O1D
29	b	501	CLA	CHA-CBD-CGD-O1D
29	b	501	CLA	CHA-CBD-CGD-O2D
29	b	506	CLA	CHA-CBD-CGD-O1D
29	b	506	CLA	CHA-CBD-CGD-O2D
29	n	604	CLA	CHA-CBD-CGD-O1D
29	n	604	CLA	CHA-CBD-CGD-O2D
29	s	303	CLA	CHA-CBD-CGD-O1D
29	s	303	CLA	CHA-CBD-CGD-O2D
46	R	304	CHL	CHA-CBD-CGD-O1D
46	R	304	CHL	CHA-CBD-CGD-O2D
46	g	605	CHL	CHA-CBD-CGD-O1D
46	g	605	CHL	CHA-CBD-CGD-O2D
46	r	305	CHL	CHA-CBD-CGD-O1D
46	r	305	CHL	CHA-CBD-CGD-O2D
39	o	301	SQD	C24-C25-C26-C27
29	y	314	CLA	C3-C5-C6-C7
29	B	505	CLA	O1A-CGA-O2A-C1
29	Y	314	CLA	O1A-CGA-O2A-C1
29	Y	315	CLA	O1A-CGA-O2A-C1
29	c	505	CLA	O1A-CGA-O2A-C1
37	S	301	LHG	O10-C23-O8-C6
36	C	519	DGD	C2E-C1E-O5D-C6D
46	r	305	CHL	C2A-CAA-CBA-CGA
35	B	520	LMG	C31-C32-C33-C34
37	N	618	LHG	C35-C36-C37-C38
37	S	320	LHG	C24-C25-C26-C27
50	n	619	PTY	C37-C38-C39-C40
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
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
37	y	320	LHG	C26-C27-C28-C29
29	s	305	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	b	521	3PH	C32-C33-C34-C35
33	b	521	3PH	C26-C27-C28-C29
35	c	519	LMG	C33-C34-C35-C36
37	l	102	LHG	C15-C16-C17-C18
29	g	613	CLA	C5-C6-C7-C8
37	D	408	LHG	C8-C7-O7-C5
46	Y	308	CHL	C4-C3-C5-C6
37	L	101	LHG	C10-C11-C12-C13
37	c	521	LHG	C7-C8-C9-C10
33	A	412	3PH	C3B-C3C-C3D-C3E
29	N	603	CLA	C15-C16-C17-C18
29	B	503	CLA	C6-C7-C8-C9
29	B	506	CLA	C11-C10-C8-C9
29	N	602	CLA	C11-C12-C13-C14
29	Y	313	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	y	306	CLA	C14-C13-C15-C16
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
29	G	604	CLA	O1D-CGD-O2D-CED
39	c	522	SQD	C32-C33-C34-C35
29	g	603	CLA	O1D-CGD-O2D-CED
41	b	522	DGA	CB1-CB2-CB3-CB4
40	c	523	SPH	C11-C10-C9-C8
41	w	201	DGA	CDB-CEB-CFB-CGB
29	n	609	CLA	C5-C6-C7-C8
39	C	523	SQD	C5-C6-S-O8
39	M	101	SQD	C4-C5-C6-S
39	a	410	SQD	C4-C5-C6-S
33	B	522	3PH	C3B-C3C-C3D-C3E
31	a	409	BCR	C37-C22-C23-C24
29	c	507	CLA	C13-C15-C16-C17
29	r	308	CLA	C10-C11-C12-C13
37	a	413	LHG	C11-C10-C9-C8
37	y	320	LHG	C35-C36-C37-C38
31	A	410	BCR	C21-C22-C23-C24
45	H	101	RRX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
35	C	524	LMG	C15-C16-C17-C18
29	R	308	CLA	O1D-CGD-O2D-CED
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	315	CLA	C1A-C2A-CAA-CBA
29	Y	311	CLA	C1A-C2A-CAA-CBA
29	a	406	CLA	C1A-C2A-CAA-CBA
29	c	512	CLA	C1A-C2A-CAA-CBA
46	N	601	CHL	C1A-C2A-CAA-CBA
46	G	607	CHL	C1A-C2A-CAA-CBA
46	Y	302	CHL	C1A-C2A-CAA-CBA
46	n	601	CHL	C1A-C2A-CAA-CBA
46	g	609	CHL	C1A-C2A-CAA-CBA
46	Y	307	CHL	C8-C10-C11-C12
29	A	405	CLA	C2-C1-O2A-CGA
29	G	604	CLA	C2-C1-O2A-CGA
46	Y	307	CHL	C2-C1-O2A-CGA
29	C	506	CLA	CBA-CGA-O2A-C1
33	b	521	3PH	C27-C28-C29-C2A
37	G	618	LHG	C30-C31-C32-C33
41	W	202	DGA	CB7-CB8-CB9-CAB
48	r	313	NEX	C13-C14-C15-C35
37	B	523	LHG	C3-O3-P-O6
37	L	101	LHG	C3-O3-P-O6
37	S	301	LHG	C3-O3-P-O6
37	Y	319	LHG	C3-O3-P-O6
37	g	618	LHG	C3-O3-P-O6
51	s	321	LPX	C3-O1-P1-O2
37	s	301	LHG	C11-C12-C13-C14
35	C	524	LMG	C32-C33-C34-C35
41	w	201	DGA	CA8-CA9-CAA-CBA
46	Y	302	CHL	C3-C5-C6-C7
37	c	521	LHG	C2-C3-O3-P
37	s	301	LHG	C2-C3-O3-P
29	C	513	CLA	C2-C3-C5-C6
29	y	315	CLA	C2-C3-C5-C6
46	N	601	CHL	C2-C3-C5-C6
29	B	511	CLA	C4C-C3C-CAC-CBC
29	S	312	CLA	C4B-C3B-CAB-CBB
29	b	515	CLA	C4B-C3B-CAB-CBB
29	n	602	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	g	603	CLA	C4B-C3B-CAB-CBB
29	s	312	CLA	C4B-C3B-CAB-CBB
37	B	523	LHG	C4-O6-P-O4
37	D	408	LHG	C4-O6-P-O5
37	L	101	LHG	C4-O6-P-O4
37	L	101	LHG	C4-O6-P-O5
37	S	301	LHG	C3-O3-P-O5
37	S	301	LHG	C4-O6-P-O4
37	a	414	LHG	C3-O3-P-O4
37	d	406	LHG	C4-O6-P-O4
37	s	320	LHG	C4-O6-P-O5
37	y	320	LHG	C4-O6-P-O4
50	N	620	PTY	C5-O14-P1-O12
50	n	619	PTY	C3-O11-P1-O12
50	y	321	PTY	C3-O11-P1-O13
51	s	321	LPX	C3-O1-P1-O4
29	C	506	CLA	C11-C12-C13-C14
29	g	611	CLA	C16-C17-C18-C19
37	L	101	LHG	C11-C10-C9-C8
37	a	414	LHG	C34-C35-C36-C37
40	C	525	SPH	C10-C11-C12-C13
29	D	405	CLA	C10-C11-C12-C13
29	n	602	CLA	CBA-CGA-O2A-C1
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	R	306	CLA	O1D-CGD-O2D-CED
37	a	414	LHG	C11-C10-C9-C8
37	S	320	LHG	C29-C30-C31-C32
37	n	617	LHG	C26-C27-C28-C29
41	w	201	DGA	CA6-CA7-CA8-CA9
29	n	602	CLA	C15-C16-C17-C18
29	G	613	CLA	C2A-CAA-CBA-CGA
29	Y	314	CLA	C2A-CAA-CBA-CGA
29	R	306	CLA	C3-C5-C6-C7
35	C	524	LMG	C30-C31-C32-C33
35	W	203	LMG	C36-C37-C38-C39
46	N	607	CHL	C16-C17-C18-C19
35	c	519	LMG	C18-C19-C20-C21
29	B	507	CLA	CAD-CBD-CGD-O1D
29	C	505	CLA	CAD-CBD-CGD-O1D
29	n	604	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	r	310	CLA	CAD-CBD-CGD-O1D
29	r	310	CLA	C2-C3-C5-C6
29	s	303	CLA	CAD-CBD-CGD-O1D
39	C	523	SQD	C5-C6-S-O7
39	L	102	SQD	O5-C5-C6-S
46	N	609	CHL	CAD-CBD-CGD-O1D
46	R	304	CHL	CAD-CBD-CGD-O1D
46	r	305	CHL	CAD-CBD-CGD-O1D
50	n	619	PTY	C2-C3-O11-P1
50	y	321	PTY	C2-C3-O11-P1
41	b	522	DGA	CDB-CEB-CFB-CGB
41	w	201	DGA	CEB-CFB-CGB-CHB
33	b	521	3PH	C2B-C2C-C2D-C2E
30	a	407	PHO	C15-C16-C17-C18
37	D	407	LHG	C24-C23-O8-C6
39	C	501	SQD	O10-C23-O48-C46
46	N	605	CHL	C4-C3-C5-C6
29	B	512	CLA	C3A-C2A-CAA-CBA
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	614	CLA	C3A-C2A-CAA-CBA
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	b	511	CLA	C12-C13-C15-C16
29	b	515	CLA	C11-C10-C8-C7
29	c	501	CLA	C11-C12-C13-C15
29	c	505	CLA	C6-C7-C8-C10
29	c	511	CLA	C11-C12-C13-C15
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
29	y	306	CLA	C6-C7-C8-C10
37	D	408	LHG	O6-C4-C5-O7
37	N	618	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
37	l	102	LHG	O6-C4-C5-O7
46	N	605	CHL	C12-C13-C15-C16
46	N	606	CHL	C12-C13-C15-C16
46	G	601	CHL	C6-C7-C8-C10
46	Y	308	CHL	C11-C12-C13-C15
46	n	606	CHL	C11-C10-C8-C7
46	y	309	CHL	C11-C12-C13-C15
47	S	318	LUT	C25-C26-C27-C28
50	n	619	PTY	O14-C5-C6-O7
37	S	320	LHG	C15-C16-C17-C18
29	g	613	CLA	C15-C16-C17-C18
35	B	520	LMG	C18-C19-C20-C21
36	c	518	DGD	O6D-C5D-C6D-O5D
37	G	618	LHG	O8-C23-C24-C25
37	y	320	LHG	C23-C24-C25-C26
41	w	201	DGA	CB2-CB1-OG2-CG2
29	R	302	CLA	C2C-C3C-CAC-CBC
33	b	521	3PH	C35-C36-C37-C38
33	s	322	3PH	C3E-C3F-C3G-C3H
35	c	519	LMG	C32-C33-C34-C35
29	Y	303	CLA	C2A-CAA-CBA-CGA
29	B	515	CLA	C16-C17-C18-C20
37	s	320	LHG	C23-C24-C25-C26
36	C	520	DGD	O6D-C5D-C6D-O5D
35	C	522	LMG	O1-C7-C8-C9
35	C	524	LMG	O1-C7-C8-C9
40	C	525	SPH	O1-C1-C2-N2
40	I	101	SPH	O1-C1-C2-N2
40	c	523	SPH	C1-C2-C3-O3
41	w	201	DGA	OB1-CB1-OG2-CG2
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	g	602	CLA	C15-C16-C17-C18
39	c	522	SQD	C28-C29-C30-C31
39	o	301	SQD	C25-C26-C27-C28
39	C	501	SQD	C45-C44-O6-C1
39	b	523	SQD	C45-C44-O6-C1
29	N	602	CLA	C16-C17-C18-C19
35	c	519	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
37	a	414	LHG	C2-C3-O3-P
37	a	414	LHG	C24-C25-C26-C27
38	B	524	LMT	C6-C7-C8-C9
29	C	506	CLA	O1A-CGA-O2A-C1
29	Y	312	CLA	C13-C15-C16-C17
29	c	503	CLA	C8-C10-C11-C12
43	d	405	PL9	C45-C44-C46-C47
46	Y	307	CHL	C4-C3-C5-C6
35	d	408	LMG	C13-C14-C15-C16
29	B	501	CLA	C14-C13-C15-C16
29	B	504	CLA	C14-C13-C15-C16
29	B	507	CLA	C6-C7-C8-C9
29	B	510	CLA	C11-C12-C13-C14
29	B	514	CLA	C11-C10-C8-C9
29	C	509	CLA	C11-C12-C13-C14
29	N	603	CLA	C14-C13-C15-C16
29	N	613	CLA	C14-C13-C15-C16
29	G	603	CLA	C6-C7-C8-C9
29	G	613	CLA	C14-C13-C15-C16
29	S	311	CLA	C6-C7-C8-C9
29	Y	305	CLA	C14-C13-C15-C16
29	a	405	CLA	C6-C7-C8-C9
29	a	405	CLA	C11-C12-C13-C14
29	b	504	CLA	C11-C12-C13-C14
29	c	502	CLA	C11-C12-C13-C14
29	c	508	CLA	C11-C12-C13-C14
29	n	603	CLA	C14-C13-C15-C16
29	g	603	CLA	C14-C13-C15-C16
29	y	304	CLA	C6-C7-C8-C9
29	y	306	CLA	C11-C10-C8-C9
46	N	601	CHL	C14-C13-C15-C16
46	Y	307	CHL	C6-C7-C8-C9
46	n	608	CHL	C11-C12-C13-C14
46	g	601	CHL	C6-C7-C8-C9
29	B	506	CLA	O1D-CGD-O2D-CED
35	i	101	LMG	C11-C12-C13-C14
37	G	618	LHG	C28-C29-C30-C31
37	d	406	LHG	C11-C10-C9-C8
29	Y	312	CLA	C3-C5-C6-C7
35	C	522	LMG	C36-C37-C38-C39
37	G	618	LHG	C33-C34-C35-C36
37	a	413	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
37	s	320	LHG	C9-C10-C11-C12
29	n	602	CLA	O1A-CGA-O2A-C1
41	w	201	DGA	CB3-CB4-CB5-CB6
29	N	603	CLA	C16-C17-C18-C19
29	G	611	CLA	C16-C17-C18-C20
40	i	102	SPH	C9-C10-C11-C12
29	A	407	CLA	C2B-C3B-CAB-CBB
29	B	503	CLA	C2B-C3B-CAB-CBB
29	B	509	CLA	C2B-C3B-CAB-CBB
29	C	502	CLA	C2B-C3B-CAB-CBB
29	C	511	CLA	C2B-C3B-CAB-CBB
29	C	512	CLA	C2B-C3B-CAB-CBB
29	G	604	CLA	C2B-C3B-CAB-CBB
29	G	610	CLA	C2B-C3B-CAB-CBB
29	a	405	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	504	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
29	g	604	CLA	C2B-C3B-CAB-CBB
29	s	305	CLA	C2B-C3B-CAB-CBB
37	D	408	LHG	O9-C7-O7-C5
37	l	102	LHG	C30-C31-C32-C33
40	I	101	SPH	C10-C11-C12-C13
41	W	202	DGA	CBB-CAB-CB9-CB8
29	C	514	CLA	C16-C17-C18-C20
35	c	519	LMG	C19-C20-C21-C22
29	c	501	CLA	C10-C11-C12-C13
29	r	308	CLA	C8-C10-C11-C12
29	N	611	CLA	C1-C2-C3-C4
29	G	604	CLA	C1-C2-C3-C4
29	G	614	CLA	C1-C2-C3-C4
29	n	610	CLA	C1-C2-C3-C4
29	g	604	CLA	C1-C2-C3-C4
29	g	614	CLA	C1-C2-C3-C4
46	N	608	CHL	C1-C2-C3-C4
46	G	606	CHL	C1-C2-C3-C4
46	R	305	CHL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
46	n	607	CHL	C1-C2-C3-C4
46	g	606	CHL	C1-C2-C3-C4
46	r	306	CHL	C1-C2-C3-C4
37	D	407	LHG	C31-C32-C33-C34
39	l	101	SQD	O47-C7-C8-C9
40	C	525	SPH	C15-C16-C17-C18
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	R	307	CLA	C2A-CAA-CBA-CGA
29	S	306	CLA	C2A-CAA-CBA-CGA
29	S	316	CLA	C2A-CAA-CBA-CGA
46	G	607	CHL	C2A-CAA-CBA-CGA
41	w	201	DGA	CB9-CAB-CBB-CCB
29	S	311	CLA	C2-C1-O2A-CGA
29	b	508	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
46	N	607	CHL	C2-C1-O2A-CGA
46	G	607	CHL	C2-C1-O2A-CGA
46	y	301	CHL	C2-C1-O2A-CGA
46	y	308	CHL	C2-C1-O2A-CGA
41	w	201	DGA	CAA-CBA-CCA-CDA
35	w	202	LMG	C28-C29-C30-C31
37	c	521	LHG	C26-C27-C28-C29
41	w	201	DGA	CA3-CA4-CA5-CA6
39	M	101	SQD	O47-C7-C8-C9
46	S	309	CHL	CAA-CBA-CGA-O2A
29	N	602	CLA	C3-C5-C6-C7
29	Y	313	CLA	C3-C5-C6-C7
36	c	517	DGD	C6B-C7B-C8B-C9B
35	D	410	LMG	C29-C30-C31-C32
37	g	618	LHG	C29-C30-C31-C32
37	G	618	LHG	O6-C4-C5-O7
37	S	301	LHG	C29-C30-C31-C32
46	N	607	CHL	CAA-CBA-CGA-O2A
29	B	503	CLA	C4-C3-C5-C6
46	N	609	CHL	C4-C3-C5-C6
46	S	309	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	A	410	BCR	C5-C6-C7-C8
31	a	409	BCR	C5-C6-C7-C8
31	v	101	BCR	C23-C24-C25-C26
47	S	317	LUT	C1-C6-C7-C8
47	Y	316	LUT	C1-C6-C7-C8
47	n	614	LUT	C5-C6-C7-C8
46	y	309	CHL	C10-C11-C12-C13
29	B	504	CLA	C4C-C3C-CAC-CBC
37	S	320	LHG	C35-C36-C37-C38
33	A	412	3PH	C3F-C3G-C3H-C3I
35	w	202	LMG	C29-C30-C31-C32
39	a	410	SQD	C11-C10-C9-C8
41	b	522	DGA	CAB-CBB-CCB-CDB
29	B	511	CLA	C16-C17-C18-C20
29	S	314	CLA	C6-C7-C8-C9
50	N	620	PTY	C35-C36-C37-C38
29	c	511	CLA	C2A-CAA-CBA-CGA
46	G	605	CHL	C2A-CAA-CBA-CGA
35	W	203	LMG	C2-C1-O1-C7
48	S	319	NEX	C28-C29-C30-C31
50	Y	320	PTY	O4-C1-C6-O7
37	N	618	LHG	C3-O3-P-O6
37	G	618	LHG	C3-O3-P-O6
37	S	320	LHG	C3-O3-P-O6
37	a	413	LHG	C4-O6-P-O3
37	c	521	LHG	C3-O3-P-O6
37	d	406	LHG	C3-O3-P-O6
37	s	301	LHG	C4-O6-P-O3
37	s	320	LHG	C3-O3-P-O6
50	Y	320	PTY	C5-O14-P1-O11
50	n	619	PTY	C5-O14-P1-O11
50	y	321	PTY	C5-O14-P1-O11
51	s	321	LPX	C1-O2-P1-O1
35	b	520	LMG	C19-C20-C21-C22
29	s	310	CLA	C11-C12-C13-C14
30	d	402	PHO	CHA-CBD-CGD-O2D
37	n	617	LHG	C16-C17-C18-C19
39	C	523	SQD	O6-C44-C45-C46
39	C	523	SQD	C44-C45-C46-O48
33	b	521	3PH	C23-C24-C25-C26
41	w	201	DGA	CBB-CCB-CDB-CEB
29	B	507	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	B	503	CLA	C6-C7-C8-C10
29	C	509	CLA	C11-C12-C13-C15
29	G	603	CLA	C6-C7-C8-C10
29	Y	313	CLA	C12-C13-C15-C16
29	a	405	CLA	C11-C12-C13-C15
29	a	408	CLA	C11-C10-C8-C7
29	b	516	CLA	C6-C7-C8-C10
29	c	508	CLA	C11-C12-C13-C15
29	s	312	CLA	C2-C3-C5-C6
43	D	406	PL9	C13-C14-C16-C17
46	N	605	CHL	C2-C3-C5-C6
46	N	606	CHL	C11-C12-C13-C15
46	Y	307	CHL	C2-C3-C5-C6
35	C	524	LMG	C13-C14-C15-C16
37	a	413	LHG	C33-C34-C35-C36
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	G	602	CLA	C14-C13-C15-C16
29	Y	303	CLA	C6-C7-C8-C9
29	b	507	CLA	C14-C13-C15-C16
29	g	613	CLA	C11-C12-C13-C14
29	s	312	CLA	C11-C10-C8-C9
29	y	305	CLA	C14-C13-C15-C16
29	y	316	CLA	C6-C7-C8-C9
46	N	606	CHL	C14-C13-C15-C16
46	G	609	CHL	C11-C12-C13-C14
46	n	606	CHL	C11-C12-C13-C14
46	g	609	CHL	C11-C12-C13-C14
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
37	a	413	LHG	C29-C30-C31-C32
29	c	512	CLA	C10-C11-C12-C13
50	N	620	PTY	C37-C38-C39-C40
29	b	512	CLA	C2A-CAA-CBA-CGA
37	Y	319	LHG	C17-C18-C19-C20
36	B	521	DGD	C1B-C2B-C3B-C4B
35	W	203	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
41	W	202	DGA	CA9-CAA-CBA-CCA
29	S	311	CLA	C8-C10-C11-C12
29	C	506	CLA	C11-C12-C13-C15
29	N	603	CLA	C16-C17-C18-C20
39	C	523	SQD	C24-C23-O48-C46
46	s	309	CHL	CAA-CBA-CGA-O2A
29	c	506	CLA	C5-C6-C7-C8
29	b	511	CLA	CBD-CGD-O2D-CED
37	c	521	LHG	C9-C10-C11-C12
29	N	614	CLA	O2A-C1-C2-C3
29	b	509	CLA	C4-C3-C5-C6
37	d	406	LHG	O1-C1-C2-O2
37	n	617	LHG	O8-C23-C24-C25
29	s	310	CLA	C2-C3-C5-C6
46	Y	308	CHL	C2-C3-C5-C6
29	R	308	CLA	C11-C12-C13-C14
29	C	508	CLA	CBA-CGA-O2A-C1
29	c	512	CLA	CBA-CGA-O2A-C1
29	r	302	CLA	CBA-CGA-O2A-C1
36	c	517	DGD	C2B-C3B-C4B-C5B
37	S	301	LHG	C28-C29-C30-C31
46	s	302	CHL	CAA-CBA-CGA-O1A
37	g	618	LHG	C15-C16-C17-C18
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	W	202	DGA	CCB-CDB-CEB-CFB
39	C	523	SQD	O10-C23-O48-C46
29	a	406	CLA	CBA-CGA-O2A-C1
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	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	g	610	CLA	C4B-C3B-CAB-CBB
29	g	614	CLA	C4B-C3B-CAB-CBB
29	r	302	CLA	C4B-C3B-CAB-CBB
29	y	314	CLA	C4B-C3B-CAB-CBB
29	C	502	CLA	C2A-CAA-CBA-CGA
29	y	304	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
29	y	315	CLA	C2A-CAA-CBA-CGA
29	S	314	CLA	C6-C7-C8-C10
29	N	610	CLA	C5-C6-C7-C8
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
48	R	312	NEX	C13-C14-C15-C35
41	j	101	DGA	CB3-CB4-CB5-CB6
37	n	617	LHG	O6-C4-C5-C6
29	C	508	CLA	O1A-CGA-O2A-C1
29	c	512	CLA	O1A-CGA-O2A-C1
29	Y	313	CLA	C5-C6-C7-C8
29	R	307	CLA	C4C-C3C-CAC-CBC
39	b	523	SQD	C28-C29-C30-C31
29	N	602	CLA	C15-C16-C17-C18
37	s	301	LHG	C24-C25-C26-C27
29	N	610	CLA	C16-C17-C18-C20
29	b	501	CLA	CAA-CBA-CGA-O1A
29	B	505	CLA	C4-C3-C5-C6
29	Y	315	CLA	C4-C3-C5-C6
43	D	406	PL9	C45-C44-C46-C47
35	C	522	LMG	C34-C35-C36-C37
29	b	509	CLA	C2-C3-C5-C6
29	c	512	CLA	C2-C3-C5-C6
29	r	302	CLA	O1A-CGA-O2A-C1
29	a	404	CLA	C2-C1-O2A-CGA
29	n	612	CLA	C2-C1-O2A-CGA
29	r	304	CLA	C2-C1-O2A-CGA
36	c	516	DGD	C2A-C3A-C4A-C5A
40	I	101	SPH	C11-C10-C9-C8
29	B	516	CLA	C5-C6-C7-C8
29	C	502	CLA	C15-C16-C17-C18
29	C	513	CLA	C15-C16-C17-C18
29	C	511	CLA	C16-C17-C18-C20
29	n	602	CLA	C16-C17-C18-C20
29	y	312	CLA	C16-C17-C18-C20
29	B	506	CLA	C2A-CAA-CBA-CGA
29	b	505	CLA	C2A-CAA-CBA-CGA
29	y	312	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
33	A	412	3PH	O21-C2-C3-O31
35	d	408	LMG	O7-C8-C9-O8
35	w	202	LMG	C37-C38-C39-C40
46	y	301	CHL	CAA-CBA-CGA-O2A
35	i	101	LMG	C31-C32-C33-C34
37	D	407	LHG	C2-C3-O3-P
29	r	309	CLA	CBD-CGD-O2D-CED
50	n	619	PTY	C23-C24-C25-C26
29	S	303	CLA	C3A-C2A-CAA-CBA
29	c	512	CLA	C3A-C2A-CAA-CBA
46	Y	306	CHL	C3A-C2A-CAA-CBA
29	b	513	CLA	CBD-CGD-O2D-CED
29	y	314	CLA	CBA-CGA-O2A-C1
29	b	513	CLA	O1D-CGD-O2D-CED
36	c	518	DGD	C4A-C5A-C6A-C7A
37	l	102	LHG	C11-C10-C9-C8
39	a	410	SQD	C29-C30-C31-C32
46	R	304	CHL	C2A-CAA-CBA-CGA
46	n	608	CHL	C4-C3-C5-C6
29	n	603	CLA	C8-C10-C11-C12
37	D	407	LHG	C29-C30-C31-C32
37	G	618	LHG	C26-C27-C28-C29
37	c	521	LHG	C25-C26-C27-C28
41	w	201	DGA	CCA-CDA-CEA-CFA
29	B	503	CLA	C14-C13-C15-C16
29	C	504	CLA	C11-C10-C8-C9
29	a	404	CLA	C11-C12-C13-C14
29	b	504	CLA	C6-C7-C8-C9
29	g	613	CLA	C14-C13-C15-C16
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
46	N	609	CHL	C11-C12-C13-C14
46	n	608	CHL	C11-C10-C8-C9
29	n	604	CLA	C15-C16-C17-C18
29	g	612	CLA	C4C-C3C-CAC-CBC
37	D	408	LHG	C30-C31-C32-C33
37	c	521	LHG	C31-C32-C33-C34
35	W	201	LMG	C7-C8-C9-O8
35	d	408	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
37	L	101	LHG	C4-C5-C6-O8
39	b	523	SQD	O6-C44-C45-C46
47	G	616	LUT	C21-C26-C27-C28
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
48	y	319	NEX	C39-C29-C30-C31
35	C	522	LMG	C15-C16-C17-C18
29	B	504	CLA	O1D-CGD-O2D-CED
29	b	506	CLA	C2A-CAA-CBA-CGA
29	y	310	CLA	C2A-CAA-CBA-CGA
39	a	410	SQD	C15-C16-C17-C18
35	w	202	LMG	O9-C10-C11-C12
29	C	514	CLA	C16-C17-C18-C19
29	G	611	CLA	C16-C17-C18-C19
46	s	309	CHL	C11-C12-C13-C14
29	b	505	CLA	CBA-CGA-O2A-C1
29	C	506	CLA	O1D-CGD-O2D-CED
39	b	523	SQD	C12-C13-C14-C15
41	w	201	DGA	CFA-CGA-CHA-CIA
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	b	502	CLA	C5-C6-C7-C8
29	C	510	CLA	CBD-CGD-O2D-CED
50	n	619	PTY	C17-C18-C19-C20
39	C	523	SQD	C7-C8-C9-C10
40	I	101	SPH	O3-C3-C4-C5
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
46	N	608	CHL	C1A-C2A-CAA-CBA
46	G	601	CHL	C1A-C2A-CAA-CBA
46	G	605	CHL	C1A-C2A-CAA-CBA
46	g	606	CHL	C1A-C2A-CAA-CBA
29	A	406	CLA	C11-C10-C8-C7
29	B	504	CLA	C11-C10-C8-C7
29	B	508	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
29	C	504	CLA	C12-C13-C15-C16
29	C	507	CLA	C11-C10-C8-C7
29	S	312	CLA	C6-C7-C8-C10
29	Y	305	CLA	C11-C12-C13-C15
29	Y	313	CLA	C6-C7-C8-C10
29	b	502	CLA	C11-C10-C8-C7
29	b	502	CLA	C12-C13-C15-C16
29	b	507	CLA	C11-C12-C13-C15
29	c	509	CLA	C11-C10-C8-C7
29	n	612	CLA	C11-C10-C8-C7
29	s	312	CLA	C11-C12-C13-C15
29	y	306	CLA	C12-C13-C15-C16
29	y	312	CLA	C12-C13-C15-C16
43	d	405	PL9	C43-C44-C46-C47
46	Y	307	CHL	C11-C12-C13-C15
46	g	607	CHL	C11-C10-C8-C7
29	a	406	CLA	O1A-CGA-O2A-C1
29	C	506	CLA	C2A-CAA-CBA-CGA
29	N	602	CLA	C2A-CAA-CBA-CGA
36	C	518	DGD	O6D-C5D-C6D-O5D
29	b	501	CLA	C8-C10-C11-C12
37	D	408	LHG	C32-C33-C34-C35
29	D	404	CLA	O1D-CGD-O2D-CED
46	N	608	CHL	O2A-C1-C2-C3
29	B	509	CLA	C15-C16-C17-C18
29	r	307	CLA	C5-C6-C7-C8
29	y	313	CLA	C13-C15-C16-C17
29	b	511	CLA	O1D-CGD-O2D-CED
29	b	504	CLA	C16-C17-C18-C20
29	s	311	CLA	C10-C11-C12-C13
29	n	611	CLA	CAA-CBA-CGA-O2A
29	Y	304	CLA	C4-C3-C5-C6
29	b	513	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
29	C	510	CLA	C13-C15-C16-C17
29	R	308	CLA	C2B-C3B-CAB-CBB
29	Y	311	CLA	C2B-C3B-CAB-CBB
29	c	501	CLA	C2B-C3B-CAB-CBB
29	y	315	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	b	511	CLA	C4C-C3C-CAC-CBC
46	y	307	CHL	CAA-CBA-CGA-O2A
29	y	314	CLA	O1A-CGA-O2A-C1
37	D	407	LHG	O10-C23-O8-C6
29	A	406	CLA	C4C-C3C-CAC-CBC
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
46	S	302	CHL	CAA-CBA-CGA-O1A
46	S	302	CHL	CAA-CBA-CGA-O2A
46	s	302	CHL	CAA-CBA-CGA-O2A
41	J	101	DGA	OG1-CG1-CG2-OG2
37	s	301	LHG	C26-C27-C28-C29
35	W	201	LMG	C11-C12-C13-C14
31	C	515	BCR	C15-C16-C17-C18
31	C	515	BCR	C19-C20-C21-C22
31	K	101	BCR	C9-C10-C11-C12
31	v	101	BCR	C9-C10-C11-C12
36	c	517	DGD	C3A-C4A-C5A-C6A
33	b	521	3PH	C21-C22-C23-C24
37	S	301	LHG	C24-C25-C26-C27
37	n	617	LHG	C18-C19-C20-C21
37	s	301	LHG	C30-C31-C32-C33
39	b	523	SQD	C11-C10-C9-C8
39	c	522	SQD	O5-C1-O6-C44
29	c	512	CLA	C15-C16-C17-C18
29	b	505	CLA	O1A-CGA-O2A-C1
41	D	402	DGA	CG1-CG2-CG3-OXT
41	W	202	DGA	CG1-CG2-CG3-OXT
29	C	510	CLA	O1D-CGD-O2D-CED
29	S	303	CLA	C4-C3-C5-C6
41	b	522	DGA	CBA-CCA-CDA-CEA
29	B	508	CLA	C2-C1-O2A-CGA
29	C	513	CLA	C2-C1-O2A-CGA
29	r	310	CLA	C2-C1-O2A-CGA
29	s	315	CLA	C2-C1-O2A-CGA
46	N	609	CHL	C2-C3-C5-C6
29	B	511	CLA	CBD-CGD-O2D-CED
39	b	523	SQD	C11-C12-C13-C14
41	b	522	DGA	CB7-CB8-CB9-CAB
29	S	312	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	s	310	CLA	C11-C12-C13-C15
29	A	406	CLA	C6-C7-C8-C9
29	B	501	CLA	C11-C12-C13-C14
29	C	508	CLA	C6-C7-C8-C9
29	n	611	CLA	CAA-CBA-CGA-O1A
46	N	607	CHL	C13-C15-C16-C17
29	r	310	CLA	C4-C3-C5-C6
35	D	410	LMG	C34-C35-C36-C37
37	d	406	LHG	C31-C32-C33-C34
29	B	503	CLA	C13-C15-C16-C17
29	b	504	CLA	C13-C15-C16-C17
29	y	315	CLA	C5-C6-C7-C8
29	a	406	CLA	C2A-CAA-CBA-CGA
29	c	503	CLA	C2A-CAA-CBA-CGA
29	s	306	CLA	C2A-CAA-CBA-CGA
29	g	614	CLA	O2A-C1-C2-C3
29	s	314	CLA	C4C-C3C-CAC-CBC
33	a	415	3PH	C2B-C2C-C2D-C2E
36	C	520	DGD	C9A-CAA-CBA-CCA
41	j	101	DGA	OA1-CA1-OG1-CG1
31	A	410	BCR	C1-C6-C7-C8
31	B	517	BCR	C23-C24-C25-C30
31	a	409	BCR	C1-C6-C7-C8
31	b	517	BCR	C23-C24-C25-C30
31	b	518	BCR	C23-C24-C25-C30
31	v	101	BCR	C23-C24-C25-C30
31	c	515	BCR	C1-C6-C7-C8
31	c	515	BCR	C23-C24-C25-C26
31	c	515	BCR	C23-C24-C25-C30
47	N	616	LUT	C1-C6-C7-C8
47	R	310	LUT	C1-C6-C7-C8
47	S	318	LUT	C1-C6-C7-C8
47	n	614	LUT	C1-C6-C7-C8
47	g	615	LUT	C1-C6-C7-C8
47	s	317	LUT	C1-C6-C7-C8
47	y	317	LUT	C1-C6-C7-C8
47	y	317	LUT	C5-C6-C7-C8
33	s	322	3PH	C33-C34-C35-C36
35	W	201	LMG	O7-C10-C11-C12
37	g	618	LHG	O8-C23-C24-C25
39	L	102	SQD	O6-C44-C45-C46
46	y	307	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
29	Y	314	CLA	C13-C15-C16-C17
29	b	503	CLA	C13-C15-C16-C17
37	d	406	LHG	C12-C13-C14-C15
37	g	618	LHG	C30-C31-C32-C33
31	C	516	BCR	C13-C14-C15-C16
47	g	615	LUT	C29-C30-C31-C32
29	b	514	CLA	C4-C3-C5-C6
29	c	511	CLA	C4-C3-C5-C6
31	a	409	BCR	C21-C22-C23-C24
35	C	522	LMG	C11-C12-C13-C14
29	C	511	CLA	C2-C3-C5-C6
30	A	408	PHO	C2-C3-C5-C6
46	S	309	CHL	C2-C3-C5-C6
29	r	308	CLA	C4C-C3C-CAC-CBC
39	b	523	SQD	C9-C10-C11-C12
41	D	402	DGA	CA9-CAA-CBA-CCA
36	B	521	DGD	C2G-C3G-O3G-C1D
29	Y	304	CLA	C2C-C3C-CAC-CBC
39	o	301	SQD	C10-C11-C12-C13
50	n	619	PTY	C11-C12-C13-C14
46	S	309	CHL	C11-C12-C13-C15
29	R	301	CLA	C10-C11-C12-C13
29	n	602	CLA	C13-C15-C16-C17
29	B	511	CLA	O1D-CGD-O2D-CED
35	D	410	LMG	O9-C10-C11-C12
29	n	604	CLA	C2A-CAA-CBA-CGA
29	n	610	CLA	C2A-CAA-CBA-CGA
29	c	502	CLA	C13-C15-C16-C17
36	C	519	DGD	C3B-C4B-C5B-C6B
39	L	102	SQD	O47-C7-C8-C9
41	j	101	DGA	CA2-CA1-OG1-CG1
41	W	202	DGA	CAA-CBA-CCA-CDA
50	N	620	PTY	C22-C23-C24-C25
46	G	609	CHL	C3-C5-C6-C7
29	A	409	CLA	C4B-C3B-CAB-CBB
29	C	512	CLA	C4B-C3B-CAB-CBB
29	G	602	CLA	C4B-C3B-CAB-CBB
29	R	301	CLA	C4B-C3B-CAB-CBB
29	b	503	CLA	C4B-C3B-CAB-CBB
29	b	514	CLA	C4B-C3B-CAB-CBB
29	g	604	CLA	C4B-C3B-CAB-CBB
29	s	314	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	s	315	CLA	C4B-C3B-CAB-CBB
29	R	302	CLA	C11-C12-C13-C15
29	B	502	CLA	C4-C3-C5-C6
35	c	519	LMG	C21-C22-C23-C24
39	L	102	SQD	C24-C25-C26-C27
29	B	513	CLA	C11-C10-C8-C7
29	C	506	CLA	C2-C3-C5-C6
29	C	508	CLA	C6-C7-C8-C10
29	Y	304	CLA	C2-C3-C5-C6
29	Y	305	CLA	C12-C13-C15-C16
29	c	511	CLA	C2-C3-C5-C6
29	g	613	CLA	C12-C13-C15-C16
46	n	608	CHL	C2-C3-C5-C6
29	c	501	CLA	C15-C16-C17-C18
37	G	618	LHG	C34-C35-C36-C37
41	j	101	DGA	CA7-CA8-CA9-CAA
37	c	521	LHG	O1-C1-C2-O2
33	A	412	3PH	C33-C34-C35-C36
37	l	102	LHG	C11-C12-C13-C14
47	N	615	LUT	C29-C30-C31-C32
29	S	306	CLA	CBD-CGD-O2D-CED
29	C	513	CLA	C16-C17-C18-C20
37	s	320	LHG	C2-C3-O3-P
36	B	521	DGD	O2G-C2G-C3G-O3G
29	S	304	CLA	C13-C15-C16-C17
46	N	607	CHL	C15-C16-C17-C18
29	S	313	CLA	CAA-CBA-CGA-O2A
46	G	606	CHL	O2A-C1-C2-C3
46	n	607	CHL	O2A-C1-C2-C3
29	a	405	CLA	CAA-CBA-CGA-O2A
29	b	513	CLA	CAA-CBA-CGA-O2A
29	g	614	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	b	522	DGA	CA2-CA3-CA4-CA5
46	G	606	CHL	C2A-CAA-CBA-CGA
29	S	303	CLA	C11-C12-C13-C14
41	j	101	DGA	OG1-CA1-CA2-CA3
46	n	605	CHL	CAA-CBA-CGA-O2A
36	C	519	DGD	C2B-C3B-C4B-C5B
29	B	513	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
46	G	601	CHL	C4-C3-C5-C6
29	r	308	CLA	C5-C6-C7-C8
43	D	406	PL9	C43-C44-C46-C47
43	d	405	PL9	C38-C39-C41-C42
46	y	311	CHL	C2-C3-C5-C6
29	N	610	CLA	C16-C17-C18-C19
29	B	507	CLA	CAA-CBA-CGA-O2A
35	c	519	LMG	C14-C15-C16-C17
41	w	201	DGA	CFB-CGB-CHB-CIB
29	B	506	CLA	C14-C13-C15-C16
29	B	508	CLA	C6-C7-C8-C9
29	N	602	CLA	C6-C7-C8-C9
29	N	602	CLA	C14-C13-C15-C16
29	R	302	CLA	C6-C7-C8-C9
29	Y	312	CLA	C6-C7-C8-C9
29	b	501	CLA	C14-C13-C15-C16
29	b	503	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	C11-C12-C13-C14
29	g	611	CLA	C14-C13-C15-C16
29	y	312	CLA	C14-C13-C15-C16
46	N	605	CHL	C11-C10-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
46	y	309	CHL	C11-C12-C13-C14
37	c	521	LHG	C16-C17-C18-C19
37	D	407	LHG	C28-C29-C30-C31
37	G	618	LHG	C11-C10-C9-C8
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	513	CLA	CAA-CBA-CGA-O2A
37	G	618	LHG	O7-C7-C8-C9
37	n	617	LHG	O7-C7-C8-C9
29	B	509	CLA	CAD-CBD-CGD-O2D
29	B	512	CLA	CAD-CBD-CGD-O2D
29	B	516	CLA	CAD-CBD-CGD-O2D
29	C	504	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	G	612	CLA	CAD-CBD-CGD-O2D
29	G	614	CLA	CAD-CBD-CGD-O2D
29	R	301	CLA	CAD-CBD-CGD-O2D
29	S	312	CLA	CAD-CBD-CGD-O2D
29	S	313	CLA	CAD-CBD-CGD-O2D
29	S	316	CLA	CAD-CBD-CGD-O2D
29	Y	305	CLA	CAD-CBD-CGD-O2D
29	b	505	CLA	CAD-CBD-CGD-O2D
29	b	508	CLA	CAD-CBD-CGD-O2D
29	b	512	CLA	CAD-CBD-CGD-O2D
29	b	516	CLA	CAD-CBD-CGD-O2D
29	c	505	CLA	CAD-CBD-CGD-O2D
29	c	512	CLA	CAD-CBD-CGD-O2D
29	n	603	CLA	CAD-CBD-CGD-O2D
29	g	603	CLA	CAD-CBD-CGD-O2D
29	s	306	CLA	CAD-CBD-CGD-O2D
29	s	314	CLA	CAD-CBD-CGD-O2D
29	y	306	CLA	CAD-CBD-CGD-O2D
30	A	408	PHO	CAD-CBD-CGD-O2D
29	B	511	CLA	C16-C17-C18-C19
29	S	312	CLA	C16-C17-C18-C20
29	y	312	CLA	C16-C17-C18-C19
37	L	101	LHG	C29-C30-C31-C32
37	d	406	LHG	C35-C36-C37-C38
40	C	525	SPH	C12-C13-C14-C15
37	D	408	LHG	C25-C26-C27-C28
37	d	406	LHG	C30-C31-C32-C33
30	d	402	PHO	C2-C1-O2A-CGA
35	D	409	LMG	C10-C11-C12-C13
29	R	307	CLA	CAA-CBA-CGA-O2A
29	R	309	CLA	CAA-CBA-CGA-O2A
29	S	312	CLA	CAA-CBA-CGA-O2A
29	b	506	CLA	CAA-CBA-CGA-O2A
29	s	304	CLA	CAA-CBA-CGA-O2A
39	c	522	SQD	O47-C7-C8-C9
46	N	605	CHL	CAA-CBA-CGA-O2A
35	d	408	LMG	C31-C32-C33-C34
29	C	511	CLA	C4-C3-C5-C6
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	S	304	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
29	y	314	CLA	CAA-CBA-CGA-O2A
33	a	415	3PH	O31-C31-C32-C33
35	C	521	LMG	O7-C10-C11-C12
39	a	410	SQD	O48-C23-C24-C25
41	D	402	DGA	OG2-CB1-CB2-CB3
35	i	101	LMG	C18-C19-C20-C21
41	w	201	DGA	CB5-CB6-CB7-CB8
34	B	519	C7Z	C27-C28-C29-C30
47	R	310	LUT	C27-C28-C29-C30
35	b	520	LMG	C22-C23-C24-C25
35	w	202	LMG	C7-C8-C9-O8
49	g	619	XAT	O24-C26-C27-C28
29	B	511	CLA	C10-C11-C12-C13
29	N	613	CLA	CAA-CBA-CGA-O2A
29	R	303	CLA	CAA-CBA-CGA-O2A
29	c	507	CLA	CAA-CBA-CGA-O2A
36	c	516	DGD	O2G-C1B-C2B-C3B
29	B	507	CLA	C16-C17-C18-C20
37	S	320	LHG	C12-C13-C14-C15
39	l	101	SQD	C23-C24-C25-C26
37	N	618	LHG	C19-C20-C21-C22
29	N	603	CLA	O2A-C1-C2-C3
29	r	308	CLA	O2A-C1-C2-C3
29	s	315	CLA	O2A-C1-C2-C3
29	y	310	CLA	O2A-C1-C2-C3
46	n	605	CHL	O2A-C1-C2-C3
46	y	309	CHL	O2A-C1-C2-C3
50	n	619	PTY	C38-C39-C40-C41
29	B	515	CLA	CBA-CGA-O2A-C1
29	S	312	CLA	C2A-CAA-CBA-CGA
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	B	506	CLA	C13-C15-C16-C17
29	B	514	CLA	CAA-CBA-CGA-O2A
37	N	618	LHG	O7-C7-C8-C9
41	b	522	DGA	OG2-CB1-CB2-CB3
37	D	408	LHG	C24-C25-C26-C27
40	i	102	SPH	C4-C5-C6-C7
29	B	507	CLA	C16-C17-C18-C19
29	b	504	CLA	C16-C17-C18-C19
29	n	602	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	S	306	CLA	O1D-CGD-O2D-CED
36	c	518	DGD	C2A-C3A-C4A-C5A
29	B	501	CLA	CHA-CBD-CGD-O1D
29	B	501	CLA	CHA-CBD-CGD-O2D
29	C	505	CLA	CHA-CBD-CGD-O2D
29	C	508	CLA	CHA-CBD-CGD-O2D
29	N	612	CLA	CHA-CBD-CGD-O1D
29	N	612	CLA	CHA-CBD-CGD-O2D
29	Y	303	CLA	CHA-CBD-CGD-O1D
29	Y	314	CLA	CHA-CBD-CGD-O1D
29	Y	314	CLA	CHA-CBD-CGD-O2D
29	b	510	CLA	CHA-CBD-CGD-O2D
29	b	515	CLA	CHA-CBD-CGD-O1D
29	b	515	CLA	CHA-CBD-CGD-O2D
29	c	504	CLA	CHA-CBD-CGD-O1D
29	c	506	CLA	CHA-CBD-CGD-O1D
29	c	507	CLA	CHA-CBD-CGD-O2D
29	c	511	CLA	CHA-CBD-CGD-O1D
29	c	511	CLA	CHA-CBD-CGD-O2D
29	n	602	CLA	CHA-CBD-CGD-O1D
29	n	611	CLA	CHA-CBD-CGD-O1D
29	n	611	CLA	CHA-CBD-CGD-O2D
29	n	612	CLA	CHA-CBD-CGD-O1D
29	n	612	CLA	CHA-CBD-CGD-O2D
29	g	604	CLA	CHA-CBD-CGD-O1D
29	r	307	CLA	CHA-CBD-CGD-O2D
29	s	305	CLA	CHA-CBD-CGD-O1D
29	s	313	CLA	CHA-CBD-CGD-O1D
29	s	313	CLA	CHA-CBD-CGD-O2D
29	y	304	CLA	CHA-CBD-CGD-O2D
31	C	515	BCR	C13-C14-C15-C16
31	b	518	BCR	C9-C10-C11-C12
46	R	305	CHL	CHA-CBD-CGD-O1D
46	R	305	CHL	CHA-CBD-CGD-O2D
46	n	601	CHL	CHA-CBD-CGD-O1D
46	r	306	CHL	CHA-CBD-CGD-O1D
46	r	306	CHL	CHA-CBD-CGD-O2D
46	s	302	CHL	CHA-CBD-CGD-O2D
49	n	618	XAT	C29-C30-C31-C32
46	Y	308	CHL	C10-C11-C12-C13
30	A	408	PHO	C4-C3-C5-C6
37	d	406	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
43	D	406	PL9	C38-C39-C41-C42
39	M	101	SQD	C11-C12-C13-C14
29	A	405	CLA	CAA-CBA-CGA-O2A
29	B	516	CLA	CAA-CBA-CGA-O2A
29	G	603	CLA	CAA-CBA-CGA-O2A
29	S	315	CLA	CAA-CBA-CGA-O2A
29	b	512	CLA	CAA-CBA-CGA-O2A
29	r	304	CLA	CAA-CBA-CGA-O2A
41	D	402	DGA	OG1-CA1-CA2-CA3
46	G	605	CHL	CAA-CBA-CGA-O2A
35	d	407	LMG	C15-C16-C17-C18
29	c	512	CLA	CAA-CBA-CGA-O2A
35	c	519	LMG	O8-C28-C29-C30
36	B	521	DGD	O1G-C1A-C2A-C3A
37	Y	319	LHG	O8-C23-C24-C25
46	n	606	CHL	CAA-CBA-CGA-O2A
29	r	309	CLA	O1D-CGD-O2D-CED
29	C	511	CLA	C16-C17-C18-C19
30	D	401	PHO	CHA-CBD-CGD-O2D
30	a	407	PHO	CHA-CBD-CGD-O2D
30	d	402	PHO	CHA-CBD-CGD-O1D
40	I	101	SPH	N2-C2-C3-O3
35	c	519	LMG	O9-C10-C11-C12
35	C	524	LMG	O8-C28-C29-C30
35	i	101	LMG	O7-C10-C11-C12
37	L	101	LHG	C31-C32-C33-C34
36	c	517	DGD	C1A-C2A-C3A-C4A
37	n	617	LHG	C19-C20-C21-C22
29	B	503	CLA	C2-C3-C5-C6
29	S	312	CLA	C11-C10-C8-C7
29	Y	311	CLA	C12-C13-C15-C16
29	b	514	CLA	C11-C12-C13-C15
29	c	505	CLA	C11-C10-C8-C7
29	g	613	CLA	C6-C7-C8-C10
29	C	504	CLA	C10-C11-C12-C13
29	C	511	CLA	CAA-CBA-CGA-O2A
37	c	521	LHG	O7-C7-C8-C9
50	n	619	PTY	O4-C30-C31-C32
29	S	313	CLA	CAA-CBA-CGA-O1A
29	A	406	CLA	C11-C10-C8-C9
29	A	409	CLA	C11-C10-C8-C9
29	C	503	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	C	507	CLA	C11-C10-C8-C9
29	C	510	CLA	C11-C10-C8-C9
29	Y	304	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
29	n	612	CLA	C11-C10-C8-C9
29	g	613	CLA	C6-C7-C8-C9
29	s	312	CLA	C11-C12-C13-C14
46	G	607	CHL	C11-C12-C13-C14
46	y	301	CHL	C11-C12-C13-C14
31	z	101	BCR	C15-C16-C17-C18
29	Y	313	CLA	C2B-C3B-CAB-CBB
29	b	513	CLA	C2B-C3B-CAB-CBB
29	c	502	CLA	C2B-C3B-CAB-CBB
29	c	509	CLA	C2B-C3B-CAB-CBB
46	N	608	CHL	C2B-C3B-CAB-CBB
46	G	607	CHL	C2B-C3B-CAB-CBB
46	Y	302	CHL	C2B-C3B-CAB-CBB
46	Y	308	CHL	C2B-C3B-CAB-CBB
46	n	607	CHL	C2B-C3B-CAB-CBB
46	g	607	CHL	C2B-C3B-CAB-CBB
46	y	301	CHL	C2B-C3B-CAB-CBB
46	y	308	CHL	C2B-C3B-CAB-CBB
37	N	618	LHG	C18-C19-C20-C21
49	N	619	XAT	C14-C15-C35-C34
46	Y	306	CHL	CAA-CBA-CGA-O2A
50	n	619	PTY	C13-C14-C15-C16
29	Y	303	CLA	CBA-CGA-O2A-C1
29	A	406	CLA	CAA-CBA-CGA-O2A
35	b	520	LMG	O7-C10-C11-C12
37	L	101	LHG	O7-C7-C8-C9
39	m	101	SQD	O47-C7-C8-C9
39	C	523	SQD	C4-C5-C6-S
39	b	523	SQD	C4-C5-C6-S
39	c	522	SQD	C4-C5-C6-S
29	B	515	CLA	O1A-CGA-O2A-C1
29	c	506	CLA	C10-C11-C12-C13
35	C	522	LMG	O9-C10-C11-C12
39	a	410	SQD	O10-C23-C24-C25
35	C	524	LMG	C11-C12-C13-C14
29	c	510	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
33	s	322	3PH	O21-C21-C22-C23
35	W	203	LMG	O8-C28-C29-C30
39	o	301	SQD	C19-C20-C21-C22
41	D	402	DGA	CA2-CA3-CA4-CA5
50	N	620	PTY	O30-C30-C31-C32
51	s	321	LPX	O7-C6-C7-C8
29	R	303	CLA	CAA-CBA-CGA-O1A
29	R	309	CLA	CAA-CBA-CGA-O1A
29	c	510	CLA	CAA-CBA-CGA-O1A
29	y	314	CLA	CAA-CBA-CGA-O1A
33	s	322	3PH	O22-C21-C22-C23
37	n	617	LHG	O9-C7-C8-C9
46	n	605	CHL	CAA-CBA-CGA-O1A
31	C	517	BCR	C7-C8-C9-C10
31	K	101	BCR	C17-C18-C19-C20
34	b	519	C7Z	C27-C28-C29-C30
37	g	618	LHG	C33-C34-C35-C36
29	s	304	CLA	C8-C10-C11-C12
29	A	406	CLA	C2C-C3C-CAC-CBC
29	g	612	CLA	C1A-C2A-CAA-CBA
29	y	313	CLA	C1A-C2A-CAA-CBA
46	y	301	CHL	C1A-C2A-CAA-CBA
46	y	307	CHL	C1A-C2A-CAA-CBA
29	B	507	CLA	CAA-CBA-CGA-O1A
29	a	405	CLA	CAA-CBA-CGA-O1A
29	g	614	CLA	CAA-CBA-CGA-O1A
29	r	303	CLA	C2-C1-O2A-CGA
35	W	203	LMG	C32-C33-C34-C35
39	b	523	SQD	C24-C23-O48-C46
29	b	506	CLA	CAA-CBA-CGA-O1A
33	a	415	3PH	O32-C31-C32-C33
36	c	516	DGD	O1B-C1B-C2B-C3B
37	N	618	LHG	O9-C7-C8-C9
37	G	618	LHG	O9-C7-C8-C9
37	a	413	LHG	C30-C31-C32-C33
41	j	101	DGA	CB7-CB8-CB9-CAB
29	C	513	CLA	CAA-CBA-CGA-O2A
41	b	522	DGA	OG1-CA1-CA2-CA3
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

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Mol	Chain	Res	Type	Atoms
29	S	304	CLA	C16-C17-C18-C19
29	b	515	CLA	C16-C17-C18-C20
29	A	406	CLA	CAA-CBA-CGA-O1A
36	C	518	DGD	CCB-CDB-CEB-CFB
39	b	523	SQD	O10-C23-O48-C46
39	m	101	SQD	C11-C10-C9-C8
29	C	506	CLA	C4-C3-C5-C6
41	J	101	DGA	OG1-CA1-CA2-CA3
29	b	511	CLA	C8-C10-C11-C12
29	g	610	CLA	C8-C10-C11-C12
46	N	601	CHL	C8-C10-C11-C12
37	S	301	LHG	C2-C3-O3-P
37	Y	319	LHG	C32-C33-C34-C35
29	B	513	CLA	CAA-CBA-CGA-O1A
41	D	402	DGA	OA1-CA1-CA2-CA3
46	G	605	CHL	CAA-CBA-CGA-O1A
29	B	506	CLA	C8-C10-C11-C12
41	j	101	DGA	CB4-CB5-CB6-CB7
37	S	320	LHG	C3-O3-P-O5
37	a	413	LHG	C4-O6-P-O4
50	n	619	PTY	C5-O14-P1-O13
51	S	321	LPX	C1-O2-P1-O4
29	Y	312	CLA	C16-C17-C18-C19
37	a	414	LHG	C29-C30-C31-C32
29	B	514	CLA	CAA-CBA-CGA-O1A
29	S	304	CLA	CAA-CBA-CGA-O1A
29	b	512	CLA	CAA-CBA-CGA-O1A
29	b	513	CLA	CAA-CBA-CGA-O1A
41	j	101	DGA	OA1-CA1-CA2-CA3
50	n	619	PTY	O30-C30-C31-C32
29	R	303	CLA	O2A-C1-C2-C3
29	r	304	CLA	O2A-C1-C2-C3
29	n	612	CLA	CAA-CBA-CGA-O2A
35	i	101	LMG	C13-C14-C15-C16
35	w	202	LMG	C30-C31-C32-C33
31	B	517	BCR	C23-C24-C25-C26
31	b	518	BCR	C23-C24-C25-C26
47	s	317	LUT	C5-C6-C7-C8
29	N	613	CLA	CAA-CBA-CGA-O1A
29	s	304	CLA	CAA-CBA-CGA-O1A
35	W	203	LMG	O10-C28-C29-C30
39	c	522	SQD	O49-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
41	b	522	DGA	OB1-CB1-CB2-CB3
35	D	410	LMG	C37-C38-C39-C40
29	C	502	CLA	CAA-CBA-CGA-O2A
39	o	301	SQD	C11-C12-C13-C14
29	G	602	CLA	C2A-CAA-CBA-CGA
29	R	301	CLA	C2A-CAA-CBA-CGA
29	S	312	CLA	CAA-CBA-CGA-O1A
29	Y	303	CLA	O1A-CGA-O2A-C1
33	B	522	3PH	C2E-C2F-C2G-C2H
29	B	506	CLA	CAA-CBA-CGA-O2A
46	y	303	CHL	C13-C15-C16-C17
33	b	521	3PH	C2C-C2D-C2E-C2F
40	i	102	SPH	C15-C16-C17-C18
29	r	304	CLA	CAA-CBA-CGA-O1A
41	D	402	DGA	OB1-CB1-CB2-CB3
29	S	305	CLA	O1D-CGD-O2D-CED
29	Y	315	CLA	C2-C3-C5-C6
29	B	501	CLA	C5-C6-C7-C8
29	C	507	CLA	CAD-CBD-CGD-O1D
29	C	512	CLA	CAD-CBD-CGD-O1D
29	G	604	CLA	CAD-CBD-CGD-O1D
29	S	305	CLA	CAD-CBD-CGD-O1D
29	b	506	CLA	C3-C5-C6-C7
29	b	507	CLA	CAD-CBD-CGD-O1D
29	b	515	CLA	CAD-CBD-CGD-O1D
29	c	503	CLA	CAD-CBD-CGD-O1D
29	c	504	CLA	CAD-CBD-CGD-O1D
29	c	506	CLA	CAD-CBD-CGD-O1D
29	g	604	CLA	CAD-CBD-CGD-O1D
29	g	614	CLA	CAD-CBD-CGD-O1D
33	b	521	3PH	C3-C2-O21-C21
39	C	523	SQD	O5-C5-C6-S
39	b	523	SQD	O5-C5-C6-S
39	m	101	SQD	O5-C5-C6-S
46	N	601	CHL	CAD-CBD-CGD-O1D
46	R	305	CHL	CAD-CBD-CGD-O1D
46	n	601	CHL	CAD-CBD-CGD-O1D
50	N	620	PTY	C2-C3-O11-P1
29	B	516	CLA	CAA-CBA-CGA-O1A
29	C	511	CLA	CAA-CBA-CGA-O1A
29	c	507	CLA	CAA-CBA-CGA-O1A
36	B	521	DGD	O1A-C1A-C2A-C3A

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Mol	Chain	Res	Type	Atoms
36	c	516	DGD	C4A-C5A-C6A-C7A
39	c	522	SQD	C27-C28-C29-C30
29	a	405	CLA	C15-C16-C17-C18
29	B	502	CLA	C11-C12-C13-C14
29	C	514	CLA	C6-C7-C8-C9
29	Y	315	CLA	C11-C10-C8-C9
29	b	505	CLA	C11-C12-C13-C14
29	b	508	CLA	C11-C12-C13-C14
29	b	512	CLA	C11-C10-C8-C9
29	c	505	CLA	C11-C12-C13-C14
29	c	509	CLA	C11-C10-C8-C9
46	Y	308	CHL	C11-C12-C13-C14
46	s	309	CHL	C6-C7-C8-C9
37	n	617	LHG	O1-C1-C2-O2
37	s	301	LHG	O1-C1-C2-O2
29	c	512	CLA	CAA-CBA-CGA-O1A
46	n	606	CHL	CAA-CBA-CGA-O1A
29	a	404	CLA	CAA-CBA-CGA-O2A
35	B	520	LMG	O7-C10-C11-C12
41	W	202	DGA	OG1-CA1-CA2-CA3
29	B	506	CLA	C10-C11-C12-C13
46	Y	306	CHL	CAA-CBA-CGA-O1A
38	b	524	LMT	C2-C3-C4-C5
29	G	603	CLA	CAA-CBA-CGA-O1A
29	S	315	CLA	CAA-CBA-CGA-O1A
29	B	514	CLA	C5-C6-C7-C8
37	B	523	LHG	C27-C28-C29-C30
29	B	512	CLA	CAA-CBA-CGA-O2A
29	G	614	CLA	CAA-CBA-CGA-O2A
29	c	501	CLA	CAA-CBA-CGA-O2A
33	b	521	3PH	O21-C21-C22-C23
36	C	518	DGD	O2G-C1B-C2B-C3B
37	y	320	LHG	O8-C23-C24-C25
41	J	101	DGA	OG2-CB1-CB2-CB3
41	b	522	DGA	OA1-CA1-OG1-CG1
29	c	509	CLA	C13-C15-C16-C17
35	c	519	LMG	O10-C28-C29-C30
37	L	101	LHG	O9-C7-C8-C9
37	Y	319	LHG	O10-C23-C24-C25
33	B	522	3PH	C2-C1-O11-P
29	g	613	CLA	C4-C3-C5-C6
46	g	601	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	B	509	CLA	C8-C10-C11-C12
29	B	501	CLA	C3A-C2A-CAA-CBA
29	B	505	CLA	C2-C3-C5-C6
29	B	506	CLA	C11-C12-C13-C15
29	B	507	CLA	C6-C7-C8-C10
29	Y	312	CLA	C11-C10-C8-C7
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	b	513	CLA	C2-C3-C5-C6
29	c	505	CLA	C11-C12-C13-C15
29	c	508	CLA	C6-C7-C8-C10
29	s	311	CLA	C11-C10-C8-C7
29	y	310	CLA	C3A-C2A-CAA-CBA
29	y	314	CLA	C6-C7-C8-C10
46	G	607	CHL	C3A-C2A-CAA-CBA
29	A	405	CLA	CAA-CBA-CGA-O1A
33	b	521	3PH	O22-C21-C22-C23
35	i	101	LMG	O9-C10-C11-C12
41	J	101	DGA	OA1-CA1-CA2-CA3
41	b	522	DGA	OA1-CA1-CA2-CA3
29	b	514	CLA	CAA-CBA-CGA-O2A
29	g	603	CLA	CAA-CBA-CGA-O2A
39	a	410	SQD	O47-C7-C8-C9
31	b	518	BCR	C11-C12-C13-C14
34	B	519	C7Z	C11-C12-C13-C14
47	n	614	LUT	C27-C28-C29-C30
47	r	311	LUT	C11-C12-C13-C14
48	Y	318	NEX	C11-C12-C13-C14
48	y	319	NEX	C11-C12-C13-C14
29	g	603	CLA	CAA-CBA-CGA-O1A
48	G	617	NEX	C9-C10-C11-C12
48	G	617	NEX	C13-C14-C15-C35
29	S	314	CLA	C2C-C3C-CAC-CBC
35	C	521	LMG	C12-C13-C14-C15
37	n	617	LHG	C27-C28-C29-C30
29	n	613	CLA	CAA-CBA-CGA-O2A
39	C	501	SQD	O47-C7-C8-C9
46	G	607	CHL	CAA-CBA-CGA-O2A
29	y	305	CLA	C5-C6-C7-C8
29	y	316	CLA	C5-C6-C7-C8
46	y	301	CHL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
35	B	520	LMG	O9-C10-C11-C12
35	b	520	LMG	O9-C10-C11-C12
37	c	521	LHG	O9-C7-C8-C9
41	W	202	DGA	OA1-CA1-CA2-CA3
29	Y	303	CLA	C10-C11-C12-C13
41	J	101	DGA	CA5-CA6-CA7-CA8
29	g	613	CLA	CAA-CBA-CGA-O2A
29	s	315	CLA	CAA-CBA-CGA-O2A
46	g	606	CHL	CAA-CBA-CGA-O2A
29	Y	303	CLA	C5-C6-C7-C8
29	C	513	CLA	CAA-CBA-CGA-O1A
29	b	514	CLA	CAA-CBA-CGA-O1A
29	C	504	CLA	C2A-CAA-CBA-CGA
29	g	614	CLA	C2A-CAA-CBA-CGA
29	S	303	CLA	C11-C12-C13-C15
29	N	602	CLA	C13-C15-C16-C17
46	N	605	CHL	C15-C16-C17-C18
39	M	101	SQD	C12-C13-C14-C15
39	m	101	SQD	C26-C27-C28-C29
33	b	521	3PH	C31-C32-C33-C34
35	C	524	LMG	O10-C28-C29-C30
33	b	521	3PH	C29-C2A-C2B-C2C
29	s	314	CLA	CAA-CBA-CGA-O2A

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	Y	304	CLA	3	0
37	S	320	LHG	3	0
46	S	308	CHL	3	0
46	Y	310	CHL	4	0
39	b	523	SQD	4	0
31	c	515	BCR	3	0
29	g	613	CLA	1	0
47	G	616	LUT	4	0
29	y	314	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	W	201	LMG	1	0
49	Y	301	XAT	3	0
49	R	311	XAT	1	0
29	s	304	CLA	5	0
35	c	520	LMG	9	0
43	D	406	PL9	2	0
29	C	514	CLA	6	0
36	C	520	DGD	3	0
29	N	610	CLA	3	0
29	c	510	CLA	3	0
29	B	516	CLA	4	0
49	G	619	XAT	3	0
36	c	516	DGD	5	0
46	y	307	CHL	1	0
29	A	406	CLA	6	0
46	g	608	CHL	2	0
46	r	305	CHL	3	0
46	N	609	CHL	5	0
29	c	503	CLA	1	0
37	n	617	LHG	5	0
41	W	202	DGA	4	0
46	n	605	CHL	4	0
29	B	505	CLA	4	0
46	G	605	CHL	1	0
29	b	501	CLA	2	0
46	R	305	CHL	1	0
46	g	605	CHL	1	0
46	y	311	CHL	5	0
29	B	513	CLA	3	0
46	g	607	CHL	3	0
48	n	616	NEX	1	0
29	c	501	CLA	1	0
30	A	408	PHO	5	0
37	D	407	LHG	7	0
46	N	607	CHL	4	0
29	B	514	CLA	4	0
26	A	401	OEX	1	0
43	d	405	PL9	2	0
29	r	308	CLA	3	0
39	o	301	SQD	1	0
48	s	319	NEX	3	0
29	B	509	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	D	402	DGA	3	0
46	y	301	CHL	5	0
29	B	511	CLA	1	0
35	C	524	LMG	2	0
29	c	512	CLA	4	0
46	S	307	CHL	3	0
46	s	307	CHL	2	0
29	G	613	CLA	3	0
31	b	517	BCR	10	0
29	C	503	CLA	1	0
29	R	308	CLA	5	0
47	g	615	LUT	2	0
31	v	101	BCR	3	0
31	A	410	BCR	3	0
31	B	517	BCR	6	0
29	G	602	CLA	5	0
46	n	607	CHL	1	0
29	A	409	CLA	5	0
46	Y	307	CHL	3	0
35	b	520	LMG	4	0
41	b	522	DGA	2	0
47	S	317	LUT	5	0
39	c	522	SQD	3	0
46	g	609	CHL	1	0
29	c	504	CLA	2	0
29	S	312	CLA	7	0
29	s	306	CLA	2	0
29	S	304	CLA	4	0
37	N	618	LHG	4	0
29	Y	313	CLA	2	0
35	B	520	LMG	3	0
46	G	609	CHL	3	0
29	B	504	CLA	4	0
36	c	518	DGD	1	0
40	i	102	SPH	1	0
29	N	614	CLA	1	0
29	b	515	CLA	7	0
29	D	405	CLA	3	0
29	r	307	CLA	3	0
35	C	521	LMG	1	0
49	y	302	XAT	4	0
29	B	512	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	n	606	CHL	5	0
29	B	507	CLA	4	0
50	N	620	PTY	8	0
29	y	306	CLA	2	0
49	r	312	XAT	4	0
29	R	307	CLA	1	0
29	n	611	CLA	1	0
36	C	519	DGD	2	0
29	B	501	CLA	2	0
29	r	310	CLA	1	0
29	N	611	CLA	2	0
37	S	301	LHG	3	0
33	s	322	3PH	3	0
29	N	602	CLA	2	0
29	s	311	CLA	3	0
39	M	101	SQD	2	0
29	N	603	CLA	3	0
29	y	316	CLA	3	0
46	G	608	CHL	1	0
29	b	506	CLA	3	0
29	y	305	CLA	5	0
29	Y	303	CLA	2	0
46	y	309	CHL	6	0
29	S	303	CLA	3	0
29	S	316	CLA	3	0
41	J	101	DGA	2	0
29	S	305	CLA	1	0
39	m	101	SQD	1	0
46	N	605	CHL	7	0
46	G	607	CHL	5	0
29	R	306	CLA	4	0
45	H	101	RRX	3	0
31	a	409	BCR	2	0
46	r	306	CHL	1	0
31	f	101	BCR	2	0
46	g	606	CHL	3	0
29	N	604	CLA	3	0
37	B	523	LHG	3	0
37	d	406	LHG	5	0
29	n	604	CLA	2	0
48	Y	318	NEX	3	0
37	L	101	LHG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	g	610	CLA	2	0
40	C	525	SPH	1	0
31	F	101	BCR	2	0
35	d	408	LMG	2	0
29	b	507	CLA	4	0
35	c	519	LMG	1	0
39	L	102	SQD	5	0
35	C	522	LMG	2	0
29	n	610	CLA	2	0
40	I	101	SPH	3	0
26	a	401	OEX	1	0
46	Y	302	CHL	2	0
38	B	524	LMT	2	0
46	y	303	CHL	1	0
48	G	617	NEX	3	0
47	y	318	LUT	3	0
37	Y	319	LHG	8	0
35	W	203	LMG	3	0
29	D	404	CLA	6	0
29	b	510	CLA	2	0
39	l	101	SQD	3	0
35	D	410	LMG	3	0
46	G	606	CHL	2	0
37	g	618	LHG	4	0
47	n	614	LUT	3	0
31	C	517	BCR	2	0
29	G	610	CLA	2	0
30	a	407	PHO	4	0
29	c	508	CLA	4	0
29	b	502	CLA	3	0
46	S	309	CHL	6	0
29	b	511	CLA	1	0
29	g	604	CLA	2	0
29	r	309	CLA	5	0
49	n	618	XAT	4	0
29	c	513	CLA	6	0
29	s	316	CLA	1	0
29	s	305	CLA	2	0
46	R	304	CHL	2	0
48	r	313	NEX	1	0
29	c	502	CLA	2	0
29	b	513	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	d	404	CLA	3	0
31	z	101	BCR	5	0
44	e	101	HEM	3	0
31	C	515	BCR	8	0
29	s	315	CLA	1	0
33	B	522	3PH	3	0
41	j	101	DGA	3	0
29	C	502	CLA	2	0
29	N	612	CLA	1	0
29	b	508	CLA	3	0
29	g	603	CLA	3	0
37	a	414	LHG	3	0
37	y	320	LHG	3	0
29	C	510	CLA	1	0
37	G	618	LHG	1	0
46	N	601	CHL	2	0
48	R	312	NEX	3	0
29	c	507	CLA	2	0
29	y	313	CLA	4	0
29	s	312	CLA	6	0
45	h	101	RRX	2	0
47	g	616	LUT	4	0
36	C	518	DGD	4	0
47	s	318	LUT	3	0
36	B	521	DGD	1	0
49	g	619	XAT	2	0
29	n	609	CLA	6	0
31	B	518	BCR	1	0
47	y	317	LUT	1	0
29	b	509	CLA	5	0
29	S	313	CLA	4	0
29	n	612	CLA	2	0
38	b	524	LMT	4	0
35	D	409	LMG	2	0
33	A	412	3PH	1	0
29	r	304	CLA	3	0
46	s	309	CHL	4	0
37	D	408	LHG	2	0
48	g	617	NEX	2	0
29	a	404	CLA	5	0
29	A	407	CLA	1	0
30	d	402	PHO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	c	514	BCR	5	0
29	G	612	CLA	2	0
29	B	502	CLA	2	0
37	l	102	LHG	3	0
35	w	202	LMG	2	0
37	c	521	LHG	7	0
29	C	506	CLA	2	0
29	s	310	CLA	3	0
29	N	613	CLA	3	0
29	S	306	CLA	1	0
40	c	523	SPH	4	0
46	G	601	CHL	2	0
39	C	501	SQD	2	0
50	n	619	PTY	5	0
29	b	514	CLA	3	0
29	R	303	CLA	2	0
29	C	511	CLA	1	0
29	B	503	CLA	1	0
47	r	311	LUT	3	0
29	R	302	CLA	2	0
30	D	401	PHO	3	0
46	Y	306	CHL	1	0
29	b	505	CLA	3	0
36	c	517	DGD	5	0
48	S	319	NEX	4	0
29	s	303	CLA	3	0
29	b	504	CLA	2	0
29	n	603	CLA	6	0
35	d	407	LMG	2	0
29	C	507	CLA	4	0
29	n	613	CLA	1	0
46	S	302	CHL	1	0
29	a	406	CLA	1	0
37	s	301	LHG	2	0
47	N	616	LUT	4	0
47	R	310	LUT	4	0
29	g	611	CLA	3	0
47	Y	317	LUT	3	0
29	n	602	CLA	4	0
47	N	615	LUT	2	0
29	Y	309	CLA	1	0
29	Y	315	CLA	4	0

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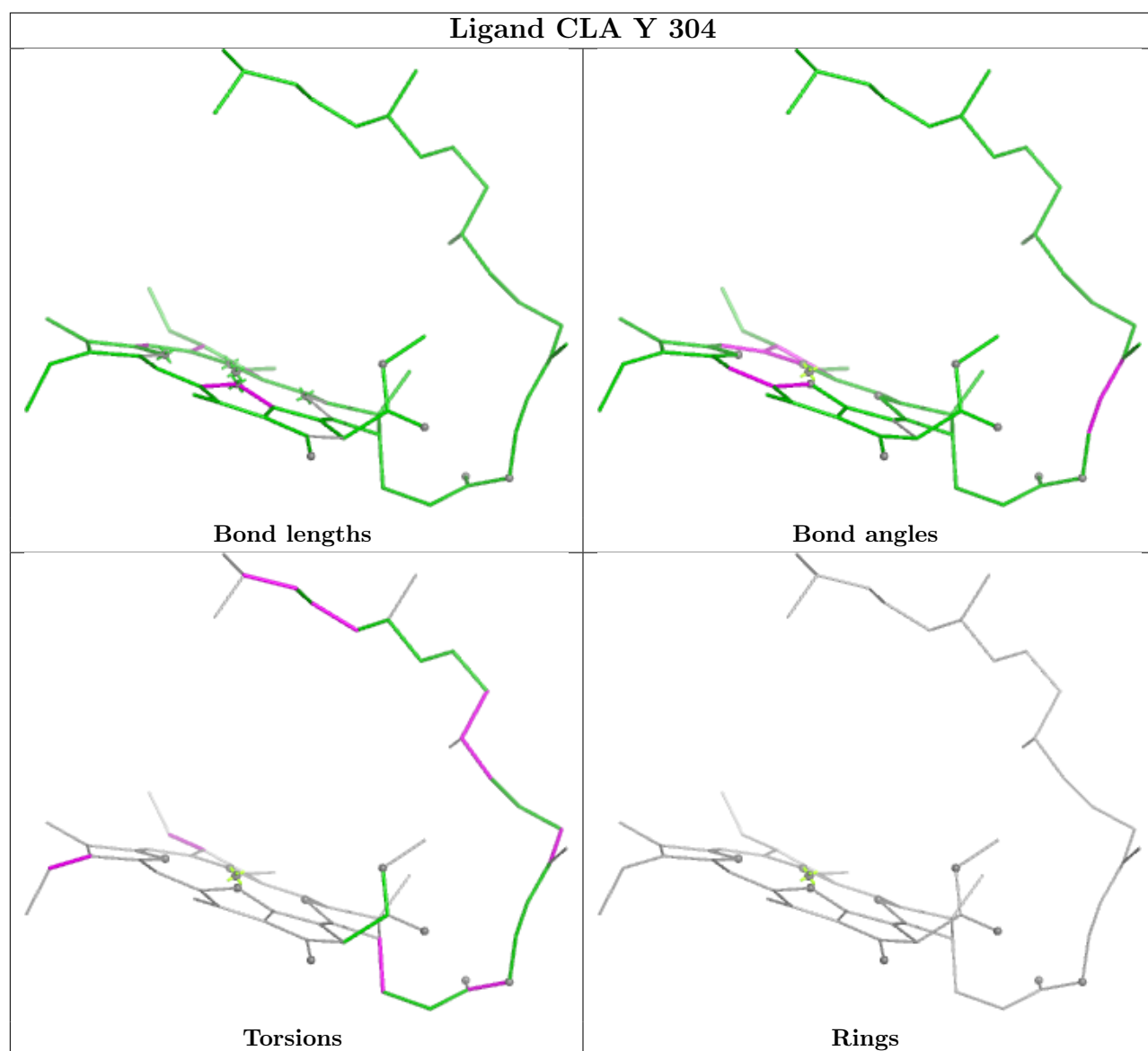
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	b	512	CLA	3	0
29	G	614	CLA	1	0
29	a	408	CLA	5	0
47	S	318	LUT	3	0
33	a	415	3PH	3	0
47	s	317	LUT	3	0
46	y	308	CHL	1	0
29	G	603	CLA	6	0
29	Y	314	CLA	6	0
29	B	506	CLA	1	0
47	Y	316	LUT	3	0
46	s	302	CHL	1	0
51	S	321	LPX	3	0
29	Y	312	CLA	3	0
44	E	101	HEM	1	0
47	n	615	LUT	4	0
41	w	201	DGA	6	0
36	r	301	DGD	1	0
29	B	510	CLA	3	0
29	G	611	CLA	1	0
29	y	315	CLA	2	0
29	C	508	CLA	4	0
29	s	313	CLA	2	0
29	d	403	CLA	4	0
29	y	304	CLA	6	0
29	c	511	CLA	3	0
37	s	320	LHG	4	0
37	a	413	LHG	2	0
33	b	521	3PH	4	0
29	Y	311	CLA	1	0
29	S	311	CLA	6	0
29	A	405	CLA	9	0
47	G	615	LUT	2	0
49	N	619	XAT	5	0
46	N	608	CHL	1	0
29	c	505	CLA	5	0
29	C	513	CLA	2	0
46	Y	308	CHL	4	0
35	i	101	LMG	2	0
29	c	509	CLA	2	0
39	a	410	SQD	1	0
29	g	602	CLA	4	0

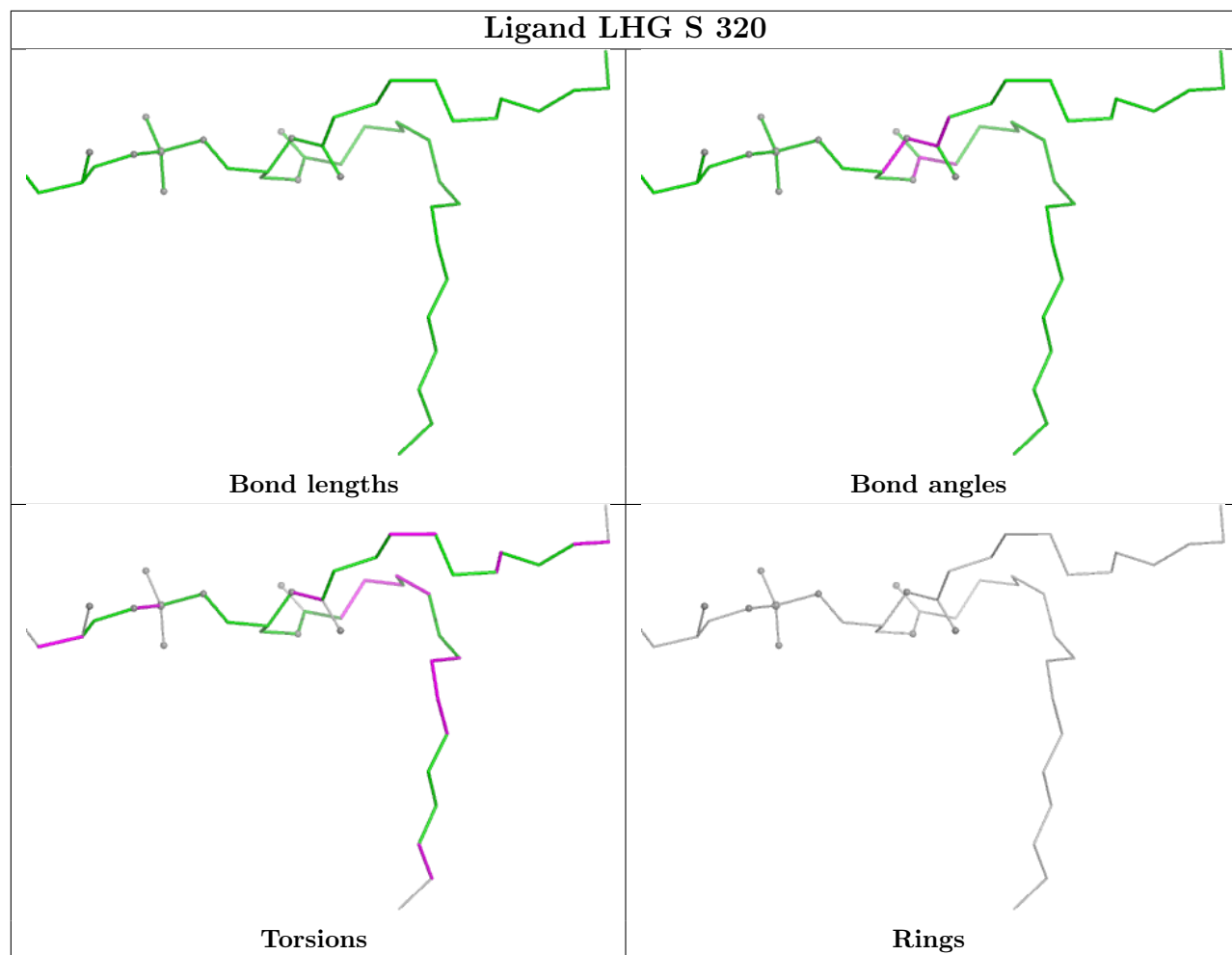
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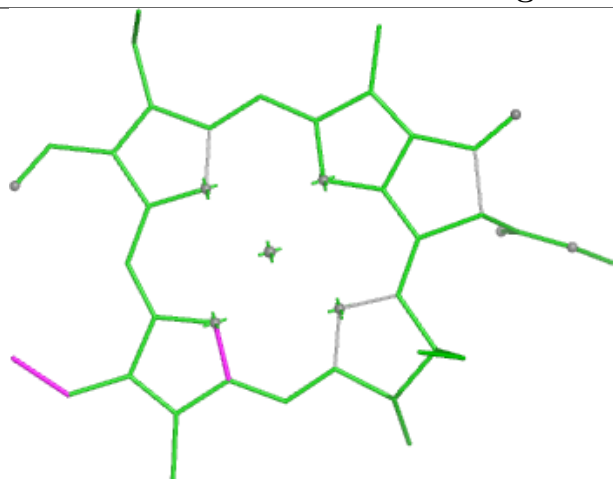
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	y	310	CLA	1	0
29	C	505	CLA	3	0
29	a	405	CLA	4	0
29	S	314	CLA	3	0
48	N	617	NEX	3	0
29	c	506	CLA	4	0
29	G	604	CLA	3	0
31	K	101	BCR	4	0
29	C	504	CLA	2	0
29	B	515	CLA	4	0
29	r	303	CLA	5	0
29	S	315	CLA	1	0
31	C	516	BCR	1	0
46	n	608	CHL	2	0
29	B	508	CLA	2	0
46	s	308	CHL	2	0
46	N	606	CHL	2	0
29	Y	305	CLA	2	0
42	D	403	BCT	1	0
33	S	322	3PH	2	0
46	n	601	CHL	4	0
48	y	319	NEX	3	0
29	C	512	CLA	3	0
29	S	310	CLA	1	0
29	g	614	CLA	1	0
46	g	601	CHL	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.

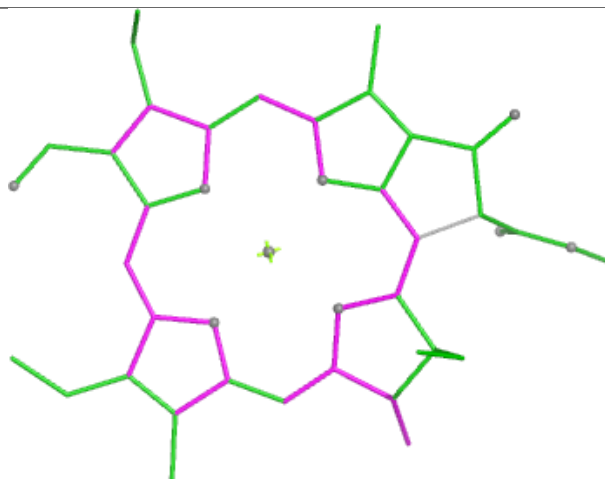




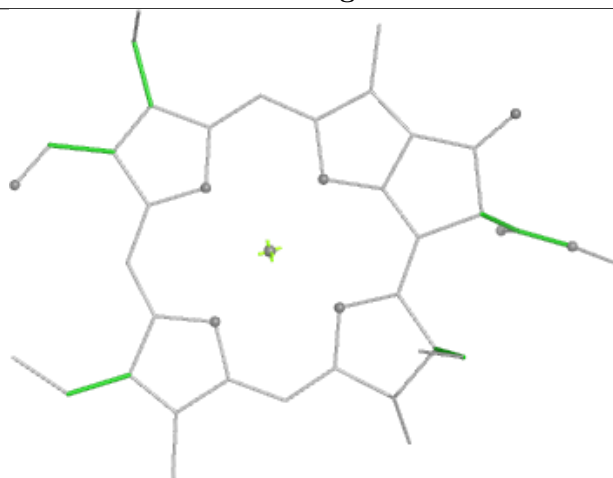
Ligand CHL S 308



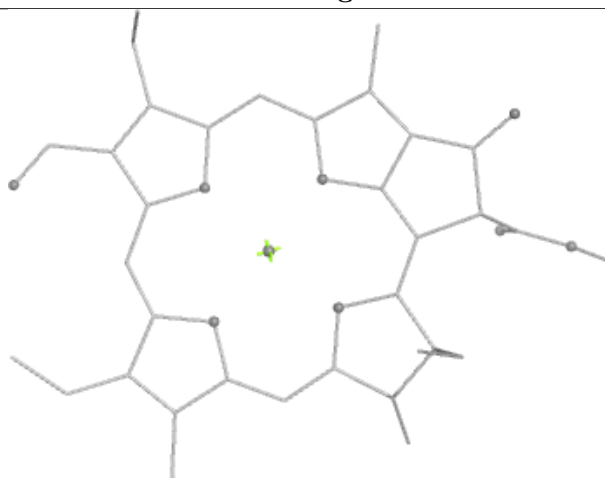
Bond lengths



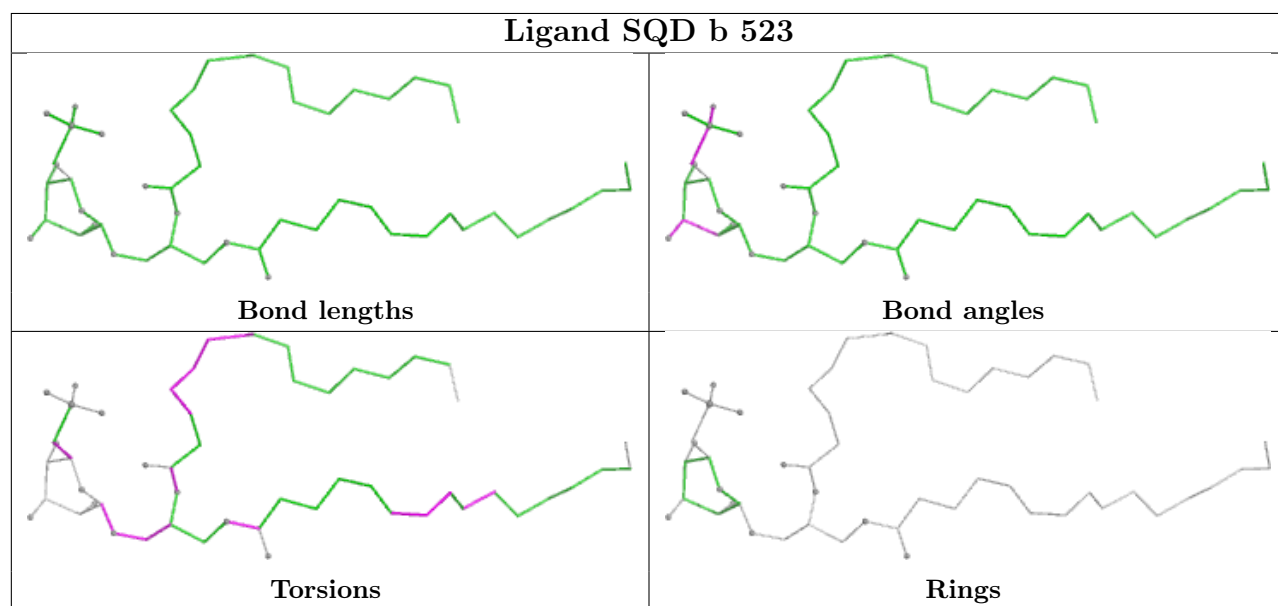
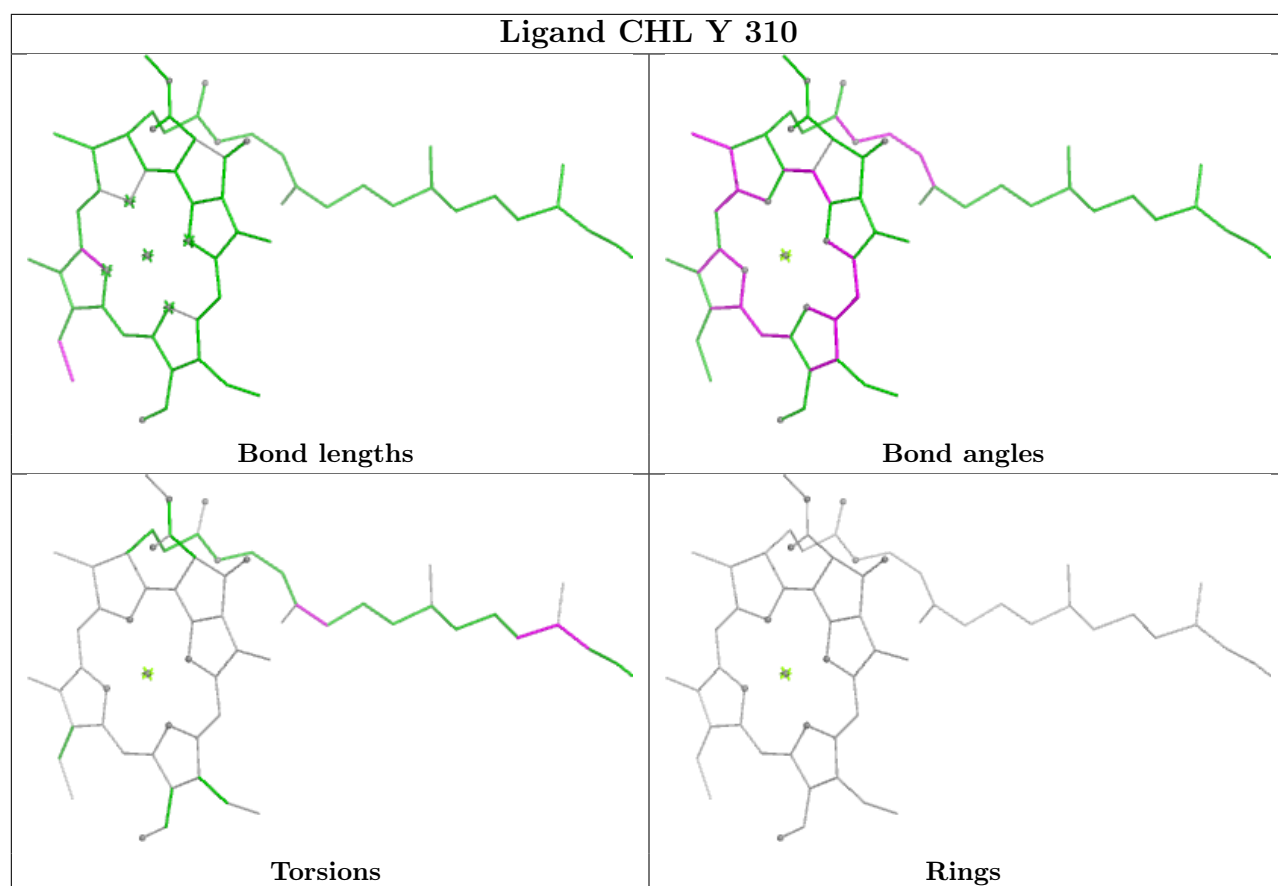
Bond angles

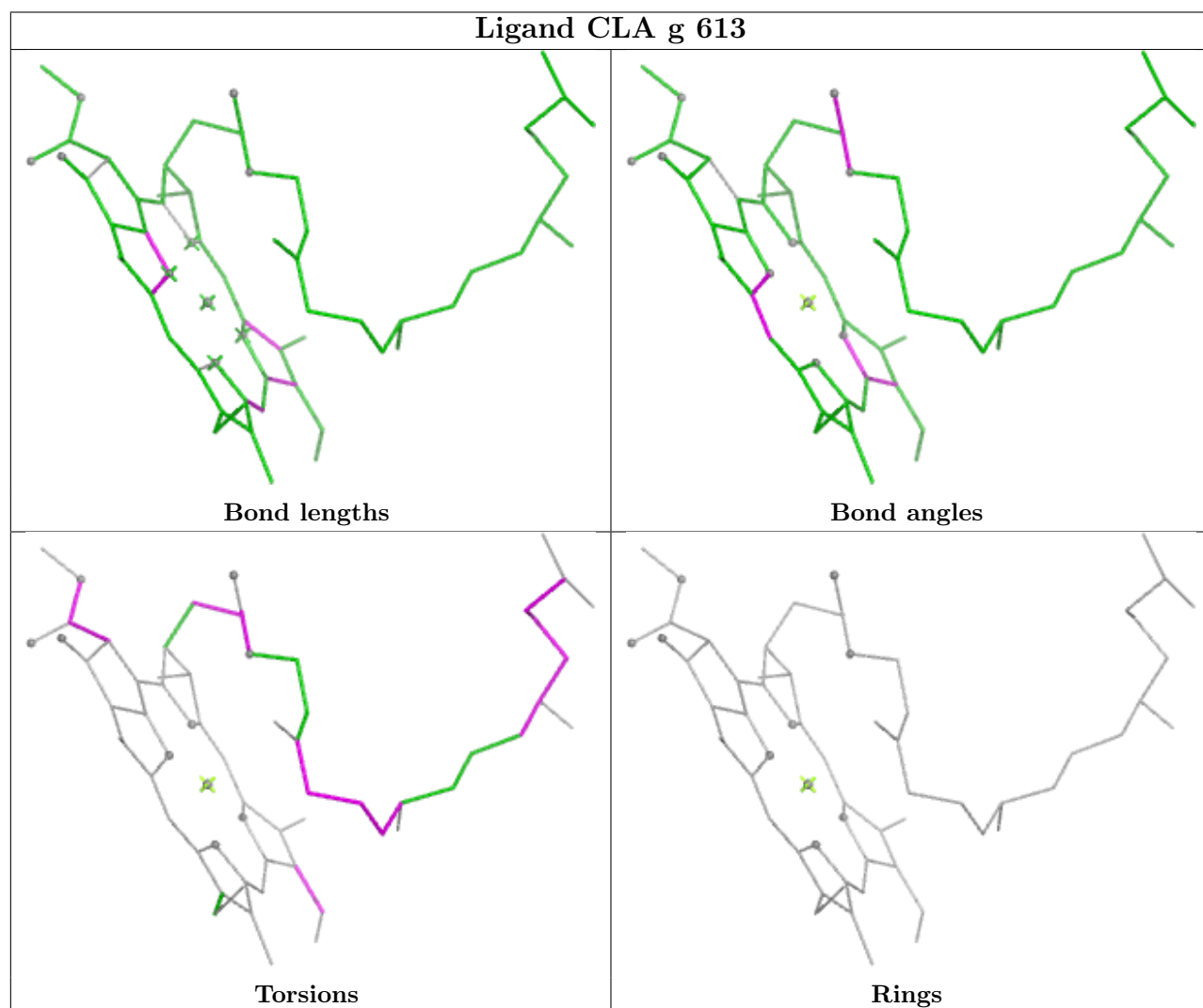
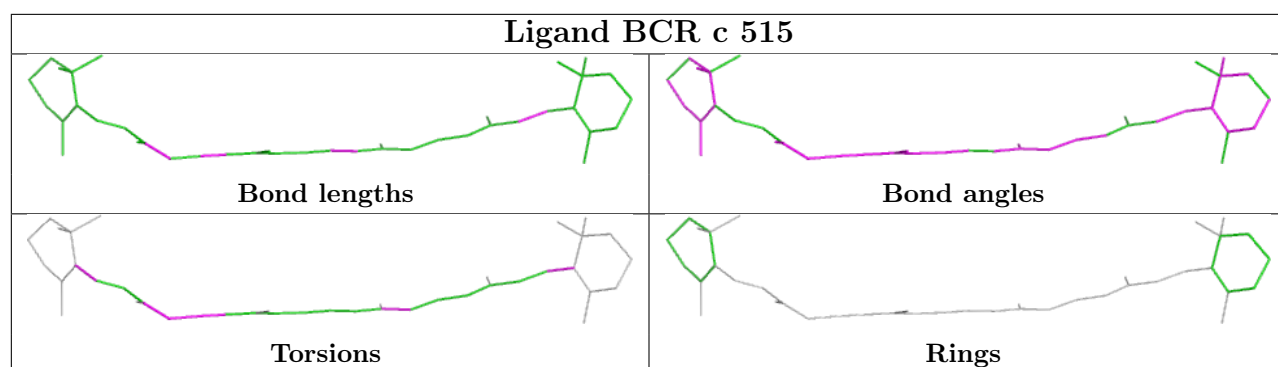


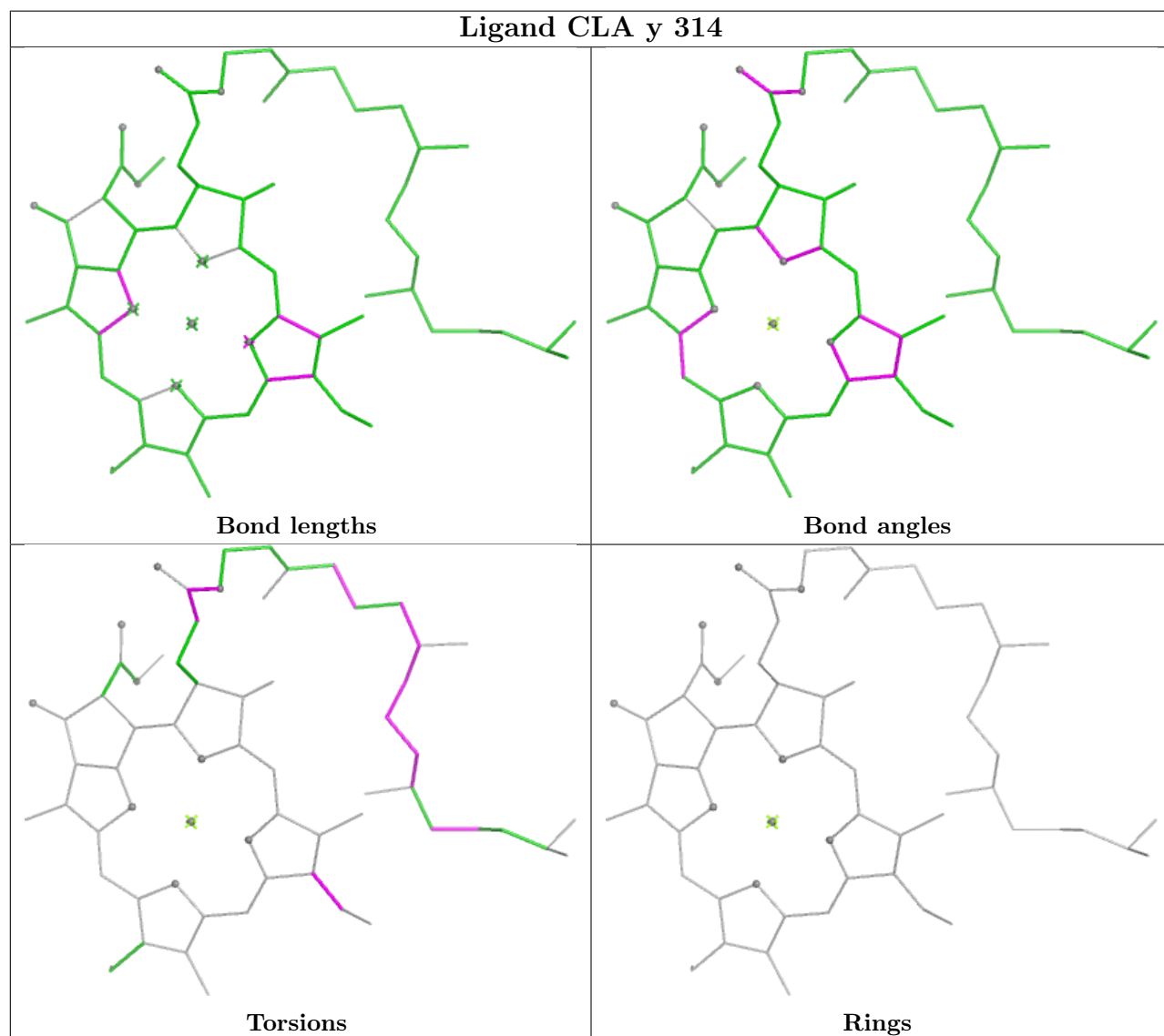
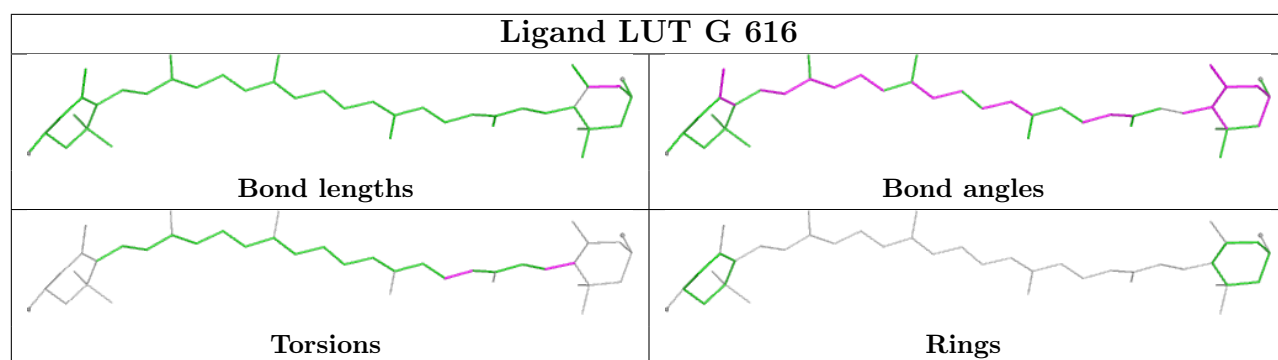
Torsions

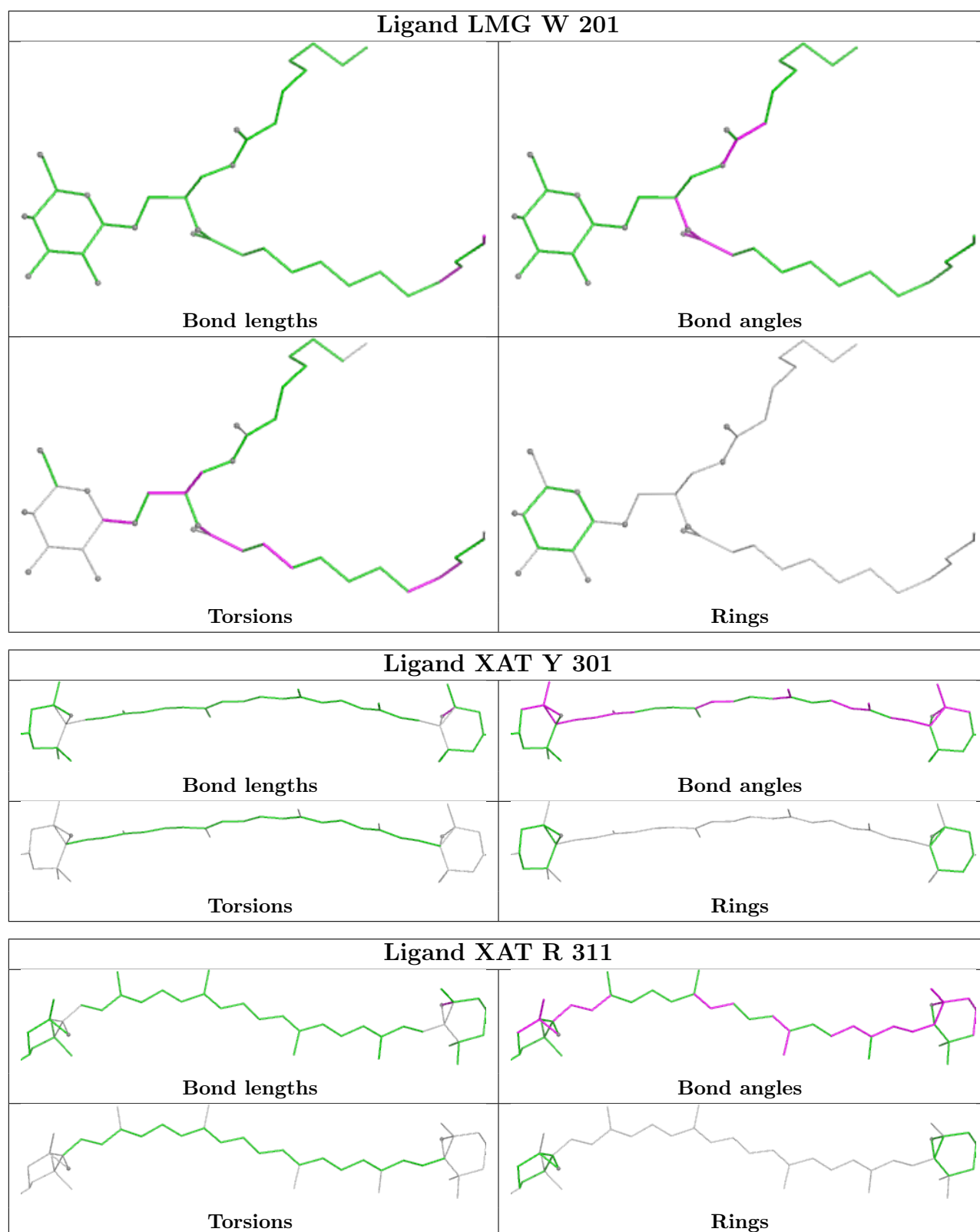


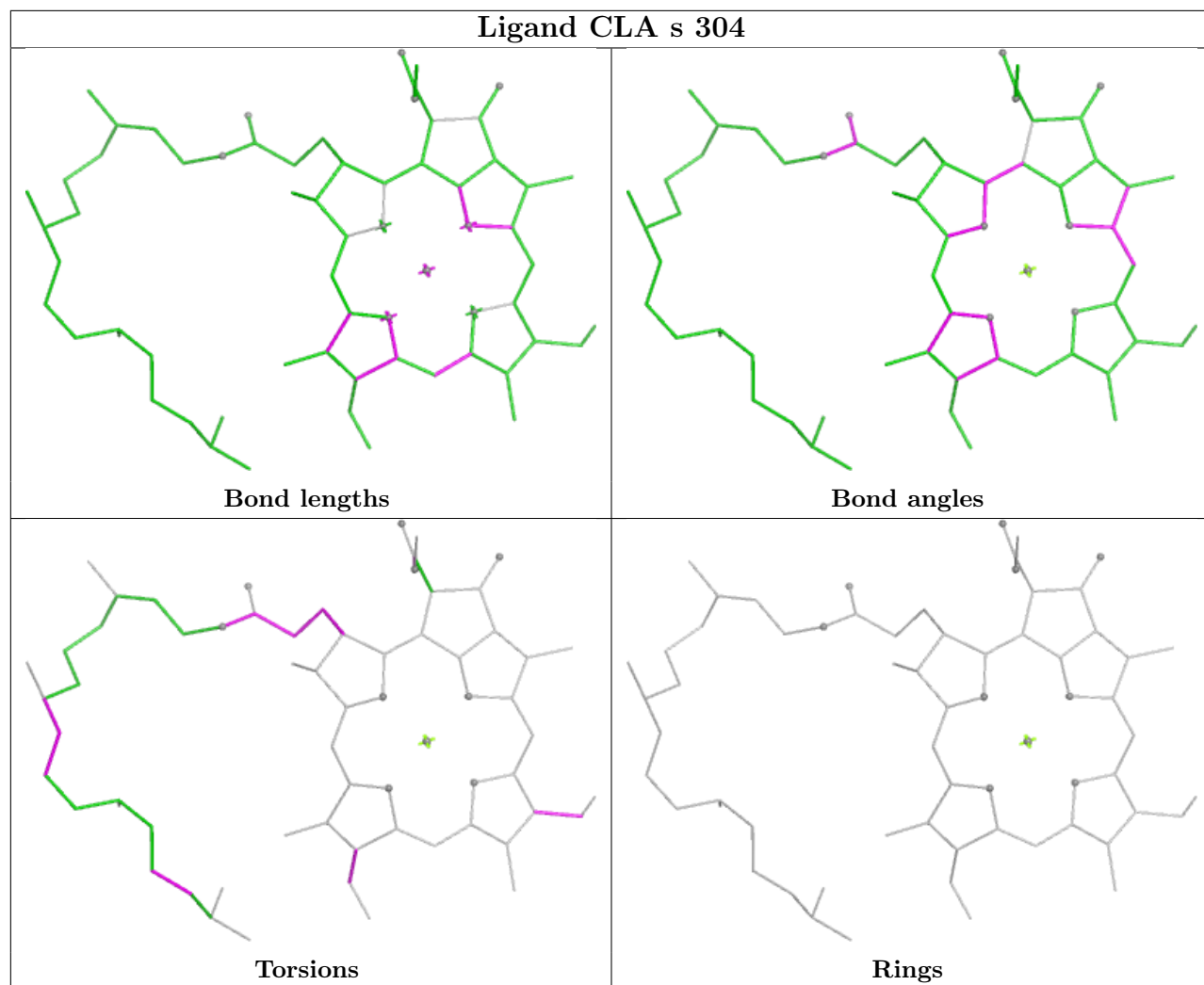
Rings

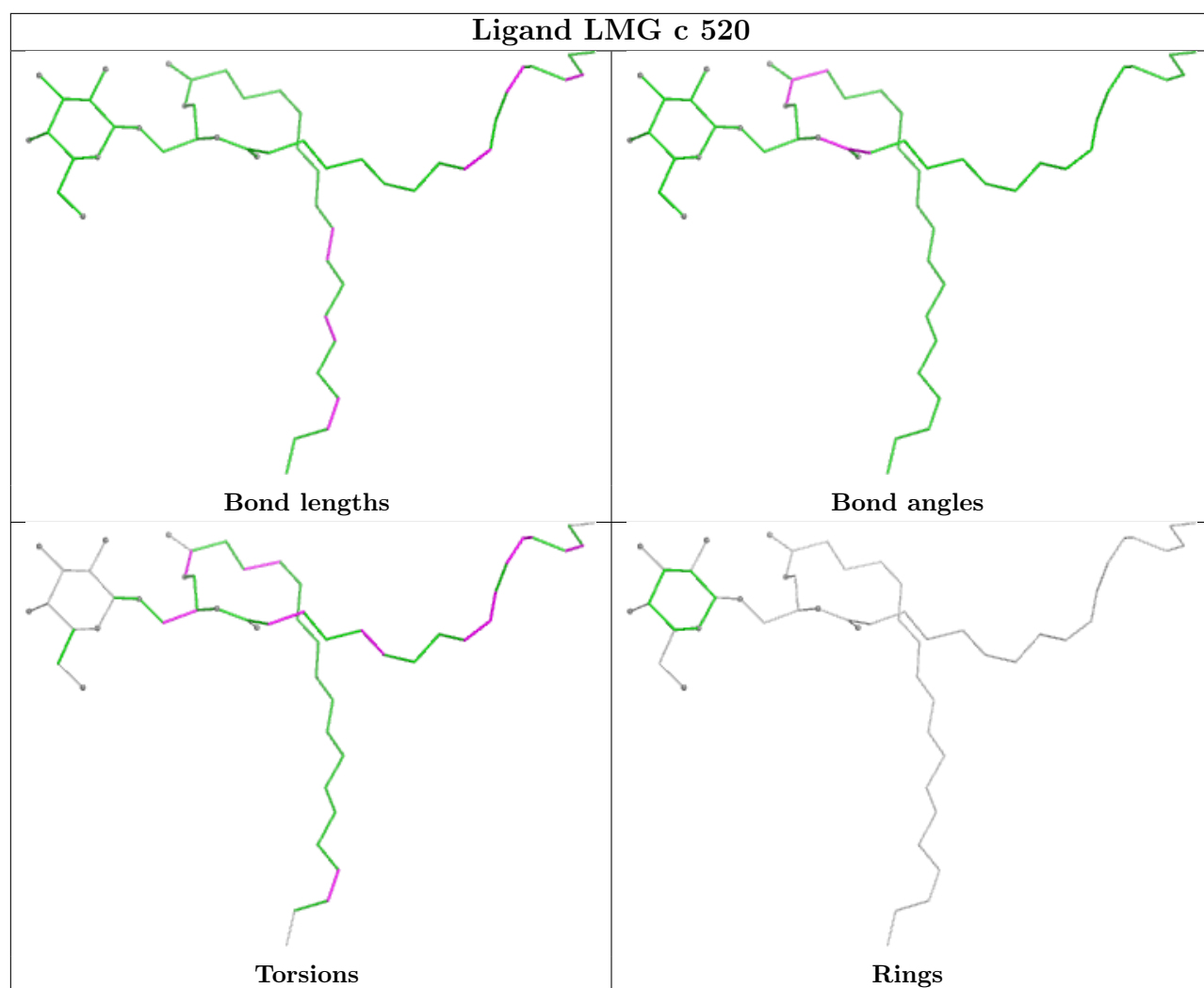


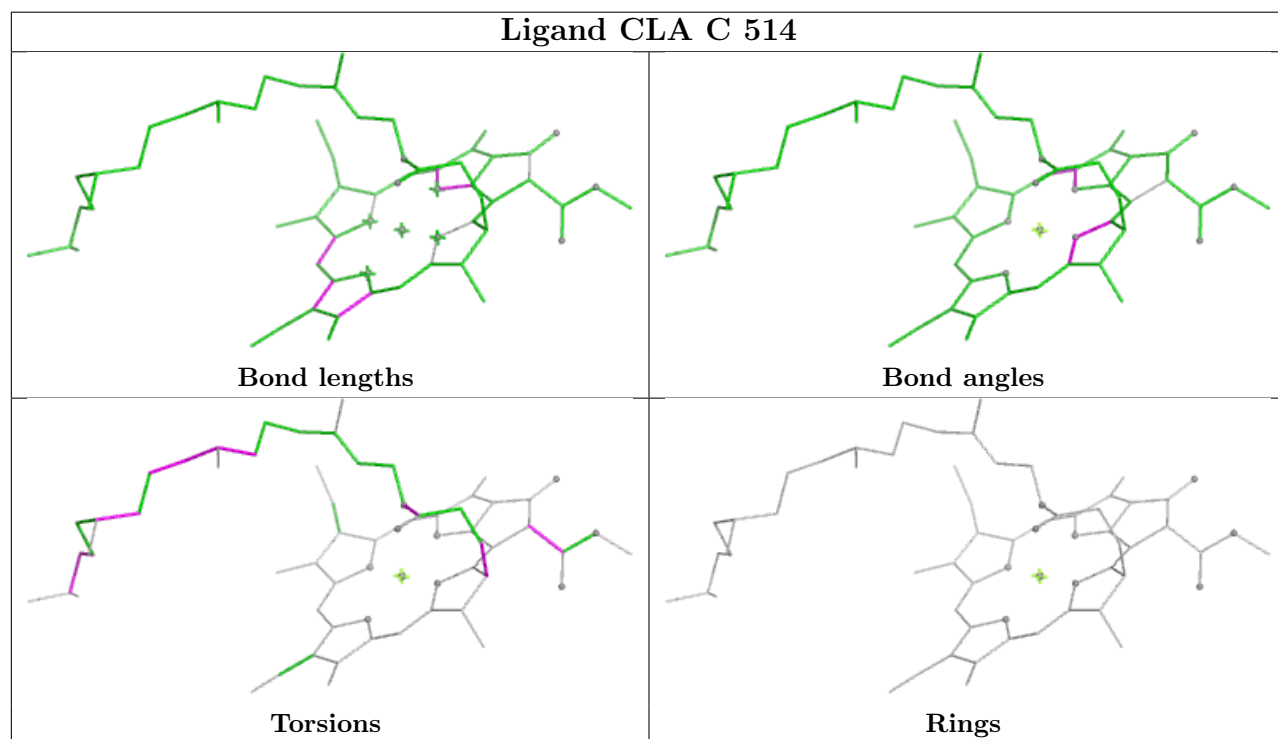
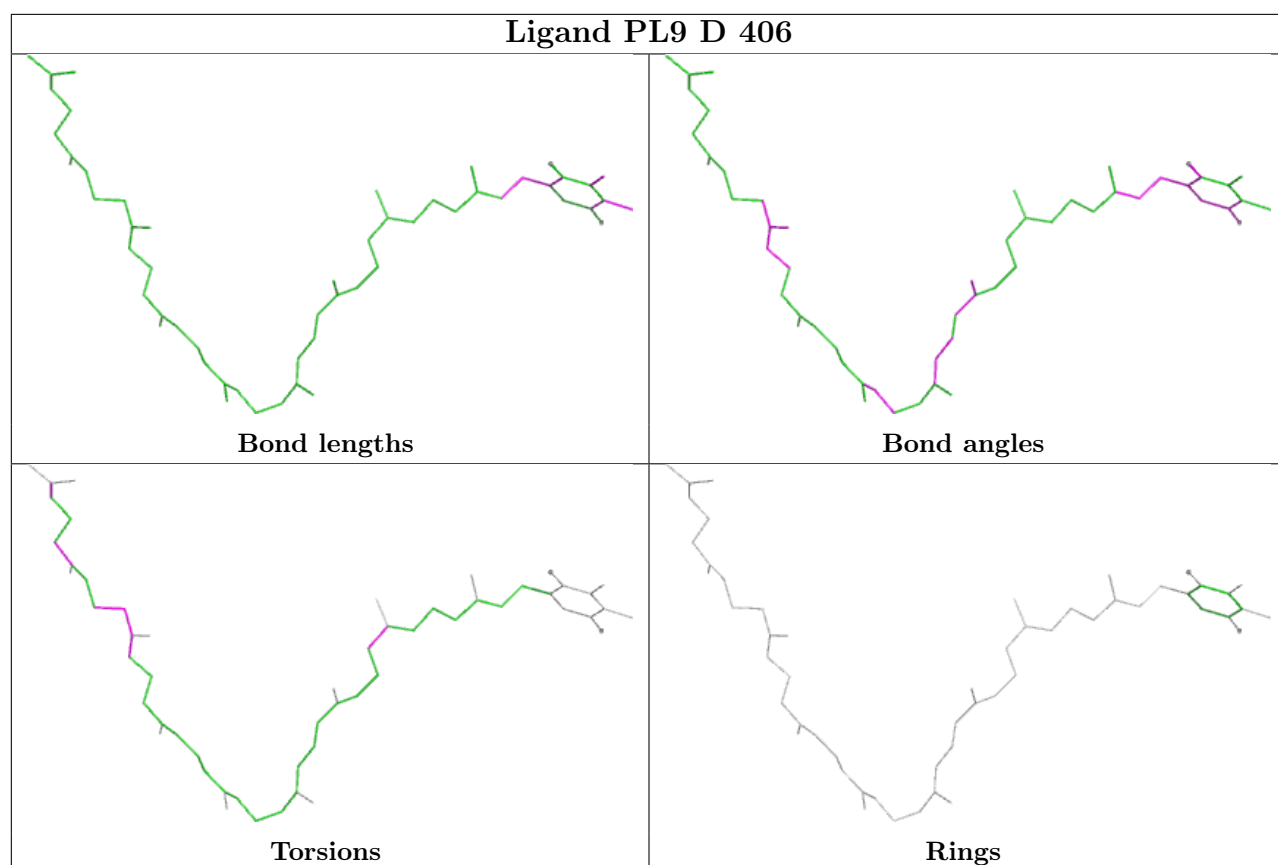


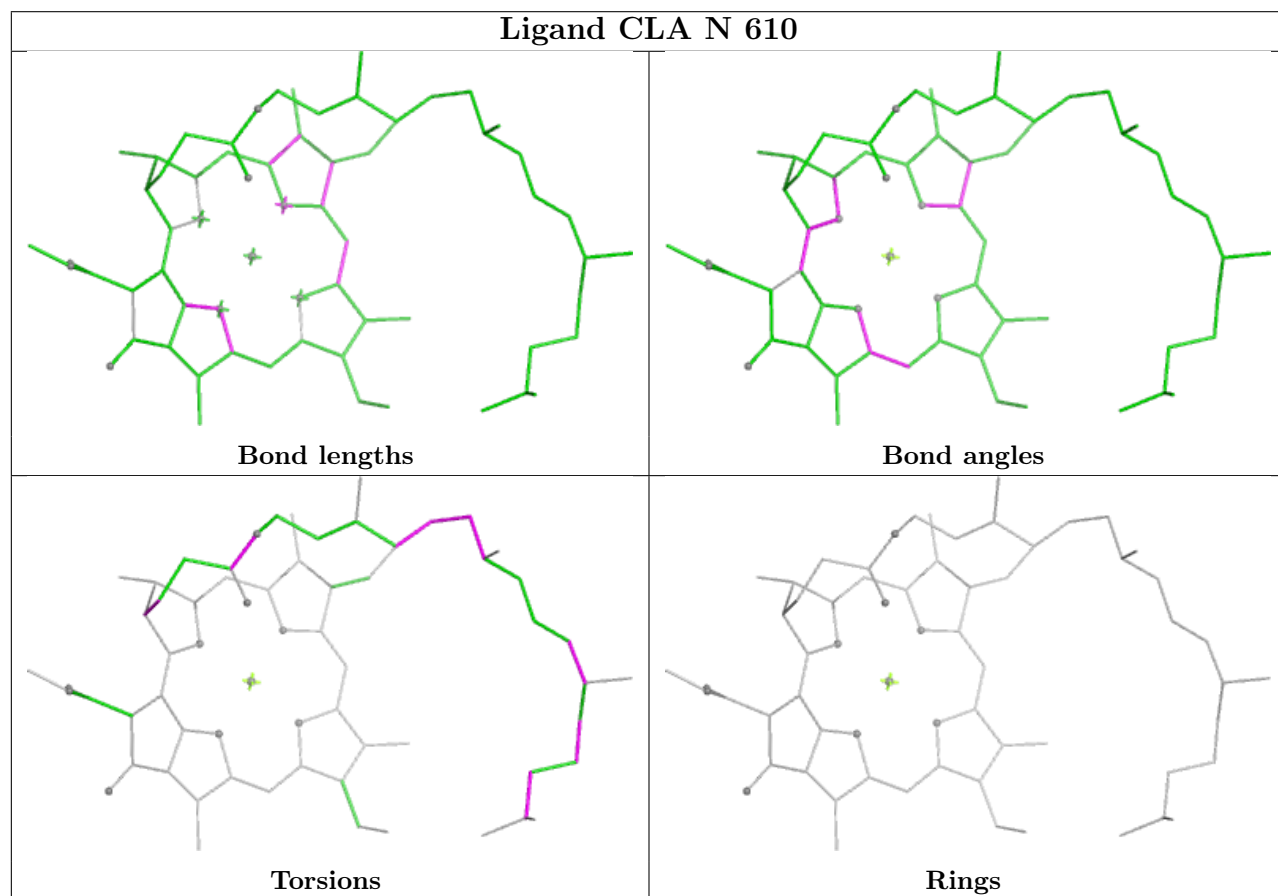
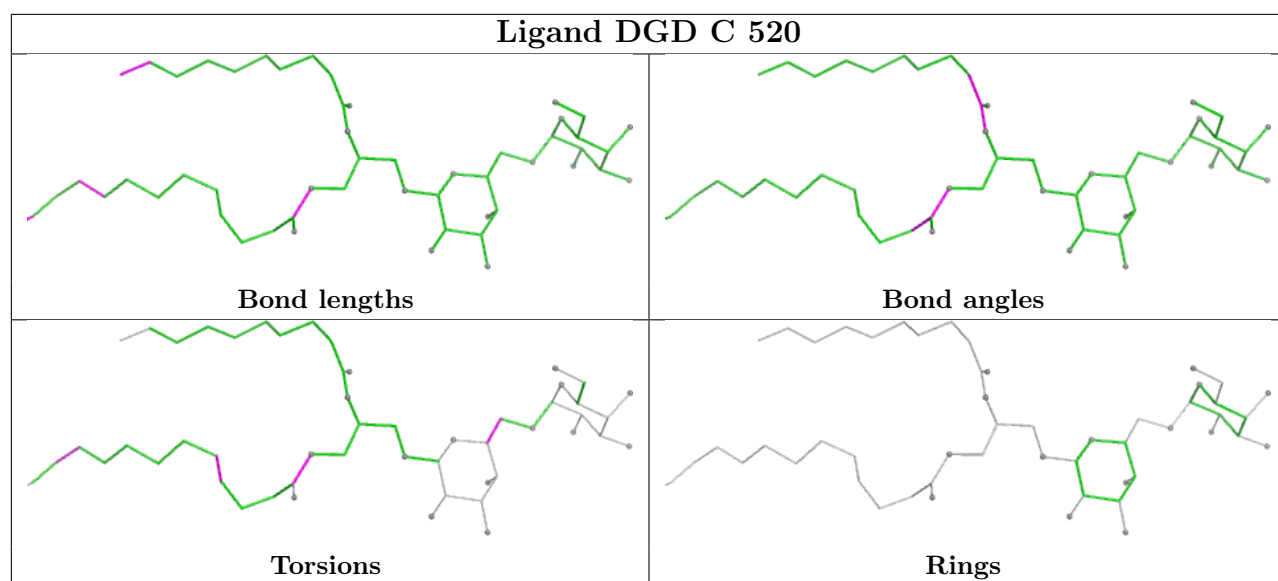




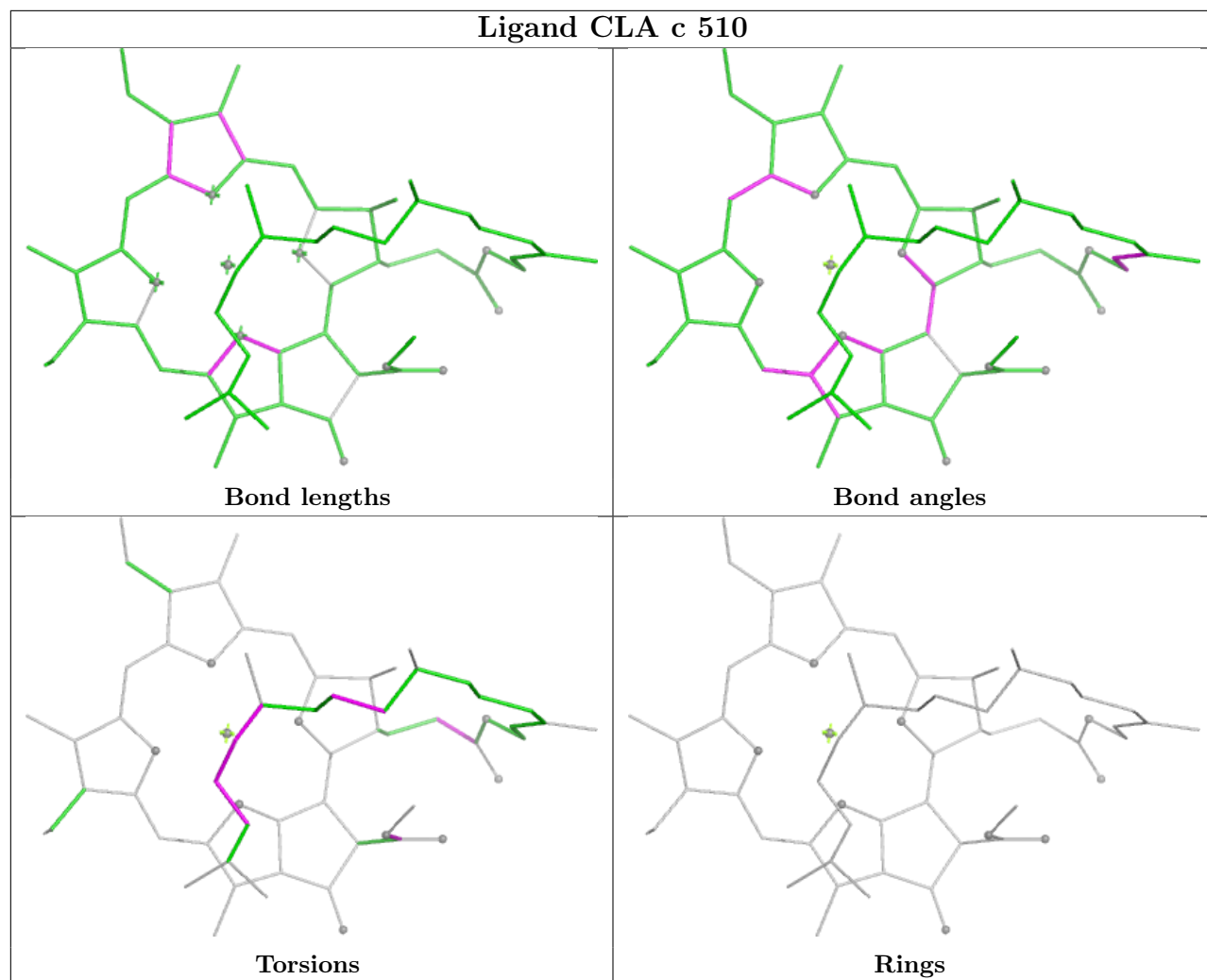


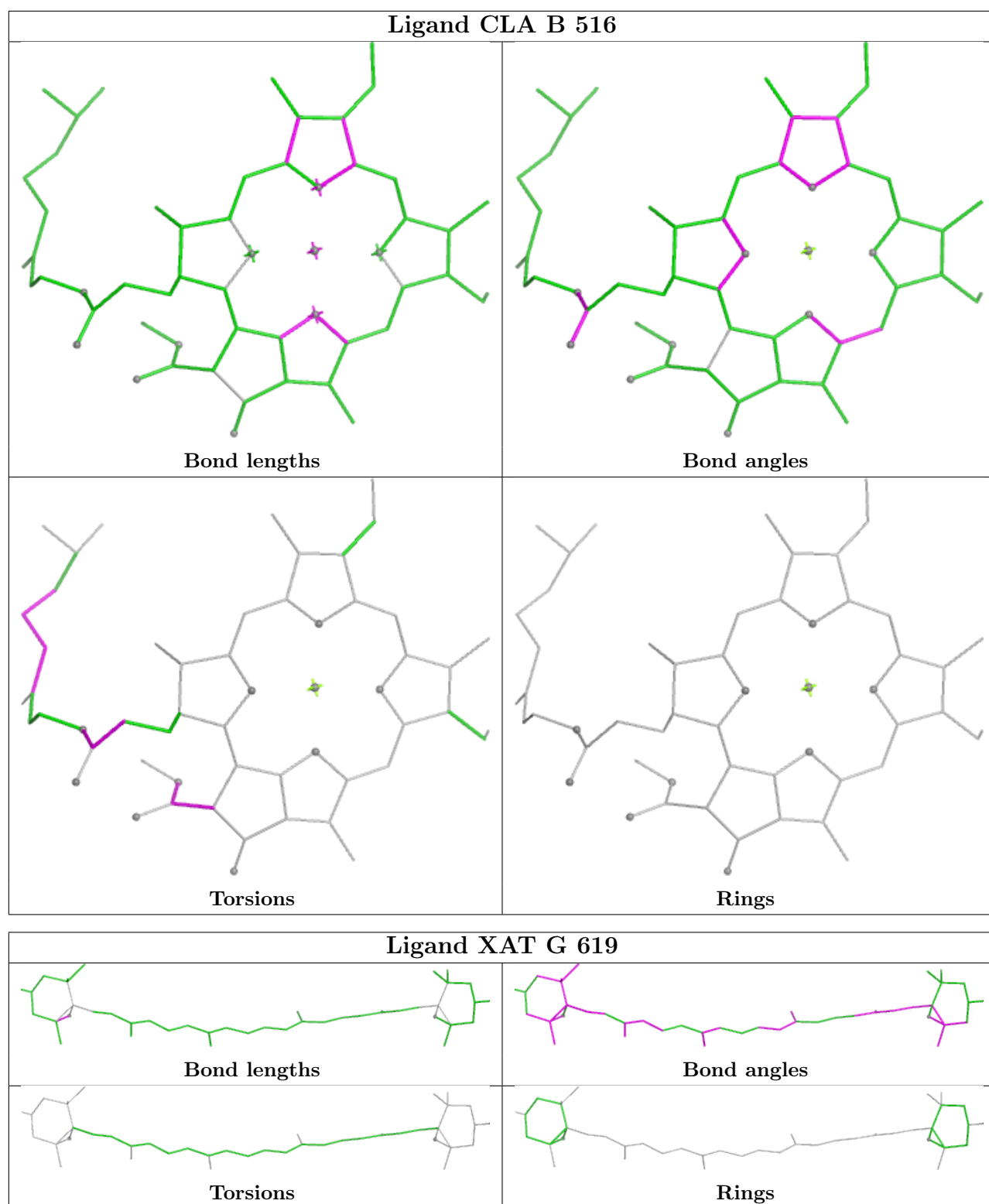


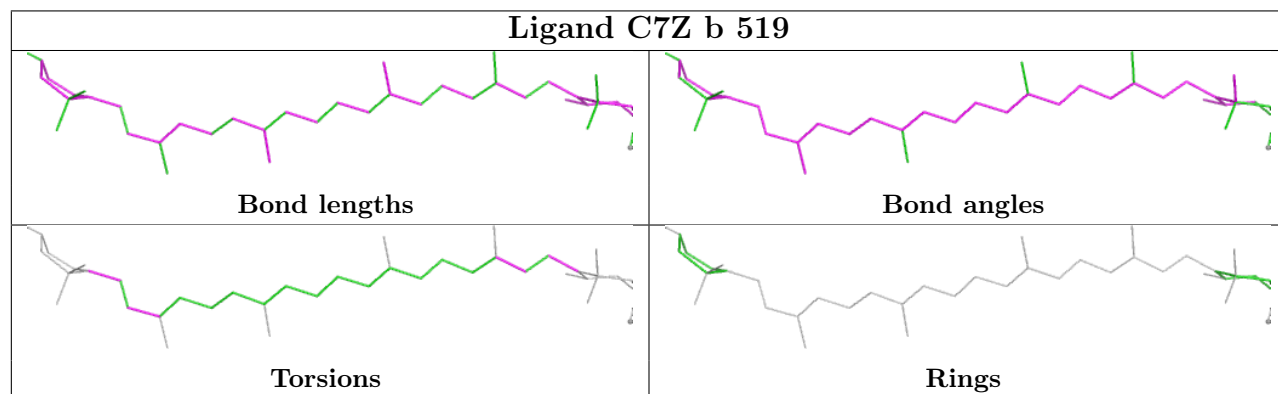
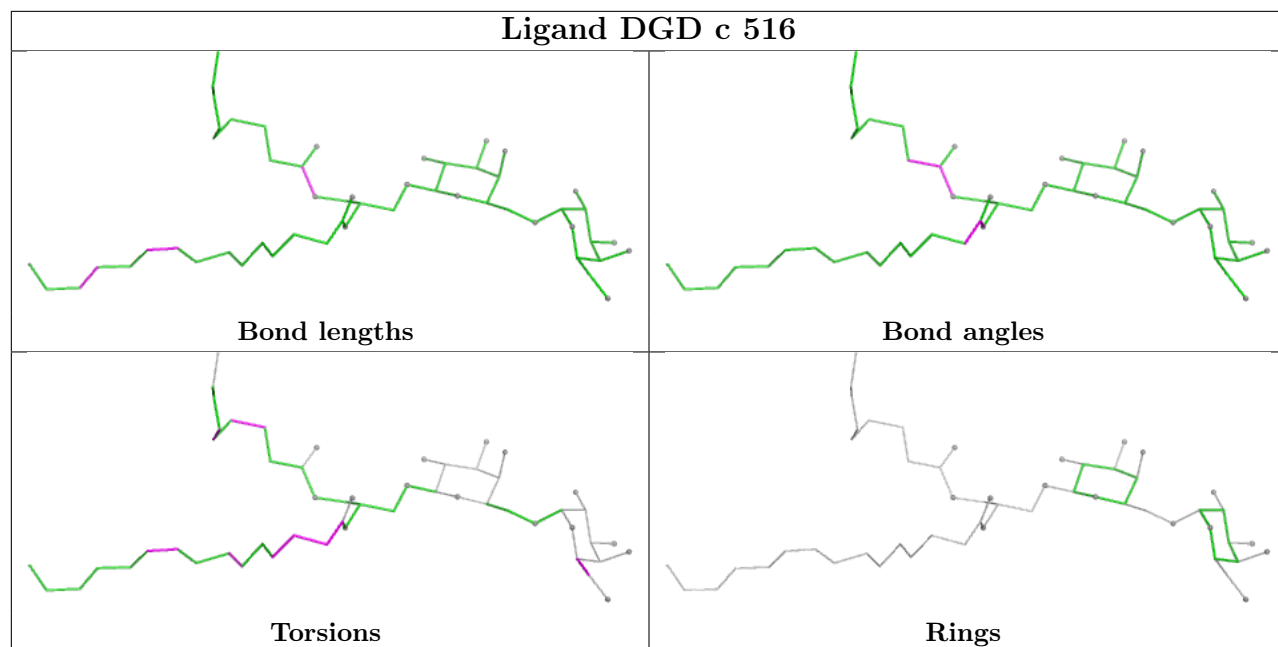


