



Full wwPDB EM Validation Report ⓘ

Jul 1, 2026 – 12:49 pm BST

PDB ID : 9I4T / pdb_00009i4t
EMDB ID : EMD-52620
Title : Photosystem II from Arabidopsis thaliana
Authors : Forsman, J.A.; Graca, A.T.; Hussein, R.; Hall, M.; Messinger, J.; Schroder, W.P.; Aydin, A.O.
Deposited on : 2025-01-26
Resolution : 2.44 Å(reported)
Based on initial model : 3JCU

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:

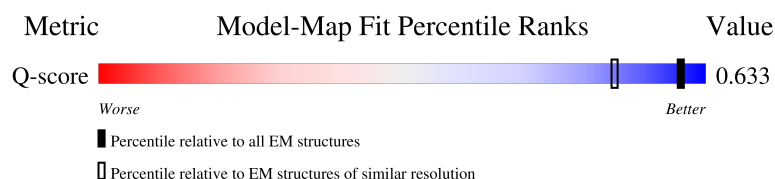
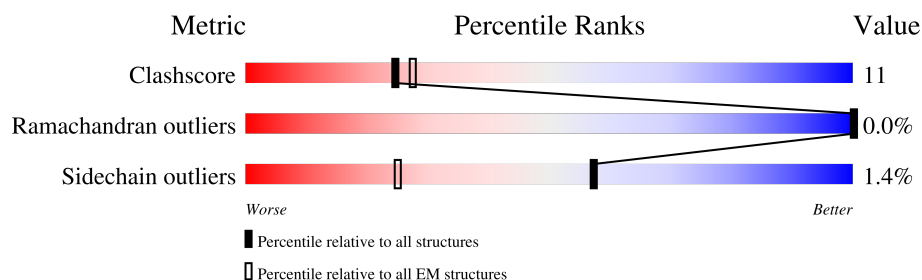
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.44 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.



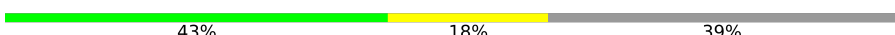
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5856 (1.94 - 2.94)

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	353	 68% 26% 5%
1	a	353	 68% 27% 5%
2	B	508	 80% 15% 5%
2	b	508	 80% 16% 5%

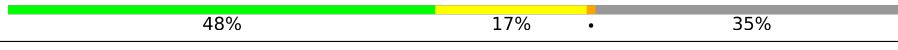
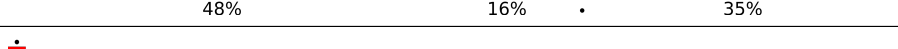
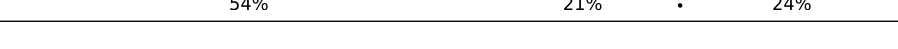
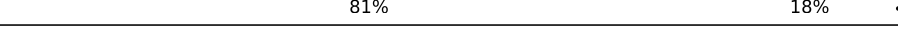
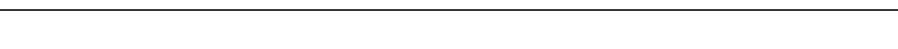
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	473	
3	c	473	
4	D	353	
4	d	353	
5	E	83	
5	e	83	
6	F	39	
6	f	39	
7	G	267	
7	N	267	
7	g	267	
7	n	267	
8	H	73	
8	h	73	
9	I	36	
9	i	36	
10	J	40	
10	j	40	
11	K	61	
11	k	61	
12	L	38	
12	l	38	
13	M	34	
13	m	34	
14	O	332	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	o	332	
15	P	263	
15	p	263	
16	Q	224	
16	q	224	
17	R	290	
17	r	290	
18	S	280	
18	s	280	
19	T	33	
19	t	33	
20	U	103	
20	u	103	
21	W	133	
21	w	133	
22	X	116	
22	x	116	
23	Y	265	
23	y	265	
24	Z	62	
24	z	62	

2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 76824 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	334	Total	C	N	O	S	0	0
			2613	1707	430	463	13		
1	a	334	Total	C	N	O	S	0	0
			2613	1707	430	463	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	485	Total	C	N	O	S	0	0
			3800	2489	642	657	12		
2	b	485	Total	C	N	O	S	0	0
			3800	2489	642	657	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	447	Total	C	N	O	S	0	0
			3468	2279	579	599	11		
3	c	447	Total	C	N	O	S	0	0
			3468	2279	579	599	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2713	1795	444	462	12		
4	d	341	Total	C	N	O	S	0	0
			2713	1795	444	462	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	74	Total	C	N	O	0	0
			604	395	99	110		
5	e	74	Total	C	N	O	0	0
			604	395	99	110		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	30	Total	C	N	O	S	0	0
			241	162	41	37	1		
6	f	30	Total	C	N	O	S	0	0
			241	162	41	37	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	33	PHE	SER	variant	UNP P62095
f	33	PHE	SER	variant	UNP P62095

- Molecule 7 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	211	Total	C	N	O	S	0	0
			1606	1037	264	300	5		
7	N	202	Total	C	N	O	S	0	0
			1536	994	251	286	5		
7	g	211	Total	C	N	O	S	0	0
			1606	1037	264	300	5		
7	n	202	Total	C	N	O	S	0	0
			1536	994	251	286	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	59	Total	C	N	O	S	0	0
			438	289	68	79	2		
8	h	59	Total	C	N	O	S	0	0
			438	289	68	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	33	Total	C	N	O	S	0	0
			266	184	39	42	1		
9	i	33	Total	C	N	O	S	0	0
			266	184	39	42	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	35	Total	C	N	O	S	0	0
			255	174	39	42			
10	j	35	Total	C	N	O	S	0	0
			255	174	39	42			

- 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	S	0	0
			302	211	44	46	1		
11	k	37	Total	C	N	O	S	0	0
			302	211	44	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	35	Total	C	N	O	S	0	0
			293	195	45	53			
12	l	35	Total	C	N	O	S	0	0
			293	195	45	53			

- 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	S	0	0
			242	168	34	40			
13	m	31	Total	C	N	O	S	0	0
			242	168	34	40			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	241	Total	C	N	O	S	0	0
			1829	1157	297	371	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
14	o	241	Total	C	N	O	S	0	0
			1829	1157	297	371	4		

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 2-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	171	Total	C	N	O	S	0	0
			1319	836	217	264	2		
15	p	171	Total	C	N	O	S	0	0
			1319	836	217	264	2		

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 3-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	146	Total	C	N	O	S	0	0
			1139	726	193	220			
16	q	146	Total	C	N	O	S	0	0
			1139	726	193	220			

- Molecule 17 is a protein called Chlorophyll a-b binding protein CP29.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	220	Total	C	N	O	S	0	0
			1710	1109	281	317	3		
17	r	220	Total	C	N	O	S	0	0
			1710	1109	281	317	3		

- Molecule 18 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	214	Total	C	N	O	S	0	0
			1653	1082	270	297	4		
18	s	214	Total	C	N	O	S	0	0
			1653	1082	270	297	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	32	Total	C	N	O	S	0	0
			261	181	37	42	1		
19	t	32	Total	C	N	O	S	0	0
			261	181	37	42	1		

- Molecule 20 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	28	Total	C	N	O	S	0	0
			219	138	40	38	3		
20	u	28	Total	C	N	O	S	0	0
			219	138	40	38	3		

- Molecule 21 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	54	Total	C	N	O	S	0	0
			427	282	61	83	1		
21	w	54	Total	C	N	O	S	0	0
			427	282	61	83	1		

- Molecule 22 is a protein called Expressed protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	39	Total	C	N	O	0	0
			279	183	46	50		
22	x	39	Total	C	N	O	0	0
			279	183	46	50		

- Molecule 23 is a protein called Chlorophyll a-b binding protein 2.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	214	Total	C	N	O	S	0	0
			1652	1075	265	307	5		
23	y	214	Total	C	N	O	S	0	0
			1652	1075	265	307	5		

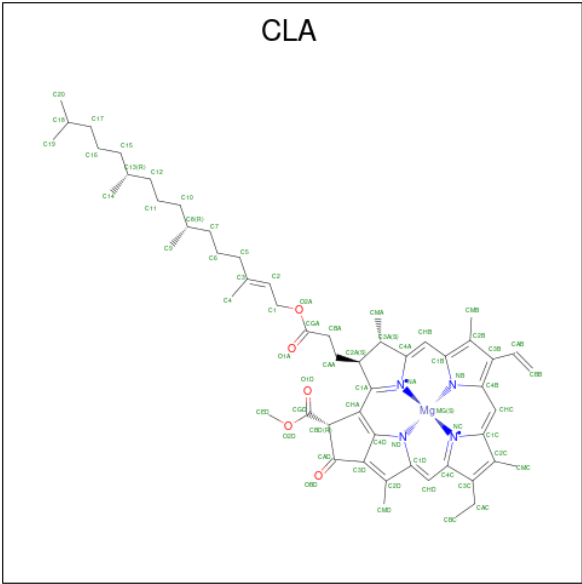
- Molecule 24 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Z	61	Total	C	N	O	0	0
			456	308	68	80		
24	z	61	Total	C	N	O	0	0
			456	308	68	80		

- Molecule 25 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 26 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	C	1	Total 64	C 55	Mg 1	N 3	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
26	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	D	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	R	1	Total 49	C 39	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
26	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 64	C 55	Mg 1	N 3	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	d	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	g	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

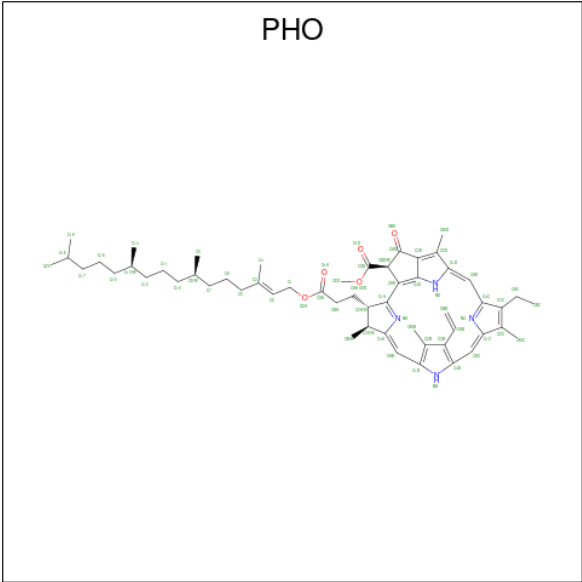
Mol	Chain	Residues	Atoms					AltConf
26	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	n	1	Total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

Continued on next page...

Continued from previous page...

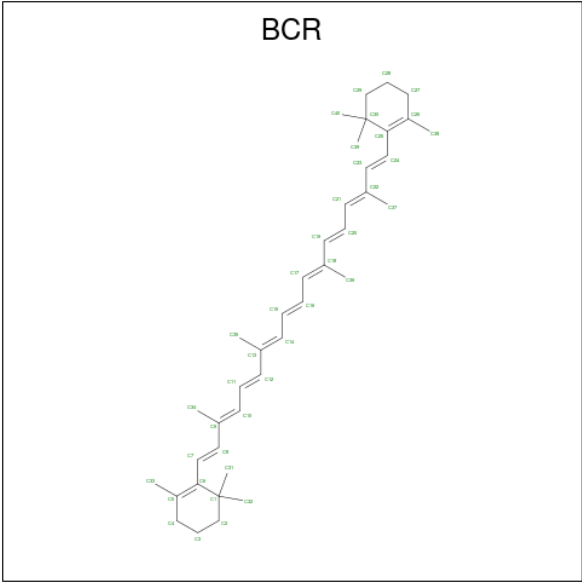
Mol	Chain	Residues	Atoms					AltConf
26	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



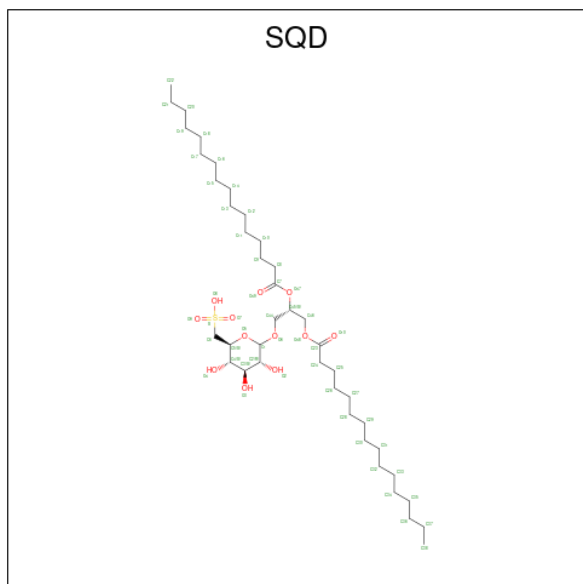
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	N	O	0
			64	55	4	5	
27	D	1	Total	C	N	O	0
			64	55	4	5	
27	a	1	Total	C	N	O	0
			64	55	4	5	
27	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 28 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



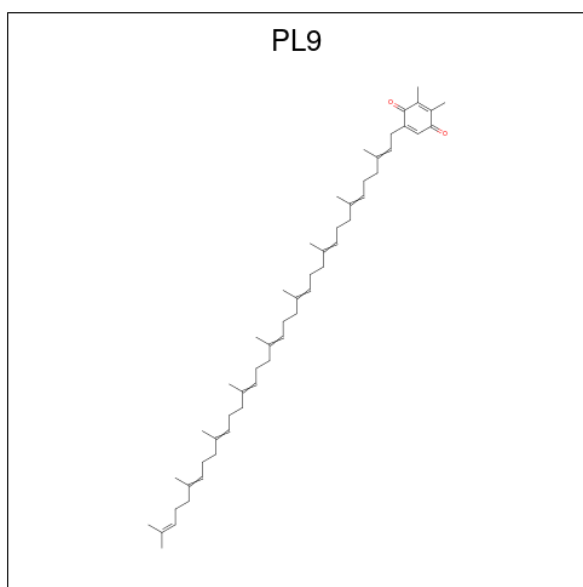
Mol	Chain	Residues	Atoms	AltConf
28	A	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	C	1	Total C 40 40	0
28	C	1	Total C 40 40	0
28	D	1	Total C 40 40	0
28	H	1	Total C 40 40	0
28	J	1	Total C 40 40	0
28	K	1	Total C 40 40	0
28	T	1	Total C 40 40	0
28	a	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	c	1	Total C 40 40	0
28	c	1	Total C 40 40	0
28	d	1	Total C 40 40	0
28	h	1	Total C 40 40	0
28	j	1	Total C 40 40	0
28	k	1	Total C 40 40	0
28	t	1	Total C 40 40	0

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	O	S	0
			54	41	12	1	
29	A	1	Total	C	O	S	0
			50	37	12	1	
29	B	1	Total	C	O	S	0
			54	41	12	1	
29	W	1	Total	C	O	S	0
			33	20	12	1	
29	a	1	Total	C	O	S	0
			54	41	12	1	
29	a	1	Total	C	O	S	0
			50	37	12	1	
29	b	1	Total	C	O	S	0
			54	41	12	1	
29	w	1	Total	C	O	S	0
			33	20	12	1	

- Molecule 30 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).

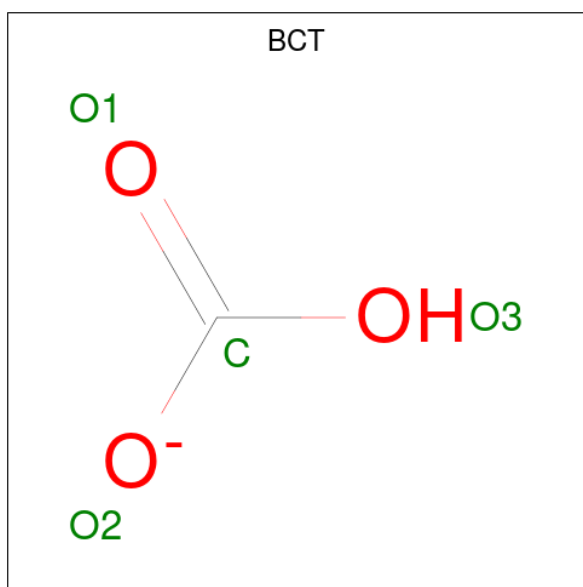


Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			22	20	2	
30	D	1	Total	C	O	0
			55	53	2	
30	a	1	Total	C	O	0
			22	20	2	
30	d	1	Total	C	O	0
			55	53	2	

- Molecule 31 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

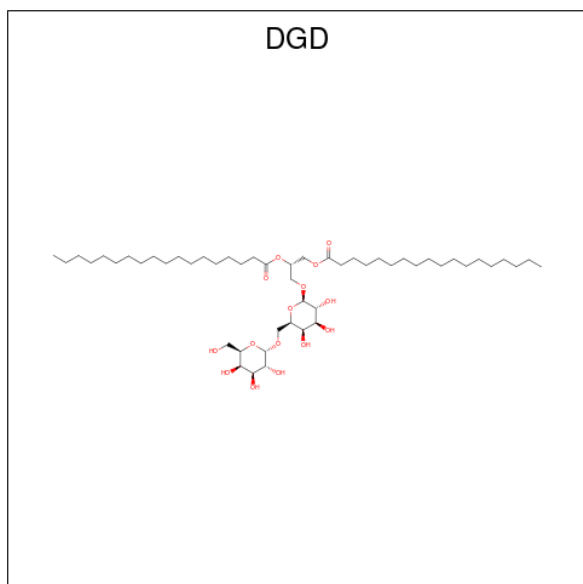
Mol	Chain	Residues	Atoms		AltConf
31	A	1	Total	Fe	0
			1	1	
31	a	1	Total	Fe	0
			1	1	

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



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

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



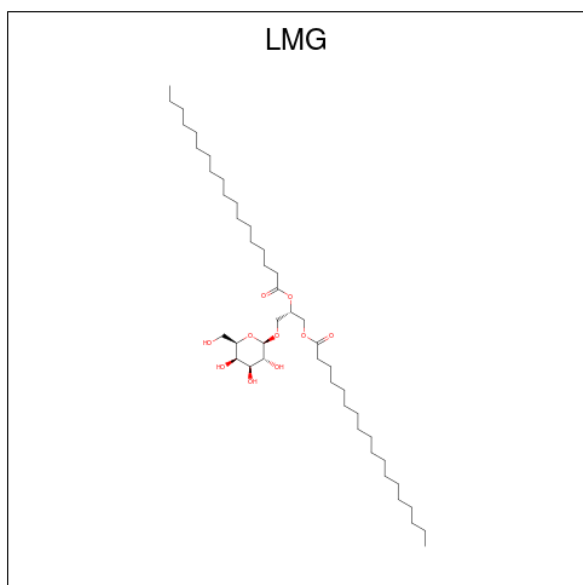
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			62	47	15	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			55	40	15	
33	C	1	Total	C	O	0
			62	47	15	
33	C	1	Total	C	O	0
			62	47	15	
33	Y	1	Total	C	O	0
			43	28	15	
33	b	1	Total	C	O	0
			62	47	15	
33	c	1	Total	C	O	0
			62	47	15	
33	c	1	Total	C	O	0
			55	40	15	
33	c	1	Total	C	O	0
			62	47	15	
33	y	1	Total	C	O	0
			43	28	15	

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



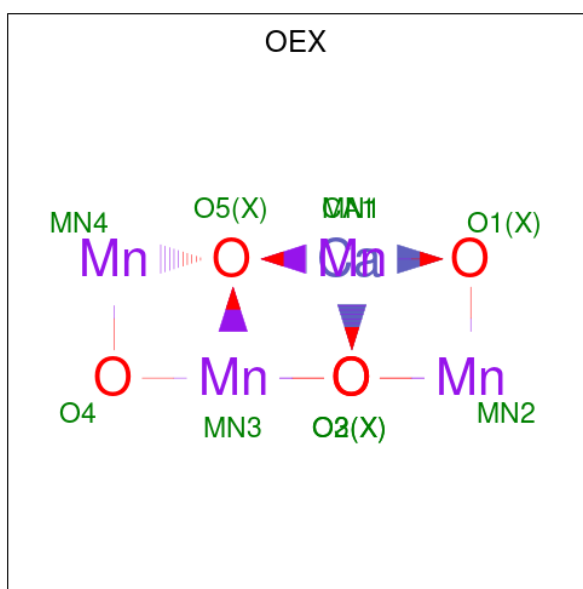
Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			51	41	10	
34	C	1	Total	C	O	0
			51	41	10	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
34	C	1	Total	C	O	0
			51	41	10	
34	D	1	Total	C	O	0
			46	36	10	
34	W	1	Total	C	O	0
			48	38	10	
34	b	1	Total	C	O	0
			51	41	10	
34	c	1	Total	C	O	0
			51	41	10	
34	c	1	Total	C	O	0
			51	41	10	
34	d	1	Total	C	O	0
			46	36	10	
34	w	1	Total	C	O	0
			48	38	10	

- Molecule 35 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
35	C	1	Total	Ca	Mn	O	0
			10	1	4	5	
35	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 36 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$).



Mol	Chain	Residues	Atoms			AltConf
36	D	1	Total 35	C 24	O 11	0
36	d	1	Total 35	C 24	O 11	0

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



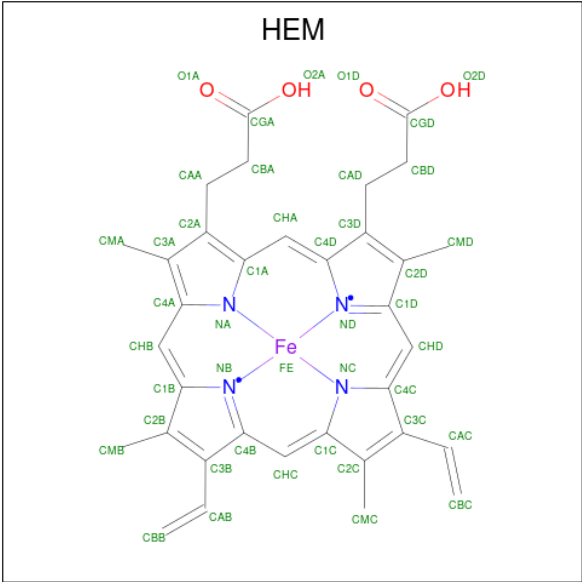
Mol	Chain	Residues	Atoms				AltConf
37	D	1	Total	C	O	P	0
			43	32	10	1	

Continued on next page...

Continued from previous page...

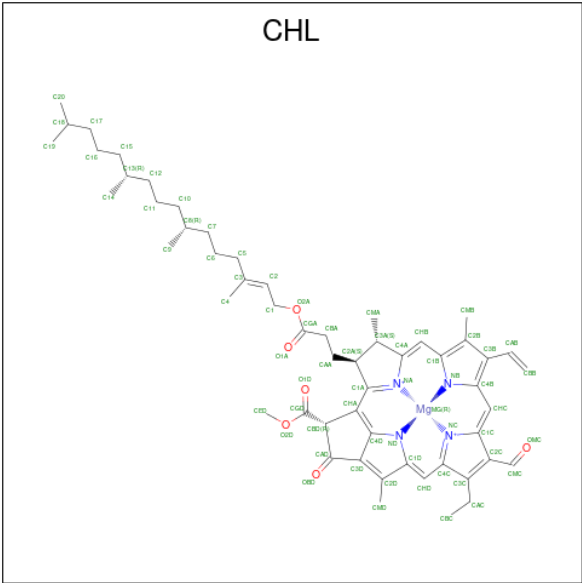
Mol	Chain	Residues	Atoms				AltConf
37	D	1	Total	C	O	P	0
			49	38	10	1	
37	D	1	Total	C	O	P	0
			37	26	10	1	
37	G	1	Total	C	O	P	0
			49	38	10	1	
37	L	1	Total	C	O	P	0
			49	38	10	1	
37	N	1	Total	C	O	P	0
			49	38	10	1	
37	R	1	Total	C	O	P	0
			49	38	10	1	
37	S	1	Total	C	O	P	0
			49	38	10	1	
37	Y	1	Total	C	O	P	0
			49	38	10	1	
37	d	1	Total	C	O	P	0
			43	32	10	1	
37	d	1	Total	C	O	P	0
			49	38	10	1	
37	d	1	Total	C	O	P	0
			37	26	10	1	
37	g	1	Total	C	O	P	0
			49	38	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	r	1	Total	C	O	P	0
			49	38	10	1	
37	s	1	Total	C	O	P	0
			49	38	10	1	
37	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 39 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
39	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	G	1	Total 48	C 37	Mg 1	N 4	O 6	0
39	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	N	1	Total 48	C 37	Mg 1	N 4	O 6	0
39	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	R	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	R	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	R	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	R	1	Total 48	C 37	Mg 1	N 4	O 6	0
39	S	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	S	1	Total 49	C 38	Mg 1	N 4	O 6	0
39	S	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	S	1	Total 52	C 41	Mg 1	N 4	O 6	0
39	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

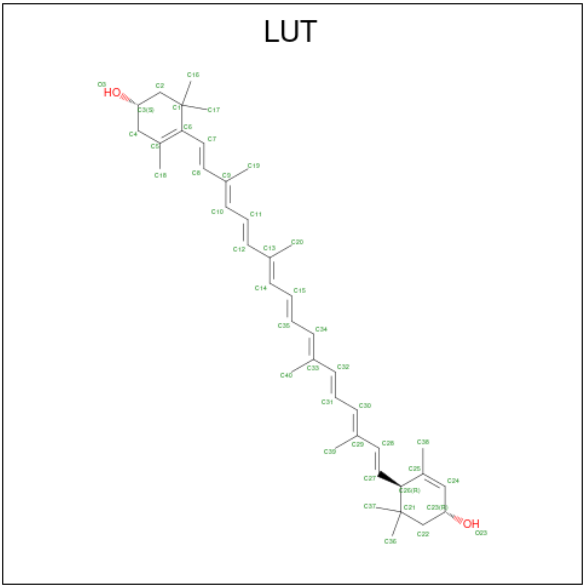
Mol	Chain	Residues	Atoms					AltConf
39	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	g	1	Total 48	C 37	Mg 1	N 4	O 6	0
39	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	n	1	Total 48	C 37	Mg 1	N 4	O 6	0
39	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	r	1	Total 48	C 37	Mg 1	N 4	O 6	0
39	r	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	r	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	r	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	s	1	Total 52	C 41	Mg 1	N 4	O 6	0
39	s	1	Total 49	C 38	Mg 1	N 4	O 6	0
39	s	1	Total 50	C 39	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	s	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 40 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



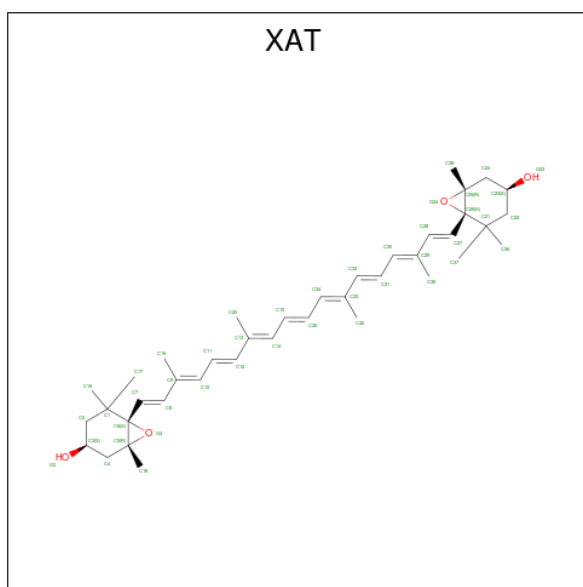
Mol	Chain	Residues	Atoms			AltConf
40	G	1	Total	C	O	0
			42	40	2	
40	G	1	Total	C	O	0
			42	40	2	
40	N	1	Total	C	O	0
			42	40	2	
40	N	1	Total	C	O	0
			42	40	2	
40	R	1	Total	C	O	0
			42	40	2	

Continued on next page...

Continued from previous page...

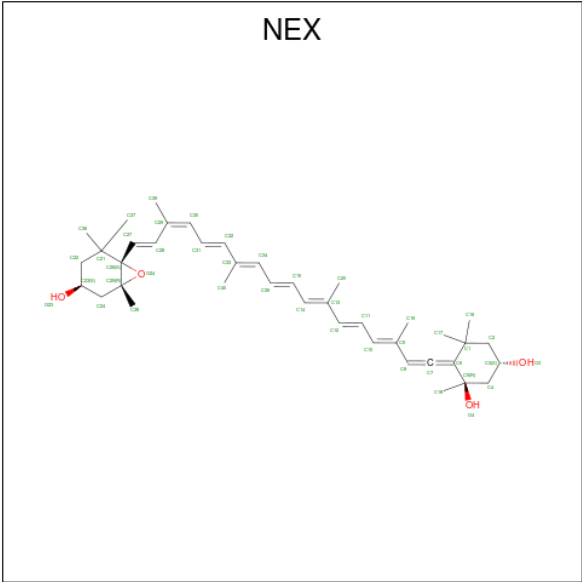
Mol	Chain	Residues	Atoms			AltConf
40	S	1	Total	C	O	0
			42	40	2	
40	S	1	Total	C	O	0
			42	40	2	
40	Y	1	Total	C	O	0
			42	40	2	
40	Y	1	Total	C	O	0
			42	40	2	
40	g	1	Total	C	O	0
			42	40	2	
40	g	1	Total	C	O	0
			42	40	2	
40	n	1	Total	C	O	0
			42	40	2	
40	n	1	Total	C	O	0
			42	40	2	
40	r	1	Total	C	O	0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

- Molecule 41 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
41	G	1	Total	C	O	0
			44	40	4	
41	G	1	Total	C	O	0
			44	40	4	
41	N	1	Total	C	O	0
			44	40	4	
41	R	1	Total	C	O	0
			44	40	4	
41	g	1	Total	C	O	0
			44	40	4	
41	g	1	Total	C	O	0
			44	40	4	
41	n	1	Total	C	O	0
			44	40	4	
41	r	1	Total	C	O	0
			44	40	4	

- Molecule 42 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
42	G	1	Total	C	O	0
			44	40	4	
42	N	1	Total	C	O	0
			44	40	4	
42	R	1	Total	C	O	0
			44	40	4	
42	S	1	Total	C	O	0
			44	40	4	
42	Y	1	Total	C	O	0
			44	40	4	
42	g	1	Total	C	O	0
			44	40	4	
42	n	1	Total	C	O	0
			44	40	4	
42	r	1	Total	C	O	0
			44	40	4	
42	s	1	Total	C	O	0
			44	40	4	
42	y	1	Total	C	O	0
			44	40	4	

- Molecule 43 is water.

Mol	Chain	Residues	Atoms		AltConf
43	A	82	Total	O	0
			82	82	
43	B	115	Total	O	0
			115	115	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
43	C	104	Total 104	O 104	0
43	D	78	Total 78	O 78	0
43	E	19	Total 19	O 19	0
43	F	3	Total 3	O 3	0
43	G	5	Total 5	O 5	0
43	H	15	Total 15	O 15	0
43	I	6	Total 6	O 6	0
43	J	4	Total 4	O 4	0
43	K	5	Total 5	O 5	0
43	L	9	Total 9	O 9	0
43	M	3	Total 3	O 3	0
43	N	5	Total 5	O 5	0
43	O	39	Total 39	O 39	0
43	P	17	Total 17	O 17	0
43	Q	1	Total 1	O 1	0
43	R	19	Total 19	O 19	0
43	S	5	Total 5	O 5	0
43	T	7	Total 7	O 7	0
43	U	1	Total 1	O 1	0
43	W	18	Total 18	O 18	0
43	X	5	Total 5	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
43	Y	36	Total 36	O 36	0
43	Z	2	Total 2	O 2	0
43	a	90	Total 90	O 90	0
43	b	114	Total 114	O 114	0
43	c	100	Total 100	O 100	0
43	d	76	Total 76	O 76	0
43	e	19	Total 19	O 19	0
43	f	3	Total 3	O 3	0
43	g	5	Total 5	O 5	0
43	h	15	Total 15	O 15	0
43	i	6	Total 6	O 6	0
43	j	4	Total 4	O 4	0
43	k	5	Total 5	O 5	0
43	l	9	Total 9	O 9	0
43	m	3	Total 3	O 3	0
43	n	5	Total 5	O 5	0
43	o	38	Total 38	O 38	0
43	p	17	Total 17	O 17	0
43	q	1	Total 1	O 1	0
43	r	19	Total 19	O 19	0
43	s	5	Total 5	O 5	0

Continued on next page...

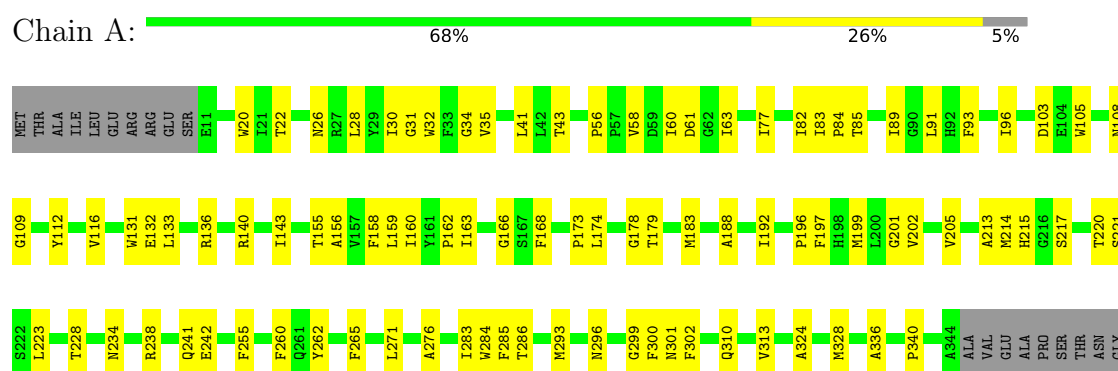
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
43	t	7	Total 7	O 7	0
43	u	1	Total 1	O 1	0
43	w	18	Total 18	O 18	0
43	x	5	Total 5	O 5	0
43	y	36	Total 36	O 36	0
43	z	2	Total 2	O 2	0

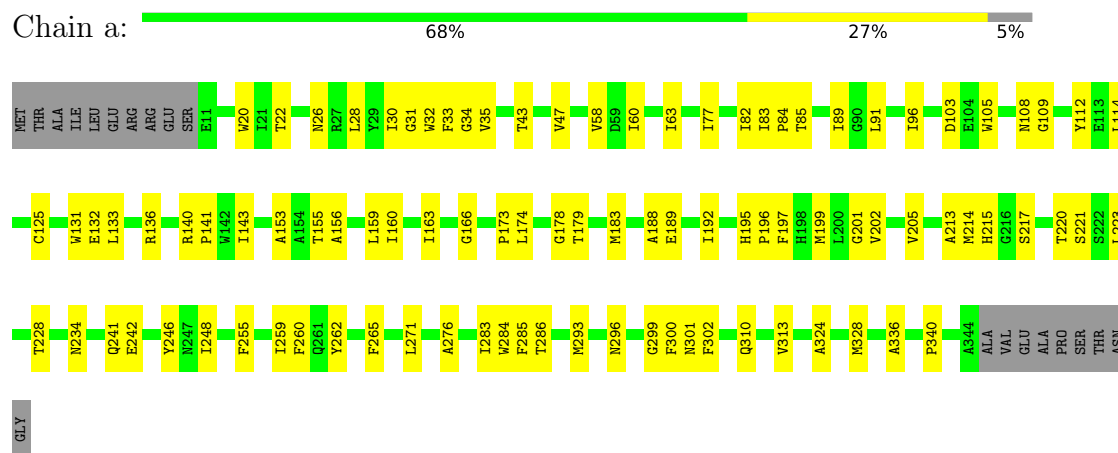
3 Residue-property plots

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.

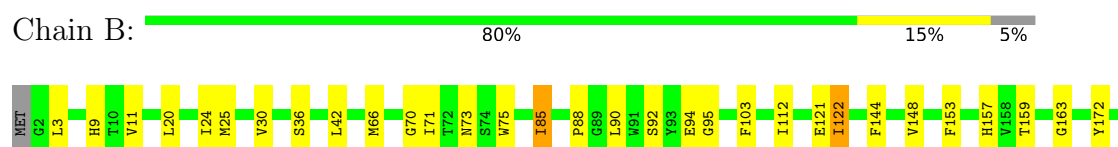
• Molecule 1: Photosystem II protein D1

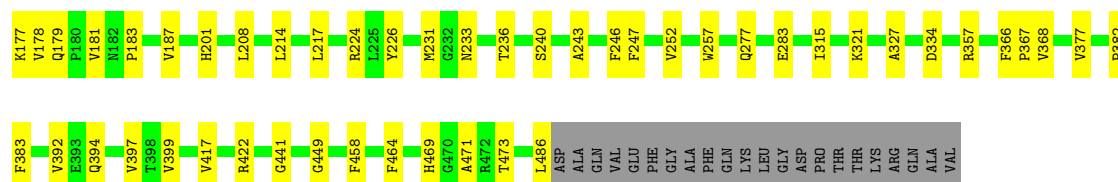


• Molecule 1: Photosystem II protein D1



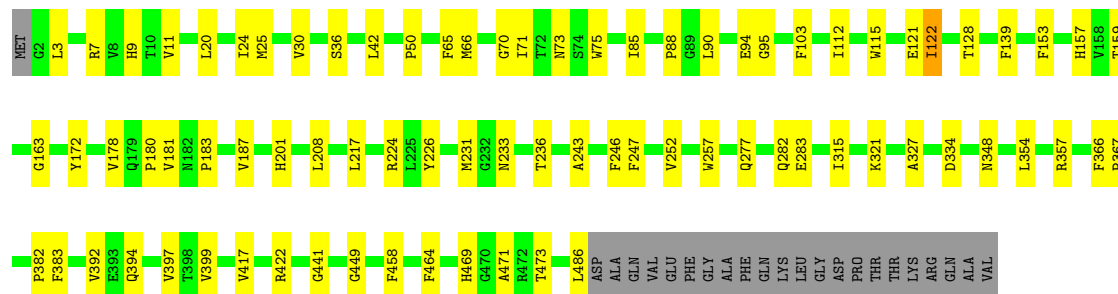
• Molecule 2: Photosystem II CP47 reaction center protein





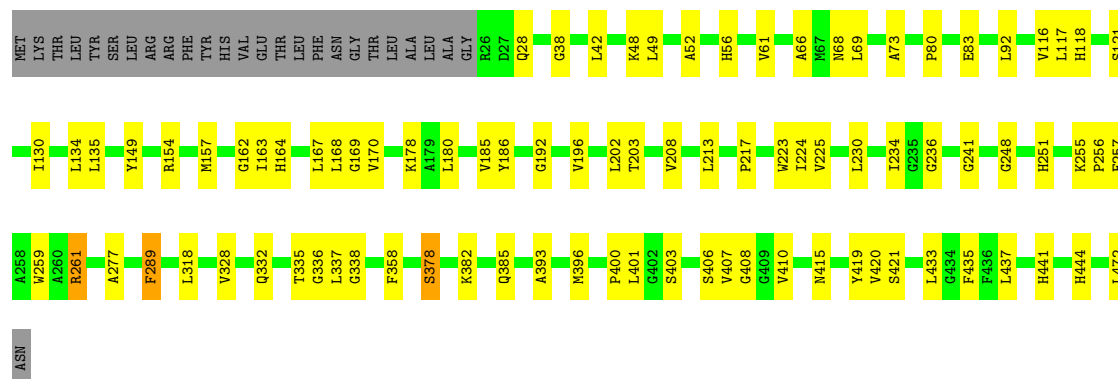
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 80% 16% 5%



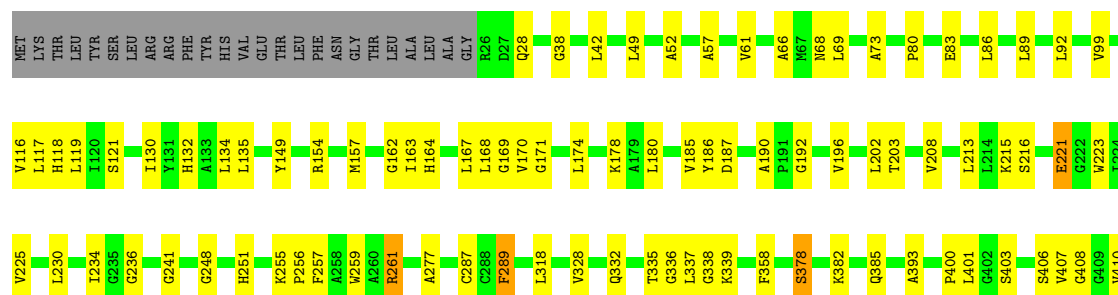
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 76% 18% 5%



• Molecule 3: Photosystem II CP43 reaction center protein

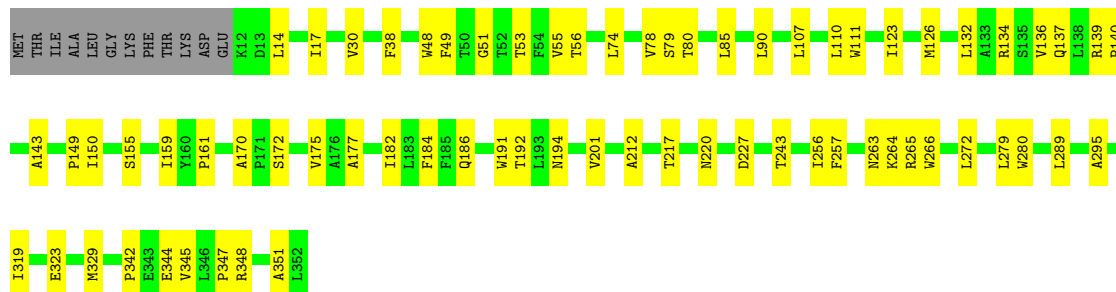
Chain c: 74% 20% 5%





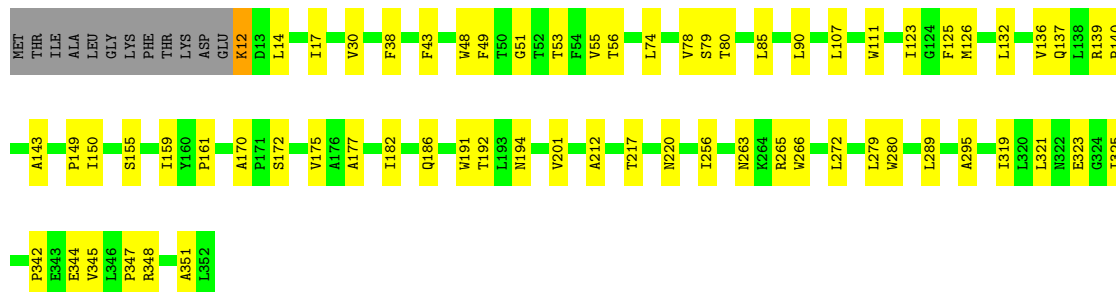
• Molecule 4: Photosystem II D2 protein

Chain D: 77% 20% .



• Molecule 4: Photosystem II D2 protein

Chain d: 78% 18% .



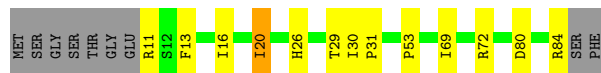
• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 72% 17% 11%



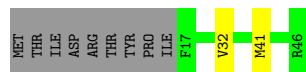
• Molecule 5: Cytochrome b559 subunit alpha

Chain e: 73% 14% 11%



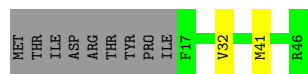
• Molecule 6: Cytochrome b559 subunit beta

Chain F: 72% 5% 23%



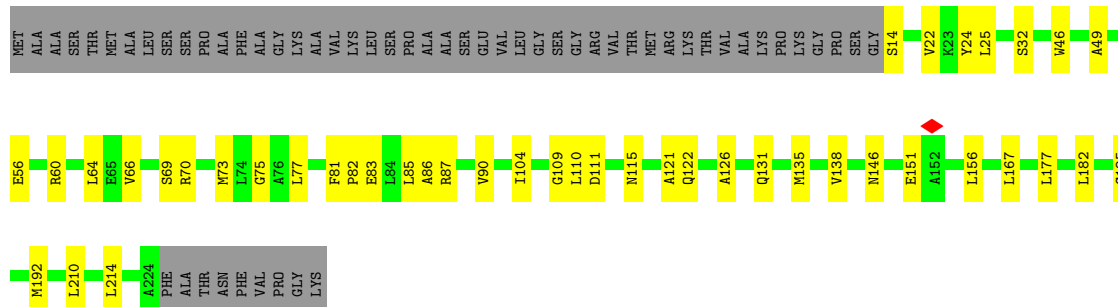
- Molecule 6: Cytochrome b559 subunit beta

Chain f:  72% 5% 23%



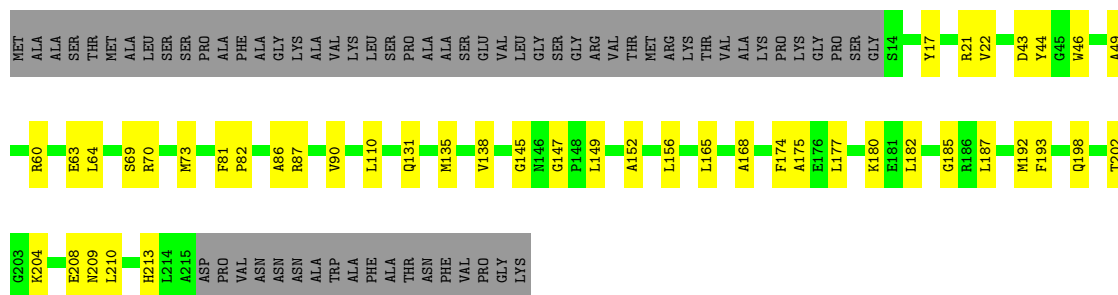
- Molecule 7: Chlorophyll a-b binding protein 1, chloroplastic

Chain G:  63% 16% 21%



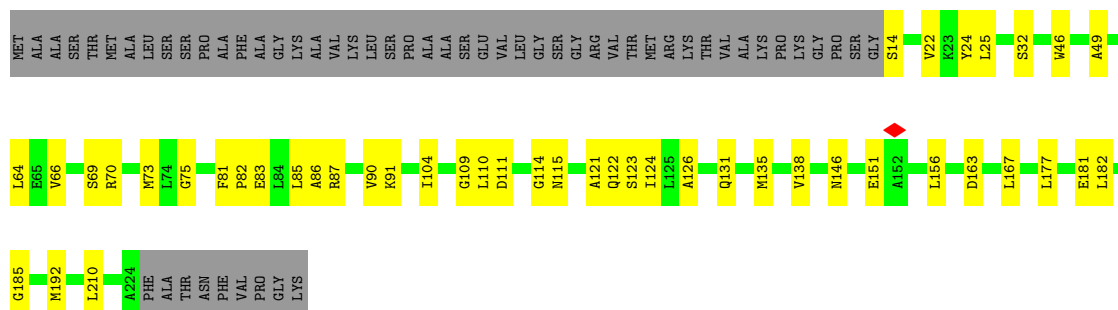
- Molecule 7: Chlorophyll a-b binding protein 1, chloroplastic

Chain N:  59% 17% 24%



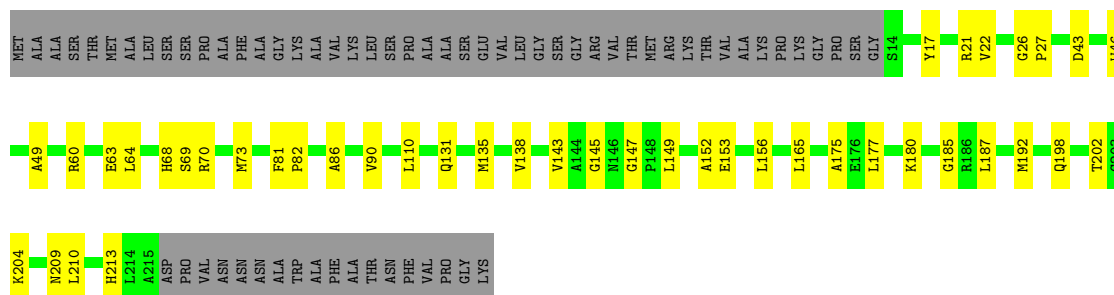
- Molecule 7: Chlorophyll a-b binding protein 1, chloroplastic

Chain g:  62% 17% 21%



- Molecule 7: Chlorophyll a-b binding protein 1, chloroplastic

Chain n:  60% 16% 24%



• Molecule 8: Photosystem II reaction center protein H

Chain H:  71% 10% 19%



• Molecule 8: Photosystem II reaction center protein H

Chain h:  71% 10% 19%



• Molecule 9: Photosystem II reaction center protein I

Chain I:  86% 6% 8%



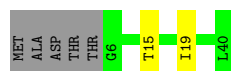
• Molecule 9: Photosystem II reaction center protein I

Chain i:  86% 6% 8%



• Molecule 10: Photosystem II reaction center protein J

Chain J:  82% 5% 12%



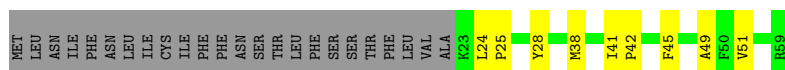
• Molecule 10: Photosystem II reaction center protein J

Chain j:  78% 10% 12%



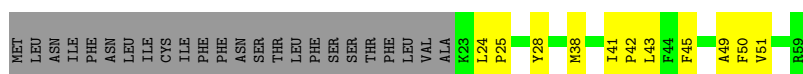
- Molecule 11: Photosystem II reaction center protein K

Chain K: 46% 15% 39%



- Molecule 11: Photosystem II reaction center protein K

Chain k: 43% 18% 39%



- Molecule 12: Photosystem II reaction center protein L

Chain L: 76% 16% 8%



- Molecule 12: Photosystem II reaction center protein L

Chain l: 71% 21% 8%



- Molecule 13: Photosystem II reaction center protein M

Chain M: 68% 24% 9%



- Molecule 13: Photosystem II reaction center protein M

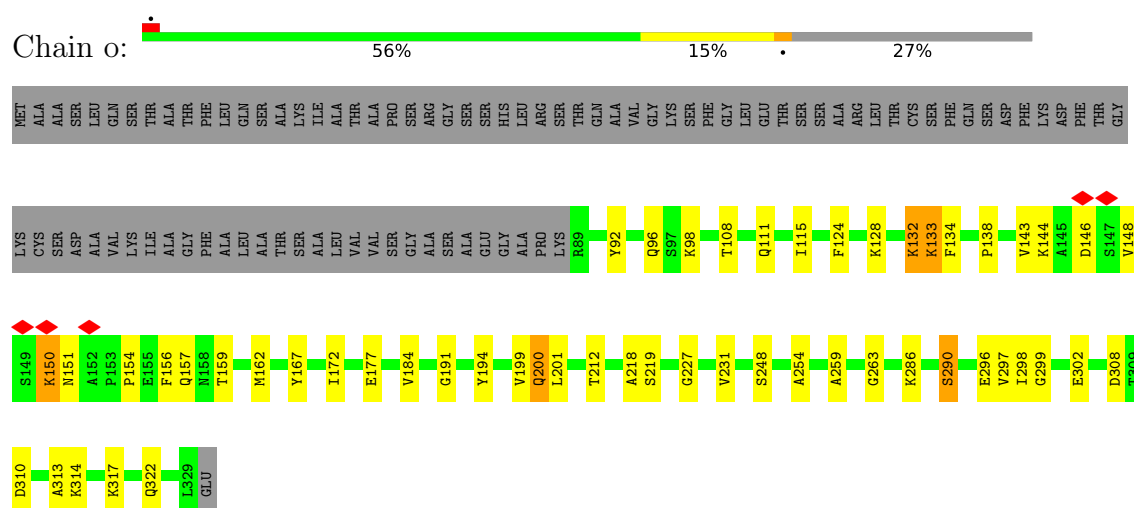
Chain m: 71% 21% 9%



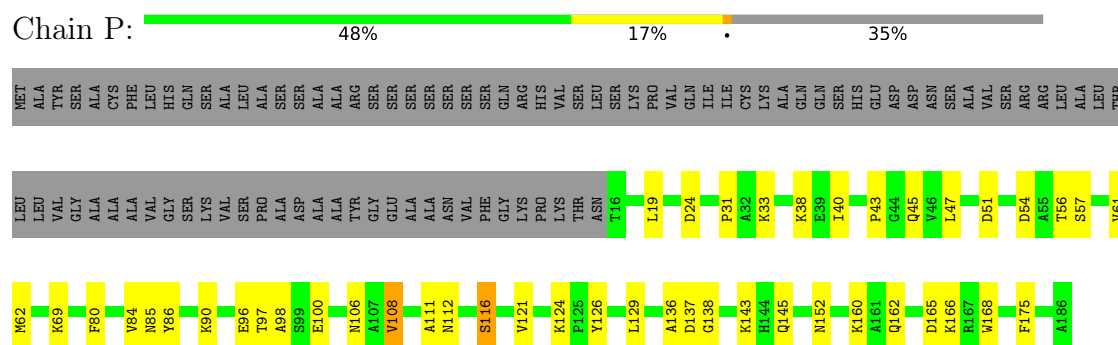
- Molecule 14: Oxygen-evolving enhancer protein 1-1, chloroplastic

Chain O: 57% 15% 27%

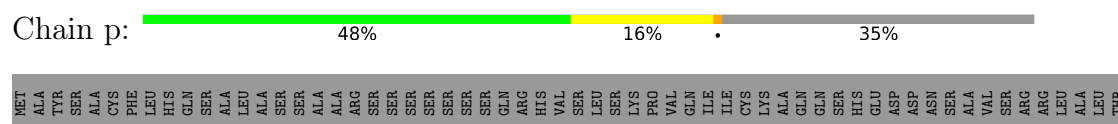
- Molecule 14: Oxygen-evolving enhancer protein 1-1, chloroplastic

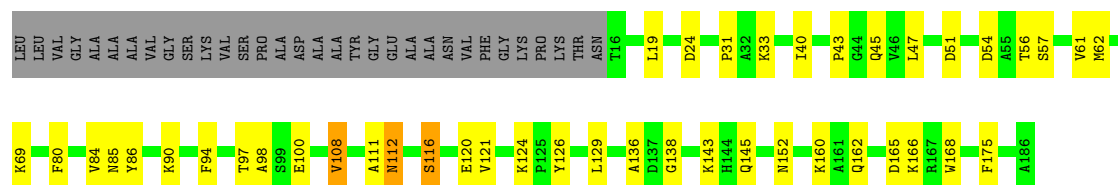


- Molecule 15: Oxygen-evolving enhancer protein 2-1, chloroplastic

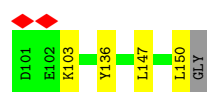
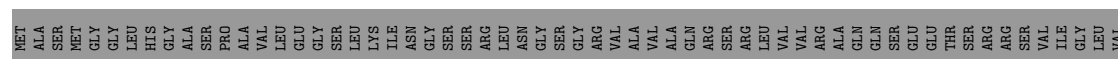


- Molecule 15: Oxygen-evolving enhancer protein 2-1, chloroplastic





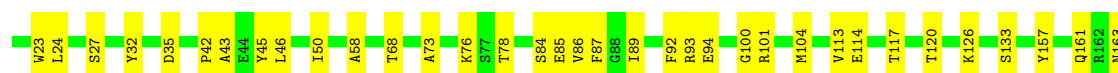
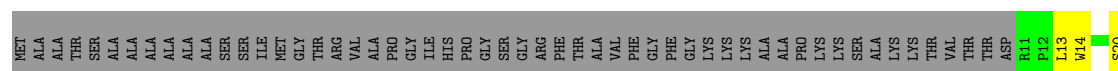
- Molecule 16: Oxygen-evolving enhancer protein 3-1, chloroplastic



- Molecule 16: Oxygen-evolving enhancer protein 3-1, chloroplastic

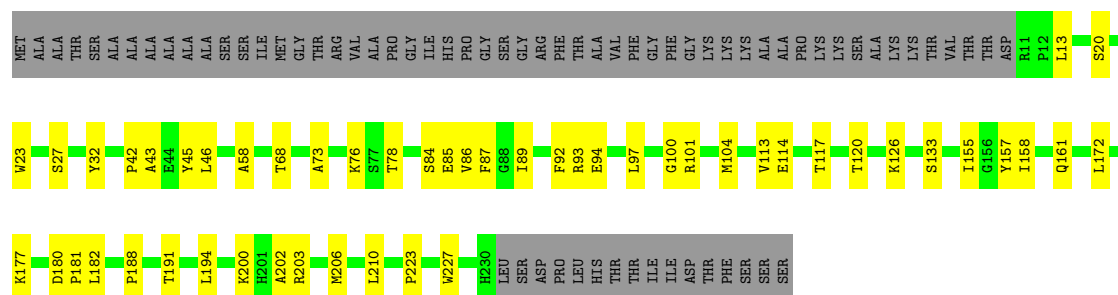


- Molecule 17: Chlorophyll a-b binding protein CP29.1, chloroplastic

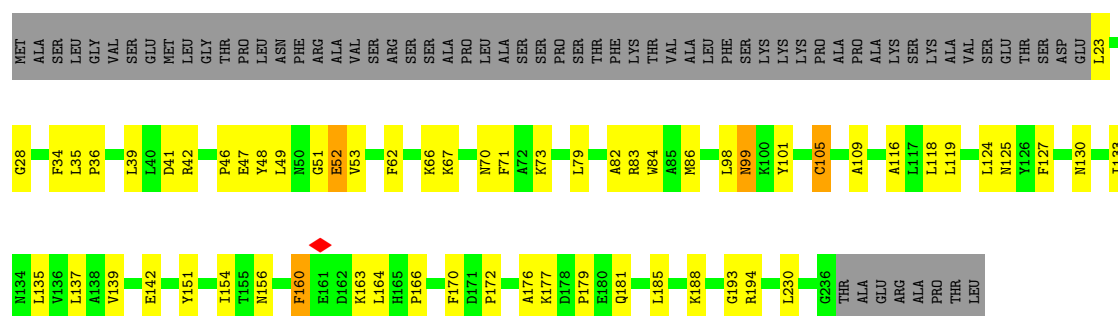


- Molecule 17: Chlorophyll a-b binding protein CP29.1, chloroplastic

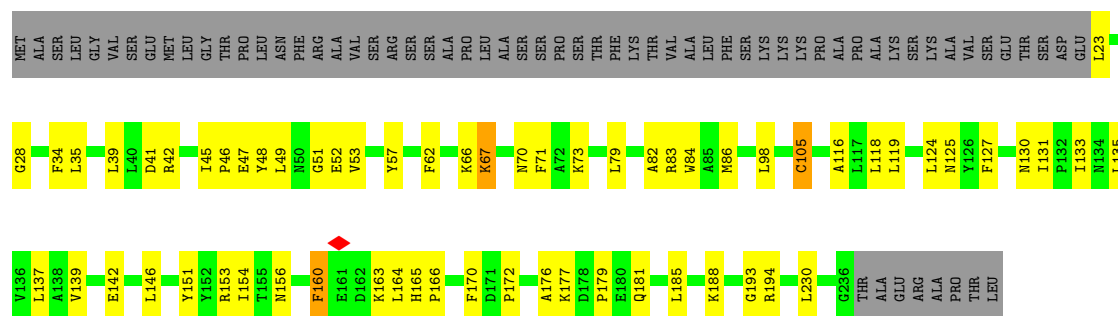




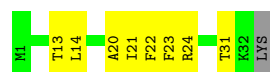
- Molecule 18: Chlorophyll a-b binding protein CP26, chloroplastic



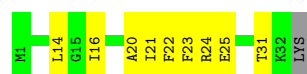
- Molecule 18: Chlorophyll a-b binding protein CP26, chloroplastic



- Molecule 19: Photosystem II reaction center protein T

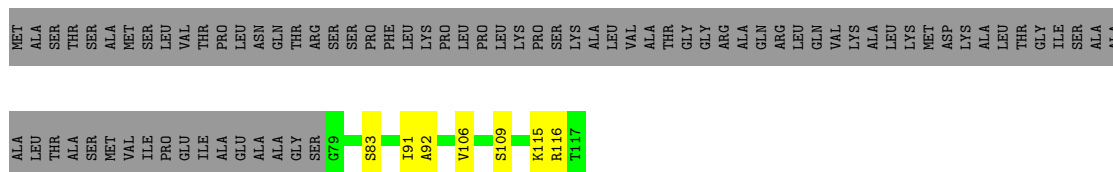


- Molecule 19: Photosystem II reaction center protein T



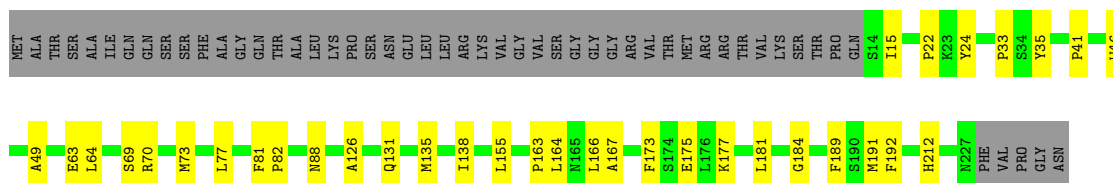
- Molecule 22: Expressed protein

Chain x:  28% 6% 66%



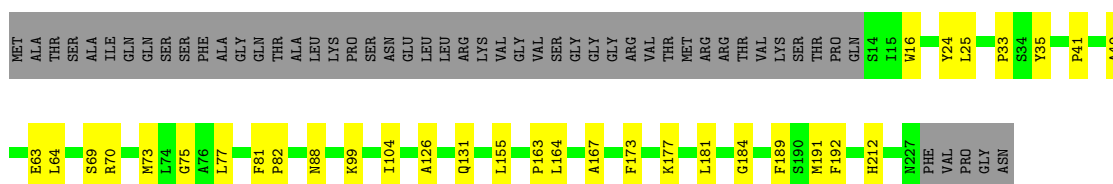
- Molecule 23: Chlorophyll a-b binding protein 2.1, chloroplastic

Chain Y:  68% 13% 19%



- Molecule 23: Chlorophyll a-b binding protein 2.1, chloroplastic

Chain y:  68% 12% 19%



- Molecule 24: Photosystem II reaction center protein Z

Chain Z:  81% 18% .



- Molecule 24: Photosystem II reaction center protein Z

Chain z:  79% 19% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	72301	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.641	Depositor
Minimum map value	-0.646	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.149	Depositor
Map size (Å)	560.952, 560.952, 560.952	wwPDB
Map dimensions	784, 784, 784	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.71550006, 0.71550006, 0.71550006	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CHL, LUT, BCT, SQD, OEX, NEX, HEM, XAT, PL9, LMG, FE2, BCR, CLA, CL, DGD, LMT, LHG, PHO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/2694	0.36	0/3674
1	a	0.26	0/2694	0.36	0/3674
2	B	0.25	0/3930	0.33	0/5354
2	b	0.25	0/3930	0.34	0/5354
3	C	0.24	0/3583	0.33	0/4883
3	c	0.24	0/3583	0.33	0/4883
4	D	0.26	0/2806	0.35	0/3825
4	d	0.26	0/2806	0.35	0/3825
5	E	0.20	0/622	0.29	0/846
5	e	0.19	0/622	0.29	0/846
6	F	0.21	0/248	0.32	0/335
6	f	0.21	0/248	0.33	0/335
7	G	0.16	0/1653	0.29	0/2249
7	N	0.18	0/1580	0.31	0/2146
7	g	0.16	0/1653	0.28	0/2249
7	n	0.18	0/1580	0.31	0/2146
8	H	0.24	0/447	0.33	0/608
8	h	0.24	0/447	0.34	0/608
9	I	0.23	0/274	0.30	0/371
9	i	0.23	0/274	0.30	0/371
10	J	0.14	0/261	0.26	0/354
10	j	0.14	0/261	0.24	0/354
11	K	0.20	0/313	0.33	0/428
11	k	0.20	0/313	0.33	0/428
12	L	0.24	0/301	0.28	0/409
12	l	0.25	0/301	0.27	0/409
13	M	0.21	0/246	0.34	0/337
13	m	0.21	0/246	0.34	0/337
14	O	0.21	0/1867	0.37	0/2525
14	o	0.21	0/1867	0.37	0/2525
15	P	0.19	0/1349	0.34	0/1827

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	p	0.19	0/1349	0.35	0/1827
16	Q	0.18	0/1162	0.35	0/1575
16	q	0.18	0/1162	0.35	0/1575
17	R	0.19	0/1758	0.34	0/2395
17	r	0.19	0/1758	0.34	0/2395
18	S	0.18	0/1698	0.39	0/2305
18	s	0.18	0/1698	0.38	0/2305
19	T	0.20	0/268	0.28	0/362
19	t	0.21	0/268	0.28	0/362
20	U	0.18	0/222	0.37	0/296
20	u	0.17	0/222	0.39	0/296
21	W	0.20	0/438	0.37	0/594
21	w	0.20	0/438	0.36	0/594
22	X	0.19	0/282	0.32	0/383
22	x	0.19	0/282	0.32	0/383
23	Y	0.20	0/1704	0.32	0/2319
23	y	0.20	0/1704	0.32	0/2319
24	Z	0.17	0/466	0.37	0/639
24	z	0.18	0/466	0.33	0/639
All	All	0.22	0/60344	0.34	0/82078

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
24	z	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	z	3	ILE	Peptide

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	2613	0	2521	78	0
1	a	2613	0	2521	79	0
2	B	3800	0	3681	70	0
2	b	3800	0	3681	72	0
3	C	3468	0	3400	73	0
3	c	3468	0	3400	76	0
4	D	2713	0	2609	59	0
4	d	2713	0	2609	61	0
5	E	604	0	586	10	0
5	e	604	0	586	9	0
6	F	241	0	246	2	0
6	f	241	0	246	2	0
7	G	1606	0	1538	34	0
7	N	1536	0	1480	35	0
7	g	1606	0	1538	35	0
7	n	1536	0	1480	34	0
8	H	438	0	465	7	0
8	h	438	0	465	7	0
9	I	266	0	276	2	0
9	i	266	0	276	2	0
10	J	255	0	269	2	0
10	j	255	0	269	2	0
11	K	302	0	313	8	0
11	k	302	0	313	10	0
12	L	293	0	283	7	0
12	l	293	0	283	8	0
13	M	242	0	267	10	0
13	m	242	0	267	9	0
14	O	1829	0	1792	38	0
14	o	1829	0	1792	37	0
15	P	1319	0	1262	30	0
15	p	1319	0	1262	28	0
16	Q	1139	0	1171	21	0
16	q	1139	0	1171	27	0
17	R	1710	0	1668	41	0
17	r	1710	0	1668	38	0
18	S	1653	0	1639	56	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	s	1653	0	1639	54	0
19	T	261	0	280	9	0
19	t	261	0	280	9	0
20	U	219	0	235	6	0
20	u	219	0	235	7	0
21	W	427	0	405	5	0
21	w	427	0	405	4	0
22	X	279	0	307	5	0
22	x	279	0	307	7	0
23	Y	1652	0	1581	33	0
23	y	1652	0	1581	34	0
24	Z	456	0	483	8	0
24	z	456	0	483	7	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	125	0	131	3	0
26	B	1040	0	1152	60	0
26	C	828	0	903	42	0
26	D	244	0	255	15	0
26	G	424	0	378	17	0
26	N	424	0	378	15	0
26	R	522	0	456	21	0
26	S	441	0	351	21	0
26	Y	472	0	477	27	0
26	a	190	0	203	5	0
26	b	1040	0	1152	60	0
26	c	828	0	903	47	0
26	d	179	0	183	15	0
26	g	424	0	378	16	0
26	n	424	0	378	13	0
26	r	522	0	456	23	0
26	s	441	0	351	20	0
26	y	472	0	477	27	0
27	A	64	0	74	2	0
27	D	64	0	74	7	0
27	a	64	0	74	1	0
27	d	64	0	74	8	0
28	A	40	0	56	1	0
28	B	120	0	168	11	0
28	C	80	0	112	6	0
28	D	40	0	56	0	0
28	H	40	0	56	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	J	40	0	56	4	0
28	K	40	0	56	5	0
28	T	40	0	56	6	0
28	a	40	0	56	1	0
28	b	120	0	168	13	0
28	c	80	0	112	7	0
28	d	40	0	56	0	0
28	h	40	0	56	3	0
28	j	40	0	56	4	0
28	k	40	0	56	5	0
28	t	40	0	56	6	0
29	A	104	0	145	7	0
29	B	54	0	78	2	0
29	W	33	0	30	0	0
29	a	104	0	145	8	0
29	b	54	0	78	3	0
29	w	33	0	30	0	0
30	A	22	0	25	3	0
30	D	55	0	80	3	0
30	a	22	0	25	4	0
30	d	55	0	80	2	0
31	A	1	0	0	0	0
31	a	1	0	0	0	0
32	A	4	0	0	0	0
32	a	4	0	0	0	0
33	B	62	0	82	3	0
33	C	179	0	232	10	0
33	Y	43	0	44	3	0
33	b	62	0	82	3	0
33	c	179	0	232	8	0
33	y	43	0	44	2	0
34	B	51	0	72	2	0
34	C	102	0	144	3	0
34	D	46	0	62	1	0
34	W	48	0	66	3	0
34	b	51	0	72	3	0
34	c	102	0	144	2	0
34	d	46	0	62	2	0
34	w	48	0	66	2	0
35	C	10	0	0	2	0
35	a	10	0	0	3	0
36	D	35	0	46	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	d	35	0	46	0	0
37	D	129	0	177	11	0
37	G	49	0	74	6	0
37	L	49	0	74	2	0
37	N	49	0	74	5	0
37	R	49	0	74	0	0
37	S	49	0	74	2	0
37	Y	49	0	74	4	0
37	d	129	0	177	10	0
37	g	49	0	74	8	0
37	l	49	0	74	3	0
37	n	49	0	74	5	0
37	r	49	0	74	2	0
37	s	49	0	74	2	0
37	y	49	0	74	4	0
38	E	43	0	30	5	0
38	e	43	0	30	4	0
39	G	314	0	251	24	0
39	N	314	0	251	17	0
39	R	198	0	144	7	0
39	S	201	0	147	14	0
39	Y	282	0	251	17	0
39	g	314	0	251	26	0
39	n	314	0	251	19	0
39	r	198	0	144	8	0
39	s	201	0	147	15	0
39	y	282	0	251	16	0
40	G	84	0	112	5	0
40	N	84	0	112	7	0
40	R	42	0	56	5	0
40	S	84	0	112	6	0
40	Y	84	0	112	12	0
40	g	84	0	112	7	0
40	n	84	0	112	7	0
40	r	42	0	56	6	0
40	s	84	0	112	5	0
40	y	84	0	112	11	0
41	G	88	0	112	10	0
41	N	44	0	56	6	0
41	R	44	0	56	1	0
41	g	88	0	112	10	0
41	n	44	0	56	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	r	44	0	56	2	0
42	G	44	0	56	4	0
42	N	44	0	56	2	0
42	R	44	0	56	3	0
42	S	44	0	56	7	0
42	Y	44	0	56	3	0
42	g	44	0	56	4	0
42	n	44	0	56	1	0
42	r	44	0	56	4	0
42	s	44	0	56	6	0
42	y	44	0	56	3	0
43	A	82	0	0	0	0
43	B	115	0	0	0	0
43	C	104	0	0	0	0
43	D	78	0	0	1	0
43	E	19	0	0	1	0
43	F	3	0	0	0	0
43	G	5	0	0	0	0
43	H	15	0	0	1	0
43	I	6	0	0	0	0
43	J	4	0	0	0	0
43	K	5	0	0	0	0
43	L	9	0	0	0	0
43	M	3	0	0	0	0
43	N	5	0	0	0	0
43	O	39	0	0	0	0
43	P	17	0	0	0	0
43	Q	1	0	0	0	0
43	R	19	0	0	1	0
43	S	5	0	0	0	0
43	T	7	0	0	0	0
43	U	1	0	0	0	0
43	W	18	0	0	0	0
43	X	5	0	0	0	0
43	Y	36	0	0	0	0
43	Z	2	0	0	0	0
43	a	90	0	0	1	0
43	b	114	0	0	0	0
43	c	100	0	0	0	0
43	d	76	0	0	1	0
43	e	19	0	0	1	0
43	f	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	g	5	0	0	0	0
43	h	15	0	0	1	0
43	i	6	0	0	0	0
43	j	4	0	0	0	0
43	k	5	0	0	0	0
43	l	9	0	0	0	0
43	m	3	0	0	0	0
43	n	5	0	0	0	0
43	o	38	0	0	0	0
43	p	17	0	0	0	0
43	q	1	0	0	0	0
43	r	19	0	0	1	0
43	s	5	0	0	0	0
43	t	7	0	0	0	0
43	u	1	0	0	0	0
43	w	18	0	0	0	0
43	x	5	0	0	0	0
43	y	36	0	0	0	0
43	z	2	0	0	0	0
All	All	76824	0	75622	1602	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 11.