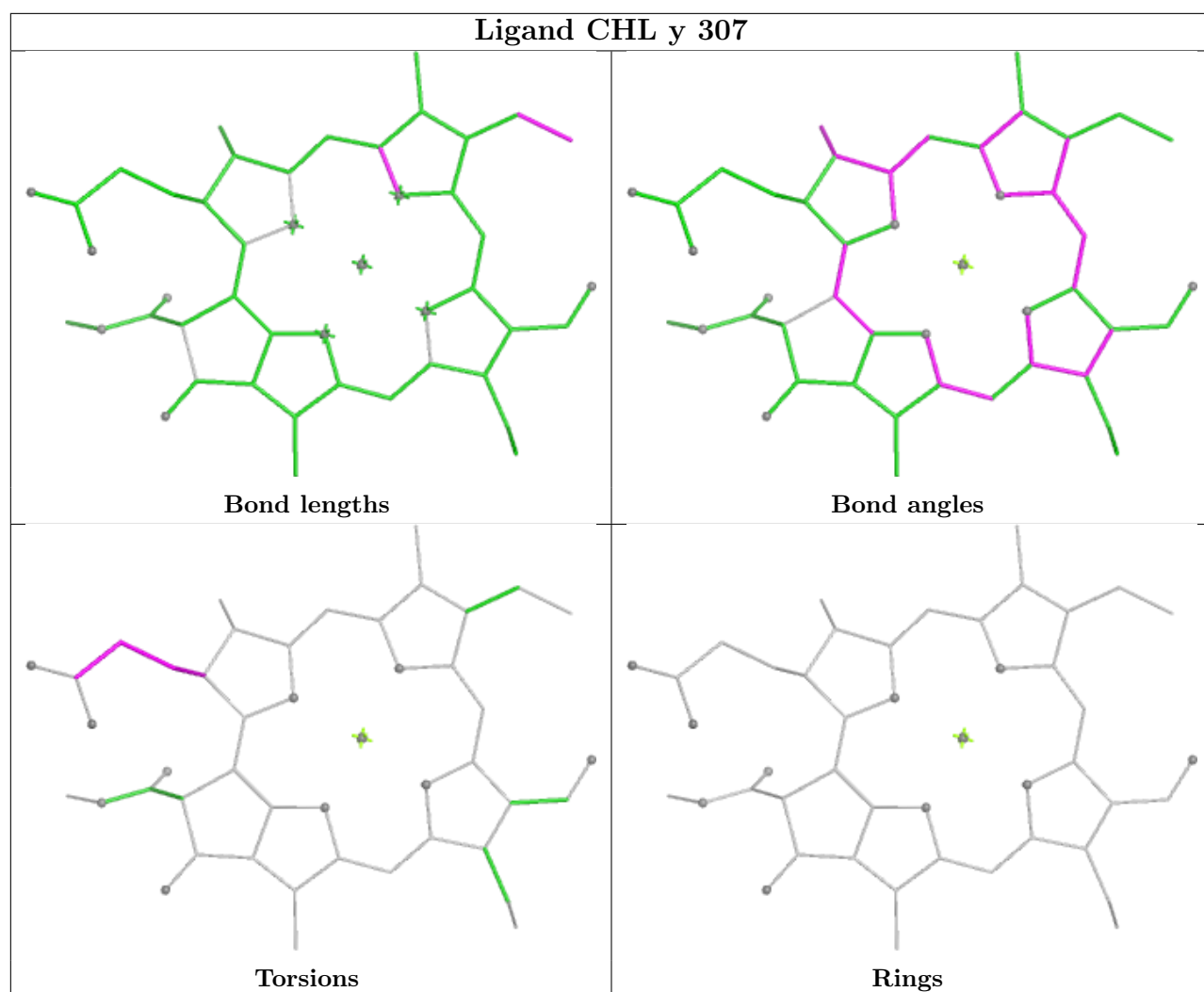


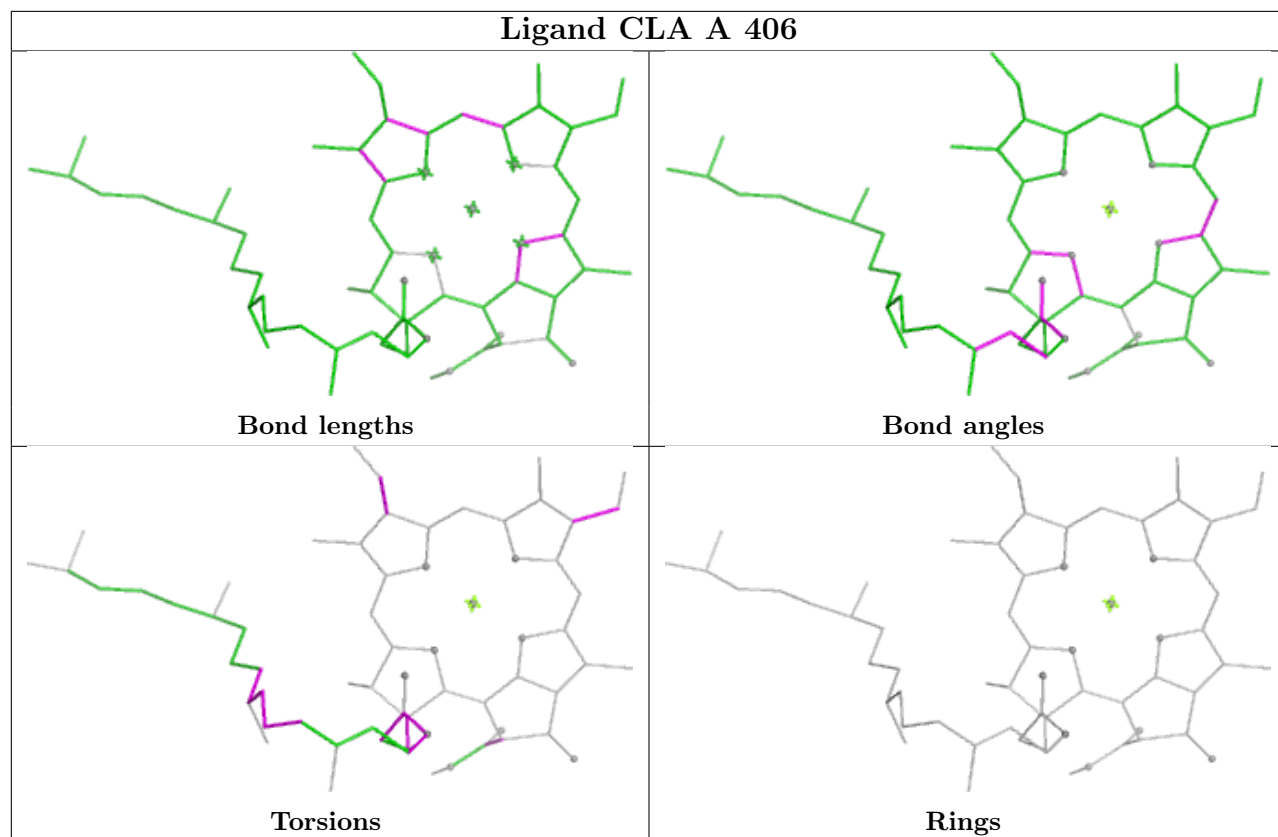
Ligand CLA c 510

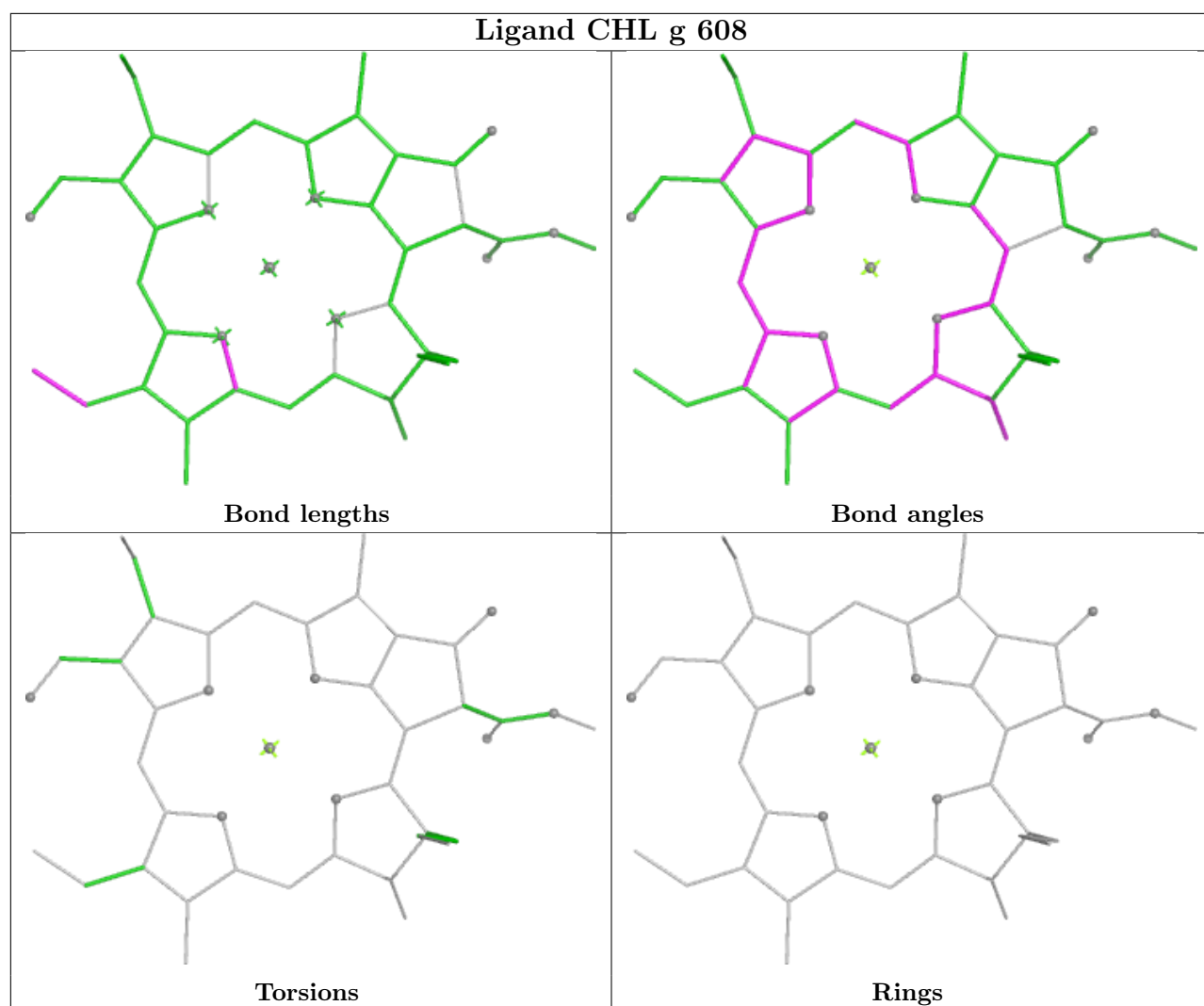




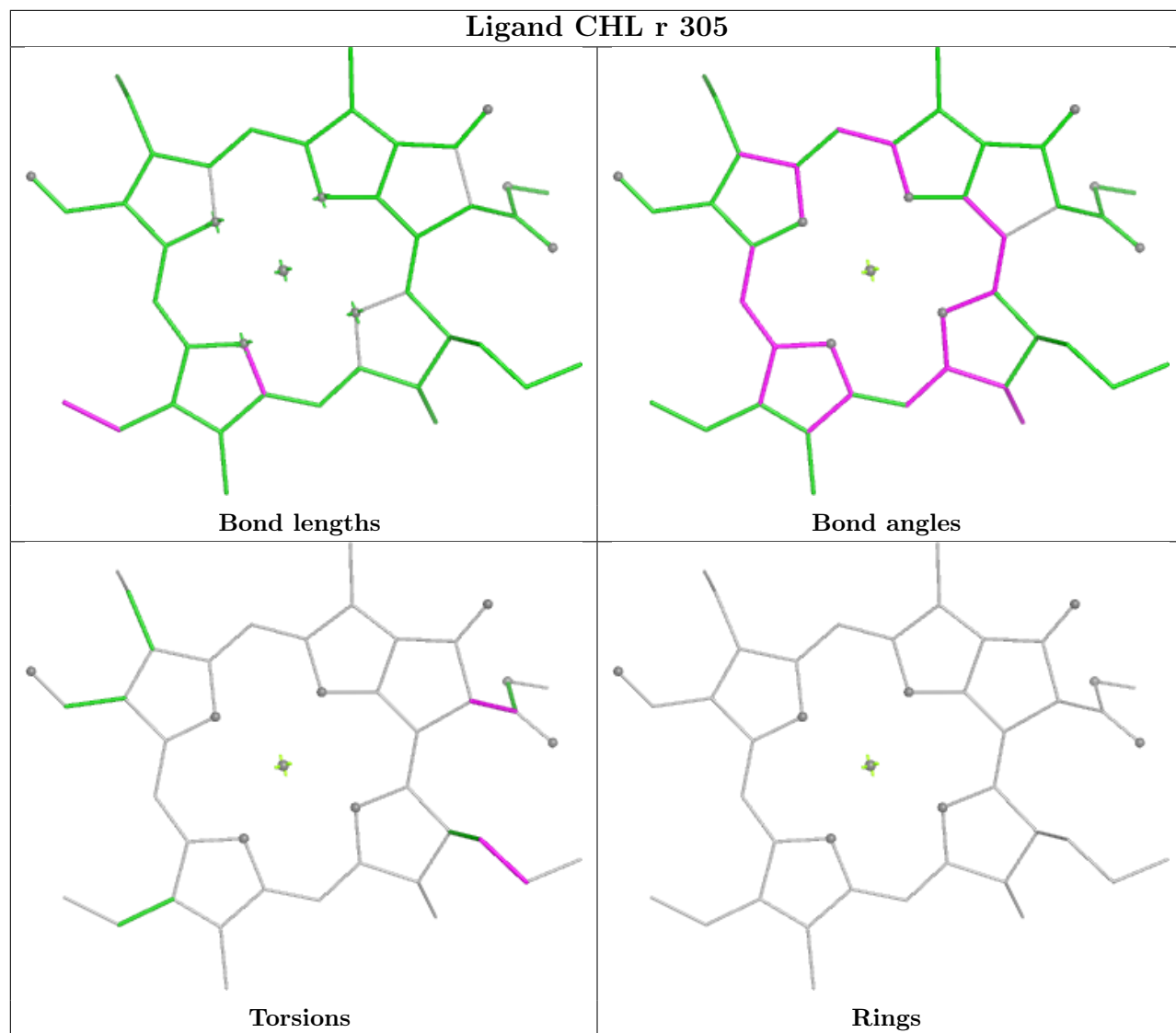




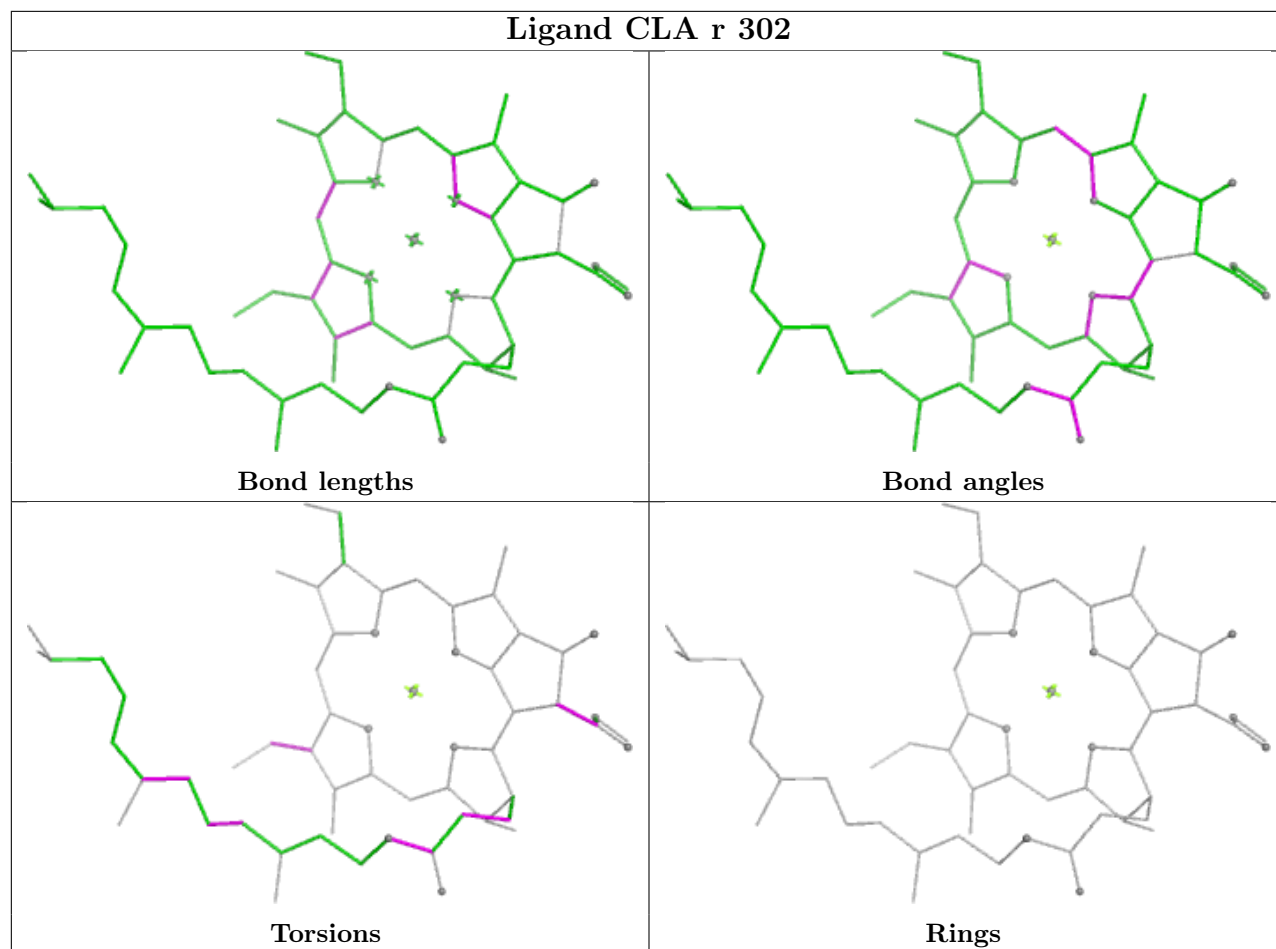




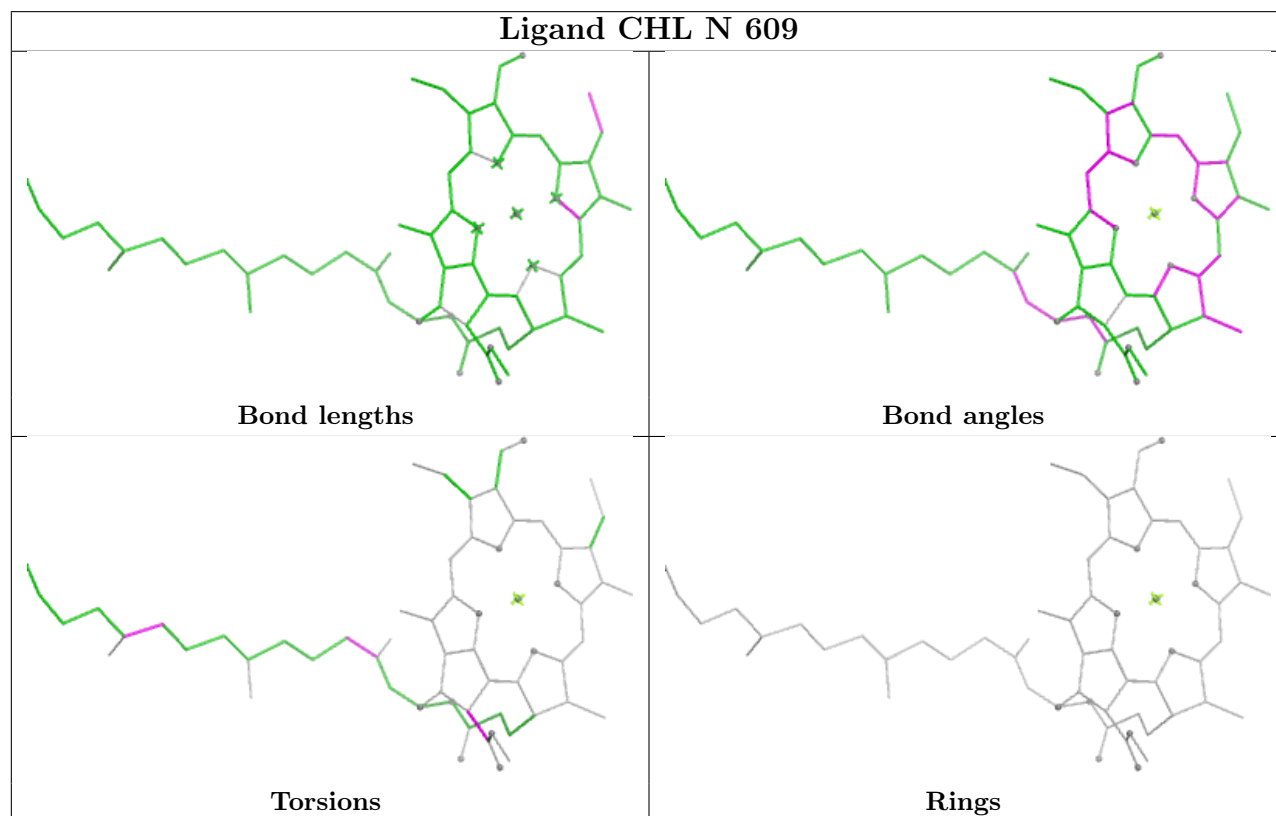
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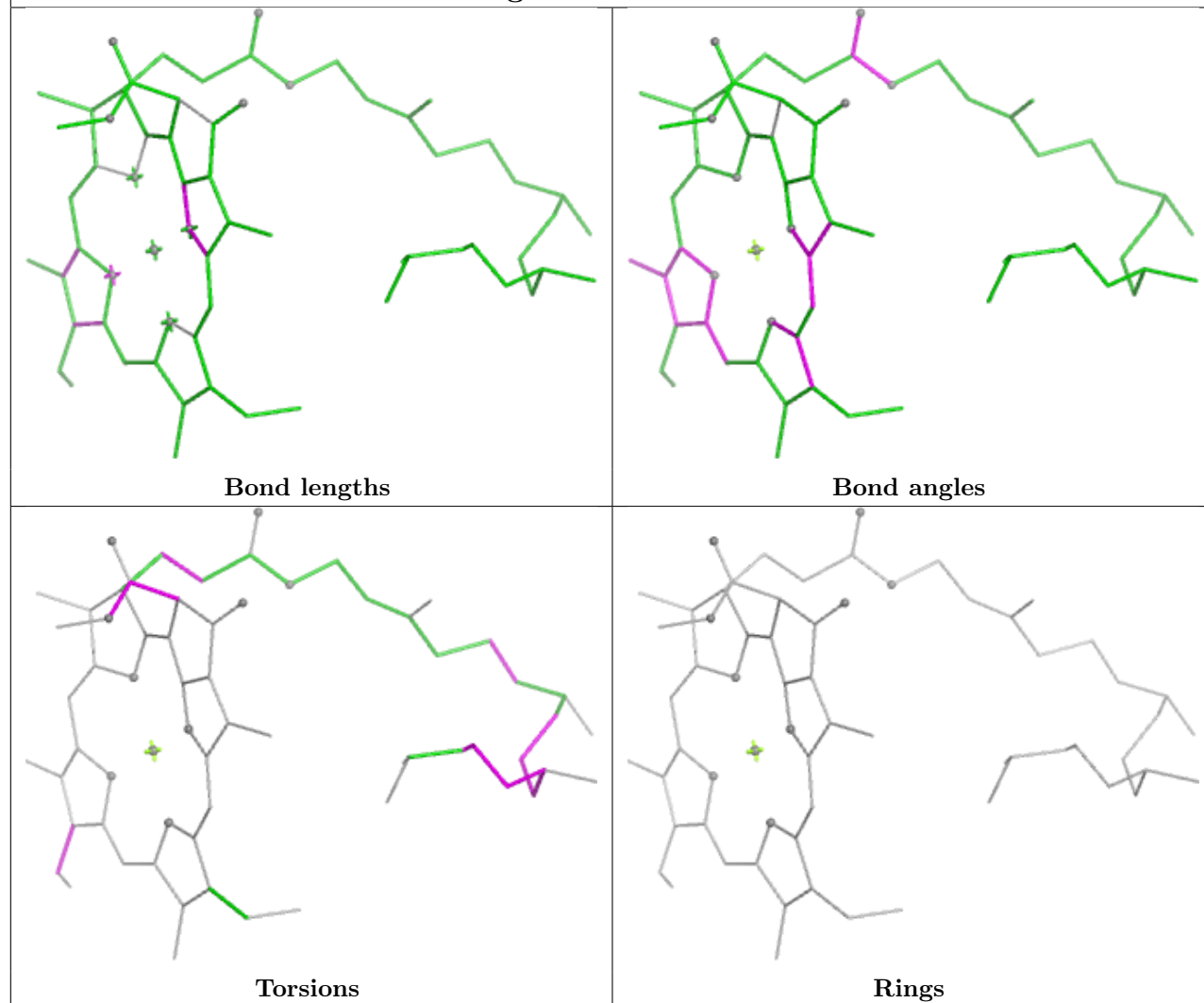
Ligand CLA r 302



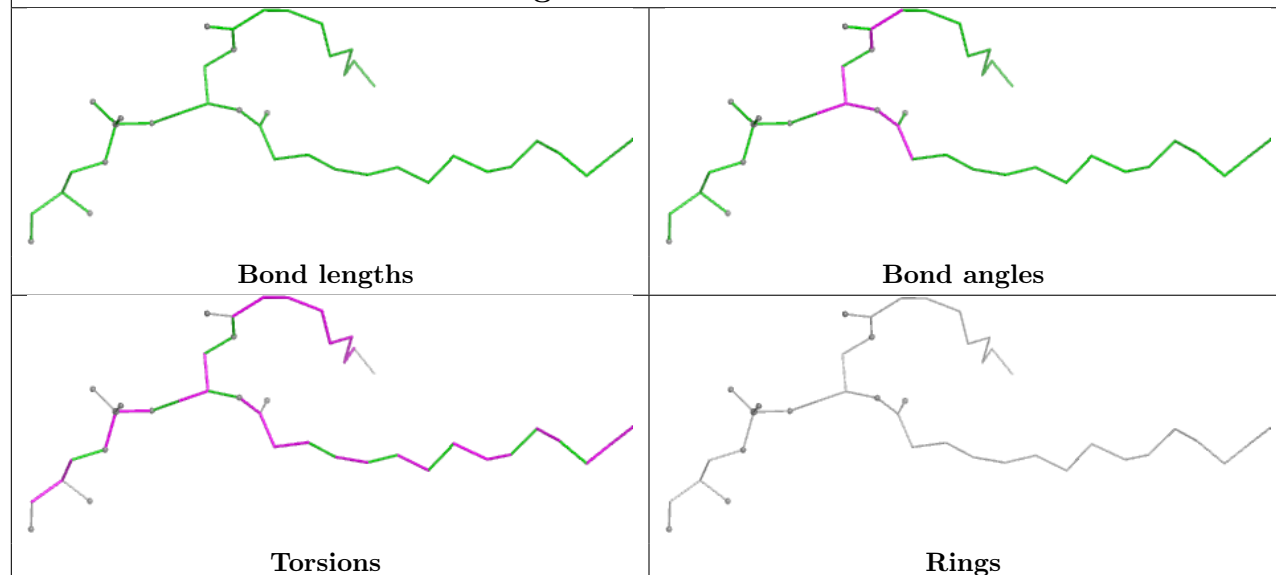
Ligand CHL N 609

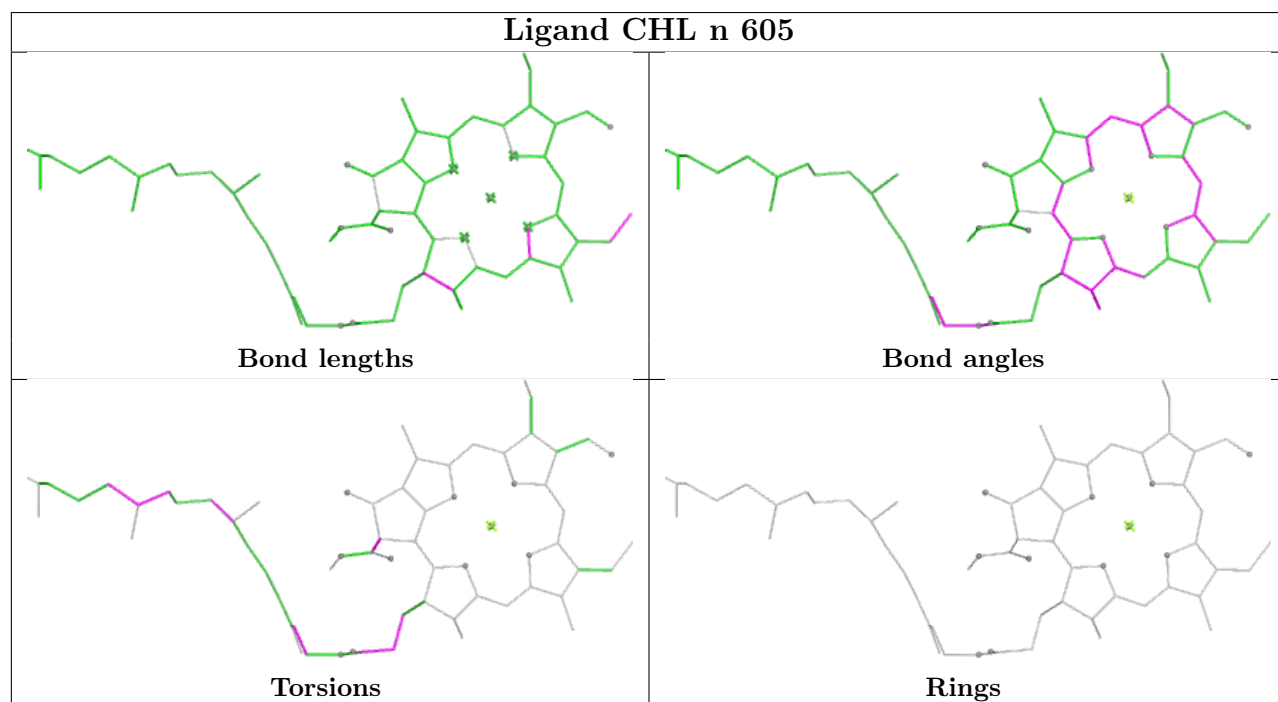
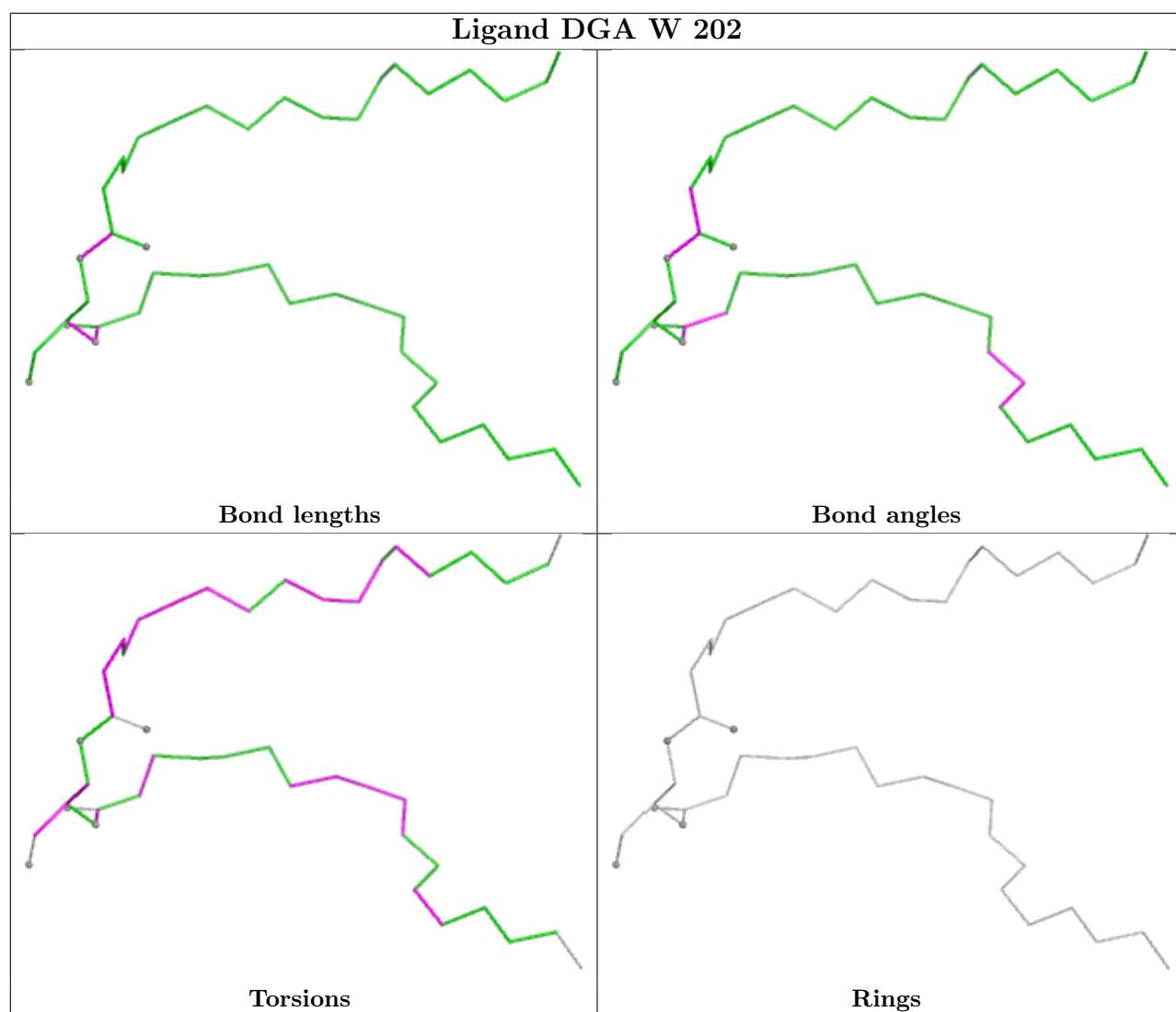


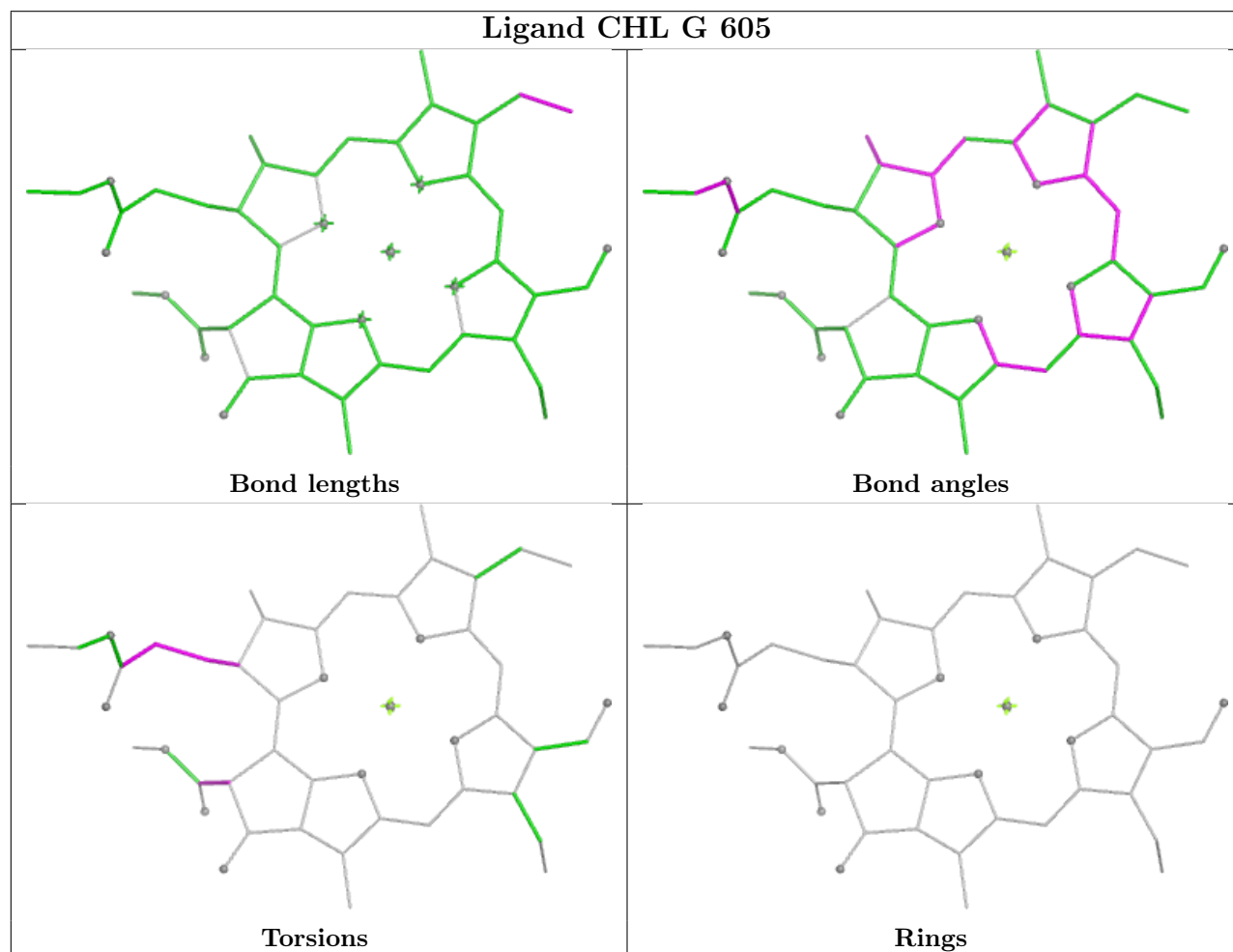
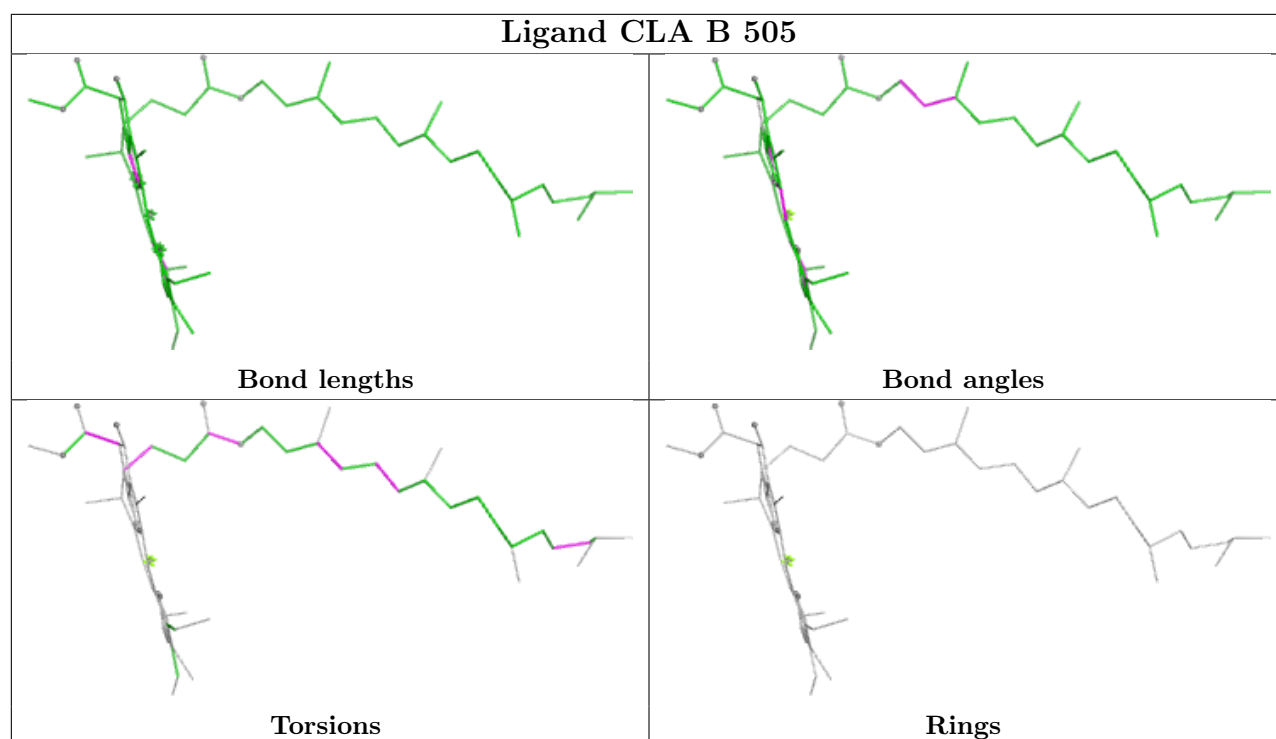
Ligand CLA c 503

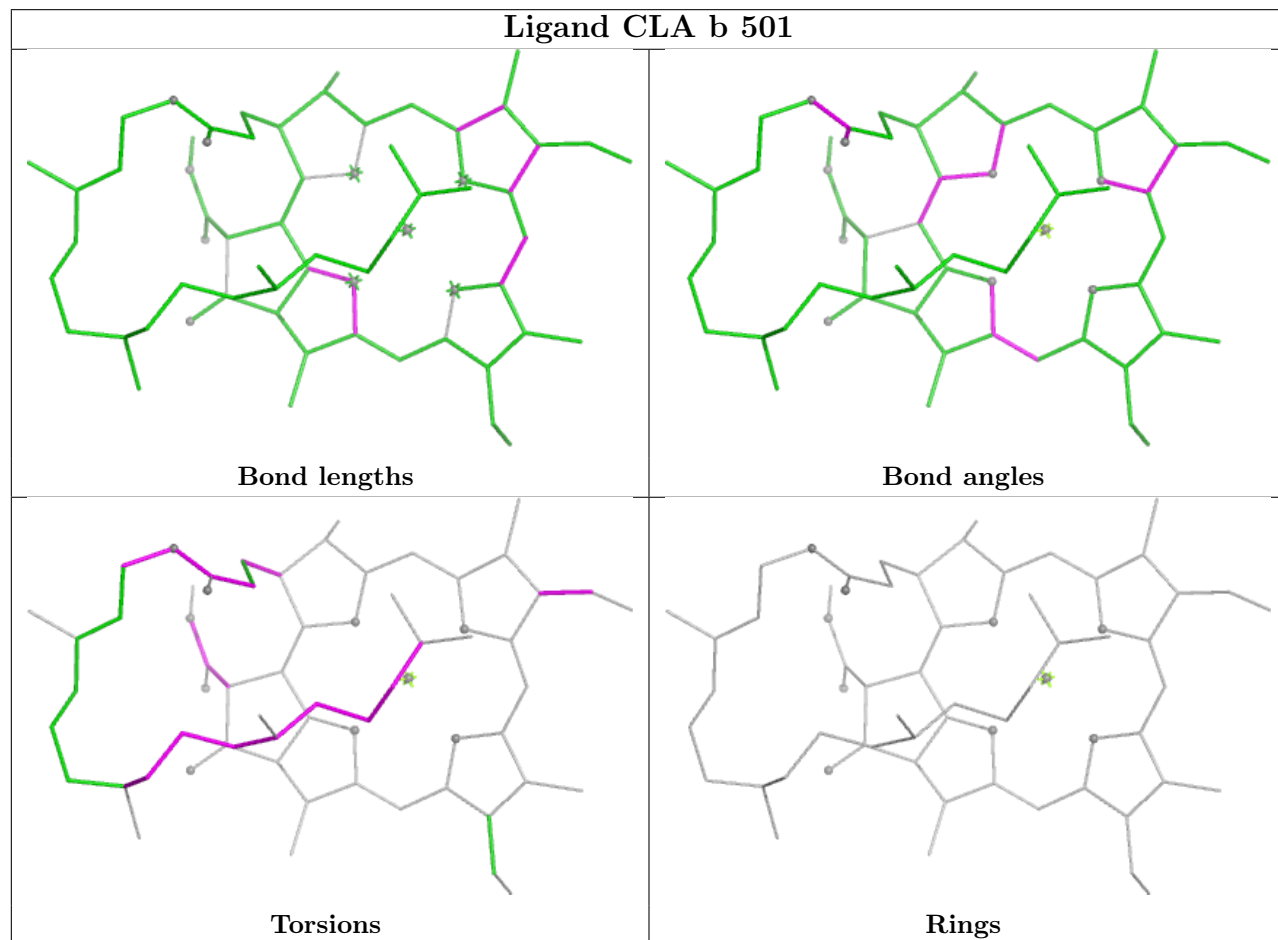
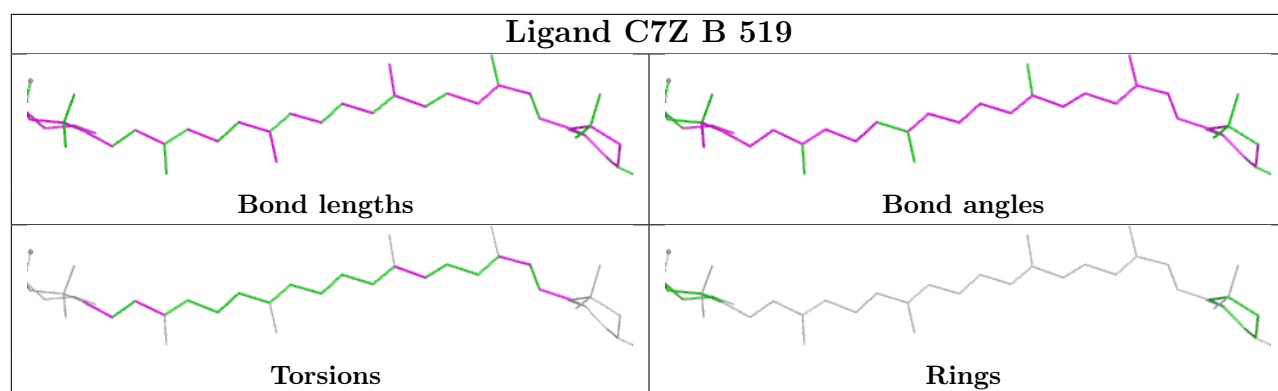


Ligand LHG n 617

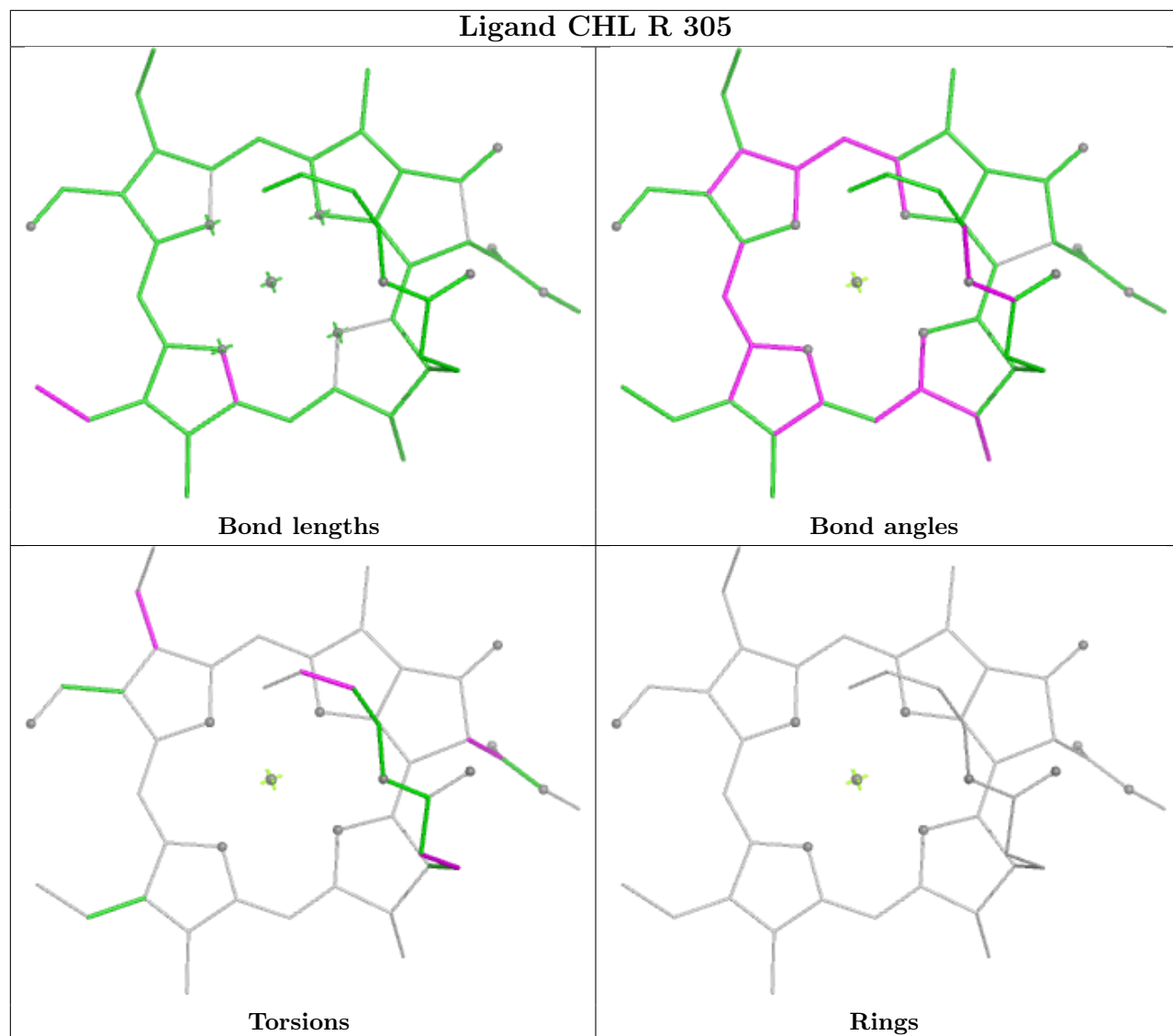


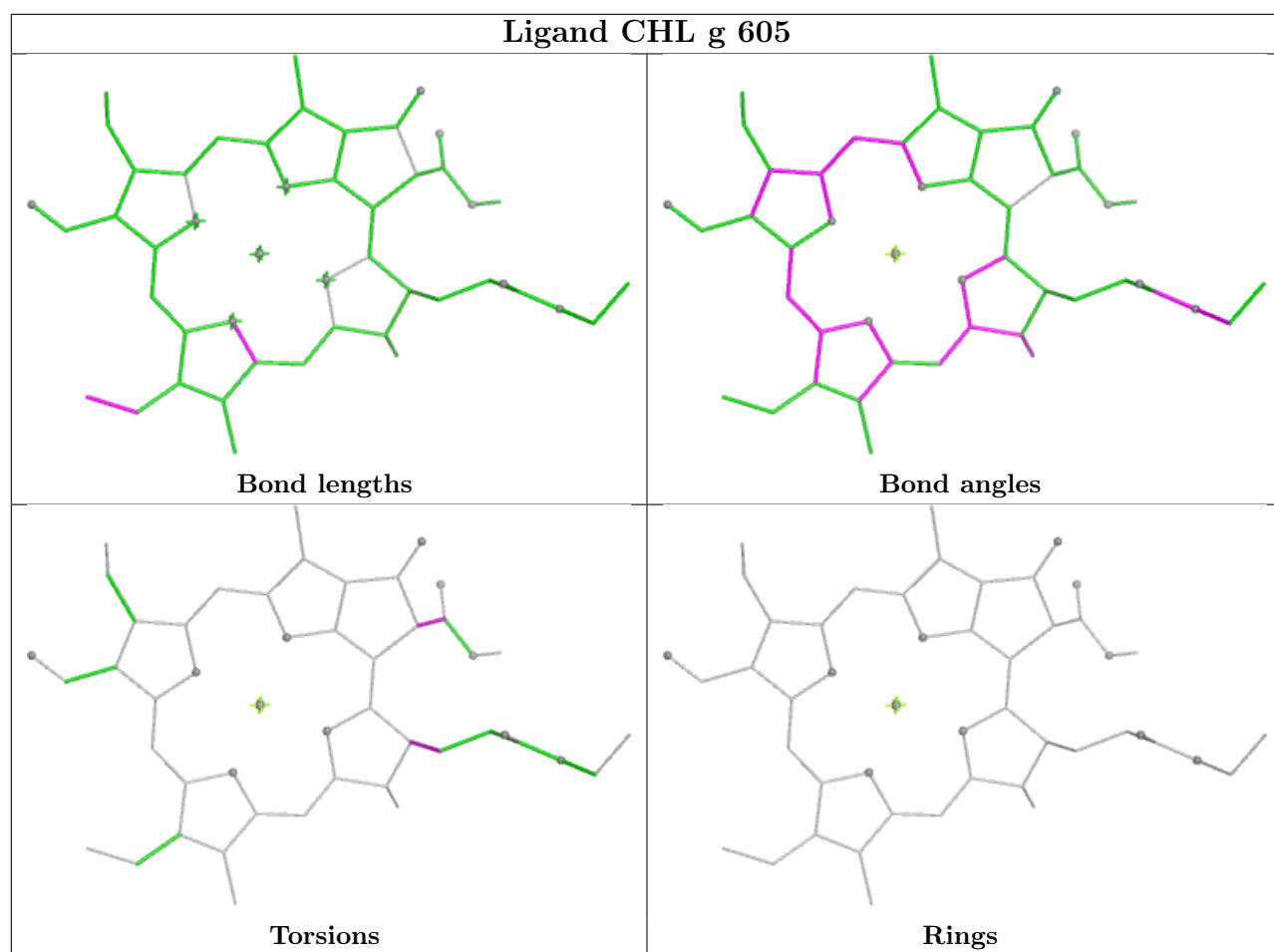


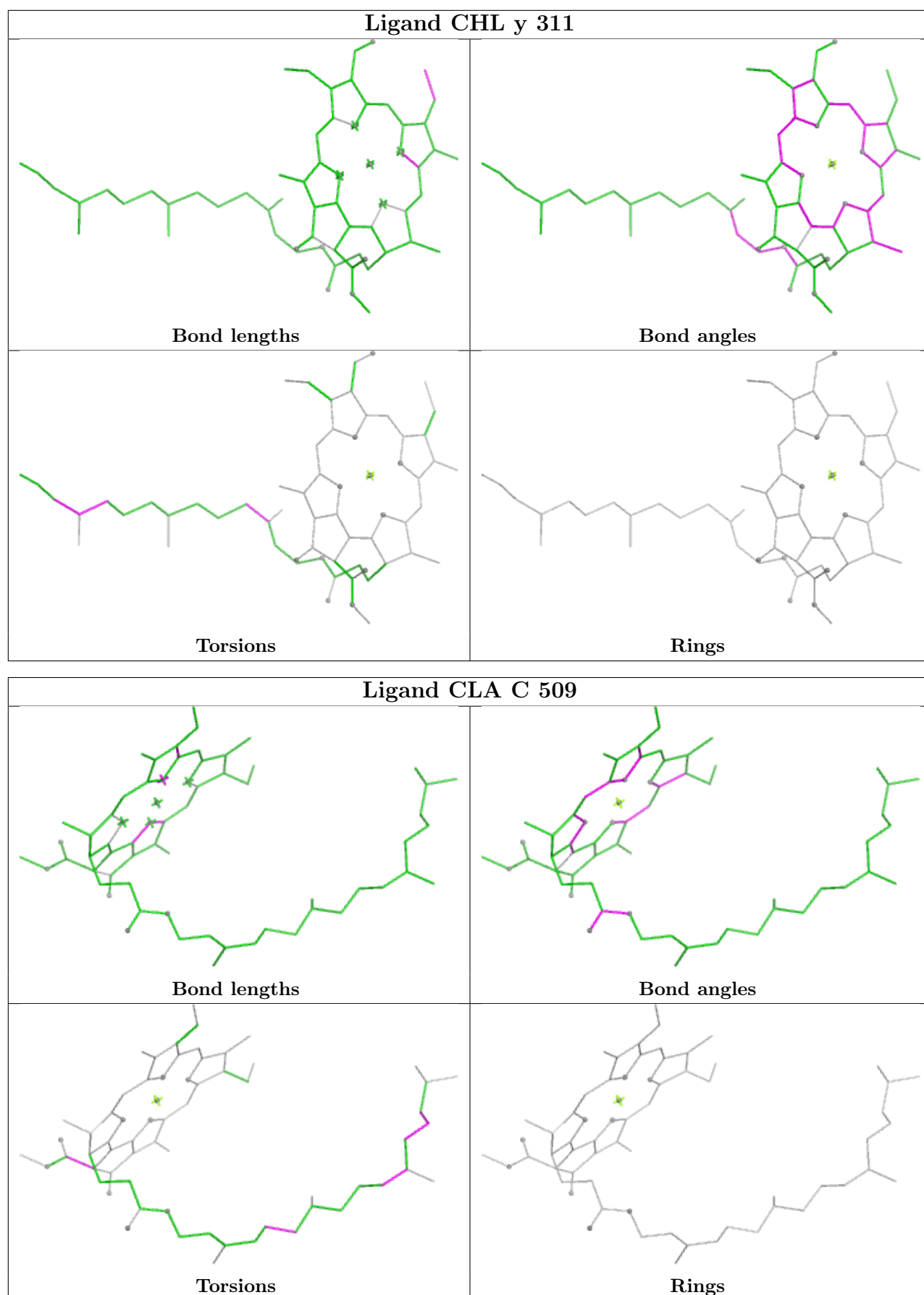


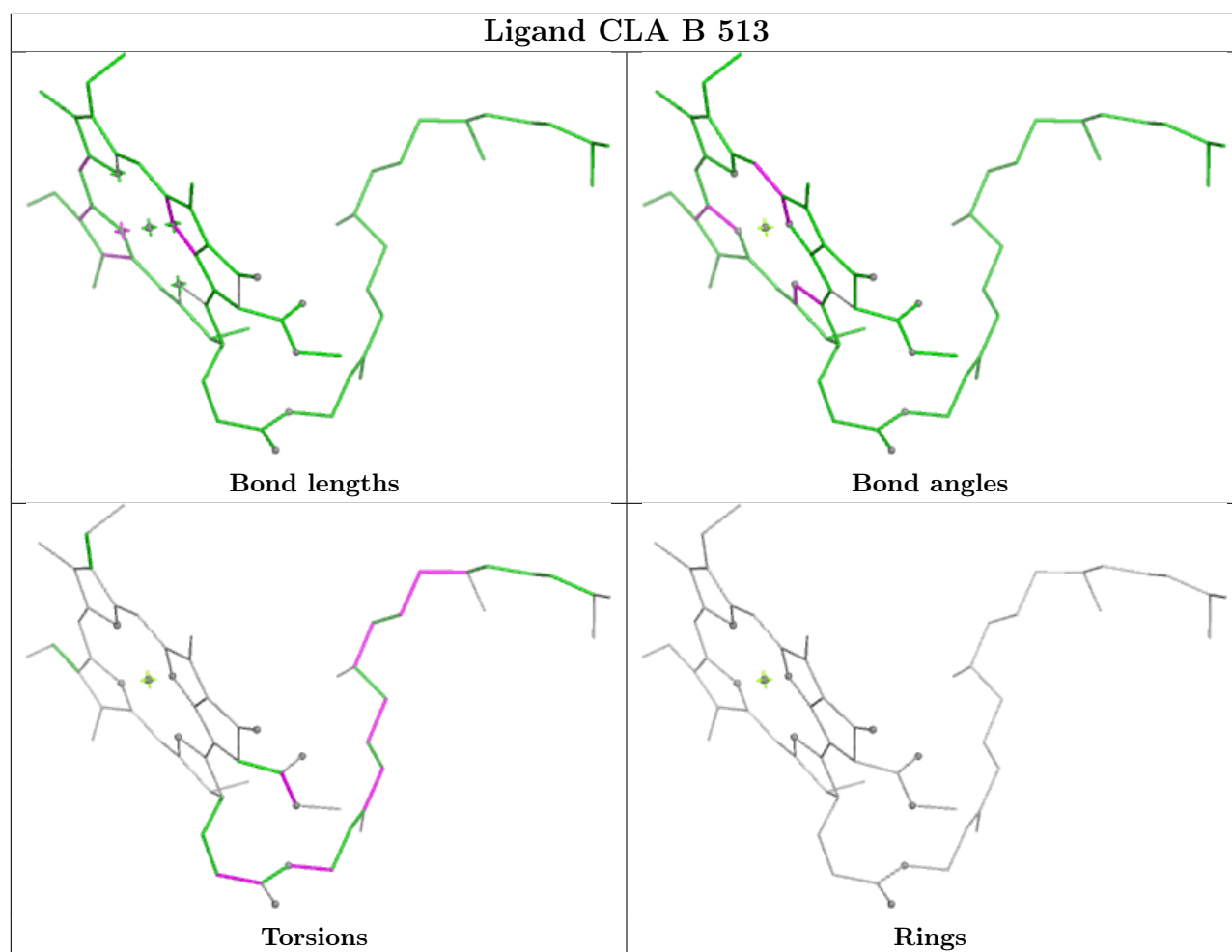


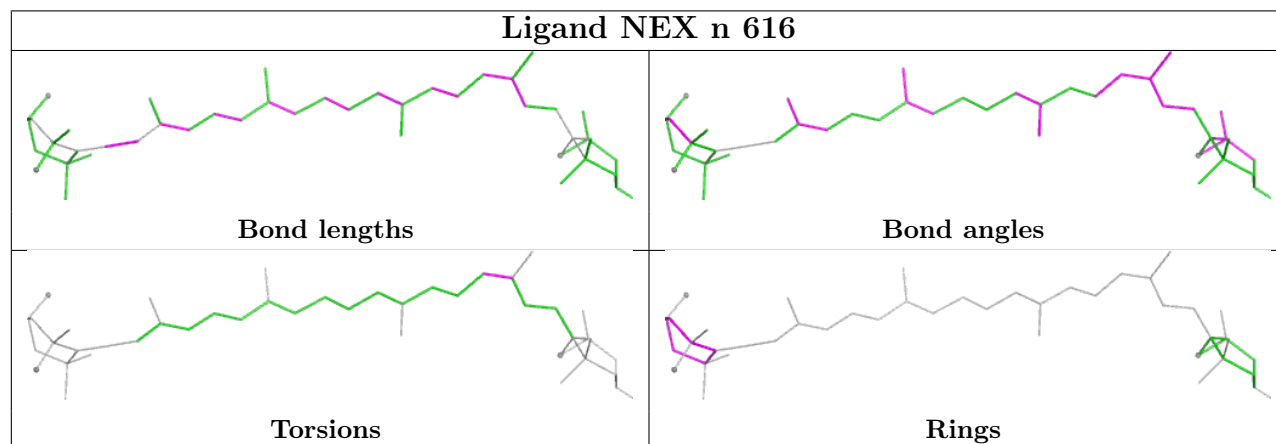
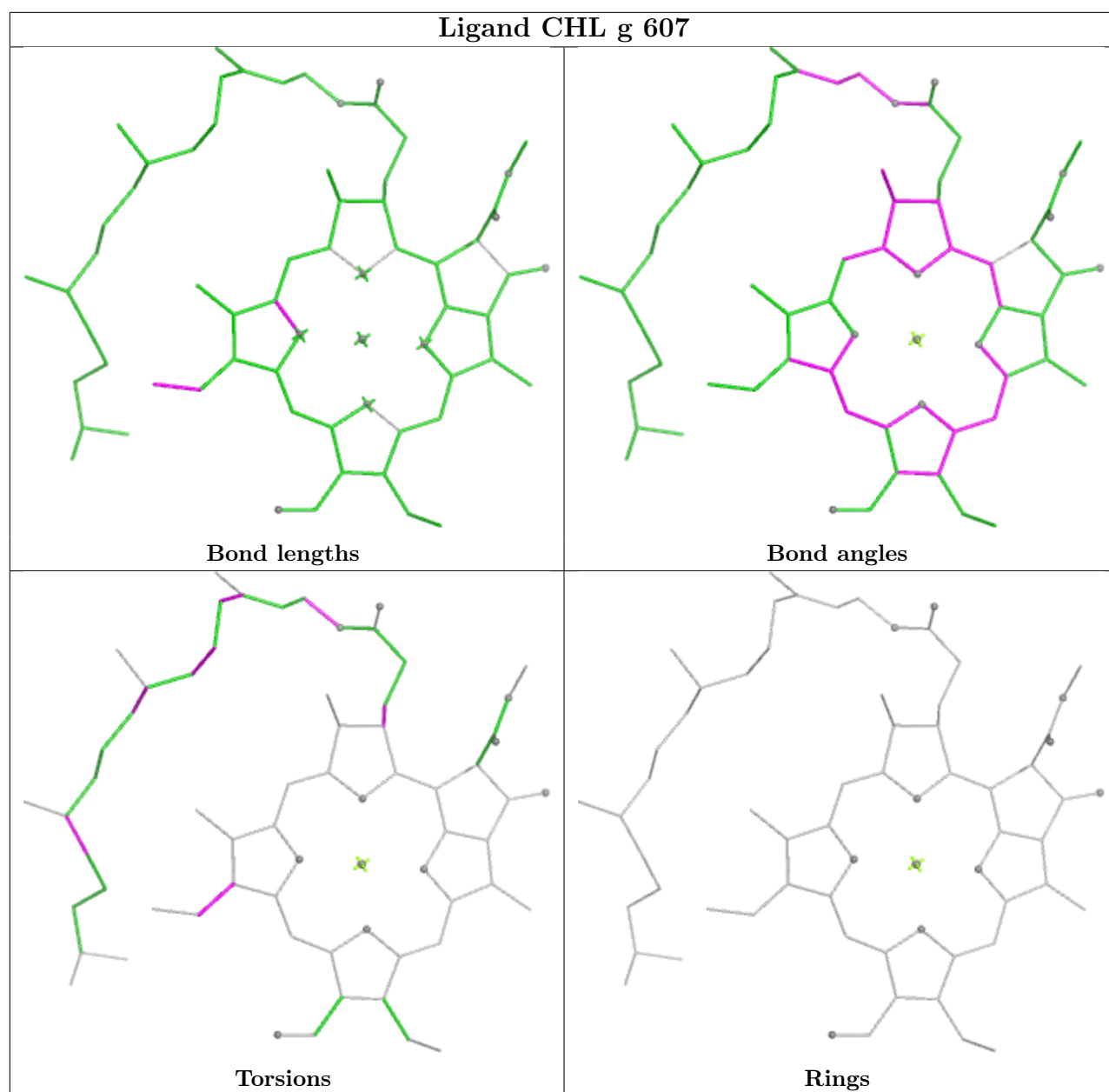
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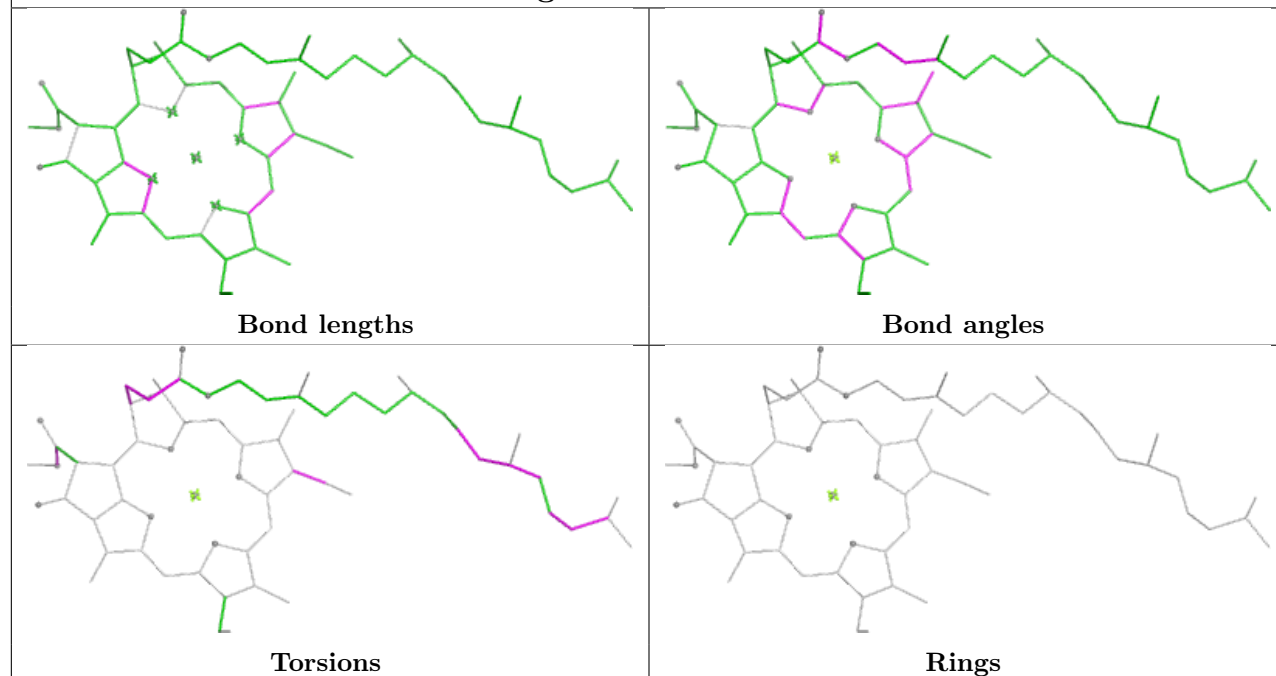
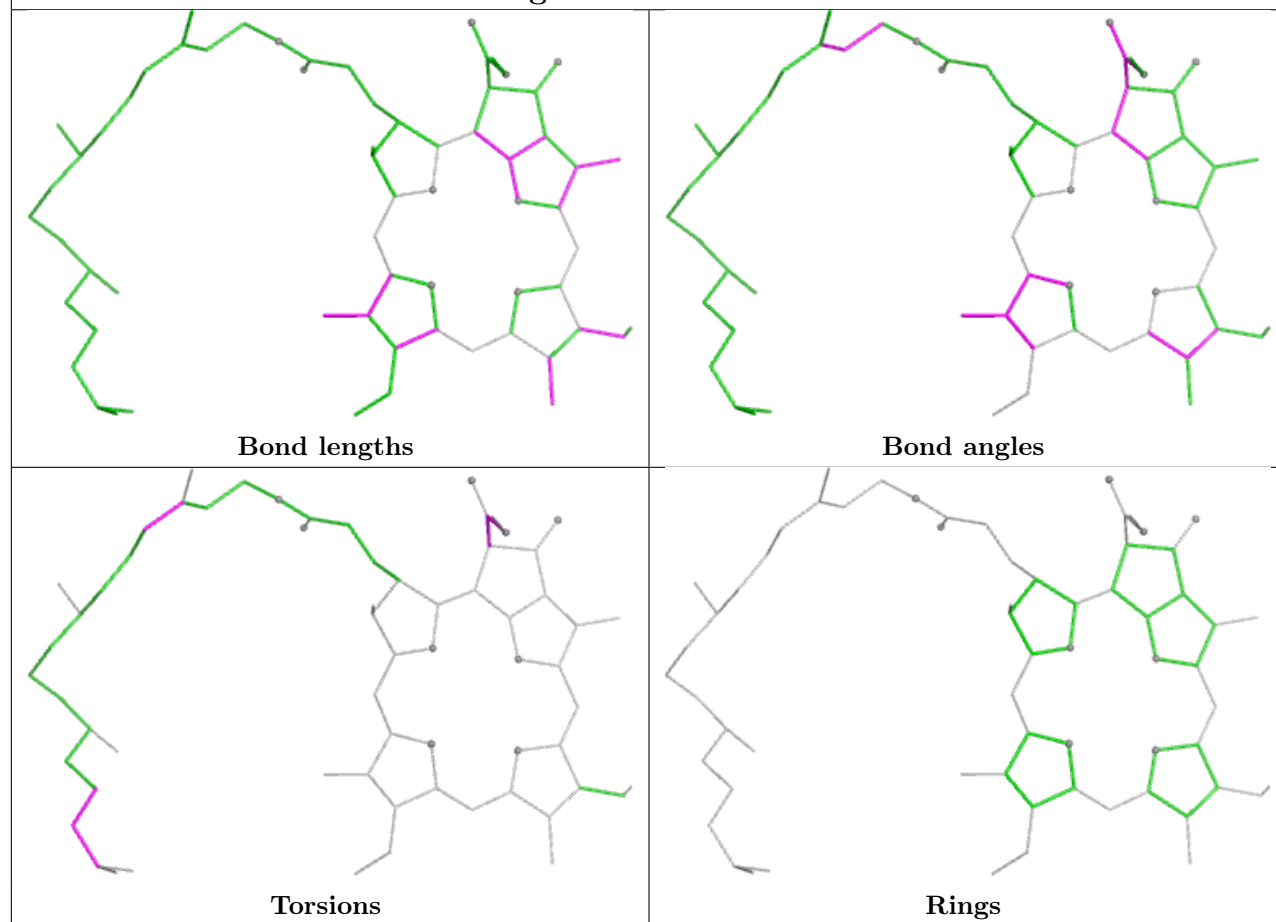


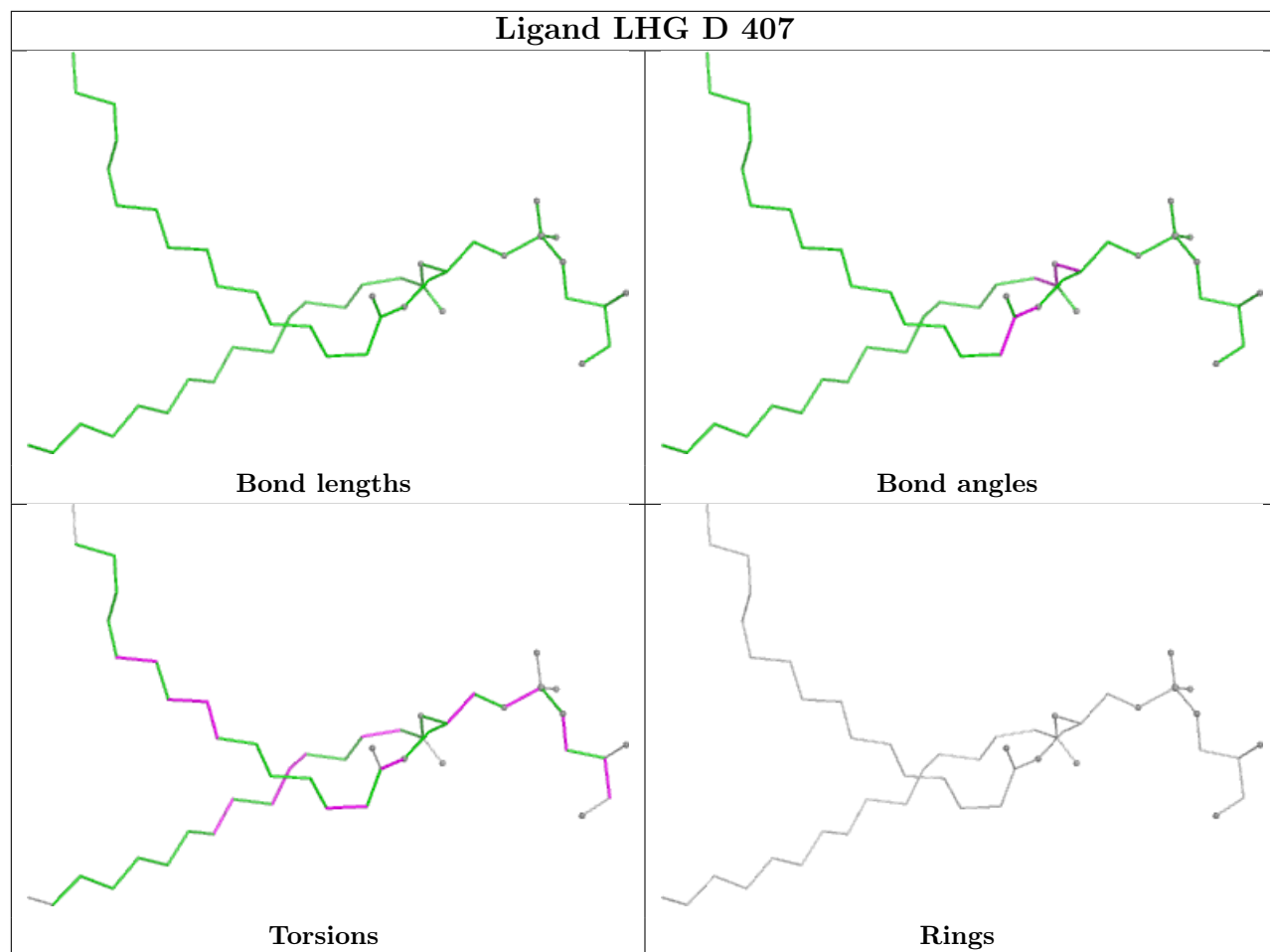


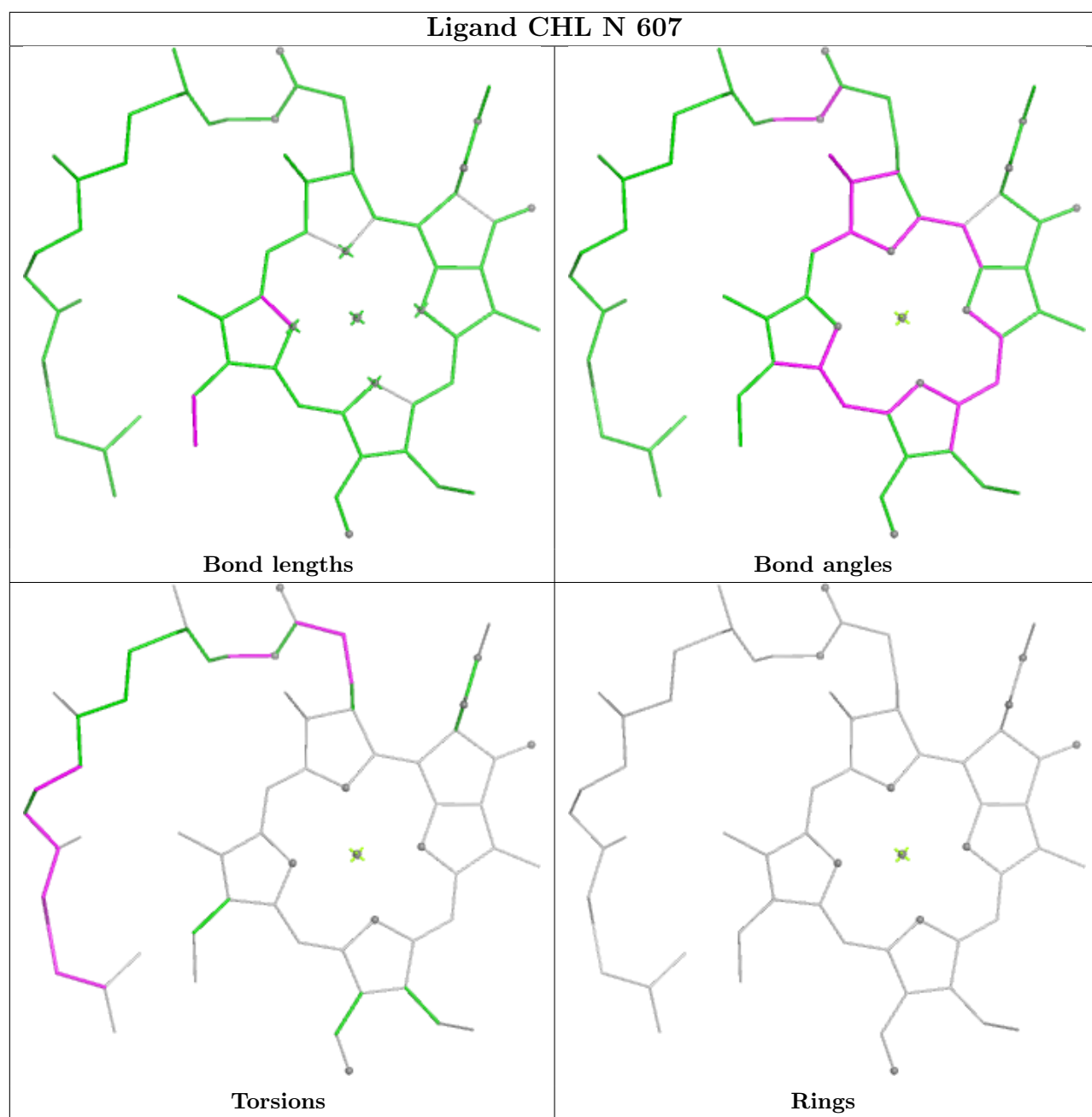


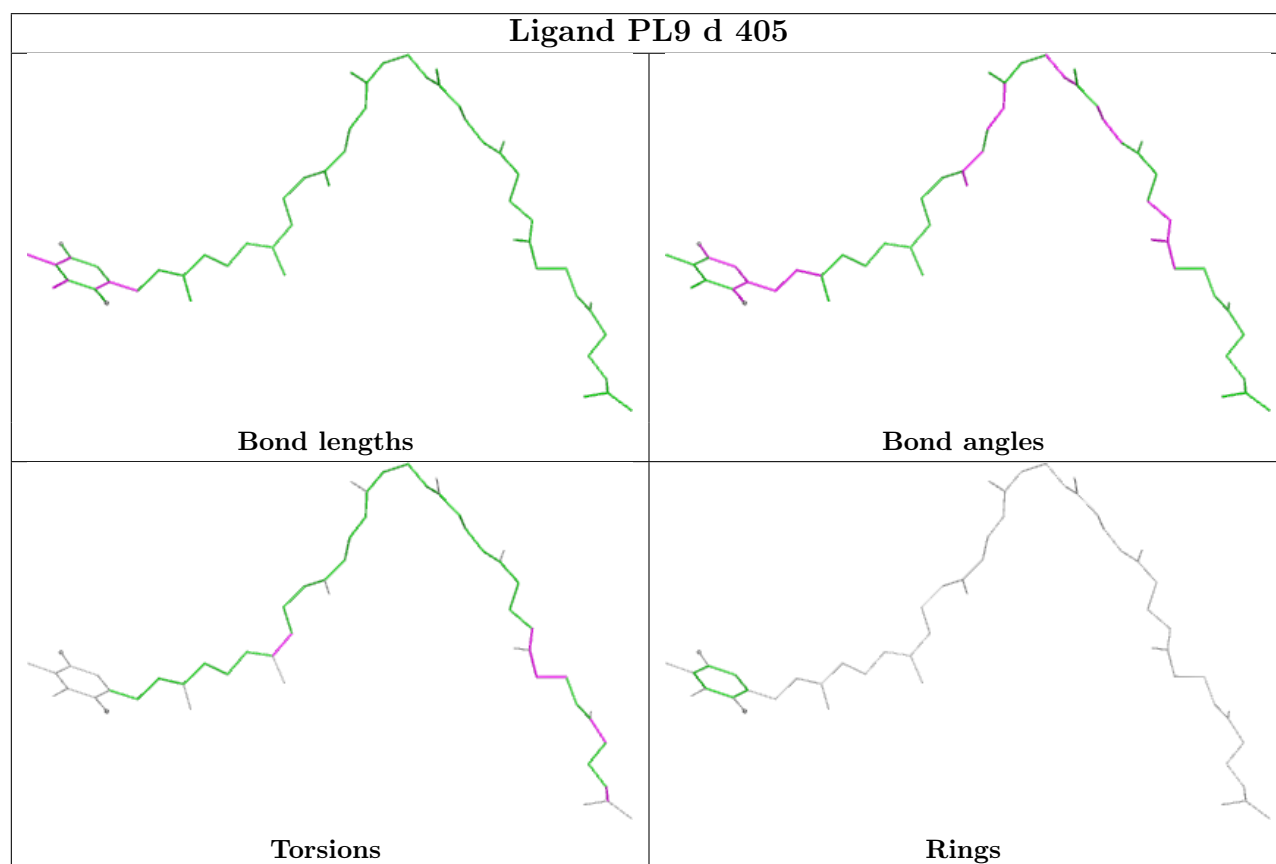
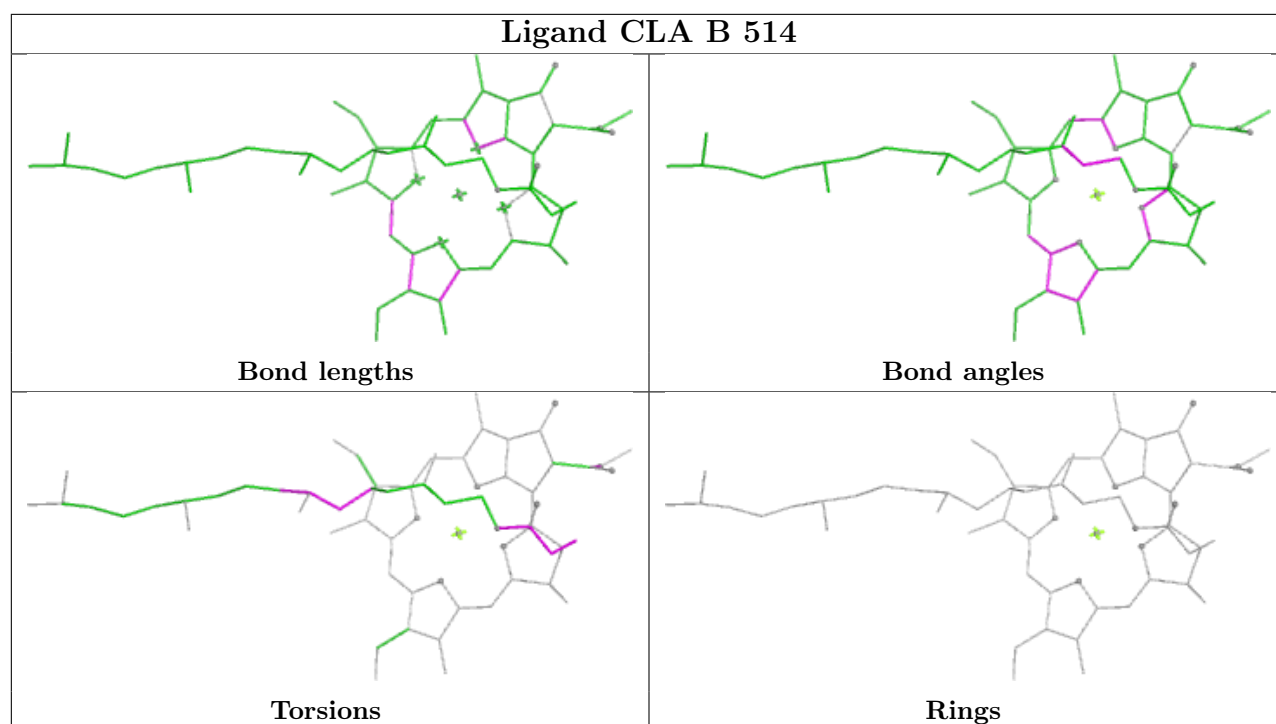




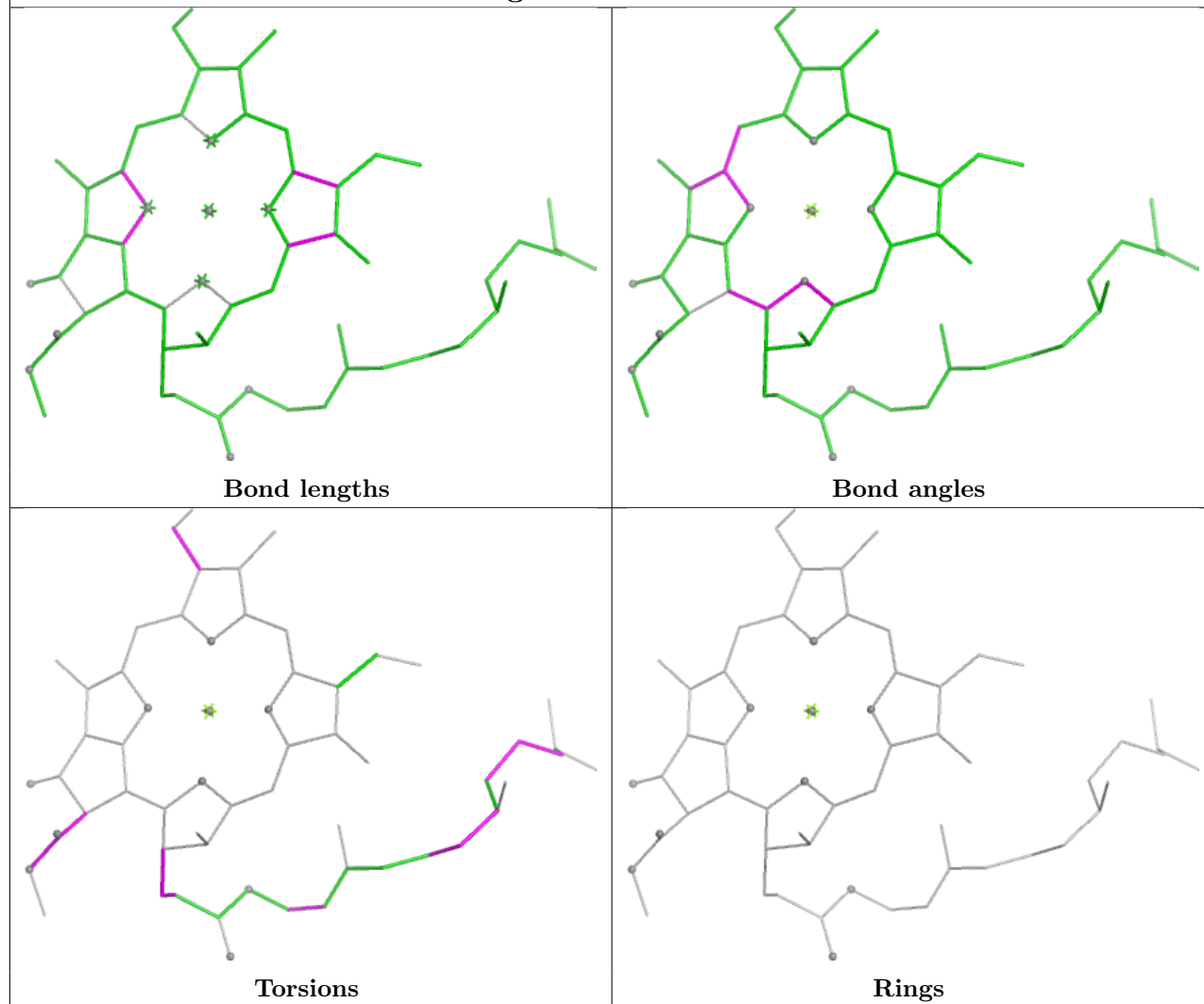
Ligand CLA c 501**Ligand PHO A 408**



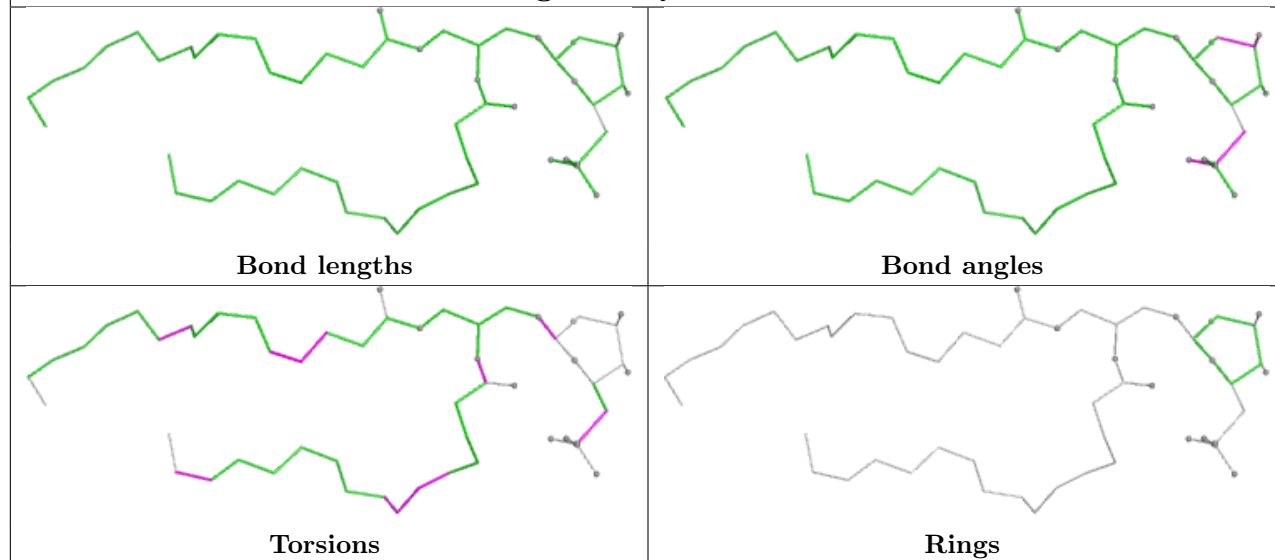


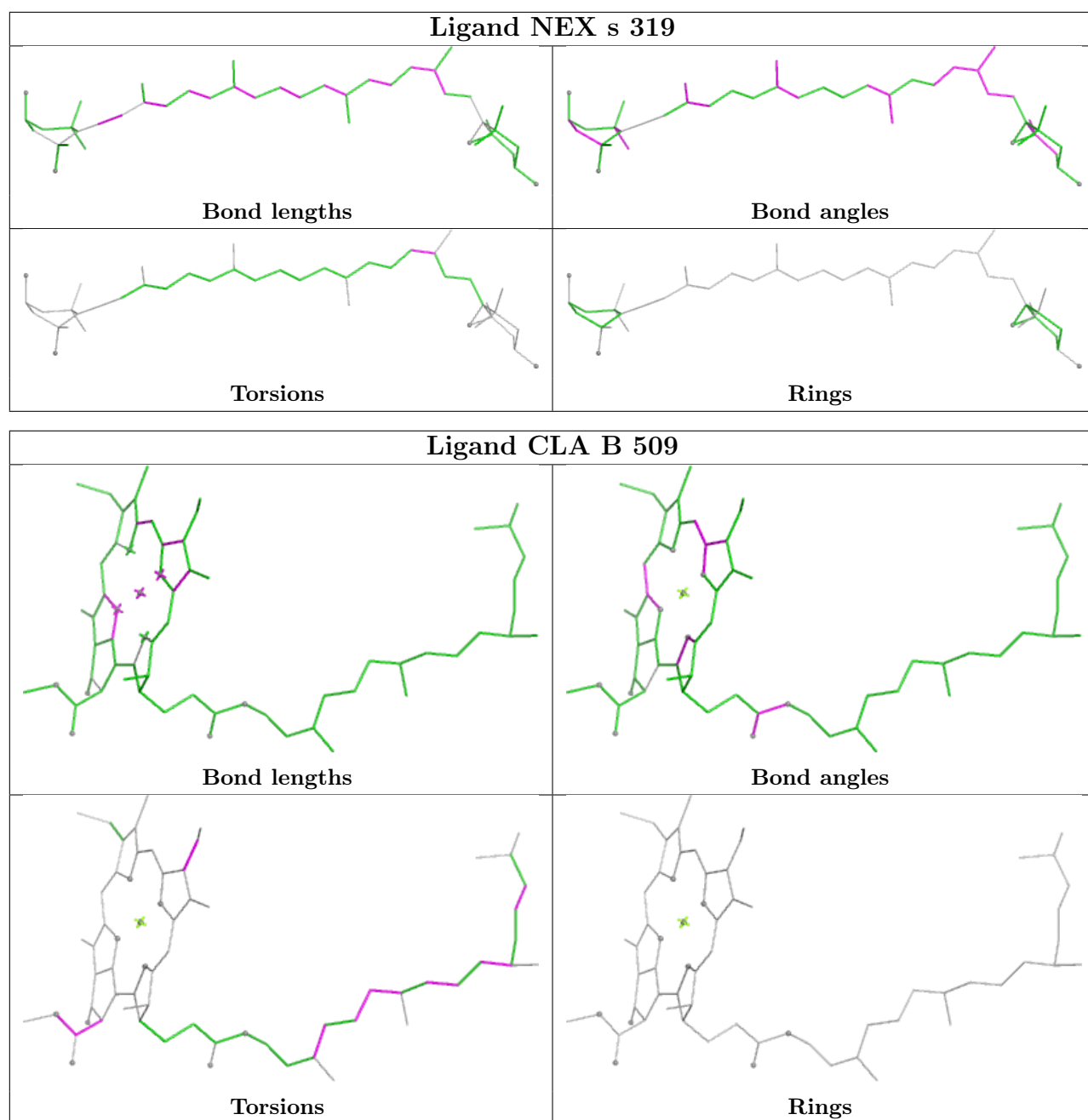


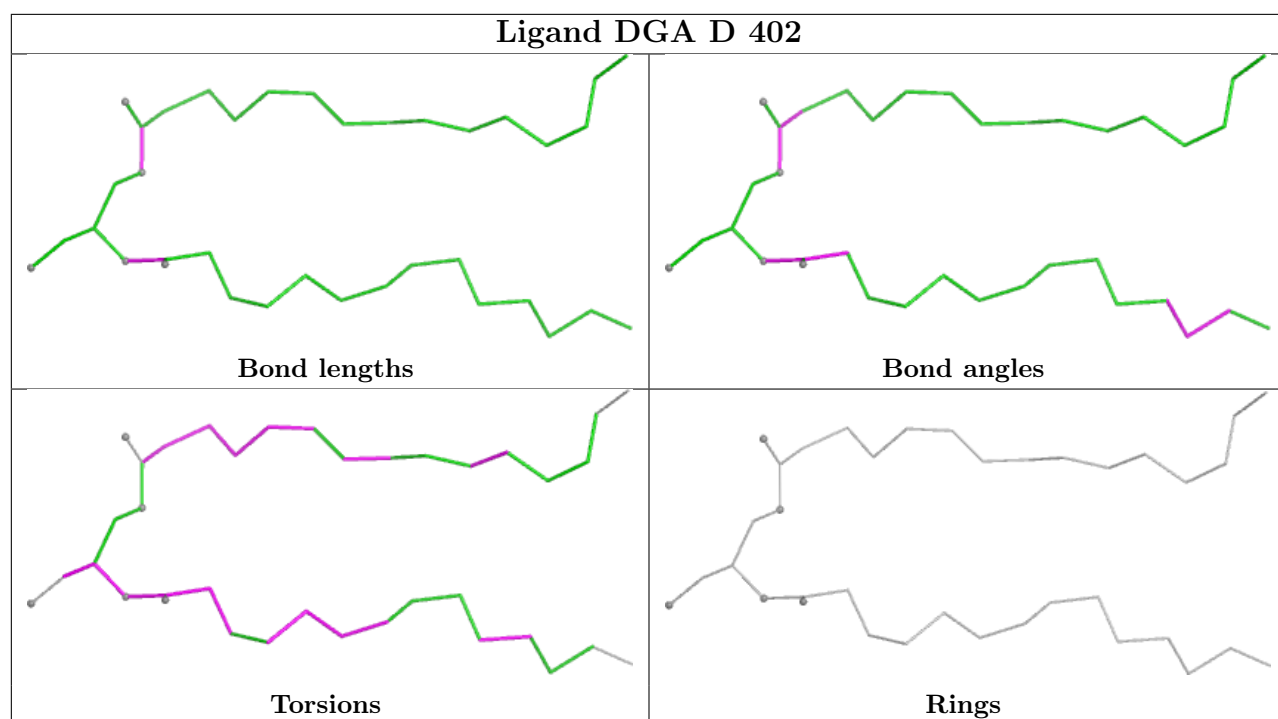
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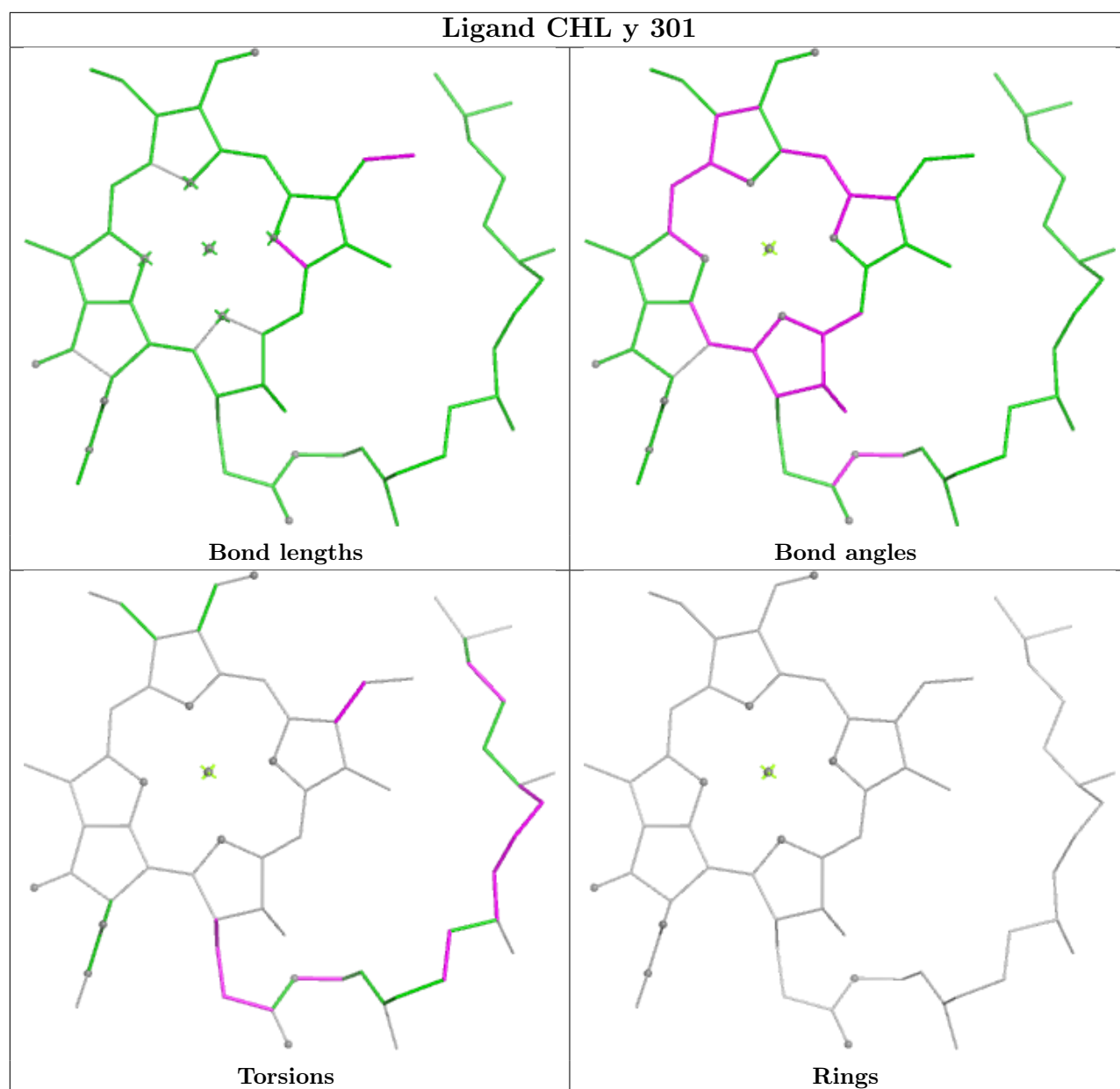


Ligand SQD o 301

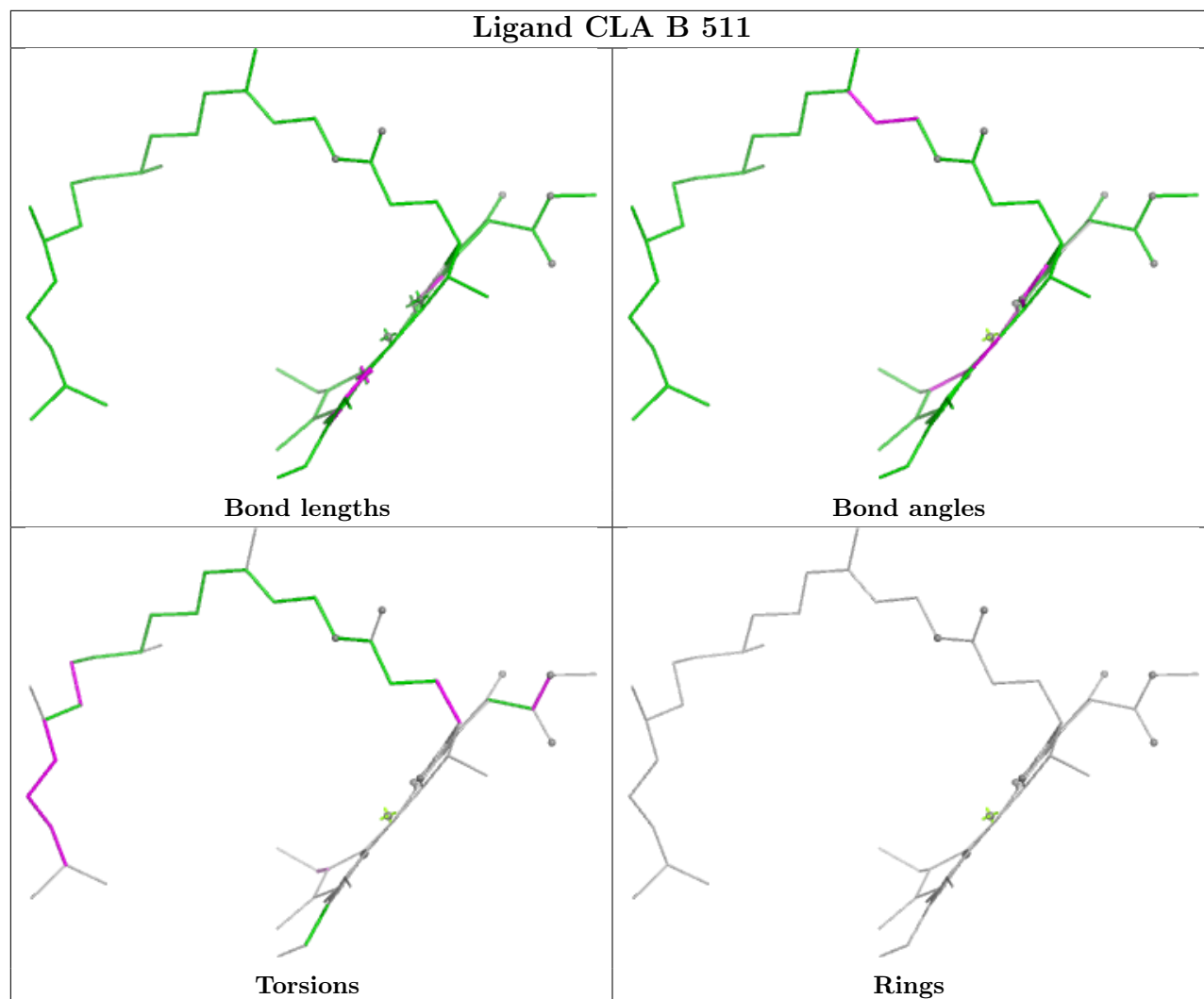




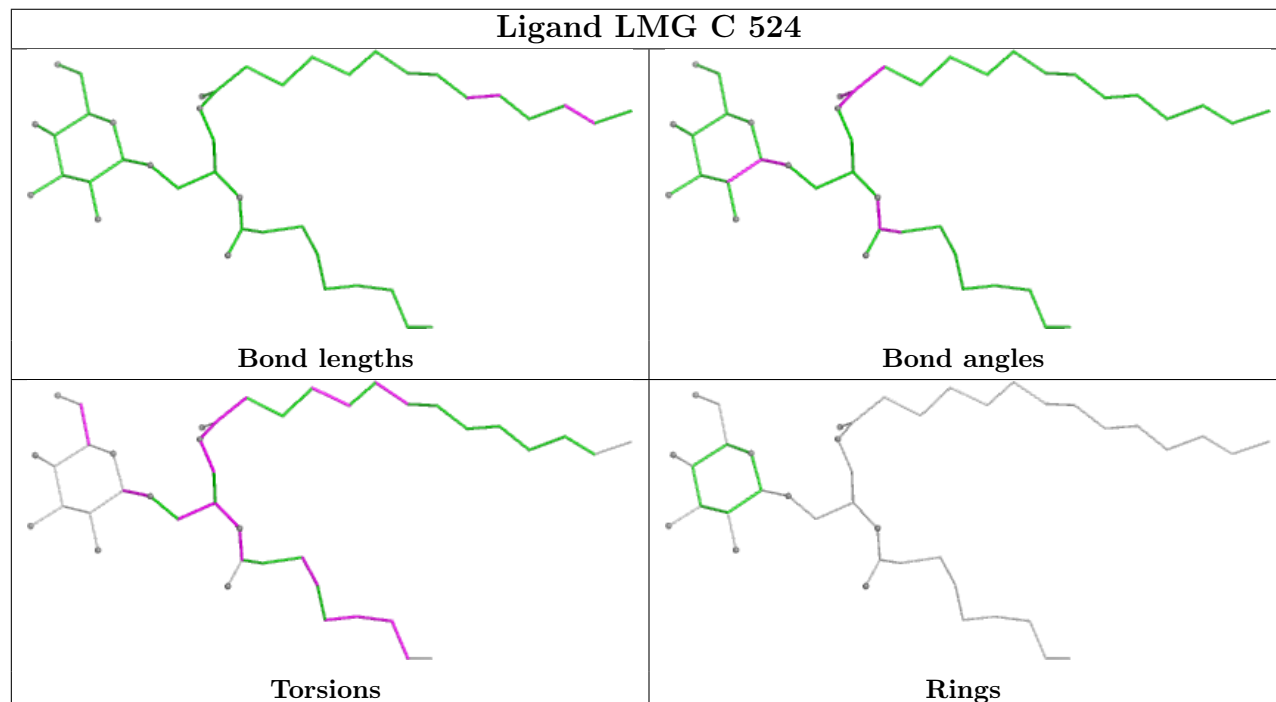




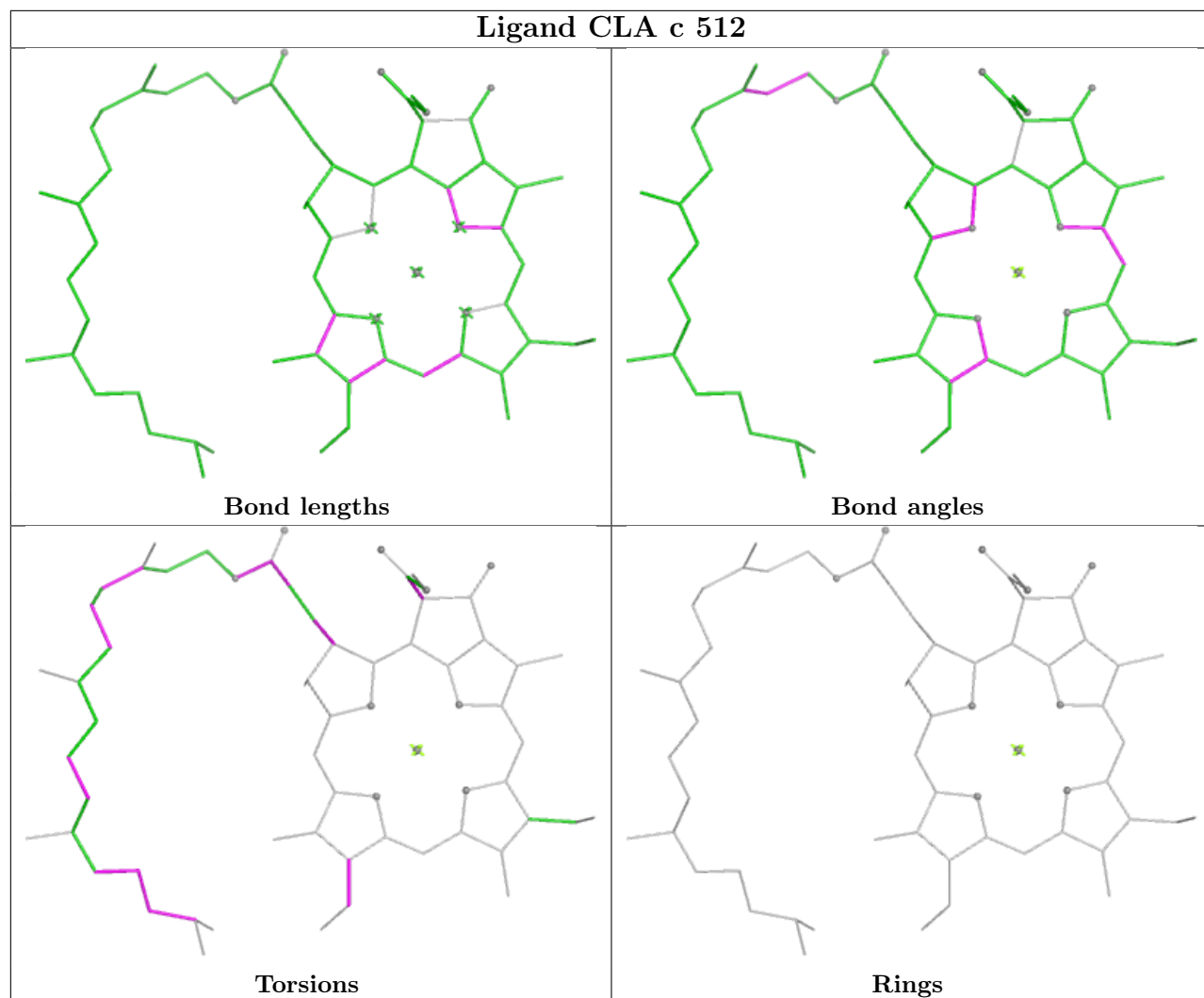
Ligand CLA B 511



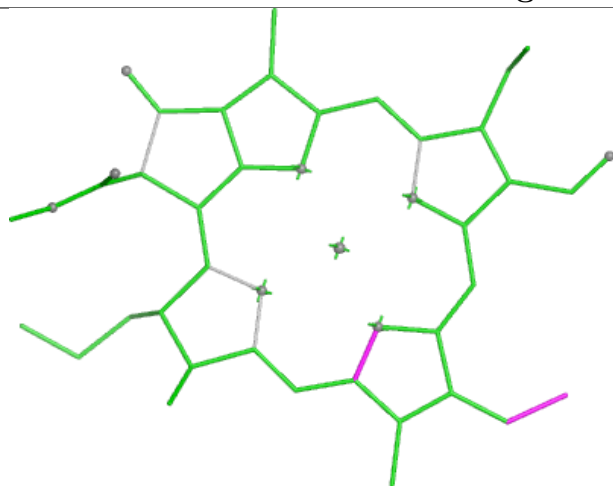
Ligand LMG C 524



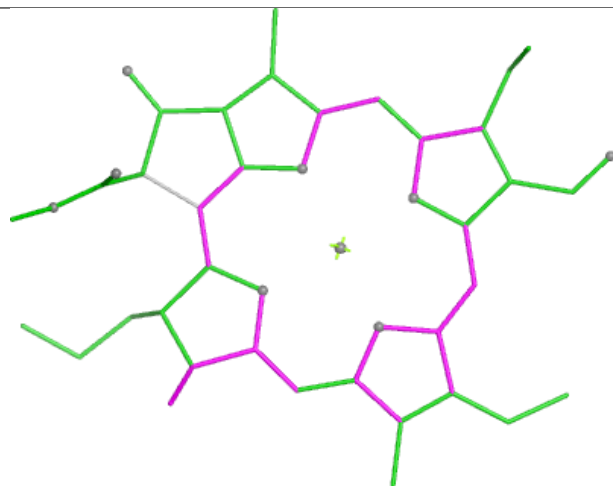
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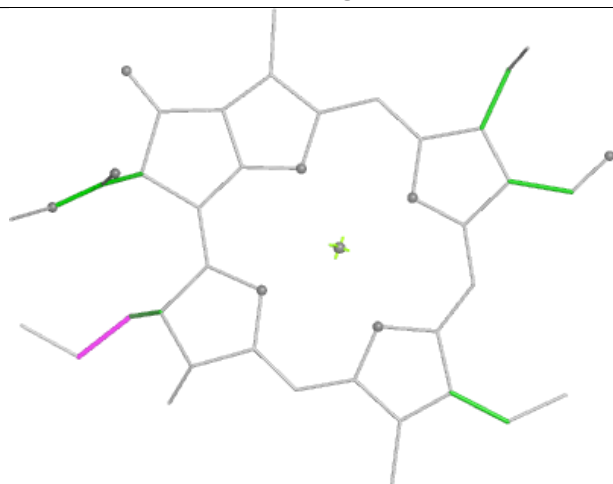
Ligand CHL S 307



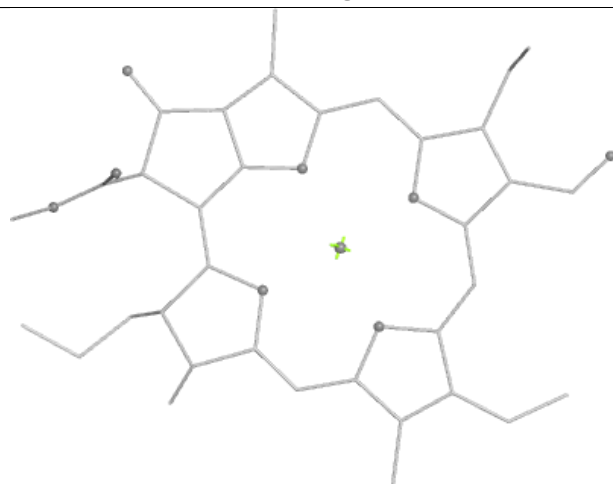
Bond lengths



Bond angles

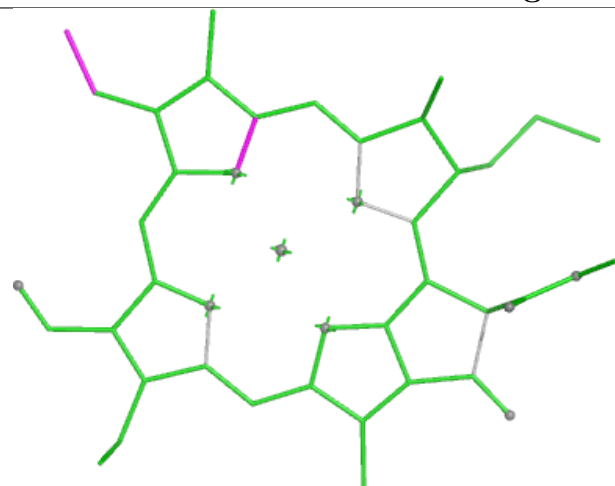


Torsions

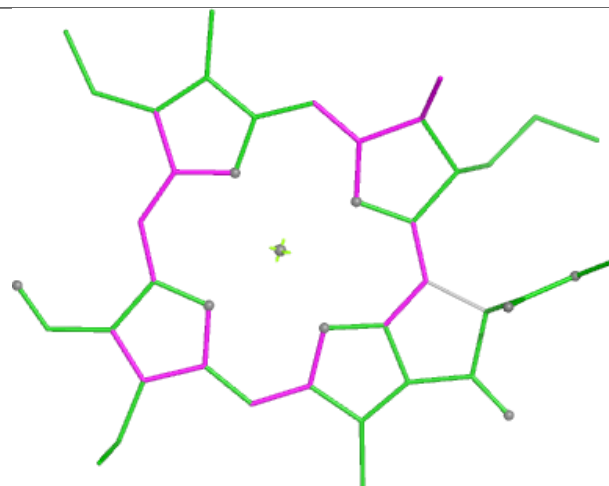


Rings

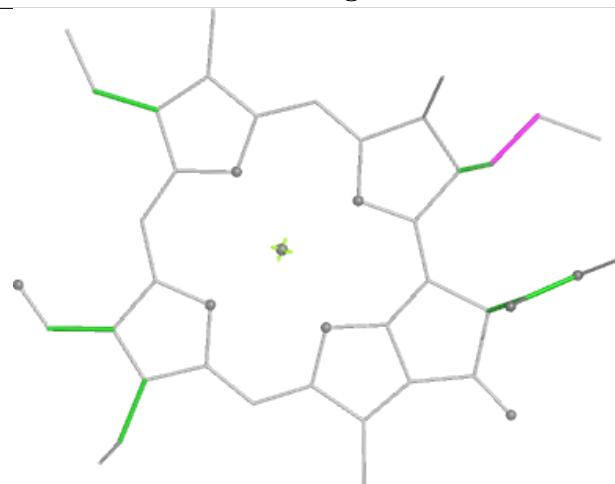
Ligand CHL s 307



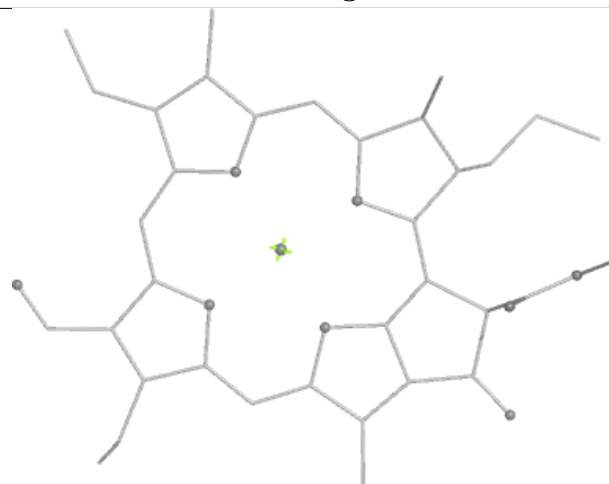
Bond lengths



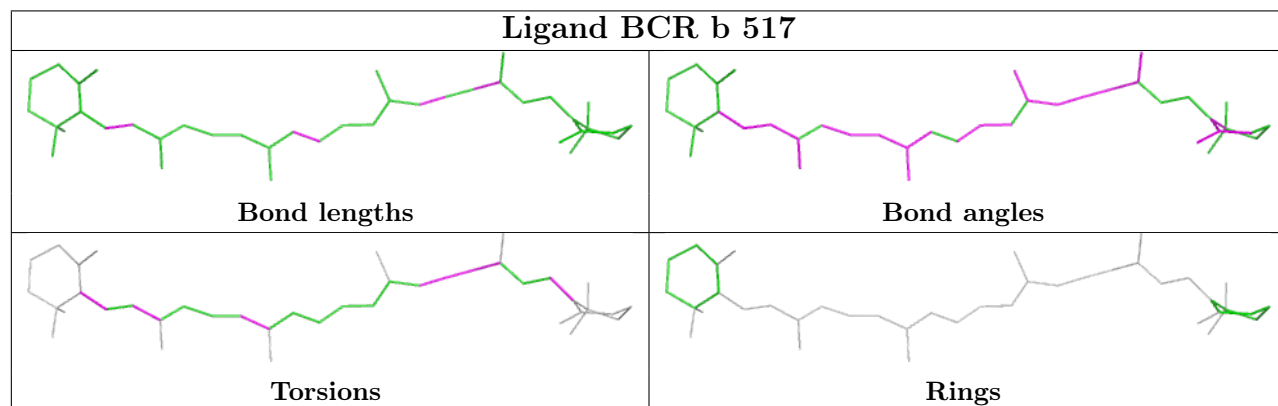
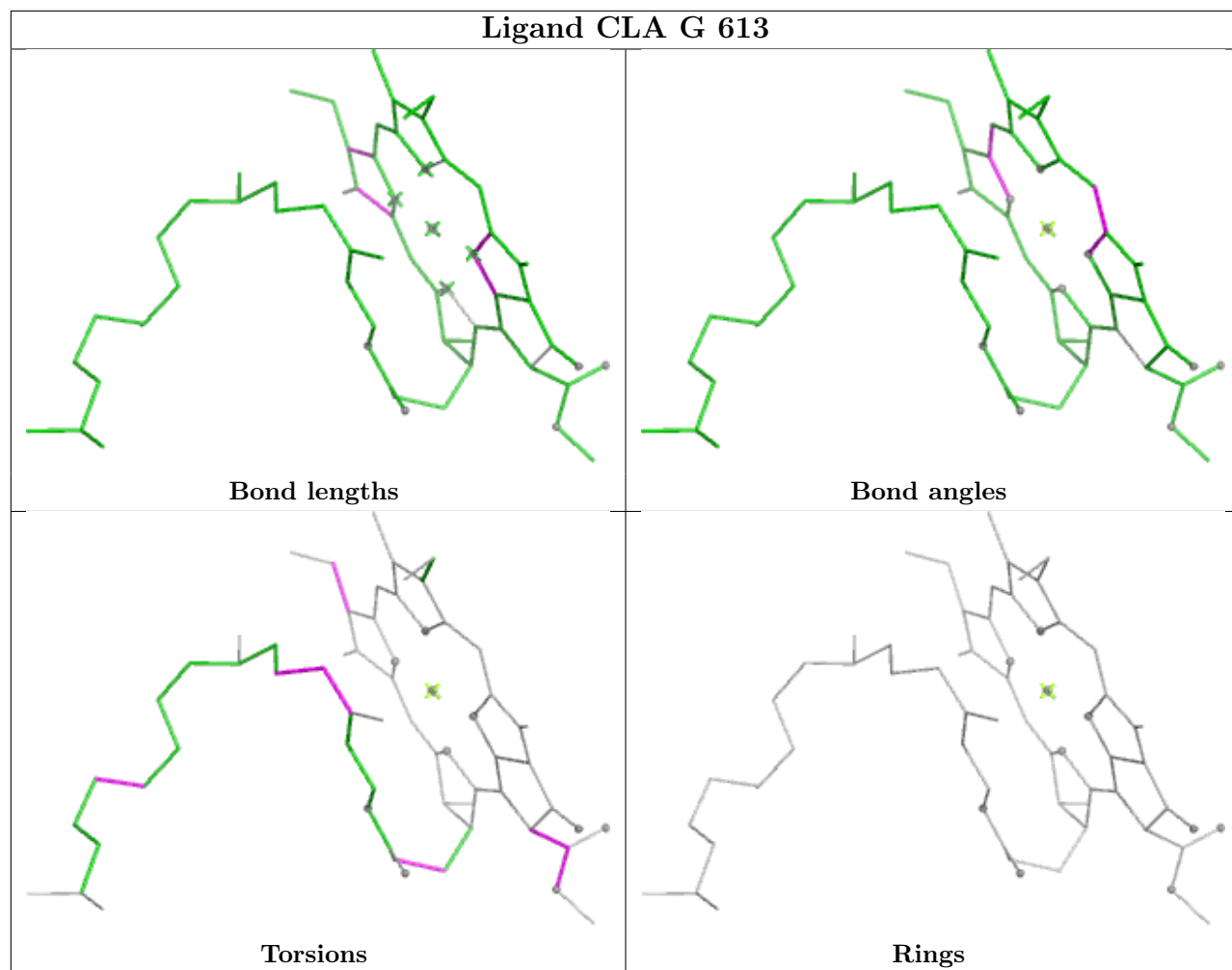
Bond angles

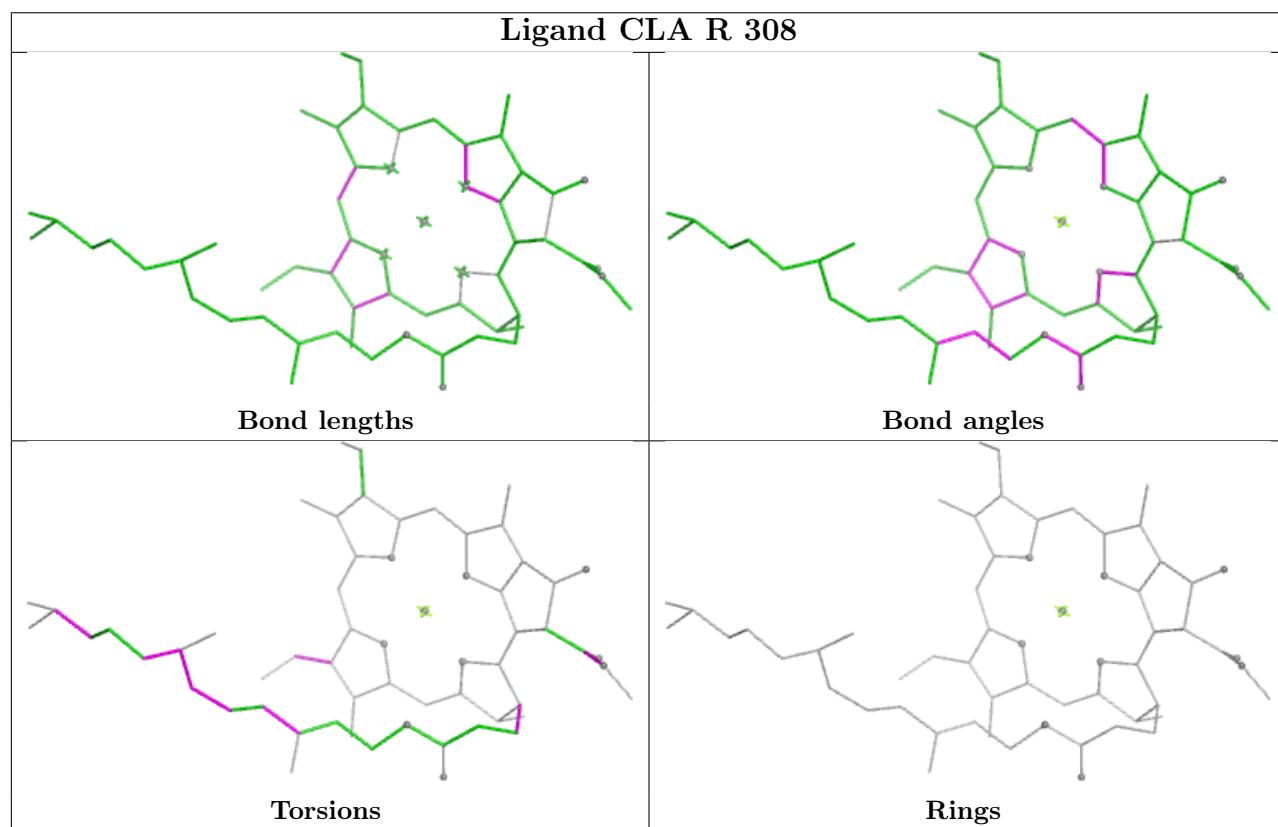
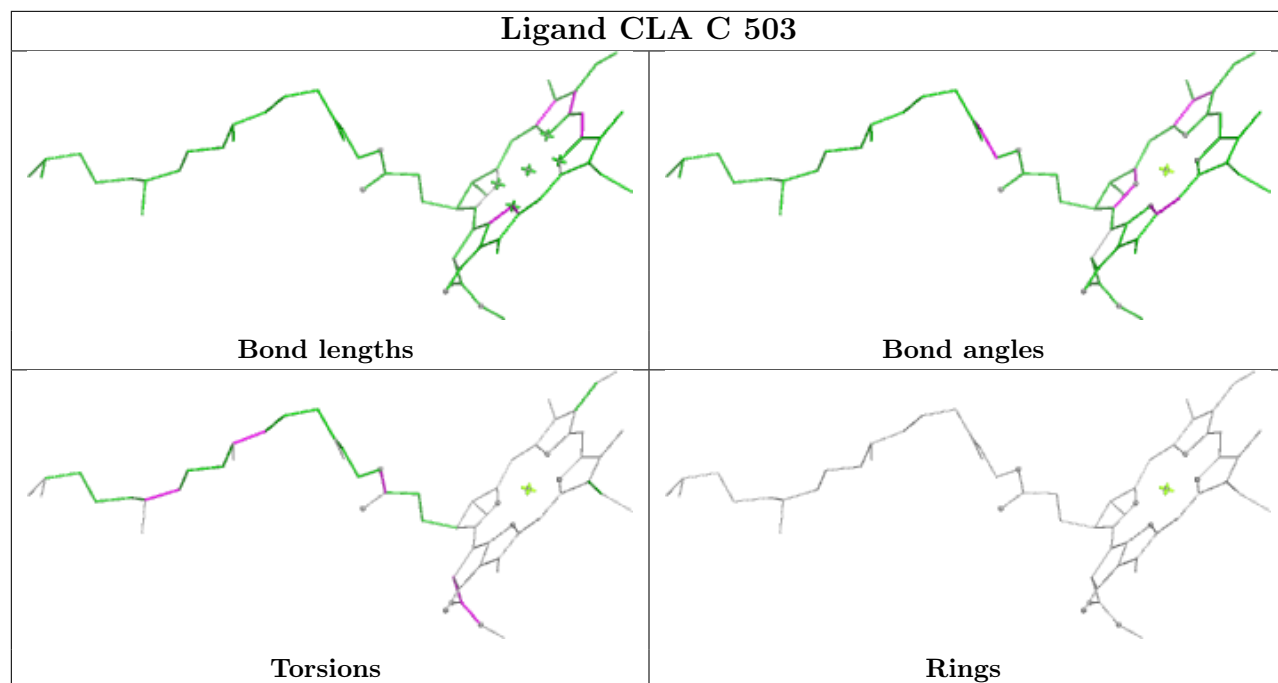