All (1602) 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)
35:a:408:OEX:CA1	35:a:408:OEX:O1	1.31	1.05
35:C:501:OEX:O1	35:C:501:OEX:CA1	1.40	0.96
3:c:68:ASN:HD21	3:c:92:LEU:HD11	1.34	0.92
4:D:175:VAL:HG13	26:D:412:CLA:HED1	1.56	0.87
39:s:316:CHL:HBB2	39:s:317:CHL:HBB1	1.55	0.86
4:d:175:VAL:HG13	26:d:411:CLA:HED1	1.57	0.86
39:S:302:CHL:HBB2	39:S:313:CHL:HBB1	1.57	0.86
18:s:188:LYS:HD3	26:s:304:CLA:HBA1	1.59	0.84
18:S:188:LYS:HD3	26:S:309:CLA:HBA1	1.60	0.83
26:n:305:CLA:HAB	40:n:317:LUT:H32	1.60	0.83
18:S:28:GLY:H	18:S:51:GLY:HA3	1.43	0.81
18:s:139:VAL:HG22	39:s:317:CHL:HBC1	1.62	0.81
18:S:139:VAL:HG22	39:S:313:CHL:HBC1	1.62	0.81
18:s:28:GLY:H	18:s:51:GLY:HA3	1.42	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:192:MET:HE2	40:n:317:LUT:H10	1.63	0.80
40:N:305:LUT:H32	26:N:307:CLA:HAB	1.63	0.80
7:N:192:MET:HE2	40:N:305:LUT:H10	1.64	0.80
18:S:99:ASN:HD22	18:S:109:ALA:HB2	1.48	0.78
18:s:82:ALA:HB1	18:s:193:GLY:HA3	1.64	0.78
39:g:313:CHL:HBB2	39:g:319:CHL:HBB1	1.64	0.78
18:S:82:ALA:HB1	18:S:193:GLY:HA3	1.65	0.77
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.67	0.76
14:O:143:VAL:HB	14:O:201:LEU:HD21	1.67	0.76
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.66	0.76
17:r:100:GLY:HA3	17:r:202:ALA:HB1	1.66	0.76
17:R:100:GLY:HA3	17:R:202:ALA:HB1	1.66	0.76
14:o:143:VAL:HB	14:o:201:LEU:HD21	1.66	0.75
3:c:121:SER:HA	28:c:507:BCR:H16C	1.68	0.75
30:d:408:PL9:H111	37:d:409:LHG:HC92	1.70	0.74
26:b:606:CLA:H2	26:b:613:CLA:H91	1.70	0.73
18:S:67:LYS:HB2	18:S:70:ASN:HB2	1.68	0.73
28:T:101:BCR:H402	2:b:36:SER:HB2	1.69	0.73
35:a:408:OEX:MN3	35:a:408:OEX:O2	1.44	0.73
28:C:502:BCR:H16C	26:C:516:CLA:H142	1.71	0.72
3:c:38:GLY:HA3	26:c:518:CLA:HMD2	1.69	0.72
2:B:36:SER:HB2	28:t:101:BCR:H402	1.70	0.72
26:B:611:CLA:H2	26:B:618:CLA:H91	1.70	0.72
37:D:408:LHG:HC92	30:D:411:PL9:H111	1.69	0.72
18:s:194:ARG:HB3	26:s:311:CLA:HBC3	1.72	0.72
3:C:42:LEU:HD21	26:C:504:CLA:H2A	1.71	0.72
3:c:163:ILE:HD13	26:c:503:CLA:HAB	1.72	0.72
3:C:38:GLY:HA3	26:C:504:CLA:HMD2	1.71	0.72
38:e:101:HEM:HBC2	38:e:101:HEM:HHD	1.71	0.72
39:G:301:CHL:HBB2	39:G:305:CHL:HBB1	1.71	0.72
14:o:150:LYS:HA	14:o:150:LYS:HZ2	1.54	0.72
18:s:176:ALA:HB2	26:s:315:CLA:H2A	1.72	0.72
3:c:42:LEU:HD21	26:c:518:CLA:H2A	1.72	0.71
3:C:121:SER:HA	28:C:514:BCR:H16C	1.73	0.71
18:S:176:ALA:HB2	26:S:314:CLA:H2A	1.73	0.71
18:s:177:LYS:O	18:s:179:PRO:HD3	1.90	0.71
3:C:163:ILE:HD13	26:C:511:CLA:HAB	1.73	0.70
26:c:508:CLA:H142	28:c:511:BCR:H16C	1.72	0.70
26:Y:301:CLA:HBA1	33:Y:303:DGD:HG31	1.74	0.70
38:E:101:HEM:HBC2	38:E:101:HEM:HHD	1.72	0.70
16:Q:5:ILE:HG12	16:Q:6:SER:H	1.57	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:y:304:CLA:HBA1	33:y:308:DGD:HG31	1.74	0.69
1:A:221:SER:HA	4:D:139:ARG:HB2	1.73	0.69
17:R:113:VAL:HG21	26:R:308:CLA:HED2	1.73	0.69
18:S:177:LYS:O	18:S:179:PRO:HD3	1.90	0.69
16:q:5:ILE:HG12	16:q:6:SER:H	1.56	0.69
18:S:194:ARG:HB3	26:S:307:CLA:HBC3	1.73	0.69
2:b:153:PHE:HB2	26:b:617:CLA:HBB1	1.74	0.69
26:B:611:CLA:HAB	26:B:618:CLA:H152	1.75	0.69
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.75	0.69
17:r:113:VAL:HG21	26:r:311:CLA:HED2	1.73	0.68
18:s:118:LEU:HD13	18:s:135:LEU:HA	1.75	0.68
4:d:107:LEU:HD23	5:e:69:ILE:HD13	1.75	0.68
4:d:279:LEU:HD22	27:d:407:PHO:HBC3	1.76	0.68
4:D:107:LEU:HD23	5:E:69:ILE:HD13	1.75	0.68
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.76	0.68
1:A:296:ASN:HB3	3:C:401:LEU:HA	1.75	0.68
17:R:13:LEU:HD21	17:R:20:SER:HB2	1.75	0.68
26:Y:305:CLA:H52	40:Y:315:LUT:H30	1.76	0.68
1:A:228:THR:HA	17:R:58:ALA:HA	1.76	0.68
26:b:606:CLA:HAB	26:b:613:CLA:H152	1.75	0.67
1:a:221:SER:HA	4:d:139:ARG:HB2	1.76	0.67
1:a:241:GLN:HA	19:t:31:THR:HA	1.77	0.67
17:r:13:LEU:HD21	17:r:20:SER:HB2	1.76	0.67
7:n:202:THR:HG22	7:n:204:LYS:HD2	1.77	0.67
4:d:192:THR:HG23	26:d:404:CLA:HBC2	1.77	0.67
2:B:153:PHE:HB2	26:B:610:CLA:HBB1	1.75	0.67
7:G:192:MET:HE2	40:G:308:LUT:H10	1.76	0.66
18:s:53:VAL:HG21	18:s:71:PHE:HE2	1.60	0.66
1:A:241:GLN:HA	19:T:31:THR:HA	1.78	0.66
3:c:116:VAL:HG22	28:k:101:BCR:HC21	1.77	0.66
16:q:19:LEU:HG	16:q:20:PRO:HD3	1.77	0.66
2:B:334:ASP:HB3	14:O:259:ALA:HB1	1.77	0.66
1:a:296:ASN:HB3	3:c:401:LEU:HA	1.76	0.66
4:D:192:THR:HG23	26:D:409:CLA:HBC2	1.78	0.66
7:N:202:THR:HG22	7:N:204:LYS:HD2	1.77	0.66
3:c:472:LEU:HD23	19:t:24:ARG:HH21	1.60	0.66
16:Q:19:LEU:HG	16:Q:20:PRO:HD3	1.76	0.65
2:b:315:ILE:HG12	2:b:321:LYS:HG3	1.78	0.65
7:g:192:MET:HE2	40:g:310:LUT:H10	1.76	0.65
35:C:501:OEX:MN3	35:C:501:OEX:O2	1.54	0.65
39:G:301:CHL:HBA2	42:G:315:NEX:H403	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:332:GLN:HG2	3:c:336:GLY:HA2	1.78	0.65
23:y:73:MET:SD	26:y:309:CLA:HAB	2.37	0.65
18:S:79:LEU:HD23	18:S:164:LEU:HB3	1.79	0.65
14:O:150:LYS:HA	14:O:150:LYS:HZ2	1.62	0.64
18:S:118:LEU:HD13	18:S:135:LEU:HA	1.77	0.64
4:D:279:LEU:HD22	27:D:403:PHO:HBC3	1.77	0.64
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.80	0.64
2:B:458:PHE:HB3	26:B:615:CLA:HBC2	1.79	0.64
1:a:228:THR:HA	17:r:58:ALA:HA	1.79	0.64
2:b:334:ASP:HB3	14:o:259:ALA:HB1	1.78	0.64
3:C:472:LEU:HD23	19:T:24:ARG:HH21	1.62	0.64
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.79	0.64
18:S:53:VAL:HG21	18:S:71:PHE:HE2	1.63	0.64
23:y:191:MET:HE2	40:y:318:LUT:H10	1.79	0.64
1:a:234:ASN:HD21	37:d:402:LHG:HC11	1.62	0.64
3:c:80:PRO:HD3	16:q:36:LEU:HD13	1.79	0.64
16:Q:65:LYS:HB2	16:Q:136:TYR:CZ	2.33	0.64
1:a:313:VAL:HG23	15:p:33:LYS:HG3	1.79	0.63
14:o:310:ASP:HB3	14:o:313:ALA:HB3	1.79	0.63
2:B:315:ILE:HG12	2:B:321:LYS:HG3	1.80	0.63
7:n:152:ALA:HB2	39:n:307:CHL:HBC1	1.80	0.63
3:C:332:GLN:HG2	3:C:336:GLY:HA2	1.81	0.63
1:A:271:LEU:HD11	30:A:408:PL9:HC8	1.81	0.63
23:Y:191:MET:HE2	40:Y:309:LUT:H10	1.81	0.63
7:g:69:SER:HB3	7:g:185:GLY:HA3	1.80	0.63
1:A:234:ASN:HD21	37:D:407:LHG:HC11	1.64	0.63
3:C:116:VAL:HG22	28:K:101:BCR:HC21	1.79	0.63
1:a:77:ILE:HD13	12:l:30:VAL:HG13	1.80	0.63
16:q:65:LYS:HB2	16:q:136:TYR:CZ	2.33	0.63
24:z:33:TRP:O	24:z:37:LYS:HB3	1.99	0.63
2:b:103:PHE:HB2	26:b:617:CLA:H62	1.81	0.63
33:c:519:DGD:HBT1	33:c:519:DGD:HB52	1.81	0.63
3:C:80:PRO:HD3	16:Q:36:LEU:HD13	1.81	0.62
4:D:79:SER:HA	4:D:172:SER:HB3	1.81	0.62
23:Y:73:MET:SD	26:Y:305:CLA:HAB	2.39	0.62
24:z:57:LEU:HD23	24:z:60:LEU:HD12	1.81	0.62
19:T:22:PHE:HB3	28:b:615:BCR:H271	1.81	0.62
2:b:458:PHE:HB3	26:b:611:CLA:HBC2	1.80	0.62
3:c:185:VAL:HG23	3:c:230:LEU:HD13	1.81	0.62
14:O:310:ASP:HB3	14:O:313:ALA:HB3	1.81	0.62
2:b:236:THR:HB	2:b:473:THR:HG21	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:PHE:HB2	26:B:610:CLA:H62	1.80	0.62
23:y:24:TYR:HD2	39:y:303:CHL:HAA1	1.63	0.62
1:A:340:PRO:HB2	15:P:166:LYS:HB3	1.81	0.62
1:a:271:LEU:HD11	30:a:407:PL9:HC8	1.81	0.62
4:d:79:SER:HA	4:d:172:SER:HB3	1.81	0.62
26:B:602:CLA:H162	26:B:616:CLA:H71	1.82	0.61
28:B:608:BCR:H271	19:t:22:PHE:HB3	1.81	0.61
23:Y:24:TYR:HD2	39:Y:302:CHL:HAA1	1.65	0.61
14:o:302:GLU:HG3	14:o:322:GLN:HG2	1.82	0.61
15:p:124:LYS:HE3	15:p:152:ASN:HB2	1.83	0.61
14:O:148:VAL:HA	14:O:154:PRO:HB3	1.83	0.61
4:D:48:TRP:HA	4:D:78:VAL:HG21	1.83	0.61
37:n:301:LHG:HC61	26:n:310:CLA:HBC3	1.82	0.61
23:y:69:SER:HB3	23:y:184:GLY:HA3	1.83	0.61
16:q:51:ALA:O	16:q:55:LYS:HG2	2.01	0.60
1:A:242:GLU:H	19:T:31:THR:HG23	1.66	0.60
23:Y:69:SER:HB3	23:Y:184:GLY:HA3	1.83	0.60
26:c:518:CLA:HBA1	28:k:101:BCR:H271	1.83	0.60
2:b:157:HIS:HA	2:b:163:GLY:HA3	1.83	0.60
26:b:605:CLA:H162	26:b:609:CLA:H71	1.83	0.60
3:C:185:VAL:HG23	3:C:230:LEU:HD13	1.83	0.60
37:N:301:LHG:HC61	26:N:319:CLA:HBC3	1.81	0.60
24:Z:34:SER:HA	24:Z:37:LYS:HE3	1.84	0.60
28:b:619:BCR:H14C	37:l:101:LHG:H382	1.84	0.60
1:a:340:PRO:HB2	15:p:166:LYS:HB3	1.83	0.60
1:a:26:ASN:HB3	29:a:403:SQD:H112	1.84	0.60
26:C:504:CLA:HBA1	28:K:101:BCR:H271	1.83	0.60
8:H:65:VAL:HA	22:X:83:SER:HB3	1.83	0.60
4:d:186:GLN:HB2	26:d:404:CLA:HBC1	1.84	0.59
7:N:152:ALA:HB2	39:N:311:CHL:HBC1	1.83	0.59
15:P:124:LYS:HE3	15:P:152:ASN:HB2	1.83	0.59
7:G:167:LEU:HD11	26:G:307:CLA:H11	1.85	0.59
7:n:147:GLY:H	39:n:307:CHL:HMC	1.66	0.59
26:B:607:CLA:HAC2	28:t:101:BCR:H391	1.85	0.59
3:C:164:HIS:HA	3:C:167:LEU:HD12	1.84	0.59
35:a:408:OEX:MN1	35:a:408:OEX:O3	1.59	0.59
7:G:69:SER:HB3	7:G:185:GLY:HA3	1.83	0.59
7:G:167:LEU:HD23	7:G:167:LEU:H	1.67	0.59
7:N:69:SER:HB3	7:N:185:GLY:HA3	1.85	0.59
7:N:147:GLY:H	39:N:311:CHL:HMC	1.67	0.59
1:a:155:THR:HG21	33:c:517:DGD:HBE1	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:149:LEU:HG	39:n:307:CHL:HAB	1.84	0.59
1:a:84:PRO:HA	1:a:112:TYR:CG	2.38	0.59
26:y:309:CLA:H52	40:y:311:LUT:H30	1.85	0.59
33:C:510:DGD:HBT1	33:C:510:DGD:HB52	1.84	0.59
16:Q:51:ALA:O	16:Q:55:LYS:HG2	2.03	0.59
3:c:164:HIS:HA	3:c:167:LEU:HD12	1.85	0.59
1:A:155:THR:HG21	33:C:509:DGD:HBE1	1.84	0.59
27:D:403:PHO:H61	26:D:409:CLA:H111	1.84	0.59
17:R:86:VAL:HG22	26:R:302:CLA:CGA	2.33	0.59
2:b:392:VAL:HG13	2:b:397:VAL:HB	1.85	0.59
7:g:110:LEU:HD21	26:g:302:CLA:HAA1	1.83	0.59
7:G:110:LEU:HD21	26:G:302:CLA:HAA1	1.84	0.58
7:N:64:LEU:HD11	23:Y:49:ALA:HA	1.86	0.58
8:h:65:VAL:HA	22:x:83:SER:HB3	1.83	0.58
14:o:148:VAL:HA	14:o:154:PRO:HB3	1.83	0.58
1:A:301:ASN:HB3	3:C:407:VAL:HG21	1.84	0.58
2:B:217:LEU:O	26:R:302:CLA:H12	2.03	0.58
28:B:614:BCR:H14C	37:L:101:LHG:H382	1.84	0.58
7:G:85:LEU:HB3	7:G:90:VAL:HB	1.85	0.58
18:s:79:LEU:HD23	18:s:164:LEU:HB3	1.84	0.58
7:g:66:VAL:HB	7:g:156:LEU:HD11	1.84	0.58
39:G:311:CHL:HHC	39:G:311:CHL:HBB1	1.84	0.58
7:N:149:LEU:HG	39:N:311:CHL:HAB	1.85	0.58
18:S:179:PRO:HD2	18:S:181:GLN:H	1.69	0.58
23:Y:166:LEU:HD22	40:Y:315:LUT:H221	1.85	0.58
4:d:48:TRP:HA	4:d:78:VAL:HG21	1.85	0.58
18:S:185:LEU:HB3	26:S:314:CLA:H3A	1.85	0.58
3:C:69:LEU:HD12	11:K:38:MET:HE1	1.86	0.58
42:g:306:NEX:H403	39:g:313:CHL:HBA2	1.84	0.58
1:A:313:VAL:HG23	15:P:33:LYS:HG3	1.86	0.58
2:B:157:HIS:HA	2:B:163:GLY:HA3	1.85	0.58
39:g:311:CHL:HHC	39:g:311:CHL:HBB1	1.85	0.58
2:B:464:PHE:HD2	26:B:617:CLA:HAC2	1.68	0.57
15:P:56:THR:HG23	15:P:143:LYS:HE3	1.86	0.57
23:Y:41:PRO:HG3	23:Y:177:LYS:HB3	1.85	0.57
23:Y:77:LEU:HD13	26:Y:313:CLA:HBB2	1.86	0.57
26:C:506:CLA:CMD	26:C:516:CLA:HAB	2.34	0.57
39:G:318:CHL:HHC	39:G:318:CHL:HBB1	1.87	0.57
18:s:185:LEU:HB3	26:s:315:CLA:H3A	1.86	0.57
7:g:109:GLY:HA3	7:g:122:GLN:HE21	1.70	0.57
7:g:167:LEU:HD23	7:g:167:LEU:H	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:146:ASN:O	39:G:303:CHL:HMC	2.05	0.57
2:b:382:PRO:HB3	4:d:344:GLU:HB2	1.87	0.57
2:b:11:VAL:HG11	26:b:607:CLA:HED2	1.87	0.57
26:c:502:CLA:CMD	26:c:508:CLA:HAB	2.34	0.57
15:p:145:GLN:HG2	15:p:160:LYS:HE2	1.87	0.57
18:S:151:TYR:HA	18:S:154:ILE:HG22	1.86	0.57
1:a:28:LEU:HB2	29:a:403:SQD:H122	1.85	0.57
2:b:217:LEU:O	26:r:313:CLA:H12	2.03	0.57
26:n:303:CLA:H52	40:n:314:LUT:H30	1.87	0.57
4:D:186:GLN:HB2	26:D:409:CLA:HBC1	1.86	0.57
15:P:111:ALA:O	16:Q:11:PRO:HA	2.04	0.57
1:a:301:ASN:HB3	3:c:407:VAL:HG21	1.86	0.57
26:d:404:CLA:H72	26:d:411:CLA:HAB	1.87	0.57
26:C:520:CLA:H2	26:C:520:CLA:HMA2	1.86	0.57
37:G:312:LHG:H131	41:G:320:XAT:H403	1.86	0.57
39:N:317:CHL:HHC	39:N:317:CHL:HBB1	1.87	0.57
2:b:464:PHE:HD2	26:b:610:CLA:HAC2	1.69	0.57
7:g:146:ASN:O	39:g:307:CHL:HMC	2.04	0.57
18:s:151:TYR:HA	18:s:154:ILE:HG22	1.87	0.57
18:s:179:PRO:HD2	18:s:181:GLN:H	1.69	0.56
3:C:154:ARG:HH22	21:W:132:GLU:HA	1.69	0.56
7:g:85:LEU:HB3	7:g:90:VAL:HB	1.87	0.56
26:s:311:CLA:HAB	40:s:312:LUT:H32	1.87	0.56
1:A:84:PRO:HA	1:A:112:TYR:CG	2.40	0.56
2:B:11:VAL:HG11	26:B:601:CLA:HED2	1.87	0.56
1:a:63:ILE:HB	3:c:335:THR:HG21	1.88	0.56
2:b:30:VAL:HG12	26:b:613:CLA:HHD	1.87	0.56
34:d:405:LMG:H232	34:d:405:LMG:H331	1.87	0.56
7:n:69:SER:HB3	7:n:185:GLY:HA3	1.86	0.56
17:r:86:VAL:HG22	26:r:313:CLA:CGA	2.35	0.56
16:Q:56:GLU:HA	16:Q:59:LYS:HE2	1.86	0.56
23:y:77:LEU:HD13	26:y:316:CLA:HBB2	1.86	0.56
3:c:61:VAL:HG13	3:c:118:HIS:HD2	1.69	0.56
15:p:56:THR:HG23	15:p:143:LYS:HE3	1.88	0.56
1:A:20:TRP:HE1	29:A:407:SQD:H81	1.71	0.56
7:G:66:VAL:HB	7:G:156:LEU:HD11	1.88	0.56
1:A:63:ILE:HB	3:C:335:THR:HG21	1.87	0.56
39:n:319:CHL:HHC	39:n:319:CHL:HBB1	1.87	0.56
3:c:154:ARG:HH22	21:w:132:GLU:HA	1.71	0.56
37:n:301:LHG:HC41	39:n:306:CHL:HMD3	1.88	0.56
18:s:142:GLU:OE1	39:s:317:CHL:HMC	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:76:LYS:HE2	17:R:84:SER:HB3	1.88	0.56
7:n:64:LEU:HD11	23:y:49:ALA:HA	1.87	0.56
27:D:403:PHO:H143	26:D:409:CLA:H141	1.88	0.55
18:S:142:GLU:OE1	39:S:313:CHL:HMC	2.06	0.55
40:S:306:LUT:H32	26:S:307:CLA:HAB	1.87	0.55
2:B:236:THR:HB	2:B:473:THR:HG21	1.87	0.55
7:G:135:MET:HA	7:G:138:VAL:HG22	1.88	0.55
1:a:201:GLY:HA3	1:a:286:THR:HB	1.89	0.55
26:d:404:CLA:H111	27:d:407:PHO:H61	1.87	0.55
15:p:47:LEU:HB3	15:p:61:VAL:HB	1.88	0.55
4:D:182:ILE:HG23	26:D:409:CLA:CHD	2.36	0.55
26:d:404:CLA:H141	27:d:407:PHO:H143	1.87	0.55
14:O:302:GLU:HG3	14:O:322:GLN:HG2	1.88	0.55
39:S:312:CHL:HBB1	39:S:312:CHL:HHC	1.88	0.55
17:r:126:LYS:HB2	39:r:318:CHL:CGD	2.37	0.55
14:O:115:ILE:HG23	14:O:298:ILE:HG23	1.89	0.55
2:b:70:GLY:HA2	2:b:178:VAL:HG11	1.89	0.55
4:d:182:ILE:HG23	26:d:404:CLA:CHD	2.37	0.55
3:C:117:LEU:HD21	34:C:503:LMG:H332	1.89	0.55
17:R:46:LEU:HA	17:R:68:THR:HA	1.88	0.55
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.42	0.54
3:C:68:ASN:HD21	3:C:92:LEU:HD11	1.72	0.54
3:C:154:ARG:HB3	3:C:256:PRO:HG2	1.90	0.54
28:T:101:BCR:H391	26:b:616:CLA:HAC2	1.90	0.54
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.42	0.54
37:g:301:LHG:H131	41:g:320:XAT:H403	1.88	0.54
26:y:310:CLA:HBB1	40:y:311:LUT:H192	1.88	0.54
1:A:340:PRO:HA	4:D:351:ALA:O	2.08	0.54
1:a:20:TRP:HE1	29:a:403:SQD:H81	1.72	0.54
7:g:135:MET:HA	7:g:138:VAL:HG22	1.89	0.54
4:d:51:GLY:HA3	4:d:78:VAL:HG22	1.89	0.54
39:y:305:CHL:HBB1	26:y:313:CLA:HMB2	1.89	0.54
2:B:30:VAL:HG12	26:B:618:CLA:HHD	1.88	0.54
2:B:392:VAL:HG13	2:B:397:VAL:HB	1.88	0.54
3:C:61:VAL:HG12	3:C:118:HIS:O	2.08	0.54
26:b:602:CLA:HED3	26:b:602:CLA:H2	1.89	0.54
26:b:608:CLA:HBA2	26:b:608:CLA:H142	1.90	0.54
17:r:46:LEU:HA	17:r:68:THR:HA	1.88	0.54
1:A:201:GLY:HA3	1:A:286:THR:HB	1.87	0.54
4:D:51:GLY:HA3	4:D:78:VAL:HG22	1.89	0.54
41:G:310:XAT:H12	37:N:301:LHG:H211	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:340:PRO:HA	4:d:351:ALA:O	2.08	0.54
3:c:69:LEU:HD12	11:k:38:MET:HE1	1.88	0.54
4:d:126:MET:HE3	4:d:143:ALA:O	2.07	0.54
7:g:64:LEU:HD11	7:n:49:ALA:HA	1.90	0.54
26:C:505:CLA:C3D	26:C:507:CLA:H2	2.37	0.54
7:G:210:LEU:HD22	40:G:316:LUT:H163	1.89	0.54
7:g:177:LEU:HB3	26:g:317:CLA:H3A	1.89	0.54
23:y:41:PRO:HG3	23:y:177:LYS:HB3	1.90	0.54
1:A:310:GLN:HB3	15:P:19:LEU:HD21	1.90	0.54
7:G:177:LEU:HB3	26:G:307:CLA:H3A	1.90	0.54
39:g:314:CHL:HHC	39:g:314:CHL:HBB1	1.90	0.54
7:n:135:MET:HA	7:n:138:VAL:HG22	1.89	0.54
1:A:77:ILE:HD13	12:L:30:VAL:HG13	1.89	0.54
26:b:601:CLA:H12	33:b:620:DGD:HB41	1.90	0.54
7:g:167:LEU:HD11	26:g:317:CLA:H11	1.89	0.54
3:C:66:ALA:HB1	11:K:38:MET:HB3	1.90	0.54
7:G:151:GLU:HB2	39:G:303:CHL:HBC1	1.90	0.54
3:c:225:VAL:HG13	3:c:289:PHE:HA	1.90	0.54
4:d:155:SER:HA	4:d:159:ILE:HB	1.90	0.54
7:G:64:LEU:HD11	7:N:49:ALA:HA	1.90	0.53
11:K:25:PRO:HB2	11:K:28:TYR:HD2	1.73	0.53
26:N:312:CLA:H52	40:N:314:LUT:H30	1.89	0.53
17:R:126:LYS:HB2	39:R:315:CHL:CGD	2.38	0.53
1:a:91:LEU:HD11	1:a:163:ILE:HA	1.90	0.53
18:S:118:LEU:HG	18:S:124:LEU:HD13	1.91	0.53
7:g:22:VAL:HB	39:g:311:CHL:HBC1	1.89	0.53
41:g:309:XAT:H12	37:n:301:LHG:H211	1.90	0.53
18:s:125:ASN:HA	18:s:130:ASN:HA	1.90	0.53
7:G:109:GLY:HA3	7:G:122:GLN:HE21	1.74	0.53
1:a:213:ALA:HA	4:d:272:LEU:HA	1.89	0.53
1:a:242:GLU:H	19:t:31:THR:HG23	1.72	0.53
1:a:310:GLN:HB3	15:p:19:LEU:HD21	1.90	0.53
26:B:605:CLA:HBA2	26:B:605:CLA:H142	1.89	0.53
4:D:126:MET:HE3	4:D:143:ALA:O	2.08	0.53
13:M:25:ILE:HA	13:M:28:LYS:HG2	1.88	0.53
26:Y:312:CLA:HBB1	40:Y:315:LUT:H192	1.89	0.53
2:b:327:ALA:HB1	34:b:622:LMG:HC8	1.91	0.53
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.91	0.53
1:A:213:ALA:HA	4:D:272:LEU:HA	1.90	0.53
3:c:154:ARG:HB3	3:c:256:PRO:HG2	1.91	0.53
4:d:263:ASN:HB3	4:d:266:TRP:HB3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:r:306:CLA:H52	40:r:307:LUT:H30	1.91	0.53
37:N:301:LHG:HC41	39:N:316:CHL:HMD3	1.89	0.53
26:c:505:CLA:H2	26:c:520:CLA:C3D	2.38	0.53
1:A:131:TRP:CH2	26:C:506:CLA:HAA2	2.44	0.53
2:b:277:GLN:HB3	20:u:24:LYS:HB2	1.90	0.53
3:c:66:ALA:HB1	11:k:38:MET:HB3	1.91	0.53
4:d:49:PHE:HZ	34:d:405:LMG:H341	1.74	0.53
3:C:385:GLN:HG3	16:Q:82:SER:O	2.09	0.53
26:C:512:CLA:HBB2	26:C:520:CLA:H193	1.90	0.53
37:D:408:LHG:H161	12:L:23:LEU:HD21	1.90	0.53
7:g:151:GLU:HB2	39:g:307:CHL:HBC1	1.90	0.53
1:A:159:LEU:HD11	33:C:509:DGD:HA41	1.90	0.53
7:G:22:VAL:HB	39:G:318:CHL:HBC1	1.91	0.53
14:O:124:PHE:HE1	14:O:290:SER:HB2	1.74	0.53
26:c:506:CLA:HMA2	26:c:506:CLA:H2	1.90	0.53
26:c:510:CLA:H41	26:s:301:CLA:HAB	1.90	0.53
23:y:63:GLU:HA	23:y:155:LEU:HD21	1.90	0.53
1:a:58:VAL:HB	1:a:83:ILE:HB	1.91	0.53
3:c:86:LEU:HD13	3:c:89:LEU:HD12	1.90	0.53
3:c:251:HIS:CE1	26:c:516:CLA:NA	2.77	0.53
2:b:277:GLN:HA	20:u:23:ALA:HA	1.92	0.52
26:C:519:CLA:H41	26:S:308:CLA:HAB	1.91	0.52
7:N:210:LEU:HD22	40:N:314:LUT:H163	1.91	0.52
39:R:312:CHL:HHC	39:R:312:CHL:HBB1	1.90	0.52
23:Y:63:GLU:HA	23:Y:155:LEU:HD21	1.90	0.52
39:s:303:CHL:HHC	39:s:303:CHL:HBB1	1.90	0.52
4:D:155:SER:HA	4:D:159:ILE:HB	1.91	0.52
26:Y:316:CLA:HMB2	39:Y:317:CHL:HBB1	1.91	0.52
1:a:131:TRP:CH2	26:c:502:CLA:HAA2	2.44	0.52
11:k:49:ALA:HB2	28:k:101:BCR:H391	1.92	0.52
7:n:63:GLU:HG3	7:n:156:LEU:HD13	1.91	0.52
2:B:327:ALA:HB1	34:B:622:LMG:HC8	1.90	0.52
26:B:603:CLA:H2	26:B:603:CLA:HED3	1.91	0.52
7:N:135:MET:HA	7:N:138:VAL:HG22	1.90	0.52
14:O:128:LYS:HG3	14:O:177:GLU:HG3	1.91	0.52
11:k:25:PRO:HB2	11:k:28:TYR:HD2	1.73	0.52
16:q:63:ASN:O	16:q:66:PRO:HD2	2.10	0.52
26:y:309:CLA:H121	40:y:311:LUT:H403	1.91	0.52
3:C:61:VAL:HG13	3:C:118:HIS:HD2	1.74	0.52
3:C:162:GLY:HA2	3:C:248:GLY:HA2	1.91	0.52
28:C:502:BCR:HC32	9:I:23:PHE:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:263:ASN:HB3	4:D:266:TRP:HB3	1.90	0.52
26:g:308:CLA:HMD3	39:g:312:CHL:HBA2	1.91	0.52
18:s:105:CYS:HA	18:s:127:PHE:HA	1.91	0.52
39:G:309:CHL:HHC	39:G:309:CHL:HBB1	1.90	0.52
14:o:290:SER:HB3	14:o:297:VAL:HG12	1.91	0.52
39:r:309:CHL:HHC	39:r:309:CHL:HBB1	1.91	0.52
18:s:166:PRO:HG3	39:s:313:CHL:HBC2	1.92	0.52
15:P:145:GLN:HG2	15:P:160:LYS:HE2	1.91	0.52
1:a:217:SER:HB3	4:d:272:LEU:HD12	1.91	0.52
7:n:60:ARG:HH21	23:y:33:PRO:HG3	1.75	0.52
26:C:507:CLA:H203	26:C:520:CLA:HAB	1.92	0.52
39:g:307:CHL:HAA1	26:g:317:CLA:HBC1	1.91	0.52
2:B:177:LYS:HG3	2:B:179:GLN:HG2	1.92	0.52
26:a:409:CLA:H52	30:d:408:PL9:H151	1.91	0.52
37:d:409:LHG:H161	12:l:23:LEU:HD21	1.91	0.52
14:o:172:ILE:HG13	14:o:191:GLY:O	2.10	0.52
15:p:97:THR:HG23	15:p:98:ALA:H	1.75	0.52
1:A:28:LEU:HB2	29:A:407:SQD:H122	1.92	0.52
26:B:606:CLA:H191	33:B:620:DGD:HBT1	1.91	0.52
3:C:225:VAL:HG13	3:C:289:PHE:HA	1.93	0.52
3:C:251:HIS:CE1	26:C:508:CLA:NA	2.77	0.52
39:N:316:CHL:HHC	39:N:316:CHL:HBB1	1.92	0.52
26:g:302:CLA:H11	42:g:306:NEX:H241	1.92	0.52
1:A:58:VAL:HB	1:A:83:ILE:HB	1.92	0.51
26:b:601:CLA:H191	33:b:620:DGD:HBT1	1.91	0.51
3:c:180:LEU:HD11	3:c:202:LEU:HD21	1.92	0.51
4:d:53:THR:HG22	6:f:41:MET:HE1	1.93	0.51
18:s:46:PRO:HD2	18:s:49:LEU:HD12	1.92	0.51
39:G:305:CHL:CGA	39:G:305:CHL:H3A	2.41	0.51
15:P:47:LEU:HB3	15:P:61:VAL:HB	1.91	0.51
17:R:85:GLU:HA	26:R:302:CLA:H41	1.92	0.51
19:T:14:LEU:HD22	28:T:101:BCR:H332	1.92	0.51
7:g:210:LEU:HD22	40:g:316:LUT:H163	1.92	0.51
14:o:92:TYR:O	14:o:96:GLN:HG2	2.10	0.51
2:B:277:GLN:HA	20:U:23:ALA:HA	1.92	0.51
26:D:409:CLA:H72	26:D:412:CLA:HAB	1.91	0.51
13:m:25:ILE:HA	13:m:28:LYS:HG2	1.91	0.51
2:B:224:ARG:HB2	43:H:202:HOH:O	2.10	0.51
26:G:302:CLA:H11	42:G:315:NEX:H241	1.92	0.51
39:g:312:CHL:HHC	39:g:312:CHL:HBB1	1.92	0.51
17:r:32:TYR:OH	17:r:200:LYS:HE2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:r:227:TRP:HE3	26:r:308:CLA:HMA1	1.76	0.51
23:y:77:LEU:HD21	26:y:316:CLA:H202	1.91	0.51
26:C:511:CLA:H42	26:C:512:CLA:H61	1.92	0.51
7:G:111:ASP:HB3	7:G:115:ASN:O	2.10	0.51
18:s:118:LEU:HG	18:s:124:LEU:HD13	1.92	0.51
3:C:406:SER:HA	3:C:420:VAL:HG23	1.93	0.51
7:G:126:ALA:HB3	39:G:309:CHL:HMC	1.91	0.51
7:N:110:LEU:HD22	39:N:304:CHL:HMD2	1.93	0.51
14:O:92:TYR:O	14:O:96:GLN:HG2	2.10	0.51
15:P:80:PHE:O	15:P:84:VAL:HG22	2.11	0.51
18:S:125:ASN:HA	18:S:130:ASN:HA	1.91	0.51
2:b:73:ASN:HB3	2:b:85:ILE:HG21	1.91	0.51
3:c:61:VAL:HG12	3:c:118:HIS:O	2.09	0.51
26:c:504:CLA:HBB1	26:c:504:CLA:HMB1	1.93	0.51
1:a:214:MET:HE2	1:a:255:PHE:CD1	2.45	0.51
26:b:605:CLA:H172	28:b:615:BCR:H331	1.92	0.51
26:c:503:CLA:H42	26:c:515:CLA:H61	1.92	0.51
7:g:111:ASP:HB3	7:g:115:ASN:O	2.11	0.51
23:Y:164:LEU:HD12	40:Y:315:LUT:H222	1.92	0.51
1:a:43:THR:HG23	28:a:404:BCR:H362	1.93	0.51
3:c:117:LEU:HD21	34:c:512:LMG:H332	1.92	0.51
7:n:177:LEU:HB3	26:n:303:CLA:H3A	1.93	0.51
17:R:227:TRP:HE3	26:R:307:CLA:HMA1	1.76	0.51
1:a:30:ILE:O	1:a:34:GLY:HA3	2.11	0.51
3:c:385:GLN:HG3	16:q:82:SER:O	2.10	0.51
1:A:30:ILE:O	1:A:34:GLY:HA3	2.11	0.51
14:O:159:THR:HG22	14:O:201:LEU:HD23	1.92	0.51
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.93	0.50
1:A:283:ILE:HA	1:A:286:THR:HG22	1.93	0.50
2:B:75:TRP:CD1	2:B:92:SER:HG	2.29	0.50
3:C:180:LEU:HD11	3:C:202:LEU:HD21	1.92	0.50
40:S:301:LUT:H181	26:S:303:CLA:HBB1	1.92	0.50
39:Y:302:CHL:HHC	39:Y:302:CHL:HBB1	1.92	0.50
1:a:265:PHE:HE2	29:a:413:SQD:H92	1.75	0.50
28:c:511:BCR:HC32	9:i:23:PHE:HB3	1.92	0.50
7:g:126:ALA:HB3	39:g:314:CHL:HMC	1.92	0.50
1:A:220:THR:HA	1:A:223:LEU:HG	1.94	0.50
26:A:405:CLA:HAA2	34:W:201:LMG:H111	1.93	0.50
4:d:56:THR:HG21	5:e:53:PRO:HD3	1.92	0.50
39:g:319:CHL:CGA	39:g:319:CHL:H3A	2.40	0.50
7:n:22:VAL:HB	39:n:306:CHL:HBC1	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:p:40:ILE:HG23	15:p:45:GLN:HB3	1.92	0.50
40:r:307:LUT:H10	40:r:307:LUT:H203	1.94	0.50
1:A:132:GLU:O	1:A:136:ARG:HG2	2.11	0.50
1:A:214:MET:HE2	1:A:255:PHE:CD1	2.46	0.50
39:G:303:CHL:HAA1	26:G:307:CLA:HBC1	1.91	0.50
18:s:166:PRO:HB2	18:s:170:PHE:HD2	1.77	0.50
26:s:307:CLA:HBB1	40:s:308:LUT:H181	1.93	0.50
39:y:303:CHL:HHC	39:y:303:CHL:HBB1	1.92	0.50
26:B:616:CLA:H172	26:B:616:CLA:H112	1.93	0.50
37:N:301:LHG:H312	37:N:301:LHG:HC91	1.93	0.50
1:a:132:GLU:O	1:a:136:ARG:HG2	2.11	0.50
7:g:49:ALA:HA	23:y:64:LEU:HD11	1.93	0.50
37:g:301:LHG:HC92	41:g:320:XAT:H361	1.94	0.50
1:A:56:PRO:HB2	14:O:206:ARG:NH2	2.27	0.50
26:B:606:CLA:H12	33:B:620:DGD:HB41	1.92	0.50
39:G:311:CHL:HBA2	26:G:317:CLA:HMD3	1.92	0.50
40:R:311:LUT:H10	40:R:311:LUT:H203	1.93	0.50
14:o:115:ILE:HG23	14:o:298:ILE:HG23	1.91	0.50
19:t:14:LEU:HD22	28:t:101:BCR:H332	1.94	0.50
1:A:91:LEU:HD11	1:A:163:ILE:HA	1.94	0.50
2:B:233:ASN:O	2:B:236:THR:HG22	2.11	0.50
26:R:306:CLA:H52	40:R:311:LUT:H30	1.94	0.50
18:s:83:ARG:HA	18:s:86:MET:HE3	1.93	0.50
18:S:83:ARG:HA	18:S:86:MET:HE3	1.94	0.50
26:b:609:CLA:H112	26:b:609:CLA:H172	1.93	0.50
37:d:409:LHG:H302	19:t:21:ILE:HD11	1.92	0.50
14:o:115:ILE:HG21	14:o:296:GLU:HB3	1.94	0.50
1:A:43:THR:HG23	28:A:406:BCR:H362	1.94	0.50
26:B:605:CLA:H162	28:H:101:BCR:H19C	1.93	0.50
4:D:126:MET:SD	4:D:150:ILE:HD12	2.52	0.50
7:N:63:GLU:HG3	7:N:156:LEU:HD13	1.93	0.50
18:S:166:PRO:HB2	18:S:170:PHE:HD2	1.76	0.50
2:b:224:ARG:HB2	43:h:201:HOH:O	2.10	0.50
7:n:210:LEU:HD22	40:n:314:LUT:H163	1.92	0.50
1:A:166:GLY:HA3	3:C:358:PHE:CE1	2.47	0.50
1:A:214:MET:HG2	30:A:408:PL9:H102	1.93	0.50
2:B:382:PRO:HB3	4:D:344:GLU:HB2	1.93	0.50
38:E:101:HEM:HMB1	38:E:101:HEM:HBB2	1.92	0.50
14:O:172:ILE:HG13	14:O:191:GLY:O	2.12	0.50
1:a:89:ILE:HD11	1:a:108:ASN:HB3	1.93	0.50
1:a:299:GLY:O	3:c:403:SER:HB2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:464:PHE:HB2	4:d:280:TRP:CZ2	2.47	0.50
23:y:24:TYR:CD2	39:y:303:CHL:HAA1	2.46	0.50
2:B:247:PHE:HB2	26:B:604:CLA:HBC1	1.94	0.49
4:D:53:THR:HG22	6:F:41:MET:HE1	1.94	0.49
42:S:305:NEX:H34	39:S:312:CHL:HMA1	1.93	0.49
1:a:133:LEU:HD23	4:d:256:ILE:HG12	1.94	0.49
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.47	0.49
33:c:501:DGD:HB52	26:c:514:CLA:H51	1.94	0.49
17:r:101:ARG:HA	17:r:104:MET:HE3	1.93	0.49
42:s:302:NEX:H222	26:s:310:CLA:C1C	2.42	0.49
2:B:9:HIS:HB3	26:B:609:CLA:HAB	1.93	0.49
26:D:401:CLA:H52	30:D:411:PL9:H151	1.94	0.49
18:S:46:PRO:HD2	18:S:49:LEU:HD12	1.94	0.49
3:c:171:GLY:HA2	3:c:174:LEU:HD12	1.94	0.49
26:c:506:CLA:H193	26:c:515:CLA:HBB2	1.92	0.49
26:y:306:CLA:H202	40:y:318:LUT:H402	1.94	0.49
2:B:486:LEU:HD11	4:D:137:GLN:HB2	1.94	0.49
15:P:31:PRO:HG3	15:P:175:PHE:HB3	1.93	0.49
2:b:157:HIS:HE1	26:b:617:CLA:NA	2.10	0.49
15:p:57:SER:HA	15:p:162:GLN:O	2.12	0.49
15:p:80:PHE:O	15:p:84:VAL:HG22	2.13	0.49
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.93	0.49
33:C:513:DGD:HB52	26:C:521:CLA:H51	1.95	0.49
4:D:279:LEU:HD21	27:D:403:PHO:HMC2	1.95	0.49
13:M:28:LYS:HB3	13:m:27:VAL:HG12	1.93	0.49
18:S:47:GLU:O	18:S:48:TYR:CD2	2.66	0.49
1:a:159:LEU:HD11	33:c:517:DGD:HA41	1.94	0.49
1:a:166:GLY:HA3	3:c:358:PHE:CE1	2.48	0.49
26:c:505:CLA:H2	26:c:520:CLA:C4D	2.42	0.49
29:B:621:SQD:H241	19:t:23:PHE:HB3	1.95	0.49
26:C:505:CLA:C4D	26:C:507:CLA:H2	2.43	0.49
7:G:110:LEU:HD22	39:G:301:CHL:HMD2	1.94	0.49
7:N:131:GLN:OE1	39:N:303:CHL:HMC	2.11	0.49
1:a:60:ILE:HD12	1:a:84:PRO:HD2	1.94	0.49
2:b:112:ILE:HG12	28:b:619:BCR:H271	1.95	0.49
2:b:233:ASN:O	2:b:236:THR:HG22	2.13	0.49
18:S:230:LEU:HD13	26:S:303:CLA:HMD3	1.94	0.49
21:W:107:TRP:HE1	23:Y:88:ASN:CG	2.21	0.49
1:a:196:PRO:HG3	1:a:300:PHE:CE2	2.48	0.49
12:l:13:LEU:HD22	13:m:25:ILE:HG13	1.94	0.49
7:n:21:ARG:HD2	7:n:43:ASP:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LEU:HD23	4:D:256:ILE:HG12	1.93	0.49
1:A:217:SER:HB3	4:D:272:LEU:HD12	1.93	0.49
3:C:393:ALA:HB1	16:Q:30:ARG:HG3	1.94	0.49
7:N:209:ASN:HB3	26:N:318:CLA:O1D	2.13	0.49
2:b:9:HIS:HB3	26:b:618:CLA:HAB	1.95	0.49
2:b:25:MET:HG2	28:b:619:BCR:H23C	1.94	0.49
4:d:201:VAL:HG22	26:d:404:CLA:C1B	2.42	0.49
14:o:108:THR:HA	14:o:111:GLN:HG3	1.95	0.49
2:B:159:THR:HG22	2:B:183:PRO:HD3	1.93	0.49
14:O:218:ALA:HA	14:O:227:GLY:HA3	1.94	0.49
17:R:101:ARG:HA	17:R:104:MET:HE3	1.94	0.49
17:R:194:LEU:HB3	26:R:306:CLA:H3A	1.95	0.49
14:o:134:PHE:HB2	14:o:172:ILE:O	2.13	0.49
2:B:464:PHE:HB2	4:D:280:TRP:CZ2	2.48	0.49
33:B:620:DGD:HAE2	4:D:123:ILE:HD11	1.95	0.49
7:N:22:VAL:HB	39:N:316:CHL:HBC1	1.95	0.49
41:N:315:XAT:H12	37:Y:306:LHG:H202	1.95	0.49
14:O:159:THR:HB	14:O:199:VAL:HB	1.94	0.49
1:a:143:ILE:HD11	4:d:217:THR:HA	1.94	0.49
2:b:247:PHE:HB2	26:b:612:CLA:HBC1	1.95	0.49
28:j:101:BCR:HC8	11:k:41:ILE:HD13	1.95	0.49
16:q:104:LYS:HA	16:q:107:LYS:HD2	1.95	0.49
3:C:408:GLY:HA2	3:C:419:TYR:O	2.13	0.49
11:K:49:ALA:HB2	28:K:101:BCR:H391	1.94	0.49
17:R:210:LEU:HD13	26:R:317:CLA:HBB2	1.95	0.49
18:S:124:LEU:HD23	26:S:310:CLA:HAA2	1.95	0.49
26:a:402:CLA:HAA2	34:w:201:LMG:H111	1.93	0.49
26:r:303:CLA:HBA1	26:r:306:CLA:H43	1.95	0.49
1:A:173:PRO:HB2	1:A:178:GLY:HA3	1.95	0.48
1:A:196:PRO:HG3	1:A:300:PHE:CE2	2.48	0.48
26:B:602:CLA:HMA3	26:B:616:CLA:H122	1.95	0.48
4:D:348:ARG:HD2	43:D:520:HOH:O	2.13	0.48
16:Q:63:ASN:O	16:Q:66:PRO:HD2	2.13	0.48
26:R:309:CLA:H3A	26:R:309:CLA:HBA1	1.59	0.48
3:c:406:SER:HA	3:c:420:VAL:HG23	1.95	0.48
15:p:85:ASN:HD22	16:q:8:LYS:HE3	1.78	0.48
2:B:187:VAL:HG12	26:B:605:CLA:HBC3	1.95	0.48
37:D:408:LHG:H302	19:T:21:ILE:HD11	1.94	0.48
15:P:40:ILE:HG23	15:P:45:GLN:HB3	1.96	0.48
22:X:80:ILE:HG23	22:X:84:LEU:HD23	1.95	0.48
3:c:407:VAL:HG13	3:c:415:ASN:HA	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:g:316:LUT:H32	26:g:317:CLA:HAB	1.95	0.48
4:D:201:VAL:HG22	26:D:409:CLA:C1B	2.43	0.48
7:N:177:LEU:HB3	26:N:312:CLA:H3A	1.94	0.48
15:P:97:THR:HG23	15:P:98:ALA:H	1.78	0.48
17:R:32:TYR:OH	17:R:200:LYS:HE2	2.13	0.48
23:Y:173:PHE:CZ	26:Y:305:CLA:HED3	2.47	0.48
24:Z:33:TRP:O	24:Z:37:LYS:HB3	2.13	0.48
26:b:607:CLA:H61	26:b:607:CLA:H41	1.67	0.48
3:c:393:ALA:HB1	16:q:30:ARG:HG3	1.94	0.48
17:r:194:LEU:HB3	26:r:306:CLA:H3A	1.96	0.48
23:y:173:PHE:CZ	23:y:177:LYS:HE2	2.48	0.48
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.48	0.48
4:D:319:ILE:O	4:D:323:GLU:HG3	2.14	0.48
18:S:166:PRO:HG3	39:S:312:CHL:HBC2	1.94	0.48
39:S:316:CHL:HHC	39:S:316:CHL:HBB1	1.94	0.48
1:a:103:ASP:HB2	14:o:162:MET:HE1	1.95	0.48
18:s:47:GLU:O	18:s:48:TYR:CD2	2.66	0.48
21:w:114:GLY:O	21:w:118:THR:HG23	2.14	0.48
1:A:85:THR:HA	1:A:109:GLY:HA3	1.94	0.48
1:A:103:ASP:HB2	14:O:162:MET:HE1	1.96	0.48
1:A:265:PHE:HE2	29:A:410:SQD:H92	1.78	0.48
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.95	0.48
14:O:134:PHE:HB2	14:O:172:ILE:O	2.14	0.48
28:T:101:BCR:H403	28:b:603:BCR:H14C	1.94	0.48
21:W:114:GLY:O	21:W:118:THR:HG23	2.14	0.48
2:b:187:VAL:HG12	26:b:608:CLA:HBC3	1.95	0.48
33:b:620:DGD:HAE2	4:d:123:ILE:HD11	1.94	0.48
3:c:80:PRO:HG2	3:c:83:GLU:HG3	1.95	0.48
14:o:124:PHE:HE1	14:o:290:SER:HB2	1.78	0.48
23:y:164:LEU:HD12	40:y:311:LUT:H222	1.95	0.48
1:A:299:GLY:O	3:C:403:SER:HB2	2.13	0.48
2:B:25:MET:HG2	28:B:614:BCR:H23C	1.96	0.48
28:J:101:BCR:HC8	11:K:41:ILE:HD13	1.96	0.48
2:b:42:LEU:HD13	2:b:94:GLU:HG3	1.95	0.48
4:d:126:MET:SD	4:d:150:ILE:HD12	2.53	0.48
26:d:403:CLA:H161	22:x:91:ILE:HG22	1.95	0.48
39:n:306:CHL:HHC	39:n:306:CHL:HBB1	1.95	0.48
17:r:76:LYS:HE2	17:r:84:SER:HB3	1.94	0.48
39:s:313:CHL:HHC	39:s:313:CHL:HBB1	1.95	0.48
4:D:161:PRO:HB3	4:D:170:ALA:HB2	1.96	0.48
12:L:13:LEU:HD22	13:M:25:ILE:HG13	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:166:PRO:HB3	39:S:312:CHL:HBC2	1.96	0.48
26:b:608:CLA:H143	26:b:608:CLA:H161	1.75	0.48
7:n:131:GLN:OE1	39:n:318:CHL:HMC	2.13	0.48
14:o:128:LYS:HG3	14:o:177:GLU:HG3	1.96	0.48
16:q:56:GLU:HA	16:q:59:LYS:HE2	1.95	0.48
26:s:301:CLA:C4C	37:s:309:LHG:HC61	2.44	0.48
28:B:619:BCR:HC42	34:B:622:LMG:H341	1.95	0.48
42:S:305:NEX:H241	26:S:310:CLA:O1A	2.13	0.48
40:g:310:LUT:H161	39:g:313:CHL:HBB1	1.96	0.48
14:o:159:THR:HG22	14:o:201:LEU:HD23	1.96	0.48
42:s:302:NEX:H241	26:s:310:CLA:O1A	2.14	0.48
17:R:114:GLU:HG3	17:R:120:THR:HA	1.96	0.48
2:b:159:THR:HG22	2:b:183:PRO:HD3	1.95	0.48
17:r:210:LEU:HD13	26:r:315:CLA:HBB2	1.96	0.48
1:A:202:VAL:HA	1:A:205:VAL:HG22	1.96	0.48
2:B:71:ILE:HG12	26:B:610:CLA:HMA2	1.96	0.48
3:C:49:LEU:HD11	26:C:515:CLA:C1C	2.44	0.48
23:Y:24:TYR:CD2	39:Y:302:CHL:HAA1	2.46	0.48
1:a:173:PRO:HB2	1:a:178:GLY:HA3	1.94	0.48
1:a:220:THR:HA	1:a:223:LEU:HG	1.95	0.48
3:c:73:ALA:HB2	11:k:24:LEU:HG	1.96	0.48
38:e:101:HEM:HBB2	38:e:101:HEM:HMB2	1.96	0.48
42:g:306:NEX:H11	42:g:306:NEX:H191	1.74	0.48
37:n:301:LHG:H312	37:n:301:LHG:HC91	1.96	0.48
18:s:230:LEU:HD13	26:s:307:CLA:HMD3	1.95	0.48
26:B:602:CLA:H172	28:B:608:BCR:H331	1.94	0.47
28:B:619:BCR:H14C	28:t:101:BCR:H403	1.95	0.47
39:G:301:CHL:HBB1	40:G:308:LUT:H161	1.95	0.47
26:R:308:CLA:HBA1	26:R:308:CLA:CHA	2.44	0.47
24:Z:3:ILE:HG22	24:Z:3:ILE:O	2.14	0.47
1:a:85:THR:HA	1:a:109:GLY:HA3	1.95	0.47
1:a:214:MET:HG2	30:a:407:PL9:H102	1.96	0.47
26:n:303:CLA:HAB	40:n:314:LUT:H32	1.96	0.47
14:o:218:ALA:HA	14:o:227:GLY:HA3	1.96	0.47
18:s:118:LEU:HB3	18:s:135:LEU:HB2	1.96	0.47
2:B:90:LEU:HD11	26:B:610:CLA:H141	1.96	0.47
7:N:70:ARG:HA	7:N:73:MET:HE3	1.96	0.47
42:S:305:NEX:H30	42:S:305:NEX:H402	1.96	0.47
4:d:279:LEU:HD21	27:d:407:PHO:HMC2	1.96	0.47
39:y:314:CHL:HBA1	39:y:314:CHL:H3A	1.56	0.47
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:49:ALA:HA	23:Y:64:LEU:HD11	1.97	0.47
7:G:81:PHE:HB3	7:G:82:PRO:HD3	1.95	0.47
26:Y:301:CLA:HAC1	37:Y:306:LHG:H321	1.96	0.47
2:b:90:LEU:HD11	26:b:617:CLA:H141	1.96	0.47
2:b:357:ARG:CZ	20:u:21:PRO:HD2	2.44	0.47
4:d:161:PRO:HB3	4:d:170:ALA:HB2	1.95	0.47
7:g:81:PHE:HB3	7:g:82:PRO:HD3	1.95	0.47
16:q:94:ILE:HG21	16:q:150:LEU:HD22	1.96	0.47
18:s:62:PHE:CD2	40:s:312:LUT:H222	2.49	0.47
18:s:166:PRO:HB3	39:s:313:CHL:HBC2	1.96	0.47
1:A:276:ALA:HA	4:D:212:ALA:HA	1.94	0.47
40:R:311:LUT:H383	39:R:312:CHL:H12	1.96	0.47
39:S:302:CHL:HHC	39:S:302:CHL:HBB1	1.96	0.47
1:a:60:ILE:HB	1:a:83:ILE:HG22	1.96	0.47
1:a:215:HIS:HA	30:a:407:PL9:O1	2.14	0.47
1:a:276:ALA:HA	4:d:212:ALA:HA	1.96	0.47
4:d:348:ARG:HD2	43:d:517:HOH:O	2.13	0.47
16:q:55:LYS:HD3	16:q:147:LEU:HD22	1.97	0.47
37:G:312:LHG:O4	26:G:313:CLA:NA	2.47	0.47
15:P:116:SER:HB2	15:P:129:LEU:HD23	1.97	0.47
19:T:20:ALA:O	19:T:24:ARG:HB3	2.14	0.47
1:a:202:VAL:HA	1:a:205:VAL:HG22	1.96	0.47
26:b:608:CLA:H162	28:h:101:BCR:H19C	1.97	0.47
3:c:49:LEU:HD11	26:c:504:CLA:C1C	2.44	0.47
3:c:178:LYS:HD3	26:c:515:CLA:H192	1.97	0.47
7:g:182:LEU:HD23	7:g:182:LEU:HA	1.74	0.47
15:p:31:PRO:HG3	15:p:175:PHE:HB3	1.96	0.47
17:r:43:ALA:HB1	17:r:45:TYR:CE2	2.49	0.47
1:A:26:ASN:HB3	29:A:407:SQD:H112	1.96	0.47
29:A:407:SQD:H361	28:b:603:BCR:H281	1.95	0.47
2:B:112:ILE:HG12	28:B:614:BCR:H271	1.96	0.47
26:C:507:CLA:H101	26:C:507:CLA:H62	1.50	0.47
13:M:27:VAL:HG12	13:m:28:LYS:HB3	1.96	0.47
26:b:610:CLA:H112	26:b:610:CLA:H72	1.72	0.47
42:s:302:NEX:H403	39:s:316:CHL:HMA2	1.97	0.47
3:C:407:VAL:HG13	3:C:415:ASN:HA	1.96	0.47
26:C:504:CLA:H142	28:J:101:BCR:H353	1.97	0.47
4:D:49:PHE:HZ	34:D:404:LMG:H341	1.79	0.47
18:S:99:ASN:ND2	18:S:109:ALA:HB2	2.24	0.47
19:T:23:PHE:HB3	29:b:621:SQD:H241	1.96	0.47
26:Y:305:CLA:H121	40:Y:315:LUT:H403	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:179:THR:O	1:a:183:MET:HG3	2.15	0.47
2:b:201:HIS:HB2	26:b:601:CLA:CHB	2.45	0.47
2:b:486:LEU:HD11	4:d:137:GLN:HB2	1.96	0.47
7:n:165:LEU:HD12	40:n:314:LUT:H222	1.97	0.47
41:n:316:XAT:H363	37:y:301:LHG:HC41	1.95	0.47
14:o:115:ILE:HG12	14:o:298:ILE:HG12	1.96	0.47
17:r:85:GLU:HA	26:r:313:CLA:H41	1.95	0.47
17:r:114:GLU:HG3	17:r:120:THR:HA	1.96	0.47
26:r:311:CLA:CHA	26:r:311:CLA:HBA1	2.44	0.47
26:r:313:CLA:HMA2	26:r:313:CLA:H11	1.97	0.47
39:s:316:CHL:HBB1	39:s:316:CHL:HHC	1.95	0.47
23:y:99:LYS:HA	39:y:312:CHL:HED3	1.96	0.47
3:C:56:HIS:HB2	26:C:515:CLA:HMB1	1.96	0.47
3:C:338:GLY:HA2	14:O:194:TYR:OH	2.15	0.47
27:D:403:PHO:H41	27:D:403:PHO:H62	1.66	0.47
27:D:403:PHO:H42	27:D:403:PHO:O1A	2.15	0.47
18:S:39:LEU:HD22	24:Z:41:PHE:CE1	2.49	0.47
1:a:22:THR:HB	1:a:136:ARG:HE	1.80	0.47
2:b:30:VAL:HG11	26:b:618:CLA:H112	1.97	0.47
7:n:209:ASN:HB3	26:n:302:CLA:O1D	2.15	0.47
14:o:212:THR:HG21	14:o:231:VAL:HA	1.97	0.47
15:p:111:ALA:O	16:q:11:PRO:HA	2.14	0.47
39:r:309:CHL:H3A	39:r:309:CHL:HBA2	1.48	0.47
37:y:301:LHG:H321	26:y:304:CLA:HAC1	1.96	0.47
26:y:315:CLA:HAB	40:y:318:LUT:C35	2.45	0.47
1:A:215:HIS:HA	30:A:408:PL9:O1	2.14	0.47
26:S:308:CLA:C4C	37:S:317:LHG:HC61	2.45	0.47
26:b:605:CLA:HMA3	26:b:609:CLA:H122	1.97	0.47
3:c:400:PRO:HA	3:c:421:SER:HB2	1.97	0.47
4:d:342:PRO:O	4:d:345:VAL:HG22	2.15	0.47
8:h:33:VAL:O	17:r:45:TYR:HD1	1.98	0.47
26:y:310:CLA:H2	26:y:310:CLA:H61	1.73	0.47
2:B:357:ARG:CZ	20:U:21:PRO:HD2	2.44	0.47
4:D:56:THR:HG21	5:E:53:PRO:HD3	1.96	0.47
7:N:165:LEU:HD12	40:N:314:LUT:H222	1.96	0.47
39:N:310:CHL:H3A	18:S:101:TYR:HB3	1.97	0.47
26:R:302:CLA:HMA2	26:R:302:CLA:H11	1.97	0.47
2:b:3:LEU:HD22	12:l:9:GLN:HB2	1.97	0.47
26:c:505:CLA:H203	26:c:506:CLA:HAB	1.96	0.47
7:n:70:ARG:HA	7:n:73:MET:HE3	1.96	0.47
33:y:308:DGD:HG12	33:y:308:DGD:HB52	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:HIS:HE1	26:B:610:CLA:NA	2.13	0.46
2:B:399:VAL:HG12	2:B:417:VAL:HG22	1.97	0.46
26:G:314:CLA:H151	26:G:314:CLA:H112	1.80	0.46
23:Y:63:GLU:HA	23:Y:155:LEU:HD11	1.97	0.46
26:Y:305:CLA:HMD2	39:Y:318:CHL:O1A	2.15	0.46
2:b:7:ARG:HD3	26:b:610:CLA:HED1	1.97	0.46
2:b:399:VAL:HG12	2:b:417:VAL:HG22	1.98	0.46
26:c:502:CLA:H111	26:c:502:CLA:H152	1.38	0.46
7:g:86:ALA:HA	7:g:90:VAL:O	2.15	0.46
39:g:314:CHL:H3A	39:g:314:CHL:HBA2	1.34	0.46
14:o:248:SER:HB3	15:p:108:VAL:HG21	1.98	0.46
42:r:302:NEX:H15	42:r:302:NEX:H201	1.72	0.46
26:r:311:CLA:O2D	26:r:311:CLA:H2A	2.15	0.46
1:A:60:ILE:HB	1:A:83:ILE:HG22	1.98	0.46
2:B:277:GLN:HB3	20:U:24:LYS:HB2	1.97	0.46
4:D:30:VAL:HA	4:D:38:PHE:HE2	1.81	0.46
8:H:33:VAL:O	17:R:45:TYR:HD1	1.98	0.46
41:N:315:XAT:H15	41:N:315:XAT:H201	1.76	0.46
26:Y:308:CLA:H202	40:Y:309:LUT:H402	1.97	0.46
18:s:156:ASN:OD1	39:s:313:CHL:HAC1	2.14	0.46
1:A:63:ILE:HG21	1:A:336:ALA:HA	1.98	0.46
3:C:255:LYS:HB3	3:C:255:LYS:HE2	1.73	0.46
17:R:94:GLU:HA	17:R:172:LEU:HD21	1.98	0.46
3:c:163:ILE:HG21	26:c:503:CLA:C3B	2.46	0.46
4:d:175:VAL:HG22	26:d:411:CLA:HED3	1.96	0.46
23:y:173:PHE:CZ	26:y:309:CLA:HED3	2.50	0.46
1:A:223:LEU:HD13	4:D:265:ARG:HD3	1.97	0.46
3:C:400:PRO:HA	3:C:421:SER:HB2	1.97	0.46
4:D:342:PRO:O	4:D:345:VAL:HG22	2.15	0.46
37:D:408:LHG:H202	30:D:411:PL9:H401	1.97	0.46
12:L:25:ILE:HG13	13:M:18:PRO:HB2	1.98	0.46
14:O:290:SER:HB3	14:O:297:VAL:HG12	1.97	0.46
16:Q:57:SER:HB3	16:Q:84:ALA:HA	1.97	0.46
26:R:308:CLA:O2D	26:R:308:CLA:H2A	2.15	0.46
18:S:156:ASN:OD1	39:S:312:CHL:HAC1	2.15	0.46
42:S:305:NEX:H222	26:S:310:CLA:C1C	2.45	0.46
4:d:319:ILE:O	4:d:323:GLU:HG3	2.15	0.46
23:y:63:GLU:HA	23:y:155:LEU:HD11	1.98	0.46
1:A:179:THR:O	1:A:183:MET:HG3	2.16	0.46
28:K:101:BCR:H24C	28:K:101:BCR:H371	1.70	0.46
17:R:87:PHE:HA	17:R:92:PHE:CZ	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:62:PHE:CD2	40:S:306:LUT:H222	2.50	0.46
2:b:65:PHE:HE1	26:b:611:CLA:HED2	1.80	0.46
26:b:618:CLA:H193	26:b:618:CLA:H162	1.74	0.46
2:B:187:VAL:HG13	26:B:605:CLA:HMD2	1.98	0.46
2:B:257:TRP:HZ3	2:B:449:GLY:HA2	1.81	0.46
26:C:504:CLA:H152	24:Z:24:PRO:HG3	1.97	0.46
26:C:521:CLA:H92	26:C:521:CLA:H62	1.76	0.46
42:N:302:NEX:H11	42:N:302:NEX:H191	1.80	0.46
17:R:188:PRO:O	17:R:191:THR:HG22	2.16	0.46
26:r:313:CLA:H12	26:r:313:CLA:HBA1	1.69	0.46
39:y:303:CHL:H142	39:y:303:CHL:H111	1.81	0.46
2:B:377:VAL:H	15:P:38:LYS:HZ1	1.63	0.46
17:R:43:ALA:HB1	17:R:45:TYR:CE2	2.51	0.46
23:Y:77:LEU:HD21	26:Y:313:CLA:H202	1.98	0.46
33:Y:303:DGD:HG12	33:Y:303:DGD:HB52	1.98	0.46
3:c:149:TYR:CD2	3:c:157:MET:HE1	2.51	0.46
4:d:30:VAL:HA	4:d:38:PHE:HE2	1.80	0.46
1:A:260:PHE:CE2	1:A:262:TYR:HB2	2.50	0.46
26:B:602:CLA:HED1	26:B:616:CLA:H143	1.98	0.46
3:C:163:ILE:HG21	26:C:511:CLA:C3B	2.46	0.46
4:D:17:ILE:HG22	22:X:109:SER:HB2	1.98	0.46
17:R:24:LEU:HD11	17:R:35:ASP:HB2	1.98	0.46
17:R:45:TYR:O	17:R:46:LEU:HB2	2.16	0.46
20:U:3:LYS:HE2	20:U:28:TYR:CG	2.51	0.46
26:b:601:CLA:HBA2	26:b:601:CLA:HBD	1.98	0.46
23:y:33:PRO:HB3	23:y:35:TYR:CZ	2.51	0.46
1:A:143:ILE:HD11	4:D:217:THR:HA	1.98	0.46
15:P:45:GLN:HA	15:P:62:MET:HG3	1.97	0.46
15:P:57:SER:HA	15:P:162:GLN:O	2.16	0.46
39:Y:302:CHL:H142	39:Y:302:CHL:H111	1.80	0.46
3:c:277:ALA:HB2	3:c:441:HIS:CG	2.49	0.46
26:r:313:CLA:C1	26:r:313:CLA:H2A	2.46	0.46
42:s:302:NEX:H30	42:s:302:NEX:H402	1.97	0.46
1:A:166:GLY:HA3	3:C:358:PHE:HE1	1.80	0.46
3:C:80:PRO:HG2	3:C:83:GLU:HG3	1.97	0.46
3:C:277:ALA:HB2	3:C:441:HIS:CG	2.51	0.46
4:D:134:ARG:HD2	4:D:134:ARG:HA	1.66	0.46
7:G:182:LEU:HD23	7:G:182:LEU:HA	1.73	0.46
18:S:70:ASN:HA	18:S:73:LYS:HG2	1.98	0.46
23:Y:212:HIS:CG	26:Y:312:CLA:HAA2	2.51	0.46
1:a:166:GLY:HA3	3:c:358:PHE:HE1	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:284:TRP:CD1	3:c:435:PHE:HZ	2.34	0.46
3:c:338:GLY:HA2	14:o:194:TYR:OH	2.16	0.46
17:r:188:PRO:O	17:r:191:THR:HG22	2.16	0.46
37:r:312:LHG:H142	37:r:312:LHG:H351	1.98	0.46
18:s:67:LYS:HE2	18:s:70:ASN:CG	2.40	0.46
19:t:20:ALA:O	19:t:24:ARG:HB3	2.16	0.46
20:u:6:THR:HG22	20:u:8:ALA:H	1.80	0.46
39:y:305:CHL:HBA1	42:y:307:NEX:H403	1.97	0.46
3:C:236:GLY:HA3	28:C:502:BCR:H402	1.98	0.45
28:H:101:BCR:H24C	28:H:101:BCR:H371	1.79	0.45
27:d:407:PHO:H42	27:d:407:PHO:O1A	2.16	0.45
39:y:314:CHL:H161	26:y:315:CLA:HBB1	1.98	0.45
1:A:22:THR:HB	1:A:136:ARG:HE	1.81	0.45
28:B:619:BCR:H281	29:a:403:SQD:H361	1.97	0.45
7:G:75:GLY:HA2	40:G:308:LUT:H181	1.99	0.45
16:Q:64:VAL:HG12	16:Q:79:ASP:HB3	1.99	0.45
17:R:93:ARG:O	17:R:93:ARG:HD3	2.17	0.45
39:R:312:CHL:H3A	39:R:312:CHL:HBA2	1.47	0.45
18:S:105:CYS:HA	18:S:127:PHE:HA	1.98	0.45
39:S:302:CHL:HMA2	42:S:305:NEX:H403	1.99	0.45
23:Y:131:GLN:OE1	39:Y:314:CHL:HMC	2.16	0.45
2:b:157:HIS:CE1	26:b:617:CLA:NA	2.84	0.45
26:c:505:CLA:H101	26:c:505:CLA:H62	1.51	0.45
26:c:506:CLA:H71	26:c:513:CLA:HBC3	1.98	0.45
38:e:101:HEM:HMC2	6:f:32:VAL:HG21	1.97	0.45
7:n:17:TYR:CE2	7:n:175:ALA:HB1	2.51	0.45
14:o:162:MET:HE3	14:o:200:GLN:HB2	1.98	0.45
1:A:31:GLY:O	1:A:35:VAL:HG13	2.17	0.45
1:A:32:TRP:O	1:A:35:VAL:HG22	2.16	0.45
2:B:122:ILE:HA	8:H:24:LYS:HD2	1.97	0.45
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.51	0.45
26:C:507:CLA:H193	26:C:507:CLA:H161	1.79	0.45
7:N:60:ARG:HH21	23:Y:33:PRO:HG3	1.82	0.45
15:P:85:ASN:HD22	16:Q:8:LYS:HE3	1.81	0.45
26:b:606:CLA:H61	26:b:606:CLA:H41	1.69	0.45
3:c:318:LEU:HG	3:c:328:VAL:HG11	1.98	0.45
26:d:403:CLA:H172	22:x:92:ALA:HB2	1.97	0.45
17:r:87:PHE:HA	17:r:92:PHE:CZ	2.50	0.45
1:A:82:ILE:HB	1:A:174:LEU:HB2	1.99	0.45
26:B:602:CLA:H102	26:B:616:CLA:H121	1.97	0.45
14:O:108:THR:HA	14:O:111:GLN:HG3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:313:CLA:H72	26:R:313:CLA:H111	1.74	0.45
28:T:101:BCR:H392	28:T:101:BCR:H24C	1.72	0.45
2:b:122:ILE:HA	8:h:24:LYS:HD2	1.98	0.45
2:b:187:VAL:HG13	26:b:608:CLA:HMD2	1.98	0.45
3:c:203:THR:HG21	3:c:208:VAL:HG11	1.99	0.45
12:l:22:LEU:HB3	19:t:16:ILE:HD13	1.97	0.45
39:y:302:CHL:O1A	26:y:309:CLA:HMD2	2.15	0.45
1:A:284:TRP:CD1	3:C:435:PHE:HZ	2.34	0.45
3:C:52:ALA:HB2	26:C:504:CLA:HMA2	1.98	0.45
4:D:51:GLY:HA2	4:D:55:VAL:HB	1.99	0.45
14:O:98:LYS:O	16:Q:74:PRO:HG3	2.17	0.45
39:Y:302:CHL:H62	39:Y:302:CHL:H41	1.85	0.45
42:Y:304:NEX:H403	39:Y:317:CHL:HBA1	1.97	0.45
1:a:260:PHE:CE2	1:a:262:TYR:HB2	2.51	0.45
2:b:36:SER:OG	28:b:603:BCR:H362	2.16	0.45
37:g:301:LHG:H142	39:g:311:CHL:HED3	1.99	0.45
37:g:301:LHG:HC41	41:g:320:XAT:H363	1.97	0.45
16:q:57:SER:HB3	16:q:84:ALA:HA	1.99	0.45
26:y:310:CLA:HMA1	40:y:311:LUT:H3	1.99	0.45
2:B:394:GLN:HA	16:Q:5:ILE:HG13	1.99	0.45
26:B:609:CLA:H162	26:B:609:CLA:H193	1.72	0.45
37:G:312:LHG:HC61	39:G:318:CHL:HMD3	1.99	0.45
7:N:81:PHE:HB3	7:N:82:PRO:HD3	1.99	0.45
15:P:43:PRO:HD2	15:P:86:TYR:CD1	2.52	0.45
18:S:48:TYR:CD2	18:S:66:LYS:HA	2.51	0.45
1:a:63:ILE:HG21	1:a:336:ALA:HA	1.99	0.45
26:g:308:CLA:HBC1	39:g:312:CHL:HAC2	1.99	0.45
15:p:116:SER:HB2	15:p:129:LEU:HD23	1.99	0.45
41:r:304:XAT:H35	41:r:304:XAT:H401	1.81	0.45
18:s:133:ILE:HG23	18:s:137:LEU:HB3	1.99	0.45
21:w:107:TRP:HE1	23:y:88:ASN:CG	2.23	0.45
3:C:203:THR:HG21	3:C:208:VAL:HG11	1.99	0.45
26:G:307:CLA:H112	26:G:307:CLA:H152	1.63	0.45
11:K:42:PRO:O	11:K:45:PHE:HB2	2.16	0.45
7:N:46:TRP:CZ3	39:N:316:CHL:HBD	2.51	0.45
41:N:315:XAT:H363	37:Y:306:LHG:HC41	1.98	0.45
16:Q:94:ILE:HG21	16:Q:150:LEU:HD22	1.99	0.45
17:R:180:ASP:HA	40:R:311:LUT:H24	1.99	0.45
26:R:306:CLA:H43	26:R:316:CLA:HBA1	1.97	0.45
18:S:133:ILE:HG23	18:S:137:LEU:HB3	1.98	0.45
26:Y:305:CLA:HBB1	26:Y:313:CLA:H3A	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:g:307:CHL:HHC	39:g:307:CHL:HBB1	1.99	0.45
18:s:48:TYR:CE2	18:s:66:LYS:HA	2.52	0.45
2:B:30:VAL:HG11	26:B:609:CLA:H112	1.99	0.45
2:B:469:HIS:CE1	26:B:617:CLA:NA	2.85	0.45
3:C:170:VAL:HG11	26:C:511:CLA:H112	1.98	0.45
3:C:202:LEU:HD22	3:C:234:ILE:HB	1.98	0.45
3:C:401:LEU:HD22	3:C:410:VAL:HG12	1.99	0.45
14:O:115:ILE:HG21	14:O:296:GLU:HB3	1.99	0.45
26:R:302:CLA:C1	26:R:302:CLA:H2A	2.46	0.45
42:R:305:NEX:H11	42:R:305:NEX:H191	1.77	0.45
40:Y:309:LUT:C35	26:Y:311:CLA:HAB	2.47	0.45
26:a:409:CLA:H151	26:a:411:CLA:H151	1.98	0.45
27:a:410:PHO:H92	27:a:410:PHO:H62	1.79	0.45
7:g:24:TYR:CZ	7:g:25:LEU:HG	2.52	0.45
40:r:307:LUT:H383	39:r:309:CHL:H12	1.99	0.45
26:r:314:CLA:H111	26:r:314:CLA:H72	1.69	0.45
2:B:441:GLY:C	14:O:259:ALA:HB3	2.42	0.45
4:D:175:VAL:HG22	26:D:412:CLA:HED3	1.98	0.45
38:E:101:HEM:HMC2	6:F:32:VAL:HG21	1.98	0.45
7:G:86:ALA:HA	7:G:90:VAL:O	2.17	0.45
42:G:315:NEX:H35	42:G:315:NEX:H401	1.81	0.45
15:P:100:GLU:OE1	15:P:136:ALA:HB1	2.17	0.45
26:Y:312:CLA:HMA1	40:Y:315:LUT:H3	1.99	0.45
2:b:226:TYR:CD2	2:b:231:MET:HB2	2.52	0.45
3:c:57:ALA:O	3:c:61:VAL:HG23	2.17	0.45
7:g:110:LEU:HD22	39:g:313:CHL:HMD1	1.99	0.45
26:g:303:CLA:H172	26:g:303:CLA:H13	1.77	0.45
16:q:95:ILE:HD11	16:q:110:THR:HG21	1.99	0.45
18:s:116:ALA:HA	18:s:119:LEU:HG	1.98	0.45
23:y:212:HIS:CG	26:y:310:CLA:HAA2	2.51	0.45
26:y:309:CLA:H92	26:y:309:CLA:H61	1.81	0.45
2:B:201:HIS:HB2	26:B:606:CLA:CHB	2.47	0.45
3:C:149:TYR:CD2	3:C:157:MET:HE1	2.52	0.45
3:C:169:GLY:HA2	3:C:241:GLY:HA2	1.98	0.45
26:D:406:CLA:H172	22:X:92:ALA:HB2	1.99	0.45
7:N:17:TYR:CE2	7:N:175:ALA:HB1	2.52	0.45
14:O:286:LYS:O	14:O:299:GLY:HA3	2.17	0.45
4:d:149:PRO:HB3	26:d:404:CLA:H41	1.98	0.45
37:g:301:LHG:O4	26:g:315:CLA:NA	2.50	0.45
26:y:306:CLA:HBA1	40:y:318:LUT:H382	1.99	0.45
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:LEU:HD22	12:L:9:GLN:HB2	1.98	0.44
2:B:214:LEU:HB3	26:R:317:CLA:HED1	1.99	0.44
26:C:521:CLA:H201	37:D:410:LHG:H331	1.99	0.44
18:S:98:LEU:HD13	18:S:127:PHE:CE2	2.51	0.44
26:c:514:CLA:H201	37:d:410:LHG:H331	1.98	0.44
23:y:131:GLN:OE1	39:y:312:CHL:HMC	2.17	0.44
3:C:42:LEU:HD22	3:C:48:LYS:HB3	1.99	0.44
33:C:510:DGD:HB91	26:C:521:CLA:C4B	2.47	0.44
1:a:31:GLY:O	1:a:35:VAL:HG13	2.16	0.44
1:a:32:TRP:O	1:a:35:VAL:HG22	2.16	0.44
7:n:86:ALA:HA	7:n:90:VAL:O	2.18	0.44
23:y:75:GLY:HA2	40:y:318:LUT:H181	2.00	0.44
26:A:403:CLA:H151	26:D:401:CLA:H151	1.98	0.44
2:B:36:SER:OG	28:B:619:BCR:H362	2.17	0.44
2:B:73:ASN:HB3	2:B:85:ILE:HG21	1.99	0.44
26:B:606:CLA:H92	26:B:606:CLA:H61	1.78	0.44
26:C:517:CLA:HBC3	26:C:520:CLA:H71	1.99	0.44
7:G:46:TRP:CZ3	39:G:318:CHL:HBD	2.52	0.44
14:O:238:SER:HB2	15:P:137:ASP:HB3	1.99	0.44
14:O:248:SER:HB3	15:P:108:VAL:HG21	1.99	0.44
23:Y:33:PRO:HB3	23:Y:35:TYR:CZ	2.52	0.44
1:a:223:LEU:HD13	4:d:265:ARG:HD3	1.98	0.44
1:a:234:ASN:ND2	37:d:402:LHG:HC11	2.30	0.44
2:b:469:HIS:CE1	26:b:610:CLA:NA	2.86	0.44
28:b:619:BCR:H322	34:b:622:LMG:H111	1.99	0.44
20:u:3:LYS:HE2	20:u:28:TYR:CG	2.53	0.44
23:y:181:LEU:HA	23:y:181:LEU:HD23	1.85	0.44
2:B:383:PHE:CG	4:D:347:PRO:HA	2.53	0.44
26:B:607:CLA:H111	26:B:607:CLA:H91	1.65	0.44
14:O:138:PRO:HD2	14:O:167:TYR:HD1	1.83	0.44
18:S:41:ASP:O	18:S:42:ARG:HB2	2.18	0.44
39:Y:307:CHL:HBA1	39:Y:307:CHL:H3A	1.57	0.44
1:a:199:MET:HB3	33:c:501:DGD:HAE1	1.99	0.44
26:b:609:CLA:H162	8:h:19:VAL:HG11	2.00	0.44
3:c:378:SER:O	3:c:382:LYS:HG2	2.17	0.44
5:e:11:ARG:CZ	5:e:16:ILE:HG12	2.47	0.44
7:g:83:GLU:O	7:g:87:ARG:HG3	2.18	0.44
7:n:46:TRP:CZ3	39:n:306:CHL:HBD	2.52	0.44
18:s:163:LYS:HE3	18:s:165:HIS:H	1.81	0.44
37:y:301:LHG:HC81	39:y:303:CHL:C1D	2.47	0.44
26:B:601:CLA:HMD1	13:M:21:PHE:HE1	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:607:CLA:H93	26:B:607:CLA:H62	1.67	0.44
14:O:177:GLU:O	14:O:184:VAL:HA	2.18	0.44
29:a:403:SQD:H102	29:a:403:SQD:H132	1.80	0.44
2:b:471:ALA:HB1	4:d:140:PRO:CG	2.48	0.44
26:b:607:CLA:H122	26:b:607:CLA:H161	1.59	0.44
26:b:611:CLA:HBA2	26:b:613:CLA:H11	1.99	0.44
3:c:187:ASP:HB3	3:c:190:ALA:HB2	1.99	0.44
26:c:503:CLA:H202	26:c:503:CLA:H161	1.81	0.44
28:c:507:BCR:H361	28:c:507:BCR:H20C	1.76	0.44
7:g:70:ARG:HA	7:g:73:MET:HE3	2.00	0.44
28:j:101:BCR:H19C	11:k:51:VAL:HG21	1.99	0.44
7:n:81:PHE:HB3	7:n:82:PRO:HD3	1.99	0.44
14:o:148:VAL:HG11	14:o:151:ASN:O	2.18	0.44
26:r:305:CLA:HBA1	26:r:305:CLA:H3A	1.62	0.44
18:s:70:ASN:O	18:s:73:LYS:HG2	2.17	0.44
3:C:135:LEU:HD21	24:Z:33:TRP:CD2	2.53	0.44
3:C:378:SER:O	3:C:382:LYS:HG2	2.18	0.44
3:C:433:LEU:HD22	26:C:512:CLA:HMC3	1.99	0.44
28:C:514:BCR:H361	28:C:514:BCR:H20C	1.75	0.44
15:P:90:LYS:HB3	16:Q:6:SER:HB2	2.00	0.44
17:R:104:MET:SD	26:R:306:CLA:HAB	2.58	0.44
18:S:116:ALA:HA	18:S:119:LEU:HG	1.99	0.44
1:a:197:PHE:HB3	1:a:285:PHE:O	2.18	0.44
29:a:413:SQD:H242	37:d:410:LHG:H121	2.00	0.44
2:b:90:LEU:O	2:b:95:GLY:HA3	2.18	0.44
3:c:52:ALA:HB2	26:c:518:CLA:HMA2	1.98	0.44
3:c:192:GLY:C	16:q:85:SER:HA	2.43	0.44
17:r:94:GLU:HA	17:r:172:LEU:HD21	1.99	0.44
18:s:48:TYR:CD2	18:s:66:LYS:HA	2.52	0.44
12:L:19:TYR:HE1	29:b:621:SQD:H302	1.83	0.44
13:M:27:VAL:HA	13:M:30:VAL:HG22	2.00	0.44
14:O:162:MET:HE3	14:O:200:GLN:HB2	1.99	0.44
16:Q:5:ILE:HG12	16:Q:6:SER:N	2.31	0.44
1:a:131:TRP:CZ3	26:c:502:CLA:HAA2	2.53	0.44
3:c:215:LYS:HG3	3:c:223:TRP:HA	1.99	0.44
4:d:51:GLY:HA2	4:d:55:VAL:HB	1.99	0.44
11:k:42:PRO:O	11:k:45:PHE:HB2	2.18	0.44
26:n:304:CLA:OBD	26:n:310:CLA:HBD	2.18	0.44
39:n:318:CHL:H91	39:n:318:CHL:H112	1.77	0.44
14:o:98:LYS:O	16:q:74:PRO:HG3	2.17	0.44
14:o:286:LYS:O	14:o:299:GLY:HA3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:r:302:NEX:H11	42:r:302:NEX:H191	1.76	0.44
18:s:124:LEU:HD23	26:s:310:CLA:HAA2	1.98	0.44
3:C:68:ASN:ND2	3:C:92:LEU:HD11	2.31	0.44
4:D:110:LEU:HD12	4:D:110:LEU:HA	1.82	0.44
7:G:70:ARG:HA	7:G:73:MET:HE3	2.00	0.44
15:P:165:ASP:HA	15:P:168:TRP:HB3	2.00	0.44
17:R:73:ALA:HA	43:R:402:HOH:O	2.18	0.44
23:Y:189:PHE:CD2	26:Y:308:CLA:H201	2.53	0.44
1:a:283:ILE:HA	1:a:286:THR:HG22	1.98	0.44
29:a:413:SQD:H292	11:k:50:PHE:CE1	2.53	0.44
26:b:613:CLA:H162	26:b:613:CLA:H193	1.78	0.44
10:j:15:THR:O	10:j:19:ILE:HG12	2.18	0.44
7:n:131:GLN:HE22	39:n:318:CHL:CMC	2.31	0.44
15:p:165:ASP:HA	15:p:168:TRP:HB3	1.99	0.44
17:r:180:ASP:HA	40:r:307:LUT:H24	2.00	0.44
3:C:186:TYR:HA	3:C:196:VAL:HA	1.99	0.44
34:C:503:LMG:HC1	34:C:503:LMG:HC8	1.78	0.44
42:G:315:NEX:H191	42:G:315:NEX:H11	1.74	0.44
7:N:131:GLN:HE22	39:N:303:CHL:CMC	2.30	0.44
18:S:160:PHE:O	18:S:163:LYS:HG2	2.18	0.44
28:T:101:BCR:H21C	28:b:603:BCR:H363	2.00	0.44
23:Y:126:ALA:HB3	39:r:301:CHL:HMC	2.00	0.44
23:Y:173:PHE:CZ	23:Y:177:LYS:HE2	2.53	0.44
39:Y:307:CHL:HHC	39:Y:307:CHL:HBB1	2.00	0.44
3:c:230:LEU:O	3:c:234:ILE:HG12	2.17	0.44
7:g:121:ALA:HA	39:g:314:CHL:C1C	2.48	0.44
39:g:311:CHL:H202	39:g:311:CHL:H161	1.82	0.44
41:g:320:XAT:H401	41:g:320:XAT:H35	1.71	0.44
8:h:29:GLU:OE1	26:r:313:CLA:H42	2.18	0.44
1:A:61:ASP:HB2	1:A:63:ILE:HG12	2.00	0.43
2:B:42:LEU:HD13	2:B:94:GLU:HG3	1.99	0.43
2:B:90:LEU:O	2:B:95:GLY:HA3	2.18	0.43
26:C:520:CLA:H112	26:C:520:CLA:H151	1.81	0.43
41:R:304:XAT:H15	41:R:304:XAT:H201	1.87	0.43
1:a:82:ILE:HB	1:a:174:LEU:HB2	2.00	0.43
2:b:20:LEU:O	2:b:24:ILE:HG13	2.18	0.43
2:b:71:ILE:HG12	26:b:617:CLA:HMA2	2.00	0.43
37:d:402:LHG:H321	37:d:402:LHG:H272	2.00	0.43
41:g:309:XAT:H31	41:g:309:XAT:H391	1.80	0.43
7:n:110:LEU:HD22	39:n:311:CHL:HMD2	2.00	0.43
17:r:93:ARG:O	17:r:93:ARG:HD3	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s:41:ASP:O	18:s:42:ARG:HB2	2.18	0.43
28:t:101:BCR:H24C	28:t:101:BCR:H392	1.71	0.43
34:w:201:LMG:H341	34:w:201:LMG:H312	1.91	0.43
4:D:14:LEU:HD11	22:X:106:VAL:HG13	2.00	0.43
5:E:11:ARG:CZ	5:E:16:ILE:HG12	2.48	0.43
7:N:86:ALA:HA	7:N:90:VAL:O	2.18	0.43
26:b:605:CLA:H102	26:b:609:CLA:H121	2.00	0.43
3:c:135:LEU:HD21	24:z:33:TRP:CD2	2.54	0.43
26:c:514:CLA:C4B	33:c:519:DGD:HB91	2.48	0.43
14:o:310:ASP:H	14:o:314:LYS:HG2	1.83	0.43
23:y:189:PHE:CD2	26:y:306:CLA:H201	2.53	0.43
26:y:316:CLA:H141	26:y:316:CLA:H162	1.76	0.43
2:B:471:ALA:HB1	4:D:140:PRO:CG	2.48	0.43
26:B:605:CLA:H91	26:B:605:CLA:H111	1.68	0.43
3:C:178:LYS:HD3	26:C:512:CLA:H192	1.99	0.43
3:C:230:LEU:O	3:C:234:ILE:HG12	2.18	0.43
26:G:314:CLA:H71	26:G:317:CLA:HHB	1.99	0.43
7:N:44:TYR:HB2	26:N:307:CLA:HMD1	2.00	0.43
7:N:187:LEU:HD13	26:N:319:CLA:HBC1	2.00	0.43
15:P:96:GLU:HA	15:P:106:ASN:ND2	2.33	0.43
40:S:306:LUT:H382	26:S:307:CLA:HBA1	2.00	0.43
20:U:6:THR:HG22	20:U:8:ALA:H	1.83	0.43
1:a:140:ARG:HB2	4:d:220:ASN:HA	1.99	0.43
2:b:75:TRP:HA	2:b:88:PRO:HG3	2.00	0.43
3:c:168:LEU:HD21	26:c:504:CLA:H61	2.00	0.43
3:c:169:GLY:HA2	3:c:241:GLY:HA2	2.00	0.43
3:c:170:VAL:HG11	26:c:503:CLA:H112	1.98	0.43
3:c:236:GLY:HA3	28:c:511:BCR:H402	1.99	0.43
41:g:309:XAT:H11	41:g:309:XAT:H191	1.85	0.43
41:n:316:XAT:H35	41:n:316:XAT:H401	1.80	0.43
14:o:146:ASP:HB2	14:o:317:LYS:NZ	2.33	0.43
15:p:69:LYS:HD2	15:p:69:LYS:N	2.33	0.43
15:p:90:LYS:HB3	16:q:6:SER:HB2	2.00	0.43
1:A:324:ALA:O	1:A:328:MET:HG3	2.17	0.43
29:B:621:SQD:H302	12:l:19:TYR:HE1	1.82	0.43
4:D:149:PRO:HB3	26:D:409:CLA:H41	2.00	0.43
7:G:104:ILE:HD13	7:G:104:ILE:HA	1.82	0.43
14:O:143:VAL:O	14:O:157:GLN:HG2	2.19	0.43
39:Y:302:CHL:C1D	37:Y:306:LHG:HC81	2.47	0.43
1:a:141:PRO:HG3	3:c:446:GLY:C	2.44	0.43
2:b:366:PHE:CD1	2:b:367:PRO:HD2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:441:GLY:C	14:o:259:ALA:HB3	2.44	0.43
7:g:104:ILE:HD13	7:g:104:ILE:HA	1.83	0.43
7:n:187:LEU:HD13	26:n:310:CLA:HBC1	2.00	0.43
15:p:100:GLU:OE1	15:p:136:ALA:HB1	2.19	0.43
2:B:157:HIS:CE1	26:B:610:CLA:NA	2.86	0.43
3:C:192:GLY:C	16:Q:85:SER:HA	2.44	0.43
33:C:510:DGD:HA72	34:C:518:LMG:H362	2.00	0.43
26:c:514:CLA:H92	26:c:514:CLA:H62	1.76	0.43
26:c:515:CLA:H141	26:c:515:CLA:H161	1.80	0.43
28:h:101:BCR:H24C	28:h:101:BCR:H371	1.82	0.43
7:n:149:LEU:HD23	7:n:149:LEU:HA	1.78	0.43
14:o:159:THR:HB	14:o:199:VAL:HB	2.01	0.43
18:s:137:LEU:HD23	18:s:137:LEU:HA	1.77	0.43
42:s:302:NEX:H34	39:s:313:CHL:HMA1	2.00	0.43
26:B:616:CLA:H162	8:H:19:VAL:HG11	2.00	0.43
3:C:259:TRP:HE1	33:Y:303:DGD:HB21	1.83	0.43
14:O:148:VAL:HG11	14:O:151:ASN:O	2.18	0.43
26:c:514:CLA:H42	33:c:519:DGD:HB51	1.99	0.43
10:j:19:ILE:HD11	28:j:101:BCR:H361	2.01	0.43
41:n:316:XAT:H41	39:n:318:CHL:HAA1	2.00	0.43
26:r:314:CLA:H141	26:r:314:CLA:H161	1.75	0.43
18:s:34:PHE:CE2	18:s:35:LEU:HG	2.53	0.43
18:s:160:PHE:O	18:s:163:LYS:HG2	2.18	0.43
39:y:314:CHL:HHC	39:y:314:CHL:HBB1	2.00	0.43
1:A:234:ASN:ND2	37:D:407:LHG:HC11	2.32	0.43
26:B:615:CLA:HBA2	26:B:618:CLA:H11	2.01	0.43
41:G:310:XAT:H11	41:G:310:XAT:H191	1.84	0.43
8:H:25:PRO:HG2	17:R:78:THR:HB	2.00	0.43
26:Y:308:CLA:HBA1	40:Y:309:LUT:H382	2.00	0.43
2:b:115:TRP:CG	28:b:619:BCR:H291	2.54	0.43
2:b:383:PHE:CG	4:d:347:PRO:HA	2.54	0.43
26:b:607:CLA:HMD1	13:m:21:PHE:HE1	1.84	0.43
41:n:316:XAT:H12	37:y:301:LHG:H202	2.00	0.43
17:r:182:LEU:HD12	40:r:307:LUT:H222	2.01	0.43
18:s:39:LEU:HD22	24:z:41:PHE:CE1	2.54	0.43
23:y:104:ILE:HD12	23:y:104:ILE:HA	1.90	0.43
42:y:307:NEX:H15	42:y:307:NEX:H201	1.80	0.43
29:A:407:SQD:H102	29:A:407:SQD:H132	1.80	0.43
2:B:20:LEU:O	2:B:24:ILE:HG13	2.18	0.43
2:B:75:TRP:HA	2:B:88:PRO:HG3	2.01	0.43
2:B:159:THR:HA	2:B:181:VAL:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:24:TYR:CZ	7:G:25:LEU:HG	2.53	0.43
7:G:121:ALA:HA	39:G:309:CHL:C1C	2.48	0.43
7:N:21:ARG:HD2	7:N:43:ASP:O	2.19	0.43
15:P:145:GLN:HG3	15:P:162:GLN:HB2	2.01	0.43
5:e:30:ILE:HB	5:e:31:PRO:HD3	2.00	0.43
7:g:46:TRP:CZ3	39:g:311:CHL:HBD	2.53	0.43
14:o:132:LYS:HB3	14:o:133:LYS:H	1.62	0.43
15:p:51:ASP:HB3	15:p:54:ASP:O	2.18	0.43
26:y:317:CLA:CHA	26:y:317:CLA:HBA1	2.45	0.43
26:B:601:CLA:H122	26:B:601:CLA:H161	1.61	0.43
26:G:314:CLA:H13	26:G:314:CLA:H172	1.85	0.43
18:S:118:LEU:HB3	18:S:135:LEU:HB2	2.00	0.43
26:Y:301:CLA:H62	26:Y:301:CLA:H2	1.78	0.43
2:b:66:MET:HG3	26:b:613:CLA:O1D	2.19	0.43
5:e:13:PHE:CE1	38:e:101:HEM:HBD2	2.54	0.43
39:g:313:CHL:O2D	39:g:313:CHL:H2A	2.18	0.43
8:h:25:PRO:HG2	17:r:78:THR:HB	2.01	0.43
12:l:25:ILE:HG13	13:m:18:PRO:HB2	1.99	0.43
13:m:17:VAL:HB	13:m:18:PRO:HD3	2.01	0.43
41:r:304:XAT:H15	41:r:304:XAT:H201	1.88	0.43
24:z:36:ASN:O	24:z:39:VAL:HG12	2.19	0.43
4:D:56:THR:HG22	43:E:202:HOH:O	2.18	0.43
4:D:132:LEU:O	4:D:136:VAL:HG22	2.19	0.43
9:I:28:PRO:HB3	21:W:135:LEU:HD22	2.00	0.43
39:N:310:CHL:HAA2	18:S:98:LEU:HD23	2.01	0.43
41:N:315:XAT:H31	41:N:315:XAT:H391	1.77	0.43
14:O:310:ASP:H	14:O:314:LYS:HG2	1.84	0.43
17:R:133:SER:HB2	39:R:301:CHL:CMD	2.49	0.43
1:a:195:HIS:CE1	1:a:197:PHE:HB2	2.54	0.43
4:d:80:THR:HG22	4:d:111:TRP:CE2	2.53	0.43
37:g:301:LHG:HC61	39:g:311:CHL:HMD3	2.01	0.43
39:n:306:CHL:HBA1	39:n:306:CHL:H3A	1.88	0.43
26:n:315:CLA:HMD3	39:n:319:CHL:HBA2	2.00	0.43
16:q:106:LEU:HD21	16:q:150:LEU:HD23	2.01	0.43
39:y:302:CHL:HHC	39:y:302:CHL:HBB1	2.00	0.43
26:B:606:CLA:HBA2	26:B:606:CLA:HBD	2.00	0.42
26:B:609:CLA:H162	26:B:609:CLA:H122	1.76	0.42
3:C:69:LEU:HD11	28:K:101:BCR:H322	2.01	0.42
5:E:30:ILE:HB	5:E:31:PRO:HD3	2.01	0.42
17:R:180:ASP:N	17:R:181:PRO:HD3	2.34	0.42
42:R:305:NEX:H35	42:R:305:NEX:H401	1.92	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:R:318:CHL:HMC	23:y:126:ALA:HB3	2.00	0.42
18:S:48:TYR:CE2	18:S:66:LYS:HA	2.53	0.42
39:S:302:CHL:C1D	26:S:310:CLA:HBA1	2.49	0.42
23:Y:22:PRO:HB2	39:Y:302:CHL:HBC1	2.00	0.42
1:a:300:PHE:HB3	1:a:302:PHE:CE2	2.54	0.42
3:c:130:ILE:O	3:c:134:LEU:HB2	2.19	0.42
3:c:213:LEU:HD11	28:c:511:BCR:H373	2.01	0.42
26:d:403:CLA:H152	22:x:92:ALA:HA	2.00	0.42
7:g:131:GLN:HE22	39:g:319:CHL:CMC	2.32	0.42
7:n:180:LYS:HD3	26:n:304:CLA:HAA2	2.00	0.42
7:n:198:GLN:HB3	7:n:209:ASN:ND2	2.34	0.42
3:C:130:ILE:O	3:C:134:LEU:HB2	2.19	0.42
4:D:80:THR:HG22	4:D:111:TRP:CE2	2.54	0.42
37:D:408:LHG:H201	19:T:13:THR:HG21	2.01	0.42
41:G:310:XAT:H15	41:G:310:XAT:H201	1.82	0.42
7:N:198:GLN:HE21	7:N:209:ASN:HD22	1.67	0.42
14:O:212:THR:HG21	14:O:231:VAL:HA	2.00	0.42
17:R:14:TRP:O	26:R:309:CLA:NC	2.52	0.42
17:R:114:GLU:OE2	17:R:223:PRO:HD2	2.19	0.42
1:a:156:ALA:HA	1:a:160:ILE:HB	2.01	0.42
1:a:324:ALA:O	1:a:328:MET:HG3	2.18	0.42
28:b:615:BCR:H20C	28:b:615:BCR:H361	1.86	0.42
3:c:255:LYS:HB3	3:c:255:LYS:HE2	1.77	0.42
26:s:310:CLA:H2	39:s:316:CHL:HBD	2.02	0.42
1:A:131:TRP:CZ3	26:C:506:CLA:HAA2	2.54	0.42
39:G:318:CHL:H12	39:Y:307:CHL:C1B	2.50	0.42
39:G:318:CHL:H161	39:G:318:CHL:H202	1.80	0.42
24:Z:36:ASN:O	24:Z:39:VAL:HG12	2.19	0.42
26:b:605:CLA:HED1	26:b:609:CLA:H143	1.99	0.42
26:b:605:CLA:NC	26:b:609:CLA:H171	2.34	0.42
3:c:119:LEU:HD23	28:k:101:BCR:H321	2.01	0.42
4:d:14:LEU:HD11	22:x:106:VAL:HG13	1.99	0.42
5:e:26:HIS:HA	5:e:29:THR:OG1	2.19	0.42
7:g:75:GLY:HA2	40:g:310:LUT:H181	2.00	0.42
16:q:95:ILE:HG22	16:q:103:LYS:HG3	2.02	0.42
26:s:311:CLA:HBA1	40:s:312:LUT:H382	2.00	0.42
23:y:155:LEU:HD23	23:y:155:LEU:HA	1.89	0.42
26:B:602:CLA:H161	26:B:602:CLA:H202	1.80	0.42
7:G:131:GLN:HE22	39:G:305:CHL:CMC	2.32	0.42
37:G:312:LHG:HC41	41:G:320:XAT:H363	2.00	0.42
18:S:67:LYS:HD3	18:S:70:ASN:ND2	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S:304:CLA:H12	26:S:304:CLA:C4D	2.50	0.42
28:b:603:BCR:HC42	34:b:622:LMG:H341	2.01	0.42
26:b:605:CLA:H202	26:b:605:CLA:H161	1.79	0.42
3:c:437:LEU:HA	26:c:513:CLA:HMC2	2.01	0.42
26:g:303:CLA:H71	26:g:308:CLA:HHB	2.02	0.42
28:k:101:BCR:H20C	28:k:101:BCR:H361	1.94	0.42
39:n:308:CHL:HAA2	18:s:98:LEU:HD23	2.01	0.42
42:n:313:NEX:H15	42:n:313:NEX:H201	1.74	0.42
15:p:45:GLN:HA	15:p:62:MET:HG3	2.00	0.42
15:p:121:VAL:HB	15:p:126:TYR:CE1	2.54	0.42
17:r:45:TYR:O	17:r:46:LEU:HB2	2.18	0.42
26:N:307:CLA:H141	26:N:307:CLA:H161	1.71	0.42
26:N:313:CLA:OBD	26:N:319:CLA:HBD	2.19	0.42
42:S:305:NEX:H11	42:S:305:NEX:H191	1.71	0.42
23:Y:167:ALA:HB1	23:Y:173:PHE:CD1	2.54	0.42
2:b:159:THR:HA	2:b:181:VAL:O	2.19	0.42
2:b:236:THR:CB	2:b:473:THR:HG21	2.49	0.42
18:s:42:ARG:HA	18:s:45:ILE:HG12	2.02	0.42
23:y:163:PRO:HD2	40:y:311:LUT:H23	2.00	0.42
1:A:197:PHE:HB3	1:A:285:PHE:O	2.19	0.42
2:B:70:GLY:HA2	2:B:178:VAL:HG11	2.01	0.42
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.54	0.42
26:B:611:CLA:H61	26:B:611:CLA:H41	1.68	0.42
41:G:320:XAT:H31	41:G:320:XAT:H391	1.88	0.42
15:P:121:VAL:HB	15:P:126:TYR:CE1	2.55	0.42
17:R:182:LEU:HD12	40:R:311:LUT:H222	2.01	0.42
17:R:203:ARG:HA	17:R:206:MET:HE3	2.01	0.42
18:S:36:PRO:HD2	18:S:39:LEU:HD12	2.00	0.42
23:Y:70:ARG:HA	23:Y:73:MET:HE3	2.01	0.42
23:Y:81:PHE:HB3	23:Y:82:PRO:HD3	2.02	0.42
3:c:401:LEU:HD22	3:c:410:VAL:HG12	2.01	0.42
15:p:43:PRO:HD2	15:p:86:TYR:CD1	2.54	0.42
17:r:155:ILE:HA	17:r:158:ILE:HG12	2.02	0.42
18:s:98:LEU:HD13	18:s:127:PHE:CE2	2.55	0.42
1:A:238:ARG:HA	1:A:238:ARG:HD3	1.87	0.42
1:A:300:PHE:HB3	1:A:302:PHE:CE2	2.54	0.42
26:C:516:CLA:H92	26:C:516:CLA:H61	1.87	0.42
42:N:302:NEX:H15	42:N:302:NEX:H201	1.73	0.42
14:O:175:PRO:HG2	14:O:187:LYS:HB2	2.02	0.42
18:S:118:LEU:HD12	39:S:302:CHL:HBC3	2.02	0.42
18:S:135:LEU:O	18:S:139:VAL:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:47:VAL:HG21	1:a:114:LEU:HD22	2.02	0.42
2:b:257:TRP:HZ3	2:b:449:GLY:HA2	1.83	0.42
3:c:216:SER:O	3:c:221:GLU:HB2	2.19	0.42
26:c:520:CLA:H202	26:c:520:CLA:H161	1.85	0.42
9:i:28:PRO:HB3	21:w:135:LEU:HD22	2.00	0.42
14:o:254:ALA:HB3	14:o:263:GLY:HA2	2.02	0.42
17:r:94:GLU:HA	17:r:172:LEU:HD11	2.02	0.42
26:y:309:CLA:HBB1	26:y:316:CLA:H3A	2.02	0.42
5:E:26:HIS:HA	5:E:29:THR:OG1	2.20	0.42
12:L:25:ILE:HG22	13:M:15:ILE:HD13	2.02	0.42
12:l:24:LEU:HD13	37:l:101:LHG:H151	2.02	0.42
37:r:312:LHG:HC81	37:r:312:LHG:H112	1.91	0.42
26:r:314:CLA:H112	26:r:314:CLA:H142	1.76	0.42
1:A:260:PHE:HE2	1:A:262:TYR:HB2	1.83	0.42
2:B:66:MET:HG3	26:B:618:CLA:O1D	2.19	0.42
26:B:603:CLA:H141	26:B:603:CLA:H161	1.88	0.42
26:B:605:CLA:H193	26:B:605:CLA:H141	2.01	0.42
28:B:619:BCR:H363	28:t:101:BCR:H21C	2.01	0.42
3:C:257:PHE:O	3:C:261:ARG:HG3	2.20	0.42
41:G:310:XAT:H393	37:N:301:LHG:H101	2.02	0.42
28:J:101:BCR:H19C	11:K:51:VAL:HG21	2.00	0.42
7:N:182:LEU:HD23	7:N:182:LEU:HA	1.77	0.42
14:O:200:GLN:HE21	14:O:200:GLN:HB3	1.67	0.42
26:S:309:CLA:HBA2	26:S:309:CLA:CGD	2.50	0.42
39:Y:318:CHL:HHC	39:Y:318:CHL:HBB1	2.01	0.42
26:c:506:CLA:H151	26:c:506:CLA:H112	1.76	0.42
17:r:114:GLU:OE2	17:r:223:PRO:HD2	2.19	0.42
17:r:133:SER:HB2	39:r:316:CHL:CMD	2.49	0.42
1:A:156:ALA:HA	1:A:160:ILE:HB	2.01	0.42
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.55	0.42
3:C:437:LEU:HA	26:C:517:CLA:HMC2	2.02	0.42
26:N:312:CLA:HAB	40:N:314:LUT:H32	2.01	0.42
2:b:282:GLN:HG2	20:u:13:TYR:CE1	2.55	0.42
3:c:38:GLY:HA3	26:c:518:CLA:CMD	2.44	0.42
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.54	0.42
39:n:318:CHL:H2	39:n:318:CHL:H62	1.93	0.42
15:p:94:PHE:CE1	16:q:6:SER:HA	2.55	0.42
18:s:118:LEU:HD23	18:s:118:LEU:HA	1.85	0.42
18:s:146:LEU:HD22	39:s:316:CHL:HMB3	2.02	0.42
1:A:199:MET:HB3	33:C:513:DGD:HAE1	2.02	0.41
2:B:85:ILE:HG12	2:B:88:PRO:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:602:CLA:H11	26:B:602:CLA:H51	1.92	0.41
4:D:194:ASN:HA	4:D:295:ALA:HB3	2.01	0.41
41:G:310:XAT:H35	41:G:310:XAT:H401	1.81	0.41
41:N:315:XAT:H401	41:N:315:XAT:H35	1.78	0.41
14:O:146:ASP:HB2	14:O:317:LYS:NZ	2.34	0.41
15:P:51:ASP:HB2	15:P:57:SER:HB2	2.02	0.41
15:P:51:ASP:HB3	15:P:54:ASP:O	2.20	0.41
30:a:407:PL9:H121	30:a:407:PL9:H161	1.85	0.41
26:a:411:CLA:H201	37:d:409:LHG:H312	2.02	0.41
4:d:56:THR:HG22	43:e:202:HOH:O	2.19	0.41
4:d:351:ALA:HA	15:p:138:GLY:C	2.45	0.41
39:r:318:CHL:HHC	39:r:318:CHL:HBB1	2.02	0.41
18:s:166:PRO:HB2	18:s:170:PHE:CD2	2.55	0.41
23:y:16:TRP:CE2	26:y:304:CLA:HED3	2.55	0.41
26:y:310:CLA:H111	26:y:310:CLA:H91	1.73	0.41
7:G:214:LEU:HD11	26:G:304:CLA:HMC3	2.02	0.41
26:N:306:CLA:HMD3	39:N:317:CHL:HBA2	2.01	0.41
23:Y:163:PRO:HD2	40:Y:315:LUT:H23	2.01	0.41
1:a:214:MET:HE2	1:a:255:PHE:HD1	1.84	0.41
26:c:518:CLA:H152	24:z:24:PRO:HG3	2.02	0.41
26:g:303:CLA:HBA1	40:g:310:LUT:H382	2.02	0.41
41:g:320:XAT:H31	41:g:320:XAT:H391	1.83	0.41
28:h:101:BCR:H361	28:h:101:BCR:H20C	1.83	0.41
17:r:203:ARG:HA	17:r:206:MET:HE3	2.02	0.41
2:B:144:PHE:O	2:B:148:VAL:HG23	2.20	0.41
3:C:396:MET:HE3	3:C:396:MET:HB2	1.99	0.41
4:D:85:LEU:HD23	5:E:72:ARG:HA	2.02	0.41
7:N:180:LYS:HD3	26:N:313:CLA:HAA2	2.02	0.41
40:N:305:LUT:H382	26:N:307:CLA:HBA1	2.01	0.41
14:O:150:LYS:HE2	2:b:50:PRO:HD2	2.02	0.41
15:P:69:LYS:HD2	15:P:69:LYS:N	2.35	0.41
17:R:94:GLU:HA	17:R:172:LEU:HD11	2.02	0.41
17:R:163:ASN:HD22	26:R:302:CLA:HBC3	1.85	0.41
42:S:305:NEX:H31	42:S:305:NEX:H391	1.70	0.41
34:W:201:LMG:H362	34:W:201:LMG:H331	1.86	0.41
2:b:394:GLN:HA	16:q:5:ILE:HG13	2.02	0.41
4:d:12:LYS:HB3	4:d:12:LYS:NZ	2.35	0.41
5:e:80:ASP:O	5:e:84:ARG:HG3	2.20	0.41
7:n:68:HIS:NE2	26:n:315:CLA:ND	2.69	0.41
17:r:73:ALA:HA	43:r:401:HOH:O	2.19	0.41
26:s:305:CLA:C4D	26:s:305:CLA:H12	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:608:BCR:H20C	28:B:608:BCR:H361	1.87	0.41
26:C:505:CLA:H2	26:C:505:CLA:C1B	2.51	0.41
4:D:48:TRP:NE1	27:D:403:PHO:H172	2.36	0.41
37:D:407:LHG:O9	37:L:101:LHG:HC81	2.20	0.41
39:G:318:CHL:H142	39:G:318:CHL:H111	1.83	0.41
14:O:157:GLN:HG3	14:O:201:LEU:HD22	2.03	0.41
26:Y:308:CLA:H8	26:Y:308:CLA:H51	1.89	0.41
1:a:246:TYR:CE2	1:a:248:ILE:HG12	2.56	0.41
1:a:259:ILE:HG22	1:a:260:PHE:H	1.85	0.41
26:b:602:CLA:OBD	26:b:607:CLA:HHC	2.20	0.41
26:c:505:CLA:H193	26:c:505:CLA:H161	1.77	0.41
26:c:513:CLA:H171	11:k:43:LEU:HD11	2.02	0.41
37:g:301:LHG:H301	26:g:305:CLA:HBB2	2.02	0.41
14:o:138:PRO:HD2	14:o:167:TYR:HD1	1.85	0.41
16:q:130:SER:O	16:q:133:GLU:HG2	2.20	0.41
17:r:157:TYR:O	17:r:161:GLN:HG2	2.20	0.41
18:s:118:LEU:HD12	39:s:316:CHL:HBC3	2.01	0.41
1:A:174:LEU:HD22	27:A:404:PHO:H151	2.01	0.41
2:B:172:TYR:CE1	2:B:283:GLU:HB2	2.55	0.41
26:B:612:CLA:H18	26:B:612:CLA:H151	1.79	0.41
4:D:351:ALA:HA	15:P:138:GLY:C	2.45	0.41
40:G:308:LUT:H382	26:G:314:CLA:HBA1	2.03	0.41
37:G:312:LHG:H141	37:G:312:LHG:H171	1.93	0.41
23:Y:192:PHE:CD2	26:Y:312:CLA:HAC1	2.56	0.41
3:c:61:VAL:HG13	3:c:118:HIS:CD2	2.52	0.41
3:c:186:TYR:HA	3:c:196:VAL:HA	2.02	0.41
41:g:309:XAT:H201	41:g:309:XAT:H15	1.81	0.41
41:g:320:XAT:H15	41:g:320:XAT:H201	1.83	0.41
14:o:177:GLU:O	14:o:184:VAL:HA	2.20	0.41
17:r:97:LEU:HD23	17:r:172:LEU:HD22	2.03	0.41
17:r:104:MET:SD	26:r:306:CLA:HAB	2.60	0.41
17:r:180:ASP:N	17:r:181:PRO:HD3	2.34	0.41
17:r:188:PRO:HA	17:r:191:THR:HG22	2.03	0.41
39:r:301:CHL:CHA	39:r:301:CHL:HBA1	2.50	0.41
40:r:307:LUT:H15	40:r:307:LUT:H201	1.92	0.41
26:r:317:CLA:HBA2	26:r:317:CLA:H3A	1.28	0.41
18:s:118:LEU:HG	18:s:124:LEU:CD1	2.51	0.41
26:s:304:CLA:HBA2	26:s:304:CLA:CGD	2.50	0.41
1:A:116:VAL:HG13	1:A:158:PHE:HB3	2.02	0.41
10:J:15:THR:O	10:J:19:ILE:HG12	2.20	0.41
18:S:172:PRO:HD2	40:S:301:LUT:H23	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:S:301:LUT:H35	40:S:301:LUT:H401	1.94	0.41
23:Y:46:TRP:CE3	40:Y:309:LUT:H383	2.55	0.41
26:Y:310:CLA:CHA	26:Y:310:CLA:HBA1	2.46	0.41
1:a:260:PHE:HE2	1:a:262:TYR:HB2	1.86	0.41
3:c:257:PHE:O	3:c:261:ARG:HG3	2.21	0.41
26:c:505:CLA:HMA1	34:c:512:LMG:H182	2.02	0.41
39:g:312:CHL:C1B	39:n:306:CHL:H12	2.51	0.41
14:o:143:VAL:O	14:o:157:GLN:HG2	2.19	0.41
18:s:153:ARG:NH2	26:s:314:CLA:HMA3	2.35	0.41
23:y:167:ALA:HB1	23:y:173:PHE:CD1	2.56	0.41
23:y:192:PHE:CD2	26:y:310:CLA:HAC1	2.56	0.41
39:y:303:CHL:HBA1	39:y:303:CHL:H3A	1.78	0.41
26:B:601:CLA:HHC	26:B:603:CLA:OBD	2.20	0.41
7:G:77:LEU:HD13	26:G:319:CLA:HBB2	2.02	0.41
13:M:17:VAL:HB	13:M:18:PRO:HD3	2.02	0.41
18:S:160:PHE:HD1	18:S:160:PHE:HA	1.78	0.41
2:b:208:LEU:HD23	26:b:601:CLA:HAC2	2.03	0.41
2:b:231:MET:HE2	26:b:614:CLA:HMC1	2.03	0.41
26:b:611:CLA:CHA	26:b:611:CLA:HBA1	2.50	0.41
29:b:621:SQD:H342	29:b:621:SQD:H371	1.90	0.41
3:c:259:TRP:HZ3	26:c:516:CLA:H42	1.86	0.41
4:d:85:LEU:HD23	5:e:72:ARG:HA	2.01	0.41
4:d:161:PRO:HG3	4:d:170:ALA:HB2	2.03	0.41
37:n:301:LHG:HC91	37:n:301:LHG:H122	1.86	0.41
18:s:84:TRP:CD1	26:s:314:CLA:HMD3	2.55	0.41
26:B:615:CLA:CHA	26:B:615:CLA:HBA1	2.50	0.41
33:C:513:DGD:HA62	4:D:74:LEU:HD21	2.03	0.41
7:G:56:GLU:O	7:G:60:ARG:HG2	2.21	0.41
26:G:307:CLA:H43	26:G:319:CLA:HBA1	2.03	0.41
39:G:311:CHL:HAC2	26:G:317:CLA:HBC1	2.02	0.41
37:G:312:LHG:HC31	26:G:313:CLA:C1B	2.51	0.41
7:N:213:HIS:CG	26:N:318:CLA:HAA2	2.55	0.41
39:N:316:CHL:HBA1	39:N:316:CHL:H3A	1.85	0.41
33:c:501:DGD:HA62	4:d:74:LEU:HD21	2.02	0.41
4:d:43:PHE:HE2	26:d:403:CLA:C2C	2.33	0.41
7:g:146:ASN:H	7:g:151:GLU:HB3	1.86	0.41
26:g:304:CLA:HBA1	26:g:317:CLA:H43	2.03	0.41
13:m:27:VAL:HA	13:m:30:VAL:HG22	2.02	0.41
42:r:302:NEX:H173	42:r:302:NEX:H3	1.92	0.41
1:A:41:LEU:HD23	1:A:41:LEU:HA	1.94	0.41
2:B:208:LEU:HD23	26:B:606:CLA:HAC2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:601:CLA:H41	26:B:601:CLA:H61	1.68	0.41
26:B:604:CLA:HMB3	4:D:126:MET:HB3	2.03	0.41
26:B:618:CLA:H193	26:B:618:CLA:H162	1.77	0.41
3:C:223:TRP:CE3	3:C:224:ILE:HG12	2.55	0.41
26:C:512:CLA:H161	26:C:512:CLA:H141	1.86	0.41
4:D:182:ILE:HG23	26:D:409:CLA:HHD	2.02	0.41
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.56	0.41
39:N:303:CHL:HAA1	41:N:315:XAT:H41	2.03	0.41
17:R:76:LYS:HB2	17:R:76:LYS:HE3	1.82	0.41
17:R:133:SER:HB2	39:R:301:CHL:HMD2	2.03	0.41
17:R:188:PRO:HA	17:R:191:THR:HG22	2.03	0.41
18:S:84:TRP:CD1	26:S:311:CLA:HMD3	2.56	0.41
26:S:311:CLA:HMD2	26:S:315:CLA:HBC2	2.03	0.41
42:Y:304:NEX:H222	26:Y:316:CLA:C1C	2.51	0.41
26:Y:305:CLA:H92	26:Y:305:CLA:H61	1.76	0.41
26:Y:316:CLA:CMB	39:Y:317:CHL:HBB1	2.51	0.41
1:a:189:GLU:HG2	43:a:579:HOH:O	2.21	0.41
2:b:30:VAL:HG13	26:b:602:CLA:HMC2	2.02	0.41
2:b:121:GLU:HG3	8:h:14:PRO:HB2	2.03	0.41
26:b:608:CLA:H91	26:b:608:CLA:H111	1.66	0.41
3:c:186:TYR:O	3:c:230:LEU:HD11	2.20	0.41
4:d:125:PHE:CE2	27:d:407:PHO:HBD	2.56	0.41
4:d:194:ASN:HA	4:d:295:ALA:HB3	2.02	0.41
27:d:407:PHO:H41	27:d:407:PHO:H62	1.65	0.41
7:g:104:ILE:HG21	7:g:124:ILE:HB	2.02	0.41
42:g:306:NEX:H401	42:g:306:NEX:H35	1.81	0.41
13:m:21:PHE:O	13:m:25:ILE:HG12	2.21	0.41
7:n:26:GLY:HA3	7:n:27:PRO:HD3	1.94	0.41
26:n:305:CLA:HBA1	40:n:317:LUT:H382	2.03	0.41
14:o:144:LYS:HA	14:o:156:PHE:HA	2.02	0.41
14:o:308:ASP:O	14:o:314:LYS:HE3	2.21	0.41
15:p:112:ASN:HA	16:q:12:PRO:O	2.21	0.41
18:s:172:PRO:HD2	40:s:308:LUT:H23	2.03	0.41
26:s:301:CLA:C3C	37:s:309:LHG:HC61	2.51	0.41
23:y:70:ARG:HA	23:y:73:MET:HE3	2.02	0.41
26:B:605:CLA:H143	26:B:605:CLA:H161	1.75	0.41
3:C:213:LEU:HD11	28:C:502:BCR:H373	2.03	0.41
26:C:515:CLA:H152	26:C:516:CLA:OBD	2.21	0.41
39:G:309:CHL:H3A	39:G:309:CHL:HBA2	1.32	0.41
7:N:87:ARG:NH2	7:N:208:GLU:HB2	2.36	0.41
18:S:118:LEU:HG	18:S:124:LEU:CD1	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:4:ARG:HB3	20:U:27:ARG:O	2.21	0.41
23:Y:181:LEU:HD23	23:Y:181:LEU:HA	1.84	0.41
42:Y:304:NEX:H15	42:Y:304:NEX:H201	1.80	0.41
39:Y:318:CHL:H3A	39:Y:318:CHL:HBA2	1.71	0.41
2:b:348:ASN:OD1	2:b:354:LEU:HD11	2.20	0.41
26:b:612:CLA:HMB3	4:d:126:MET:HB3	2.03	0.41
4:d:17:ILE:HG22	22:x:109:SER:HB2	2.03	0.41
4:d:48:TRP:NE1	27:d:407:PHO:H172	2.36	0.41
7:g:91:LYS:O	7:g:114:GLY:HA3	2.21	0.41
39:g:311:CHL:H142	39:g:311:CHL:H111	1.85	0.41
18:s:57:TYR:HB2	26:s:311:CLA:HMD1	2.03	0.41
22:x:115:LYS:O	22:x:116:ARG:HB3	2.21	0.41
2:B:368:VAL:HG21	2:B:422:ARG:HG3	2.03	0.40
3:C:168:LEU:HD21	26:C:515:CLA:H61	2.03	0.40
33:C:509:DGD:HBF1	33:C:509:DGD:HBE2	1.89	0.40
26:C:515:CLA:H161	26:C:515:CLA:H141	1.77	0.40
4:D:257:PHE:O	37:D:408:LHG:H321	2.21	0.40
5:E:54:ARG:HB2	5:E:57:GLU:HG3	2.03	0.40
16:Q:73:TRP:N	16:Q:74:PRO:HD2	2.36	0.40
17:R:23:TRP:HB3	17:R:42:PRO:HD3	2.03	0.40
26:R:313:CLA:H112	26:R:313:CLA:H142	1.72	0.40
26:b:614:CLA:H151	26:b:614:CLA:H18	1.87	0.40
3:c:339:LYS:HE3	3:c:339:LYS:HB2	1.93	0.40
3:c:408:GLY:HA2	3:c:419:TYR:O	2.21	0.40
26:c:504:CLA:H143	26:c:504:CLA:CHA	2.51	0.40
26:c:518:CLA:H171	24:z:20:LEU:HD12	2.03	0.40
5:e:20:ILE:HD13	5:e:20:ILE:HA	1.91	0.40
7:g:163:ASP:HA	40:g:316:LUT:H24	2.02	0.40
37:g:301:LHG:HC31	26:g:315:CLA:C1B	2.51	0.40
17:r:23:TRP:HB3	17:r:42:PRO:HD3	2.02	0.40
42:s:302:NEX:H31	42:s:302:NEX:H391	1.70	0.40
39:s:313:CHL:HHD	39:s:313:CHL:HAC2	1.91	0.40
1:A:93:PHE:HZ	26:A:405:CLA:HAA1	1.87	0.40
2:B:252:VAL:HG11	26:B:615:CLA:OBD	2.21	0.40
3:C:217:PRO:HB2	33:C:509:DGD:HA21	2.03	0.40
4:D:184:PHE:HB2	4:D:329:MET:HE1	2.03	0.40
5:E:13:PHE:CE1	38:E:101:HEM:HBD2	2.57	0.40
39:G:301:CHL:O2D	39:G:301:CHL:H2A	2.21	0.40
41:G:310:XAT:H391	41:G:310:XAT:H31	1.80	0.40
7:N:168:ALA:HB1	7:N:174:PHE:CD1	2.57	0.40
16:Q:55:LYS:HD3	16:Q:147:LEU:HD22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:157:TYR:O	17:R:161:GLN:HG2	2.20	0.40
23:Y:155:LEU:HD23	23:Y:155:LEU:HA	1.90	0.40
1:a:33:PHE:O	1:a:125:CYS:HB3	2.22	0.40
2:b:252:VAL:HG11	26:b:611:CLA:OBD	2.21	0.40
3:c:132:HIS:CE1	26:c:510:CLA:NA	2.89	0.40
28:c:507:BCR:H24C	28:c:507:BCR:H371	1.94	0.40
37:d:402:LHG:O9	37:l:101:LHG:HC81	2.22	0.40
7:n:213:HIS:CG	26:n:302:CLA:HAA2	2.57	0.40
16:q:73:TRP:N	16:q:74:PRO:HD2	2.36	0.40
42:r:302:NEX:H222	26:r:311:CLA:CHC	2.51	0.40
18:s:49:LEU:HD23	18:s:49:LEU:HA	1.91	0.40
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.03	0.40
2:B:30:VAL:HG13	26:B:603:CLA:HMC2	2.02	0.40
3:C:73:ALA:HB2	11:K:24:LEU:HG	2.02	0.40
3:C:337:LEU:HD23	3:C:337:LEU:HA	1.89	0.40
5:E:33:LEU:HD11	38:E:101:HEM:HAB	2.02	0.40
7:G:146:ASN:H	7:G:151:GLU:HB3	1.87	0.40
41:G:320:XAT:H35	41:G:320:XAT:H401	1.71	0.40
10:J:19:ILE:HD11	28:J:101:BCR:H361	2.03	0.40
18:S:34:PHE:CE2	18:S:35:LEU:HG	2.56	0.40
18:S:52:GLU:H	18:S:52:GLU:HG3	1.55	0.40
21:W:91:THR:O	34:W:201:LMG:HC62	2.22	0.40
26:Y:312:CLA:H2	26:Y:312:CLA:H61	1.73	0.40
2:b:464:PHE:HB2	4:d:280:TRP:CH2	2.57	0.40
26:b:602:CLA:H141	26:b:602:CLA:H161	1.88	0.40
26:c:518:CLA:H142	28:j:101:BCR:H353	2.02	0.40
4:d:132:LEU:O	4:d:136:VAL:HG22	2.21	0.40
7:g:181:GLU:HB2	26:g:317:CLA:CHB	2.51	0.40
17:r:180:ASP:HB2	26:r:306:CLA:HBD	2.02	0.40
23:y:81:PHE:HB3	23:y:82:PRO:HD3	2.02	0.40
42:y:307:NEX:H11	42:y:307:NEX:H191	1.97	0.40
27:A:404:PHO:H61	27:A:404:PHO:H2	1.87	0.40
2:B:121:GLU:HG3	8:H:14:PRO:HB2	2.02	0.40
26:B:610:CLA:H3A	26:B:618:CLA:HMA1	2.04	0.40
26:B:612:CLA:H51	26:B:612:CLA:H8	1.96	0.40
3:C:444:HIS:CE1	26:C:517:CLA:NA	2.89	0.40
26:D:401:CLA:H202	26:D:401:CLA:H162	1.90	0.40
13:M:15:ILE:HD13	13:M:15:ILE:HA	1.94	0.40
7:N:193:PHE:HD2	26:N:318:CLA:HMC1	1.86	0.40
39:S:302:CHL:HBA2	39:S:302:CHL:H11	1.86	0.40
26:S:308:CLA:C3C	37:S:317:LHG:HC61	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:159:THR:O	2:b:180:PRO:HB3	2.22	0.40
2:b:172:TYR:CE1	2:b:283:GLU:HB2	2.56	0.40
26:b:611:CLA:H11	26:b:613:CLA:ND	2.36	0.40
3:c:337:LEU:HD23	3:c:337:LEU:HA	1.90	0.40
7:n:143:VAL:HG11	23:y:25:LEU:HD12	2.02	0.40
16:q:10:GLY:HA2	16:q:11:PRO:HD3	1.83	0.40
20:u:4:ARG:HB3	20:u:27:ARG:O	2.21	0.40
39:y:305:CHL:HBB1	26:y:313:CLA:CMB	2.50	0.40
29:A:410:SQD:H242	37:D:410:LHG:H121	2.04	0.40
26:C:504:CLA:H171	24:Z:20:LEU:HD12	2.04	0.40
5:E:20:ILE:HD13	5:E:20:ILE:HA	1.91	0.40
7:G:83:GLU:O	7:G:87:ARG:HG3	2.21	0.40
8:H:30:TYR:HE1	17:R:50:ILE:HA	1.85	0.40
7:N:145:GLY:HA2	39:N:311:CHL:HAC1	2.02	0.40
42:R:305:NEX:H222	26:R:308:CLA:CHC	2.51	0.40
18:S:86:MET:SD	26:S:314:CLA:HAB	2.62	0.40
18:S:99:ASN:HD22	18:S:109:ALA:CB	2.28	0.40
18:S:163:LYS:HD2	18:S:163:LYS:HA	1.64	0.40
18:S:170:PHE:HB3	26:S:314:CLA:HMD1	2.04	0.40
23:Y:135:MET:SD	23:Y:138:ILE:HD11	2.62	0.40
26:Y:305:CLA:H91	26:Y:305:CLA:H111	1.81	0.40
1:a:153:ALA:HB1	26:a:411:CLA:HED1	2.03	0.40
2:b:139:PHE:HB2	26:b:614:CLA:C1D	2.52	0.40
26:b:601:CLA:H92	26:b:601:CLA:H61	1.79	0.40
26:c:504:CLA:H152	26:c:508:CLA:OBD	2.20	0.40
4:d:182:ILE:HG23	26:d:404:CLA:HHD	2.03	0.40
4:d:321:LEU:O	4:d:325:ILE:HG13	2.22	0.40
7:n:145:GLY:HA2	39:n:307:CHL:HAC1	2.03	0.40
15:p:51:ASP:HB2	15:p:57:SER:HB2	2.03	0.40
18:s:131:ILE:HG22	18:s:133:ILE:H	1.87	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	332/353 (94%)	328 (99%)	4 (1%)	0	100	100
1	a	332/353 (94%)	327 (98%)	5 (2%)	0	100	100
2	B	483/508 (95%)	476 (99%)	7 (1%)	0	100	100
2	b	483/508 (95%)	477 (99%)	6 (1%)	0	100	100
3	C	445/473 (94%)	437 (98%)	8 (2%)	0	100	100
3	c	445/473 (94%)	438 (98%)	7 (2%)	0	100	100
4	D	339/353 (96%)	332 (98%)	7 (2%)	0	100	100
4	d	339/353 (96%)	332 (98%)	7 (2%)	0	100	100
5	E	72/83 (87%)	71 (99%)	1 (1%)	0	100	100
5	e	72/83 (87%)	71 (99%)	1 (1%)	0	100	100
6	F	28/39 (72%)	28 (100%)	0	0	100	100
6	f	28/39 (72%)	28 (100%)	0	0	100	100
7	G	209/267 (78%)	206 (99%)	3 (1%)	0	100	100
7	N	200/267 (75%)	195 (98%)	5 (2%)	0	100	100
7	g	209/267 (78%)	206 (99%)	3 (1%)	0	100	100
7	n	200/267 (75%)	195 (98%)	5 (2%)	0	100	100
8	H	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
8	h	57/73 (78%)	55 (96%)	2 (4%)	0	100	100
9	I	31/36 (86%)	31 (100%)	0	0	100	100
9	i	31/36 (86%)	31 (100%)	0	0	100	100
10	J	33/40 (82%)	33 (100%)	0	0	100	100
10	j	33/40 (82%)	33 (100%)	0	0	100	100
11	K	35/61 (57%)	35 (100%)	0	0	100	100
11	k	35/61 (57%)	35 (100%)	0	0	100	100
12	L	33/38 (87%)	33 (100%)	0	0	100	100
12	l	33/38 (87%)	33 (100%)	0	0	100	100
13	M	29/34 (85%)	28 (97%)	1 (3%)	0	100	100
13	m	29/34 (85%)	28 (97%)	1 (3%)	0	100	100
14	O	239/332 (72%)	228 (95%)	11 (5%)	0	100	100
14	o	239/332 (72%)	228 (95%)	11 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	P	169/263 (64%)	161 (95%)	8 (5%)	0	100	100
15	p	169/263 (64%)	162 (96%)	7 (4%)	0	100	100
16	Q	144/224 (64%)	136 (94%)	8 (6%)	0	100	100
16	q	144/224 (64%)	136 (94%)	8 (6%)	0	100	100
17	R	218/290 (75%)	210 (96%)	8 (4%)	0	100	100
17	r	218/290 (75%)	211 (97%)	7 (3%)	0	100	100
18	S	212/280 (76%)	204 (96%)	8 (4%)	0	100	100
18	s	212/280 (76%)	203 (96%)	9 (4%)	0	100	100
19	T	30/33 (91%)	29 (97%)	1 (3%)	0	100	100
19	t	30/33 (91%)	29 (97%)	1 (3%)	0	100	100
20	U	26/103 (25%)	24 (92%)	2 (8%)	0	100	100
20	u	26/103 (25%)	23 (88%)	3 (12%)	0	100	100
21	W	52/133 (39%)	47 (90%)	4 (8%)	1 (2%)	6	4
21	w	52/133 (39%)	47 (90%)	4 (8%)	1 (2%)	6	4
22	X	37/116 (32%)	36 (97%)	1 (3%)	0	100	100
22	x	37/116 (32%)	36 (97%)	1 (3%)	0	100	100
23	Y	212/265 (80%)	206 (97%)	6 (3%)	0	100	100
23	y	212/265 (80%)	206 (97%)	6 (3%)	0	100	100
24	Z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
24	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
All	All	7448/9452 (79%)	7256 (97%)	190 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	W	86	ASP
21	w	86	ASP