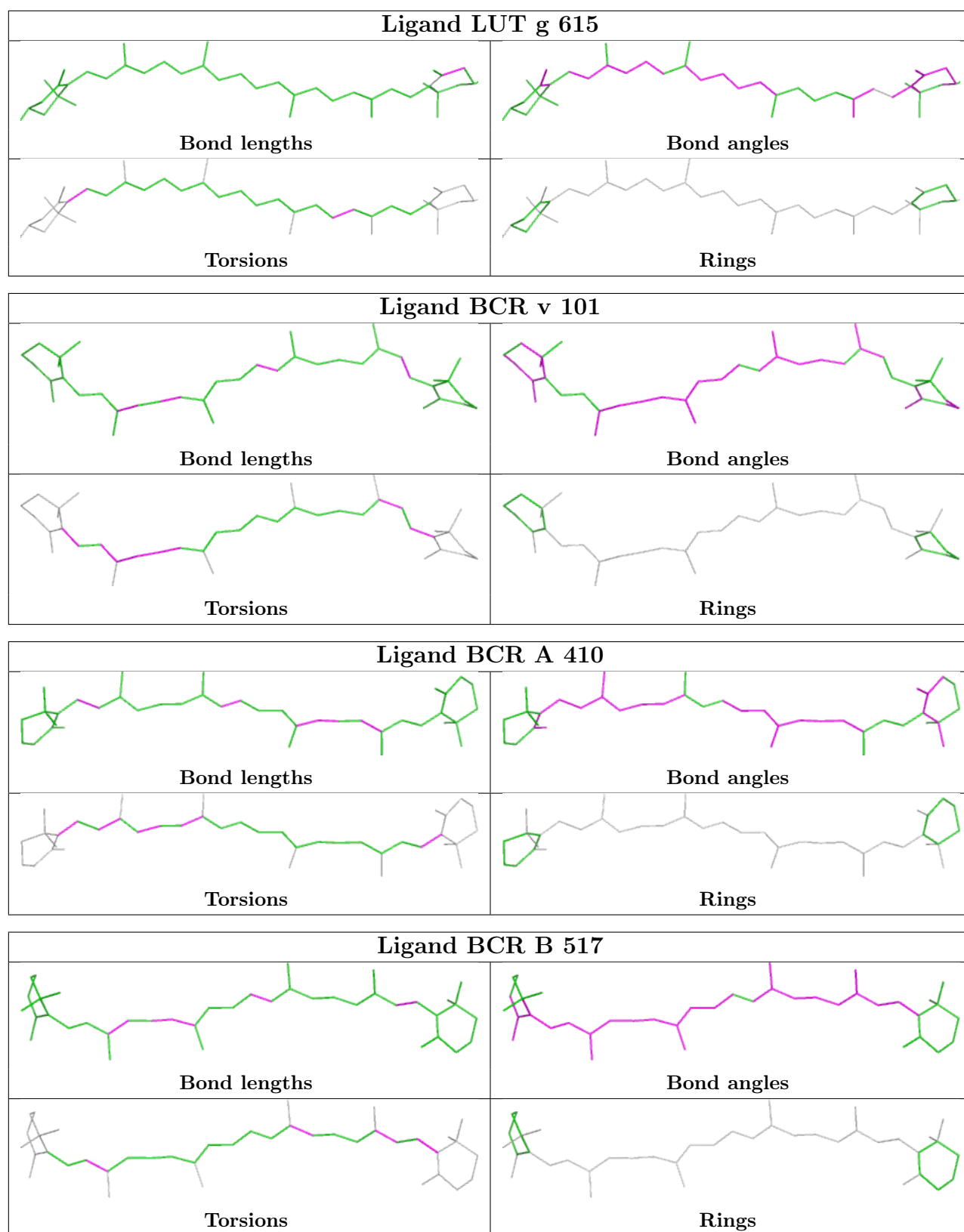
Torsions

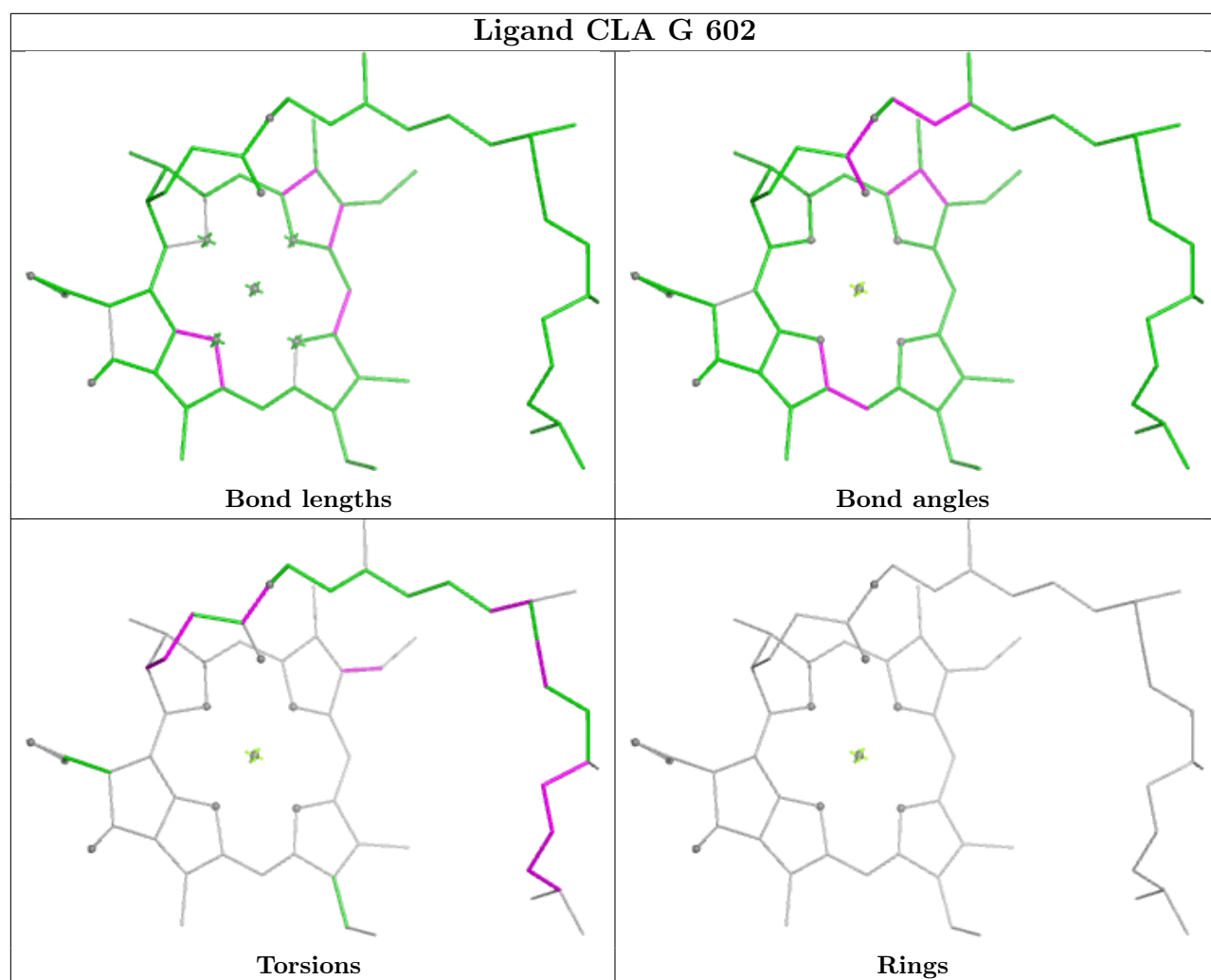


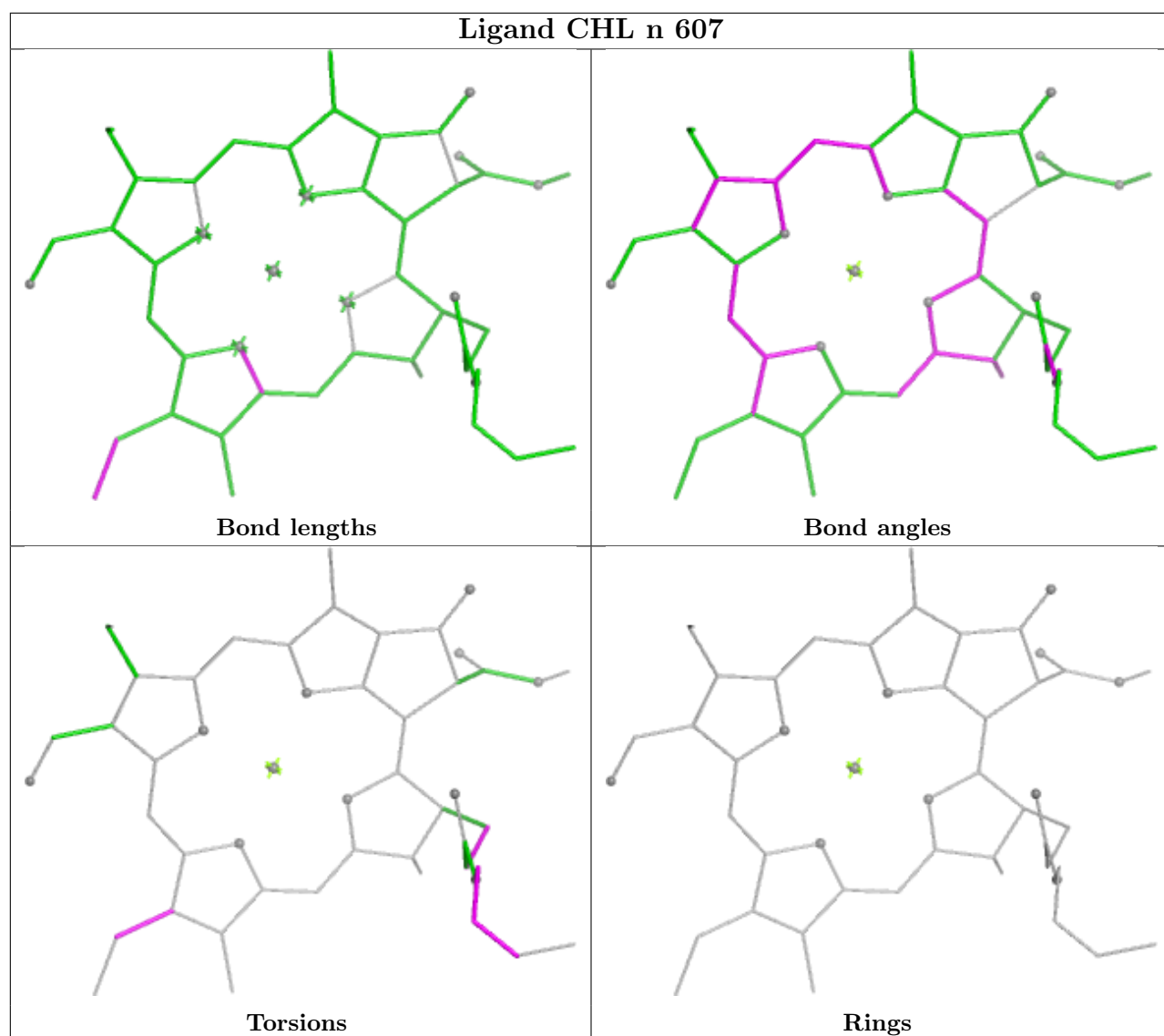
Rings

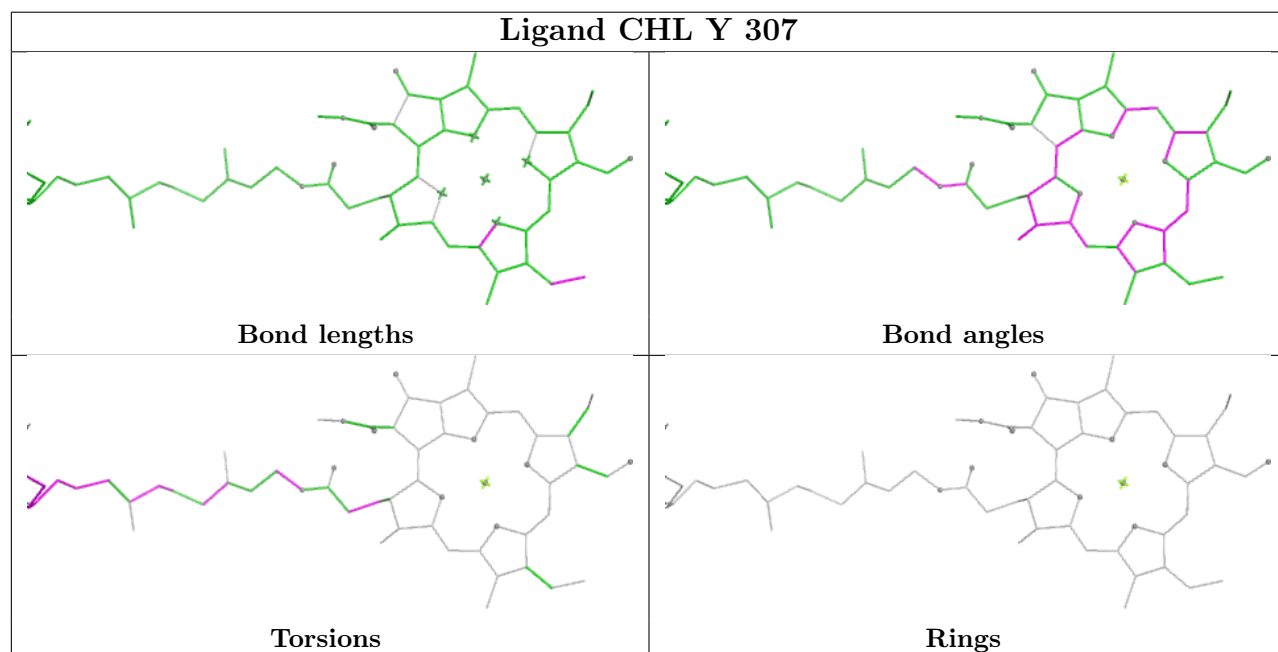
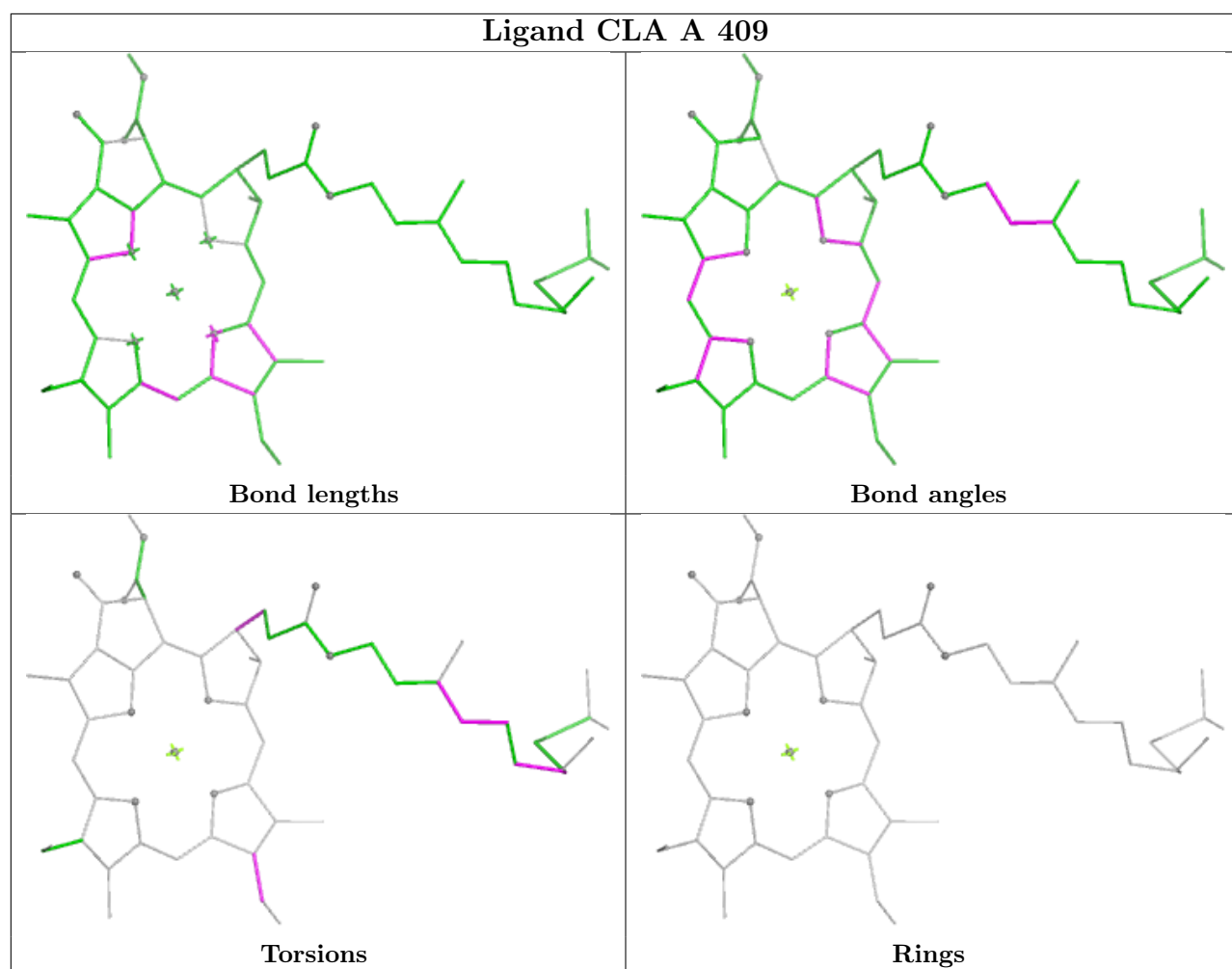


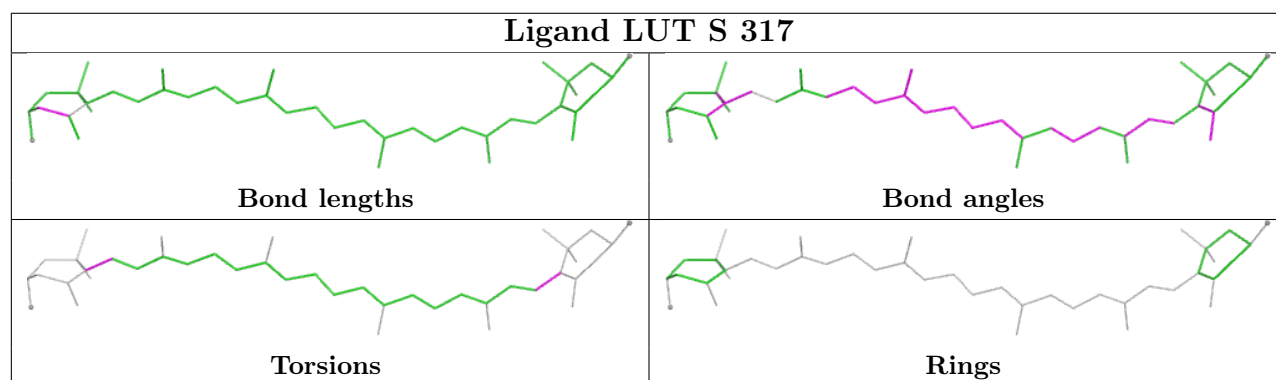
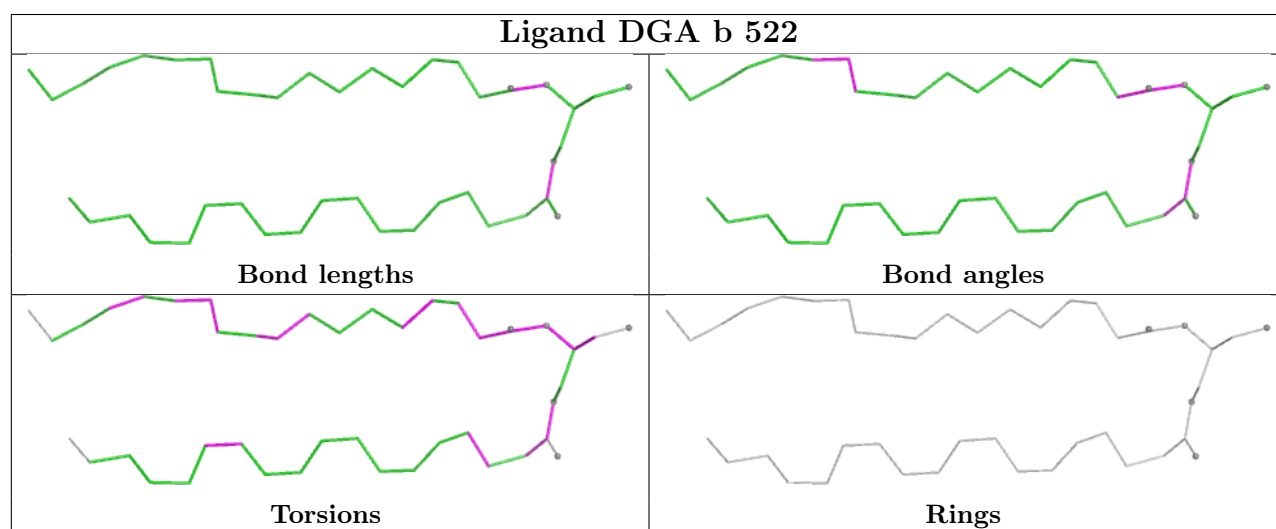
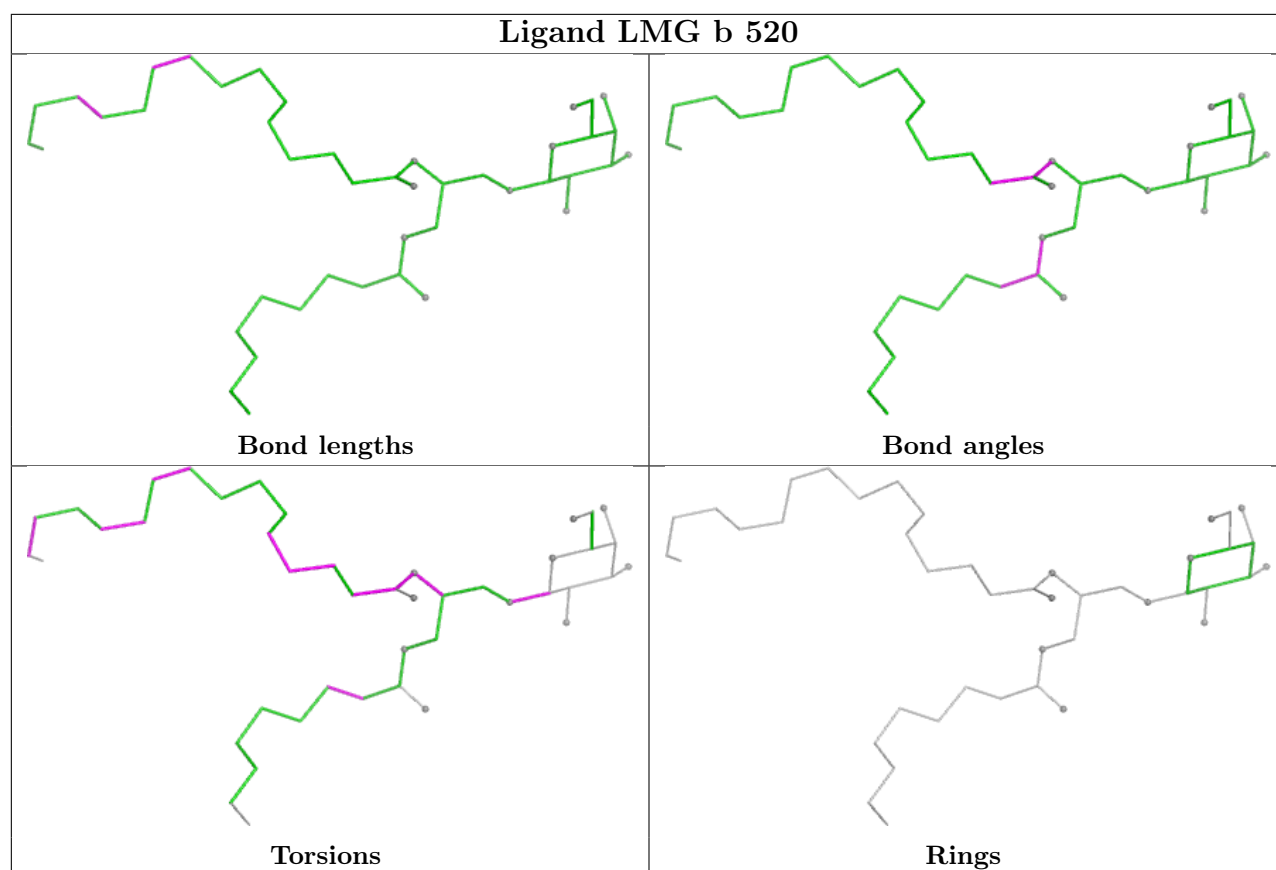


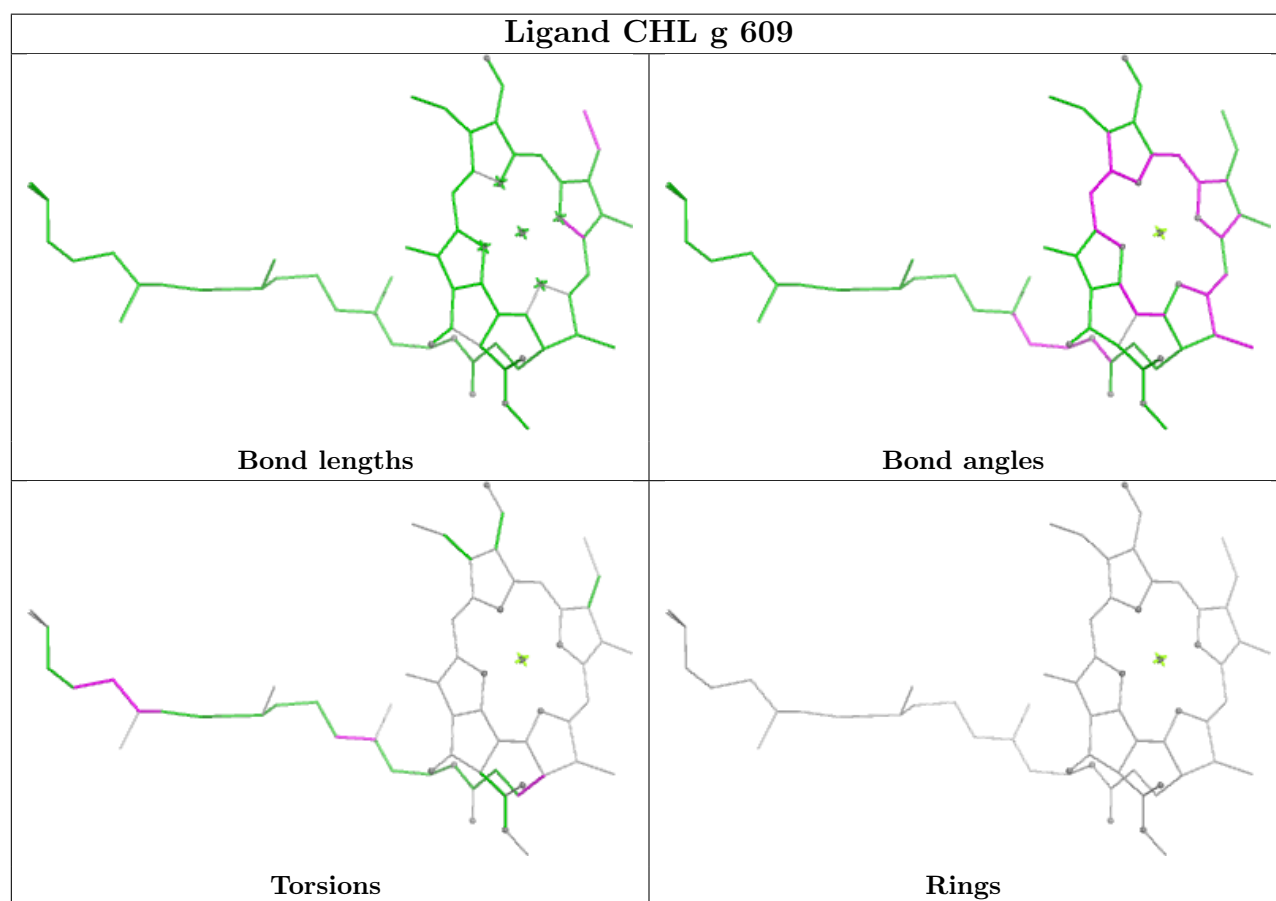
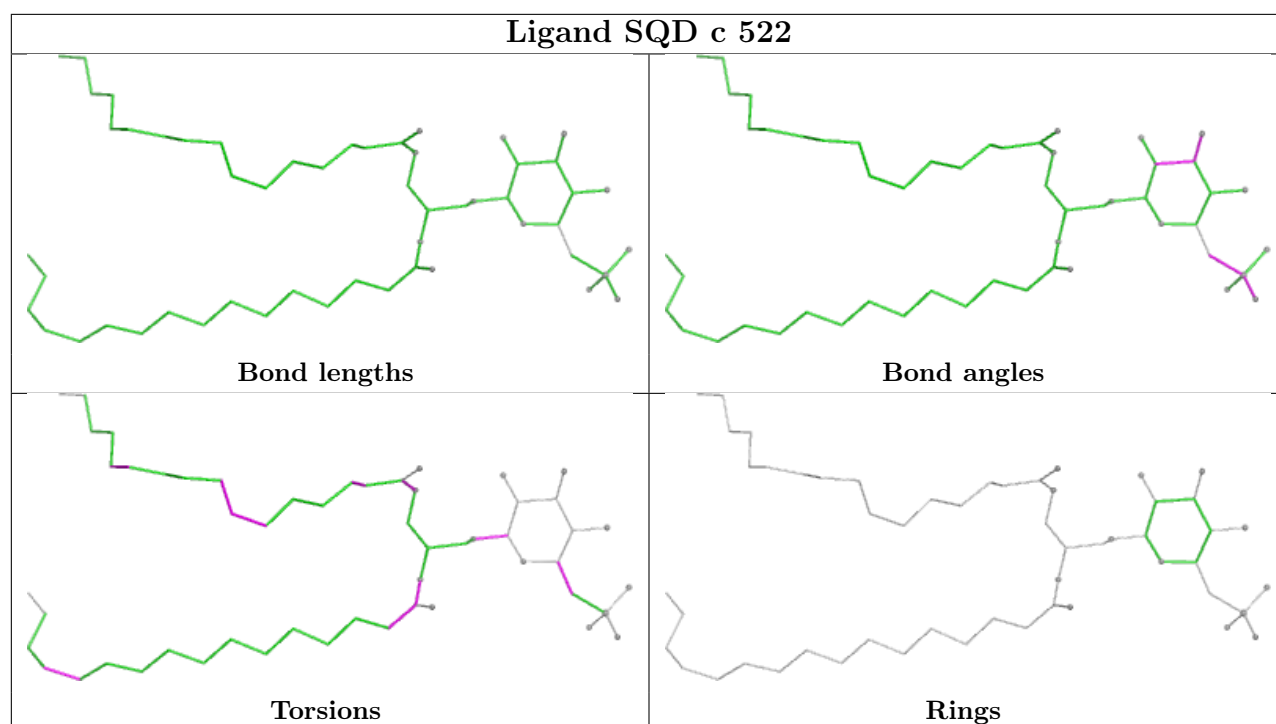


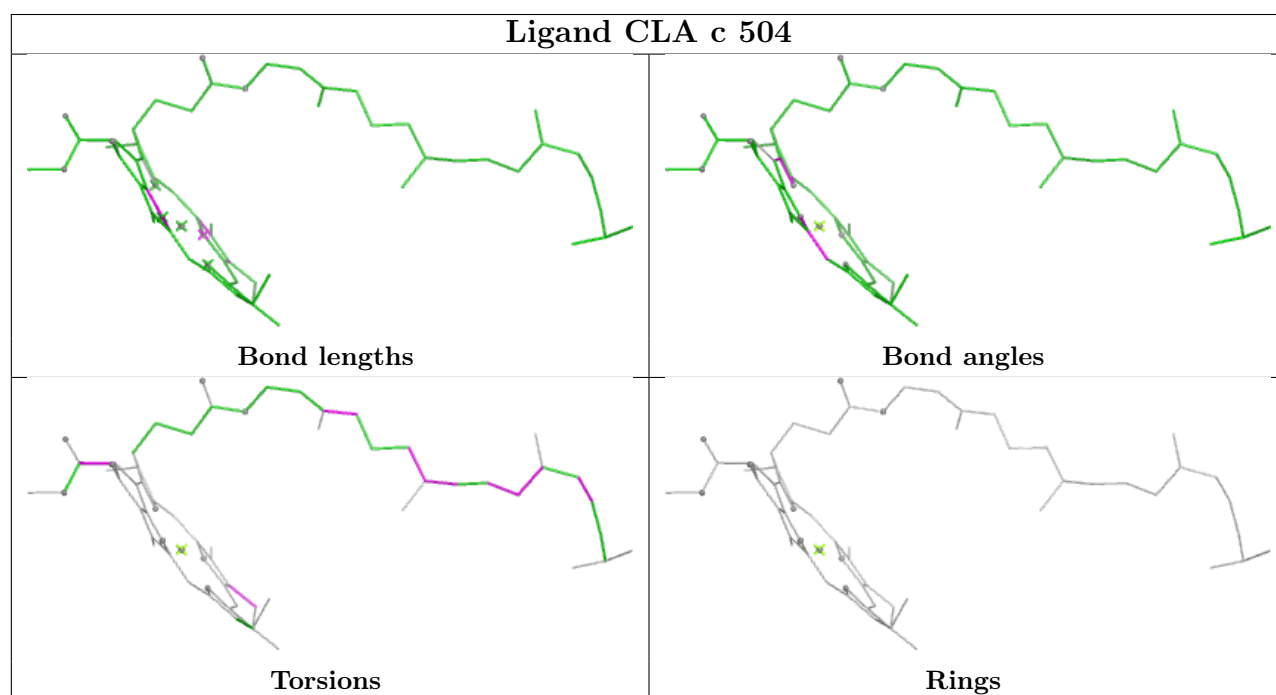
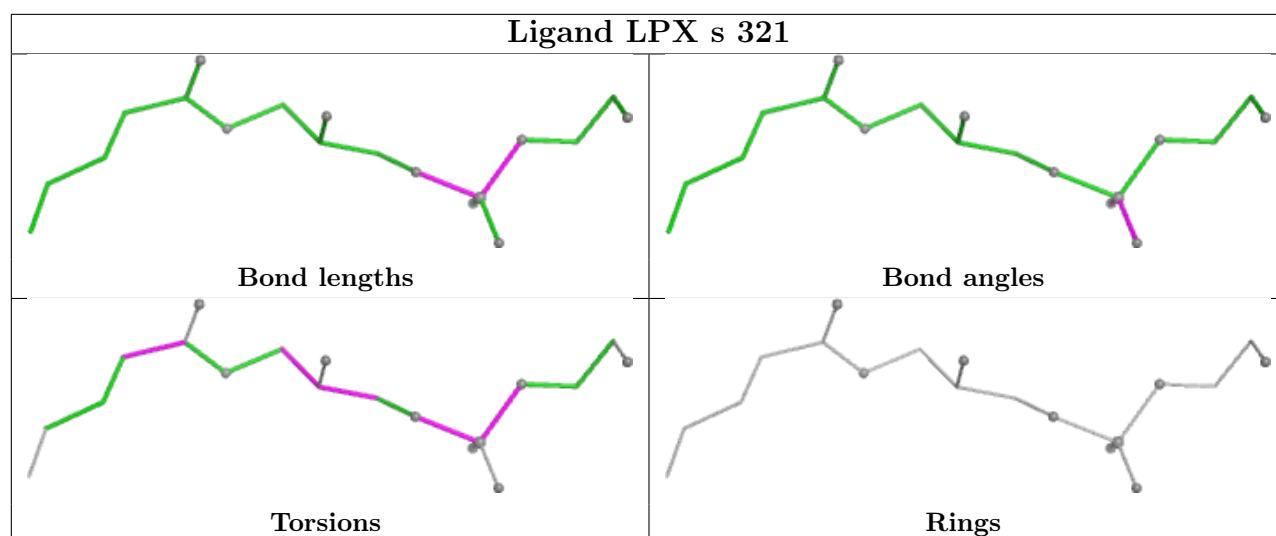


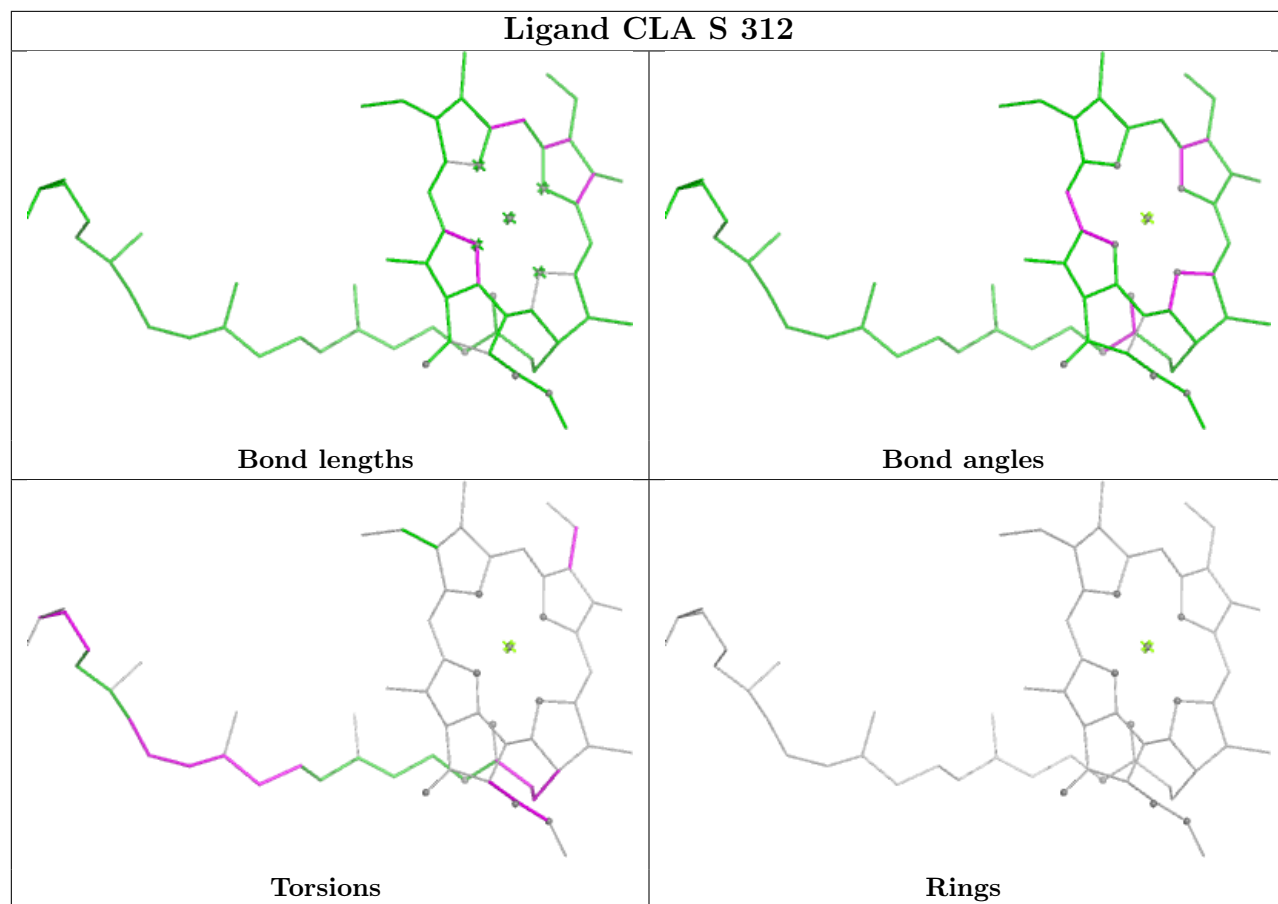


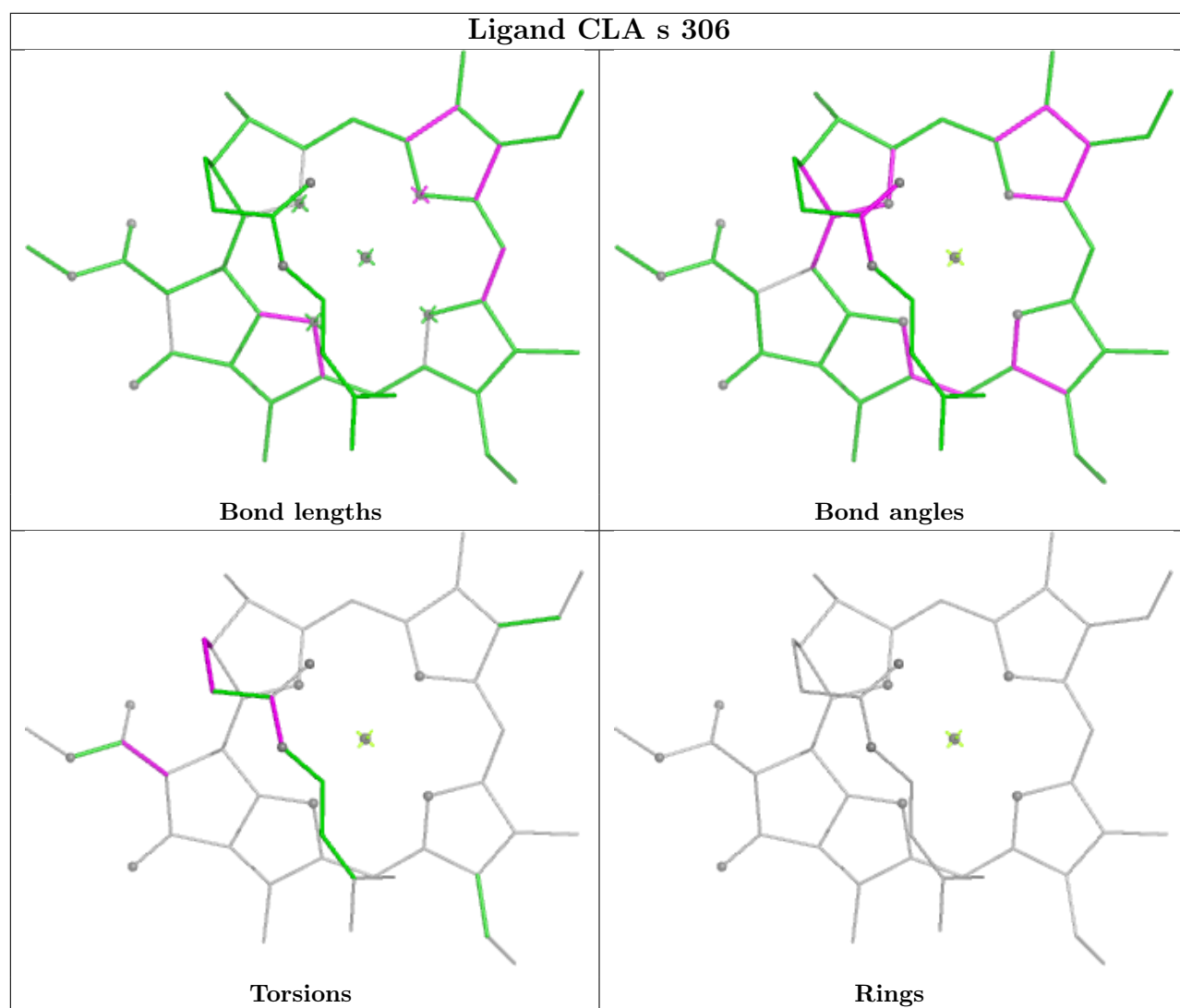


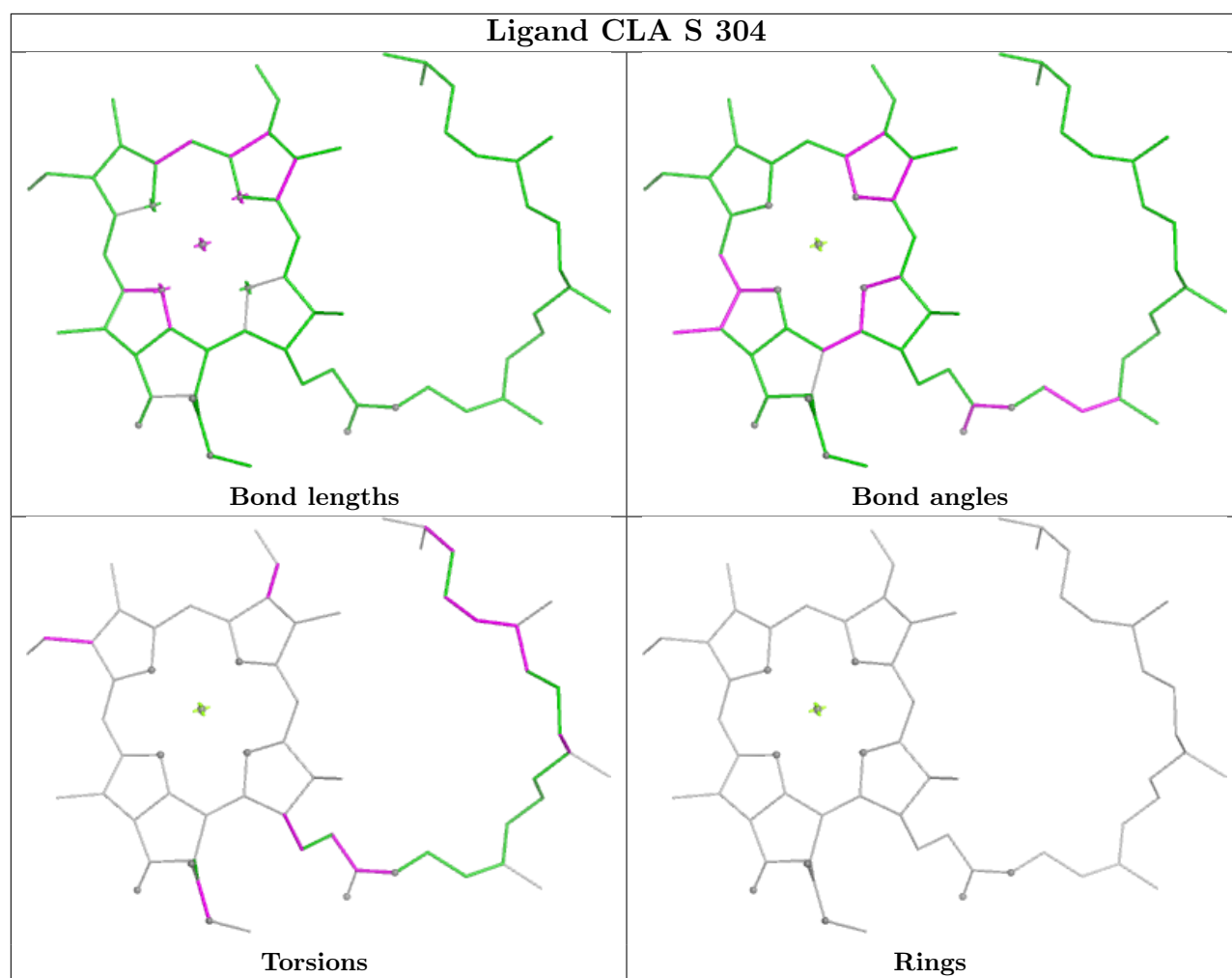


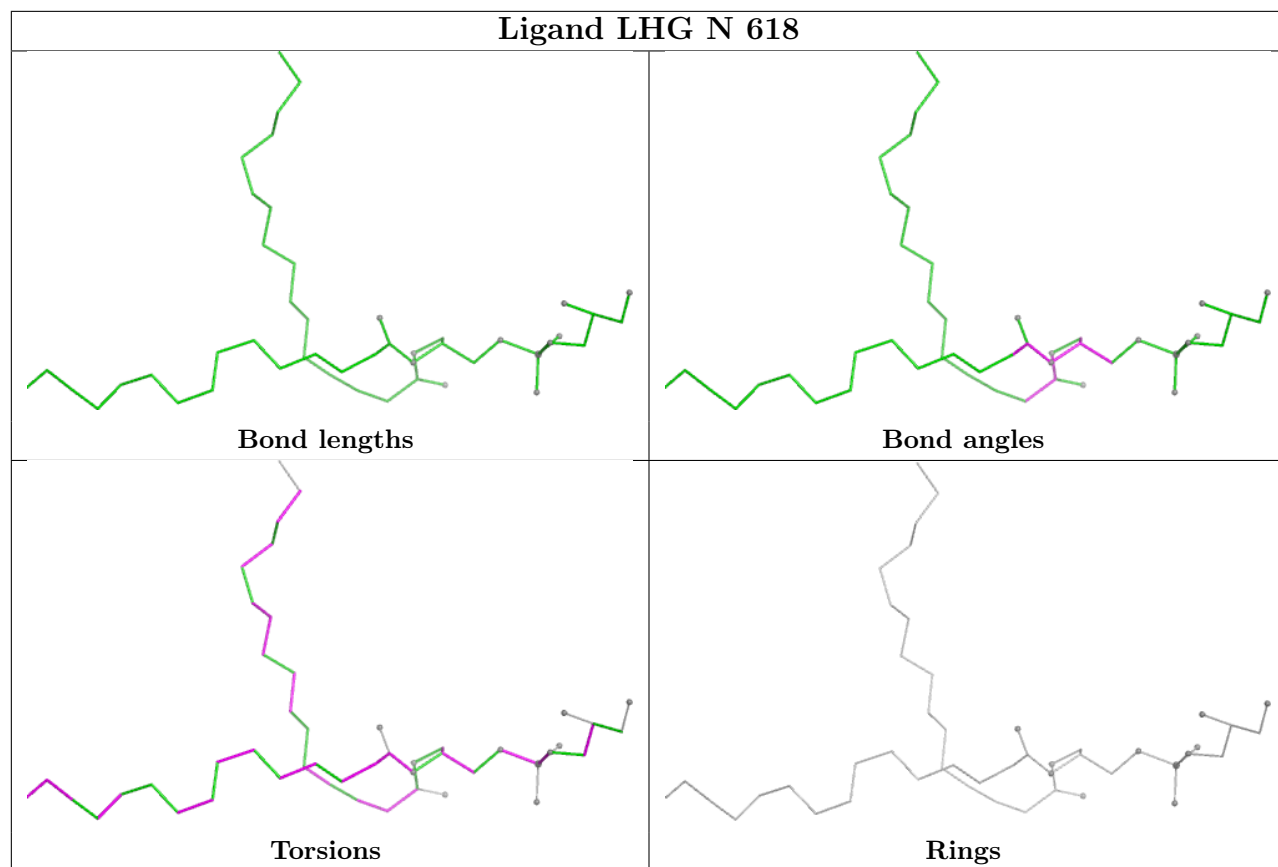




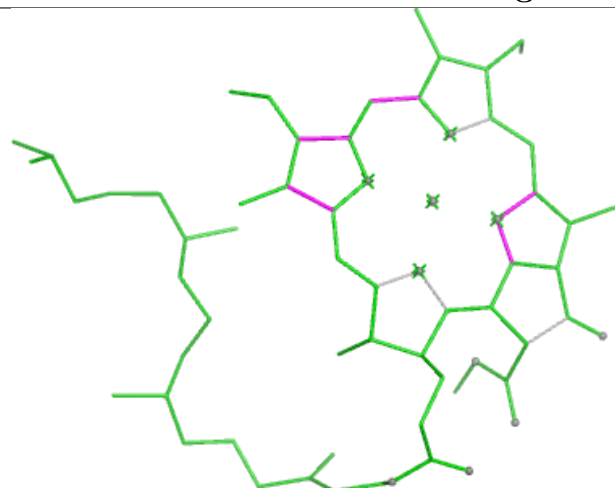




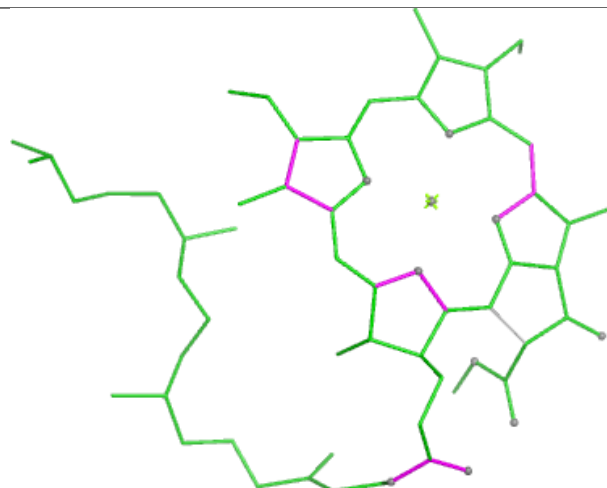




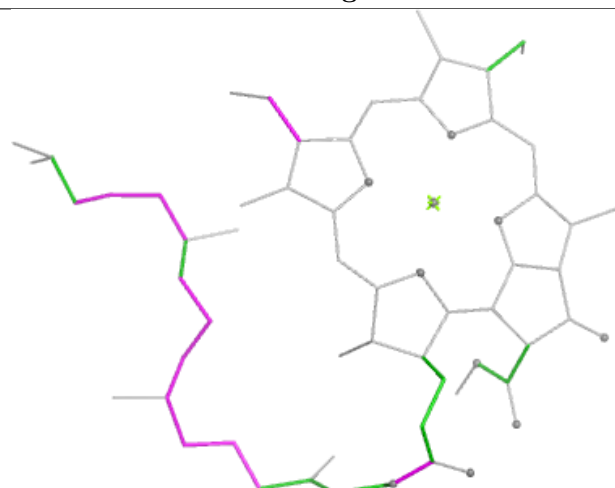
Ligand CLA Y 313



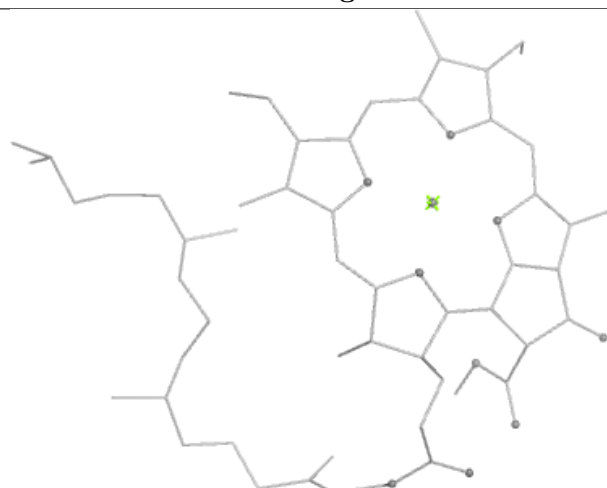
Bond lengths



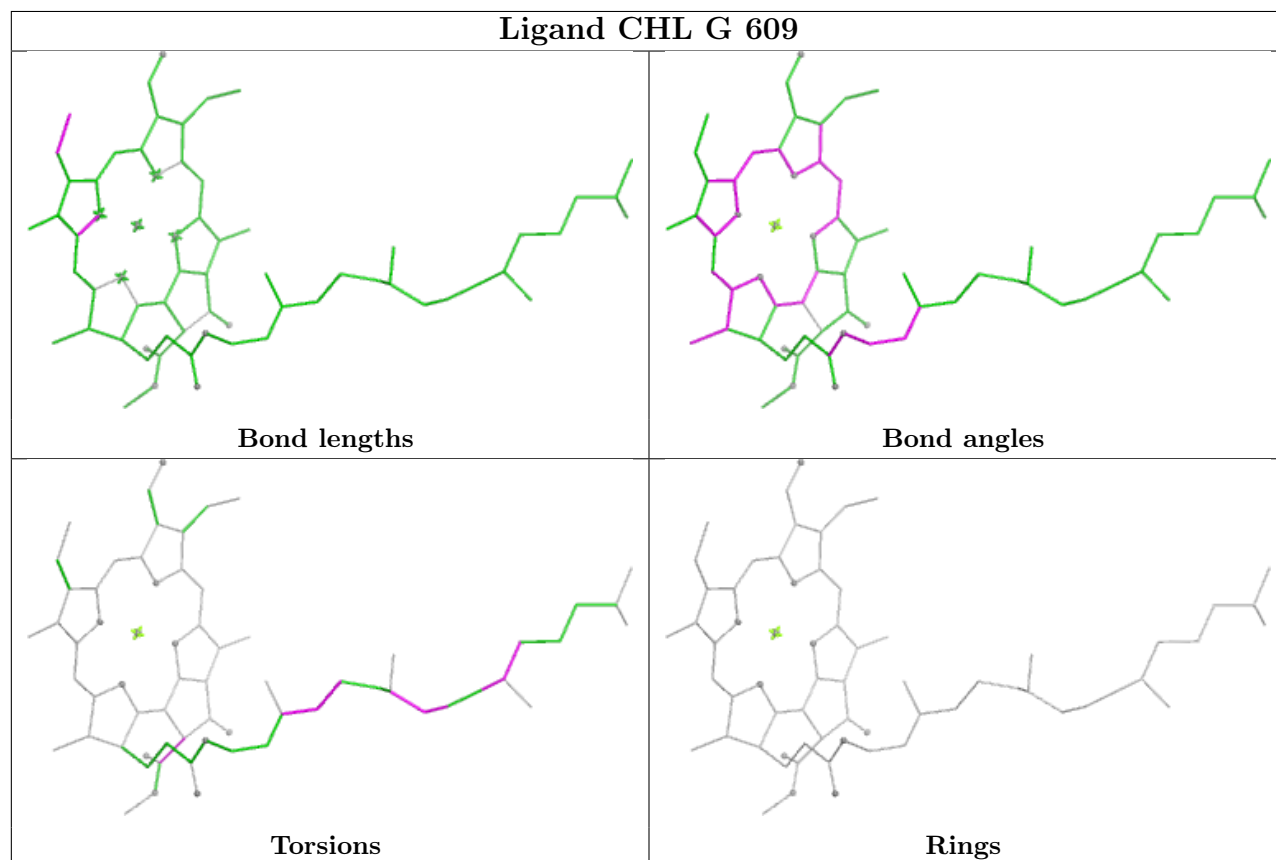
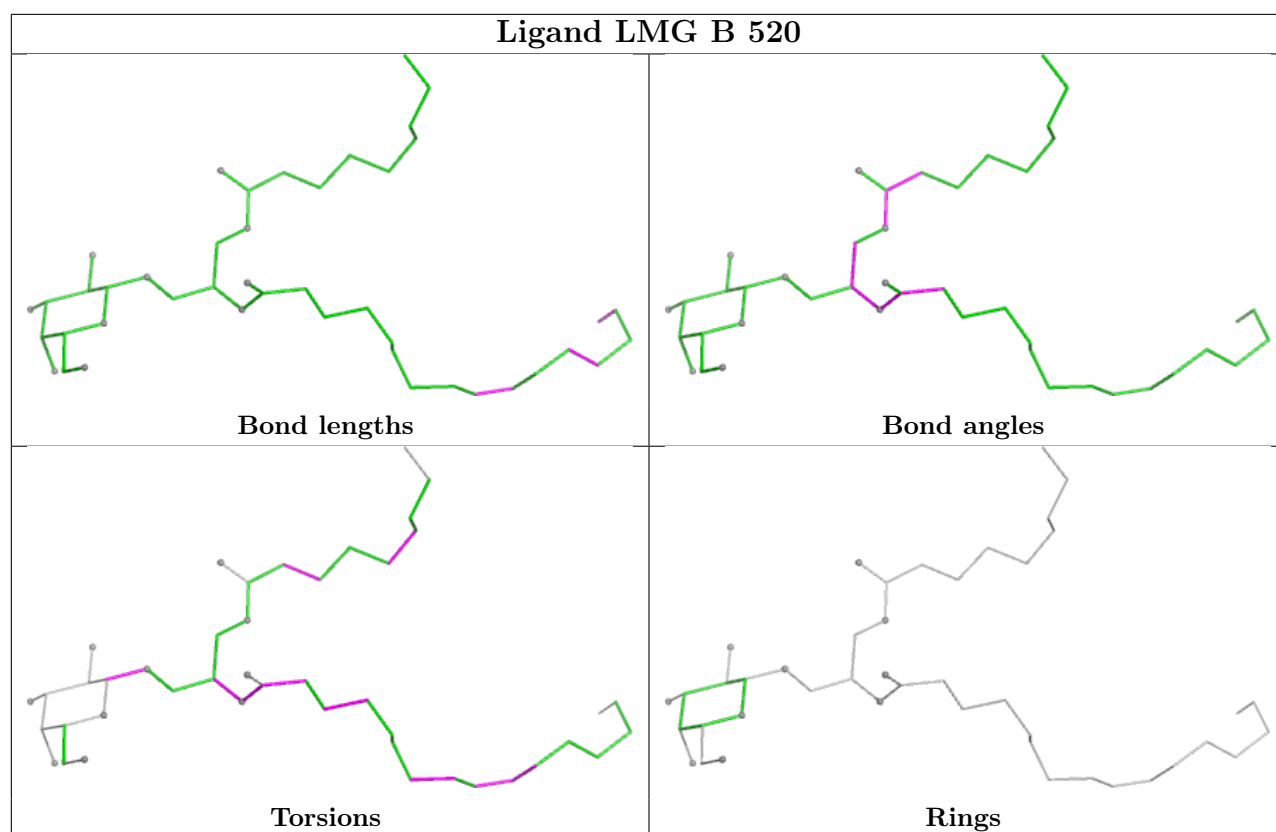
Bond angles

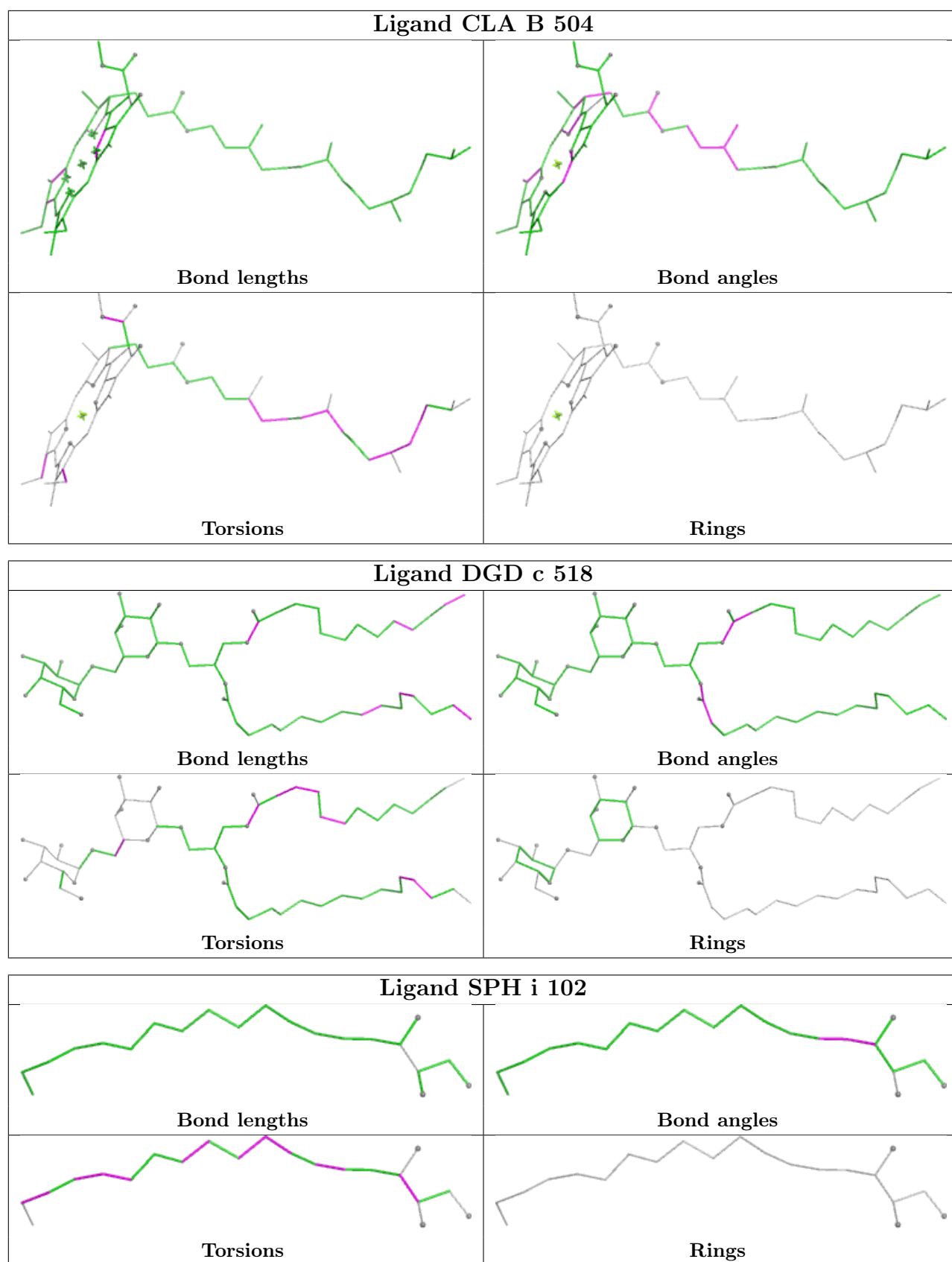


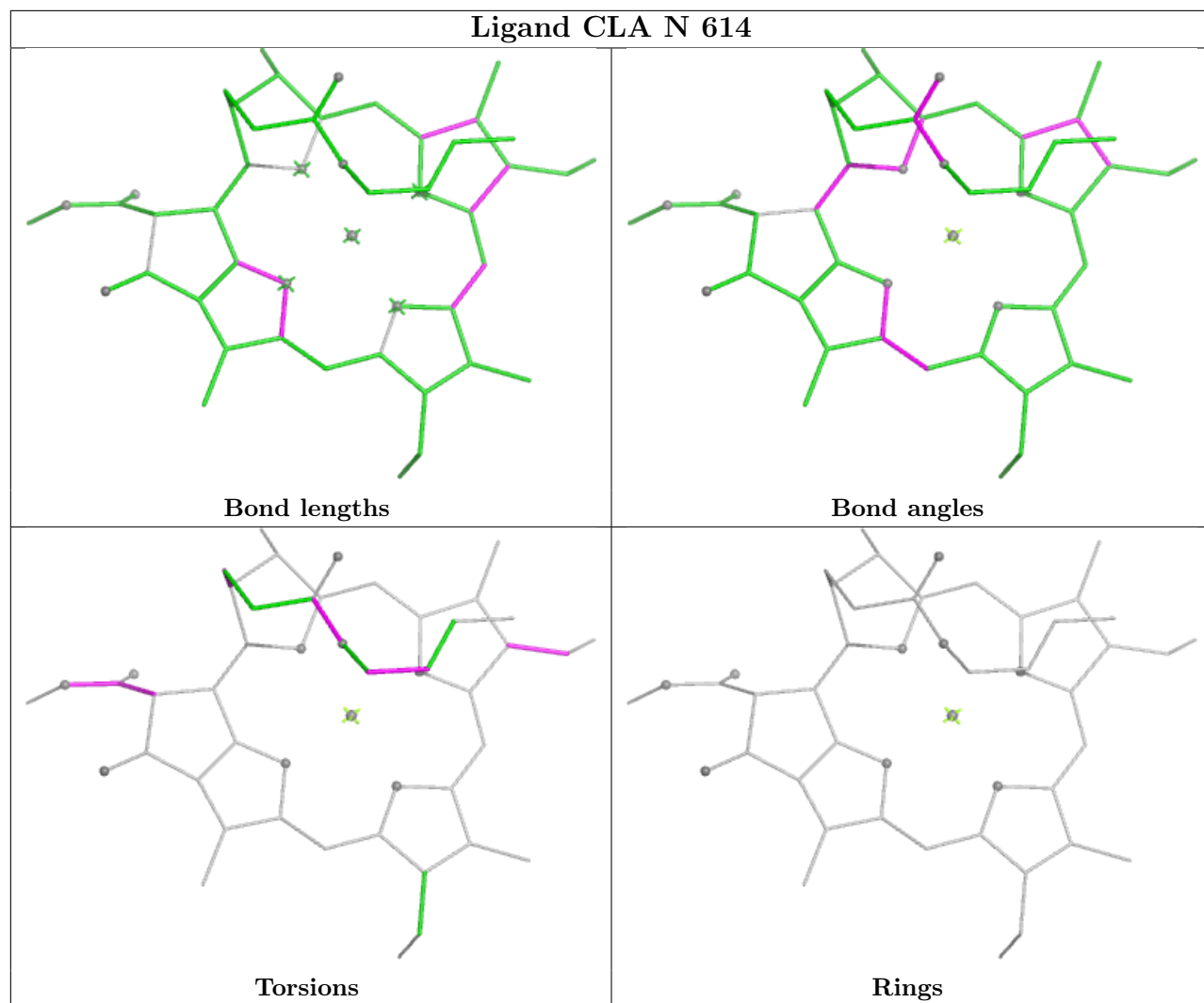
Torsions



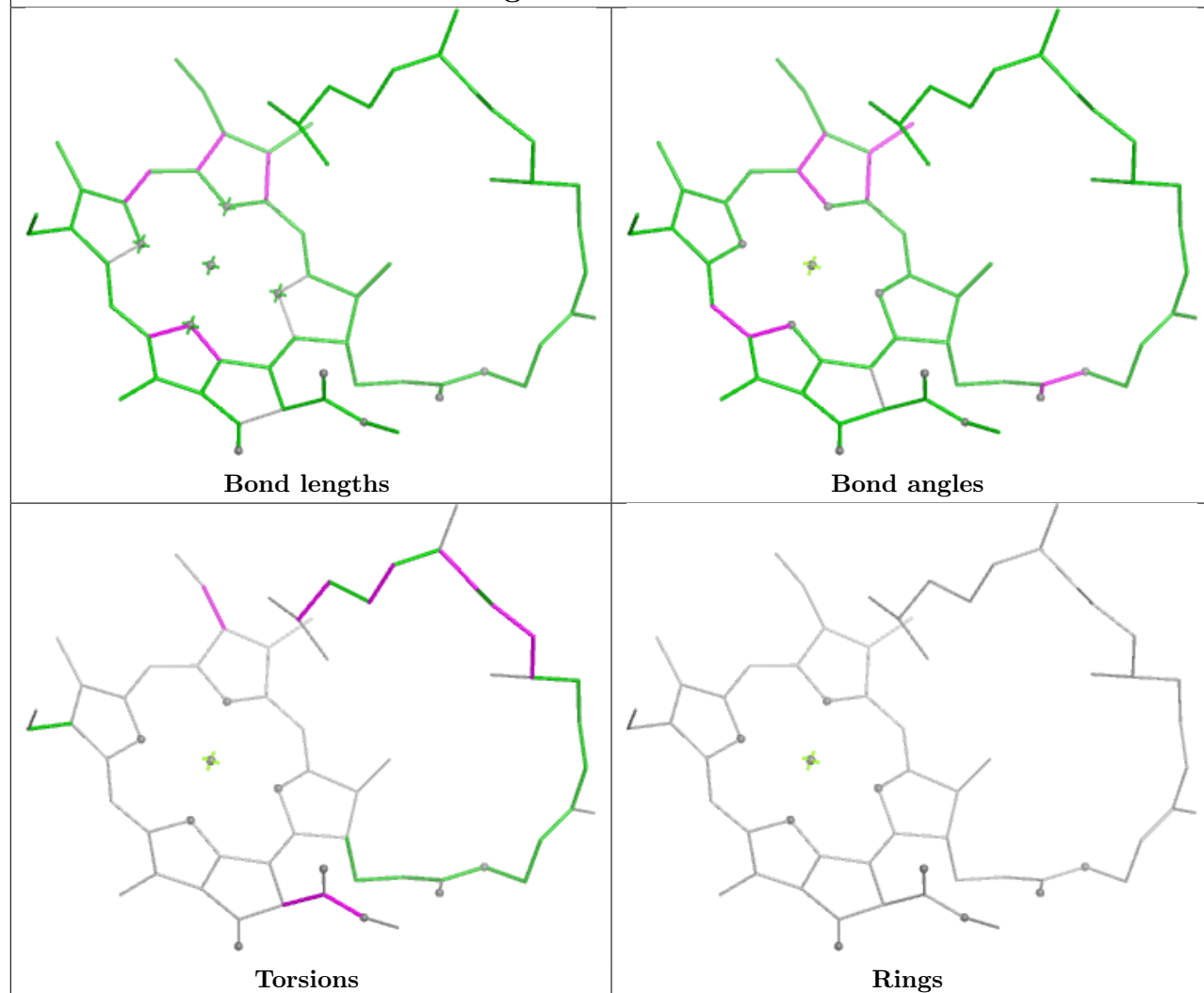
Rings



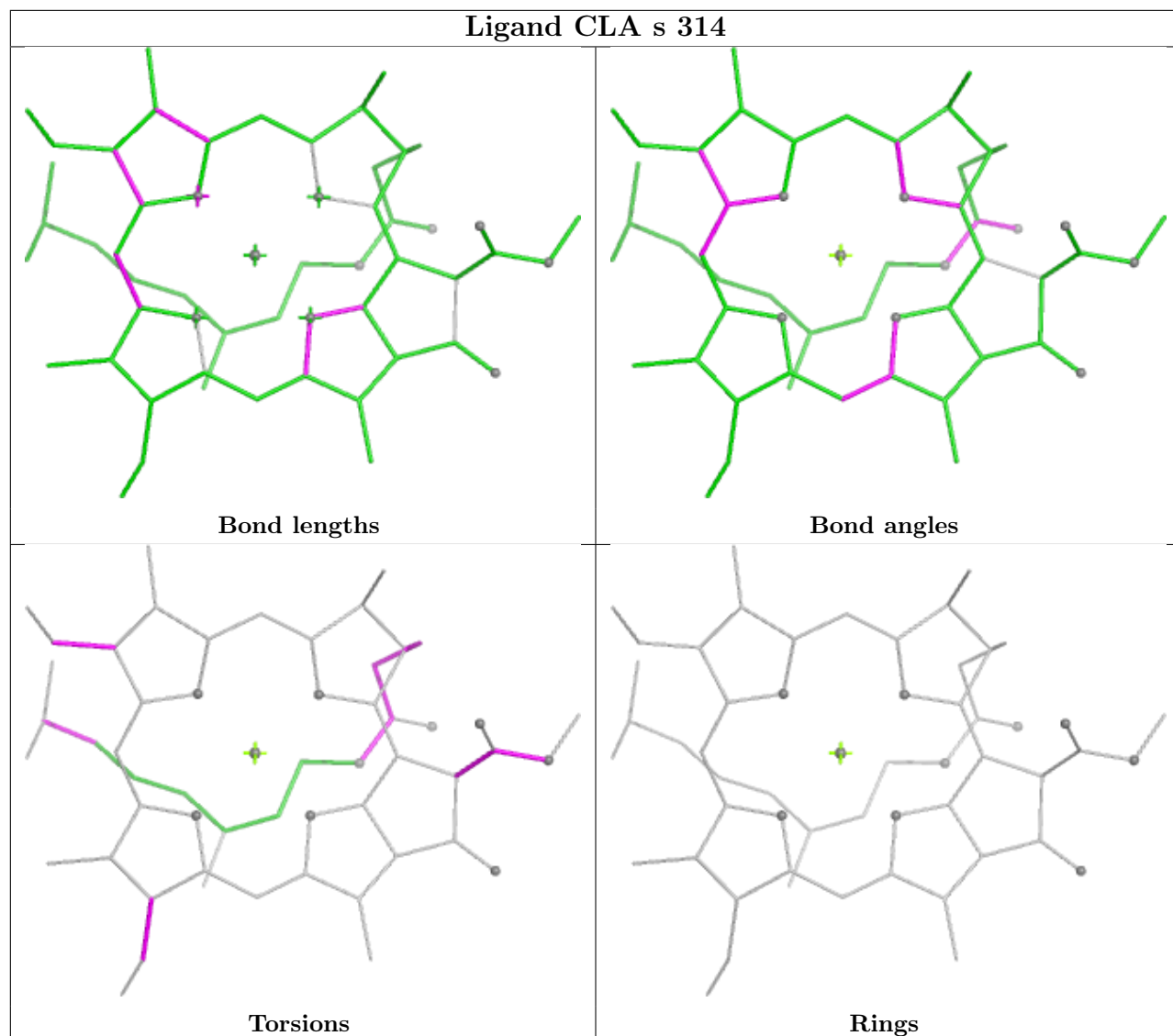




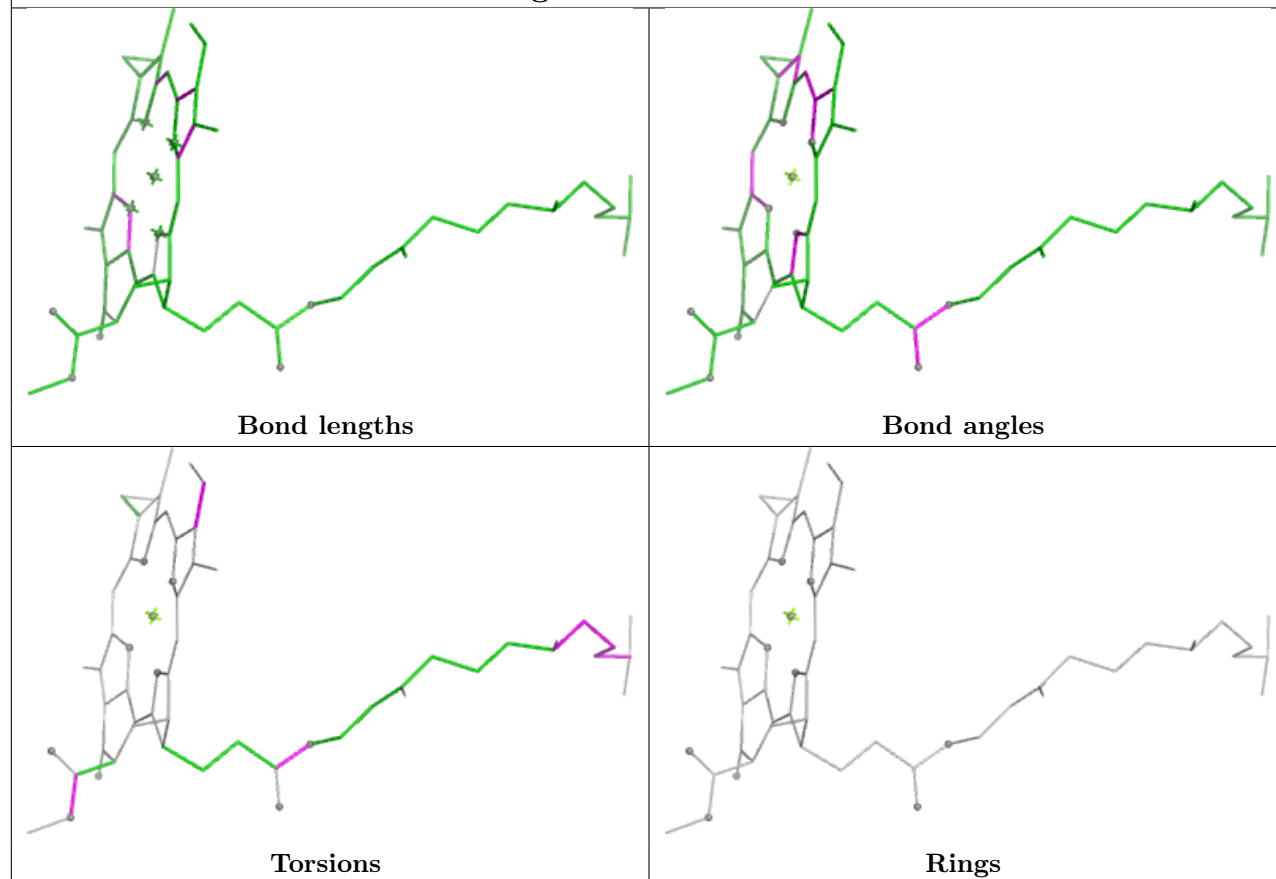
Ligand CLA b 515



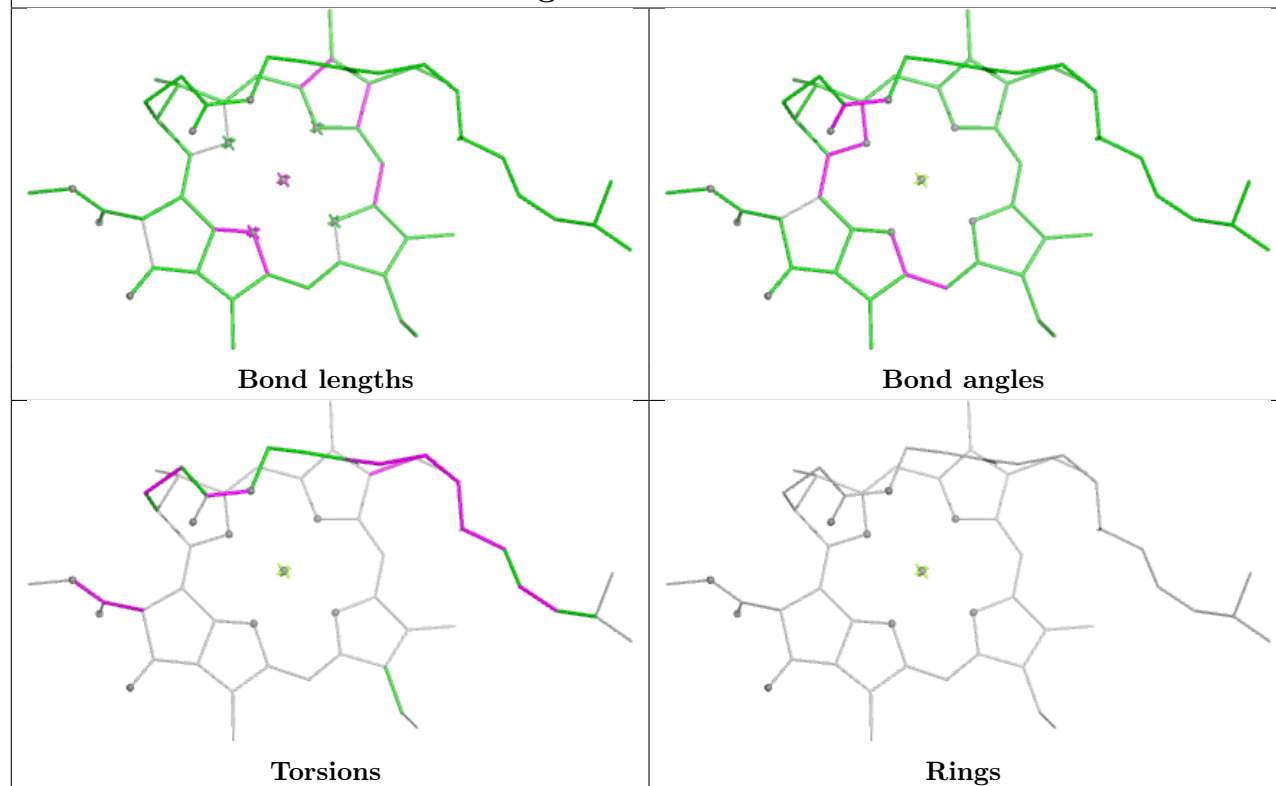
Ligand CLA s 314

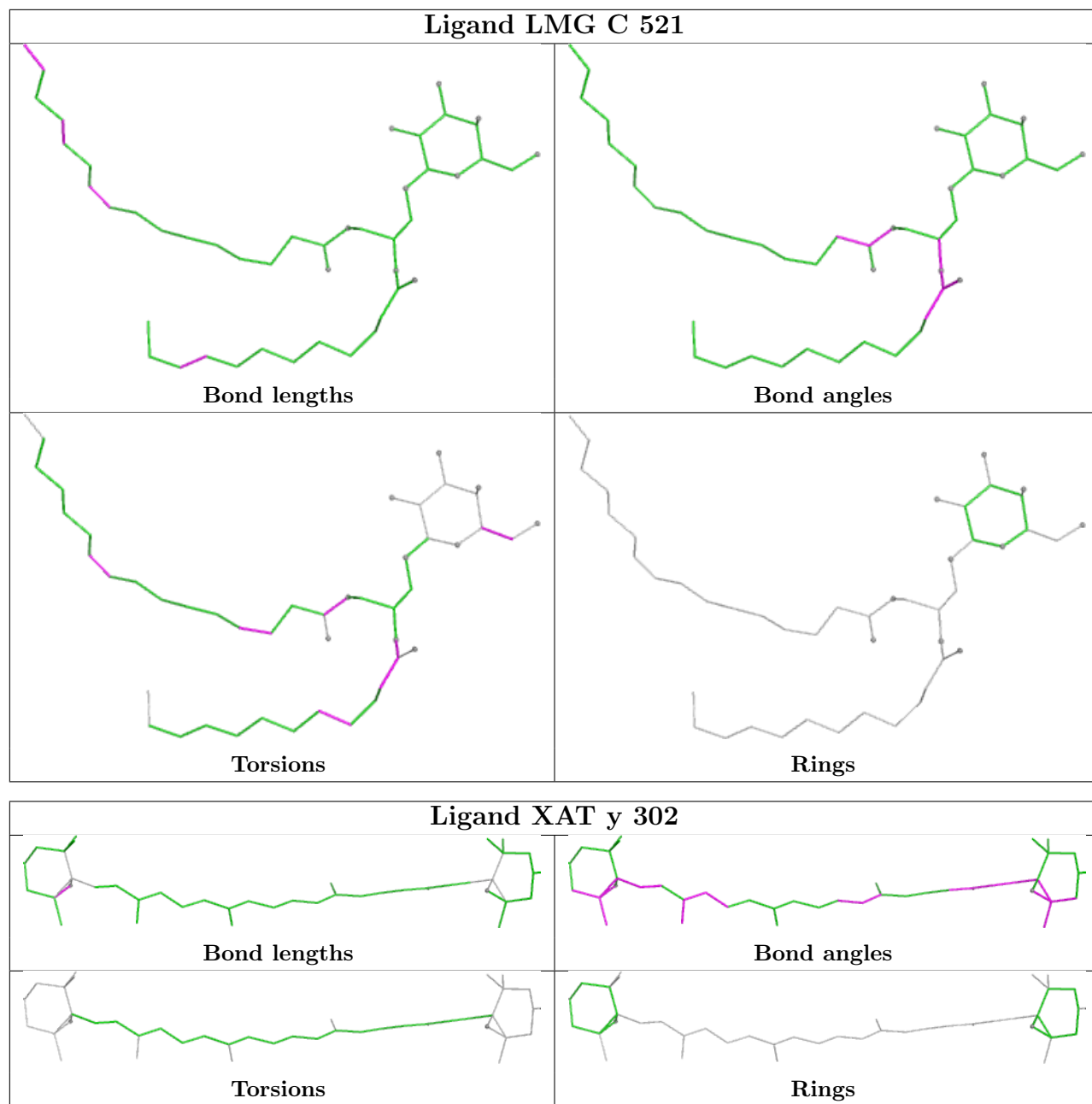


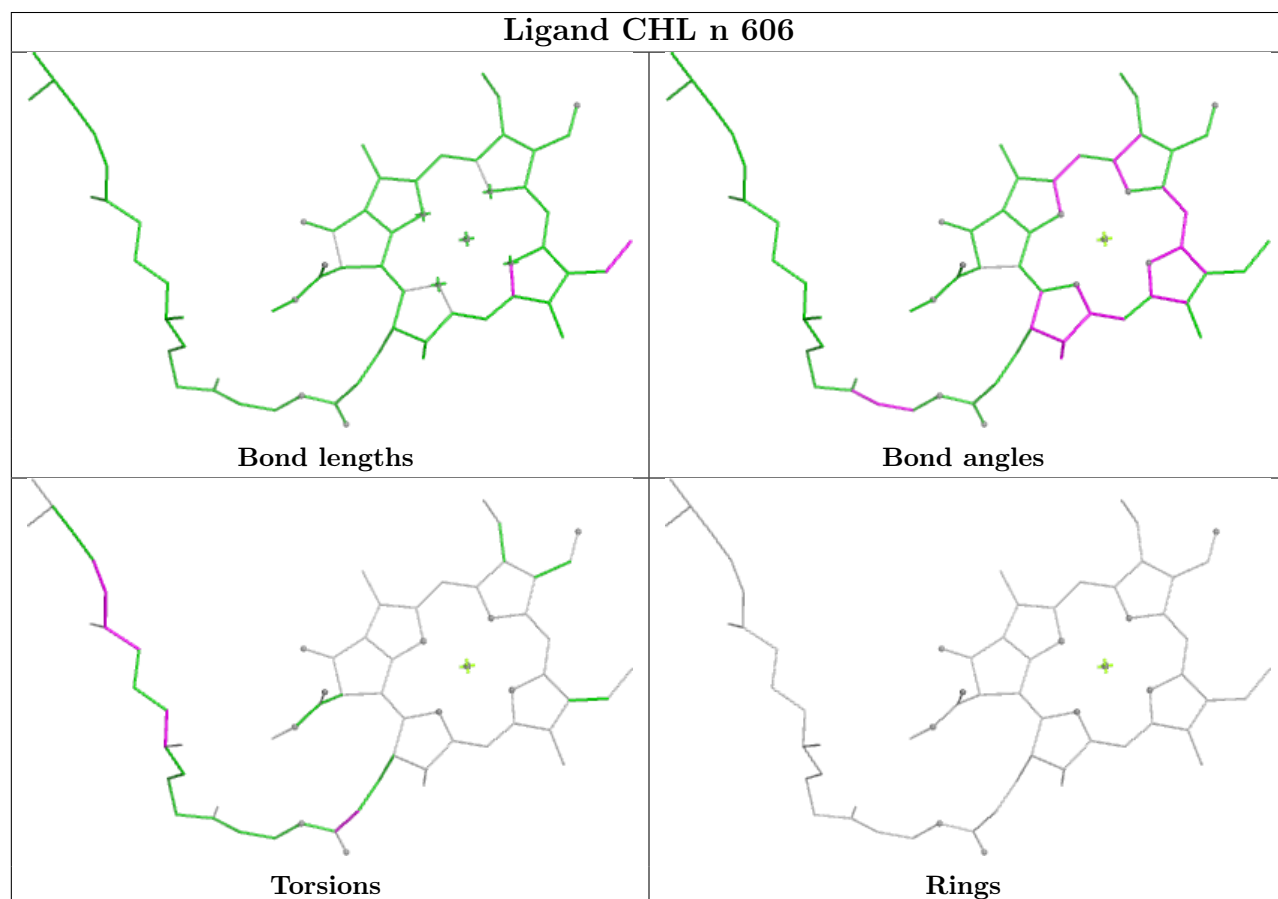
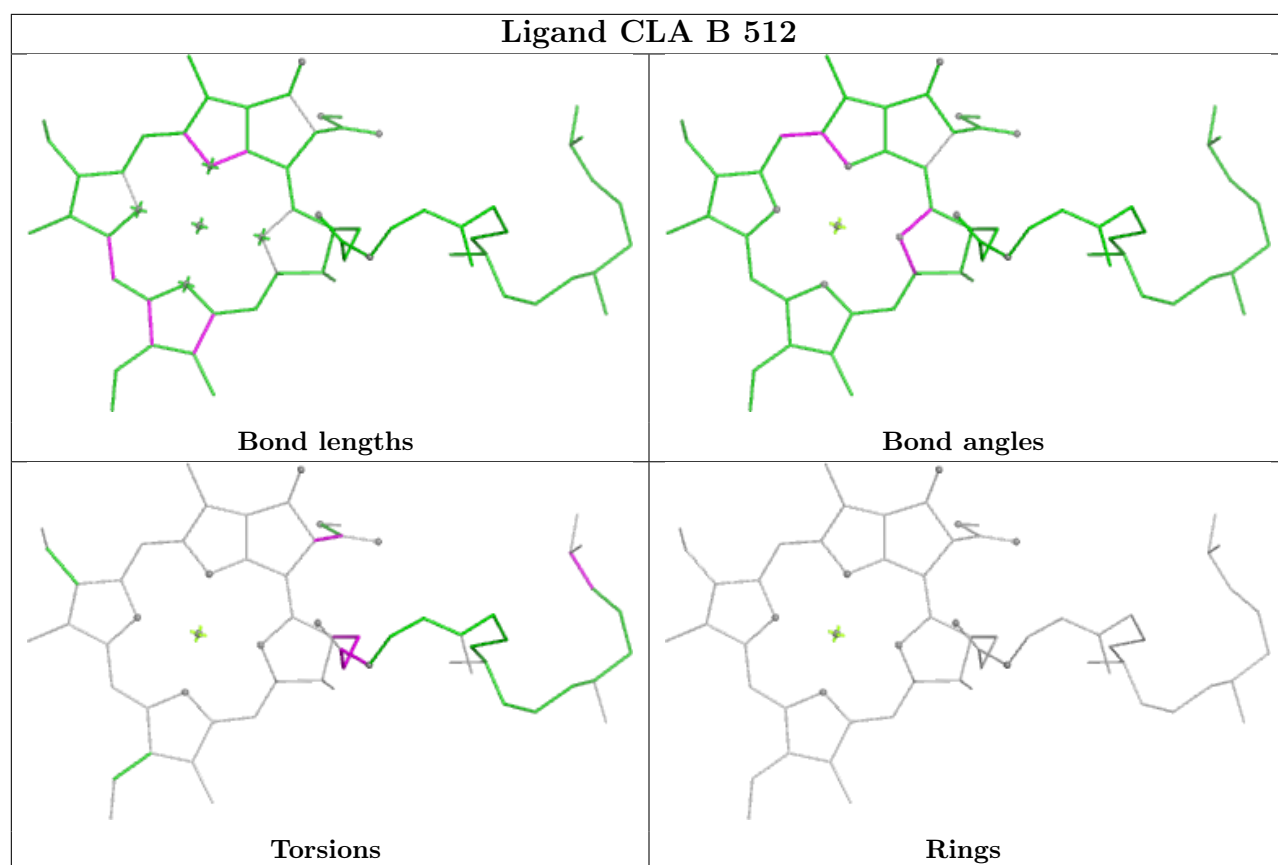
Ligand CLA D 405



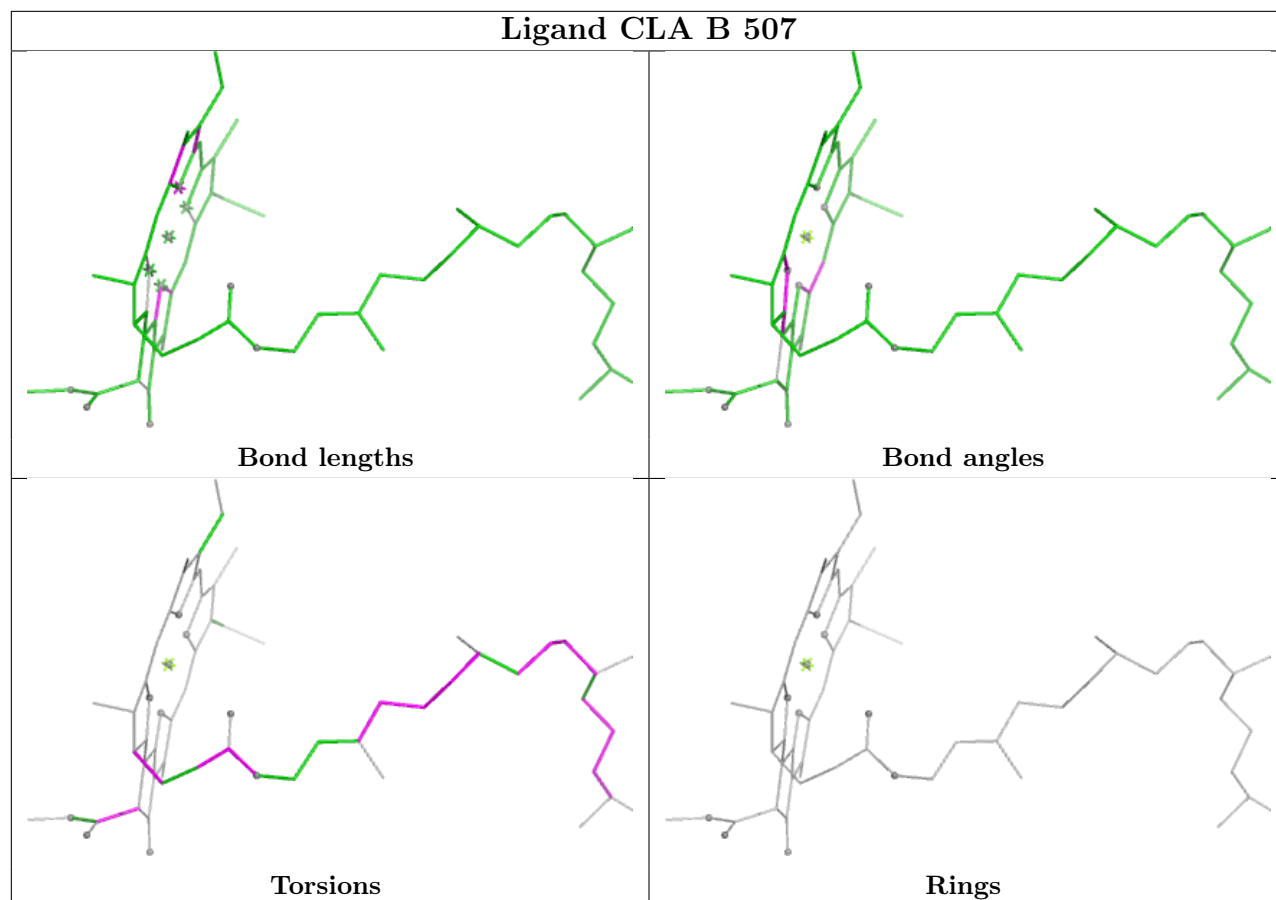
Ligand CLA r 307



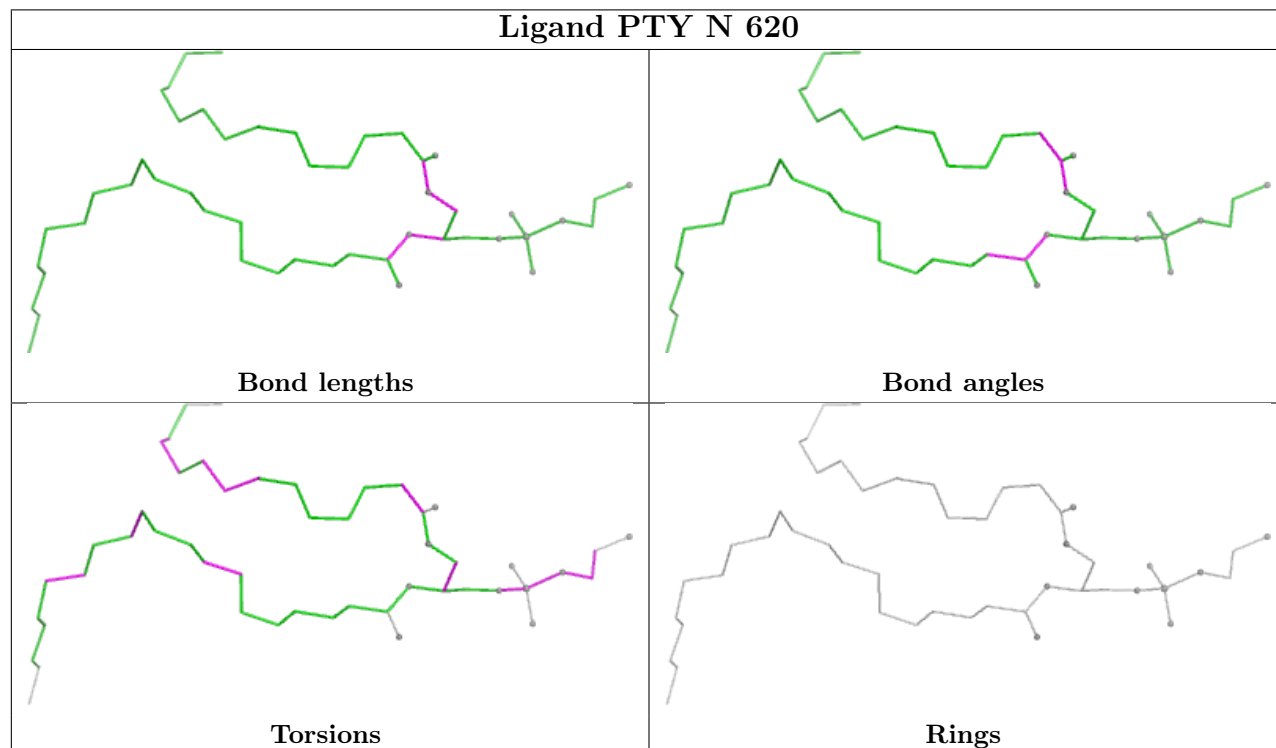


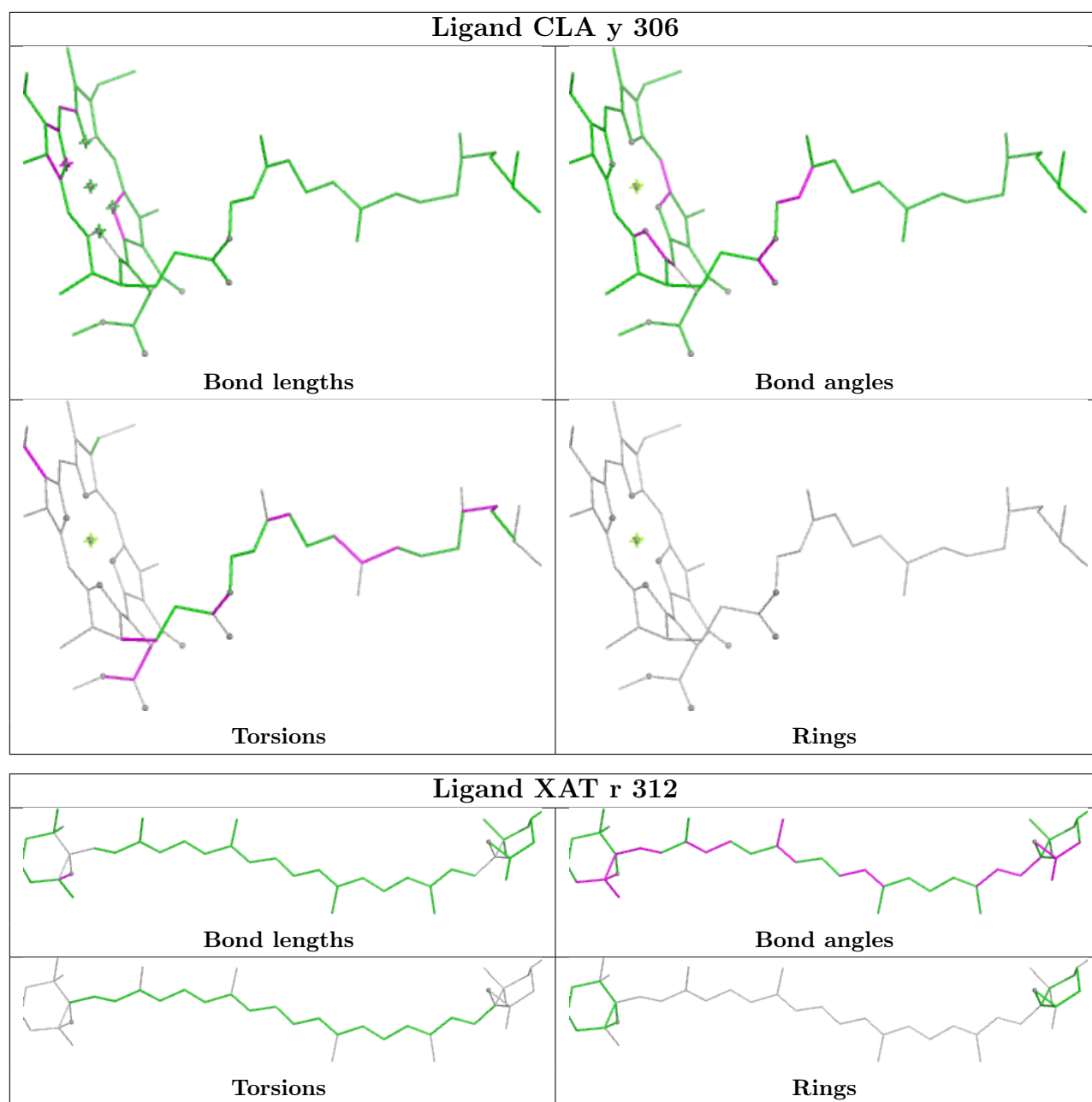


Ligand CLA B 507

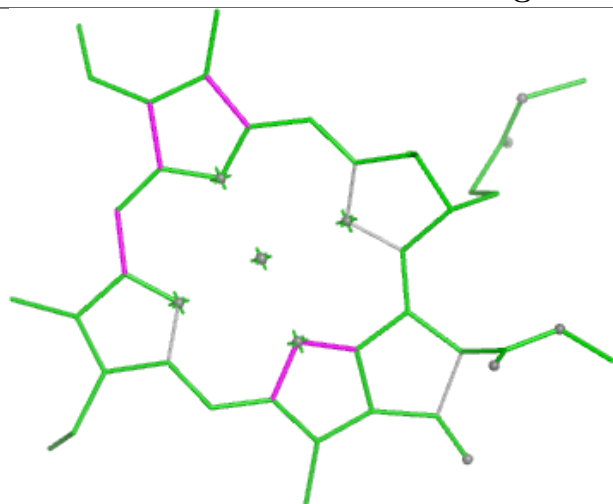


Ligand PTY N 620

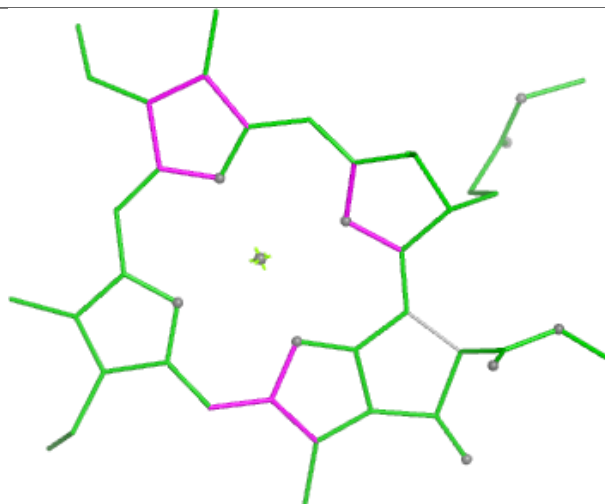




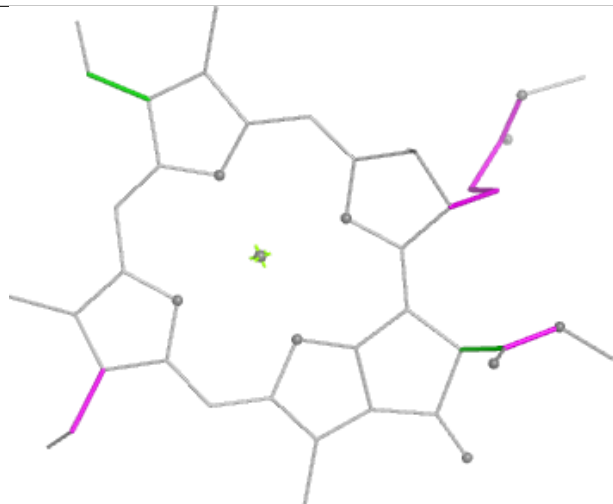
Ligand CLA R 307



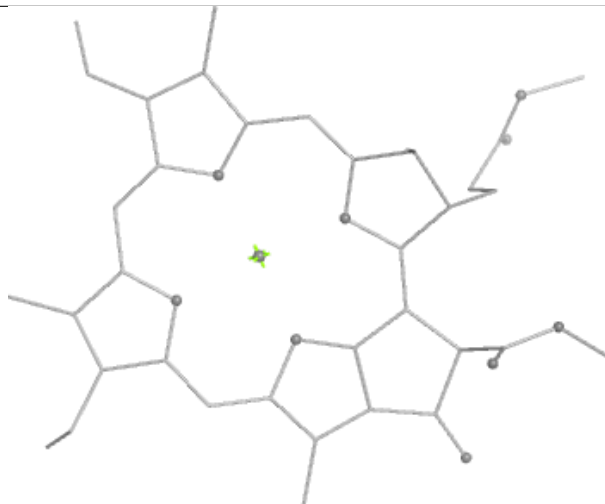
Bond lengths



Bond angles

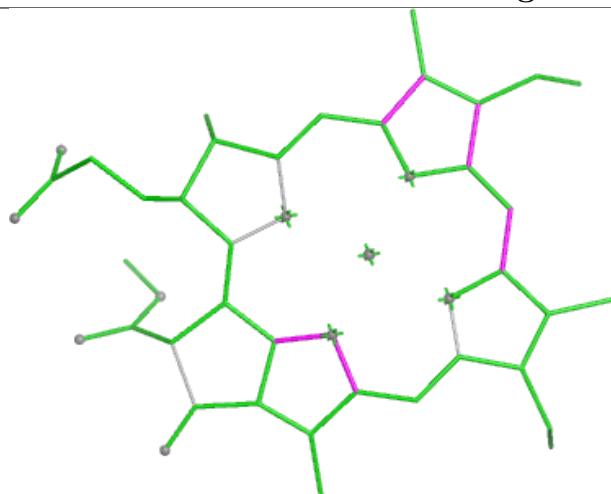


Torsions

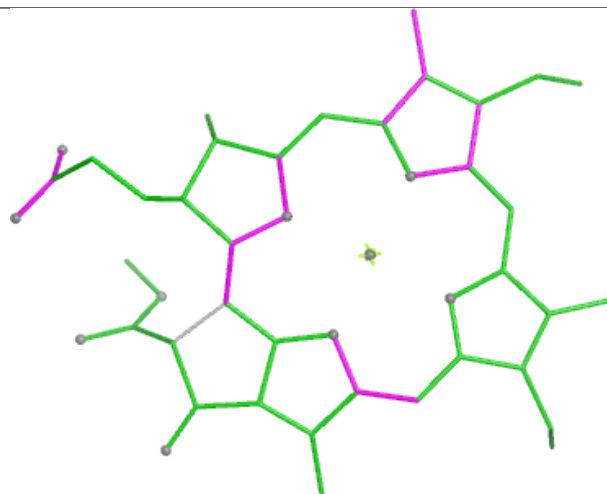


Rings

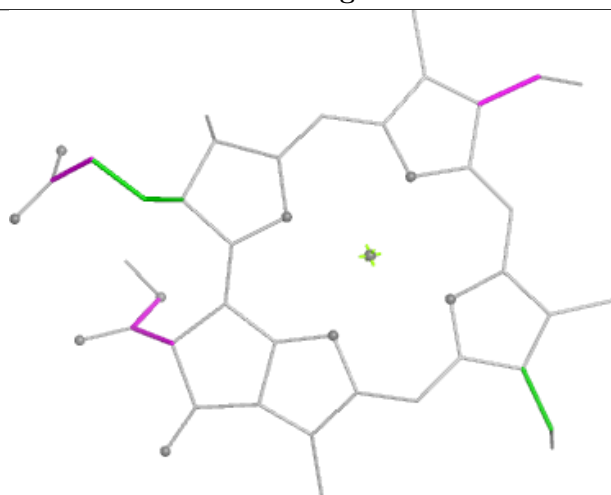
Ligand CLA n 611



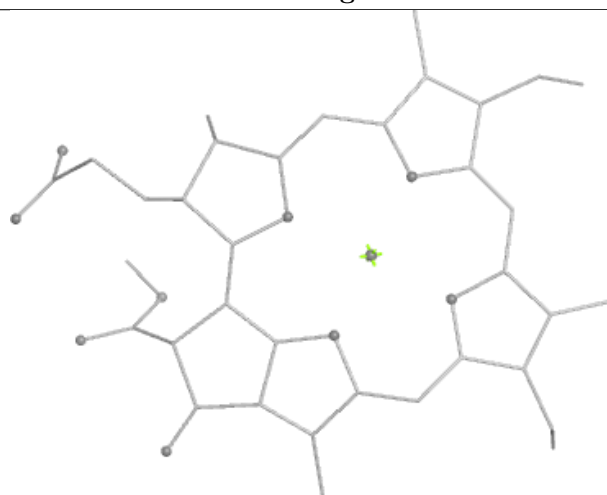
Bond lengths



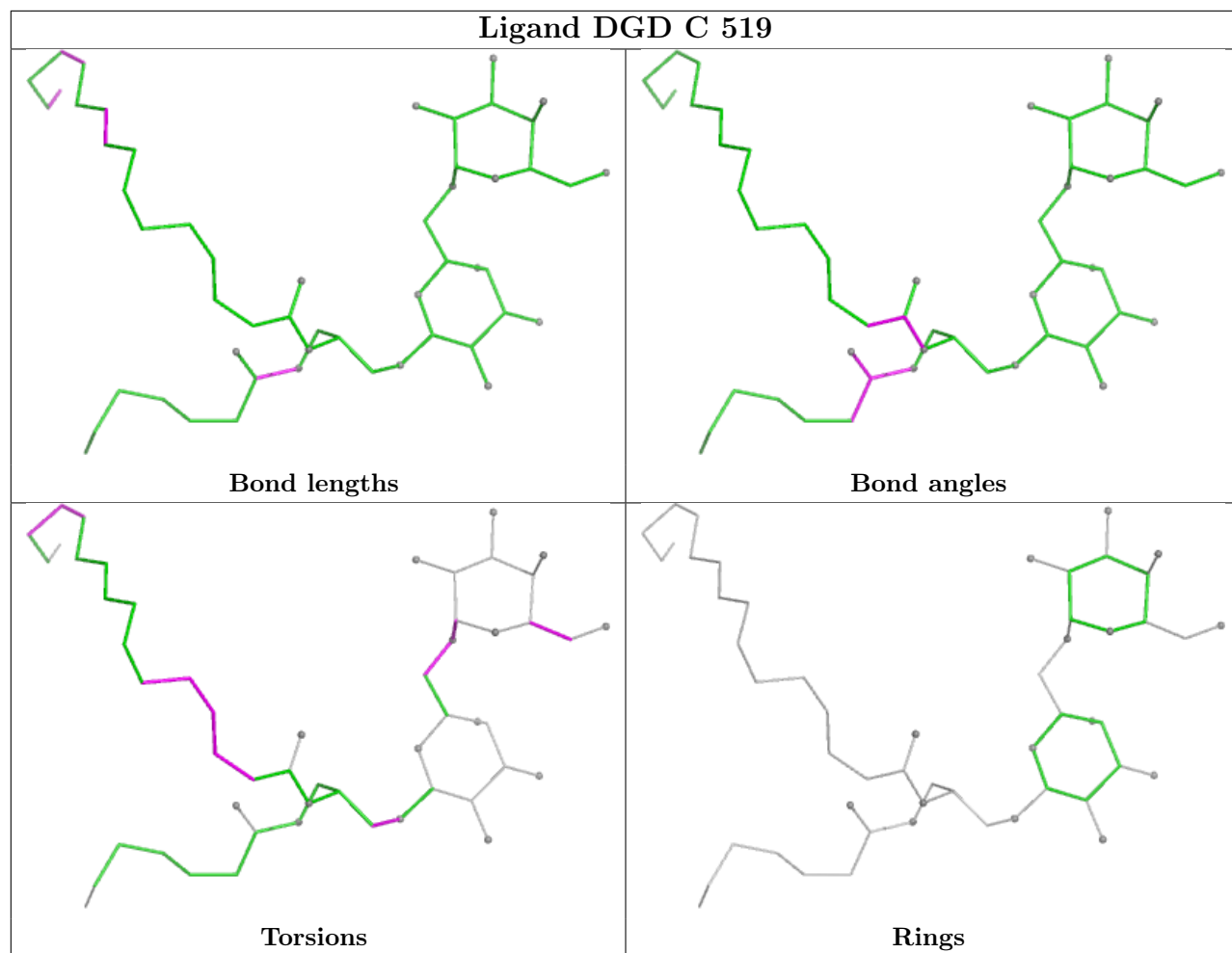
Bond angles



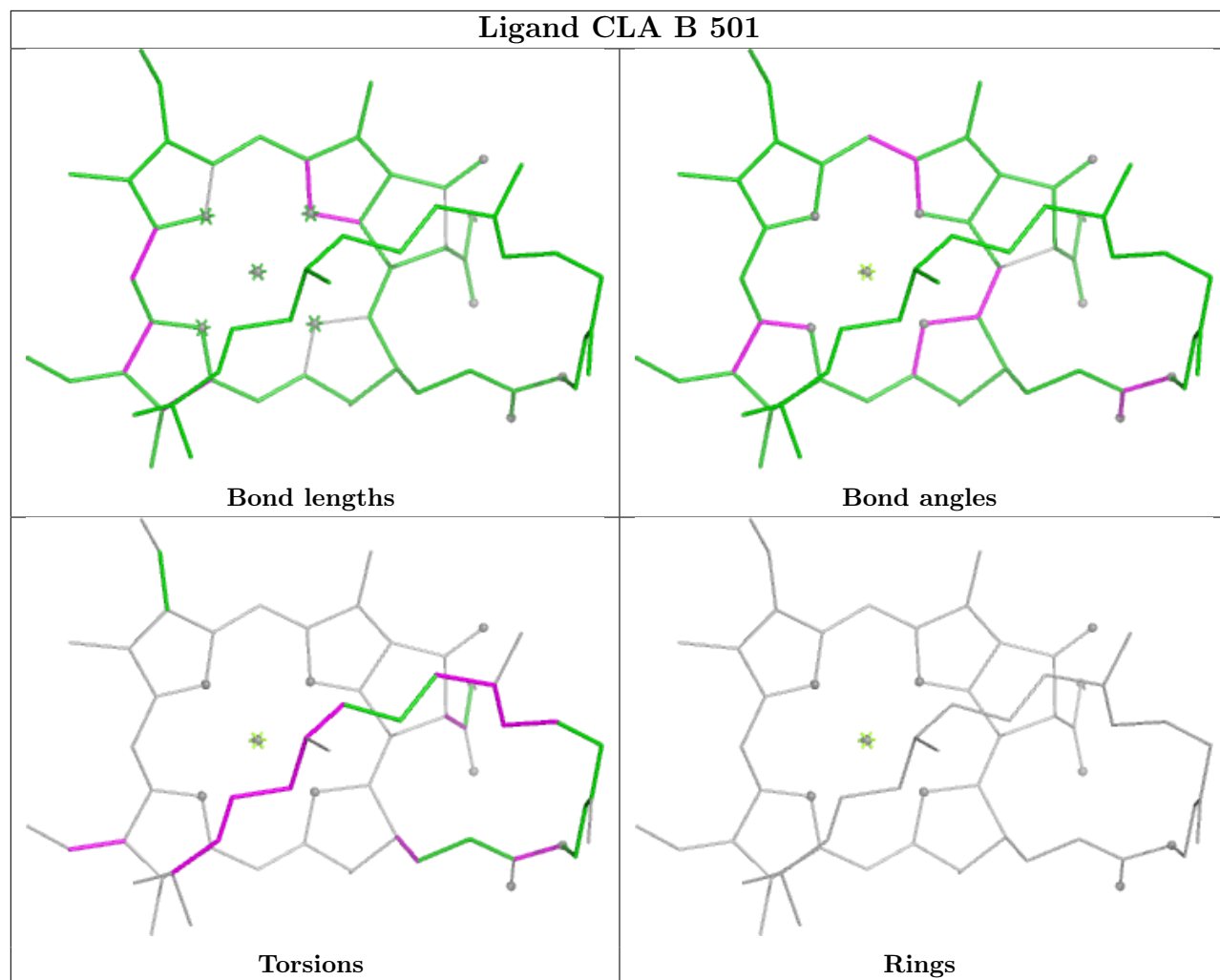
Torsions

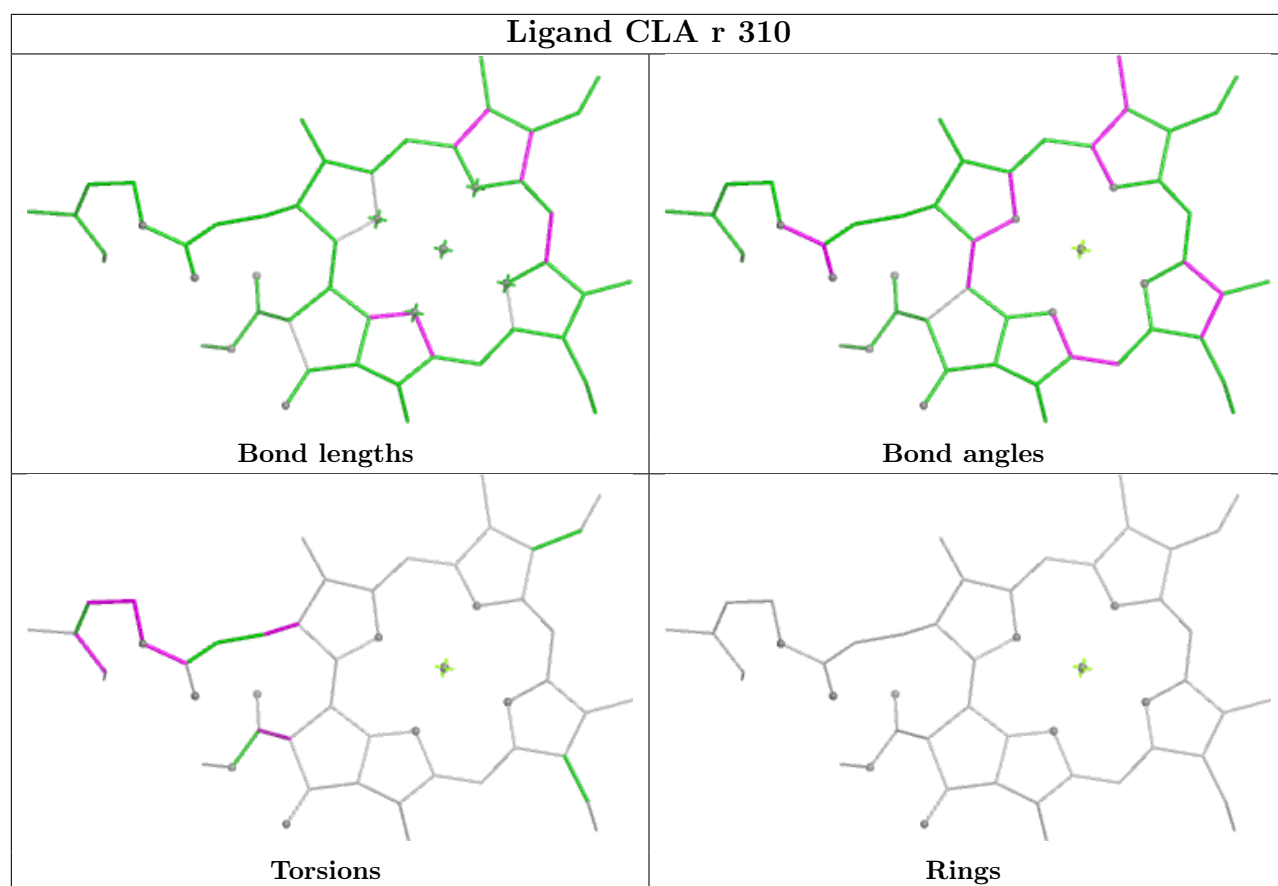


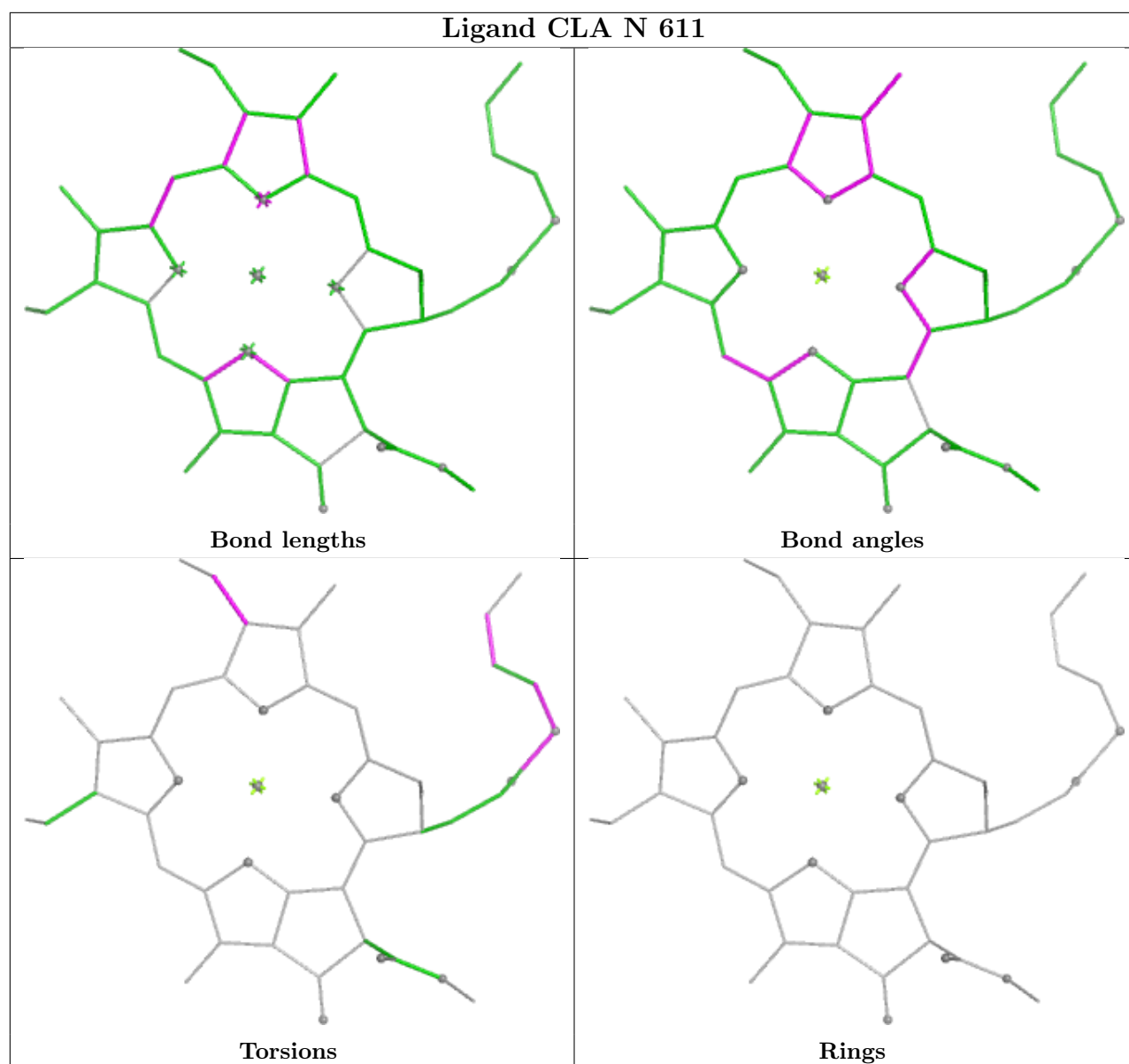
Rings

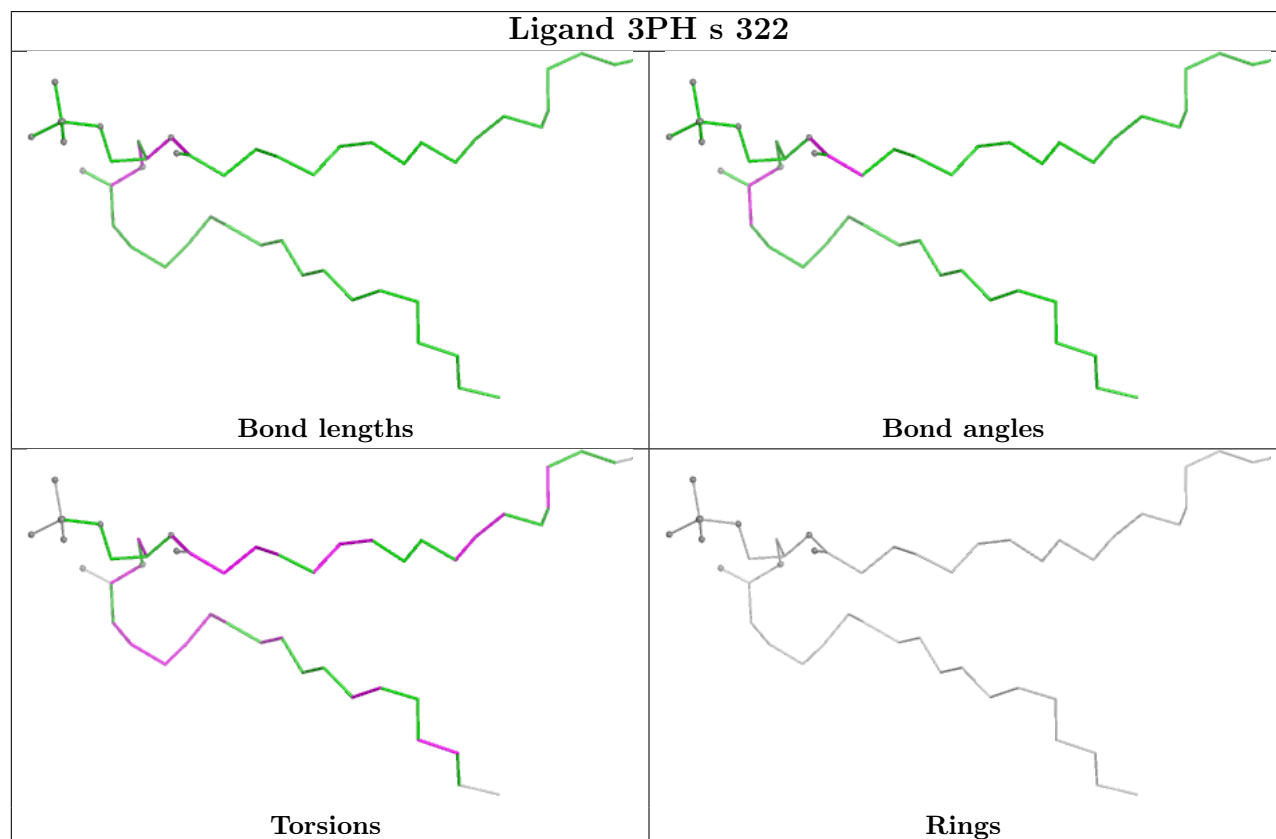
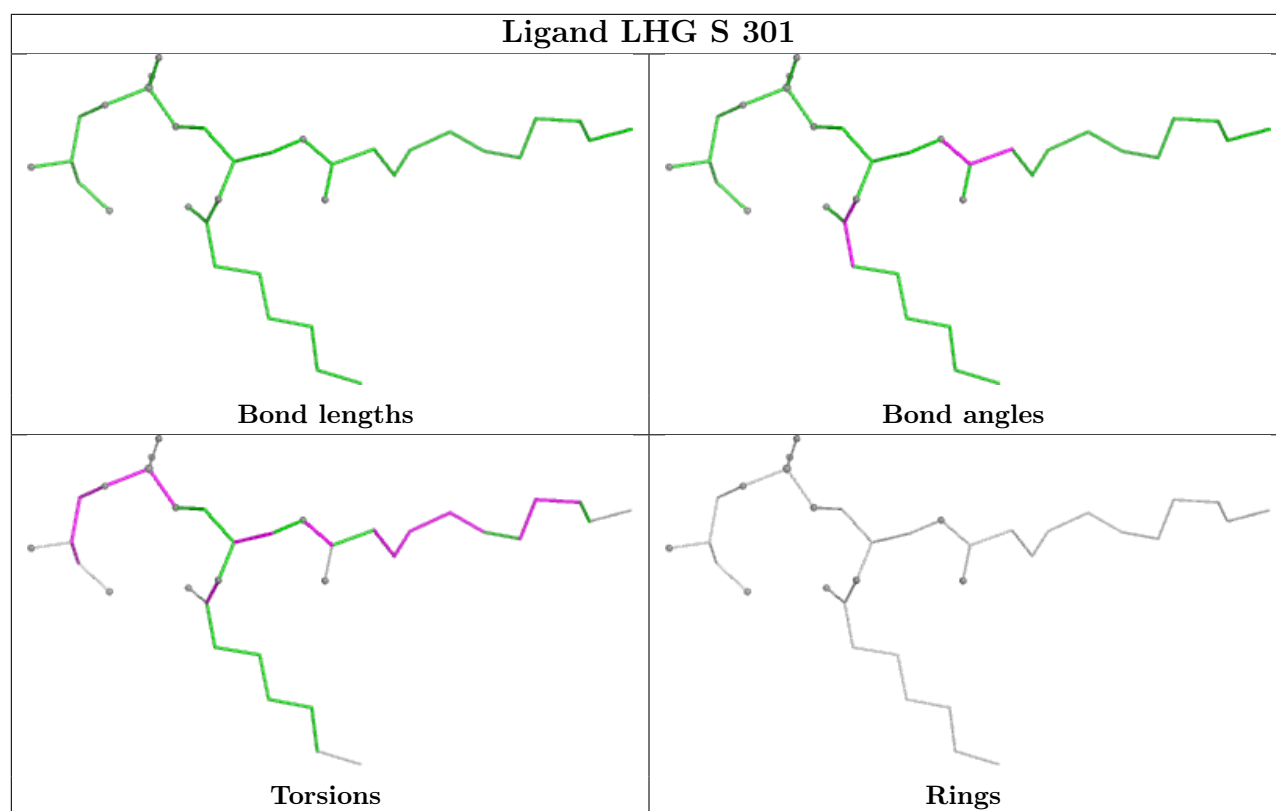


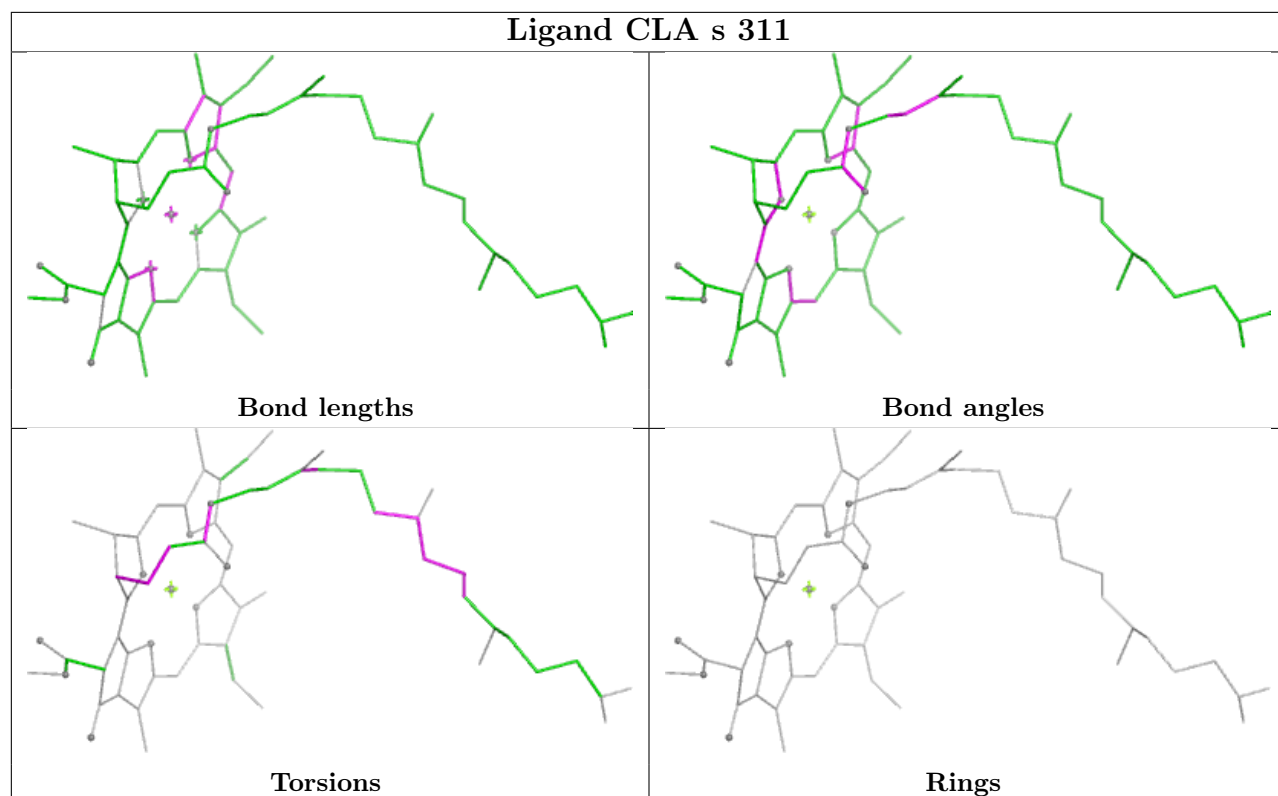
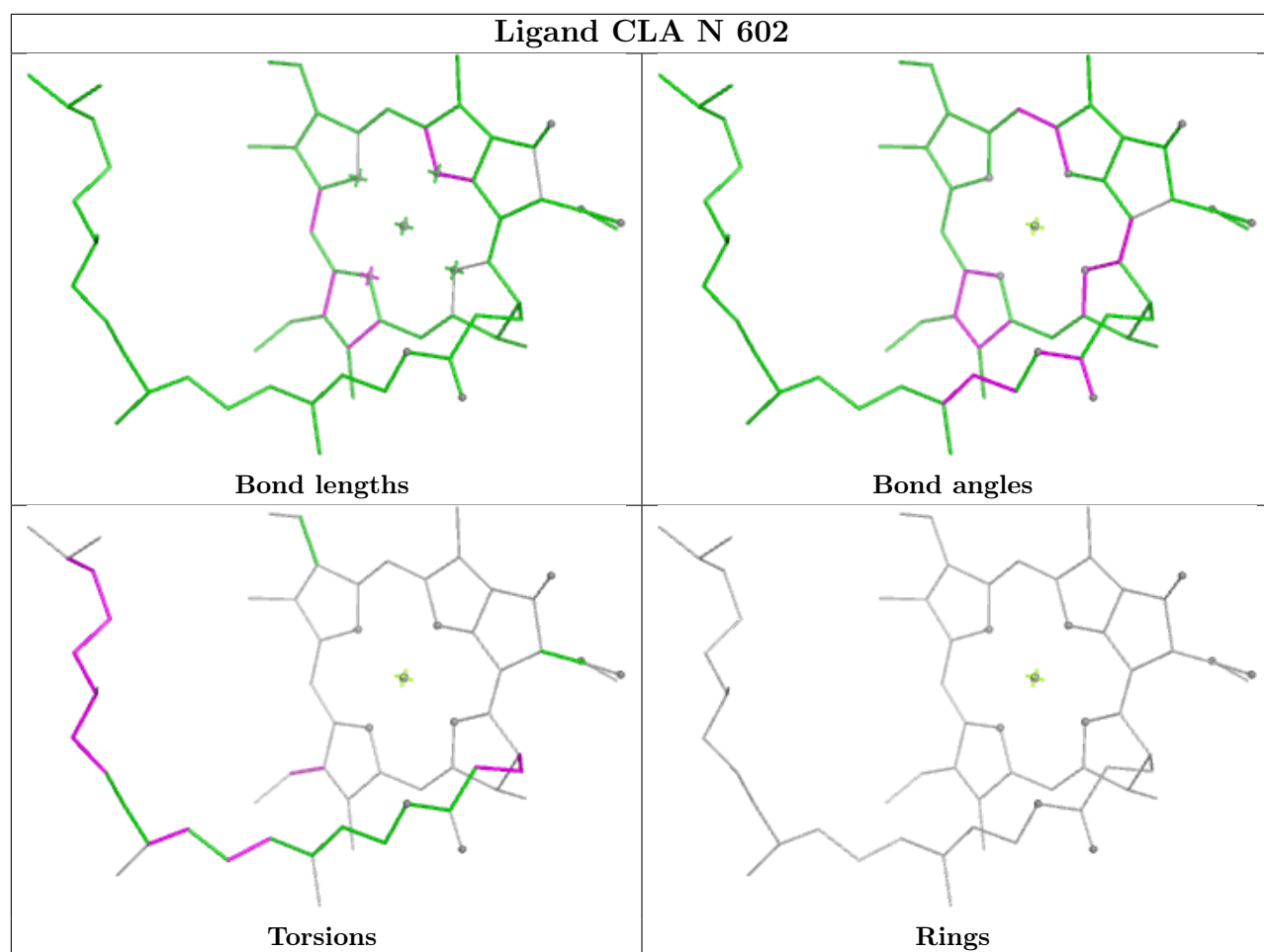
Ligand CLA B 501