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	270/285 (95%)	270 (100%)	0	100	100
1	a	270/285 (95%)	270 (100%)	0	100	100
2	B	384/402 (96%)	381 (99%)	3 (1%)	73	81
2	b	384/402 (96%)	381 (99%)	3 (1%)	73	81
3	C	351/373 (94%)	347 (99%)	4 (1%)	65	75
3	c	351/373 (94%)	344 (98%)	7 (2%)	48	62
4	D	273/283 (96%)	269 (98%)	4 (2%)	57	69
4	d	273/283 (96%)	271 (99%)	2 (1%)	76	83
5	E	66/73 (90%)	66 (100%)	0	100	100
5	e	66/73 (90%)	65 (98%)	1 (2%)	57	69
6	F	25/34 (74%)	25 (100%)	0	100	100
6	f	25/34 (74%)	25 (100%)	0	100	100
7	G	161/201 (80%)	159 (99%)	2 (1%)	63	74
7	N	154/201 (77%)	154 (100%)	0	100	100
7	g	161/201 (80%)	158 (98%)	3 (2%)	50	63
7	n	154/201 (77%)	153 (99%)	1 (1%)	78	85
8	H	49/61 (80%)	49 (100%)	0	100	100
8	h	49/61 (80%)	49 (100%)	0	100	100
9	I	30/33 (91%)	30 (100%)	0	100	100
9	i	30/33 (91%)	30 (100%)	0	100	100
10	J	26/30 (87%)	26 (100%)	0	100	100
10	j	26/30 (87%)	24 (92%)	2 (8%)	12	14
11	K	32/55 (58%)	32 (100%)	0	100	100
11	k	32/55 (58%)	32 (100%)	0	100	100
12	L	33/36 (92%)	33 (100%)	0	100	100
12	l	33/36 (92%)	33 (100%)	0	100	100
13	M	27/30 (90%)	27 (100%)	0	100	100
13	m	27/30 (90%)	27 (100%)	0	100	100
14	O	200/268 (75%)	195 (98%)	5 (2%)	42	54
14	o	200/268 (75%)	194 (97%)	6 (3%)	36	48
15	P	139/210 (66%)	135 (97%)	4 (3%)	37	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	p	139/210 (66%)	134 (96%)	5 (4%)	31	42
16	Q	124/178 (70%)	121 (98%)	3 (2%)	43	56
16	q	124/178 (70%)	121 (98%)	3 (2%)	43	56
17	R	174/225 (77%)	170 (98%)	4 (2%)	44	57
17	r	174/225 (77%)	170 (98%)	4 (2%)	44	57
18	S	165/219 (75%)	160 (97%)	5 (3%)	36	48
18	s	165/219 (75%)	160 (97%)	5 (3%)	36	48
19	T	29/30 (97%)	29 (100%)	0	100	100
19	t	29/30 (97%)	28 (97%)	1 (3%)	32	45
20	U	23/82 (28%)	23 (100%)	0	100	100
20	u	23/82 (28%)	23 (100%)	0	100	100
21	W	47/102 (46%)	47 (100%)	0	100	100
21	w	47/102 (46%)	47 (100%)	0	100	100
22	X	33/92 (36%)	33 (100%)	0	100	100
22	x	33/92 (36%)	33 (100%)	0	100	100
23	Y	168/209 (80%)	166 (99%)	2 (1%)	63	74
23	y	168/209 (80%)	168 (100%)	0	100	100
24	Z	53/54 (98%)	51 (96%)	2 (4%)	29	41
24	z	53/54 (98%)	51 (96%)	2 (4%)	29	41
All	All	6072/7532 (81%)	5989 (99%)	83 (1%)	57	70

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	85	ILE
2	B	122	ILE
2	B	240	SER
3	C	28	GLN
3	C	261	ARG
3	C	289	PHE
3	C	378	SER
4	D	90	LEU
4	D	227	ASP
4	D	243	THR
4	D	264	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	14	SER
7	G	32	SER
14	O	132	LYS
14	O	133	LYS
14	O	150	LYS
14	O	200	GLN
14	O	219	SER
15	P	24	ASP
15	P	108	VAL
15	P	112	ASN
15	P	116	SER
16	Q	8	LYS
16	Q	48	THR
16	Q	103	LYS
17	R	27	SER
17	R	89	ILE
17	R	117	THR
17	R	177	LYS
18	S	23	LEU
18	S	52	GLU
18	S	99	ASN
18	S	105	CYS
18	S	160	PHE
23	Y	15	ILE
23	Y	175	GLU
24	Z	31	ASP
24	Z	40	VAL
2	b	122	ILE
2	b	128	THR
2	b	422	ARG
3	c	28	GLN
3	c	99	VAL
3	c	221	GLU
3	c	261	ARG
3	c	287	CYS
3	c	289	PHE
3	c	378	SER
4	d	12	LYS
4	d	90	LEU
5	e	20	ILE
7	g	14	SER
7	g	32	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	g	123	SER
10	j	7	ARG
10	j	20	LEU
7	n	153	GLU
14	o	132	LYS
14	o	133	LYS
14	o	150	LYS
14	o	200	GLN
14	o	219	SER
14	o	290	SER
15	p	24	ASP
15	p	108	VAL
15	p	112	ASN
15	p	116	SER
15	p	120	GLU
16	q	8	LYS
16	q	48	THR
16	q	64	VAL
17	r	27	SER
17	r	89	ILE
17	r	117	THR
17	r	177	LYS
18	s	23	LEU
18	s	52	GLU
18	s	67	LYS
18	s	105	CYS
18	s	160	PHE
19	t	25	GLU
24	z	31	ASP
24	z	40	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	165	GLN
1	A	234	ASN
1	A	304	GLN
1	A	315	ASN
2	B	157	HIS
2	B	343	HIS
2	B	394	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	68	ASN
4	D	83	ASN
4	D	142	ASN
4	D	263	ASN
4	D	332	GLN
4	D	336	HIS
7	G	209	ASN
12	L	7	ASN
14	O	111	GLN
14	O	158	ASN
15	P	35	ASN
15	P	52	ASN
15	P	106	ASN
15	P	112	ASN
18	S	99	ASN
18	S	104	ASN
23	Y	31	ASN
24	Z	38	ASN
1	a	108	ASN
1	a	165	GLN
1	a	234	ASN
1	a	304	GLN
1	a	315	ASN
3	c	68	ASN
3	c	332	GLN
4	d	83	ASN
4	d	142	ASN
4	d	263	ASN
4	d	332	GLN
6	f	45	GLN
7	g	209	ASN
13	m	4	ASN
14	o	111	GLN
15	p	35	ASN
15	p	52	ASN
17	r	226	ASN
18	s	192	ASN
18	s	228	ASN
23	y	31	ASN
24	z	38	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 332 ligands modelled in this entry, 6 are monoatomic - leaving 326 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	$\# Z > 2$
26	CLA	S	308	37	53,57,73	1.38	9 (16%)	62,93,113	1.35	5 (8%)
26	CLA	c	518	3	69,73,73	1.22	7 (10%)	83,113,113	1.37	5 (6%)
42	NEX	G	315	-	38,46,46	1.55	8 (21%)	50,70,70	2.36	15 (30%)
26	CLA	R	317	17	53,57,73	1.37	8 (15%)	62,93,113	1.42	9 (14%)
36	LMT	d	406	-	36,36,36	0.57	0	47,47,47	0.68	0
26	CLA	G	314	7	69,73,73	1.26	10 (14%)	83,113,113	1.23	7 (8%)
26	CLA	c	515	3	69,73,73	1.20	7 (10%)	83,113,113	1.29	6 (7%)
26	CLA	Y	305	23	69,73,73	1.22	8 (11%)	83,113,113	1.17	10 (12%)
26	CLA	b	605	2	69,73,73	1.22	8 (11%)	83,113,113	1.22	7 (8%)
26	CLA	B	605	43	69,73,73	1.23	8 (11%)	83,113,113	1.27	5 (6%)
26	CLA	b	610	2	69,73,73	1.22	8 (11%)	83,113,113	1.24	8 (9%)
37	LHG	g	301	26	48,48,48	0.52	0	51,54,54	0.52	0
40	LUT	Y	315	-	42,43,43	0.48	0	51,60,60	0.87	0
28	BCR	b	619	-	41,41,41	0.33	0	56,56,56	0.56	0
39	CHL	n	311	43	49,58,74	2.30	13 (26%)	38,94,114	3.08	17 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	LUT	g	310	-	42,43,43	0.46	0	51,60,60	0.75	0
39	CHL	S	316	18	51,60,74	2.32	14 (27%)	42,97,114	3.00	17 (40%)
26	CLA	D	401	43	69,73,73	1.21	8 (11%)	83,113,113	1.21	7 (8%)
26	CLA	C	505	3	69,73,73	1.22	8 (11%)	83,113,113	1.22	7 (8%)
39	CHL	Y	307	23	65,74,74	2.04	14 (21%)	59,114,114	2.50	18 (30%)
39	CHL	r	316	43	49,58,74	2.28	12 (24%)	38,94,114	3.13	18 (47%)
33	DGD	C	509	-	56,56,67	0.69	0	70,70,81	0.75	1 (1%)
37	LHG	N	301	26	48,48,48	0.52	0	51,54,54	0.47	0
28	BCR	t	101	-	41,41,41	0.32	0	56,56,56	1.40	10 (17%)
36	LMT	D	402	-	36,36,36	0.57	0	47,47,47	0.68	0
26	CLA	g	315	37	53,57,73	1.41	9 (16%)	62,93,113	1.38	7 (11%)
39	CHL	Y	318	-	49,58,74	2.31	13 (26%)	38,94,114	3.11	18 (47%)
26	CLA	y	304	37	69,73,73	1.24	7 (10%)	83,113,113	1.24	6 (7%)
26	CLA	R	313	17	69,73,73	1.21	8 (11%)	83,113,113	1.23	8 (9%)
28	BCR	d	401	-	41,41,41	0.33	0	56,56,56	0.72	1 (1%)
27	PHO	d	407	-	58,69,69	1.98	10 (17%)	56,99,99	1.55	6 (10%)
40	LUT	n	317	-	42,43,43	0.48	0	51,60,60	0.84	1 (1%)
28	BCR	b	615	-	41,41,41	0.32	0	56,56,56	0.52	0
26	CLA	b	608	43	69,73,73	1.23	8 (11%)	83,113,113	1.25	6 (7%)
26	CLA	B	613	-	69,73,73	1.24	8 (11%)	83,113,113	1.23	7 (8%)
26	CLA	n	312	43	53,57,73	1.43	9 (16%)	62,93,113	1.27	7 (11%)
27	PHO	D	403	-	58,69,69	1.97	10 (17%)	56,99,99	1.55	7 (12%)
33	DGD	b	620	-	63,63,67	0.58	0	77,77,81	0.79	1 (1%)
26	CLA	c	516	3	69,73,73	1.24	9 (13%)	83,113,113	1.24	9 (10%)
26	CLA	s	305	18	53,57,73	1.38	7 (13%)	62,93,113	1.29	6 (9%)
28	BCR	j	101	-	41,41,41	0.31	0	56,56,56	0.68	1 (1%)
26	CLA	D	406	4	69,73,73	1.21	7 (10%)	83,113,113	1.24	6 (7%)
39	CHL	R	318	23	47,56,74	2.33	14 (29%)	37,92,114	3.10	18 (48%)
42	NEX	Y	304	-	38,46,46	1.59	9 (23%)	50,70,70	2.15	11 (22%)
37	LHG	D	410	-	36,36,48	0.61	0	39,42,54	0.59	0
26	CLA	S	314	18	53,57,73	1.36	7 (13%)	62,93,113	1.16	5 (8%)
26	CLA	B	609	2	69,73,73	1.23	8 (11%)	83,113,113	1.26	8 (9%)
37	LHG	l	101	-	48,48,48	0.52	0	51,54,54	0.54	0
26	CLA	r	310	17	53,57,73	1.34	6 (11%)	62,93,113	1.29	5 (8%)
26	CLA	G	304	7	53,57,73	1.40	7 (13%)	62,93,113	1.39	7 (11%)
35	OEX	a	408	1,43,3	0,15,15	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PL9	A	408	-	22,22,55	1.24	3 (13%)	28,29,69	1.48	6 (21%)
34	LMG	D	404	-	46,46,55	0.60	0	54,54,63	0.69	1 (1%)
39	CHL	y	314	23	65,74,74	2.04	15 (23%)	59,114,114	2.51	18 (30%)
26	CLA	B	601	2	69,73,73	1.23	8 (11%)	83,113,113	1.18	7 (8%)
26	CLA	y	316	23	69,73,73	1.23	8 (11%)	83,113,113	1.31	7 (8%)
41	XAT	G	320	-	39,47,47	1.13	5 (12%)	54,74,74	2.50	18 (33%)
34	LMG	c	509	-	51,51,55	0.52	0	59,59,63	0.60	0
26	CLA	G	307	7	69,73,73	1.22	9 (13%)	83,113,113	1.11	7 (8%)
26	CLA	G	319	7	53,57,73	1.40	8 (15%)	62,93,113	1.36	6 (9%)
37	LHG	D	407	-	42,42,48	0.56	0	45,48,54	0.50	0
34	LMG	W	201	-	48,48,55	0.57	0	56,56,63	0.63	1 (1%)
26	CLA	B	615	2	69,73,73	1.30	8 (11%)	83,113,113	1.45	9 (10%)
40	LUT	Y	309	-	42,43,43	0.50	0	51,60,60	0.86	1 (1%)
26	CLA	c	508	43	69,73,73	1.25	9 (13%)	83,113,113	1.34	6 (7%)
42	NEX	r	302	-	38,46,46	1.56	9 (23%)	50,70,70	2.27	16 (32%)
39	CHL	G	311	7	49,58,74	2.33	14 (28%)	38,94,114	3.10	17 (44%)
26	CLA	N	309	7	53,57,73	1.39	6 (11%)	62,93,113	1.33	5 (8%)
34	LMG	b	622	-	51,51,55	0.52	0	59,59,63	0.65	0
30	PL9	a	407	-	22,22,55	1.25	3 (13%)	28,29,69	1.51	6 (21%)
39	CHL	n	307	-	49,58,74	2.28	13 (26%)	38,94,114	3.06	17 (44%)
28	BCR	J	101	-	41,41,41	0.32	0	56,56,56	0.67	1 (1%)
26	CLA	C	508	3	69,73,73	1.23	8 (11%)	83,113,113	1.24	9 (10%)
26	CLA	d	403	4	69,73,73	1.22	8 (11%)	83,113,113	1.24	7 (8%)
28	BCR	b	603	-	41,41,41	0.36	0	56,56,56	0.74	0
42	NEX	g	306	-	38,46,46	1.55	9 (23%)	50,70,70	2.36	14 (28%)
26	CLA	S	310	-	53,57,73	1.44	9 (16%)	62,93,113	1.29	7 (11%)
26	CLA	C	506	3	69,73,73	1.20	9 (13%)	83,113,113	1.22	6 (7%)
37	LHG	s	309	26	48,48,48	0.52	0	51,54,54	0.52	0
33	DGD	C	510	-	63,63,67	0.63	0	77,77,81	0.69	0
37	LHG	n	301	26	48,48,48	0.51	0	51,54,54	0.47	0
26	CLA	C	515	3	69,73,73	1.22	8 (11%)	83,113,113	1.27	8 (9%)
26	CLA	s	311	18	53,57,73	1.40	8 (15%)	62,93,113	1.26	7 (11%)
26	CLA	r	315	17	53,57,73	1.37	8 (15%)	62,93,113	1.40	8 (12%)
26	CLA	C	521	43	69,73,73	1.21	8 (11%)	83,113,113	1.23	7 (8%)
39	CHL	N	310	7	47,56,74	2.36	14 (29%)	37,92,114	3.05	17 (45%)
26	CLA	B	611	2	69,73,73	1.23	9 (13%)	83,113,113	1.22	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	s	314	18	53,57,73	1.38	7 (13%)	62,93,113	1.36	8 (12%)
26	CLA	s	304	18	53,57,73	1.39	8 (15%)	62,93,113	1.42	6 (9%)
29	SQD	A	410	-	49,50,54	0.80	1 (2%)	58,61,65	1.03	3 (5%)
39	CHL	n	306	7	49,58,74	2.35	13 (26%)	38,94,114	3.16	18 (47%)
26	CLA	r	311	43	53,57,73	1.41	10 (18%)	62,93,113	1.42	9 (14%)
39	CHL	Y	314	43	49,58,74	2.29	14 (28%)	38,94,114	3.06	17 (44%)
35	OEX	C	501	1,43,3	0,15,15	-	-	-	-	-
29	SQD	a	403	-	53,54,54	0.78	1 (1%)	62,65,65	0.99	3 (4%)
26	CLA	B	606	2	69,73,73	1.21	8 (11%)	83,113,113	1.16	6 (7%)
42	NEX	n	313	-	38,46,46	1.55	9 (23%)	50,70,70	2.23	11 (22%)
29	SQD	a	413	-	49,50,54	0.79	1 (2%)	58,61,65	1.02	3 (5%)
26	CLA	S	303	18	53,57,73	1.39	9 (16%)	62,93,113	1.32	6 (9%)
26	CLA	B	612	43	69,73,73	1.23	8 (11%)	83,113,113	1.25	7 (8%)
26	CLA	y	309	23	69,73,73	1.22	8 (11%)	83,113,113	1.14	8 (9%)
26	CLA	b	609	2	69,73,73	1.19	7 (10%)	83,113,113	1.33	6 (7%)
39	CHL	n	319	7	49,58,74	2.33	14 (28%)	38,94,114	3.11	17 (44%)
26	CLA	r	305	17	53,57,73	1.41	7 (13%)	62,93,113	1.31	5 (8%)
33	DGD	Y	303	-	44,44,67	0.68	0	58,58,81	0.87	2 (3%)
26	CLA	d	411	43	53,57,73	1.43	9 (16%)	62,93,113	1.25	8 (12%)
33	DGD	C	513	-	63,63,67	0.63	0	77,77,81	0.70	0
28	BCR	C	514	-	41,41,41	0.37	0	56,56,56	0.74	2 (3%)
39	CHL	N	316	7	49,58,74	2.36	13 (26%)	38,94,114	3.17	18 (47%)
26	CLA	C	504	3	69,73,73	1.22	8 (11%)	83,113,113	1.31	5 (6%)
26	CLA	n	303	7	69,73,73	1.20	7 (10%)	83,113,113	1.08	7 (8%)
39	CHL	s	316	-	49,58,74	2.39	13 (26%)	38,94,114	3.12	17 (44%)
26	CLA	g	318	7	53,57,73	1.40	8 (15%)	62,93,113	1.38	7 (11%)
26	CLA	s	307	18	53,57,73	1.39	8 (15%)	62,93,113	1.33	6 (9%)
28	BCR	a	404	-	41,41,41	0.33	0	56,56,56	0.51	0
39	CHL	Y	302	23	65,74,74	2.03	15 (23%)	59,114,114	2.58	18 (30%)
26	CLA	C	520	3	63,70,73	1.29	6 (9%)	73,103,113	0.98	3 (4%)
39	CHL	g	311	7	65,74,74	2.04	15 (23%)	59,114,114	2.52	18 (30%)
39	CHL	Y	317	43	49,58,74	2.29	13 (26%)	38,94,114	3.08	17 (44%)
32	BCT	A	411	31	2,3,3	1.16	0	2,3,3	1.79	1 (50%)
29	SQD	A	407	-	53,54,54	0.78	1 (1%)	62,65,65	0.99	4 (6%)
26	CLA	s	315	18	53,57,73	1.36	7 (13%)	62,93,113	1.16	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	A	406	-	41,41,41	0.32	0	56,56,56	0.51	0
29	SQD	b	621	-	53,54,54	0.78	1 (1%)	62,65,65	0.85	2 (3%)
29	SQD	W	202	-	32,33,54	1.03	2 (6%)	41,44,65	1.14	4 (9%)
26	CLA	r	303	17	53,57,73	1.40	9 (16%)	62,93,113	1.30	5 (8%)
33	DGD	c	501	-	63,63,67	0.63	0	77,77,81	0.71	0
39	CHL	S	312	-	48,57,74	2.36	13 (27%)	38,93,114	3.13	16 (42%)
26	CLA	a	402	1	64,68,73	1.25	9 (14%)	77,107,113	1.21	7 (9%)
26	CLA	N	307	7	69,73,73	1.22	7 (10%)	83,113,113	1.24	7 (8%)
26	CLA	s	301	37	53,57,73	1.38	9 (16%)	62,93,113	1.36	5 (8%)
40	LUT	S	306	-	42,43,43	0.48	0	51,60,60	0.88	1 (1%)
37	LHG	r	312	26	48,48,48	0.51	0	51,54,54	0.52	0
26	CLA	s	310	-	53,57,73	1.43	8 (15%)	62,93,113	1.30	7 (11%)
30	PL9	d	408	-	55,55,55	1.38	7 (12%)	68,69,69	1.51	10 (14%)
26	CLA	Y	310	23	53,57,73	1.40	7 (13%)	62,93,113	1.28	6 (9%)
39	CHL	N	311	-	49,58,74	2.28	13 (26%)	38,94,114	3.04	17 (44%)
33	DGD	c	519	-	63,63,67	0.62	0	77,77,81	0.70	0
28	BCR	D	405	-	41,41,41	0.33	0	56,56,56	0.70	1 (1%)
34	LMG	C	503	-	51,51,55	0.48	0	59,59,63	0.64	0
37	LHG	G	312	26	48,48,48	0.52	0	51,54,54	0.52	0
26	CLA	N	312	7	69,73,73	1.20	7 (10%)	83,113,113	1.08	7 (8%)
26	CLA	g	308	7	53,57,73	1.40	9 (16%)	62,93,113	1.38	6 (9%)
26	CLA	R	307	17	53,57,73	2.71	11 (20%)	62,93,113	1.43	5 (8%)
28	BCR	h	101	-	41,41,41	0.33	0	56,56,56	0.68	0
39	CHL	N	303	-	65,74,74	2.00	15 (23%)	59,114,114	2.49	18 (30%)
40	LUT	N	314	-	42,43,43	0.47	0	51,60,60	0.84	0
37	LHG	R	303	26	48,48,48	0.51	0	51,54,54	0.52	0
26	CLA	c	504	3	69,73,73	1.22	8 (11%)	83,113,113	1.28	9 (10%)
26	CLA	d	404	4	69,73,73	1.21	8 (11%)	83,113,113	1.15	5 (6%)
41	XAT	g	320	-	39,47,47	1.13	4 (10%)	54,74,74	2.49	19 (35%)
26	CLA	S	304	18	53,57,73	1.38	7 (13%)	62,93,113	1.28	6 (9%)
39	CHL	G	301	-	49,58,74	2.38	13 (26%)	38,94,114	3.08	16 (42%)
26	CLA	B	607	43	69,73,73	1.21	8 (11%)	83,113,113	1.24	7 (8%)
40	LUT	n	314	-	42,43,43	0.48	0	51,60,60	0.85	0
40	LUT	R	311	-	42,43,43	0.53	0	51,60,60	1.04	3 (5%)
26	CLA	b	602	2	69,73,73	1.21	8 (11%)	83,113,113	1.25	6 (7%)
28	BCR	B	608	-	41,41,41	0.31	0	56,56,56	0.52	0
26	CLA	B	617	2	69,73,73	1.21	8 (11%)	83,113,113	1.26	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	Y	316	43	53,57,73	1.44	8 (15%)	62,93,113	1.29	8 (12%)
26	CLA	s	306	18	53,57,73	1.39	8 (15%)	62,93,113	1.30	6 (9%)
26	CLA	C	512	3	69,73,73	1.20	7 (10%)	83,113,113	1.30	6 (7%)
26	CLA	N	313	7	53,57,73	1.40	9 (16%)	62,93,113	1.36	6 (9%)
26	CLA	S	315	18	53,57,73	1.39	8 (15%)	62,93,113	1.30	6 (9%)
26	CLA	G	313	37	53,57,73	1.42	9 (16%)	62,93,113	1.39	7 (11%)
26	CLA	R	310	17	53,57,73	1.34	6 (11%)	62,93,113	1.29	5 (8%)
40	LUT	g	316	-	42,43,43	0.49	0	51,60,60	0.95	0
26	CLA	r	306	17	69,73,73	1.20	9 (13%)	83,113,113	1.11	7 (8%)
28	BCR	H	101	-	41,41,41	0.33	0	56,56,56	0.69	0
26	CLA	b	601	2	69,73,73	1.21	8 (11%)	83,113,113	1.18	7 (8%)
39	CHL	R	315	43	49,58,74	2.31	15 (30%)	38,94,114	3.08	19 (50%)
26	CLA	B	610	2	69,73,73	1.20	9 (13%)	83,113,113	1.26	7 (8%)
28	BCR	K	101	-	41,41,41	0.33	0	56,56,56	0.87	3 (5%)
26	CLA	R	309	17	53,57,73	1.41	8 (15%)	62,93,113	1.31	7 (11%)
26	CLA	C	519	3	53,57,73	1.38	9 (16%)	62,93,113	1.38	7 (11%)
26	CLA	n	309	7	53,57,73	1.39	6 (11%)	62,93,113	1.33	5 (8%)
37	LHG	D	408	-	48,48,48	0.51	0	51,54,54	0.58	0
26	CLA	C	516	43	69,73,73	1.24	7 (10%)	83,113,113	1.32	6 (7%)
37	LHG	d	409	-	48,48,48	0.51	0	51,54,54	0.57	0
39	CHL	G	303	-	49,58,74	2.31	14 (28%)	38,94,114	3.01	18 (47%)
26	CLA	b	614	43	69,73,73	1.24	7 (10%)	83,113,113	1.28	8 (9%)
39	CHL	S	302	-	49,58,74	2.38	14 (28%)	38,94,114	3.12	17 (44%)
37	LHG	S	317	26	48,48,48	0.52	0	51,54,54	0.52	0
42	NEX	S	305	-	38,46,46	1.56	9 (23%)	50,70,70	2.34	16 (32%)
40	LUT	r	307	-	42,43,43	0.53	0	51,60,60	1.05	3 (5%)
40	LUT	G	316	-	42,43,43	0.49	0	51,60,60	0.96	0
26	CLA	y	313	43	53,57,73	1.45	8 (15%)	62,93,113	1.29	8 (12%)
26	CLA	b	613	2	69,73,73	1.22	9 (13%)	83,113,113	1.24	8 (9%)
26	CLA	b	604	-	69,73,73	1.25	8 (11%)	83,113,113	1.23	8 (9%)
33	DGD	y	308	-	44,44,67	0.69	0	58,58,81	0.88	2 (3%)
26	CLA	b	618	2	69,73,73	1.23	8 (11%)	83,113,113	1.25	8 (9%)
40	LUT	N	305	-	42,43,43	0.48	0	51,60,60	0.81	0
26	CLA	S	311	18	53,57,73	1.37	8 (15%)	62,93,113	1.36	8 (12%)
26	CLA	C	517	3	69,73,73	1.23	7 (10%)	83,113,113	1.27	6 (7%)
26	CLA	Y	312	23	69,73,73	1.24	7 (10%)	83,113,113	1.26	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	XAT	g	309	-	39,47,47	1.14	4 (10%)	54,74,74	2.32	12 (22%)
26	CLA	N	318	7	53,57,73	1.39	9 (16%)	62,93,113	1.42	5 (8%)
34	LMG	c	512	-	51,51,55	0.48	0	59,59,63	0.64	0
33	DGD	c	517	-	56,56,67	0.69	0	70,70,81	0.76	1 (1%)
26	CLA	A	403	1	69,73,73	1.22	8 (11%)	83,113,113	1.16	7 (8%)
39	CHL	G	305	-	49,58,74	2.36	14 (28%)	38,94,114	3.00	18 (47%)
26	CLA	c	514	43	69,73,73	1.21	9 (13%)	83,113,113	1.23	9 (10%)
41	XAT	n	316	-	39,47,47	1.14	4 (10%)	54,74,74	2.30	13 (24%)
40	LUT	y	318	-	42,43,43	0.49	0	51,60,60	0.86	1 (1%)
26	CLA	r	317	37	53,57,73	1.41	8 (15%)	62,93,113	1.39	6 (9%)
26	CLA	n	305	7	69,73,73	1.22	7 (10%)	83,113,113	1.24	7 (8%)
42	NEX	N	302	-	38,46,46	1.57	9 (23%)	50,70,70	2.26	11 (22%)
26	CLA	N	308	43	53,57,73	1.43	9 (16%)	62,93,113	1.27	7 (11%)
39	CHL	g	312	7	49,58,74	2.34	13 (26%)	38,94,114	3.09	17 (44%)
26	CLA	n	304	7	53,57,73	1.41	10 (18%)	62,93,113	1.38	7 (11%)
26	CLA	G	302	-	53,57,73	1.42	8 (15%)	62,93,113	1.33	6 (9%)
39	CHL	N	317	7	49,58,74	2.33	14 (28%)	38,94,114	3.12	17 (44%)
26	CLA	Y	308	23	69,73,73	1.21	6 (8%)	83,113,113	1.28	10 (12%)
39	CHL	y	303	23	65,74,74	2.03	15 (23%)	59,114,114	2.58	18 (30%)
26	CLA	c	506	3	63,70,73	1.29	6 (9%)	73,103,113	0.98	3 (4%)
39	CHL	G	309	7	47,56,74	2.44	14 (29%)	37,92,114	3.05	17 (45%)
26	CLA	R	302	17	53,57,73	1.38	8 (15%)	62,93,113	1.57	12 (19%)
26	CLA	g	302	-	53,57,73	1.42	9 (16%)	62,93,113	1.32	6 (9%)
39	CHL	s	317	-	49,58,74	2.35	14 (28%)	38,94,114	3.11	17 (44%)
26	CLA	R	316	17	53,57,73	1.39	8 (15%)	62,93,113	1.30	5 (8%)
39	CHL	r	301	23	47,56,74	2.34	14 (29%)	37,92,114	3.12	18 (48%)
37	LHG	Y	306	26	48,48,48	0.51	0	51,54,54	0.52	0
33	DGD	B	620	-	63,63,67	0.58	0	77,77,81	0.77	1 (1%)
42	NEX	R	305	-	38,46,46	1.57	9 (23%)	50,70,70	2.26	16 (32%)
26	CLA	g	317	7	69,73,73	1.22	9 (13%)	83,113,113	1.11	7 (8%)
39	CHL	n	318	-	65,74,74	2.02	15 (23%)	59,114,114	2.47	18 (30%)
26	CLA	N	319	37	53,57,73	1.40	8 (15%)	62,93,113	1.37	6 (9%)
39	CHL	y	305	43	49,58,74	2.29	13 (26%)	38,94,114	3.08	17 (44%)
34	LMG	B	622	-	51,51,55	0.52	0	59,59,63	0.65	0
26	CLA	r	313	17	53,57,73	1.37	7 (13%)	62,93,113	1.56	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	LUT	S	301	-	42,43,43	0.51	0	51,60,60	0.74	0
28	BCR	k	101	-	41,41,41	0.34	0	56,56,56	0.86	3 (5%)
26	CLA	b	611	2	69,73,73	1.30	9 (13%)	83,113,113	1.46	10 (12%)
26	CLA	S	309	18	53,57,73	1.39	8 (15%)	62,93,113	1.41	6 (9%)
26	CLA	a	409	43	69,73,73	1.21	7 (10%)	83,113,113	1.20	6 (7%)
32	BCT	a	405	31	2,3,3	0.89	0	2,3,3	3.23	2 (100%)
26	CLA	B	603	2	69,73,73	1.20	8 (11%)	83,113,113	1.24	6 (7%)
26	CLA	b	607	2	69,73,73	1.23	9 (13%)	83,113,113	1.20	8 (9%)
38	HEM	e	101	6,5	50,50,50	1.38	7 (14%)	66,82,82	1.26	7 (10%)
26	CLA	B	602	2	69,73,73	1.21	9 (13%)	83,113,113	1.21	7 (8%)
26	CLA	r	314	17	69,73,73	1.21	8 (11%)	83,113,113	1.23	8 (9%)
30	PL9	D	411	-	55,55,55	1.37	7 (12%)	68,69,69	1.52	10 (14%)
39	CHL	y	302	-	49,58,74	2.32	14 (28%)	38,94,114	3.10	18 (47%)
39	CHL	S	313	-	49,58,74	2.35	14 (28%)	38,94,114	3.10	17 (44%)
39	CHL	N	304	43	49,58,74	2.30	13 (26%)	38,94,114	3.09	18 (47%)
39	CHL	s	313	-	48,57,74	2.36	13 (27%)	38,93,114	3.15	17 (44%)
26	CLA	c	520	3	69,73,73	1.22	8 (11%)	83,113,113	1.23	8 (9%)
26	CLA	a	411	1	69,73,73	1.22	9 (13%)	83,113,113	1.17	7 (8%)
26	CLA	G	317	7	53,57,73	1.39	9 (16%)	62,93,113	1.38	6 (9%)
28	BCR	T	101	-	41,41,41	0.32	0	56,56,56	1.46	10 (17%)
39	CHL	g	314	7	47,56,74	2.43	14 (29%)	37,92,114	3.05	17 (45%)
34	LMG	C	518	-	51,51,55	0.52	0	59,59,63	0.59	0
39	CHL	r	318	43	49,58,74	2.29	15 (30%)	38,94,114	3.08	19 (50%)
28	BCR	B	614	-	41,41,41	0.33	0	56,56,56	0.55	0
26	CLA	n	315	7	53,57,73	1.43	10 (18%)	62,93,113	1.39	6 (9%)
26	CLA	c	503	3	69,73,73	1.18	8 (11%)	83,113,113	1.23	7 (8%)
41	XAT	R	304	-	39,47,47	1.16	4 (10%)	54,74,74	2.22	13 (24%)
39	CHL	R	301	43	49,58,74	2.29	12 (24%)	38,94,114	3.14	19 (50%)
26	CLA	N	306	7	53,57,73	1.43	10 (18%)	62,93,113	1.40	6 (9%)
39	CHL	n	308	7	47,56,74	2.37	14 (29%)	37,92,114	3.04	17 (45%)
26	CLA	R	308	43	53,57,73	1.41	9 (16%)	62,93,113	1.41	9 (14%)
39	CHL	s	303	18	51,60,74	2.34	14 (27%)	42,97,114	3.01	16 (38%)
26	CLA	g	303	7	69,73,73	1.26	10 (14%)	83,113,113	1.22	7 (8%)
26	CLA	C	511	3	69,73,73	1.18	8 (11%)	83,113,113	1.23	7 (8%)
37	LHG	d	410	-	36,36,48	0.61	0	39,42,54	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	A	405	1	64,68,73	1.25	7 (10%)	77,107,113	1.23	7 (9%)
26	CLA	b	606	2	69,73,73	1.24	8 (11%)	83,113,113	1.23	8 (9%)
28	BCR	c	511	-	41,41,41	0.34	0	56,56,56	0.83	2 (3%)
26	CLA	n	310	37	53,57,73	1.42	8 (15%)	62,93,113	1.39	6 (9%)
26	CLA	g	305	7	53,57,73	1.42	9 (16%)	62,93,113	1.34	7 (11%)
26	CLA	B	616	2	69,73,73	1.20	7 (10%)	83,113,113	1.31	6 (7%)
28	BCR	C	502	-	41,41,41	0.36	0	56,56,56	0.87	2 (3%)
27	PHO	A	404	-	58,69,69	1.98	11 (18%)	56,99,99	1.49	8 (14%)
26	CLA	c	510	3	53,57,73	1.37	9 (16%)	62,93,113	1.39	7 (11%)
41	XAT	N	315	-	39,47,47	1.14	4 (10%)	54,74,74	2.32	15 (27%)
26	CLA	C	507	3	69,73,73	1.25	10 (14%)	83,113,113	1.29	7 (8%)
26	CLA	b	616	43	69,73,73	1.21	7 (10%)	83,113,113	1.24	7 (8%)
27	PHO	a	410	-	58,69,69	1.97	11 (18%)	56,99,99	1.47	8 (14%)
37	LHG	y	301	26	48,48,48	0.51	0	51,54,54	0.52	0
38	HEM	E	101	6,5	50,50,50	1.37	6 (12%)	66,82,82	1.25	7 (10%)
29	SQD	w	202	-	32,33,54	1.02	2 (6%)	41,44,65	1.14	3 (7%)
26	CLA	B	618	2	69,73,73	1.22	8 (11%)	83,113,113	1.22	8 (9%)
26	CLA	y	317	23	53,57,73	1.41	9 (16%)	62,93,113	1.29	6 (9%)
26	CLA	c	502	3	69,73,73	1.21	8 (11%)	83,113,113	1.21	6 (7%)
26	CLA	D	412	43	53,57,73	1.43	9 (16%)	62,93,113	1.26	8 (12%)
39	CHL	G	318	7	65,74,74	2.04	15 (23%)	59,114,114	2.52	18 (30%)
26	CLA	Y	311	23	53,57,73	1.37	8 (15%)	62,93,113	1.45	6 (9%)
26	CLA	b	612	2	69,73,73	1.27	9 (13%)	83,113,113	1.22	9 (10%)
26	CLA	c	513	3	69,73,73	1.22	6 (8%)	83,113,113	1.27	7 (8%)
37	LHG	d	402	-	42,42,48	0.57	0	45,48,54	0.49	0
39	CHL	g	313	-	49,58,74	2.39	13 (26%)	38,94,114	3.07	16 (42%)
40	LUT	s	312	-	42,43,43	0.49	0	51,60,60	0.90	1 (1%)
26	CLA	R	306	17	69,73,73	1.21	9 (13%)	83,113,113	1.12	7 (8%)
34	LMG	d	405	-	46,46,55	0.60	0	54,54,63	0.68	1 (1%)
26	CLA	r	308	17	53,57,73	1.39	8 (15%)	62,93,113	1.32	6 (9%)
26	CLA	S	307	18	53,57,73	1.41	9 (16%)	62,93,113	1.26	7 (11%)
26	CLA	Y	313	23	69,73,73	1.20	9 (13%)	83,113,113	1.33	9 (10%)
41	XAT	r	304	-	39,47,47	1.16	4 (10%)	54,74,74	2.20	12 (22%)
26	CLA	R	314	37	53,57,73	1.41	8 (15%)	62,93,113	1.39	6 (9%)
39	CHL	r	309	43	49,58,74	2.33	14 (28%)	38,94,114	3.05	16 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	SQD	B	621	-	53,54,54	0.79	1 (1%)	62,65,65	0.85	2 (3%)
42	NEX	y	307	-	38,46,46	1.59	9 (23%)	50,70,70	2.14	11 (22%)
26	CLA	D	409	4	69,73,73	1.21	8 (11%)	83,113,113	1.16	5 (6%)
40	LUT	G	308	-	42,43,43	0.47	0	51,60,60	0.74	0
42	NEX	s	302	-	38,46,46	1.56	9 (23%)	50,70,70	2.28	16 (32%)
26	CLA	Y	301	37	69,73,73	1.22	8 (11%)	83,113,113	1.26	6 (7%)
26	CLA	y	315	23	53,57,73	1.36	8 (15%)	62,93,113	1.44	7 (11%)
26	CLA	y	310	23	69,73,73	1.24	7 (10%)	83,113,113	1.27	7 (8%)
26	CLA	G	306	7	53,57,73	1.42	9 (16%)	62,93,113	1.34	6 (9%)
26	CLA	n	302	7	53,57,73	1.40	9 (16%)	62,93,113	1.41	5 (8%)
26	CLA	c	505	3	69,73,73	1.24	8 (11%)	83,113,113	1.30	6 (7%)
26	CLA	y	306	23	69,73,73	1.21	6 (8%)	83,113,113	1.27	9 (10%)
26	CLA	g	304	7	53,57,73	1.40	8 (15%)	62,93,113	1.36	6 (9%)
37	LHG	L	101	-	48,48,48	0.52	0	51,54,54	0.55	0
40	LUT	s	308	-	42,43,43	0.51	0	51,60,60	0.73	0
39	CHL	g	307	-	49,58,74	2.32	14 (28%)	38,94,114	2.99	18 (47%)
39	CHL	g	319	-	49,58,74	2.36	15 (30%)	38,94,114	3.02	18 (47%)
28	BCR	c	507	-	41,41,41	0.36	0	56,56,56	0.75	2 (3%)
39	CHL	y	312	43	49,58,74	2.28	14 (28%)	38,94,114	3.06	17 (44%)
41	XAT	G	310	-	39,47,47	1.14	4 (10%)	54,74,74	2.33	12 (22%)
39	CHL	R	312	43	49,58,74	2.32	14 (28%)	38,94,114	3.05	16 (42%)
26	CLA	B	604	2	69,73,73	1.27	9 (13%)	83,113,113	1.22	8 (9%)
34	LMG	w	201	-	48,48,55	0.58	0	56,56,63	0.65	1 (1%)
40	LUT	y	311	-	42,43,43	0.48	0	51,60,60	0.86	0
26	CLA	b	617	2	69,73,73	1.20	9 (13%)	83,113,113	1.25	7 (8%)
28	BCR	B	619	-	41,41,41	0.37	0	56,56,56	0.73	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
26	CLA	S	308	37	-	11/20/96/115	-
26	CLA	c	518	3	-	7/39/115/115	-
42	NEX	G	315	-	-	2/27/83/83	0/3/3/3
26	CLA	R	317	17	-	4/20/96/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LMT	d	406	-	-	7/21/61/61	0/2/2/2
26	CLA	G	314	7	-	7/39/115/115	-
26	CLA	c	515	3	-	12/39/115/115	-
26	CLA	Y	305	23	-	12/39/115/115	-
26	CLA	b	605	2	-	14/39/115/115	-
26	CLA	B	605	43	-	19/39/115/115	-
26	CLA	b	610	2	-	7/39/115/115	-
37	LHG	g	301	26	-	18/53/53/53	-
40	LUT	Y	315	-	-	2/29/67/67	0/2/2/2
28	BCR	b	619	-	-	5/29/63/63	0/2/2/2
39	CHL	n	311	43	-	7/20/118/137	-
40	LUT	g	310	-	-	2/29/67/67	0/2/2/2
39	CHL	S	316	18	-	5/23/121/137	-
26	CLA	D	401	43	-	3/39/115/115	-
26	CLA	C	505	3	-	11/39/115/115	-
39	CHL	Y	307	23	-	12/39/137/137	-
39	CHL	r	316	43	-	10/20/118/137	-
33	DGD	C	509	-	-	17/44/84/95	0/2/2/2
37	LHG	N	301	26	-	14/53/53/53	-
28	BCR	t	101	-	-	16/29/63/63	0/2/2/2
36	LMT	D	402	-	-	7/21/61/61	0/2/2/2
26	CLA	g	315	37	-	6/20/96/115	-
39	CHL	Y	318	-	-	6/20/118/137	-
26	CLA	y	304	37	-	12/39/115/115	-
26	CLA	R	313	17	-	11/39/115/115	-
28	BCR	d	401	-	-	9/29/63/63	0/2/2/2
27	PHO	d	407	-	-	13/37/103/103	0/5/6/6
40	LUT	n	317	-	-	3/29/67/67	0/2/2/2
28	BCR	b	615	-	-	1/29/63/63	0/2/2/2
26	CLA	b	608	43	-	20/39/115/115	-
26	CLA	B	613	-	-	10/39/115/115	-
26	CLA	n	312	43	-	7/20/96/115	-
27	PHO	D	403	-	-	13/37/103/103	0/5/6/6
33	DGD	b	620	-	-	18/51/91/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	c	516	3	-	13/39/115/115	-
26	CLA	s	305	18	-	6/20/96/115	-
28	BCR	j	101	-	-	10/29/63/63	0/2/2/2
26	CLA	D	406	4	-	12/39/115/115	-
39	CHL	R	318	23	-	8/18/116/137	-
42	NEX	Y	304	-	-	2/27/83/83	0/3/3/3
37	LHG	D	410	-	-	9/41/41/53	-
26	CLA	S	314	18	-	6/20/96/115	-
26	CLA	B	609	2	-	11/39/115/115	-
37	LHG	l	101	-	-	13/53/53/53	-
26	CLA	r	310	17	-	10/20/96/115	-
26	CLA	G	304	7	-	7/20/96/115	-
30	PL9	A	408	-	-	4/14/34/73	0/1/1/1
34	LMG	D	404	-	-	10/41/61/70	0/1/1/1
39	CHL	y	314	23	-	11/39/137/137	-
26	CLA	B	601	2	-	14/39/115/115	-
26	CLA	y	316	23	-	14/39/115/115	-
41	XAT	G	320	-	-	4/31/93/93	0/4/4/4
34	LMG	c	509	-	-	19/46/66/70	0/1/1/1
26	CLA	G	307	7	-	12/39/115/115	-
26	CLA	G	319	7	-	11/20/96/115	-
37	LHG	D	407	-	-	15/47/47/53	-
34	LMG	W	201	-	-	13/43/63/70	0/1/1/1
26	CLA	B	615	2	-	17/39/115/115	-
40	LUT	Y	309	-	-	3/29/67/67	0/2/2/2
26	CLA	c	508	43	-	10/39/115/115	-
42	NEX	r	302	-	-	2/27/83/83	0/3/3/3
39	CHL	G	311	7	-	8/20/118/137	-
26	CLA	N	309	7	-	11/20/96/115	-
34	LMG	b	622	-	-	16/46/66/70	0/1/1/1
30	PL9	a	407	-	-	4/14/34/73	0/1/1/1
39	CHL	n	307	-	-	10/20/118/137	-
28	BCR	J	101	-	-	9/29/63/63	0/2/2/2
26	CLA	C	508	3	-	13/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	d	403	4	-	12/39/115/115	-
28	BCR	b	603	-	-	0/29/63/63	0/2/2/2
42	NEX	g	306	-	-	2/27/83/83	0/3/3/3
26	CLA	S	310	-	-	15/20/96/115	-
26	CLA	C	506	3	-	13/39/115/115	-
37	LHG	s	309	26	-	24/53/53/53	-
33	DGD	C	510	-	-	14/51/91/95	0/2/2/2
37	LHG	n	301	26	-	14/53/53/53	-
26	CLA	C	515	3	-	8/39/115/115	-
26	CLA	s	311	18	-	8/20/96/115	-
26	CLA	r	315	17	-	4/20/96/115	-
26	CLA	C	521	43	-	9/39/115/115	-
39	CHL	N	310	7	-	5/18/116/137	-
26	CLA	B	611	2	-	15/39/115/115	-
26	CLA	s	314	18	-	11/20/96/115	-
26	CLA	s	304	18	-	7/20/96/115	-
29	SQD	A	410	-	-	17/45/65/69	0/1/1/1
39	CHL	n	306	7	-	6/20/118/137	-
26	CLA	r	311	43	-	12/20/96/115	-
39	CHL	Y	314	43	-	9/20/118/137	-
29	SQD	a	403	-	-	21/49/69/69	0/1/1/1
26	CLA	B	606	2	-	16/39/115/115	-
42	NEX	n	313	-	-	3/27/83/83	0/3/3/3
29	SQD	a	413	-	-	17/45/65/69	0/1/1/1
26	CLA	S	303	18	-	6/20/96/115	-
26	CLA	B	612	43	-	5/39/115/115	-
26	CLA	y	309	23	-	11/39/115/115	-
26	CLA	b	609	2	-	10/39/115/115	-
39	CHL	n	319	7	-	6/20/118/137	-
26	CLA	r	305	17	-	11/20/96/115	-
33	DGD	Y	303	-	-	13/32/72/95	0/2/2/2
26	CLA	d	411	43	-	9/20/96/115	-
33	DGD	C	513	-	-	17/51/91/95	0/2/2/2
28	BCR	C	514	-	-	4/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	N	316	7	-	6/20/118/137	-
26	CLA	C	504	3	-	8/39/115/115	-
26	CLA	n	303	7	-	10/39/115/115	-
39	CHL	s	316	-	-	15/20/118/137	-
26	CLA	g	318	7	-	7/20/96/115	-
26	CLA	s	307	18	-	6/20/96/115	-
28	BCR	a	404	-	-	2/29/63/63	0/2/2/2
39	CHL	Y	302	23	-	12/39/137/137	-
26	CLA	C	520	3	-	16/51/101/115	-
39	CHL	g	311	7	-	18/39/137/137	-
39	CHL	Y	317	43	-	5/20/118/137	-
29	SQD	A	407	-	-	22/49/69/69	0/1/1/1
26	CLA	s	315	18	-	6/20/96/115	-
28	BCR	A	406	-	-	2/29/63/63	0/2/2/2
29	SQD	b	621	-	-	26/49/69/69	0/1/1/1
29	SQD	W	202	-	-	12/28/48/69	0/1/1/1
26	CLA	r	303	17	-	6/20/96/115	-
33	DGD	c	501	-	-	18/51/91/95	0/2/2/2
39	CHL	S	312	-	-	10/19/117/137	-
26	CLA	a	402	1	-	4/33/109/115	-
26	CLA	N	307	7	-	5/39/115/115	-
26	CLA	s	301	37	-	11/20/96/115	-
40	LUT	S	306	-	-	2/29/67/67	0/2/2/2
37	LHG	r	312	26	-	16/53/53/53	-
26	CLA	s	310	-	-	15/20/96/115	-
30	PL9	d	408	-	-	5/53/73/73	0/1/1/1
26	CLA	Y	310	23	-	11/20/96/115	-
39	CHL	N	311	-	-	10/20/118/137	-
33	DGD	c	519	-	-	18/51/91/95	0/2/2/2
28	BCR	D	405	-	-	9/29/63/63	0/2/2/2
34	LMG	C	503	-	-	19/46/66/70	0/1/1/1
37	LHG	G	312	26	-	15/53/53/53	-
26	CLA	N	312	7	-	9/39/115/115	-
26	CLA	g	308	7	-	9/20/96/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	R	307	17	-	7/20/96/115	-
28	BCR	h	101	-	-	2/29/63/63	0/2/2/2
39	CHL	N	303	-	-	12/39/137/137	-
40	LUT	N	314	-	-	1/29/67/67	0/2/2/2
37	LHG	R	303	26	-	17/53/53/53	-
26	CLA	c	504	3	-	8/39/115/115	-
26	CLA	d	404	4	-	10/39/115/115	-
41	XAT	g	320	-	-	3/31/93/93	0/4/4/4
26	CLA	S	304	18	-	7/20/96/115	-
39	CHL	G	301	-	-	11/20/118/137	-
26	CLA	B	607	43	-	11/39/115/115	-
40	LUT	n	314	-	-	1/29/67/67	0/2/2/2
40	LUT	R	311	-	-	8/29/67/67	0/2/2/2
26	CLA	b	602	2	-	10/39/115/115	-
28	BCR	B	608	-	-	1/29/63/63	0/2/2/2
26	CLA	B	617	2	-	8/39/115/115	-
26	CLA	Y	316	43	-	7/20/96/115	-
26	CLA	s	306	18	-	10/20/96/115	-
26	CLA	C	512	3	-	12/39/115/115	-
26	CLA	N	313	7	-	9/20/96/115	-
26	CLA	S	315	18	-	10/20/96/115	-
26	CLA	G	313	37	-	6/20/96/115	-
26	CLA	R	310	17	-	10/20/96/115	-
40	LUT	g	316	-	-	1/29/67/67	0/2/2/2
26	CLA	r	306	17	-	6/39/115/115	-
28	BCR	H	101	-	-	2/29/63/63	0/2/2/2
26	CLA	b	601	2	-	17/39/115/115	-
39	CHL	R	315	43	-	8/20/118/137	-
26	CLA	B	610	2	-	12/39/115/115	-
28	BCR	K	101	-	-	2/29/63/63	0/2/2/2
26	CLA	R	309	17	-	11/20/96/115	-
26	CLA	C	519	3	-	6/20/96/115	-
26	CLA	n	309	7	-	11/20/96/115	-
37	LHG	D	408	-	-	14/53/53/53	-
26	CLA	C	516	43	-	10/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LHG	d	409	-	-	13/53/53/53	-
39	CHL	G	303	-	-	9/20/118/137	-
26	CLA	b	614	43	-	5/39/115/115	-
39	CHL	S	302	-	-	15/20/118/137	-
37	LHG	S	317	26	-	24/53/53/53	-
42	NEX	S	305	-	-	7/27/83/83	0/3/3/3
40	LUT	r	307	-	-	8/29/67/67	0/2/2/2
40	LUT	G	316	-	-	0/29/67/67	0/2/2/2
26	CLA	y	313	43	-	6/20/96/115	-
26	CLA	b	613	2	-	11/39/115/115	-
26	CLA	b	604	-	-	10/39/115/115	-
33	DGD	y	308	-	-	14/32/72/95	0/2/2/2
26	CLA	b	618	2	-	12/39/115/115	-
40	LUT	N	305	-	-	3/29/67/67	0/2/2/2
26	CLA	S	311	18	-	8/20/96/115	-
26	CLA	C	517	3	-	4/39/115/115	-
26	CLA	Y	312	23	-	12/39/115/115	-
41	XAT	g	309	-	-	0/31/93/93	0/4/4/4
26	CLA	N	318	7	-	8/20/96/115	-
34	LMG	c	512	-	-	19/46/66/70	0/1/1/1
33	DGD	c	517	-	-	17/44/84/95	0/2/2/2
26	CLA	A	403	1	-	8/39/115/115	-
39	CHL	G	305	-	-	7/20/118/137	-
26	CLA	c	514	43	-	9/39/115/115	-
41	XAT	n	316	-	-	0/31/93/93	0/4/4/4
40	LUT	y	318	-	-	3/29/67/67	0/2/2/2
26	CLA	r	317	37	-	10/20/96/115	-
26	CLA	n	305	7	-	5/39/115/115	-
42	NEX	N	302	-	-	2/27/83/83	0/3/3/3
26	CLA	N	308	43	-	7/20/96/115	-
39	CHL	g	312	7	-	8/20/118/137	-
26	CLA	n	304	7	-	9/20/96/115	-
26	CLA	G	302	-	-	10/20/96/115	-
39	CHL	N	317	7	-	7/20/118/137	-
26	CLA	Y	308	23	-	10/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	y	303	23	-	12/39/137/137	-
26	CLA	c	506	3	-	15/51/101/115	-
39	CHL	G	309	7	-	12/18/116/137	-
26	CLA	R	302	17	-	10/20/96/115	-
26	CLA	g	302	-	-	10/20/96/115	-
39	CHL	r	301	23	-	7/18/116/137	-
26	CLA	R	316	17	-	6/20/96/115	-
39	CHL	s	317	-	-	7/20/118/137	-
37	LHG	Y	306	26	-	29/53/53/53	-
33	DGD	B	620	-	-	15/51/91/95	0/2/2/2
42	NEX	R	305	-	-	2/27/83/83	0/3/3/3
26	CLA	g	317	7	-	11/39/115/115	-
39	CHL	n	318	-	-	14/39/137/137	-
26	CLA	N	319	37	-	12/20/96/115	-
39	CHL	y	305	43	-	5/20/118/137	-
34	LMG	B	622	-	-	17/46/66/70	0/1/1/1
26	CLA	r	313	17	-	10/20/96/115	-
40	LUT	S	301	-	-	3/29/67/67	0/2/2/2
28	BCR	k	101	-	-	2/29/63/63	0/2/2/2
26	CLA	b	611	2	-	19/39/115/115	-
26	CLA	S	309	18	-	7/20/96/115	-
26	CLA	a	409	43	-	3/39/115/115	-
26	CLA	B	603	2	-	10/39/115/115	-
26	CLA	b	607	2	-	14/39/115/115	-
38	HEM	e	101	6,5	-	2/14/54/54	-
26	CLA	B	602	2	-	14/39/115/115	-
26	CLA	r	314	17	-	13/39/115/115	-
30	PL9	D	411	-	-	6/53/73/73	0/1/1/1
39	CHL	y	302	-	-	6/20/118/137	-
39	CHL	S	313	-	-	8/20/118/137	-
39	CHL	N	304	43	-	7/20/118/137	-
39	CHL	s	313	-	-	9/19/117/137	-
26	CLA	c	520	3	-	10/39/115/115	-
26	CLA	a	411	1	-	8/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	G	317	7	-	9/20/96/115	-
28	BCR	T	101	-	-	16/29/63/63	0/2/2/2
39	CHL	g	314	7	-	11/18/116/137	-
34	LMG	C	518	-	-	19/46/66/70	0/1/1/1
39	CHL	r	318	43	-	7/20/118/137	-
28	BCR	B	614	-	-	4/29/63/63	0/2/2/2
26	CLA	n	315	7	-	11/20/96/115	-
26	CLA	c	503	3	-	16/39/115/115	-
41	XAT	R	304	-	-	1/31/93/93	0/4/4/4
39	CHL	R	301	43	-	11/20/118/137	-
26	CLA	N	306	7	-	11/20/96/115	-
39	CHL	n	308	7	-	5/18/116/137	-
26	CLA	R	308	43	-	12/20/96/115	-
39	CHL	s	303	18	-	6/23/121/137	-
26	CLA	g	303	7	-	8/39/115/115	-
26	CLA	C	511	3	-	14/39/115/115	-
37	LHG	d	410	-	-	10/41/41/53	-
26	CLA	A	405	1	-	4/33/109/115	-
26	CLA	b	606	2	-	15/39/115/115	-
28	BCR	c	511	-	-	3/29/63/63	0/2/2/2
26	CLA	n	310	37	-	12/20/96/115	-
26	CLA	g	305	7	-	11/20/96/115	-
26	CLA	B	616	2	-	10/39/115/115	-
28	BCR	C	502	-	-	1/29/63/63	0/2/2/2
27	PHO	A	404	-	-	11/37/103/103	0/5/6/6
26	CLA	c	510	3	-	6/20/96/115	-
41	XAT	N	315	-	-	0/31/93/93	0/4/4/4
26	CLA	C	507	3	-	14/39/115/115	-
26	CLA	b	616	43	-	11/39/115/115	-
27	PHO	a	410	-	-	10/37/103/103	0/5/6/6
37	LHG	y	301	26	-	28/53/53/53	-
38	HEM	E	101	6,5	-	2/14/54/54	-
29	SQD	w	202	-	-	12/28/48/69	0/1/1/1
26	CLA	B	618	2	-	12/39/115/115	-
26	CLA	y	317	23	-	11/20/96/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	c	502	3	-	13/39/115/115	-
26	CLA	D	412	43	-	9/20/96/115	-
39	CHL	G	318	7	-	20/39/137/137	-
26	CLA	Y	311	23	-	7/20/96/115	-
26	CLA	b	612	2	-	4/39/115/115	-
26	CLA	c	513	3	-	4/39/115/115	-
37	LHG	d	402	-	-	15/47/47/53	-
39	CHL	g	313	-	-	11/20/118/137	-
40	LUT	s	312	-	-	2/29/67/67	0/2/2/2
26	CLA	R	306	17	-	6/39/115/115	-
34	LMG	d	405	-	-	9/41/61/70	0/1/1/1
26	CLA	r	308	17	-	7/20/96/115	-
26	CLA	S	307	18	-	7/20/96/115	-
26	CLA	Y	313	23	-	16/39/115/115	-
41	XAT	r	304	-	-	1/31/93/93	0/4/4/4
26	CLA	R	314	37	-	10/20/96/115	-
39	CHL	r	309	43	-	10/20/118/137	-
29	SQD	B	621	-	-	25/49/69/69	0/1/1/1
42	NEX	y	307	-	-	2/27/83/83	0/3/3/3
26	CLA	D	409	4	-	10/39/115/115	-
40	LUT	G	308	-	-	1/29/67/67	0/2/2/2
42	NEX	s	302	-	-	6/27/83/83	0/3/3/3
26	CLA	Y	301	37	-	12/39/115/115	-
26	CLA	y	315	23	-	7/20/96/115	-
26	CLA	y	310	23	-	12/39/115/115	-
26	CLA	G	306	7	-	10/20/96/115	-
26	CLA	n	302	7	-	8/20/96/115	-
26	CLA	c	505	3	-	14/39/115/115	-
26	CLA	y	306	23	-	10/39/115/115	-
26	CLA	g	304	7	-	11/20/96/115	-
37	LHG	L	101	-	-	11/53/53/53	-
40	LUT	s	308	-	-	4/29/67/67	0/2/2/2
39	CHL	g	307	-	-	8/20/118/137	-
39	CHL	g	319	-	-	7/20/118/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	BCR	c	507	-	-	5/29/63/63	0/2/2/2
39	CHL	y	312	43	-	8/20/118/137	-
41	XAT	G	310	-	-	0/31/93/93	0/4/4/4
39	CHL	R	312	43	-	10/20/118/137	-
26	CLA	B	604	2	-	3/39/115/115	-
34	LMG	w	201	-	-	14/43/63/70	0/1/1/1
40	LUT	y	311	-	-	0/29/67/67	0/2/2/2
26	CLA	b	617	2	-	12/39/115/115	-
28	BCR	B	619	-	-	0/29/63/63	0/2/2/2