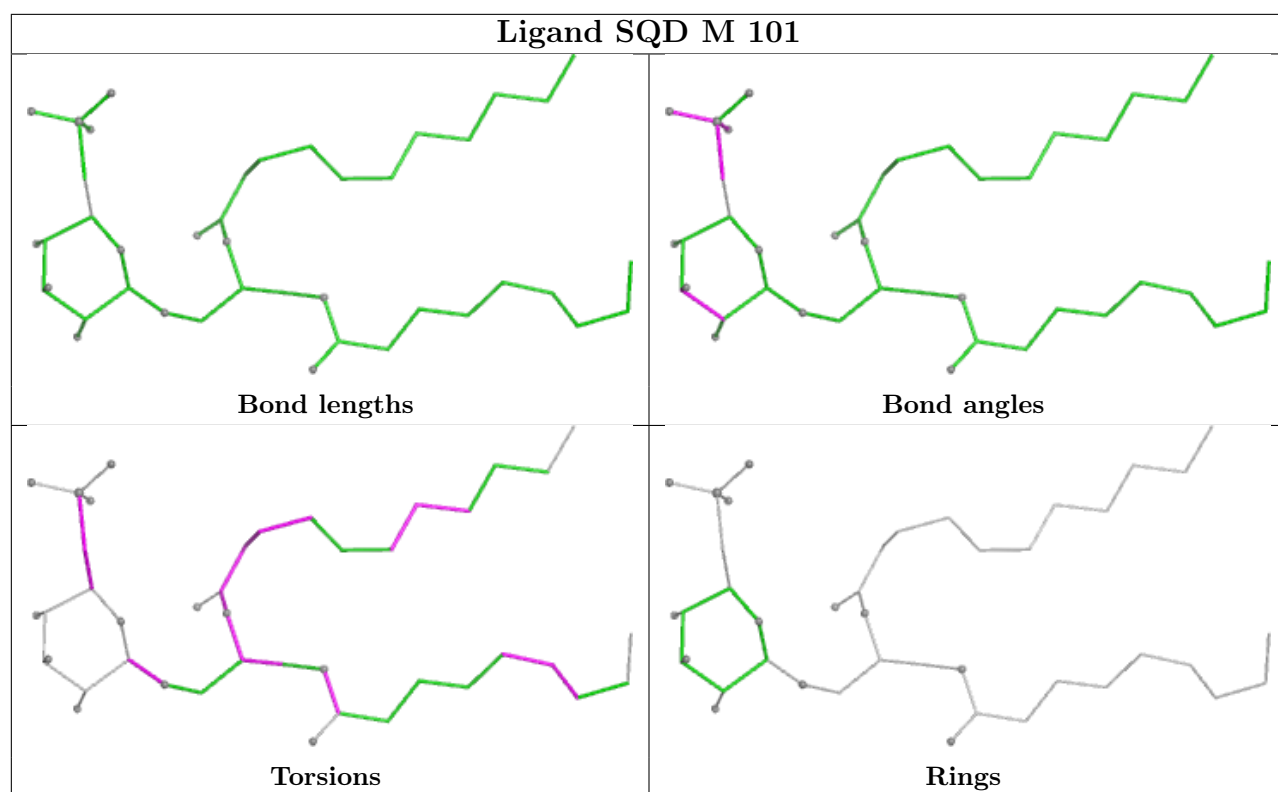


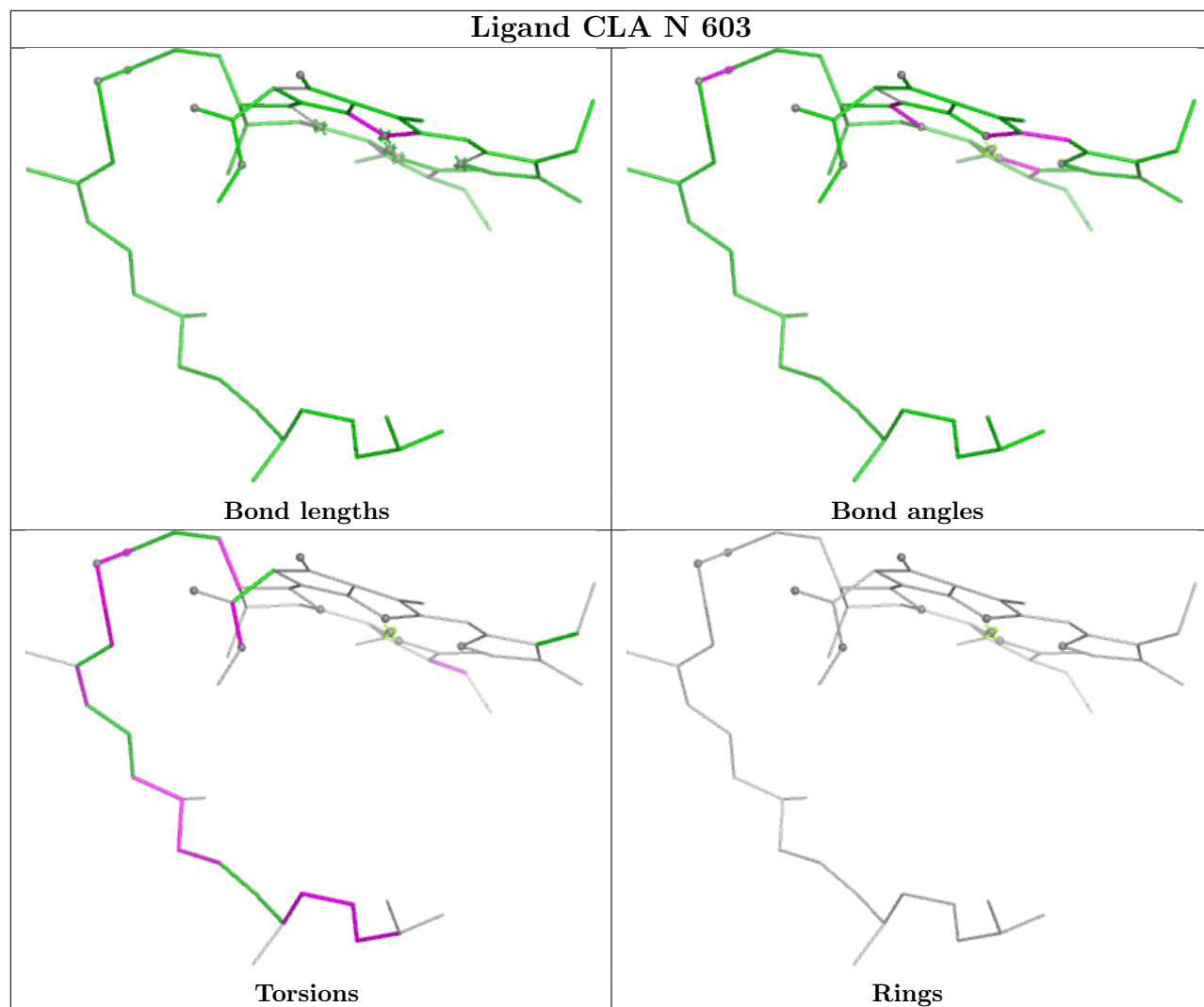


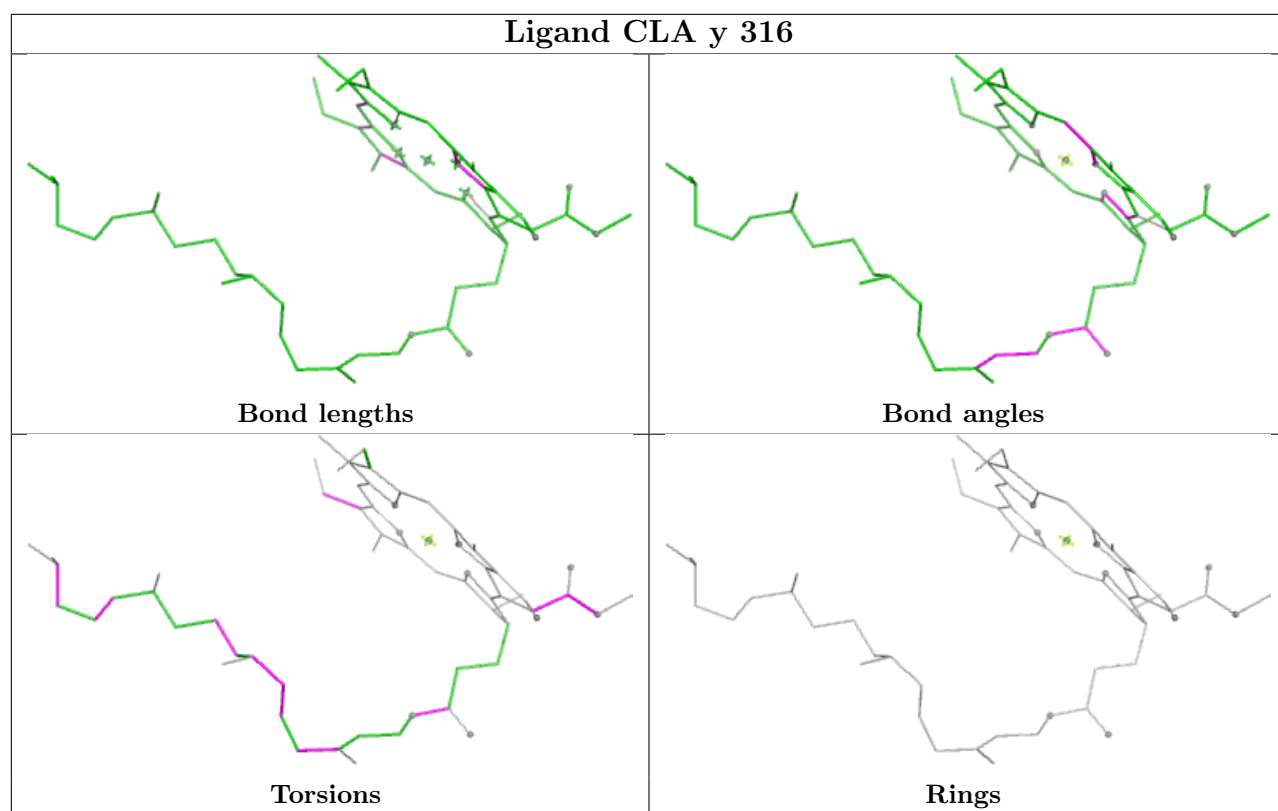


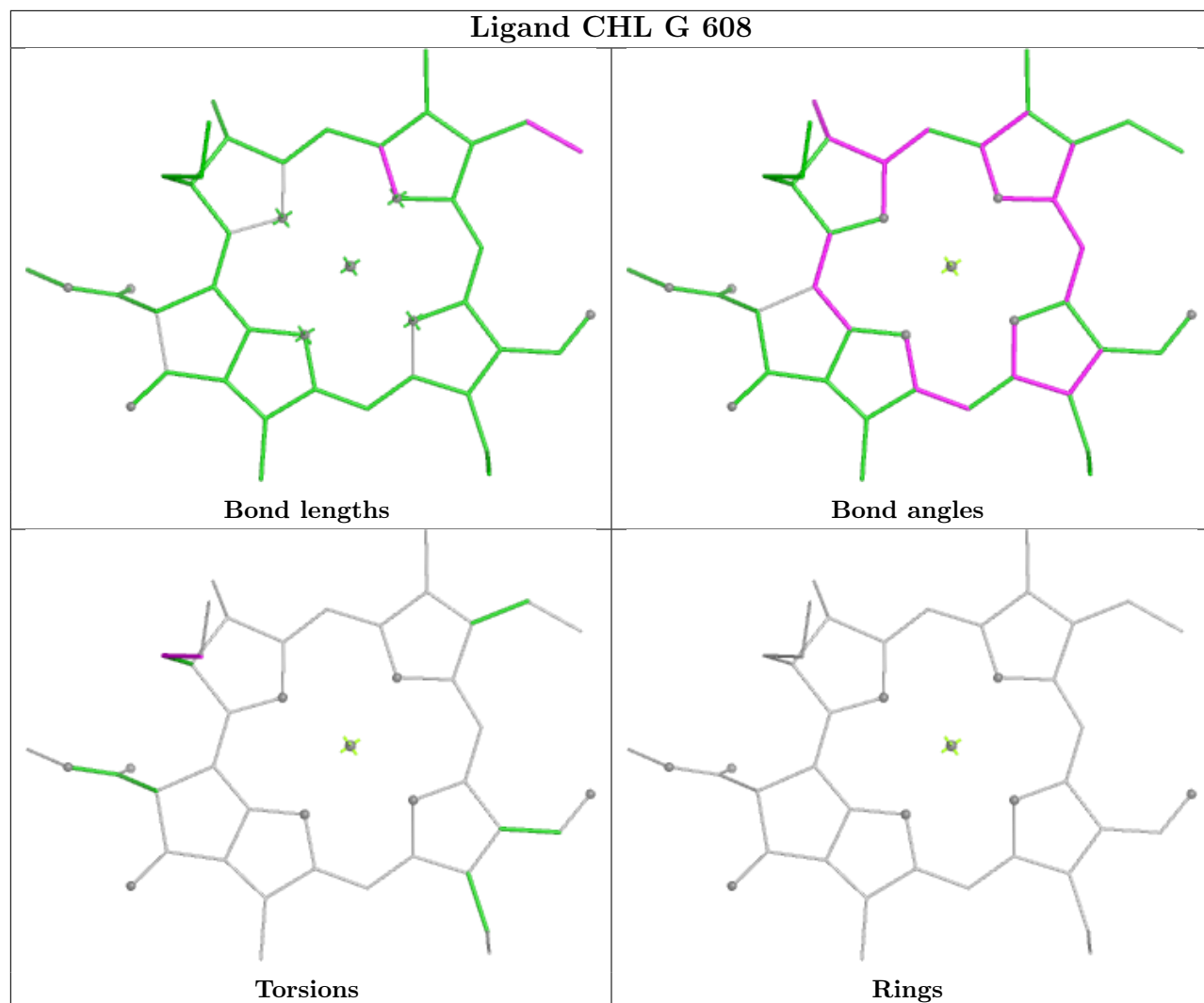


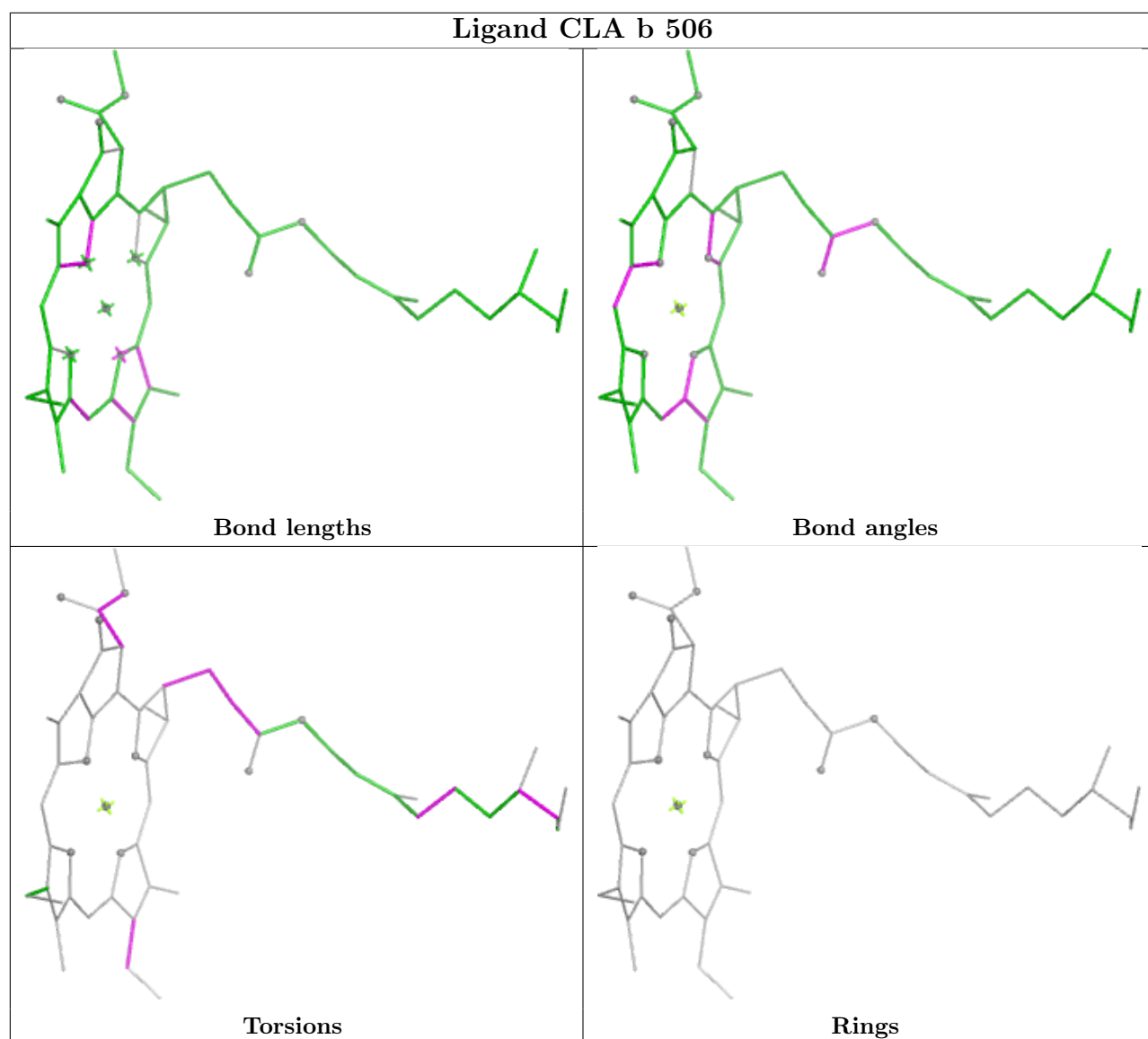


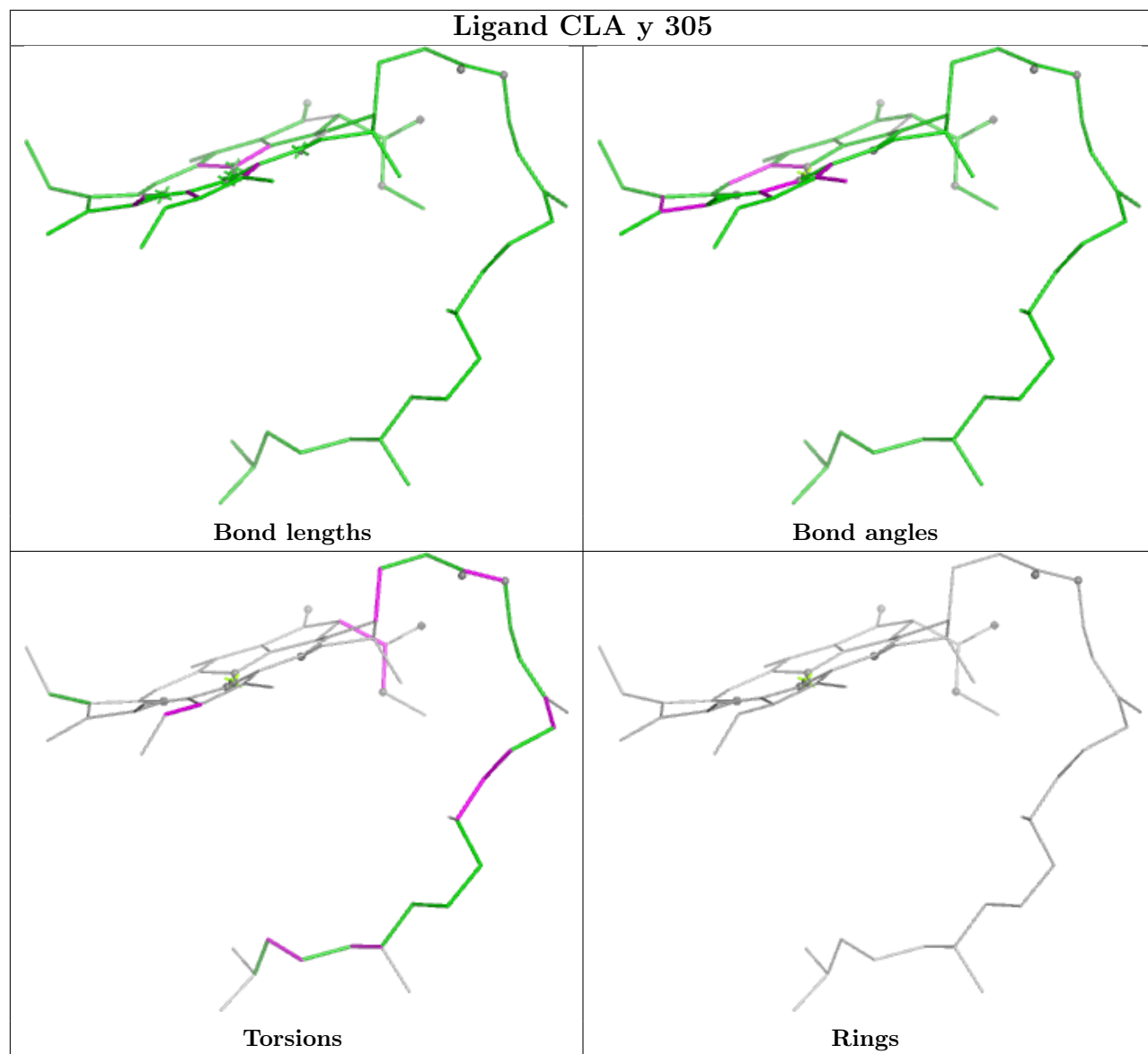


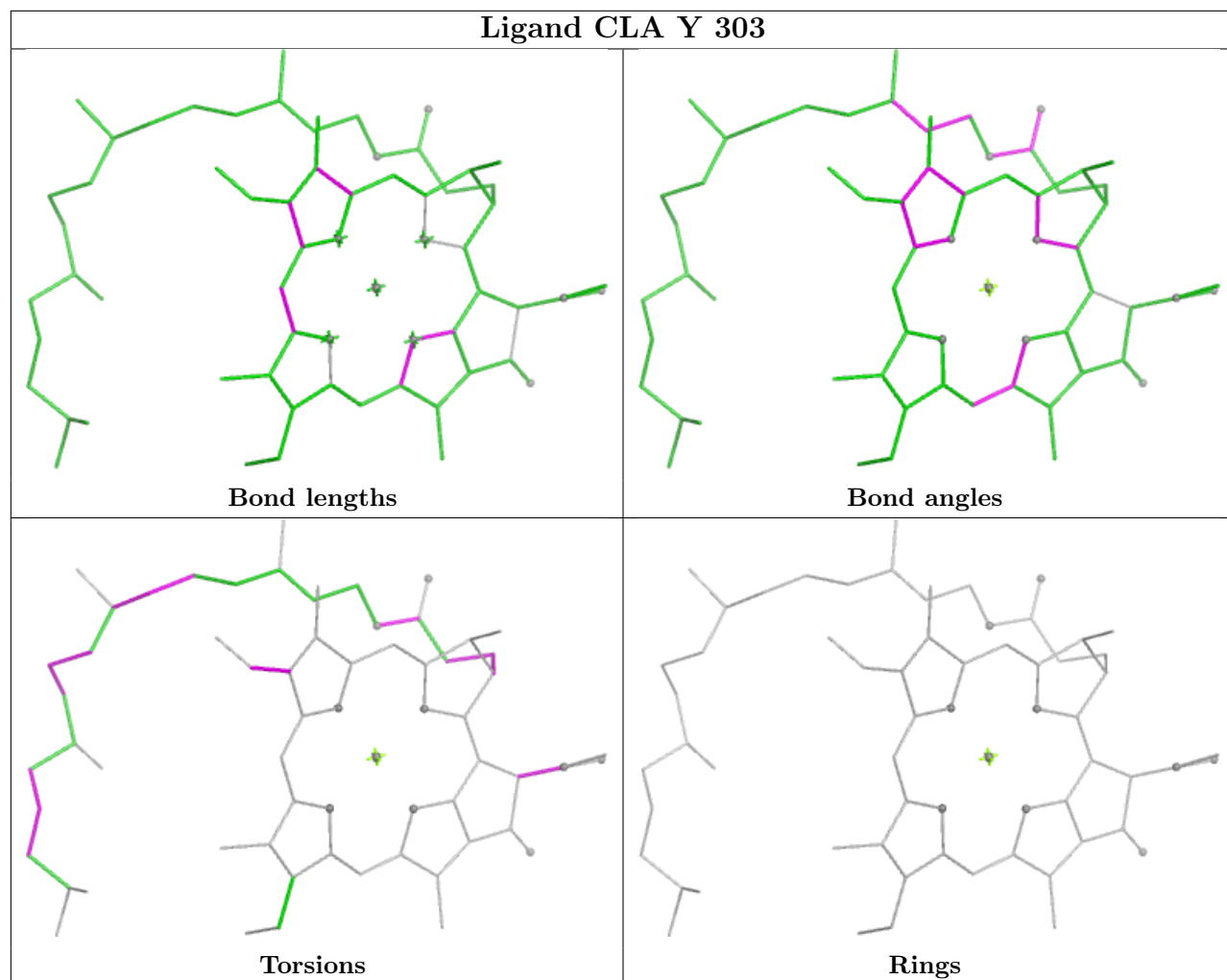


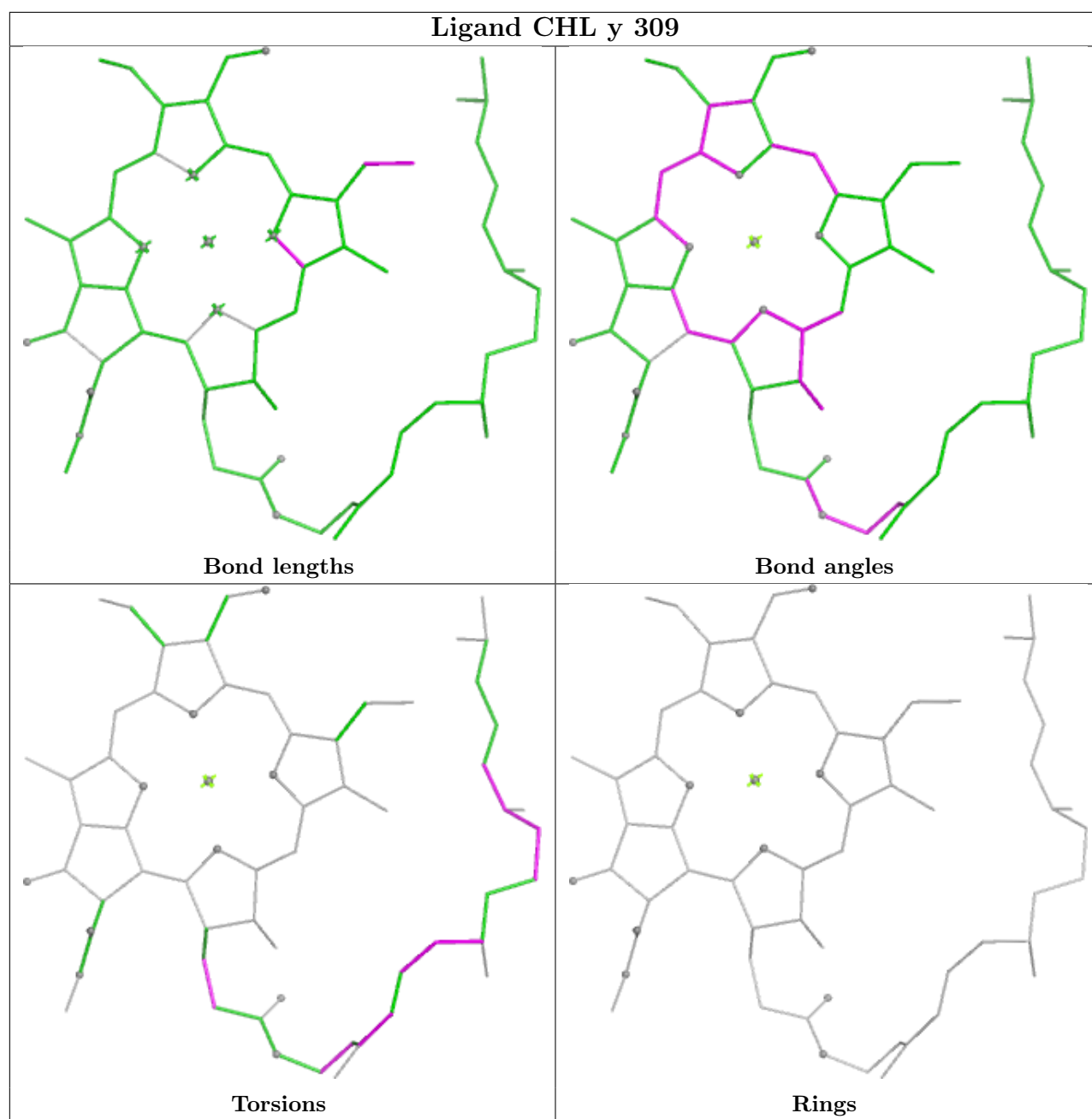




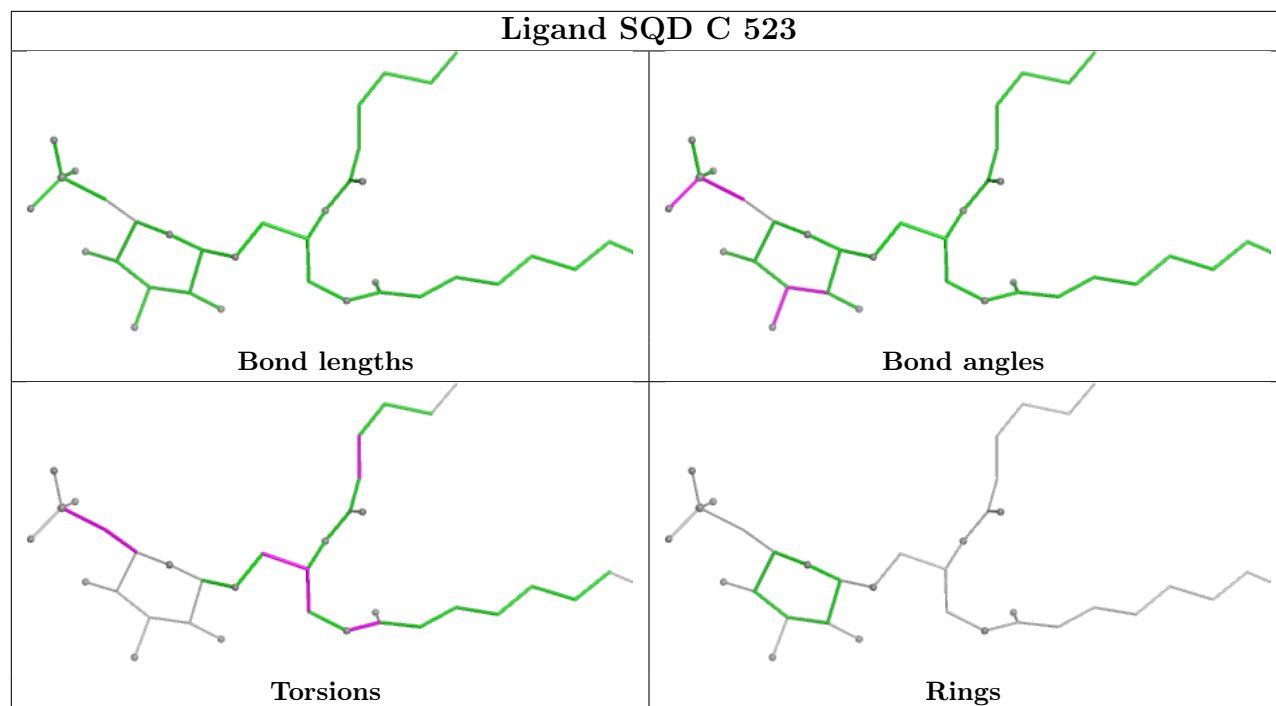




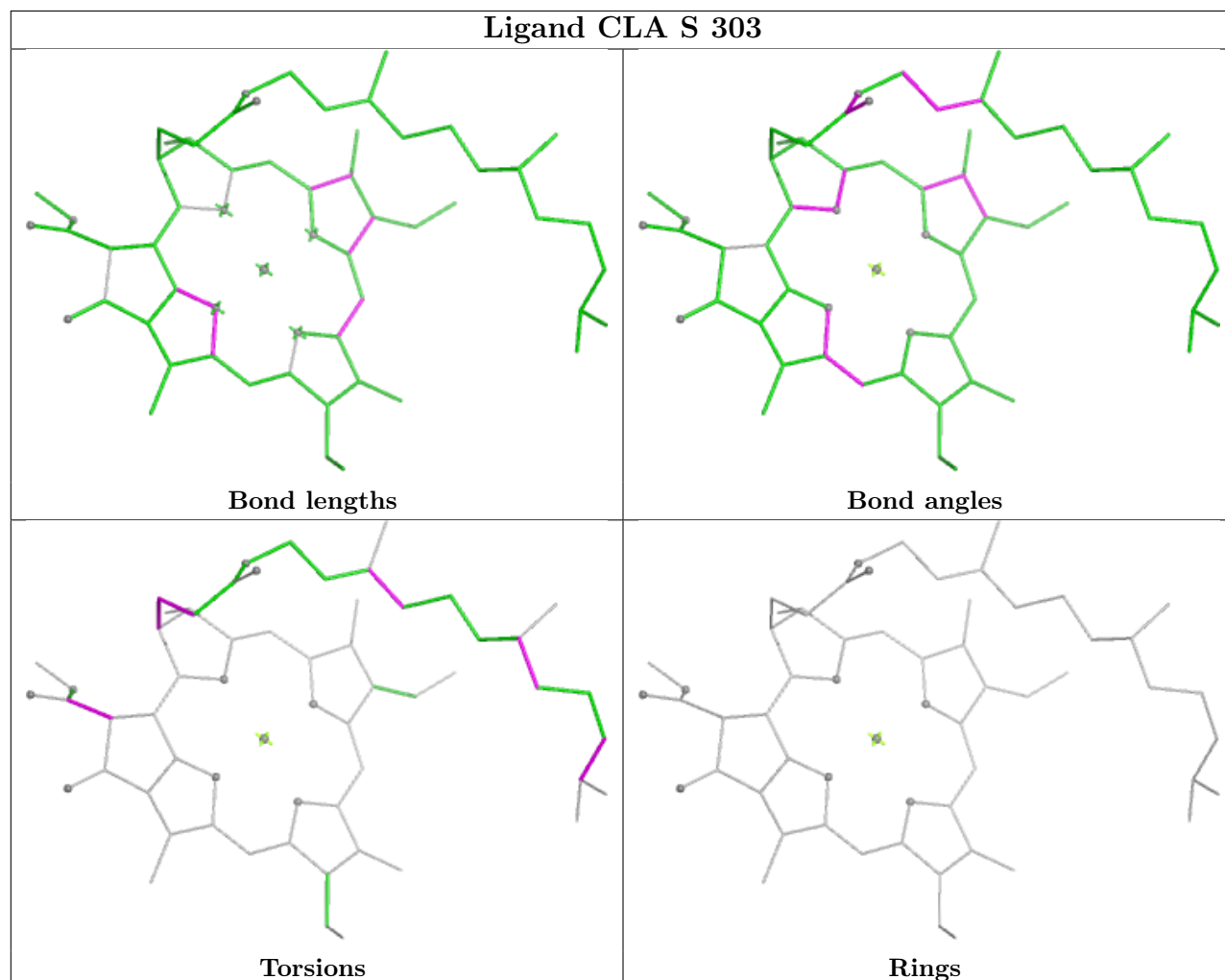




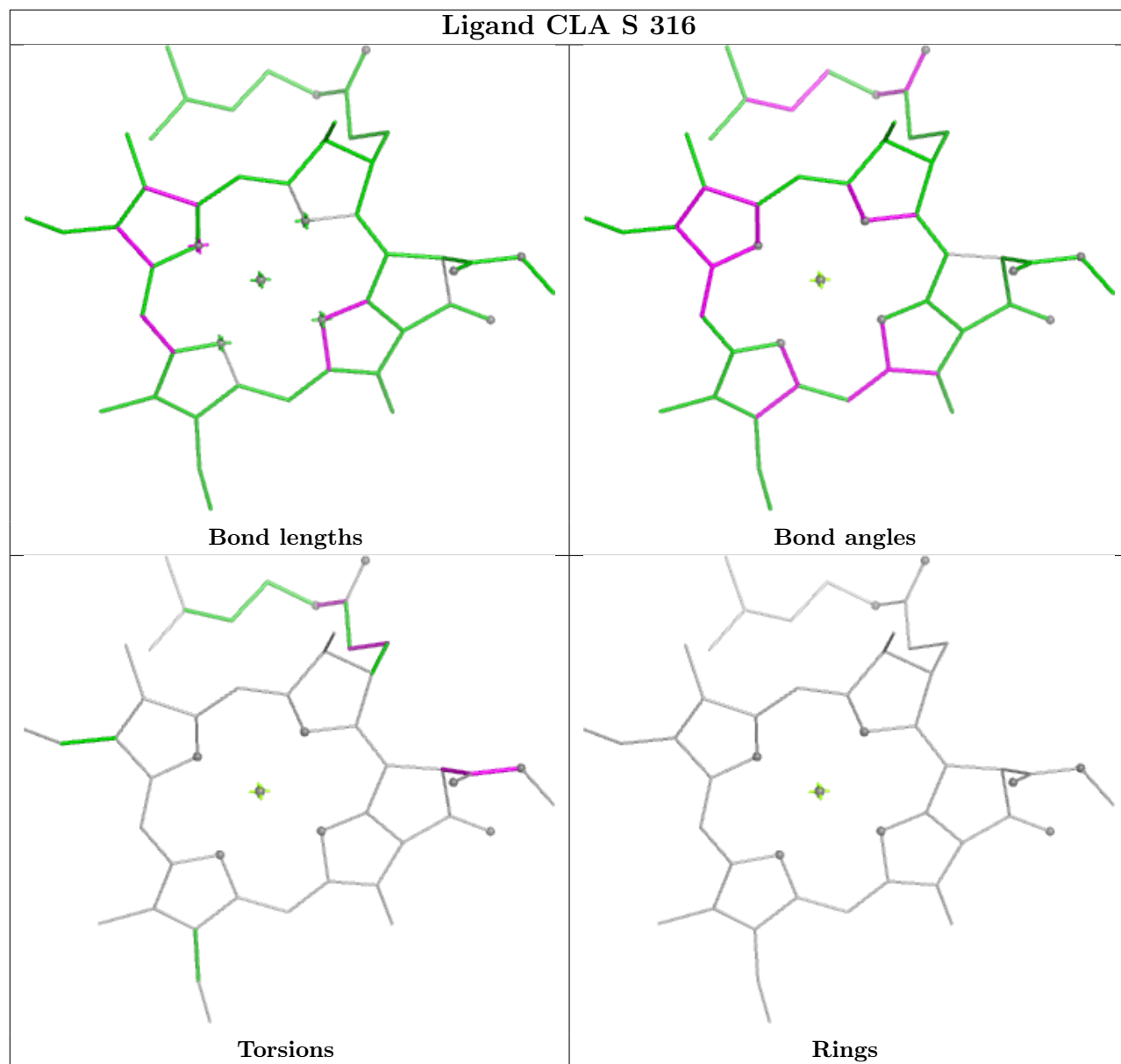
Ligand SQD C 523

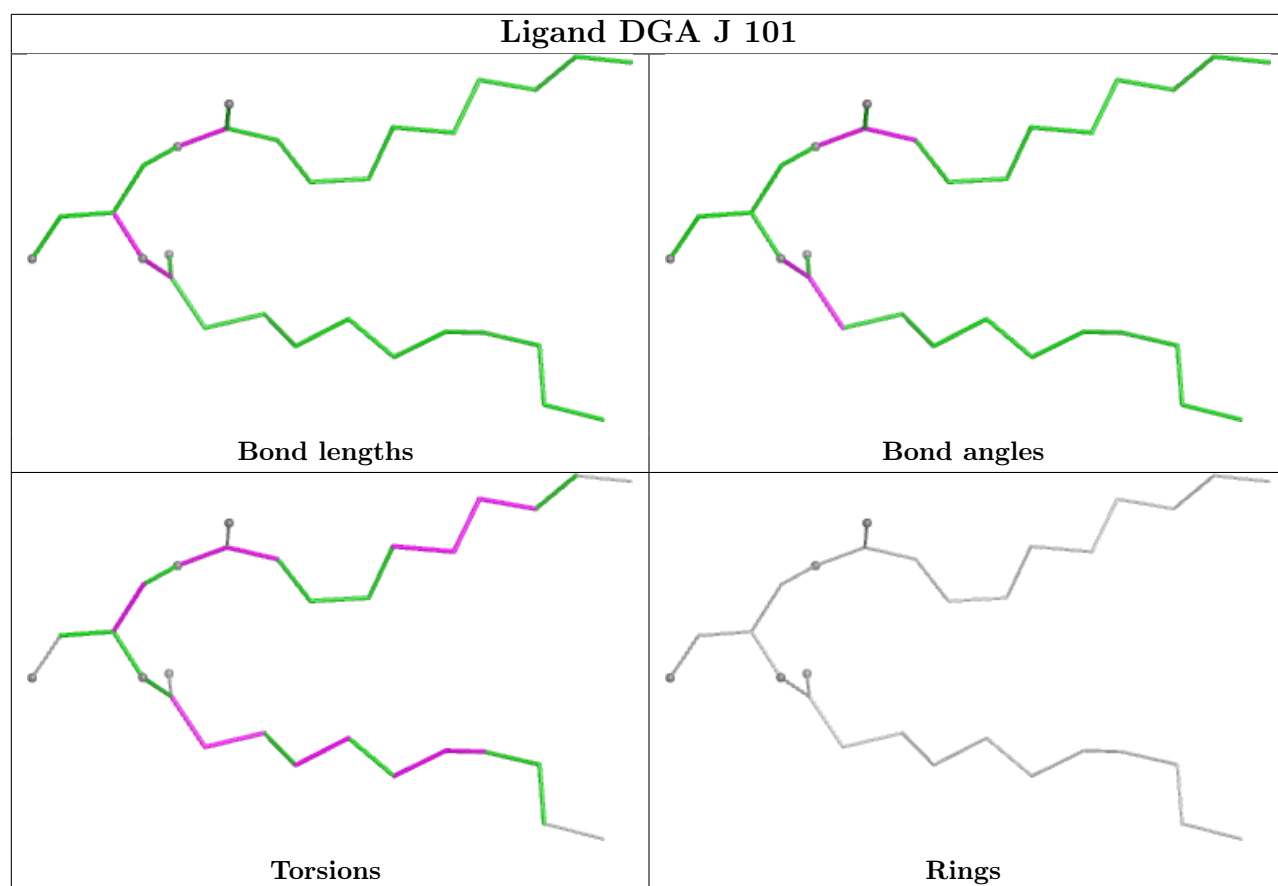


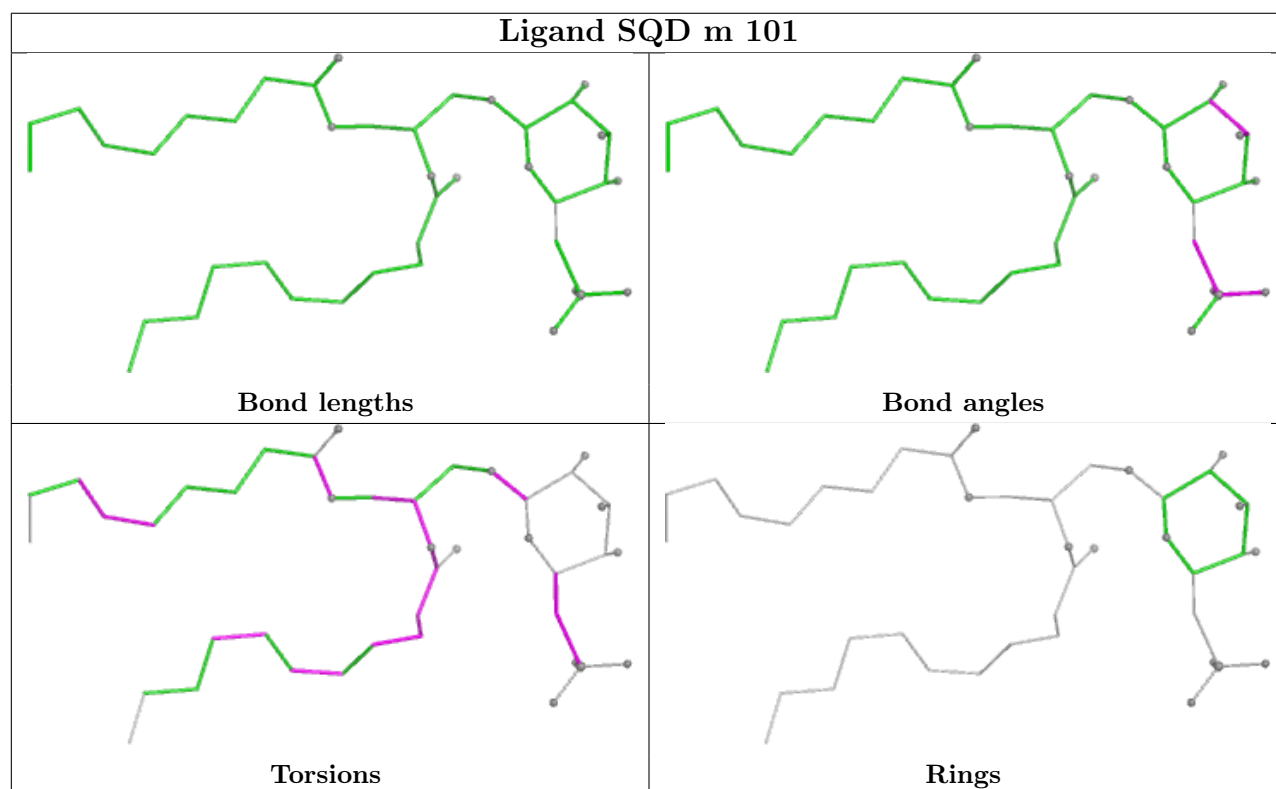
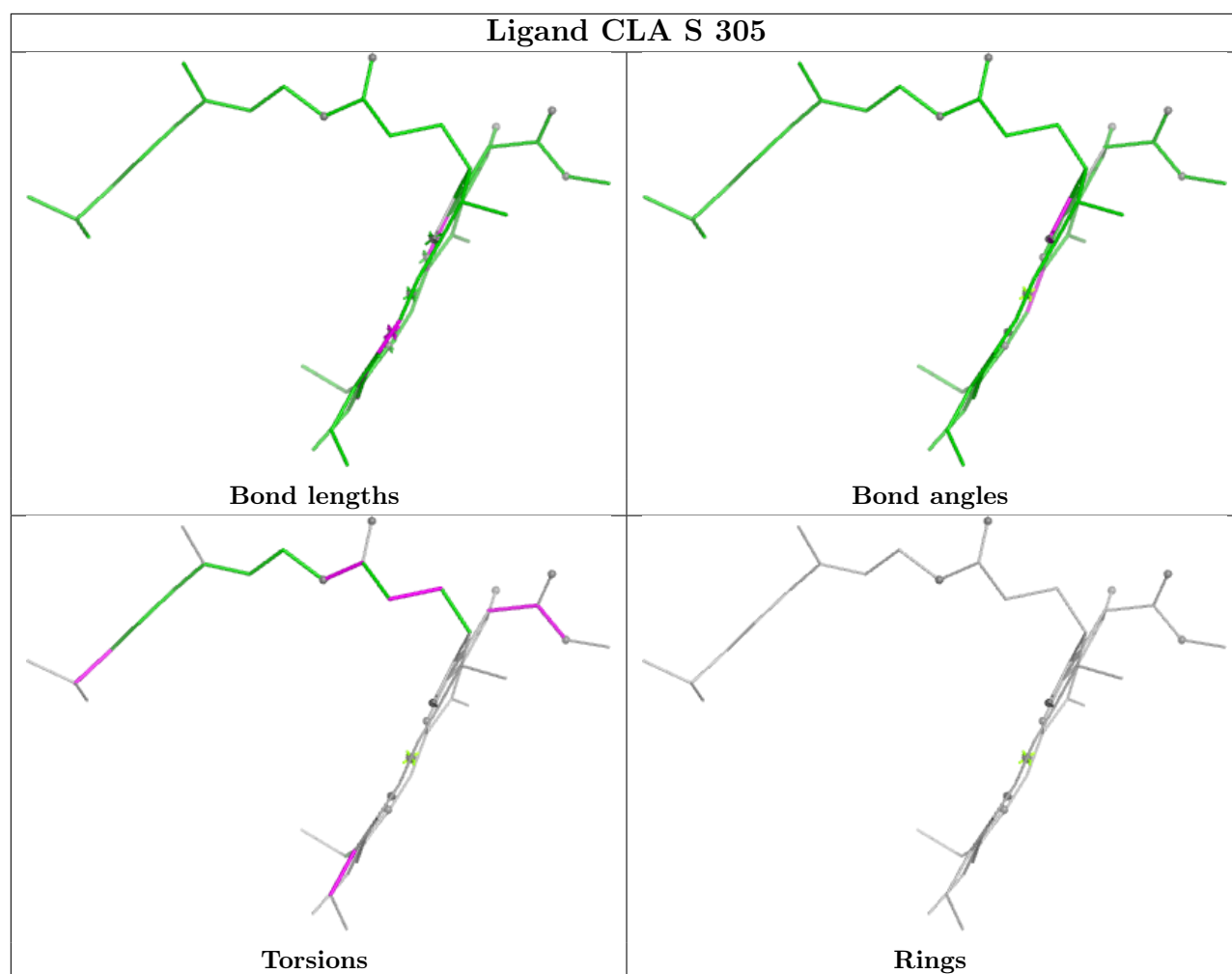
Ligand CLA S 303

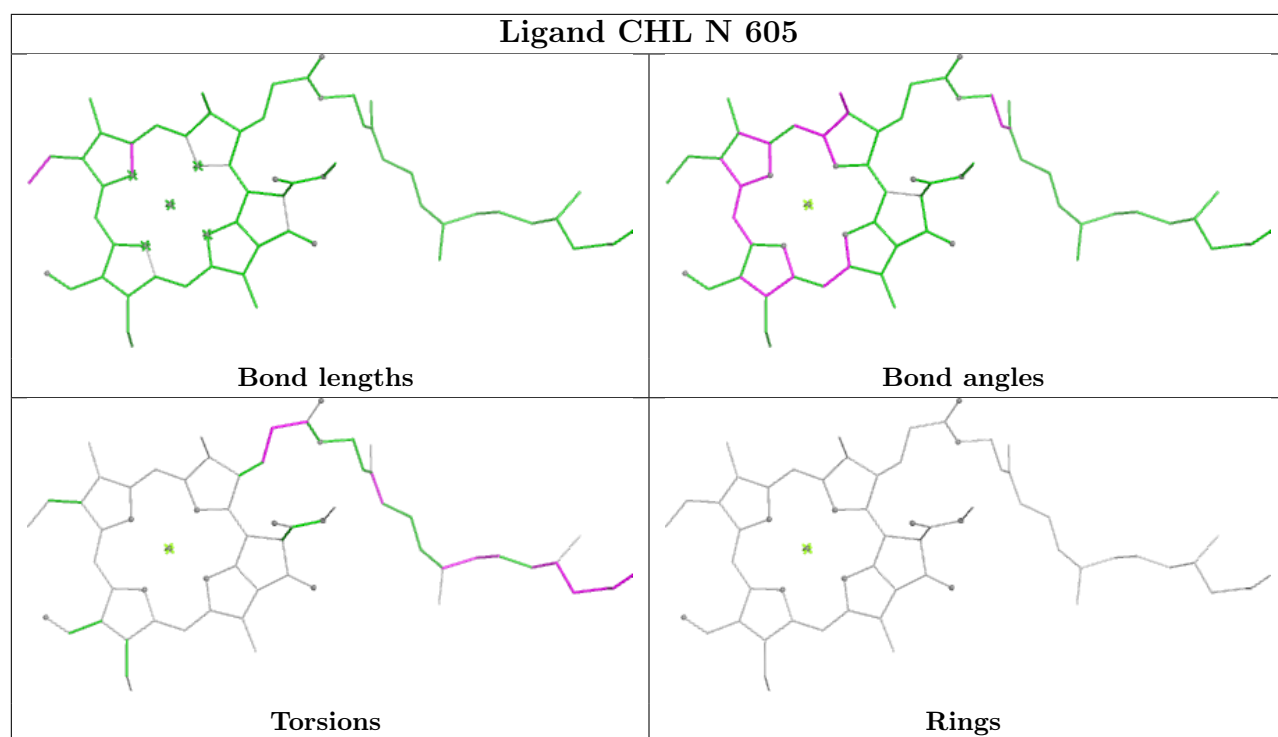


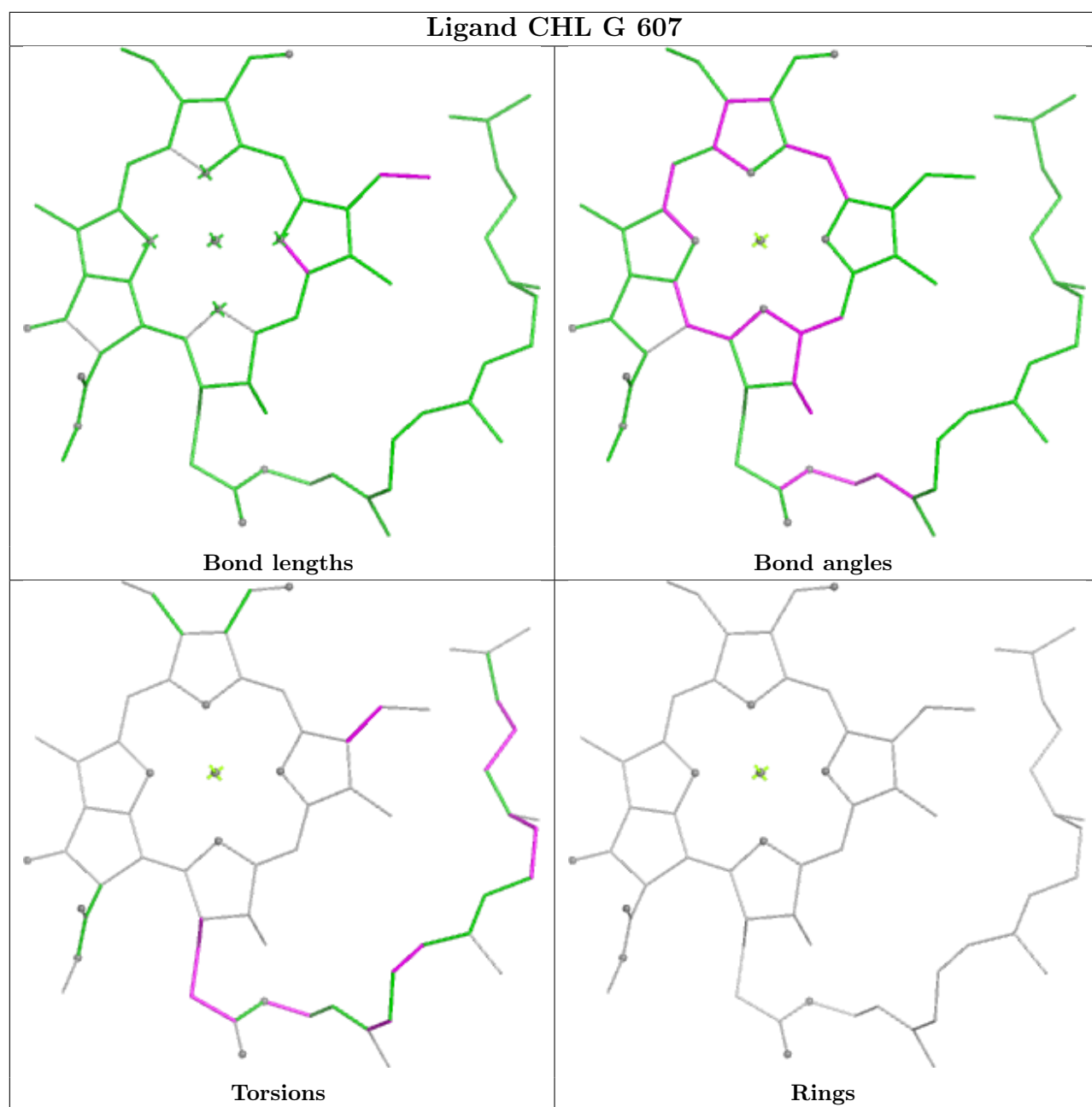
Ligand CLA S 316

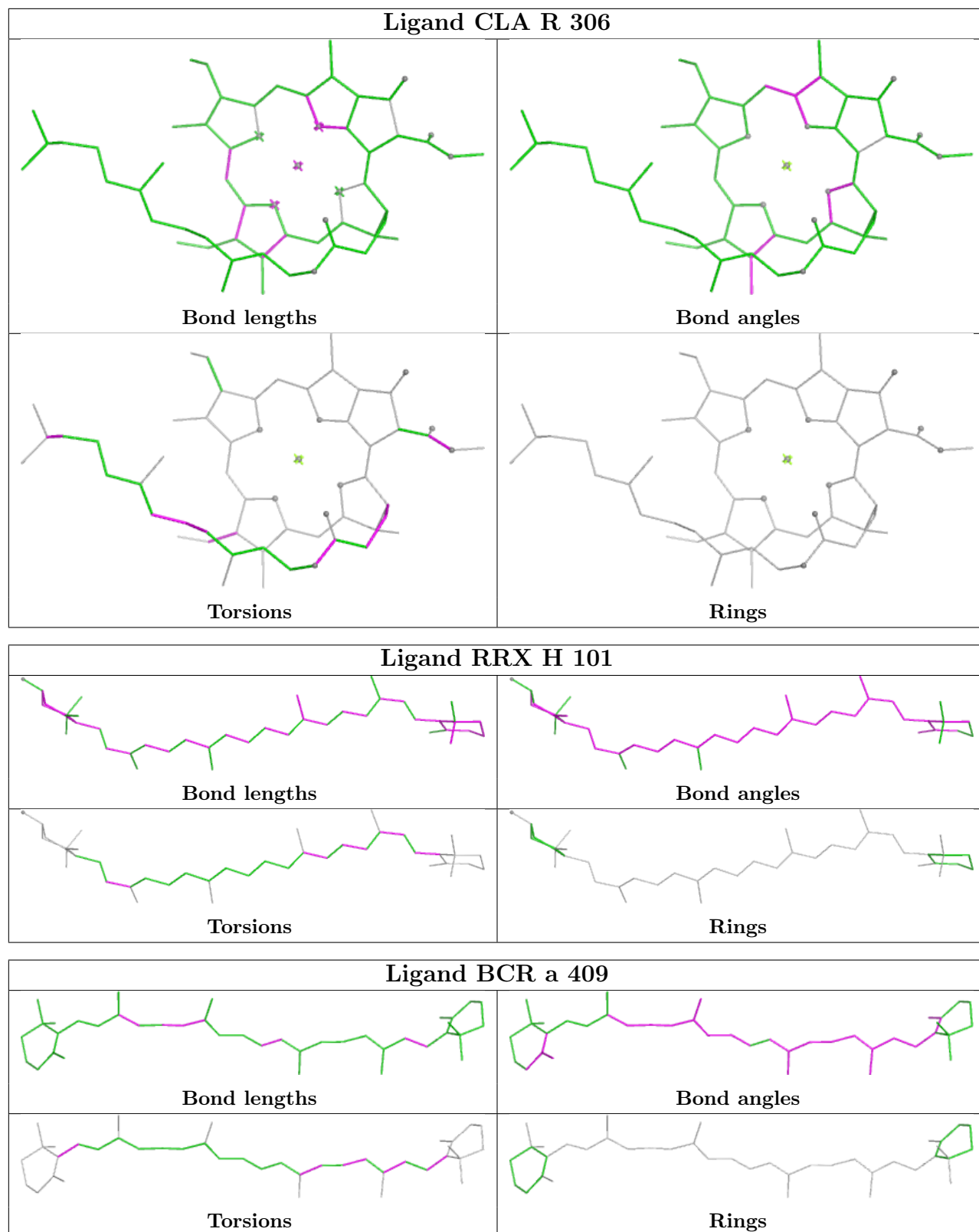




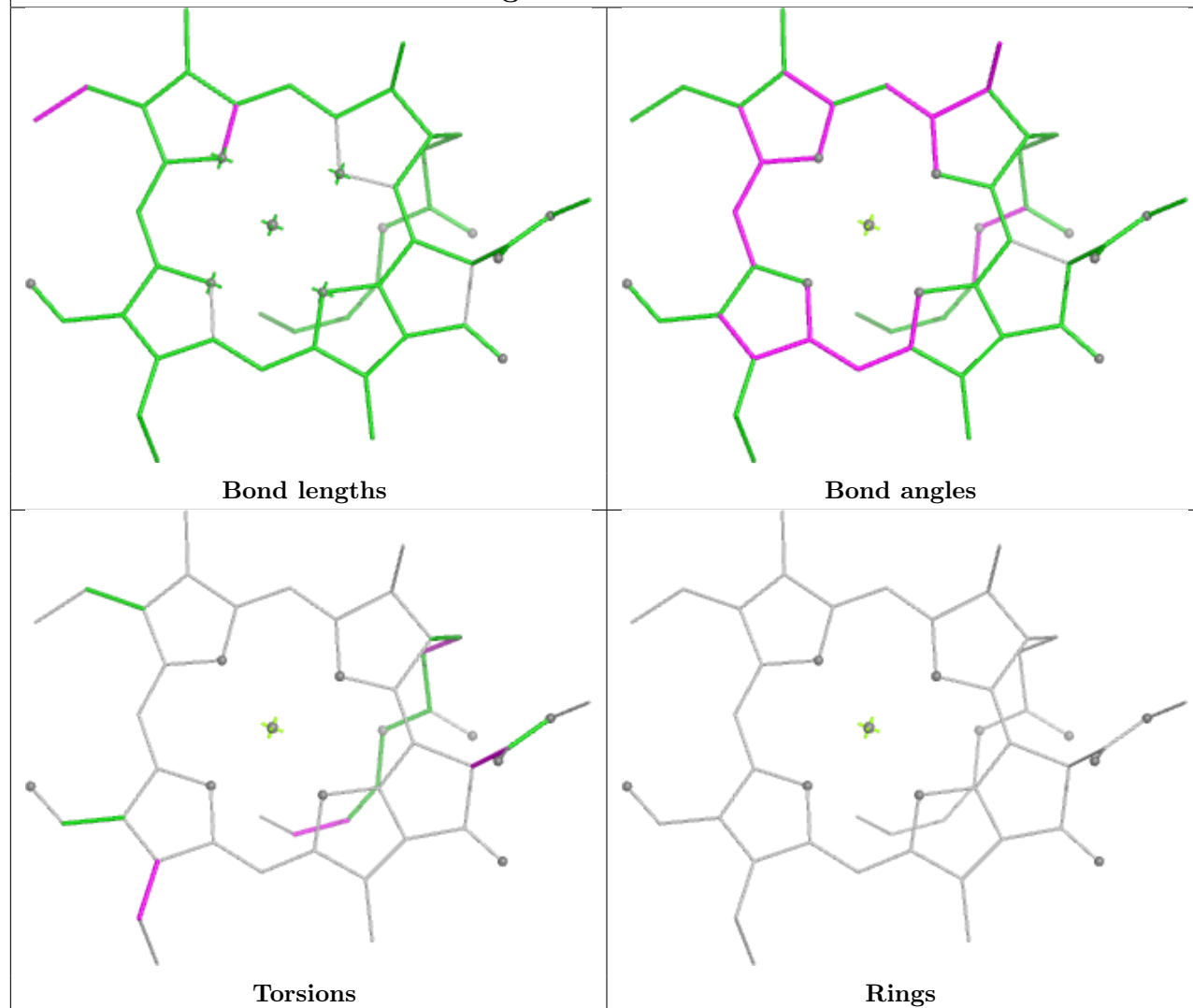




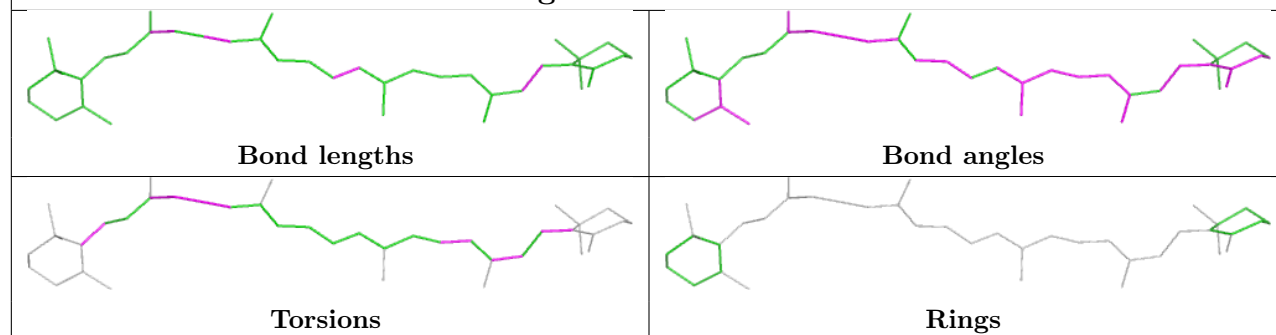


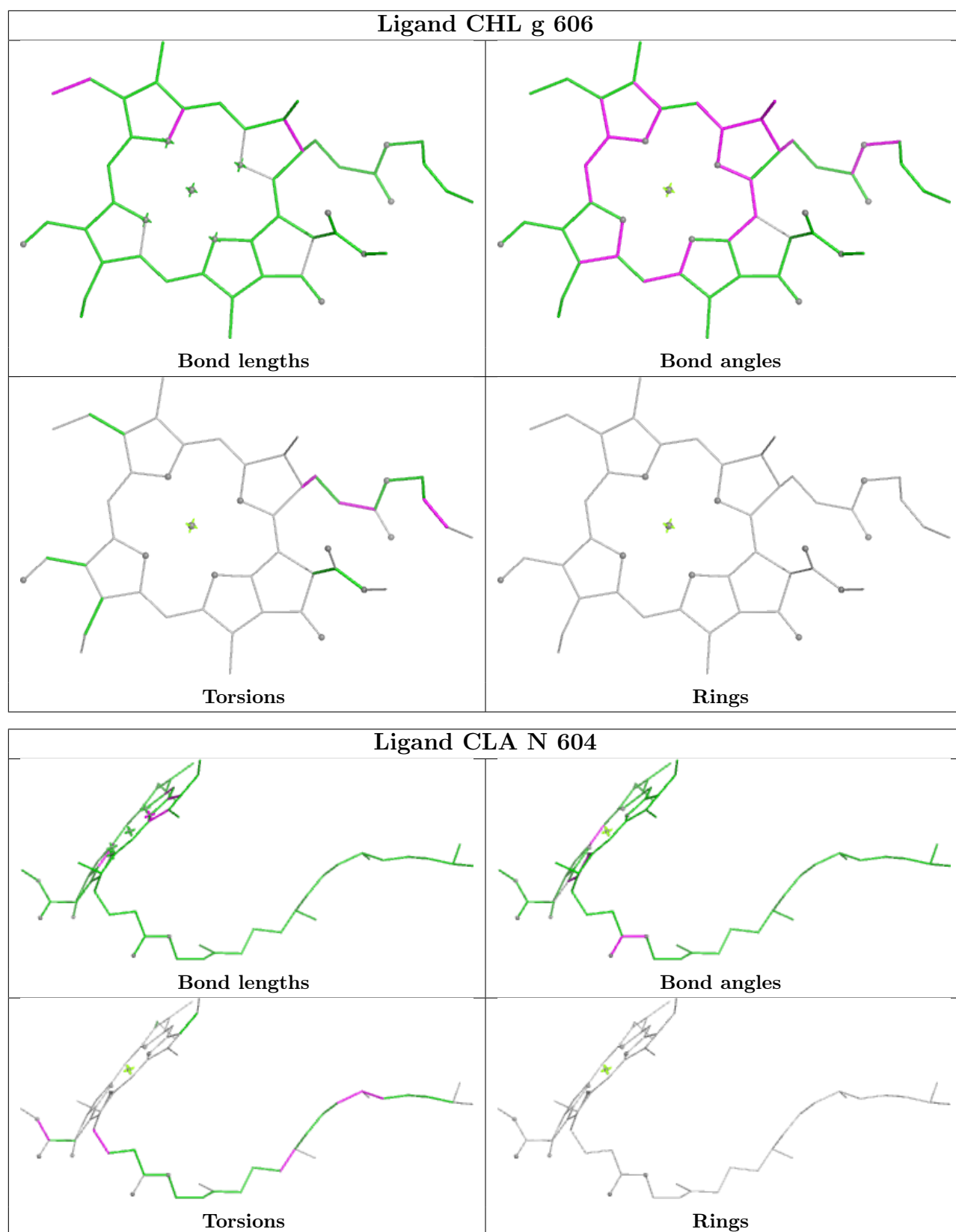


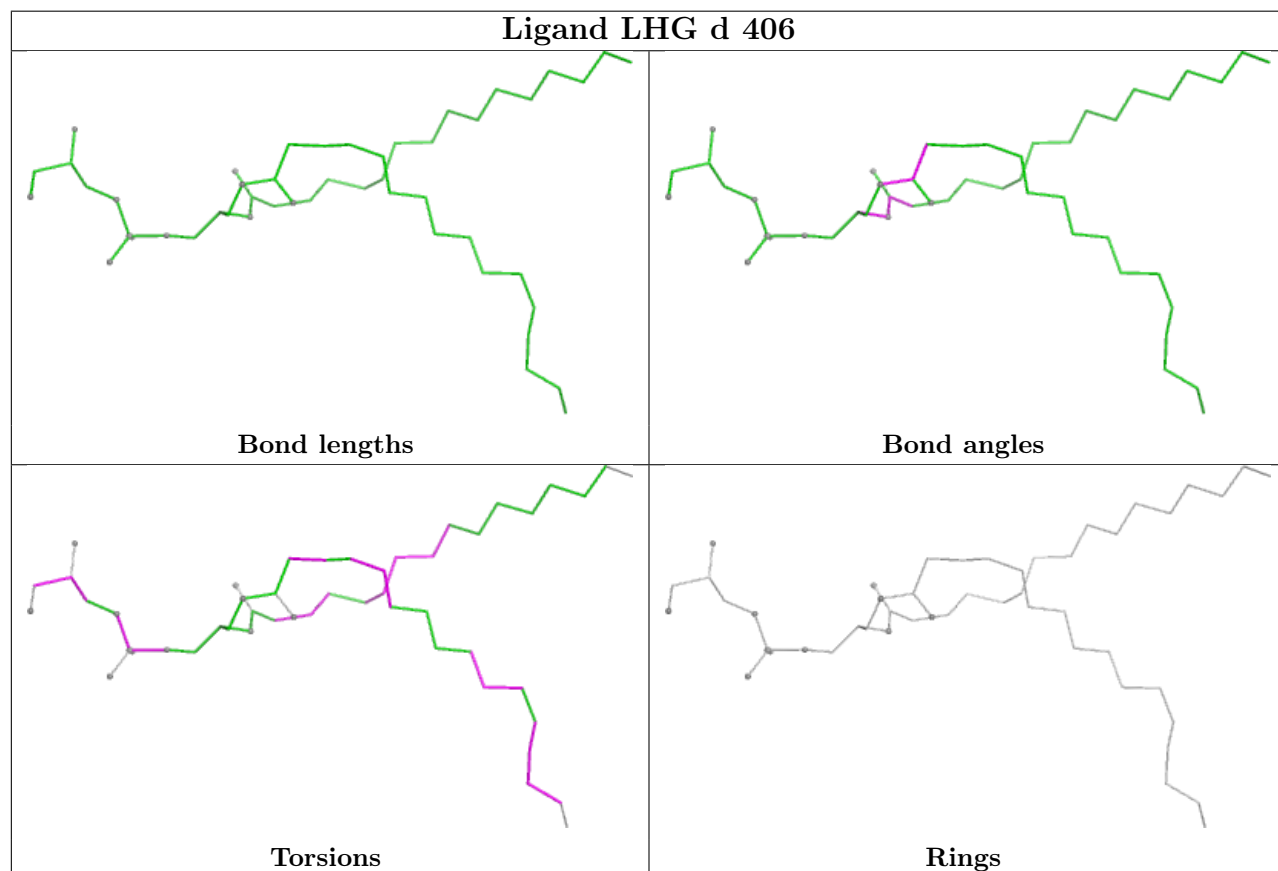
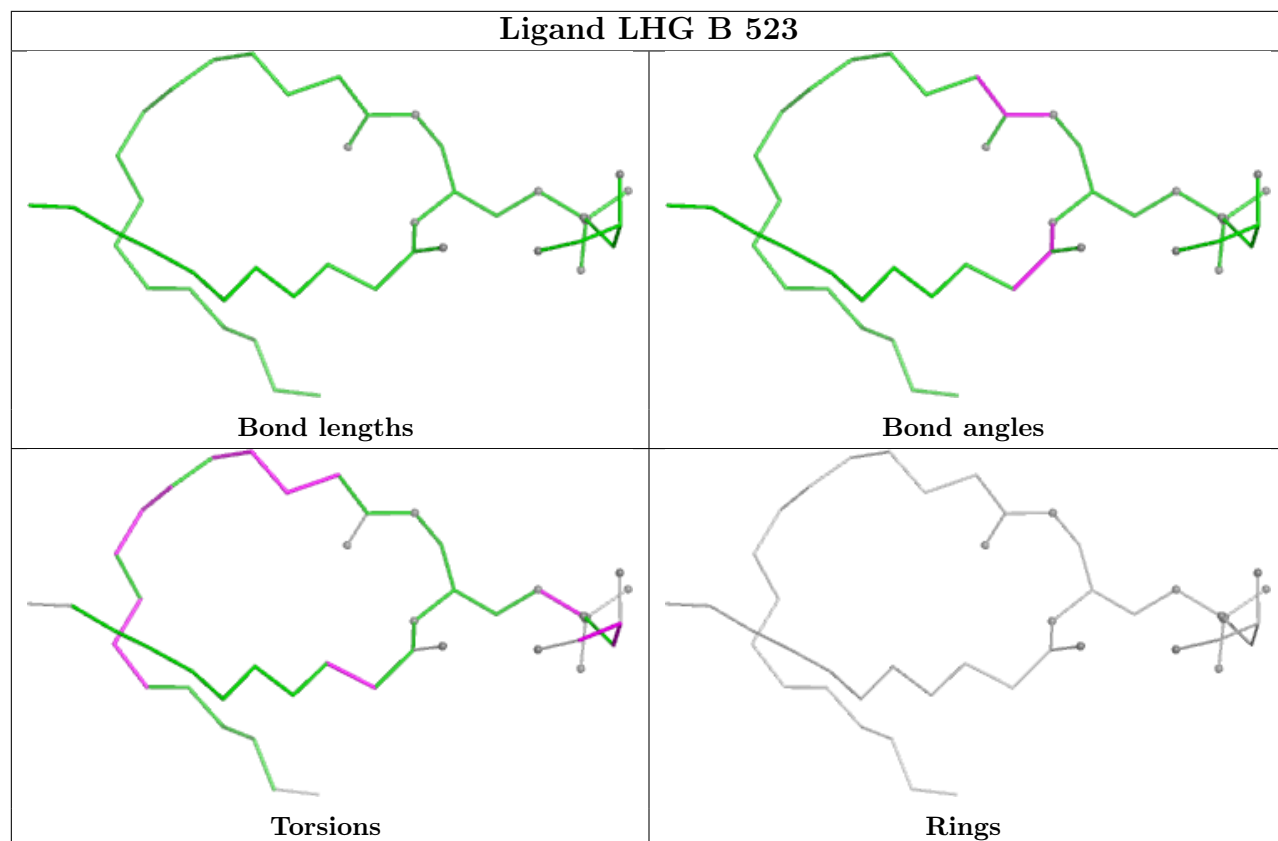
Ligand CHL r 306

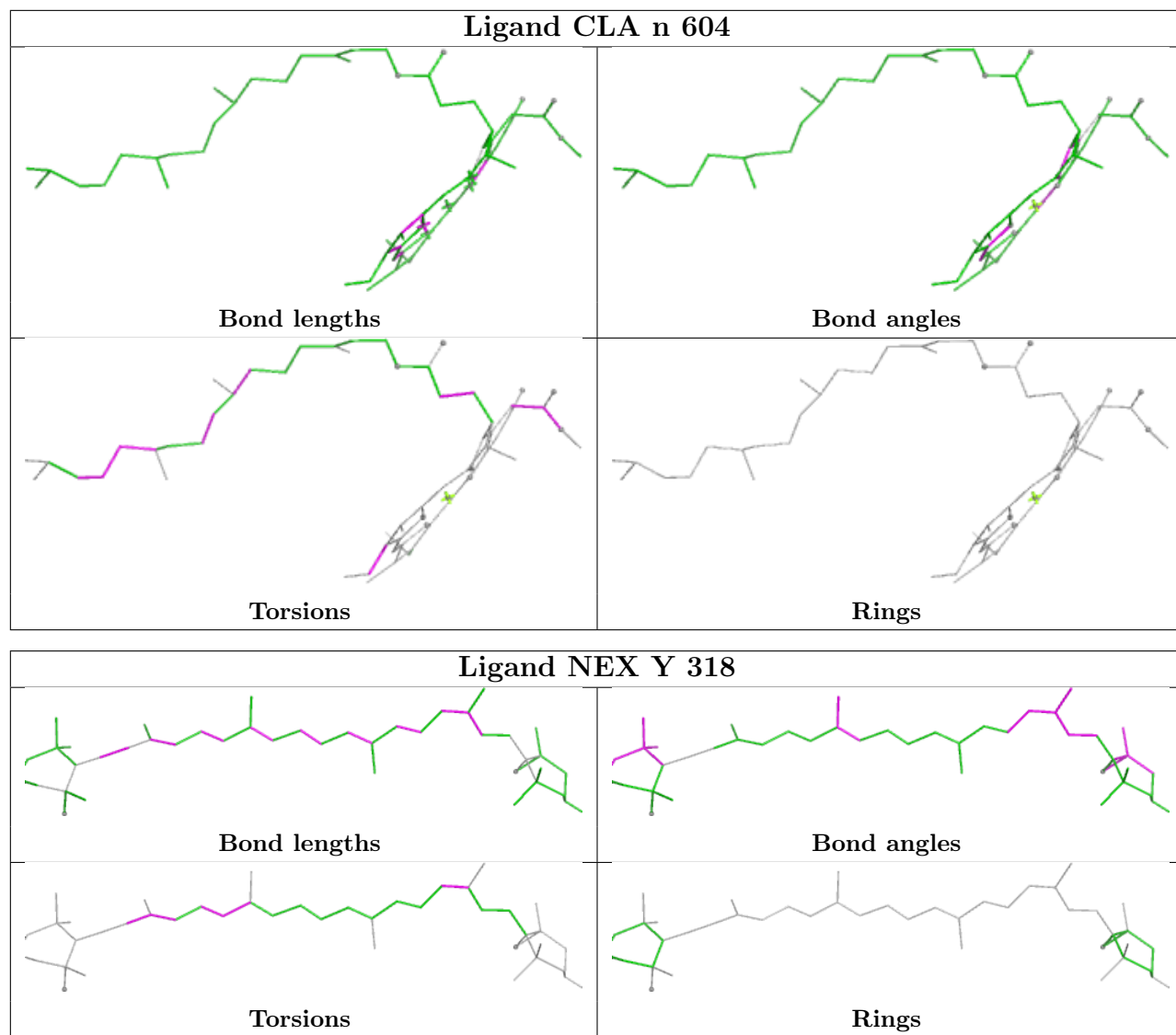


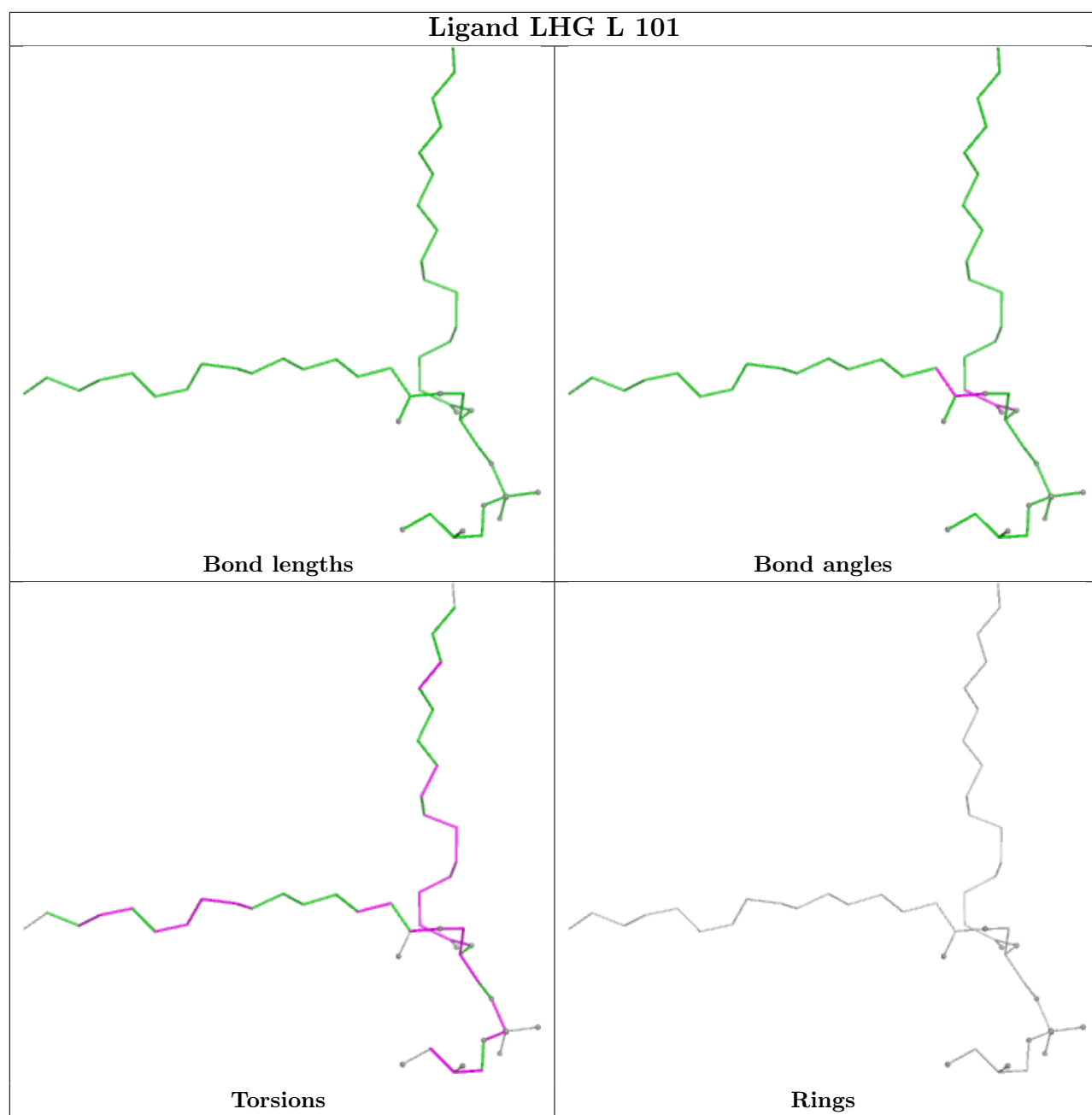
Ligand BCR f 101

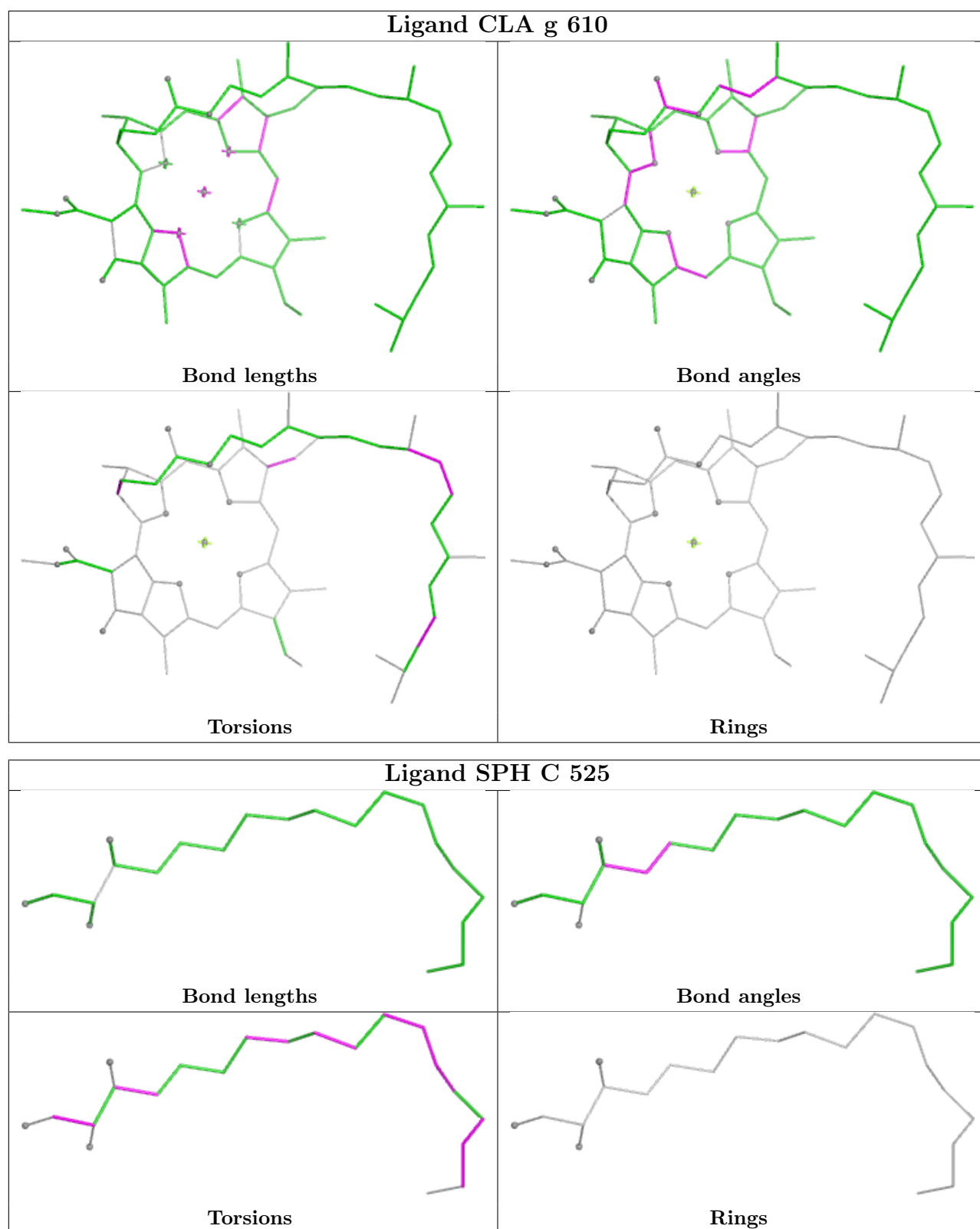


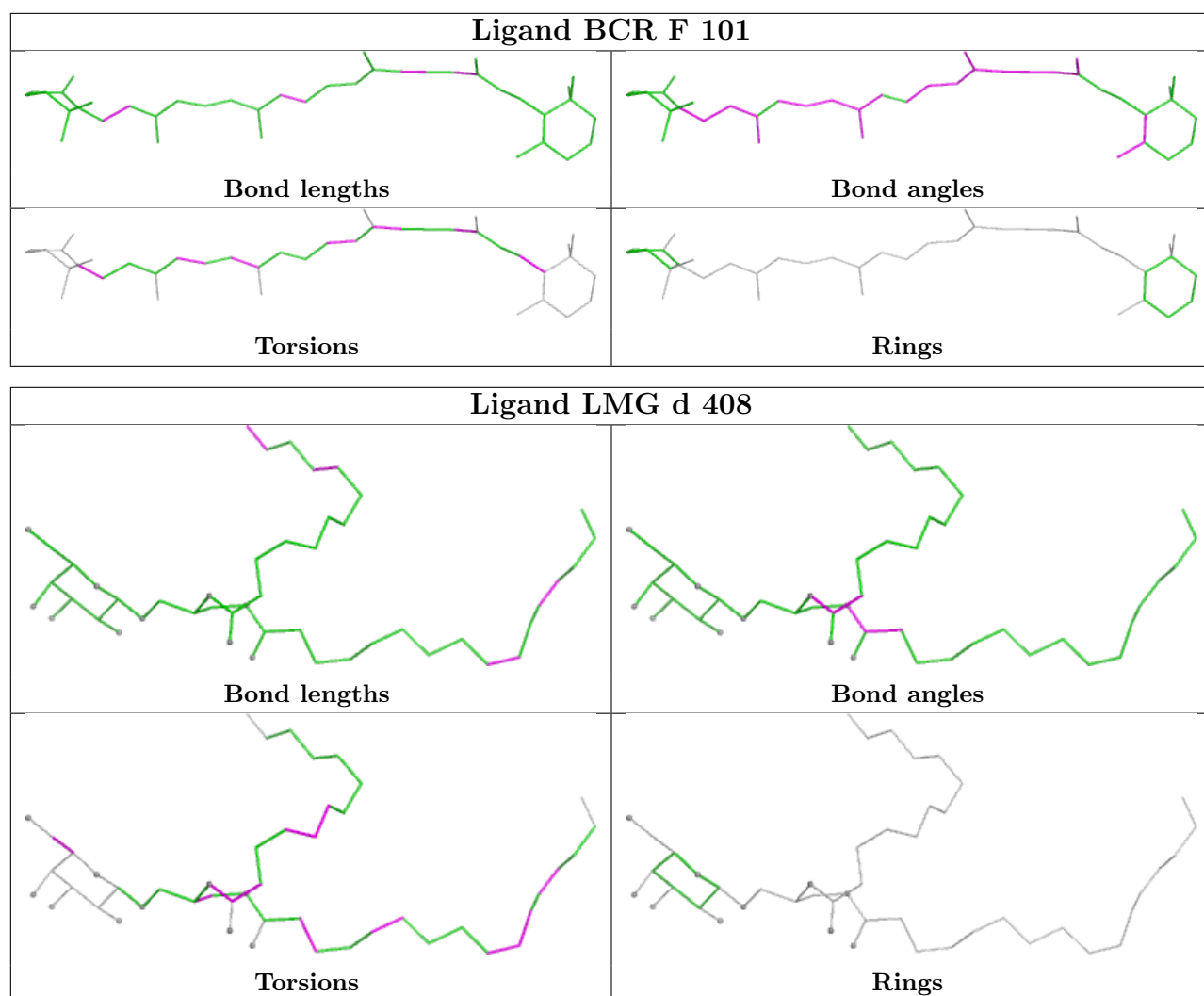


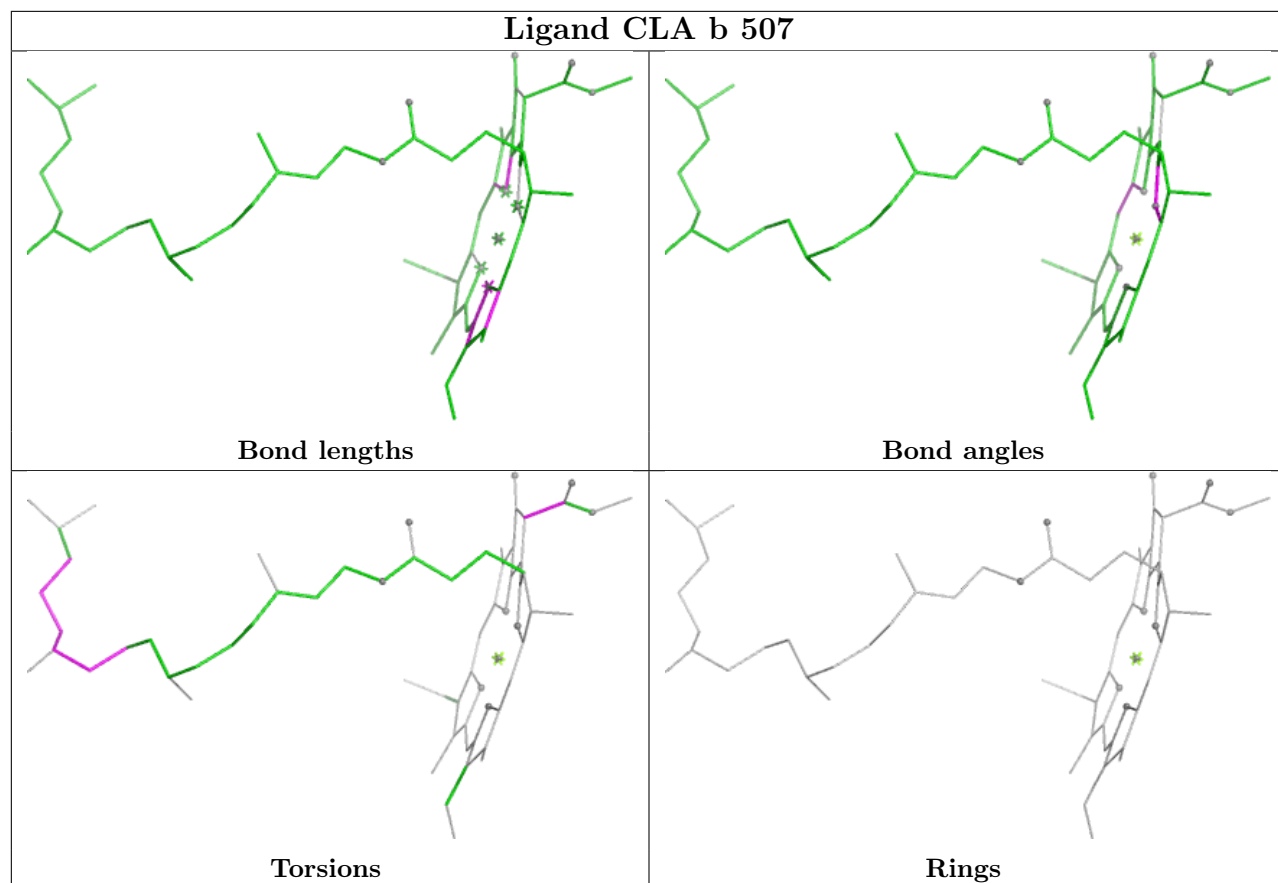


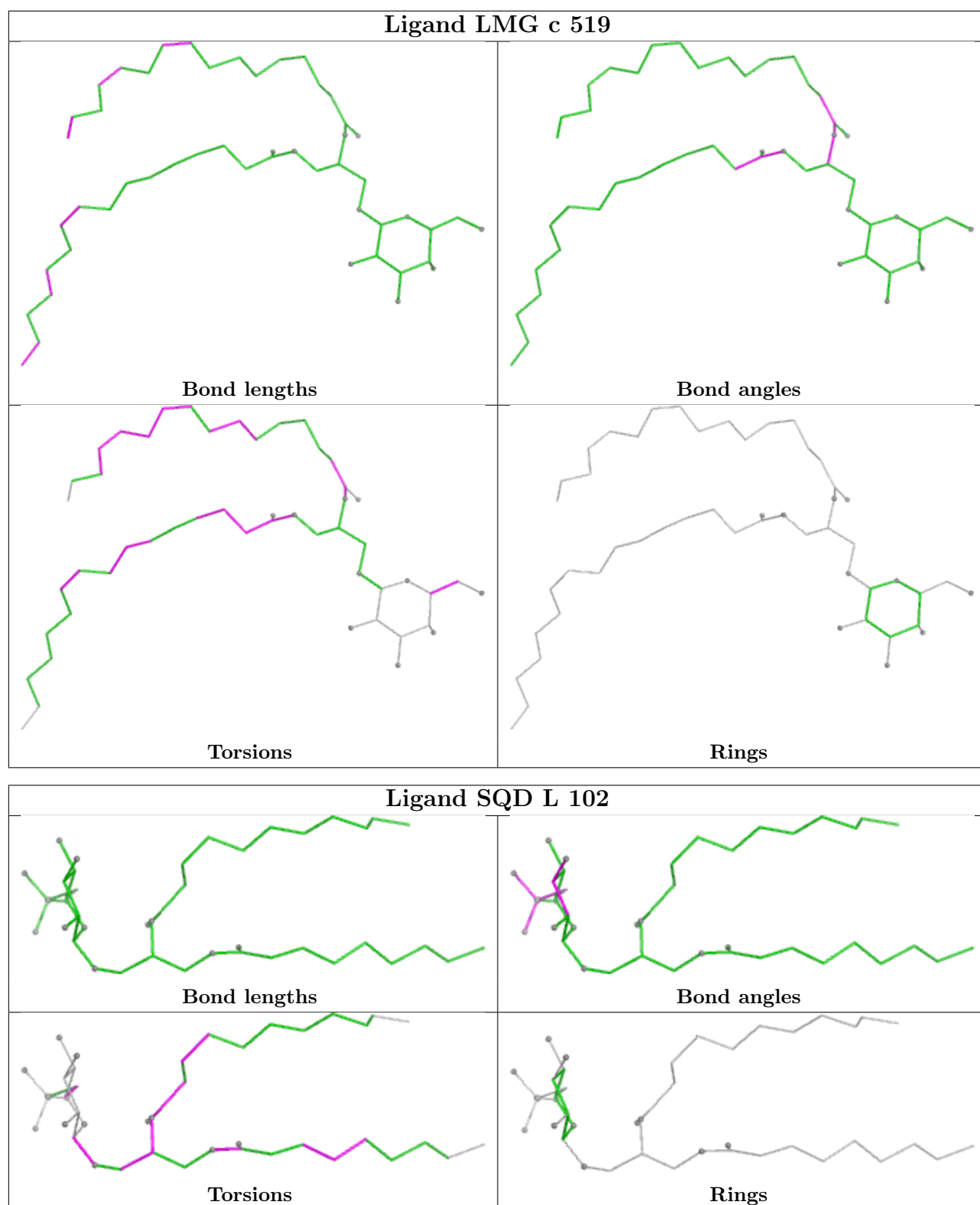




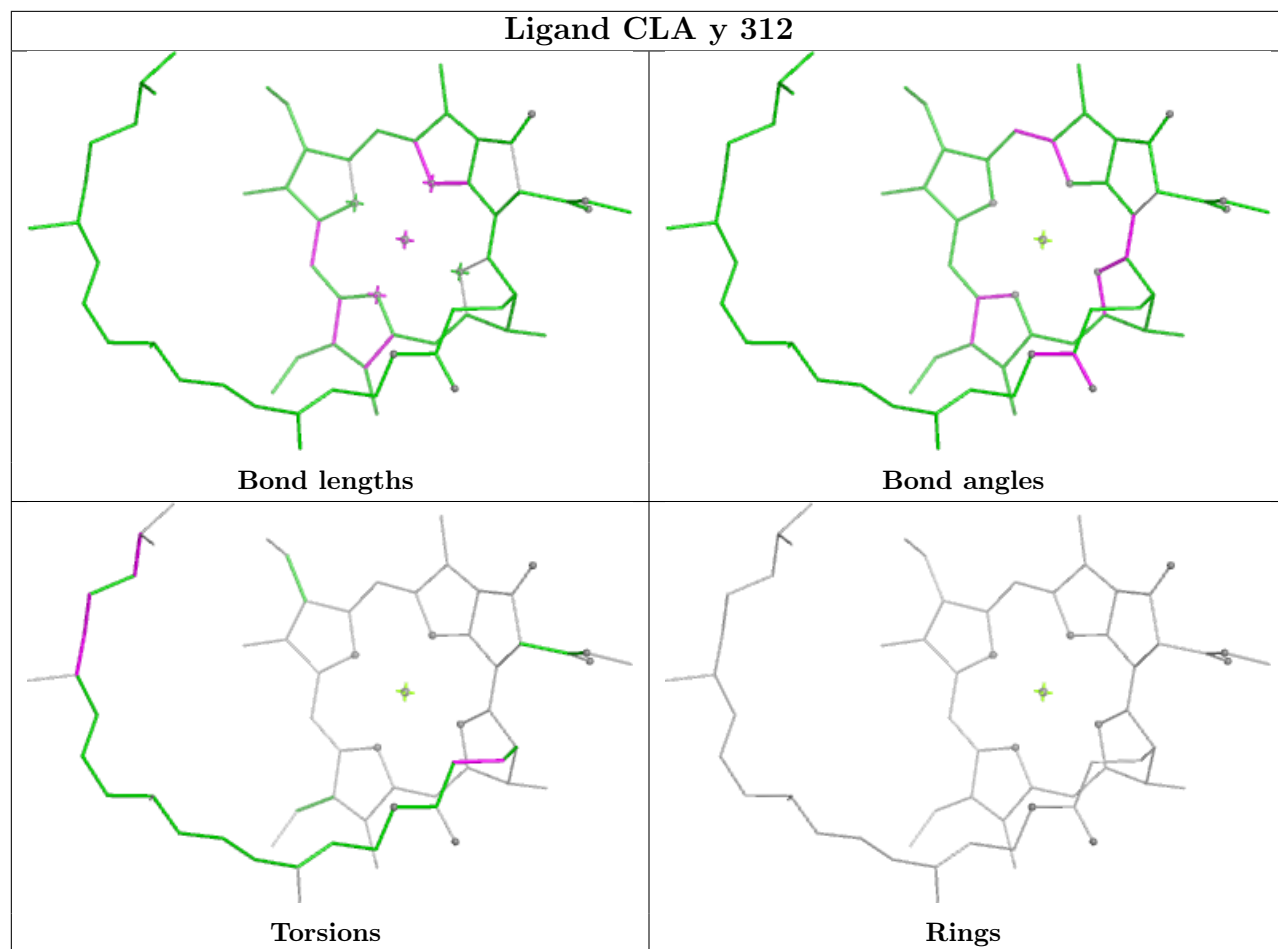


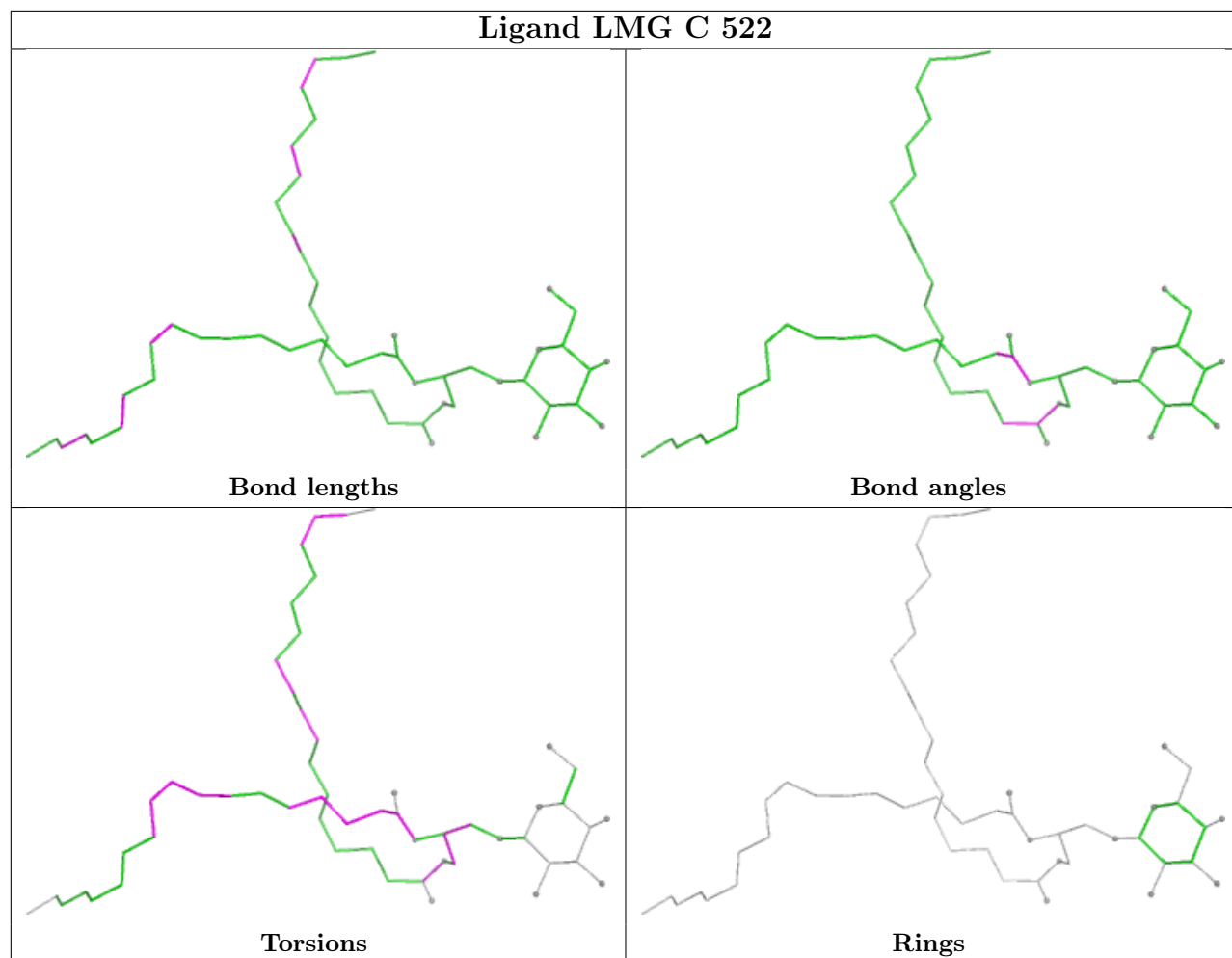


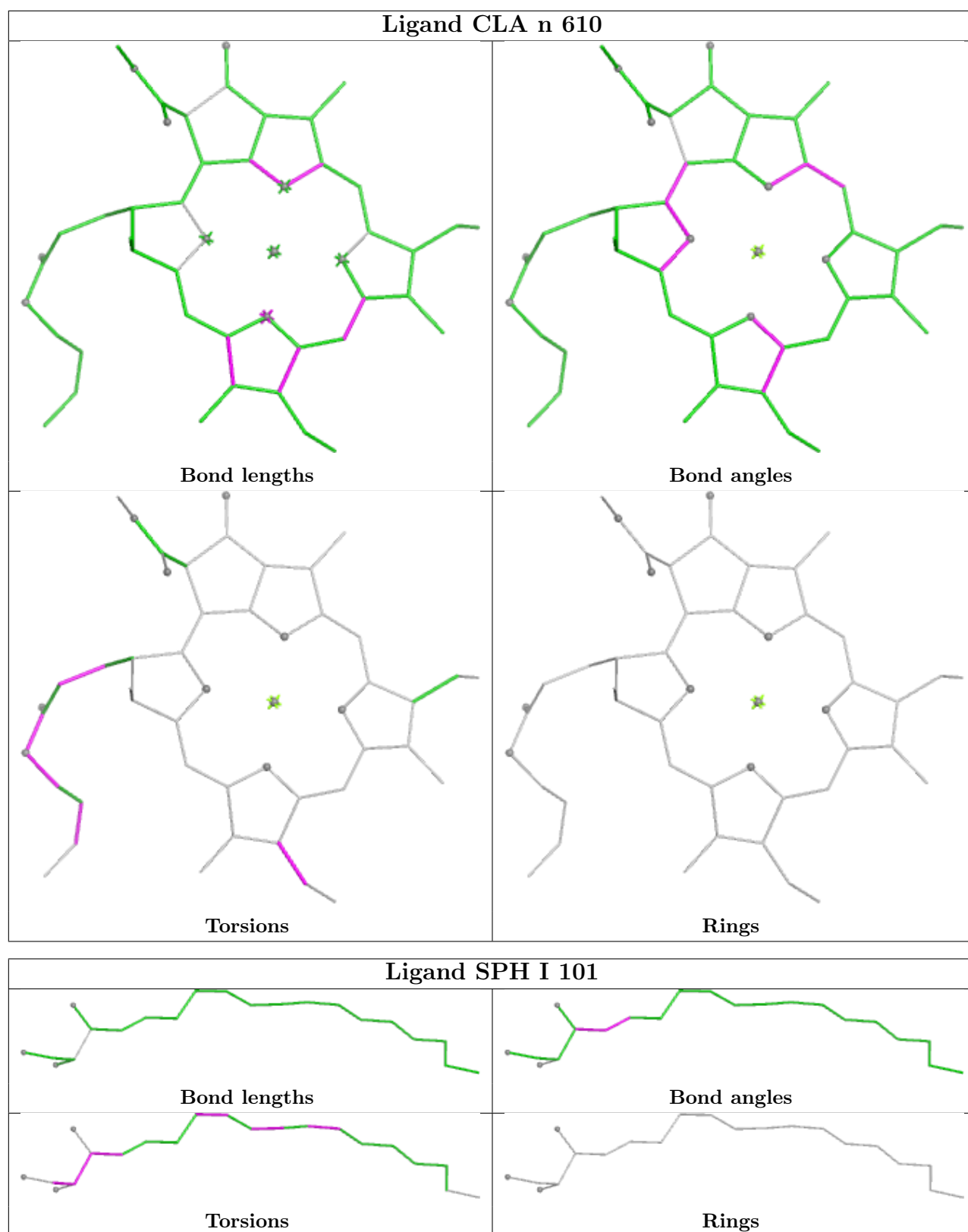


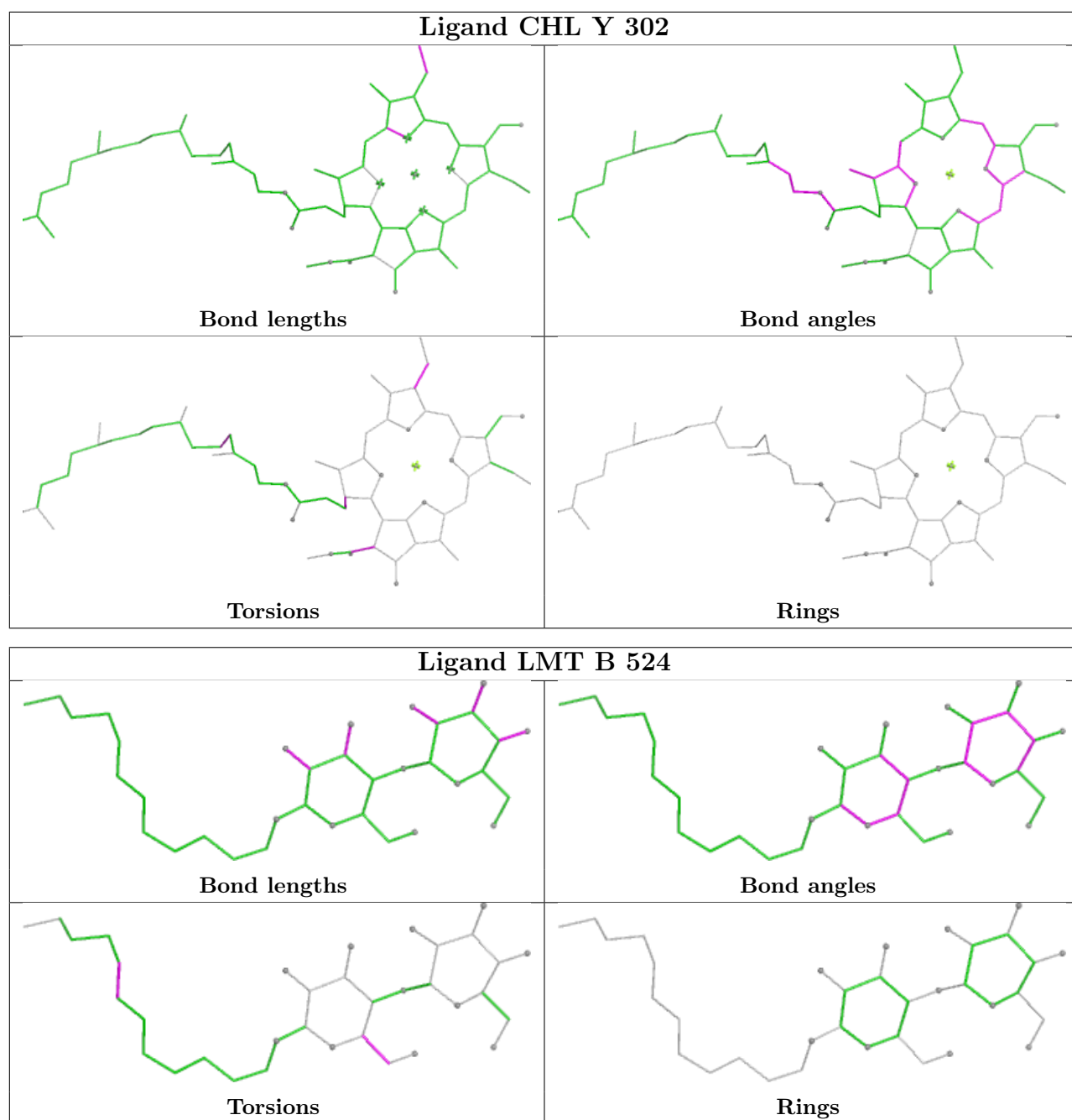


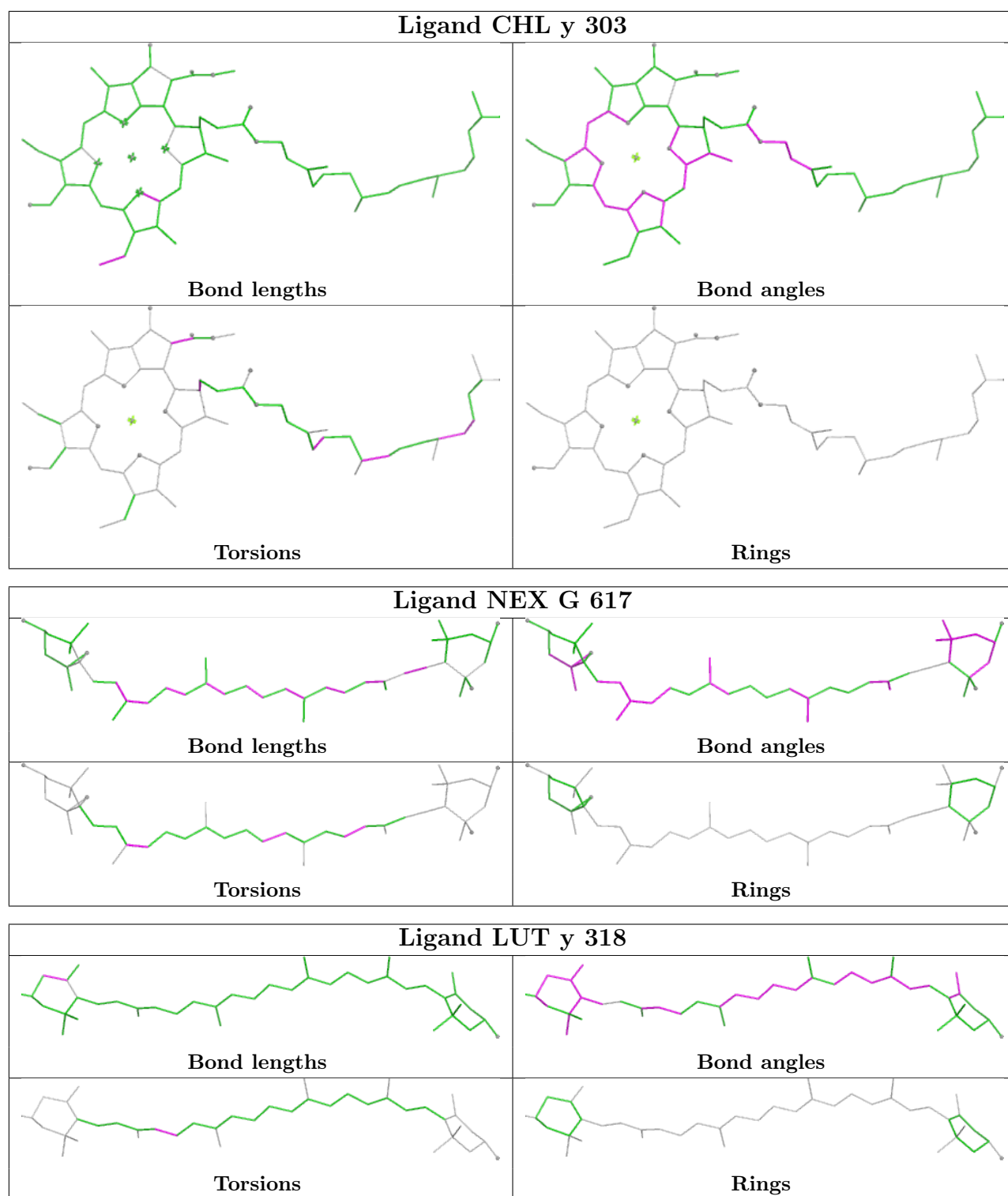
Ligand CLA y 312

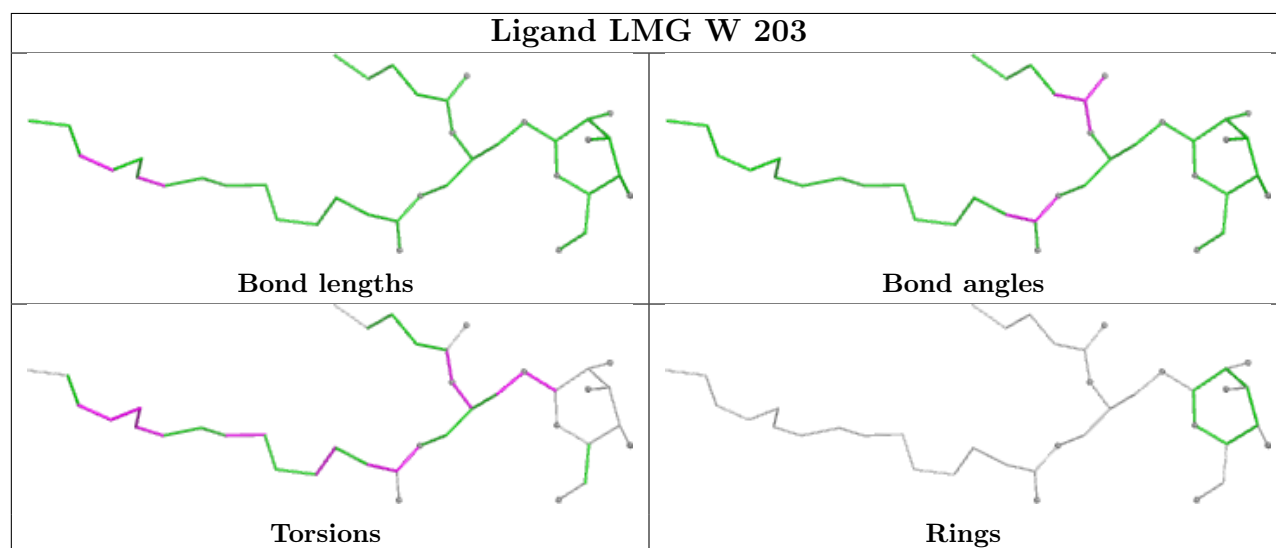
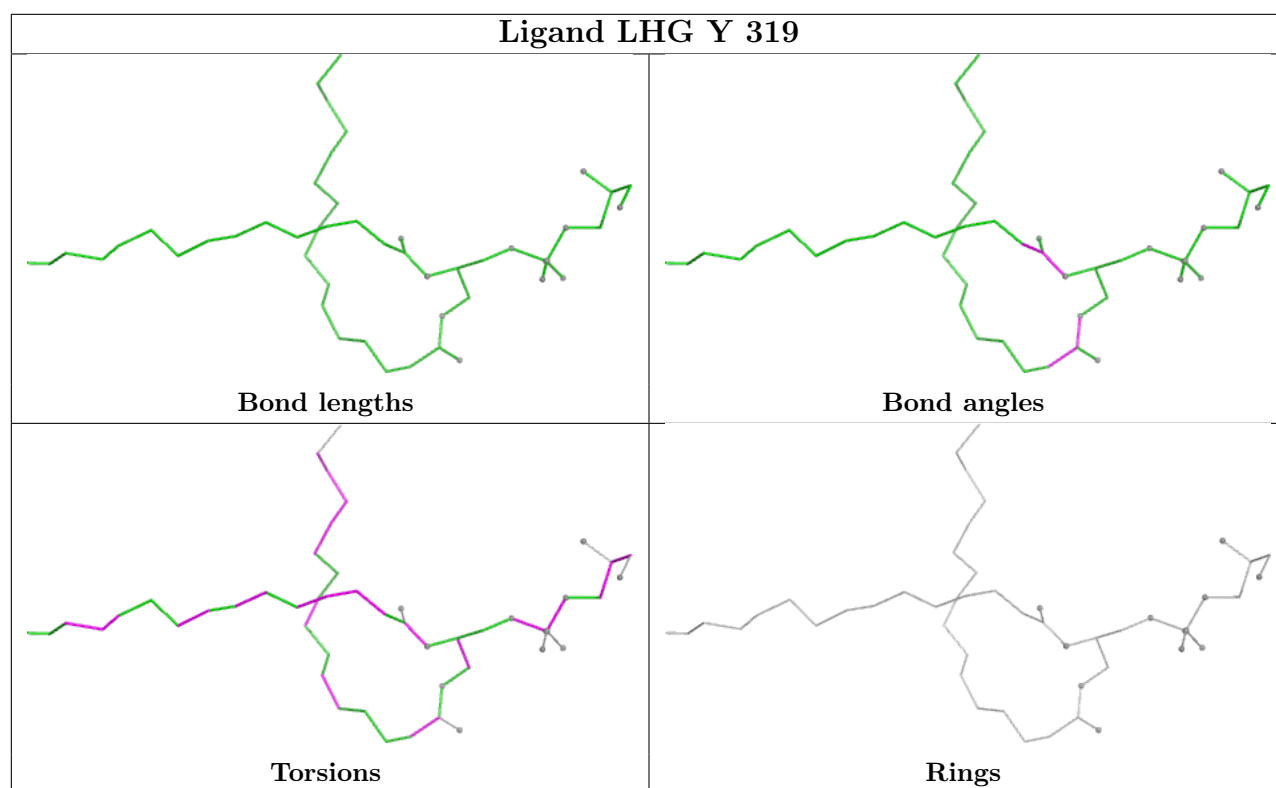


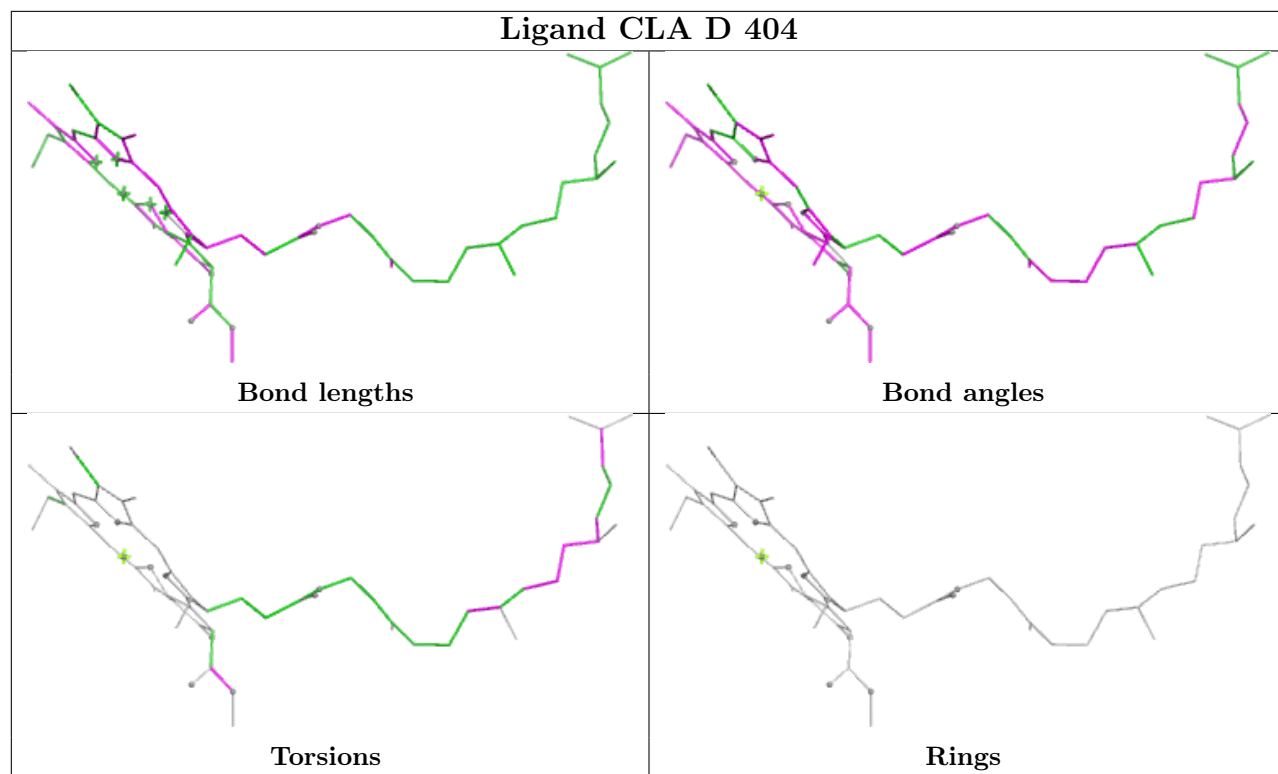


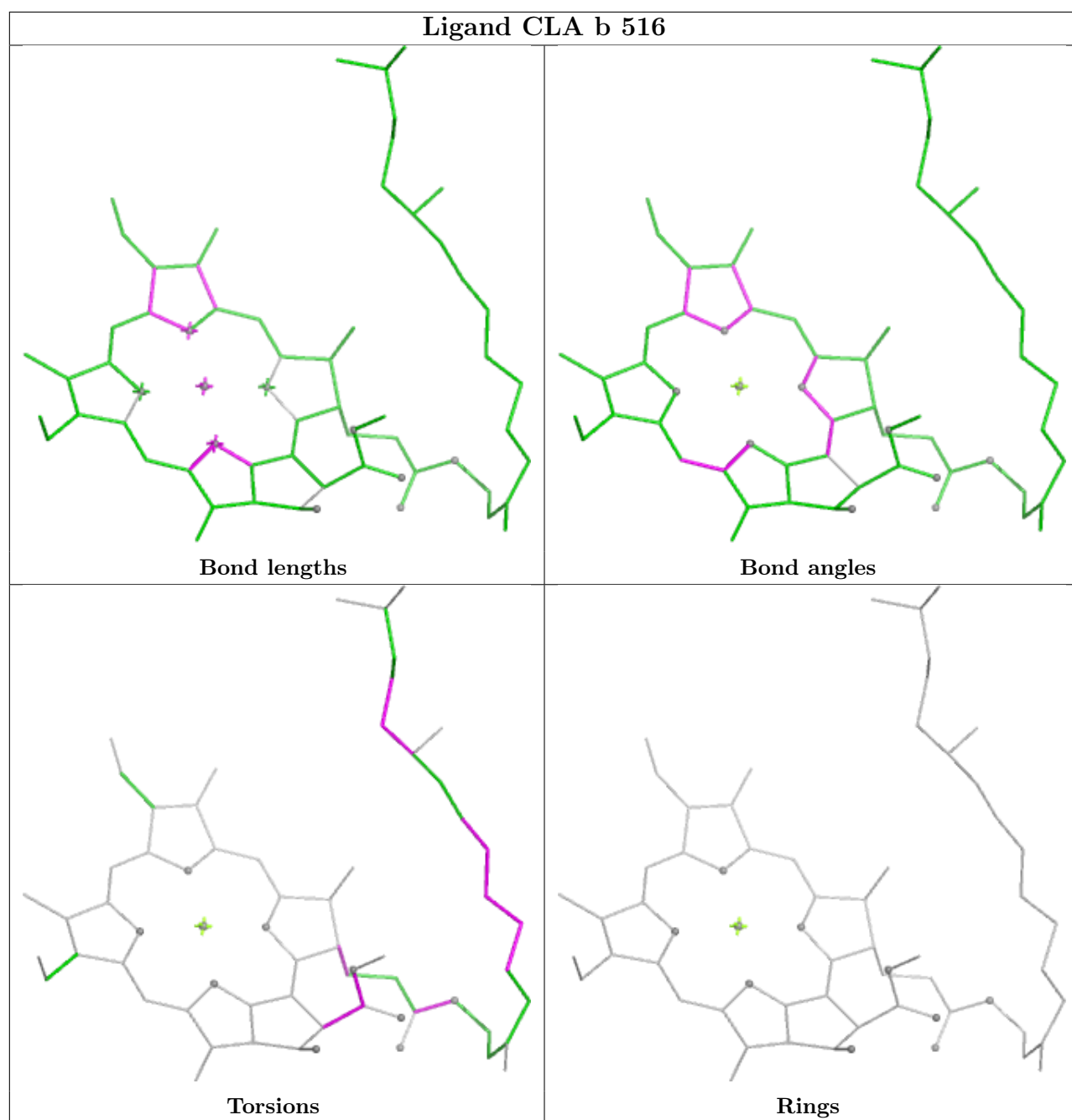


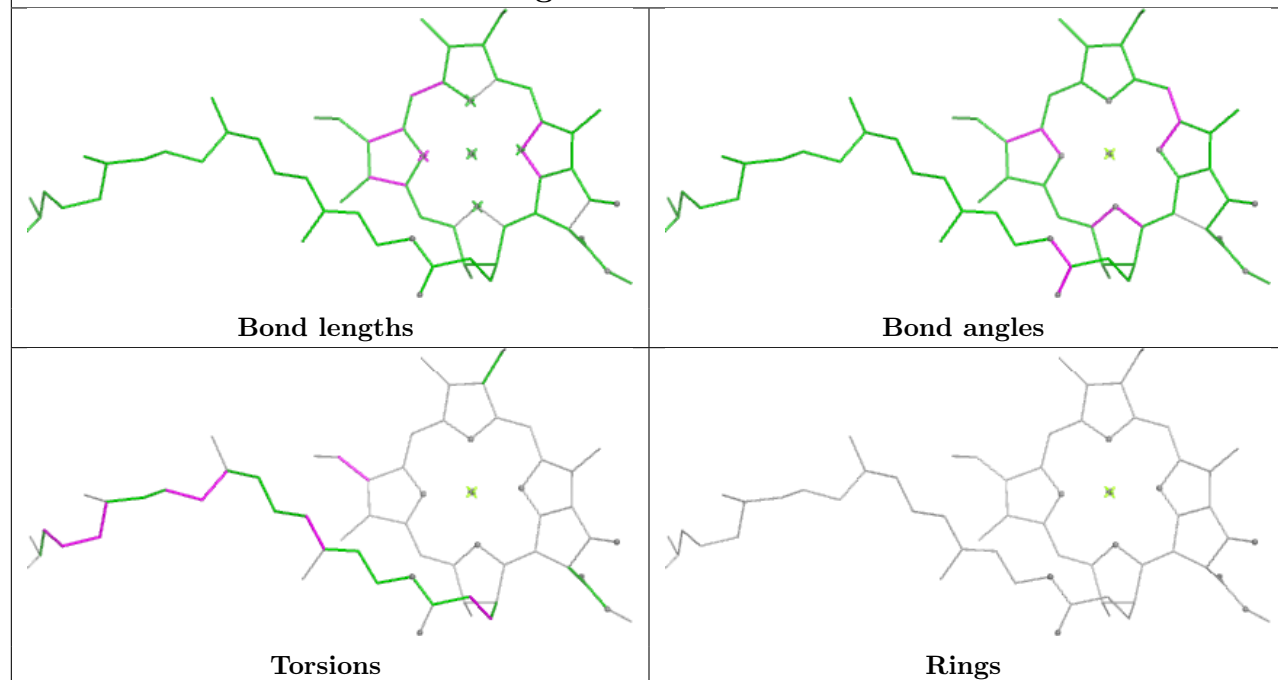
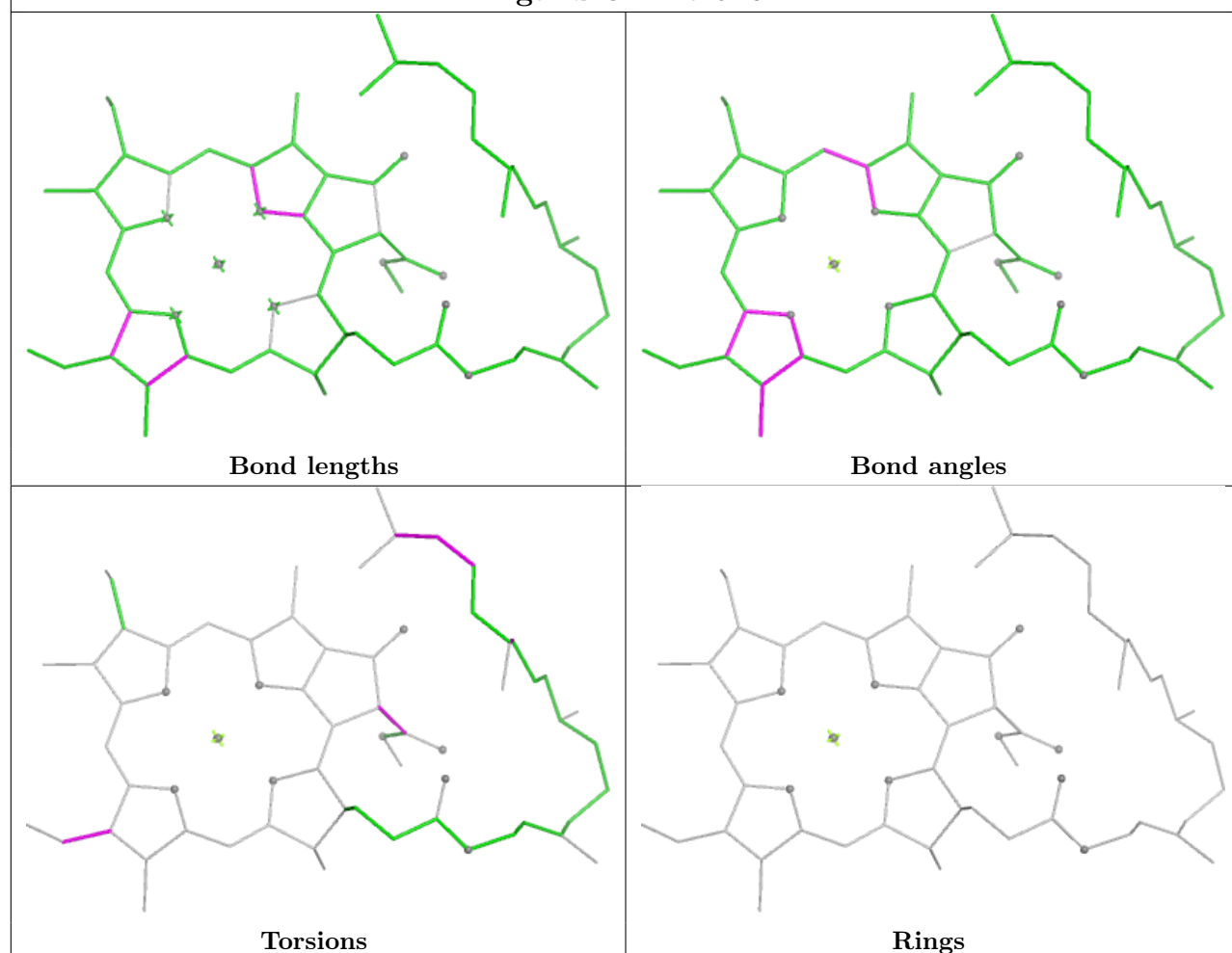