All (2161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	307	CLA	MG-NC	14.46	2.40	2.06
27	d	407	PHO	C1B-C2B	8.83	1.49	1.39
27	A	404	PHO	C1B-C2B	8.80	1.49	1.39
27	D	403	PHO	C1B-C2B	8.80	1.49	1.39
27	a	410	PHO	C1B-C2B	8.74	1.49	1.39
27	d	407	PHO	C3B-C4B	7.66	1.50	1.41
27	D	403	PHO	C3B-C4B	7.62	1.50	1.41
27	A	404	PHO	C3B-C4B	7.46	1.50	1.41
27	a	410	PHO	C3B-C4B	7.42	1.50	1.41
39	G	309	CHL	CMC-C2C	7.19	1.56	1.44
39	s	303	CHL	C3B-C4B	7.18	1.47	1.41
39	g	314	CHL	CMC-C2C	7.18	1.56	1.44
39	g	311	CHL	CMC-C2C	7.16	1.56	1.44
39	s	316	CHL	CMC-C2C	7.12	1.56	1.44
39	G	318	CHL	CMC-C2C	7.11	1.56	1.44
39	Y	317	CHL	C3B-C4B	7.08	1.47	1.41
39	N	316	CHL	CMC-C2C	7.08	1.56	1.44
39	G	305	CHL	C3B-C4B	7.07	1.47	1.41
39	G	309	CHL	C3B-C4B	7.07	1.47	1.41
39	g	313	CHL	CMC-C2C	7.06	1.56	1.44
39	S	302	CHL	CMC-C2C	7.06	1.56	1.44
39	r	309	CHL	C3B-C4B	7.04	1.47	1.41
39	G	301	CHL	CMC-C2C	7.04	1.56	1.44
39	Y	318	CHL	C3B-C4B	7.04	1.47	1.41
39	n	306	CHL	CMC-C2C	7.04	1.56	1.44
39	G	301	CHL	C3B-C4B	7.04	1.47	1.41
39	g	312	CHL	CMC-C2C	7.03	1.56	1.44
39	s	313	CHL	CMC-C2C	7.03	1.56	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	S	312	CHL	CMC-C2C	7.02	1.56	1.44
39	g	319	CHL	C3B-C4B	7.02	1.47	1.41
39	S	316	CHL	C3B-C4B	7.01	1.47	1.41
39	g	313	CHL	C3B-C4B	7.01	1.47	1.41
39	N	316	CHL	C3B-C4B	7.01	1.47	1.41
39	n	306	CHL	C3B-C4B	7.00	1.47	1.41
39	s	313	CHL	C3B-C4B	7.00	1.47	1.41
39	N	304	CHL	CMC-C2C	7.00	1.56	1.44
39	S	313	CHL	CMC-C2C	7.00	1.56	1.44
39	N	317	CHL	CMC-C2C	7.00	1.56	1.44
39	n	319	CHL	CMC-C2C	7.00	1.56	1.44
39	n	308	CHL	CMC-C2C	7.00	1.56	1.44
39	G	311	CHL	CMC-C2C	6.99	1.56	1.44
39	g	314	CHL	C3B-C4B	6.99	1.46	1.41
39	y	302	CHL	C3B-C4B	6.99	1.46	1.41
39	N	310	CHL	CMC-C2C	6.99	1.56	1.44
39	y	305	CHL	C3B-C4B	6.98	1.46	1.41
39	s	303	CHL	CMC-C2C	6.98	1.56	1.44
39	S	316	CHL	CMC-C2C	6.97	1.56	1.44
39	R	312	CHL	C3B-C4B	6.97	1.46	1.41
39	n	311	CHL	CMC-C2C	6.96	1.56	1.44
39	y	303	CHL	CMC-C2C	6.96	1.56	1.44
39	S	312	CHL	C3B-C4B	6.96	1.46	1.41
39	s	317	CHL	CMC-C2C	6.95	1.56	1.44
39	S	302	CHL	C3B-C4B	6.95	1.46	1.41
39	y	314	CHL	CMC-C2C	6.95	1.56	1.44
39	Y	307	CHL	CMC-C2C	6.95	1.56	1.44
39	r	309	CHL	CMC-C2C	6.95	1.56	1.44
39	Y	302	CHL	CMC-C2C	6.92	1.56	1.44
39	Y	317	CHL	CMC-C2C	6.91	1.56	1.44
39	N	304	CHL	C3B-C4B	6.90	1.46	1.41
39	R	312	CHL	CMC-C2C	6.90	1.56	1.44
39	r	301	CHL	CMC-C2C	6.90	1.56	1.44
39	s	316	CHL	C3B-C4B	6.89	1.46	1.41
39	R	315	CHL	CMC-C2C	6.87	1.56	1.44
39	R	318	CHL	CMC-C2C	6.87	1.56	1.44
39	y	305	CHL	CMC-C2C	6.87	1.56	1.44
39	R	315	CHL	C3B-C4B	6.86	1.46	1.41
39	g	307	CHL	C3B-C4B	6.84	1.46	1.41
39	r	318	CHL	CMC-C2C	6.84	1.56	1.44
39	R	301	CHL	CMC-C2C	6.82	1.56	1.44
39	g	319	CHL	CMC-C2C	6.80	1.56	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	G	303	CHL	C3B-C4B	6.80	1.46	1.41
39	G	305	CHL	CMC-C2C	6.79	1.56	1.44
39	Y	314	CHL	CMC-C2C	6.78	1.56	1.44
39	s	317	CHL	C3B-C4B	6.77	1.46	1.41
39	Y	302	CHL	C3B-C4B	6.77	1.46	1.41
39	r	316	CHL	C3B-C4B	6.76	1.46	1.41
39	r	316	CHL	CMC-C2C	6.76	1.56	1.44
39	y	314	CHL	C3B-C4B	6.76	1.46	1.41
39	y	312	CHL	CMC-C2C	6.75	1.56	1.44
39	Y	307	CHL	C3B-C4B	6.75	1.46	1.41
39	N	317	CHL	C3B-C4B	6.74	1.46	1.41
39	R	301	CHL	C3B-C4B	6.74	1.46	1.41
39	n	318	CHL	CMC-C2C	6.74	1.56	1.44
39	g	307	CHL	CMC-C2C	6.74	1.56	1.44
39	S	313	CHL	C3B-C4B	6.73	1.46	1.41
39	y	303	CHL	C3B-C4B	6.73	1.46	1.41
39	n	311	CHL	C3B-C4B	6.73	1.46	1.41
39	N	311	CHL	C3B-C4B	6.72	1.46	1.41
39	G	303	CHL	CMC-C2C	6.71	1.55	1.44
39	n	308	CHL	C3B-C4B	6.71	1.46	1.41
39	N	310	CHL	C3B-C4B	6.70	1.46	1.41
39	r	318	CHL	C3B-C4B	6.70	1.46	1.41
39	n	319	CHL	C3B-C4B	6.69	1.46	1.41
39	n	307	CHL	C3B-C4B	6.69	1.46	1.41
39	N	303	CHL	CMC-C2C	6.68	1.55	1.44
39	y	302	CHL	CMC-C2C	6.67	1.55	1.44
39	g	312	CHL	C3B-C4B	6.66	1.46	1.41
39	G	311	CHL	C3B-C4B	6.62	1.46	1.41
39	Y	318	CHL	CMC-C2C	6.61	1.55	1.44
39	R	318	CHL	C3B-C4B	6.59	1.46	1.41
39	r	301	CHL	C3B-C4B	6.57	1.46	1.41
39	g	311	CHL	C3B-C4B	6.51	1.46	1.41
39	G	318	CHL	C3B-C4B	6.50	1.46	1.41
39	N	311	CHL	CMC-C2C	6.48	1.55	1.44
39	n	307	CHL	CMC-C2C	6.47	1.55	1.44
26	R	307	CLA	MG-NB	6.43	2.18	2.05
39	n	318	CHL	C3B-C4B	6.33	1.46	1.41
39	N	303	CHL	C3B-C4B	6.29	1.46	1.41
39	Y	314	CHL	C3B-C4B	6.21	1.46	1.41
39	y	312	CHL	C3B-C4B	6.19	1.46	1.41
26	c	506	CLA	C1B-C2B	5.10	1.49	1.34
26	C	520	CLA	C1B-C2B	5.08	1.49	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	307	CLA	MG-NA	-4.96	1.94	2.06
39	s	316	CHL	C1D-C2D	4.82	1.45	1.39
30	d	408	PL9	C7-C3	-4.79	1.46	1.51
39	g	311	CHL	C1D-C2D	4.77	1.45	1.39
39	N	316	CHL	C1D-C2D	4.74	1.45	1.39
30	D	411	PL9	C7-C3	-4.73	1.46	1.51
39	N	317	CHL	C1D-C2D	4.72	1.45	1.39
39	y	302	CHL	C1D-C2D	4.72	1.45	1.39
39	S	302	CHL	C1D-C2D	4.71	1.45	1.39
39	R	301	CHL	C1C-NC	4.69	1.39	1.35
39	y	314	CHL	C1D-C2D	4.69	1.45	1.39
39	n	319	CHL	C1D-C2D	4.68	1.45	1.39
39	G	311	CHL	C1D-C2D	4.67	1.45	1.39
42	Y	304	NEX	C10-C9	4.67	1.42	1.35
39	g	312	CHL	C1D-C2D	4.66	1.45	1.39
42	y	307	NEX	C10-C9	4.66	1.42	1.35
39	n	311	CHL	C1D-C2D	4.66	1.45	1.39
39	n	306	CHL	C1D-C2D	4.66	1.45	1.39
39	r	316	CHL	C1C-NC	4.65	1.39	1.35
42	S	305	NEX	C10-C9	4.65	1.41	1.35
39	N	316	CHL	C1C-NC	4.64	1.39	1.35
39	g	319	CHL	C1C-NC	4.64	1.39	1.35
39	G	318	CHL	C1D-C2D	4.64	1.45	1.39
42	s	302	NEX	C10-C9	4.63	1.41	1.35
39	Y	307	CHL	C1D-C2D	4.63	1.45	1.39
39	S	313	CHL	C1D-C2D	4.62	1.45	1.39
42	R	305	NEX	C10-C9	4.61	1.41	1.35
39	g	314	CHL	C1D-C2D	4.61	1.45	1.39
39	y	303	CHL	C1D-C2D	4.60	1.45	1.39
39	s	317	CHL	C1C-NC	4.60	1.39	1.35
39	n	306	CHL	C1C-NC	4.60	1.39	1.35
39	G	309	CHL	C1D-C2D	4.59	1.45	1.39
39	s	317	CHL	C1D-C2D	4.59	1.45	1.39
42	N	302	NEX	C10-C9	4.58	1.41	1.35
42	r	302	NEX	C10-C9	4.58	1.41	1.35
39	S	313	CHL	C1C-NC	4.57	1.39	1.35
39	n	307	CHL	C1D-C2D	4.57	1.45	1.39
39	N	311	CHL	C1D-C2D	4.57	1.45	1.39
39	G	301	CHL	C1C-NC	4.56	1.39	1.35
39	G	305	CHL	C1C-NC	4.56	1.39	1.35
39	g	313	CHL	C1D-C2D	4.56	1.45	1.39
39	Y	302	CHL	C1D-C2D	4.56	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	g	313	CHL	C1C-NC	4.56	1.39	1.35
39	S	312	CHL	C1D-C2D	4.56	1.45	1.39
39	Y	318	CHL	C1D-C2D	4.56	1.45	1.39
29	B	621	SQD	O8-S	4.55	1.63	1.47
42	G	315	NEX	C10-C9	4.55	1.41	1.35
42	g	306	NEX	C10-C9	4.54	1.41	1.35
39	N	304	CHL	C1D-C2D	4.54	1.45	1.39
29	b	621	SQD	O8-S	4.53	1.63	1.47
39	s	313	CHL	C1D-C2D	4.52	1.45	1.39
39	N	310	CHL	C1D-C2D	4.52	1.45	1.39
39	n	308	CHL	C1D-C2D	4.52	1.45	1.39
29	W	202	SQD	O8-S	4.52	1.63	1.47
39	G	309	CHL	C1C-NC	4.51	1.39	1.35
39	S	316	CHL	C1D-C2D	4.50	1.45	1.39
39	s	316	CHL	C1C-NC	4.50	1.39	1.35
29	w	202	SQD	O8-S	4.49	1.63	1.47
29	A	410	SQD	O8-S	4.49	1.63	1.47
39	s	303	CHL	C1D-C2D	4.48	1.45	1.39
39	g	314	CHL	C1C-NC	4.48	1.39	1.35
39	N	317	CHL	C1C-NC	4.47	1.39	1.35
39	G	301	CHL	C1D-C2D	4.46	1.44	1.39
39	n	308	CHL	C1B-C2B	4.46	1.44	1.39
39	G	305	CHL	C1D-C2D	4.45	1.44	1.39
29	a	413	SQD	O8-S	4.45	1.63	1.47
39	r	309	CHL	C1C-NC	4.44	1.39	1.35
39	Y	314	CHL	C1D-C2D	4.44	1.44	1.39
39	r	318	CHL	C1D-C2D	4.43	1.44	1.39
39	R	315	CHL	C1D-C2D	4.43	1.44	1.39
39	y	302	CHL	C1C-NC	4.42	1.39	1.35
39	G	318	CHL	C1B-C2B	4.42	1.44	1.39
39	n	319	CHL	C1C-NC	4.41	1.39	1.35
39	S	302	CHL	C1C-NC	4.41	1.39	1.35
39	S	312	CHL	C1B-C2B	4.41	1.44	1.39
39	R	312	CHL	C1C-NC	4.40	1.39	1.35
42	n	313	NEX	C10-C9	4.40	1.41	1.35
39	g	312	CHL	C1C-NC	4.40	1.39	1.35
39	r	301	CHL	C1D-C2D	4.38	1.44	1.39
39	N	310	CHL	C1B-C2B	4.38	1.44	1.39
39	R	318	CHL	C1D-C2D	4.38	1.44	1.39
29	A	407	SQD	O8-S	4.36	1.63	1.47
39	g	319	CHL	C1D-C2D	4.36	1.44	1.39
39	Y	318	CHL	C1C-NC	4.36	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	g	307	CHL	C1D-C2D	4.35	1.44	1.39
39	y	312	CHL	C1D-C2D	4.35	1.44	1.39
39	R	315	CHL	C1C-NC	4.35	1.39	1.35
29	a	403	SQD	O8-S	4.35	1.63	1.47
39	R	312	CHL	C1D-C2D	4.35	1.44	1.39
39	s	313	CHL	C1B-C2B	4.34	1.44	1.39
39	G	309	CHL	C1B-C2B	4.32	1.44	1.39
39	S	316	CHL	C1C-NC	4.32	1.39	1.35
39	g	311	CHL	C1C-NC	4.32	1.39	1.35
39	r	309	CHL	C1D-C2D	4.32	1.44	1.39
39	n	306	CHL	C1B-C2B	4.31	1.44	1.39
39	n	318	CHL	C1D-C2D	4.31	1.44	1.39
39	G	318	CHL	C1C-NC	4.31	1.39	1.35
39	N	316	CHL	C1B-C2B	4.30	1.44	1.39
39	N	303	CHL	C1D-C2D	4.30	1.44	1.39
39	Y	314	CHL	C1B-C2B	4.29	1.44	1.39
39	N	311	CHL	C1C-NC	4.29	1.39	1.35
39	G	303	CHL	C1D-C2D	4.29	1.44	1.39
39	G	311	CHL	C1C-NC	4.29	1.39	1.35
39	n	307	CHL	C1B-C2B	4.28	1.44	1.39
39	g	313	CHL	C1B-C2B	4.28	1.44	1.39
39	N	311	CHL	C1B-C2B	4.28	1.44	1.39
39	g	314	CHL	C1B-C2B	4.28	1.44	1.39
39	r	316	CHL	C1D-C2D	4.27	1.44	1.39
39	g	311	CHL	C1B-C2B	4.27	1.44	1.39
39	s	316	CHL	C1B-C2B	4.26	1.44	1.39
39	R	301	CHL	C1D-C2D	4.26	1.44	1.39
39	y	305	CHL	C1D-C2D	4.26	1.44	1.39
39	R	318	CHL	C1B-C2B	4.26	1.44	1.39
39	s	303	CHL	C1C-NC	4.26	1.39	1.35
39	n	311	CHL	C1C-NC	4.25	1.39	1.35
39	r	318	CHL	C1C-NC	4.25	1.39	1.35
39	Y	302	CHL	C1B-C2B	4.25	1.44	1.39
39	y	314	CHL	C1C-NC	4.25	1.39	1.35
39	r	301	CHL	C1B-C2B	4.25	1.44	1.39
39	y	312	CHL	C1B-C2B	4.25	1.44	1.39
39	n	307	CHL	C1C-NC	4.23	1.39	1.35
39	N	304	CHL	C1C-NC	4.23	1.39	1.35
39	y	303	CHL	C1B-C2B	4.23	1.44	1.39
39	y	303	CHL	C1C-NC	4.22	1.39	1.35
39	G	301	CHL	C1B-C2B	4.22	1.44	1.39
39	R	301	CHL	C1B-C2B	4.21	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	G	303	CHL	C1C-NC	4.21	1.39	1.35
39	Y	317	CHL	C1B-C2B	4.20	1.44	1.39
39	s	317	CHL	C1B-C2B	4.20	1.44	1.39
39	s	303	CHL	C1B-C2B	4.19	1.44	1.39
39	G	311	CHL	C1B-C2B	4.19	1.44	1.39
39	g	312	CHL	C1B-C2B	4.19	1.44	1.39
39	Y	302	CHL	C1C-NC	4.19	1.38	1.35
39	y	305	CHL	C1B-C2B	4.19	1.44	1.39
39	Y	307	CHL	C1C-NC	4.19	1.38	1.35
39	S	302	CHL	C1B-C2B	4.18	1.44	1.39
39	g	307	CHL	C1C-NC	4.18	1.38	1.35
39	n	308	CHL	C1C-NC	4.18	1.38	1.35
39	g	307	CHL	C1B-C2B	4.18	1.44	1.39
39	S	316	CHL	C1B-C2B	4.17	1.44	1.39
39	Y	317	CHL	C1C-NC	4.17	1.38	1.35
39	Y	317	CHL	C1D-C2D	4.17	1.44	1.39
39	Y	314	CHL	C1C-NC	4.17	1.38	1.35
39	y	312	CHL	C1C-NC	4.17	1.38	1.35
39	S	313	CHL	C1B-C2B	4.16	1.44	1.39
39	r	316	CHL	C1B-C2B	4.15	1.44	1.39
39	N	303	CHL	C1B-C2B	4.15	1.44	1.39
39	n	318	CHL	C1B-C2B	4.15	1.44	1.39
39	R	318	CHL	C1C-NC	4.14	1.38	1.35
39	r	301	CHL	C1C-NC	4.14	1.38	1.35
39	G	303	CHL	C1B-C2B	4.14	1.44	1.39
39	N	310	CHL	C1C-NC	4.14	1.38	1.35
39	n	318	CHL	C1C-NC	4.14	1.38	1.35
39	R	315	CHL	C1B-C2B	4.12	1.44	1.39
39	n	311	CHL	C1B-C2B	4.11	1.44	1.39
39	y	305	CHL	C1C-NC	4.11	1.38	1.35
39	r	318	CHL	C1B-C2B	4.09	1.44	1.39
26	R	307	CLA	C1D-ND	4.08	1.42	1.37
39	R	312	CHL	C1B-C2B	4.08	1.44	1.39
39	S	312	CHL	C1C-NC	4.07	1.38	1.35
39	s	313	CHL	C1C-NC	4.06	1.38	1.35
39	N	303	CHL	C1C-NC	4.02	1.38	1.35
39	y	314	CHL	C1B-C2B	4.02	1.44	1.39
39	Y	318	CHL	C1B-C2B	4.01	1.44	1.39
26	N	318	CLA	C1D-ND	4.00	1.42	1.37
39	y	302	CHL	C1B-C2B	4.00	1.44	1.39
39	r	309	CHL	C1B-C2B	4.00	1.44	1.39
39	N	304	CHL	C1B-C2B	3.99	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Y	307	CHL	C1B-C2B	3.98	1.44	1.39
26	R	307	CLA	C4B-NB	3.96	1.42	1.37
26	n	302	CLA	C1D-ND	3.94	1.42	1.37
39	G	305	CHL	C1B-C2B	3.94	1.44	1.39
39	g	319	CHL	C1B-C2B	3.93	1.44	1.39
26	b	611	CLA	C1D-ND	3.93	1.42	1.37
39	N	317	CHL	C1B-C2B	3.91	1.44	1.39
26	r	305	CLA	C1D-ND	3.91	1.42	1.37
27	a	410	PHO	C1D-C2D	3.89	1.43	1.39
39	n	319	CHL	C1B-C2B	3.88	1.44	1.39
39	g	319	CHL	C4C-NC	3.88	1.38	1.35
27	d	407	PHO	C1D-C2D	3.86	1.43	1.39
27	D	403	PHO	C1D-C2D	3.86	1.43	1.39
26	B	615	CLA	C1D-ND	3.86	1.42	1.37
39	G	309	CHL	C4C-NC	3.86	1.38	1.35
39	G	305	CHL	C4C-NC	3.85	1.38	1.35
39	S	313	CHL	C4C-NC	3.85	1.38	1.35
27	A	404	PHO	C1D-C2D	3.84	1.43	1.39
39	s	317	CHL	C4C-NC	3.83	1.38	1.35
26	n	310	CLA	C1D-ND	3.83	1.42	1.37
26	g	305	CLA	C1D-ND	3.82	1.42	1.37
26	R	309	CLA	C1D-ND	3.81	1.42	1.37
26	s	306	CLA	C1D-ND	3.81	1.42	1.37
26	G	313	CLA	C1D-ND	3.80	1.42	1.37
26	y	317	CLA	C1D-ND	3.80	1.42	1.37
26	G	306	CLA	C1D-ND	3.80	1.42	1.37
26	C	507	CLA	C1D-ND	3.79	1.42	1.37
39	S	302	CHL	C4C-NC	3.79	1.38	1.35
26	c	508	CLA	C1D-ND	3.79	1.42	1.37
26	B	605	CLA	C1D-ND	3.79	1.42	1.37
39	g	314	CHL	CHA-CBD	3.78	1.56	1.51
26	S	308	CLA	C1D-ND	3.77	1.42	1.37
39	s	316	CHL	C4C-NC	3.77	1.38	1.35
26	G	304	CLA	C1D-ND	3.77	1.42	1.37
26	y	316	CLA	C1D-ND	3.76	1.42	1.37
39	r	309	CHL	C4C-NC	3.76	1.38	1.35
39	g	314	CHL	C4C-NC	3.76	1.38	1.35
39	y	302	CHL	C4C-NC	3.76	1.38	1.35
26	C	516	CLA	C1D-ND	3.76	1.42	1.37
26	N	309	CLA	C1D-ND	3.76	1.42	1.37
26	c	505	CLA	C1D-ND	3.76	1.42	1.37
39	Y	318	CHL	C4C-NC	3.75	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	G	309	CHL	CHA-CBD	3.75	1.56	1.51
39	g	307	CHL	C4C-NC	3.75	1.38	1.35
26	S	315	CLA	C1D-ND	3.74	1.42	1.37
26	B	616	CLA	C1D-ND	3.74	1.42	1.37
26	D	412	CLA	C1D-ND	3.74	1.42	1.37
26	N	306	CLA	C1D-ND	3.74	1.42	1.37
39	s	316	CHL	C3B-C2B	-3.74	1.35	1.40
26	R	314	CLA	C1D-ND	3.74	1.42	1.37
26	b	608	CLA	C1D-ND	3.74	1.42	1.37
26	S	310	CLA	C1D-ND	3.73	1.42	1.37
26	G	319	CLA	C1D-ND	3.73	1.42	1.37
26	N	319	CLA	C1D-ND	3.73	1.42	1.37
26	n	309	CLA	C1D-ND	3.73	1.42	1.37
26	g	318	CLA	C1D-ND	3.73	1.42	1.37
26	b	613	CLA	C1D-ND	3.71	1.42	1.37
26	Y	310	CLA	C1D-ND	3.71	1.42	1.37
39	Y	307	CHL	C3B-C2B	-3.71	1.35	1.40
39	n	319	CHL	C4C-NC	3.71	1.38	1.35
26	n	315	CLA	C1D-ND	3.71	1.42	1.37
26	r	317	CLA	C1D-ND	3.71	1.42	1.37
26	B	618	CLA	C1D-ND	3.70	1.42	1.37
26	g	315	CLA	C1D-ND	3.70	1.42	1.37
26	s	301	CLA	C1D-ND	3.70	1.42	1.37
39	Y	318	CHL	C3B-C2B	-3.70	1.35	1.40
26	d	411	CLA	C1D-ND	3.70	1.42	1.37
39	G	301	CHL	C4C-NC	3.69	1.38	1.35
39	y	314	CHL	C3B-C2B	-3.69	1.35	1.40
39	g	313	CHL	C4C-NC	3.69	1.38	1.35
39	g	312	CHL	C3B-C2B	-3.69	1.35	1.40
26	R	317	CLA	C1D-ND	3.69	1.42	1.37
39	y	302	CHL	C3B-C2B	-3.68	1.35	1.40
26	g	304	CLA	C1D-ND	3.68	1.42	1.37
26	s	310	CLA	C1D-ND	3.67	1.42	1.37
39	Y	307	CHL	C4C-NC	3.67	1.38	1.35
39	y	312	CHL	C4C-NC	3.67	1.38	1.35
39	N	317	CHL	C4C-NC	3.67	1.38	1.35
26	b	609	CLA	C1D-ND	3.67	1.42	1.37
26	g	308	CLA	C1D-ND	3.66	1.42	1.37
26	S	307	CLA	C1D-ND	3.66	1.42	1.37
26	c	516	CLA	C1D-ND	3.66	1.42	1.37
26	y	310	CLA	C1D-ND	3.66	1.42	1.37
39	R	318	CHL	C3B-C2B	-3.66	1.35	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	302	CLA	C1D-ND	3.65	1.42	1.37
26	y	315	CLA	C1D-ND	3.65	1.42	1.37
39	G	311	CHL	C3B-C2B	-3.65	1.35	1.40
39	N	317	CHL	C3B-C2B	-3.65	1.35	1.40
26	C	515	CLA	C1D-ND	3.65	1.42	1.37
39	Y	302	CHL	C3B-C2B	-3.65	1.35	1.40
39	G	303	CHL	C4C-NC	3.65	1.38	1.35
26	r	314	CLA	C1D-ND	3.65	1.42	1.37
26	G	317	CLA	C1D-ND	3.65	1.42	1.37
26	r	315	CLA	C1D-ND	3.65	1.42	1.37
26	n	305	CLA	C1D-ND	3.65	1.42	1.37
26	B	606	CLA	C1D-ND	3.64	1.42	1.37
26	G	314	CLA	C1D-ND	3.64	1.42	1.37
26	b	605	CLA	C1D-ND	3.64	1.42	1.37
26	g	303	CLA	C1D-ND	3.64	1.42	1.37
26	c	504	CLA	C1D-ND	3.64	1.42	1.37
26	y	304	CLA	C1D-ND	3.64	1.42	1.37
39	R	312	CHL	C4C-NC	3.64	1.38	1.35
26	Y	301	CLA	C1D-ND	3.64	1.42	1.37
26	Y	312	CLA	C1D-ND	3.64	1.42	1.37
26	s	311	CLA	C1D-ND	3.64	1.42	1.37
26	y	309	CLA	C1D-ND	3.64	1.42	1.37
39	N	310	CHL	C4C-NC	3.64	1.38	1.35
39	R	301	CHL	CHA-CBD	3.64	1.55	1.51
39	Y	314	CHL	CHA-CBD	3.64	1.55	1.51
39	y	314	CHL	C4C-NC	3.64	1.38	1.35
26	Y	313	CLA	C1D-ND	3.64	1.42	1.37
26	r	303	CLA	C1D-ND	3.63	1.42	1.37
39	r	318	CHL	C3B-C2B	-3.63	1.35	1.40
26	s	314	CLA	C1D-ND	3.63	1.42	1.37
39	g	312	CHL	C4C-NC	3.63	1.38	1.35
39	S	302	CHL	C3B-C2B	-3.63	1.35	1.40
39	G	301	CHL	CHA-CBD	3.63	1.55	1.51
26	s	304	CLA	C1D-ND	3.63	1.42	1.37
39	n	306	CHL	C4C-NC	3.63	1.38	1.35
26	B	602	CLA	C1D-ND	3.63	1.42	1.37
26	C	505	CLA	C1D-ND	3.63	1.42	1.37
39	G	305	CHL	CHA-CBD	3.62	1.55	1.51
39	G	303	CHL	C3B-C2B	-3.62	1.35	1.40
26	c	510	CLA	C1D-ND	3.62	1.42	1.37
26	g	317	CLA	C1D-ND	3.62	1.42	1.37
26	C	521	CLA	C1D-ND	3.61	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	G	311	CHL	C4C-NC	3.61	1.38	1.35
26	a	409	CLA	C4D-ND	-3.61	1.32	1.37
26	r	308	CLA	C1D-ND	3.61	1.42	1.37
26	R	316	CLA	C1D-ND	3.61	1.42	1.37
39	s	303	CHL	C3B-C2B	-3.61	1.35	1.40
26	s	305	CLA	C1D-ND	3.61	1.42	1.37
26	D	412	CLA	C4D-ND	-3.61	1.32	1.37
39	R	315	CHL	C4C-NC	3.61	1.38	1.35
39	n	319	CHL	C3B-C2B	-3.61	1.35	1.40
39	S	316	CHL	C3B-C2B	-3.60	1.35	1.40
39	r	318	CHL	C4C-NC	3.60	1.38	1.35
39	g	319	CHL	CHA-CBD	3.60	1.55	1.51
26	s	307	CLA	C1D-ND	3.60	1.42	1.37
26	Y	311	CLA	C1D-ND	3.60	1.42	1.37
26	b	614	CLA	C1D-ND	3.60	1.42	1.37
39	n	318	CHL	C4C-NC	3.59	1.38	1.35
26	B	604	CLA	C1D-ND	3.59	1.42	1.37
26	N	307	CLA	C1D-ND	3.59	1.42	1.37
26	R	313	CLA	C1D-ND	3.59	1.42	1.37
26	G	302	CLA	C1D-ND	3.59	1.42	1.37
26	y	306	CLA	C1D-ND	3.59	1.42	1.37
39	y	303	CHL	C3B-C2B	-3.58	1.35	1.40
26	c	514	CLA	C1D-ND	3.58	1.42	1.37
26	S	309	CLA	C1D-ND	3.58	1.42	1.37
26	S	311	CLA	C1D-ND	3.58	1.42	1.37
26	y	313	CLA	C1D-ND	3.58	1.42	1.37
39	N	316	CHL	C4C-NC	3.58	1.38	1.35
26	C	517	CLA	C1D-ND	3.58	1.42	1.37
39	r	301	CHL	C3B-C2B	-3.58	1.35	1.40
39	n	307	CHL	C4C-NC	3.58	1.38	1.35
26	B	607	CLA	C1D-ND	3.58	1.42	1.37
26	C	508	CLA	C1D-ND	3.58	1.42	1.37
26	r	313	CLA	C1D-ND	3.58	1.42	1.37
26	s	315	CLA	C1D-ND	3.58	1.42	1.37
26	d	411	CLA	C4D-ND	-3.58	1.32	1.37
39	N	310	CHL	C3B-C2B	-3.58	1.35	1.40
26	b	616	CLA	C1D-ND	3.57	1.42	1.37
26	r	310	CLA	C1D-ND	3.57	1.42	1.37
39	N	303	CHL	C4C-NC	3.57	1.38	1.35
26	b	612	CLA	C1D-ND	3.57	1.42	1.37
39	R	312	CHL	C3B-C2B	-3.57	1.35	1.40
39	n	311	CHL	C4C-NC	3.57	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	307	CLA	C1D-ND	3.57	1.42	1.37
39	n	308	CHL	C3B-C2B	-3.57	1.35	1.40
26	S	304	CLA	C1D-ND	3.57	1.42	1.37
26	g	302	CLA	C1D-ND	3.57	1.42	1.37
39	Y	314	CHL	C4C-NC	3.57	1.38	1.35
26	C	512	CLA	C4D-ND	-3.57	1.32	1.37
39	N	311	CHL	C4C-NC	3.57	1.38	1.35
39	n	308	CHL	C4C-NC	3.56	1.38	1.35
26	R	307	CLA	C4D-ND	-3.56	1.32	1.37
39	g	307	CHL	C3B-C2B	-3.56	1.35	1.40
26	C	519	CLA	C1D-ND	3.56	1.42	1.37
26	D	401	CLA	C4D-ND	-3.56	1.32	1.37
39	s	303	CHL	C4C-NC	3.56	1.38	1.35
26	n	312	CLA	C1D-ND	3.56	1.42	1.37
42	Y	304	NEX	C12-C13	-3.56	1.38	1.45
26	Y	316	CLA	C1D-ND	3.56	1.42	1.37
26	b	601	CLA	C1D-ND	3.56	1.42	1.37
39	g	313	CHL	C3B-C2B	-3.55	1.35	1.40
39	N	304	CHL	C4C-NC	3.55	1.38	1.35
26	c	520	CLA	C1D-ND	3.55	1.42	1.37
26	S	314	CLA	C1D-ND	3.55	1.42	1.37
39	S	312	CHL	O2D-CGD	3.55	1.41	1.33
26	d	403	CLA	C1D-ND	3.55	1.42	1.37
39	G	301	CHL	C3B-C2B	-3.55	1.35	1.40
26	D	406	CLA	C1D-ND	3.54	1.42	1.37
26	S	303	CLA	C1D-ND	3.54	1.42	1.37
26	c	518	CLA	C1D-ND	3.54	1.42	1.37
42	y	307	NEX	C12-C13	-3.54	1.38	1.45
39	r	301	CHL	CHA-CBD	3.53	1.55	1.51
26	C	504	CLA	C1D-ND	3.53	1.42	1.37
26	c	515	CLA	C4D-ND	-3.53	1.32	1.37
39	G	303	CHL	CHA-CBD	3.53	1.55	1.51
26	B	612	CLA	C1D-ND	3.53	1.42	1.37
26	R	310	CLA	C1D-ND	3.53	1.42	1.37
39	s	303	CHL	CHA-CBD	3.53	1.55	1.51
39	R	318	CHL	C4C-NC	3.53	1.38	1.35
42	r	302	NEX	C12-C13	-3.53	1.38	1.45
39	S	302	CHL	O2D-CGD	3.52	1.41	1.33
39	r	309	CHL	C3B-C2B	-3.52	1.35	1.40
39	S	313	CHL	C3B-C2B	-3.52	1.35	1.40
26	B	617	CLA	C4D-ND	-3.52	1.32	1.37
39	g	313	CHL	CHA-CBD	3.52	1.55	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	610	CLA	C4D-ND	-3.52	1.32	1.37
39	R	301	CHL	C4C-NC	3.52	1.38	1.35
26	c	515	CLA	C1D-ND	3.52	1.42	1.37
26	b	607	CLA	C1D-ND	3.51	1.42	1.37
39	y	312	CHL	CHA-CBD	3.51	1.55	1.51
26	c	513	CLA	C1D-ND	3.51	1.42	1.37
39	s	313	CHL	O2D-CGD	3.51	1.41	1.33
39	s	317	CHL	C3B-C2B	-3.51	1.35	1.40
26	Y	308	CLA	C1D-ND	3.51	1.42	1.37
26	Y	305	CLA	C1D-ND	3.51	1.42	1.37
26	n	303	CLA	C1D-ND	3.51	1.42	1.37
26	n	304	CLA	C1D-ND	3.50	1.42	1.37
26	N	308	CLA	C1D-ND	3.50	1.42	1.37
42	R	305	NEX	C12-C13	-3.50	1.38	1.45
39	g	314	CHL	O2D-CGD	3.50	1.41	1.33
26	d	403	CLA	C4D-ND	-3.50	1.32	1.37
42	g	306	NEX	C12-C13	-3.50	1.38	1.45
39	S	316	CHL	CHA-CBD	3.50	1.55	1.51
42	N	302	NEX	C12-C13	-3.50	1.38	1.45
39	n	318	CHL	CHA-CBD	3.49	1.55	1.51
26	B	610	CLA	C1D-ND	3.49	1.42	1.37
39	G	309	CHL	O2D-CGD	3.49	1.41	1.33
39	r	316	CHL	C4C-NC	3.49	1.38	1.35
39	s	316	CHL	O2D-CGD	3.49	1.41	1.33
39	S	316	CHL	C4C-NC	3.49	1.38	1.35
39	g	312	CHL	CHA-CBD	3.49	1.55	1.51
26	R	308	CLA	C1D-ND	3.48	1.42	1.37
39	g	307	CHL	CHA-CBD	3.48	1.55	1.51
26	d	411	CLA	MG-ND	-3.48	1.98	2.05
39	r	316	CHL	CHA-CBD	3.47	1.55	1.51
26	B	613	CLA	C4D-ND	-3.47	1.32	1.37
39	G	305	CHL	C3B-C2B	-3.47	1.35	1.40
39	R	315	CHL	C3B-C2B	-3.47	1.35	1.40
39	r	316	CHL	O2D-CGD	3.47	1.41	1.33
26	r	306	CLA	C1D-ND	3.47	1.42	1.37
26	B	601	CLA	C1D-ND	3.47	1.42	1.37
26	N	312	CLA	C1D-ND	3.47	1.42	1.37
26	b	602	CLA	C1D-ND	3.47	1.42	1.37
39	r	301	CHL	C4C-NC	3.46	1.38	1.35
26	b	605	CLA	C4D-ND	-3.46	1.32	1.37
42	n	313	NEX	C12-C13	-3.46	1.38	1.45
26	b	604	CLA	C4D-ND	-3.46	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	G	311	CHL	CHA-CBD	3.46	1.55	1.51
42	s	302	NEX	C12-C13	-3.46	1.38	1.45
39	g	319	CHL	C3B-C2B	-3.45	1.35	1.40
39	N	303	CHL	CHA-CBD	3.45	1.55	1.51
39	N	311	CHL	O2D-CGD	3.45	1.41	1.33
26	B	602	CLA	C4D-ND	-3.45	1.33	1.37
39	G	318	CHL	O2D-CGD	3.45	1.41	1.33
39	S	313	CHL	O2D-CGD	3.44	1.41	1.33
26	b	617	CLA	C1D-ND	3.44	1.42	1.37
26	r	311	CLA	C1D-ND	3.44	1.42	1.37
39	R	301	CHL	O2D-CGD	3.44	1.41	1.33
26	D	409	CLA	C4D-ND	-3.44	1.33	1.37
42	G	315	NEX	C12-C13	-3.43	1.38	1.45
42	S	305	NEX	C12-C13	-3.43	1.38	1.45
26	R	306	CLA	C1D-ND	3.43	1.42	1.37
39	Y	318	CHL	O2D-CGD	3.43	1.41	1.33
39	N	316	CHL	C3B-C2B	-3.43	1.35	1.40
39	g	313	CHL	O2D-CGD	3.43	1.41	1.33
26	C	512	CLA	C1D-ND	3.43	1.42	1.37
39	R	318	CHL	CHA-CBD	3.43	1.55	1.51
39	g	311	CHL	O2D-CGD	3.43	1.41	1.33
26	C	508	CLA	C4D-ND	-3.42	1.33	1.37
39	G	305	CHL	O2D-CGD	3.42	1.41	1.33
26	D	406	CLA	C4D-ND	-3.42	1.33	1.37
26	N	313	CLA	C1D-ND	3.42	1.42	1.37
39	G	318	CHL	C3B-C2B	-3.42	1.35	1.40
26	B	617	CLA	C1D-ND	3.41	1.42	1.37
26	b	610	CLA	C1D-ND	3.41	1.42	1.37
39	y	302	CHL	O2D-CGD	3.41	1.41	1.33
26	d	404	CLA	C4D-ND	-3.41	1.33	1.37
39	g	319	CHL	O2D-CGD	3.41	1.41	1.33
39	n	307	CHL	O2D-CGD	3.41	1.41	1.33
39	N	303	CHL	C3B-C2B	-3.41	1.35	1.40
39	g	311	CHL	C4C-NC	3.41	1.38	1.35
26	c	502	CLA	C1D-ND	3.40	1.42	1.37
39	s	317	CHL	O2D-CGD	3.40	1.41	1.33
26	a	411	CLA	C1D-ND	3.40	1.42	1.37
39	G	301	CHL	O2D-CGD	3.40	1.41	1.33
26	B	613	CLA	C1D-ND	3.40	1.42	1.37
26	b	604	CLA	C1D-ND	3.40	1.42	1.37
39	n	318	CHL	C3B-C2B	-3.39	1.35	1.40
26	B	611	CLA	C1D-ND	3.39	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	S	302	CHL	CHA-CBD	3.39	1.55	1.51
39	Y	302	CHL	CHA-CBD	3.39	1.55	1.51
26	D	401	CLA	C1D-ND	3.39	1.41	1.37
26	A	405	CLA	C1D-ND	3.39	1.41	1.37
39	s	317	CHL	CHA-CBD	3.38	1.55	1.51
26	b	606	CLA	C1D-ND	3.38	1.41	1.37
39	n	306	CHL	C3B-C2B	-3.38	1.35	1.40
39	y	303	CHL	O2D-CGD	3.38	1.41	1.33
39	n	311	CHL	O2D-CGD	3.38	1.41	1.33
39	n	319	CHL	O2D-CGD	3.38	1.41	1.33
30	d	408	PL9	C3-C4	-3.37	1.44	1.49
26	A	403	CLA	C4D-ND	-3.37	1.33	1.37
39	Y	314	CHL	O2D-CGD	3.37	1.41	1.33
39	g	311	CHL	C3B-C2B	-3.37	1.35	1.40
26	B	611	CLA	C4D-ND	-3.37	1.33	1.37
39	n	307	CHL	CHA-CBD	3.37	1.55	1.51
26	c	513	CLA	C4D-ND	-3.37	1.33	1.37
26	D	412	CLA	MG-ND	-3.37	1.99	2.05
39	S	313	CHL	CHA-CBD	3.37	1.55	1.51
26	g	302	CLA	C4B-NB	3.37	1.41	1.37
39	N	304	CHL	CHA-CBD	3.36	1.55	1.51
39	S	312	CHL	C3B-C2B	-3.36	1.35	1.40
39	N	310	CHL	O2D-CGD	3.36	1.41	1.33
39	N	311	CHL	CHA-CBD	3.36	1.55	1.51
26	B	601	CLA	C4D-ND	-3.36	1.33	1.37
39	y	303	CHL	C4C-NC	3.36	1.38	1.35
39	n	308	CHL	O2D-CGD	3.36	1.41	1.33
39	N	317	CHL	O2D-CGD	3.36	1.41	1.33
26	A	403	CLA	C1D-ND	3.36	1.41	1.37
39	Y	302	CHL	O2D-CGD	3.36	1.41	1.33
26	c	516	CLA	C4D-ND	-3.35	1.33	1.37
26	C	517	CLA	C4D-ND	-3.35	1.33	1.37
39	y	305	CHL	CHA-CBD	3.35	1.55	1.51
26	B	603	CLA	C1D-ND	3.35	1.41	1.37
26	C	506	CLA	C1D-ND	3.35	1.41	1.37
39	g	312	CHL	O2D-CGD	3.35	1.41	1.33
39	s	313	CHL	C3B-C2B	-3.35	1.35	1.40
26	b	606	CLA	C4D-ND	-3.35	1.33	1.37
26	y	304	CLA	C4B-NB	3.35	1.41	1.37
39	G	303	CHL	O2D-CGD	3.35	1.41	1.33
26	b	601	CLA	C4D-ND	-3.35	1.33	1.37
39	Y	317	CHL	C3B-C2B	-3.34	1.35	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Y	317	CHL	O2D-CGD	3.34	1.41	1.33
39	G	318	CHL	C4C-NC	3.34	1.38	1.35
26	Y	305	CLA	C4B-NB	3.34	1.41	1.37
39	r	318	CHL	O2D-CGD	3.34	1.41	1.33
39	s	303	CHL	O2D-CGD	3.34	1.41	1.33
39	g	307	CHL	O2D-CGD	3.34	1.41	1.33
39	N	304	CHL	O2D-CGD	3.34	1.41	1.33
39	N	317	CHL	CHA-CBD	3.33	1.55	1.51
39	G	311	CHL	O2D-CGD	3.33	1.41	1.33
39	N	310	CHL	CHA-CBD	3.33	1.55	1.51
26	a	402	CLA	C4D-ND	-3.33	1.33	1.37
39	S	316	CHL	O2D-CGD	3.33	1.41	1.33
39	y	302	CHL	CHA-CBD	3.33	1.55	1.51
39	n	319	CHL	CHA-CBD	3.33	1.55	1.51
39	R	312	CHL	O2D-CGD	3.33	1.41	1.33
39	n	311	CHL	CHA-CBD	3.33	1.55	1.51
39	y	305	CHL	O2D-CGD	3.33	1.41	1.33
39	Y	318	CHL	CHA-CBD	3.33	1.55	1.51
26	c	503	CLA	C1D-ND	3.33	1.41	1.37
38	e	101	HEM	FE-NB	3.33	2.05	1.94
26	B	606	CLA	C4D-ND	-3.33	1.33	1.37
39	r	309	CHL	O2D-CGD	3.32	1.41	1.33
39	r	309	CHL	CHA-CBD	3.32	1.55	1.51
39	Y	302	CHL	C4C-NC	3.32	1.38	1.35
26	B	615	CLA	MG-ND	-3.32	1.99	2.05
39	N	311	CHL	C3B-C2B	-3.32	1.35	1.40
26	r	314	CLA	C4D-ND	-3.32	1.33	1.37
26	y	313	CLA	C4B-NB	3.32	1.41	1.37
39	R	312	CHL	CHA-CBD	3.32	1.55	1.51
26	a	409	CLA	C1D-ND	3.32	1.41	1.37
39	Y	317	CHL	CHA-CBD	3.32	1.55	1.51
26	A	405	CLA	C4D-ND	-3.32	1.33	1.37
26	g	318	CLA	C4B-NB	3.31	1.41	1.37
26	c	503	CLA	C4D-ND	-3.31	1.33	1.37
39	n	318	CHL	O2D-CGD	3.31	1.41	1.33
39	N	316	CHL	O2D-CGD	3.31	1.41	1.33
39	y	312	CHL	O2D-CGD	3.31	1.41	1.33
39	y	305	CHL	C4C-NC	3.31	1.38	1.35
26	G	302	CLA	C4B-NB	3.31	1.41	1.37
39	G	318	CHL	CHA-CBD	3.31	1.55	1.51
26	n	305	CLA	C4D-ND	-3.30	1.33	1.37
39	n	306	CHL	O2D-CGD	3.30	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	402	CLA	C1D-ND	3.30	1.41	1.37
39	Y	314	CHL	C3B-C2B	-3.30	1.35	1.40
26	b	604	CLA	MG-NB	-3.30	1.99	2.05
30	D	411	PL9	C3-C4	-3.30	1.44	1.49
26	n	310	CLA	C4B-NB	3.30	1.41	1.37
39	n	308	CHL	CHA-CBD	3.30	1.55	1.51
39	G	309	CHL	C3B-C2B	-3.30	1.35	1.40
39	n	307	CHL	C3B-C2B	-3.30	1.35	1.40
39	y	312	CHL	C3B-C2B	-3.30	1.35	1.40
39	N	303	CHL	O2D-CGD	3.30	1.41	1.33
26	a	411	CLA	C4D-ND	-3.30	1.33	1.37
39	s	316	CHL	CHA-CBD	3.29	1.55	1.51
26	r	306	CLA	C4D-ND	-3.29	1.33	1.37
26	b	607	CLA	C4D-ND	-3.29	1.33	1.37
39	R	315	CHL	O2D-CGD	3.29	1.41	1.33
39	y	305	CHL	C3B-C2B	-3.29	1.35	1.40
26	N	319	CLA	C4B-NB	3.28	1.41	1.37
26	B	603	CLA	C4D-ND	-3.28	1.33	1.37
26	b	602	CLA	C4D-ND	-3.27	1.33	1.37
39	Y	317	CHL	C4C-NC	3.27	1.38	1.35
26	B	609	CLA	C1D-ND	3.27	1.41	1.37
26	C	511	CLA	C1D-ND	3.27	1.41	1.37
39	g	314	CHL	C3B-C2B	-3.27	1.35	1.40
39	r	301	CHL	O2D-CGD	3.27	1.41	1.33
39	s	313	CHL	CHA-CBD	3.27	1.55	1.51
26	B	609	CLA	C4D-ND	-3.27	1.33	1.37
26	R	306	CLA	C4D-ND	-3.27	1.33	1.37
26	G	304	CLA	C4B-NB	3.26	1.41	1.37
26	C	505	CLA	C4D-ND	-3.26	1.33	1.37
26	C	519	CLA	C4D-ND	-3.26	1.33	1.37
26	C	511	CLA	C4D-ND	-3.26	1.33	1.37
39	g	311	CHL	CHA-CBD	3.26	1.55	1.51
26	C	515	CLA	C4D-ND	-3.26	1.33	1.37
26	N	308	CLA	C4B-NB	3.26	1.41	1.37
26	g	304	CLA	C4B-NB	3.26	1.41	1.37
26	b	613	CLA	C4D-ND	-3.26	1.33	1.37
26	C	520	CLA	C4B-C3B	3.26	1.49	1.38
39	y	303	CHL	CHA-CBD	3.26	1.55	1.51
26	R	313	CLA	C4D-ND	-3.26	1.33	1.37
26	c	504	CLA	C4D-ND	-3.26	1.33	1.37
39	S	312	CHL	CHA-CBD	3.26	1.55	1.51
26	B	618	CLA	C4D-ND	-3.26	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	313	CLA	C4B-NB	3.26	1.41	1.37
26	R	314	CLA	C4B-NB	3.26	1.41	1.37
26	Y	316	CLA	C4B-NB	3.26	1.41	1.37
26	c	506	CLA	C4D-ND	-3.25	1.33	1.37
39	R	318	CHL	O2D-CGD	3.25	1.41	1.33
39	y	314	CHL	CHA-CBD	3.25	1.55	1.51
26	R	302	CLA	C4D-ND	-3.25	1.33	1.37
39	Y	307	CHL	O2D-CGD	3.25	1.41	1.33
26	r	317	CLA	C4B-NB	3.25	1.41	1.37
26	s	305	CLA	C4D-ND	-3.25	1.33	1.37
26	B	604	CLA	MG-ND	-3.24	1.99	2.05
26	b	618	CLA	C1D-ND	3.24	1.41	1.37
26	b	611	CLA	MG-ND	-3.24	1.99	2.05
26	Y	312	CLA	C4B-NB	3.24	1.41	1.37
26	b	614	CLA	C4D-ND	-3.24	1.33	1.37
26	c	506	CLA	C4B-C3B	3.24	1.49	1.38
26	Y	301	CLA	C4B-NB	3.24	1.41	1.37
26	c	520	CLA	C4D-ND	-3.24	1.33	1.37
26	R	313	CLA	C4B-NB	3.24	1.41	1.37
39	y	314	CHL	O2D-CGD	3.24	1.41	1.33
26	Y	316	CLA	C4D-ND	-3.24	1.33	1.37
26	C	520	CLA	C4D-ND	-3.24	1.33	1.37
39	Y	307	CHL	CHA-CBD	3.23	1.55	1.51
26	r	314	CLA	C4B-NB	3.23	1.41	1.37
26	y	310	CLA	C4B-NB	3.23	1.41	1.37
26	S	311	CLA	C4D-ND	-3.23	1.33	1.37
26	N	307	CLA	C4D-ND	-3.23	1.33	1.37
26	g	315	CLA	C4B-NB	3.22	1.41	1.37
26	B	610	CLA	C4D-ND	-3.22	1.33	1.37
42	y	307	NEX	C14-C13	3.22	1.40	1.35
26	g	305	CLA	C4B-NB	3.21	1.41	1.37
26	Y	305	CLA	C4D-ND	-3.21	1.33	1.37
26	Y	311	CLA	C4D-ND	-3.21	1.33	1.37
26	c	510	CLA	C4D-ND	-3.21	1.33	1.37
26	y	309	CLA	C4D-ND	-3.21	1.33	1.37
26	b	618	CLA	C4D-ND	-3.21	1.33	1.37
26	C	520	CLA	C1D-ND	3.21	1.42	1.37
26	n	312	CLA	C4B-NB	3.20	1.41	1.37
26	G	314	CLA	MG-ND	-3.20	1.99	2.05
26	g	303	CLA	MG-ND	-3.20	1.99	2.05
26	G	319	CLA	C4B-NB	3.20	1.41	1.37
26	y	310	CLA	C4D-ND	-3.20	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	y	313	CLA	C4D-ND	-3.20	1.33	1.37
42	Y	304	NEX	C14-C13	3.19	1.40	1.35
39	R	315	CHL	CHA-CBD	3.19	1.55	1.51
26	b	617	CLA	C4D-ND	-3.19	1.33	1.37
26	y	306	CLA	C4D-ND	-3.19	1.33	1.37
26	y	315	CLA	C4D-ND	-3.19	1.33	1.37
26	N	309	CLA	C4B-NB	3.19	1.41	1.37
38	E	101	HEM	FE-NB	3.18	2.04	1.94
26	r	305	CLA	C4B-NB	3.18	1.41	1.37
26	C	521	CLA	C4D-ND	-3.18	1.33	1.37
26	G	314	CLA	C4D-ND	-3.18	1.33	1.37
26	c	508	CLA	C4D-ND	-3.18	1.33	1.37
26	c	514	CLA	C4D-ND	-3.18	1.33	1.37
26	y	309	CLA	C4B-NB	3.18	1.41	1.37
26	r	313	CLA	C4D-ND	-3.18	1.33	1.37
42	G	315	NEX	C14-C13	3.17	1.40	1.35
26	G	306	CLA	C4B-NB	3.17	1.41	1.37
26	S	304	CLA	C4D-ND	-3.17	1.33	1.37
26	S	307	CLA	C4D-ND	-3.17	1.33	1.37
26	s	311	CLA	C4D-ND	-3.17	1.33	1.37
26	B	612	CLA	C4D-ND	-3.17	1.33	1.37
26	s	314	CLA	C4D-ND	-3.17	1.33	1.37
26	n	309	CLA	C4B-NB	3.16	1.41	1.37
26	S	307	CLA	C4B-NB	3.16	1.41	1.37
39	S	312	CHL	C4C-NC	3.16	1.38	1.35
26	n	303	CLA	C4D-ND	-3.16	1.33	1.37
26	C	504	CLA	C4B-NB	3.16	1.41	1.37
26	S	314	CLA	C4B-NB	3.16	1.41	1.37
26	b	614	CLA	C4B-NB	3.16	1.41	1.37
26	Y	311	CLA	C4B-NB	3.16	1.41	1.37
26	Y	312	CLA	C4D-ND	-3.16	1.33	1.37
39	s	313	CHL	C4C-NC	3.16	1.38	1.35
26	r	308	CLA	C4B-NB	3.16	1.41	1.37
26	b	612	CLA	MG-ND	-3.16	1.99	2.05
26	c	505	CLA	C4D-ND	-3.15	1.33	1.37
26	c	506	CLA	C1D-ND	3.15	1.42	1.37
26	N	306	CLA	C4D-ND	-3.15	1.33	1.37
26	S	303	CLA	C4B-NB	3.15	1.41	1.37
26	Y	308	CLA	C4D-ND	-3.15	1.33	1.37
26	b	607	CLA	C4B-NB	3.15	1.41	1.37
26	n	315	CLA	C4D-ND	-3.15	1.33	1.37
42	g	306	NEX	C14-C13	3.14	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N	312	CLA	C4D-ND	-3.14	1.33	1.37
26	B	601	CLA	C4B-NB	3.14	1.41	1.37
26	C	516	CLA	C4D-ND	-3.14	1.33	1.37
42	s	302	NEX	C14-C13	3.14	1.39	1.35
26	Y	313	CLA	C4D-ND	-3.14	1.33	1.37
26	R	309	CLA	C4B-NB	3.14	1.41	1.37
26	N	309	CLA	C4D-ND	-3.14	1.33	1.37
26	b	612	CLA	C4D-ND	-3.14	1.33	1.37
42	n	313	NEX	C14-C13	3.14	1.39	1.35
39	n	306	CHL	CHA-CBD	3.14	1.55	1.51
26	c	502	CLA	C4D-ND	-3.14	1.33	1.37
26	S	304	CLA	C4B-NB	3.14	1.41	1.37
26	S	314	CLA	C4D-ND	-3.13	1.33	1.37
26	y	304	CLA	C4D-ND	-3.13	1.33	1.37
26	s	311	CLA	C4B-NB	3.13	1.41	1.37
26	R	317	CLA	C4B-NB	3.13	1.41	1.37
26	r	315	CLA	C4B-NB	3.13	1.41	1.37
26	S	310	CLA	C4B-NB	3.13	1.41	1.37
26	y	317	CLA	C4D-ND	-3.13	1.33	1.37
39	N	316	CHL	CHA-CBD	3.13	1.55	1.51
26	Y	310	CLA	C4B-NB	3.13	1.41	1.37
26	s	315	CLA	C4B-NB	3.12	1.41	1.37
26	C	507	CLA	C4D-ND	-3.12	1.33	1.37
26	s	307	CLA	C4B-NB	3.12	1.41	1.37
26	B	613	CLA	MG-NB	-3.12	1.99	2.05
26	n	302	CLA	C4B-NB	3.12	1.41	1.37
26	n	315	CLA	MG-ND	-3.12	1.99	2.05
26	Y	310	CLA	C4D-ND	-3.12	1.33	1.37
26	s	304	CLA	C4B-NB	3.12	1.41	1.37
26	C	505	CLA	C4B-NB	3.12	1.41	1.37
26	G	307	CLA	C4D-ND	-3.12	1.33	1.37
27	a	410	PHO	C4D-CHA	3.12	1.44	1.39
26	g	308	CLA	C4B-NB	3.12	1.41	1.37
26	S	310	CLA	C4D-ND	-3.12	1.33	1.37
26	S	308	CLA	C4B-NB	3.11	1.41	1.37
42	r	302	NEX	C14-C13	3.11	1.39	1.35
26	C	508	CLA	C4B-NB	3.11	1.41	1.37
26	b	608	CLA	C4D-ND	-3.11	1.33	1.37
26	B	604	CLA	C4B-NB	3.11	1.41	1.37
26	B	605	CLA	C4D-ND	-3.11	1.33	1.37
26	S	309	CLA	C4B-NB	3.11	1.41	1.37
26	s	306	CLA	C4B-NB	3.11	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	504	CLA	C4D-ND	-3.11	1.33	1.37
26	d	404	CLA	C1D-ND	3.11	1.41	1.37
26	g	303	CLA	C4B-NB	3.11	1.41	1.37
26	g	303	CLA	C4D-ND	-3.11	1.33	1.37
26	B	604	CLA	C4D-ND	-3.10	1.33	1.37
26	b	616	CLA	C4D-ND	-3.10	1.33	1.37
26	D	409	CLA	C1D-ND	3.10	1.41	1.37
26	N	306	CLA	C4B-NB	3.10	1.41	1.37
26	B	612	CLA	C4B-NB	3.10	1.41	1.37
26	G	314	CLA	C4B-NB	3.10	1.41	1.37
26	R	306	CLA	C4B-NB	3.10	1.41	1.37
26	s	314	CLA	C4B-NB	3.10	1.41	1.37
26	N	307	CLA	C4B-NB	3.10	1.41	1.37
26	b	609	CLA	C4D-ND	-3.10	1.33	1.37
26	n	309	CLA	C4D-ND	-3.10	1.33	1.37
26	b	612	CLA	C4B-NB	3.10	1.41	1.37
26	r	311	CLA	C4B-NB	3.10	1.41	1.37
26	g	308	CLA	C4D-ND	-3.10	1.33	1.37
26	R	308	CLA	C4B-NB	3.10	1.41	1.37
26	G	317	CLA	C4B-NB	3.10	1.41	1.37
26	s	301	CLA	C4B-NB	3.09	1.41	1.37
26	s	310	CLA	C4D-ND	-3.09	1.33	1.37
26	s	315	CLA	C4D-ND	-3.09	1.33	1.37
26	c	516	CLA	C4B-NB	3.09	1.41	1.37
26	d	404	CLA	C4B-NB	3.09	1.41	1.37
26	y	306	CLA	C4B-NB	3.09	1.41	1.37
26	y	316	CLA	C4D-ND	-3.09	1.33	1.37
26	r	310	CLA	C4D-ND	-3.09	1.33	1.37
26	R	310	CLA	C4D-ND	-3.09	1.33	1.37
39	g	307	CHL	O2A-CGA	3.09	1.42	1.33
26	B	607	CLA	C4D-ND	-3.08	1.33	1.37
26	N	306	CLA	MG-ND	-3.08	1.99	2.05
26	G	317	CLA	C4D-ND	-3.08	1.33	1.37
26	r	303	CLA	C4D-ND	-3.08	1.33	1.37
42	N	302	NEX	C14-C13	3.08	1.39	1.35
26	R	316	CLA	C4D-ND	-3.08	1.33	1.37
26	S	311	CLA	C4B-NB	3.08	1.41	1.37
26	S	315	CLA	C4B-NB	3.08	1.41	1.37
26	n	315	CLA	C4B-NB	3.08	1.41	1.37
26	g	317	CLA	C4D-ND	-3.08	1.33	1.37
26	b	617	CLA	C4B-NB	3.08	1.41	1.37
26	n	305	CLA	C4B-NB	3.08	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	S	305	NEX	C14-C13	3.08	1.39	1.35
26	s	306	CLA	C4D-ND	-3.07	1.33	1.37
26	r	303	CLA	C4B-NB	3.07	1.41	1.37
26	G	319	CLA	C4D-ND	-3.07	1.33	1.37
26	b	616	CLA	C4B-NB	3.07	1.41	1.37
42	R	305	NEX	C14-C13	3.07	1.39	1.35
26	Y	301	CLA	C4D-ND	-3.07	1.33	1.37
26	c	518	CLA	C4B-NB	3.07	1.41	1.37
26	R	316	CLA	C4B-NB	3.06	1.41	1.37
27	A	404	PHO	C4D-CHA	3.06	1.44	1.39
26	c	508	CLA	C4B-NB	3.06	1.41	1.37
30	D	411	PL9	C6-C1	-3.06	1.43	1.48
26	s	307	CLA	C4D-ND	-3.06	1.33	1.37
39	G	303	CHL	O2A-CGA	3.06	1.42	1.33
26	s	310	CLA	C4B-NB	3.06	1.41	1.37
26	n	312	CLA	C4D-ND	-3.05	1.33	1.37
26	r	311	CLA	C4D-ND	-3.05	1.33	1.37
26	B	610	CLA	C4B-NB	3.05	1.41	1.37
26	b	608	CLA	C4B-NB	3.05	1.41	1.37
26	s	305	CLA	C4B-NB	3.05	1.41	1.37
26	N	318	CLA	C4B-NB	3.05	1.41	1.37
39	G	301	CHL	O2A-CGA	3.05	1.42	1.33
26	y	316	CLA	C4B-NB	3.04	1.41	1.37
26	D	409	CLA	C4B-NB	3.04	1.41	1.37
26	c	505	CLA	C4B-NB	3.04	1.41	1.37
26	C	505	CLA	C3B-C4B	3.04	1.49	1.42
26	S	303	CLA	C4D-ND	-3.04	1.33	1.37
26	c	520	CLA	C4B-NB	3.04	1.41	1.37
26	G	302	CLA	C4D-ND	-3.04	1.33	1.37
39	g	319	CHL	O2A-CGA	3.03	1.42	1.33
26	S	311	CLA	C3B-C4B	3.03	1.49	1.42
26	R	308	CLA	C4D-ND	-3.03	1.33	1.37
26	C	512	CLA	C4B-NB	3.03	1.41	1.37
39	g	313	CHL	O2A-CGA	3.03	1.42	1.33
39	N	304	CHL	O2A-CGA	3.03	1.42	1.33
26	N	308	CLA	C4D-ND	-3.03	1.33	1.37
26	R	317	CLA	C4D-ND	-3.03	1.33	1.37
26	g	305	CLA	C4D-ND	-3.03	1.33	1.37
39	y	312	CHL	O2A-CGA	3.03	1.42	1.33
26	S	315	CLA	C4D-ND	-3.03	1.33	1.37
38	e	101	HEM	FE-NA	3.03	2.05	1.95
26	C	506	CLA	C4D-ND	-3.02	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	g	304	CLA	C4D-ND	-3.02	1.33	1.37
39	G	305	CHL	O2A-CGA	3.02	1.42	1.33
26	C	511	CLA	C4B-NB	3.02	1.41	1.37
30	d	408	PL9	C6-C1	-3.02	1.43	1.48
39	S	313	CHL	O2A-CGA	3.02	1.42	1.33
26	N	312	CLA	C4B-NB	3.02	1.41	1.37
26	y	317	CLA	C4B-NB	3.02	1.41	1.37
26	R	314	CLA	C4D-ND	-3.02	1.33	1.37
39	R	301	CHL	O2A-CGA	3.02	1.42	1.33
26	d	403	CLA	C4B-NB	3.02	1.41	1.37
26	y	315	CLA	C4B-NB	3.01	1.41	1.37
39	n	311	CHL	O2A-CGA	3.01	1.42	1.33
39	r	316	CHL	O2A-CGA	3.01	1.42	1.33
26	B	605	CLA	C4B-NB	3.01	1.41	1.37
26	D	406	CLA	C4B-NB	3.01	1.41	1.37
39	N	303	CHL	O2A-CGA	3.01	1.42	1.33
26	G	306	CLA	C4D-ND	-3.01	1.33	1.37
26	C	516	CLA	C4B-NB	3.01	1.41	1.37
26	B	606	CLA	C4B-NB	3.01	1.41	1.37
26	r	317	CLA	C4D-ND	-3.01	1.33	1.37
26	b	604	CLA	C4B-NB	3.00	1.41	1.37
39	Y	314	CHL	O2A-CGA	3.00	1.42	1.33
26	g	302	CLA	C4D-ND	-3.00	1.33	1.37
26	B	616	CLA	C4D-ND	-3.00	1.33	1.37
26	n	303	CLA	C4B-NB	3.00	1.41	1.37
26	r	306	CLA	C4B-NB	3.00	1.41	1.37
26	C	507	CLA	C4B-NB	3.00	1.41	1.37
26	r	308	CLA	C4D-ND	-2.99	1.33	1.37
26	s	304	CLA	C4D-ND	-2.99	1.33	1.37
26	Y	308	CLA	C3B-C4B	2.99	1.49	1.42
39	r	309	CHL	O2A-CGA	2.99	1.42	1.33
26	r	305	CLA	C3B-C4B	2.99	1.49	1.42
26	B	611	CLA	C4B-NB	2.99	1.41	1.37
26	Y	308	CLA	C4B-NB	2.99	1.41	1.37
26	G	304	CLA	C4D-ND	-2.99	1.33	1.37
26	c	520	CLA	C3B-C4B	2.98	1.49	1.42
39	n	311	CHL	C3B-C2B	-2.98	1.36	1.40
26	c	518	CLA	C4D-ND	-2.98	1.33	1.37
26	r	315	CLA	C4D-ND	-2.98	1.33	1.37
26	Y	305	CLA	C3B-C4B	2.98	1.49	1.42
26	S	309	CLA	C4D-ND	-2.98	1.33	1.37
26	c	515	CLA	C4B-NB	2.98	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	309	CLA	C3B-C4B	2.98	1.49	1.42
26	g	318	CLA	C4D-ND	-2.98	1.33	1.37
26	B	613	CLA	C4B-NB	2.98	1.41	1.37
26	R	310	CLA	C4B-NB	2.98	1.41	1.37
39	G	309	CHL	O2A-CGA	2.97	1.42	1.33
39	R	312	CHL	O2A-CGA	2.97	1.42	1.33
26	Y	313	CLA	C4B-NB	2.97	1.41	1.37
26	R	307	CLA	C3B-C4B	2.97	1.49	1.42
39	N	316	CHL	O2A-CGA	2.97	1.42	1.33
39	N	310	CHL	O2A-CGA	2.97	1.42	1.33
26	b	601	CLA	C4B-NB	2.97	1.41	1.37
26	R	309	CLA	C4D-ND	-2.97	1.33	1.37
26	b	606	CLA	C4B-NB	2.97	1.41	1.37
26	y	306	CLA	C3B-C4B	2.97	1.49	1.42
39	n	318	CHL	O2A-CGA	2.97	1.42	1.33
26	s	301	CLA	C4D-ND	-2.97	1.33	1.37
38	E	101	HEM	CAB-C3B	2.97	1.55	1.47
39	r	318	CHL	O2A-CGA	2.96	1.42	1.33
38	e	101	HEM	CAB-C3B	2.96	1.55	1.47
26	B	607	CLA	C4B-NB	2.96	1.41	1.37
39	s	317	CHL	O2A-CGA	2.96	1.42	1.33
39	g	314	CHL	O2A-CGA	2.96	1.42	1.33
38	E	101	HEM	FE-NA	2.96	2.05	1.95
39	R	301	CHL	C3B-C2B	-2.96	1.36	1.40
39	n	308	CHL	O2A-CGA	2.96	1.42	1.33
26	g	317	CLA	C4B-NB	2.96	1.41	1.37
26	b	602	CLA	C4B-NB	2.95	1.41	1.37
26	c	503	CLA	C4B-NB	2.95	1.41	1.37
39	n	306	CHL	O2A-CGA	2.95	1.42	1.33
26	S	308	CLA	C4D-ND	-2.95	1.33	1.37
26	N	318	CLA	C4D-ND	-2.95	1.33	1.37
26	g	315	CLA	C4D-ND	-2.95	1.33	1.37
27	d	407	PHO	C4D-CHA	2.94	1.44	1.39
26	B	617	CLA	C4B-NB	2.94	1.41	1.37
39	r	316	CHL	C3B-C2B	-2.94	1.36	1.40
26	n	302	CLA	C4D-ND	-2.94	1.33	1.37
39	g	312	CHL	O2A-CGA	2.94	1.41	1.33
26	a	402	CLA	C4B-NB	2.94	1.41	1.37
39	s	303	CHL	O2A-CGA	2.94	1.41	1.33
26	s	314	CLA	C3B-C4B	2.94	1.49	1.42
39	R	315	CHL	O2A-CGA	2.94	1.41	1.33
39	N	304	CHL	C3B-C2B	-2.94	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	610	CLA	C4B-NB	2.93	1.41	1.37
39	N	317	CHL	O2A-CGA	2.93	1.41	1.33
39	n	319	CHL	O2A-CGA	2.93	1.41	1.33
26	N	313	CLA	C4D-ND	-2.93	1.33	1.37
38	e	101	HEM	FE-ND	2.93	2.03	1.94
42	r	302	NEX	C32-C33	-2.92	1.39	1.45
39	G	311	CHL	O2A-CGA	2.92	1.41	1.33
26	b	605	CLA	C4B-NB	2.92	1.41	1.37
27	D	403	PHO	C4D-CHA	2.92	1.44	1.39
26	r	305	CLA	C4D-ND	-2.92	1.33	1.37
39	s	316	CHL	O2A-CGA	2.92	1.41	1.33
26	n	304	CLA	C4D-ND	-2.92	1.33	1.37
26	y	309	CLA	C3B-C4B	2.92	1.49	1.42
26	n	304	CLA	C4B-NB	2.92	1.41	1.37
26	g	318	CLA	C3B-C4B	2.92	1.49	1.42
26	G	313	CLA	C4D-ND	-2.92	1.33	1.37
39	s	313	CHL	O2A-CGA	2.92	1.41	1.33
39	y	305	CHL	O2A-CGA	2.92	1.41	1.33
26	b	611	CLA	C4B-NB	2.92	1.41	1.37
26	b	617	CLA	C3B-C4B	2.91	1.49	1.42
26	A	405	CLA	C4B-NB	2.91	1.41	1.37
26	N	313	CLA	C4B-NB	2.91	1.41	1.37
39	r	318	CHL	CHA-CBD	2.91	1.55	1.51
26	n	310	CLA	C4D-ND	-2.91	1.33	1.37
26	b	614	CLA	C3B-C4B	2.91	1.49	1.42
39	S	312	CHL	O2A-CGA	2.90	1.41	1.33
26	b	611	CLA	C4D-ND	-2.90	1.33	1.37
26	a	411	CLA	C4B-NB	2.90	1.41	1.37
26	A	403	CLA	C4B-NB	2.90	1.41	1.37
26	G	313	CLA	C3B-C4B	2.90	1.49	1.42
39	S	302	CHL	O2A-CGA	2.90	1.41	1.33
39	S	316	CHL	O2A-CGA	2.90	1.41	1.33
26	r	310	CLA	C4B-NB	2.90	1.41	1.37
26	g	315	CLA	C3B-C4B	2.90	1.49	1.42
39	s	313	CHL	C2C-C3C	2.89	1.39	1.36
42	N	302	NEX	C32-C33	-2.89	1.39	1.45
26	B	615	CLA	C4D-ND	-2.89	1.33	1.37
26	C	521	CLA	C4B-NB	2.89	1.41	1.37
38	e	101	HEM	FE-NC	2.89	2.04	1.95
26	B	603	CLA	C4B-NB	2.89	1.41	1.37
39	N	311	CHL	O2A-CGA	2.89	1.41	1.33
26	C	519	CLA	C4B-NB	2.89	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	307	CLA	C4B-NB	2.89	1.41	1.37
26	N	313	CLA	MG-NB	-2.89	2.00	2.05
26	G	304	CLA	C3B-C4B	2.89	1.49	1.42
26	n	302	CLA	C3B-C4B	2.89	1.49	1.42
39	Y	317	CHL	O2A-CGA	2.88	1.41	1.33
42	R	305	NEX	C32-C33	-2.88	1.39	1.45
26	S	309	CLA	C3B-C4B	2.88	1.49	1.42
26	s	304	CLA	C3B-C4B	2.88	1.49	1.42
39	n	307	CHL	O2A-CGA	2.88	1.41	1.33
26	B	610	CLA	C3B-C4B	2.88	1.49	1.42
26	D	412	CLA	C4B-NB	2.88	1.41	1.37
39	G	318	CHL	O2A-CGA	2.88	1.41	1.33
26	S	314	CLA	C3B-C4B	2.87	1.49	1.42
26	B	612	CLA	C3B-C4B	2.87	1.49	1.42
26	B	615	CLA	C4B-NB	2.87	1.41	1.37
26	N	319	CLA	C4D-ND	-2.87	1.33	1.37
26	S	307	CLA	C3B-C4B	2.86	1.49	1.42
26	s	315	CLA	C3B-C4B	2.86	1.49	1.42
26	b	618	CLA	C4B-NB	2.86	1.41	1.37
26	S	315	CLA	C3B-C4B	2.86	1.49	1.42
26	B	616	CLA	C4B-NB	2.86	1.41	1.37
26	C	517	CLA	C4B-NB	2.86	1.41	1.37
26	c	514	CLA	C4B-NB	2.86	1.41	1.37
26	r	314	CLA	C3B-C4B	2.86	1.49	1.42
39	S	312	CHL	C2C-C3C	2.86	1.39	1.36
39	Y	307	CHL	O2A-CGA	2.86	1.41	1.33
26	c	513	CLA	C4B-NB	2.85	1.41	1.37
26	n	304	CLA	MG-NB	-2.85	2.00	2.05
39	g	311	CHL	O2A-CGA	2.85	1.41	1.33
26	y	316	CLA	C3B-C4B	2.85	1.49	1.42
39	y	303	CHL	O2A-CGA	2.85	1.41	1.33
26	r	317	CLA	C3B-C4B	2.85	1.49	1.42
26	s	311	CLA	C3B-C4B	2.85	1.49	1.42
26	b	609	CLA	C4B-NB	2.85	1.41	1.37
26	b	605	CLA	C3B-C4B	2.85	1.49	1.42
26	G	306	CLA	C3B-C4B	2.85	1.49	1.42
39	Y	318	CHL	O2A-CGA	2.85	1.41	1.33
26	N	318	CLA	C3B-C4B	2.84	1.49	1.42
26	s	306	CLA	C3B-C4B	2.84	1.49	1.42
38	E	101	HEM	FE-ND	2.84	2.03	1.94
26	r	313	CLA	C3B-C4B	2.84	1.49	1.42
42	S	305	NEX	O24-C25	-2.84	1.42	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	302	CLA	C3B-C4B	2.84	1.49	1.42
26	b	607	CLA	C3B-C4B	2.84	1.49	1.42
26	g	304	CLA	C3B-C4B	2.84	1.49	1.42
26	g	305	CLA	C3B-C4B	2.84	1.49	1.42
26	d	411	CLA	C4B-NB	2.84	1.41	1.37
38	E	101	HEM	CAC-C3C	2.84	1.55	1.47
26	r	308	CLA	C3B-C4B	2.84	1.49	1.42
26	A	405	CLA	C3B-C4B	2.84	1.49	1.42
26	S	304	CLA	C3B-C4B	2.84	1.49	1.42
26	c	518	CLA	C3B-C4B	2.84	1.49	1.42
39	y	302	CHL	O2A-CGA	2.83	1.41	1.33
26	n	309	CLA	C3B-C4B	2.83	1.49	1.42
39	Y	302	CHL	O2A-CGA	2.83	1.41	1.33
26	B	601	CLA	C3B-C4B	2.83	1.49	1.42
39	y	314	CHL	O2A-CGA	2.83	1.41	1.33
38	e	101	HEM	CAC-C3C	2.83	1.55	1.47
42	n	313	NEX	C32-C33	-2.83	1.39	1.45
26	S	308	CLA	C3B-C4B	2.82	1.49	1.42
26	s	301	CLA	C3B-C4B	2.82	1.49	1.42
26	R	302	CLA	C4B-NB	2.82	1.41	1.37
41	R	304	XAT	O24-C25	-2.81	1.42	1.46
26	R	314	CLA	C3B-C4B	2.81	1.49	1.42
26	B	602	CLA	C3B-C4B	2.81	1.49	1.42
39	g	319	CHL	C1A-CHA	2.81	1.43	1.40
26	b	601	CLA	C3B-C4B	2.81	1.49	1.42
26	g	303	CLA	C3B-C4B	2.81	1.49	1.42
26	Y	313	CLA	C3B-C4B	2.81	1.49	1.42
38	E	101	HEM	FE-NC	2.81	2.04	1.95
26	B	602	CLA	C4B-NB	2.81	1.41	1.37
30	a	407	PL9	C3-C4	-2.80	1.44	1.49
26	G	314	CLA	C3B-C4B	2.80	1.49	1.42
26	r	313	CLA	C4B-NB	2.80	1.41	1.37
26	B	618	CLA	C4B-NB	2.80	1.41	1.37
26	c	510	CLA	C4B-NB	2.80	1.41	1.37
26	G	319	CLA	C3B-C4B	2.80	1.49	1.42
26	C	504	CLA	C3B-C4B	2.79	1.49	1.42
26	D	412	CLA	C3B-C4B	2.79	1.49	1.42
26	r	303	CLA	MG-ND	-2.79	2.00	2.05
26	C	506	CLA	C4B-NB	2.79	1.41	1.37
39	N	303	CHL	C1A-CHA	2.79	1.43	1.40
26	g	302	CLA	C3B-C4B	2.79	1.49	1.42
26	s	305	CLA	C3B-C4B	2.79	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	313	CLA	C3B-C4B	2.79	1.49	1.42
26	c	504	CLA	C4B-NB	2.78	1.41	1.37
42	s	302	NEX	O24-C25	-2.78	1.42	1.46
26	b	618	CLA	MG-ND	-2.78	2.00	2.05
26	N	309	CLA	C3B-C4B	2.78	1.49	1.42
26	R	316	CLA	C3B-C4B	2.78	1.49	1.42
42	R	305	NEX	O24-C25	-2.78	1.42	1.46
30	A	408	PL9	C3-C4	-2.78	1.45	1.49
26	a	402	CLA	C3B-C4B	2.78	1.49	1.42
26	R	302	CLA	C3B-C4B	2.78	1.49	1.42
26	r	303	CLA	C3B-C4B	2.77	1.49	1.42
26	y	310	CLA	C3B-C4B	2.77	1.49	1.42
26	N	307	CLA	C3B-C4B	2.77	1.49	1.42
39	r	301	CHL	C1A-CHA	2.77	1.43	1.40
39	G	305	CHL	C1A-CHA	2.77	1.43	1.40
39	n	318	CHL	C1A-CHA	2.77	1.43	1.40
26	B	609	CLA	C4B-NB	2.77	1.41	1.37
26	d	411	CLA	C3B-C4B	2.77	1.49	1.42
42	g	306	NEX	C32-C33	-2.77	1.40	1.45
26	r	315	CLA	C3B-C4B	2.76	1.49	1.42
39	R	318	CHL	O2A-CGA	2.76	1.41	1.33
26	B	609	CLA	C3B-C4B	2.76	1.49	1.42
26	N	312	CLA	C3B-C4B	2.76	1.49	1.42
42	r	302	NEX	O24-C25	-2.76	1.42	1.46
26	B	606	CLA	C3B-C4B	2.76	1.49	1.42
42	Y	304	NEX	C32-C33	-2.76	1.40	1.45
26	c	502	CLA	C4B-NB	2.76	1.41	1.37
26	G	317	CLA	C3B-C4B	2.76	1.49	1.42
26	n	310	CLA	C3B-C4B	2.76	1.49	1.42
26	C	515	CLA	C4B-NB	2.76	1.41	1.37
26	b	608	CLA	C3B-C4B	2.76	1.49	1.42
41	R	304	XAT	O4-C5	-2.75	1.42	1.46
42	Y	304	NEX	O24-C25	-2.75	1.42	1.46
39	r	301	CHL	O2A-CGA	2.75	1.41	1.33
39	g	314	CHL	C1A-CHA	2.75	1.43	1.40
26	s	310	CLA	C3B-C4B	2.75	1.49	1.42
26	d	403	CLA	C3B-C4B	2.75	1.49	1.42
26	n	305	CLA	C3B-C4B	2.75	1.49	1.42
26	C	521	CLA	C3B-C4B	2.75	1.49	1.42
42	y	307	NEX	C32-C33	-2.75	1.40	1.45
26	N	319	CLA	C3B-C4B	2.74	1.49	1.42
41	r	304	XAT	O24-C25	-2.74	1.42	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	G	309	CHL	C1A-CHA	2.74	1.43	1.40
42	G	315	NEX	C32-C33	-2.74	1.40	1.45
26	G	307	CLA	C3B-C4B	2.74	1.49	1.42
26	Y	312	CLA	C3B-C4B	2.74	1.49	1.42
27	D	403	PHO	CMC-C2C	-2.74	1.46	1.50
39	S	302	CHL	C2C-C3C	2.74	1.38	1.36
26	s	307	CLA	C3B-C4B	2.74	1.49	1.42
26	n	304	CLA	C3B-C4B	2.73	1.49	1.42
26	n	303	CLA	C3B-C4B	2.73	1.49	1.42
26	y	304	CLA	C3B-C4B	2.73	1.49	1.42
26	R	306	CLA	C3B-C4B	2.73	1.49	1.42
26	r	306	CLA	C3B-C4B	2.73	1.49	1.42
26	N	306	CLA	C3B-C4B	2.73	1.49	1.42
26	c	514	CLA	C3B-C4B	2.73	1.49	1.42
26	r	310	CLA	C3B-C4B	2.73	1.49	1.42
26	B	605	CLA	C3B-C4B	2.73	1.49	1.42
26	a	409	CLA	C4B-NB	2.72	1.41	1.37
26	b	613	CLA	C4B-NB	2.72	1.41	1.37
26	y	304	CLA	C1B-C2B	2.72	1.49	1.43
26	S	310	CLA	C3B-C4B	2.72	1.49	1.42
26	b	618	CLA	C3B-C4B	2.72	1.49	1.42
26	S	303	CLA	C3B-C4B	2.72	1.49	1.42
26	r	311	CLA	C3B-C4B	2.72	1.49	1.42
26	g	308	CLA	C3B-C4B	2.72	1.49	1.42
42	y	307	NEX	O24-C25	-2.72	1.42	1.46
42	N	302	NEX	O24-C25	-2.71	1.42	1.46
26	y	313	CLA	MG-ND	-2.71	2.00	2.05
26	B	609	CLA	MG-ND	-2.71	2.00	2.05
26	D	401	CLA	C4B-NB	2.71	1.41	1.37
26	y	317	CLA	C1B-C2B	2.71	1.49	1.43
26	R	310	CLA	C3B-C4B	2.71	1.49	1.42
26	n	310	CLA	C1B-C2B	2.71	1.49	1.43
26	D	406	CLA	C3B-C4B	2.71	1.49	1.42
26	n	315	CLA	C3B-C4B	2.71	1.49	1.42
26	Y	301	CLA	C3B-C4B	2.71	1.49	1.42
26	g	317	CLA	C3B-C4B	2.71	1.49	1.42
26	A	403	CLA	C3B-C4B	2.70	1.49	1.42
26	b	611	CLA	C1B-C2B	2.70	1.49	1.43
26	R	317	CLA	C3B-C4B	2.70	1.49	1.42
27	D	403	PHO	C4D-ND	-2.70	1.34	1.38
27	d	407	PHO	C4D-ND	-2.70	1.34	1.38
26	R	308	CLA	C3B-C4B	2.70	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	604	CLA	C3B-C4B	2.69	1.49	1.42
26	c	503	CLA	C3B-C4B	2.69	1.49	1.42
26	n	309	CLA	C1B-C2B	2.69	1.49	1.43
27	d	407	PHO	CMC-C2C	-2.69	1.46	1.50
26	R	308	CLA	MG-ND	-2.69	2.00	2.05
26	b	612	CLA	C3B-C4B	2.69	1.49	1.42
26	N	309	CLA	C1B-C2B	2.68	1.49	1.43
26	a	411	CLA	C3B-C4B	2.68	1.49	1.42
26	S	315	CLA	C1B-C2B	2.68	1.49	1.43
42	n	313	NEX	O24-C25	-2.68	1.42	1.46
26	N	313	CLA	C3B-C4B	2.68	1.49	1.42
26	C	511	CLA	C3B-C4B	2.68	1.49	1.42
26	r	311	CLA	MG-ND	-2.68	2.00	2.05
26	N	319	CLA	C1B-C2B	2.68	1.49	1.43
26	g	303	CLA	C1B-C2B	2.67	1.49	1.43
26	b	606	CLA	C3B-C4B	2.67	1.49	1.42
26	C	504	CLA	C1B-C2B	2.67	1.49	1.43
41	r	304	XAT	O4-C5	-2.67	1.42	1.46
26	B	615	CLA	C1B-C2B	2.67	1.49	1.43
26	a	411	CLA	C1B-C2B	2.67	1.49	1.43
26	s	305	CLA	C1B-C2B	2.67	1.49	1.43
39	g	313	CHL	C1A-CHA	2.67	1.43	1.40
26	Y	301	CLA	C1B-C2B	2.67	1.49	1.43
26	Y	311	CLA	C1B-C2B	2.67	1.49	1.43
39	R	318	CHL	C1A-CHA	2.66	1.43	1.40
26	S	304	CLA	C1B-C2B	2.66	1.49	1.43
41	R	304	XAT	C12-C13	-2.66	1.40	1.45
27	a	410	PHO	CMC-C2C	-2.66	1.46	1.50
26	c	505	CLA	C3B-C4B	2.66	1.49	1.42
26	G	314	CLA	C1B-C2B	2.66	1.49	1.43
26	n	312	CLA	C3B-C4B	2.66	1.49	1.42
26	C	507	CLA	C3B-C4B	2.66	1.49	1.42
26	s	315	CLA	C1B-C2B	2.66	1.49	1.43
26	C	519	CLA	C3B-C4B	2.66	1.49	1.42
26	r	310	CLA	C1B-C2B	2.66	1.49	1.43
26	r	308	CLA	C1B-C2B	2.65	1.49	1.43
26	N	308	CLA	C3B-C4B	2.65	1.49	1.42
26	A	403	CLA	C1B-C2B	2.65	1.49	1.43
26	N	306	CLA	C1B-C2B	2.65	1.49	1.43
26	c	518	CLA	C1B-C2B	2.65	1.49	1.43
26	B	611	CLA	C3B-C4B	2.65	1.49	1.42
26	s	310	CLA	MG-ND	-2.65	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y	311	CLA	C3B-C4B	2.65	1.49	1.42
26	s	306	CLA	C1B-C2B	2.64	1.49	1.43
26	y	315	CLA	C1B-C2B	2.64	1.49	1.43
26	R	310	CLA	C1B-C2B	2.64	1.49	1.43
26	r	314	CLA	C1B-C2B	2.64	1.49	1.43
26	R	316	CLA	C1B-C2B	2.64	1.49	1.43
26	c	510	CLA	C3B-C4B	2.64	1.48	1.42
26	Y	316	CLA	MG-ND	-2.64	2.00	2.05
26	R	313	CLA	C1B-C2B	2.64	1.49	1.43
26	c	510	CLA	C1B-C2B	2.64	1.49	1.43
26	r	305	CLA	C1B-C2B	2.64	1.49	1.43
27	A	404	PHO	CMC-C2C	-2.63	1.46	1.50
26	b	616	CLA	C3B-C4B	2.63	1.48	1.42
26	n	305	CLA	C1B-C2B	2.63	1.49	1.43
39	Y	314	CHL	C1A-CHA	2.63	1.43	1.40
26	b	610	CLA	C3B-C4B	2.63	1.48	1.42
39	G	301	CHL	C2C-C3C	2.63	1.38	1.36
39	G	301	CHL	C1A-CHA	2.63	1.43	1.40
41	n	316	XAT	O4-C5	-2.63	1.42	1.46
26	S	314	CLA	C1B-C2B	2.62	1.49	1.43
41	r	304	XAT	C12-C13	-2.62	1.40	1.45
26	d	404	CLA	C1B-C2B	2.62	1.49	1.43
26	c	504	CLA	C1B-C2B	2.62	1.49	1.43
26	r	303	CLA	C1B-C2B	2.62	1.49	1.43
26	g	315	CLA	C1B-C2B	2.62	1.49	1.43
26	y	315	CLA	C3B-C4B	2.62	1.48	1.42
26	b	613	CLA	C3B-C4B	2.62	1.48	1.42
26	C	519	CLA	C1B-C2B	2.62	1.49	1.43
26	b	604	CLA	C3B-C4B	2.62	1.48	1.42
39	s	316	CHL	C2C-C3C	2.62	1.38	1.36
26	B	611	CLA	MG-ND	-2.62	2.00	2.05
26	s	314	CLA	C1B-C2B	2.62	1.49	1.43
26	Y	310	CLA	C1B-C2B	2.62	1.49	1.43
26	C	515	CLA	C1B-C2B	2.61	1.49	1.43
39	G	309	CHL	MG-NB	2.61	2.11	2.05
26	b	602	CLA	C3B-C4B	2.61	1.48	1.42
26	n	315	CLA	C1B-C2B	2.61	1.49	1.43
42	G	315	NEX	O24-C25	-2.61	1.42	1.46
26	G	317	CLA	C1B-C2B	2.61	1.49	1.43
26	S	303	CLA	C1B-C2B	2.61	1.49	1.43
26	B	617	CLA	C3B-C4B	2.61	1.48	1.42
26	N	313	CLA	C1B-C2B	2.61	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	606	CLA	MG-ND	-2.61	2.00	2.05
39	g	314	CHL	MG-NB	2.61	2.11	2.05
26	R	309	CLA	C1B-C2B	2.61	1.49	1.43
41	G	310	XAT	O24-C25	-2.61	1.42	1.46
26	B	607	CLA	C3B-C4B	2.61	1.48	1.42
39	g	313	CHL	C2C-C3C	2.60	1.38	1.36
26	C	506	CLA	C3B-C4B	2.60	1.48	1.42
26	D	401	CLA	C3B-C4B	2.60	1.48	1.42
26	y	313	CLA	MG-NB	-2.60	2.00	2.05
26	c	502	CLA	C3B-C4B	2.60	1.48	1.42
26	y	310	CLA	C1B-C2B	2.60	1.49	1.43
41	n	316	XAT	C12-C13	-2.60	1.40	1.45
39	y	312	CHL	C1A-CHA	2.60	1.43	1.40
41	G	320	XAT	O24-C25	-2.60	1.42	1.46
41	g	320	XAT	O4-C5	-2.60	1.42	1.46
26	s	307	CLA	C1B-C2B	2.60	1.49	1.43
26	D	409	CLA	C1B-C2B	2.60	1.49	1.43
41	n	316	XAT	O24-C25	-2.60	1.42	1.46
26	G	313	CLA	C1B-C2B	2.59	1.49	1.43
39	y	314	CHL	MG-NB	2.59	2.10	2.05
41	G	310	XAT	O4-C5	-2.59	1.42	1.46
26	C	506	CLA	C1B-C2B	2.59	1.49	1.43
26	B	618	CLA	C1B-C2B	2.59	1.49	1.43
26	y	317	CLA	C3B-C4B	2.59	1.48	1.42
26	B	605	CLA	C1B-C2B	2.59	1.49	1.43
26	B	603	CLA	C3B-C4B	2.59	1.48	1.42
41	N	315	XAT	O24-C25	-2.59	1.42	1.46
26	B	613	CLA	C3B-C4B	2.59	1.48	1.42
26	Y	316	CLA	C3B-C4B	2.59	1.48	1.42
26	N	307	CLA	C1B-C2B	2.59	1.49	1.43
26	B	618	CLA	C3B-C4B	2.59	1.48	1.42
41	N	315	XAT	O4-C5	-2.59	1.42	1.46
26	b	613	CLA	C1B-C2B	2.58	1.49	1.43
26	n	304	CLA	C1B-C2B	2.58	1.49	1.43
26	B	616	CLA	C1B-C2B	2.58	1.49	1.43
26	C	512	CLA	C1B-C2B	2.58	1.49	1.43
26	c	516	CLA	C3B-C4B	2.58	1.48	1.42
26	Y	310	CLA	C3B-C4B	2.58	1.48	1.42
39	y	302	CHL	MG-NB	2.58	2.10	2.05
26	C	512	CLA	C3B-C4B	2.57	1.48	1.42
41	N	315	XAT	C12-C13	-2.57	1.40	1.45
39	g	312	CHL	MG-NB	2.57	2.10	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	404	PHO	C4D-ND	-2.57	1.35	1.38
26	S	309	CLA	C1B-C2B	2.57	1.49	1.43
26	B	617	CLA	C1B-C2B	2.57	1.49	1.43
26	b	602	CLA	C1B-C2B	2.57	1.49	1.43
26	n	302	CLA	C1B-C2B	2.57	1.49	1.43
42	g	306	NEX	O24-C25	-2.57	1.42	1.46
26	s	301	CLA	C1B-C2B	2.57	1.49	1.43
26	S	308	CLA	C1B-C2B	2.57	1.49	1.43
26	B	603	CLA	C1B-C2B	2.56	1.49	1.43
26	g	308	CLA	C1B-C2B	2.56	1.49	1.43
39	Y	318	CHL	MG-NB	2.56	2.10	2.05
26	Y	312	CLA	C1B-C2B	2.56	1.49	1.43
39	Y	307	CHL	MG-NB	2.56	2.10	2.05
26	G	306	CLA	C1B-C2B	2.56	1.49	1.43
26	R	317	CLA	C1B-C2B	2.56	1.49	1.43
41	r	304	XAT	C32-C33	-2.56	1.40	1.45
26	s	304	CLA	C1B-C2B	2.56	1.49	1.43
41	R	304	XAT	C32-C33	-2.56	1.40	1.45
26	c	515	CLA	C3B-C4B	2.56	1.48	1.42
26	y	313	CLA	C3B-C4B	2.56	1.48	1.42
26	B	610	CLA	C1B-C2B	2.55	1.49	1.43
26	g	305	CLA	C1B-C2B	2.55	1.49	1.43
26	S	310	CLA	MG-ND	-2.55	2.00	2.05
27	A	404	PHO	CMB-C2B	-2.55	1.46	1.51
26	G	307	CLA	C1B-C2B	2.55	1.49	1.43
26	r	315	CLA	C1B-C2B	2.55	1.49	1.43
26	C	517	CLA	C1B-C2B	2.55	1.49	1.43
41	G	320	XAT	O4-C5	-2.55	1.42	1.46
27	a	410	PHO	C4D-ND	-2.55	1.35	1.38
26	N	318	CLA	C1B-C2B	2.55	1.49	1.43
26	r	317	CLA	C1B-C2B	2.55	1.49	1.43
26	S	311	CLA	C1B-C2B	2.55	1.49	1.43
26	a	409	CLA	C3B-C4B	2.55	1.48	1.42
26	R	306	CLA	C1B-C2B	2.55	1.49	1.43
26	b	609	CLA	C1B-C2B	2.55	1.49	1.43
26	S	307	CLA	C1B-C2B	2.54	1.49	1.43
26	N	312	CLA	C1B-C2B	2.54	1.49	1.43
39	G	311	CHL	MG-NB	2.54	2.10	2.05
26	b	610	CLA	C1B-C2B	2.54	1.49	1.43
26	c	513	CLA	C3B-C4B	2.54	1.48	1.42
26	n	312	CLA	MG-NB	-2.54	2.00	2.05
26	C	508	CLA	C3B-C4B	2.54	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	307	CLA	C1B-C2B	2.54	1.49	1.43
41	g	309	XAT	O24-C25	-2.54	1.42	1.46
26	r	306	CLA	C1B-C2B	2.54	1.49	1.43
26	g	318	CLA	C1B-C2B	2.54	1.49	1.43
39	s	317	CHL	MG-NB	2.54	2.10	2.05
26	R	314	CLA	C1B-C2B	2.54	1.49	1.43
26	c	502	CLA	C1B-C2B	2.53	1.49	1.43
26	b	605	CLA	C1B-C2B	2.53	1.49	1.43
26	G	304	CLA	C1B-C2B	2.53	1.49	1.43
26	b	611	CLA	CMD-C2D	-2.53	1.45	1.50
26	s	311	CLA	C1B-C2B	2.53	1.49	1.43
26	C	516	CLA	C1B-C2B	2.53	1.49	1.43
26	G	302	CLA	C1B-C2B	2.53	1.49	1.43
39	S	313	CHL	C1A-CHA	2.53	1.42	1.40
26	c	520	CLA	C1B-C2B	2.52	1.49	1.43
26	a	402	CLA	MG-ND	-2.52	2.00	2.05
39	s	303	CHL	C1A-CHA	2.52	1.42	1.40
41	g	320	XAT	O24-C25	-2.52	1.42	1.46
26	g	317	CLA	MG-ND	-2.52	2.00	2.05
26	C	515	CLA	C3B-C4B	2.52	1.48	1.42
26	C	517	CLA	C3B-C4B	2.52	1.48	1.42
27	a	410	PHO	CMB-C2B	-2.52	1.46	1.51
39	s	317	CHL	C1A-CHA	2.52	1.42	1.40
26	c	508	CLA	C1B-C2B	2.52	1.49	1.43
39	R	315	CHL	MG-NB	2.52	2.10	2.05
39	G	311	CHL	C1A-CHA	2.52	1.42	1.40
26	c	513	CLA	C1B-C2B	2.52	1.49	1.43
39	n	311	CHL	C2C-C3C	2.52	1.38	1.36
39	S	312	CHL	C1A-CHA	2.52	1.42	1.40
39	Y	314	CHL	C2C-C3C	2.51	1.38	1.36
26	S	310	CLA	C1B-C2B	2.51	1.49	1.43
26	b	616	CLA	C1B-C2B	2.51	1.49	1.43
26	b	617	CLA	C1B-C2B	2.51	1.49	1.43
39	N	304	CHL	C2C-C3C	2.51	1.38	1.36
39	G	305	CHL	MG-NB	2.51	2.10	2.05
26	B	602	CLA	C1B-C2B	2.51	1.49	1.43
26	g	317	CLA	C1B-C2B	2.51	1.49	1.43
39	S	313	CHL	MG-NB	2.51	2.10	2.05
26	C	507	CLA	C1B-C2B	2.51	1.49	1.43
26	g	302	CLA	MG-NB	-2.51	2.00	2.05
41	g	309	XAT	O4-C5	-2.51	1.42	1.46
39	n	319	CHL	MG-NB	2.51	2.10	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	608	CLA	C1B-C2B	2.50	1.49	1.43
26	n	303	CLA	C1B-C2B	2.50	1.49	1.43
26	D	409	CLA	C3B-C4B	2.50	1.48	1.42
26	N	308	CLA	MG-NB	-2.50	2.00	2.05
26	g	302	CLA	C1B-C2B	2.50	1.49	1.43
26	B	615	CLA	CMD-C2D	-2.50	1.45	1.50
39	G	318	CHL	C2C-C3C	2.50	1.38	1.36
26	d	404	CLA	C3B-C4B	2.50	1.48	1.42
26	s	310	CLA	C1B-C2B	2.50	1.49	1.43
39	G	303	CHL	MG-NB	2.50	2.10	2.05
26	c	504	CLA	C3B-C4B	2.50	1.48	1.42
26	B	601	CLA	C1B-C2B	2.49	1.49	1.43
26	c	515	CLA	C1B-C2B	2.49	1.49	1.43
26	b	618	CLA	C1B-C2B	2.49	1.49	1.43
26	Y	316	CLA	MG-NB	-2.49	2.00	2.05
39	g	319	CHL	MG-NB	2.49	2.10	2.05
39	r	316	CHL	C1A-CHA	2.49	1.42	1.40
39	g	307	CHL	MG-NB	2.49	2.10	2.05
39	s	316	CHL	MG-NB	2.49	2.10	2.05
39	Y	302	CHL	C2C-C3C	2.49	1.38	1.36
27	D	403	PHO	CMD-C2D	-2.49	1.46	1.51
27	d	407	PHO	CMD-C2D	-2.49	1.46	1.51
30	d	408	PL9	C53-C6	-2.49	1.45	1.50
39	n	307	CHL	MG-NB	2.48	2.10	2.05
39	g	313	CHL	MG-NB	2.48	2.10	2.05
27	A	404	PHO	CMD-C2D	-2.48	1.46	1.51
26	G	302	CLA	MG-NB	-2.48	2.00	2.05
26	b	607	CLA	C1B-C2B	2.48	1.49	1.43
26	B	609	CLA	CMD-C2D	-2.48	1.45	1.50
26	y	306	CLA	C1B-C2B	2.48	1.49	1.43
26	s	301	CLA	MG-ND	-2.48	2.00	2.05
39	N	317	CHL	MG-NB	2.48	2.10	2.05
39	S	302	CHL	MG-NB	2.48	2.10	2.05
27	a	410	PHO	CMD-C2D	-2.48	1.46	1.51
39	y	305	CHL	C2C-C3C	2.47	1.38	1.36
26	C	505	CLA	C1B-C2B	2.47	1.49	1.43
26	c	514	CLA	C1B-C2B	2.47	1.49	1.43
26	b	618	CLA	CMD-C2D	-2.47	1.45	1.50
26	y	313	CLA	CMB-C2B	-2.47	1.45	1.50
39	y	312	CHL	C2C-C3C	2.47	1.38	1.36
30	a	407	PL9	C53-C6	-2.47	1.45	1.50
39	r	301	CHL	MG-NB	2.47	2.10	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	609	CLA	C1B-C2B	2.47	1.49	1.43
26	g	304	CLA	C1B-C2B	2.47	1.49	1.43
26	C	521	CLA	C1B-C2B	2.47	1.49	1.43
39	n	308	CHL	MG-NB	2.46	2.10	2.05
26	G	319	CLA	C1B-C2B	2.46	1.49	1.43
26	Y	308	CLA	C1B-C2B	2.46	1.49	1.43
41	n	316	XAT	C32-C33	-2.46	1.40	1.45
39	s	303	CHL	C2-C3	2.46	1.38	1.33
42	s	302	NEX	C32-C33	-2.46	1.40	1.45
26	b	609	CLA	C3B-C4B	2.46	1.48	1.42
39	S	316	CHL	C1A-CHA	2.46	1.42	1.40
26	G	307	CLA	MG-ND	-2.45	2.00	2.05
42	y	307	NEX	C11-C12	2.45	1.40	1.34
26	n	312	CLA	C1B-C2B	2.45	1.49	1.43
39	R	301	CHL	C1A-CHA	2.45	1.42	1.40
26	b	606	CLA	C1B-C2B	2.45	1.49	1.43
39	g	312	CHL	C1A-CHA	2.45	1.42	1.40
41	N	315	XAT	C32-C33	-2.45	1.40	1.45
26	C	511	CLA	C1B-C2B	2.45	1.49	1.43
39	S	316	CHL	C2-C3	2.45	1.38	1.33
26	B	607	CLA	C1B-C2B	2.45	1.49	1.43
26	N	308	CLA	C1B-C2B	2.45	1.49	1.43
26	c	503	CLA	C1B-C2B	2.44	1.49	1.43
39	g	311	CHL	C2C-C3C	2.44	1.38	1.36
26	c	508	CLA	MG-NB	-2.44	2.00	2.05
26	a	411	CLA	CMC-C2C	-2.44	1.45	1.50
39	y	312	CHL	MG-NB	2.44	2.10	2.05
26	a	409	CLA	C1B-C2B	2.44	1.49	1.43
39	G	301	CHL	MG-NB	2.44	2.10	2.05
39	R	318	CHL	MG-NB	2.44	2.10	2.05
26	S	310	CLA	CMB-C2B	-2.44	1.45	1.50
26	c	505	CLA	C1B-C2B	2.44	1.49	1.43
26	B	616	CLA	C3B-C4B	2.44	1.48	1.42
39	N	303	CHL	C2-C3	2.44	1.38	1.33
39	s	313	CHL	C1A-CHA	2.44	1.42	1.40
26	A	403	CLA	CMC-C2C	-2.43	1.45	1.50
26	b	614	CLA	C1B-C2B	2.43	1.49	1.43
39	n	318	CHL	MG-NB	2.43	2.10	2.05
39	S	312	CHL	MG-NB	2.43	2.10	2.05
26	Y	316	CLA	CMB-C2B	-2.43	1.45	1.50
42	y	307	NEX	C34-C33	2.43	1.39	1.35
39	s	316	CHL	C1A-CHA	2.43	1.42	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	401	CLA	C1B-C2B	2.43	1.49	1.43
39	n	318	CHL	C2-C3	2.43	1.38	1.33
30	D	411	PL9	C53-C6	-2.43	1.45	1.50
42	Y	304	NEX	C11-C12	2.43	1.40	1.34
30	A	408	PL9	C53-C6	-2.43	1.45	1.50
39	N	311	CHL	MG-NB	2.42	2.10	2.05
26	B	611	CLA	C1B-C2B	2.42	1.49	1.43
41	G	310	XAT	C12-C13	-2.42	1.40	1.45
41	g	309	XAT	C12-C13	-2.42	1.40	1.45
39	n	306	CHL	MG-NB	2.42	2.10	2.05
26	B	613	CLA	C1B-C2B	2.42	1.48	1.43
26	y	316	CLA	C1B-C2B	2.42	1.48	1.43
42	S	305	NEX	C32-C33	-2.42	1.40	1.45
26	B	615	CLA	C3B-C4B	2.42	1.48	1.42
26	B	606	CLA	C1B-C2B	2.41	1.48	1.43
39	Y	314	CHL	MG-NB	2.41	2.10	2.05
26	c	508	CLA	C3B-C4B	2.41	1.48	1.42
39	n	307	CHL	C1A-CHA	2.41	1.42	1.40
39	y	303	CHL	C2C-C3C	2.41	1.38	1.36
39	s	303	CHL	MG-NB	2.41	2.10	2.05
26	Y	316	CLA	C1B-C2B	2.41	1.48	1.43
39	G	309	CHL	C2C-C3C	2.40	1.38	1.36
39	g	314	CHL	C2C-C3C	2.40	1.38	1.36
39	y	314	CHL	C2-C3	2.40	1.38	1.33
41	G	310	XAT	C32-C33	-2.40	1.40	1.45
26	s	310	CLA	CMB-C2B	-2.40	1.45	1.50
39	N	310	CHL	MG-NB	2.40	2.10	2.05
42	n	313	NEX	C11-C12	2.40	1.40	1.34
41	g	309	XAT	C32-C33	-2.40	1.40	1.45
39	N	310	CHL	C2C-C3C	2.40	1.38	1.36
39	s	313	CHL	MG-NB	2.40	2.10	2.05
39	N	316	CHL	MG-NB	2.40	2.10	2.05
26	Y	313	CLA	C1B-C2B	2.39	1.48	1.43
26	b	604	CLA	C1B-C2B	2.39	1.48	1.43
39	S	316	CHL	MG-NB	2.39	2.10	2.05
39	N	303	CHL	MG-NB	2.39	2.10	2.05
39	R	315	CHL	C1A-CHA	2.39	1.42	1.40
26	b	611	CLA	C3B-C4B	2.39	1.48	1.42
42	Y	304	NEX	C34-C33	2.39	1.38	1.35
26	C	506	CLA	MG-ND	-2.39	2.01	2.05
39	Y	317	CHL	MG-NB	2.39	2.10	2.05
26	C	516	CLA	C3B-C4B	2.39	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	g	311	CHL	MG-NB	2.38	2.10	2.05
26	C	508	CLA	CMB-C2B	-2.38	1.45	1.50
26	C	519	CLA	MG-ND	-2.38	2.01	2.05
26	C	507	CLA	MG-NC	2.38	2.11	2.06
26	n	312	CLA	CMB-C2B	-2.38	1.45	1.50
26	B	602	CLA	CMC-C2C	-2.38	1.45	1.50
26	N	308	CLA	CMB-C2B	-2.38	1.45	1.50
26	c	516	CLA	CMB-C2B	-2.38	1.45	1.50
39	n	311	CHL	MG-NB	2.38	2.10	2.05
39	Y	307	CHL	C2-C3	2.37	1.38	1.33
39	S	302	CHL	C1A-CHA	2.37	1.42	1.40
26	c	502	CLA	CMD-C2D	-2.37	1.45	1.50
26	B	612	CLA	C1B-C2B	2.37	1.48	1.43
39	N	304	CHL	MG-NB	2.37	2.10	2.05
26	B	615	CLA	CMB-C2B	-2.37	1.45	1.50
26	C	516	CLA	MG-NB	-2.37	2.01	2.05
39	R	301	CHL	MG-NB	2.37	2.10	2.05
39	r	316	CHL	MG-NB	2.37	2.10	2.05
26	a	402	CLA	C1B-C2B	2.37	1.48	1.43
26	y	313	CLA	C1B-C2B	2.37	1.48	1.43
39	N	316	CHL	C1A-CHA	2.36	1.42	1.40
39	r	318	CHL	MG-NB	2.36	2.10	2.05
30	D	411	PL9	C52-C5	-2.36	1.45	1.50
39	y	305	CHL	MG-NB	2.36	2.10	2.05
39	Y	307	CHL	C1A-CHA	2.36	1.42	1.40
39	Y	317	CHL	C1A-CHA	2.36	1.42	1.40
39	N	317	CHL	C2C-C3C	2.36	1.38	1.36
30	d	408	PL9	C52-C5	-2.36	1.45	1.50
30	a	407	PL9	C6-C1	-2.36	1.44	1.48
26	C	508	CLA	C1B-C2B	2.36	1.48	1.43
26	D	412	CLA	C1B-C2B	2.36	1.48	1.43
39	g	311	CHL	C2-C3	2.36	1.38	1.33
26	r	313	CLA	C1B-C2B	2.35	1.48	1.43
26	n	304	CLA	MG-NA	2.35	2.11	2.06
39	n	308	CHL	C2C-C3C	2.35	1.38	1.36
39	y	305	CHL	C1A-CHA	2.35	1.42	1.40
39	N	311	CHL	C1A-CHA	2.35	1.42	1.40
26	b	605	CLA	CMC-C2C	-2.35	1.45	1.50
42	s	302	NEX	C11-C12	2.35	1.40	1.34
42	n	313	NEX	C34-C33	2.35	1.38	1.35
39	n	306	CHL	C1A-CHA	2.34	1.42	1.40
26	c	516	CLA	C1B-C2B	2.34	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	403	CLA	CMD-C2D	-2.34	1.45	1.50
26	b	601	CLA	C1B-C2B	2.34	1.48	1.43
39	n	319	CHL	C2C-C3C	2.34	1.38	1.36
26	R	308	CLA	C1B-C2B	2.34	1.48	1.43
26	d	403	CLA	C1B-C2B	2.34	1.48	1.43
42	g	306	NEX	C34-C33	2.34	1.38	1.35
26	B	611	CLA	CMB-C2B	-2.34	1.45	1.50
26	B	604	CLA	CMB-C2B	-2.34	1.45	1.50
26	B	618	CLA	MG-ND	-2.34	2.01	2.05
39	n	306	CHL	C2C-C3C	2.34	1.38	1.36
39	y	314	CHL	C1A-CHA	2.34	1.42	1.40
42	N	302	NEX	C34-C33	2.34	1.38	1.35
26	S	303	CLA	MG-ND	-2.33	2.01	2.05
26	D	406	CLA	C1B-C2B	2.33	1.48	1.43
26	C	506	CLA	CMD-C2D	-2.33	1.45	1.50
39	G	311	CHL	C2C-C3C	2.33	1.38	1.36
39	r	301	CHL	C2C-C3C	2.33	1.38	1.36
39	y	303	CHL	MG-NB	2.33	2.10	2.05
39	g	307	CHL	C1A-CHA	2.33	1.42	1.40
26	C	507	CLA	MG-ND	-2.33	2.01	2.05
42	G	315	NEX	C11-C12	2.33	1.40	1.34
26	d	411	CLA	C1B-C2B	2.33	1.48	1.43
42	g	306	NEX	C11-C12	2.33	1.40	1.34
26	r	311	CLA	C1B-C2B	2.33	1.48	1.43
26	A	405	CLA	MG-ND	-2.32	2.01	2.05
26	N	308	CLA	MG-ND	-2.32	2.01	2.05
39	N	316	CHL	C2C-C3C	2.32	1.38	1.36
39	Y	317	CHL	C2C-C3C	2.32	1.38	1.36
26	n	312	CLA	MG-ND	-2.32	2.01	2.05
26	B	607	CLA	CMB-C2B	-2.32	1.45	1.50
39	G	318	CHL	C2-C3	2.32	1.38	1.33
26	A	405	CLA	C1B-C2B	2.32	1.48	1.43
26	b	606	CLA	CMB-C2B	-2.32	1.45	1.50
26	N	313	CLA	MG-NA	2.32	2.11	2.06
26	R	302	CLA	C1B-C2B	2.32	1.48	1.43
39	r	309	CHL	MG-NB	2.32	2.10	2.05
42	r	302	NEX	C11-C12	2.32	1.40	1.34
42	s	302	NEX	C34-C33	2.32	1.38	1.35
39	G	318	CHL	MG-NB	2.32	2.10	2.05
39	n	319	CHL	C1A-CHA	2.32	1.42	1.40
42	R	305	NEX	C11-C12	2.31	1.40	1.34
42	G	315	NEX	C34-C33	2.31	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Y	302	CHL	C2-C3	2.31	1.38	1.33
26	g	305	CLA	MG-ND	-2.31	2.01	2.05
42	S	305	NEX	C34-C33	2.31	1.38	1.35
39	Y	302	CHL	MG-NB	2.31	2.10	2.05
42	N	302	NEX	C11-C12	2.31	1.40	1.34
39	R	312	CHL	MG-NB	2.30	2.10	2.05
26	c	505	CLA	MG-ND	-2.30	2.01	2.05
26	b	611	CLA	CMB-C2B	-2.30	1.45	1.50
39	r	318	CHL	C1A-CHA	2.30	1.42	1.40
26	b	614	CLA	CHC-C1C	2.30	1.43	1.38
39	s	303	CHL	C2C-C3C	2.30	1.38	1.36
26	g	315	CLA	MG-ND	-2.30	2.01	2.05
39	N	317	CHL	C1A-CHA	2.30	1.42	1.40
39	n	308	CHL	C1A-CHA	2.29	1.42	1.40
39	y	303	CHL	C2-C3	2.29	1.38	1.33
41	g	320	XAT	C32-C33	-2.29	1.41	1.45
26	C	520	CLA	CMD-C2D	-2.29	1.45	1.50
26	b	612	CLA	CMD-C2D	-2.29	1.45	1.50
26	G	306	CLA	MG-ND	-2.29	2.01	2.05
26	R	306	CLA	MG-ND	-2.29	2.01	2.05
41	G	320	XAT	C32-C33	-2.29	1.41	1.45
26	A	405	CLA	CHC-C1C	2.29	1.43	1.38
26	B	604	CLA	CMD-C2D	-2.28	1.46	1.50
26	c	502	CLA	MG-ND	-2.28	2.01	2.05
42	S	305	NEX	C11-C12	2.28	1.40	1.34
26	s	311	CLA	CHC-C1C	2.28	1.43	1.38
39	n	318	CHL	C2C-C3C	2.28	1.38	1.36
26	Y	305	CLA	CHC-C1C	2.28	1.43	1.38
39	g	312	CHL	C2C-C3C	2.28	1.38	1.36
26	c	506	CLA	CMD-C2D	-2.27	1.46	1.50
26	r	311	CLA	CMB-C2B	-2.27	1.46	1.50
26	b	616	CLA	CMB-C2B	-2.27	1.46	1.50
26	S	311	CLA	CHC-C1C	2.27	1.43	1.38
26	b	606	CLA	CMD-C2D	-2.27	1.46	1.50
26	b	612	CLA	CMB-C2B	-2.27	1.46	1.50
26	G	313	CLA	MG-ND	-2.27	2.01	2.05
26	a	411	CLA	CMD-C2D	-2.27	1.46	1.50
30	A	408	PL9	C6-C1	-2.27	1.44	1.48
26	B	611	CLA	CMD-C2D	-2.27	1.46	1.50
39	R	312	CHL	C2C-C3C	2.27	1.38	1.36
26	r	314	CLA	CHC-C1C	2.26	1.43	1.38
26	y	306	CLA	CHC-C1C	2.26	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	R	318	CHL	C2C-C3C	2.26	1.38	1.36
27	d	407	PHO	CMB-C2B	-2.26	1.46	1.51
39	N	310	CHL	C1A-CHA	2.26	1.42	1.40
39	n	311	CHL	C1A-CHA	2.26	1.42	1.40
26	Y	305	CLA	C1B-C2B	2.26	1.48	1.43
39	N	304	CHL	C1A-CHA	2.25	1.42	1.40
39	G	303	CHL	C1A-CHA	2.25	1.42	1.40
26	S	307	CLA	CHC-C1C	2.25	1.43	1.38
39	Y	307	CHL	C2C-C3C	2.25	1.38	1.36
26	a	402	CLA	CHC-C1C	2.25	1.43	1.38
26	Y	305	CLA	CMB-C2B	-2.25	1.46	1.50
26	y	309	CLA	CMB-C2B	-2.25	1.46	1.50
27	D	403	PHO	CMB-C2B	-2.25	1.47	1.51
26	R	308	CLA	CMB-C2B	-2.24	1.46	1.50
39	R	315	CHL	C2C-C3C	2.24	1.38	1.36
39	r	318	CHL	C2C-C3C	2.24	1.38	1.36
26	c	510	CLA	MG-ND	-2.24	2.01	2.05
26	y	310	CLA	CHC-C1C	2.24	1.43	1.38
26	C	516	CLA	MG-ND	-2.24	2.01	2.05
26	Y	308	CLA	CHC-C1C	2.24	1.43	1.38
39	r	309	CHL	C2C-C3C	2.24	1.38	1.36
42	R	305	NEX	C34-C33	2.23	1.38	1.35
26	r	308	CLA	CHC-C1C	2.23	1.43	1.38
39	S	316	CHL	C2C-C3C	2.23	1.38	1.36
26	R	317	CLA	CHC-C1C	2.23	1.43	1.38
26	R	313	CLA	CMD-C2D	-2.23	1.46	1.50
39	y	314	CHL	C2C-C3C	2.23	1.38	1.36
26	D	409	CLA	CMD-C2D	-2.23	1.46	1.50
26	c	518	CLA	CHC-C1C	2.23	1.43	1.38
26	y	309	CLA	CHC-C1C	2.22	1.43	1.38
26	B	618	CLA	CMD-C2D	-2.22	1.46	1.50
26	G	302	CLA	CMB-C2B	-2.22	1.46	1.50
26	R	313	CLA	CHC-C1C	2.22	1.43	1.38
26	s	306	CLA	CHC-C1C	2.22	1.43	1.38
26	b	601	CLA	CHC-C1C	2.22	1.43	1.38
26	c	505	CLA	MG-NC	2.22	2.11	2.06
26	C	505	CLA	CHC-C1C	2.22	1.43	1.38
26	C	517	CLA	CMB-C2B	-2.22	1.46	1.50
26	B	604	CLA	C1B-C2B	2.22	1.48	1.43
26	S	315	CLA	CHC-C1C	2.21	1.43	1.38
26	r	317	CLA	MG-ND	-2.21	2.01	2.05
26	b	613	CLA	CMD-C2D	-2.21	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	520	CLA	CMD-C2D	-2.21	1.46	1.50
42	R	305	NEX	C11-C10	-2.21	1.36	1.43
26	s	314	CLA	CHC-C1C	2.21	1.43	1.38
26	y	309	CLA	C1B-C2B	2.21	1.48	1.43
26	B	612	CLA	CHC-C1C	2.20	1.43	1.38
26	N	307	CLA	CHC-C1C	2.20	1.43	1.38
26	R	314	CLA	CHC-C1C	2.20	1.43	1.38
26	g	302	CLA	CMB-C2B	-2.20	1.46	1.50
26	r	314	CLA	CMD-C2D	-2.20	1.46	1.50
26	c	520	CLA	CHC-C1C	2.20	1.43	1.38
39	N	303	CHL	C2C-C3C	2.20	1.38	1.36
26	C	505	CLA	CMD-C2D	-2.20	1.46	1.50
26	n	305	CLA	CHC-C1C	2.20	1.43	1.38
42	r	302	NEX	C34-C33	2.20	1.38	1.35
42	r	302	NEX	C11-C10	-2.19	1.36	1.43
26	G	306	CLA	CHC-C1C	2.19	1.43	1.38
26	b	612	CLA	C1B-C2B	2.19	1.48	1.43
26	C	517	CLA	MG-ND	-2.19	2.01	2.05
26	D	412	CLA	CHC-C1C	2.19	1.43	1.38
42	N	302	NEX	C11-C10	-2.19	1.36	1.43
27	a	410	PHO	CAC-C3C	-2.18	1.47	1.51
42	S	305	NEX	C11-C10	-2.18	1.36	1.43
26	S	309	CLA	CHC-C1C	2.18	1.43	1.38
26	Y	312	CLA	CHC-C1C	2.18	1.42	1.38
26	b	607	CLA	CHC-C1C	2.18	1.42	1.38
39	S	313	CHL	C2C-C3C	2.18	1.38	1.36
26	C	512	CLA	CMB-C2B	-2.18	1.46	1.50
26	y	316	CLA	CMD-C2D	-2.18	1.46	1.50
42	s	302	NEX	C11-C10	-2.17	1.36	1.43
26	r	313	CLA	CMD-C2D	-2.17	1.46	1.50
26	B	601	CLA	CHC-C1C	2.17	1.42	1.38
26	d	404	CLA	CMD-C2D	-2.17	1.46	1.50
26	r	315	CLA	CHC-C1C	2.17	1.42	1.38
26	D	401	CLA	CMB-C2B	-2.17	1.46	1.50
26	g	308	CLA	MG-ND	-2.17	2.01	2.05
42	y	307	NEX	C11-C10	-2.17	1.36	1.43
26	G	304	CLA	MG-NB	-2.17	2.01	2.05
39	y	303	CHL	C1A-CHA	2.17	1.42	1.40
26	B	610	CLA	CMC-C2C	-2.17	1.46	1.50
39	g	319	CHL	C2C-C3C	2.17	1.38	1.36
27	A	404	PHO	CAC-C3C	-2.17	1.47	1.51
26	c	515	CLA	CMB-C2B	-2.16	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	Y	304	NEX	C11-C10	-2.16	1.36	1.43
26	s	304	CLA	CHC-C1C	2.16	1.42	1.38
26	r	311	CLA	MG-NB	-2.16	2.01	2.05
26	b	610	CLA	CMC-C2C	-2.16	1.46	1.50
26	b	613	CLA	MG-ND	-2.16	2.01	2.05
39	G	305	CHL	C2C-C3C	2.16	1.38	1.36
26	c	513	CLA	CMB-C2B	-2.16	1.46	1.50
26	R	309	CLA	CHC-C1C	2.16	1.42	1.38
26	g	305	CLA	CHC-C1C	2.16	1.42	1.38
26	r	317	CLA	CHC-C1C	2.16	1.42	1.38
26	b	610	CLA	CMB-C2B	-2.16	1.46	1.50
29	W	202	SQD	O6-C1	2.16	1.43	1.40
26	C	504	CLA	CHC-C1C	2.16	1.42	1.38
26	S	304	CLA	CHC-C1C	2.15	1.42	1.38
42	r	302	NEX	C28-C29	-2.15	1.41	1.45
26	r	305	CLA	CMD-C2D	-2.15	1.46	1.50
26	C	515	CLA	CMD-C2D	-2.15	1.46	1.50
42	G	315	NEX	C11-C10	-2.15	1.36	1.43
26	n	309	CLA	CHC-C1C	2.15	1.42	1.38
26	d	404	CLA	CMC-C2C	-2.15	1.46	1.50
26	b	617	CLA	CMC-C2C	-2.15	1.46	1.50
30	d	408	PL9	C7-C8	-2.15	1.47	1.50
26	R	316	CLA	MG-ND	-2.15	2.01	2.05
26	a	409	CLA	MG-ND	-2.15	2.01	2.05
26	B	618	CLA	CMC-C2C	-2.15	1.46	1.50
26	Y	313	CLA	CMD-C2D	-2.15	1.46	1.50
26	a	409	CLA	CMB-C2B	-2.15	1.46	1.50
39	Y	318	CHL	C1A-CHA	2.15	1.42	1.40
26	R	307	CLA	CHC-C1C	2.15	1.42	1.38
26	r	305	CLA	CHC-C1C	2.15	1.42	1.38
26	N	318	CLA	CHC-C1C	2.15	1.42	1.38
26	R	309	CLA	CMD-C2D	-2.15	1.46	1.50
26	g	304	CLA	CHC-C1C	2.15	1.42	1.38
26	B	601	CLA	MG-NB	-2.15	2.01	2.05
26	n	310	CLA	CHC-C1C	2.14	1.42	1.38
26	B	613	CLA	CMB-C2B	-2.14	1.46	1.50
26	D	409	CLA	CMC-C2C	-2.14	1.46	1.50
26	G	304	CLA	CHC-C1C	2.14	1.42	1.38
26	g	318	CLA	CHC-C1C	2.14	1.42	1.38
26	G	302	CLA	CHC-C1C	2.14	1.42	1.38
26	y	316	CLA	CHC-C1C	2.14	1.42	1.38
26	S	314	CLA	CHC-C1C	2.14	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	411	CLA	CHC-C1C	2.14	1.42	1.38
26	g	302	CLA	CHC-C1C	2.14	1.42	1.38
42	g	306	NEX	C11-C10	-2.14	1.36	1.43
39	r	318	CHL	C3B-CAB	-2.14	1.43	1.47
39	s	317	CHL	C2C-C3C	2.14	1.38	1.36
26	b	613	CLA	CMC-C2C	-2.14	1.46	1.50
26	b	605	CLA	CHC-C1C	2.14	1.42	1.38
26	B	603	CLA	CMD-C2D	-2.14	1.46	1.50
26	R	308	CLA	MG-NB	-2.14	2.01	2.05
26	S	310	CLA	MG-NB	-2.14	2.01	2.05
42	R	305	NEX	C28-C29	-2.14	1.41	1.45
26	c	510	CLA	CHC-C1C	2.13	1.42	1.38
26	b	604	CLA	CMC-C2C	-2.13	1.46	1.50
26	c	504	CLA	CMD-C2D	-2.13	1.46	1.50
26	s	315	CLA	CHC-C1C	2.13	1.42	1.38
26	C	512	CLA	CHC-C1C	2.13	1.42	1.38
30	d	408	PL9	C31-C29	-2.13	1.46	1.51
26	N	312	CLA	CHC-C1C	2.13	1.42	1.38
39	n	308	CHL	C3B-CAB	-2.13	1.43	1.47
39	n	318	CHL	C3B-CAB	-2.13	1.43	1.47
26	R	314	CLA	MG-ND	-2.13	2.01	2.05
26	G	313	CLA	CHC-C1C	2.13	1.42	1.38
29	w	202	SQD	O6-C1	2.13	1.43	1.40
26	n	304	CLA	CMC-C2C	-2.13	1.46	1.50
26	n	302	CLA	CHC-C1C	2.13	1.42	1.38
26	b	612	CLA	CHC-C1C	2.13	1.42	1.38
26	R	306	CLA	CMB-C2B	-2.13	1.46	1.50
26	d	411	CLA	CMB-C2B	-2.13	1.46	1.50
26	b	607	CLA	CMD-C2D	-2.13	1.46	1.50
26	G	317	CLA	MG-ND	-2.12	2.01	2.05
26	G	314	CLA	CMD-C2D	-2.12	1.46	1.50
39	r	309	CHL	C3B-CAB	-2.12	1.43	1.47
26	s	305	CLA	CMD-C2D	-2.12	1.46	1.50
26	B	606	CLA	CHC-C1C	2.12	1.42	1.38
26	R	306	CLA	CHC-C1C	2.12	1.42	1.38
26	g	303	CLA	CHC-C1C	2.12	1.42	1.38
26	B	602	CLA	CHC-C1C	2.12	1.42	1.38
26	G	319	CLA	CHC-C1C	2.12	1.42	1.38
41	G	320	XAT	C14-C13	2.12	1.38	1.35
26	r	306	CLA	CMB-C2B	-2.12	1.46	1.50
26	y	304	CLA	CMD-C2D	-2.12	1.46	1.50
39	N	303	CHL	C3B-CAB	-2.12	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	302	CLA	CMD-C2D	-2.12	1.46	1.50
26	g	315	CLA	CHC-C1C	2.12	1.42	1.38
39	r	301	CHL	C3B-CAB	-2.12	1.43	1.47
26	B	617	CLA	CMC-C2C	-2.12	1.46	1.50
26	n	303	CLA	CHC-C1C	2.12	1.42	1.38
26	C	519	CLA	CHC-C1C	2.12	1.42	1.38
26	S	308	CLA	MG-ND	-2.12	2.01	2.05
42	n	313	NEX	C11-C10	-2.12	1.36	1.43
26	G	314	CLA	CHC-C1C	2.11	1.42	1.38
26	B	613	CLA	CMC-C2C	-2.11	1.46	1.50
26	B	617	CLA	CMB-C2B	-2.11	1.46	1.50
26	b	617	CLA	CMD-C2D	-2.11	1.46	1.50
26	y	316	CLA	CMC-C2C	-2.11	1.46	1.50
39	N	310	CHL	C3B-CAB	-2.11	1.43	1.47
26	R	316	CLA	CHC-C1C	2.11	1.42	1.38
26	S	308	CLA	CMD-C2D	-2.11	1.46	1.50
26	Y	313	CLA	CHC-C1C	2.11	1.42	1.38
26	D	409	CLA	CMB-C2B	-2.11	1.46	1.50
26	C	515	CLA	CHC-C1C	2.11	1.42	1.38
26	A	403	CLA	CMB-C2B	-2.11	1.46	1.50
26	c	510	CLA	CMC-C2C	-2.11	1.46	1.50
26	N	319	CLA	CHC-C1C	2.10	1.42	1.38
26	b	604	CLA	CMB-C2B	-2.10	1.46	1.50
27	D	403	PHO	CAC-C3C	-2.10	1.47	1.51
26	S	304	CLA	CMD-C2D	-2.10	1.46	1.50
26	d	404	CLA	CMB-C2B	-2.10	1.46	1.50
26	r	311	CLA	CMD-C2D	-2.10	1.46	1.50
26	r	303	CLA	CHC-C1C	2.10	1.42	1.38
27	a	410	PHO	C3B-C2B	-2.10	1.37	1.40
26	g	308	CLA	CHC-C1C	2.10	1.42	1.38
26	c	515	CLA	CHC-C1C	2.10	1.42	1.38
26	c	508	CLA	MG-ND	-2.10	2.01	2.05
26	R	307	CLA	MG-ND	2.10	2.10	2.05
26	C	508	CLA	CMD-C2D	-2.10	1.46	1.50
42	S	305	NEX	C28-C29	-2.10	1.41	1.45
42	s	302	NEX	C28-C29	-2.10	1.41	1.45
26	N	309	CLA	CHC-C1C	2.10	1.42	1.38
26	s	307	CLA	CMB-C2B	-2.10	1.46	1.50
39	y	302	CHL	C1A-CHA	2.10	1.42	1.40
26	B	609	CLA	CHC-C1C	2.10	1.42	1.38
26	B	610	CLA	CHC-C1C	2.10	1.42	1.38
39	G	318	CHL	C1A-CHA	2.10	1.42	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	514	CLA	MG-NB	-2.10	2.01	2.05
26	N	313	CLA	CMC-C2C	-2.10	1.46	1.50
26	C	520	CLA	CHC-C1C	2.09	1.43	1.38
39	s	317	CHL	C3B-CAB	-2.09	1.43	1.47
26	C	511	CLA	CMD-C2D	-2.09	1.46	1.50
26	g	303	CLA	CMC-C2C	-2.09	1.46	1.50
27	d	407	PHO	CAC-C3C	-2.09	1.47	1.51
26	Y	305	CLA	CMD-C2D	-2.09	1.46	1.50
26	n	312	CLA	CMD-C2D	-2.09	1.46	1.50
39	r	309	CHL	C1A-CHA	2.09	1.42	1.40
26	c	504	CLA	CHC-C1C	2.09	1.42	1.38
26	R	308	CLA	CMD-C2D	-2.09	1.46	1.50
30	D	411	PL9	C7-C8	-2.09	1.47	1.50
26	D	401	CLA	MG-ND	-2.09	2.01	2.05
26	y	309	CLA	CMD-C2D	-2.09	1.46	1.50
26	B	610	CLA	CMD-C2D	-2.09	1.46	1.50
26	S	303	CLA	CHC-C1C	2.09	1.42	1.38
26	D	406	CLA	CMD-C2D	-2.09	1.46	1.50
39	G	303	CHL	C2C-C3C	2.09	1.38	1.36
42	y	307	NEX	C28-C29	-2.09	1.41	1.45
26	r	310	CLA	CHC-C1C	2.09	1.42	1.38
39	S	313	CHL	C3B-CAB	-2.09	1.43	1.47
26	r	313	CLA	CMB-C2B	-2.08	1.46	1.50
26	S	308	CLA	CHC-C1C	2.08	1.42	1.38
26	R	302	CLA	CMB-C2B	-2.08	1.46	1.50
26	Y	301	CLA	CMD-C2D	-2.08	1.46	1.50
26	g	308	CLA	CMD-C2D	-2.08	1.46	1.50
39	G	318	CHL	C3B-CAB	-2.08	1.43	1.47
26	B	601	CLA	CMD-C2D	-2.08	1.46	1.50
26	S	310	CLA	CMD-C2D	-2.08	1.46	1.50
26	d	411	CLA	CMD-C2D	-2.08	1.46	1.50
27	A	404	PHO	C3D-C4D	2.08	1.44	1.41
26	b	602	CLA	CMD-C2D	-2.08	1.46	1.50
26	G	317	CLA	CMD-C2D	-2.08	1.46	1.50
39	R	318	CHL	C3B-CAB	-2.08	1.43	1.47
30	D	411	PL9	C31-C29	-2.08	1.47	1.51
26	b	608	CLA	CMB-C2B	-2.08	1.46	1.50
26	g	317	CLA	CMD-C2D	-2.08	1.46	1.50
26	n	315	CLA	CHC-C1C	2.08	1.42	1.38
26	G	307	CLA	CMB-C2B	-2.08	1.46	1.50
42	Y	304	NEX	C28-C29	-2.08	1.41	1.45
26	D	412	CLA	CMB-C2B	-2.08	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	520	CLA	CMB-C2B	-2.08	1.46	1.50
26	s	311	CLA	MG-ND	-2.08	2.01	2.05
39	g	311	CHL	C3B-CAB	-2.08	1.43	1.47
26	G	307	CLA	CMD-C2D	-2.08	1.46	1.50
26	g	304	CLA	CMD-C2D	-2.07	1.46	1.50
26	G	313	CLA	CMD-C2D	-2.07	1.46	1.50
26	G	314	CLA	CMB-C2B	-2.07	1.46	1.50
26	S	309	CLA	CMD-C2D	-2.07	1.46	1.50
26	r	306	CLA	CHC-C1C	2.07	1.42	1.38
26	R	307	CLA	CMB-C2B	-2.07	1.46	1.50
26	S	303	CLA	CMB-C2B	-2.07	1.46	1.50
26	G	317	CLA	CHC-C1C	2.07	1.42	1.38
26	S	307	CLA	CMD-C2D	-2.07	1.46	1.50
26	b	602	CLA	CMB-C2B	-2.07	1.46	1.50
26	R	313	CLA	CMC-C2C	-2.07	1.46	1.50
26	s	307	CLA	CMD-C2D	-2.07	1.46	1.50
39	n	319	CHL	C3B-CAB	-2.07	1.43	1.47
39	Y	302	CHL	C1A-CHA	2.07	1.42	1.40
26	R	306	CLA	CMD-C2D	-2.07	1.46	1.50
26	R	314	CLA	CMD-C2D	-2.07	1.46	1.50
26	n	315	CLA	CMD-C2D	-2.07	1.46	1.50
26	B	604	CLA	CHC-C1C	2.07	1.42	1.38
26	s	315	CLA	CMB-C2B	-2.07	1.46	1.50
26	b	607	CLA	MG-NB	-2.07	2.01	2.05
26	g	318	CLA	MG-NB	-2.07	2.01	2.05
26	R	310	CLA	CHC-C1C	2.07	1.42	1.38
26	d	403	CLA	CMB-C2B	-2.07	1.46	1.50
26	y	310	CLA	CMD-C2D	-2.07	1.46	1.50
26	y	317	CLA	CMB-C2B	-2.07	1.46	1.50
26	b	601	CLA	CMB-C2B	-2.07	1.46	1.50
26	s	304	CLA	CMD-C2D	-2.07	1.46	1.50
26	a	411	CLA	CMB-C2B	-2.07	1.46	1.50
26	b	618	CLA	CHC-C1C	2.07	1.42	1.38
26	B	606	CLA	CMB-C2B	-2.07	1.46	1.50
26	a	402	CLA	CMD-C2D	-2.07	1.46	1.50
27	A	404	PHO	C3B-C2B	-2.07	1.37	1.40
26	s	305	CLA	CHC-C1C	2.07	1.42	1.38
26	D	412	CLA	CMD-C2D	-2.07	1.46	1.50
26	s	301	CLA	CHC-C1C	2.07	1.42	1.38
39	g	307	CHL	C3B-CAB	-2.06	1.43	1.47
26	N	319	CLA	CMD-C2D	-2.06	1.46	1.50
26	y	315	CLA	CMB-C2B	-2.06	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	602	CLA	CMD-C2D	-2.06	1.46	1.50
26	B	616	CLA	CMD-C2D	-2.06	1.46	1.50
26	r	306	CLA	CMD-C2D	-2.06	1.46	1.50
27	a	410	PHO	C3D-C4D	2.06	1.44	1.41
26	b	617	CLA	CHC-C1C	2.06	1.42	1.38
26	c	516	CLA	CMD-C2D	-2.06	1.46	1.50
26	g	303	CLA	CMB-C2B	-2.06	1.46	1.50
39	G	303	CHL	C3B-CAB	-2.06	1.43	1.47
39	g	319	CHL	C3B-CAB	-2.06	1.43	1.47
26	n	304	CLA	CHC-C1C	2.06	1.42	1.38
26	S	308	CLA	CMB-C2B	-2.06	1.46	1.50
26	B	607	CLA	CMD-C2D	-2.06	1.46	1.50
39	R	315	CHL	CBA-CGA	2.06	1.56	1.50
26	N	306	CLA	CMD-C2D	-2.06	1.46	1.50
26	b	610	CLA	CMD-C2D	-2.06	1.46	1.50
41	g	320	XAT	C14-C13	2.06	1.38	1.35
26	C	507	CLA	CMD-C2D	-2.06	1.46	1.50
26	S	309	CLA	CMC-C2C	-2.06	1.46	1.50
26	S	314	CLA	CMB-C2B	-2.06	1.46	1.50
26	g	315	CLA	CMB-C2B	-2.06	1.46	1.50
26	Y	310	CLA	CMD-C2D	-2.06	1.46	1.50
41	G	320	XAT	C34-C33	2.06	1.38	1.35
26	g	304	CLA	CMB-C2B	-2.06	1.46	1.50
26	G	314	CLA	CMC-C2C	-2.06	1.46	1.50
26	y	315	CLA	CHC-C1C	2.05	1.42	1.38
39	G	305	CHL	C3B-CAB	-2.05	1.43	1.47
26	R	317	CLA	CMD-C2D	-2.05	1.46	1.50
42	N	302	NEX	C28-C29	-2.05	1.41	1.45
26	d	403	CLA	CHC-C1C	2.05	1.42	1.38
26	Y	313	CLA	CMC-C2C	-2.05	1.46	1.50
26	C	521	CLA	CHC-C1C	2.05	1.42	1.38
39	R	312	CHL	C3B-CAB	-2.05	1.43	1.47
26	g	303	CLA	CMD-C2D	-2.05	1.46	1.50
26	B	617	CLA	CMD-C2D	-2.05	1.46	1.50
26	s	311	CLA	CMD-C2D	-2.05	1.46	1.50
26	c	506	CLA	CHC-C1C	2.05	1.43	1.38
39	g	319	CHL	CBA-CGA	2.05	1.56	1.50
26	c	502	CLA	CMC-C2C	-2.05	1.46	1.50
26	n	315	CLA	CMB-C2B	-2.05	1.46	1.50
26	s	301	CLA	CMD-C2D	-2.05	1.46	1.50
26	C	519	CLA	CMC-C2C	-2.05	1.46	1.50
26	G	319	CLA	CMD-C2D	-2.05	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	R	312	CHL	C1A-CHA	2.05	1.42	1.40
26	b	611	CLA	MG-NC	2.05	2.11	2.06
26	G	306	CLA	CMB-C2B	-2.05	1.46	1.50
26	s	306	CLA	CMD-C2D	-2.05	1.46	1.50
26	C	507	CLA	CHC-C1C	2.05	1.42	1.38
26	c	503	CLA	CHC-C1C	2.05	1.42	1.38
26	d	403	CLA	CMD-C2D	-2.05	1.46	1.50
26	c	505	CLA	CMD-C2D	-2.04	1.46	1.50
26	B	603	CLA	CMB-C2B	-2.04	1.46	1.50
26	G	319	CLA	CMB-C2B	-2.04	1.46	1.50
26	Y	311	CLA	CMD-C2D	-2.04	1.46	1.50
26	s	307	CLA	CHC-C1C	2.04	1.42	1.38
26	b	616	CLA	CMD-C2D	-2.04	1.46	1.50
26	g	315	CLA	CMD-C2D	-2.04	1.46	1.50
26	y	315	CLA	CMD-C2D	-2.04	1.46	1.50
26	B	605	CLA	CMB-C2B	-2.04	1.46	1.50
26	N	308	CLA	CMD-C2D	-2.04	1.46	1.50
26	r	317	CLA	CMD-C2D	-2.04	1.46	1.50
42	n	313	NEX	C28-C29	-2.04	1.41	1.45
39	N	317	CHL	C3B-CAB	-2.04	1.43	1.47
26	g	305	CLA	CMB-C2B	-2.04	1.46	1.50
26	N	307	CLA	CMC-C2C	-2.04	1.46	1.50
26	b	609	CLA	CMB-C2B	-2.04	1.46	1.50
26	r	306	CLA	MG-ND	-2.04	2.01	2.05
26	Y	310	CLA	CMB-C2B	-2.04	1.46	1.50
26	S	303	CLA	CMD-C2D	-2.04	1.46	1.50
26	c	503	CLA	CMD-C2D	-2.04	1.46	1.50
26	Y	311	CLA	CMB-C2B	-2.04	1.46	1.50
26	y	317	CLA	CMD-C2D	-2.03	1.46	1.50
26	B	603	CLA	CMC-C2C	-2.03	1.46	1.50
26	s	304	CLA	CMC-C2C	-2.03	1.46	1.50
26	B	612	CLA	CMD-C2D	-2.03	1.46	1.50
26	c	514	CLA	CMD-C2D	-2.03	1.46	1.50
26	r	314	CLA	CMC-C2C	-2.03	1.46	1.50
26	C	515	CLA	CMB-C2B	-2.03	1.46	1.50
26	n	302	CLA	CMD-C2D	-2.03	1.46	1.50
27	d	407	PHO	C3D-C4D	2.03	1.44	1.41
26	c	514	CLA	CHC-C1C	2.03	1.42	1.38
26	C	504	CLA	CMD-C2D	-2.03	1.46	1.50
26	s	314	CLA	CMB-C2B	-2.03	1.46	1.50
26	B	605	CLA	CHC-C1C	2.03	1.42	1.38
39	g	311	CHL	C1A-CHA	2.03	1.42	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	519	CLA	CMD-C2D	-2.03	1.46	1.50
26	G	306	CLA	CMD-C2D	-2.03	1.46	1.50
26	n	303	CLA	CMB-C2B	-2.03	1.46	1.50
26	N	313	CLA	CMD-C2D	-2.03	1.46	1.50
26	S	311	CLA	CMB-C2B	-2.03	1.46	1.50
26	b	605	CLA	CMB-C2B	-2.03	1.46	1.50
26	N	318	CLA	MG-ND	-2.03	2.01	2.05
26	B	612	CLA	CMC-C2C	-2.03	1.46	1.50
26	B	616	CLA	CMB-C2B	-2.03	1.46	1.50
39	Y	318	CHL	O1D-CGD	2.03	1.26	1.21
26	D	406	CLA	CMB-C2B	-2.03	1.46	1.50
26	G	313	CLA	CMB-C2B	-2.03	1.46	1.50
26	b	614	CLA	CMC-C2C	-2.03	1.46	1.50
39	R	315	CHL	C3B-CAB	-2.03	1.43	1.47
26	N	306	CLA	CMB-C2B	-2.03	1.46	1.50
26	g	305	CLA	CMD-C2D	-2.03	1.46	1.50
26	s	301	CLA	CMB-C2B	-2.03	1.46	1.50
27	D	403	PHO	C3D-C4D	2.03	1.44	1.41
26	S	307	CLA	MG-ND	-2.03	2.01	2.05
26	N	306	CLA	CMC-C2C	-2.03	1.46	1.50
26	R	316	CLA	CMB-C2B	-2.03	1.46	1.50
26	N	318	CLA	CMD-C2D	-2.03	1.46	1.50
26	Y	312	CLA	CMD-C2D	-2.03	1.46	1.50
26	b	601	CLA	CMD-C2D	-2.02	1.46	1.50
26	r	308	CLA	CMB-C2B	-2.02	1.46	1.50
26	r	315	CLA	CMD-C2D	-2.02	1.46	1.50
39	y	303	CHL	C3B-CAB	-2.02	1.43	1.47
26	n	310	CLA	CMD-C2D	-2.02	1.46	1.50
26	r	315	CLA	CMB-C2B	-2.02	1.46	1.50
26	r	303	CLA	CMB-C2B	-2.02	1.46	1.50
26	n	302	CLA	MG-ND	-2.02	2.01	2.05
26	s	310	CLA	CMD-C2D	-2.02	1.46	1.50
38	e	101	HEM	CMB-C2B	2.02	1.55	1.50
26	y	317	CLA	MG-ND	-2.02	2.01	2.05
26	N	306	CLA	CHC-C1C	2.02	1.42	1.38
26	c	516	CLA	MG-ND	-2.02	2.01	2.05
42	g	306	NEX	C28-C29	-2.02	1.41	1.45
26	n	304	CLA	CMD-C2D	-2.02	1.46	1.50
26	c	518	CLA	CMD-C2D	-2.02	1.46	1.50
39	r	318	CHL	CBA-CGA	2.02	1.56	1.50
26	C	507	CLA	CMB-C2B	-2.02	1.46	1.50
26	b	608	CLA	CHC-C1C	2.02	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	n	315	CLA	CMC-C2C	-2.02	1.46	1.50
26	C	508	CLA	MG-ND	-2.02	2.01	2.05
26	Y	301	CLA	CMB-C2B	-2.02	1.46	1.50
39	n	307	CHL	C3B-CAB	-2.02	1.43	1.47
26	a	402	CLA	CMB-C2B	-2.02	1.46	1.50
39	N	311	CHL	C3B-CAB	-2.02	1.43	1.47
26	C	506	CLA	CMB-C2B	-2.02	1.46	1.50
26	c	508	CLA	CMB-C2B	-2.02	1.46	1.50
26	c	516	CLA	CMC-C2C	-2.02	1.46	1.50
26	r	311	CLA	CHC-C1C	2.02	1.42	1.38
39	y	314	CHL	C3B-CAB	-2.02	1.43	1.47
26	b	613	CLA	CMB-C2B	-2.02	1.46	1.50
39	g	307	CHL	C2C-C3C	2.01	1.38	1.36
26	B	605	CLA	CMD-C2D	-2.01	1.46	1.50
26	C	504	CLA	CMC-C2C	-2.01	1.46	1.50
26	B	606	CLA	CMD-C2D	-2.01	1.46	1.50
26	C	505	CLA	CMB-C2B	-2.01	1.46	1.50
26	Y	301	CLA	CHC-C1C	2.01	1.42	1.38
39	y	302	CHL	C2C-C3C	2.01	1.38	1.36
26	g	302	CLA	CMD-C2D	-2.01	1.46	1.50
26	B	610	CLA	CMB-C2B	-2.01	1.46	1.50
26	B	611	CLA	CMC-C2C	-2.01	1.46	1.50
26	n	302	CLA	CMB-C2B	-2.01	1.46	1.50
26	Y	311	CLA	CHC-C1C	2.01	1.42	1.38
26	G	307	CLA	CHC-C1C	2.01	1.42	1.38
26	g	317	CLA	CMB-C2B	-2.01	1.46	1.50
26	r	308	CLA	MG-ND	-2.01	2.01	2.05
26	D	401	CLA	CMD-C2D	-2.01	1.46	1.50
26	n	305	CLA	CMD-C2D	-2.01	1.46	1.50
26	n	310	CLA	CMB-C2B	-2.01	1.46	1.50
39	y	312	CHL	C3B-CAB	-2.01	1.43	1.47
26	B	607	CLA	CMC-C2C	-2.01	1.46	1.50
26	r	303	CLA	CMD-C2D	-2.01	1.46	1.50
26	B	602	CLA	CMB-C2B	-2.01	1.46	1.50
26	b	609	CLA	CMD-C2D	-2.01	1.46	1.50
26	c	503	CLA	CMB-C2B	-2.01	1.46	1.50
39	G	309	CHL	O1D-CGD	2.01	1.26	1.21
26	C	521	CLA	CMD-C2D	-2.01	1.46	1.50
26	g	308	CLA	CMC-C2C	-2.01	1.46	1.50
39	G	311	CHL	C3B-CAB	-2.01	1.43	1.47
26	R	317	CLA	CMB-C2B	-2.01	1.46	1.50
39	g	314	CHL	O1D-CGD	2.01	1.26	1.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	511	CLA	CMB-C2B	-2.01	1.46	1.50
26	C	521	CLA	CMB-C2B	-2.01	1.46	1.50
26	S	315	CLA	CMB-C2B	-2.01	1.46	1.50
26	c	510	CLA	CMD-C2D	-2.01	1.46	1.50
26	b	617	CLA	CMB-C2B	-2.01	1.46	1.50
26	G	317	CLA	CMC-C2C	-2.01	1.46	1.50
26	N	319	CLA	CMB-C2B	-2.01	1.46	1.50
26	R	302	CLA	CMC-C2C	-2.01	1.46	1.50
26	c	504	CLA	CMB-C2B	-2.01	1.46	1.50
39	Y	302	CHL	C3B-CAB	-2.01	1.43	1.47
26	b	608	CLA	CMD-C2D	-2.01	1.46	1.50
26	C	506	CLA	CMC-C2C	-2.01	1.46	1.50
26	b	602	CLA	CMC-C2C	-2.01	1.46	1.50
26	c	508	CLA	CMD-C2D	-2.01	1.46	1.50
26	c	514	CLA	CMB-C2B	-2.01	1.46	1.50
26	S	307	CLA	CMB-C2B	-2.01	1.46	1.50
26	y	317	CLA	CHC-C1C	2.01	1.42	1.38
26	N	312	CLA	CMB-C2B	-2.00	1.46	1.50
26	N	318	CLA	CMB-C2B	-2.00	1.46	1.50
26	g	317	CLA	CHC-C1C	2.00	1.42	1.38
26	R	309	CLA	CMB-C2B	-2.00	1.46	1.50
26	y	304	CLA	CHC-C1C	2.00	1.42	1.38
39	y	302	CHL	O1D-CGD	2.00	1.26	1.21
26	S	311	CLA	CMD-C2D	-2.00	1.46	1.50
26	g	318	CLA	CMB-C2B	-2.00	1.46	1.50
39	S	302	CHL	C3B-CAB	-2.00	1.43	1.47
26	Y	313	CLA	CMB-C2B	-2.00	1.46	1.50
26	b	607	CLA	CMB-C2B	-2.00	1.46	1.50
26	s	306	CLA	CMB-C2B	-2.00	1.46	1.50
26	a	411	CLA	CHC-C1C	2.00	1.42	1.38
39	Y	314	CHL	C3B-CAB	-2.00	1.43	1.47
26	S	315	CLA	CMD-C2D	-2.00	1.46	1.50
26	C	511	CLA	CHC-C1C	2.00	1.42	1.38

All (2351) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	y	303	CHL	C1B-CHB-C4A	13.41	129.61	121.39
39	Y	302	CHL	C1B-CHB-C4A	13.39	129.59	121.39
39	N	316	CHL	C1B-CHB-C4A	13.36	129.57	121.39
39	n	306	CHL	C1B-CHB-C4A	13.30	129.54	121.39
39	g	311	CHL	C1B-CHB-C4A	13.19	129.47	121.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	318	CHL	C1B-CHB-C4A	13.18	129.47	121.39
39	G	301	CHL	C1B-CHB-C4A	13.00	129.35	121.39
39	g	313	CHL	C1B-CHB-C4A	12.93	129.31	121.39
39	s	316	CHL	C1B-CHB-C4A	12.91	129.30	121.39
39	S	302	CHL	C1B-CHB-C4A	12.90	129.29	121.39
39	R	301	CHL	C1B-CHB-C4A	12.88	129.28	121.39
39	r	316	CHL	C1B-CHB-C4A	12.87	129.27	121.39
39	R	312	CHL	C1B-CHB-C4A	12.82	129.24	121.39
39	r	309	CHL	C1B-CHB-C4A	12.81	129.24	121.39
39	N	317	CHL	C1B-CHB-C4A	12.73	129.19	121.39
39	n	319	CHL	C1B-CHB-C4A	12.69	129.16	121.39
39	N	304	CHL	C1B-CHB-C4A	12.66	129.15	121.39
39	s	303	CHL	C1B-CHB-C4A	12.64	129.13	121.39
39	n	311	CHL	C1B-CHB-C4A	12.60	129.11	121.39
39	s	313	CHL	C1B-CHB-C4A	12.58	129.09	121.39
39	S	316	CHL	C1B-CHB-C4A	12.56	129.08	121.39
39	Y	314	CHL	C1B-CHB-C4A	12.55	129.08	121.39
39	y	312	CHL	C1B-CHB-C4A	12.52	129.06	121.39
39	r	301	CHL	C1B-CHB-C4A	12.49	129.04	121.39
39	g	314	CHL	C1B-CHB-C4A	12.49	129.04	121.39
39	y	314	CHL	C1B-CHB-C4A	12.48	129.03	121.39
39	G	309	CHL	C1B-CHB-C4A	12.47	129.03	121.39
39	S	312	CHL	C1B-CHB-C4A	12.47	129.03	121.39
39	Y	318	CHL	C1B-CHB-C4A	12.46	129.02	121.39
39	Y	317	CHL	C1B-CHB-C4A	12.43	129.00	121.39
39	g	312	CHL	C1B-CHB-C4A	12.43	129.00	121.39
39	G	311	CHL	C1B-CHB-C4A	12.42	129.00	121.39
39	R	318	CHL	C1B-CHB-C4A	12.41	128.99	121.39
39	y	302	CHL	C1B-CHB-C4A	12.40	128.99	121.39
39	y	305	CHL	C1B-CHB-C4A	12.38	128.98	121.39
39	S	313	CHL	C1B-CHB-C4A	12.36	128.96	121.39
39	s	317	CHL	C1B-CHB-C4A	12.34	128.95	121.39
39	Y	307	CHL	C1B-CHB-C4A	12.34	128.95	121.39
39	r	318	CHL	C1B-CHB-C4A	12.32	128.94	121.39
39	N	303	CHL	C1B-CHB-C4A	12.29	128.92	121.39
39	N	310	CHL	C1B-CHB-C4A	12.28	128.91	121.39
39	n	308	CHL	C1B-CHB-C4A	12.21	128.87	121.39
39	R	315	CHL	C1B-CHB-C4A	12.17	128.84	121.39
39	n	318	CHL	C1B-CHB-C4A	12.10	128.81	121.39
39	n	307	CHL	C1B-CHB-C4A	11.88	128.67	121.39
39	g	319	CHL	C1B-CHB-C4A	11.83	128.64	121.39
39	N	311	CHL	C1B-CHB-C4A	11.79	128.62	121.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	303	CHL	C1B-CHB-C4A	11.74	128.59	121.39
39	g	307	CHL	C1B-CHB-C4A	11.69	128.55	121.39
39	G	305	CHL	C1B-CHB-C4A	11.63	128.52	121.39
42	G	315	NEX	O24-C25-C24	9.23	120.32	113.38
42	g	306	NEX	O24-C25-C24	9.21	120.30	113.38
42	N	302	NEX	O24-C25-C24	9.15	120.25	113.38
42	n	313	NEX	O24-C25-C24	9.13	120.24	113.38
42	r	302	NEX	O24-C25-C24	8.62	119.86	113.38
42	R	305	NEX	O24-C25-C24	8.53	119.79	113.38
42	Y	304	NEX	O24-C25-C24	8.52	119.78	113.38
42	y	307	NEX	O24-C25-C24	8.48	119.75	113.38
41	N	315	XAT	O24-C25-C24	8.07	119.45	113.38
41	n	316	XAT	O24-C25-C24	7.98	119.37	113.38
41	G	310	XAT	O4-C5-C4	7.93	119.34	113.38
26	b	611	CLA	C4A-NA-C1A	7.90	110.26	106.71
41	G	320	XAT	O4-C5-C4	7.87	119.29	113.38
41	g	309	XAT	O4-C5-C4	7.81	119.25	113.38
41	g	320	XAT	O4-C5-C4	7.81	119.25	113.38
42	S	305	NEX	O24-C25-C24	7.67	119.14	113.38
41	G	310	XAT	O24-C25-C24	7.64	119.12	113.38
26	B	615	CLA	C4A-NA-C1A	7.64	110.14	106.71
41	r	304	XAT	O24-C25-C24	7.61	119.10	113.38
26	c	518	CLA	C4A-NA-C1A	7.57	110.11	106.71
41	g	309	XAT	O24-C25-C24	7.55	119.06	113.38
41	R	304	XAT	O24-C25-C24	7.49	119.00	113.38
41	G	320	XAT	O24-C25-C24	7.14	118.75	113.38
42	s	302	NEX	O24-C25-C24	7.10	118.72	113.38
41	g	320	XAT	O24-C25-C24	7.08	118.70	113.38
26	R	307	CLA	C4A-NA-C1A	6.95	109.83	106.71
26	C	504	CLA	C4A-NA-C1A	6.90	109.81	106.71
26	c	508	CLA	C4A-NA-C1A	6.88	109.80	106.71
26	C	516	CLA	C4A-NA-C1A	6.78	109.75	106.71
27	D	403	PHO	C4D-CHA-CBD	-6.68	105.49	108.52
39	Y	318	CHL	O2D-CGD-CBD	6.61	119.37	111.00
27	d	407	PHO	C4D-CHA-CBD	-6.61	105.53	108.52
39	G	311	CHL	O2D-CGD-CBD	6.54	119.28	111.00
39	g	312	CHL	O2D-CGD-CBD	6.52	119.26	111.00
39	y	302	CHL	O2D-CGD-CBD	6.46	119.18	111.00
41	r	304	XAT	O4-C5-C4	6.41	118.20	113.38
41	R	304	XAT	O4-C5-C4	6.38	118.17	113.38
39	S	312	CHL	O2D-CGD-CBD	6.37	119.07	111.00
39	n	307	CHL	O2D-CGD-CBD	6.36	119.05	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	609	CLA	C4A-NA-C1A	6.35	109.56	106.71
26	N	318	CLA	C4A-NA-C1A	6.31	109.54	106.71
26	c	510	CLA	C4A-NA-C1A	6.28	109.53	106.71
26	B	616	CLA	C4A-NA-C1A	6.27	109.53	106.71
26	n	302	CLA	C4A-NA-C1A	6.24	109.51	106.71
26	C	519	CLA	C4A-NA-C1A	6.21	109.50	106.71
26	N	306	CLA	C4A-NA-C1A	6.21	109.50	106.71
39	N	311	CHL	O2D-CGD-CBD	6.21	118.87	111.00
39	s	317	CHL	O2D-CGD-CBD	6.21	118.87	111.00
26	G	313	CLA	C4A-NA-C1A	6.17	109.48	106.71
26	c	505	CLA	C4A-NA-C1A	6.17	109.48	106.71
39	R	318	CHL	O2D-CGD-CBD	6.16	118.80	111.00
39	S	313	CHL	O2D-CGD-CBD	6.15	118.78	111.00
26	S	309	CLA	C4A-NA-C1A	6.15	109.47	106.71
26	C	507	CLA	C4A-NA-C1A	6.14	109.47	106.71
26	s	304	CLA	C4A-NA-C1A	6.13	109.46	106.71
39	r	301	CHL	O2D-CGD-CBD	6.13	118.76	111.00
39	Y	314	CHL	O2D-CGD-CBD	6.13	118.76	111.00
39	N	303	CHL	O2D-CGD-CBD	6.12	118.75	111.00
26	B	605	CLA	C4A-NA-C1A	6.11	109.45	106.71
39	n	318	CHL	O2D-CGD-CBD	6.08	118.70	111.00
26	C	512	CLA	C4A-NA-C1A	6.08	109.44	106.71
26	y	310	CLA	C4A-NA-C1A	6.07	109.44	106.71
26	g	315	CLA	C4A-NA-C1A	6.06	109.43	106.71
39	s	313	CHL	O2D-CGD-CBD	6.06	118.68	111.00
26	r	317	CLA	C4A-NA-C1A	6.05	109.43	106.71
39	R	315	CHL	O2D-CGD-CBD	6.05	118.66	111.00
26	y	315	CLA	C4A-NA-C1A	6.02	109.41	106.71
26	R	314	CLA	C4A-NA-C1A	6.01	109.41	106.71
26	n	310	CLA	C4A-NA-C1A	6.01	109.41	106.71
39	N	310	CHL	O2D-CGD-CBD	6.01	118.61	111.00
26	Y	311	CLA	C4A-NA-C1A	6.01	109.41	106.71
39	N	317	CHL	O2D-CGD-CBD	6.00	118.60	111.00
26	n	315	CLA	C4A-NA-C1A	5.99	109.40	106.71
39	N	304	CHL	O2D-CGD-CBD	5.94	118.52	111.00
39	y	312	CHL	O2D-CGD-CBD	5.94	118.52	111.00
26	c	515	CLA	C4A-NA-C1A	5.93	109.37	106.71
26	b	602	CLA	C4A-NA-C1A	5.92	109.37	106.71
39	G	305	CHL	O2D-CGD-CBD	5.92	118.49	111.00
39	n	319	CHL	O2D-CGD-CBD	5.92	118.49	111.00
39	y	305	CHL	O2D-CGD-CBD	5.91	118.49	111.00
39	n	308	CHL	O2D-CGD-CBD	5.91	118.48	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	Y	307	CHL	O2D-CGD-CBD	5.91	118.48	111.00
39	y	314	CHL	O2D-CGD-CBD	5.91	118.48	111.00
39	Y	317	CHL	O2D-CGD-CBD	5.90	118.47	111.00
39	r	318	CHL	O2D-CGD-CBD	5.90	118.47	111.00
26	B	603	CLA	C4A-NA-C1A	5.90	109.36	106.71
39	n	311	CHL	O2D-CGD-CBD	5.90	118.47	111.00
39	g	319	CHL	O2D-CGD-CBD	5.89	118.45	111.00
41	n	316	XAT	O4-C5-C4	5.89	117.80	113.38
26	Y	312	CLA	C4A-NA-C1A	5.88	109.35	106.71
39	S	316	CHL	O2D-CGD-CBD	5.88	118.44	111.00
26	G	317	CLA	C4A-NA-C1A	5.88	109.35	106.71
26	g	308	CLA	C4A-NA-C1A	5.87	109.35	106.71
39	R	301	CHL	O2D-CGD-CBD	5.87	118.44	111.00
26	c	504	CLA	C4A-NA-C1A	5.86	109.34	106.71
26	G	304	CLA	C4A-NA-C1A	5.85	109.34	106.71
26	s	301	CLA	C4A-NA-C1A	5.85	109.34	106.71
39	g	314	CHL	O2D-CGD-CBD	5.84	118.39	111.00
26	S	308	CLA	C4A-NA-C1A	5.83	109.33	106.71
39	s	303	CHL	O2D-CGD-CBD	5.81	118.36	111.00
26	N	319	CLA	C4A-NA-C1A	5.80	109.31	106.71
26	g	318	CLA	C4A-NA-C1A	5.80	109.31	106.71
26	y	304	CLA	C4A-NA-C1A	5.79	109.31	106.71
41	N	315	XAT	O4-C5-C4	5.78	117.72	113.38
42	R	305	NEX	C15-C14-C13	-5.77	119.08	127.31
39	S	302	CHL	O2D-CGD-CBD	5.76	118.30	111.00
39	s	316	CHL	O2D-CGD-CBD	5.76	118.30	111.00
39	G	309	CHL	O2D-CGD-CBD	5.76	118.29	111.00
27	A	404	PHO	C4D-CHA-CBD	-5.73	105.92	108.52
26	C	515	CLA	C4A-NA-C1A	5.73	109.28	106.71
26	b	608	CLA	C4A-NA-C1A	5.73	109.28	106.71
39	r	309	CHL	O2D-CGD-CBD	5.73	118.25	111.00
26	Y	313	CLA	C4A-NA-C1A	5.71	109.27	106.71
26	R	317	CLA	C4A-NA-C1A	5.70	109.27	106.71
26	Y	301	CLA	C4A-NA-C1A	5.69	109.26	106.71
42	r	302	NEX	C15-C14-C13	-5.67	119.21	127.31
26	g	304	CLA	C4A-NA-C1A	5.67	109.25	106.71
26	y	316	CLA	C4A-NA-C1A	5.67	109.25	106.71
42	S	305	NEX	C11-C10-C9	-5.66	119.23	127.31
27	a	410	PHO	C4D-CHA-CBD	-5.65	105.96	108.52
26	b	613	CLA	C4A-NA-C1A	5.64	109.24	106.71
26	N	309	CLA	C4A-NA-C1A	5.63	109.24	106.71
26	n	304	CLA	C4A-NA-C1A	5.62	109.23	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	r	315	CLA	C4A-NA-C1A	5.61	109.23	106.71
26	G	319	CLA	C4A-NA-C1A	5.60	109.22	106.71
26	B	617	CLA	C4A-NA-C1A	5.55	109.20	106.71
26	n	309	CLA	C4A-NA-C1A	5.54	109.20	106.71
39	R	312	CHL	O2D-CGD-CBD	5.54	118.02	111.00
39	y	303	CHL	O2D-CGD-CBD	5.54	118.02	111.00
26	b	614	CLA	C4A-NA-C1A	5.54	109.20	106.71
26	B	609	CLA	C4A-NA-C1A	5.53	109.19	106.71
39	g	313	CHL	O2D-CGD-CBD	5.53	118.00	111.00
39	Y	302	CHL	O2D-CGD-CBD	5.52	117.99	111.00
26	s	307	CLA	C4A-NA-C1A	5.51	109.18	106.71
26	g	303	CLA	C4A-NA-C1A	5.50	109.18	106.71
26	B	602	CLA	C4A-NA-C1A	5.49	109.18	106.71
26	B	613	CLA	C4A-NA-C1A	5.49	109.18	106.71
26	Y	308	CLA	C4A-NA-C1A	5.49	109.17	106.71
26	r	305	CLA	C4A-NA-C1A	5.47	109.17	106.71
26	N	313	CLA	C4A-NA-C1A	5.47	109.17	106.71
26	b	605	CLA	C4A-NA-C1A	5.47	109.16	106.71
39	G	301	CHL	O2D-CGD-CBD	5.46	117.91	111.00
26	r	303	CLA	C4A-NA-C1A	5.45	109.16	106.71
26	R	316	CLA	C4A-NA-C1A	5.45	109.15	106.71
26	B	618	CLA	C4A-NA-C1A	5.44	109.15	106.71
26	b	618	CLA	C4A-NA-C1A	5.42	109.14	106.71
26	S	303	CLA	C4A-NA-C1A	5.41	109.14	106.71
26	b	604	CLA	C4A-NA-C1A	5.39	109.13	106.71
26	c	516	CLA	C4A-NA-C1A	5.39	109.13	106.71
26	R	302	CLA	C4A-NA-C1A	5.38	109.12	106.71
26	b	616	CLA	C4A-NA-C1A	5.38	109.12	106.71
26	G	314	CLA	C4A-NA-C1A	5.38	109.12	106.71
39	r	316	CHL	O2D-CGD-CBD	5.37	117.80	111.00
26	g	305	CLA	C4A-NA-C1A	5.36	109.12	106.71
39	g	307	CHL	O2D-CGD-CBD	5.36	117.79	111.00
42	g	306	NEX	C27-C28-C29	-5.36	117.22	125.53
26	c	503	CLA	C4A-NA-C1A	5.35	109.11	106.71
39	G	303	CHL	O2D-CGD-CBD	5.34	117.77	111.00
42	G	315	NEX	C27-C28-C29	-5.34	117.25	125.53
26	G	302	CLA	C4A-NA-C1A	5.33	109.10	106.71
26	g	302	CLA	C4A-NA-C1A	5.33	109.10	106.71
26	n	305	CLA	C4A-NA-C1A	5.33	109.10	106.71
26	G	306	CLA	C4A-NA-C1A	5.33	109.10	106.71
26	B	612	CLA	C4A-NA-C1A	5.32	109.10	106.71
26	N	307	CLA	C4A-NA-C1A	5.32	109.10	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	610	CLA	C4A-NA-C1A	5.32	109.10	106.71
26	C	508	CLA	C4A-NA-C1A	5.32	109.10	106.71
26	y	306	CLA	C4A-NA-C1A	5.31	109.09	106.71
26	d	404	CLA	C4A-NA-C1A	5.29	109.09	106.71
26	B	610	CLA	C4A-NA-C1A	5.28	109.08	106.71
26	r	313	CLA	C4A-NA-C1A	5.28	109.08	106.71
26	r	308	CLA	C4A-NA-C1A	5.27	109.08	106.71
26	D	409	CLA	C4A-NA-C1A	5.27	109.07	106.71
26	B	607	CLA	C4A-NA-C1A	5.25	109.07	106.71
26	C	511	CLA	C4A-NA-C1A	5.18	109.03	106.71
42	G	315	NEX	C15-C14-C13	-5.16	119.94	127.31
42	n	313	NEX	C27-C28-C29	-5.14	117.56	125.53
42	s	302	NEX	C31-C30-C29	-5.13	119.99	127.31
26	S	315	CLA	C4A-NA-C1A	5.12	109.01	106.71
42	y	307	NEX	C35-C34-C33	-5.10	120.03	127.31
26	d	403	CLA	C4A-NA-C1A	5.09	108.99	106.71
30	D	411	PL9	C7-C3-C4	5.09	121.01	116.88
42	Y	304	NEX	C35-C34-C33	-5.09	120.05	127.31
26	R	309	CLA	C4A-NA-C1A	5.06	108.98	106.71
42	r	302	NEX	C11-C10-C9	-5.06	120.08	127.31
26	D	406	CLA	C4A-NA-C1A	5.06	108.98	106.71
41	r	304	XAT	C6-C7-C8	-5.06	115.30	125.99
41	R	304	XAT	C6-C7-C8	-5.05	115.31	125.99
42	Y	304	NEX	C27-C28-C29	-5.05	117.69	125.53
26	s	306	CLA	C4A-NA-C1A	5.04	108.97	106.71
26	b	617	CLA	C4A-NA-C1A	5.03	108.97	106.71
26	r	314	CLA	C4A-NA-C1A	5.02	108.97	106.71
42	N	302	NEX	C15-C14-C13	-5.02	120.14	127.31
26	R	313	CLA	C4A-NA-C1A	5.02	108.96	106.71
42	S	305	NEX	C31-C30-C29	-5.01	120.15	127.31
42	g	306	NEX	C15-C14-C13	-5.01	120.16	127.31
26	C	521	CLA	C4A-NA-C1A	5.00	108.95	106.71
42	g	306	NEX	C11-C10-C9	-5.00	120.17	127.31
42	y	307	NEX	C27-C28-C29	-5.00	117.77	125.53
30	d	408	PL9	C7-C3-C4	5.00	120.94	116.88
42	g	306	NEX	C35-C34-C33	-4.99	120.19	127.31
41	g	320	XAT	C7-C8-C9	-4.98	117.80	125.53
26	R	310	CLA	C4A-NA-C1A	4.97	108.94	106.71
41	G	320	XAT	C7-C8-C9	-4.96	117.84	125.53
41	G	320	XAT	C35-C34-C33	-4.95	120.24	127.31
39	N	316	CHL	O2D-CGD-CBD	4.94	117.26	111.00
42	s	302	NEX	C11-C10-C9	-4.94	120.26	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	g	320	XAT	C35-C34-C33	-4.94	120.26	127.31
26	c	514	CLA	C4A-NA-C1A	4.94	108.92	106.71
26	C	506	CLA	C4A-NA-C1A	4.93	108.92	106.71
26	r	310	CLA	C4A-NA-C1A	4.92	108.92	106.71
42	G	315	NEX	C35-C34-C33	-4.92	120.29	127.31
39	n	306	CHL	O2D-CGD-CBD	4.92	117.22	111.00
39	s	313	CHL	C4D-CHA-CBD	-4.88	103.86	108.89
26	s	310	CLA	C4A-NA-C1A	4.88	108.90	106.71
42	N	302	NEX	C27-C28-C29	-4.84	118.02	125.53
26	c	502	CLA	C4A-NA-C1A	4.84	108.88	106.71
42	G	315	NEX	C11-C10-C9	-4.83	120.41	127.31
26	S	310	CLA	C4A-NA-C1A	4.83	108.88	106.71
39	G	318	CHL	O2D-CGD-CBD	4.82	117.10	111.00
26	r	311	CLA	C4A-NA-C1A	4.82	108.87	106.71
39	S	312	CHL	C4D-CHA-CBD	-4.80	103.94	108.89
42	n	313	NEX	C15-C14-C13	-4.78	120.48	127.31
26	R	308	CLA	C4A-NA-C1A	4.78	108.86	106.71
26	a	411	CLA	C4A-NA-C1A	4.78	108.86	106.71
42	R	305	NEX	C11-C10-C9	-4.78	120.49	127.31
29	A	407	SQD	O8-S-C6	-4.78	98.13	105.74
39	s	317	CHL	CBC-CAC-C3C	-4.78	105.89	112.88
29	a	403	SQD	O8-S-C6	-4.75	98.17	105.74
41	N	315	XAT	C15-C14-C13	-4.71	120.58	127.31
39	S	316	CHL	C3D-C4D-CHA	4.67	115.64	108.54
41	R	304	XAT	C26-C27-C28	-4.67	116.13	125.99
39	s	303	CHL	C3D-C4D-CHA	4.65	115.61	108.54
39	g	319	CHL	C3D-C4D-CHA	4.64	115.59	108.54
39	y	305	CHL	C3D-C4D-CHA	4.64	115.59	108.54
39	n	318	CHL	C3D-C4D-CHA	4.63	115.58	108.54
39	S	313	CHL	CBC-CAC-C3C	-4.63	106.10	112.88
39	Y	317	CHL	C3D-C4D-CHA	4.63	115.57	108.54
39	y	312	CHL	C3D-C4D-CHA	4.62	115.56	108.54
39	r	318	CHL	C3D-C4D-CHA	4.62	115.56	108.54
39	N	303	CHL	C3D-C4D-CHA	4.61	115.56	108.54
26	C	517	CLA	C4A-NA-C1A	4.61	108.78	106.71
26	s	305	CLA	C4A-NA-C1A	4.60	108.78	106.71
39	G	305	CHL	C3D-C4D-CHA	4.60	115.53	108.54
39	R	315	CHL	C3D-C4D-CHA	4.59	115.52	108.54
41	n	316	XAT	C15-C14-C13	-4.58	120.77	127.31
41	g	320	XAT	C20-C13-C12	4.58	125.29	118.08
26	c	513	CLA	C4A-NA-C1A	4.57	108.76	106.71
26	C	505	CLA	C4A-NA-C1A	4.57	108.76	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	s	317	CHL	C3D-C4D-CHA	4.57	115.48	108.54
39	Y	314	CHL	C3D-C4D-CHA	4.56	115.48	108.54
41	G	320	XAT	C20-C13-C12	4.56	125.26	118.08
39	R	318	CHL	C3D-C4D-CHA	4.55	115.45	108.54
26	A	403	CLA	C4A-NA-C1A	4.55	108.75	106.71
39	g	311	CHL	O2D-CGD-CBD	4.54	116.75	111.00
39	Y	307	CHL	C3D-C4D-CHA	4.54	115.45	108.54
30	a	407	PL9	C7-C3-C4	4.54	120.56	116.88
39	r	301	CHL	C3D-C4D-CHA	4.54	115.44	108.54
39	G	309	CHL	C3D-C4D-CHA	4.53	115.43	108.54
39	N	317	CHL	C3D-C4D-CHA	4.53	115.43	108.54
41	r	304	XAT	C26-C27-C28	-4.53	116.41	125.99
26	S	304	CLA	C4A-NA-C1A	4.53	108.74	106.71
42	s	302	NEX	C26-C27-C28	-4.52	116.43	125.99
39	S	312	CHL	C3D-C4D-CHA	4.52	115.42	108.54
39	g	314	CHL	C3D-C4D-CHA	4.52	115.41	108.54
39	n	306	CHL	C3D-C4D-CHA	4.52	115.41	108.54
39	G	311	CHL	C3D-C4D-CHA	4.52	115.40	108.54
39	N	316	CHL	C3D-C4D-CHA	4.51	115.40	108.54
39	N	304	CHL	C3D-C4D-CHA	4.51	115.40	108.54
39	Y	302	CHL	C3D-C4D-CHA	4.51	115.40	108.54
26	c	520	CLA	C4A-NA-C1A	4.51	108.73	106.71
39	n	319	CHL	C3D-C4D-CHA	4.51	115.39	108.54
39	g	313	CHL	C3D-C4D-CHA	4.51	115.39	108.54
39	G	301	CHL	C3D-C4D-CHA	4.50	115.39	108.54
39	s	313	CHL	C3D-C4D-CHA	4.50	115.38	108.54
39	n	311	CHL	C3D-C4D-CHA	4.50	115.38	108.54
39	g	312	CHL	C3D-C4D-CHA	4.49	115.37	108.54
26	b	606	CLA	C4A-NA-C1A	4.49	108.72	106.71
39	S	313	CHL	C3D-C4D-CHA	4.49	115.36	108.54
39	y	314	CHL	C3D-C4D-CHA	4.48	115.34	108.54
42	R	305	NEX	C27-C28-C29	-4.48	118.58	125.53
28	T	101	BCR	C24-C23-C22	-4.47	119.47	126.23
39	y	303	CHL	C3D-C4D-CHA	4.47	115.34	108.54
39	N	310	CHL	C3D-C4D-CHA	4.47	115.34	108.54
39	r	316	CHL	C4D-CHA-CBD	-4.47	104.28	108.89
41	n	316	XAT	C31-C30-C29	-4.47	120.93	127.31
39	n	308	CHL	C3D-C4D-CHA	4.47	115.33	108.54
39	g	311	CHL	C3D-C4D-CHA	4.46	115.33	108.54
26	B	611	CLA	C4A-NA-C1A	4.46	108.71	106.71
39	G	318	CHL	C3D-C4D-CHA	4.45	115.31	108.54
26	y	313	CLA	C4A-NA-C1A	4.44	108.70	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	N	302	NEX	C35-C34-C33	-4.44	120.98	127.31
26	y	317	CLA	C4A-NA-C1A	4.44	108.70	106.71
42	S	305	NEX	C35-C34-C33	-4.42	121.00	127.31
26	n	312	CLA	C4A-NA-C1A	4.42	108.69	106.71
41	N	315	XAT	C31-C30-C29	-4.41	121.01	127.31
39	s	316	CHL	C3D-C4D-CHA	4.41	115.25	108.54
39	R	312	CHL	C3D-C4D-CHA	4.41	115.25	108.54
39	S	302	CHL	C3D-C4D-CHA	4.41	115.24	108.54
29	W	202	SQD	O8-S-C6	-4.41	98.71	105.74
39	r	309	CHL	C3D-C4D-CHA	4.41	115.24	108.54
39	G	303	CHL	C3D-C4D-CHA	4.41	115.24	108.54
39	g	307	CHL	C3D-C4D-CHA	4.40	115.22	108.54
29	B	621	SQD	O8-S-C6	-4.39	98.74	105.74
42	r	302	NEX	C27-C28-C29	-4.39	118.72	125.53
26	N	308	CLA	C4A-NA-C1A	4.39	108.68	106.71
29	b	621	SQD	O8-S-C6	-4.38	98.76	105.74
42	n	313	NEX	C35-C34-C33	-4.38	121.06	127.31
42	N	302	NEX	C11-C10-C9	-4.37	121.07	127.31
39	n	307	CHL	C3D-C4D-CHA	4.37	115.19	108.54
39	R	301	CHL	C4D-CHA-CBD	-4.37	104.38	108.89
39	N	311	CHL	C3D-C4D-CHA	4.36	115.16	108.54
39	R	301	CHL	C3D-C4D-CHA	4.35	115.15	108.54
39	n	306	CHL	CBC-CAC-C3C	-4.35	106.51	112.88
39	r	316	CHL	C3D-C4D-CHA	4.35	115.14	108.54
28	t	101	BCR	C24-C23-C22	-4.34	119.67	126.23
26	Y	316	CLA	C4A-NA-C1A	4.34	108.66	106.71
39	y	302	CHL	C3D-C4D-CHA	4.33	115.12	108.54
30	A	408	PL9	C7-C3-C4	4.33	120.40	116.88
42	Y	304	NEX	C15-C14-C13	-4.33	121.13	127.31
42	y	307	NEX	C15-C14-C13	-4.33	121.14	127.31
39	Y	318	CHL	C3D-C4D-CHA	4.30	115.08	108.54
29	w	202	SQD	O8-S-C6	-4.29	98.90	105.74
41	n	316	XAT	C6-C7-C8	-4.28	116.95	125.99
42	S	305	NEX	C15-C14-C13	-4.26	121.23	127.31
41	R	304	XAT	C35-C34-C33	-4.26	121.24	127.31
39	g	319	CHL	C4D-CHA-CBD	-4.25	104.51	108.89
42	S	305	NEX	C26-C27-C28	-4.25	117.01	125.99
41	G	320	XAT	C31-C30-C29	-4.25	121.25	127.31
26	Y	310	CLA	C4A-NA-C1A	4.23	108.61	106.71
26	c	513	CLA	O2D-CGD-O1D	-4.23	115.57	123.84
39	S	316	CHL	C4D-CHA-CBD	-4.23	104.53	108.89
26	C	517	CLA	O2D-CGD-O1D	-4.20	115.63	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	N	316	CHL	CBC-CAC-C3C	-4.19	106.74	112.88
39	s	303	CHL	C4D-CHA-CBD	-4.18	104.58	108.89
39	G	305	CHL	C4D-CHA-CBD	-4.18	104.58	108.89
26	b	612	CLA	C4A-NA-C1A	4.17	108.58	106.71
41	N	315	XAT	C35-C34-C33	-4.16	121.37	127.31
41	r	304	XAT	C35-C34-C33	-4.16	121.37	127.31
39	G	303	CHL	CBC-CAC-C3C	-4.16	106.79	112.88
39	n	318	CHL	C4D-CHA-CBD	-4.15	104.61	108.89
39	y	312	CHL	C4D-CHA-CBD	-4.15	104.61	108.89
39	N	303	CHL	C4D-CHA-CBD	-4.14	104.62	108.89
42	s	302	NEX	C35-C34-C33	-4.14	121.41	127.31
39	g	313	CHL	C4D-CHA-CBD	-4.13	104.63	108.89
39	G	301	CHL	C4D-CHA-CBD	-4.12	104.64	108.89
41	g	309	XAT	C35-C34-C33	-4.11	121.44	127.31
39	G	309	CHL	C4D-CHA-CBD	-4.10	104.66	108.89
26	b	607	CLA	C4A-NA-C1A	4.09	108.55	106.71
39	g	307	CHL	CBC-CAC-C3C	-4.09	106.89	112.88
32	a	405	BCT	O2-C-O1	4.09	130.15	119.55
39	g	314	CHL	C4D-CHA-CBD	-4.06	104.70	108.89
26	B	604	CLA	C4A-NA-C1A	4.06	108.53	106.71
41	N	315	XAT	C6-C7-C8	-4.05	117.43	125.99
42	s	302	NEX	C15-C14-C13	-4.04	121.54	127.31
41	g	320	XAT	C31-C30-C29	-4.04	121.55	127.31
41	G	310	XAT	C35-C34-C33	-4.04	121.55	127.31
39	Y	317	CHL	C4D-CHA-CBD	-4.03	104.73	108.89
39	y	305	CHL	C4D-CHA-CBD	-4.03	104.74	108.89
39	Y	314	CHL	C4D-CHA-CBD	-4.03	104.74	108.89
26	D	401	CLA	C4A-NA-C1A	4.02	108.51	106.71
39	G	311	CHL	C4D-CHA-CBD	-4.00	104.77	108.89
41	n	316	XAT	C35-C34-C33	-3.99	121.62	127.31
39	G	305	CHL	CMA-C3A-C4A	-3.98	105.65	114.38
41	G	310	XAT	C31-C30-C29	-3.98	121.63	127.31
26	Y	301	CLA	O2D-CGD-O1D	-3.98	116.06	123.84
39	S	302	CHL	C4D-CHA-CBD	-3.97	104.80	108.89
39	g	312	CHL	C4D-CHA-CBD	-3.97	104.80	108.89
39	R	315	CHL	C4D-CHA-CBD	-3.97	104.80	108.89
39	r	301	CHL	C4D-CHA-CBD	-3.96	104.81	108.89
29	A	410	SQD	O8-S-C6	-3.96	99.43	105.74
39	G	303	CHL	C4D-CHA-CBD	-3.95	104.81	108.89
39	n	307	CHL	CBC-CAC-C3C	-3.95	107.10	112.88
39	r	318	CHL	C4D-CHA-CBD	-3.94	104.83	108.89
26	B	601	CLA	C4A-NA-C1A	3.94	108.48	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	s	316	CHL	C4D-CHA-CBD	-3.94	104.83	108.89
42	G	315	NEX	C38-C25-C26	-3.93	115.67	122.26
26	A	405	CLA	C4A-NA-C1A	3.93	108.47	106.71
41	g	309	XAT	C31-C30-C29	-3.92	121.71	127.31
39	Y	302	CHL	CBC-CAC-C3C	-3.92	107.14	112.88
42	g	306	NEX	C38-C25-C26	-3.91	115.70	122.26
39	N	316	CHL	C4D-CHA-CBD	-3.91	104.86	108.89
39	n	306	CHL	C4D-CHA-CBD	-3.91	104.86	108.89
39	R	318	CHL	C4D-CHA-CBD	-3.91	104.86	108.89
39	n	307	CHL	C4D-CHA-CBD	-3.91	104.86	108.89
39	N	311	CHL	CBC-CAC-C3C	-3.91	107.16	112.88
39	y	305	CHL	CBC-CAC-C3C	-3.91	107.16	112.88
39	n	308	CHL	CMA-C3A-C4A	-3.90	105.83	114.38
39	n	319	CHL	C4D-CHA-CBD	-3.90	104.87	108.89
39	N	317	CHL	C4D-CHA-CBD	-3.89	104.88	108.89
26	s	311	CLA	C4A-NA-C1A	3.89	108.45	106.71
28	T	101	BCR	C15-C14-C13	3.88	132.85	127.31
39	Y	317	CHL	CBC-CAC-C3C	-3.87	107.21	112.88
39	g	307	CHL	C4D-CHA-CBD	-3.87	104.90	108.89
39	s	317	CHL	C4D-CHA-CBD	-3.87	104.90	108.89
26	C	506	CLA	O2D-CGD-O1D	-3.87	116.28	123.84
39	y	303	CHL	CBC-CAC-C3C	-3.85	107.24	112.88
26	a	409	CLA	C4A-NA-C1A	3.85	108.44	106.71
39	N	304	CHL	C4D-CHA-CBD	-3.84	104.94	108.89
42	r	302	NEX	C38-C25-C26	-3.82	115.85	122.26
26	b	606	CLA	O2D-CGD-O1D	-3.82	116.37	123.84
39	N	310	CHL	CMA-C3A-C4A	-3.82	106.02	114.38
39	N	311	CHL	C4D-CHA-CBD	-3.81	104.96	108.89
26	b	617	CLA	O2D-CGD-O1D	-3.81	116.39	123.84
41	g	309	XAT	C15-C14-C13	-3.81	121.88	127.31
26	B	610	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
39	n	311	CHL	C4D-CHA-CBD	-3.80	104.98	108.89
39	n	318	CHL	CMA-C3A-C4A	-3.80	106.06	114.38
42	R	305	NEX	C38-C25-C26	-3.80	115.90	122.26
39	s	313	CHL	OBD-CAD-CBD	-3.80	120.25	125.82
26	c	502	CLA	O2D-CGD-O1D	-3.79	116.43	123.84
39	S	313	CHL	C4D-CHA-CBD	-3.79	104.99	108.89
39	R	312	CHL	C4D-CHA-CBD	-3.77	105.01	108.89
39	N	310	CHL	C4D-CHA-CBD	-3.76	105.01	108.89
39	Y	307	CHL	C4D-CHA-CBD	-3.76	105.01	108.89
26	B	611	CLA	O2D-CGD-O1D	-3.76	116.48	123.84
39	Y	318	CHL	C4D-CHA-CBD	-3.76	105.01	108.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	601	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
29	a	413	SQD	O8-S-C6	-3.75	99.76	105.74
39	g	319	CHL	CMA-C3A-C4A	-3.75	106.17	114.38
39	n	308	CHL	C4D-CHA-CBD	-3.74	105.03	108.89
39	g	319	CHL	CAA-C2A-C3A	-3.73	102.55	112.78
41	G	310	XAT	C15-C14-C13	-3.73	121.98	127.31
26	c	520	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
39	r	309	CHL	C4D-CHA-CBD	-3.72	105.06	108.89
39	g	311	CHL	CBC-CAC-C3C	-3.71	107.45	112.88
39	G	318	CHL	C4D-CHA-CBD	-3.71	105.07	108.89
39	G	311	CHL	CAA-C2A-C3A	-3.71	102.63	112.78
39	g	314	CHL	CMA-C3A-C4A	-3.70	106.27	114.38
39	N	317	CHL	CAA-C2A-C3A	-3.70	102.66	112.78
42	s	302	NEX	C40-C33-C32	3.69	123.90	118.08
39	y	314	CHL	C4D-CHA-CBD	-3.69	105.09	108.89
26	R	308	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
39	R	301	CHL	CBC-CAC-C3C	-3.68	107.50	112.88
39	n	319	CHL	CBC-CAC-C3C	-3.68	107.50	112.88
39	G	309	CHL	CMA-C3A-C4A	-3.68	106.33	114.38
39	y	302	CHL	C4D-CHA-CBD	-3.68	105.10	108.89
39	n	319	CHL	CAA-C2A-C3A	-3.67	102.72	112.78
26	R	317	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
39	g	312	CHL	CAA-C2A-C3A	-3.67	102.74	112.78
39	Y	302	CHL	C4D-CHA-CBD	-3.66	105.11	108.89
26	a	402	CLA	C4A-NA-C1A	3.66	108.35	106.71
26	r	315	CLA	O2D-CGD-O1D	-3.66	116.69	123.84
41	g	309	XAT	C18-C5-C6	-3.66	116.13	122.26
26	r	311	CLA	O2D-CGD-O1D	-3.66	116.69	123.84
42	n	313	NEX	C11-C10-C9	-3.65	122.09	127.31
39	g	311	CHL	C4D-CHA-CBD	-3.65	105.13	108.89
26	s	314	CLA	CHB-C4A-NA	3.65	129.56	124.51
39	N	303	CHL	CMA-C3A-C4A	-3.65	106.39	114.38
39	R	315	CHL	CMA-C3A-C4A	-3.64	106.39	114.38
39	s	313	CHL	CMA-C3A-C4A	-3.64	106.40	114.38
39	S	312	CHL	CMA-C3A-C4A	-3.64	106.40	114.38
39	G	303	CHL	CMA-C3A-C4A	-3.64	106.41	114.38
39	s	303	CHL	OBD-CAD-CBD	-3.63	120.49	125.82
41	G	310	XAT	C18-C5-C6	-3.63	116.17	122.26
39	s	303	CHL	CBC-CAC-C3C	-3.63	107.57	112.88
39	S	302	CHL	CAA-C2A-C3A	-3.63	102.84	112.78
39	r	301	CHL	CAA-C2A-C3A	-3.63	102.85	112.78
39	Y	314	CHL	CMA-C3A-C4A	-3.62	106.44	114.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	g	307	CHL	CMA-C3A-C4A	-3.62	106.44	114.38
39	n	307	CHL	CMA-C3A-C4A	-3.62	106.44	114.38
26	S	307	CLA	C4A-NA-C1A	3.62	108.33	106.71
39	r	316	CHL	CBC-CAC-C3C	-3.61	107.59	112.88
26	S	311	CLA	CHB-C4A-NA	3.61	129.51	124.51
26	B	606	CLA	O2D-CGD-O1D	-3.61	116.77	123.84
39	s	316	CHL	CAA-C2A-C3A	-3.61	102.89	112.78
41	g	309	XAT	C26-C27-C28	-3.61	118.36	125.99
26	y	304	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
42	S	305	NEX	C40-C33-C32	3.60	123.76	118.08
39	y	303	CHL	C4D-CHA-CBD	-3.60	105.18	108.89
41	R	304	XAT	C15-C14-C13	-3.59	122.18	127.31
26	c	505	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
27	d	407	PHO	CMB-C2B-C3B	3.59	131.40	124.68
39	G	305	CHL	CAA-C2A-C3A	-3.59	102.95	112.78
26	C	512	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
39	S	312	CHL	OBD-CAD-CBD	-3.58	120.57	125.82
39	G	318	CHL	CBC-CAC-C3C	-3.57	107.65	112.88
27	D	403	PHO	CMB-C2B-C3B	3.57	131.36	124.68
39	S	316	CHL	OBD-CAD-CBD	-3.57	120.58	125.82
26	n	310	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
28	t	101	BCR	C15-C14-C13	3.57	132.40	127.31
41	N	315	XAT	C11-C10-C9	-3.57	122.22	127.31
39	n	319	CHL	CMA-C3A-C4A	-3.57	106.57	114.38
26	C	505	CLA	O2D-CGD-O1D	-3.57	116.87	123.84
26	C	507	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
39	N	311	CHL	CMA-C3A-C4A	-3.56	106.59	114.38
26	c	515	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
39	y	312	CHL	CMA-C3A-C4A	-3.54	106.62	114.38
26	s	314	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
39	s	317	CHL	CMA-C3A-C4A	-3.54	106.62	114.38
26	S	311	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
39	r	309	CHL	CMA-C3A-C4A	-3.54	106.63	114.38
39	R	312	CHL	CMA-C3A-C4A	-3.54	106.64	114.38
39	r	318	CHL	CMA-C3A-C4A	-3.53	106.64	114.38
41	G	310	XAT	C26-C27-C28	-3.53	118.53	125.99
39	S	313	CHL	CMA-C3A-C4A	-3.52	106.67	114.38
39	g	313	CHL	CBC-CAC-C3C	-3.52	107.73	112.88
39	N	317	CHL	CBC-CAC-C3C	-3.52	107.73	112.88
26	r	313	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
26	R	302	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
39	R	318	CHL	CAA-C2A-C3A	-3.51	103.16	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	516	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
39	G	301	CHL	CBC-CAC-C3C	-3.50	107.75	112.88
26	r	314	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
39	S	316	CHL	CBC-CAC-C3C	-3.49	107.77	112.88
41	G	310	XAT	C11-C10-C9	-3.49	122.34	127.31
26	A	405	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
42	N	302	NEX	C31-C30-C29	-3.48	122.34	127.31
26	b	605	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
39	G	311	CHL	CMA-C3A-C4A	-3.47	106.77	114.38
26	N	319	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
39	N	303	CHL	CAA-C2A-C3A	-3.47	103.28	112.78
42	Y	304	NEX	C38-C25-C26	-3.47	116.45	122.26
41	g	309	XAT	C11-C10-C9	-3.46	122.37	127.31
39	g	312	CHL	CMA-C3A-C4A	-3.46	106.80	114.38
26	a	402	CLA	O2D-CGD-O1D	-3.46	117.07	123.84
41	g	320	XAT	C26-C27-C28	-3.46	118.68	125.99
42	y	307	NEX	C38-C25-C26	-3.44	116.50	122.26
26	c	508	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
39	N	304	CHL	CBC-CAC-C3C	-3.44	107.85	112.88
26	B	602	CLA	O2D-CGD-O1D	-3.43	117.12	123.84
39	G	303	CHL	OBD-CAD-CBD	-3.43	120.79	125.82
39	y	314	CHL	CMA-C3A-C4A	-3.43	106.87	114.38
39	G	301	CHL	CMA-C3A-C4A	-3.43	106.87	114.38
26	R	313	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
39	y	302	CHL	CBC-CAC-C3C	-3.41	107.89	112.88
39	n	311	CHL	CBC-CAC-C3C	-3.41	107.89	112.88
39	N	317	CHL	CMA-C3A-C4A	-3.40	106.94	114.38
42	n	313	NEX	C38-C25-C26	-3.40	116.57	122.26
39	Y	307	CHL	CMA-C3A-C4A	-3.40	106.94	114.38
39	S	316	CHL	CAA-C2A-C3A	-3.39	103.48	112.78
26	B	606	CLA	C4A-NA-C1A	3.39	108.23	106.71
26	C	519	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
30	d	408	PL9	C7-C3-C2	-3.39	118.84	123.30
26	R	314	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
30	D	411	PL9	C7-C3-C2	-3.38	118.85	123.30
39	s	303	CHL	CAA-C2A-C3A	-3.38	103.52	112.78
39	S	313	CHL	CAA-C2A-C3A	-3.38	103.52	112.78
39	S	312	CHL	CAA-C2A-C3A	-3.38	103.52	112.78
26	r	317	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
26	G	313	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
39	g	307	CHL	CAA-C2A-C3A	-3.37	103.54	112.78
26	B	615	CLA	O2D-CGD-O1D	-3.37	117.25	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	R	301	CHL	CMA-C3A-C4A	-3.37	106.99	114.38
39	G	318	CHL	CMA-C3A-C4A	-3.37	107.00	114.38
26	c	510	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
39	G	303	CHL	CAA-C2A-C3A	-3.37	103.56	112.78
39	g	311	CHL	CMA-C3A-C4A	-3.37	107.00	114.38
39	r	301	CHL	CMA-C3A-C4A	-3.37	107.00	114.38
39	y	302	CHL	OMC-CMC-C2C	-3.37	119.64	125.03
42	N	302	NEX	C38-C25-C26	-3.36	116.63	122.26
39	r	316	CHL	CMA-C3A-C4A	-3.36	107.02	114.38
26	Y	310	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
42	s	302	NEX	C38-C25-C26	-3.36	116.63	122.26
39	Y	307	CHL	CBC-CAC-C3C	-3.36	107.96	112.88
26	Y	308	CLA	C1-C2-C3	-3.36	120.24	126.04
26	D	401	CLA	CHD-C1D-ND	-3.35	121.37	124.45
39	N	316	CHL	CMA-C3A-C4A	-3.35	107.05	114.38
39	n	318	CHL	CAA-C2A-C3A	-3.35	103.61	112.78
39	n	306	CHL	CMA-C3A-C4A	-3.34	107.06	114.38
39	G	311	CHL	CBC-CAC-C3C	-3.34	107.99	112.88
39	Y	318	CHL	CBC-CAC-C3C	-3.34	107.99	112.88
26	y	317	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
26	g	315	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
39	Y	318	CHL	OMC-CMC-C2C	-3.33	119.69	125.03
41	g	320	XAT	C20-C13-C14	-3.33	118.26	122.92
41	G	320	XAT	C20-C13-C14	-3.32	118.27	122.92
39	Y	318	CHL	OBD-CAD-CBD	-3.32	120.95	125.82
39	N	304	CHL	CMA-C3A-C4A	-3.32	107.10	114.38
39	y	314	CHL	CBC-CAC-C3C	-3.32	108.03	112.88
39	y	303	CHL	CMA-C3A-C4A	-3.31	107.12	114.38
26	b	601	CLA	C4A-NA-C1A	3.31	108.19	106.71
26	r	310	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
39	Y	302	CHL	CMA-C3A-C4A	-3.30	107.14	114.38
26	y	306	CLA	C1-C2-C3	-3.30	120.33	126.04
41	G	320	XAT	C26-C27-C28	-3.29	119.03	125.99
26	B	604	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
26	b	612	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
39	s	317	CHL	CAA-C2A-C3A	-3.29	103.78	112.78
26	Y	313	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
39	S	316	CHL	CMA-C3A-C4A	-3.28	107.20	114.38
41	n	316	XAT	C27-C28-C29	-3.27	120.45	125.53
39	R	318	CHL	CMA-C3A-C4A	-3.27	107.21	114.38
39	y	302	CHL	OBD-CAD-CBD	-3.27	121.02	125.82
39	Y	318	CHL	CAA-C2A-C3A	-3.27	103.82	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	Y	307	CHL	CAA-C2A-C3A	-3.27	103.83	112.78
42	S	305	NEX	C38-C25-C26	-3.27	116.78	122.26
39	g	307	CHL	OBD-CAD-CBD	-3.27	121.03	125.82
39	s	303	CHL	CMA-C3A-C4A	-3.26	107.23	114.38
26	G	304	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
39	S	302	CHL	CMA-C3A-C4A	-3.26	107.23	114.38
39	y	302	CHL	CAA-C2A-C3A	-3.26	103.84	112.78
26	c	514	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
26	R	310	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
26	a	409	CLA	CHD-C1D-ND	-3.26	121.46	124.45
41	g	320	XAT	C38-C25-C26	-3.25	116.81	122.26
39	s	316	CHL	CMA-C3A-C4A	-3.25	107.26	114.38
39	Y	302	CHL	C1C-CHC-C4B	3.25	126.50	115.73
41	G	310	XAT	C38-C25-C26	-3.25	116.81	122.26
26	S	311	CLA	CHD-C1D-ND	-3.24	121.47	124.45
39	s	313	CHL	CAA-C2A-C3A	-3.24	103.91	112.78
26	N	313	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
41	N	315	XAT	C27-C28-C29	-3.23	120.52	125.53
39	s	303	CHL	C1C-CHC-C4B	3.23	126.43	115.73
26	n	302	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
39	g	313	CHL	CMA-C3A-C4A	-3.23	107.30	114.38
26	C	521	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
39	S	316	CHL	C1C-CHC-C4B	3.23	126.42	115.73
39	g	319	CHL	CBC-CAC-C3C	-3.23	108.15	112.88
26	b	613	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
26	C	508	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
39	y	302	CHL	CMA-C3A-C4A	-3.22	107.33	114.38
26	C	504	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
39	R	318	CHL	OMC-CMC-C2C	-3.22	119.87	125.03
39	R	315	CHL	C1C-CHC-C4B	3.22	126.38	115.73
39	y	303	CHL	C1C-CHC-C4B	3.22	126.38	115.73
26	C	515	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
26	c	504	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
41	r	304	XAT	C15-C14-C13	-3.21	122.72	127.31
27	d	407	PHO	O1D-CGD-CBD	3.21	130.09	124.74
26	n	304	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
42	n	313	NEX	C31-C30-C29	-3.21	122.72	127.31
41	G	320	XAT	C11-C10-C9	-3.21	122.72	127.31
39	g	312	CHL	CBC-CAC-C3C	-3.21	108.18	112.88
39	n	311	CHL	CMA-C3A-C4A	-3.21	107.34	114.38
26	g	318	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
39	g	311	CHL	C1C-CHC-C4B	3.21	126.36	115.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	616	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
39	R	315	CHL	O1D-CGD-CBD	-3.21	119.40	124.74
26	C	511	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
26	b	609	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
39	G	318	CHL	C1C-CHC-C4B	3.20	126.34	115.73
39	y	314	CHL	CAA-C2A-C3A	-3.20	104.01	112.78
26	N	318	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
39	Y	318	CHL	CMA-C3A-C4A	-3.20	107.37	114.38
26	b	607	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
26	B	613	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
26	d	411	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
26	A	405	CLA	CHB-C4A-NA	3.19	128.93	124.51
26	S	308	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
26	B	617	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
26	R	302	CLA	CHB-C4A-NA	3.19	128.92	124.51
26	B	609	CLA	CHB-C4A-NA	3.19	128.92	124.51
39	Y	317	CHL	C1C-CHC-C4B	3.19	126.28	115.73
26	D	412	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
26	a	402	CLA	CHB-C4A-NA	3.18	128.92	124.51
39	R	312	CHL	OBD-CAD-CBD	-3.18	121.15	125.82
27	D	403	PHO	O1D-CGD-CBD	3.18	130.04	124.74
26	s	301	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
27	A	404	PHO	O2D-CGD-O1D	-3.18	117.62	123.84
39	N	316	CHL	C1C-CHC-C4B	3.18	126.26	115.73
26	R	310	CLA	CHB-C4A-NA	3.18	128.91	124.51
26	C	506	CLA	O2D-CGD-CBD	3.18	116.91	111.27
26	B	601	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
26	b	604	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
41	G	310	XAT	C6-C7-C8	-3.17	119.28	125.99
26	c	518	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
41	g	309	XAT	C7-C8-C9	-3.17	120.61	125.53
26	B	618	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
26	n	315	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
39	n	318	CHL	C1C-CHC-C4B	3.17	126.24	115.73
26	r	310	CLA	CHB-C4A-NA	3.17	128.90	124.51
39	s	316	CHL	CBC-CAC-C3C	-3.17	108.24	112.88
26	c	516	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
39	G	305	CHL	CBC-CAC-C3C	-3.17	108.24	112.88
39	r	309	CHL	OBD-CAD-CBD	-3.17	121.17	125.82
39	r	318	CHL	C1C-CHC-C4B	3.17	126.23	115.73
39	y	305	CHL	C1C-CHC-C4B	3.17	126.23	115.73
39	n	306	CHL	C1C-CHC-C4B	3.17	126.22	115.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	y	312	CHL	C1C-CHC-C4B	3.16	126.21	115.73
41	n	316	XAT	C11-C10-C9	-3.16	122.80	127.31
27	a	410	PHO	C2B-C1B-NB	-3.16	107.34	109.53
39	r	301	CHL	OMC-CMC-C2C	-3.16	119.96	125.03
41	g	309	XAT	C38-C25-C26	-3.15	116.98	122.26
41	g	320	XAT	C18-C5-C6	-3.15	116.98	122.26
39	s	313	CHL	O1D-CGD-CBD	-3.15	119.49	124.74
41	G	320	XAT	C38-C25-C26	-3.15	116.98	122.26
26	r	313	CLA	CHB-C4A-NA	3.15	128.87	124.51
39	g	313	CHL	CAA-C2A-C3A	-3.15	104.16	112.78
26	D	406	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
26	S	310	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
26	b	610	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
26	s	314	CLA	CHD-C1D-ND	-3.14	121.57	124.45
39	r	309	CHL	O2A-CGA-CBA	3.14	121.76	111.91
26	b	611	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
39	R	312	CHL	O2A-CGA-CBA	3.14	121.75	111.91
27	a	410	PHO	O2D-CGD-O1D	-3.14	117.71	123.84
39	y	305	CHL	CMA-C3A-C4A	-3.14	107.51	114.38
27	A	404	PHO	C2B-C1B-NB	-3.13	107.36	109.53
39	N	303	CHL	C1C-CHC-C4B	3.13	126.10	115.73
39	n	311	CHL	C1C-CHC-C4B	3.13	126.09	115.73
26	d	403	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
39	y	314	CHL	C1-C2-C3	3.13	131.45	126.04
39	g	313	CHL	C1C-CHC-C4B	3.12	126.08	115.73
39	Y	317	CHL	O2A-CGA-CBA	3.12	121.71	111.91
39	N	304	CHL	C1C-CHC-C4B	3.12	126.08	115.73
39	g	314	CHL	C1C-CHC-C4B	3.12	126.07	115.73
26	N	306	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
26	b	618	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
39	Y	314	CHL	CAA-C2A-C3A	-3.12	104.24	112.78
39	G	309	CHL	C1C-CHC-C4B	3.12	126.06	115.73
26	c	503	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
39	N	303	CHL	O2A-CGA-CBA	3.12	121.69	111.91
39	Y	314	CHL	C1C-CHC-C4B	3.12	126.06	115.73
26	b	618	CLA	CHB-C4A-NA	3.12	128.82	124.51
39	y	305	CHL	O2A-CGA-CBA	3.12	121.69	111.91
26	Y	311	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
39	N	310	CHL	C1C-CHC-C4B	3.12	126.05	115.73
39	Y	317	CHL	CMA-C3A-C4A	-3.12	107.55	114.38
39	Y	307	CHL	C1C-CHC-C4B	3.11	126.05	115.73
39	g	319	CHL	O2A-CGA-CBA	3.11	121.68	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	506	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
39	r	318	CHL	CAA-C2A-C3A	-3.11	104.26	112.78
39	G	301	CHL	CAA-C2A-C3A	-3.11	104.26	112.78
26	Y	305	CLA	C3B-C4B-NB	-3.11	107.63	110.52
39	n	308	CHL	C1C-CHC-C4B	3.11	126.02	115.73
26	R	306	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
39	G	305	CHL	O2A-CGA-CBA	3.11	121.65	111.91
39	N	311	CHL	OMC-CMC-C2C	-3.10	120.06	125.03
39	y	314	CHL	C1C-CHC-C4B	3.10	126.01	115.73
39	g	311	CHL	C3C-C4C-NC	-3.10	108.17	115.01
39	Y	314	CHL	O2A-CGA-CBA	3.10	121.64	111.91
39	n	318	CHL	O2A-CGA-CBA	3.10	121.64	111.91
39	n	308	CHL	CBC-CAC-C3C	-3.10	108.34	112.88
26	C	520	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
39	y	312	CHL	CAA-C2A-C3A	-3.10	104.29	112.78
26	r	306	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
39	y	312	CHL	O2A-CGA-CBA	3.10	121.63	111.91
39	r	318	CHL	O2A-CGA-CBA	3.10	121.63	111.91
26	R	306	CLA	CHB-C4A-NA	3.09	128.79	124.51
39	s	313	CHL	C1C-CHC-C4B	3.09	125.97	115.73
26	G	319	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
39	S	312	CHL	C1C-CHC-C4B	3.09	125.96	115.73
39	G	311	CHL	C1C-CHC-C4B	3.09	125.96	115.73
39	n	307	CHL	OMC-CMC-C2C	-3.09	120.08	125.03
39	r	316	CHL	C1C-CHC-C4B	3.09	125.96	115.73
39	s	303	CHL	C4C-CHD-C1D	3.09	125.96	115.73
30	D	411	PL9	C40-C39-C41	3.09	120.47	115.27
39	R	301	CHL	C1C-CHC-C4B	3.09	125.95	115.73
39	S	316	CHL	C4C-CHD-C1D	3.09	125.95	115.73
39	G	318	CHL	C3C-C4C-NC	-3.08	108.21	115.01
41	N	315	XAT	C38-C25-C26	-3.08	117.10	122.26
39	Y	317	CHL	CAA-C2A-C3A	-3.08	104.34	112.78
26	s	310	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
39	g	312	CHL	C1C-CHC-C4B	3.08	125.93	115.73
39	G	301	CHL	C1C-CHC-C4B	3.08	125.93	115.73
41	g	320	XAT	C19-C9-C10	-3.08	118.61	122.92
39	G	318	CHL	C4C-CHD-C1D	3.08	125.92	115.73
39	y	305	CHL	CAA-C2A-C3A	-3.08	104.35	112.78
39	N	316	CHL	C3C-C4C-NC	-3.08	108.22	115.01
39	n	311	CHL	CAA-C2A-C3A	-3.08	104.36	112.78
39	g	311	CHL	C4C-CHD-C1D	3.07	125.92	115.73
39	R	318	CHL	C1C-CHC-C4B	3.07	125.91	115.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	g	309	XAT	C6-C7-C8	-3.07	119.50	125.99
26	c	503	CLA	CHB-C4A-NA	3.07	128.76	124.51
39	y	303	CHL	C4C-CHD-C1D	3.07	125.90	115.73
41	n	316	XAT	C38-C25-C26	-3.07	117.12	122.26
26	s	315	CLA	CHB-C4A-NA	3.07	128.75	124.51
41	g	320	XAT	C11-C10-C9	-3.07	122.94	127.31
26	y	315	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
39	N	316	CHL	C1A-CHA-C4D	3.06	124.09	118.98
26	r	314	CLA	O2D-CGD-CBD	3.06	116.71	111.27
26	S	307	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
39	s	316	CHL	O1D-CGD-CBD	-3.06	119.64	124.74
39	N	310	CHL	CBC-CAC-C3C	-3.06	108.40	112.88
39	Y	318	CHL	C1C-CHC-C4B	3.06	125.86	115.73
39	r	301	CHL	C1C-CHC-C4B	3.06	125.86	115.73
39	g	307	CHL	C1C-CHC-C4B	3.05	125.85	115.73
39	r	309	CHL	C4C-CHD-C1D	3.05	125.85	115.73
39	s	303	CHL	C3C-C4C-NC	-3.05	108.27	115.01
39	R	312	CHL	C4C-CHD-C1D	3.05	125.84	115.73
39	R	315	CHL	O2A-CGA-CBA	3.05	121.48	111.91
26	y	316	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
41	n	316	XAT	C18-C5-C6	-3.05	117.15	122.26
39	G	305	CHL	C1C-CHC-C4B	3.05	125.83	115.73
26	n	309	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
39	S	302	CHL	O1D-CGD-CBD	-3.05	119.66	124.74
39	n	306	CHL	C3C-C4C-NC	-3.05	108.29	115.01
42	G	315	NEX	C31-C30-C29	-3.05	122.96	127.31
26	C	504	CLA	CHB-C4A-NA	3.05	128.72	124.51
26	D	406	CLA	CHB-C4A-NA	3.05	128.72	124.51
39	S	316	CHL	C3C-C4C-NC	-3.05	108.29	115.01
39	Y	302	CHL	C4C-CHD-C1D	3.05	125.82	115.73
39	N	317	CHL	C1C-CHC-C4B	3.04	125.82	115.73
39	Y	302	CHL	C3C-C4C-NC	-3.04	108.29	115.01
26	S	314	CLA	CHB-C4A-NA	3.04	128.72	124.51
30	d	408	PL9	C40-C39-C41	3.04	120.39	115.27
39	N	311	CHL	C3C-C4C-NC	-3.04	108.30	115.01
39	n	307	CHL	C3C-C4C-NC	-3.04	108.30	115.01
26	B	615	CLA	CHB-C4A-NA	3.04	128.72	124.51
39	y	303	CHL	C1-C2-C3	3.04	131.30	126.04
26	c	502	CLA	O2D-CGD-CBD	3.04	116.67	111.27
41	G	320	XAT	C19-C9-C10	-3.04	118.67	122.92
26	b	614	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
41	G	320	XAT	C18-C5-C6	-3.04	117.17	122.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	N	315	XAT	C18-C5-C6	-3.04	117.17	122.26
39	Y	307	CHL	C1-C2-C3	3.04	131.29	126.04
39	G	303	CHL	C1C-CHC-C4B	3.04	125.78	115.73
39	n	306	CHL	C1A-CHA-C4D	3.03	124.04	118.98
26	s	304	CLA	CHB-C4A-NA	3.03	128.71	124.51
39	s	313	CHL	O2A-CGA-CBA	3.03	121.42	111.91
39	y	302	CHL	C1C-CHC-C4B	3.03	125.77	115.73
26	y	313	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
39	N	304	CHL	O2A-CGA-CBA	3.03	121.42	111.91
39	n	307	CHL	O2A-CGA-CBA	3.03	121.42	111.91
26	B	609	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
28	T	101	BCR	C15-C16-C17	-3.03	117.27	123.47
39	N	311	CHL	OBD-CAD-CBD	-3.03	121.38	125.82
39	n	311	CHL	C4C-CHD-C1D	3.03	125.76	115.73
39	n	311	CHL	C3C-C4C-NC	-3.03	108.33	115.01
39	n	319	CHL	C1C-CHC-C4B	3.03	125.75	115.73
39	Y	314	CHL	C4C-CHD-C1D	3.03	125.75	115.73
39	N	311	CHL	O2A-CGA-CBA	3.03	121.40	111.91
26	S	304	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
26	C	511	CLA	CHB-C4A-NA	3.02	128.69	124.51
26	S	309	CLA	CHB-C4A-NA	3.02	128.69	124.51
39	n	307	CHL	C1C-CHC-C4B	3.02	125.74	115.73
39	S	302	CHL	CBC-CAC-C3C	-3.02	108.46	112.88
39	g	319	CHL	C1C-CHC-C4B	3.02	125.74	115.73
39	N	311	CHL	CAA-C2A-C3A	-3.02	104.50	112.78
39	n	307	CHL	CAA-C2A-C3A	-3.02	104.50	112.78
39	N	304	CHL	C4C-CHD-C1D	3.02	125.73	115.73
39	n	311	CHL	O2A-CGA-CBA	3.02	121.38	111.91
26	B	605	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
39	y	303	CHL	C3C-C4C-NC	-3.02	108.36	115.01
39	y	312	CHL	C4C-CHD-C1D	3.02	125.72	115.73
26	D	401	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
26	N	309	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
39	n	319	CHL	C3C-C4C-NC	-3.01	108.36	115.01
39	N	303	CHL	C1-C2-C3	3.01	131.25	126.04
26	s	305	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
26	r	306	CLA	CHB-C4A-NA	3.01	128.67	124.51
39	n	308	CHL	C4C-CHD-C1D	3.00	125.68	115.73
26	A	403	CLA	CHB-C4A-NA	3.00	128.66	124.51
26	Y	308	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
39	R	301	CHL	O2A-CGA-CBA	3.00	121.33	111.91
39	N	310	CHL	C4C-CHD-C1D	3.00	125.67	115.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	N	311	CHL	C1C-CHC-C4B	3.00	125.67	115.73
26	B	612	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
39	Y	307	CHL	C3C-C4C-NC	-3.00	108.39	115.01
39	n	319	CHL	C4C-CHD-C1D	3.00	125.67	115.73
26	R	307	CLA	CHB-C4A-NA	3.00	128.66	124.51
39	s	317	CHL	C3C-C4C-NC	-3.00	108.40	115.01
39	y	302	CHL	C3C-C4C-NC	-3.00	108.40	115.01
39	n	306	CHL	C4C-CHD-C1D	3.00	125.66	115.73
39	N	317	CHL	C3C-C4C-NC	-3.00	108.40	115.01
39	S	302	CHL	C1C-CHC-C4B	3.00	125.66	115.73
26	C	505	CLA	C3B-C4B-NB	-3.00	107.73	110.52
26	g	304	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
39	y	314	CHL	C3C-C4C-NC	-2.99	108.40	115.01
39	r	316	CHL	O2A-CGA-CBA	2.99	121.31	111.91
41	R	304	XAT	C35-C15-C14	-2.99	117.34	123.47
26	a	409	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
26	s	311	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
26	R	307	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
39	y	302	CHL	C4C-CHD-C1D	2.99	125.64	115.73
39	n	318	CHL	C1-C2-C3	2.99	131.21	126.04
26	y	306	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
39	y	305	CHL	C1A-CHA-C4D	2.99	123.97	118.98
39	y	314	CHL	C4C-CHD-C1D	2.99	125.63	115.73
42	r	302	NEX	C31-C30-C29	-2.99	123.05	127.31
39	Y	317	CHL	C1A-CHA-C4D	2.99	123.97	118.98
26	c	518	CLA	CHB-C4A-NA	2.99	128.64	124.51
39	N	317	CHL	C4C-CHD-C1D	2.99	125.62	115.73
26	Y	316	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
26	B	602	CLA	CHB-C4A-NA	2.98	128.64	124.51
39	s	316	CHL	C1C-CHC-C4B	2.98	125.62	115.73
39	n	307	CHL	OBD-CAD-CBD	-2.98	121.44	125.82
39	N	316	CHL	C4C-CHD-C1D	2.98	125.61	115.73
26	a	411	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
39	N	304	CHL	C3C-C4C-NC	-2.98	108.43	115.01
26	b	608	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
39	G	301	CHL	C4C-CHD-C1D	2.98	125.60	115.73
26	A	403	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
26	y	317	CLA	CHB-C4A-NA	2.98	128.63	124.51
39	Y	318	CHL	C4C-CHD-C1D	2.98	125.60	115.73
39	R	312	CHL	C3C-C4C-NC	-2.98	108.44	115.01
26	b	614	CLA	C3B-C4B-NB	-2.98	107.75	110.52
39	G	311	CHL	OBD-CAD-CBD	-2.98	121.45	125.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	g	320	XAT	C8-C9-C10	2.98	123.51	118.94
26	s	304	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
39	G	309	CHL	C4C-CHD-C1D	2.98	125.59	115.73
39	r	309	CHL	C3C-C4C-NC	-2.97	108.45	115.01
42	S	305	NEX	C40-C33-C34	-2.97	118.76	122.92
39	R	318	CHL	C1A-CHA-C4D	2.97	123.94	118.98
41	n	316	XAT	C26-C27-C28	-2.97	119.70	125.99
39	r	301	CHL	C4C-CHD-C1D	2.97	125.58	115.73
41	r	304	XAT	C18-C5-C6	-2.97	117.28	122.26
41	R	304	XAT	C18-C5-C6	-2.97	117.28	122.26
39	r	318	CHL	O1D-CGD-CBD	-2.97	119.79	124.74
39	S	313	CHL	C1C-CHC-C4B	2.97	125.57	115.73
26	d	403	CLA	CHB-C4A-NA	2.97	128.62	124.51
26	S	309	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
39	r	318	CHL	C4C-CHD-C1D	2.97	125.57	115.73
39	S	316	CHL	O2A-CGA-CBA	2.97	121.23	111.91
39	g	312	CHL	C4C-CHD-C1D	2.97	125.57	115.73
26	s	301	CLA	CHB-C4A-NA	2.97	128.62	124.51
42	R	305	NEX	C31-C30-C29	-2.97	123.08	127.31
39	s	303	CHL	O2A-CGA-CBA	2.96	121.21	111.91
39	S	312	CHL	O2A-CGA-CBA	2.96	121.21	111.91
39	g	313	CHL	C4C-CHD-C1D	2.96	125.55	115.73
39	g	307	CHL	C3C-C4C-NC	-2.96	108.47	115.01
26	Y	305	CLA	CHB-C4A-NA	2.96	128.61	124.51
39	S	313	CHL	C3C-C4C-NC	-2.96	108.48	115.01
39	g	314	CHL	C4C-CHD-C1D	2.96	125.54	115.73
26	b	611	CLA	CHB-C4A-NA	2.96	128.60	124.51
39	y	305	CHL	C3C-C4C-NC	-2.96	108.48	115.01
41	G	310	XAT	C7-C8-C9	-2.96	120.94	125.53
39	Y	317	CHL	C3C-C4C-NC	-2.96	108.49	115.01
39	r	309	CHL	C1C-CHC-C4B	2.95	125.52	115.73
39	g	311	CHL	C1A-CHA-C4D	2.95	123.91	118.98
39	n	307	CHL	C4C-CHD-C1D	2.95	125.52	115.73
26	G	317	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
39	r	301	CHL	C1A-CHA-C4D	2.95	123.91	118.98
26	g	308	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
26	a	411	CLA	CHB-C4A-NA	2.95	128.59	124.51
39	Y	318	CHL	C3C-C4C-NC	-2.95	108.50	115.01
41	r	304	XAT	C35-C15-C14	-2.95	117.43	123.47
39	r	316	CHL	C3C-C4C-NC	-2.95	108.50	115.01
26	b	605	CLA	CHB-C4A-NA	2.95	128.59	124.51
41	G	320	XAT	C8-C9-C10	2.95	123.47	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	N	317	CHL	OBD-CAD-CBD	-2.95	121.49	125.82
39	s	317	CHL	C1C-CHC-C4B	2.95	125.50	115.73
39	R	315	CHL	C1A-CHA-C4D	2.95	123.90	118.98
27	D	403	PHO	C2B-C1B-NB	-2.95	107.49	109.53
39	Y	307	CHL	C4C-CHD-C1D	2.95	125.49	115.73
39	S	302	CHL	C4C-CHD-C1D	2.95	125.49	115.73
39	R	301	CHL	C3C-C4C-NC	-2.94	108.51	115.01
27	d	407	PHO	C2B-C1B-NB	-2.94	107.49	109.53
26	B	607	CLA	CHB-C4A-NA	2.94	128.58	124.51
39	Y	302	CHL	C1-C2-C3	2.94	131.13	126.04
28	t	101	BCR	C15-C16-C17	-2.94	117.45	123.47
39	N	304	CHL	CAA-C2A-C3A	-2.94	104.72	112.78
39	y	312	CHL	C1A-CHA-C4D	2.94	123.89	118.98
41	N	315	XAT	C26-C27-C28	-2.94	119.78	125.99
26	Y	310	CLA	CHB-C4A-NA	2.94	128.58	124.51
39	S	312	CHL	O1D-CGD-CBD	-2.94	119.85	124.74
39	N	316	CHL	O2A-CGA-CBA	2.94	121.12	111.91
39	G	303	CHL	C3C-C4C-NC	-2.94	108.53	115.01
27	D	403	PHO	C1-C2-C3	-2.94	120.97	126.04
39	G	311	CHL	C4C-CHD-C1D	2.93	125.45	115.73
39	R	315	CHL	C4C-CHD-C1D	2.93	125.45	115.73
39	R	318	CHL	C4C-CHD-C1D	2.93	125.44	115.73
26	s	306	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
26	N	307	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
39	R	312	CHL	C1C-CHC-C4B	2.93	125.44	115.73
26	R	313	CLA	O2D-CGD-CBD	2.93	116.47	111.27
26	b	601	CLA	CHB-C4A-NA	2.93	128.56	124.51
26	r	317	CLA	C3B-C4B-NB	-2.93	107.80	110.52
26	r	313	CLA	CHD-C1D-ND	-2.93	121.76	124.45
39	g	311	CHL	O2A-CGA-CBA	2.93	121.09	111.91
26	b	606	CLA	O2D-CGD-CBD	2.93	116.47	111.27
39	n	306	CHL	O2A-CGA-CBA	2.93	121.09	111.91
39	s	317	CHL	C4C-CHD-C1D	2.93	125.42	115.73
39	N	311	CHL	C4C-CHD-C1D	2.92	125.42	115.73
41	g	320	XAT	C15-C14-C13	-2.92	123.14	127.31
26	S	315	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
39	G	305	CHL	C4C-CHD-C1D	2.92	125.41	115.73
39	G	309	CHL	CAA-C2A-C3A	-2.92	104.78	112.78
26	b	616	CLA	CHB-C4A-NA	2.92	128.55	124.51
41	R	304	XAT	C38-C25-C26	-2.92	117.37	122.26
39	S	313	CHL	C4C-CHD-C1D	2.92	125.39	115.73
39	s	316	CHL	C4C-CHD-C1D	2.92	125.39	115.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	520	CLA	C3B-C4B-NB	-2.92	107.81	110.52
26	y	309	CLA	C3B-C4B-NB	-2.92	107.81	110.52
39	g	319	CHL	C4C-CHD-C1D	2.92	125.39	115.73
39	R	301	CHL	C4C-CHD-C1D	2.91	125.39	115.73
29	a	403	SQD	O7-S-C6	2.91	110.40	106.94
39	g	312	CHL	OBD-CAD-CBD	-2.91	121.55	125.82
42	y	307	NEX	C39-C29-C30	-2.91	118.84	122.92
26	N	312	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
39	g	312	CHL	C3C-C4C-NC	-2.91	108.59	115.01
39	G	318	CHL	O2A-CGA-CBA	2.91	121.03	111.91
26	r	308	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
26	S	308	CLA	CHB-C4A-NA	2.91	128.53	124.51
30	d	408	PL9	C7-C8-C9	-2.91	121.95	126.79
26	b	607	CLA	C3B-C4B-NB	-2.91	107.82	110.52
26	y	310	CLA	C3B-C4B-NB	-2.91	107.82	110.52
26	B	607	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
39	s	313	CHL	C4C-CHD-C1D	2.90	125.35	115.73
26	n	305	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
26	B	601	CLA	C3B-C4B-NB	-2.90	107.82	110.52
39	r	318	CHL	CBC-CAC-C3C	-2.90	108.63	112.88
26	R	302	CLA	CHD-C1D-ND	-2.90	121.79	124.45
39	Y	317	CHL	C4C-CHD-C1D	2.90	125.34	115.73
39	n	318	CHL	C4C-CHD-C1D	2.90	125.33	115.73
39	g	314	CHL	CAA-C2A-C3A	-2.90	104.85	112.78
26	c	513	CLA	O2D-CGD-CBD	2.89	116.41	111.27
26	A	405	CLA	C3B-C4B-NB	-2.89	107.83	110.52
39	y	314	CHL	O2A-CGA-CBA	2.89	120.99	111.91
26	B	610	CLA	CHB-C4A-NA	2.89	128.51	124.51
26	y	309	CLA	CHB-C4A-NA	2.89	128.51	124.51
39	y	305	CHL	C4C-CHD-C1D	2.89	125.31	115.73
38	e	101	HEM	C4D-ND-C1D	2.89	108.06	105.07
39	S	312	CHL	C4C-CHD-C1D	2.89	125.31	115.73
39	R	315	CHL	CAA-C2A-C3A	-2.89	104.86	112.78
26	B	612	CLA	C3B-C4B-NB	-2.89	107.83	110.52
30	D	411	PL9	C7-C8-C9	-2.89	121.98	126.79
42	s	302	NEX	C40-C33-C34	-2.89	118.88	122.92
42	g	306	NEX	C31-C30-C29	-2.89	123.19	127.31
39	r	318	CHL	C3C-C4C-NC	-2.89	108.64	115.01
26	c	504	CLA	CHB-C4A-NA	2.89	128.50	124.51
39	r	316	CHL	CAA-C2A-C3A	-2.88	104.88	112.78
39	Y	307	CHL	C1A-CHA-C4D	2.88	123.79	118.98
39	r	316	CHL	C4C-CHD-C1D	2.88	125.28	115.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	r	318	CHL	C1A-CHA-C4D	2.88	123.79	118.98
26	C	515	CLA	CHB-C4A-NA	2.88	128.50	124.51
26	R	314	CLA	C3B-C4B-NB	-2.88	107.84	110.52
39	n	306	CHL	CAA-C2A-C3A	-2.88	104.89	112.78
26	C	505	CLA	CHD-C1D-ND	-2.88	121.81	124.45
26	D	409	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
42	Y	304	NEX	C39-C29-C30	-2.88	118.89	122.92
39	n	308	CHL	C3C-C4C-NC	-2.88	108.66	115.01
39	R	301	CHL	CAA-C2A-C3A	-2.88	104.90	112.78
39	Y	318	CHL	O2A-CGA-CBA	2.88	120.93	111.91
39	N	304	CHL	C1A-CHA-C4D	2.88	123.78	118.98
39	G	311	CHL	C3C-C4C-NC	-2.88	108.67	115.01
39	S	302	CHL	C3C-C4C-NC	-2.87	108.67	115.01
39	R	315	CHL	CBC-CAC-C3C	-2.87	108.67	112.88
27	A	404	PHO	CMB-C2B-C3B	2.87	130.05	124.68
29	A	407	SQD	O7-S-C6	2.87	110.35	106.94
27	a	410	PHO	CMB-C2B-C3B	2.87	130.05	124.68
26	B	615	CLA	O2D-CGD-CBD	2.87	116.37	111.27
41	G	320	XAT	C15-C14-C13	-2.87	123.22	127.31
26	C	517	CLA	O2D-CGD-CBD	2.87	116.37	111.27
26	s	307	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
26	b	617	CLA	CHB-C4A-NA	2.87	128.48	124.51
26	g	317	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
39	G	301	CHL	C3C-C4C-NC	-2.87	108.68	115.01
39	G	305	CHL	C3C-C4C-NC	-2.87	108.68	115.01
26	r	314	CLA	C3B-C4B-NB	-2.86	107.86	110.52
39	N	316	CHL	CAA-C2A-C3A	-2.86	104.94	112.78
38	E	101	HEM	C4D-ND-C1D	2.86	108.03	105.07
39	s	316	CHL	C3C-C4C-NC	-2.86	108.70	115.01
26	s	305	CLA	CHD-C1D-ND	-2.86	121.83	124.45
39	y	314	CHL	CHA-C1A-C2A	-2.86	126.59	133.31
26	B	606	CLA	CHB-C4A-NA	2.86	128.46	124.51
39	G	318	CHL	C1A-CHA-C4D	2.86	123.75	118.98
26	b	602	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
39	N	303	CHL	C4C-CHD-C1D	2.85	125.19	115.73
26	g	303	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
39	y	302	CHL	O2A-CGA-CBA	2.85	120.86	111.91
39	Y	302	CHL	C1A-CHA-C4D	2.85	123.74	118.98
26	b	611	CLA	O2D-CGD-CBD	2.85	116.33	111.27
39	N	316	CHL	OBD-CAD-CBD	-2.85	121.64	125.82
39	N	310	CHL	C3C-C4C-NC	-2.85	108.73	115.01
39	G	303	CHL	C4C-CHD-C1D	2.84	125.15	115.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	R	305	NEX	C35-C34-C33	-2.84	123.25	127.31
39	y	314	CHL	C1A-CHA-C4D	2.84	123.72	118.98
39	Y	314	CHL	C3C-C4C-NC	-2.84	108.75	115.01
39	s	316	CHL	OBD-CAD-CBD	-2.84	121.66	125.82
26	S	303	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
26	Y	312	CLA	C3B-C4B-NB	-2.83	107.89	110.52
26	G	314	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
26	R	313	CLA	C3B-C4B-NB	-2.83	107.89	110.52
26	d	404	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
26	C	520	CLA	CHD-C1D-ND	-2.83	121.85	124.45
26	r	303	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
26	Y	313	CLA	CHB-C4A-NA	2.83	128.43	124.51
39	R	315	CHL	C3C-C4C-NC	-2.83	108.76	115.01
42	r	302	NEX	C26-C27-C28	-2.83	120.01	125.99
26	b	616	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
42	r	302	NEX	C35-C34-C33	-2.83	123.27	127.31
26	a	409	CLA	CHB-C4A-NA	2.83	128.42	124.51
39	N	303	CHL	C1A-CHA-C4D	2.83	123.70	118.98
39	N	310	CHL	C1A-CHA-C4D	2.83	123.70	118.98
39	n	318	CHL	C1A-CHA-C4D	2.83	123.70	118.98
39	s	316	CHL	O2A-CGA-CBA	2.82	120.77	111.91
39	S	302	CHL	OBD-CAD-CBD	-2.82	121.68	125.82
39	g	307	CHL	C4C-CHD-C1D	2.82	125.09	115.73
39	r	301	CHL	C3C-C4C-NC	-2.82	108.78	115.01
39	g	319	CHL	C3C-C4C-NC	-2.82	108.78	115.01
26	R	316	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
39	n	308	CHL	C1A-CHA-C4D	2.82	123.69	118.98
26	c	506	CLA	CHD-C1D-ND	-2.82	121.86	124.45
39	Y	302	CHL	CHA-C1A-C2A	-2.82	126.68	133.31
39	Y	307	CHL	O2A-CGA-CBA	2.82	120.76	111.91
39	N	317	CHL	O2A-CGA-CBA	2.82	120.75	111.91
39	n	319	CHL	O2A-CGA-CBA	2.82	120.75	111.91
38	E	101	HEM	C4A-NA-C1A	2.82	108.11	105.35
26	N	307	CLA	CHD-C1D-ND	-2.82	121.86	124.45
26	y	306	CLA	C3B-C4B-NB	-2.82	107.90	110.52
26	n	312	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
39	R	301	CHL	OBD-CAD-CBD	-2.82	121.69	125.82
26	G	307	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
38	e	101	HEM	C4C-NC-C1C	2.81	108.10	105.35
39	g	313	CHL	C3C-C4C-NC	-2.81	108.80	115.01
26	Y	311	CLA	CHB-C4A-NA	2.81	128.40	124.51
26	Y	301	CLA	O2D-CGD-CBD	2.81	116.27	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	r	305	CLA	CHB-C4A-NA	2.81	128.40	124.51
39	y	312	CHL	C3C-C4C-NC	-2.81	108.81	115.01
26	y	316	CLA	CHB-C4A-NA	2.81	128.40	124.51
26	g	317	CLA	CHB-C4A-NA	2.81	128.40	124.51
39	S	302	CHL	O2A-CGA-CBA	2.81	120.72	111.91
39	N	304	CHL	OBD-CAD-CBD	-2.81	121.70	125.82
39	y	303	CHL	CHA-C1A-C2A	-2.80	126.72	133.31
39	n	319	CHL	OBD-CAD-CBD	-2.80	121.71	125.82
26	S	307	CLA	CHD-C1D-ND	-2.80	121.88	124.45
39	s	316	CHL	C1A-CHA-C4D	2.80	123.66	118.98
27	d	407	PHO	C1-C2-C3	-2.80	121.20	126.04
26	y	316	CLA	C3B-C4B-NB	-2.80	107.92	110.52
39	s	316	CHL	CHA-C1A-C2A	-2.80	126.73	133.31
39	G	309	CHL	C3C-C4C-NC	-2.80	108.83	115.01
39	n	318	CHL	C3C-C4C-NC	-2.80	108.84	115.01
26	B	603	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
39	g	314	CHL	C3C-C4C-NC	-2.80	108.84	115.01
26	Y	308	CLA	C3B-C4B-NB	-2.80	107.92	110.52
39	y	314	CHL	OBD-CAD-CBD	-2.80	121.72	125.82
26	s	306	CLA	CHB-C4A-NA	2.80	128.38	124.51
39	G	318	CHL	OBD-CAD-CBD	-2.80	121.72	125.82
39	S	302	CHL	C1A-CHA-C4D	2.79	123.64	118.98
39	g	313	CHL	O2A-CGA-CBA	2.79	120.67	111.91
39	S	302	CHL	CHA-C1A-C2A	-2.79	126.75	133.31
26	G	313	CLA	C3B-C4B-NB	-2.79	107.92	110.52
39	n	311	CHL	OBD-CAD-CBD	-2.79	121.73	125.82
39	R	318	CHL	C3C-C4C-NC	-2.79	108.85	115.01
26	D	401	CLA	CHB-C4A-NA	2.79	128.37	124.51
39	y	303	CHL	O2A-CGA-CBA	2.79	120.66	111.91
39	Y	302	CHL	O2A-CGA-CBA	2.79	120.66	111.91
26	S	315	CLA	CHB-C4A-NA	2.79	128.37	124.51
26	D	412	CLA	CHD-C1D-ND	-2.79	121.89	124.45
39	r	316	CHL	C1A-CHA-C4D	2.79	123.63	118.98
26	g	305	CLA	C3B-C4B-NB	-2.78	107.93	110.52
39	N	310	CHL	O2A-CGA-CBA	2.78	120.64	111.91
27	A	404	PHO	O1D-CGD-CBD	2.78	129.38	124.74
39	n	311	CHL	C1A-CHA-C4D	2.78	123.63	118.98