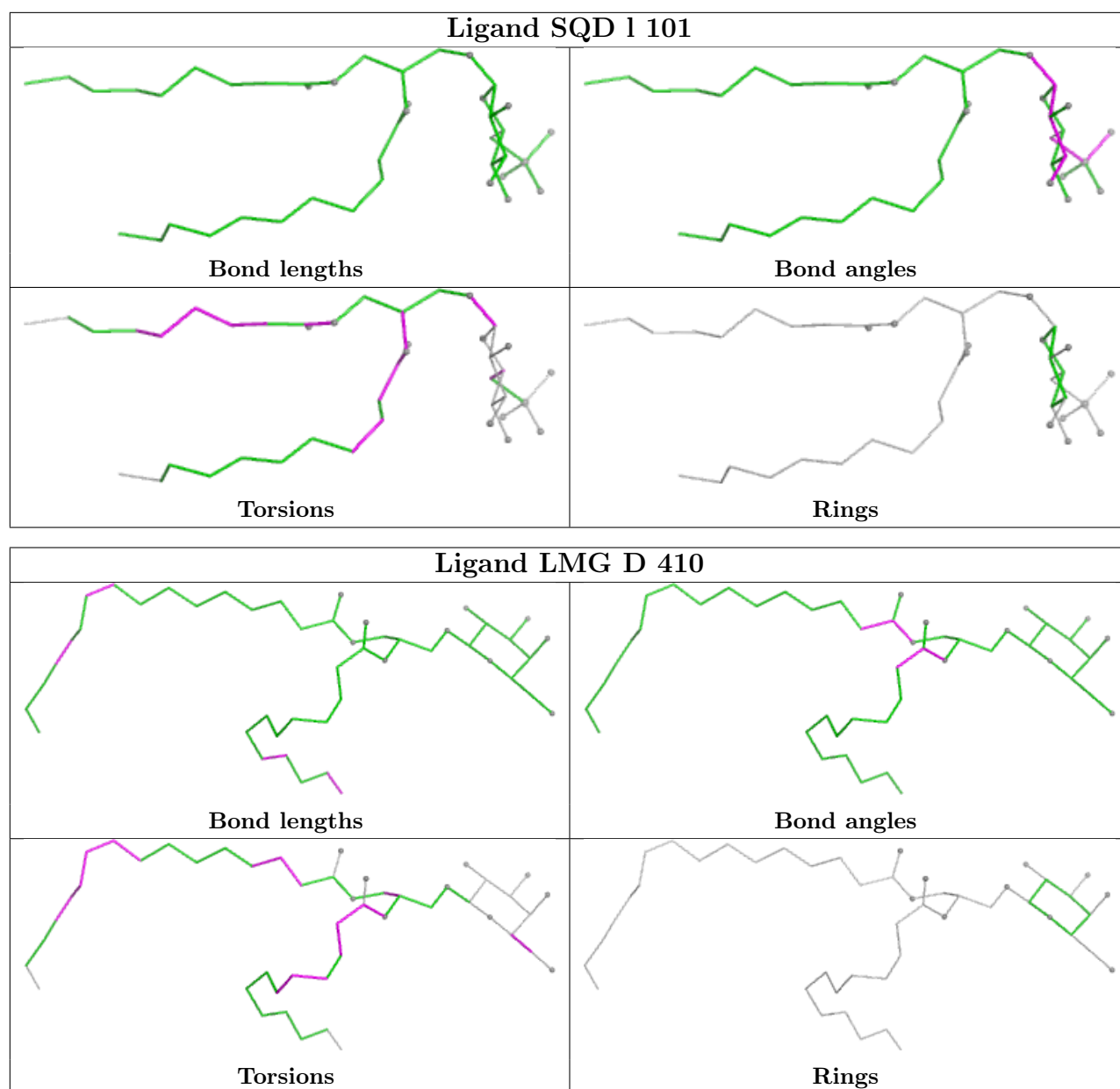


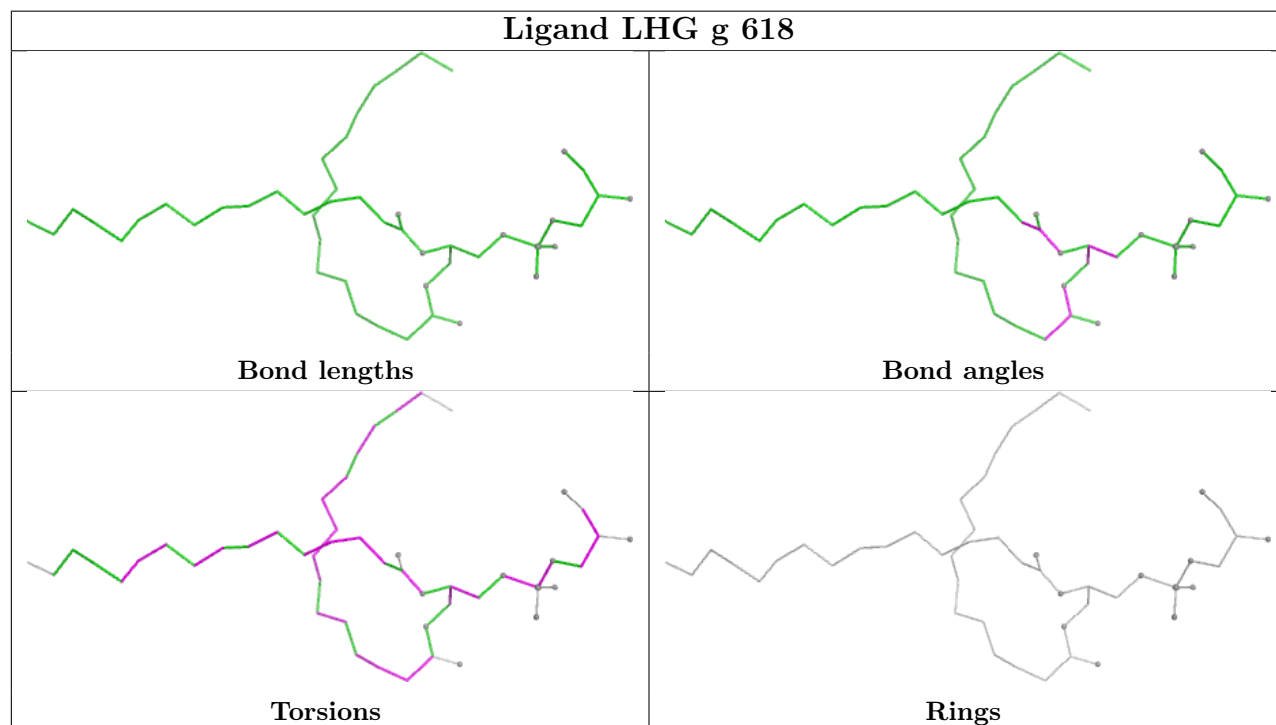
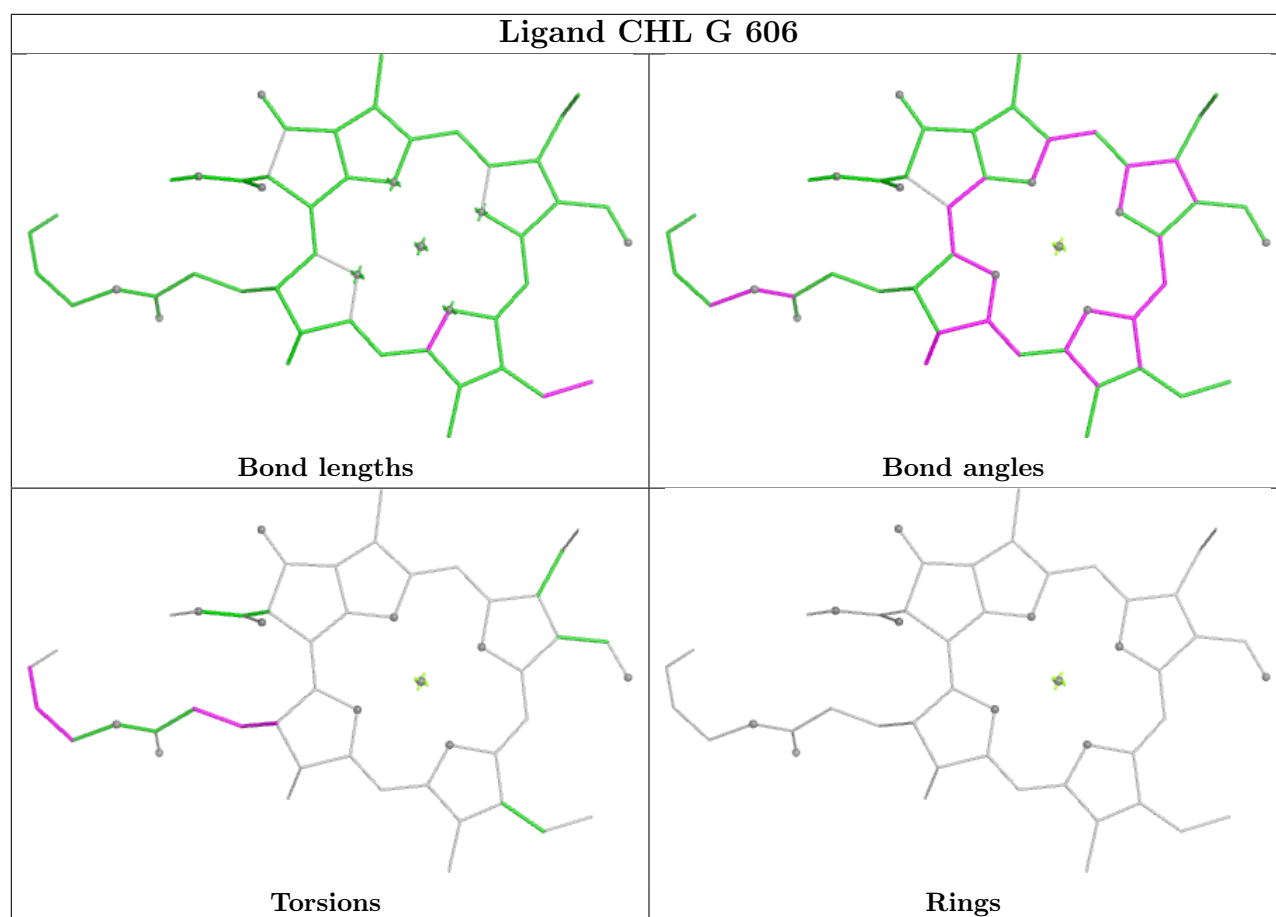


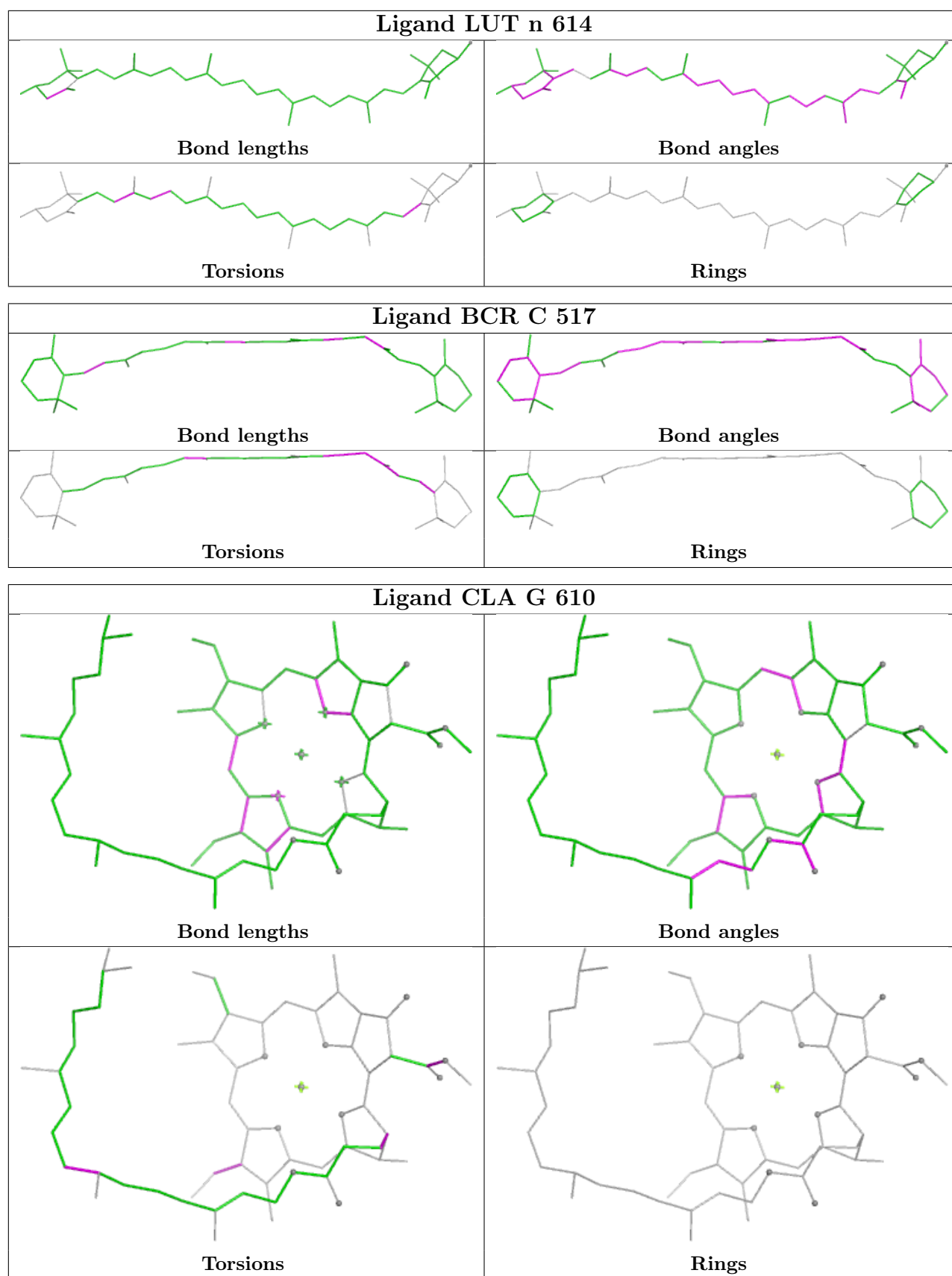


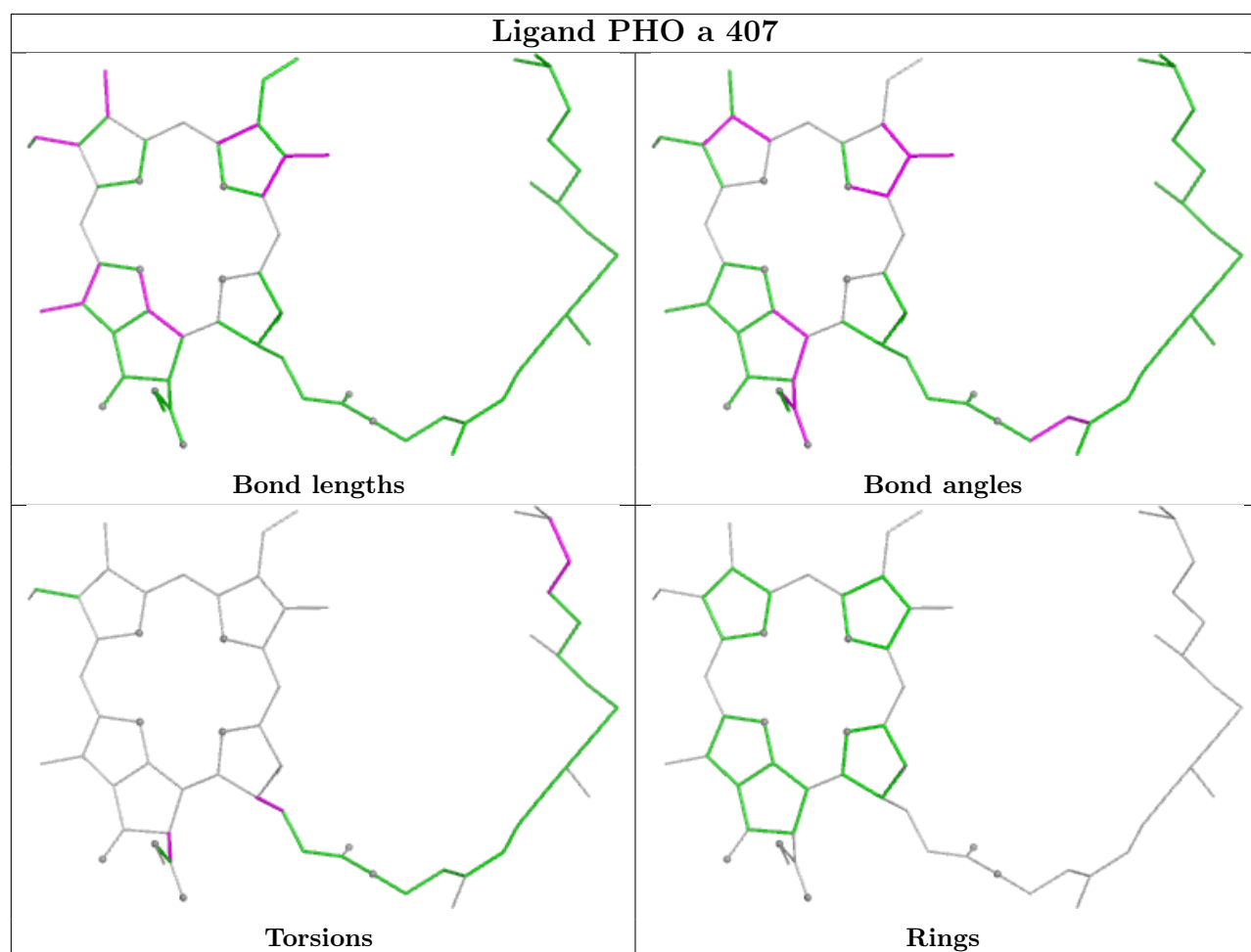


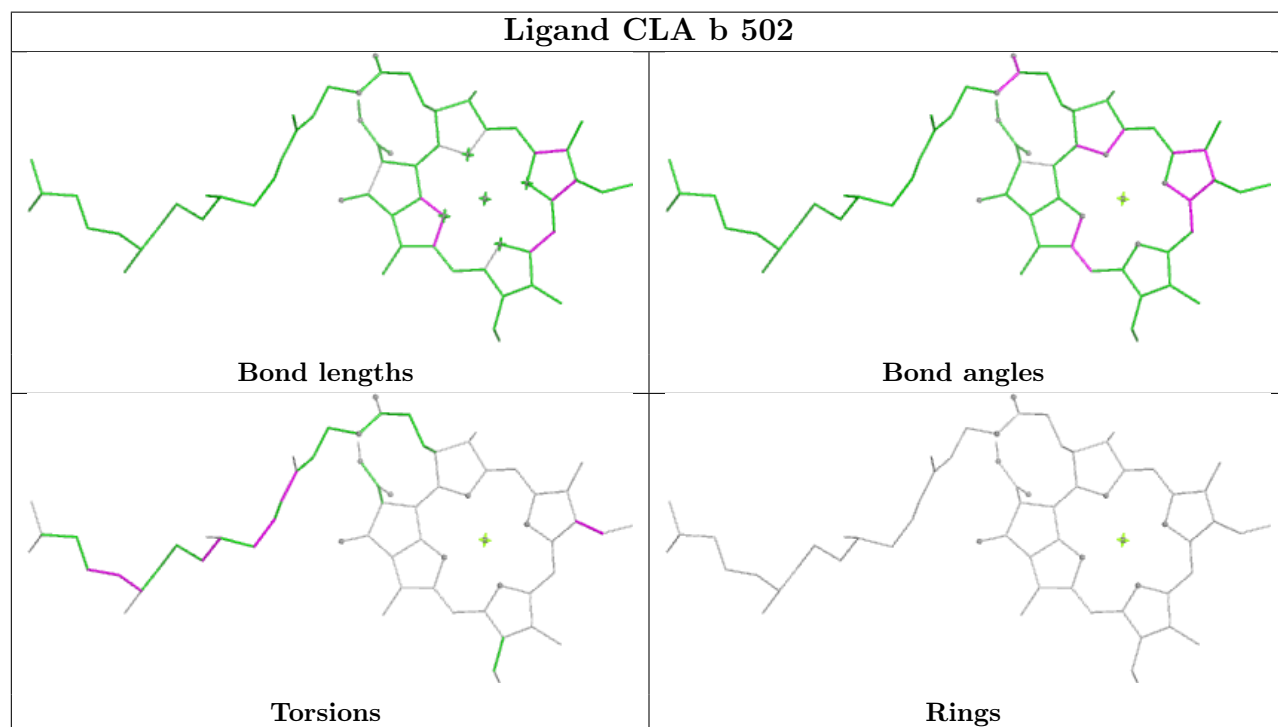
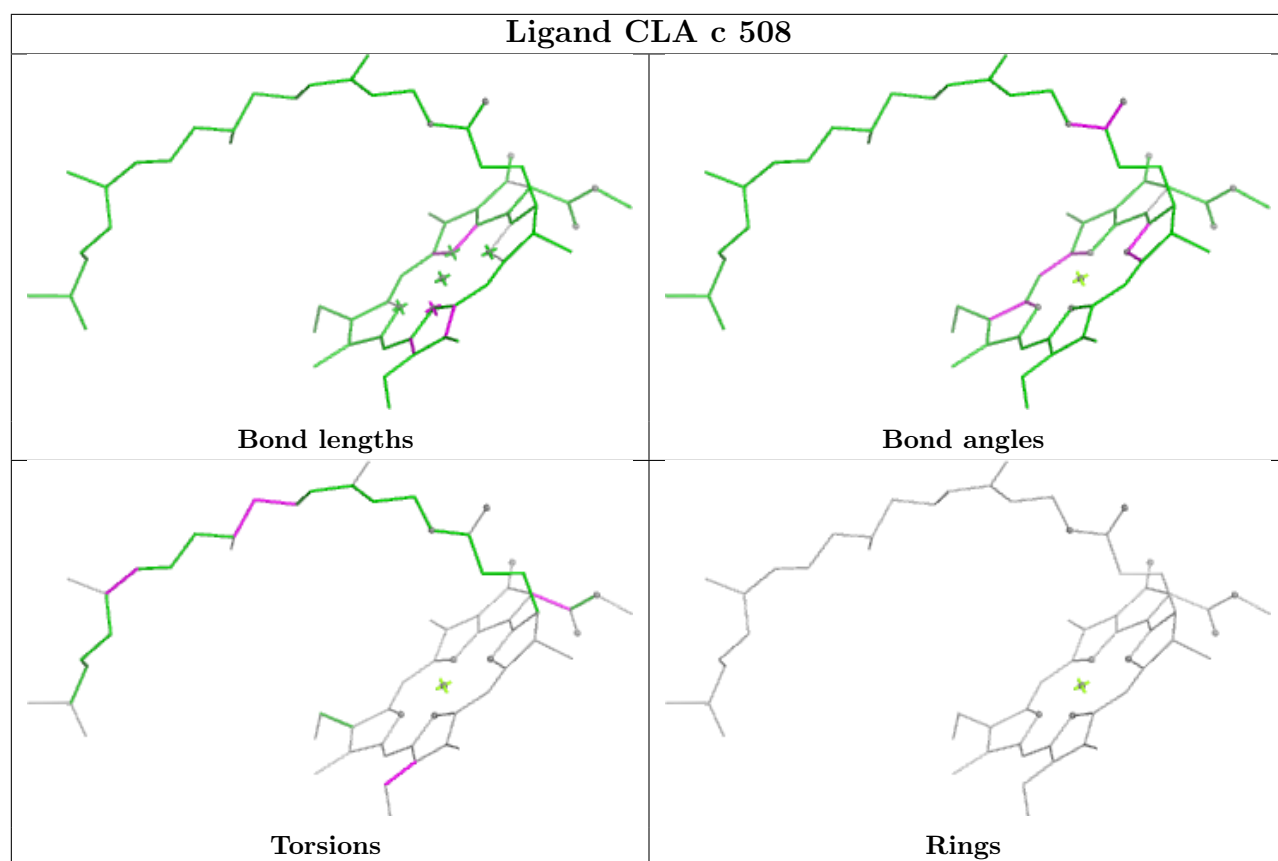
Ligand CLA b 503**Ligand CLA b 510**

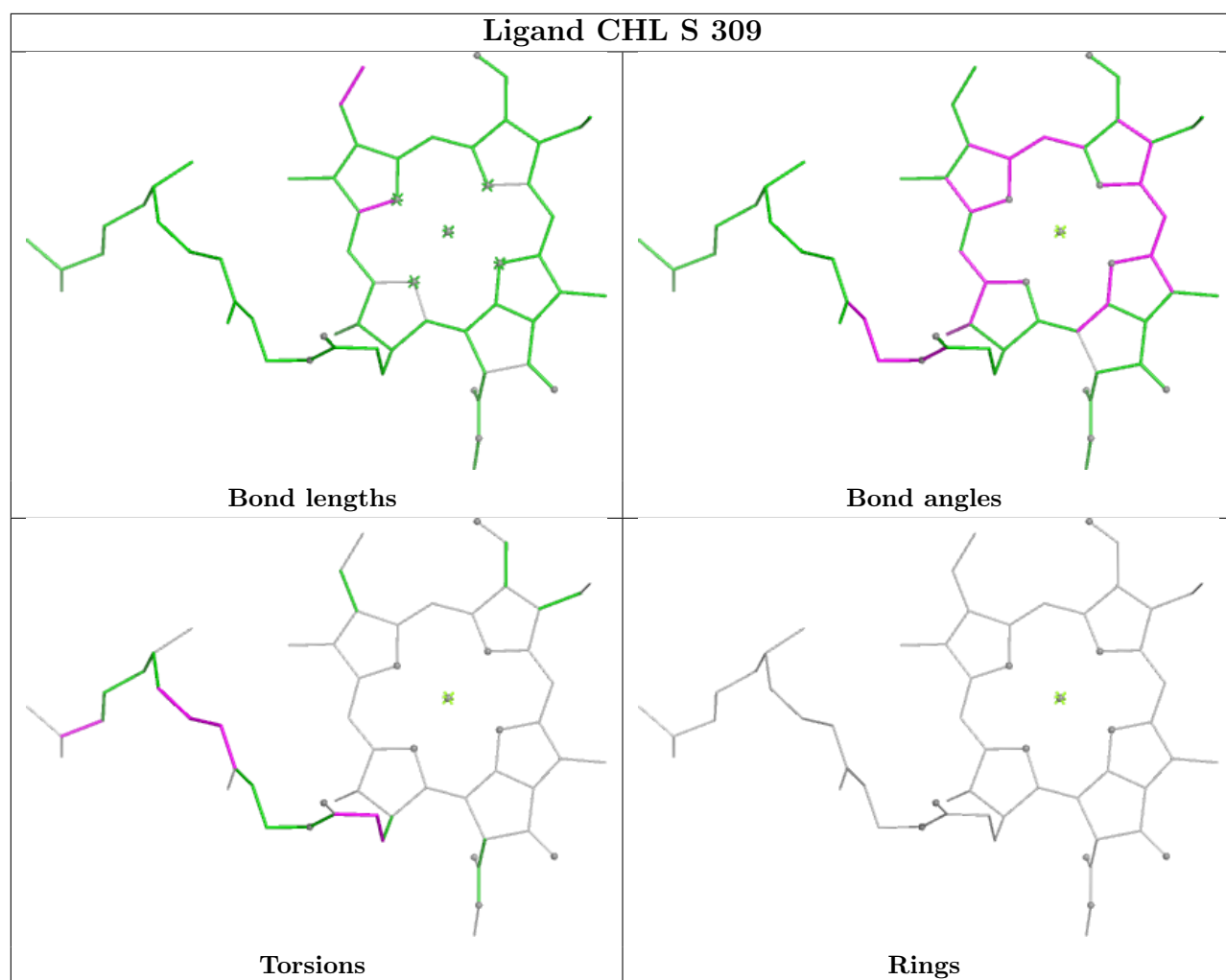


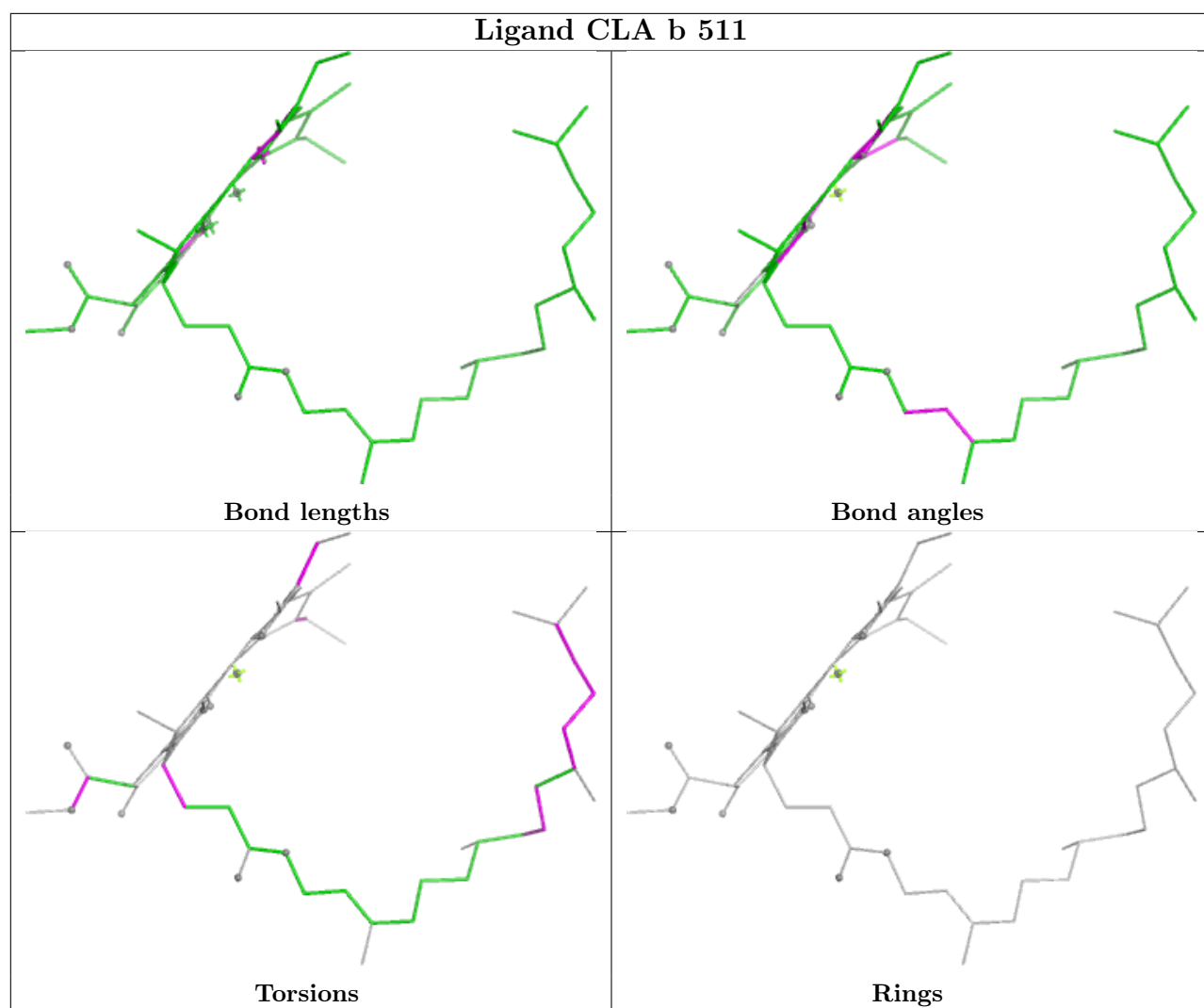


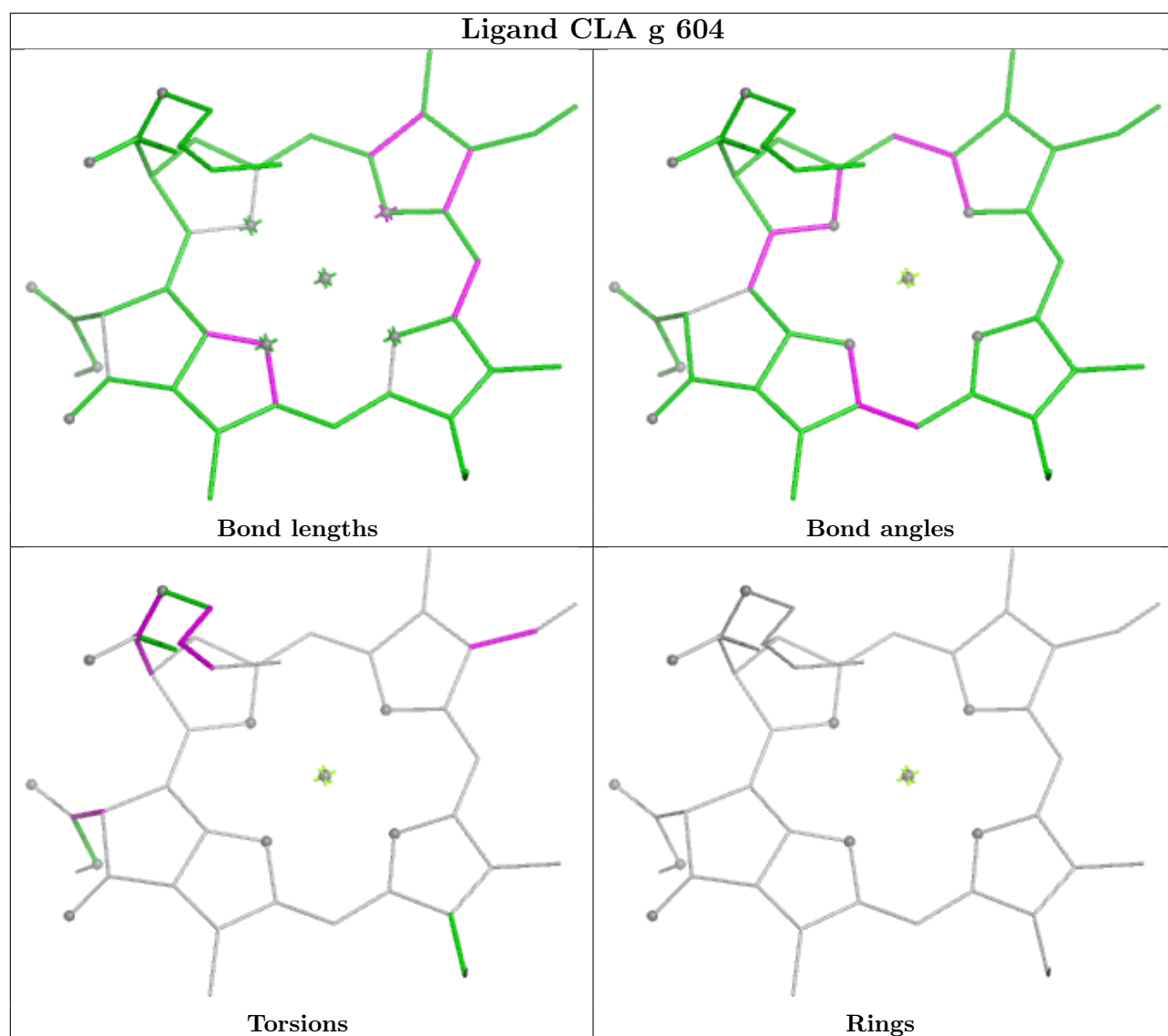


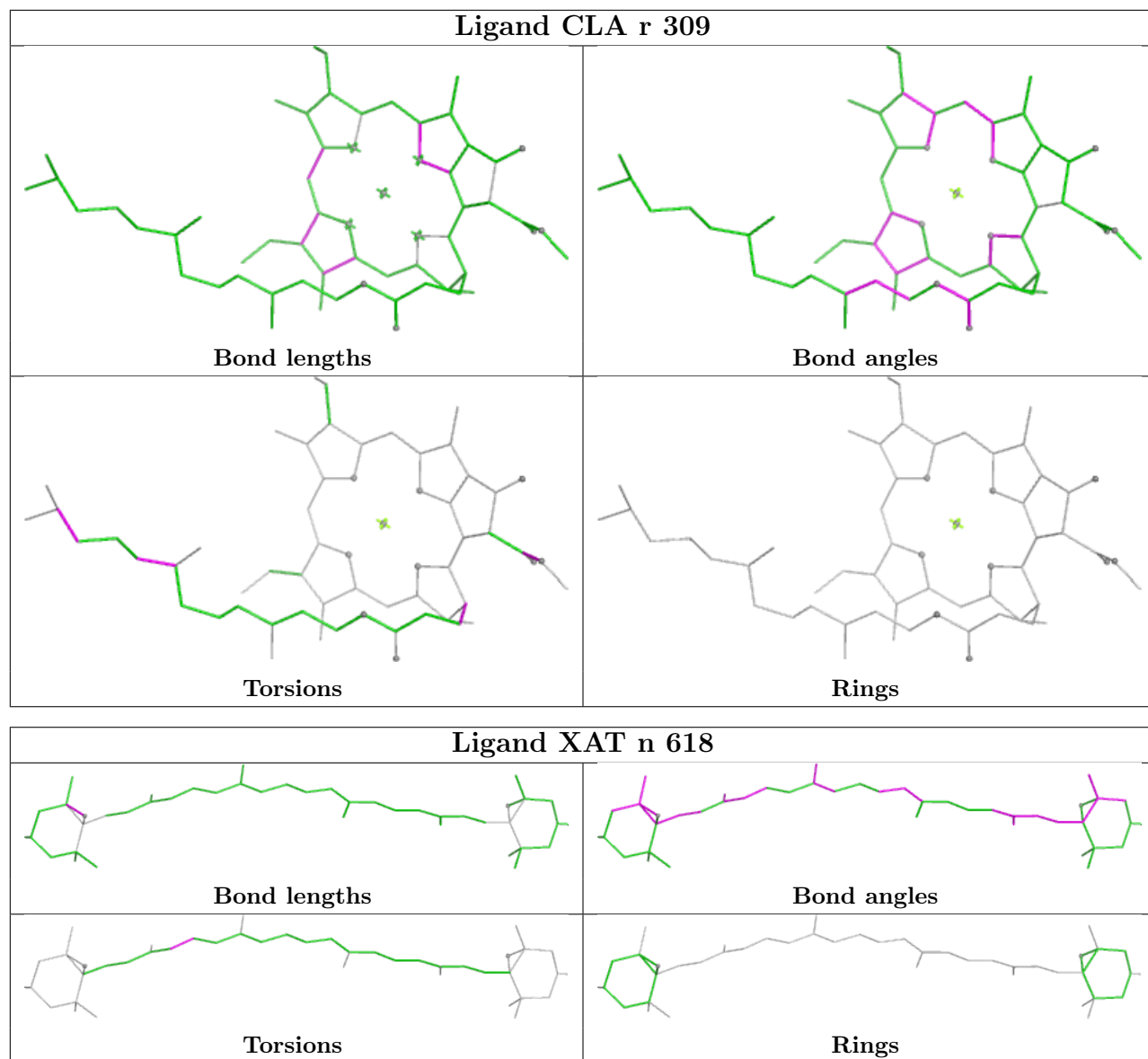


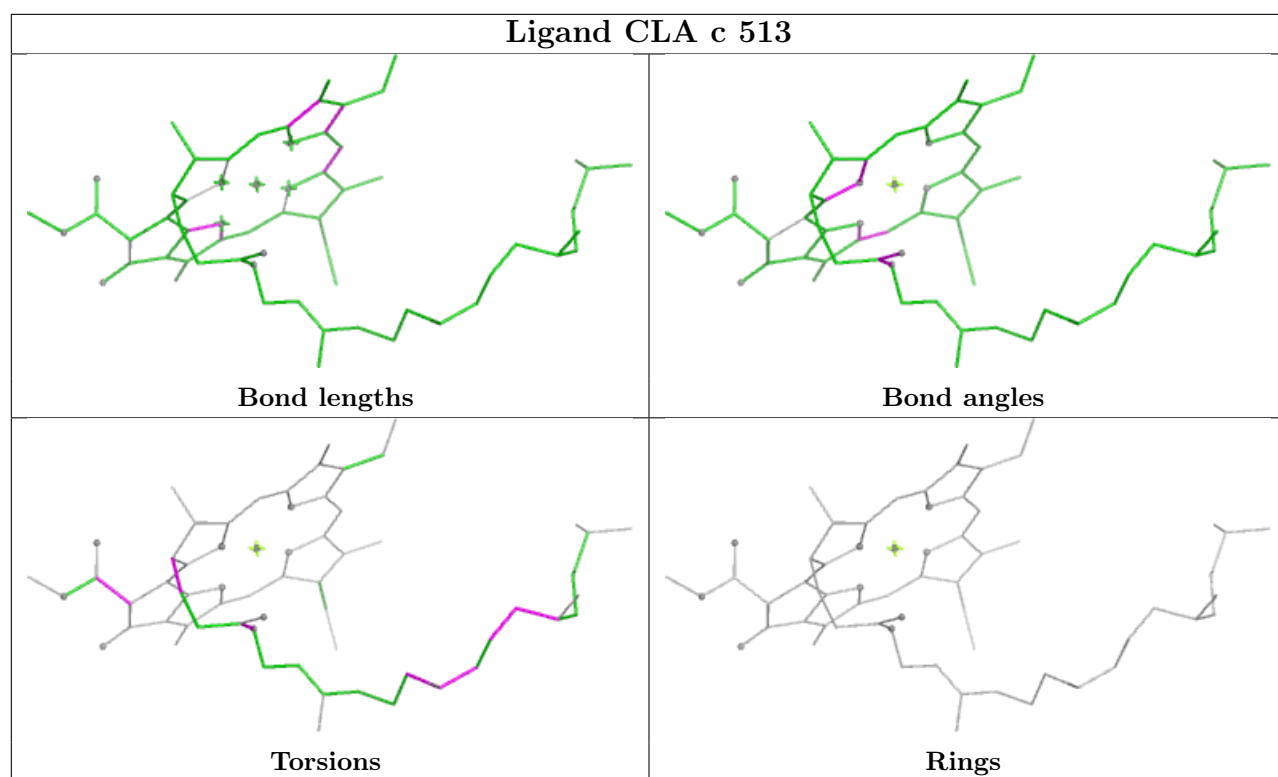


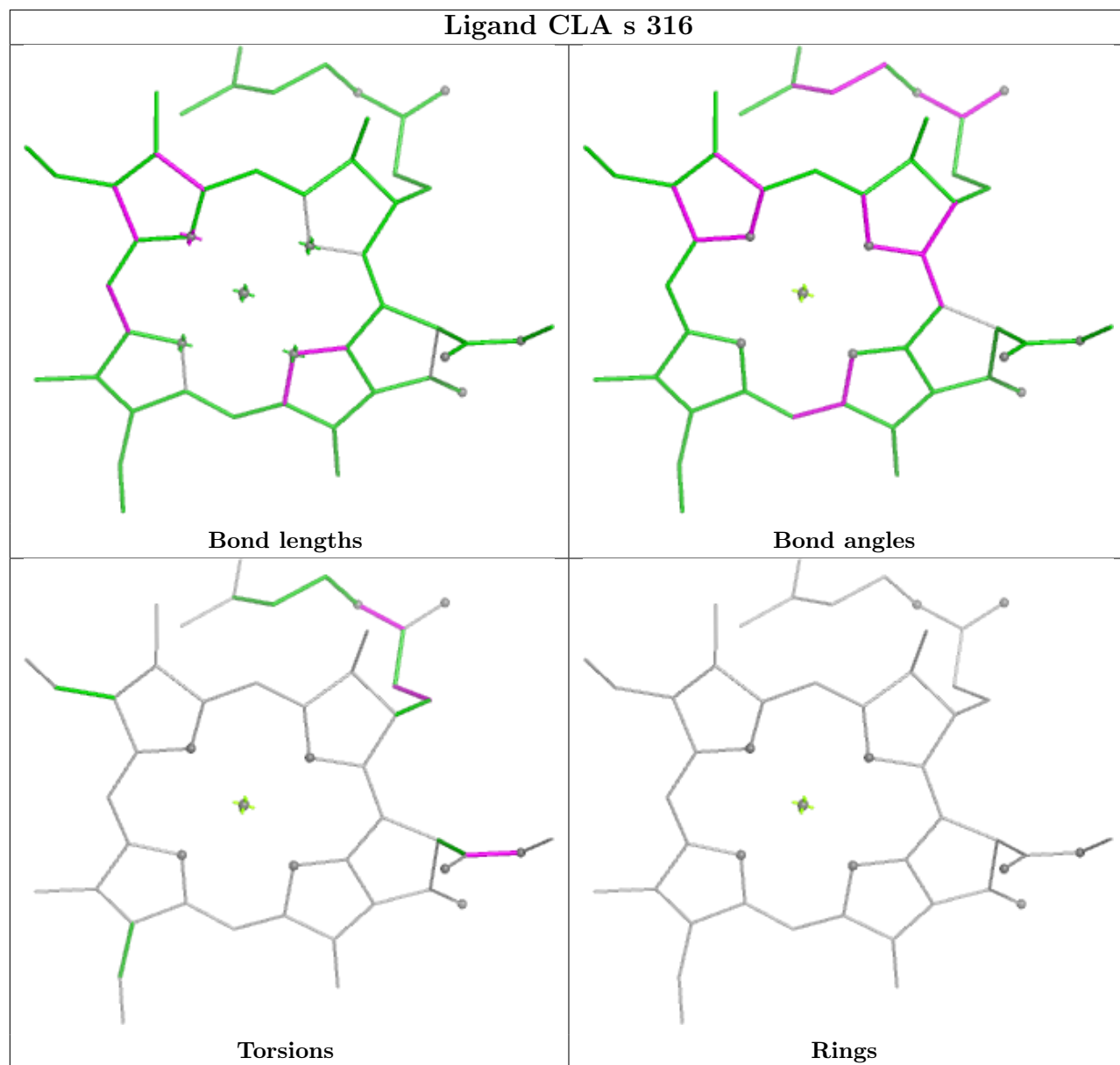


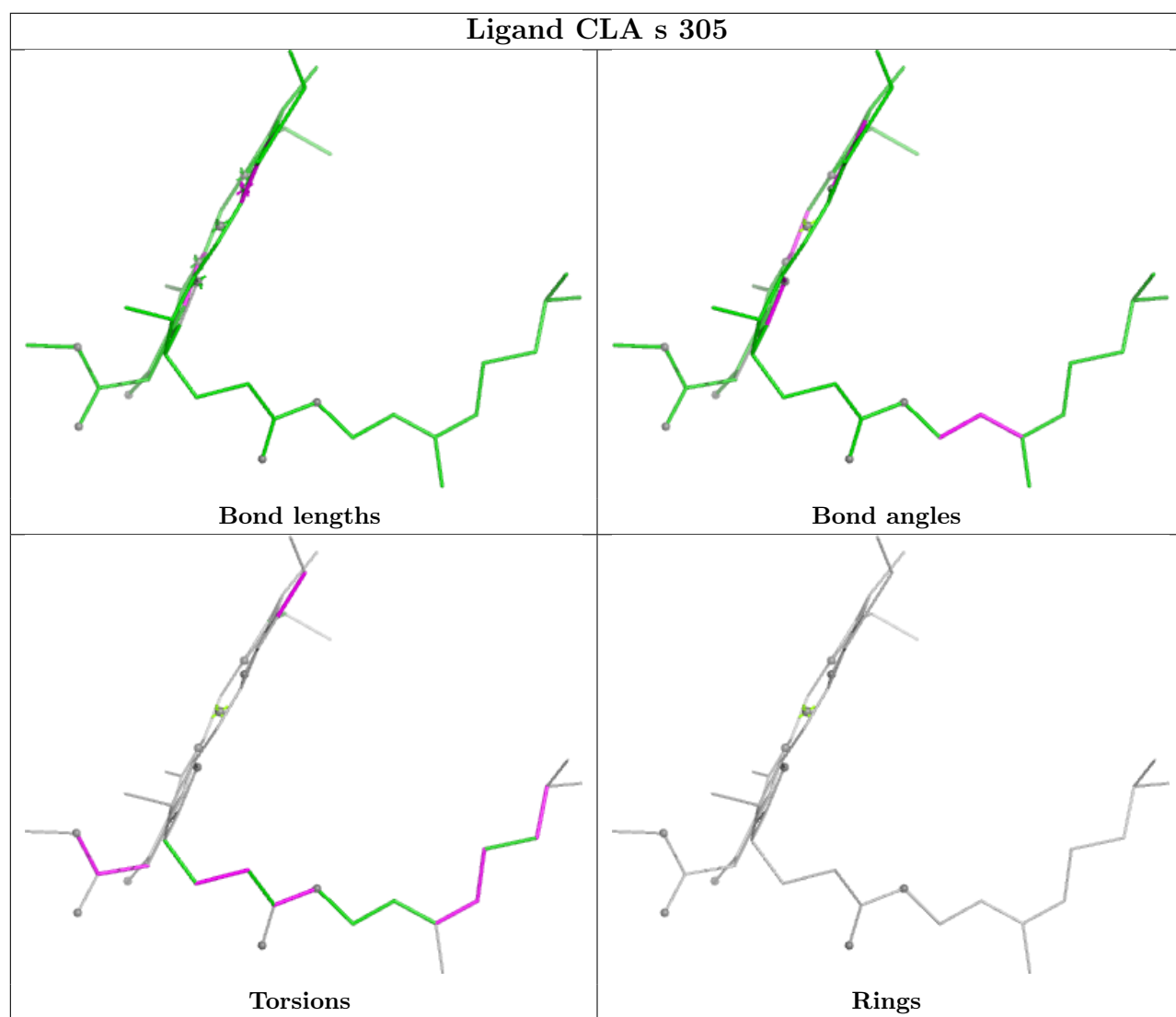




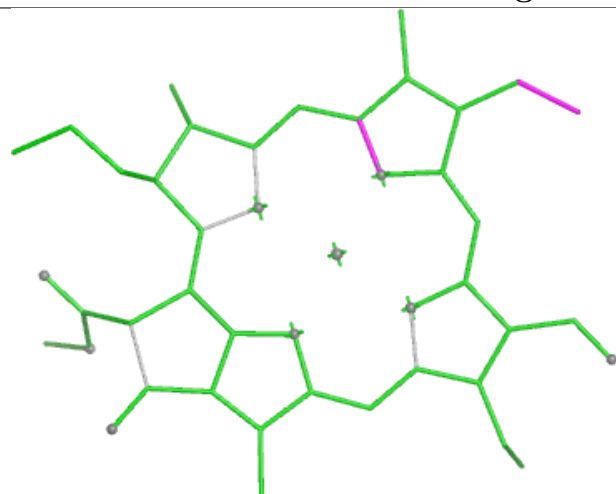




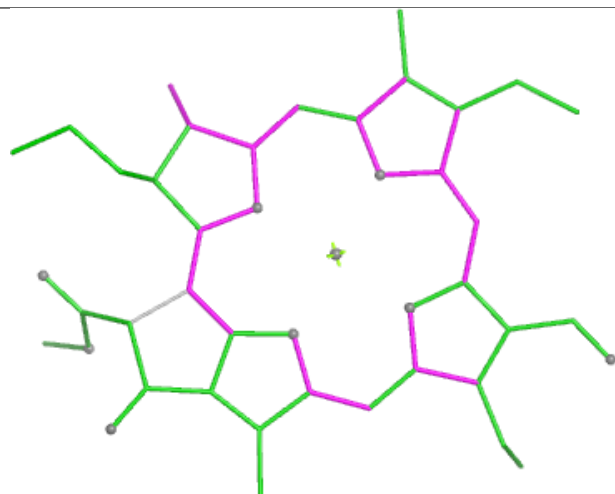




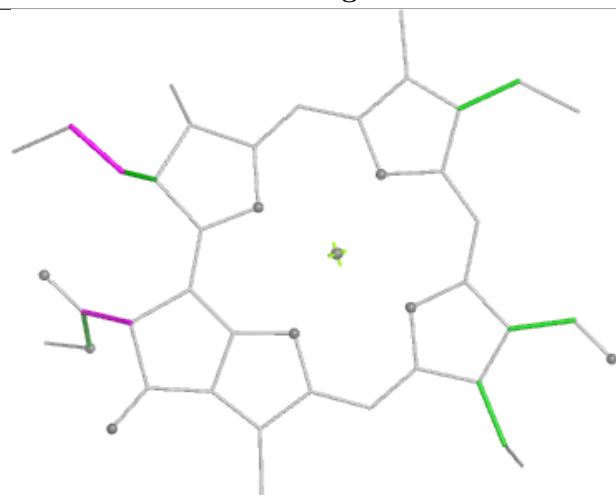
Ligand CHL R 304



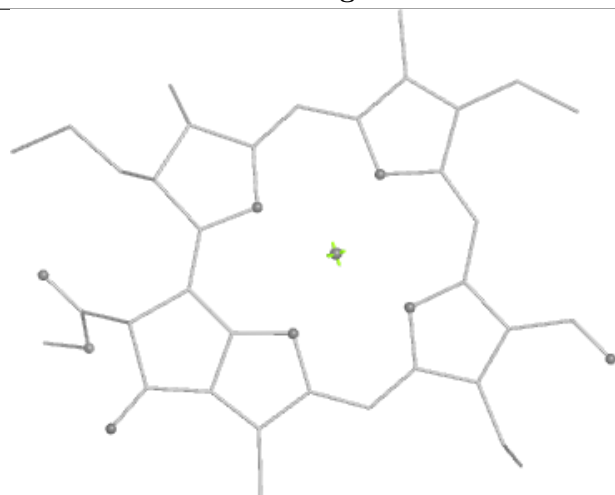
Bond lengths



Bond angles

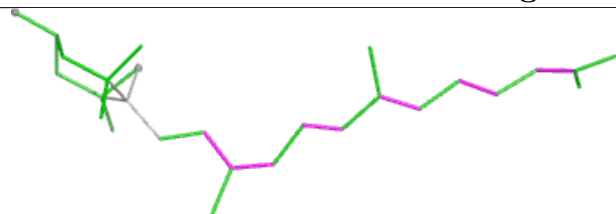


Torsions

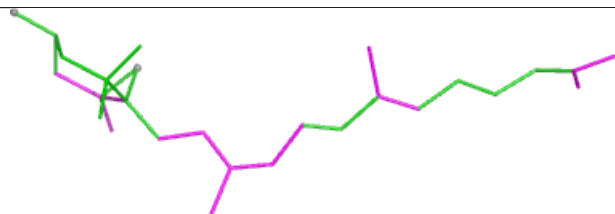


Rings

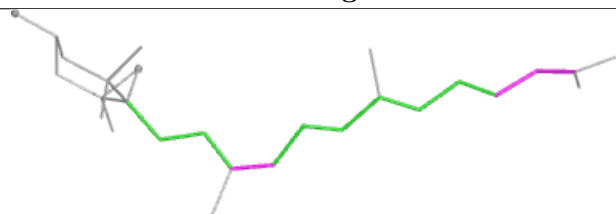
Ligand NEX r 313



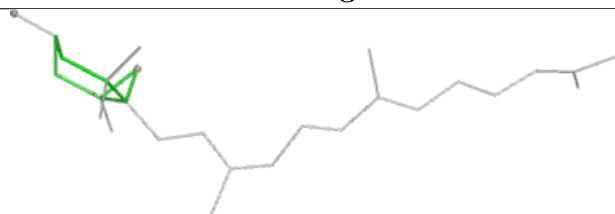
Bond lengths



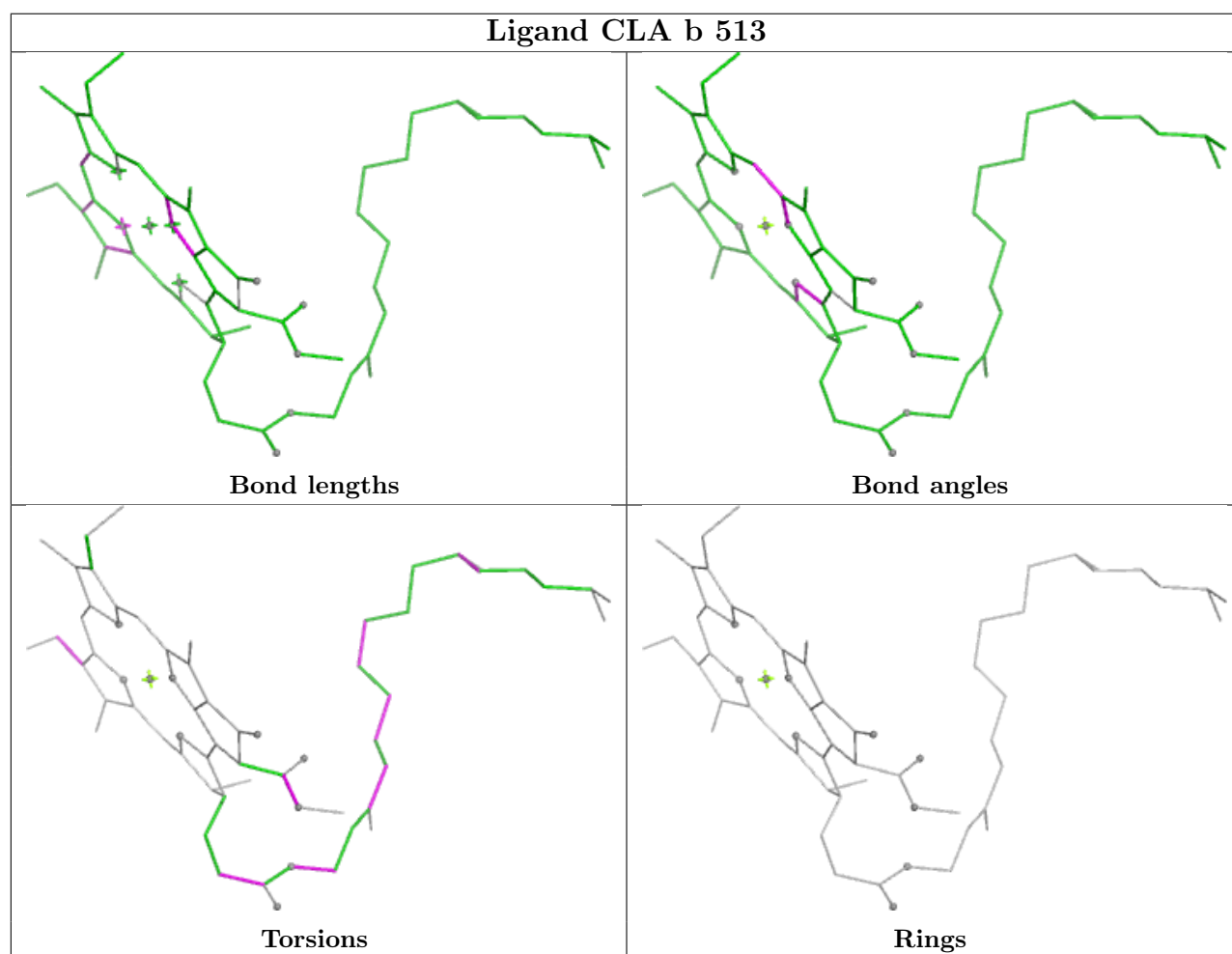
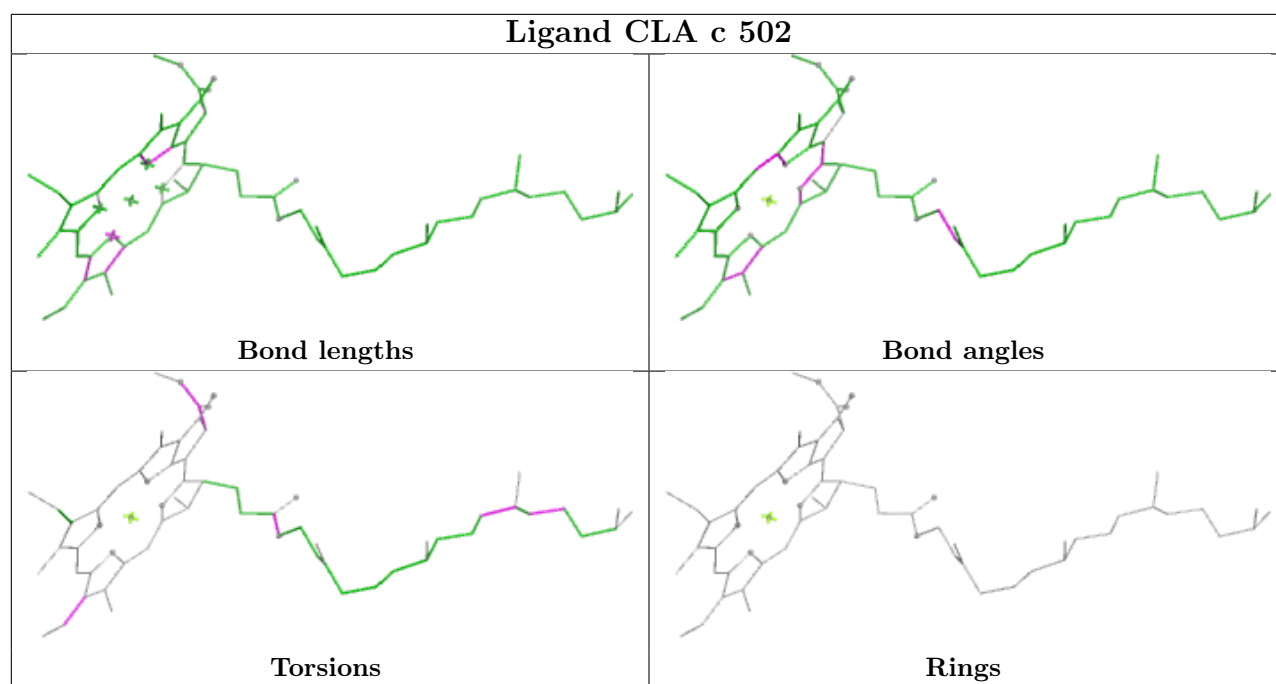
Bond angles

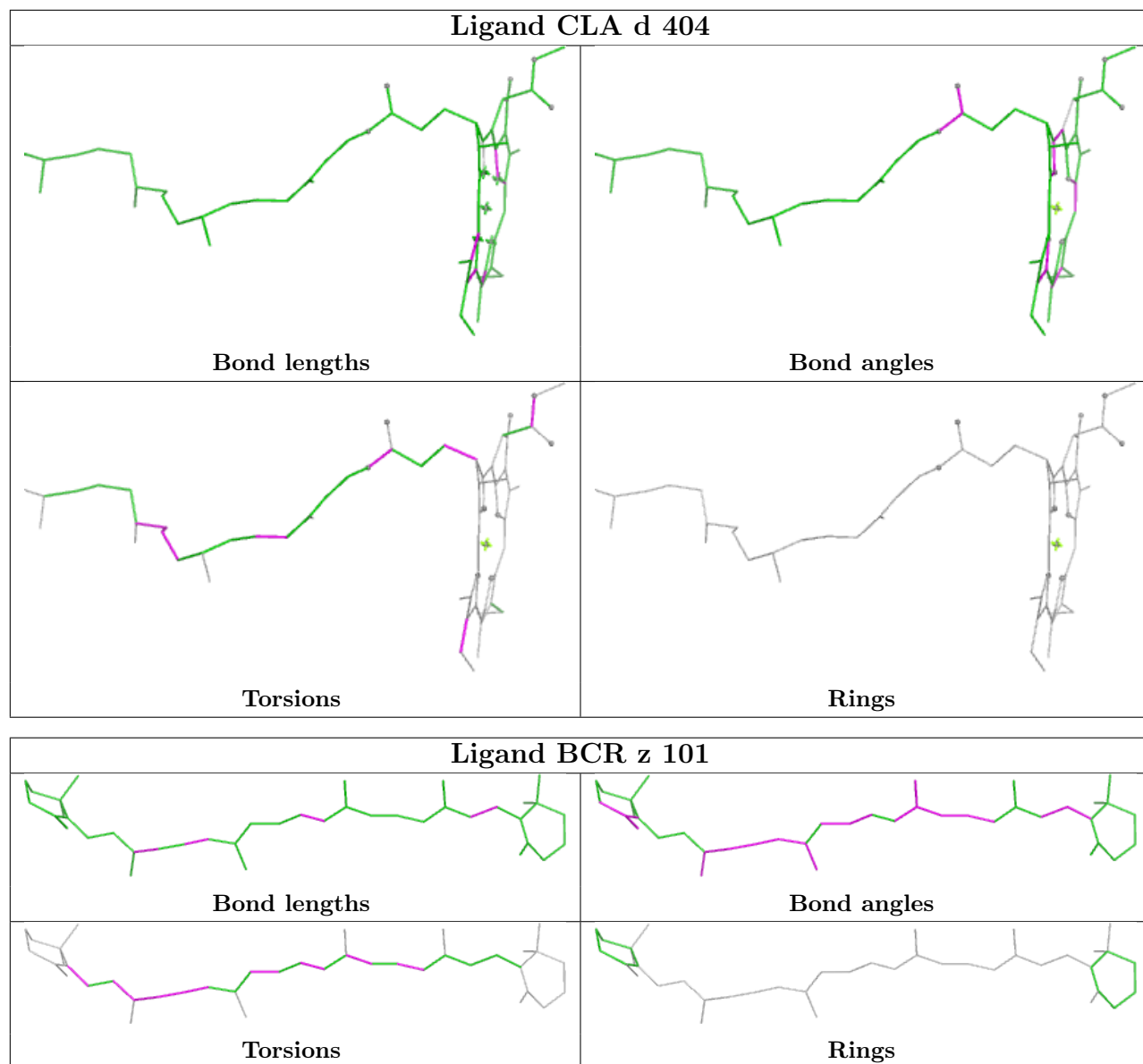


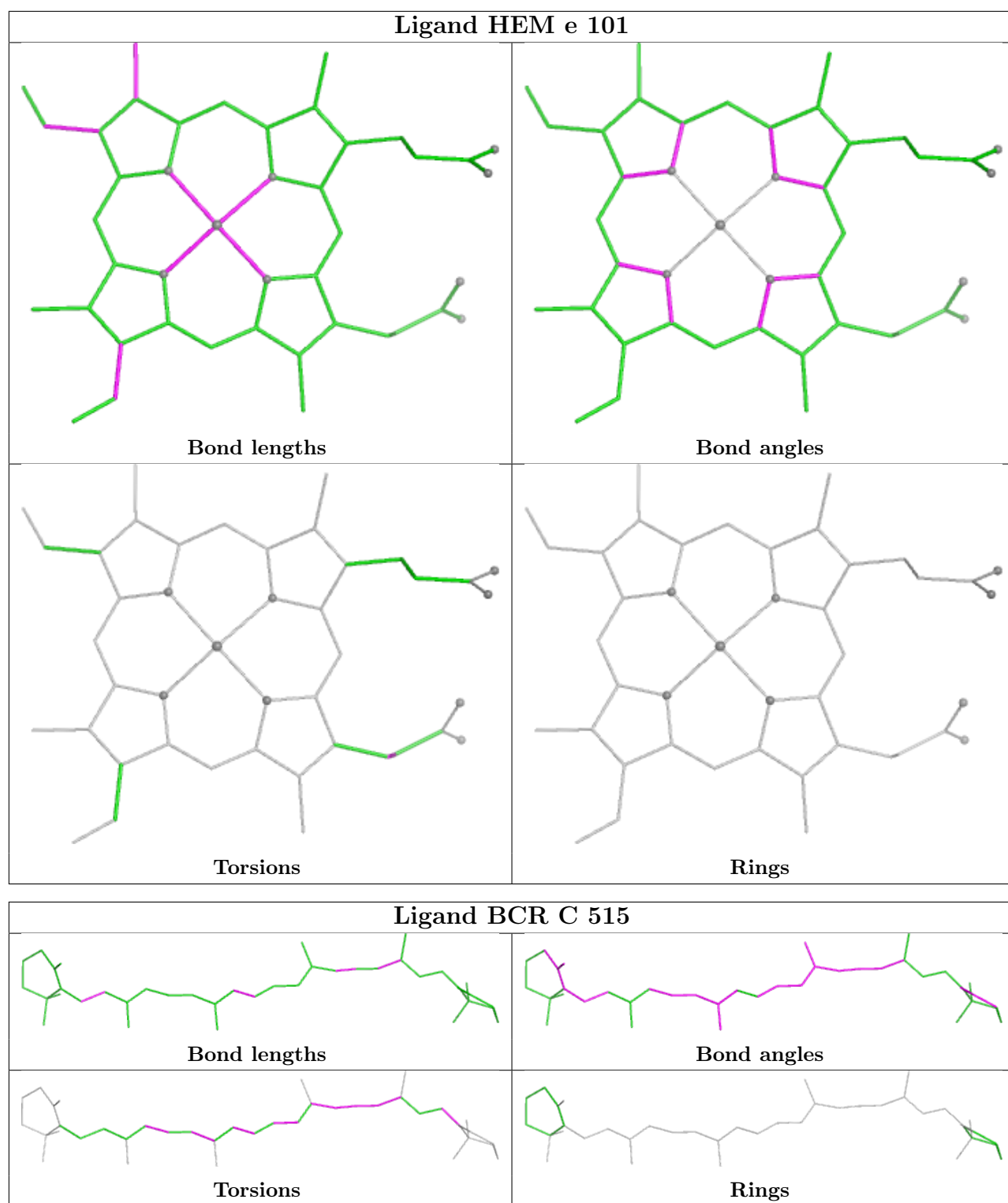
Torsions

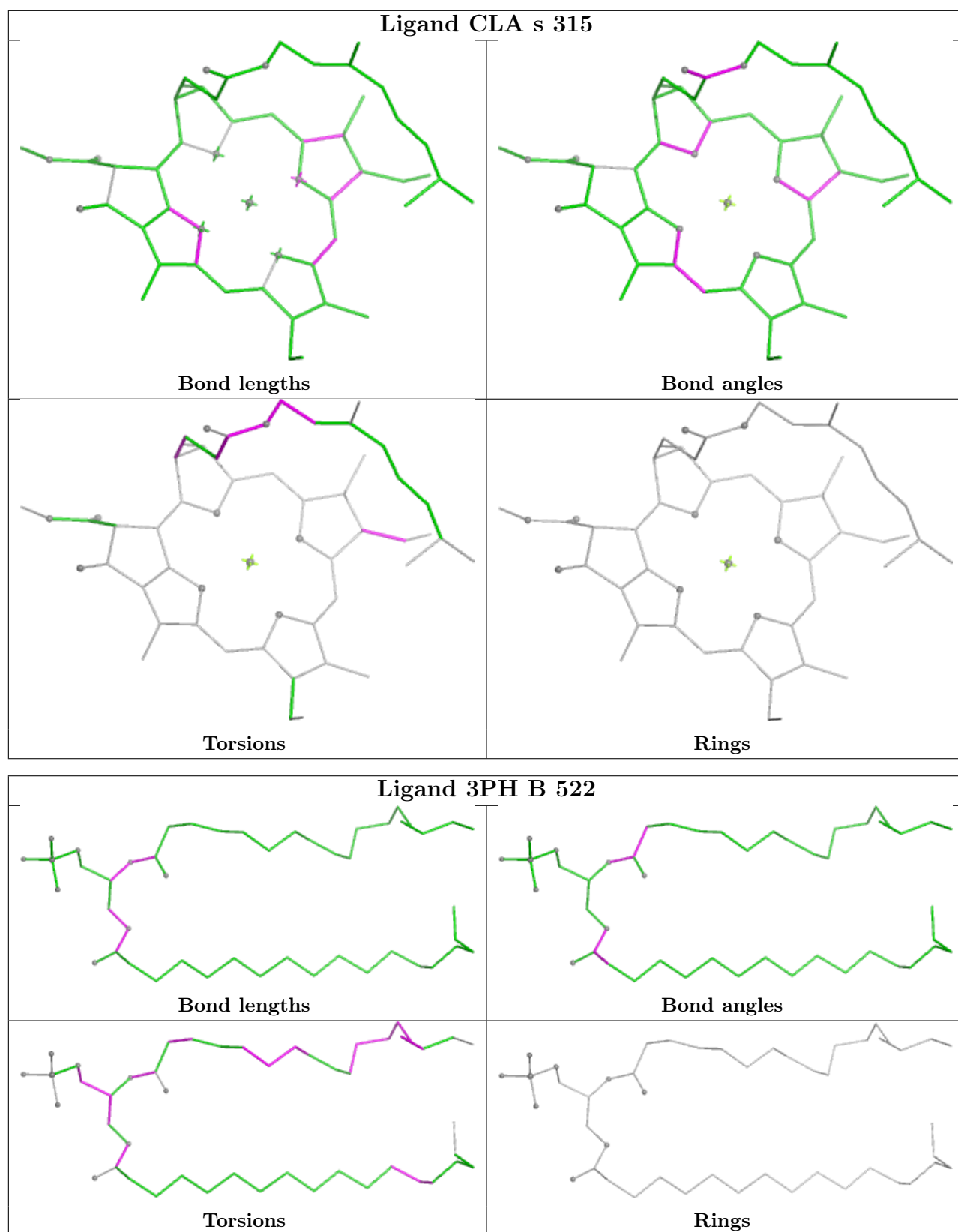


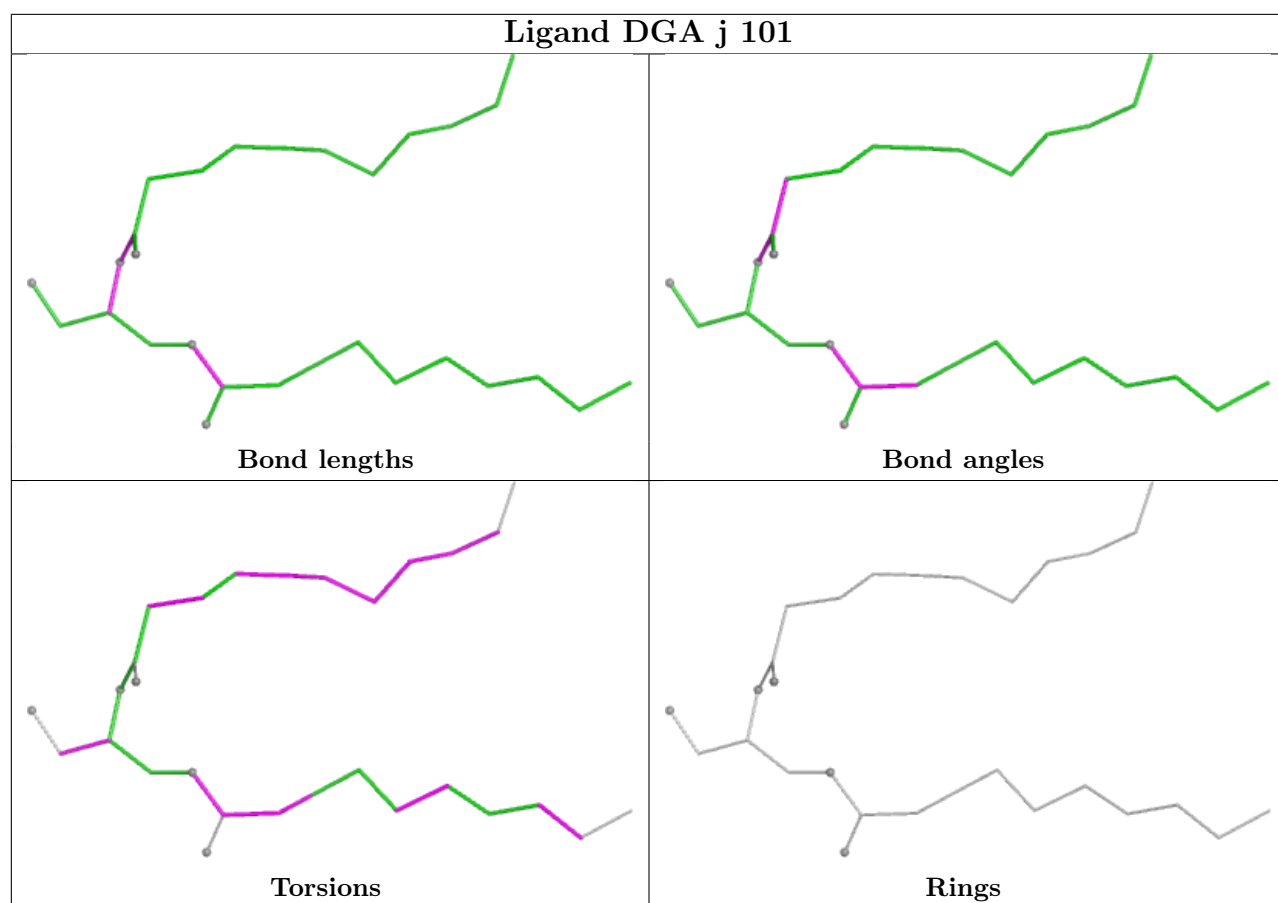
Rings



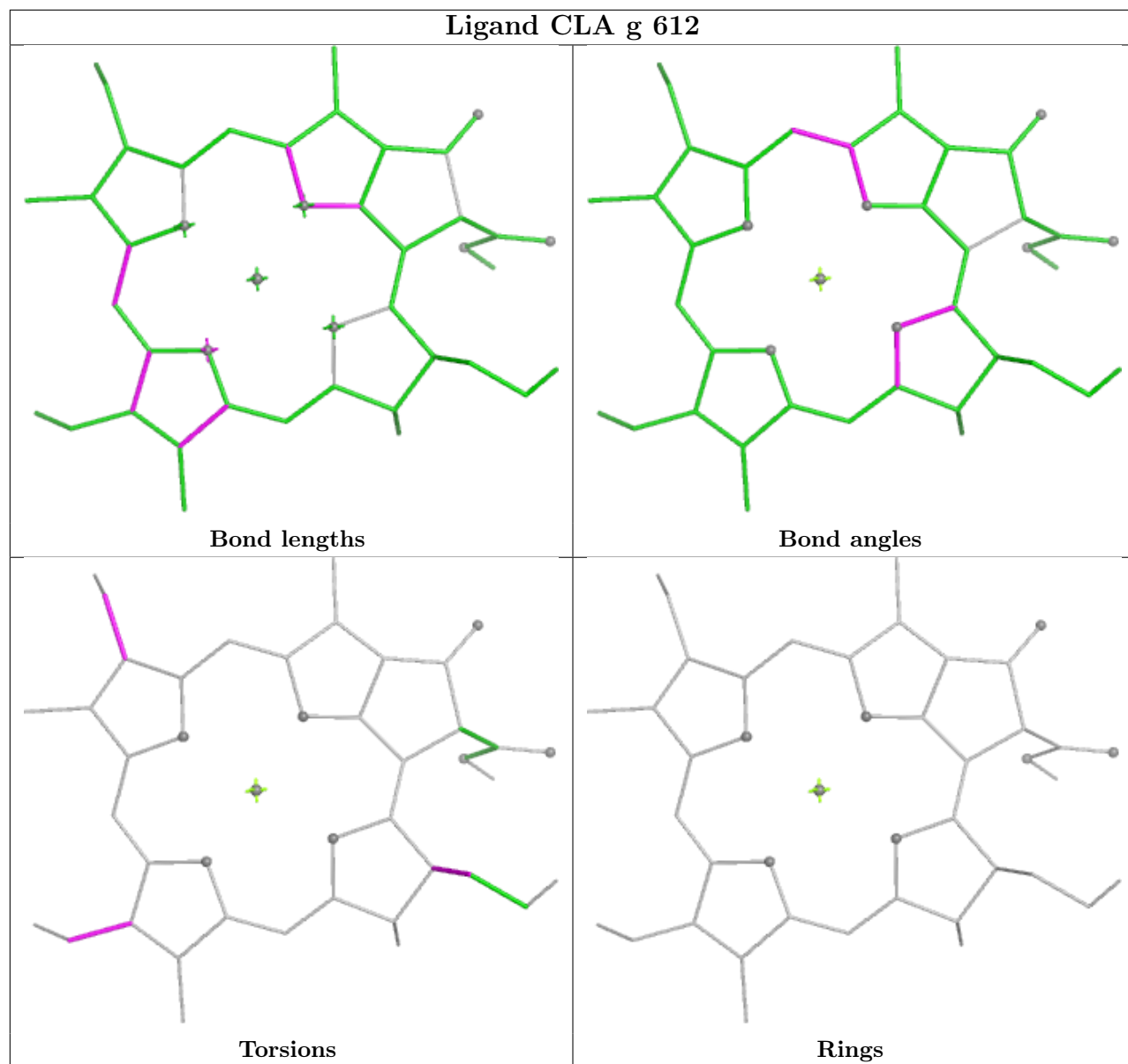


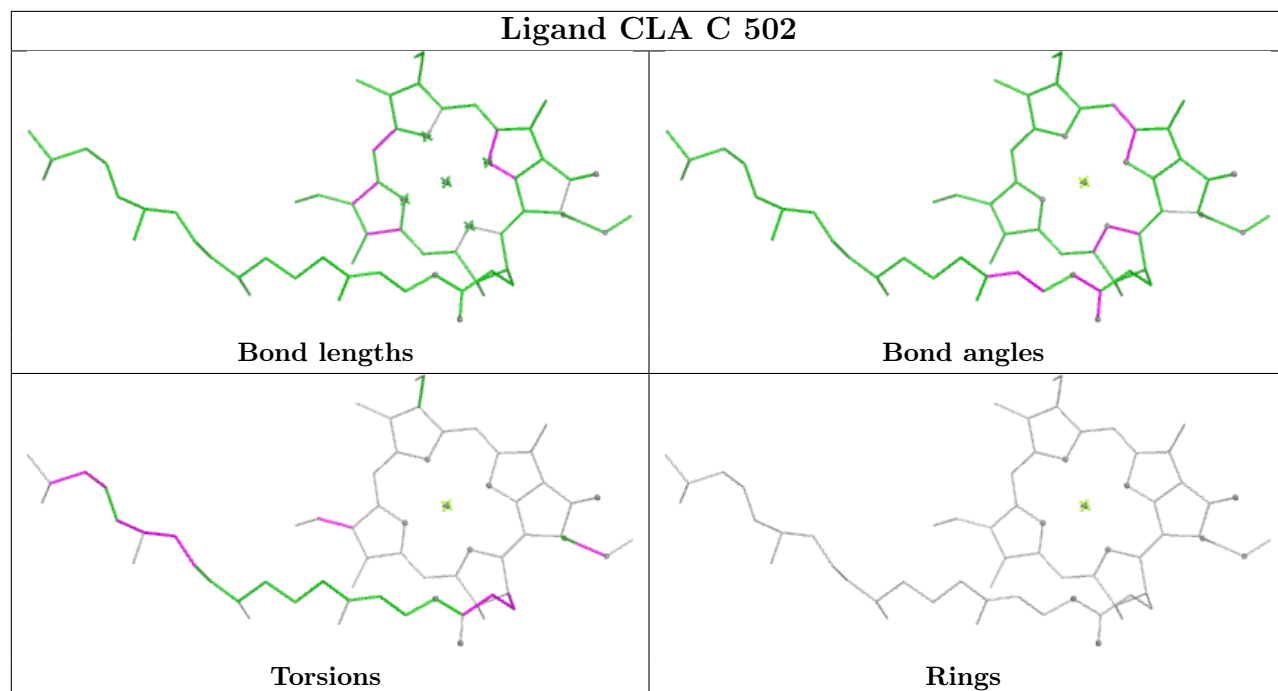




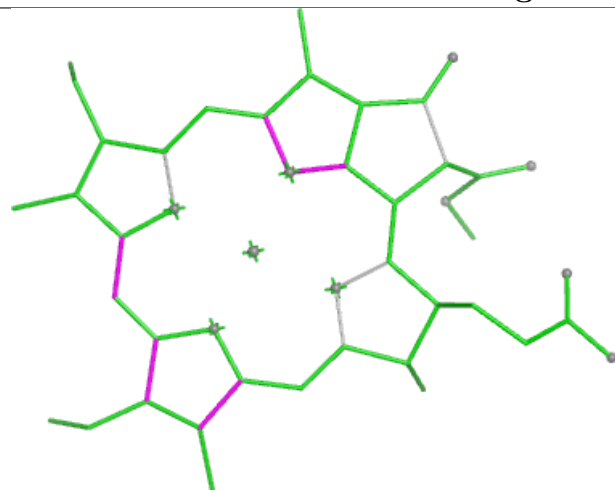


Ligand CLA g 612

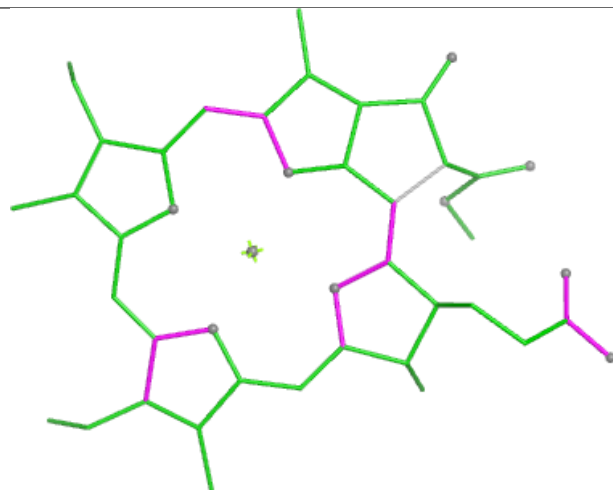




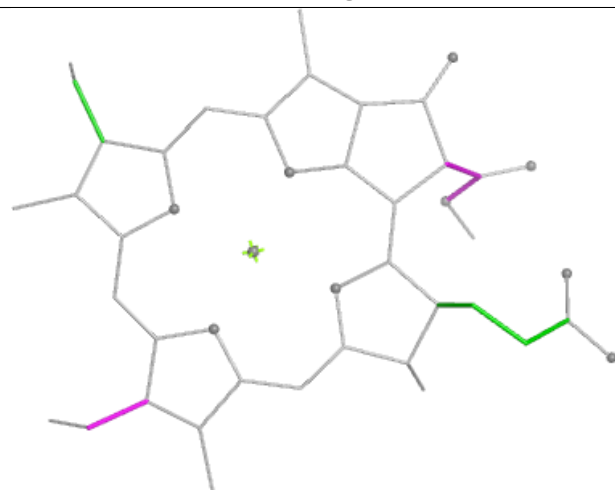
Ligand CLA N 612



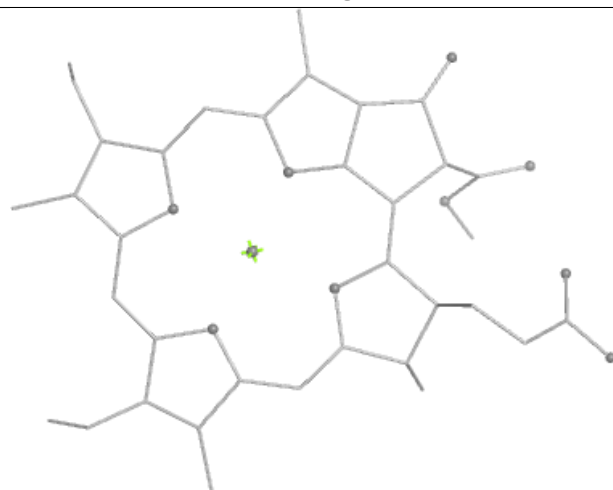
Bond lengths



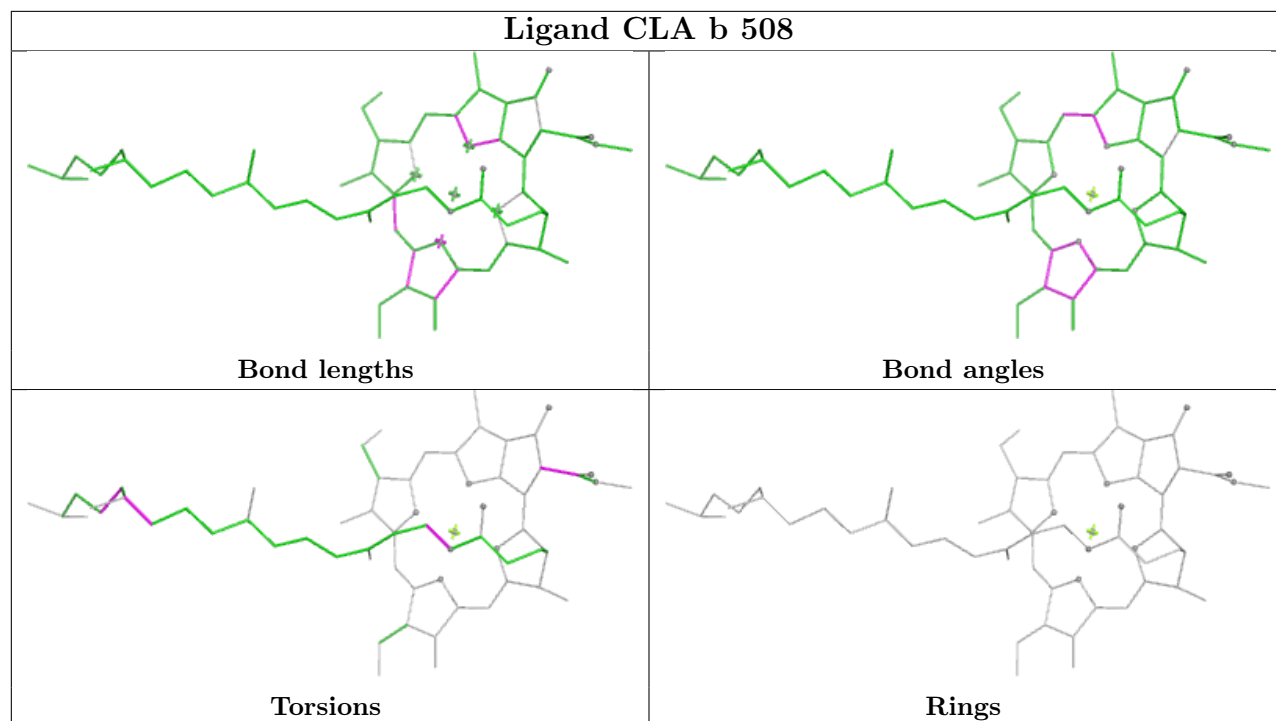
Bond angles

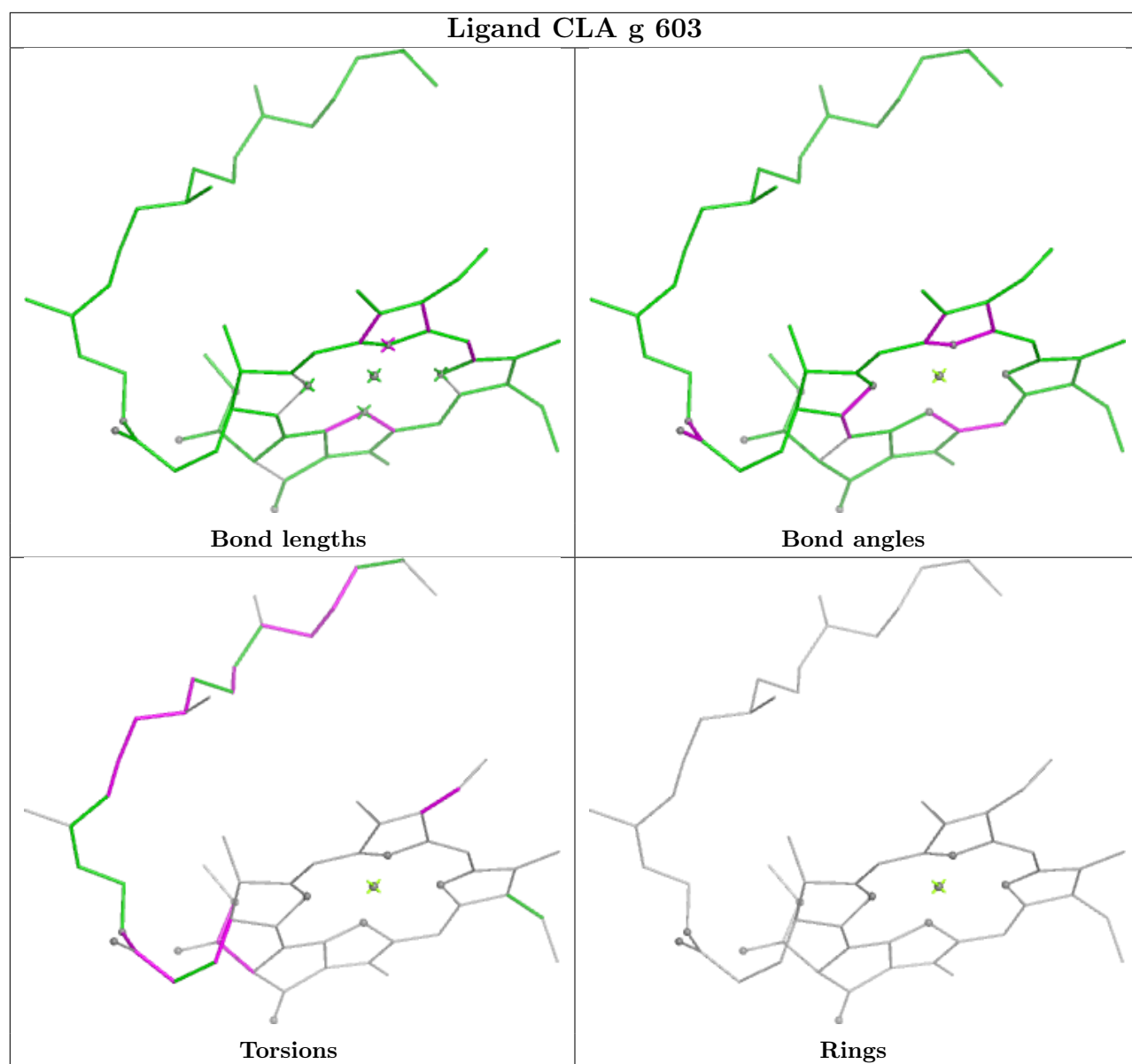


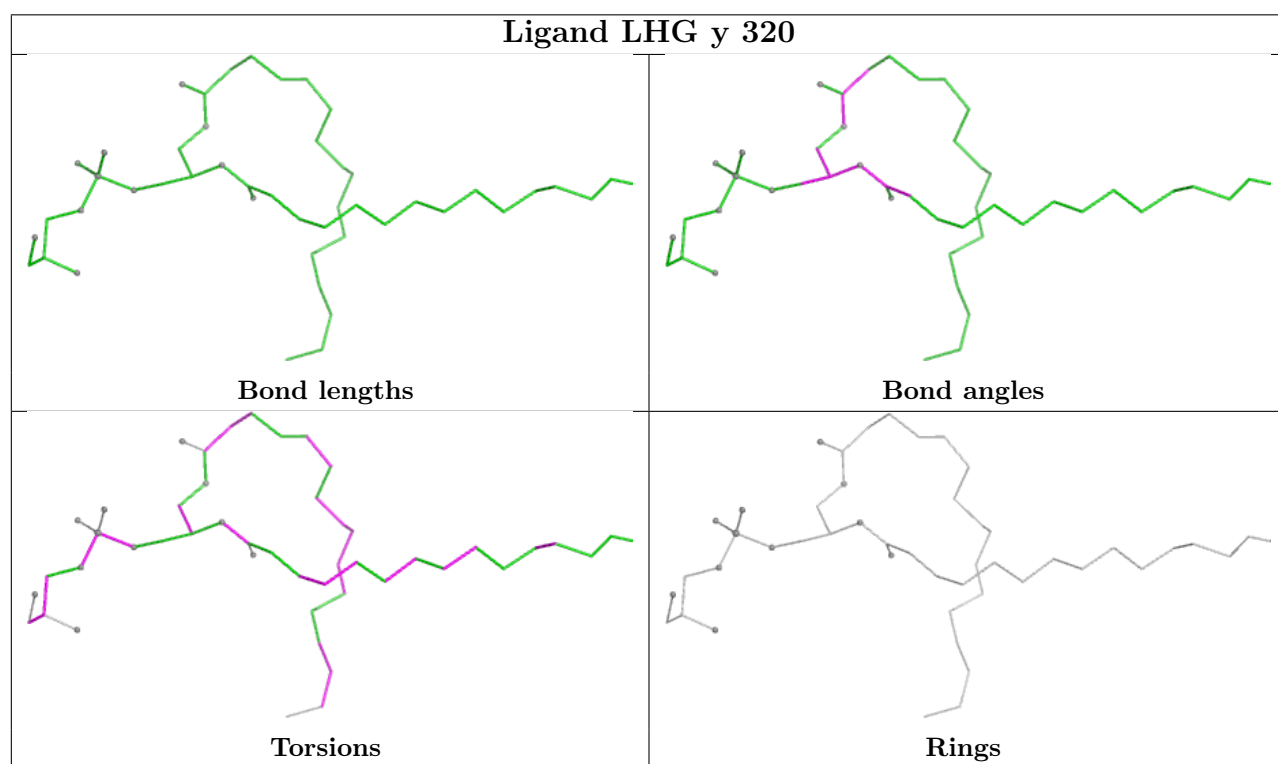
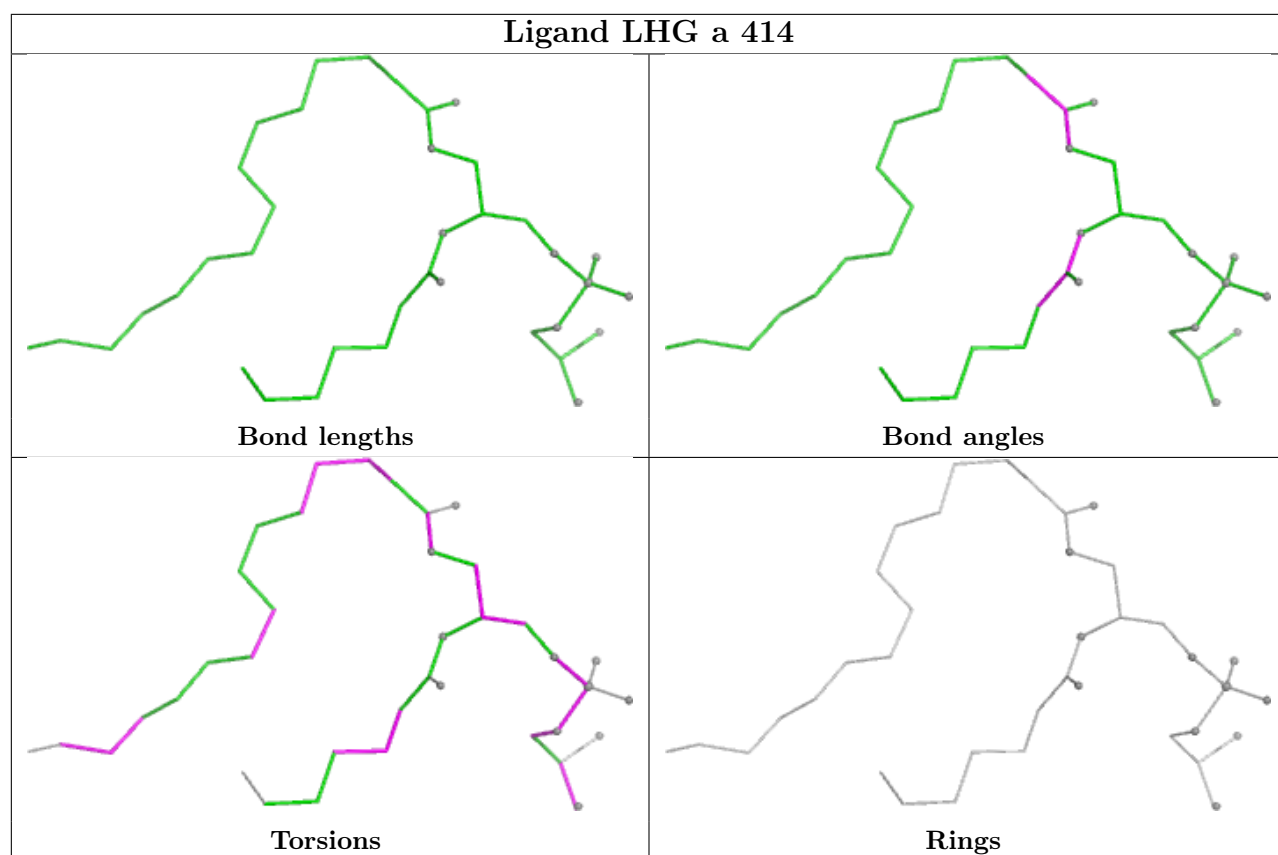
Torsions

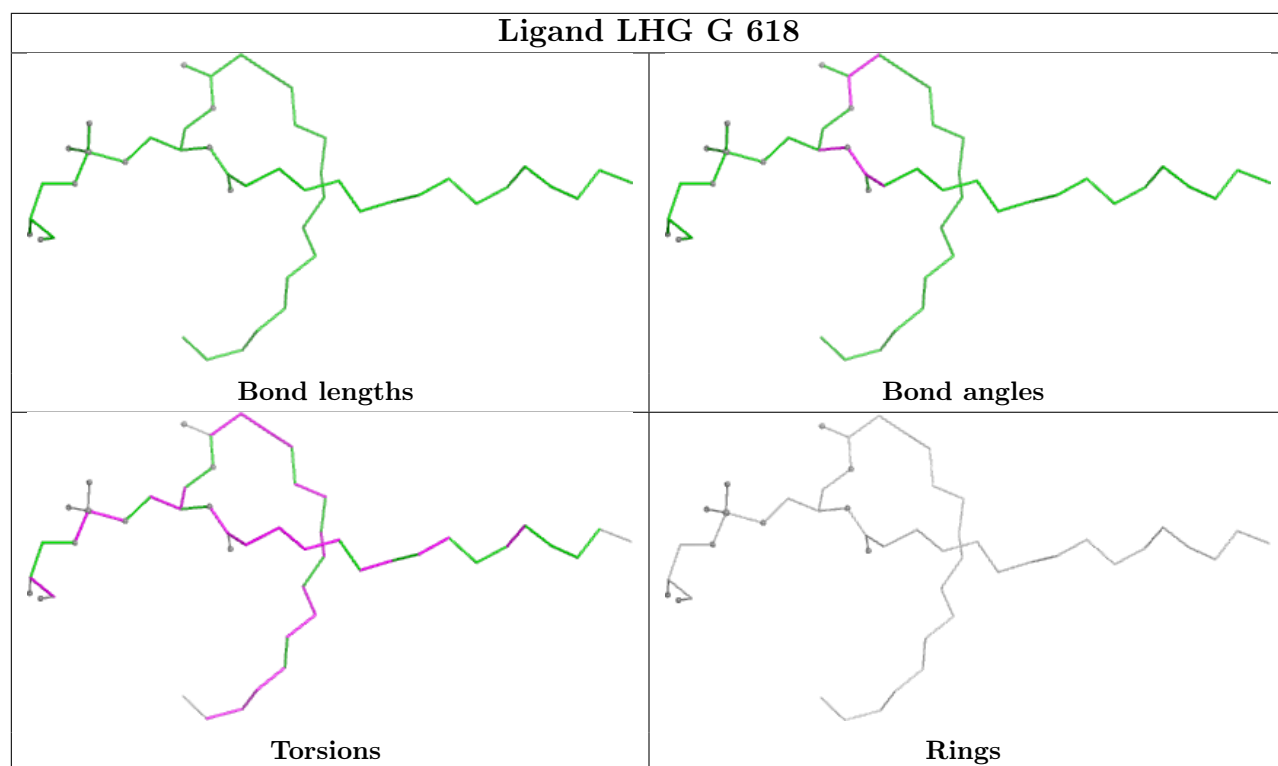
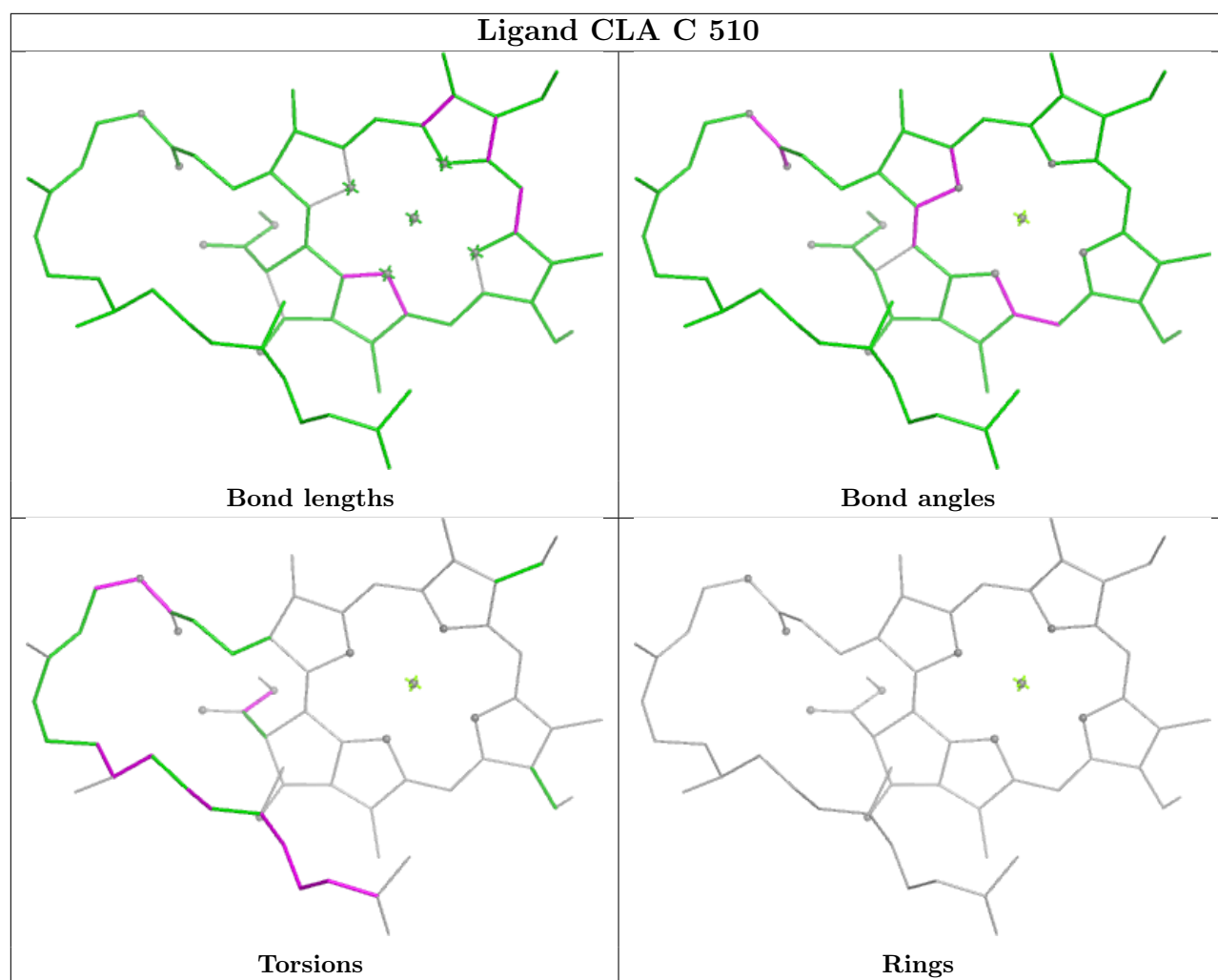


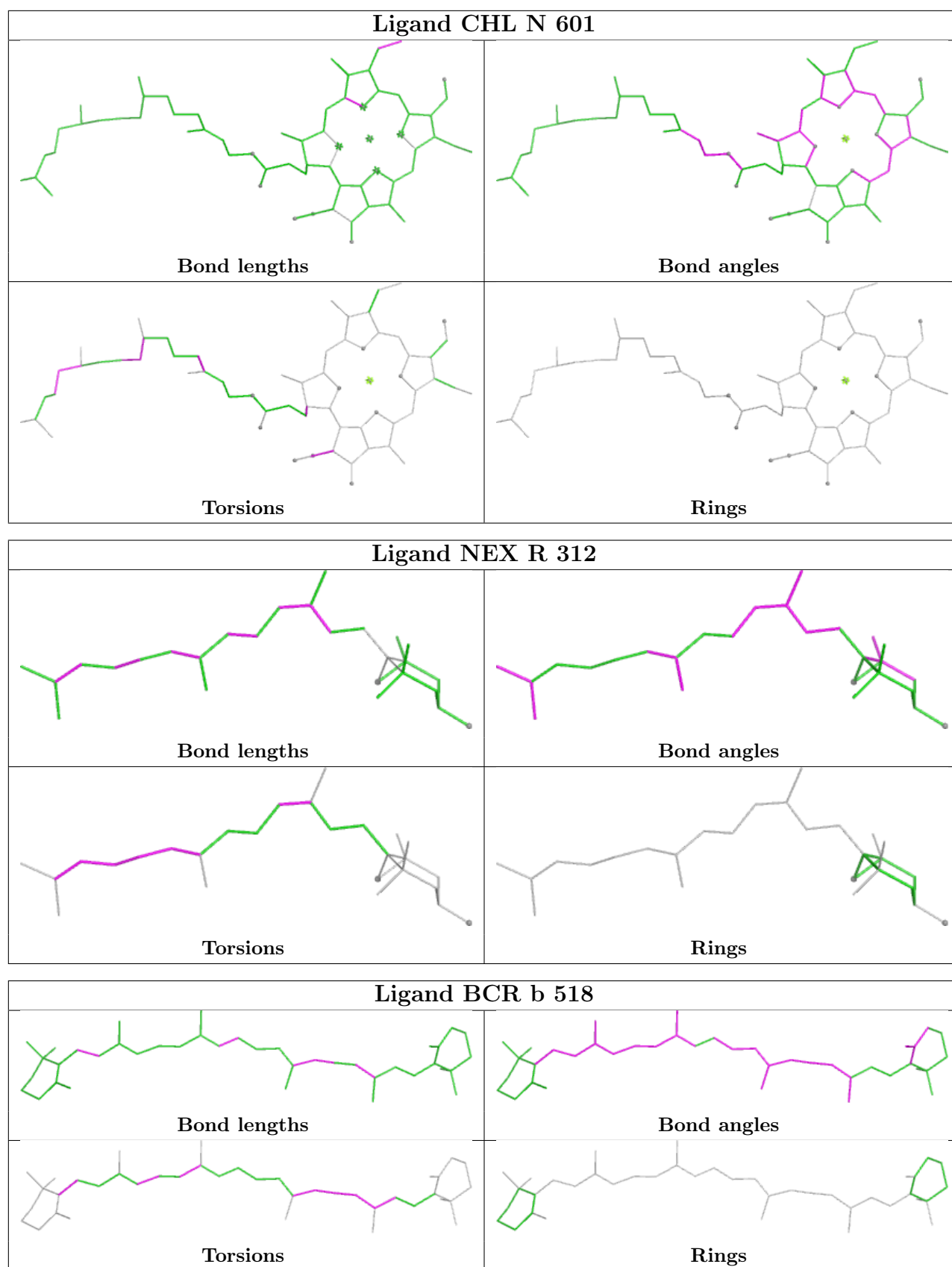
Rings

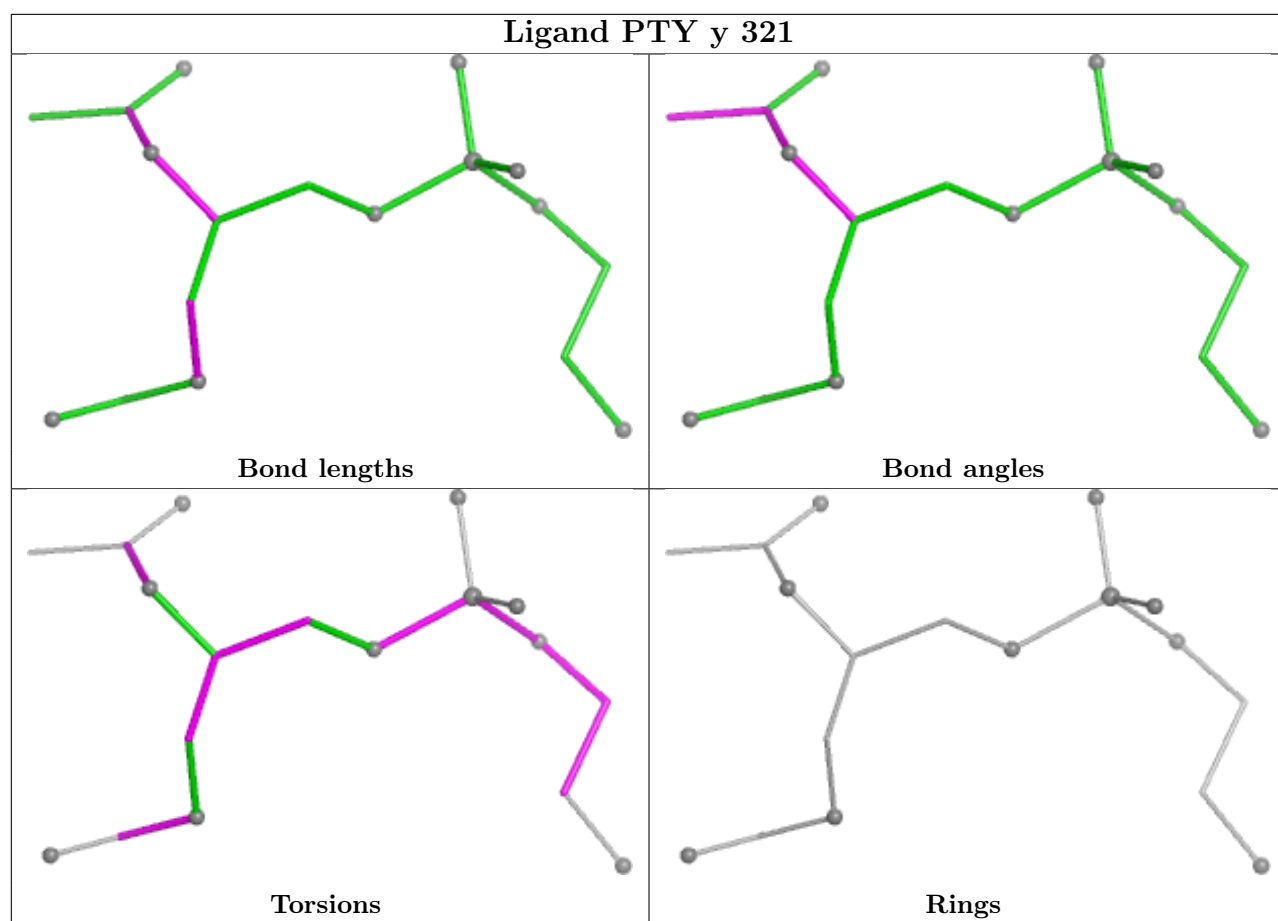




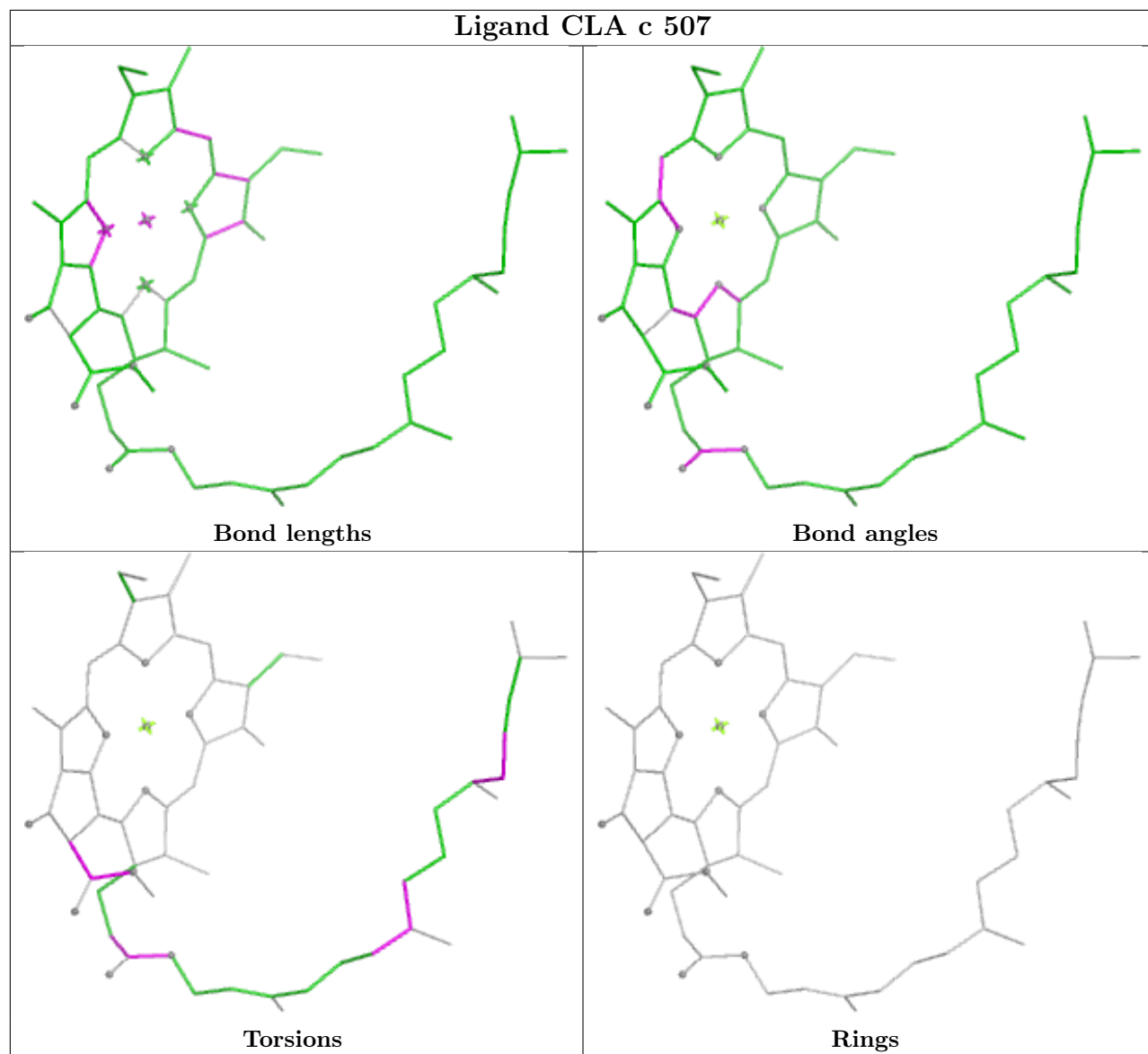


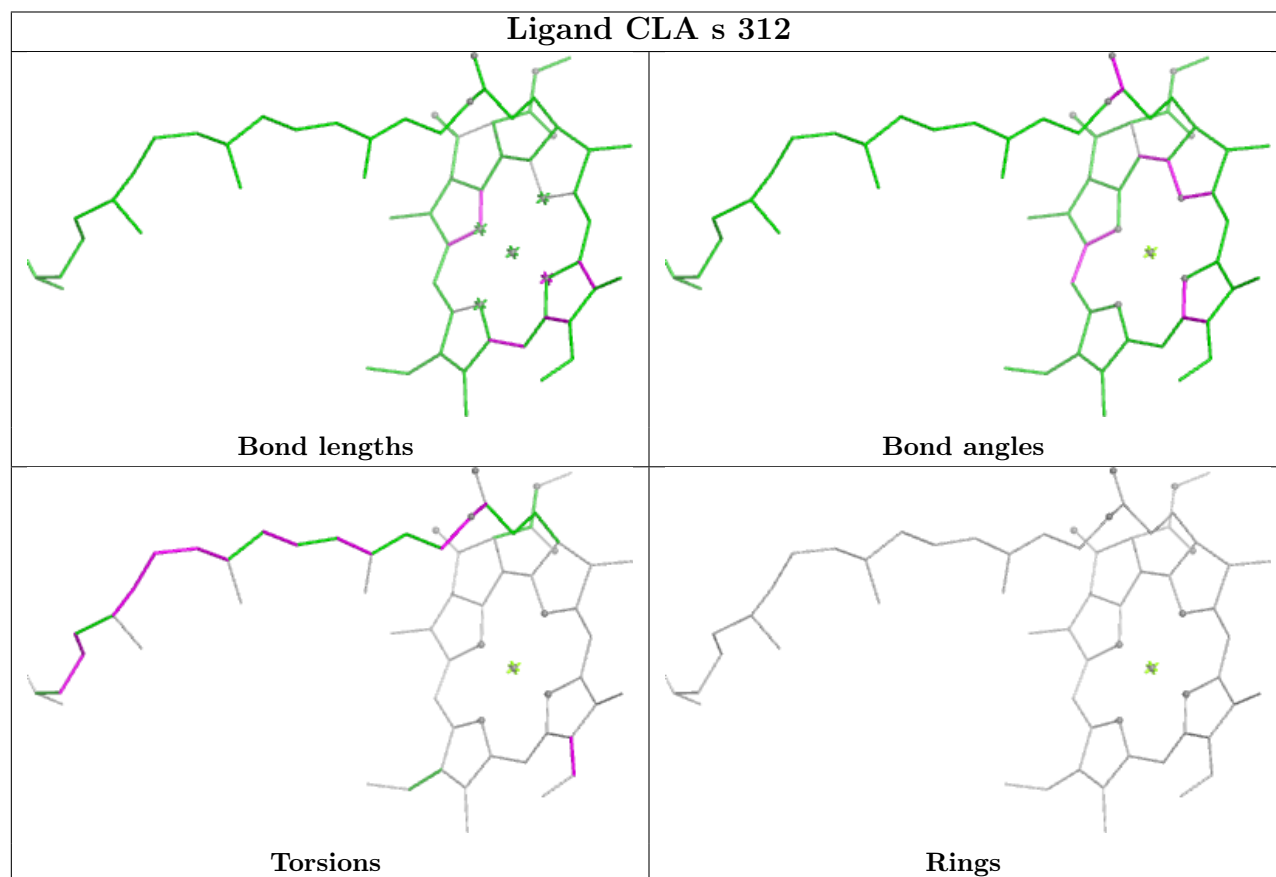
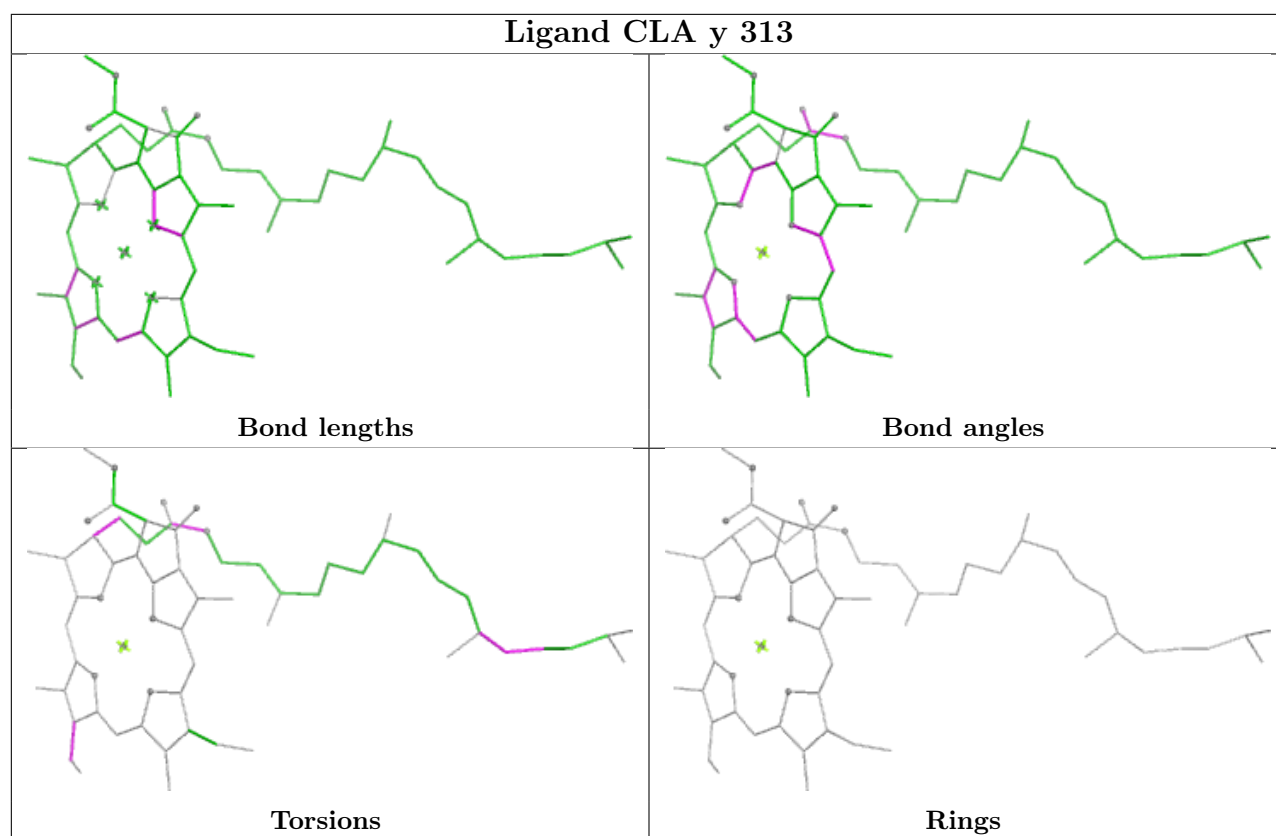


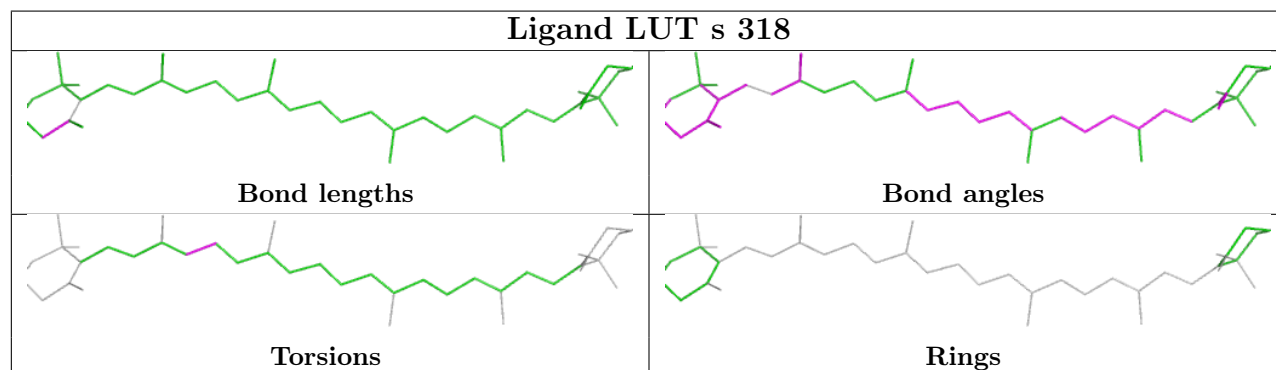
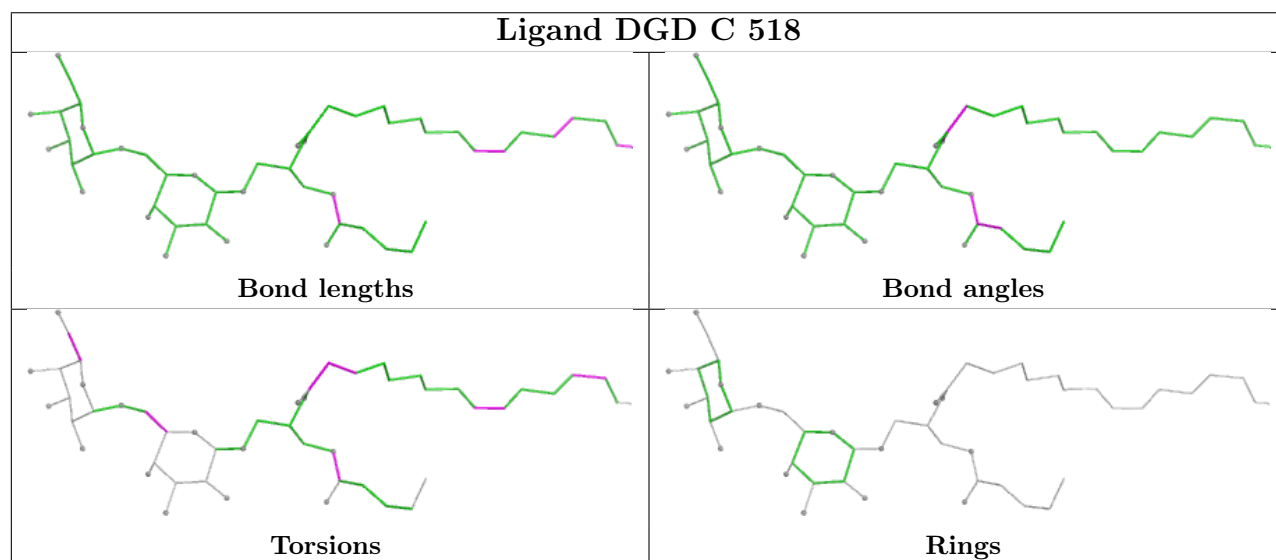
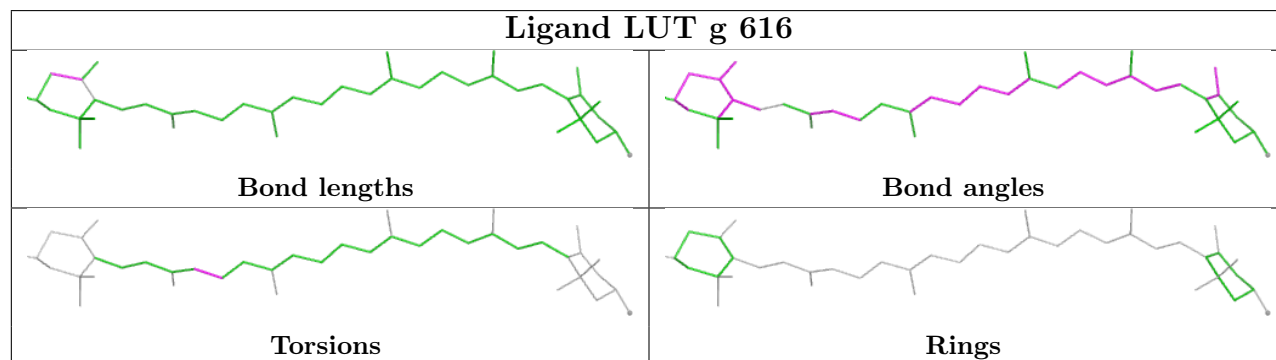
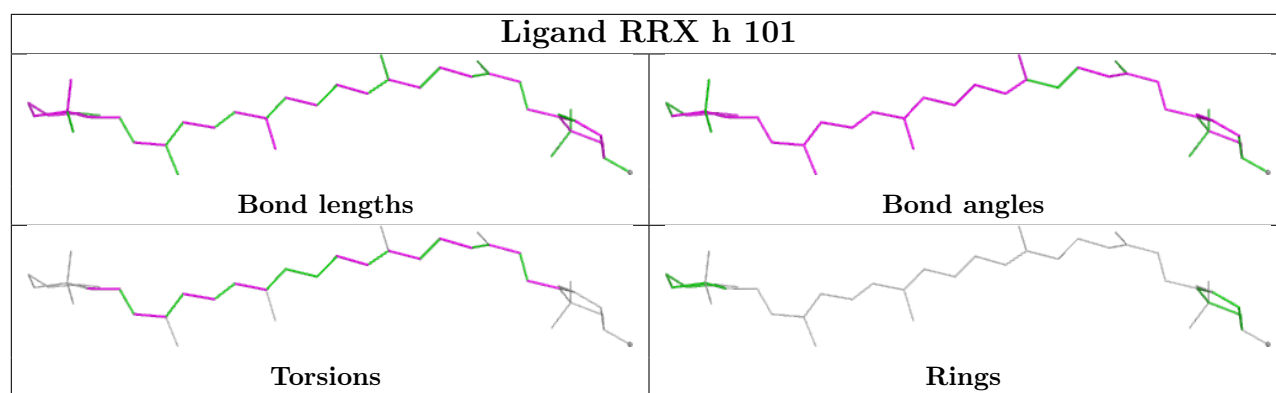


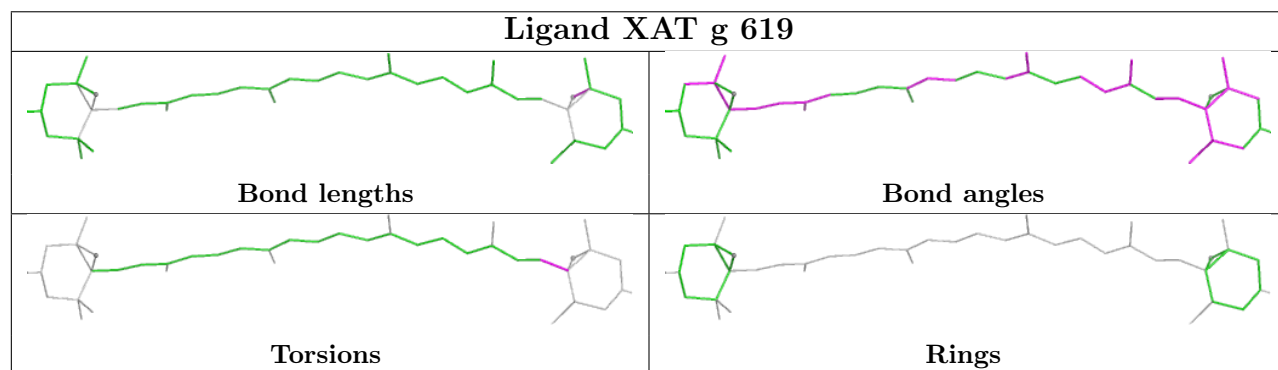
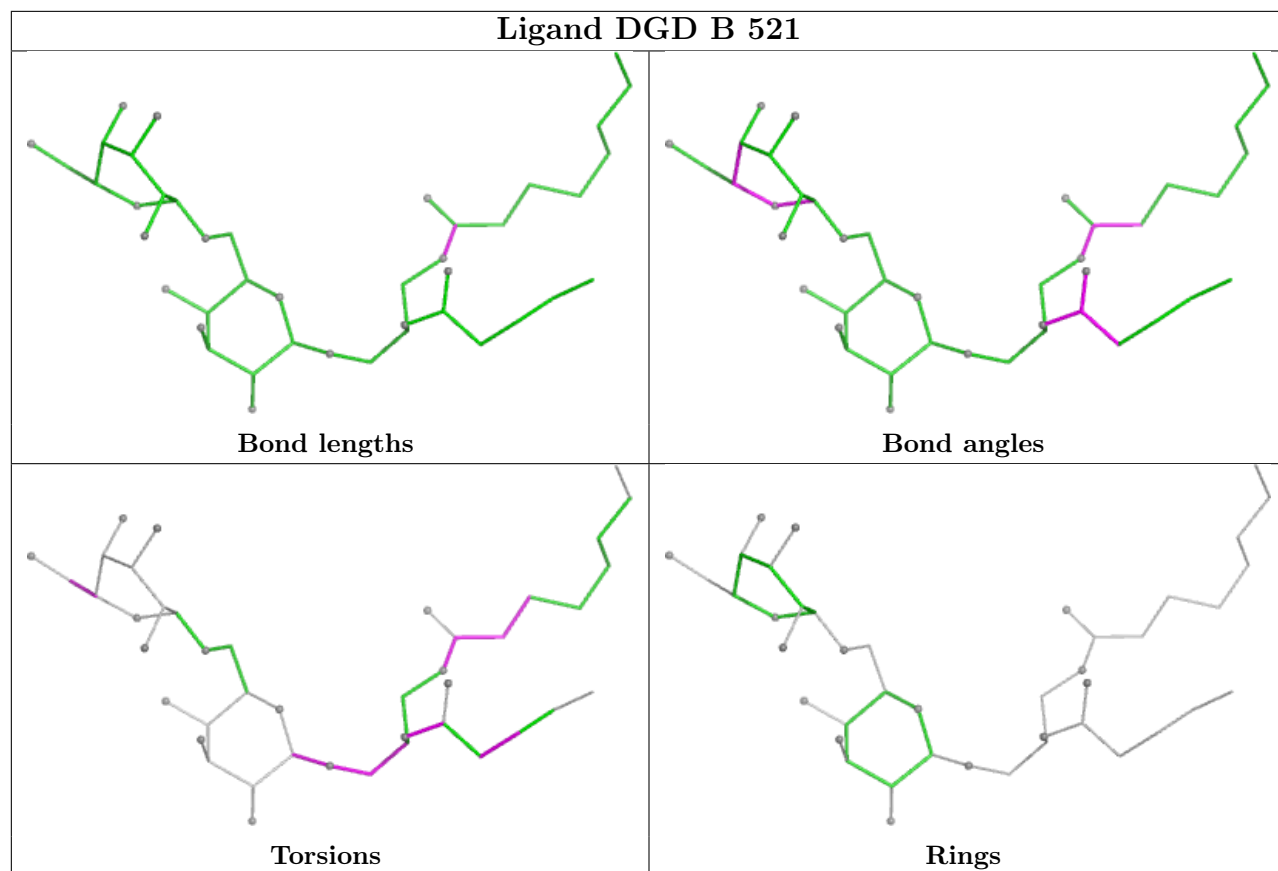