26	c	508	CLA	CHB-C4A-NA	2.78	128.36	124.51
39	S	313	CHL	O2A-CGA-CBA	2.78	120.64	111.91
26	S	311	CLA	C3B-C4B-NB	-2.78	107.94	110.52
27	a	410	PHO	O1D-CGD-CBD	2.78	129.37	124.74
26	G	306	CLA	C3B-C4B-NB	-2.78	107.94	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	N	308	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
39	y	303	CHL	C1A-CHA-C4D	2.78	123.61	118.98
39	G	318	CHL	CAA-C2A-C3A	-2.78	105.18	112.78
42	R	305	NEX	C26-C27-C28	-2.77	120.13	125.99
26	G	306	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
26	n	303	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
39	Y	307	CHL	CHA-C1A-C2A	-2.77	126.79	133.31
26	a	402	CLA	C3B-C4B-NB	-2.77	107.94	110.52
26	g	318	CLA	C3B-C4B-NB	-2.77	107.94	110.52
26	y	315	CLA	CHB-C4A-NA	2.77	128.35	124.51
38	e	101	HEM	C4A-NA-C1A	2.77	108.06	105.35
39	g	312	CHL	O2A-CGA-CBA	2.77	120.60	111.91
39	Y	314	CHL	C1A-CHA-C4D	2.77	123.60	118.98
39	G	303	CHL	O2A-CGA-CBA	2.77	120.60	111.91
39	g	319	CHL	OBD-CAD-CBD	-2.77	121.76	125.82
26	c	520	CLA	CHD-C1D-ND	-2.77	121.91	124.45
26	b	609	CLA	CHB-C4A-NA	2.77	128.34	124.51
26	D	412	CLA	C3B-C4B-NB	-2.77	107.95	110.52
26	D	412	CLA	C4A-NA-C1A	2.77	107.95	106.71
26	d	411	CLA	C4A-NA-C1A	2.77	107.95	106.71
39	s	317	CHL	C1A-CHA-C4D	2.77	123.60	118.98
38	E	101	HEM	C4C-NC-C1C	2.77	108.06	105.35
39	N	303	CHL	C3C-C4C-NC	-2.77	108.91	115.01
39	Y	317	CHL	OBD-CAD-CBD	-2.76	121.77	125.82
26	R	309	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
26	S	304	CLA	CHD-C1D-ND	-2.76	121.92	124.45
26	B	611	CLA	O2D-CGD-CBD	2.76	116.17	111.27
39	S	313	CHL	C1A-CHA-C4D	2.76	123.59	118.98
39	r	316	CHL	OBD-CAD-CBD	-2.76	121.77	125.82
39	y	305	CHL	OBD-CAD-CBD	-2.76	121.77	125.82
26	n	304	CLA	CHB-C4A-NA	2.76	128.33	124.51
26	n	315	CLA	CHB-C4A-NA	2.76	128.33	124.51
26	N	312	CLA	CHB-C4A-NA	2.76	128.33	124.51
39	r	309	CHL	CBC-CAC-C3C	-2.76	108.84	112.88
39	g	307	CHL	O2A-CGA-CBA	2.76	120.56	111.91
26	n	310	CLA	C3B-C4B-NB	-2.76	107.96	110.52
39	R	312	CHL	CBC-CAC-C3C	-2.76	108.84	112.88
39	G	305	CHL	OBD-CAD-CBD	-2.75	121.78	125.82
26	d	411	CLA	C3B-C4B-NB	-2.75	107.96	110.52
26	G	307	CLA	CHB-C4A-NA	2.75	128.32	124.51
39	S	313	CHL	OBD-CAD-CBD	-2.75	121.78	125.82
26	b	602	CLA	CHB-C4A-NA	2.75	128.32	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	g	305	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
39	G	301	CHL	O2A-CGA-CBA	2.75	120.54	111.91
42	s	302	NEX	C25-C24-C23	-2.75	107.31	112.75
26	B	616	CLA	CHB-C4A-NA	2.75	128.31	124.51
39	G	309	CHL	C1A-CHA-C4D	2.75	123.57	118.98
39	s	317	CHL	O2A-CGA-CBA	2.75	120.53	111.91
39	N	317	CHL	C1A-CHA-C4D	2.75	123.57	118.98
39	n	306	CHL	OBD-CAD-CBD	-2.75	121.79	125.82
39	Y	307	CHL	OBD-CAD-CBD	-2.75	121.79	125.82
26	b	601	CLA	C3B-C4B-NB	-2.75	107.97	110.52
39	g	311	CHL	CAA-C2A-C3A	-2.75	105.26	112.78
39	g	311	CHL	OBD-CAD-CBD	-2.74	121.80	125.82
26	y	310	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
39	R	301	CHL	C1A-CHA-C4D	2.74	123.56	118.98
26	n	303	CLA	CHB-C4A-NA	2.74	128.30	124.51
39	R	318	CHL	OBD-CAD-CBD	-2.74	121.80	125.82
28	T	101	BCR	C38-C26-C25	-2.74	121.45	124.53
26	S	307	CLA	C3B-C4B-NB	-2.74	107.97	110.52
26	c	514	CLA	CHB-C4A-NA	2.74	128.30	124.51
27	d	407	PHO	O2D-CGD-O1D	-2.74	118.48	123.84
26	g	308	CLA	CHB-C4A-NA	2.74	128.30	124.51
39	r	301	CHL	OBD-CAD-CBD	-2.74	121.81	125.82
27	D	403	PHO	O2D-CGD-O1D	-2.74	118.49	123.84
26	s	311	CLA	C3B-C4B-NB	-2.74	107.98	110.52
26	r	311	CLA	O2D-CGD-CBD	2.74	116.13	111.27
26	Y	312	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
26	N	313	CLA	CHB-C4A-NA	2.73	128.29	124.51
39	S	316	CHL	C1A-CHA-C4D	2.73	123.55	118.98
39	r	316	CHL	O1D-CGD-CBD	-2.73	120.19	124.74
26	Y	301	CLA	CHB-C4A-NA	2.73	128.29	124.51
26	g	304	CLA	CHB-C4A-NA	2.73	128.29	124.51
26	s	311	CLA	CHD-C1D-ND	-2.73	121.94	124.45
26	G	319	CLA	CHB-C4A-NA	2.73	128.29	124.51
26	n	305	CLA	CHD-C1D-ND	-2.73	121.94	124.45
39	n	308	CHL	O2A-CGA-CBA	2.73	120.47	111.91
26	C	521	CLA	CHB-C4A-NA	2.73	128.29	124.51
26	G	317	CLA	CHB-C4A-NA	2.73	128.29	124.51
26	s	314	CLA	C3B-C4B-NB	-2.73	107.98	110.52
39	s	313	CHL	C3C-C4C-NC	-2.73	108.99	115.01
26	s	315	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
39	G	311	CHL	C1A-CHA-C4D	2.72	123.52	118.98
26	b	602	CLA	CHD-C1D-ND	-2.72	121.95	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	311	CHL	O2A-CGA-CBA	2.72	120.45	111.91
26	C	516	CLA	CHB-C4A-NA	2.72	128.28	124.51
26	B	617	CLA	CHD-C1D-ND	-2.72	121.95	124.45
26	N	306	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	S	314	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
39	S	312	CHL	C3C-C4C-NC	-2.72	109.01	115.01
26	c	505	CLA	CHB-C4A-NA	2.72	128.27	124.51
39	g	311	CHL	CHA-C1A-C2A	-2.72	126.93	133.31
39	y	302	CHL	CHA-C1A-C2A	-2.71	126.93	133.31
26	N	318	CLA	CHB-C4A-NA	2.71	128.26	124.51
26	g	304	CLA	C3B-C4B-NB	-2.71	108.00	110.52
39	g	314	CHL	C1A-CHA-C4D	2.71	123.51	118.98
26	n	302	CLA	CHB-C4A-NA	2.71	128.26	124.51
26	C	505	CLA	CHB-C4A-NA	2.71	128.26	124.51
39	G	318	CHL	CHA-C1A-C2A	-2.71	126.94	133.31
26	R	307	CLA	C3B-C4B-NB	-2.71	108.00	110.52
26	Y	310	CLA	C3B-C4B-NB	-2.71	108.00	110.52
26	R	309	CLA	CHB-C4A-NA	2.71	128.26	124.51
26	R	308	CLA	O2D-CGD-CBD	2.71	116.08	111.27
26	g	302	CLA	C3B-C4B-NB	-2.71	108.00	110.52
26	S	303	CLA	CHB-C4A-NA	2.71	128.25	124.51
39	r	301	CHL	CBC-CAC-C3C	-2.70	108.92	112.88
26	B	603	CLA	CHD-C1D-ND	-2.70	121.97	124.45
26	s	307	CLA	CHB-C4A-NA	2.70	128.25	124.51
39	r	309	CHL	CHA-C1A-C2A	-2.70	126.97	133.31
39	R	318	CHL	CBC-CAC-C3C	-2.70	108.93	112.88
39	g	313	CHL	C1A-CHA-C4D	2.70	123.48	118.98
26	N	319	CLA	C3B-C4B-NB	-2.69	108.02	110.52
26	r	308	CLA	C3B-C4B-NB	-2.69	108.02	110.52
26	R	306	CLA	C4A-NA-C1A	2.69	107.92	106.71
39	Y	318	CHL	CHA-C1A-C2A	-2.69	126.98	133.31
39	s	313	CHL	C1A-CHA-C4D	2.69	123.47	118.98
39	r	316	CHL	OMC-CMC-C2C	-2.69	120.72	125.03
26	G	302	CLA	C3B-C4B-NB	-2.69	108.02	110.52
39	n	307	CHL	C1A-CHA-C4D	2.69	123.47	118.98
26	n	302	CLA	C3B-C4B-NB	-2.69	108.02	110.52
26	R	308	CLA	CHB-C4A-NA	2.69	128.23	124.51
39	s	317	CHL	OBD-CAD-CBD	-2.68	121.88	125.82
28	k	101	BCR	C2-C1-C6	2.68	114.61	110.48
26	Y	313	CLA	C3B-C4B-NB	-2.68	108.03	110.52
26	b	617	CLA	O2D-CGD-CBD	2.68	116.03	111.27
26	B	601	CLA	C1-C2-C3	-2.68	121.41	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	g	315	CLA	C3B-C4B-NB	-2.68	108.03	110.52
26	b	610	CLA	CHD-C1D-ND	-2.68	121.99	124.45
41	r	304	XAT	C38-C25-C26	-2.68	117.77	122.26
26	A	405	CLA	CHD-C1D-ND	-2.68	121.99	124.45
39	N	311	CHL	C1A-CHA-C4D	2.68	123.45	118.98
39	g	312	CHL	C1A-CHA-C4D	2.68	123.45	118.98
26	b	607	CLA	C1-C2-C3	-2.67	121.42	126.04
26	C	507	CLA	CHB-C4A-NA	2.67	128.21	124.51
39	n	319	CHL	C1A-CHA-C4D	2.67	123.44	118.98
39	R	312	CHL	CHA-C1A-C2A	-2.67	127.03	133.31
26	N	318	CLA	C3B-C4B-NB	-2.67	108.04	110.52
26	B	603	CLA	CHB-C4A-NA	2.67	128.20	124.51
26	c	508	CLA	CHC-C4B-NB	2.67	127.08	124.26
26	B	610	CLA	O2D-CGD-CBD	2.67	116.01	111.27
39	s	303	CHL	C1A-CHA-C4D	2.67	123.43	118.98
26	r	305	CLA	C3B-C4B-NB	-2.66	108.04	110.52
26	y	304	CLA	CHB-C4A-NA	2.66	128.19	124.51
26	r	311	CLA	CHB-C4A-NA	2.66	128.19	124.51
39	G	301	CHL	C1A-CHA-C4D	2.66	123.42	118.98
39	Y	314	CHL	OBD-CAD-CBD	-2.66	121.92	125.82
26	G	302	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
39	n	306	CHL	CHA-C1A-C2A	-2.66	127.06	133.31
26	G	304	CLA	C3B-C4B-NB	-2.66	108.05	110.52
26	c	508	CLA	C3B-C4B-NB	-2.66	108.05	110.52
39	r	318	CHL	OBD-CAD-CBD	-2.66	121.92	125.82
39	N	316	CHL	CHA-C1A-C2A	-2.66	127.07	133.31
26	B	604	CLA	CHB-C1B-NB	2.66	127.07	124.26
26	g	302	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
26	R	316	CLA	CHB-C4A-NA	2.65	128.18	124.51
26	G	319	CLA	C3B-C4B-NB	-2.65	108.05	110.52
39	y	303	CHL	OBD-CAD-CBD	-2.65	121.93	125.82
39	N	317	CHL	CHA-C1A-C2A	-2.65	127.08	133.31
26	b	612	CLA	CHB-C1B-NB	2.65	127.06	124.26
42	S	305	NEX	C25-C24-C23	-2.65	107.51	112.75
26	y	315	CLA	CHD-C1D-ND	-2.65	122.02	124.45
26	G	314	CLA	CHB-C4A-NA	2.65	128.18	124.51
26	S	308	CLA	C3B-C4B-NB	-2.65	108.06	110.52
39	R	301	CHL	OMC-CMC-C2C	-2.65	120.78	125.03
26	y	309	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
26	Y	305	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
26	g	317	CLA	C1-C2-C3	-2.65	121.46	126.04
39	R	315	CHL	OBD-CAD-CBD	-2.65	121.94	125.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	y	312	CHL	OBD-CAD-CBD	-2.65	121.94	125.82
26	Y	311	CLA	CHD-C1D-ND	-2.65	122.02	124.45
26	s	307	CLA	C3B-C4B-NB	-2.65	108.06	110.52
26	Y	305	CLA	CHD-C1D-ND	-2.65	122.02	124.45
39	N	316	CHL	O1D-CGD-CBD	-2.64	120.34	124.74
26	r	311	CLA	CHB-C1B-NB	2.64	127.05	124.26
26	B	609	CLA	C3B-C4B-NB	-2.64	108.07	110.52
28	t	101	BCR	C38-C26-C25	-2.64	121.56	124.53
26	r	303	CLA	CHB-C4A-NA	2.63	128.16	124.51
26	s	314	CLA	C2A-C3A-C4A	-2.63	97.61	101.87
26	s	315	CLA	C3B-C4B-NB	-2.63	108.07	110.52
39	g	314	CHL	OBD-CAD-CBD	-2.63	121.96	125.82
26	S	314	CLA	C3B-C4B-NB	-2.63	108.08	110.52
26	R	309	CLA	C3B-C4B-NB	-2.63	108.08	110.52
26	g	305	CLA	CHB-C4A-NA	2.63	128.15	124.51
39	n	306	CHL	O1D-CGD-CBD	-2.63	120.36	124.74
26	B	605	CLA	C3B-C4B-NB	-2.63	108.08	110.52
26	G	307	CLA	C1-C2-C3	-2.63	121.50	126.04
39	G	303	CHL	C1-O2A-CGA	2.62	123.33	116.44
39	g	307	CHL	C1-O2A-CGA	2.62	123.33	116.44
26	n	305	CLA	CHB-C4A-NA	2.62	128.14	124.51
26	s	314	CLA	O2D-CGD-CBD	2.62	115.93	111.27
26	Y	308	CLA	CHB-C4A-NA	2.62	128.14	124.51
39	y	312	CHL	CHA-C1A-C2A	-2.62	127.16	133.31
26	D	406	CLA	CHD-C1D-ND	-2.62	122.05	124.45
39	G	305	CHL	C1A-CHA-C4D	2.62	123.35	118.98
26	s	301	CLA	C3B-C4B-NB	-2.62	108.09	110.52
26	s	306	CLA	C3B-C4B-NB	-2.62	108.09	110.52
26	b	618	CLA	C3B-C4B-NB	-2.62	108.09	110.52
26	b	614	CLA	CHD-C1D-ND	-2.61	122.05	124.45
26	R	317	CLA	CHB-C4A-NA	2.61	128.13	124.51
26	r	308	CLA	CHB-C4A-NA	2.61	128.13	124.51
26	c	510	CLA	CHB-C4A-NA	2.61	128.12	124.51
26	N	306	CLA	C3B-C4B-NB	-2.61	108.09	110.52
26	R	314	CLA	CHB-C4A-NA	2.61	128.12	124.51
26	c	520	CLA	CHB-C4A-NA	2.61	128.12	124.51
26	d	411	CLA	CHD-C1D-ND	-2.61	122.06	124.45
39	n	319	CHL	CHA-C1A-C2A	-2.61	127.18	133.31
26	b	614	CLA	CHB-C1B-NB	2.61	127.02	124.26
26	G	317	CLA	C3B-C4B-NB	-2.61	108.10	110.52
26	Y	301	CLA	C3B-C4B-NB	-2.61	108.10	110.52
26	y	317	CLA	C3B-C4B-NB	-2.61	108.10	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	R	305	NEX	C15-C35-C34	-2.61	118.14	123.47
26	G	306	CLA	CHB-C4A-NA	2.61	128.12	124.51
26	y	315	CLA	O2A-CGA-O1A	-2.61	117.02	123.59
39	S	312	CHL	C1A-CHA-C4D	2.60	123.33	118.98
26	y	304	CLA	C3B-C4B-NB	-2.60	108.10	110.52
26	C	516	CLA	CHC-C4B-NB	2.60	127.01	124.26
39	R	315	CHL	OMC-CMC-C2C	-2.60	120.86	125.03
26	c	505	CLA	O2D-CGD-CBD	2.60	115.89	111.27
26	Y	311	CLA	C3B-C4B-NB	-2.60	108.10	110.52
28	K	101	BCR	C2-C1-C6	2.60	114.49	110.48
26	B	612	CLA	CHD-C1D-ND	-2.60	122.06	124.45
28	C	514	BCR	C15-C16-C17	2.60	128.81	123.47
28	c	507	BCR	C15-C16-C17	2.60	128.80	123.47
39	n	307	CHL	CHA-C1A-C2A	-2.60	127.20	133.31
42	s	302	NEX	C15-C35-C34	-2.60	118.15	123.47
26	Y	311	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
26	r	315	CLA	CHB-C4A-NA	2.60	128.10	124.51
28	T	101	BCR	C12-C13-C14	-2.60	114.95	118.94
26	B	604	CLA	CMB-C2B-C1B	-2.60	121.41	125.37
42	g	306	NEX	C39-C29-C30	-2.60	119.28	122.92
39	Y	314	CHL	CHA-C1A-C2A	-2.60	127.21	133.31
26	b	612	CLA	CMB-C2B-C1B	-2.60	121.42	125.37
39	N	303	CHL	CBC-CAC-C3C	-2.60	109.08	112.88
39	N	311	CHL	CHA-C1A-C2A	-2.59	127.22	133.31
26	N	307	CLA	CHB-C4A-NA	2.59	128.10	124.51
26	B	610	CLA	C3B-C4B-NB	-2.59	108.11	110.52
26	R	302	CLA	O2D-CGD-CBD	2.59	115.88	111.27
26	g	303	CLA	CHB-C4A-NA	2.59	128.10	124.51
26	R	306	CLA	C3B-C4B-NB	-2.59	108.11	110.52
39	N	310	CHL	OMC-CMC-C2C	-2.59	120.88	125.03
39	G	309	CHL	OBD-CAD-CBD	-2.59	122.03	125.82
39	S	316	CHL	C1-C2-C3	2.59	130.52	126.04
39	s	303	CHL	C1-C2-C3	2.59	130.52	126.04
26	C	515	CLA	C3B-C4B-NB	-2.59	108.11	110.52
26	S	311	CLA	C2A-C3A-C4A	-2.59	97.69	101.87
26	D	409	CLA	CHB-C4A-NA	2.59	128.09	124.51
26	r	305	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
26	g	318	CLA	CHB-C4A-NA	2.58	128.09	124.51
26	C	511	CLA	C3B-C4B-NB	-2.58	108.12	110.52
26	n	309	CLA	CHB-C4A-NA	2.58	128.08	124.51
39	r	318	CHL	OMC-CMC-C2C	-2.58	120.89	125.03
26	a	402	CLA	CHD-C1D-ND	-2.58	122.08	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	404	PHO	C1C-C2C-C3C	-2.58	106.46	108.61
26	S	311	CLA	O2D-CGD-CBD	2.58	115.85	111.27
26	n	309	CLA	C3B-C4B-NB	-2.58	108.12	110.52
26	r	306	CLA	C3B-C4B-NB	-2.58	108.12	110.52
26	C	519	CLA	CHB-C4A-NA	2.58	128.07	124.51
26	r	317	CLA	CHB-C4A-NA	2.58	128.07	124.51
39	n	308	CHL	OMC-CMC-C2C	-2.58	120.90	125.03
26	b	608	CLA	C3B-C4B-NB	-2.58	108.13	110.52
26	c	505	CLA	C3B-C4B-NB	-2.58	108.13	110.52
26	Y	316	CLA	CHB-C1B-NB	2.57	126.98	124.26
28	k	101	BCR	C4-C5-C6	-2.57	119.00	122.73
26	y	306	CLA	CHB-C4A-NA	2.57	128.07	124.51
30	a	407	PL9	C7-C3-C2	-2.57	119.92	123.30
39	G	311	CHL	O1D-CGD-CBD	-2.57	120.45	124.74
39	N	304	CHL	CHA-C1A-C2A	-2.57	127.27	133.31
26	C	507	CLA	C3B-C4B-NB	-2.57	108.13	110.52
26	D	412	CLA	CHB-C4A-NA	2.57	128.07	124.51
26	b	604	CLA	C3B-C4B-NB	-2.57	108.13	110.52
26	b	607	CLA	CHB-C4A-NA	2.57	128.06	124.51
39	R	312	CHL	OMC-CMC-C2C	-2.57	120.91	125.03
26	R	308	CLA	CHB-C1B-NB	2.57	126.97	124.26
39	Y	302	CHL	OBD-CAD-CBD	-2.57	122.06	125.82
26	b	617	CLA	C3B-C4B-NB	-2.57	108.13	110.52
26	S	303	CLA	C3B-C4B-NB	-2.57	108.14	110.52
39	G	303	CHL	OMC-CMC-C2C	-2.56	120.92	125.03
26	c	503	CLA	C3B-C4B-NB	-2.56	108.14	110.52
42	n	313	NEX	C39-C29-C30	-2.56	119.33	122.92
28	c	507	BCR	C16-C17-C18	-2.56	123.65	127.31
26	g	308	CLA	C3B-C4B-NB	-2.56	108.14	110.52
39	N	310	CHL	OBD-CAD-CBD	-2.56	122.06	125.82
26	d	403	CLA	CHD-C1D-ND	-2.56	122.10	124.45
26	C	512	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	C	512	CLA	C3B-C4B-NB	-2.56	108.14	110.52
26	y	315	CLA	C3B-C4B-NB	-2.56	108.14	110.52
26	B	601	CLA	CHB-C4A-NA	2.56	128.05	124.51
39	Y	302	CHL	OMC-CMC-C2C	-2.56	120.93	125.03
26	S	315	CLA	C3B-C4B-NB	-2.56	108.14	110.52
26	n	309	CLA	CHD-C1D-ND	-2.55	122.11	124.45
26	R	302	CLA	C1-O2A-CGA	2.55	123.14	116.44
26	d	403	CLA	C3B-C4B-NB	-2.55	108.15	110.52
39	g	312	CHL	CHA-C1A-C2A	-2.55	127.32	133.31
26	d	411	CLA	CHB-C4A-NA	2.55	128.04	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	613	CLA	CHB-C4A-NA	2.55	128.04	124.51
39	r	318	CHL	CHA-C1A-C2A	-2.55	127.32	133.31
26	N	307	CLA	C3B-C4B-NB	-2.55	108.15	110.52
26	c	515	CLA	CHB-C4A-NA	2.55	128.03	124.51
26	B	612	CLA	CHB-C4A-NA	2.55	128.03	124.51
39	S	316	CHL	OMC-CMC-C2C	-2.55	120.95	125.03
39	s	317	CHL	O1D-CGD-CBD	-2.55	120.50	124.74
26	B	618	CLA	CHB-C4A-NA	2.54	128.03	124.51
26	R	302	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
26	b	608	CLA	CHB-C4A-NA	2.54	128.03	124.51
26	N	309	CLA	CHB-C4A-NA	2.54	128.03	124.51
39	n	311	CHL	CHA-C1A-C2A	-2.54	127.34	133.31
26	n	312	CLA	CHB-C1B-NB	2.54	126.95	124.26
26	G	304	CLA	CHB-C4A-NA	2.54	128.03	124.51
26	g	315	CLA	CHB-C4A-NA	2.54	128.03	124.51
26	N	309	CLA	C3B-C4B-NB	-2.54	108.16	110.52
26	c	504	CLA	C3B-C4B-NB	-2.54	108.16	110.52
42	r	302	NEX	C15-C35-C34	-2.54	118.27	123.47
39	r	301	CHL	O2A-CGA-CBA	2.54	119.88	111.91
26	r	311	CLA	C3B-C4B-NB	-2.54	108.16	110.52
26	r	313	CLA	O2D-CGD-CBD	2.54	115.78	111.27
26	c	518	CLA	C3B-C4B-NB	-2.54	108.16	110.52
26	N	308	CLA	CHB-C1B-NB	2.54	126.94	124.26
39	n	308	CHL	OBD-CAD-CBD	-2.54	122.10	125.82
26	B	605	CLA	CHB-C4A-NA	2.54	128.02	124.51
26	n	305	CLA	C3B-C4B-NB	-2.54	108.16	110.52
26	n	315	CLA	C3B-C4B-NB	-2.54	108.16	110.52
26	r	313	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
26	b	607	CLA	CHD-C1D-ND	-2.54	122.12	124.45
42	G	315	NEX	C39-C29-C30	-2.54	119.37	122.92
39	G	311	CHL	CHA-C1A-C2A	-2.53	127.36	133.31
26	B	617	CLA	O2A-CGA-O1A	-2.53	117.20	123.59
26	c	515	CLA	C3B-C4B-NB	-2.53	108.17	110.52
39	s	303	CHL	OMC-CMC-C2C	-2.53	120.97	125.03
33	b	620	DGD	C6D-O5D-C1E	2.53	118.69	113.74
39	r	309	CHL	OMC-CMC-C2C	-2.53	120.97	125.03
39	g	312	CHL	O1D-CGD-CBD	-2.53	120.53	124.74
26	y	304	CLA	O2D-CGD-CBD	2.53	115.76	111.27
26	c	520	CLA	O2D-CGD-CBD	2.53	115.76	111.27
42	R	305	NEX	C1-C2-C3	-2.53	107.94	113.64
26	C	516	CLA	C3B-C4B-NB	-2.53	108.17	110.52
26	B	612	CLA	CHB-C1B-NB	2.52	126.93	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	R	302	CLA	CAA-CBA-CGA	-2.52	105.88	113.25
39	n	307	CHL	O1D-CGD-CBD	-2.52	120.54	124.74
26	G	313	CLA	CHB-C4A-NA	2.52	128.00	124.51
26	y	304	CLA	CHC-C4B-NB	2.52	126.93	124.26
39	R	318	CHL	CHA-C1A-C2A	-2.52	127.39	133.31
39	N	310	CHL	CHA-C1A-C2A	-2.52	127.40	133.31
39	R	315	CHL	CHA-C1A-C2A	-2.52	127.40	133.31
39	s	303	CHL	CHA-C1A-C2A	-2.52	127.40	133.31
26	B	606	CLA	C3B-C4B-NB	-2.51	108.18	110.52
39	S	316	CHL	CHA-C1A-C2A	-2.51	127.40	133.31
39	n	308	CHL	CHA-C1A-C2A	-2.51	127.40	133.31
26	y	306	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
26	D	406	CLA	C3B-C4B-NB	-2.51	108.18	110.52
39	g	319	CHL	C1A-CHA-C4D	2.51	123.17	118.98
26	y	313	CLA	CHB-C1B-NB	2.51	126.92	124.26
26	C	519	CLA	C3B-C4B-NB	-2.51	108.19	110.52
42	r	302	NEX	C39-C29-C30	-2.51	119.41	122.92
39	g	314	CHL	CBC-CAC-C3C	-2.51	109.21	112.88
26	Y	308	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
27	a	410	PHO	C1C-C2C-C3C	-2.51	106.52	108.61
26	B	613	CLA	C3B-C4B-NB	-2.51	108.19	110.52
39	r	301	CHL	CHA-C1A-C2A	-2.51	127.42	133.31
42	s	302	NEX	C35-C15-C14	-2.51	118.34	123.47
39	S	312	CHL	OMC-CMC-C2C	-2.50	121.02	125.03
26	b	601	CLA	CHD-C1D-ND	-2.50	122.15	124.45
39	y	303	CHL	OMC-CMC-C2C	-2.50	121.02	125.03
39	S	313	CHL	CHA-C1A-C2A	-2.50	127.43	133.31
28	C	502	BCR	C23-C22-C21	-2.50	115.10	118.94
26	N	319	CLA	CHB-C4A-NA	2.50	127.97	124.51
26	b	614	CLA	CHB-C4A-NA	2.50	127.97	124.51
26	R	308	CLA	C3B-C4B-NB	-2.50	108.20	110.52
26	C	521	CLA	CHD-C1D-ND	-2.50	122.16	124.45
39	g	314	CHL	O2A-CGA-CBA	2.49	119.74	111.91
39	Y	302	CHL	CAA-C2A-C3A	-2.49	105.95	112.78
39	S	313	CHL	O1D-CGD-CBD	-2.49	120.59	124.74
26	d	404	CLA	CHB-C4A-NA	2.49	127.96	124.51
26	r	313	CLA	CAA-CBA-CGA	-2.49	105.98	113.25
42	r	302	NEX	C1-C2-C3	-2.49	108.02	113.64
39	g	307	CHL	C1A-CHA-C4D	2.49	123.14	118.98
26	c	510	CLA	C3B-C4B-NB	-2.49	108.21	110.52
26	D	409	CLA	CHD-C1D-ND	-2.49	122.17	124.45
26	r	306	CLA	CHD-C1D-ND	-2.49	122.17	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	s	317	CHL	CHA-C1A-C2A	-2.49	127.47	133.31
26	b	609	CLA	C3B-C4B-NB	-2.49	108.21	110.52
42	N	302	NEX	C39-C29-C30	-2.48	119.44	122.92
39	N	304	CHL	CMB-C2B-C3B	2.48	129.32	124.68
39	y	302	CHL	O2A-CGA-O1A	-2.48	117.33	123.59
39	r	316	CHL	CHA-C1A-C2A	-2.48	127.48	133.31
39	n	306	CHL	OMC-CMC-C2C	-2.48	121.05	125.03
39	g	313	CHL	OBD-CAD-CBD	-2.48	122.18	125.82
26	S	304	CLA	C3B-C4B-NB	-2.48	108.21	110.52
26	B	617	CLA	CHB-C4A-NA	2.48	127.94	124.51
26	b	610	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
39	R	301	CHL	CHA-C1A-C2A	-2.48	127.49	133.31
26	Y	301	CLA	CHC-C4B-NB	2.48	126.88	124.26
26	r	314	CLA	CHB-C4A-NA	2.48	127.94	124.51
26	G	314	CLA	C3B-C4B-NB	-2.48	108.22	110.52
26	B	601	CLA	CHD-C1D-ND	-2.48	122.18	124.45
30	D	411	PL9	C22-C23-C24	-2.48	121.70	127.66
26	r	308	CLA	CHD-C1D-ND	-2.48	122.18	124.45
39	G	309	CHL	O2A-CGA-CBA	2.47	119.67	111.91
42	s	302	NEX	C20-C13-C14	-2.47	119.46	122.92
41	n	316	XAT	C15-C35-C34	-2.47	118.41	123.47
26	B	613	CLA	CHB-C4A-NA	2.47	127.93	124.51
26	b	610	CLA	CHB-C4A-NA	2.47	127.93	124.51
26	C	507	CLA	O2D-CGD-CBD	2.47	115.66	111.27
30	A	408	PL9	C7-C3-C2	-2.47	120.05	123.30
42	R	305	NEX	C39-C29-C30	-2.47	119.47	122.92
26	b	606	CLA	C3B-C4B-NB	-2.47	108.23	110.52
26	R	313	CLA	CHB-C4A-NA	2.47	127.92	124.51
39	R	301	CHL	CMB-C2B-C3B	2.47	129.29	124.68
26	N	309	CLA	CHD-C1D-ND	-2.46	122.19	124.45
26	c	514	CLA	CHD-C1D-ND	-2.46	122.19	124.45
28	K	101	BCR	C4-C5-C6	-2.46	119.15	122.73
42	S	305	NEX	C20-C13-C14	-2.46	119.47	122.92
42	S	305	NEX	C11-C12-C13	-2.46	119.50	126.42
39	Y	318	CHL	O1D-CGD-CBD	-2.46	120.64	124.74
26	r	306	CLA	C4A-NA-C1A	2.46	107.81	106.71
39	s	313	CHL	OMC-CMC-C2C	-2.46	121.09	125.03
26	b	612	CLA	C3B-C4B-NB	-2.46	108.23	110.52
26	g	303	CLA	C3B-C4B-NB	-2.46	108.23	110.52
38	e	101	HEM	C1B-NB-C4B	2.46	107.61	105.07
26	n	310	CLA	CHB-C4A-NA	2.46	127.91	124.51
26	s	311	CLA	CHB-C4A-NA	2.46	127.91	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	609	CLA	CHC-C4B-NB	2.46	126.86	124.26
26	Y	305	CLA	CHB-C1B-NB	2.46	126.86	124.26
26	c	510	CLA	CHD-C1D-ND	-2.45	122.20	124.45
33	Y	303	DGD	C3G-O3G-C1D	2.45	118.53	113.74
39	G	301	CHL	OBD-CAD-CBD	-2.45	122.22	125.82
39	N	316	CHL	OMC-CMC-C2C	-2.45	121.10	125.03
26	S	307	CLA	CHB-C4A-NA	2.45	127.90	124.51
26	B	616	CLA	C3B-C4B-NB	-2.45	108.24	110.52
26	B	616	CLA	CHC-C4B-NB	2.45	126.85	124.26
26	B	617	CLA	C1-C2-C3	-2.45	121.81	126.04
39	g	307	CHL	OMC-CMC-C2C	-2.45	121.11	125.03
39	R	315	CHL	O2A-CGA-O1A	-2.45	117.42	123.59
26	B	604	CLA	C3B-C4B-NB	-2.45	108.25	110.52
39	Y	302	CHL	O2D-CGD-O1D	-2.45	119.06	123.84
39	Y	318	CHL	O2A-CGA-O1A	-2.44	117.42	123.59
33	B	620	DGD	C6D-O5D-C1E	2.44	118.52	113.74
26	Y	313	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
26	C	504	CLA	C3B-C4B-NB	-2.44	108.25	110.52
26	B	611	CLA	C3B-C4B-NB	-2.44	108.25	110.52
26	R	306	CLA	CHD-C1D-ND	-2.44	122.21	124.45
39	y	302	CHL	O1D-CGD-CBD	-2.44	120.68	124.74
26	d	404	CLA	CHD-C1D-ND	-2.44	122.21	124.45
28	C	514	BCR	C16-C17-C18	-2.44	123.83	127.31
30	d	408	PL9	C27-C28-C29	-2.43	121.80	127.66
26	S	315	CLA	CHD-C1D-ND	-2.43	122.22	124.45
26	S	310	CLA	C3B-C4B-NB	-2.43	108.26	110.52
26	b	617	CLA	CHD-C1D-ND	-2.43	122.22	124.45
26	c	514	CLA	CMB-C2B-C1B	-2.43	121.67	125.37
39	y	303	CHL	O2D-CGD-O1D	-2.43	119.09	123.84
26	R	317	CLA	CHD-C1D-ND	-2.43	122.22	124.45
26	y	309	CLA	CHB-C1B-NB	2.43	126.83	124.26
26	y	316	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
26	r	313	CLA	C1-O2A-CGA	2.43	122.81	116.44
26	c	503	CLA	CHD-C1D-ND	-2.43	122.22	124.45
26	b	606	CLA	O2A-CGA-O1A	-2.42	117.47	123.59
26	R	310	CLA	C3B-C4B-NB	-2.42	108.27	110.52
26	b	610	CLA	C1-C2-C3	-2.42	121.85	126.04
39	y	305	CHL	CHA-C1A-C2A	-2.42	127.62	133.31
39	G	303	CHL	C1A-CHA-C4D	2.42	123.02	118.98
26	S	304	CLA	CHB-C4A-NA	2.42	127.86	124.51
26	b	604	CLA	CHB-C4A-NA	2.42	127.86	124.51
39	r	316	CHL	CMB-C2B-C3B	2.42	129.21	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	n	304	CLA	C3B-C4B-NB	-2.42	108.27	110.52
26	c	516	CLA	CHB-C4A-NA	2.42	127.86	124.51
26	R	316	CLA	C3B-C4B-NB	-2.42	108.27	110.52
39	Y	317	CHL	CHA-C1A-C2A	-2.42	127.63	133.31
38	E	101	HEM	C1B-NB-C4B	2.42	107.57	105.07
26	s	310	CLA	C3B-C4B-NB	-2.42	108.27	110.52
39	y	303	CHL	O1D-CGD-CBD	-2.42	120.72	124.74
26	s	305	CLA	CHB-C4A-NA	2.42	127.85	124.51
39	n	311	CHL	CMB-C2B-C3B	2.41	129.20	124.68
39	Y	318	CHL	C1A-CHA-C4D	2.41	123.01	118.98
26	B	606	CLA	CHD-C1D-ND	-2.41	122.24	124.45
26	C	511	CLA	CHD-C1D-ND	-2.41	122.24	124.45
42	s	302	NEX	C11-C12-C13	-2.41	119.64	126.42
26	B	610	CLA	CHD-C1D-ND	-2.41	122.24	124.45
39	G	309	CHL	OMC-CMC-C2C	-2.41	121.17	125.03
39	g	313	CHL	CHA-C1A-C2A	-2.41	127.64	133.31
39	G	318	CHL	O1D-CGD-CBD	-2.41	120.72	124.74
39	n	318	CHL	CBC-CAC-C3C	-2.41	109.35	112.88
26	C	512	CLA	CHD-C1D-ND	-2.41	122.24	124.45
42	S	305	NEX	C15-C35-C34	-2.41	118.54	123.47
42	N	302	NEX	C26-C27-C28	-2.41	120.90	125.99
28	c	511	BCR	C23-C22-C21	-2.41	115.25	118.94
26	y	310	CLA	CHD-C1D-ND	-2.41	122.24	124.45
30	d	408	PL9	C22-C23-C24	-2.41	121.87	127.66
41	R	304	XAT	C19-C9-C8	2.40	121.86	118.08
26	d	404	CLA	C3B-C4B-NB	-2.40	108.29	110.52
26	y	306	CLA	CMB-C2B-C1B	-2.40	121.71	125.37
26	B	607	CLA	CHD-C1D-ND	-2.40	122.25	124.45
41	r	304	XAT	C19-C9-C8	2.40	121.86	118.08
26	C	508	CLA	CHB-C4A-NA	2.40	127.83	124.51
26	y	310	CLA	CHB-C4A-NA	2.40	127.83	124.51
39	G	305	CHL	OMC-CMC-C2C	-2.40	121.18	125.03
26	Y	308	CLA	CMB-C2B-C1B	-2.40	121.72	125.37
39	G	309	CHL	CBC-CAC-C3C	-2.40	109.37	112.88
26	Y	312	CLA	CHD-C1D-ND	-2.40	122.25	124.45
26	y	309	CLA	CHD-C1D-ND	-2.40	122.25	124.45
39	N	311	CHL	O1D-CGD-CBD	-2.40	120.75	124.74
26	r	310	CLA	C3B-C4B-NB	-2.40	108.29	110.52
39	g	311	CHL	O1D-CGD-CBD	-2.40	120.75	124.74
26	Y	308	CLA	CHD-C1D-ND	-2.40	122.25	124.45
30	D	411	PL9	C27-C28-C29	-2.39	121.89	127.66
42	S	305	NEX	C27-C28-C29	-2.39	121.81	125.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	N	304	CHL	O1D-CGD-CBD	-2.39	120.75	124.74
26	R	317	CLA	CMB-C2B-C1B	-2.39	121.72	125.37
26	C	521	CLA	CMB-C2B-C1B	-2.39	121.73	125.37
26	N	313	CLA	C3B-C4B-NB	-2.39	108.30	110.52
39	r	316	CHL	O2D-CGD-O1D	-2.39	119.17	123.84
26	y	316	CLA	CHB-C1B-NB	2.39	126.79	124.26
26	r	315	CLA	CHD-C1D-ND	-2.38	122.26	124.45
39	y	302	CHL	C1A-CHA-C4D	2.38	122.95	118.98
26	n	303	CLA	CMB-C2B-C1B	-2.38	121.75	125.37
26	R	317	CLA	C3B-C4B-NB	-2.38	108.31	110.52
26	s	304	CLA	C3B-C4B-NB	-2.37	108.31	110.52
26	B	611	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
26	c	513	CLA	CHB-C4A-NA	2.37	127.79	124.51
26	G	302	CLA	CHD-C1D-ND	-2.37	122.27	124.45
26	n	310	CLA	O2D-CGD-CBD	2.37	115.48	111.27
39	g	319	CHL	OMC-CMC-C2C	-2.37	121.23	125.03
39	G	301	CHL	CHA-C1A-C2A	-2.37	127.74	133.31
26	R	313	CLA	C1-C2-C3	-2.37	121.94	126.04
26	D	401	CLA	CMB-C2B-C1B	-2.37	121.76	125.37
33	y	308	DGD	C3G-O3G-C1D	2.37	118.37	113.74
26	S	309	CLA	C3B-C4B-NB	-2.37	108.32	110.52
26	B	611	CLA	CHB-C4A-NA	2.37	127.78	124.51
26	s	310	CLA	CHB-C4A-NA	2.37	127.78	124.51
42	r	302	NEX	C30-C31-C32	-2.37	115.83	123.22
39	Y	317	CHL	OMC-CMC-C2C	-2.37	121.24	125.03
26	c	515	CLA	CHD-C1D-ND	-2.36	122.28	124.45
42	S	305	NEX	C19-C9-C10	-2.36	119.61	122.92
26	s	306	CLA	CHD-C1D-ND	-2.36	122.28	124.45
42	Y	304	NEX	C5-C4-C3	-2.36	108.95	111.75
26	B	615	CLA	C2A-C1A-CHA	2.36	127.99	123.86
26	r	303	CLA	C3B-C4B-NB	-2.36	108.33	110.52
26	N	312	CLA	C3B-C4B-NB	-2.36	108.33	110.52
39	y	303	CHL	CAA-C2A-C3A	-2.36	106.32	112.78
26	N	312	CLA	CMB-C2B-C1B	-2.36	121.78	125.37
39	G	301	CHL	O1D-CGD-CBD	-2.36	120.81	124.74
39	y	305	CHL	OMC-CMC-C2C	-2.36	121.25	125.03
26	n	303	CLA	CHD-C1D-ND	-2.36	122.29	124.45
26	B	607	CLA	C1-C2-C3	-2.36	121.97	126.04
26	B	609	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
40	r	307	LUT	C11-C10-C9	2.36	130.67	127.31
26	n	312	CLA	CHB-C4A-NA	2.35	127.77	124.51
26	n	303	CLA	C3B-C4B-NB	-2.35	108.33	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	605	CLA	C3B-C4B-NB	-2.35	108.33	110.52
26	r	310	CLA	CHD-C1D-ND	-2.35	122.29	124.45
26	r	315	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
26	y	306	CLA	CHD-C1D-ND	-2.35	122.29	124.45
39	Y	314	CHL	CBC-CAC-C3C	-2.35	109.44	112.88
26	c	514	CLA	C3B-C4B-NB	-2.35	108.34	110.52
42	N	302	NEX	C15-C35-C34	-2.35	118.66	123.47
26	N	308	CLA	CHB-C4A-NA	2.35	127.76	124.51
26	R	302	CLA	CBA-CAA-C2A	-2.35	106.93	113.86
26	Y	312	CLA	CHB-C4A-NA	2.35	127.76	124.51
42	G	315	NEX	C19-C9-C10	-2.35	119.64	122.92
26	B	618	CLA	C3B-C4B-NB	-2.34	108.34	110.52
26	r	315	CLA	C3B-C4B-NB	-2.34	108.34	110.52
26	a	409	CLA	O2D-CGD-CBD	2.34	115.43	111.27
26	Y	310	CLA	CHC-C4B-NB	2.34	126.73	124.26
26	s	310	CLA	CHB-C1B-NB	2.34	126.73	124.26
26	Y	316	CLA	C3B-C4B-NB	-2.34	108.34	110.52
39	y	305	CHL	O1D-CGD-CBD	-2.34	120.84	124.74
26	C	519	CLA	CHD-C1D-ND	-2.34	122.31	124.45
26	G	314	CLA	C1-C2-C3	-2.34	122.00	126.04
26	S	304	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
26	y	313	CLA	C3B-C4B-NB	-2.34	108.35	110.52
42	n	313	NEX	C15-C35-C34	-2.34	118.69	123.47
26	s	305	CLA	C3B-C4B-NB	-2.34	108.35	110.52
26	C	517	CLA	CHB-C4A-NA	2.34	127.74	124.51
40	r	307	LUT	C11-C12-C13	2.33	132.97	126.42
39	N	316	CHL	O2D-CGD-O1D	-2.33	119.28	123.84
26	D	409	CLA	C3B-C4B-NB	-2.33	108.35	110.52
26	G	302	CLA	CHB-C1B-NB	2.33	126.72	124.26
41	R	304	XAT	C5-C4-C3	-2.33	108.14	112.75
39	Y	302	CHL	O1D-CGD-CBD	-2.33	120.86	124.74
26	b	611	CLA	C2A-C1A-CHA	2.33	127.93	123.86
38	e	101	HEM	CHC-C1C-NC	2.33	126.96	124.44
39	R	318	CHL	O2A-CGA-CBA	2.33	119.21	111.91
26	b	616	CLA	C1-C2-C3	-2.33	122.02	126.04
39	n	306	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
39	r	309	CHL	C1A-CHA-C4D	2.33	122.86	118.98
26	R	317	CLA	O2D-CGD-CBD	2.33	115.40	111.27
26	C	516	CLA	O2D-CGD-CBD	2.32	115.40	111.27
26	B	602	CLA	C3B-C4B-NB	-2.32	108.36	110.52
26	r	314	CLA	C1-C2-C3	-2.32	122.03	126.04
39	R	312	CHL	C1A-CHA-C4D	2.32	122.86	118.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	Y	317	CHL	O1D-CGD-CBD	-2.32	120.87	124.74
42	y	307	NEX	C5-C4-C3	-2.32	109.00	111.75
26	B	605	CLA	CHD-C1D-ND	-2.32	122.32	124.45
26	S	310	CLA	CHB-C1B-NB	2.32	126.71	124.26
26	N	312	CLA	CHD-C1D-ND	-2.32	122.32	124.45
26	G	307	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
26	s	305	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
26	b	613	CLA	C3B-C4B-NB	-2.32	108.37	110.52
42	R	305	NEX	C30-C31-C32	-2.32	115.99	123.22
26	Y	316	CLA	CHB-C4A-NA	2.31	127.71	124.51
42	S	305	NEX	C35-C15-C14	-2.31	118.73	123.47
28	t	101	BCR	C12-C13-C14	-2.31	115.39	118.94
39	g	311	CHL	C1-C2-C3	2.31	130.04	126.04
26	B	604	CLA	CHB-C4A-NA	2.31	127.71	124.51
28	t	101	BCR	C30-C25-C24	-2.31	109.24	115.78
38	E	101	HEM	CHC-C1C-NC	2.31	126.94	124.44
41	G	320	XAT	C11-C12-C13	2.31	132.91	126.42
40	R	311	LUT	C11-C12-C13	2.31	132.91	126.42
30	A	408	PL9	O1-C4-C3	-2.31	118.17	120.72
26	b	618	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
26	g	302	CLA	CHD-C1D-ND	-2.31	122.33	124.45
39	r	318	CHL	O2A-CGA-O1A	-2.31	117.77	123.59
26	B	613	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
26	R	310	CLA	CHD-C1D-ND	-2.31	122.33	124.45
26	B	617	CLA	C3B-C4B-NB	-2.30	108.38	110.52
39	R	312	CHL	CAA-C2A-C3A	-2.30	106.47	112.78
39	S	302	CHL	OMC-CMC-C2C	-2.30	121.34	125.03
26	D	401	CLA	O2D-CGD-CBD	2.30	115.36	111.27
26	y	313	CLA	CHB-C4A-NA	2.30	127.69	124.51
26	r	315	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
30	a	407	PL9	O1-C4-C3	-2.30	118.19	120.72
39	g	307	CHL	O1D-CGD-CBD	-2.30	120.91	124.74
26	R	317	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
26	c	505	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
39	G	305	CHL	CHA-C1A-C2A	-2.30	127.91	133.31
39	n	311	CHL	O1D-CGD-CBD	-2.30	120.91	124.74
26	C	521	CLA	C3B-C4B-NB	-2.29	108.39	110.52
26	R	302	CLA	C3B-C4B-NB	-2.29	108.39	110.52
26	S	310	CLA	CHB-C4A-NA	2.29	127.69	124.51
39	G	309	CHL	CHA-C1A-C2A	-2.29	127.92	133.31
26	g	302	CLA	CHB-C1B-NB	2.29	126.68	124.26
39	N	317	CHL	OMC-CMC-C2C	-2.29	121.36	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	r	313	CLA	CBA-CAA-C2A	-2.29	107.11	113.86
26	y	317	CLA	O2D-CGD-CBD	2.29	115.33	111.27
26	b	607	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
26	C	517	CLA	CMB-C2B-C1B	-2.29	121.89	125.37
26	r	315	CLA	O2D-CGD-CBD	2.29	115.33	111.27
26	N	319	CLA	O2D-CGD-CBD	2.28	115.33	111.27
41	g	320	XAT	C11-C12-C13	2.28	132.83	126.42
26	b	612	CLA	CHB-C4A-NA	2.28	127.67	124.51
26	C	507	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
26	b	608	CLA	CHD-C1D-ND	-2.28	122.36	124.45
26	G	302	CLA	CHB-C4A-NA	2.28	127.67	124.51
41	r	304	XAT	C5-C4-C3	-2.28	108.23	112.75
39	G	318	CHL	C1-C2-C3	2.28	129.99	126.04
26	B	603	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
40	R	311	LUT	C20-C13-C12	2.28	121.67	118.08
26	y	309	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
26	r	314	CLA	CHD-C1D-ND	-2.28	122.36	124.45
39	s	316	CHL	OMC-CMC-C2C	-2.28	121.38	125.03
39	g	314	CHL	CHA-C1A-C2A	-2.28	127.96	133.31
26	b	602	CLA	C3B-C4B-NB	-2.28	108.40	110.52
26	g	303	CLA	C1-C2-C3	-2.28	122.11	126.04
26	G	314	CLA	CHD-C1D-ND	-2.28	122.36	124.45
26	r	313	CLA	C3B-C4B-NB	-2.27	108.41	110.52
39	R	301	CHL	O1D-CGD-CBD	-2.27	120.95	124.74
26	G	317	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
26	R	316	CLA	CHD-C1D-ND	-2.27	122.36	124.45
26	b	601	CLA	O2D-CGD-CBD	2.27	115.31	111.27
39	n	319	CHL	OMC-CMC-C2C	-2.27	121.39	125.03
40	r	307	LUT	C20-C13-C12	2.27	121.66	118.08
41	g	320	XAT	C40-C33-C34	-2.27	119.74	122.92
39	Y	314	CHL	OMC-CMC-C2C	-2.27	121.39	125.03
26	b	604	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
41	G	320	XAT	C40-C33-C34	-2.27	119.74	122.92
39	N	303	CHL	OMC-CMC-C2C	-2.27	121.39	125.03
26	g	302	CLA	CHB-C4A-NA	2.27	127.65	124.51
39	g	319	CHL	CHA-C1A-C2A	-2.27	127.98	133.31
39	y	312	CHL	CBC-CAC-C3C	-2.27	109.56	112.88
28	T	101	BCR	C30-C25-C24	-2.27	109.37	115.78
26	r	303	CLA	CHD-C1D-ND	-2.27	122.37	124.45
39	Y	307	CHL	OMC-CMC-C2C	-2.27	121.40	125.03
26	N	307	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
39	r	309	CHL	CAA-C2A-C3A	-2.26	106.58	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	N	310	CHL	O1D-CGD-CBD	-2.26	120.97	124.74
26	C	506	CLA	C3B-C4B-NB	-2.26	108.42	110.52
26	b	609	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
39	y	312	CHL	OMC-CMC-C2C	-2.26	121.41	125.03
26	B	601	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
26	B	613	CLA	CHC-C4B-NB	2.26	126.65	124.26
26	S	314	CLA	CHD-C1D-ND	-2.26	122.38	124.45
26	R	307	CLA	CHC-C4B-NB	2.26	126.65	124.26
26	a	409	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
26	c	513	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
26	B	609	CLA	C1-C2-C3	-2.26	122.14	126.04
26	n	305	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
26	R	302	CLA	C3A-C2A-C1A	2.26	104.72	101.34
41	N	315	XAT	C15-C35-C34	-2.25	118.86	123.47
39	G	318	CHL	O2D-CGD-O1D	-2.25	119.43	123.84
39	g	311	CHL	O2D-CGD-O1D	-2.25	119.43	123.84
26	a	411	CLA	O2D-CGD-CBD	2.25	115.27	111.27
41	G	310	XAT	C27-C28-C29	-2.25	122.03	125.53
39	g	314	CHL	OMC-CMC-C2C	-2.25	121.42	125.03
26	C	508	CLA	C3B-C4B-NB	-2.25	108.43	110.52
39	g	319	CHL	O1D-CGD-CBD	-2.25	120.99	124.74
26	b	606	CLA	CHB-C4A-NA	2.25	127.62	124.51
26	Y	316	CLA	CHD-C1D-ND	-2.25	122.39	124.45
42	n	313	NEX	C26-C27-C28	-2.25	121.24	125.99
42	Y	304	NEX	C40-C33-C34	-2.25	119.77	122.92
39	R	315	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
26	N	312	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
26	g	317	CLA	CMB-C2B-C1B	-2.25	121.95	125.37
39	G	303	CHL	O1D-CGD-CBD	-2.25	121.00	124.74
39	n	319	CHL	O1D-CGD-CBD	-2.25	121.00	124.74
26	b	616	CLA	CHD-C1D-ND	-2.25	122.39	124.45
40	R	311	LUT	C11-C10-C9	2.24	130.51	127.31
26	s	315	CLA	CHD-C1D-ND	-2.24	122.39	124.45
39	n	318	CHL	OMC-CMC-C2C	-2.24	121.44	125.03
42	y	307	NEX	C40-C33-C34	-2.24	119.78	122.92
39	g	313	CHL	O1D-CGD-CBD	-2.24	121.01	124.74
39	G	311	CHL	OMC-CMC-C2C	-2.24	121.44	125.03
26	y	317	CLA	CHC-C4B-NB	2.24	126.63	124.26
28	d	401	BCR	C7-C8-C9	-2.24	122.85	126.23
28	T	101	BCR	C16-C15-C14	2.24	128.06	123.47
39	N	317	CHL	O1D-CGD-CBD	-2.24	121.01	124.74
26	d	403	CLA	CMB-C2B-C1B	-2.24	121.96	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Y	305	CLA	C4A-NA-C1A	2.24	107.71	106.71
26	Y	313	CLA	CHD-C1D-ND	-2.24	122.40	124.45
26	n	303	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
40	s	312	LUT	C21-C26-C27	-2.23	109.88	112.70
26	G	314	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
26	g	317	CLA	C3B-C4B-NB	-2.23	108.44	110.52
26	g	305	CLA	CHD-C1D-ND	-2.23	122.40	124.45
39	y	314	CHL	O2D-CGD-O1D	-2.23	119.47	123.84
26	C	508	CLA	CHB-C1B-NB	2.23	126.62	124.26
26	A	403	CLA	O2D-CGD-CBD	2.23	115.23	111.27
26	g	317	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
26	B	606	CLA	O2D-CGD-CBD	2.23	115.23	111.27
42	s	302	NEX	C27-C28-C29	-2.23	122.07	125.53
26	a	402	CLA	O2D-CGD-CBD	2.23	115.23	111.27
26	d	411	CLA	CHB-C1B-NB	2.23	126.62	124.26
42	g	306	NEX	C1-C2-C3	-2.23	108.61	113.64
26	Y	310	CLA	O2D-CGD-CBD	2.23	115.23	111.27
39	r	301	CHL	O1D-CGD-CBD	-2.23	121.03	124.74
26	r	314	CLA	O2A-CGA-O1A	-2.23	117.98	123.59
26	c	515	CLA	O2D-CGD-CBD	2.23	115.22	111.27
26	r	313	CLA	C3A-C2A-C1A	2.22	104.67	101.34
26	b	604	CLA	CHC-C4B-NB	2.22	126.61	124.26
42	g	306	NEX	C19-C9-C10	-2.22	119.81	122.92
26	Y	312	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
26	s	304	CLA	CMB-C2B-C1B	-2.22	121.99	125.37
26	c	502	CLA	C3B-C4B-NB	-2.22	108.45	110.52
26	Y	305	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
26	y	313	CLA	CHD-C1D-ND	-2.22	122.42	124.45
26	C	519	CLA	O2D-CGD-CBD	2.22	115.21	111.27
26	B	615	CLA	C2D-C1D-ND	-2.22	108.47	110.10
26	C	505	CLA	O2D-CGD-CBD	2.22	115.21	111.27
26	b	602	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
26	g	318	CLA	CHD-C1D-ND	-2.22	122.42	124.45
26	C	512	CLA	O2D-CGD-CBD	2.21	115.20	111.27
26	G	307	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
26	R	313	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
26	Y	305	CLA	C1-C2-C3	-2.21	122.22	126.04
26	g	303	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
42	Y	304	NEX	C26-C27-C28	-2.21	121.32	125.99
26	b	610	CLA	C3B-C4B-NB	-2.21	108.46	110.52
42	G	315	NEX	C11-C12-C13	-2.21	120.21	126.42
39	R	318	CHL	O1D-CGD-CBD	-2.21	121.06	124.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	e	101	HEM	C2A-C1A-NA	-2.21	107.68	110.15
39	y	314	CHL	OMC-CMC-C2C	-2.21	121.49	125.03
39	G	303	CHL	CHA-C1A-C2A	-2.21	128.12	133.31
26	Y	312	CLA	CHB-C1B-NB	2.21	126.59	124.26
26	y	310	CLA	CHB-C1B-NB	2.21	126.59	124.26
39	G	305	CHL	O1D-CGD-CBD	-2.21	121.06	124.74
42	y	307	NEX	C26-C27-C28	-2.21	121.33	125.99
42	R	305	NEX	C11-C12-C13	-2.20	120.22	126.42
28	t	101	BCR	C20-C19-C18	2.20	132.60	126.42
26	G	307	CLA	CHD-C1D-ND	-2.20	122.43	124.45
26	s	307	CLA	CHD-C1D-ND	-2.20	122.43	124.45
26	d	411	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
26	r	311	CLA	CHD-C1D-ND	-2.20	122.43	124.45
26	C	506	CLA	CHB-C4A-NA	2.20	127.55	124.51
26	G	304	CLA	CHB-C1B-NB	2.20	126.58	124.26
26	N	308	CLA	C3B-C4B-NB	-2.20	108.48	110.52
28	T	101	BCR	C21-C20-C19	2.20	130.07	123.22
26	g	308	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
26	B	603	CLA	C3B-C4B-NB	-2.19	108.48	110.52
28	k	101	BCR	C24-C23-C22	-2.19	122.92	126.23
26	b	605	CLA	CHD-C1D-ND	-2.19	122.44	124.45
28	K	101	BCR	C24-C23-C22	-2.19	122.92	126.23
26	n	315	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
26	b	616	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
29	A	410	SQD	O9-S-C6	2.19	109.54	106.94
41	N	315	XAT	C7-C8-C9	-2.19	122.13	125.53
29	w	202	SQD	O9-S-C6	2.19	109.54	106.94
42	g	306	NEX	C11-C12-C13	-2.19	120.27	126.42
26	G	306	CLA	CHD-C1D-ND	-2.19	122.44	124.45
39	g	307	CHL	CHA-C1A-C2A	-2.19	128.17	133.31
26	b	613	CLA	CHD-C1D-ND	-2.19	122.44	124.45
26	c	516	CLA	CHB-C1B-NB	2.19	126.57	124.26
41	g	309	XAT	C27-C28-C29	-2.19	122.14	125.53
26	n	305	CLA	C1-C2-C3	-2.19	122.26	126.04
41	N	315	XAT	C5-C4-C3	-2.19	108.42	112.75
39	Y	307	CHL	O2D-CGD-O1D	-2.18	119.57	123.84
26	y	313	CLA	CHC-C4B-NB	2.18	126.57	124.26
26	s	310	CLA	CHD-C1D-ND	-2.18	122.45	124.45
26	A	403	CLA	C3B-C4B-NB	-2.18	108.49	110.52
26	C	504	CLA	CHD-C1D-ND	-2.18	122.45	124.45
26	S	303	CLA	CHD-C1D-ND	-2.18	122.45	124.45
39	n	308	CHL	O1D-CGD-CBD	-2.18	121.11	124.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	y	307	NEX	C28-C29-C30	2.18	122.29	118.94
26	n	312	CLA	C3B-C4B-NB	-2.18	108.49	110.52
39	n	318	CHL	CHA-C1A-C2A	-2.18	128.19	133.31
26	N	308	CLA	CHD-C1D-ND	-2.18	122.45	124.45
39	N	303	CHL	O1D-CGD-CBD	-2.18	121.11	124.74
39	G	309	CHL	O2A-CGA-O1A	-2.18	118.09	123.59
28	t	101	BCR	C16-C15-C14	2.18	127.94	123.47
39	g	312	CHL	OMC-CMC-C2C	-2.18	121.54	125.03
26	B	616	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
42	G	315	NEX	C1-C2-C3	-2.18	108.73	113.64
39	N	310	CHL	CAA-C2A-C3A	-2.18	106.82	112.78
26	S	309	CLA	CMB-C2B-C1B	-2.18	122.06	125.37
40	Y	309	LUT	O23-C23-C22	-2.18	105.24	110.74
26	R	313	CLA	CHD-C1D-ND	-2.18	122.45	124.45
39	Y	314	CHL	O1D-CGD-CBD	-2.17	121.12	124.74
30	D	411	PL9	O1-C4-C3	-2.17	118.33	120.72
26	y	310	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
26	G	304	CLA	CHD-C1D-ND	-2.17	122.46	124.45
26	C	506	CLA	C1-C2-C3	-2.17	122.28	126.04
28	D	405	BCR	C7-C8-C9	-2.17	122.95	126.23
26	c	508	CLA	O2D-CGD-CBD	2.17	115.13	111.27
26	g	315	CLA	O2D-CGD-CBD	2.17	115.13	111.27
26	B	615	CLA	CHC-C4B-NB	2.17	126.56	124.26
26	Y	316	CLA	CHC-C4B-NB	2.17	126.56	124.26
26	R	308	CLA	CHD-C1D-ND	-2.17	122.46	124.45
26	a	411	CLA	C3B-C4B-NB	-2.17	108.50	110.52
39	N	316	CHL	O2A-CGA-O1A	-2.17	118.11	123.59
26	G	304	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
26	S	310	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
26	c	516	CLA	CMB-C2B-C1B	-2.17	122.06	125.37
26	r	306	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
28	t	101	BCR	C21-C20-C19	2.17	129.99	123.22
39	R	312	CHL	O1D-CGD-CBD	-2.17	121.13	124.74
29	B	621	SQD	O9-S-O7	2.17	121.45	113.95
39	Y	307	CHL	O1D-CGD-CBD	-2.17	121.13	124.74
26	b	611	CLA	C2D-C1D-ND	-2.17	108.51	110.10
30	A	408	PL9	C8-C7-C3	2.17	118.10	111.98
39	G	318	CHL	OMC-CMC-C2C	-2.17	121.56	125.03
29	b	621	SQD	O9-S-O7	2.17	121.44	113.95
26	b	605	CLA	O2D-CGD-CBD	2.16	115.11	111.27
26	D	412	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
26	b	606	CLA	CHB-C1B-NB	2.16	126.55	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	613	CLA	CHD-C1D-ND	-2.16	122.47	124.45
40	S	306	LUT	C21-C26-C27	-2.16	109.97	112.70
26	G	307	CLA	C3B-C4B-NB	-2.16	108.51	110.52
39	s	316	CHL	O2D-CGD-O1D	-2.16	119.61	123.84
28	T	101	BCR	C20-C19-C18	2.16	132.48	126.42
26	D	406	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
38	E	101	HEM	C2A-C1A-NA	-2.16	107.73	110.15
26	b	618	CLA	C1-C2-C3	-2.16	122.31	126.04
41	G	320	XAT	C27-C28-C29	-2.16	122.18	125.53
26	R	306	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
39	S	302	CHL	O2D-CGD-O1D	-2.16	119.62	123.84
26	g	318	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
26	D	412	CLA	CHB-C1B-NB	2.16	126.54	124.26
39	n	306	CHL	O2A-CGA-O1A	-2.16	118.15	123.59
26	A	405	CLA	O2D-CGD-CBD	2.15	115.09	111.27
42	r	302	NEX	C5-C4-C3	-2.15	109.20	111.75
26	s	310	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
26	c	510	CLA	O2D-CGD-CBD	2.15	115.09	111.27
26	N	313	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
26	r	308	CLA	CHB-C1B-NB	2.15	126.53	124.26
26	y	316	CLA	C1-C2-C3	-2.15	122.32	126.04
42	r	302	NEX	C20-C13-C14	-2.15	119.91	122.92
26	N	306	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
39	s	313	CHL	O2A-CGA-O1A	-2.15	118.17	123.59
39	R	301	CHL	O2D-CGD-O1D	-2.15	119.64	123.84
42	s	302	NEX	C19-C9-C10	-2.15	119.91	122.92
26	C	515	CLA	O2D-CGD-CBD	2.15	115.08	111.27
26	Y	313	CLA	CHB-C1B-NB	2.15	126.53	124.26
26	b	605	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
26	b	611	CLA	CHC-C4B-NB	2.15	126.53	124.26
26	c	502	CLA	CHB-C4A-NA	2.15	127.48	124.51
26	B	607	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
26	s	306	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
26	B	602	CLA	CHD-C1D-ND	-2.15	122.48	124.45
26	C	508	CLA	CHD-C1D-ND	-2.15	122.48	124.45
26	R	309	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
39	g	314	CHL	O2A-CGA-O1A	-2.14	118.18	123.59
39	r	309	CHL	O1D-CGD-CBD	-2.14	121.17	124.74
39	g	311	CHL	OMC-CMC-C2C	-2.14	121.60	125.03
26	b	617	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
42	R	305	NEX	C20-C13-C14	-2.14	119.92	122.92
26	b	611	CLA	CAA-C2A-C1A	2.14	118.99	111.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	618	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
26	b	616	CLA	C3B-C4B-NB	-2.14	108.53	110.52
39	n	318	CHL	O1D-CGD-CBD	-2.14	121.17	124.74
42	r	302	NEX	C11-C12-C13	-2.14	120.41	126.42
26	B	602	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
26	b	613	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
26	n	304	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
26	Y	313	CLA	C1-C2-C3	-2.14	122.35	126.04
26	S	309	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
26	b	604	CLA	CHD-C1D-ND	-2.13	122.49	124.45
26	n	312	CLA	CHD-C1D-ND	-2.13	122.49	124.45
28	J	101	BCR	C7-C8-C9	2.13	129.46	126.23
26	G	319	CLA	CHB-C1B-NB	2.13	126.52	124.26
39	s	313	CHL	CHA-C1A-C2A	-2.13	128.30	133.31
26	c	516	CLA	O2D-CGD-CBD	2.13	115.06	111.27
26	C	517	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
38	e	101	HEM	C3D-C4D-ND	-2.13	107.79	110.17
30	d	408	PL9	O1-C4-C3	-2.13	118.37	120.72
26	B	615	CLA	CHA-C1A-NA	-2.13	121.52	126.40
26	s	304	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
39	S	312	CHL	CHA-C1A-C2A	-2.13	128.31	133.31
40	n	317	LUT	O23-C23-C22	-2.13	105.36	110.74
26	c	518	CLA	CHD-C1D-ND	-2.13	122.50	124.45
30	A	408	PL9	C12-C13-C14	-2.13	122.53	127.66
26	c	513	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
39	s	317	CHL	O2A-CGA-O1A	-2.13	118.22	123.59
30	a	407	PL9	C8-C7-C3	2.13	118.00	111.98
28	t	101	BCR	C39-C30-C25	-2.13	106.85	110.30
26	B	609	CLA	CMB-C2B-C1B	-2.13	122.13	125.37
26	b	618	CLA	CMB-C2B-C1B	-2.13	122.13	125.37
26	c	520	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
26	r	305	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
39	N	303	CHL	CHA-C1A-C2A	-2.13	128.31	133.31
26	b	611	CLA	CHA-C1A-NA	-2.12	121.53	126.40
26	S	315	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
39	n	319	CHL	O2A-CGA-O1A	-2.12	118.23	123.59
42	G	315	NEX	C5-C4-C3	-2.12	109.23	111.75
39	S	312	CHL	O2A-CGA-O1A	-2.12	118.24	123.59
39	N	317	CHL	O2A-CGA-O1A	-2.12	118.24	123.59
26	g	303	CLA	CHD-C1D-ND	-2.12	122.51	124.45
39	n	318	CHL	OBD-CAD-CBD	-2.12	122.72	125.82
40	y	318	LUT	O23-C23-C22	-2.12	105.39	110.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	n	312	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
39	g	314	CHL	O1D-CGD-CBD	-2.12	121.21	124.74
26	b	613	CLA	C1-C2-C3	-2.12	122.38	126.04
26	C	508	CLA	O2D-CGD-CBD	2.12	115.03	111.27
39	y	314	CHL	O1D-CGD-CBD	-2.12	121.21	124.74
34	w	201	LMG	C1-C2-C3	-2.12	105.59	110.00
26	B	602	CLA	O2D-CGD-CBD	2.12	115.03	111.27
39	r	318	CHL	O2D-CGD-O1D	-2.11	119.70	123.84
42	Y	304	NEX	C28-C29-C30	2.11	122.19	118.94
26	s	314	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
30	d	408	PL9	C20-C19-C21	2.11	118.83	115.27
26	C	511	CLA	C1-C2-C3	-2.11	122.39	126.04
26	A	405	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
26	n	315	CLA	CHD-C1D-ND	-2.11	122.51	124.45
26	R	306	CLA	C1-C2-C3	-2.11	122.39	126.04
26	N	308	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
26	c	504	CLA	C2D-C1D-ND	-2.11	108.55	110.10
26	c	516	CLA	CHD-C1D-ND	-2.11	122.52	124.45
30	a	407	PL9	C12-C13-C14	-2.11	122.58	127.66
26	g	304	CLA	CHB-C1B-NB	2.11	126.49	124.26
26	g	308	CLA	CHD-C1D-ND	-2.11	122.52	124.45
26	G	313	CLA	O2D-CGD-CBD	2.11	115.01	111.27
26	Y	313	CLA	O2D-CGD-CBD	2.11	115.01	111.27
29	W	202	SQD	O9-S-C6	2.11	109.44	106.94
27	A	404	PHO	C1-C2-C3	-2.11	122.40	126.04
26	G	317	CLA	CHD-C1D-ND	-2.10	122.52	124.45
39	r	301	CHL	O2D-CGD-O1D	-2.10	119.72	123.84
26	c	513	CLA	CHD-C1D-ND	-2.10	122.52	124.45
39	R	315	CHL	CMD-C2D-C3D	2.10	128.61	124.68
39	R	318	CHL	O2D-CGD-O1D	-2.10	119.73	123.84
26	B	611	CLA	CHD-C1D-ND	-2.10	122.52	124.45
26	c	502	CLA	C1-C2-C3	-2.10	122.41	126.04
26	C	505	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
26	S	314	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
26	c	504	CLA	O2D-CGD-CBD	2.10	115.00	111.27
26	S	310	CLA	CHD-C1D-ND	-2.10	122.52	124.45
26	g	317	CLA	CHD-C1D-ND	-2.10	122.52	124.45
26	c	504	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
27	a	410	PHO	C1-C2-C3	-2.10	122.41	126.04
26	a	411	CLA	CHD-C1D-ND	-2.10	122.52	124.45
26	B	611	CLA	CHB-C1B-NB	2.10	126.48	124.26
27	A	404	PHO	CBA-CAA-C2A	-2.10	107.68	113.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	y	305	CHL	CMD-C2D-C3D	2.10	128.60	124.68
26	B	610	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
39	g	307	CHL	O2D-CGD-O1D	-2.10	119.74	123.84
26	c	516	CLA	C3B-C4B-NB	-2.10	108.57	110.52
26	b	613	CLA	O2D-CGD-CBD	2.10	114.99	111.27
39	G	301	CHL	OMC-CMC-C2C	-2.10	121.67	125.03
26	B	618	CLA	CHD-C1D-ND	-2.09	122.53	124.45
29	a	413	SQD	C44-O6-C1	-2.09	109.65	113.74
27	a	410	PHO	CBA-CAA-C2A	-2.09	107.69	113.81
39	n	308	CHL	CAA-C2A-C3A	-2.09	107.05	112.78
39	s	317	CHL	OMC-CMC-C2C	-2.09	121.68	125.03
26	n	302	CLA	CHD-C1D-ND	-2.09	122.53	124.45
26	B	618	CLA	O2D-CGD-CBD	2.09	114.98	111.27
39	S	313	CHL	O2A-CGA-O1A	-2.09	118.32	123.59
26	A	403	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
26	C	515	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
26	B	607	CLA	C3B-C4B-NB	-2.09	108.58	110.52
26	c	503	CLA	C1-C2-C3	-2.09	122.43	126.04
39	y	312	CHL	O1D-CGD-CBD	-2.09	121.26	124.74
26	a	402	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
26	b	612	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
39	G	303	CHL	O2D-CGD-O1D	-2.09	119.76	123.84
29	W	202	SQD	O7-S-C6	2.08	109.42	106.94
30	D	411	PL9	O2-C1-C2	-2.08	117.00	121.78
30	D	411	PL9	C20-C19-C21	2.08	118.78	115.27
39	n	307	CHL	CMB-C2B-C3B	2.08	128.58	124.68
42	G	315	NEX	C20-C13-C14	-2.08	120.00	122.92
29	A	407	SQD	O9-S-O7	2.08	121.16	113.95
26	B	615	CLA	CAA-C2A-C1A	2.08	118.80	111.97
26	S	311	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
26	C	507	CLA	CHB-C1B-NB	2.08	126.46	124.26
26	B	618	CLA	C1-C2-C3	-2.08	122.44	126.04
26	Y	305	CLA	C2D-C1D-ND	-2.08	108.57	110.10
26	c	514	CLA	CMB-C2B-C3B	2.08	131.63	126.59
26	r	313	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
26	B	604	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
26	b	606	CLA	CHD-C1D-ND	-2.08	122.55	124.45
39	n	308	CHL	O2A-CGA-O1A	-2.08	118.35	123.59
39	G	309	CHL	O1D-CGD-CBD	-2.08	121.28	124.74
41	r	304	XAT	C31-C30-C29	-2.08	124.35	127.31
30	d	408	PL9	O2-C1-C2	-2.07	117.03	121.78
26	n	304	CLA	O2D-CGD-CBD	2.07	114.95	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	G	315	NEX	C26-C27-C28	-2.07	121.61	125.99
26	N	319	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
26	Y	305	CLA	CMB-C2B-C1B	-2.07	122.21	125.37
26	c	516	CLA	C1-C2-C3	-2.07	122.46	126.04
26	s	301	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
26	C	508	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
28	T	101	BCR	C38-C26-C27	-2.07	109.64	113.62
39	S	313	CHL	OMC-CMC-C2C	-2.07	121.72	125.03
26	a	411	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
41	R	304	XAT	C31-C30-C29	-2.06	124.36	127.31
26	S	307	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
26	b	608	CLA	CHB-C1B-NB	2.06	126.44	124.26
26	g	318	CLA	CHB-C1B-NB	2.06	126.44	124.26
26	R	302	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
26	n	310	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
39	G	311	CHL	O2A-CGA-O1A	-2.06	118.39	123.59
39	Y	317	CHL	CMD-C2D-C3D	2.06	128.53	124.68
26	r	317	CLA	CHB-C1B-NB	2.06	126.44	124.26
39	r	318	CHL	CMD-C2D-C3D	2.06	128.53	124.68
26	c	504	CLA	C1-C2-C3	-2.06	122.48	126.04
30	a	407	PL9	C7-C8-C9	-2.06	123.36	126.79
34	D	404	LMG	C1-C2-C3	-2.06	105.71	110.00
26	r	311	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
26	N	307	CLA	C1-C2-C3	-2.06	122.48	126.04
29	a	403	SQD	O9-S-O7	2.06	121.07	113.95
28	C	502	BCR	C19-C18-C17	-2.06	115.78	118.94
26	y	309	CLA	C1-C2-C3	-2.06	122.48	126.04
26	S	311	CLA	CHD-C1D-C2D	2.06	129.79	125.48
26	g	304	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
41	g	320	XAT	C27-C28-C29	-2.06	122.34	125.53
26	b	601	CLA	CMB-C2B-C1B	-2.06	122.24	125.37
26	s	315	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
39	N	304	CHL	O2D-CGD-O1D	-2.06	119.82	123.84
39	g	312	CHL	O2A-CGA-O1A	-2.06	118.40	123.59
26	c	506	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
39	r	301	CHL	O2A-CGA-O1A	-2.05	118.41	123.59
30	A	408	PL9	C7-C8-C9	-2.05	123.37	126.79
30	D	411	PL9	C31-C32-C33	-2.05	105.13	111.88
26	R	308	CLA	CMB-C2B-C1B	-2.05	122.24	125.37
34	W	201	LMG	C1-C2-C3	-2.05	105.72	110.00
42	g	306	NEX	C26-C27-C28	-2.05	121.65	125.99
28	j	101	BCR	C7-C8-C9	2.05	129.34	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	s	313	CHL	O2D-CGD-O1D	-2.05	119.83	123.84
26	S	308	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
42	y	307	NEX	C25-C24-C23	-2.05	108.69	112.75
26	C	515	CLA	C1-C2-C3	-2.05	122.50	126.04
42	N	302	NEX	C20-C13-C14	-2.05	120.05	122.92
39	N	311	CHL	CMB-C2B-C3B	2.05	128.51	124.68
26	c	514	CLA	O2D-CGD-CBD	2.05	114.91	111.27
26	G	313	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
42	r	302	NEX	C40-C33-C32	2.05	121.31	118.08
26	N	313	CLA	O2D-CGD-CBD	2.05	114.91	111.27
26	G	319	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
38	E	101	HEM	C3D-C4D-ND	-2.05	107.89	110.17
26	n	303	CLA	CMB-C2B-C3B	2.05	131.55	126.59
26	n	304	CLA	CHD-C1D-ND	-2.05	122.57	124.45
42	Y	304	NEX	C25-C24-C23	-2.05	108.70	112.75
26	C	520	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
26	C	515	CLA	C2D-C1D-ND	-2.05	108.60	110.10
26	C	511	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
39	g	319	CHL	CMD-C2D-C3D	2.05	128.50	124.68
26	b	614	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
33	c	517	DGD	C6D-O5D-C1E	2.04	117.73	113.74
26	d	411	CLA	O1D-CGD-CBD	2.04	128.67	124.48
26	D	401	CLA	CMB-C2B-C3B	2.04	131.54	126.59
26	C	519	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
39	g	319	CHL	O2A-CGA-O1A	-2.04	118.44	123.59
26	c	503	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	C	508	CLA	C1-C2-C3	-2.04	122.51	126.04
26	R	309	CLA	CHD-C1D-ND	-2.04	122.58	124.45
26	r	311	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	g	305	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	N	312	CLA	CMB-C2B-C3B	2.04	131.53	126.59
26	g	315	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	R	308	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
39	R	318	CHL	O2A-CGA-O1A	-2.04	118.44	123.59
29	A	410	SQD	O9-S-O7	2.04	121.01	113.95
30	d	408	PL9	C31-C32-C33	-2.04	105.18	111.88
39	N	303	CHL	OBD-CAD-CBD	-2.04	122.83	125.82
42	R	305	NEX	C40-C33-C32	2.04	121.29	118.08
26	s	311	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
39	y	312	CHL	O2A-CGA-O1A	-2.04	118.45	123.59
41	n	316	XAT	C5-C4-C3	-2.04	108.72	112.75
39	g	313	CHL	OMC-CMC-C2C	-2.04	121.77	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	R	317	CLA	CMB-C2B-C3B	2.03	131.52	126.59
32	A	411	BCT	O3-C-O1	-2.03	114.27	119.55
42	g	306	NEX	C40-C33-C34	-2.03	120.07	122.92
39	N	310	CHL	O2A-CGA-O1A	-2.03	118.46	123.59
41	G	320	XAT	C25-C24-C23	-2.03	108.73	112.75
26	S	307	CLA	CHB-C1B-NB	2.03	126.41	124.26
26	N	318	CLA	CHD-C1D-ND	-2.03	122.59	124.45
26	y	306	CLA	CMB-C2B-C3B	2.03	131.51	126.59
39	n	311	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
26	c	514	CLA	CHB-C1B-NB	2.03	126.41	124.26
26	b	612	CLA	O2D-CGD-CBD	2.03	114.88	111.27
26	b	611	CLA	C3B-C4B-NB	-2.03	108.63	110.52
26	D	412	CLA	O1D-CGD-CBD	2.03	128.64	124.48
32	a	405	BCT	O3-C-O1	-2.03	114.28	119.55
41	R	304	XAT	C10-C11-C12	-2.03	116.89	123.22
26	Y	308	CLA	CMB-C2B-C3B	2.03	131.49	126.59
26	N	306	CLA	CHD-C1D-ND	-2.03	122.59	124.45
26	B	617	CLA	O2D-CGD-CBD	2.02	114.87	111.27
39	G	305	CHL	CMD-C2D-C3D	2.02	128.47	124.68
29	a	413	SQD	O9-S-O7	2.02	120.95	113.95
39	G	305	CHL	O2A-CGA-O1A	-2.02	118.48	123.59
26	G	306	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
26	G	313	CLA	CHB-C1B-NB	2.02	126.40	124.26
39	n	318	CHL	O2A-CGA-O1A	-2.02	118.49	123.59
39	S	316	CHL	O1D-CGD-CBD	-2.02	121.37	124.74
26	B	604	CLA	CMB-C2B-C3B	2.02	131.48	126.59
26	s	314	CLA	CHD-C1D-C2D	2.02	129.72	125.48
26	B	612	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
26	s	311	CLA	CHB-C1B-NB	2.02	126.39	124.26
26	B	609	CLA	CMB-C2B-C3B	2.02	131.48	126.59
28	c	511	BCR	C19-C18-C17	-2.02	115.84	118.94
26	b	612	CLA	CMB-C2B-C3B	2.02	131.48	126.59
26	C	521	CLA	O2D-CGD-CBD	2.02	114.85	111.27
26	r	306	CLA	C1-C2-C3	-2.02	122.55	126.04
27	D	403	PHO	C1C-C2C-C3C	-2.02	106.93	108.61
26	c	510	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
39	N	303	CHL	O2A-CGA-O1A	-2.02	118.50	123.59
34	d	405	LMG	C1-C2-C3	-2.02	105.80	110.00
26	c	520	CLA	C1-C2-C3	-2.02	122.56	126.04
26	b	607	CLA	CHB-C1B-NB	2.02	126.39	124.26
41	g	320	XAT	C6-C7-C8	-2.02	121.73	125.99
26	r	317	CLA	O1D-CGD-CBD	2.02	128.61	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y	309	CLA	CMB-C2B-C1B	-2.02	122.30	125.37
26	R	314	CLA	CHB-C1B-NB	2.01	126.39	124.26
33	C	509	DGD	C6D-O5D-C1E	2.01	117.67	113.74
29	w	202	SQD	O7-S-C6	2.01	109.33	106.94
26	S	303	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
42	g	306	NEX	C20-C13-C14	-2.01	120.10	122.92
39	y	302	CHL	O2D-CGD-O1D	-2.01	119.91	123.84
26	g	315	CLA	CHB-C1B-NB	2.01	126.39	124.26
26	d	403	CLA	CMB-C2B-C3B	2.01	131.46	126.59
26	y	315	CLA	O2D-CGD-CBD	2.01	114.84	111.27
39	N	304	CHL	OMC-CMC-C2C	-2.01	121.81	125.03
39	Y	314	CHL	O2A-CGA-O1A	-2.01	118.52	123.59
26	b	618	CLA	CMB-C2B-C3B	2.01	131.46	126.59
26	Y	316	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
33	y	308	DGD	O3D-C3D-C2D	-2.01	105.71	110.35
26	R	309	CLA	C2D-C1D-ND	-2.01	108.62	110.10
26	Y	308	CLA	CHB-C1B-NB	2.01	126.38	124.26
42	R	305	NEX	C5-C4-C3	-2.01	109.37	111.75
29	A	407	SQD	O6-C1-C2	-2.01	105.17	108.30
42	G	315	NEX	C40-C33-C34	-2.01	120.11	122.92
26	b	604	CLA	CHB-C1B-NB	2.01	126.38	124.26
26	s	307	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
26	b	610	CLA	O2D-CGD-CBD	2.01	114.83	111.27
41	N	315	XAT	C10-C11-C12	-2.00	116.96	123.22
42	n	313	NEX	C20-C13-C14	-2.00	120.12	122.92
39	R	301	CHL	O2A-CGA-O1A	-2.00	118.53	123.59
39	Y	318	CHL	O2D-CGD-O1D	-2.00	119.92	123.84
26	g	305	CLA	CHB-C1B-NB	2.00	126.38	124.26
26	A	403	CLA	CHD-C1D-ND	-2.00	122.61	124.45
41	g	320	XAT	C25-C24-C23	-2.00	108.79	112.75
26	y	313	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
29	W	202	SQD	O9-S-O7	2.00	120.88	113.95
26	b	614	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
26	R	314	CLA	O1D-CGD-CBD	2.00	128.58	124.48
26	c	504	CLA	CHD-C1D-ND	-2.00	122.61	124.45
33	Y	303	DGD	O3D-C3D-C2D	-2.00	105.72	110.35