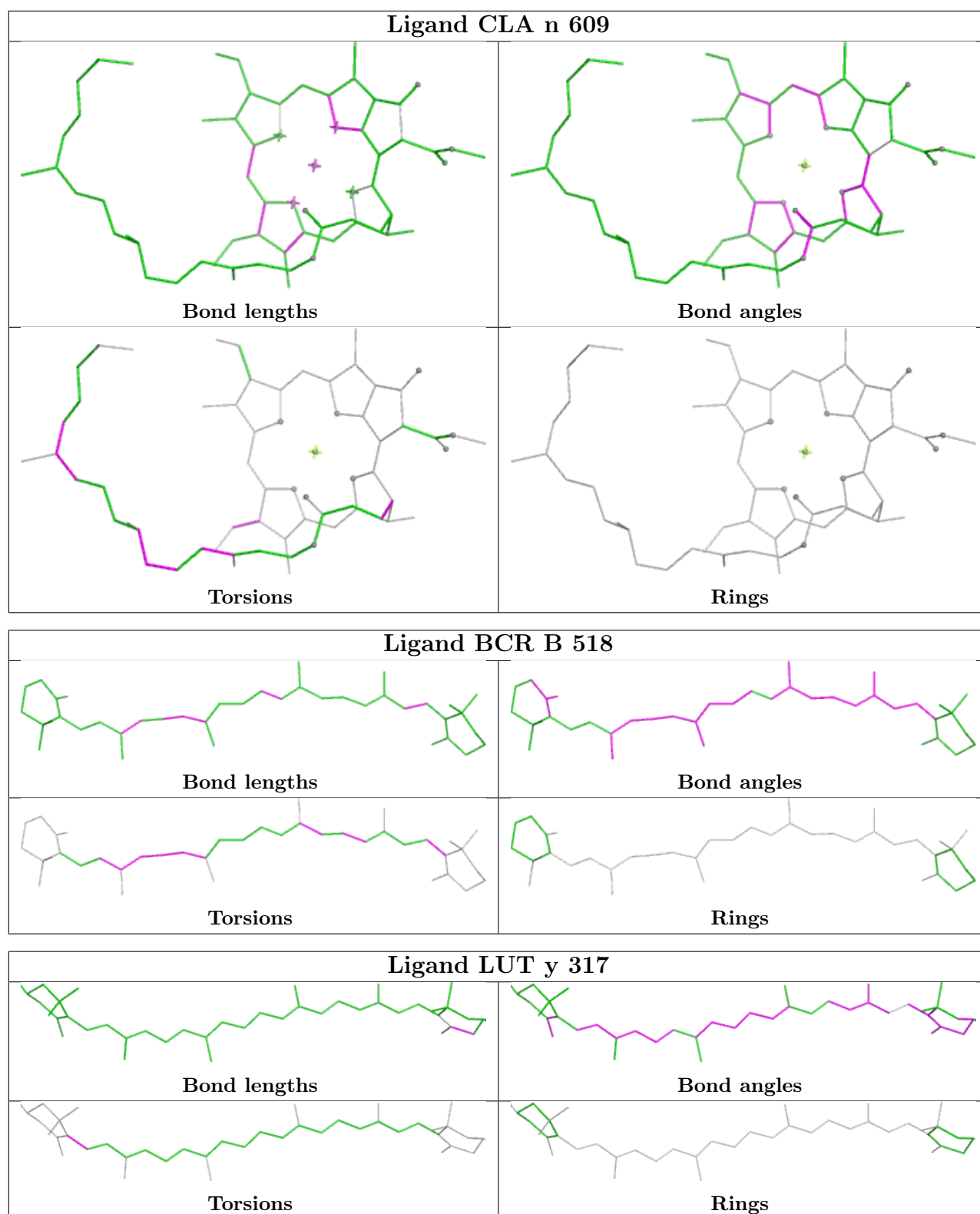
Ligand CLA c 507

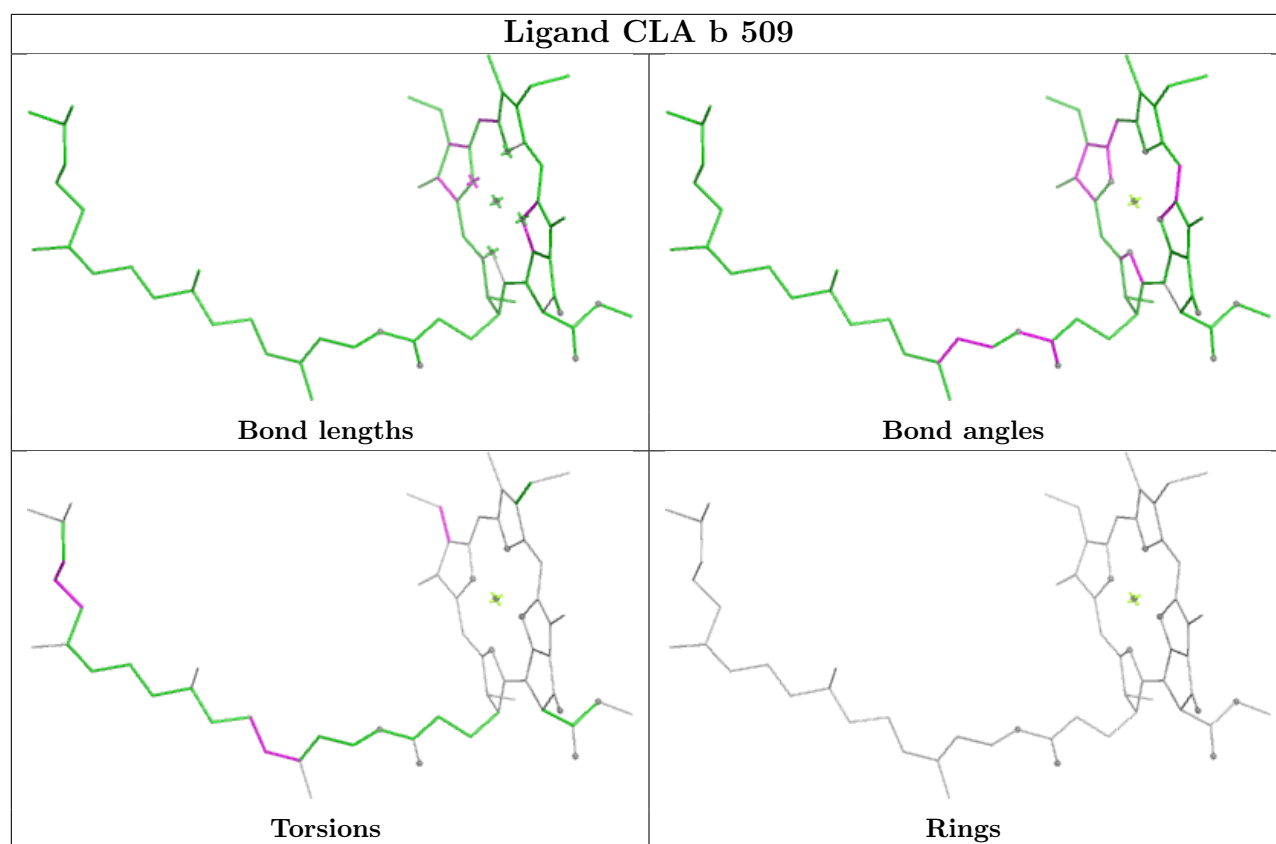




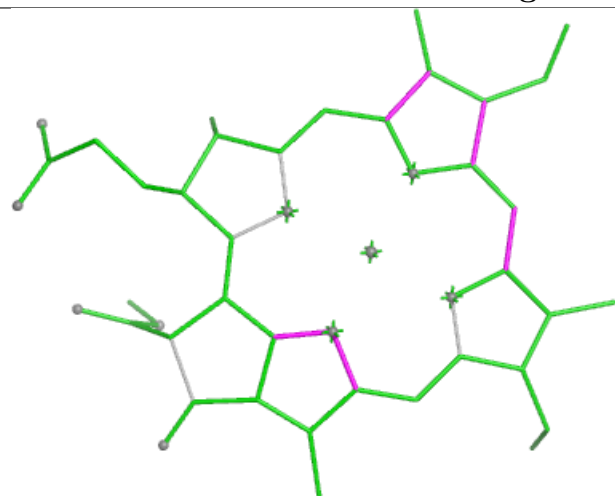




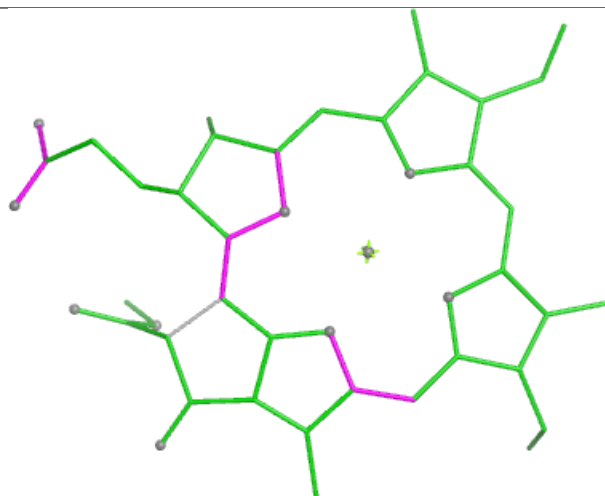




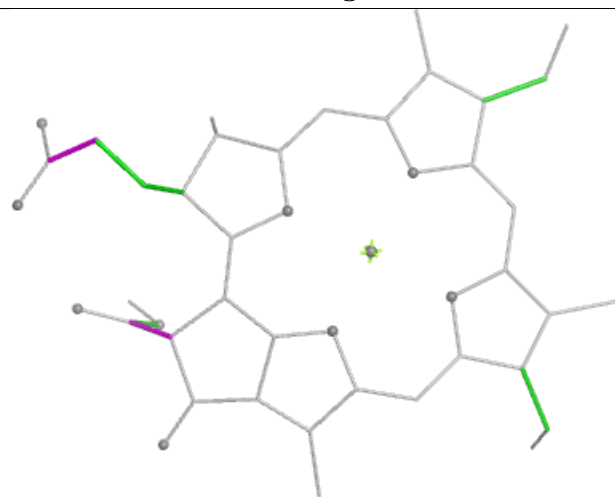
Ligand CLA S 313



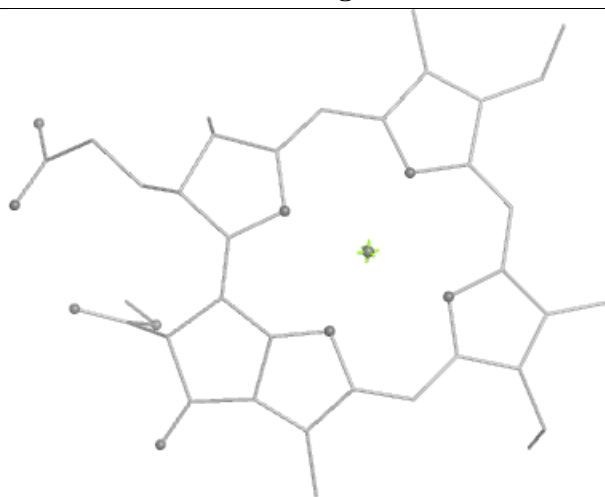
Bond lengths



Bond angles

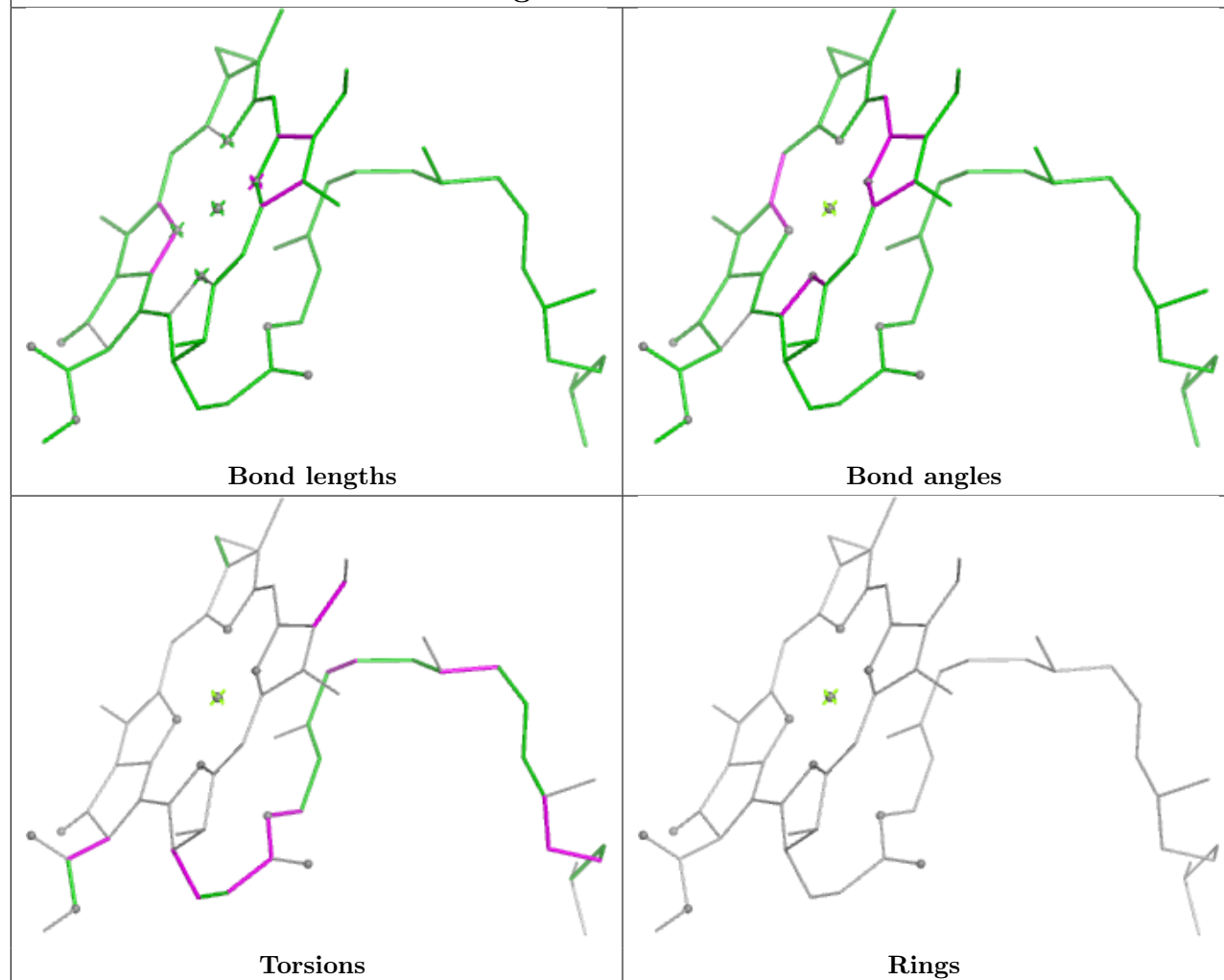


Torsions

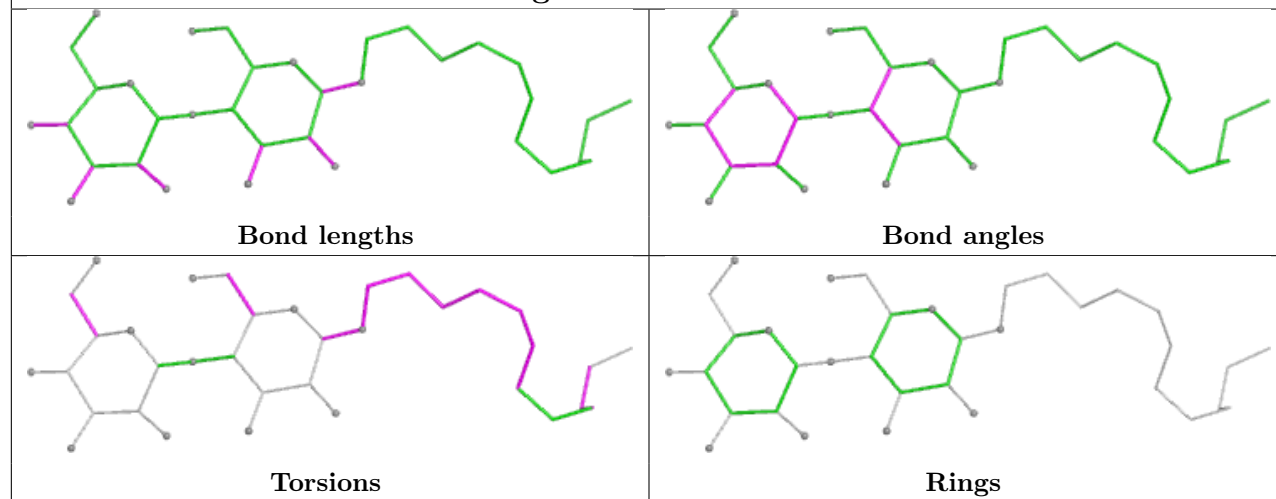


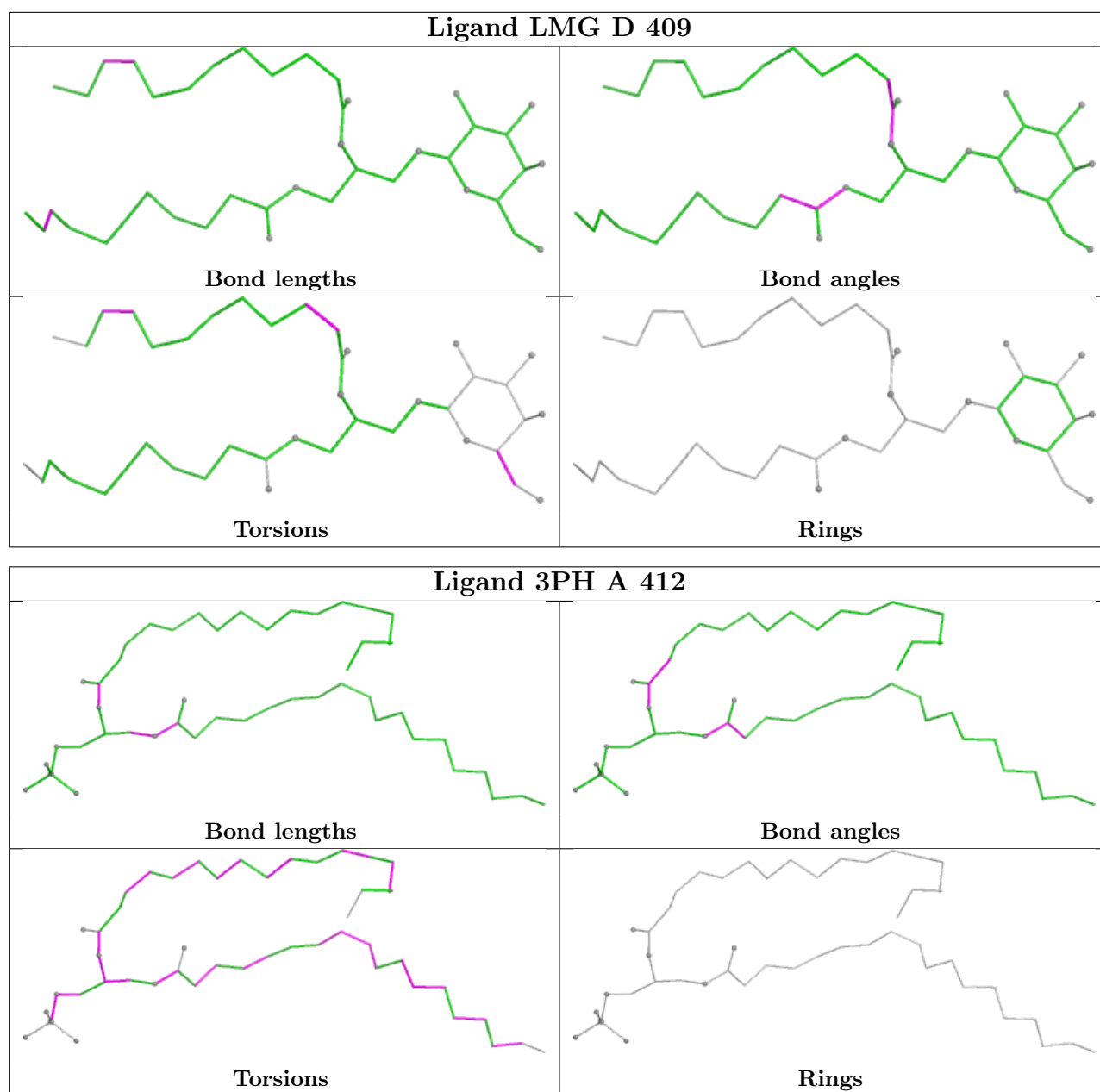
Rings

Ligand CLA n 612

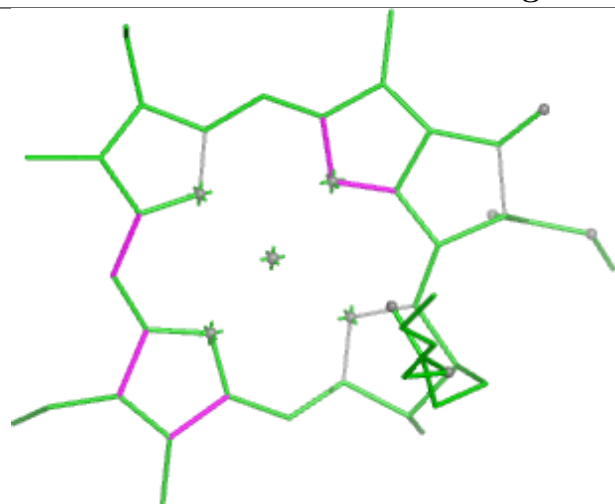


Ligand LMT b 524

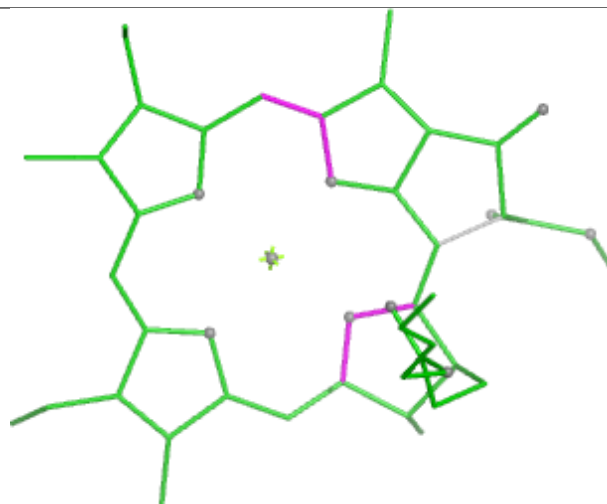




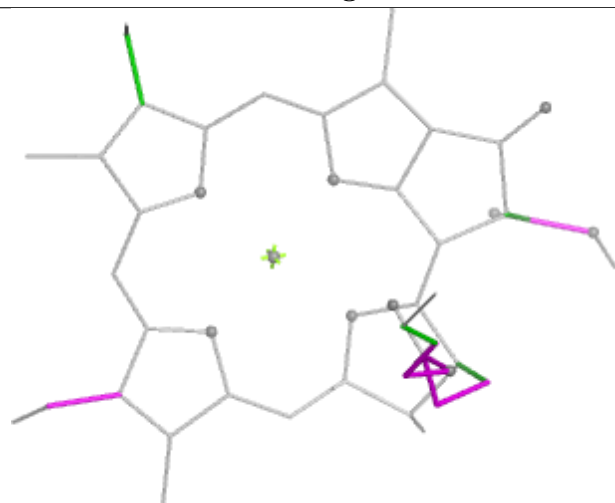
Ligand CLA r 304



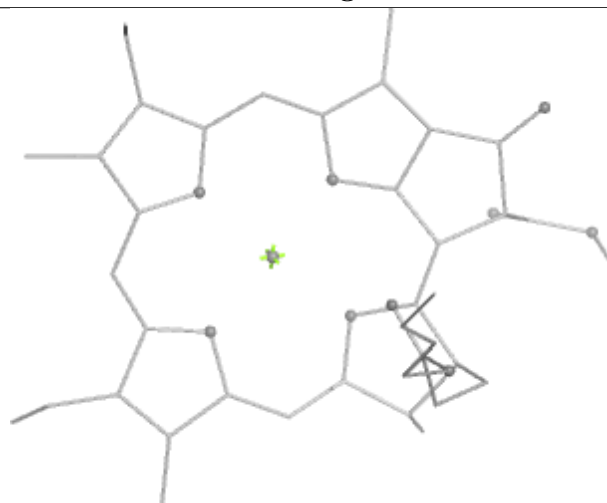
Bond lengths



Bond angles

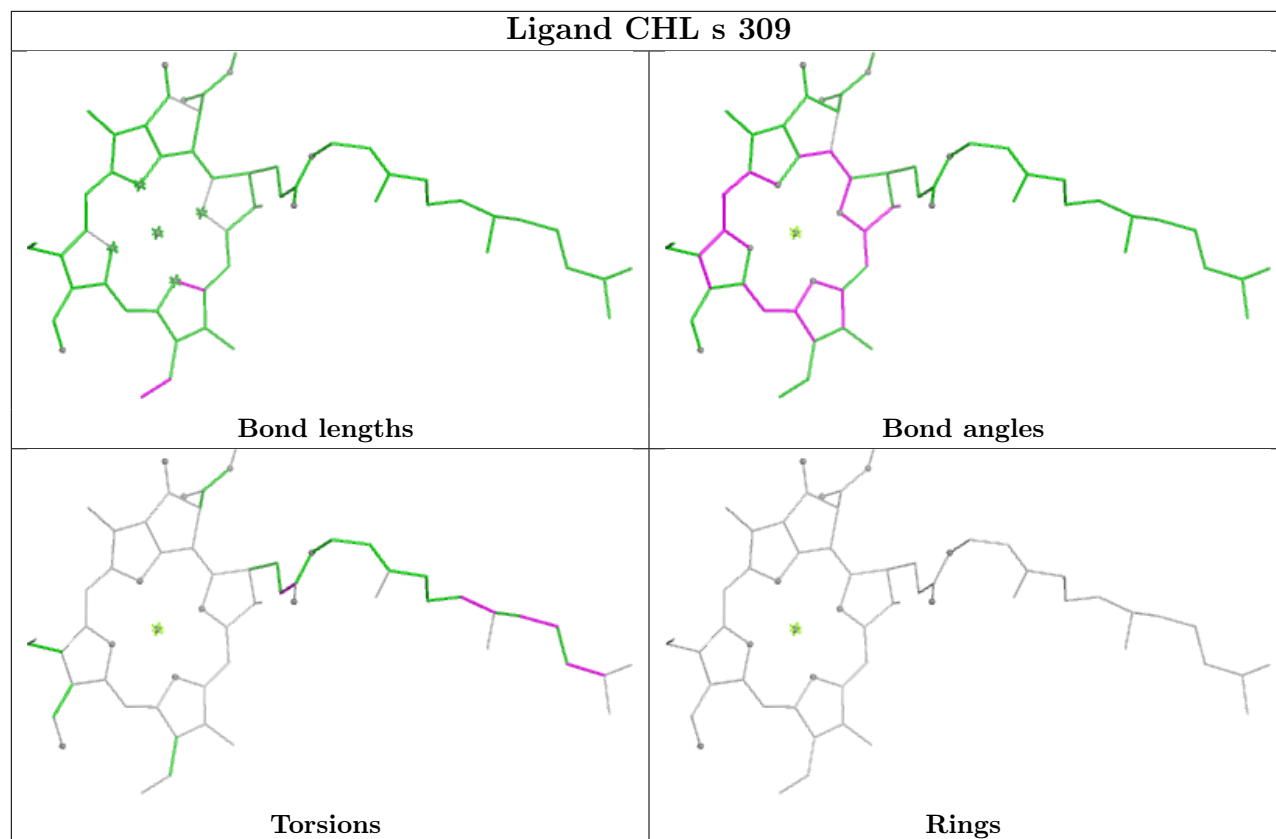


Torsions

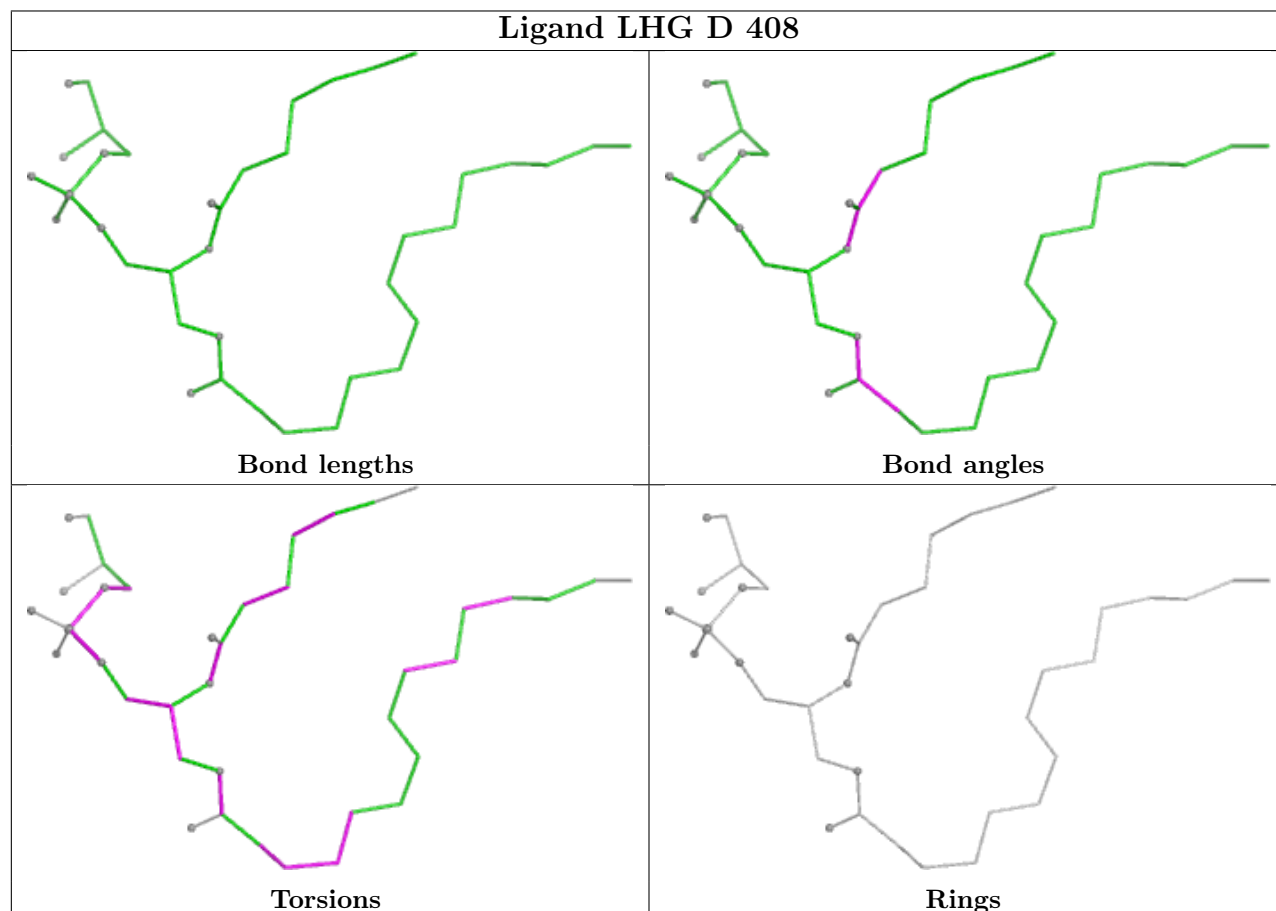


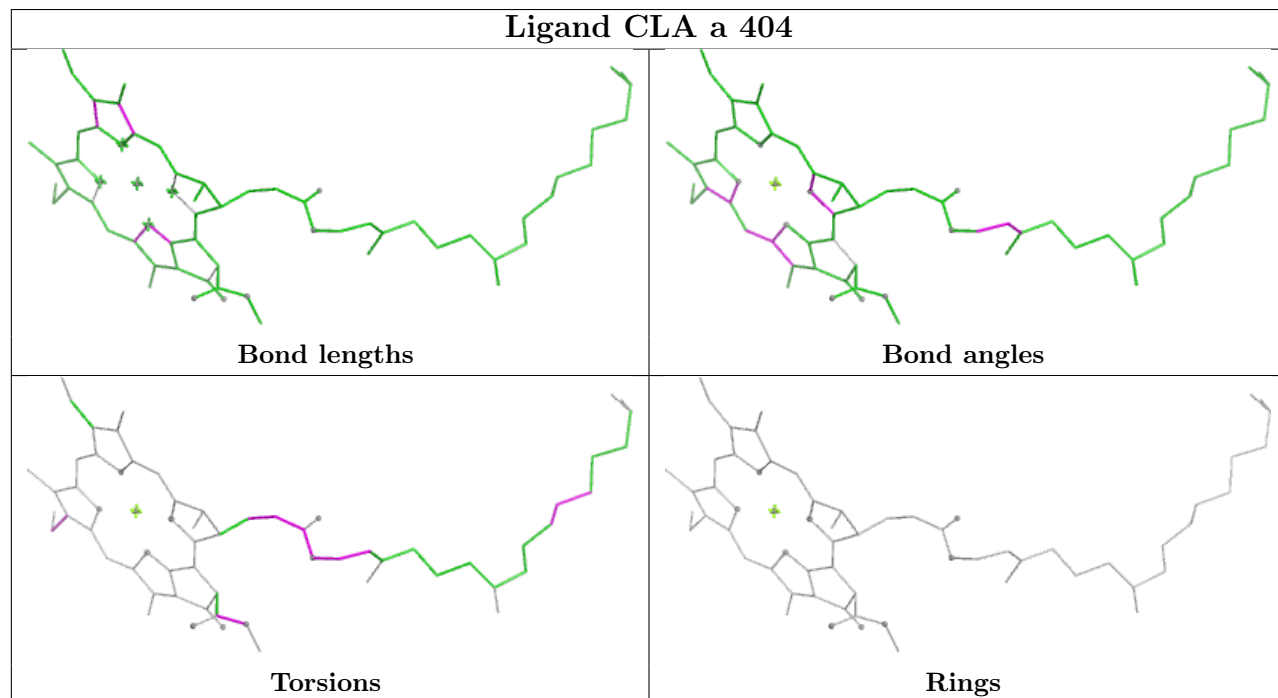
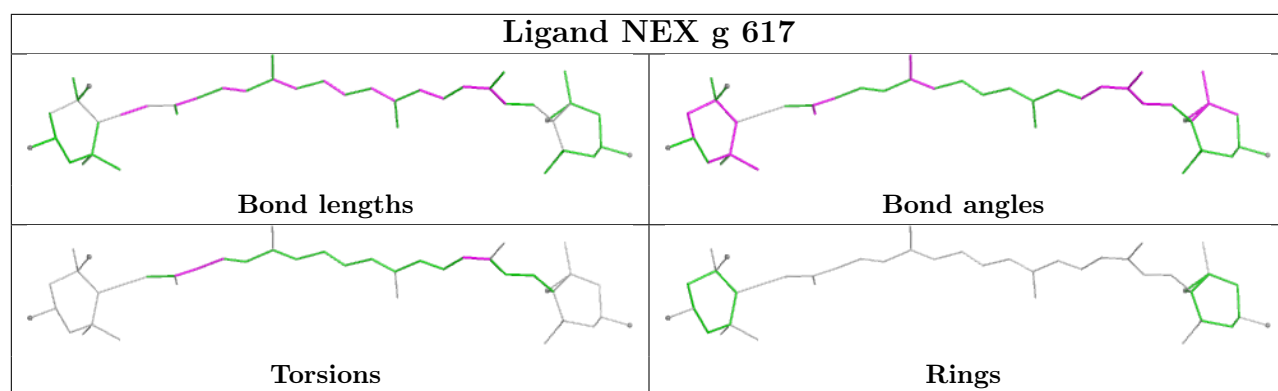
Rings

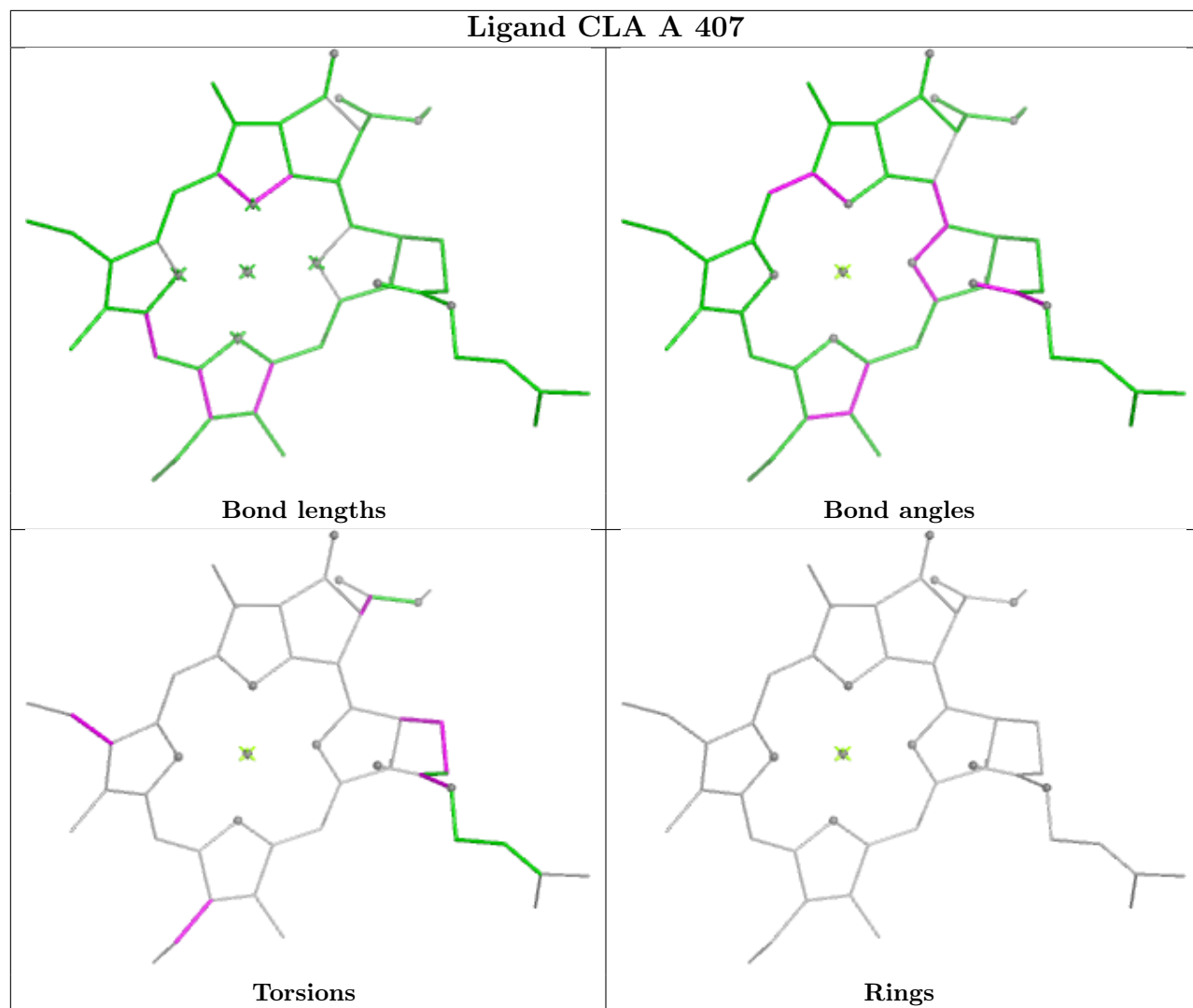
Ligand CHL s 309

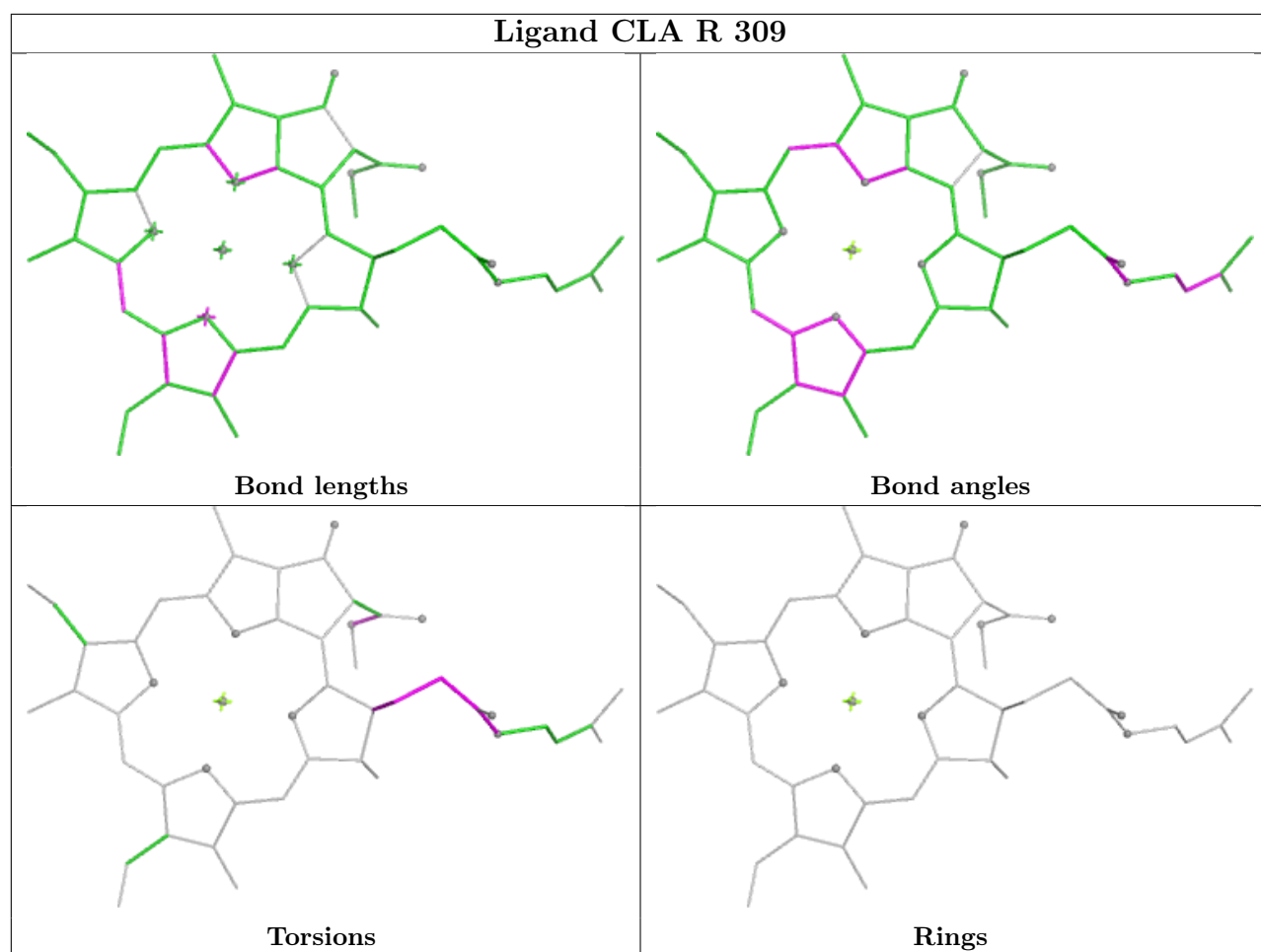


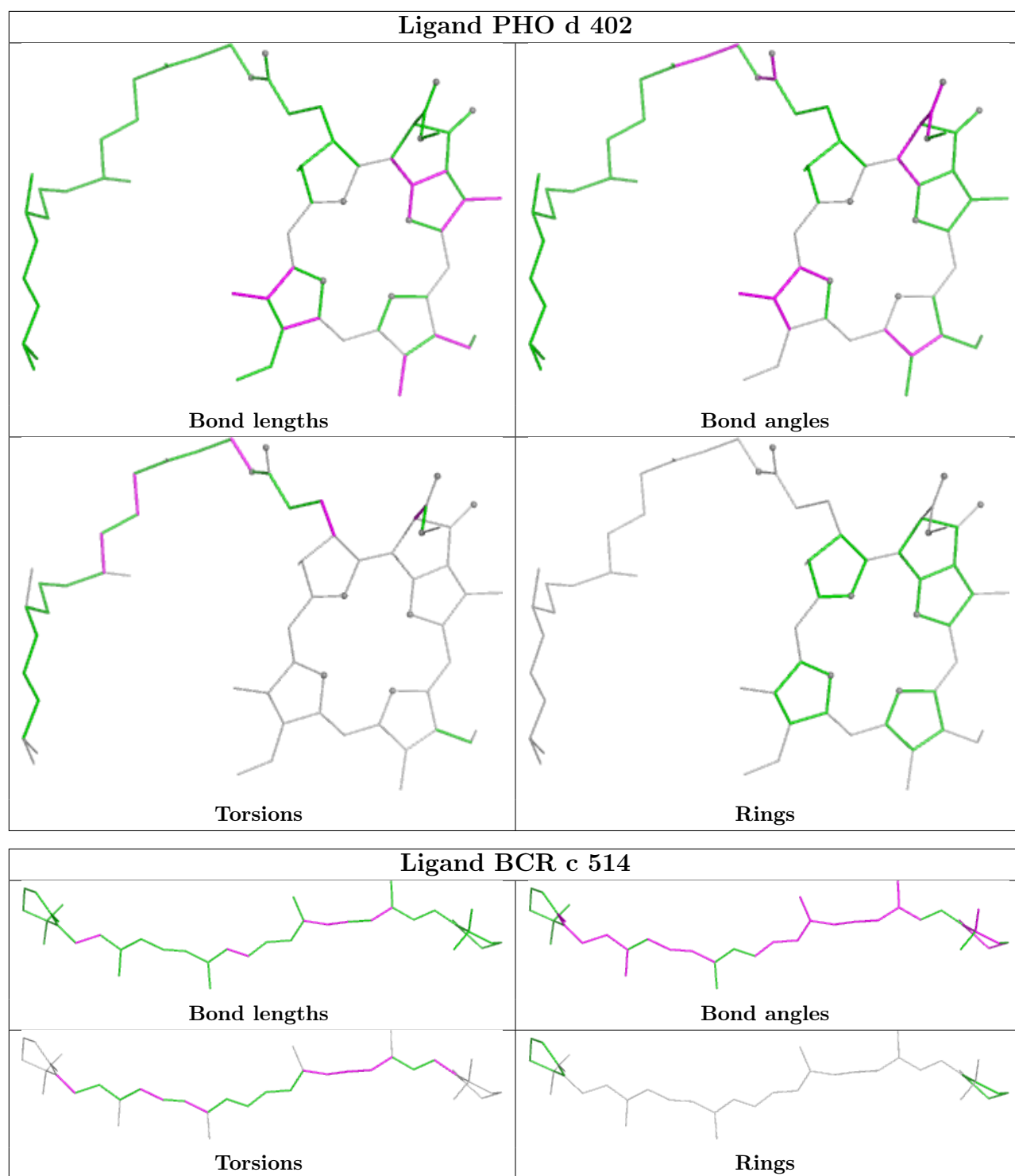
Ligand LHG D 408

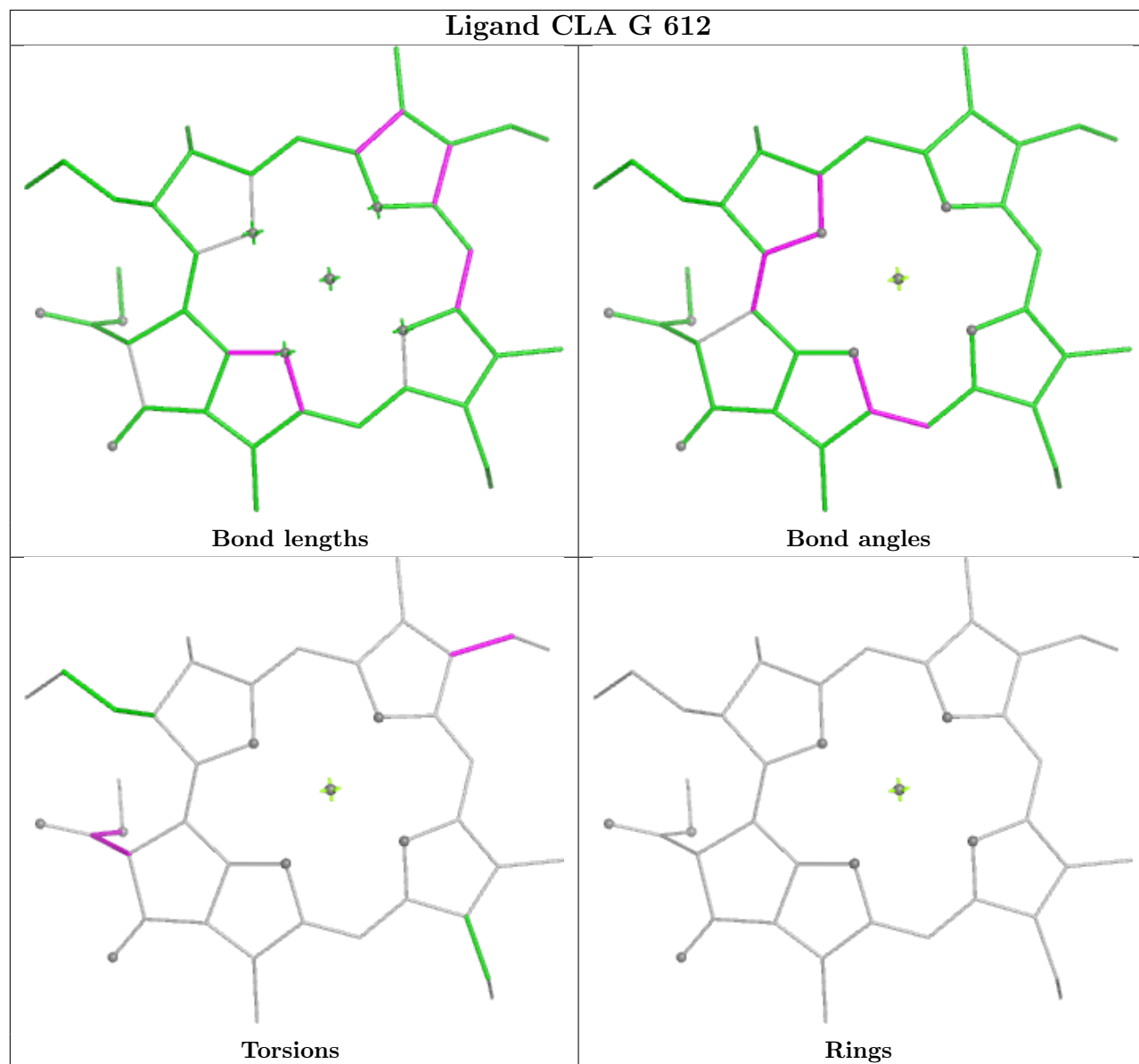


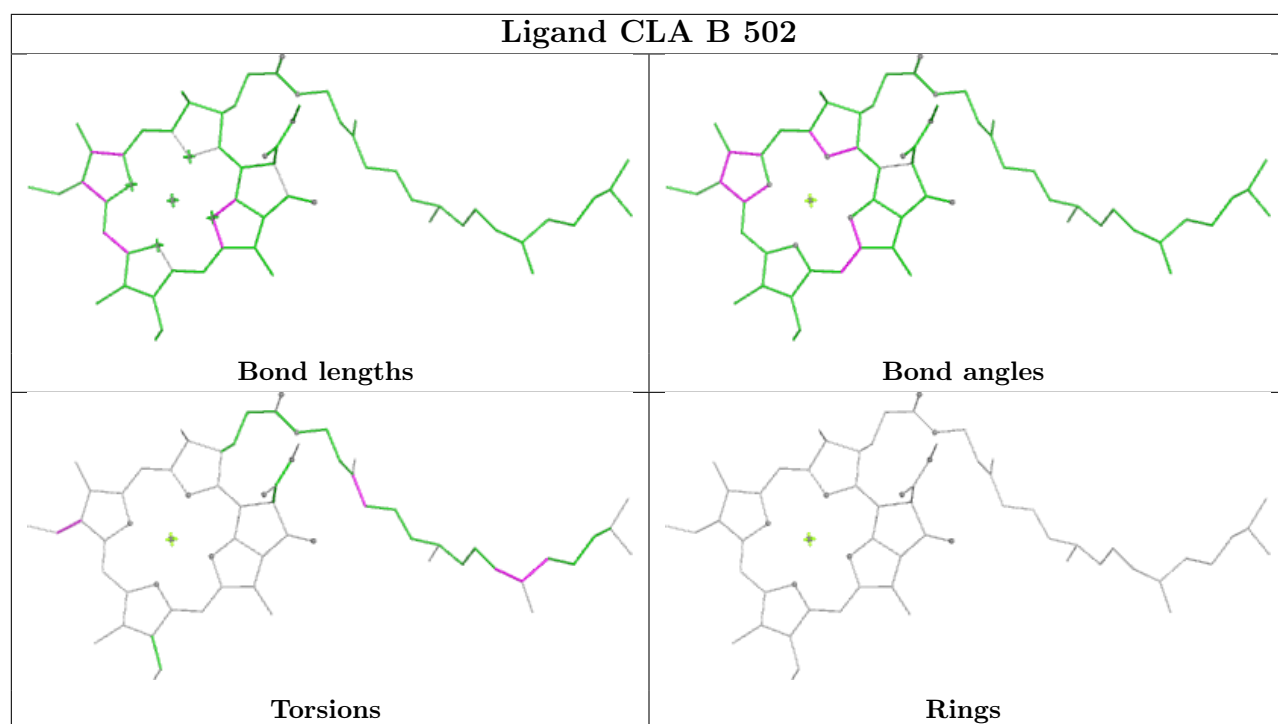


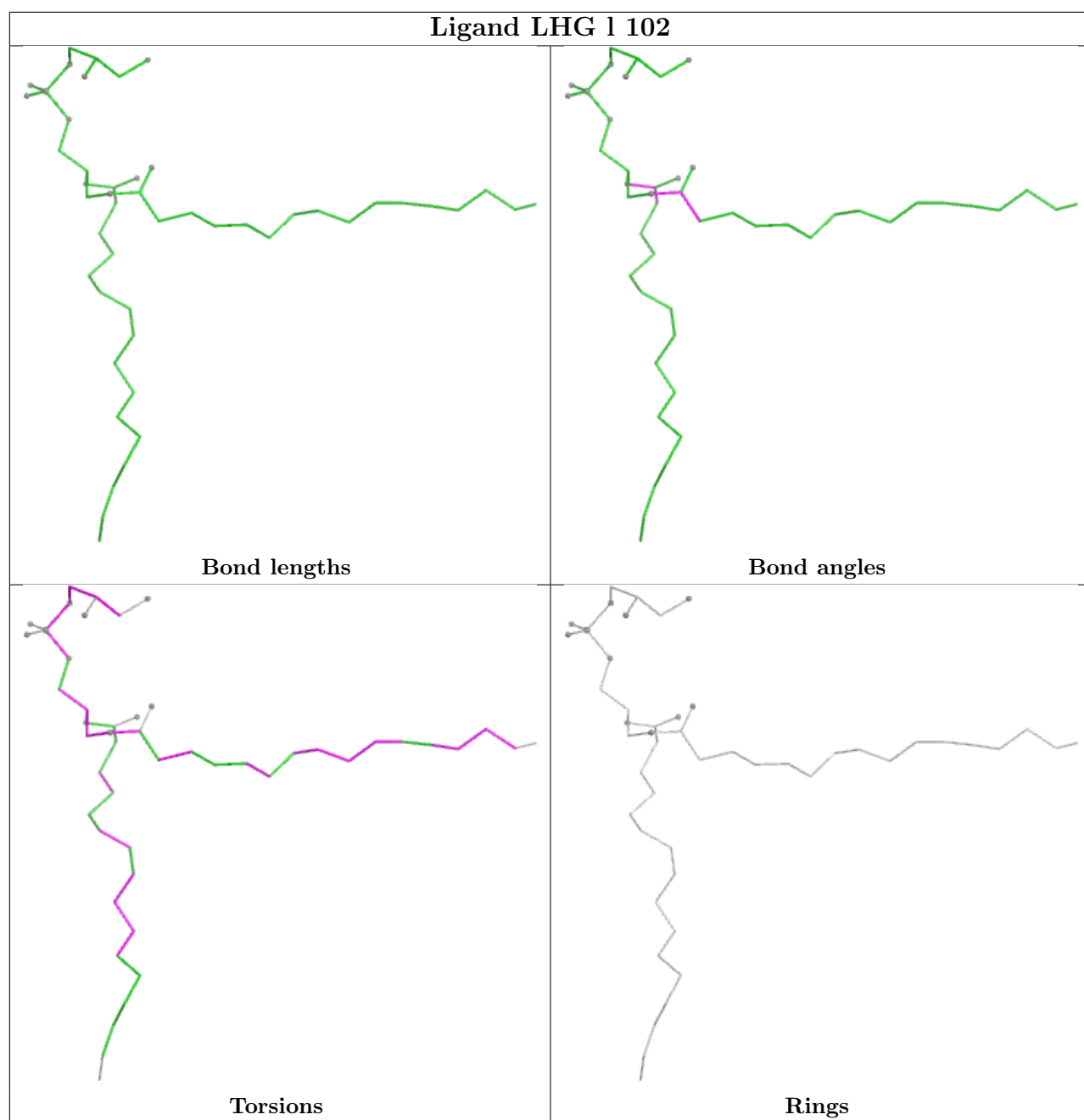


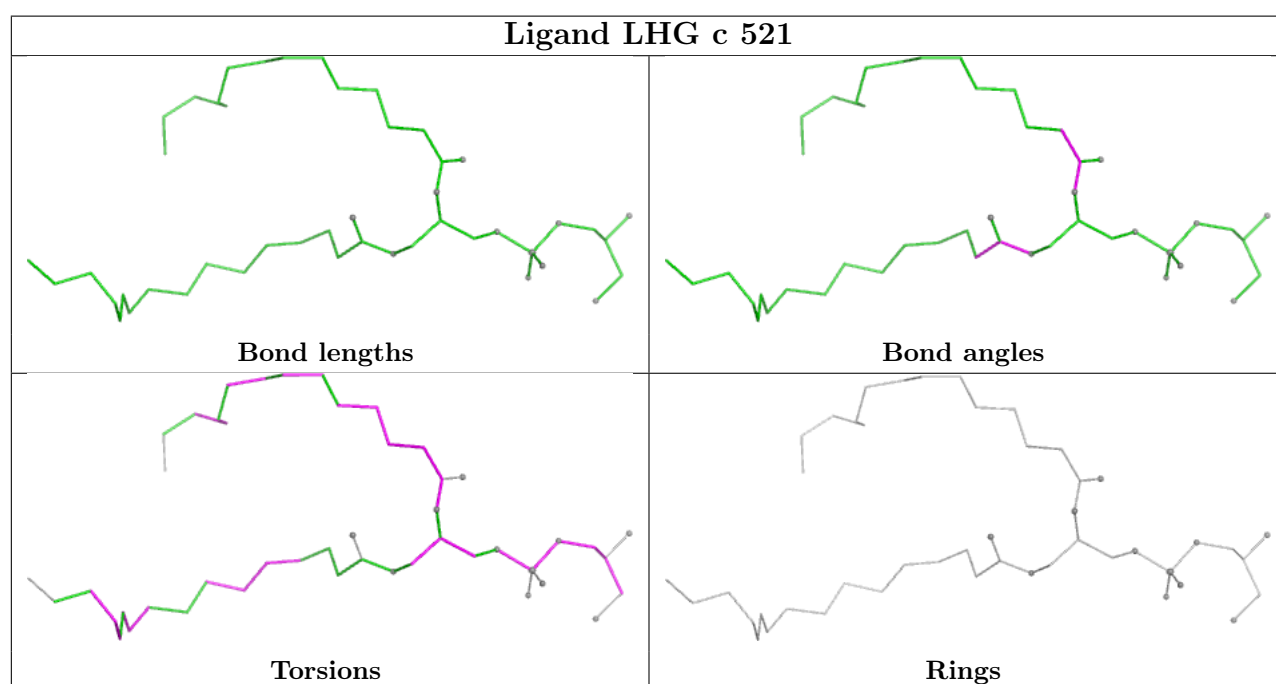
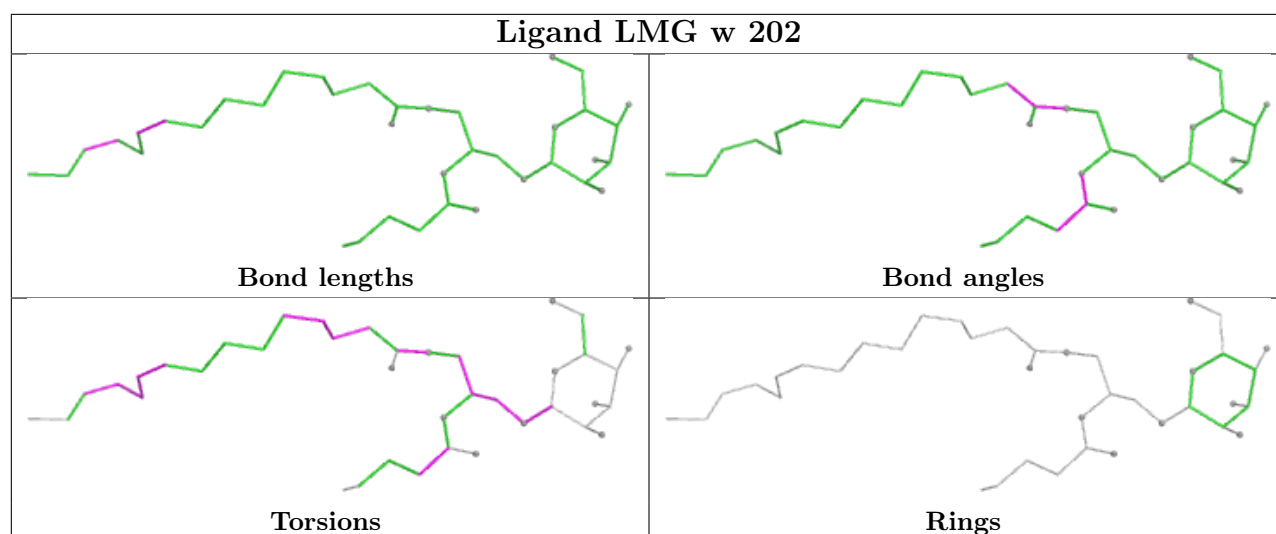


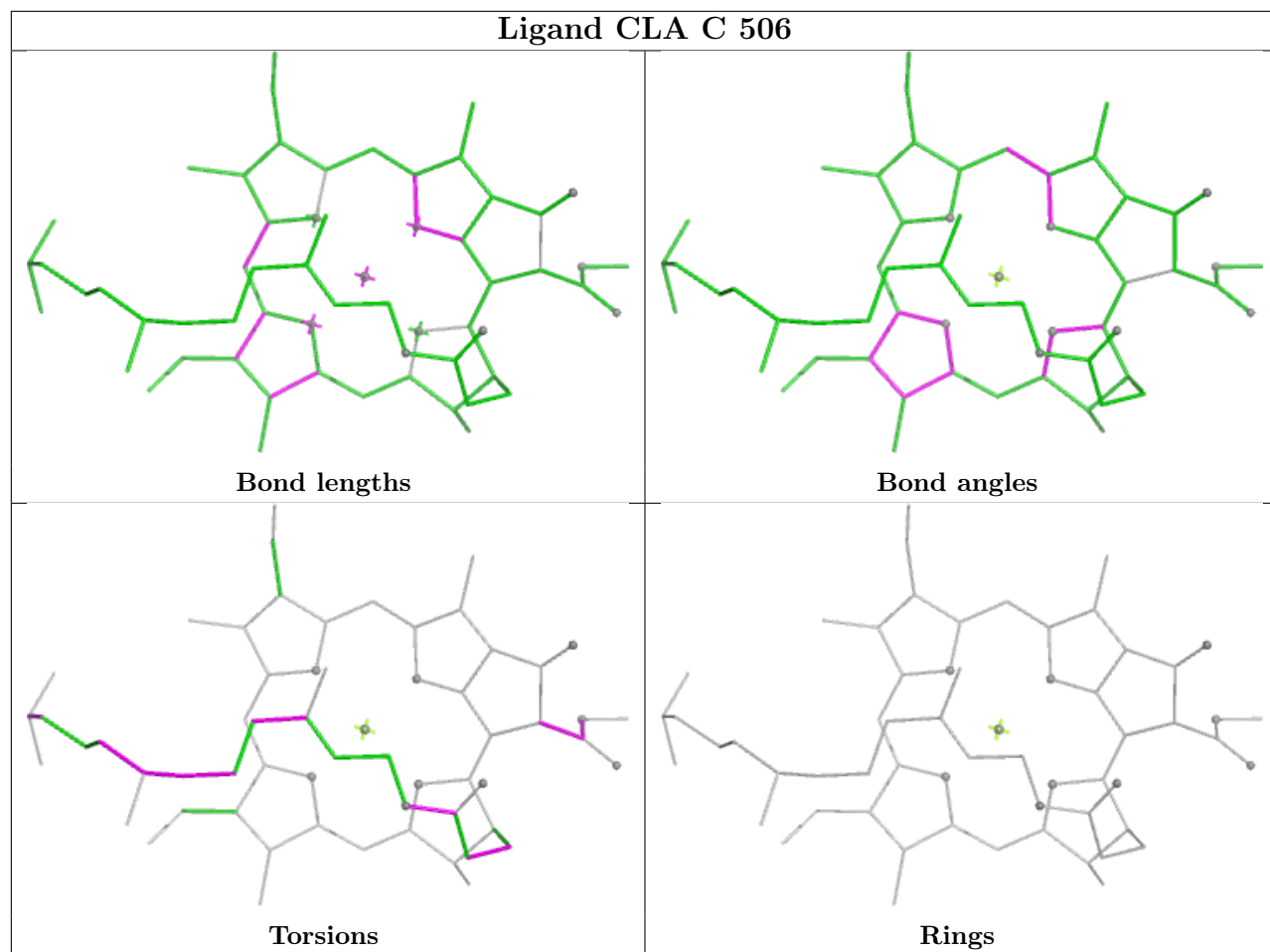




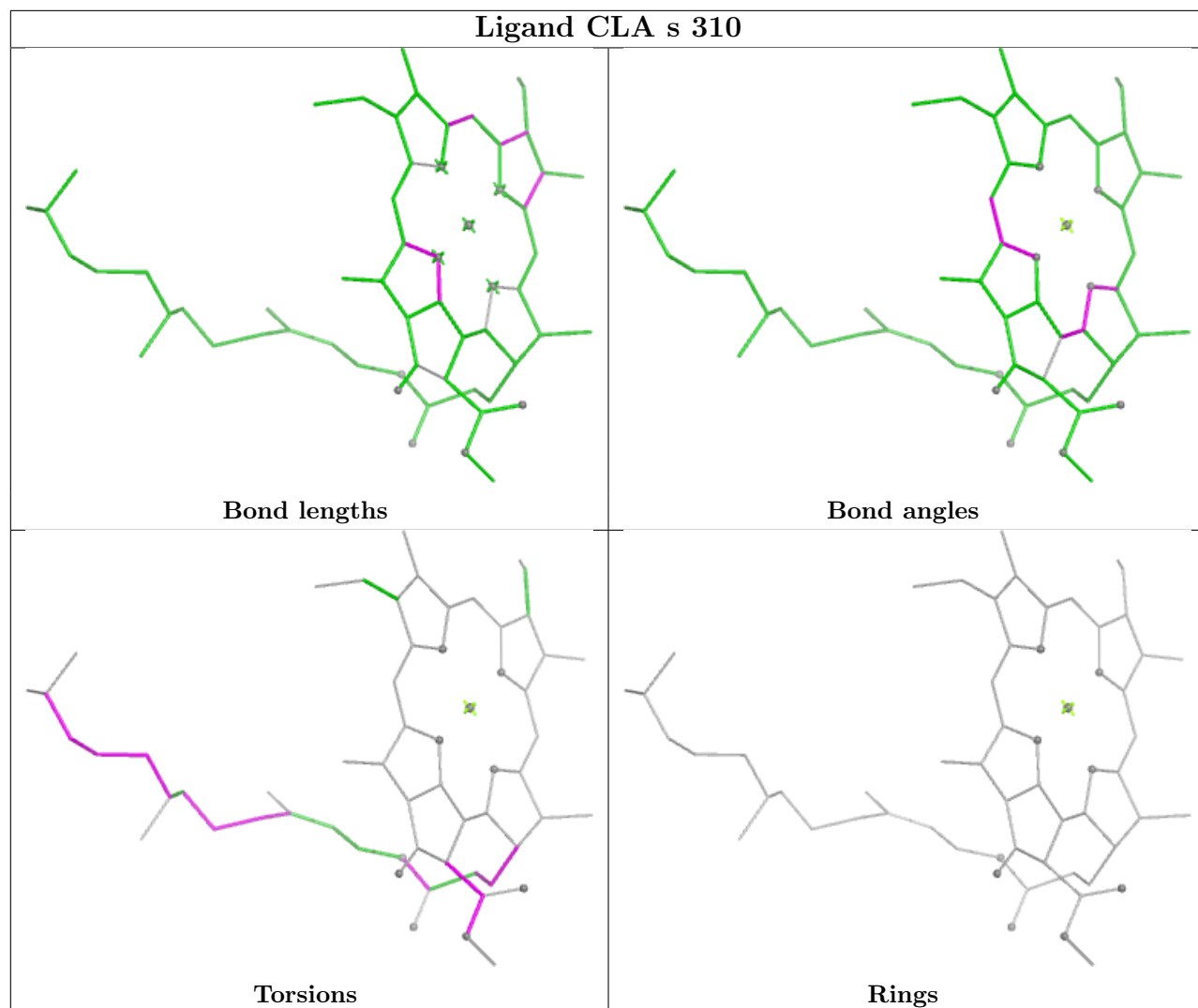


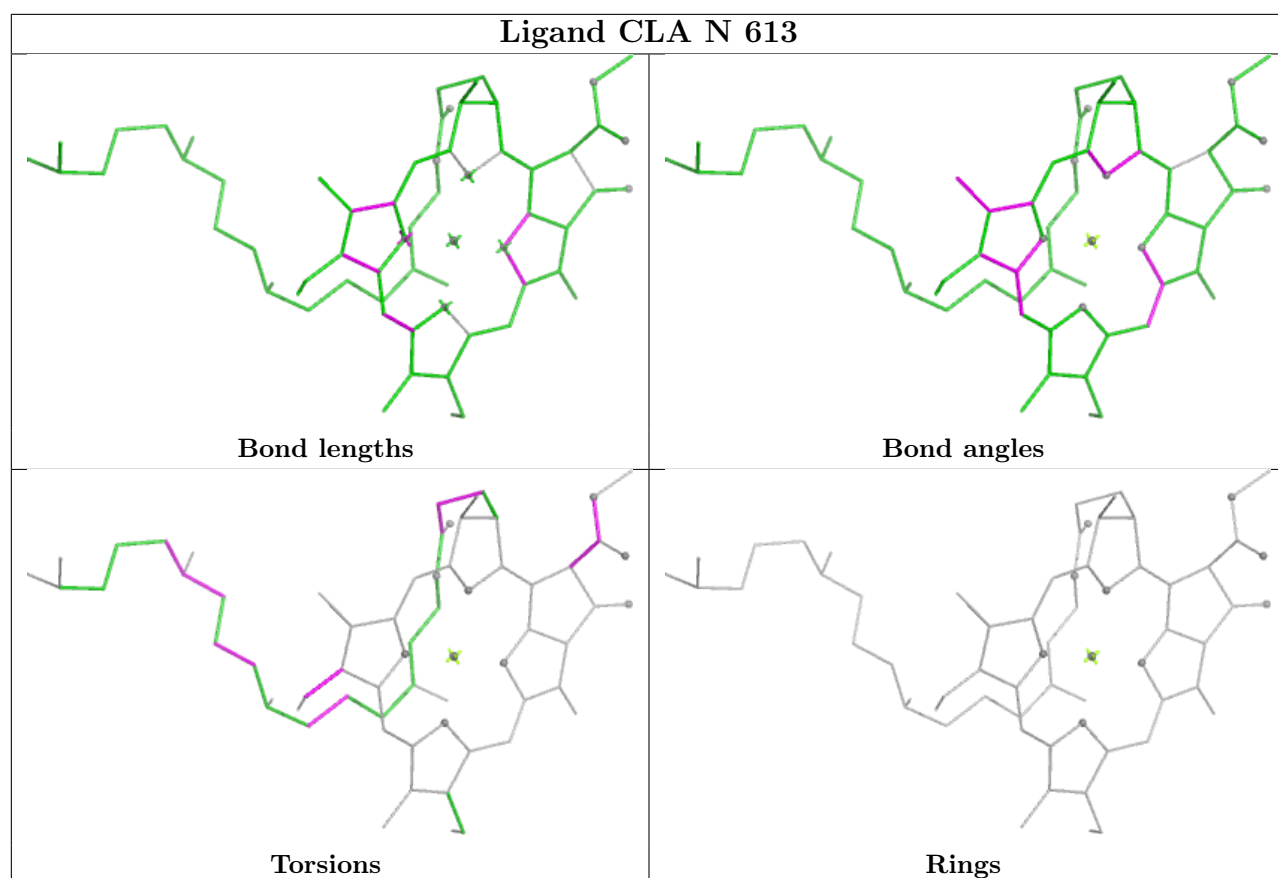




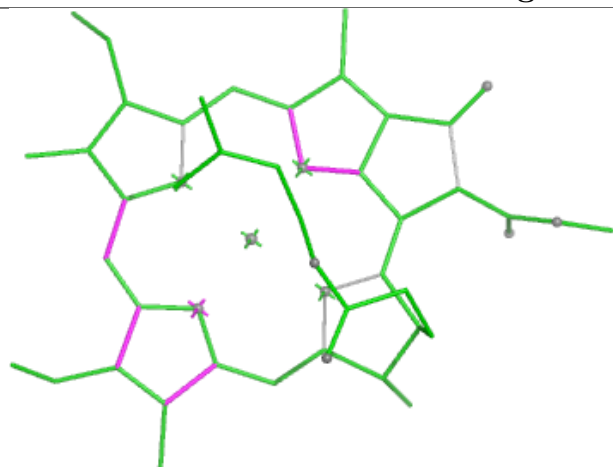


Ligand CLA s 310

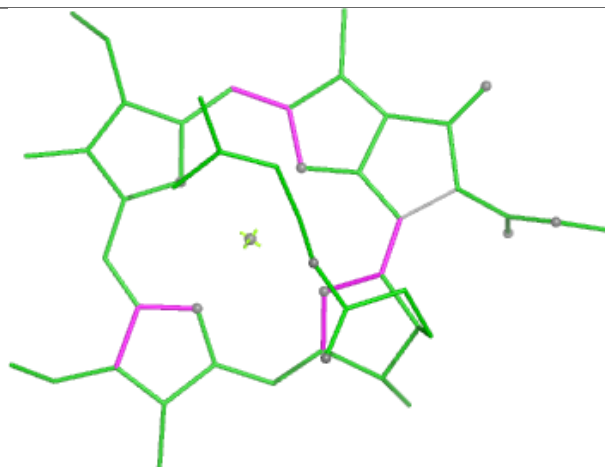




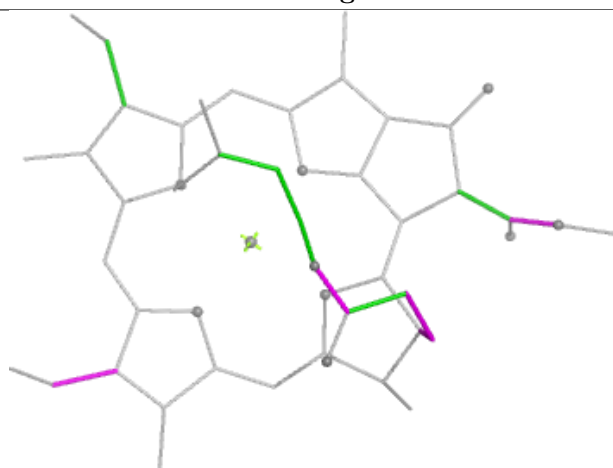
Ligand CLA S 306



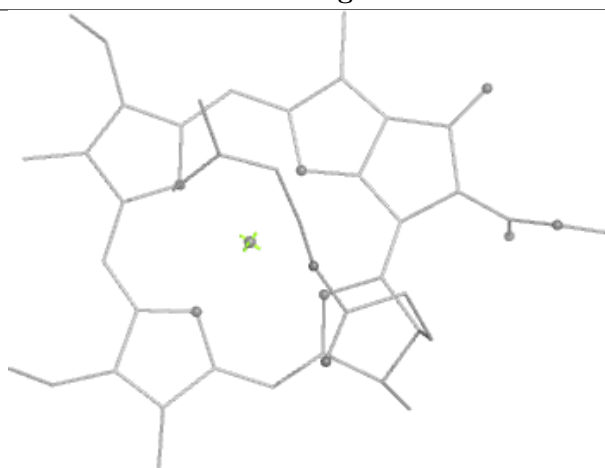
Bond lengths



Bond angles

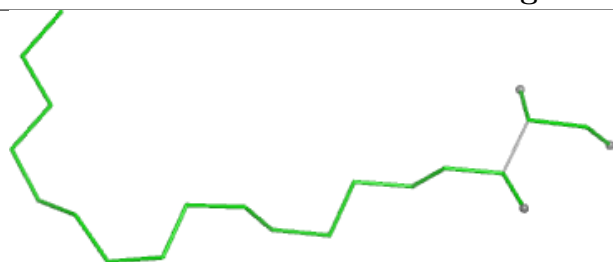


Torsions

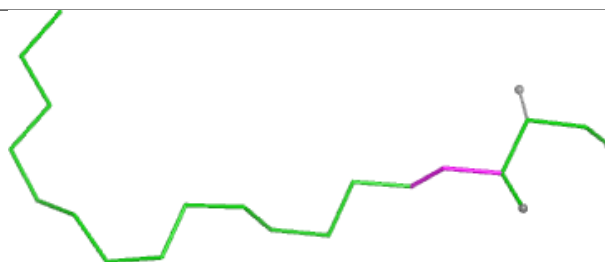


Rings

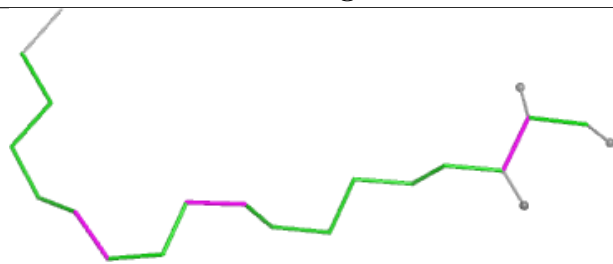
Ligand SPH c 523



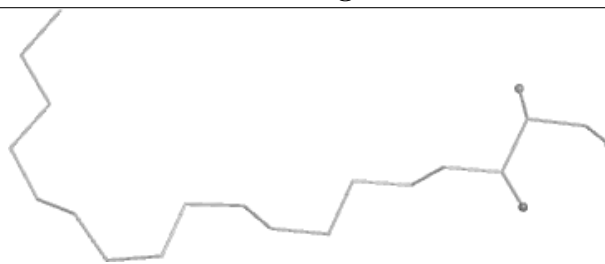
Bond lengths



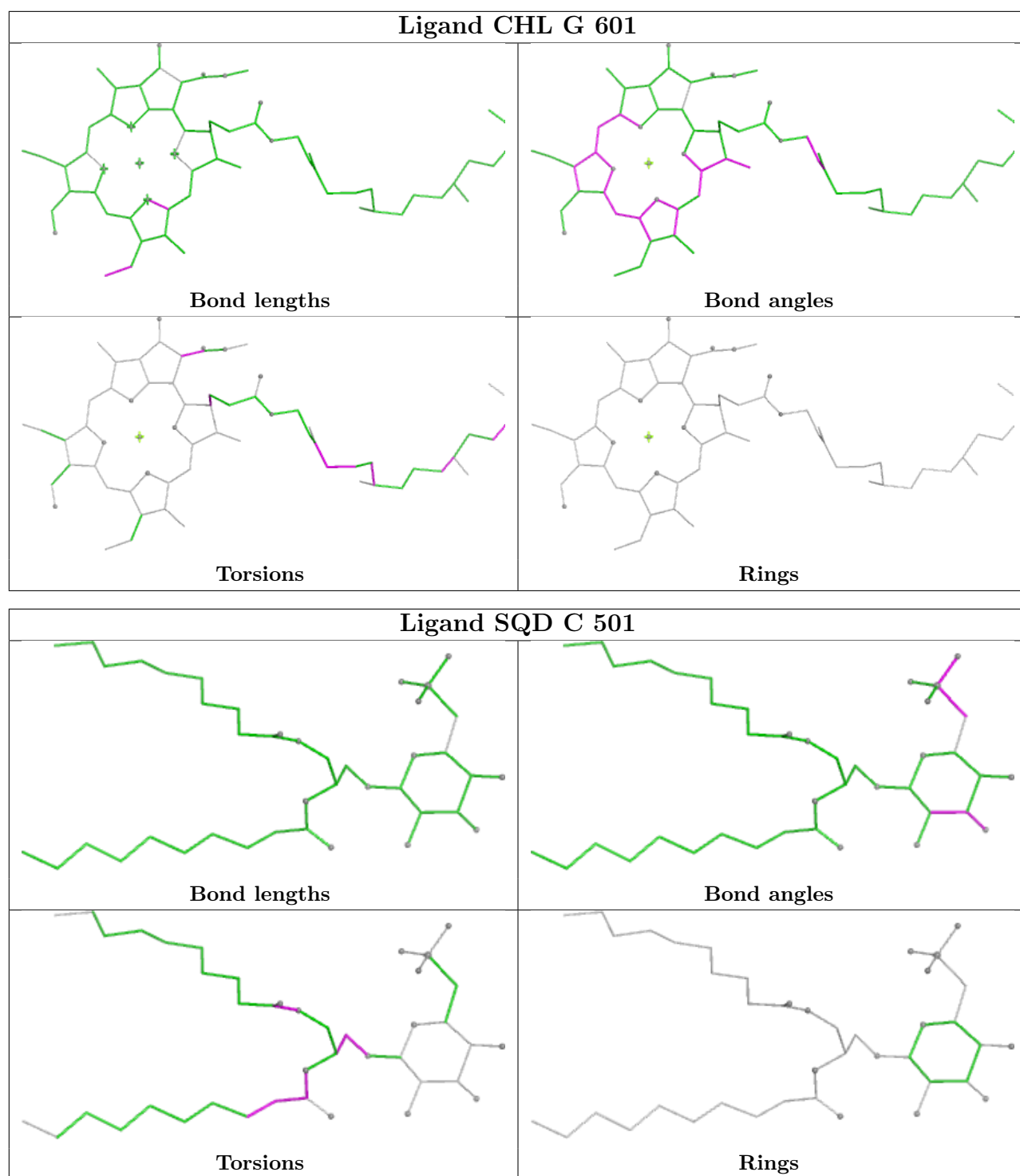
Bond angles

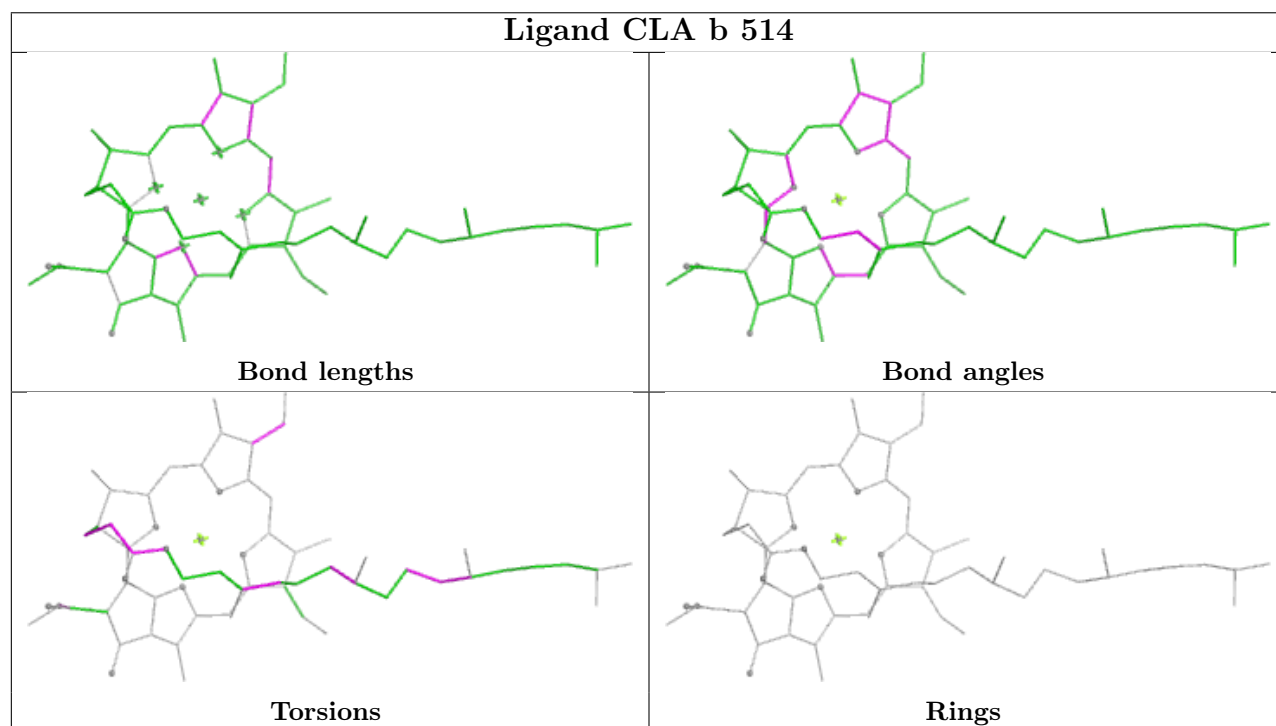
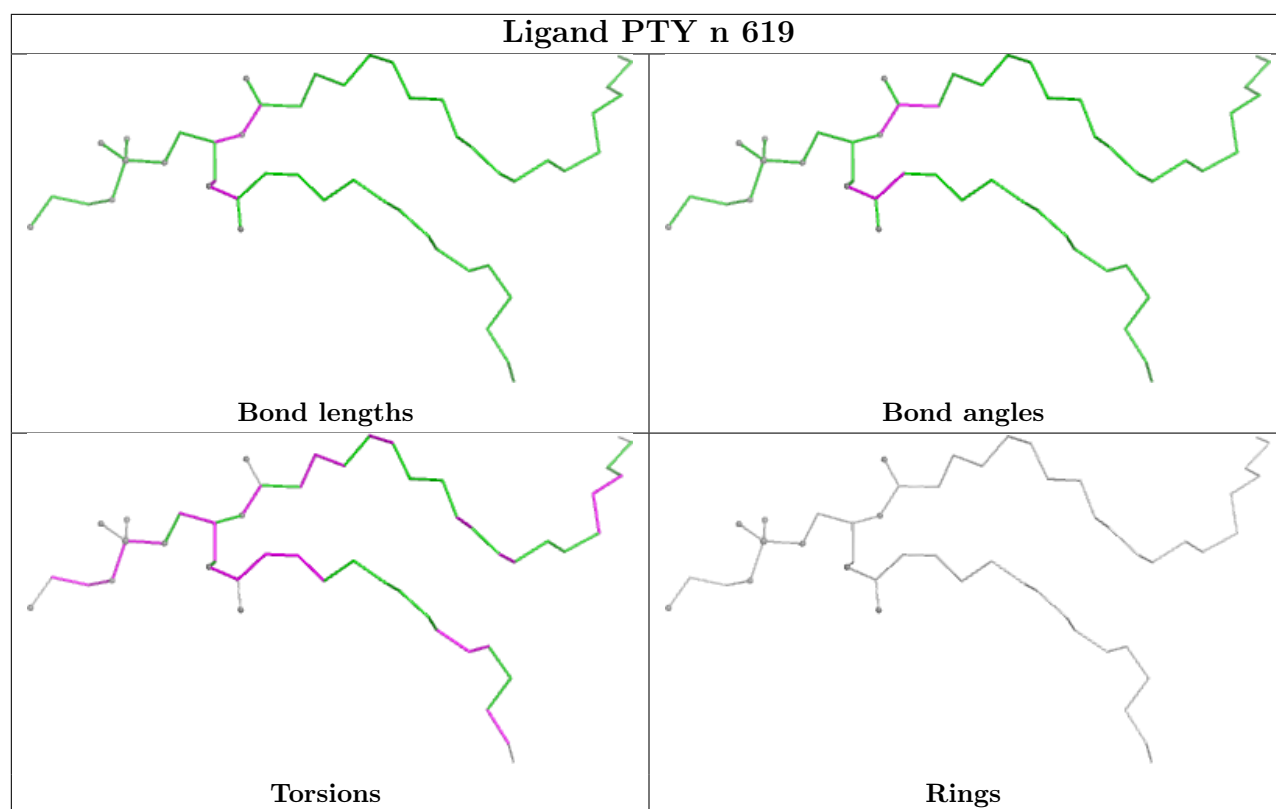


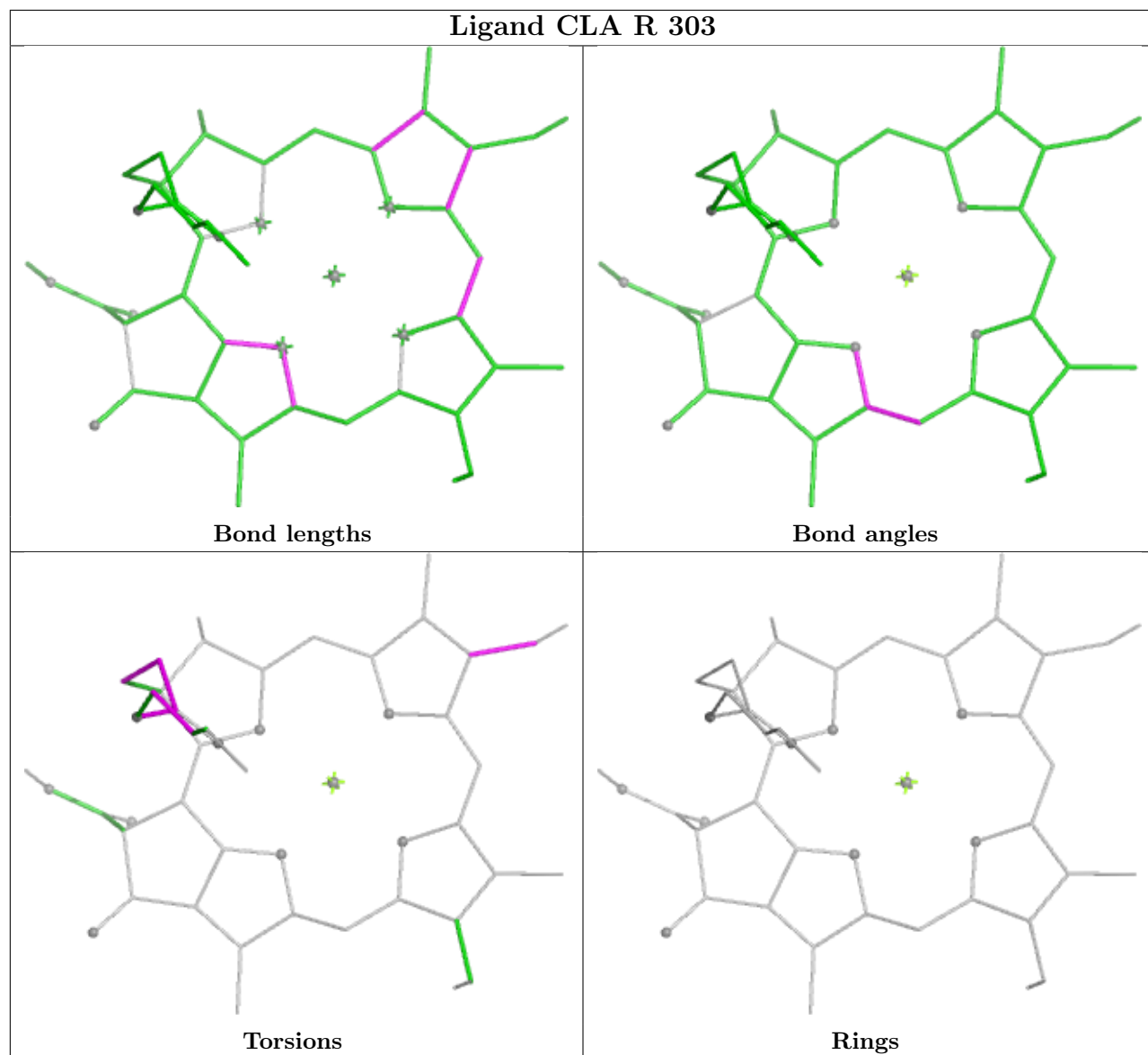
Torsions



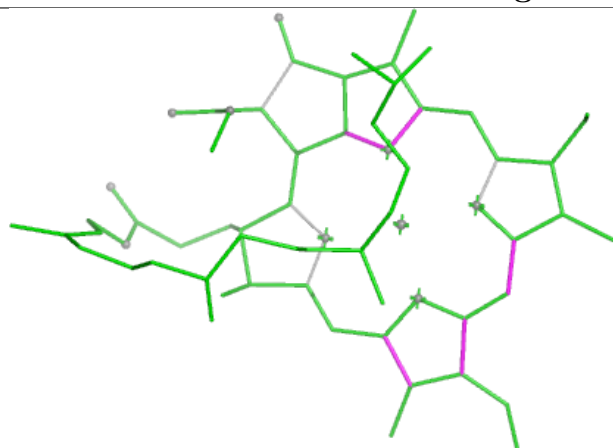
Rings



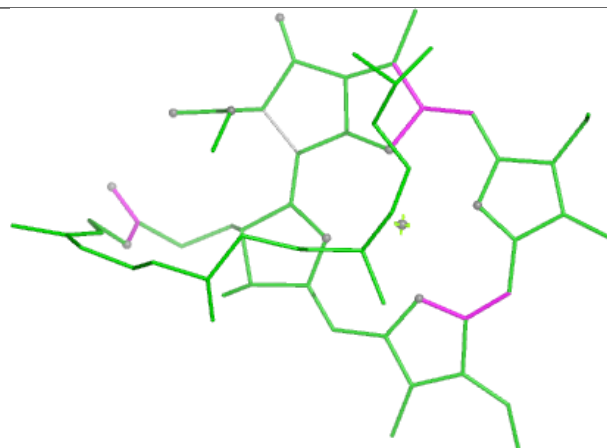




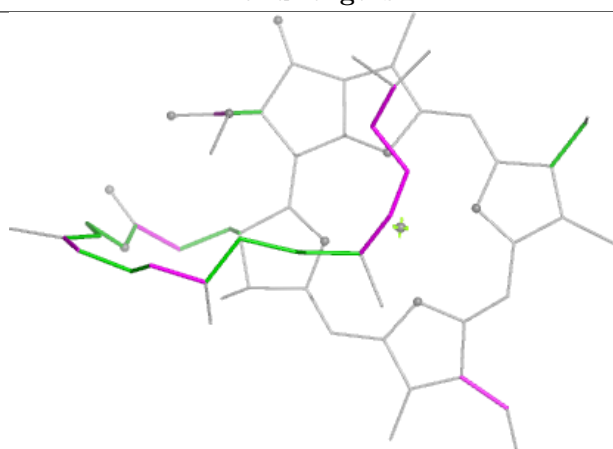
Ligand CLA C 511



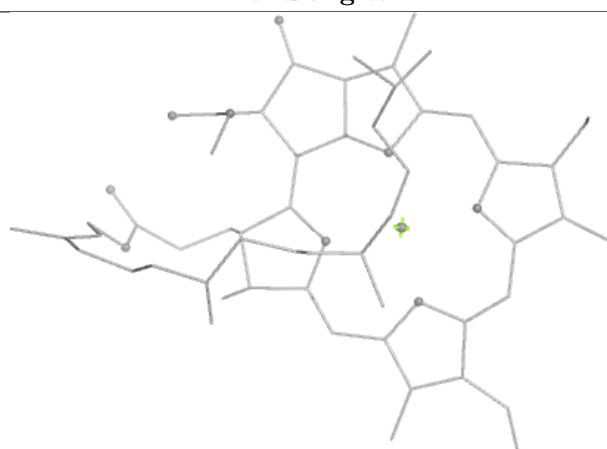
Bond lengths



Bond angles

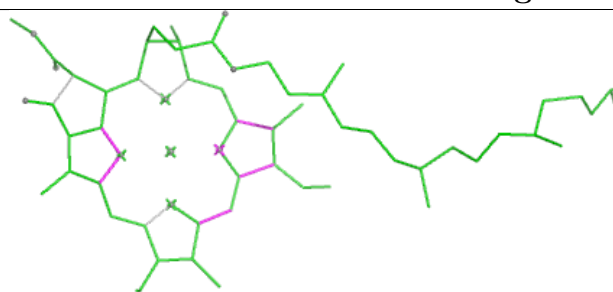


Torsions

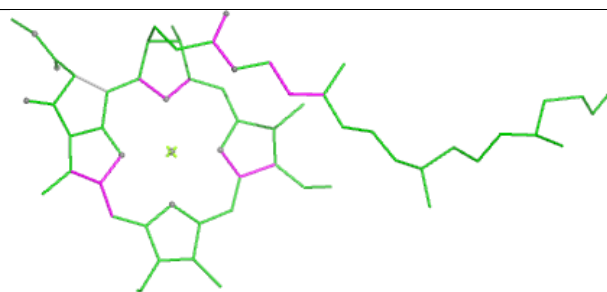


Rings

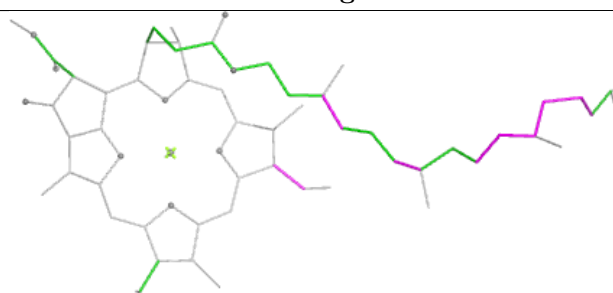
Ligand CLA B 503



Bond lengths



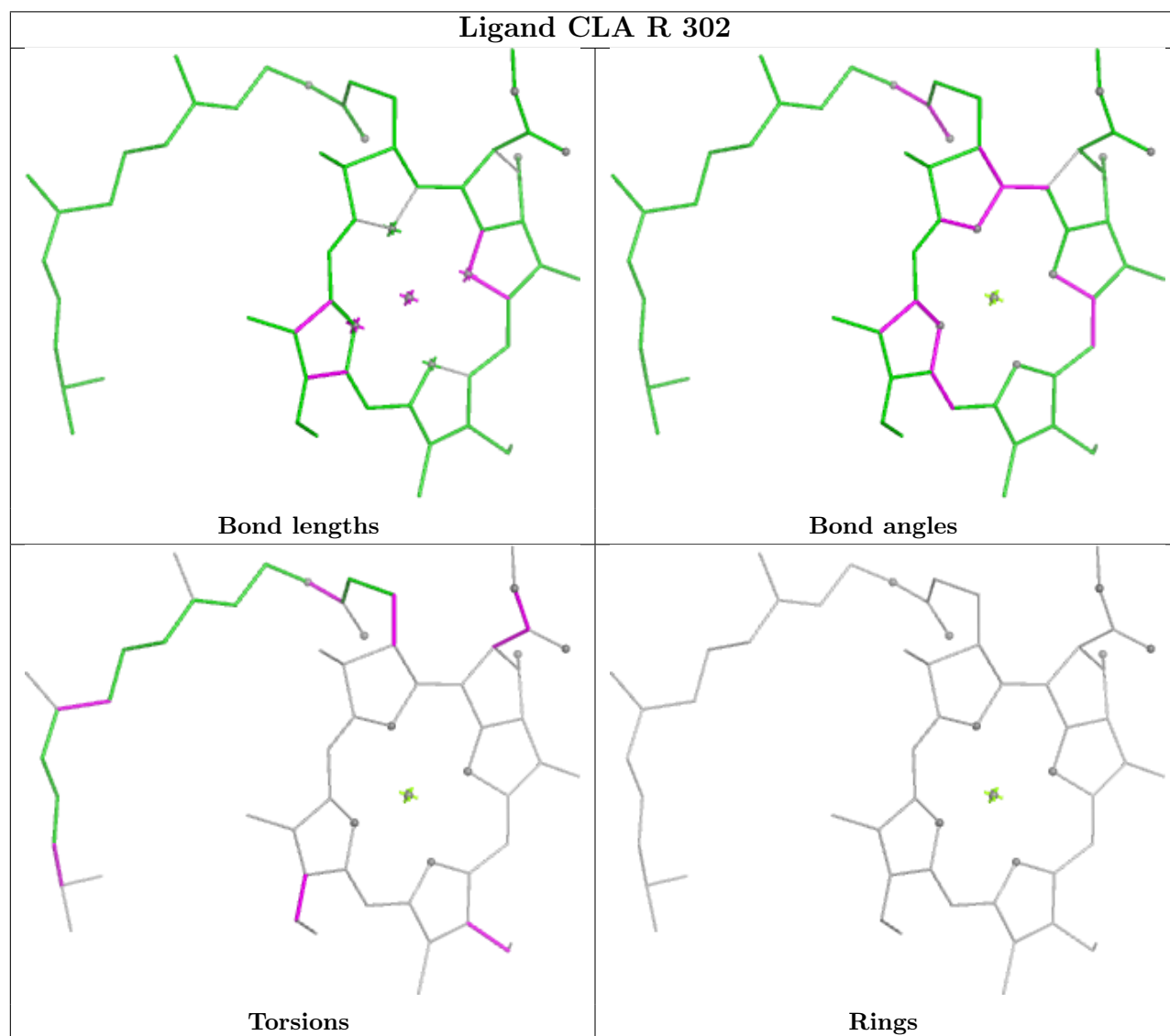
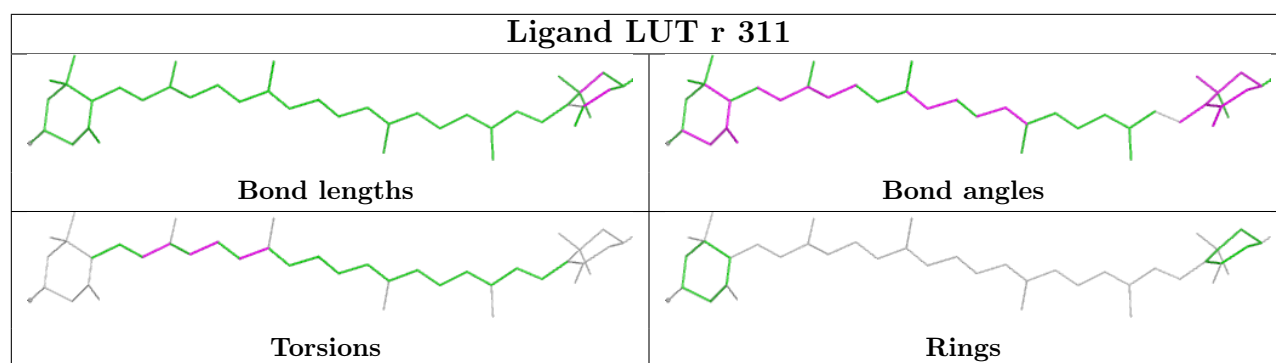
Bond angles

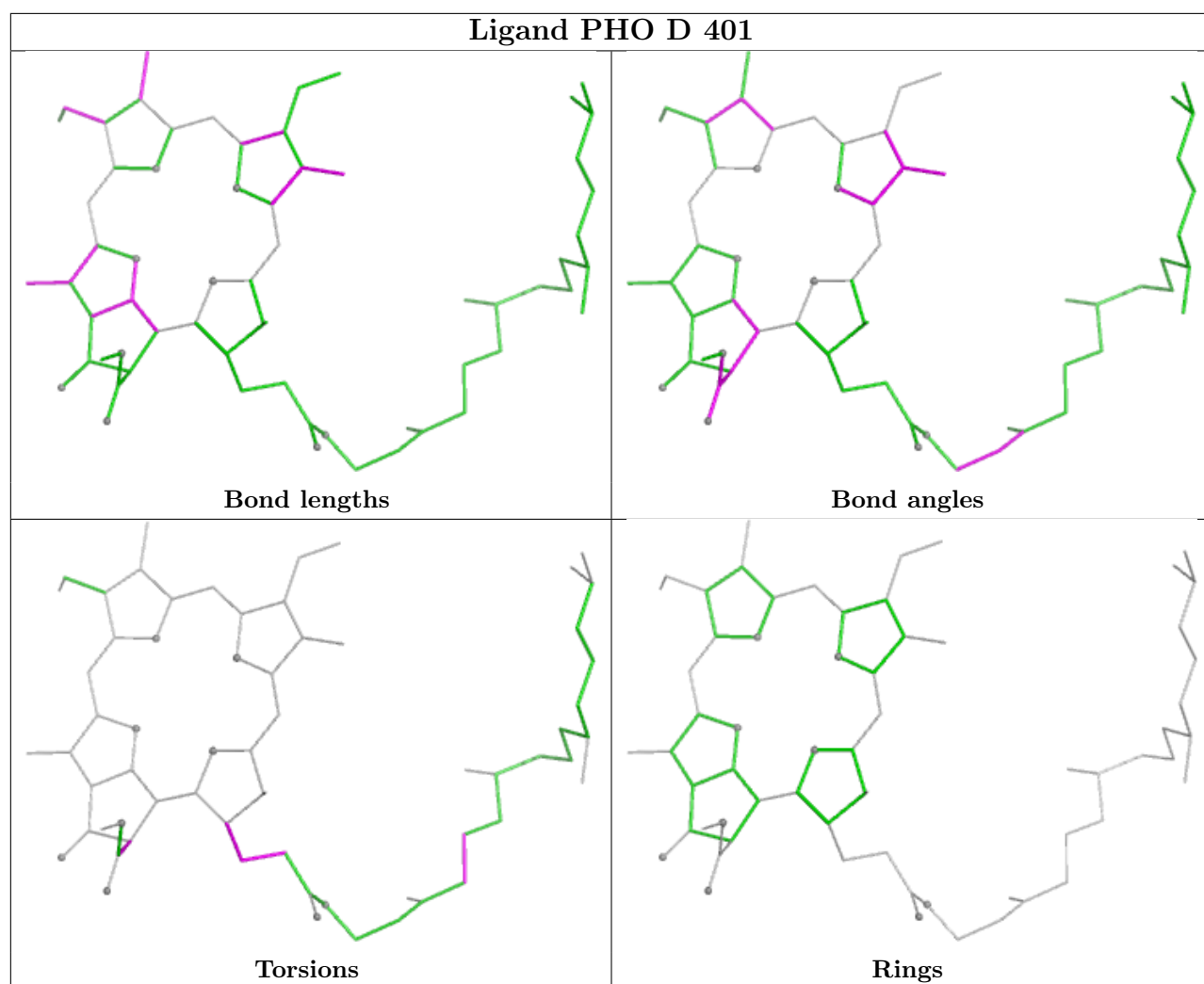


Torsions

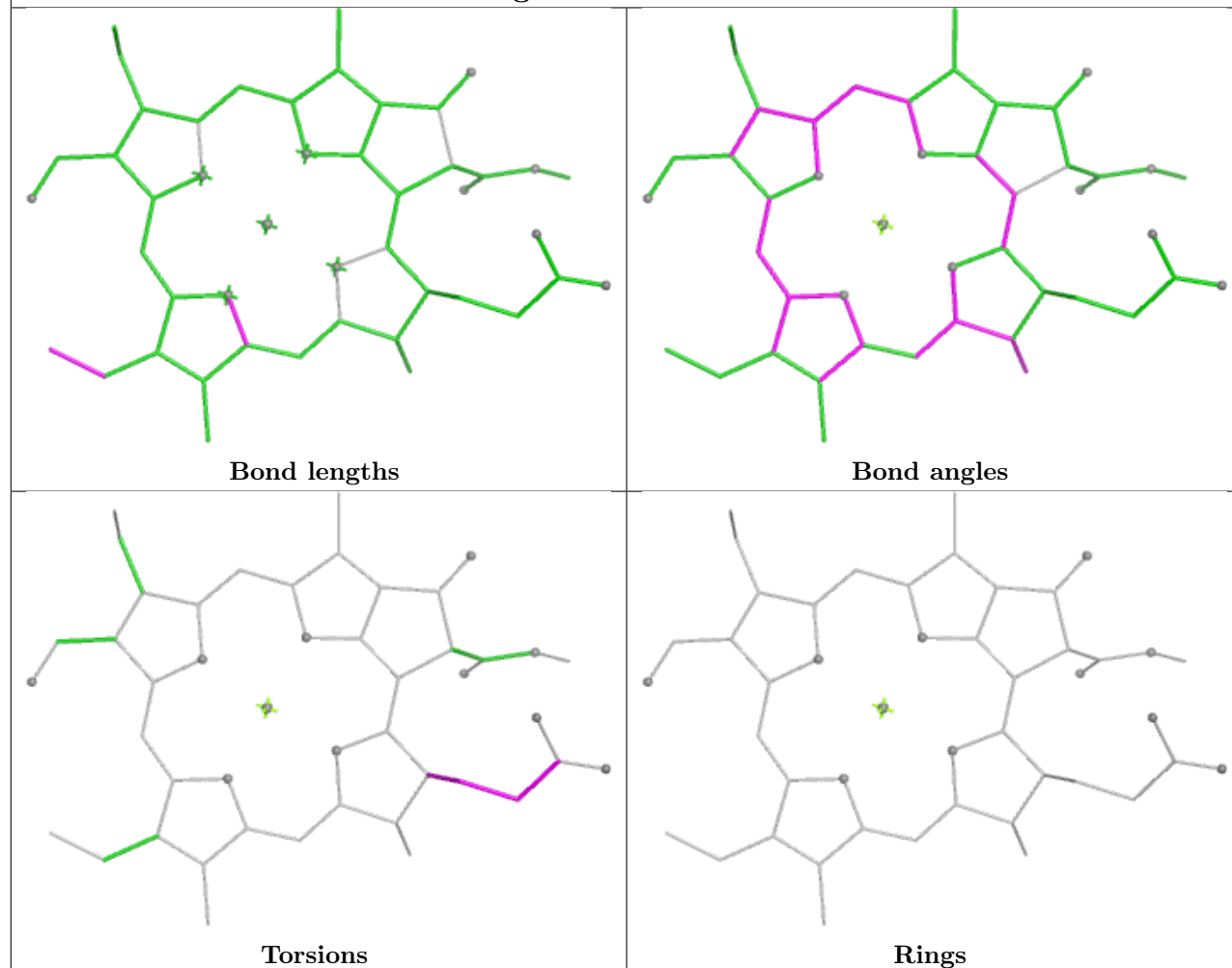


Rings

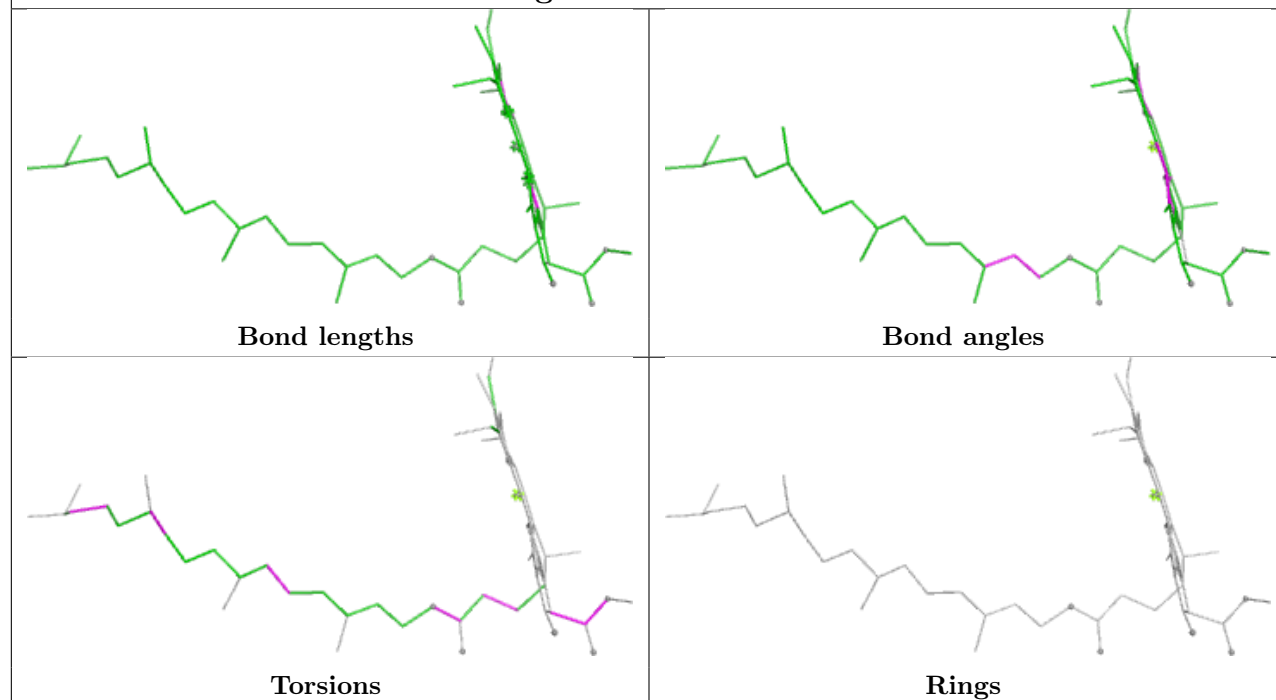


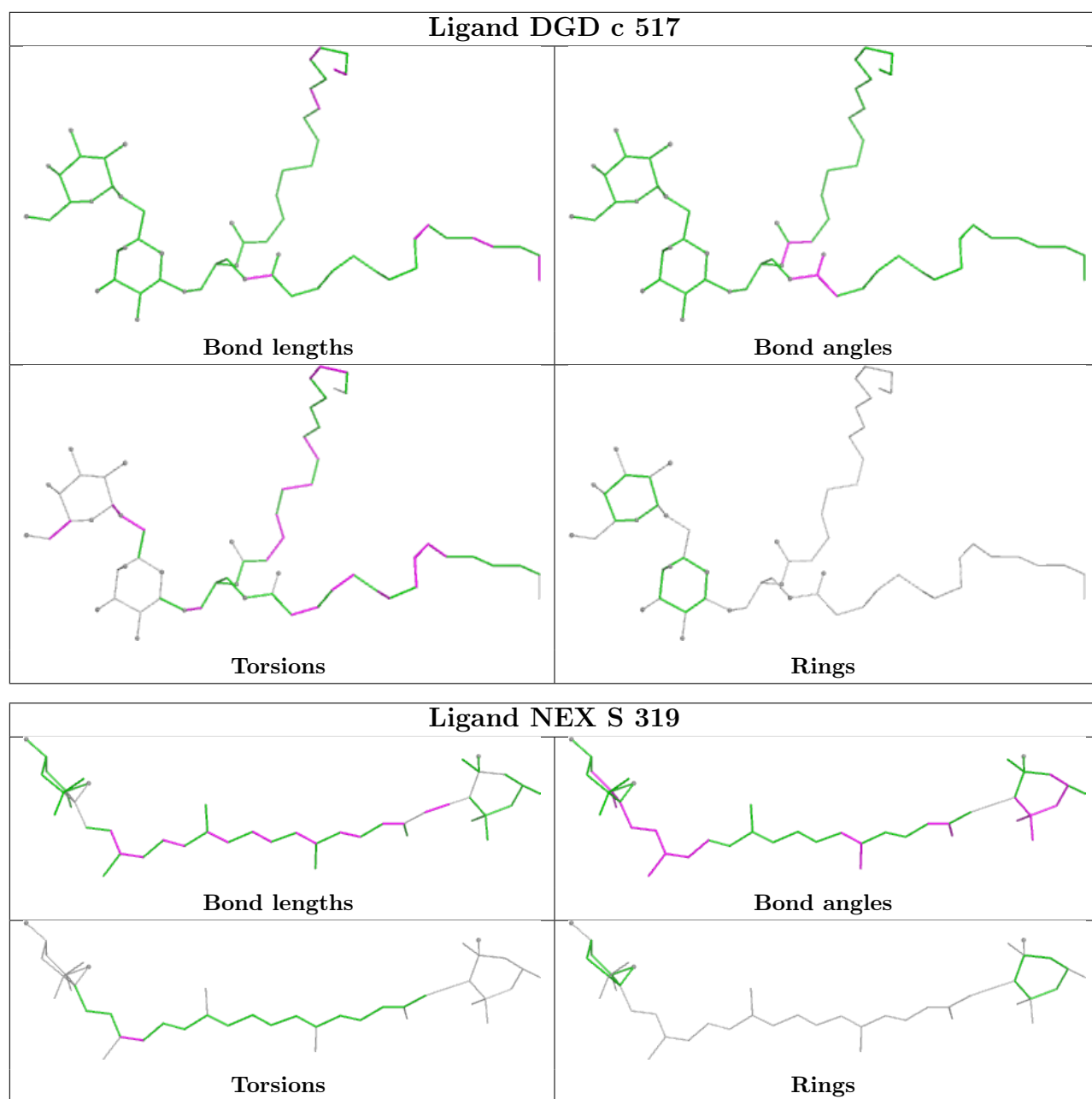


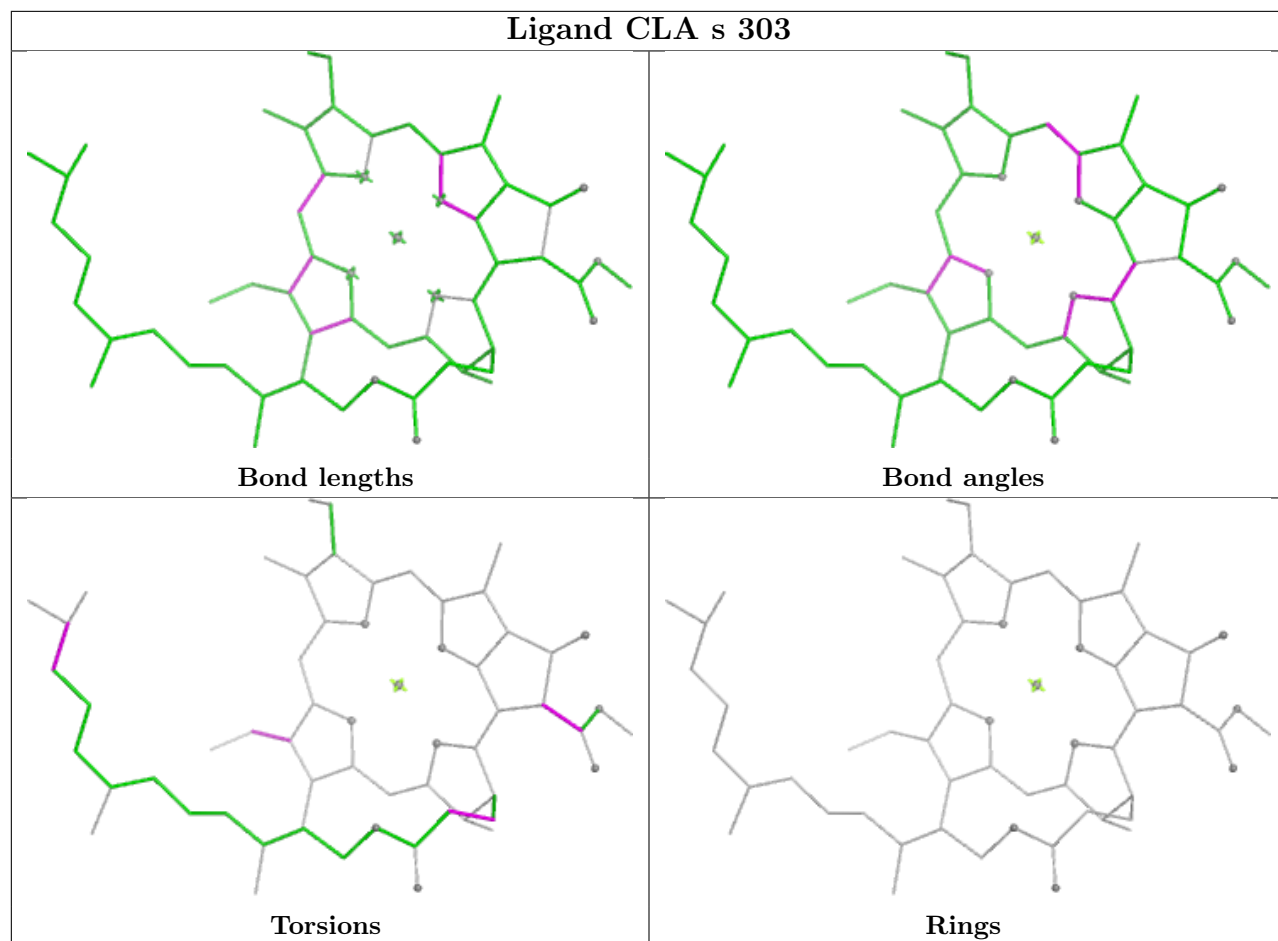
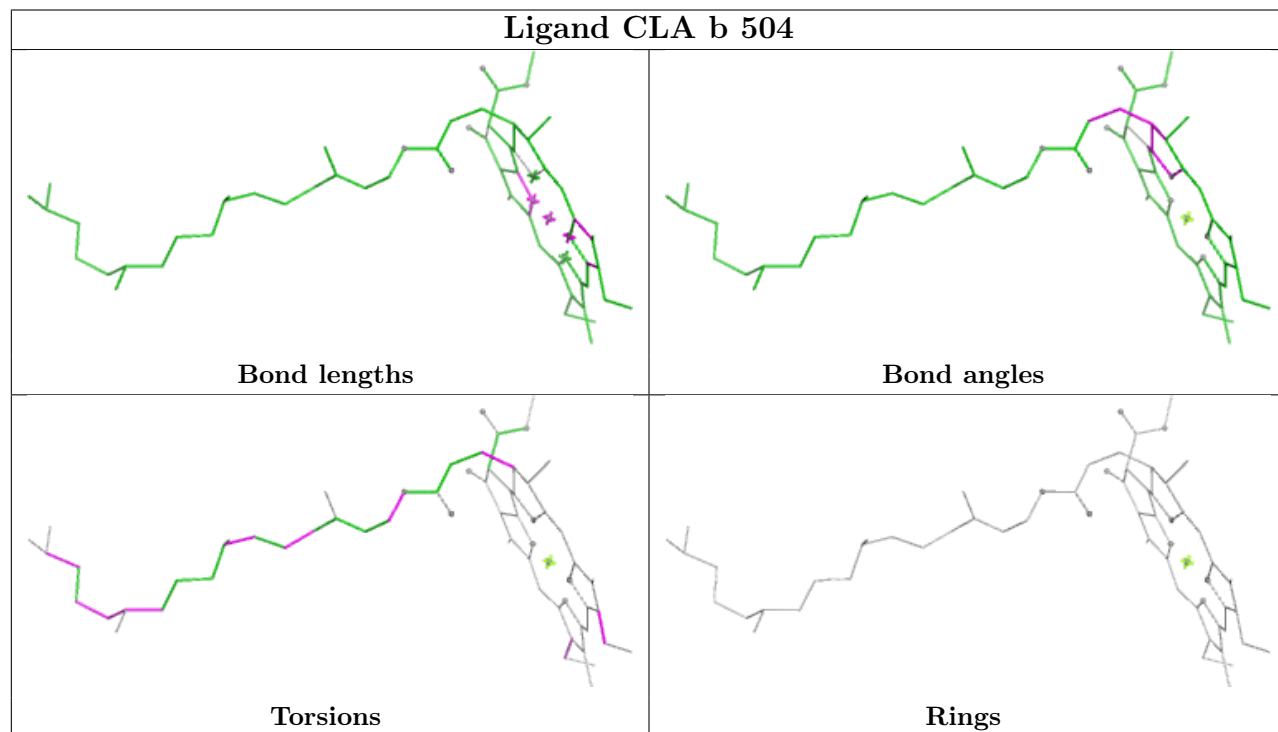
Ligand CHL Y 306

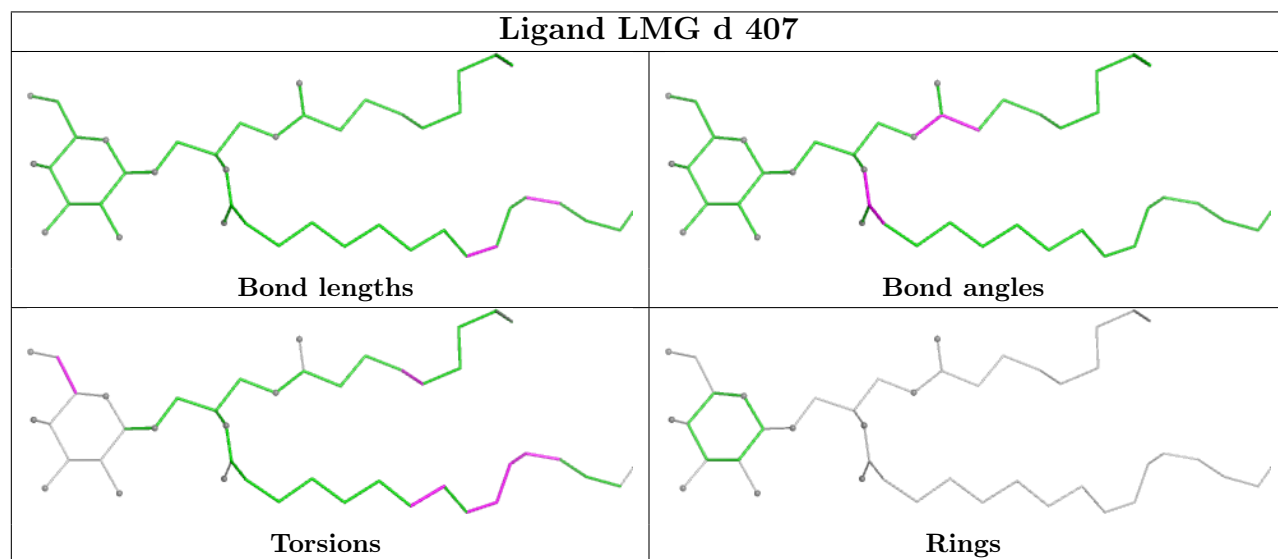
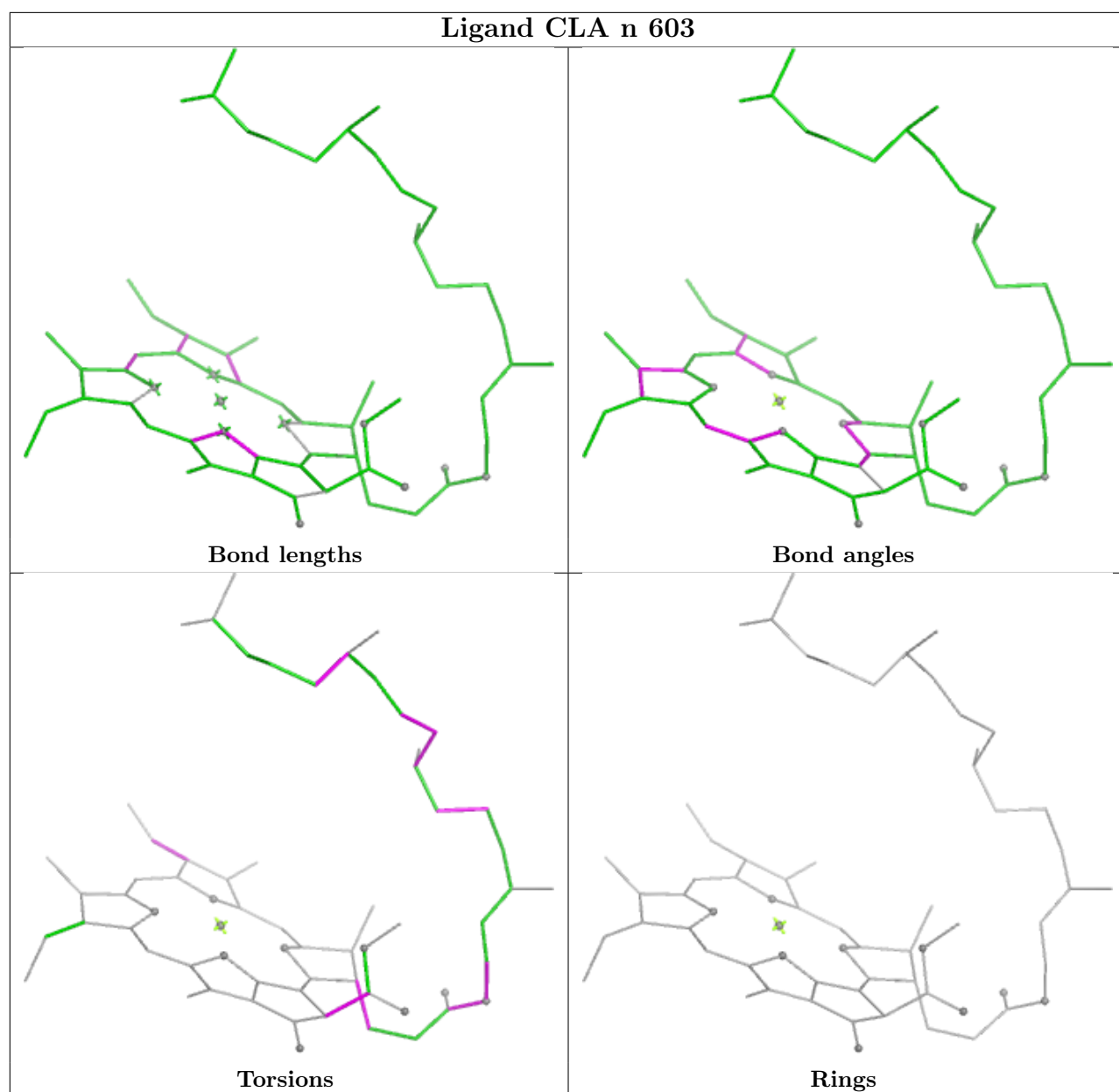


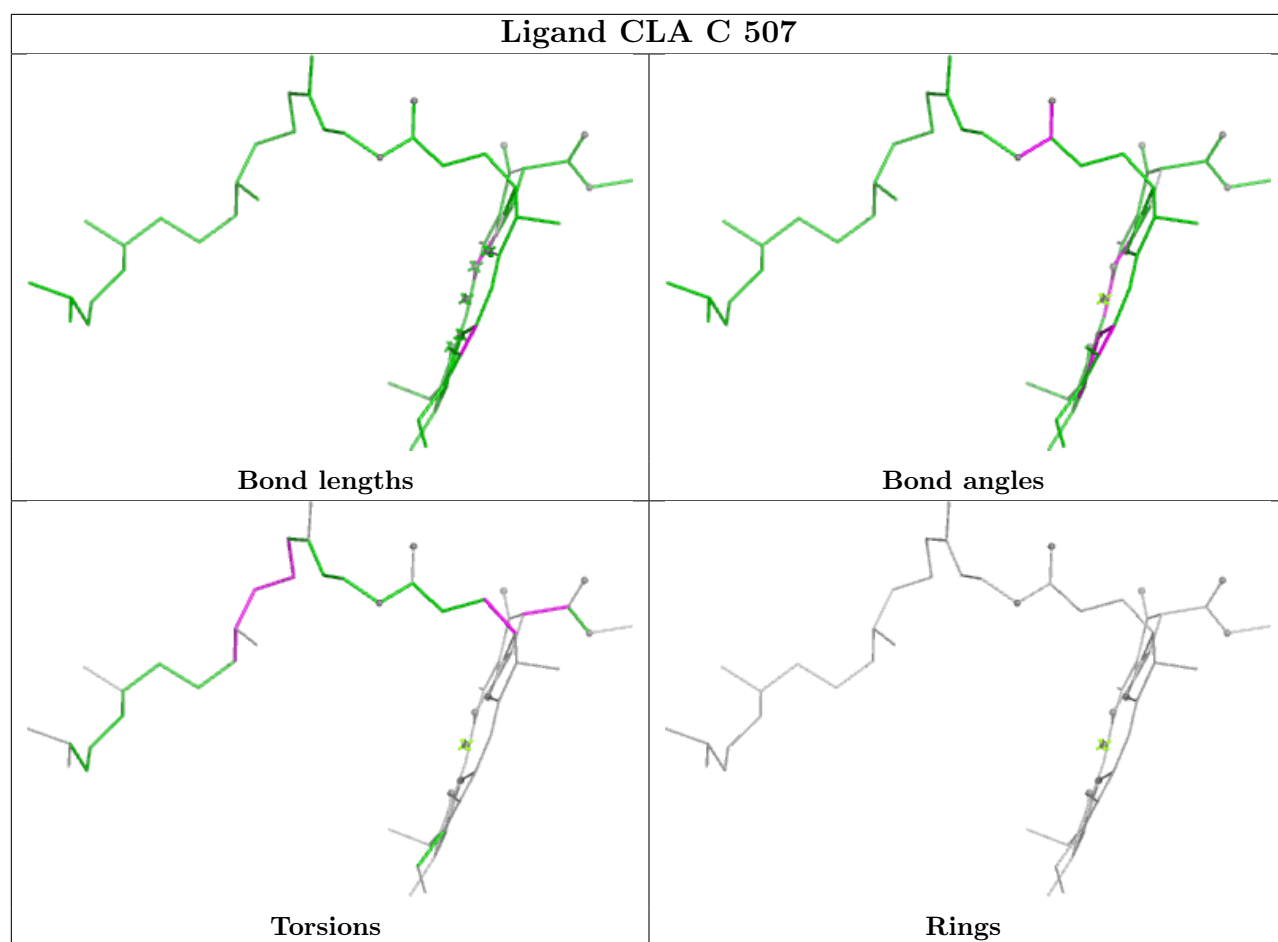
Ligand CLA b 505



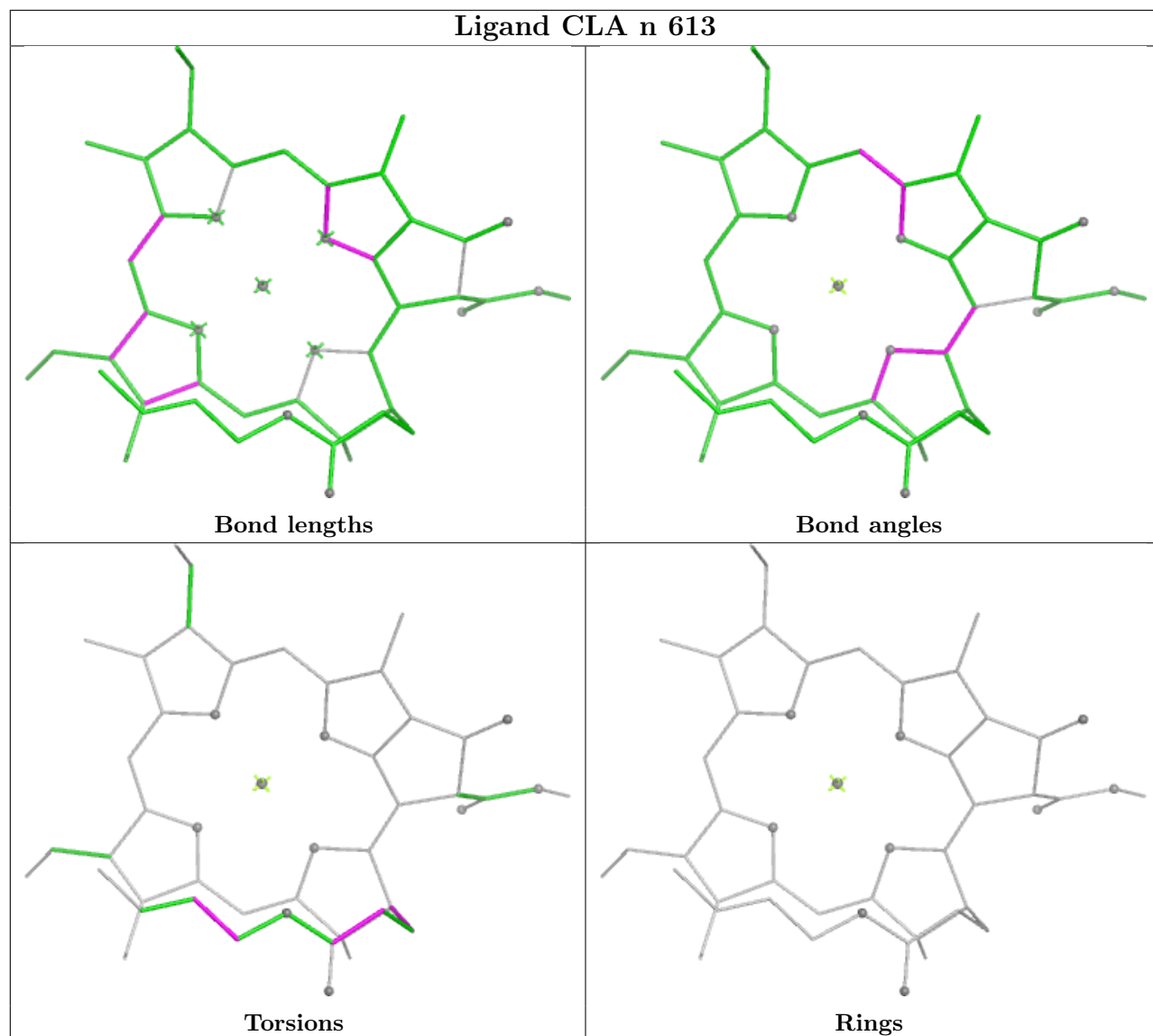


Ligand CLA s 303**Ligand CLA b 504**

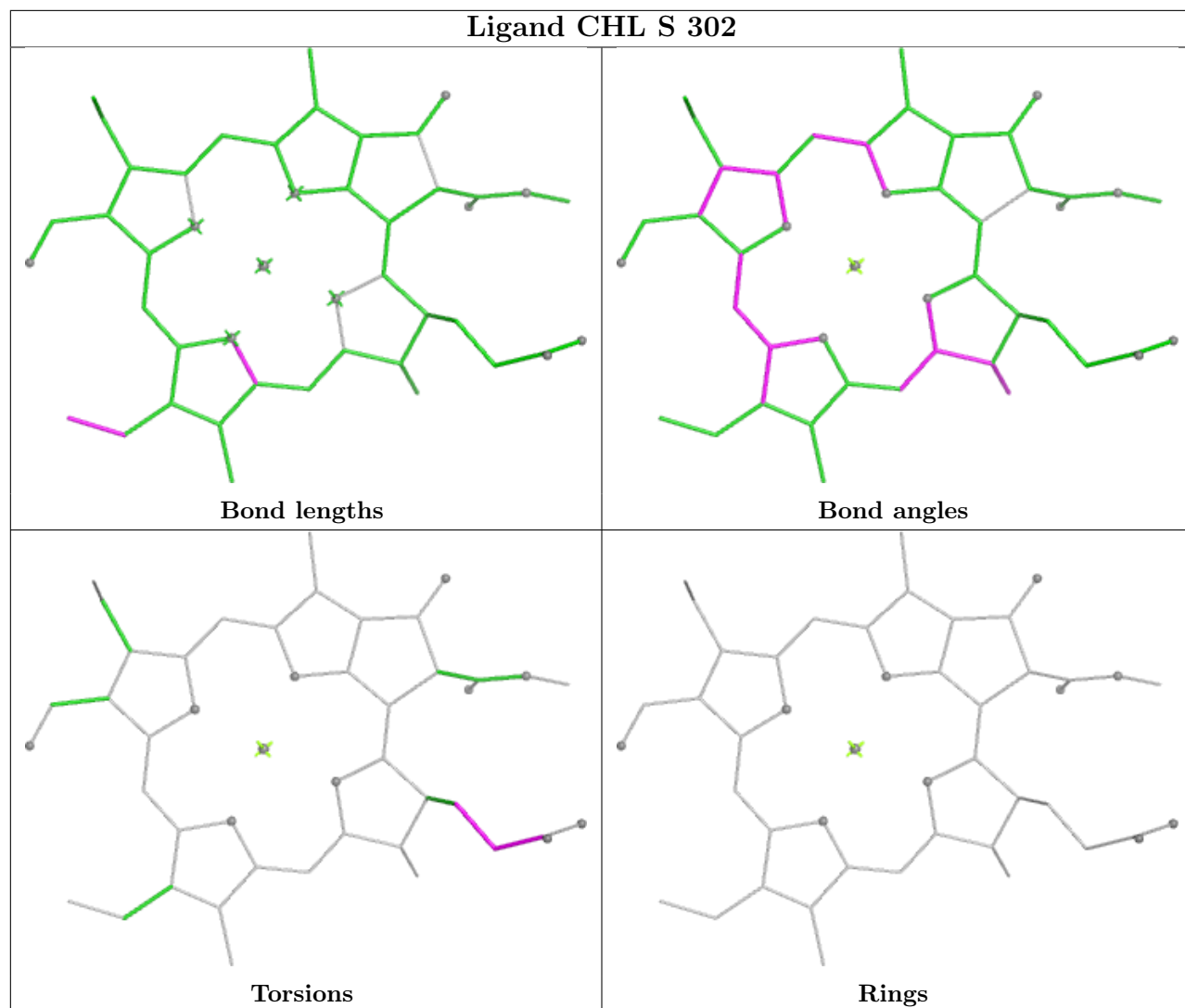




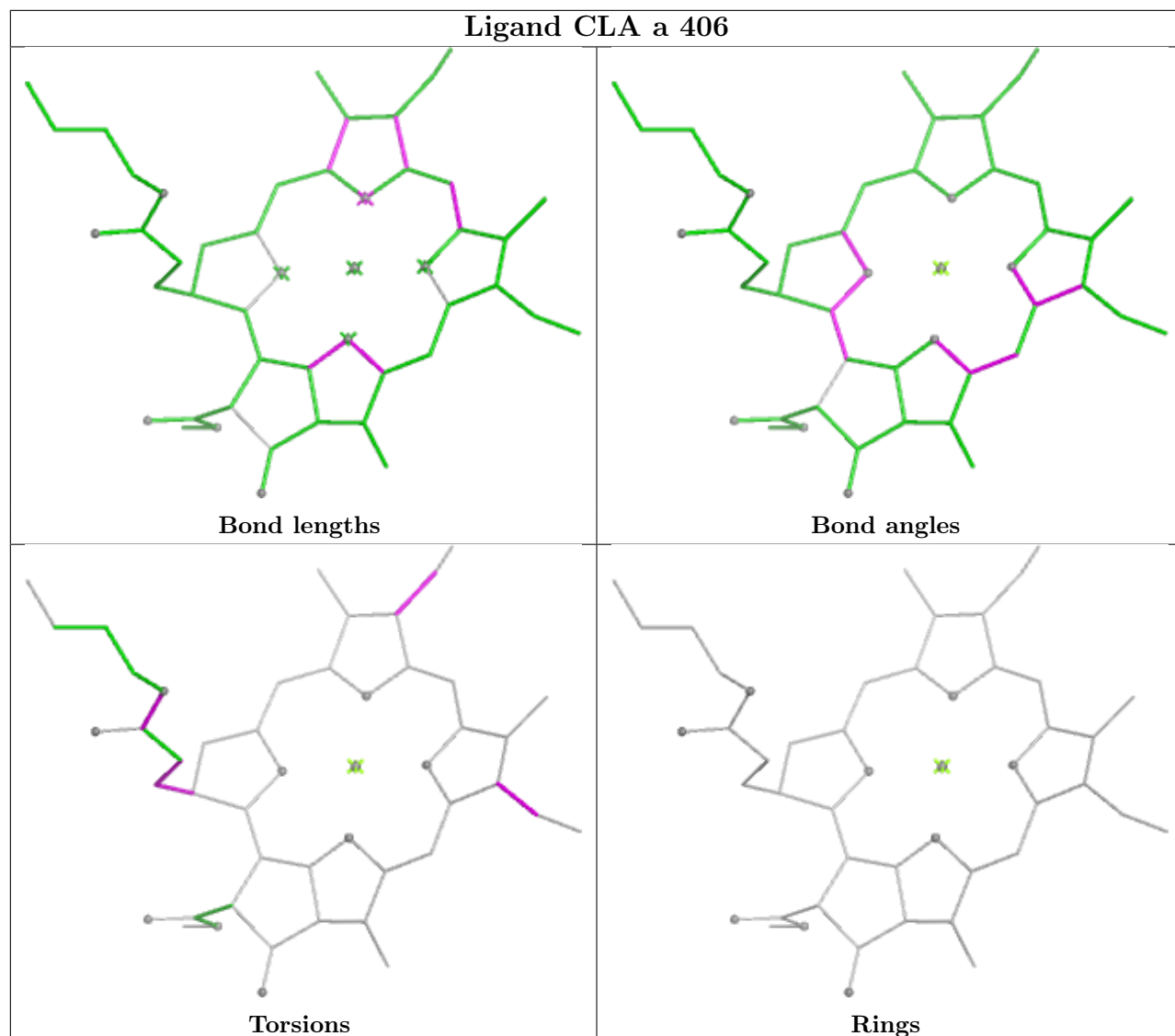
Ligand CLA n 613

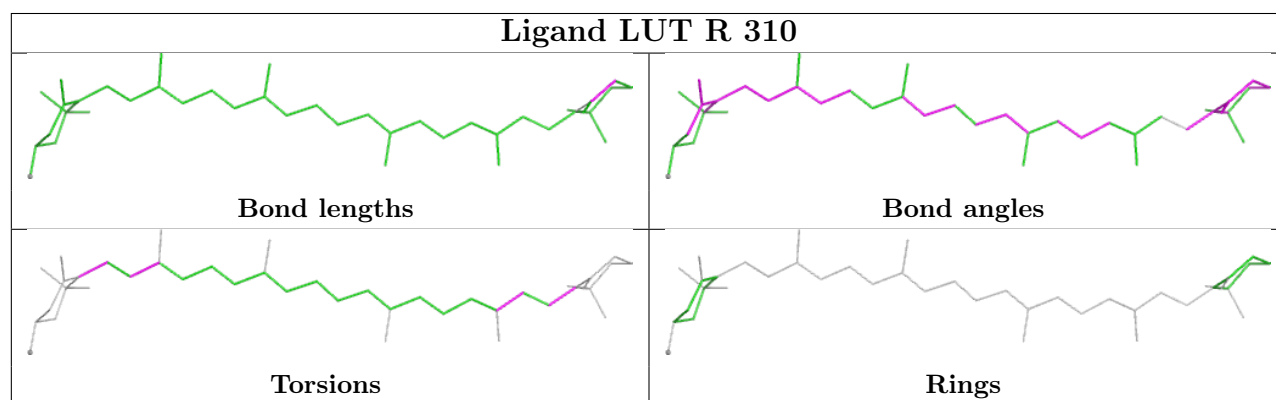
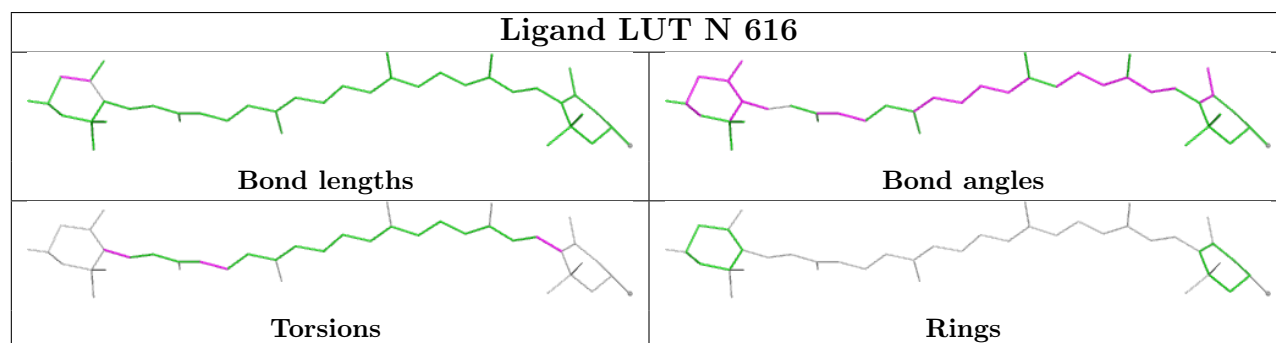
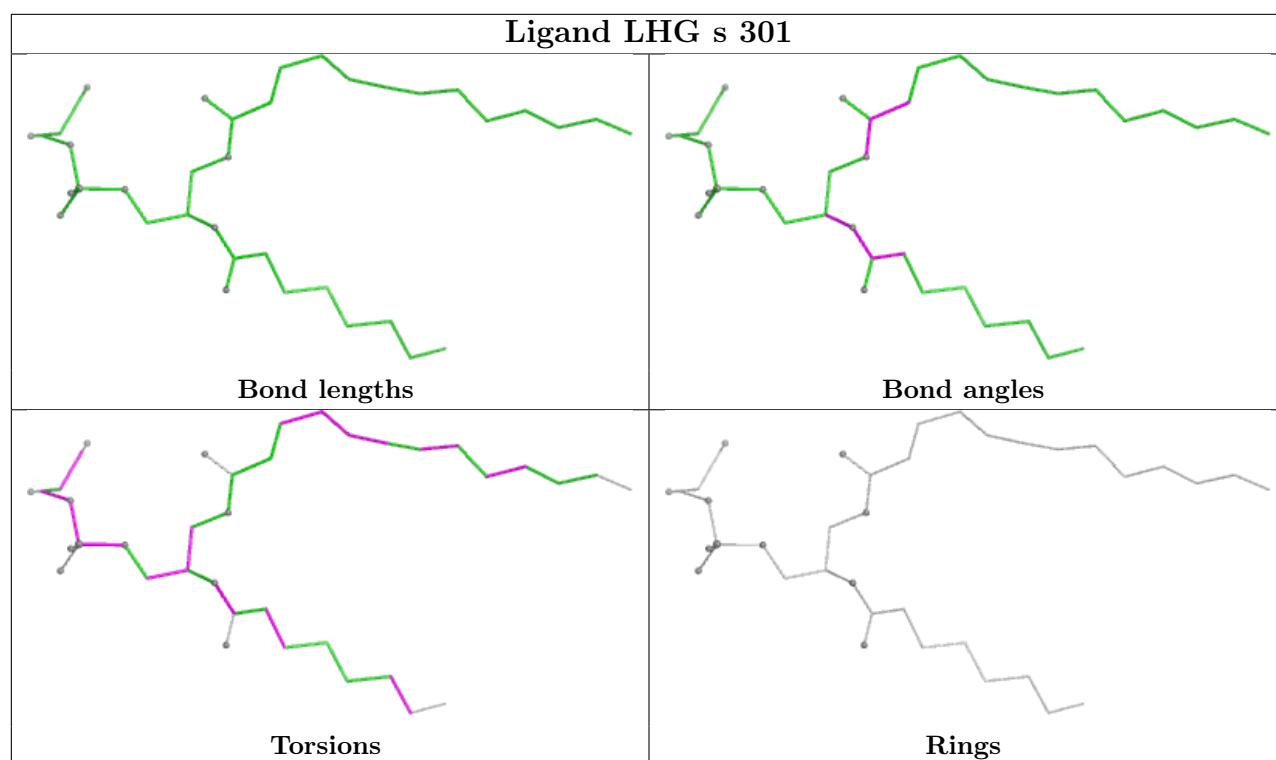


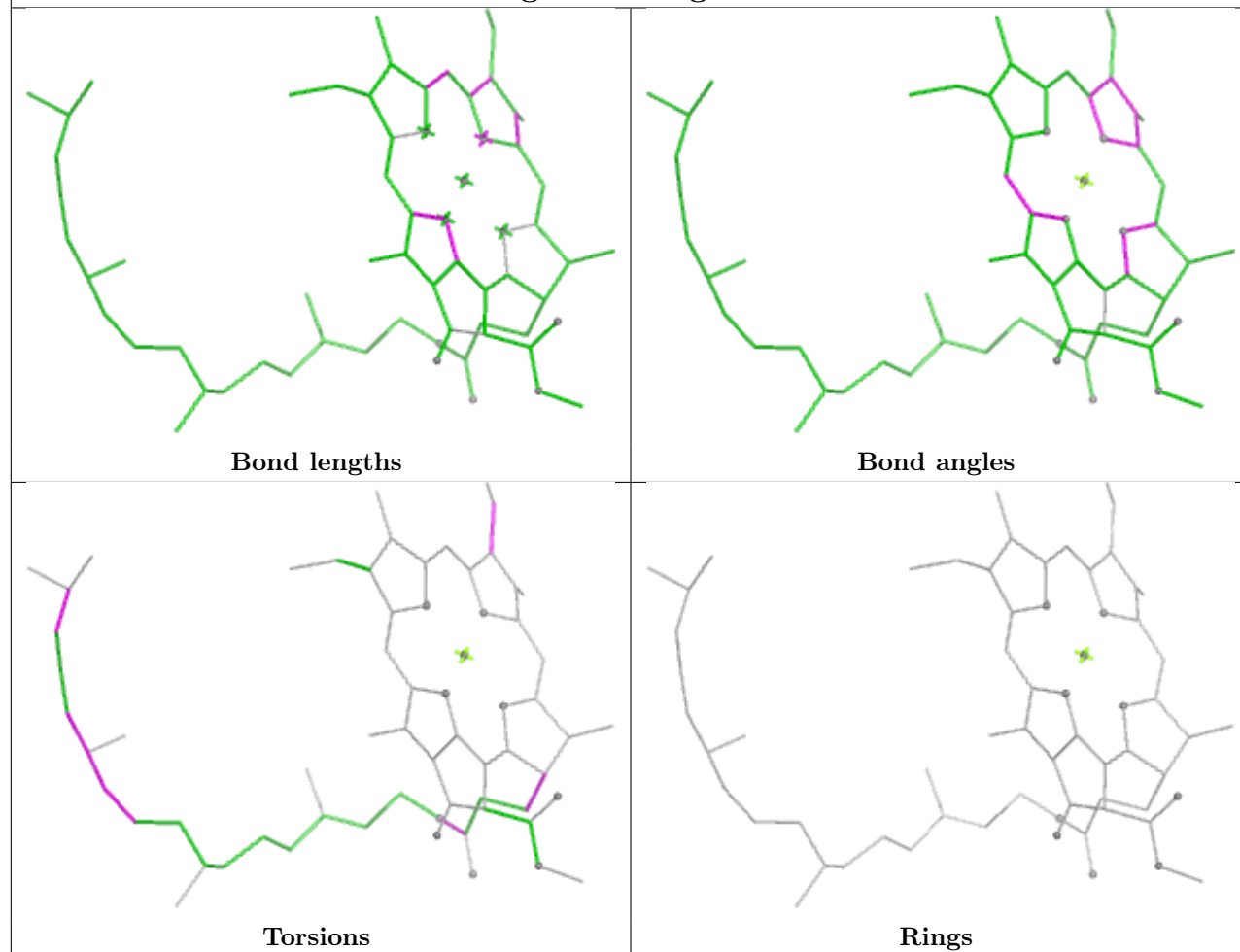
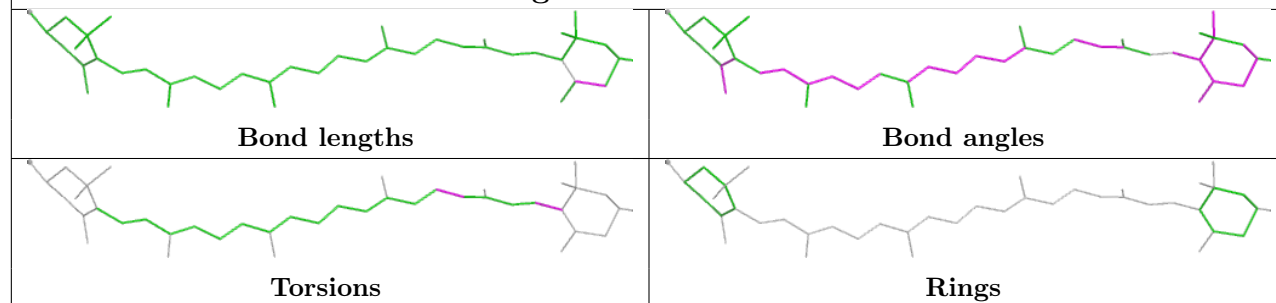
Ligand CHL S 302

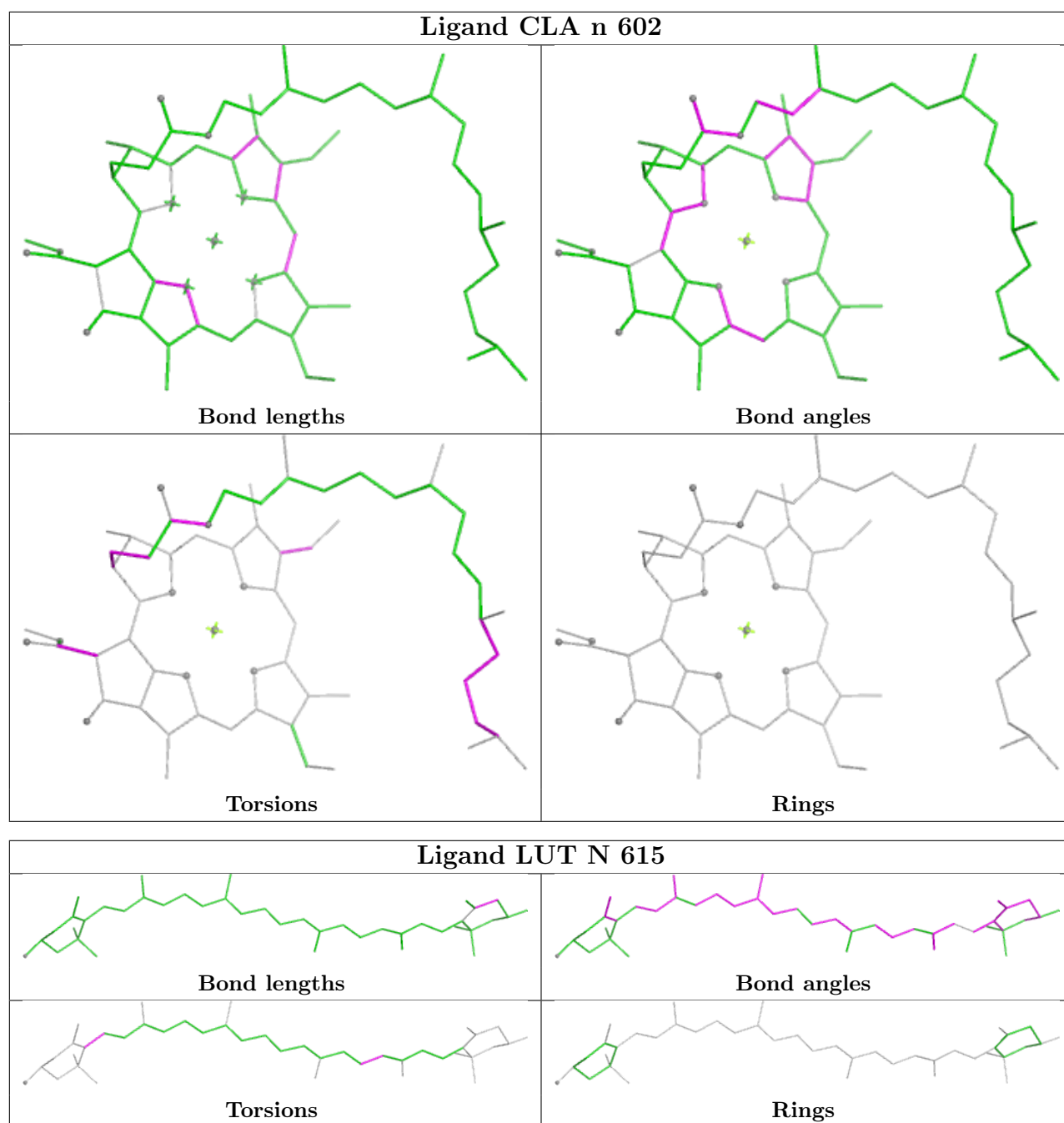


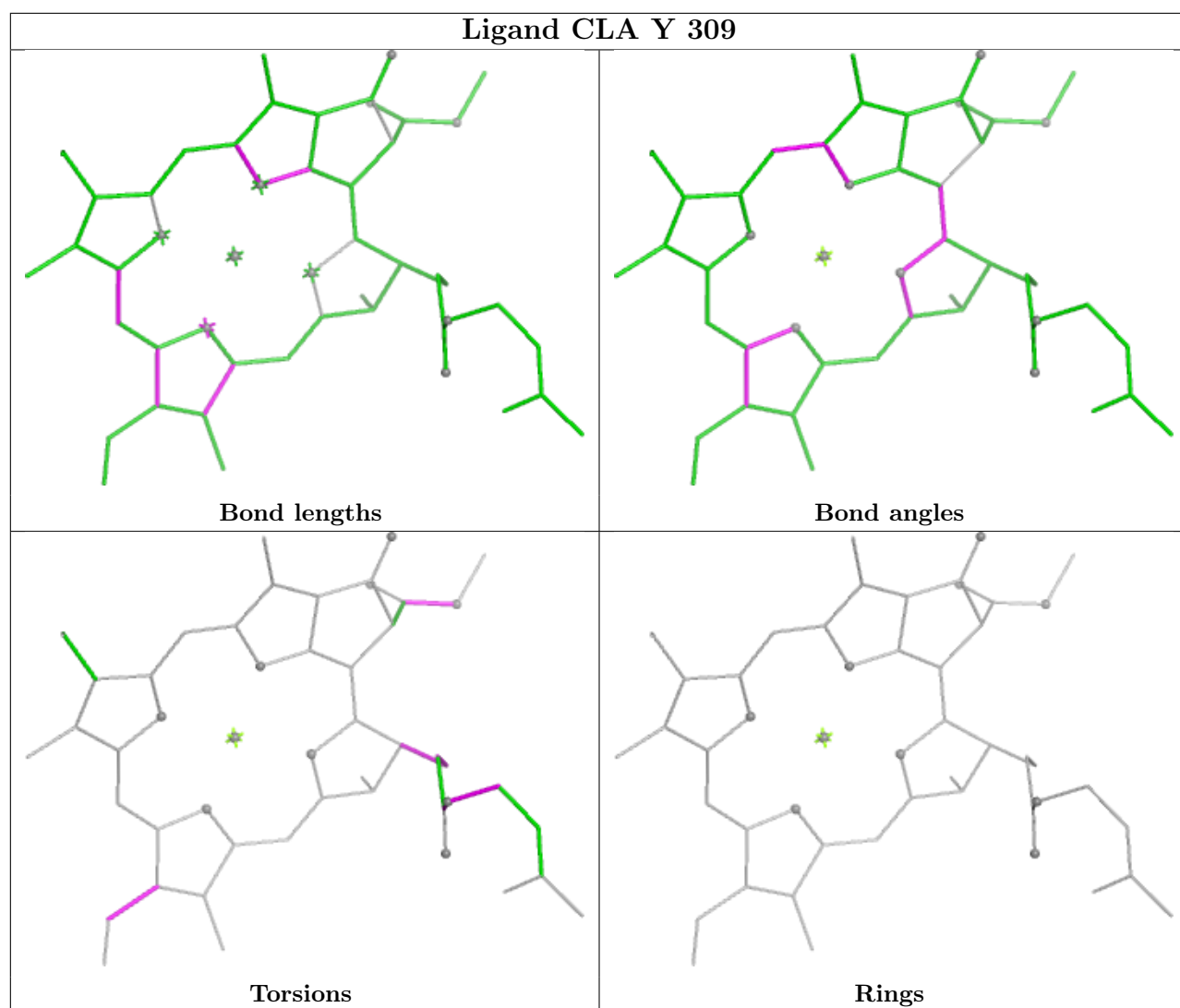
Ligand CLA a 406

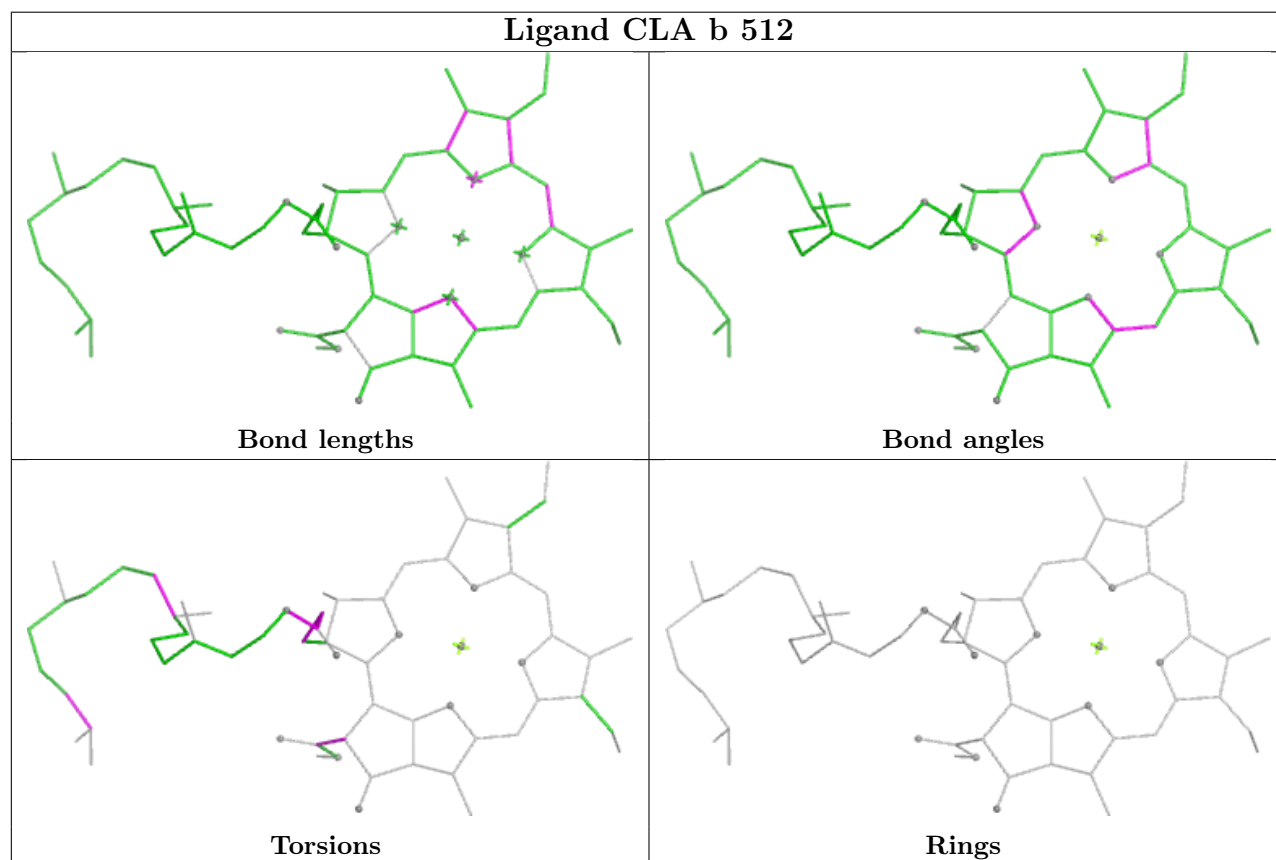
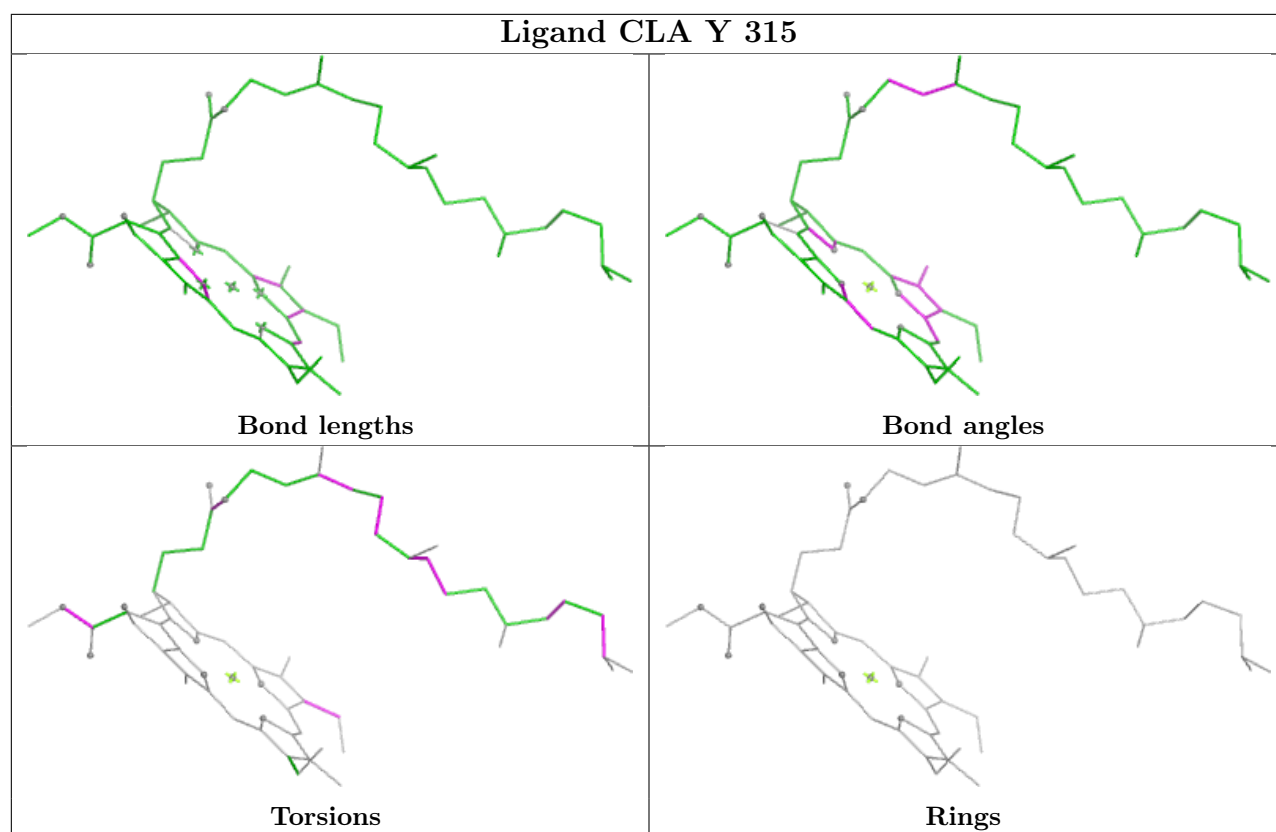




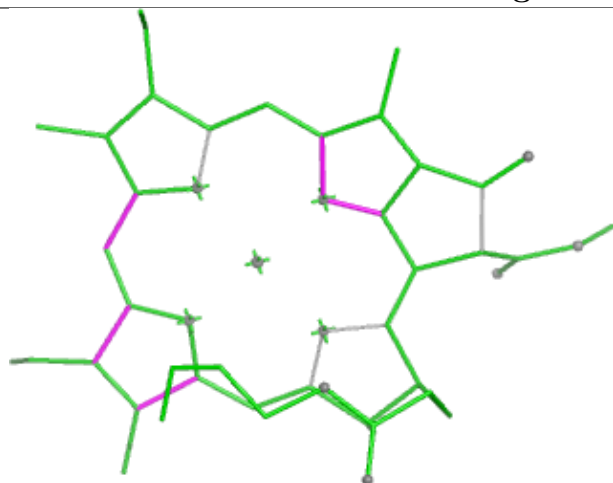
Ligand CLA g 611**Ligand LUT Y 317**



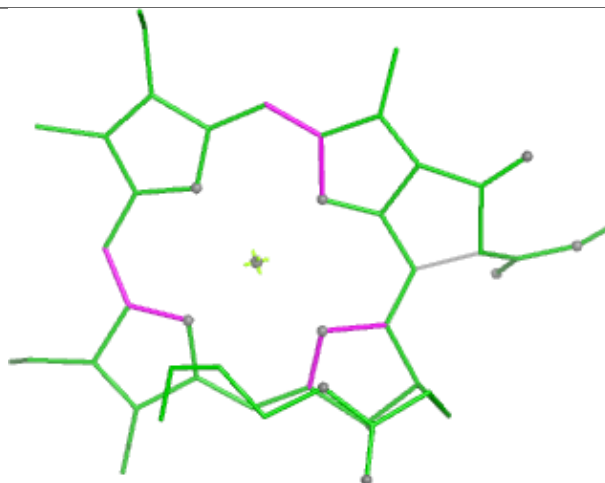




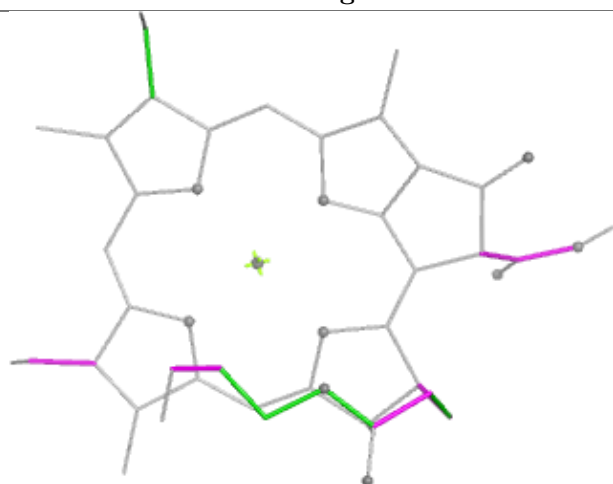
Ligand CLA G 614



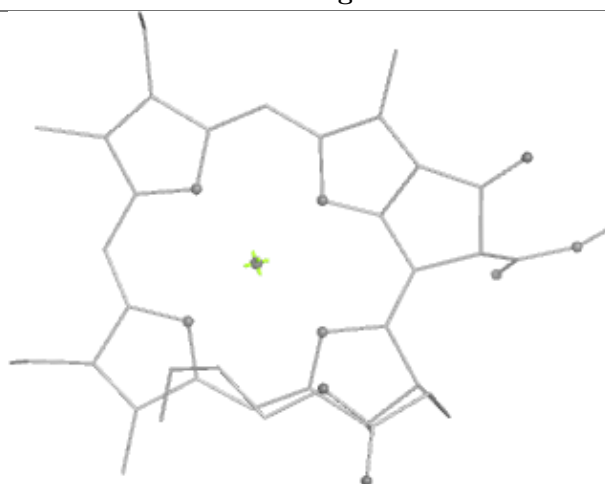
Bond lengths



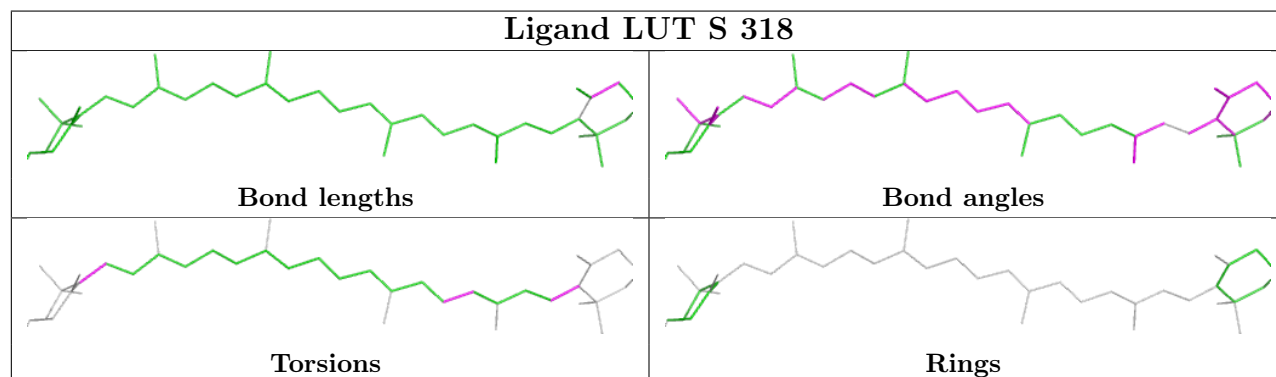
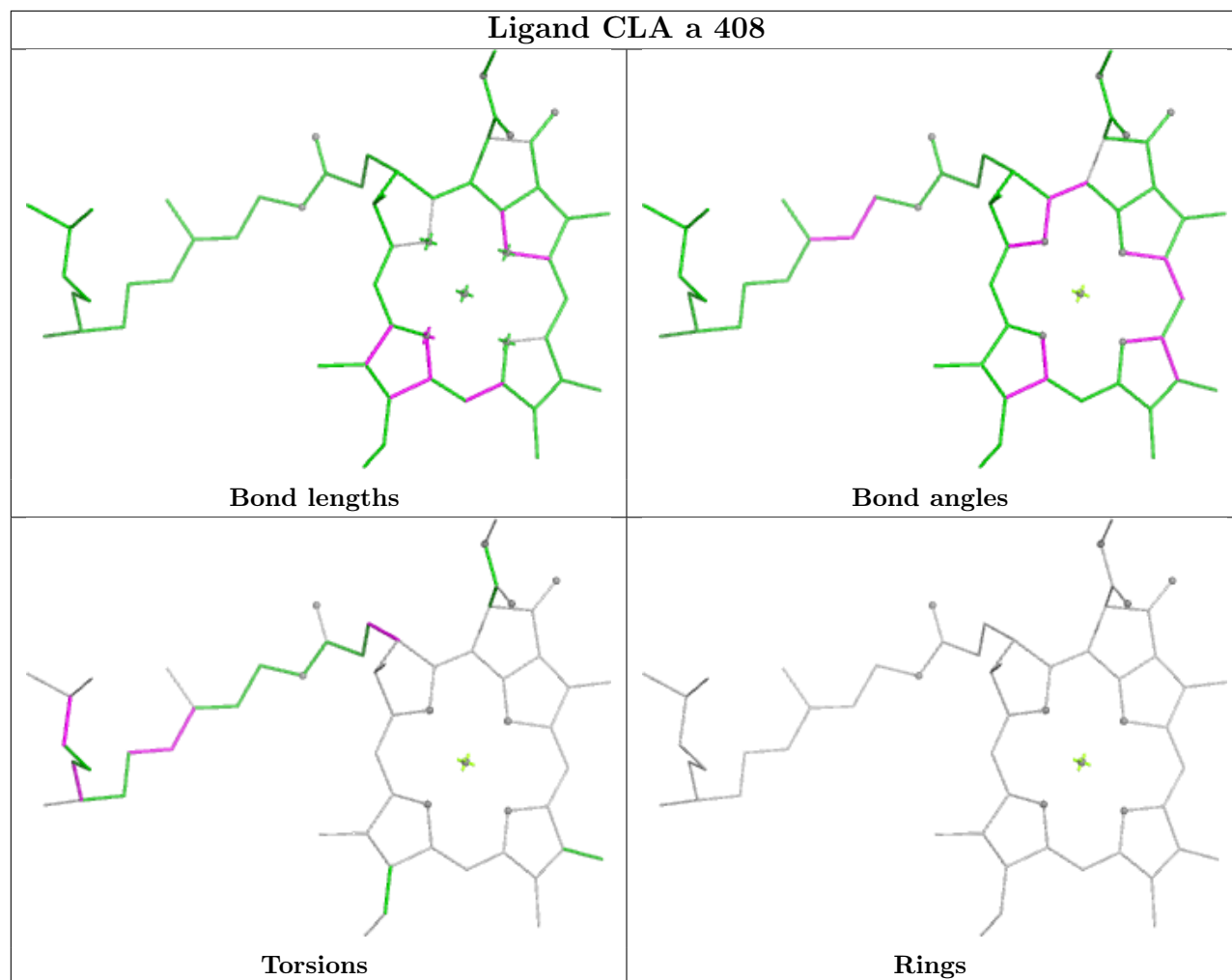
Bond angles

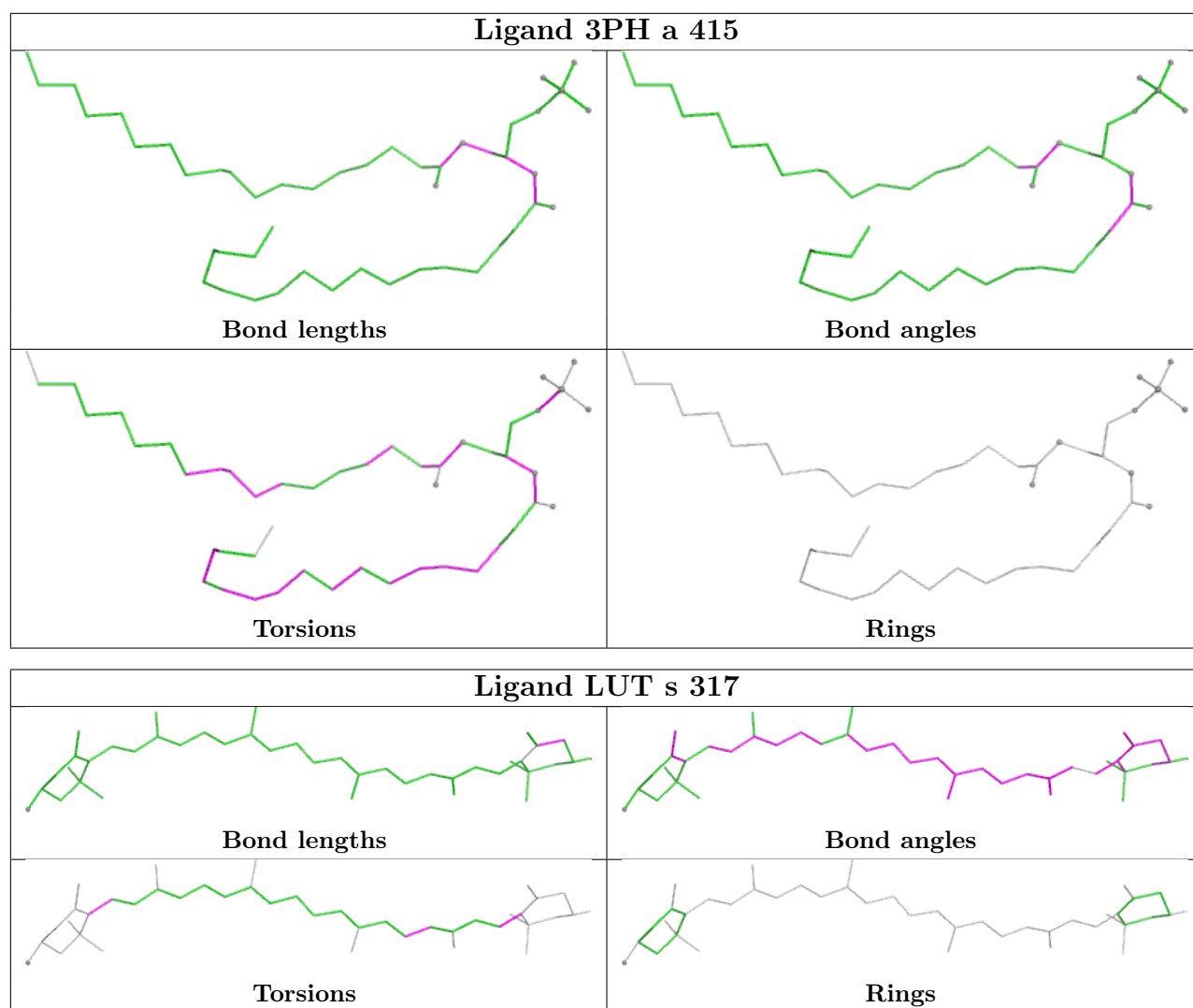


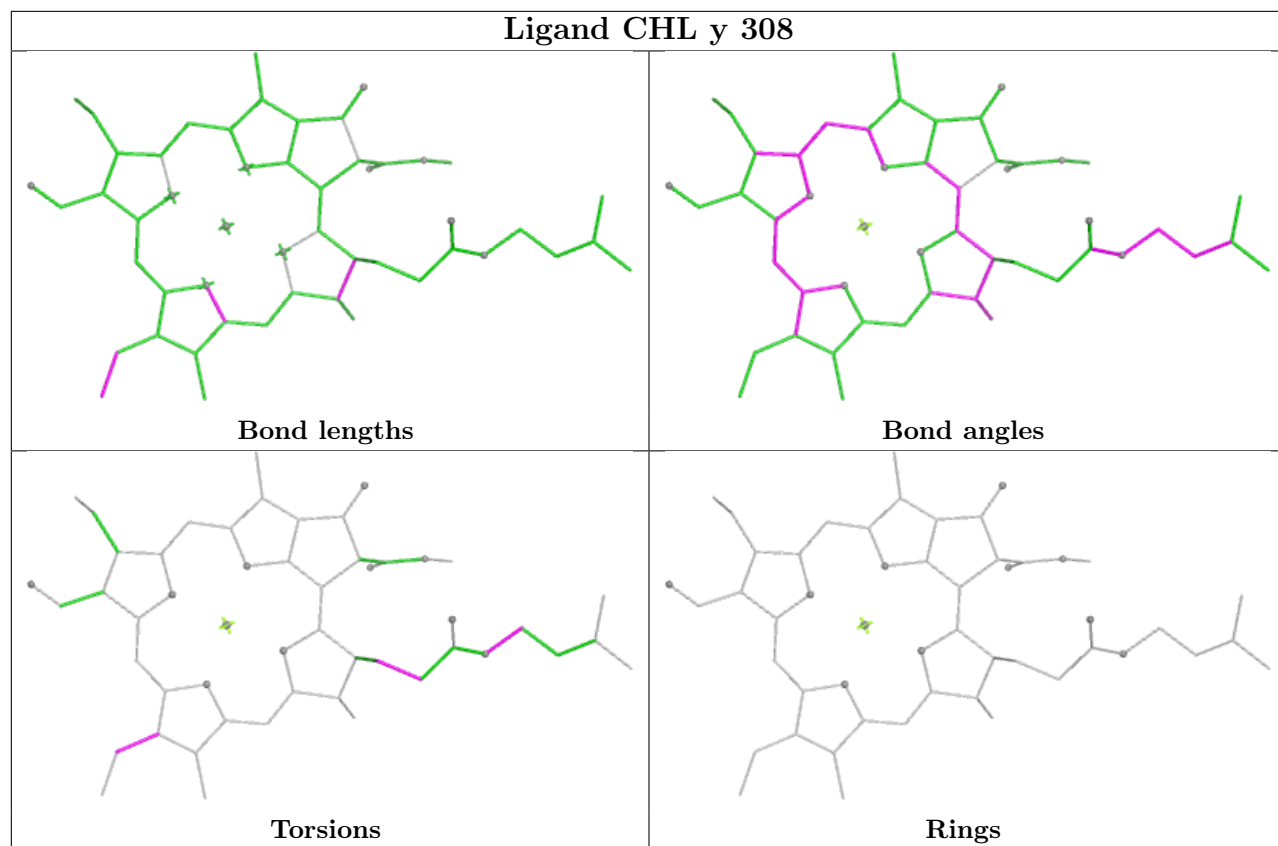
Torsions

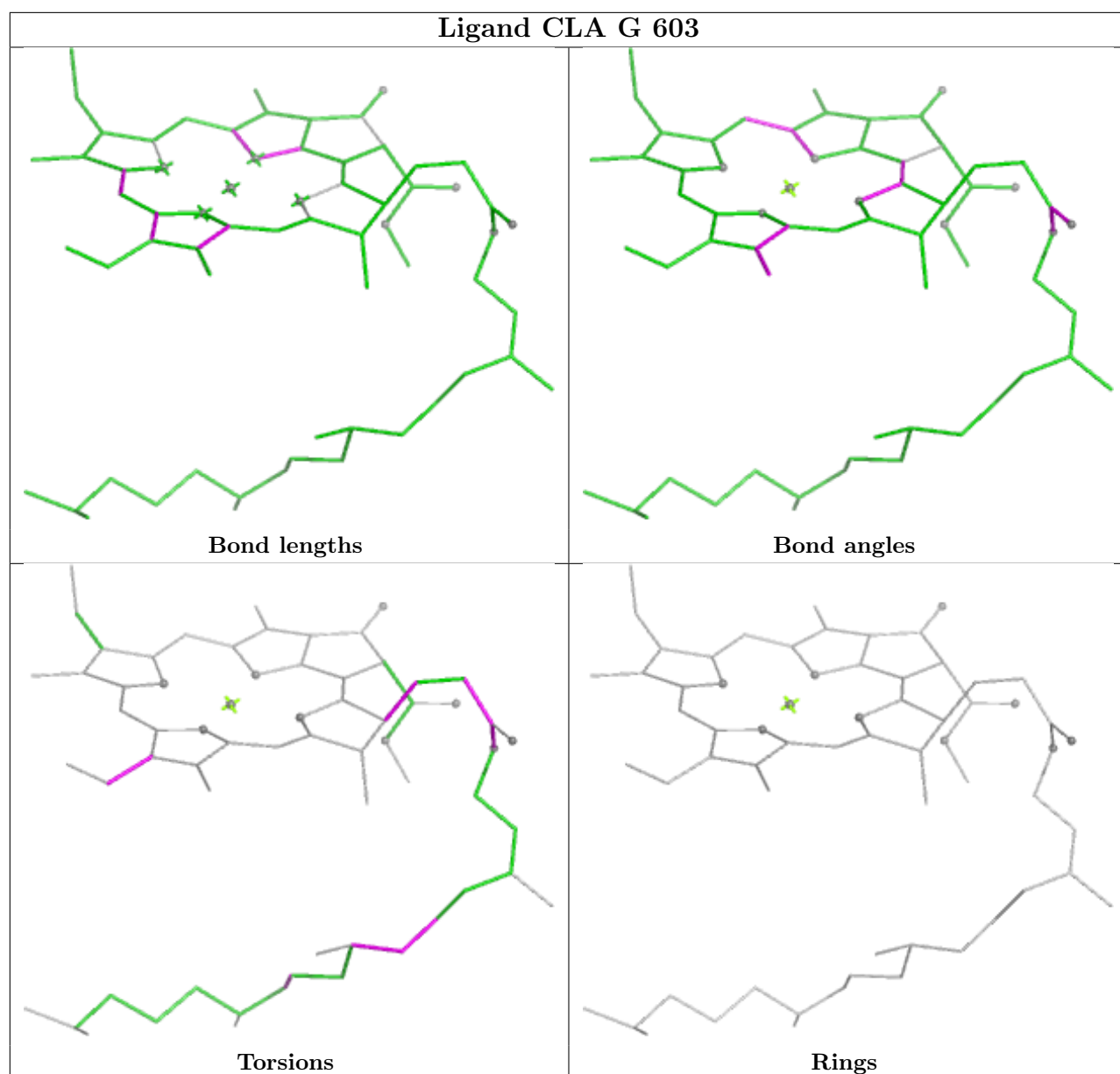


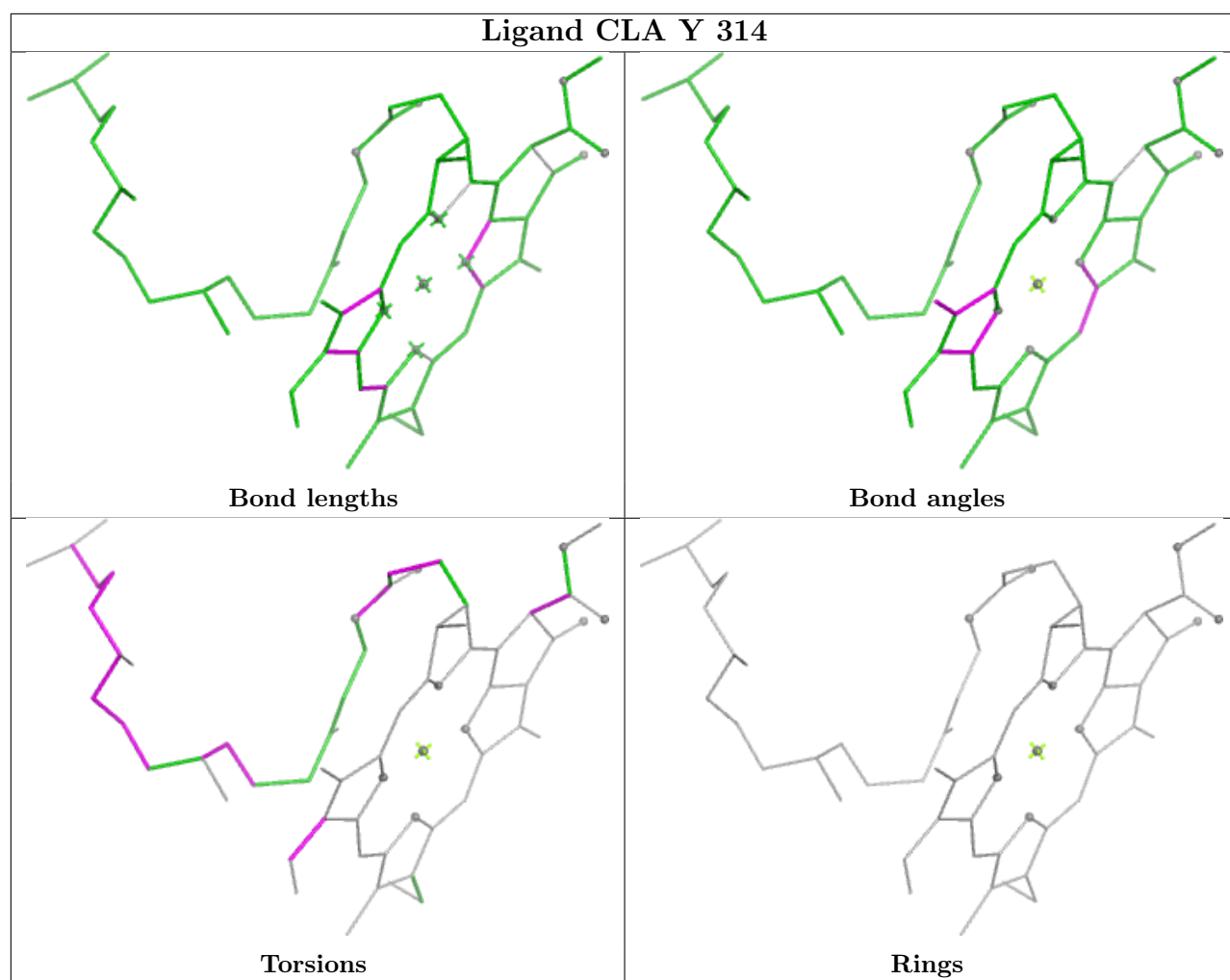
Rings



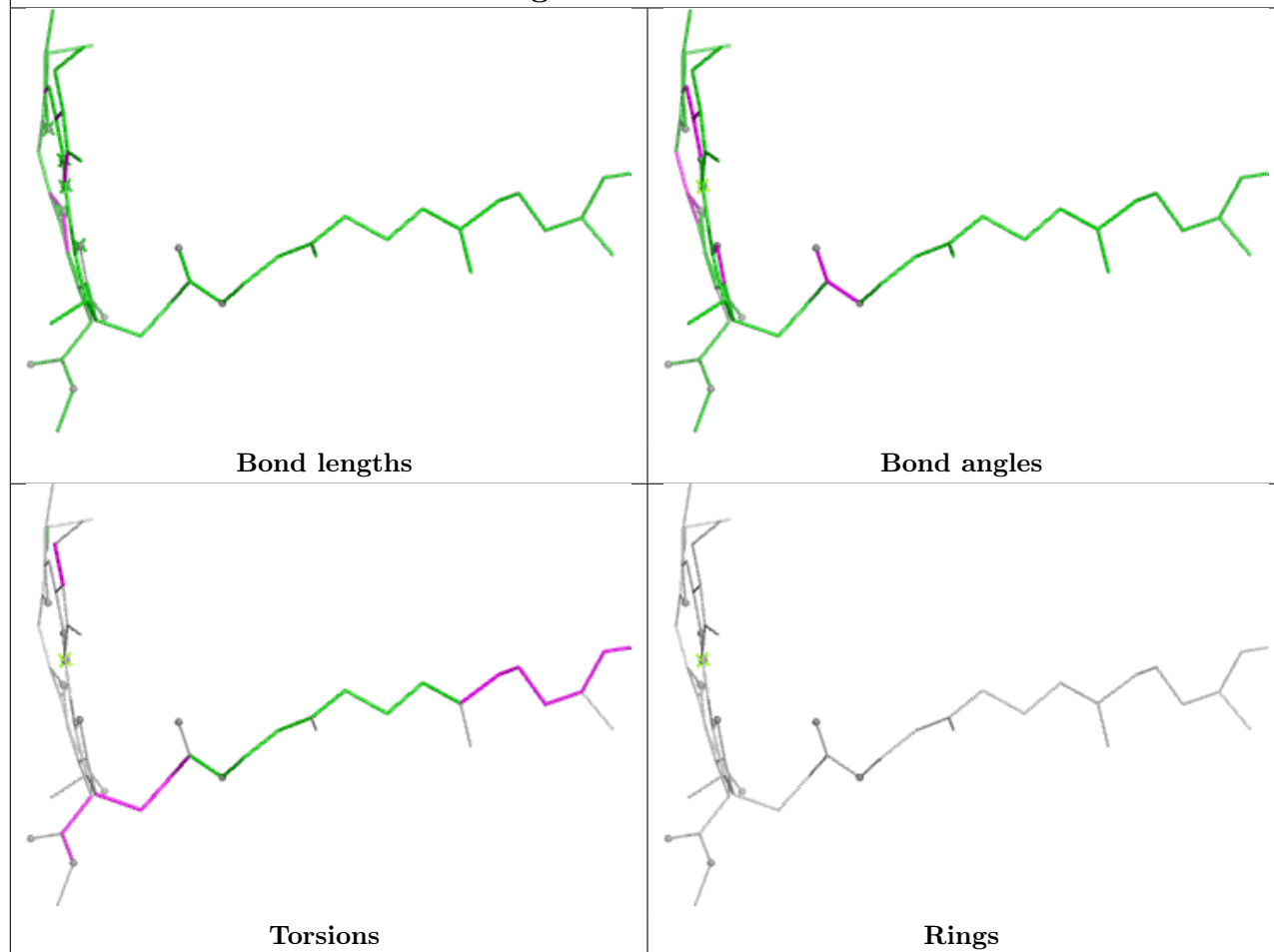




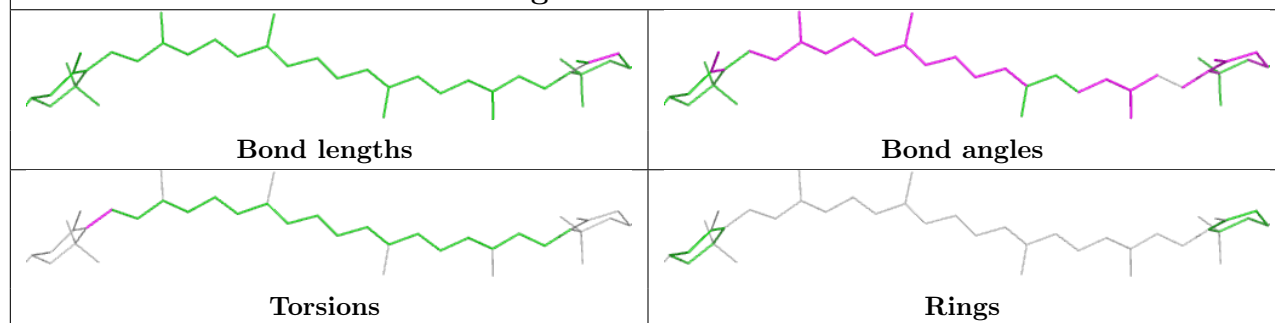




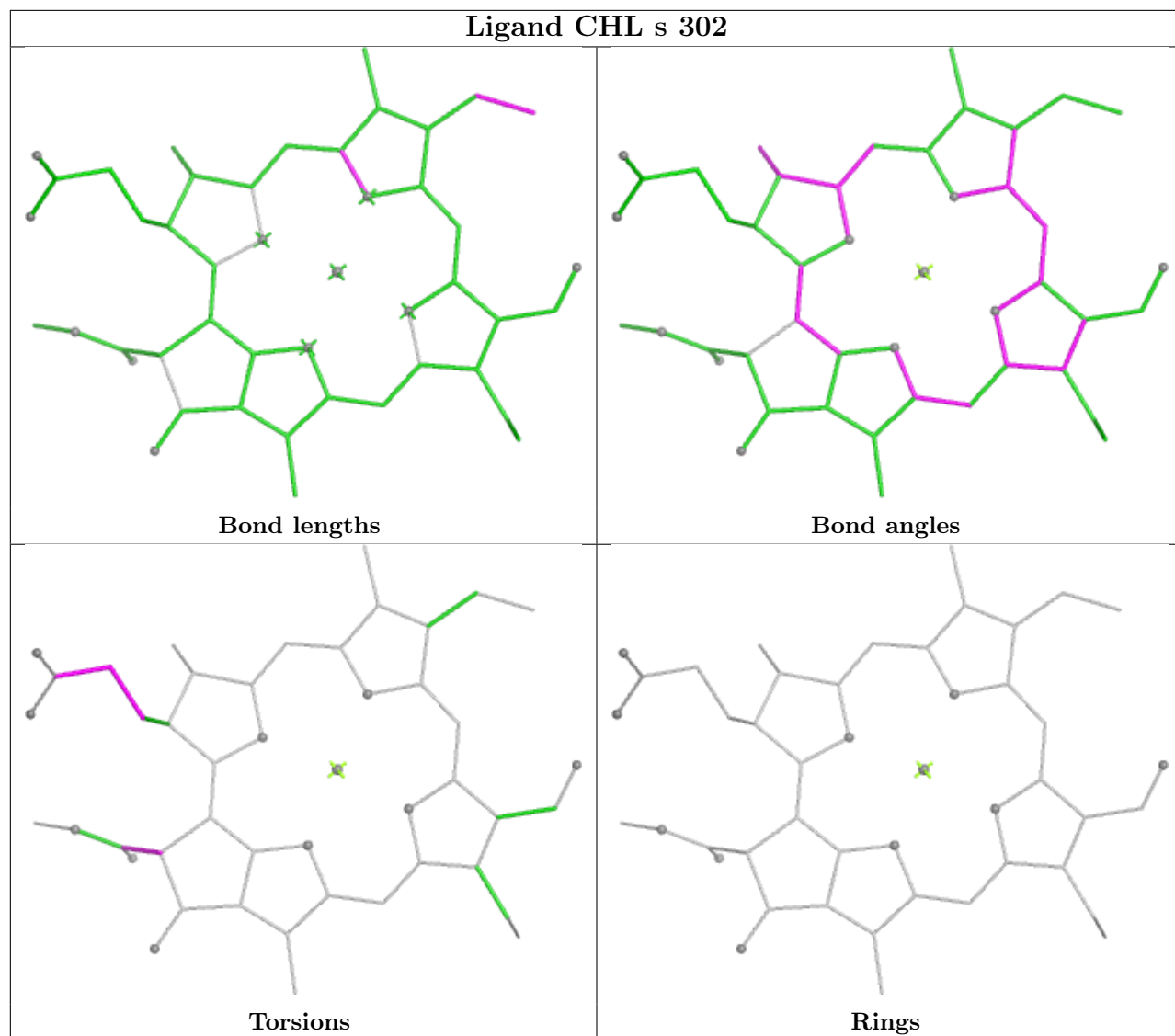
Ligand CLA B 506



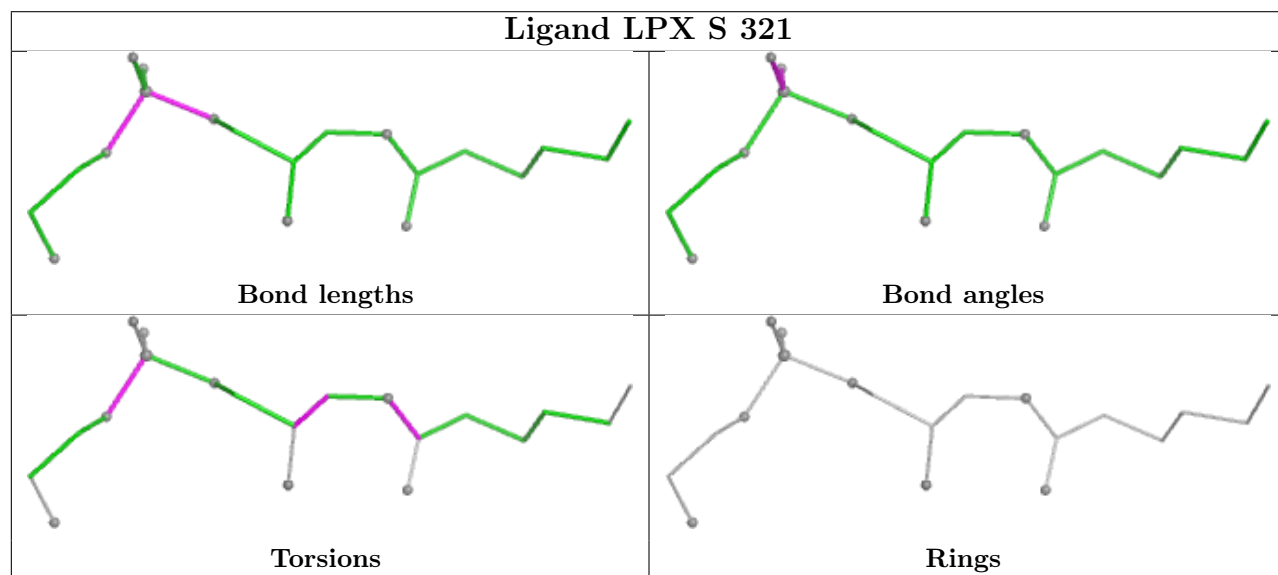
Ligand LUT Y 316

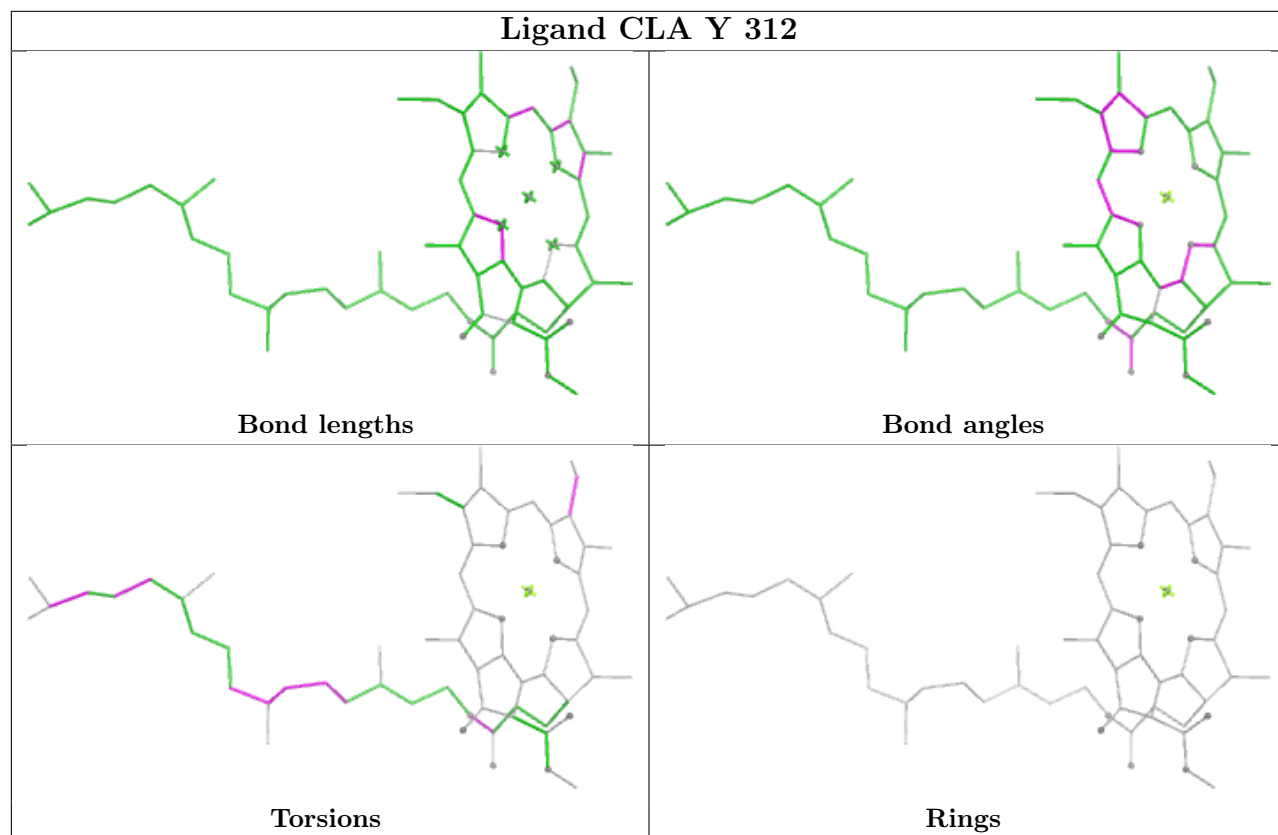


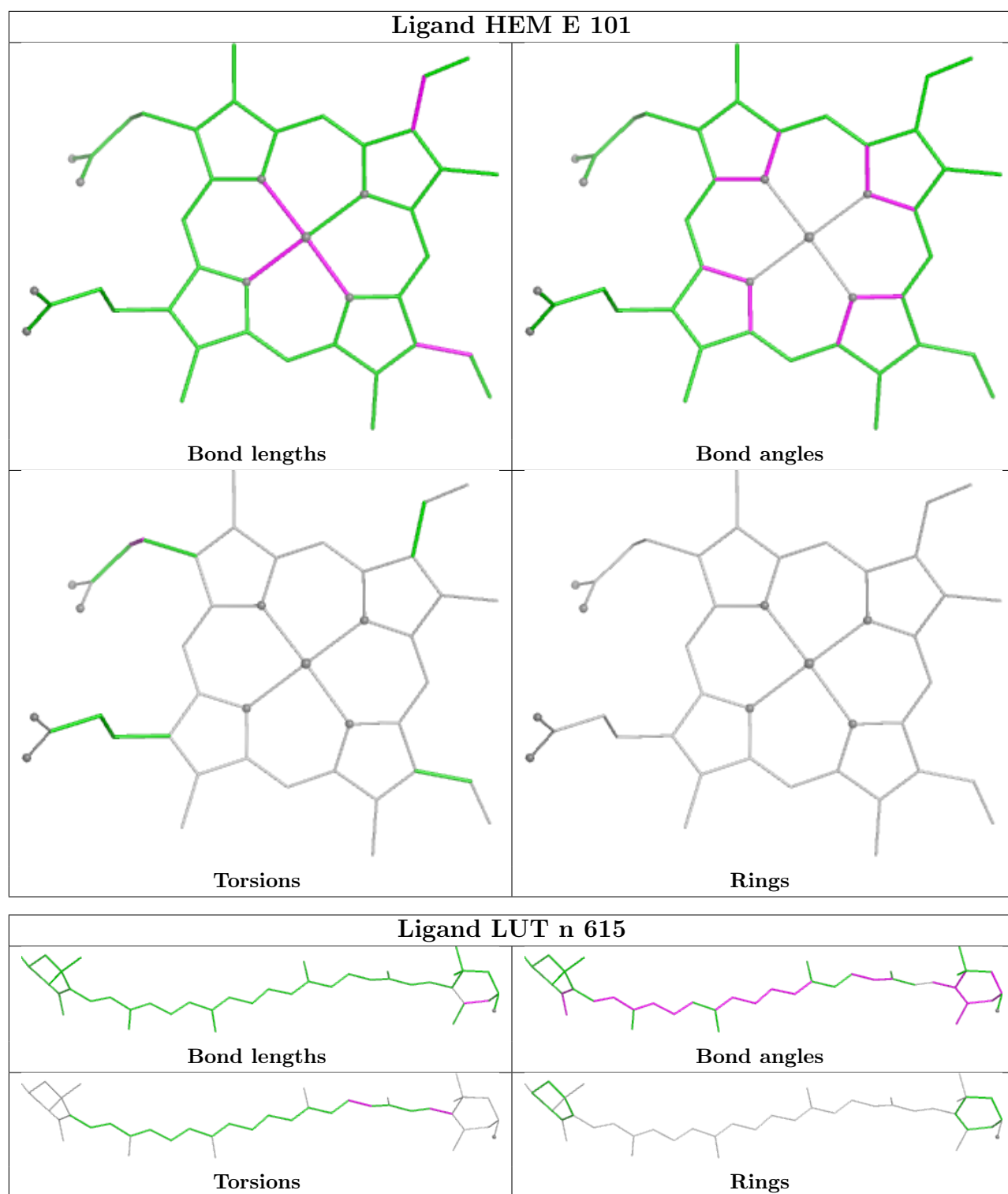
Ligand CHL s 302

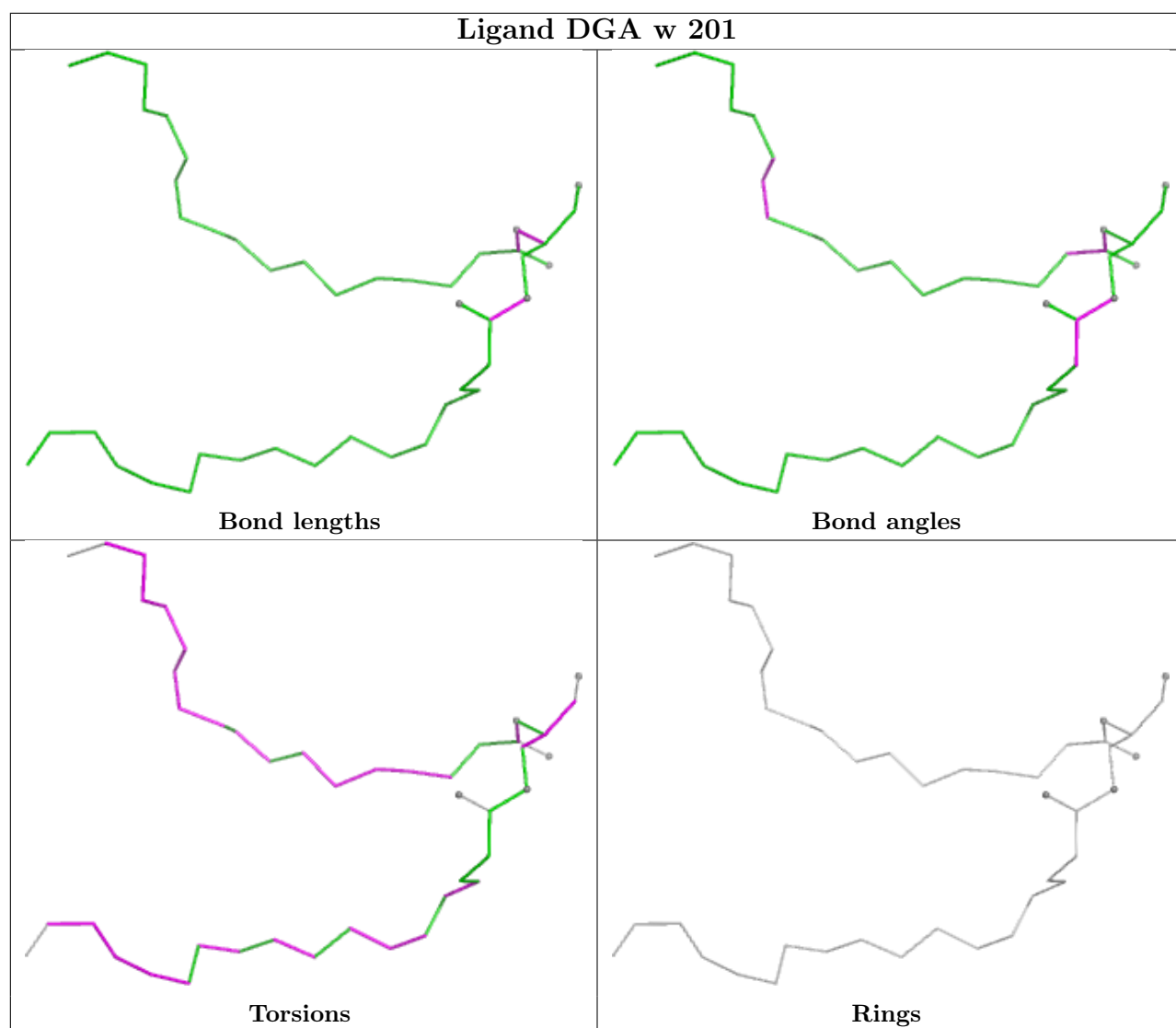


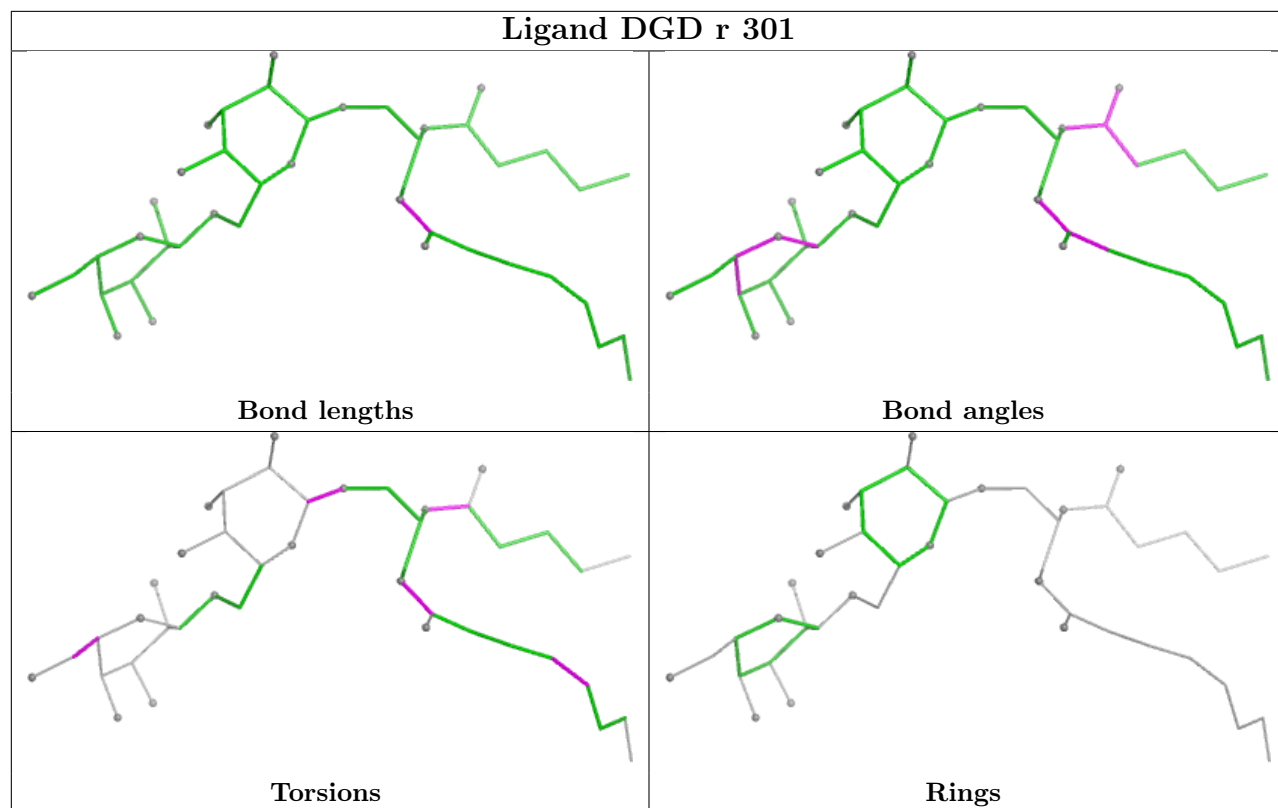
Ligand LPX S 321



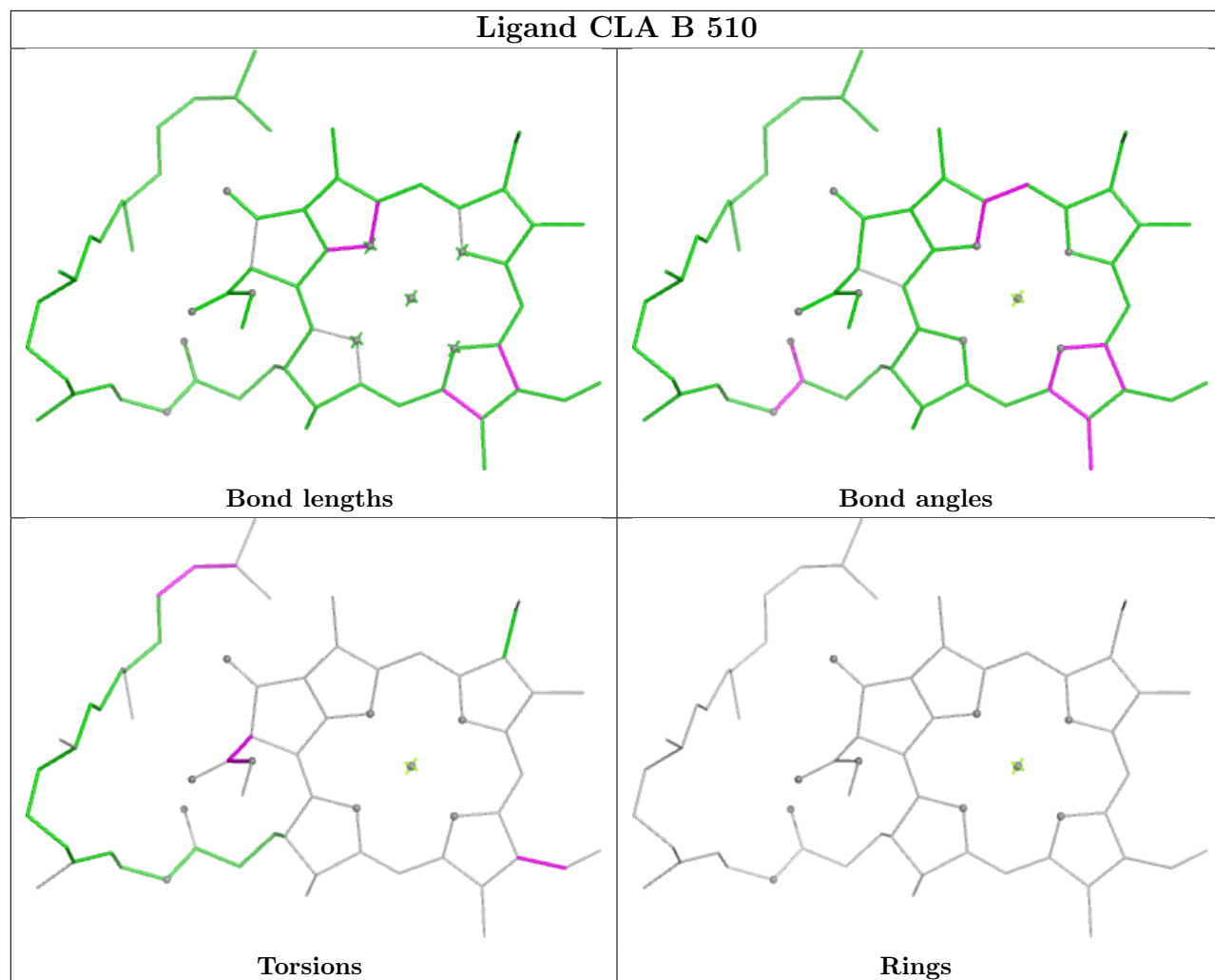


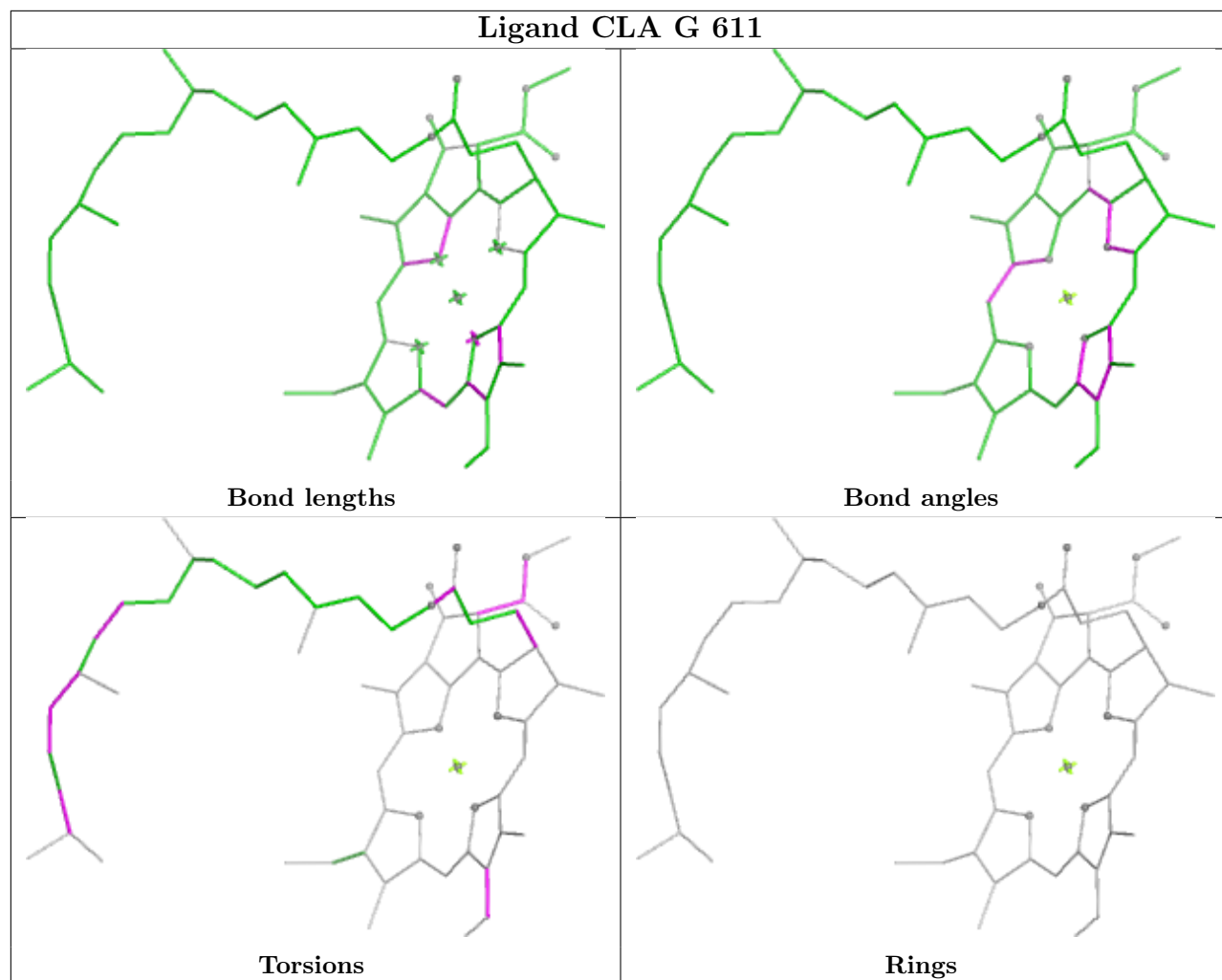


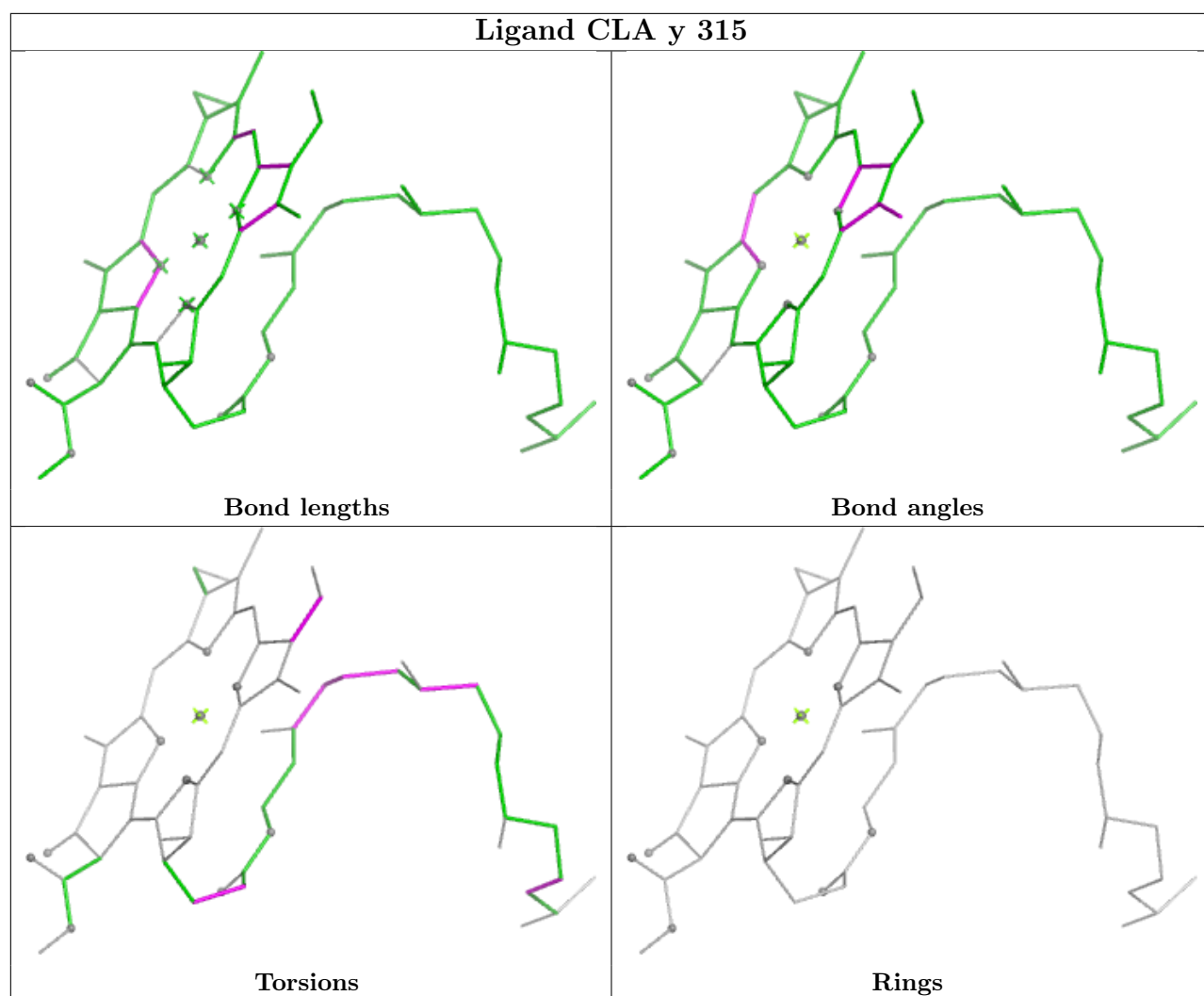


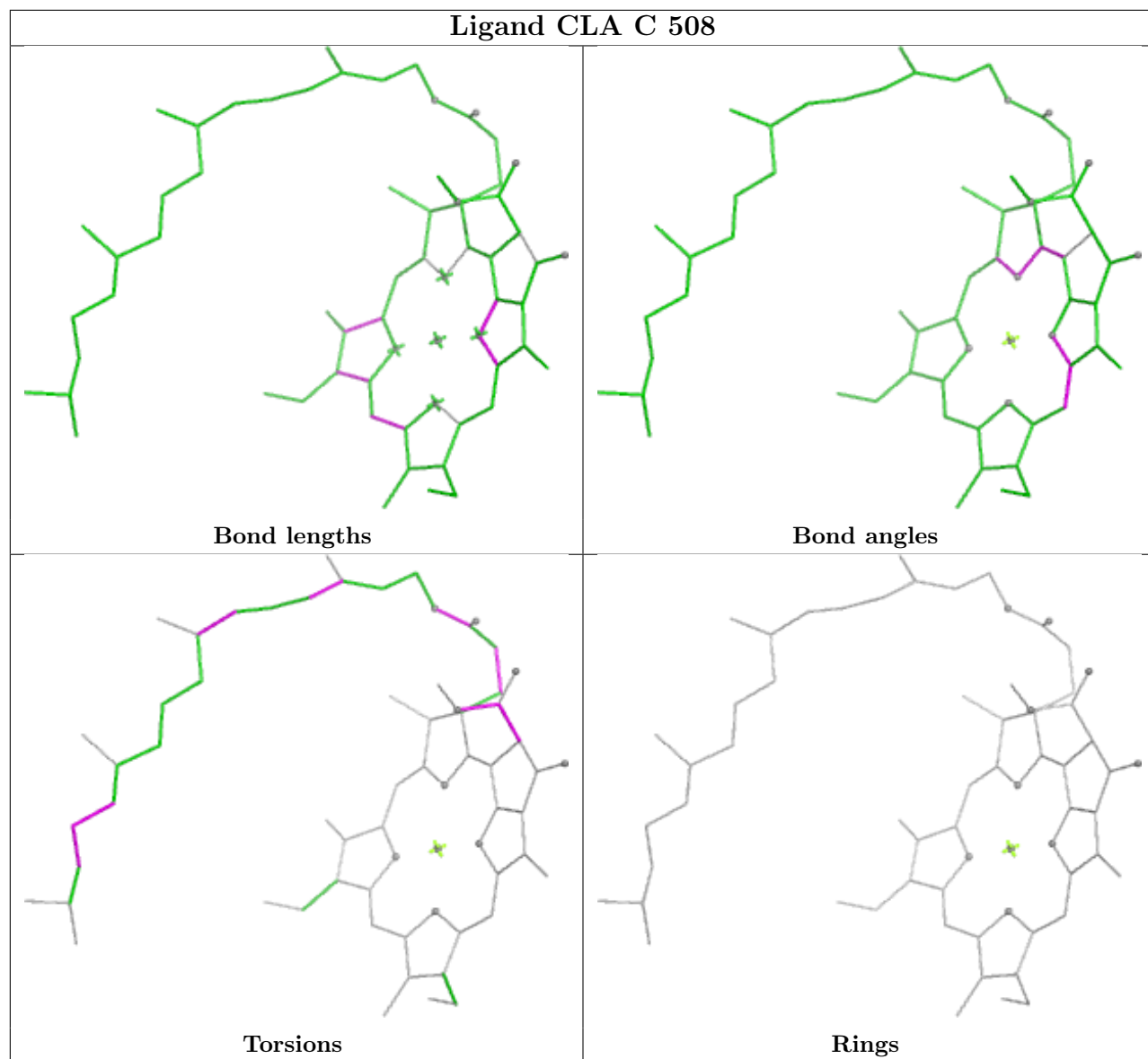


Ligand CLA B 510

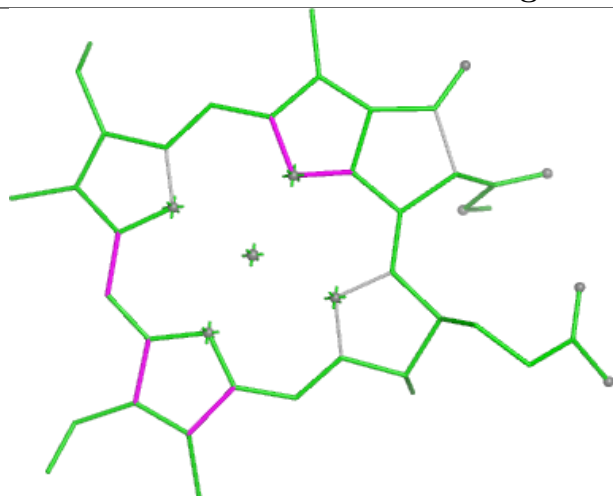




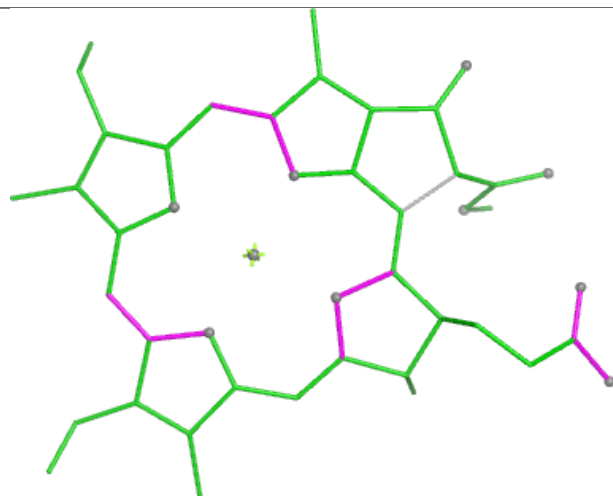




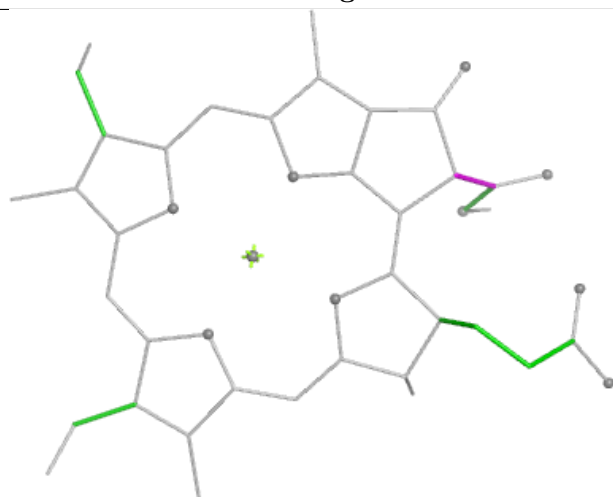
Ligand CLA s 313



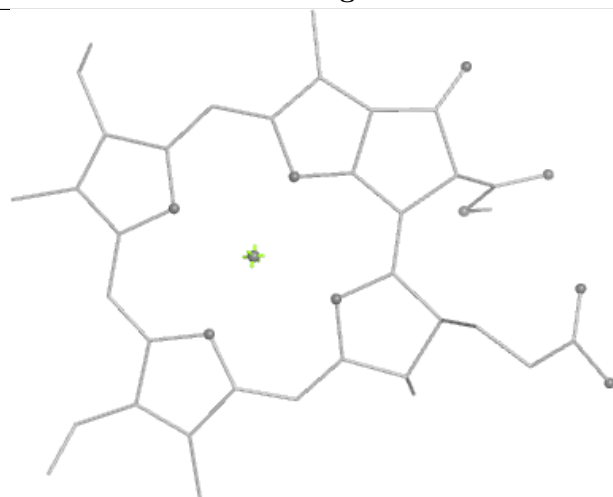
Bond lengths



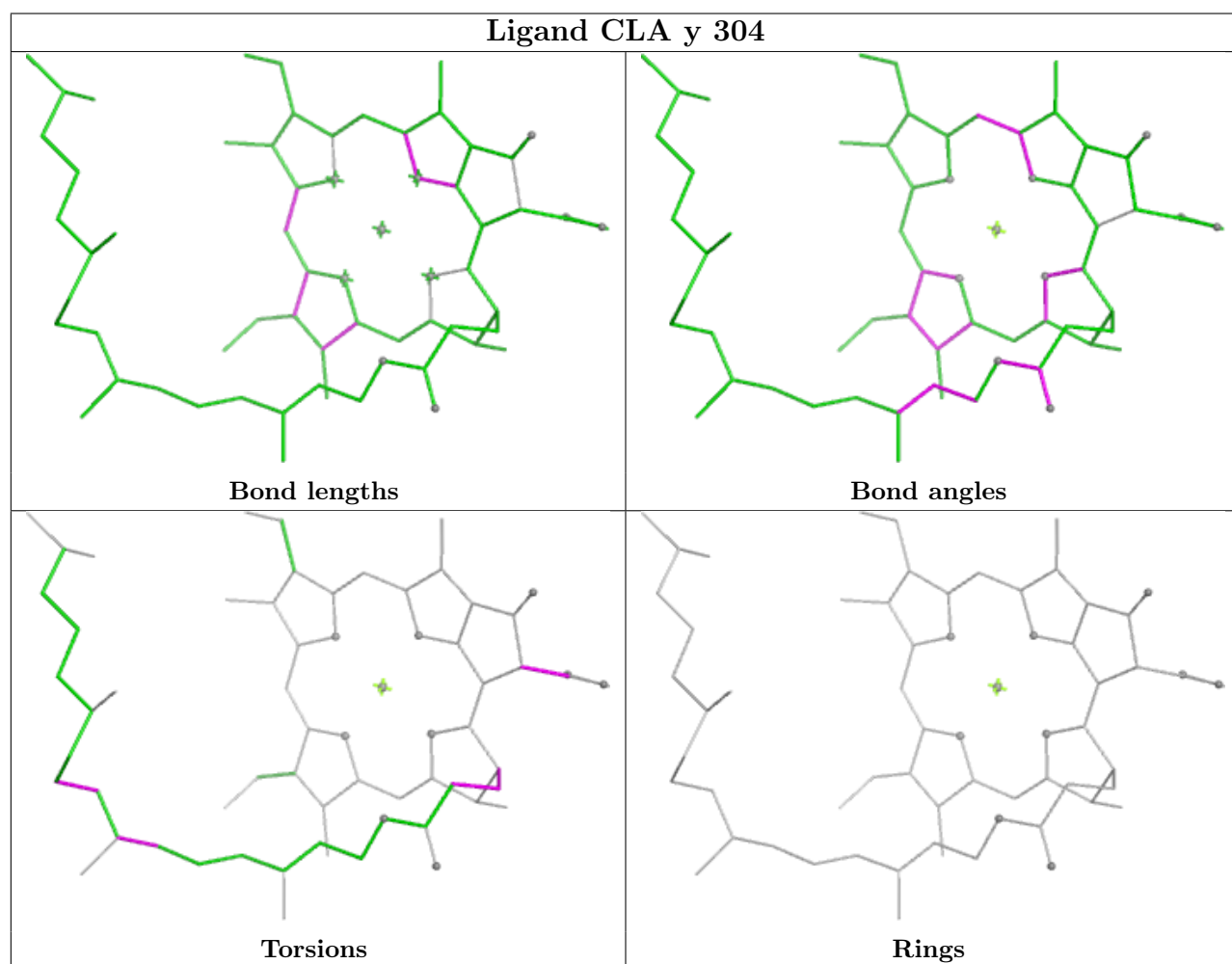
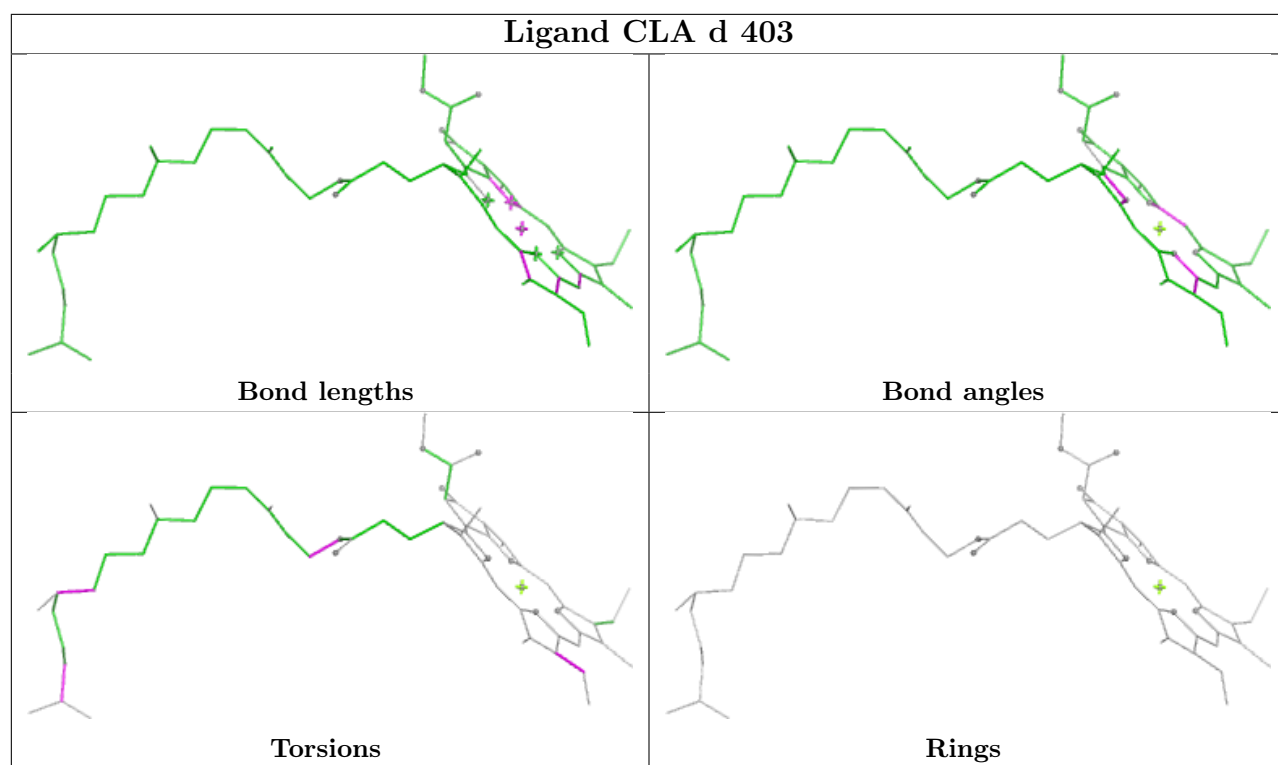
Bond angles

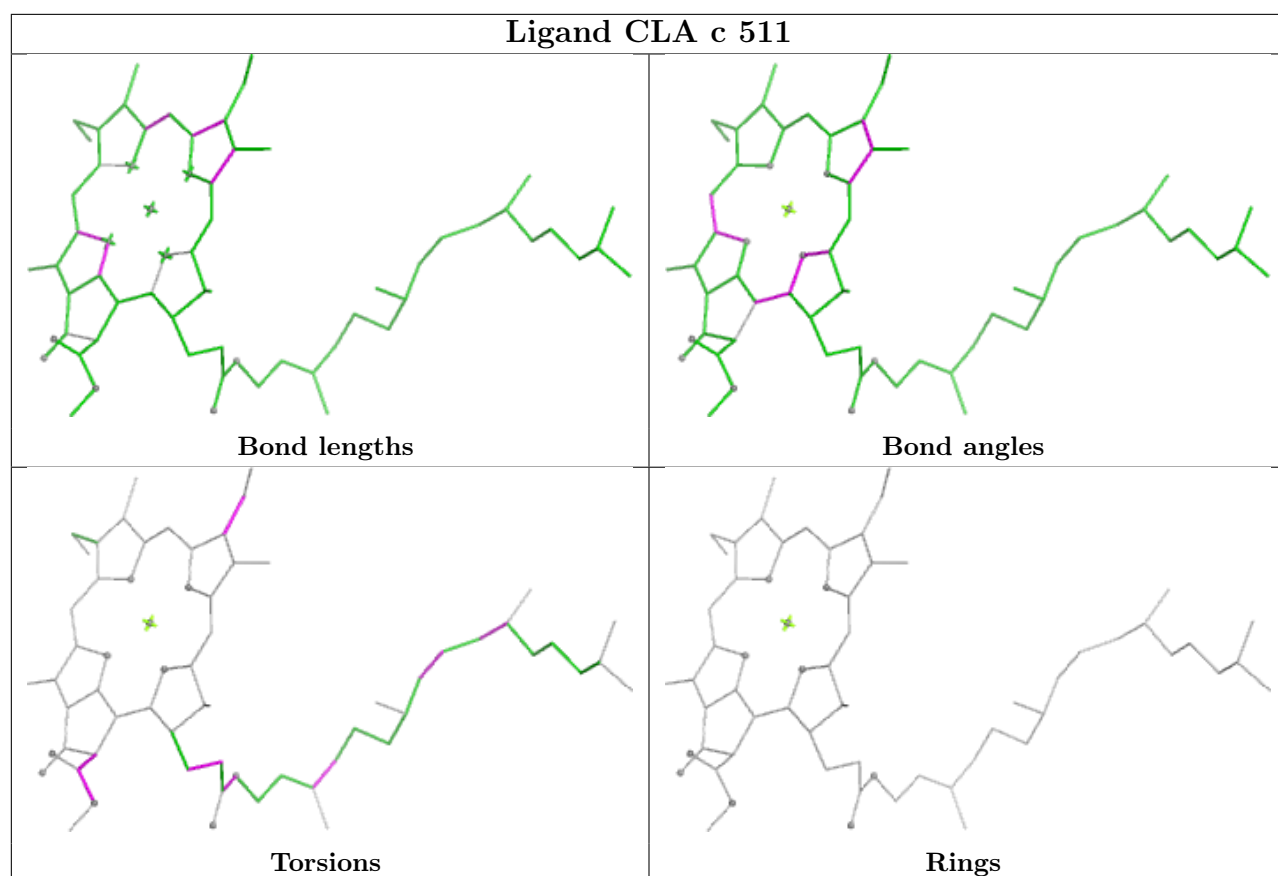


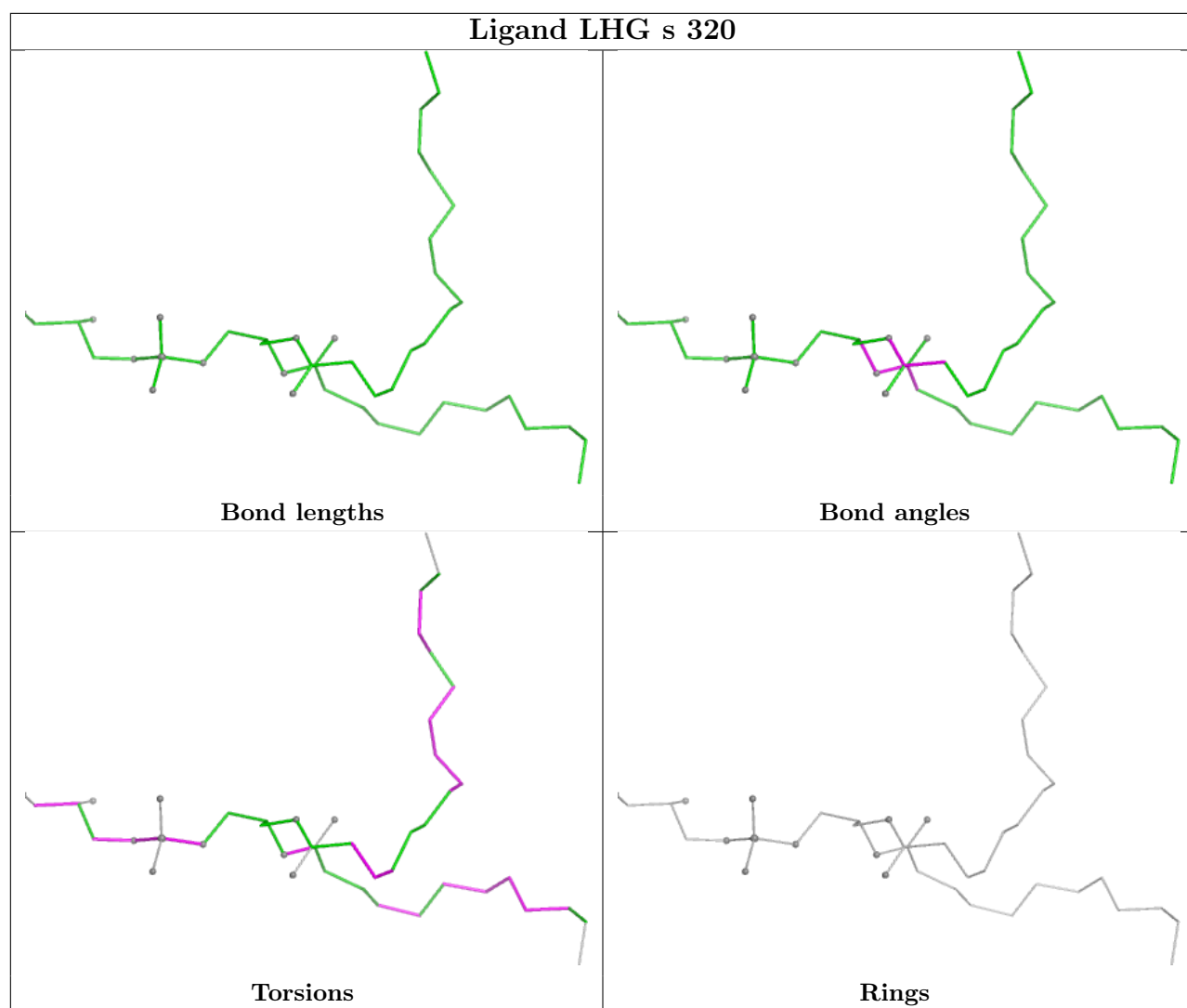
Torsions

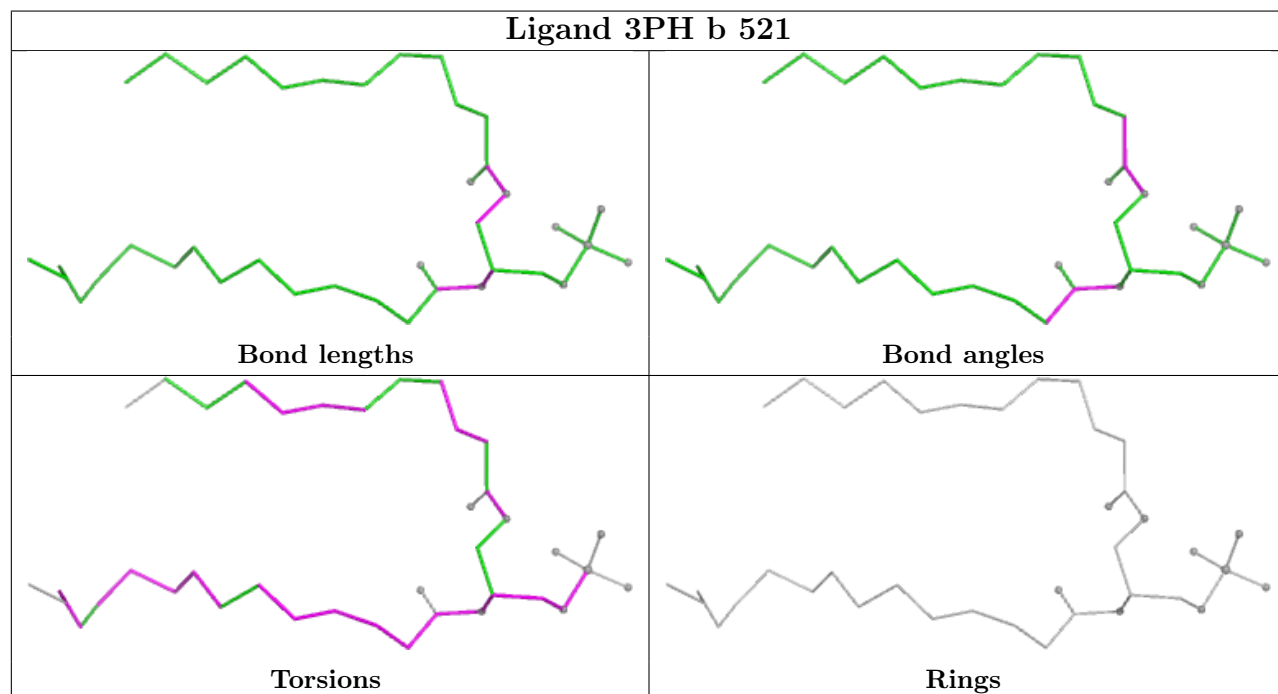
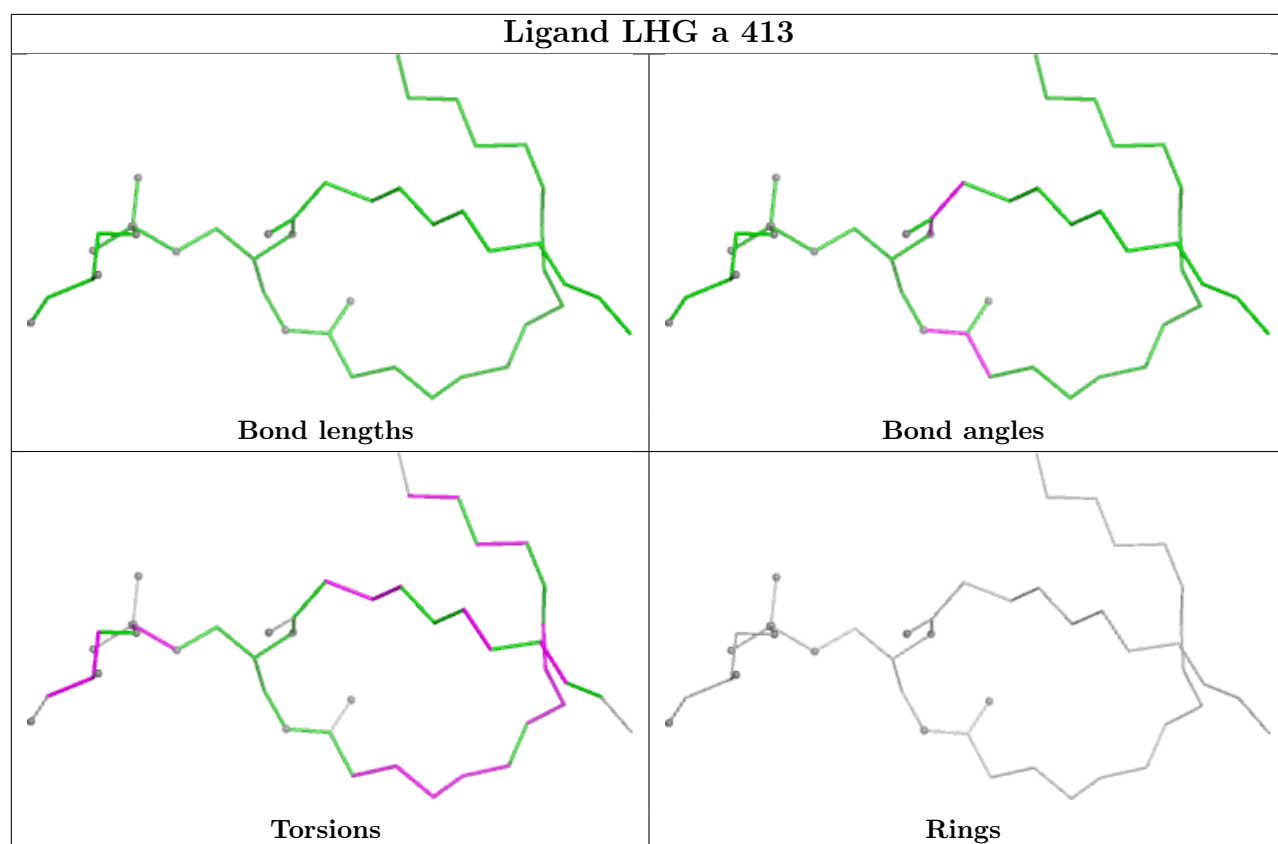


Rings

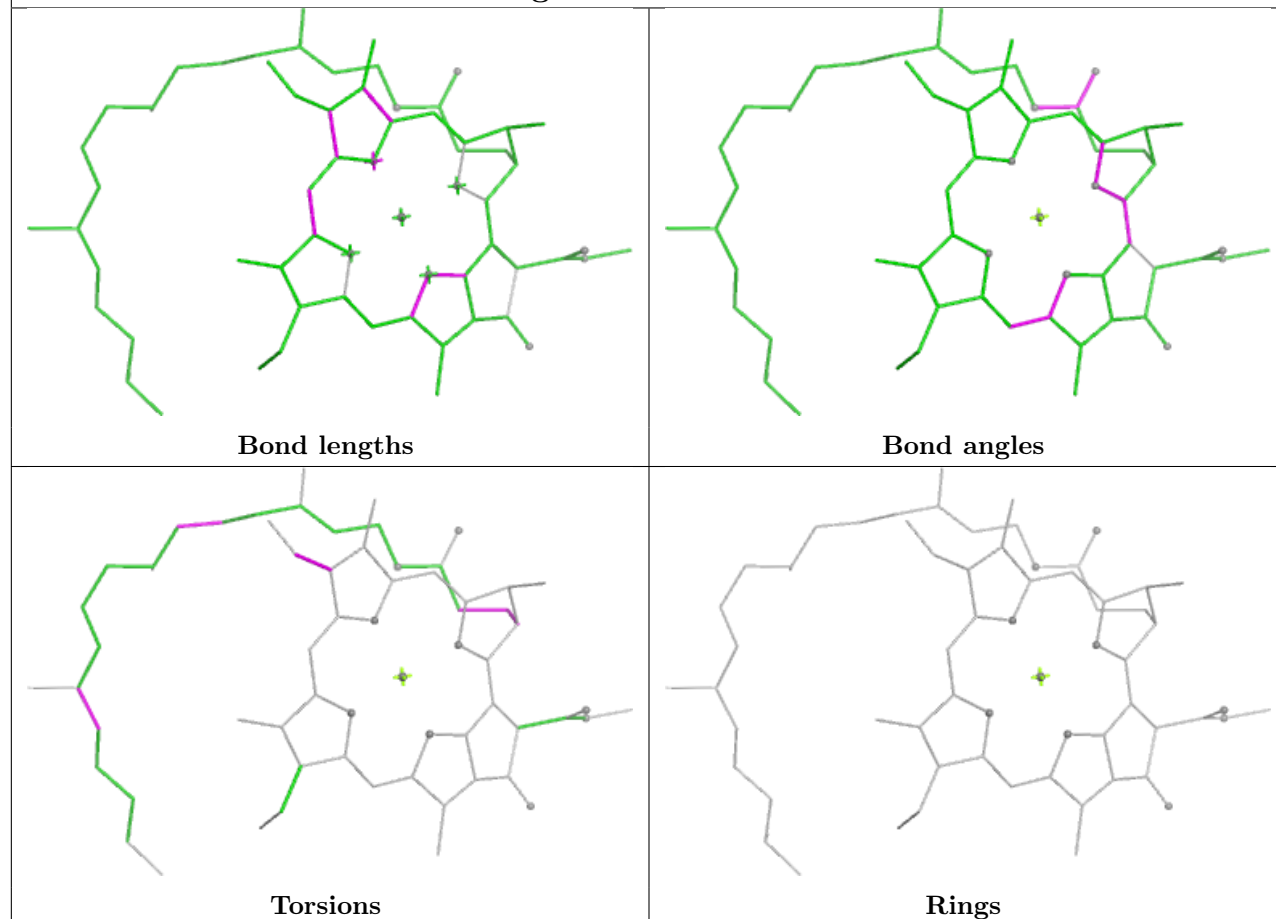




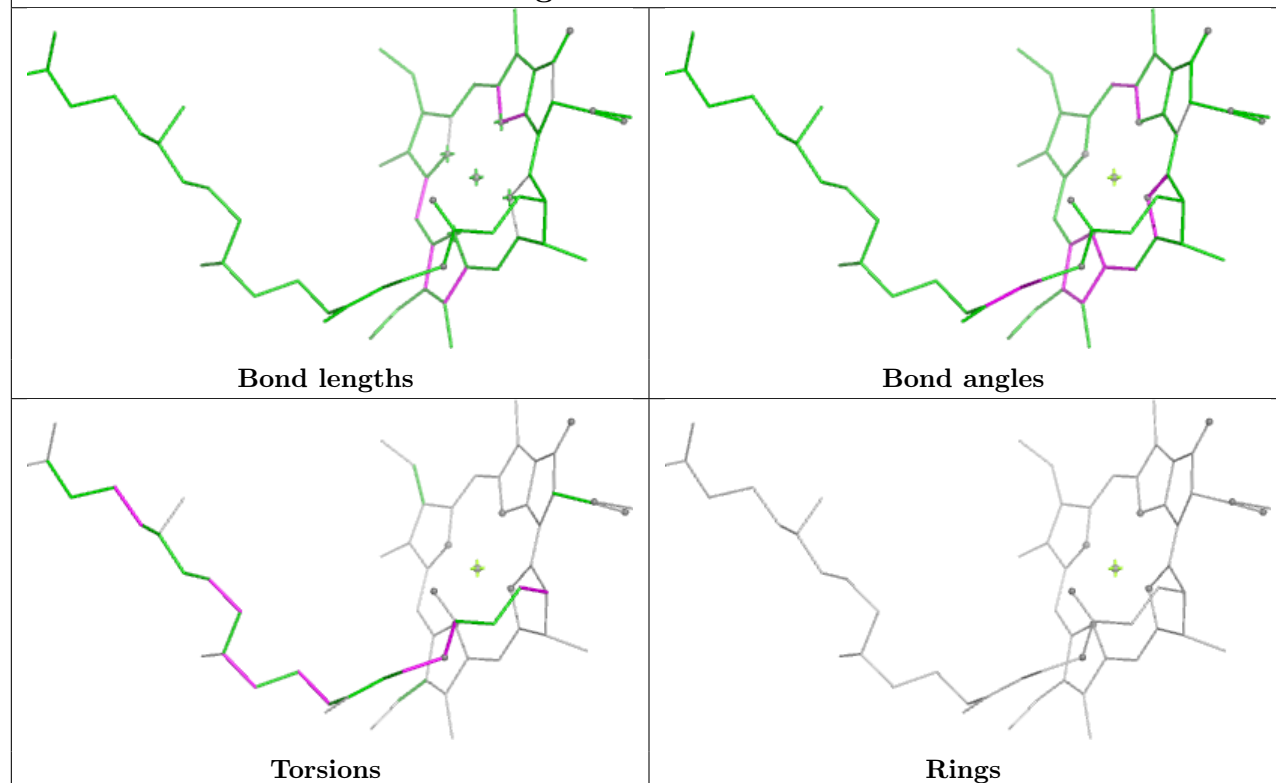


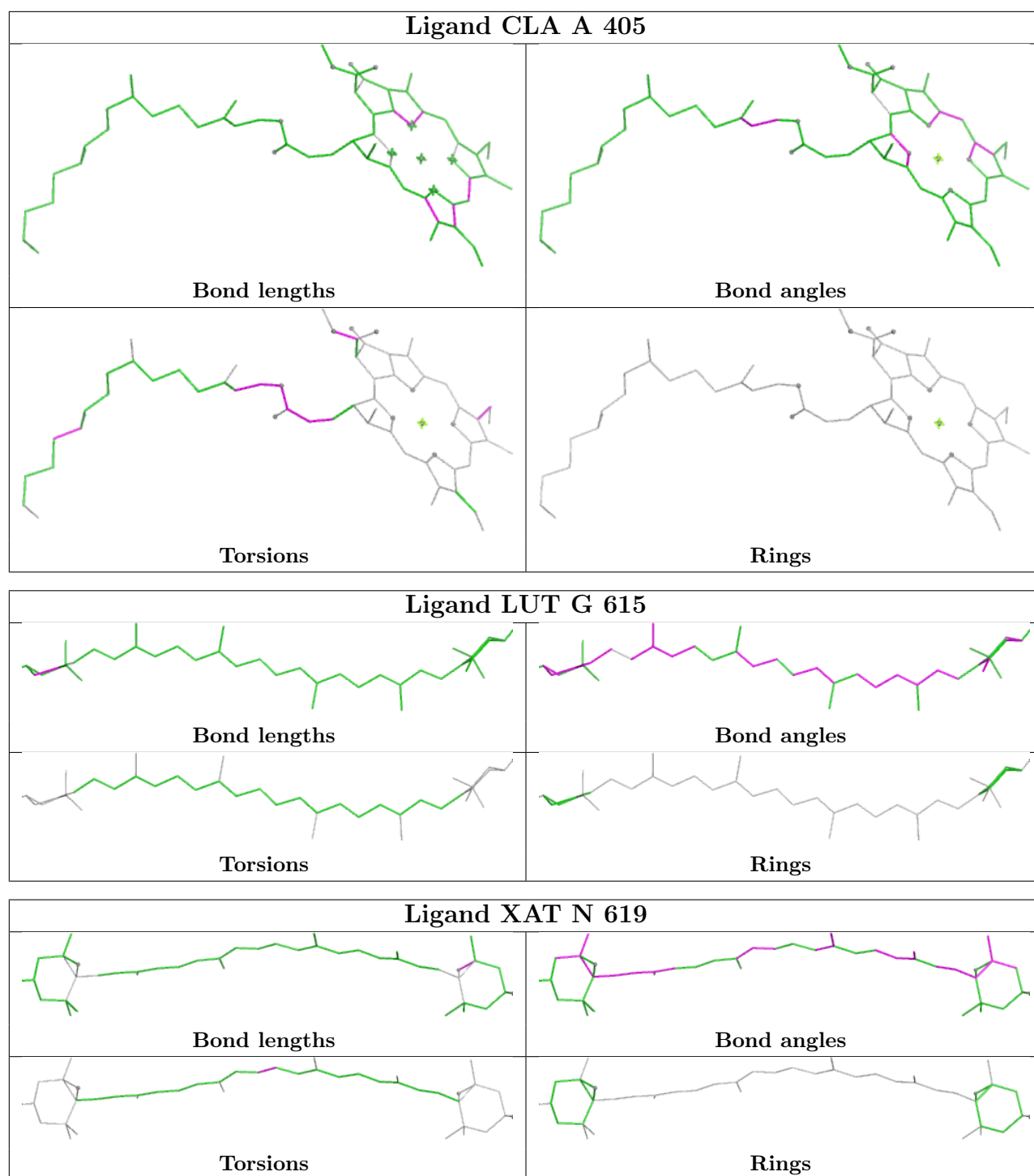


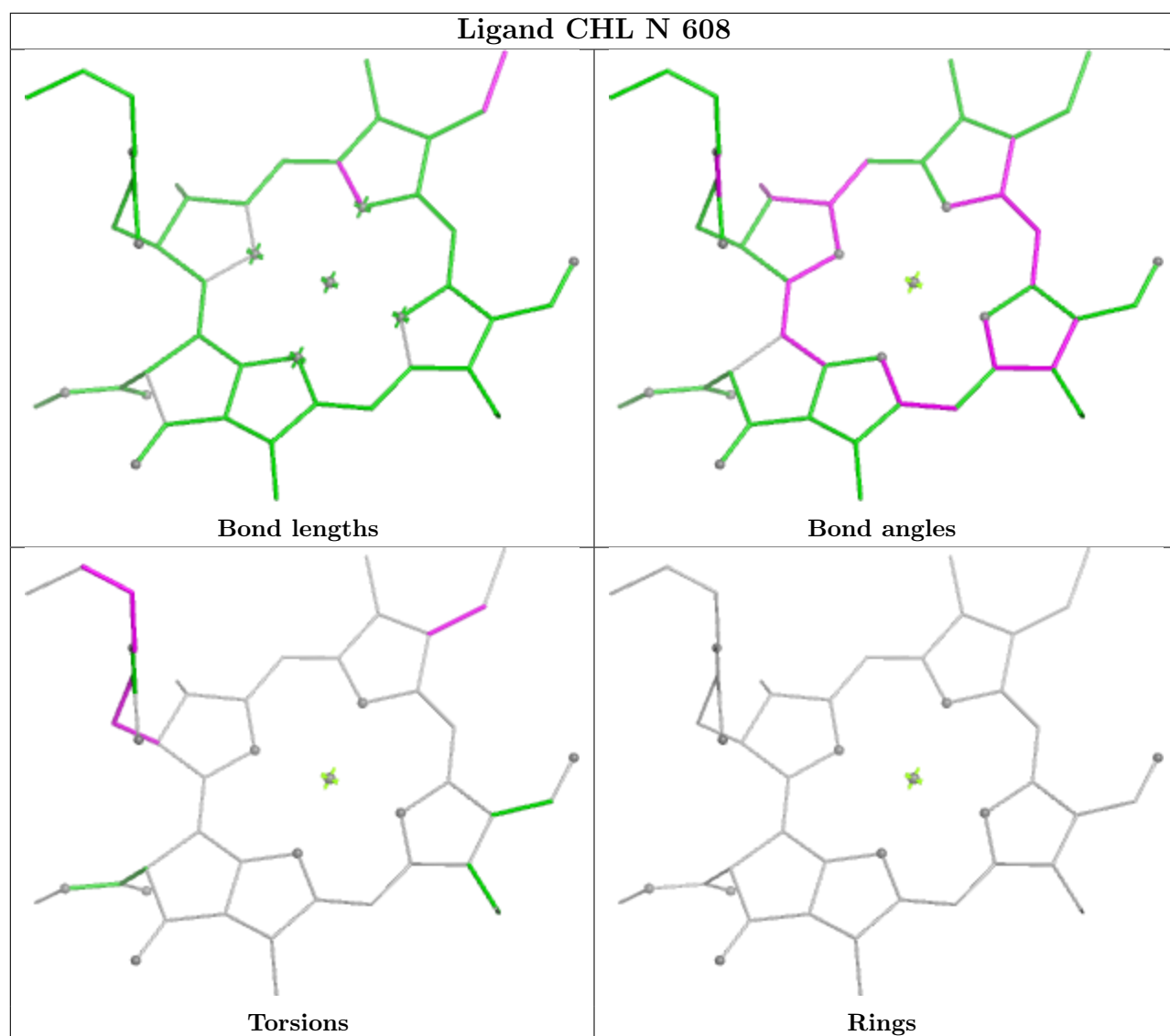
Ligand CLA Y 311

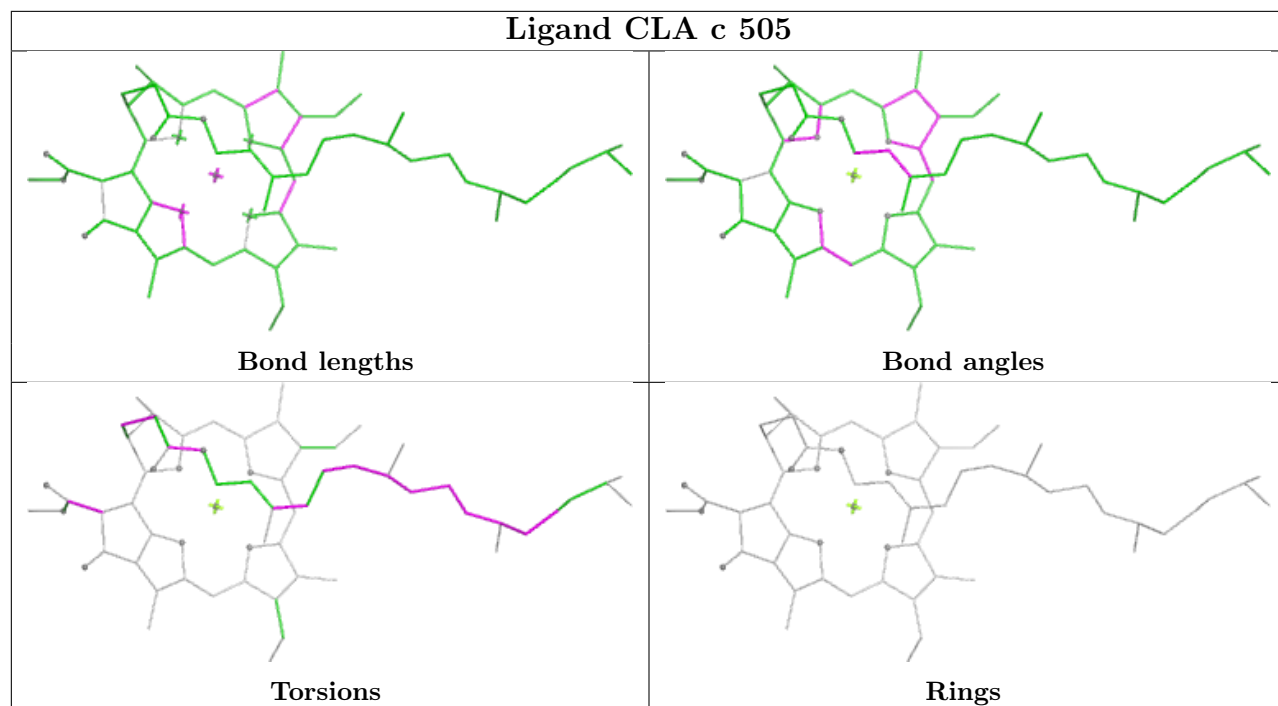


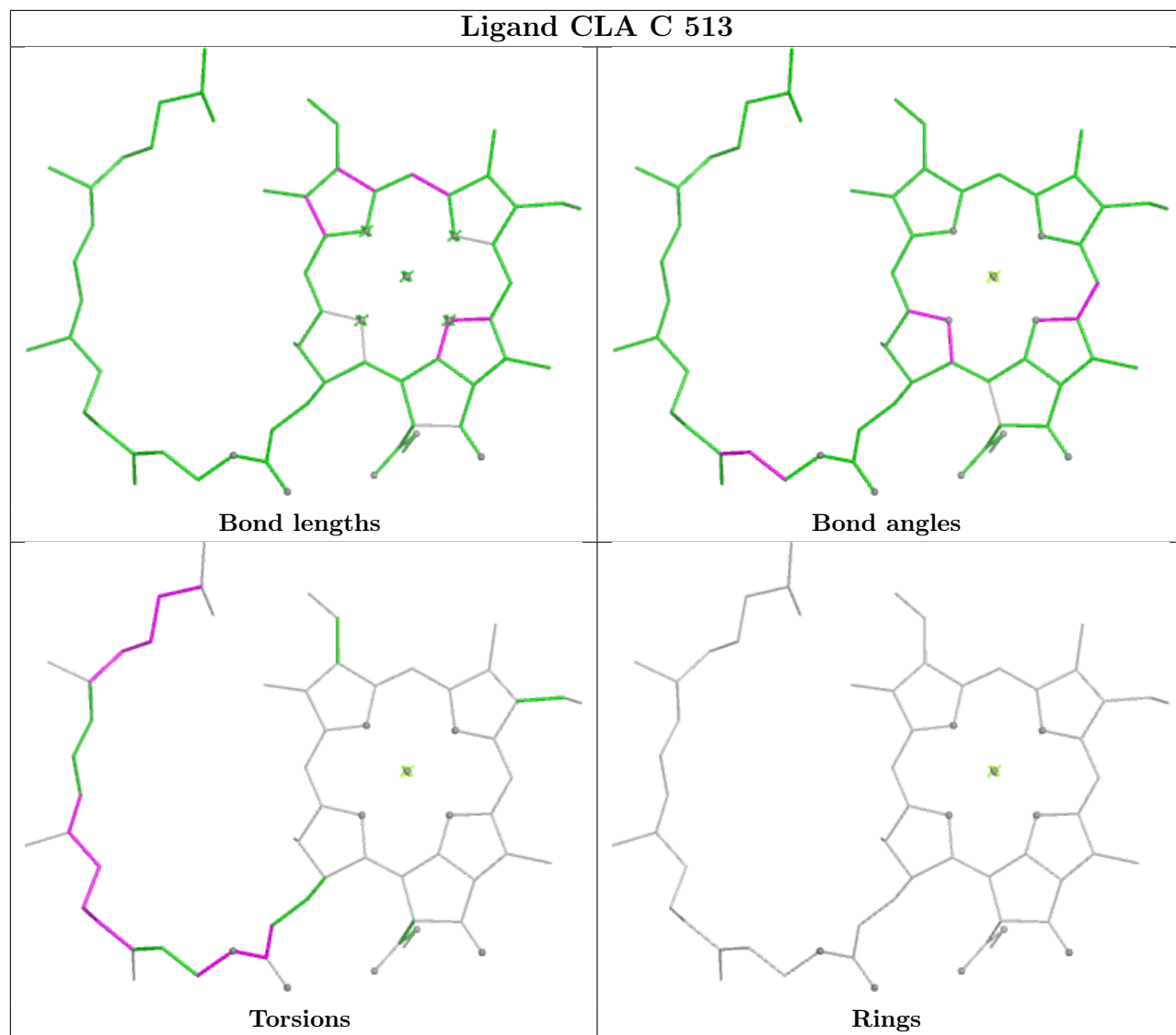
Ligand CLA S 311

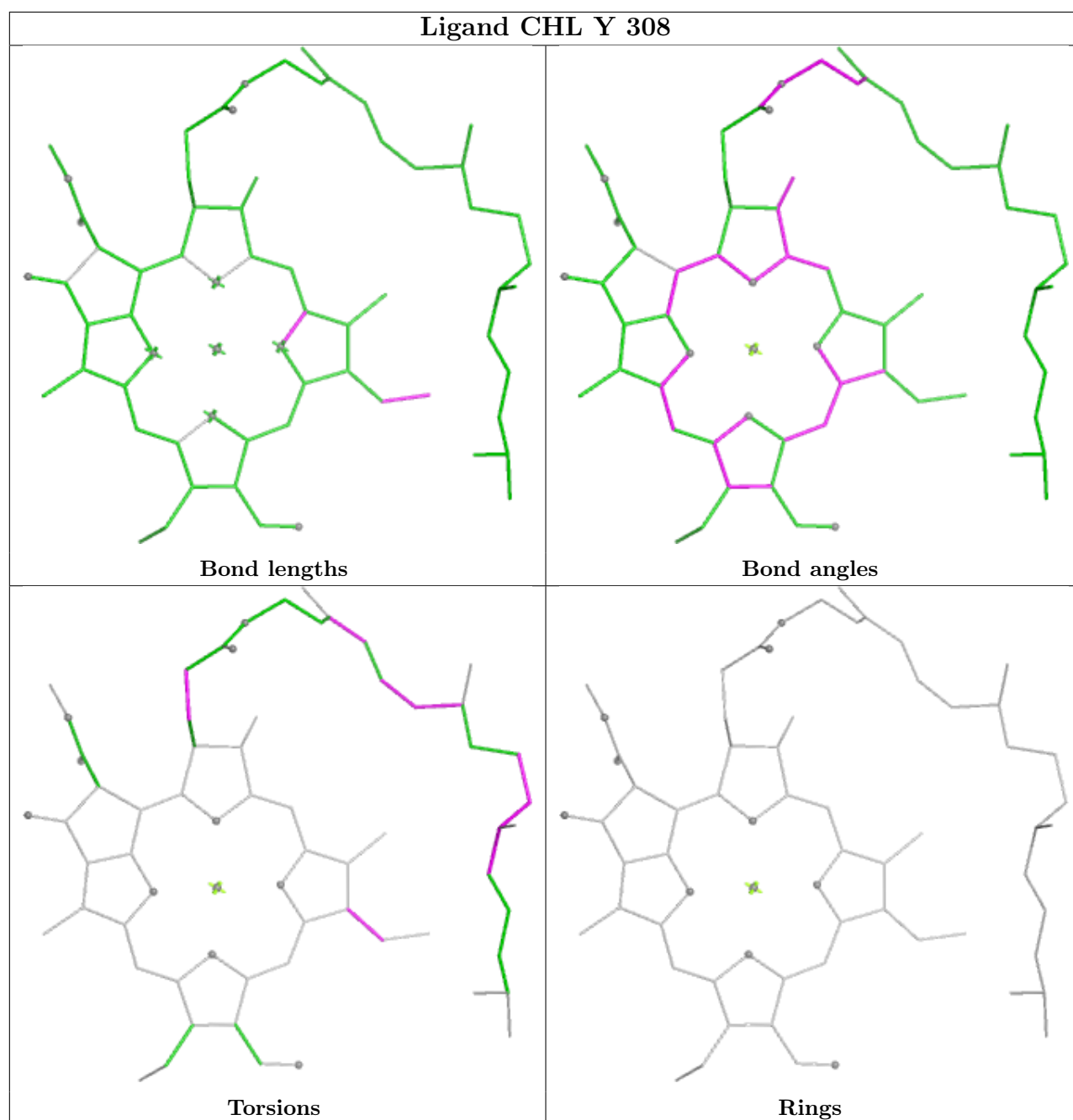


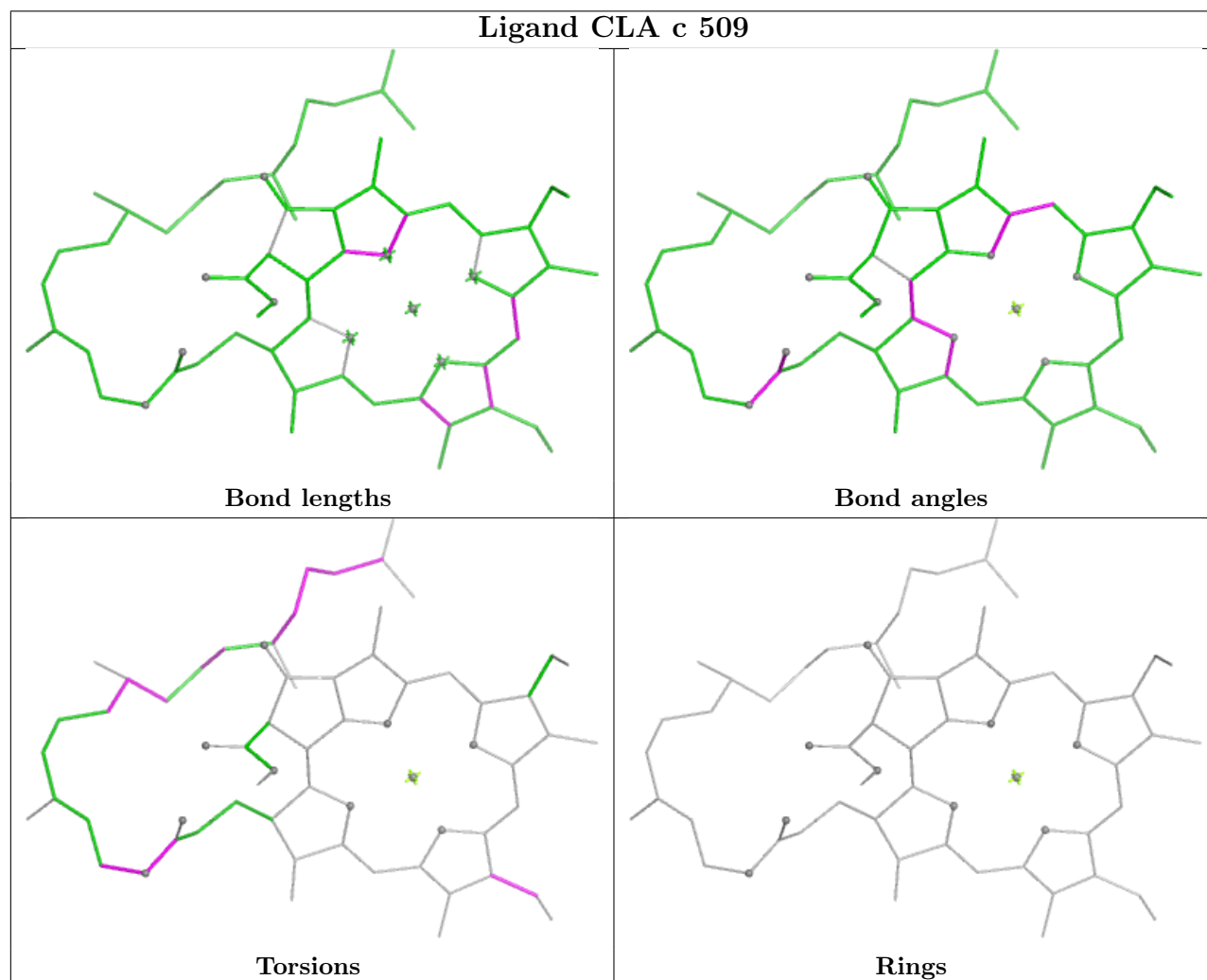
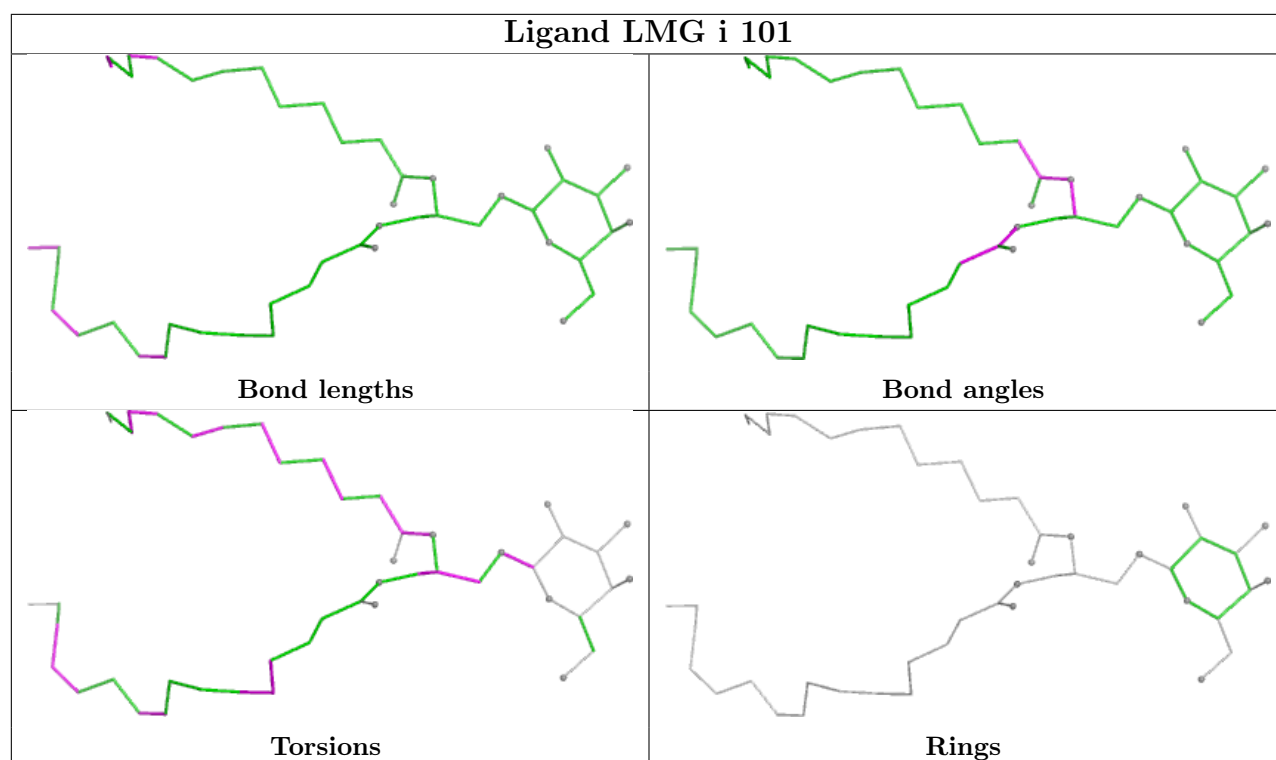


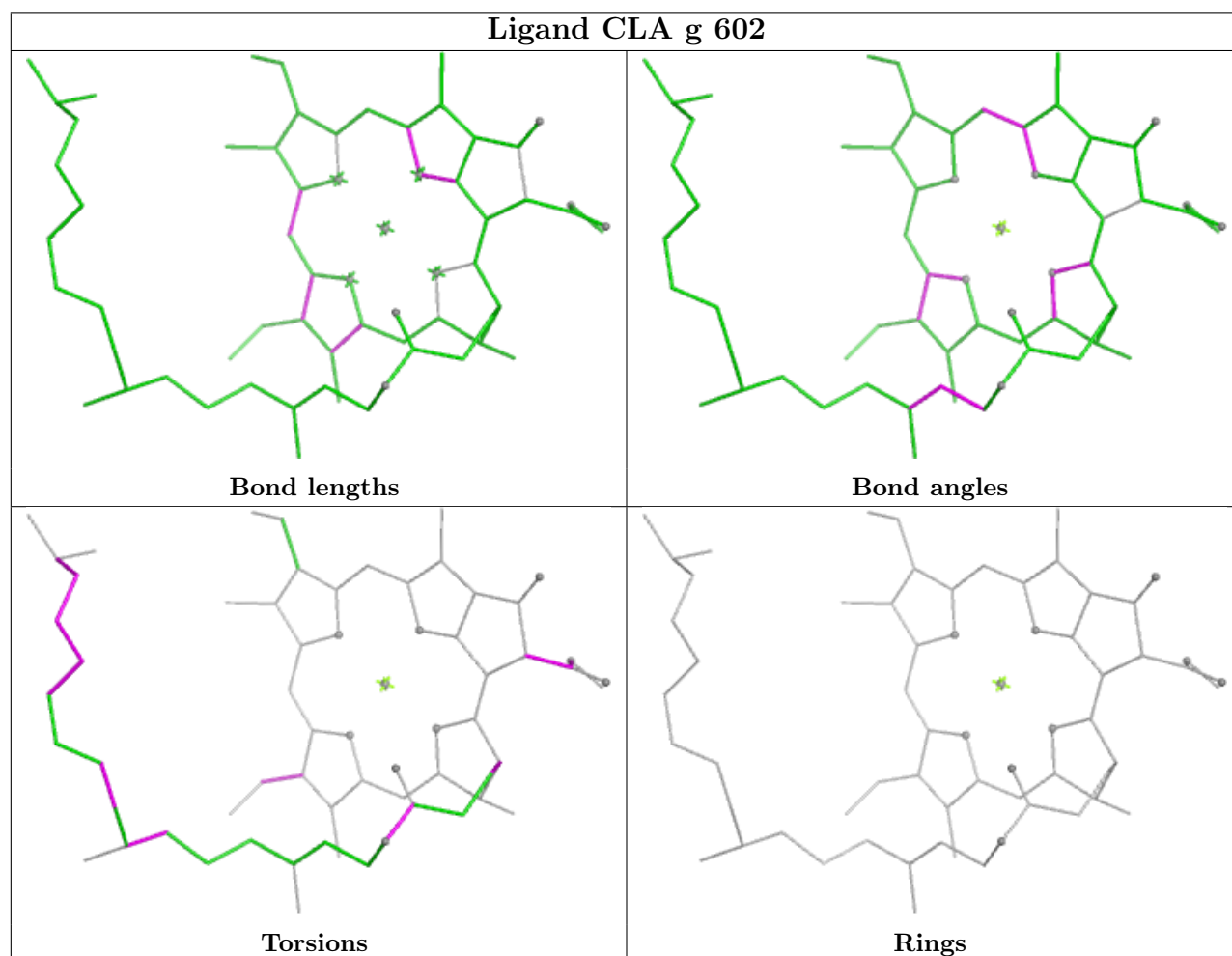
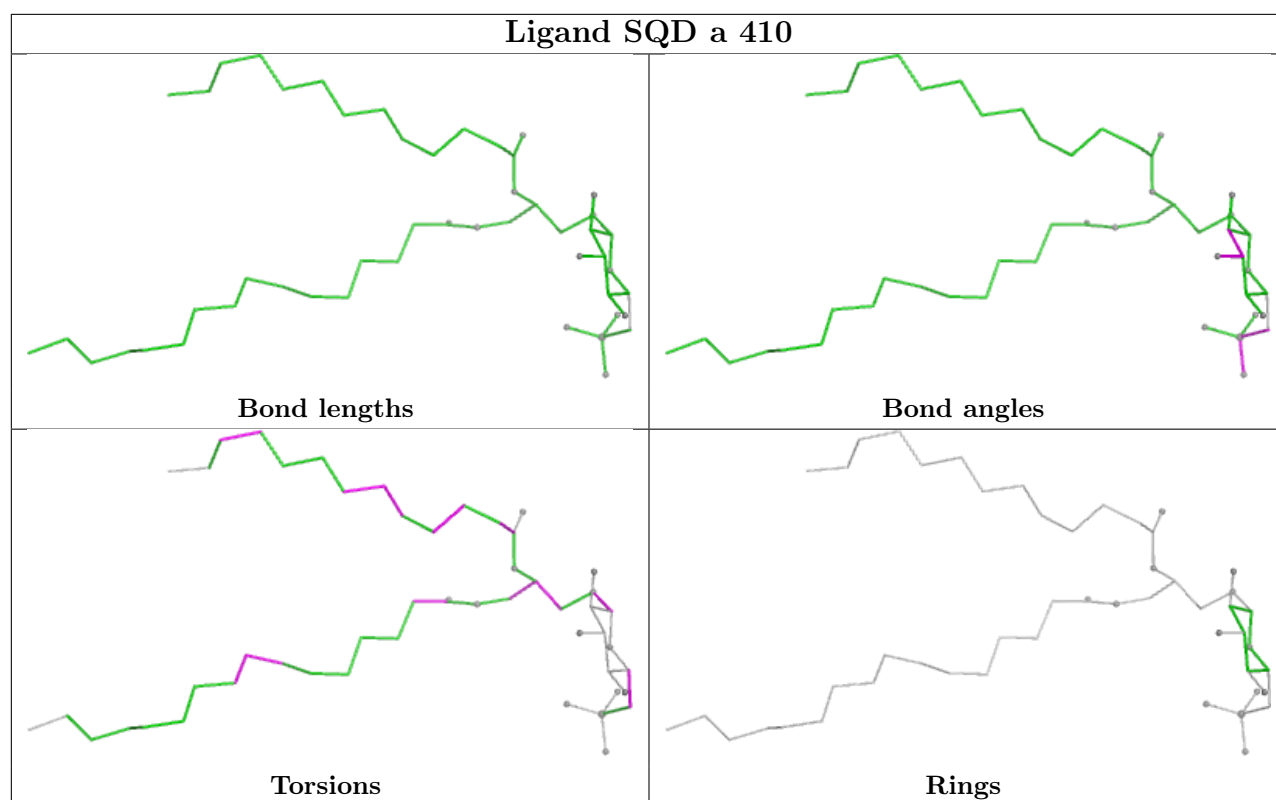


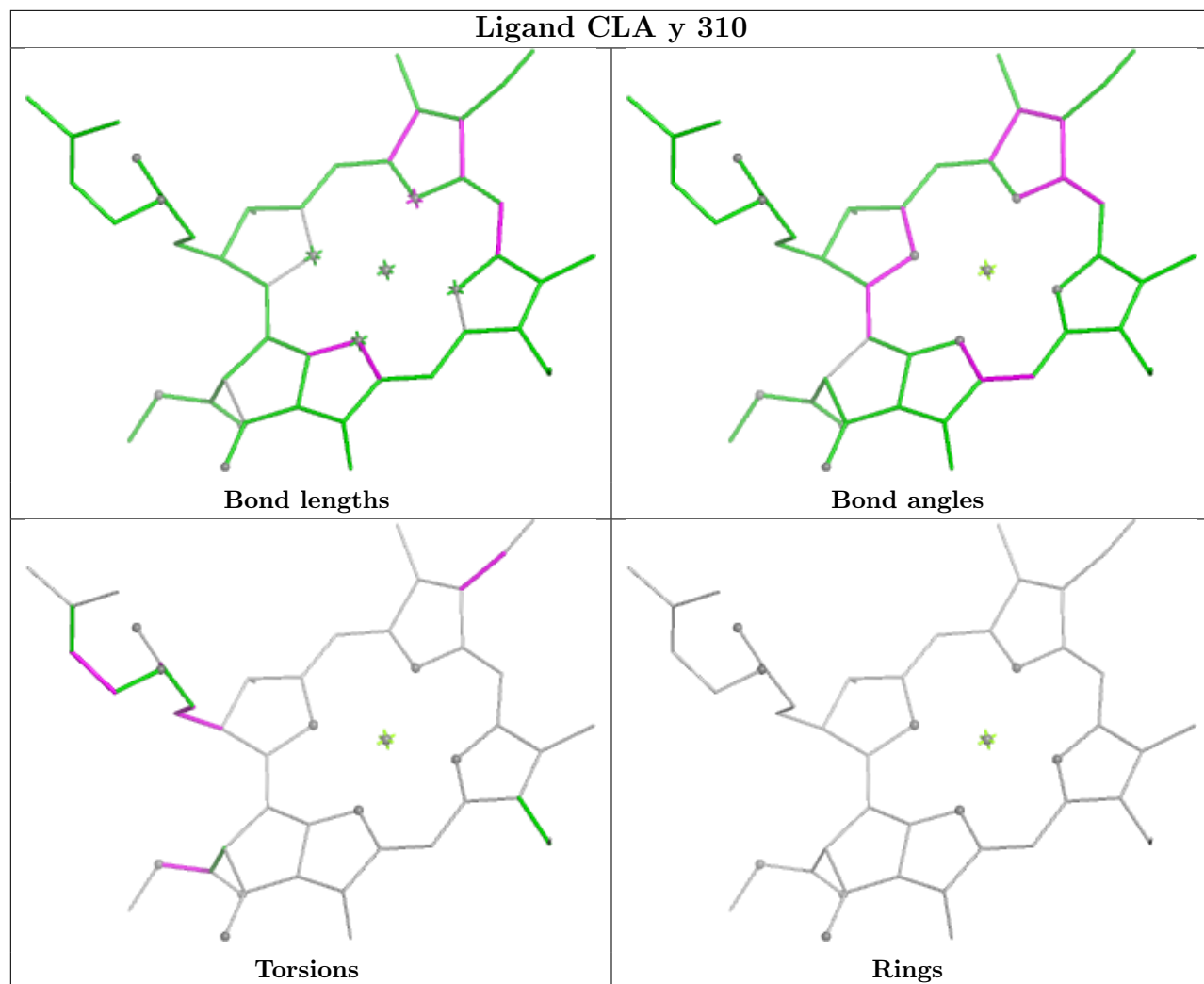


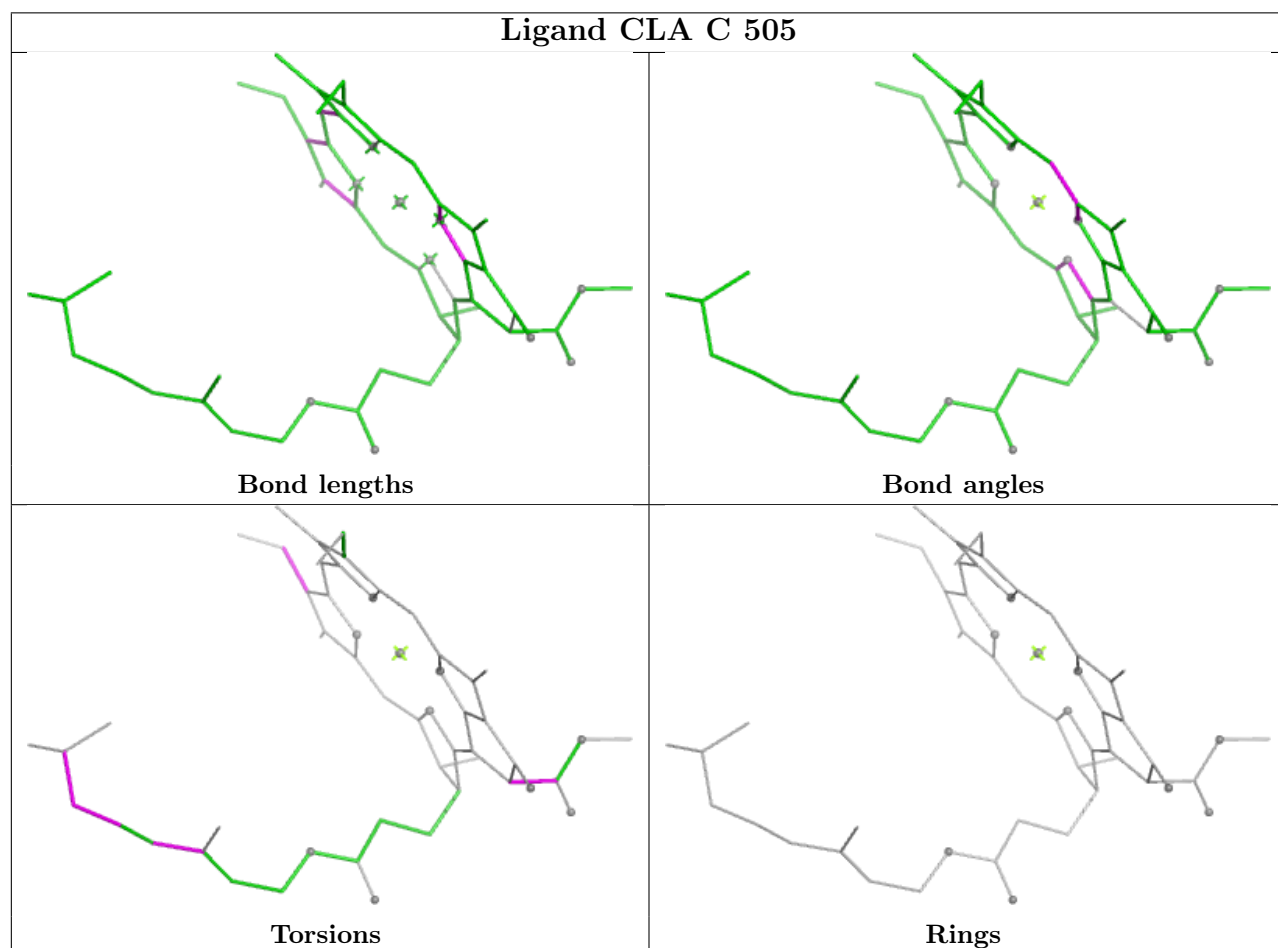
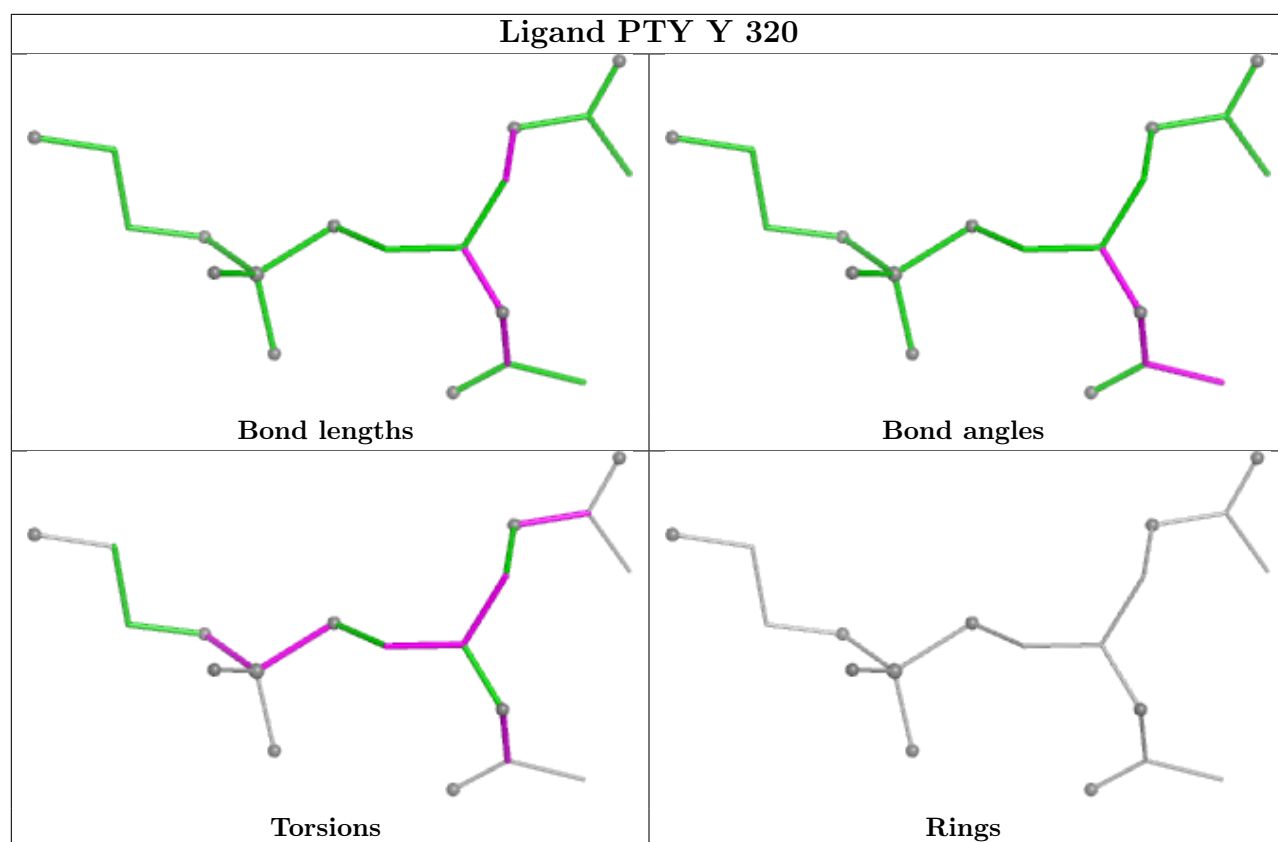


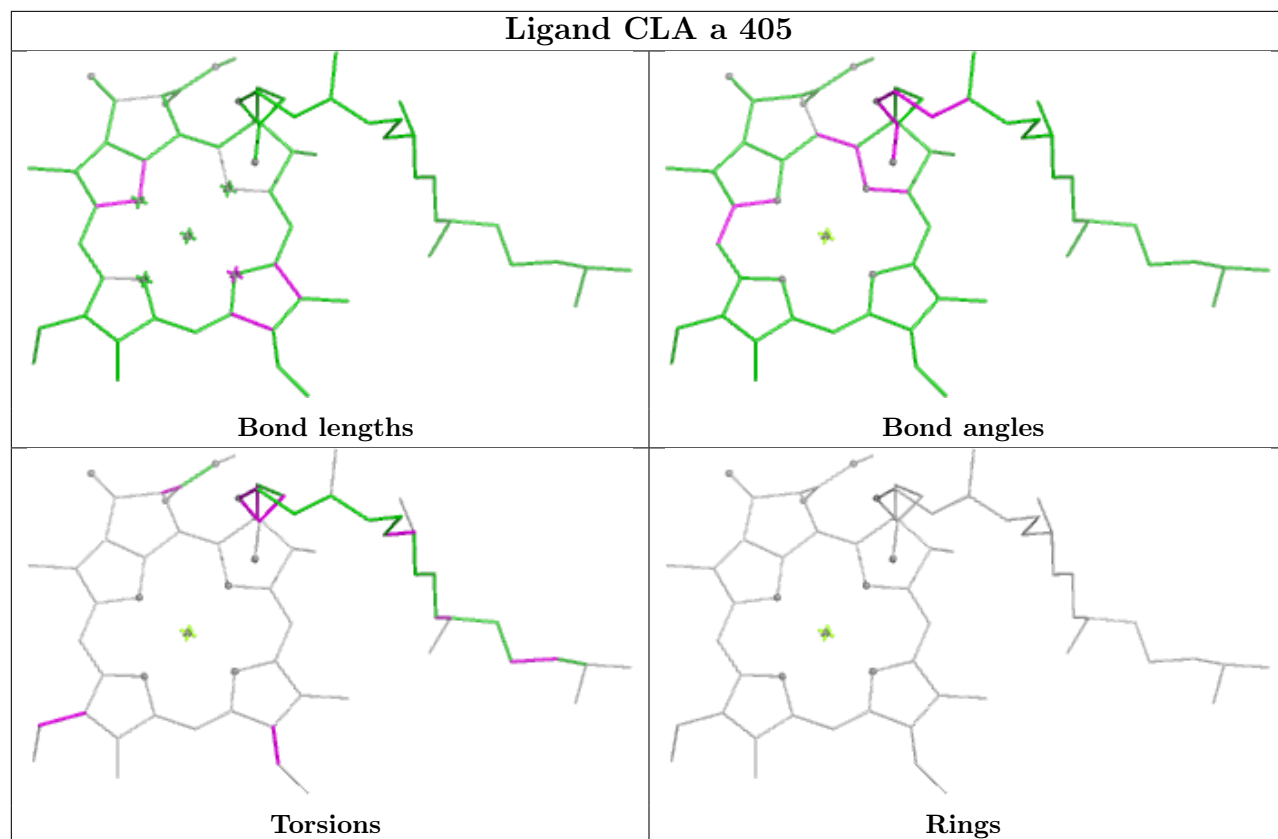




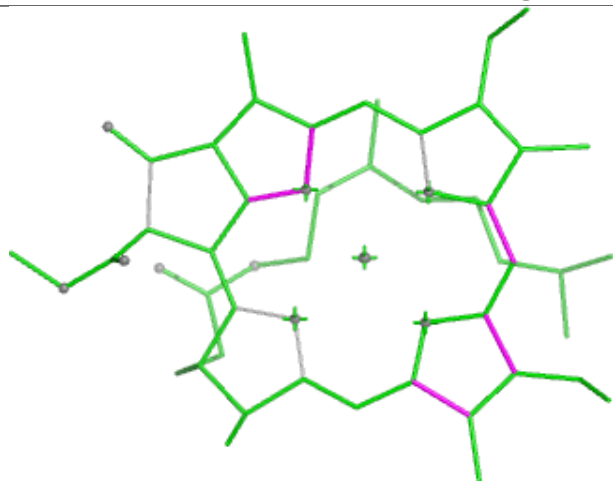




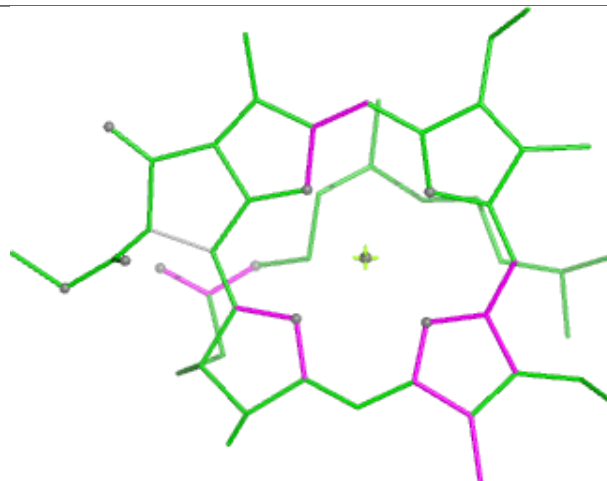




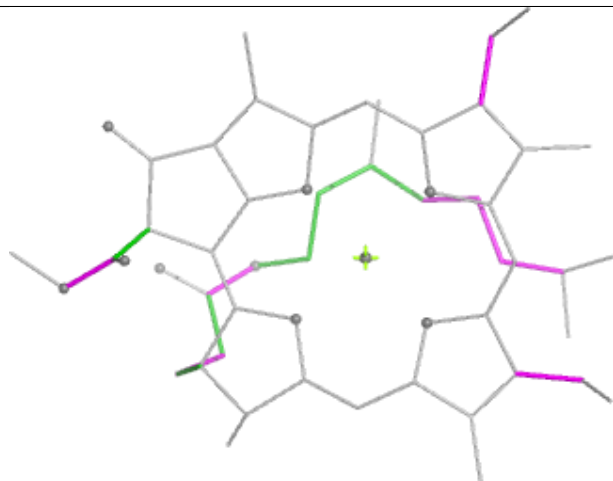
Ligand CLA S 314



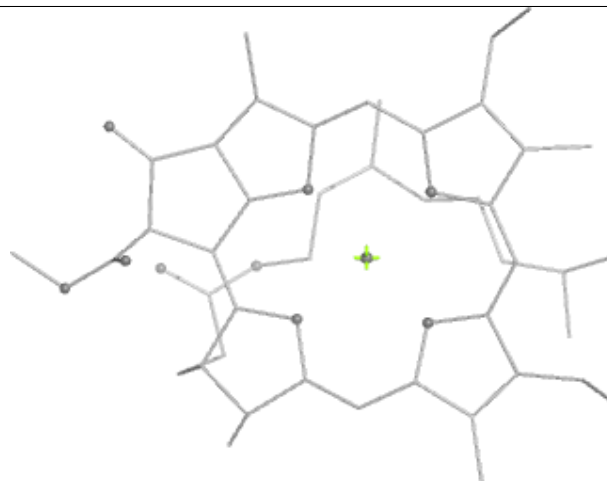
Bond lengths



Bond angles

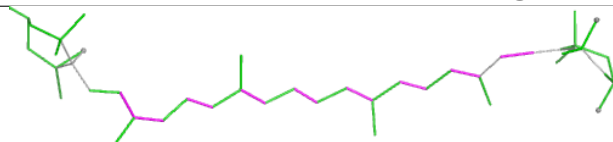


Torsions

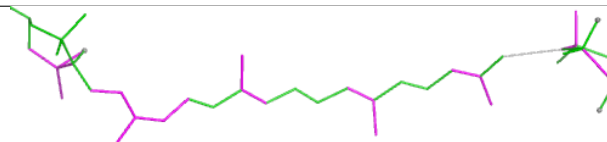


Rings

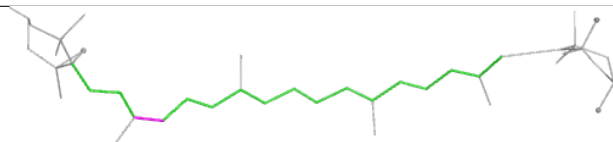
Ligand NEX N 617



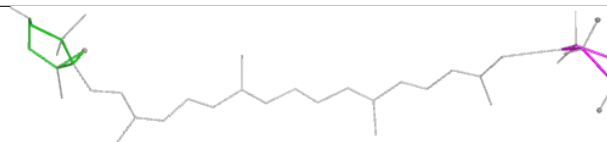
Bond lengths



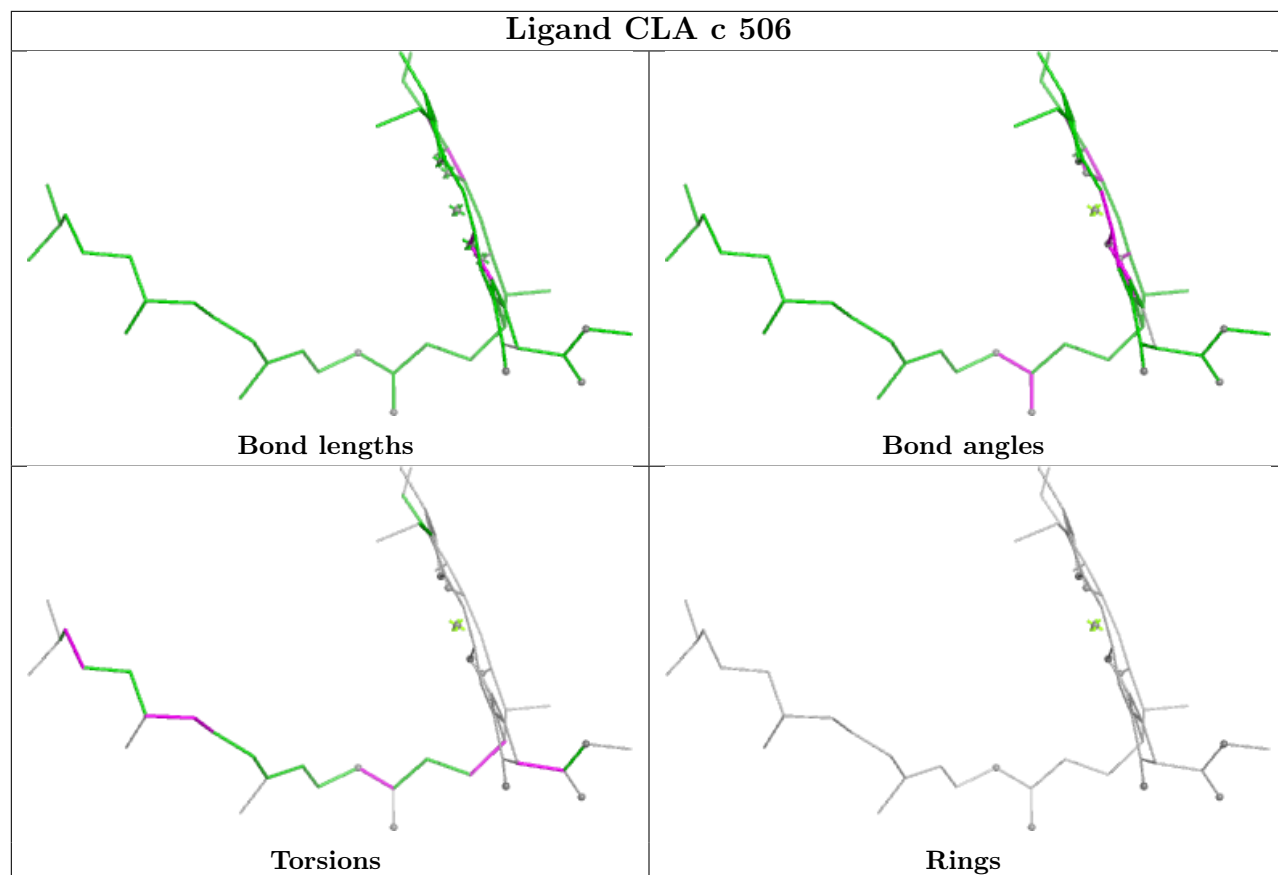
Bond angles

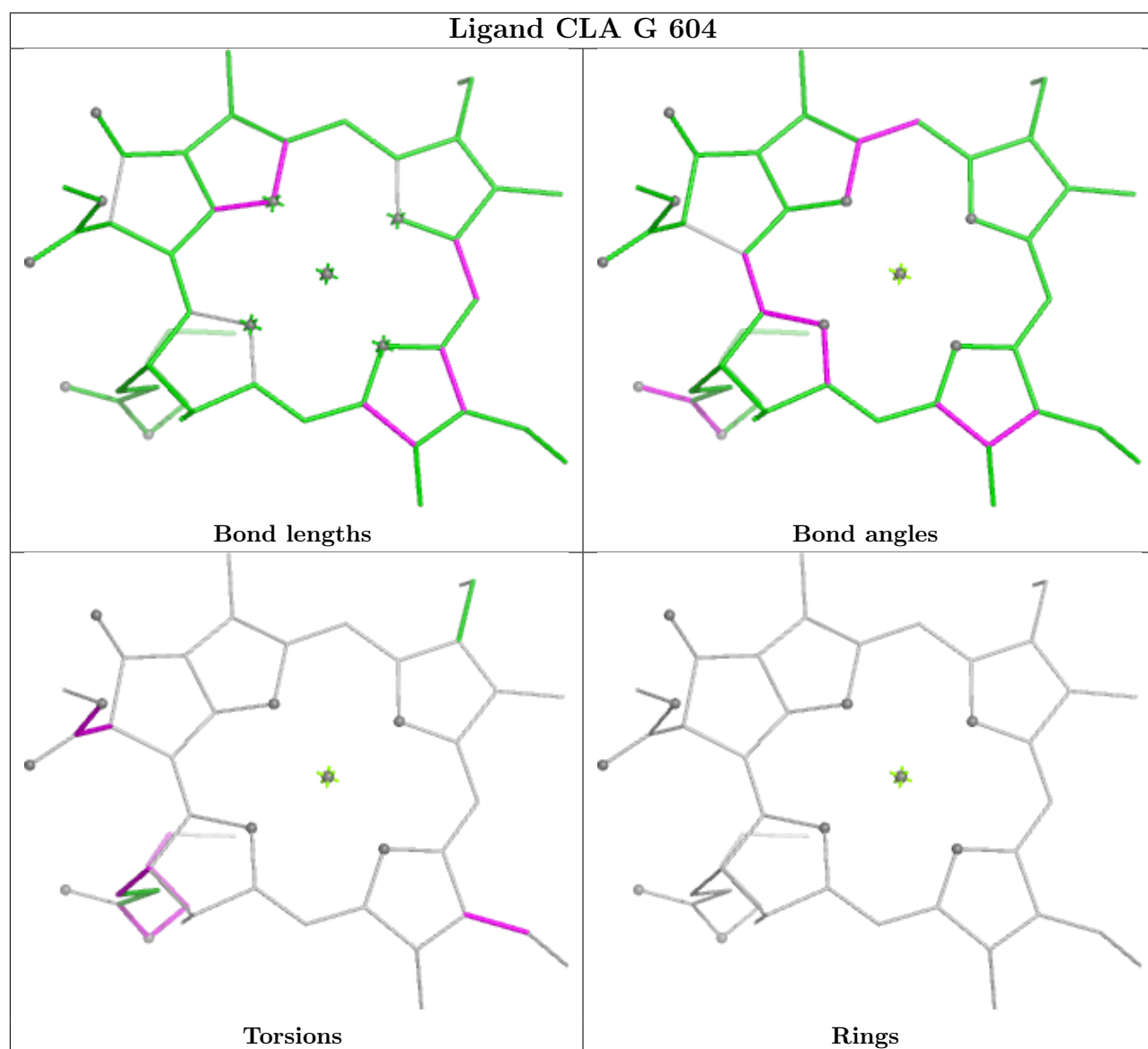


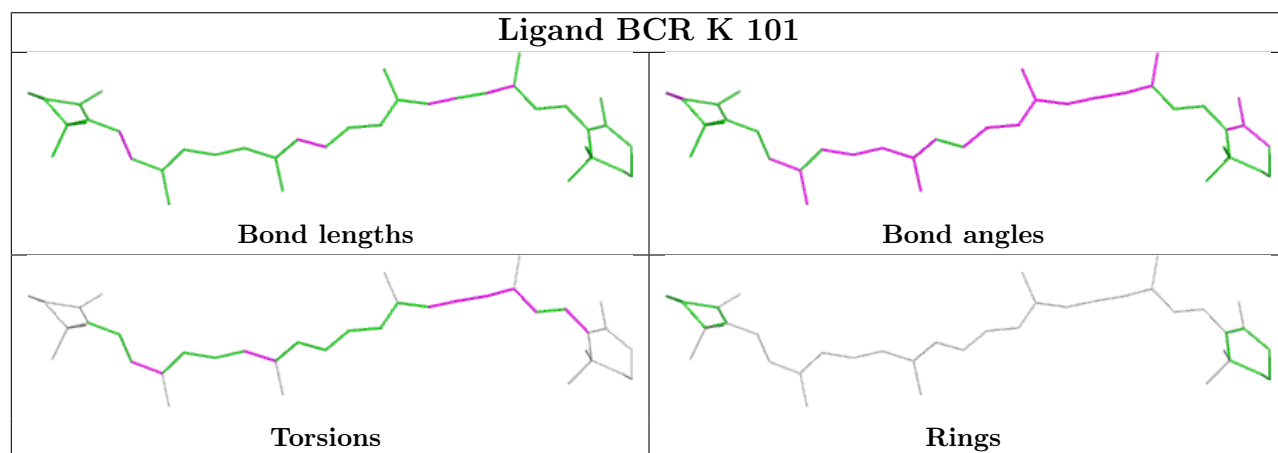
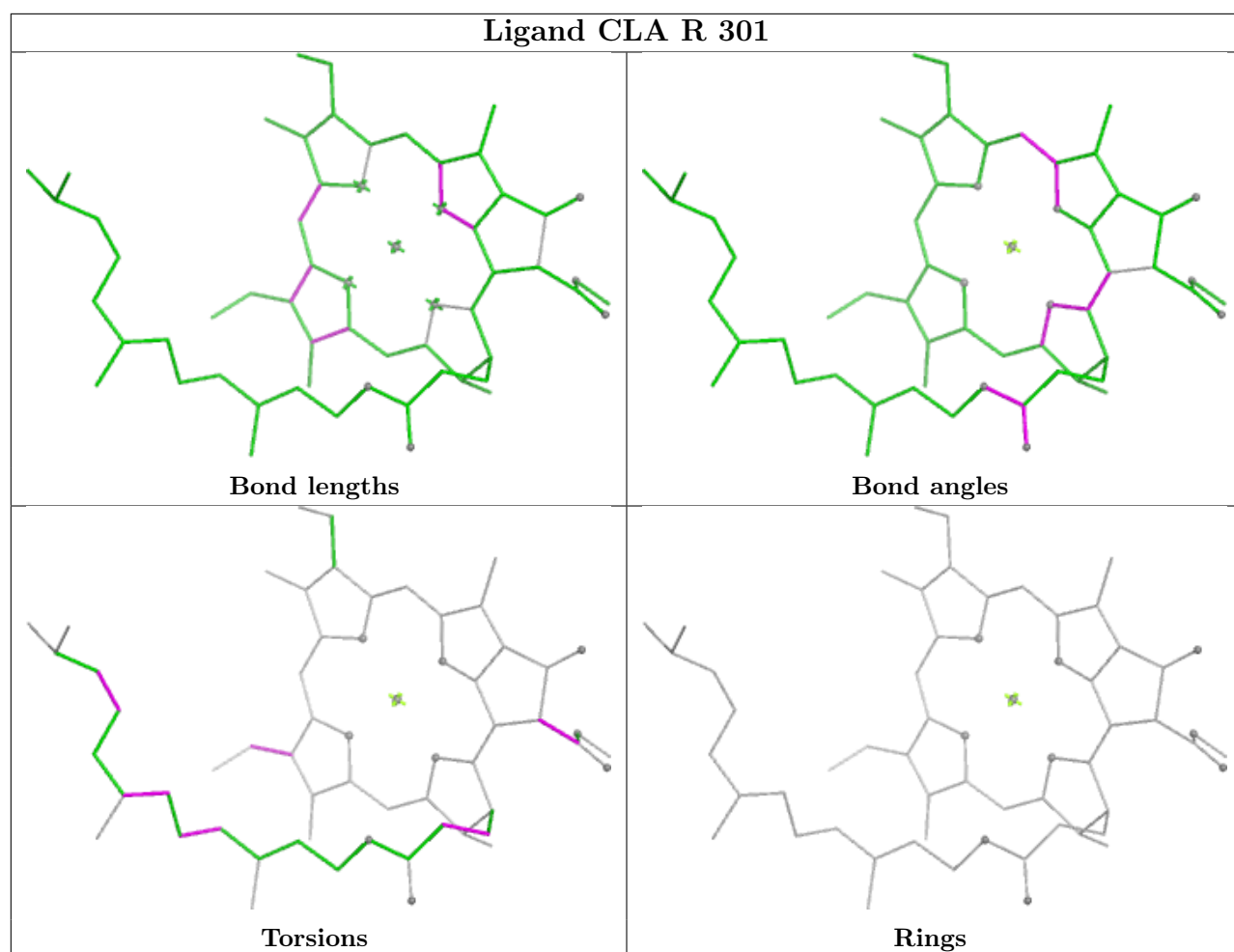
Torsions

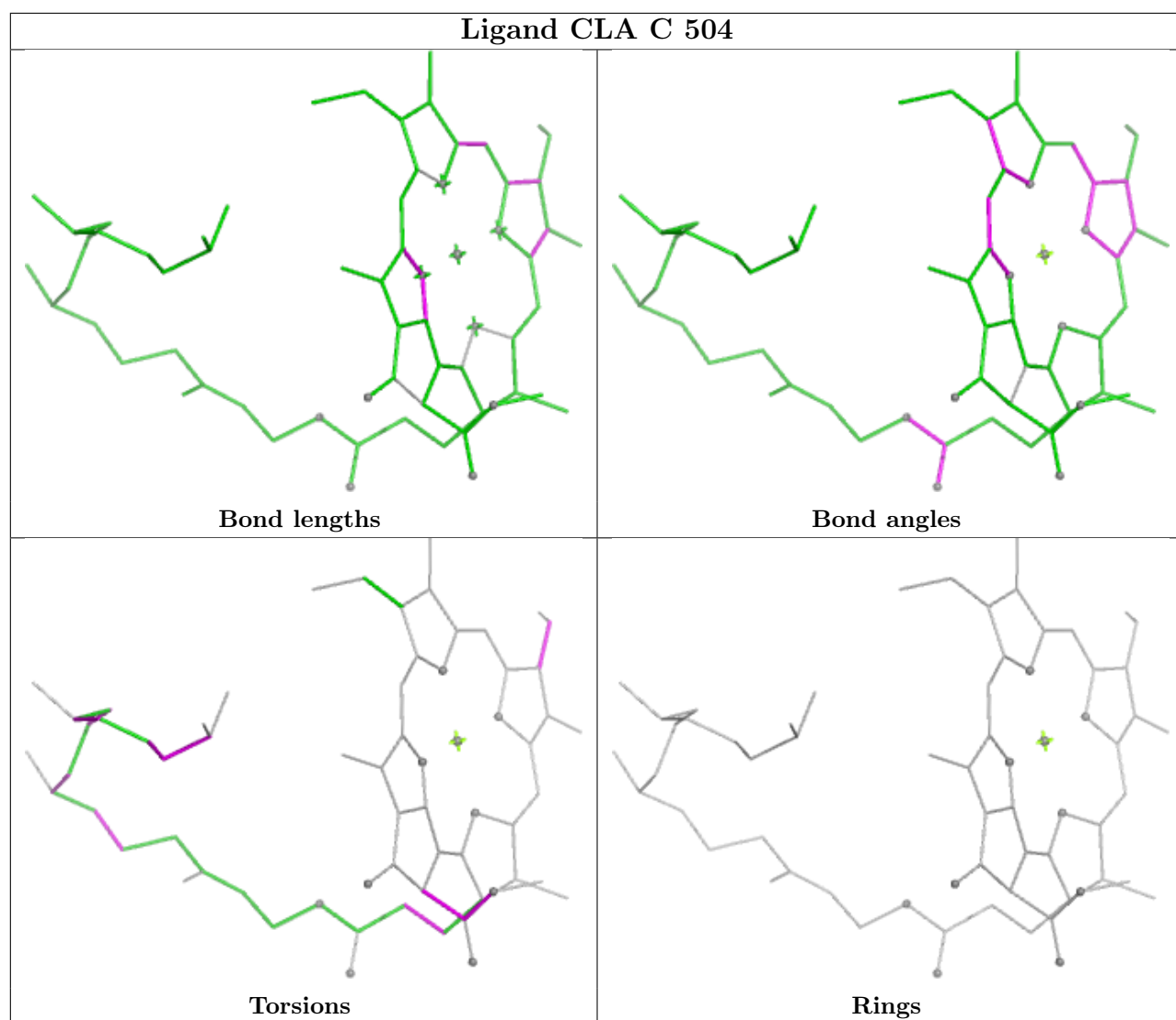


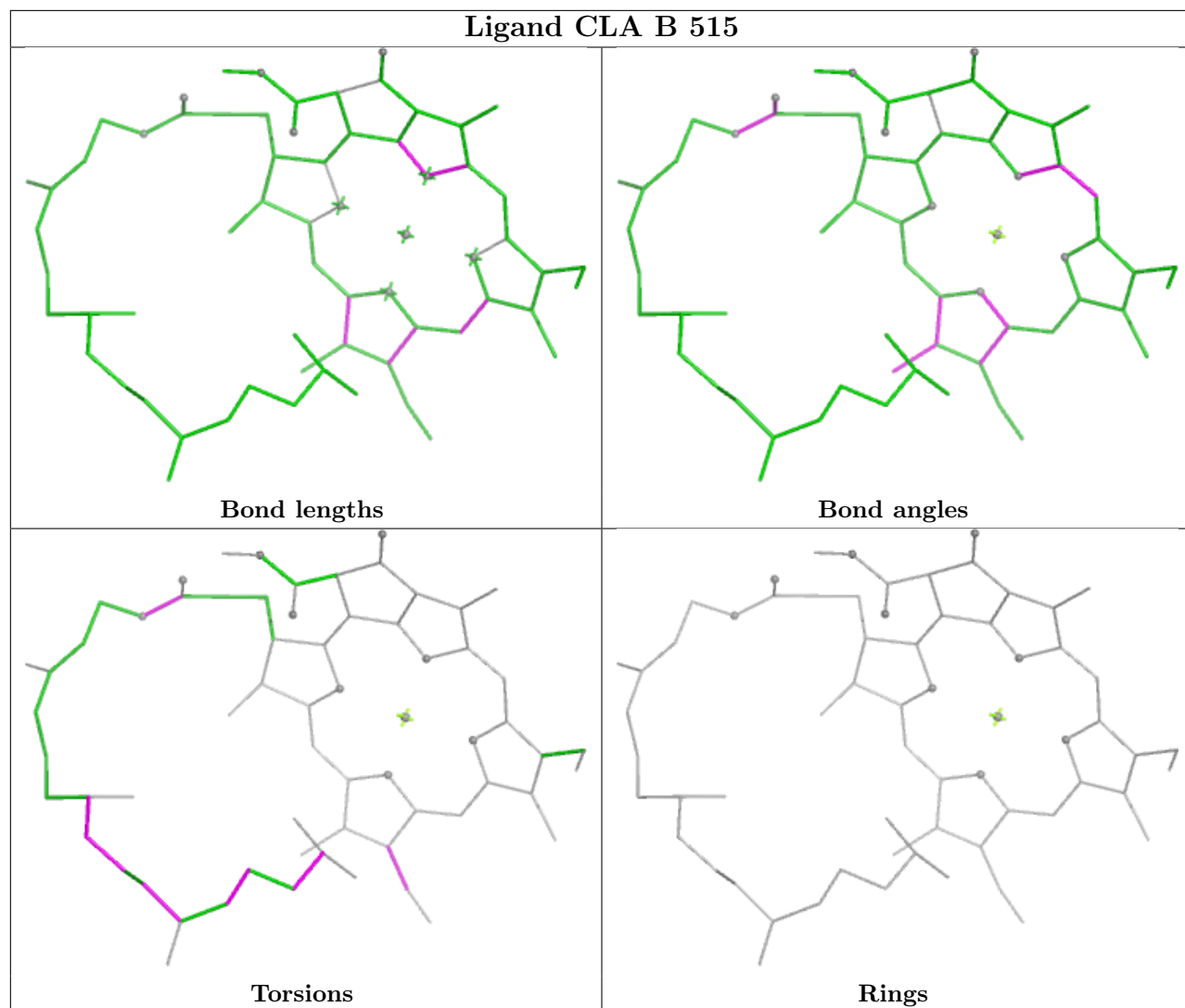
Rings



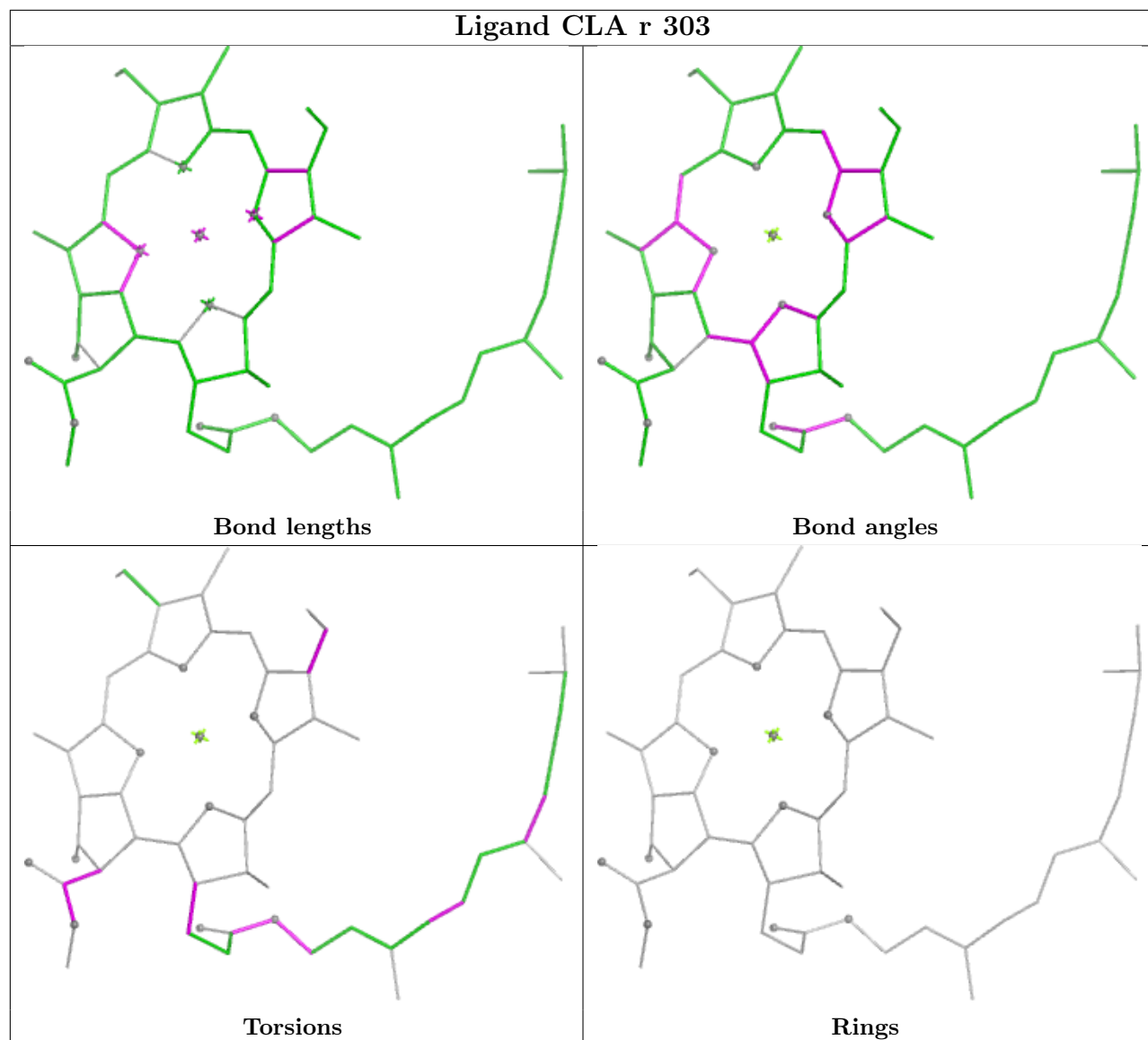




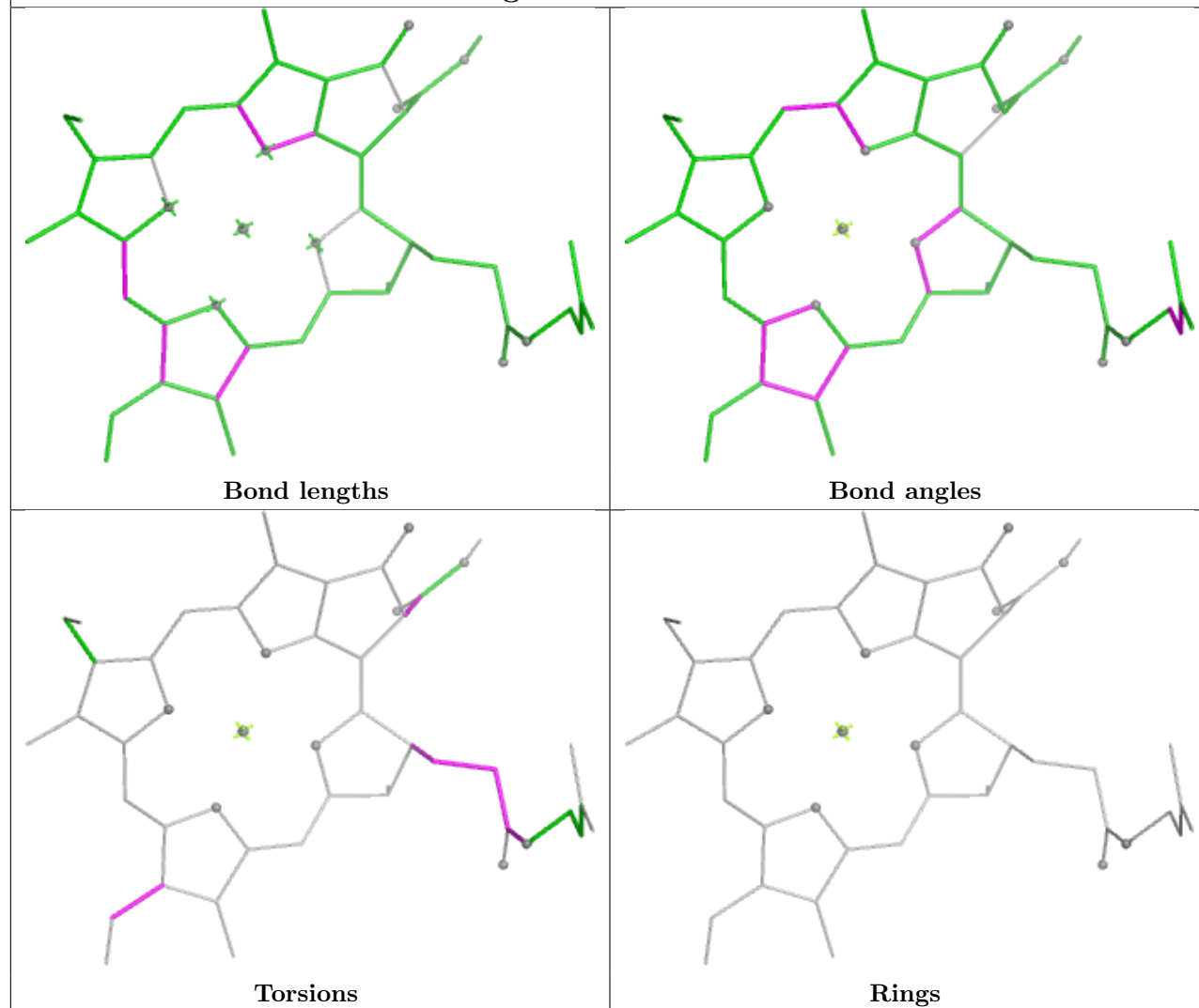




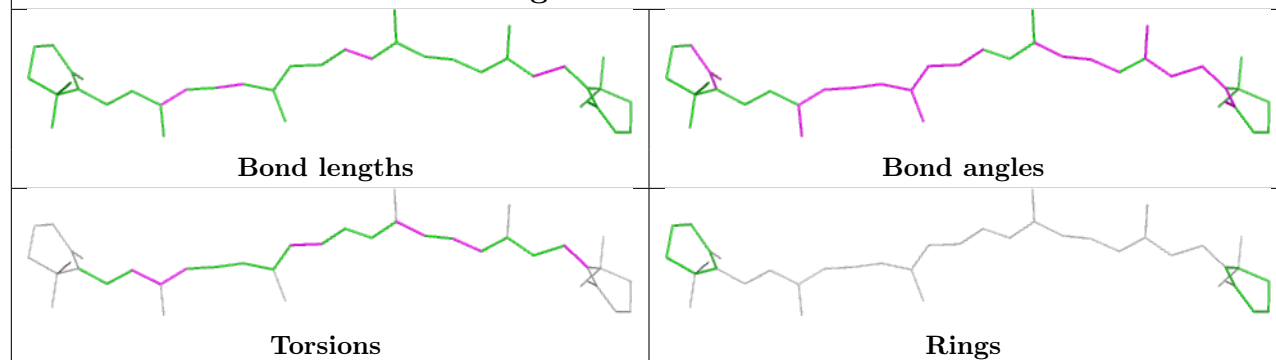
Ligand CLA r 303

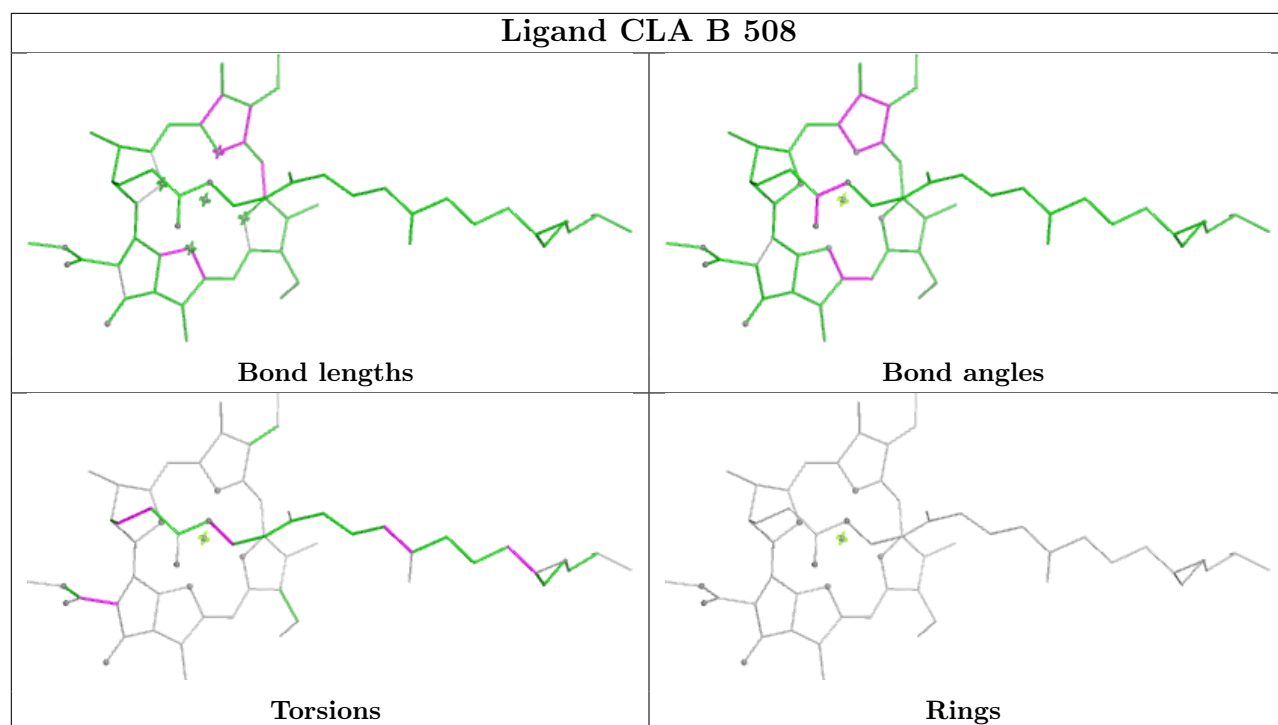
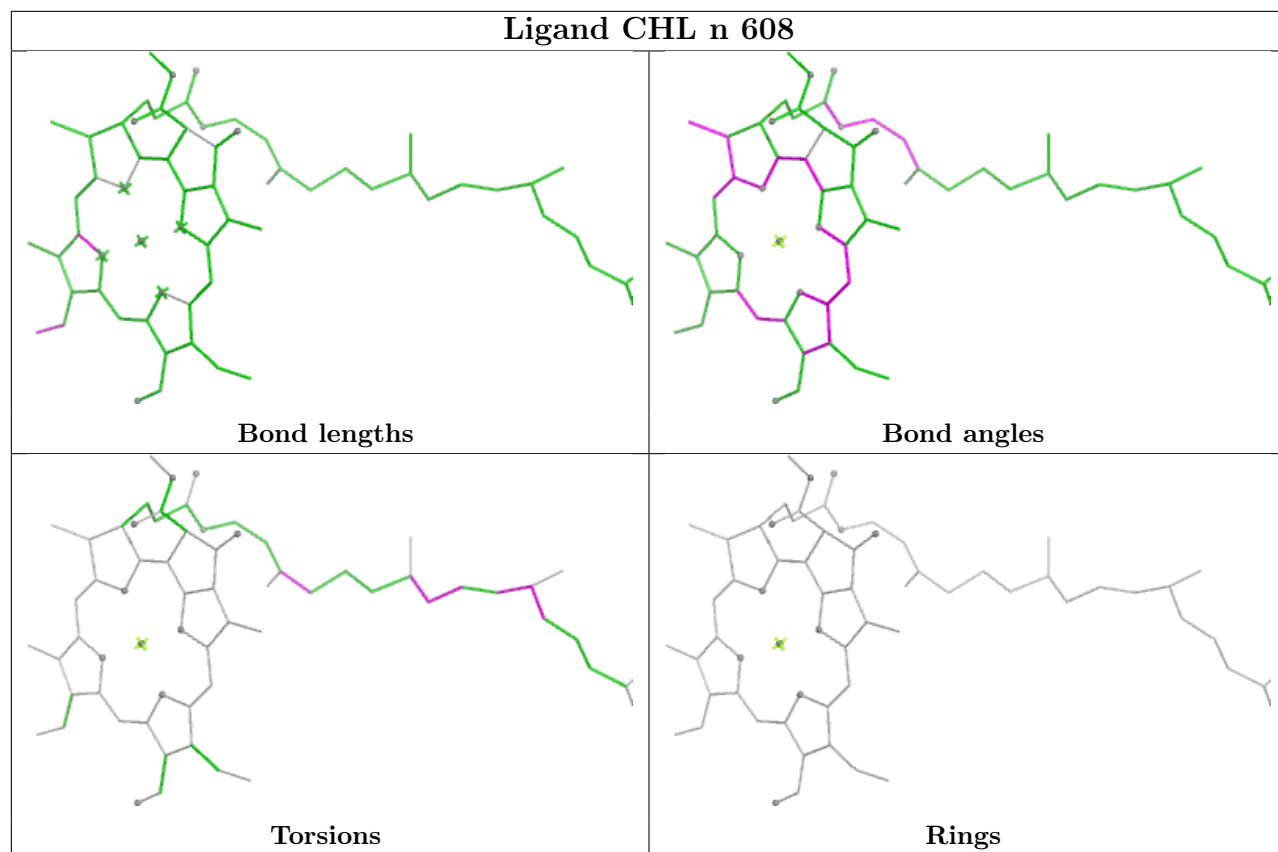


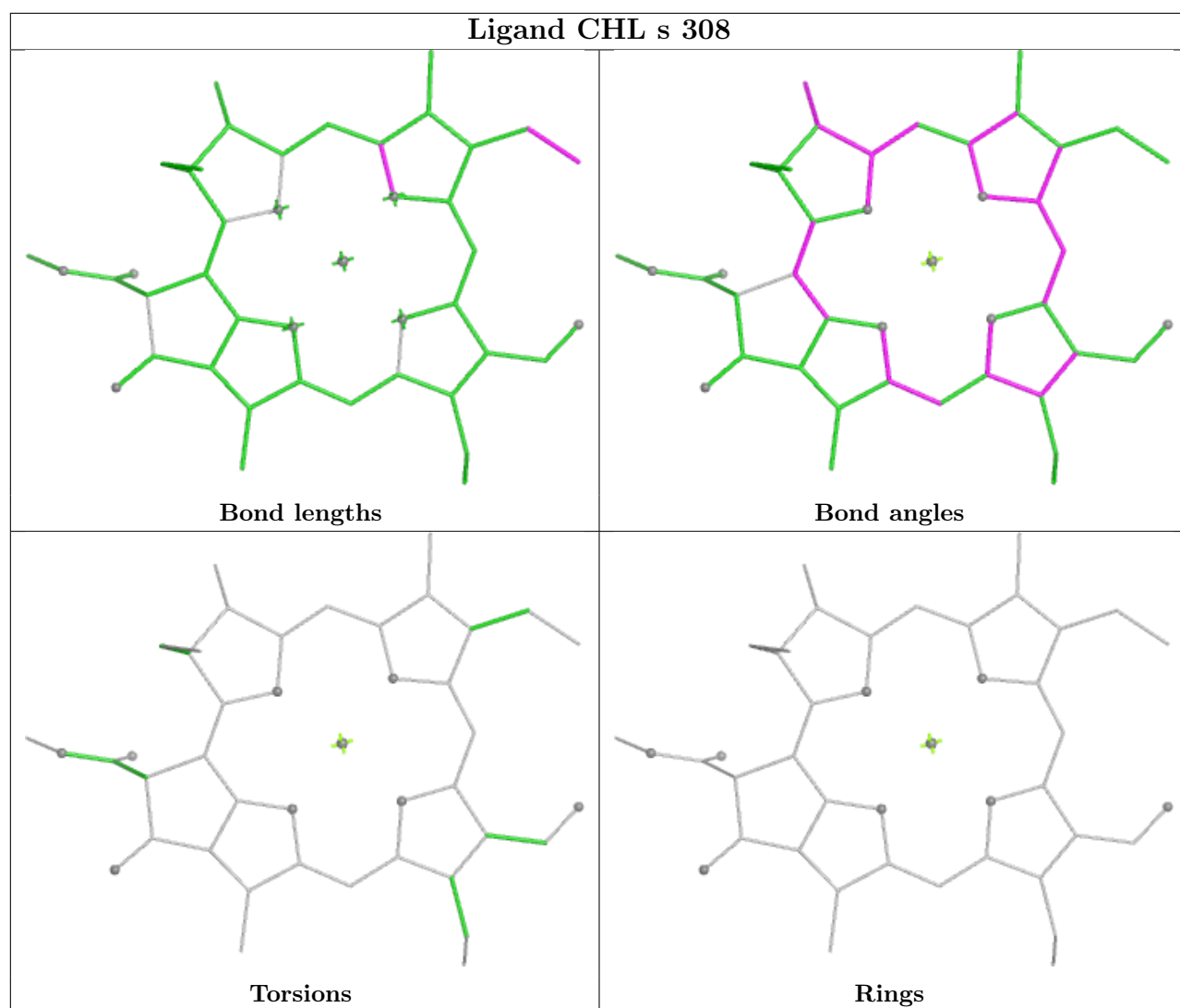
Ligand CLA S 315

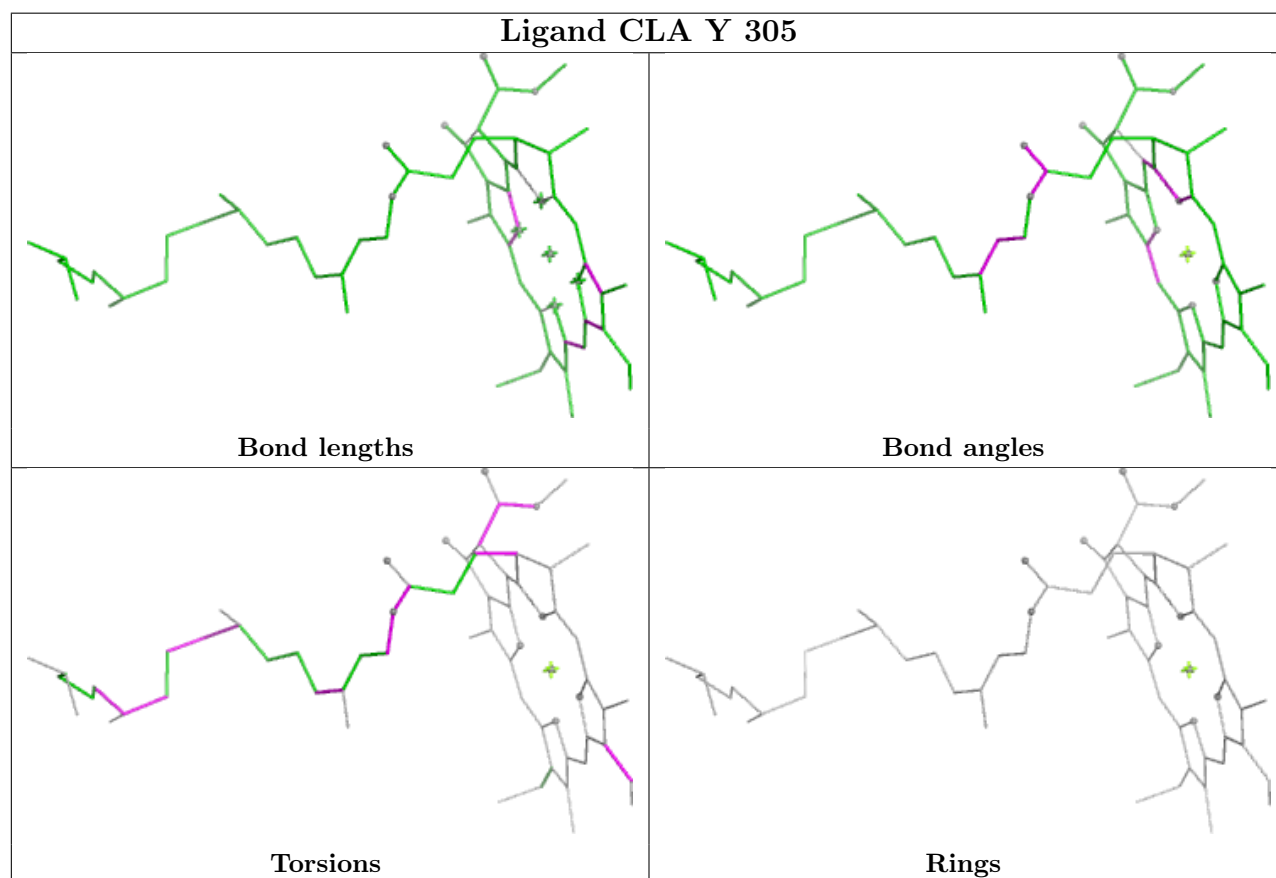
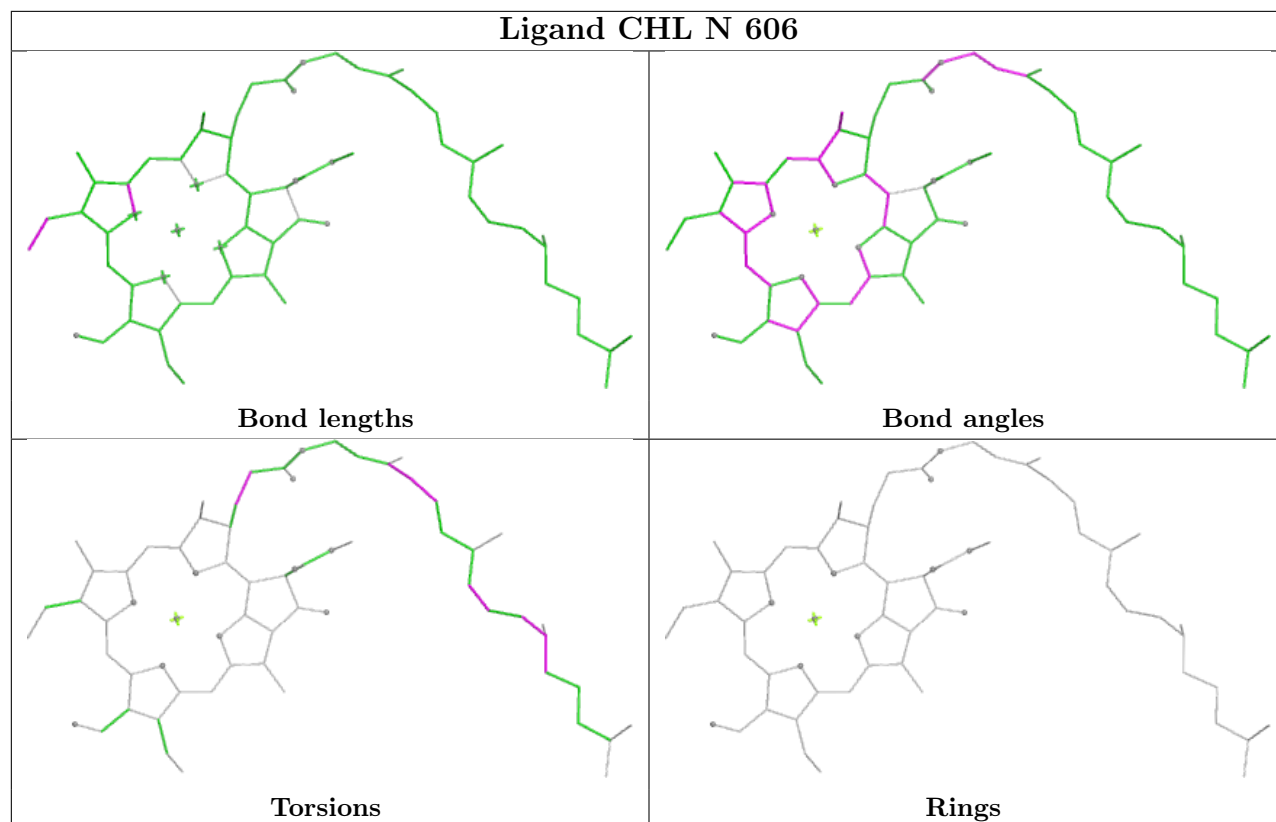


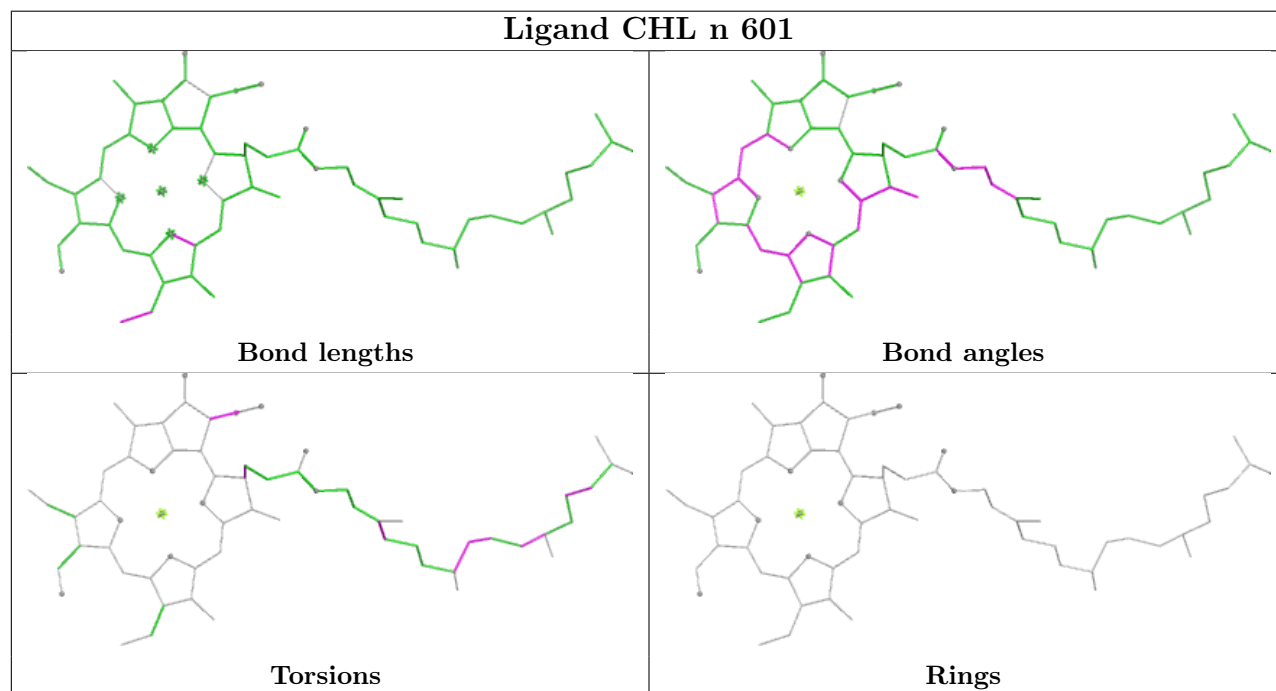
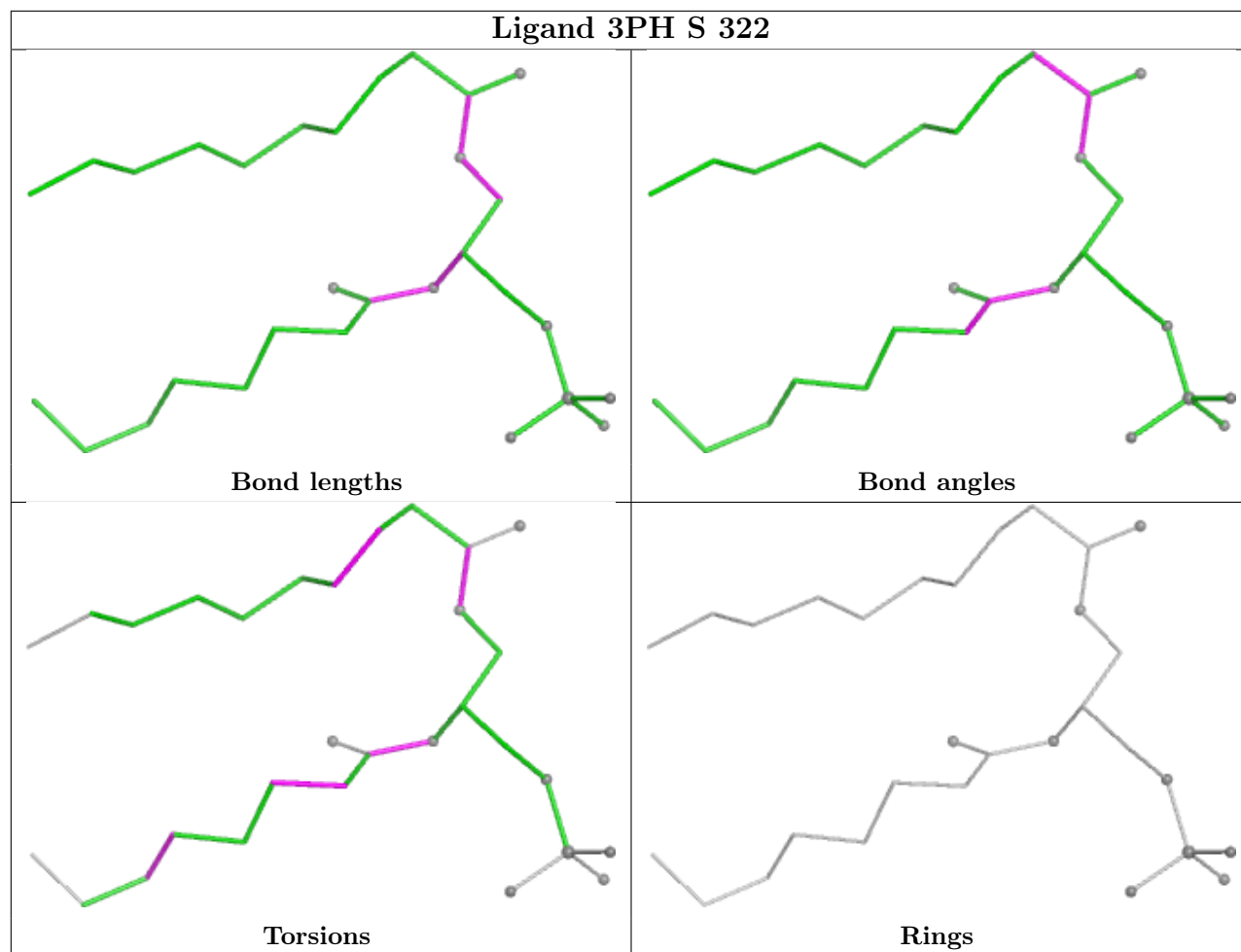
Ligand BCR C 516

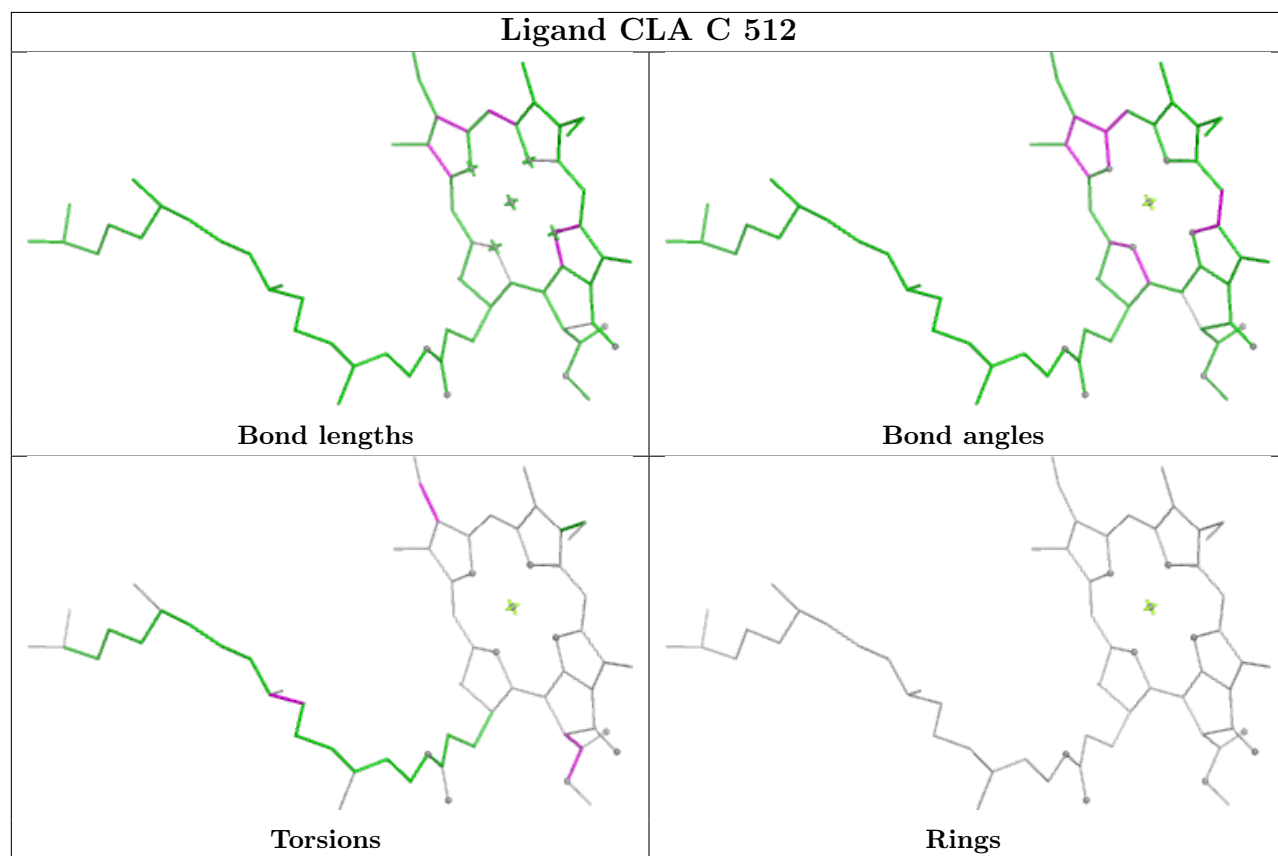
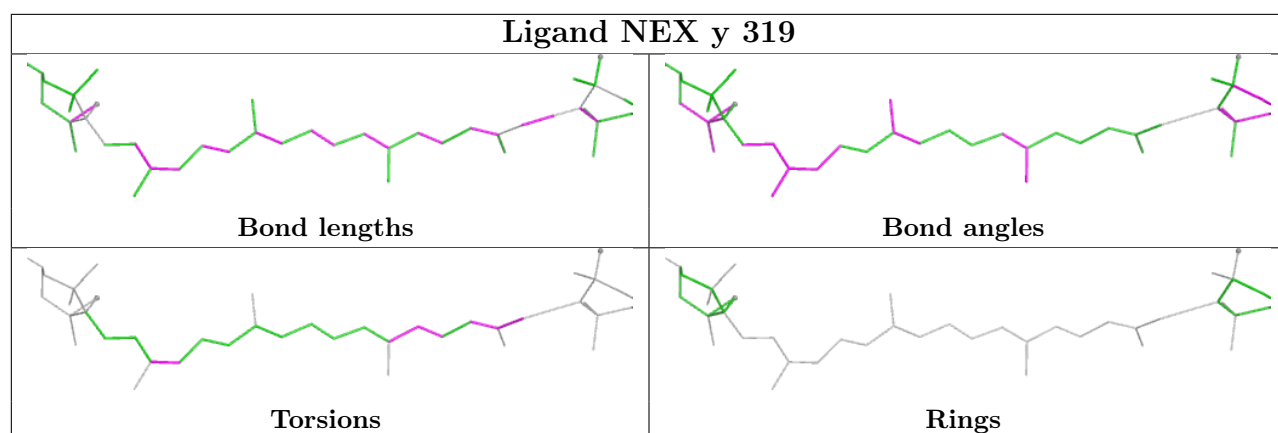




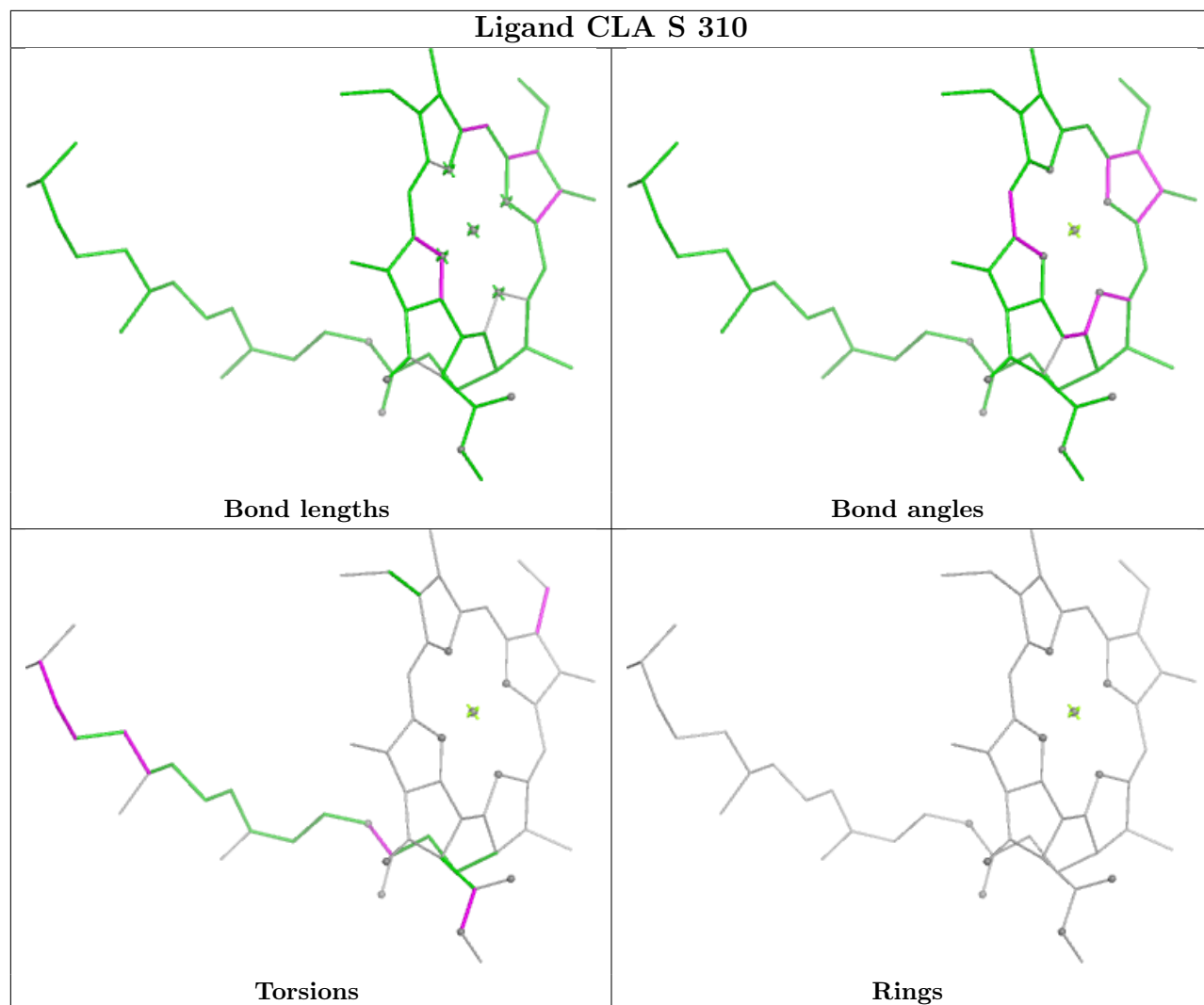




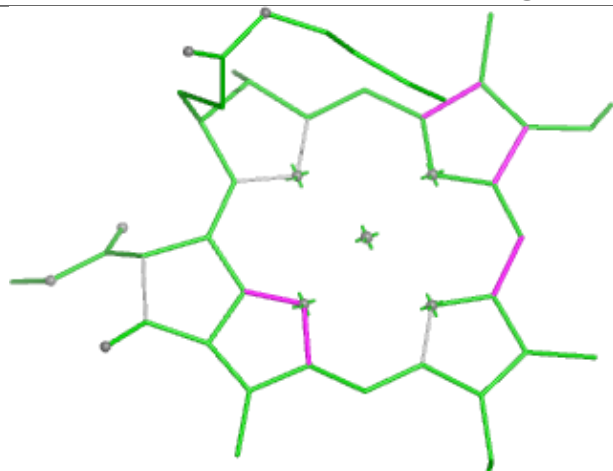




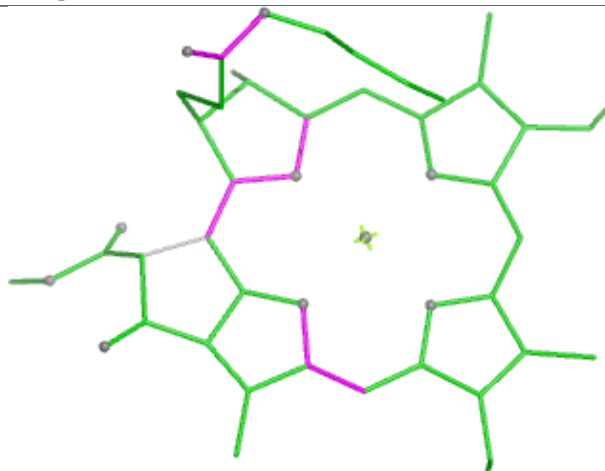
Ligand CLA S 310



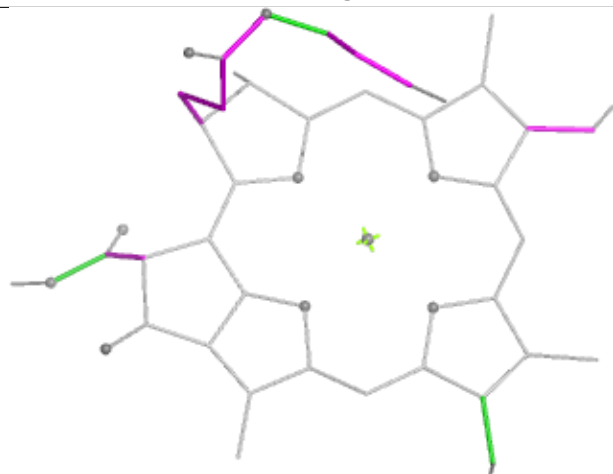
Ligand CLA g 614



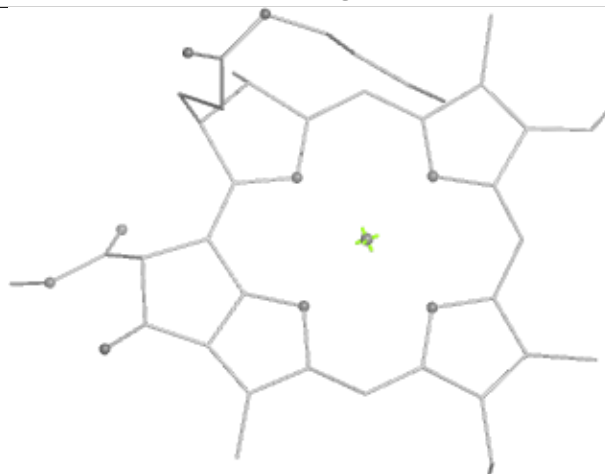
Bond lengths



Bond angles

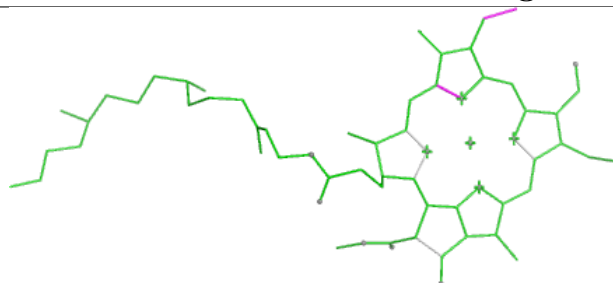


Torsions

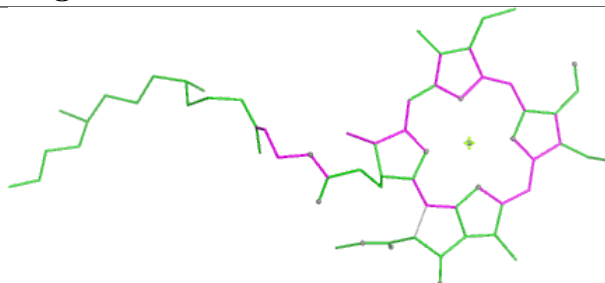


Rings

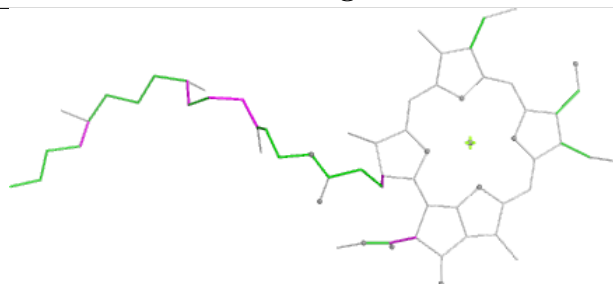
Ligand CHL g 601



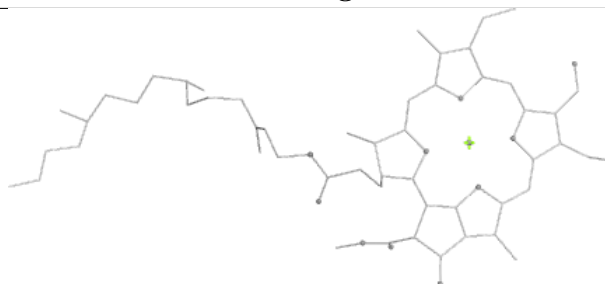
Bond lengths



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

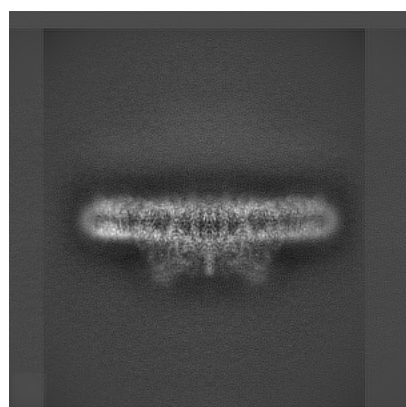
6 Map visualisation [i](#)

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.

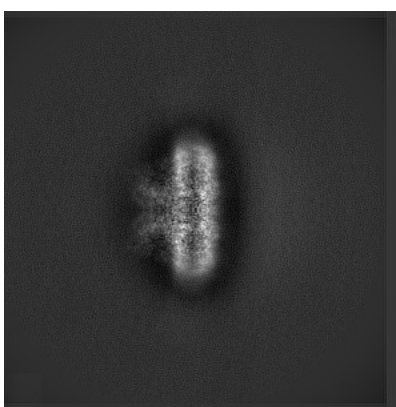
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

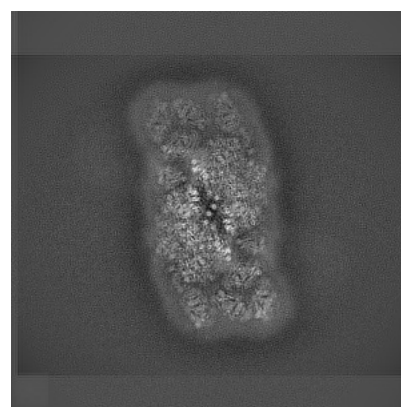
6.1.1 Primary map



X



Y

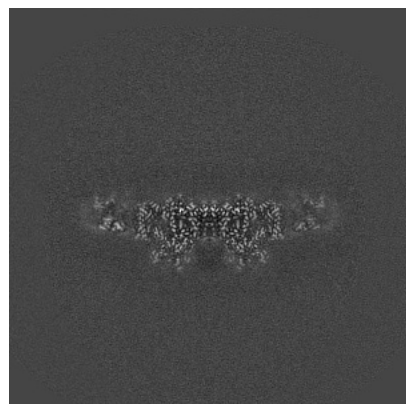


Z

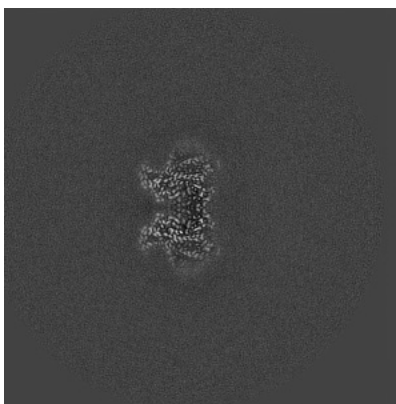
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

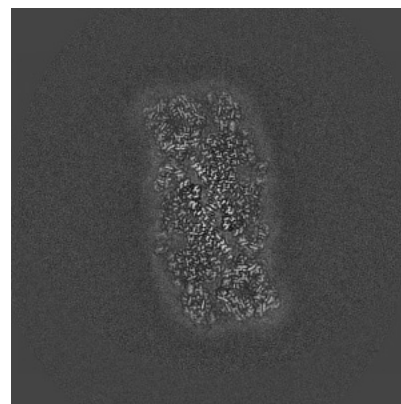
6.2.1 Primary map



X Index: 250



Y Index: 250

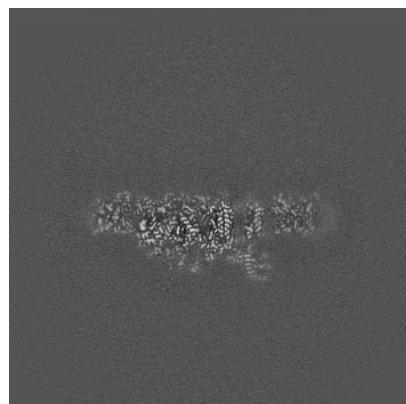


Z Index: 250

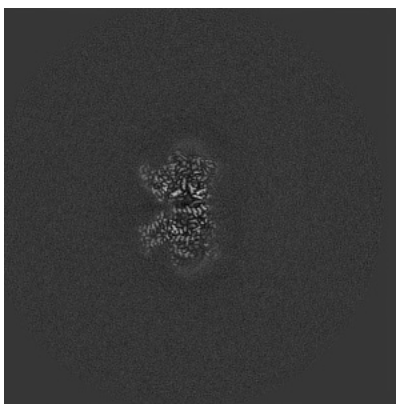
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

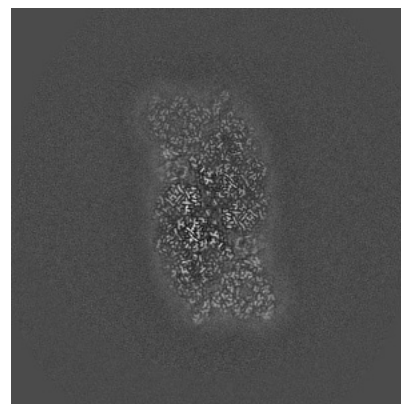
6.3.1 Primary map



X Index: 229



Y Index: 247

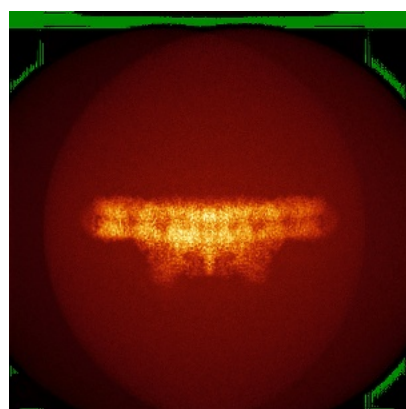


Z Index: 221

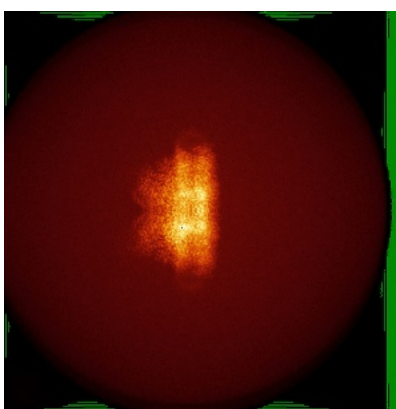
The images above show the largest variance slices of the map in three orthogonal directions.

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

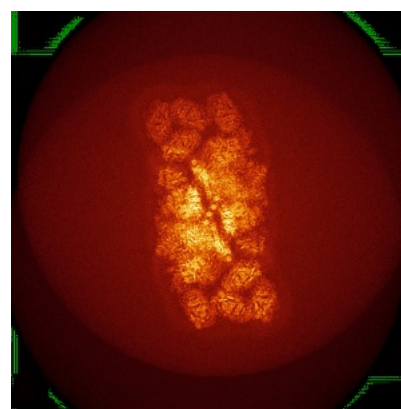
6.4.1 Primary map



X



Y

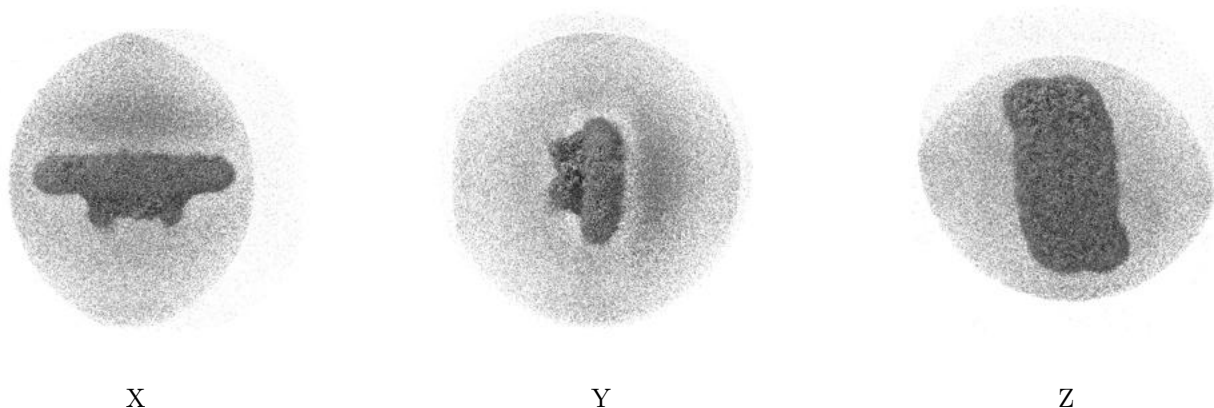


Z

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.

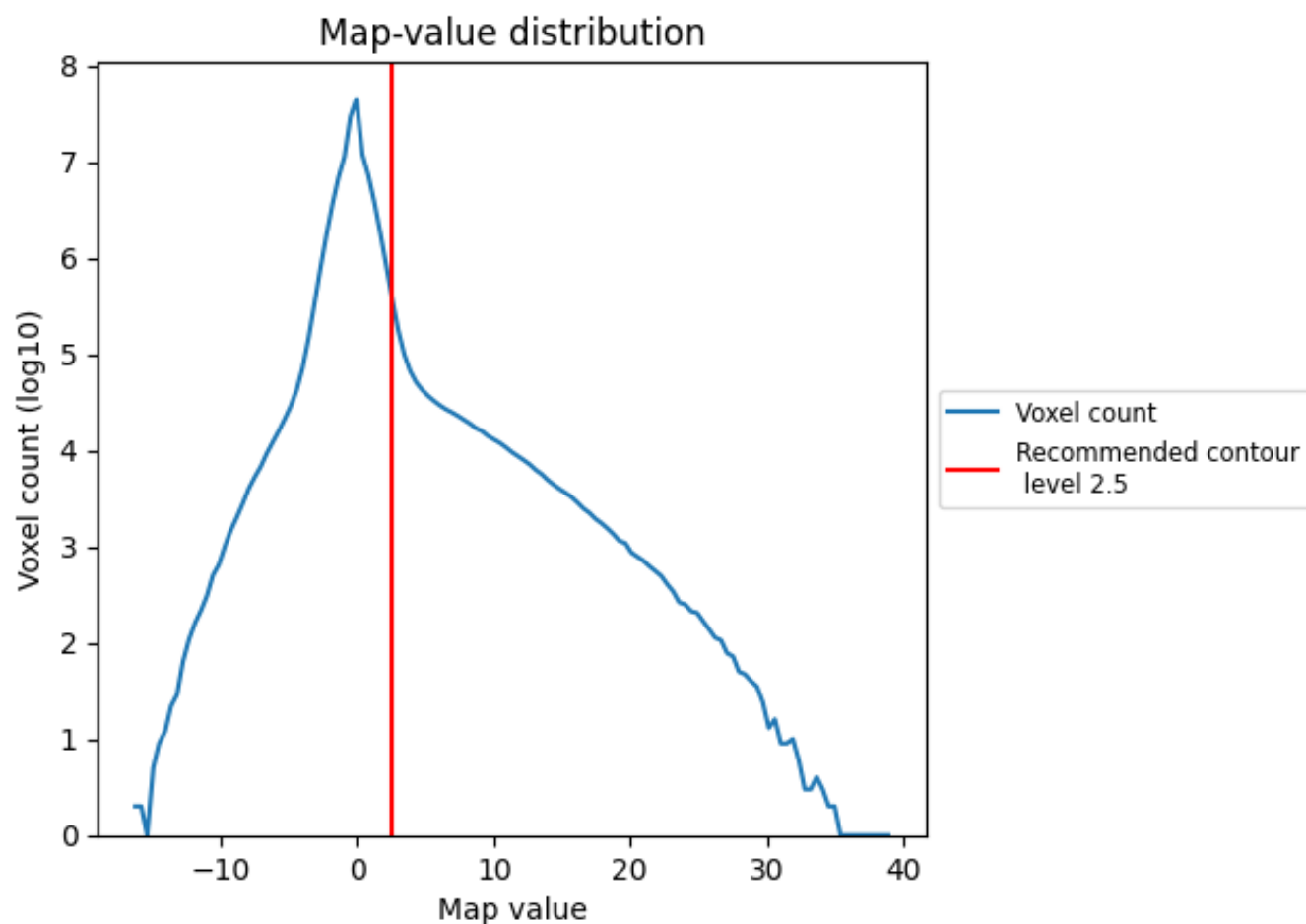
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

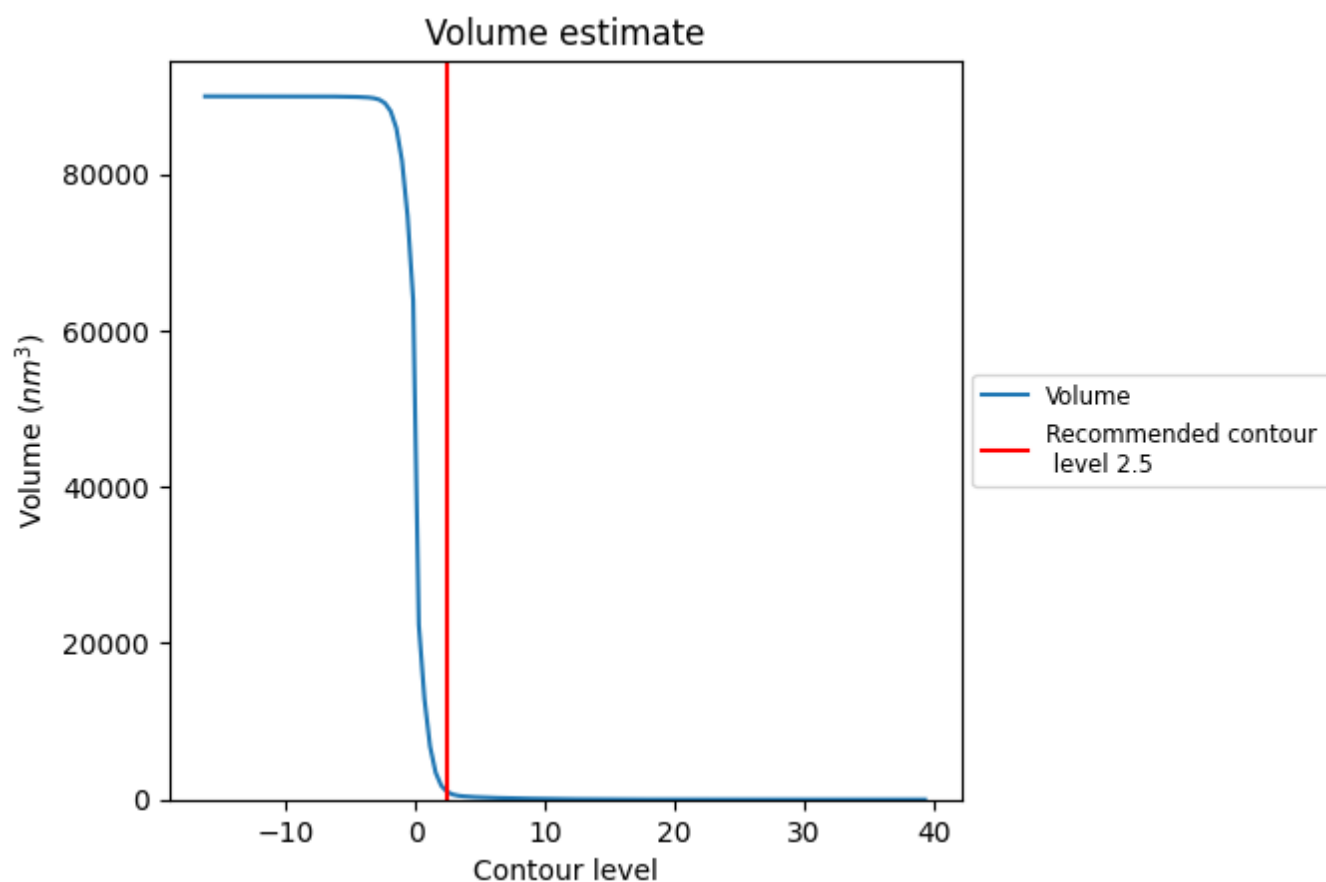
This section contains the results of statistical analysis of the map.

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.

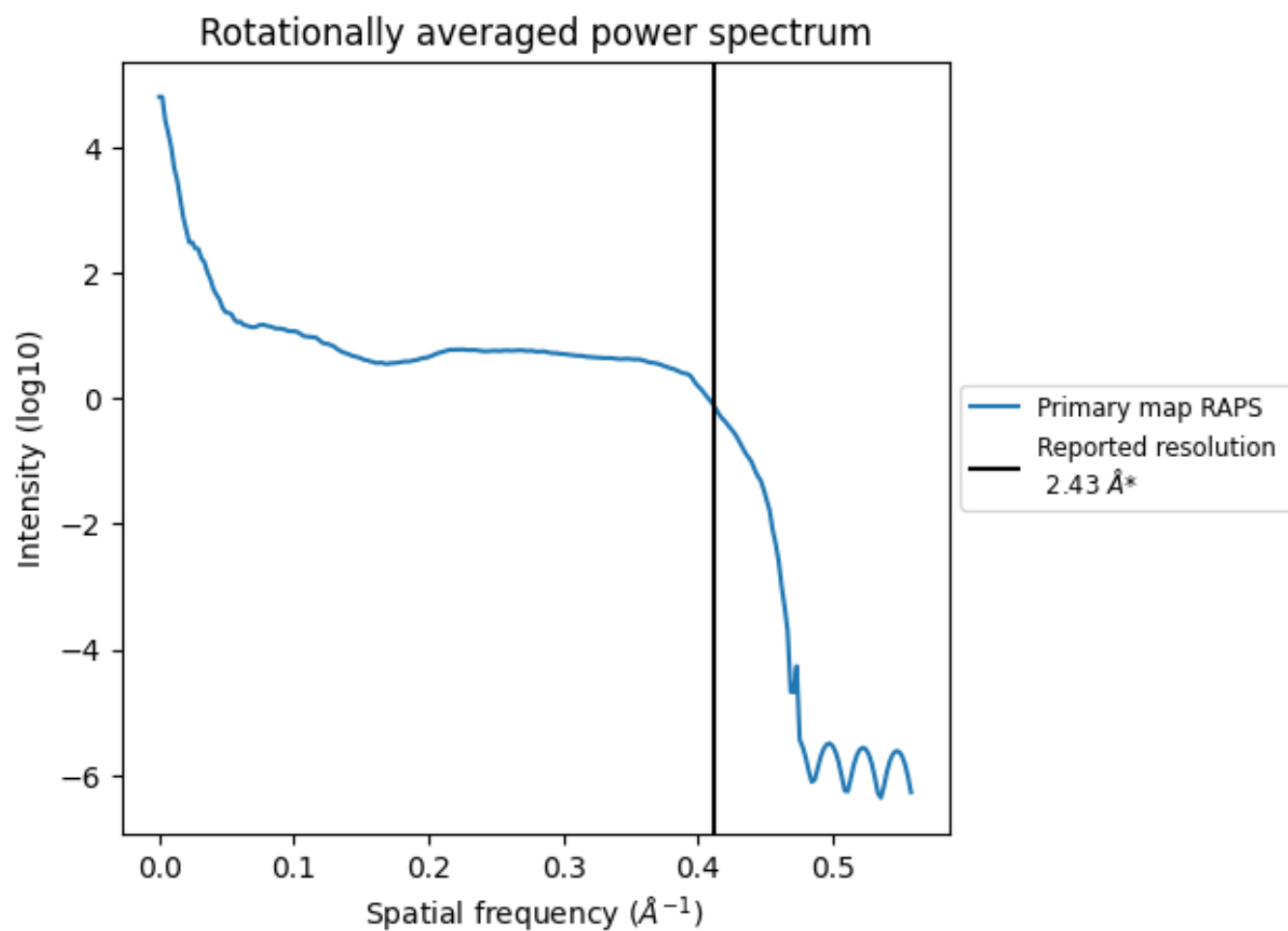
7.2 Volume estimate [i](#)



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 ⓘ

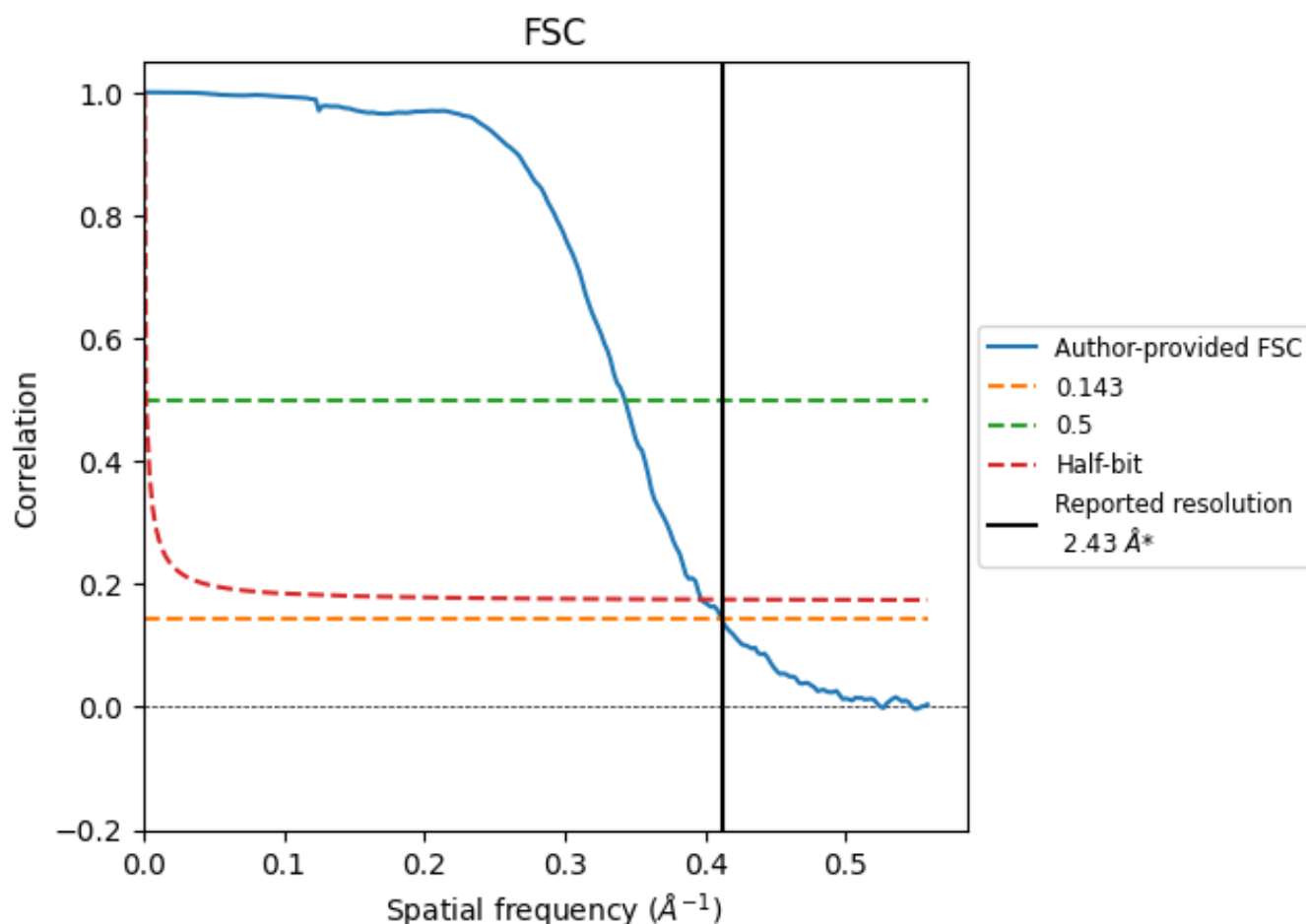


*Reported resolution corresponds to spatial frequency of 0.412 Å⁻¹

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](#)

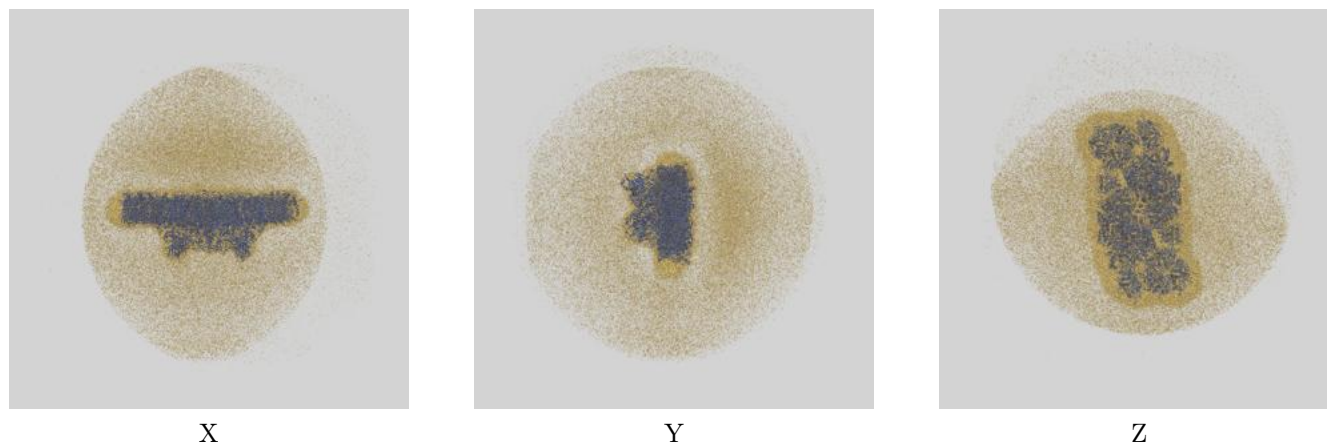
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.43	-	-
Author-provided FSC curve	2.43	2.92	2.52
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

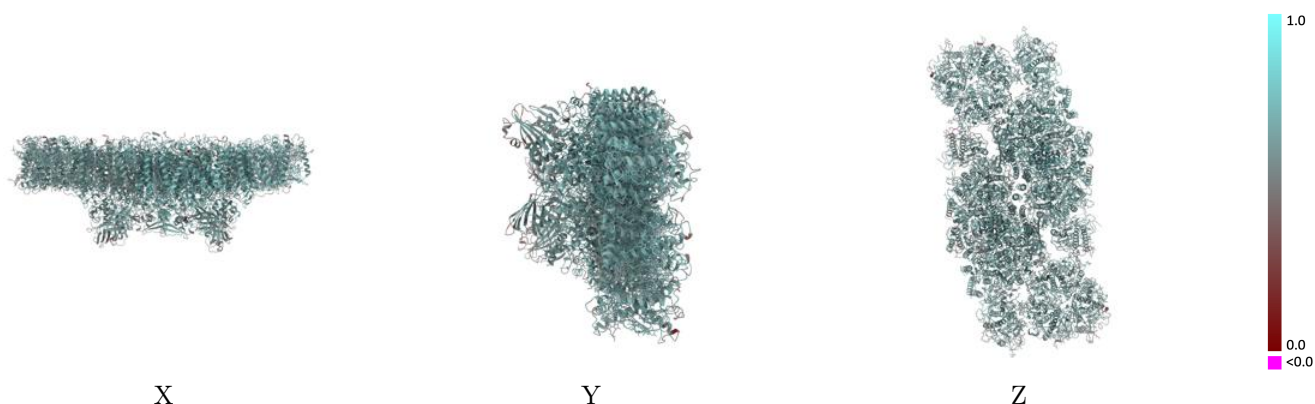
This section contains information regarding the fit between EMDB map EMD-13429 and PDB model 7PI0. Per-residue inclusion information can be found in section [3](#) on page [43](#).

9.1 Map-model overlay [i](#)



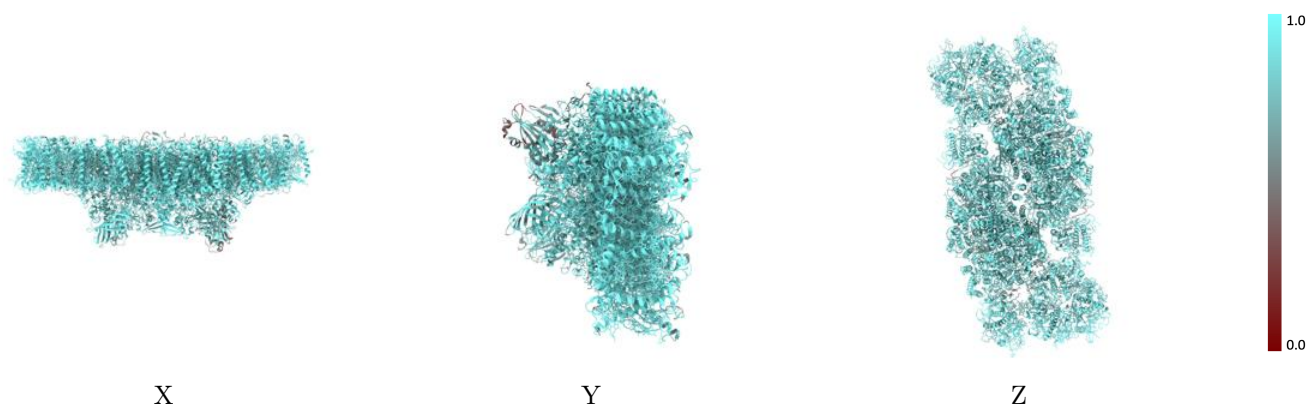
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



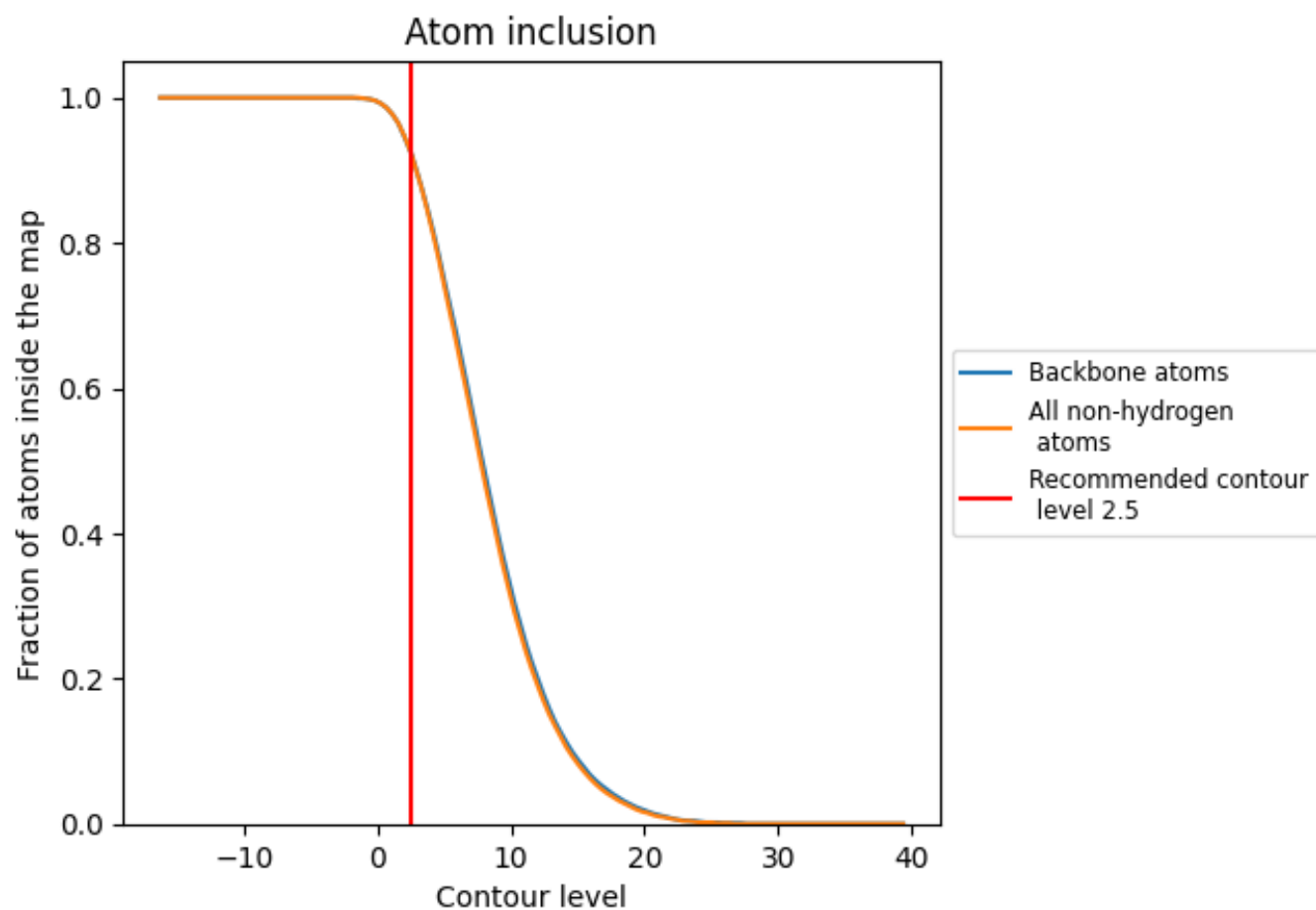
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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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