There are no chirality outliers.

All (3037) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	B	601	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	B	601	CLA	CHA-CBD-CGD-O2D
26	B	601	CLA	CAD-CBD-CGD-O1D
26	B	601	CLA	CAD-CBD-CGD-O2D
26	B	601	CLA	C2-C3-C5-C6
26	B	601	CLA	C4-C3-C5-C6
26	B	605	CLA	CHA-CBD-CGD-O1D
26	B	605	CLA	CHA-CBD-CGD-O2D
26	B	606	CLA	C1A-C2A-CAA-CBA
26	B	606	CLA	C4-C3-C5-C6
26	B	610	CLA	CHA-CBD-CGD-O1D
26	B	610	CLA	CHA-CBD-CGD-O2D
26	B	613	CLA	C1A-C2A-CAA-CBA
26	B	613	CLA	CHA-CBD-CGD-O1D
26	B	615	CLA	C1A-C2A-CAA-CBA
26	B	615	CLA	CHA-CBD-CGD-O1D
26	B	615	CLA	CHA-CBD-CGD-O2D
26	B	615	CLA	C6-C7-C8-C9
26	C	507	CLA	C2B-C3B-CAB-CBB
26	C	507	CLA	C4B-C3B-CAB-CBB
26	C	508	CLA	CBD-CGD-O2D-CED
26	C	512	CLA	CHA-CBD-CGD-O1D
26	C	515	CLA	C6-C7-C8-C9
26	C	516	CLA	C2B-C3B-CAB-CBB
26	C	516	CLA	C4B-C3B-CAB-CBB
26	C	520	CLA	NA-C4A-CHB-C1B
26	C	520	CLA	C1B-C2B-C3B-C4B
26	C	520	CLA	CMB-C2B-C3B-C4B
26	D	401	CLA	CHA-CBD-CGD-O1D
26	D	401	CLA	CHA-CBD-CGD-O2D
26	D	412	CLA	C2B-C3B-CAB-CBB
26	D	412	CLA	C4B-C3B-CAB-CBB
26	D	412	CLA	CHA-CBD-CGD-O1D
26	D	412	CLA	CHA-CBD-CGD-O2D
26	D	412	CLA	CBD-CGD-O2D-CED
26	G	302	CLA	C1A-C2A-CAA-CBA
26	G	304	CLA	C2B-C3B-CAB-CBB
26	G	304	CLA	C4B-C3B-CAB-CBB
26	G	306	CLA	CHA-CBD-CGD-O1D
26	G	306	CLA	CHA-CBD-CGD-O2D
26	G	307	CLA	C1A-C2A-CAA-CBA
26	G	307	CLA	CBD-CGD-O2D-CED
26	G	317	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	N	306	CLA	C2B-C3B-CAB-CBB
26	N	306	CLA	C4B-C3B-CAB-CBB
26	N	309	CLA	CAD-CBD-CGD-O1D
26	N	309	CLA	CAD-CBD-CGD-O2D
26	N	309	CLA	CBD-CGD-O2D-CED
26	N	313	CLA	CHA-CBD-CGD-O1D
26	N	313	CLA	CHA-CBD-CGD-O2D
26	N	319	CLA	C1A-C2A-CAA-CBA
26	N	319	CLA	C3A-C2A-CAA-CBA
26	N	319	CLA	C2B-C3B-CAB-CBB
26	N	319	CLA	C4B-C3B-CAB-CBB
26	N	319	CLA	CHA-CBD-CGD-O1D
26	N	319	CLA	CHA-CBD-CGD-O2D
26	R	302	CLA	CBA-CGA-O2A-C1
26	R	302	CLA	O1A-CGA-O2A-C1
26	R	307	CLA	C4B-C3B-CAB-CBB
26	R	308	CLA	C1A-C2A-CAA-CBA
26	R	308	CLA	CBD-CGD-O2D-CED
26	R	310	CLA	C2B-C3B-CAB-CBB
26	R	310	CLA	C4B-C3B-CAB-CBB
26	R	314	CLA	C3A-C2A-CAA-CBA
26	R	316	CLA	CBD-CGD-O2D-CED
26	S	303	CLA	C2B-C3B-CAB-CBB
26	S	303	CLA	C4B-C3B-CAB-CBB
26	S	309	CLA	C1A-C2A-CAA-CBA
26	S	310	CLA	C1A-C2A-CAA-CBA
26	S	310	CLA	C3A-C2A-CAA-CBA
26	S	310	CLA	C2A-CAA-CBA-CGA
26	S	310	CLA	C2B-C3B-CAB-CBB
26	S	310	CLA	C4B-C3B-CAB-CBB
26	S	310	CLA	CHA-CBD-CGD-O1D
26	S	310	CLA	CHA-CBD-CGD-O2D
26	S	314	CLA	C2B-C3B-CAB-CBB
26	S	314	CLA	C4B-C3B-CAB-CBB
26	Y	310	CLA	C1A-C2A-CAA-CBA
26	Y	310	CLA	C2A-CAA-CBA-CGA
26	Y	311	CLA	C2B-C3B-CAB-CBB
26	Y	311	CLA	C4B-C3B-CAB-CBB
26	Y	316	CLA	CHA-CBD-CGD-O1D
26	Y	316	CLA	CHA-CBD-CGD-O2D
26	a	409	CLA	CHA-CBD-CGD-O1D
26	a	409	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	a	411	CLA	CBD-CGD-O2D-CED
26	b	601	CLA	C1A-C2A-CAA-CBA
26	b	601	CLA	O2A-C1-C2-C3
26	b	604	CLA	CHA-CBD-CGD-O1D
26	b	607	CLA	CHA-CBD-CGD-O1D
26	b	607	CLA	CHA-CBD-CGD-O2D
26	b	607	CLA	CAD-CBD-CGD-O1D
26	b	607	CLA	CAD-CBD-CGD-O2D
26	b	607	CLA	C2-C3-C5-C6
26	b	607	CLA	C4-C3-C5-C6
26	b	608	CLA	CHA-CBD-CGD-O1D
26	b	608	CLA	CHA-CBD-CGD-O2D
26	b	611	CLA	C1A-C2A-CAA-CBA
26	b	611	CLA	C6-C7-C8-C9
26	b	617	CLA	CHA-CBD-CGD-O1D
26	b	617	CLA	CHA-CBD-CGD-O2D
26	c	502	CLA	C11-C12-C13-C15
26	c	504	CLA	C6-C7-C8-C9
26	c	505	CLA	C2B-C3B-CAB-CBB
26	c	505	CLA	CBD-CGD-O2D-CED
26	c	506	CLA	NA-C4A-CHB-C1B
26	c	506	CLA	C1B-C2B-C3B-C4B
26	c	506	CLA	CMB-C2B-C3B-C4B
26	c	508	CLA	C2B-C3B-CAB-CBB
26	c	508	CLA	C4B-C3B-CAB-CBB
26	c	515	CLA	CHA-CBD-CGD-O1D
26	c	515	CLA	CHA-CBD-CGD-O2D
26	c	515	CLA	CAD-CBD-CGD-O1D
26	c	516	CLA	CBD-CGD-O2D-CED
26	d	411	CLA	C2B-C3B-CAB-CBB
26	d	411	CLA	C4B-C3B-CAB-CBB
26	d	411	CLA	CHA-CBD-CGD-O1D
26	d	411	CLA	CHA-CBD-CGD-O2D
26	d	411	CLA	CBD-CGD-O2D-CED
26	g	302	CLA	C1A-C2A-CAA-CBA
26	g	305	CLA	CHA-CBD-CGD-O1D
26	g	305	CLA	CHA-CBD-CGD-O2D
26	g	308	CLA	C2B-C3B-CAB-CBB
26	g	308	CLA	C4B-C3B-CAB-CBB
26	g	317	CLA	C1A-C2A-CAA-CBA
26	g	317	CLA	CBD-CGD-O2D-CED
26	g	318	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	g	318	CLA	C4B-C3B-CAB-CBB
26	n	304	CLA	CHA-CBD-CGD-O1D
26	n	304	CLA	CHA-CBD-CGD-O2D
26	n	309	CLA	CAD-CBD-CGD-O1D
26	n	309	CLA	CAD-CBD-CGD-O2D
26	n	309	CLA	CBD-CGD-O2D-CED
26	n	310	CLA	C1A-C2A-CAA-CBA
26	n	310	CLA	C3A-C2A-CAA-CBA
26	n	310	CLA	C2B-C3B-CAB-CBB
26	n	310	CLA	C4B-C3B-CAB-CBB
26	n	310	CLA	CHA-CBD-CGD-O1D
26	n	310	CLA	CHA-CBD-CGD-O2D
26	n	315	CLA	C2B-C3B-CAB-CBB
26	n	315	CLA	C4B-C3B-CAB-CBB
26	r	303	CLA	CBD-CGD-O2D-CED
26	r	308	CLA	C2B-C3B-CAB-CBB
26	r	308	CLA	C4B-C3B-CAB-CBB
26	r	310	CLA	C2B-C3B-CAB-CBB
26	r	310	CLA	C4B-C3B-CAB-CBB
26	r	311	CLA	C1A-C2A-CAA-CBA
26	r	311	CLA	CBD-CGD-O2D-CED
26	r	313	CLA	CBA-CGA-O2A-C1
26	r	313	CLA	O1A-CGA-O2A-C1
26	r	314	CLA	CHA-CBD-CGD-O2D
26	r	317	CLA	C3A-C2A-CAA-CBA
26	r	317	CLA	C2A-CAA-CBA-CGA
26	s	304	CLA	C1A-C2A-CAA-CBA
26	s	307	CLA	C2B-C3B-CAB-CBB
26	s	307	CLA	C4B-C3B-CAB-CBB
26	s	310	CLA	C1A-C2A-CAA-CBA
26	s	310	CLA	C3A-C2A-CAA-CBA
26	s	310	CLA	C2A-CAA-CBA-CGA
26	s	310	CLA	C2B-C3B-CAB-CBB
26	s	310	CLA	C4B-C3B-CAB-CBB
26	s	310	CLA	CHA-CBD-CGD-O1D
26	s	315	CLA	C2B-C3B-CAB-CBB
26	s	315	CLA	C4B-C3B-CAB-CBB
26	y	313	CLA	CHA-CBD-CGD-O1D
26	y	313	CLA	CHA-CBD-CGD-O2D
26	y	315	CLA	C2B-C3B-CAB-CBB
26	y	315	CLA	C4B-C3B-CAB-CBB
26	y	317	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	y	317	CLA	C2A-CAA-CBA-CGA
28	A	406	BCR	C23-C24-C25-C30
28	B	614	BCR	C5-C6-C7-C8
28	D	405	BCR	C5-C6-C7-C8
28	D	405	BCR	C7-C8-C9-C10
28	D	405	BCR	C7-C8-C9-C34
28	D	405	BCR	C23-C24-C25-C30
28	J	101	BCR	C17-C18-C19-C20
28	J	101	BCR	C36-C18-C19-C20
28	T	101	BCR	C1-C6-C7-C8
28	T	101	BCR	C13-C14-C15-C16
28	b	619	BCR	C5-C6-C7-C8
28	c	507	BCR	C1-C6-C7-C8
28	d	401	BCR	C5-C6-C7-C8
28	d	401	BCR	C7-C8-C9-C10
28	d	401	BCR	C7-C8-C9-C34
28	d	401	BCR	C23-C24-C25-C30
28	j	101	BCR	C17-C18-C19-C20
28	j	101	BCR	C36-C18-C19-C20
28	t	101	BCR	C1-C6-C7-C8
28	t	101	BCR	C13-C14-C15-C16
28	t	101	BCR	C19-C20-C21-C22
29	A	407	SQD	O5-C5-C6-S
29	A	410	SQD	O5-C5-C6-S
29	B	621	SQD	O5-C1-O6-C44
29	B	621	SQD	C8-C7-O47-C45
29	W	202	SQD	O5-C1-O6-C44
29	W	202	SQD	C5-C6-S-O8
29	W	202	SQD	C5-C6-S-O9
29	a	403	SQD	O5-C5-C6-S
29	a	413	SQD	O49-C7-O47-C45
29	a	413	SQD	O5-C5-C6-S
29	b	621	SQD	O5-C1-O6-C44
29	b	621	SQD	C8-C7-O47-C45
29	w	202	SQD	C2-C1-O6-C44
29	w	202	SQD	O5-C1-O6-C44
29	w	202	SQD	C5-C6-S-O8
29	w	202	SQD	C5-C6-S-O9
30	A	408	PL9	C14-C16-C17-C18
30	a	407	PL9	C14-C16-C17-C18
33	B	620	DGD	C4D-C5D-C6D-O5D
33	B	620	DGD	C2E-C1E-O5D-C6D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	B	620	DGD	O6E-C1E-O5D-C6D
33	b	620	DGD	C4D-C5D-C6D-O5D
33	b	620	DGD	C2E-C1E-O5D-C6D
33	b	620	DGD	O6E-C1E-O5D-C6D
34	W	201	LMG	C11-C10-O7-C8
34	c	512	LMG	C8-C7-O1-C1
34	w	201	LMG	C11-C10-O7-C8
36	D	402	LMT	C2'-C1'-O1'-C1
36	D	402	LMT	O5'-C1'-O1'-C1
36	d	406	LMT	C2'-C1'-O1'-C1
36	d	406	LMT	O5'-C1'-O1'-C1
37	D	407	LHG	C1-C2-C3-O3
37	D	407	LHG	O2-C2-C3-O3
37	D	408	LHG	C3-O3-P-O6
37	L	101	LHG	C3-O3-P-O4
37	N	301	LHG	C4-O6-P-O3
37	R	303	LHG	C3-O3-P-O5
37	R	303	LHG	C3-O3-P-O6
37	R	303	LHG	O9-C7-O7-C5
37	R	303	LHG	C8-C7-O7-C5
37	S	317	LHG	C3-O3-P-O6
37	Y	306	LHG	O2-C2-C3-O3
37	Y	306	LHG	C3-O3-P-O4
37	Y	306	LHG	C3-O3-P-O5
37	Y	306	LHG	C3-O3-P-O6
37	Y	306	LHG	C4-O6-P-O4
37	d	402	LHG	C1-C2-C3-O3
37	d	402	LHG	O2-C2-C3-O3
37	l	101	LHG	C3-O3-P-O4
37	n	301	LHG	C4-O6-P-O3
37	r	312	LHG	C3-O3-P-O6
37	r	312	LHG	O9-C7-O7-C5
37	r	312	LHG	C8-C7-O7-C5
37	s	309	LHG	C3-O3-P-O6
37	y	301	LHG	C3-O3-P-O4
37	y	301	LHG	C3-O3-P-O5
37	y	301	LHG	C3-O3-P-O6
37	y	301	LHG	C4-O6-P-O4
39	G	301	CHL	C3A-C2A-CAA-CBA
39	G	301	CHL	C2-C1-O2A-CGA
39	G	303	CHL	C1A-C2A-CAA-CBA
39	G	309	CHL	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	G	309	CHL	C3A-C2A-CAA-CBA
39	G	309	CHL	C1C-C2C-CMC-OMC
39	G	309	CHL	C4C-C3C-CAC-CBC
39	G	309	CHL	CBD-CGD-O2D-CED
39	G	311	CHL	C4C-C3C-CAC-CBC
39	G	318	CHL	C4C-C3C-CAC-CBC
39	G	318	CHL	C2-C3-C5-C6
39	G	318	CHL	C11-C10-C8-C9
39	N	303	CHL	C4C-C3C-CAC-CBC
39	N	310	CHL	C3A-C2A-CAA-CBA
39	N	310	CHL	C1C-C2C-CMC-OMC
39	N	311	CHL	C1C-C2C-CMC-OMC
39	N	311	CHL	C4C-C3C-CAC-CBC
39	N	316	CHL	C4C-C3C-CAC-CBC
39	N	317	CHL	C4C-C3C-CAC-CBC
39	R	301	CHL	C1A-C2A-CAA-CBA
39	R	301	CHL	CBD-CGD-O2D-CED
39	R	312	CHL	C3A-C2A-CAA-CBA
39	R	312	CHL	C4C-C3C-CAC-CBC
39	R	315	CHL	C1A-C2A-CAA-CBA
39	R	318	CHL	C1A-C2A-CAA-CBA
39	R	318	CHL	C3A-C2A-CAA-CBA
39	R	318	CHL	C1C-C2C-CMC-OMC
39	R	318	CHL	C3C-C2C-CMC-OMC
39	R	318	CHL	C4C-C3C-CAC-CBC
39	S	302	CHL	C1A-C2A-CAA-CBA
39	S	302	CHL	CBA-CGA-O2A-C1
39	S	302	CHL	O1A-CGA-O2A-C1
39	S	302	CHL	C3C-C2C-CMC-OMC
39	S	302	CHL	C4C-C3C-CAC-CBC
39	S	302	CHL	CBD-CGD-O2D-CED
39	S	302	CHL	O1D-CGD-O2D-CED
39	S	312	CHL	C1C-C2C-CMC-OMC
39	S	312	CHL	CBD-CGD-O2D-CED
39	S	312	CHL	O1D-CGD-O2D-CED
39	S	313	CHL	C3A-C2A-CAA-CBA
39	S	313	CHL	C1-C2-C3-C4
39	S	316	CHL	C2-C3-C5-C6
39	Y	307	CHL	C4C-C3C-CAC-CBC
39	Y	314	CHL	C4C-C3C-CAC-CBC
39	Y	317	CHL	C3C-C2C-CMC-OMC
39	Y	318	CHL	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	g	307	CHL	C1A-C2A-CAA-CBA
39	g	311	CHL	O1A-CGA-O2A-C1
39	g	311	CHL	C4C-C3C-CAC-CBC
39	g	311	CHL	C11-C10-C8-C9
39	g	312	CHL	C4C-C3C-CAC-CBC
39	g	312	CHL	CHA-CBD-CGD-O1D
39	g	312	CHL	CHA-CBD-CGD-O2D
39	g	314	CHL	C1A-C2A-CAA-CBA
39	g	314	CHL	C3A-C2A-CAA-CBA
39	g	314	CHL	C4C-C3C-CAC-CBC
39	g	314	CHL	CBD-CGD-O2D-CED
39	n	307	CHL	C1C-C2C-CMC-OMC
39	n	307	CHL	C4C-C3C-CAC-CBC
39	n	308	CHL	C3A-C2A-CAA-CBA
39	n	308	CHL	C1C-C2C-CMC-OMC
39	n	318	CHL	C4C-C3C-CAC-CBC
39	n	319	CHL	C4C-C3C-CAC-CBC
39	r	301	CHL	C1A-C2A-CAA-CBA
39	r	301	CHL	C1C-C2C-CMC-OMC
39	r	301	CHL	C3C-C2C-CMC-OMC
39	r	301	CHL	C4C-C3C-CAC-CBC
39	r	309	CHL	C3A-C2A-CAA-CBA
39	r	309	CHL	C4C-C3C-CAC-CBC
39	r	316	CHL	C1A-C2A-CAA-CBA
39	r	316	CHL	CBD-CGD-O2D-CED
39	r	318	CHL	C1A-C2A-CAA-CBA
39	r	318	CHL	CHA-CBD-CGD-O2D
39	s	303	CHL	C2-C3-C5-C6
39	s	313	CHL	C1C-C2C-CMC-OMC
39	s	313	CHL	CBD-CGD-O2D-CED
39	s	316	CHL	C1A-C2A-CAA-CBA
39	s	316	CHL	CBA-CGA-O2A-C1
39	s	316	CHL	O1A-CGA-O2A-C1
39	s	316	CHL	C3C-C2C-CMC-OMC
39	s	316	CHL	C4C-C3C-CAC-CBC
39	s	316	CHL	CBD-CGD-O2D-CED
39	s	316	CHL	O1D-CGD-O2D-CED
39	s	317	CHL	C3A-C2A-CAA-CBA
39	s	317	CHL	C1-C2-C3-C4
39	y	302	CHL	CBD-CGD-O2D-CED
39	y	303	CHL	C2-C3-C5-C6
39	y	303	CHL	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	y	305	CHL	C3C-C2C-CMC-OMC
39	y	312	CHL	C4C-C3C-CAC-CBC
39	y	314	CHL	C3A-C2A-CAA-CBA
39	y	314	CHL	C4C-C3C-CAC-CBC
40	N	305	LUT	C7-C8-C9-C10
40	N	305	LUT	C7-C8-C9-C19
40	S	306	LUT	C7-C8-C9-C19
40	n	317	LUT	C7-C8-C9-C10
40	n	317	LUT	C7-C8-C9-C19
40	s	312	LUT	C7-C8-C9-C10
40	s	312	LUT	C7-C8-C9-C19
42	S	305	NEX	C31-C32-C33-C34
42	S	305	NEX	C31-C32-C33-C40
42	s	302	NEX	C31-C32-C33-C34
42	s	302	NEX	C31-C32-C33-C40
26	C	507	CLA	O1D-CGD-O2D-CED
26	R	307	CLA	O1D-CGD-O2D-CED
26	R	316	CLA	O1D-CGD-O2D-CED
26	a	411	CLA	O1D-CGD-O2D-CED
26	n	304	CLA	O1D-CGD-O2D-CED
26	r	303	CLA	O1D-CGD-O2D-CED
39	G	309	CHL	O1D-CGD-O2D-CED
39	N	311	CHL	O1D-CGD-O2D-CED
39	R	301	CHL	O1D-CGD-O2D-CED
39	g	314	CHL	O1D-CGD-O2D-CED
39	n	307	CHL	O1D-CGD-O2D-CED
39	r	316	CHL	O1D-CGD-O2D-CED
39	s	313	CHL	O1D-CGD-O2D-CED
26	A	403	CLA	O1D-CGD-O2D-CED
26	B	618	CLA	O1D-CGD-O2D-CED
26	D	412	CLA	O1D-CGD-O2D-CED
26	N	313	CLA	O1D-CGD-O2D-CED
26	R	308	CLA	O1D-CGD-O2D-CED
26	c	505	CLA	O1D-CGD-O2D-CED
26	d	411	CLA	O1D-CGD-O2D-CED
26	r	311	CLA	O1D-CGD-O2D-CED
39	Y	318	CHL	O1D-CGD-O2D-CED
39	y	302	CHL	O1D-CGD-O2D-CED
26	A	403	CLA	CBD-CGD-O2D-CED
26	B	607	CLA	CBD-CGD-O2D-CED
26	B	618	CLA	CBD-CGD-O2D-CED
26	C	507	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	N	312	CLA	CBD-CGD-O2D-CED
26	N	313	CLA	CBD-CGD-O2D-CED
26	R	307	CLA	CBD-CGD-O2D-CED
26	S	303	CLA	CBD-CGD-O2D-CED
26	S	310	CLA	CBD-CGD-O2D-CED
26	S	315	CLA	CBD-CGD-O2D-CED
26	Y	313	CLA	CBD-CGD-O2D-CED
26	b	613	CLA	CBD-CGD-O2D-CED
26	b	616	CLA	CBD-CGD-O2D-CED
26	n	304	CLA	CBD-CGD-O2D-CED
26	n	312	CLA	CBD-CGD-O2D-CED
26	r	308	CLA	CBD-CGD-O2D-CED
26	s	306	CLA	CBD-CGD-O2D-CED
26	s	307	CLA	CBD-CGD-O2D-CED
26	y	310	CLA	CBD-CGD-O2D-CED
39	N	311	CHL	CBD-CGD-O2D-CED
39	n	307	CHL	CBD-CGD-O2D-CED
26	G	306	CLA	O1A-CGA-O2A-C1
26	g	305	CLA	O1A-CGA-O2A-C1
37	S	317	LHG	O10-C23-O8-C6
37	s	309	LHG	O10-C23-O8-C6
39	G	318	CHL	O1A-CGA-O2A-C1
26	b	613	CLA	O1D-CGD-O2D-CED
26	n	309	CLA	O1D-CGD-O2D-CED
26	r	308	CLA	O1D-CGD-O2D-CED
26	N	309	CLA	O1D-CGD-O2D-CED
37	S	317	LHG	C24-C23-O8-C6
37	s	309	LHG	C24-C23-O8-C6
26	B	601	CLA	CBD-CGD-O2D-CED
26	B	613	CLA	CBD-CGD-O2D-CED
26	C	512	CLA	CBD-CGD-O2D-CED
26	C	517	CLA	CBD-CGD-O2D-CED
26	C	519	CLA	CBD-CGD-O2D-CED
26	N	308	CLA	CBD-CGD-O2D-CED
26	S	308	CLA	CBD-CGD-O2D-CED
26	Y	312	CLA	CBD-CGD-O2D-CED
26	b	604	CLA	CBD-CGD-O2D-CED
26	b	607	CLA	CBD-CGD-O2D-CED
26	c	510	CLA	CBD-CGD-O2D-CED
26	c	513	CLA	CBD-CGD-O2D-CED
26	s	301	CLA	CBD-CGD-O2D-CED
26	s	310	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	y	316	CLA	CBD-CGD-O2D-CED
39	G	303	CHL	CBD-CGD-O2D-CED
39	r	309	CHL	CBD-CGD-O2D-CED
26	G	304	CLA	O1A-CGA-O2A-C1
26	N	313	CLA	O1A-CGA-O2A-C1
26	R	309	CLA	O1A-CGA-O2A-C1
26	R	314	CLA	O1A-CGA-O2A-C1
26	S	304	CLA	O1A-CGA-O2A-C1
26	S	315	CLA	O1A-CGA-O2A-C1
26	g	318	CLA	O1A-CGA-O2A-C1
26	n	304	CLA	O1A-CGA-O2A-C1
26	r	305	CLA	O1A-CGA-O2A-C1
26	r	317	CLA	O1A-CGA-O2A-C1
26	s	305	CLA	O1A-CGA-O2A-C1
34	C	503	LMG	O10-C28-O8-C9
34	c	512	LMG	O10-C28-O8-C9
37	N	301	LHG	O10-C23-O8-C6
37	n	301	LHG	O10-C23-O8-C6
39	N	311	CHL	O1A-CGA-O2A-C1
39	N	316	CHL	O1A-CGA-O2A-C1
39	n	306	CHL	O1A-CGA-O2A-C1
39	n	307	CHL	O1A-CGA-O2A-C1
26	C	508	CLA	O1D-CGD-O2D-CED
26	c	516	CLA	O1D-CGD-O2D-CED
26	g	317	CLA	O1D-CGD-O2D-CED
26	G	307	CLA	O1D-CGD-O2D-CED
39	G	301	CHL	CBD-CGD-O2D-CED
39	g	307	CHL	CBD-CGD-O2D-CED
39	g	313	CHL	CBD-CGD-O2D-CED
29	A	410	SQD	O49-C7-O47-C45
29	B	621	SQD	O49-C7-O47-C45
29	b	621	SQD	O49-C7-O47-C45
34	W	201	LMG	O9-C10-O7-C8
34	w	201	LMG	O9-C10-O7-C8
26	s	306	CLA	O1A-CGA-O2A-C1
39	S	313	CHL	O1A-CGA-O2A-C1
26	Y	312	CLA	C3-C5-C6-C7
39	G	318	CHL	C3-C5-C6-C7
39	N	303	CHL	C3-C5-C6-C7
39	n	318	CHL	C3-C5-C6-C7
26	G	304	CLA	CBA-CGA-O2A-C1
26	G	306	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	R	314	CLA	CBA-CGA-O2A-C1
26	S	304	CLA	CBA-CGA-O2A-C1
26	g	305	CLA	CBA-CGA-O2A-C1
26	g	318	CLA	CBA-CGA-O2A-C1
26	n	310	CLA	CBA-CGA-O2A-C1
26	r	305	CLA	CBA-CGA-O2A-C1
26	r	317	CLA	CBA-CGA-O2A-C1
26	s	305	CLA	CBA-CGA-O2A-C1
33	y	308	DGD	C2A-C1A-O1G-C1G
34	C	503	LMG	C29-C28-O8-C9
34	c	512	LMG	C29-C28-O8-C9
37	N	301	LHG	C24-C23-O8-C6
37	n	301	LHG	C24-C23-O8-C6
39	N	316	CHL	CBA-CGA-O2A-C1
39	S	313	CHL	CBA-CGA-O2A-C1
39	n	306	CHL	CBA-CGA-O2A-C1
29	A	410	SQD	C8-C7-O47-C45
29	a	413	SQD	C8-C7-O47-C45
26	s	314	CLA	CBD-CGD-O2D-CED
26	B	611	CLA	C4-C3-C5-C6
26	G	307	CLA	C4-C3-C5-C6
26	b	601	CLA	C4-C3-C5-C6
26	b	606	CLA	C4-C3-C5-C6
26	g	317	CLA	C4-C3-C5-C6
39	Y	302	CHL	C4-C3-C5-C6
26	B	606	CLA	C2-C3-C5-C6
26	B	611	CLA	C2-C3-C5-C6
39	g	311	CHL	C2-C3-C5-C6
26	S	311	CLA	CBD-CGD-O2D-CED
26	c	520	CLA	CBD-CGD-O2D-CED
26	n	303	CLA	CBD-CGD-O2D-CED
26	B	610	CLA	C2A-CAA-CBA-CGA
26	G	302	CLA	C2A-CAA-CBA-CGA
26	G	307	CLA	C2A-CAA-CBA-CGA
26	R	314	CLA	C2A-CAA-CBA-CGA
26	b	617	CLA	C2A-CAA-CBA-CGA
26	g	302	CLA	C2A-CAA-CBA-CGA
26	g	317	CLA	C2A-CAA-CBA-CGA
39	R	301	CHL	C2A-CAA-CBA-CGA
39	R	312	CHL	C2A-CAA-CBA-CGA
39	R	318	CHL	C2A-CAA-CBA-CGA
39	Y	318	CHL	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	g	313	CHL	C2A-CAA-CBA-CGA
39	r	309	CHL	C2A-CAA-CBA-CGA
39	r	316	CHL	C2A-CAA-CBA-CGA
39	y	302	CHL	C2A-CAA-CBA-CGA
26	g	302	CLA	O1A-CGA-O2A-C1
26	s	306	CLA	O1D-CGD-O2D-CED
26	B	602	CLA	C3-C5-C6-C7
26	B	605	CLA	C3-C5-C6-C7
26	B	607	CLA	C3-C5-C6-C7
26	b	605	CLA	C3-C5-C6-C7
26	b	608	CLA	C3-C5-C6-C7
26	b	616	CLA	C3-C5-C6-C7
26	y	310	CLA	C3-C5-C6-C7
39	g	311	CHL	C3-C5-C6-C7
26	B	602	CLA	CBA-CGA-O2A-C1
26	N	313	CLA	CBA-CGA-O2A-C1
26	R	309	CLA	CBA-CGA-O2A-C1
26	S	315	CLA	CBA-CGA-O2A-C1
26	b	605	CLA	CBA-CGA-O2A-C1
26	n	304	CLA	CBA-CGA-O2A-C1
26	s	306	CLA	CBA-CGA-O2A-C1
33	Y	303	DGD	C2A-C1A-O1G-C1G
39	G	318	CHL	CBA-CGA-O2A-C1
39	N	311	CHL	CBA-CGA-O2A-C1
39	S	316	CHL	CBA-CGA-O2A-C1
39	g	311	CHL	CBA-CGA-O2A-C1
39	g	319	CHL	CBA-CGA-O2A-C1
39	n	307	CHL	CBA-CGA-O2A-C1
39	s	303	CHL	CBA-CGA-O2A-C1
39	s	317	CHL	CBA-CGA-O2A-C1
33	B	620	DGD	O6D-C5D-C6D-O5D
33	b	620	DGD	O6D-C5D-C6D-O5D
26	S	315	CLA	O1D-CGD-O2D-CED
26	b	616	CLA	O1D-CGD-O2D-CED
26	Y	305	CLA	CBD-CGD-O2D-CED
26	Y	310	CLA	CBD-CGD-O2D-CED
26	y	313	CLA	CBD-CGD-O2D-CED
39	R	312	CHL	CBD-CGD-O2D-CED
26	B	607	CLA	O1D-CGD-O2D-CED
26	Y	313	CLA	O1D-CGD-O2D-CED
26	y	310	CLA	O1D-CGD-O2D-CED
26	B	602	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	G	302	CLA	O1A-CGA-O2A-C1
26	N	319	CLA	O1A-CGA-O2A-C1
26	S	308	CLA	O1A-CGA-O2A-C1
26	b	605	CLA	O1A-CGA-O2A-C1
26	n	310	CLA	O1A-CGA-O2A-C1
26	s	301	CLA	O1A-CGA-O2A-C1
29	B	621	SQD	O10-C23-O48-C46
29	b	621	SQD	O10-C23-O48-C46
33	Y	303	DGD	O1A-C1A-O1G-C1G
39	G	301	CHL	O1A-CGA-O2A-C1
39	G	305	CHL	O1A-CGA-O2A-C1
39	S	316	CHL	O1A-CGA-O2A-C1
39	g	319	CHL	O1A-CGA-O2A-C1
39	s	303	CHL	O1A-CGA-O2A-C1
39	s	317	CHL	O1A-CGA-O2A-C1
26	s	307	CLA	O1D-CGD-O2D-CED
28	T	101	BCR	C19-C20-C21-C22
42	S	305	NEX	C33-C34-C35-C15
42	s	302	NEX	C33-C34-C35-C15
26	B	610	CLA	CBD-CGD-O2D-CED
26	Y	316	CLA	CBD-CGD-O2D-CED
26	b	617	CLA	CBD-CGD-O2D-CED
26	c	515	CLA	CBD-CGD-O2D-CED
26	y	317	CLA	CBD-CGD-O2D-CED
37	G	312	LHG	O2-C2-C3-O3
37	g	301	LHG	O2-C2-C3-O3
37	y	301	LHG	O2-C2-C3-O3
26	B	606	CLA	CBA-CGA-O2A-C1
26	N	319	CLA	CBA-CGA-O2A-C1
26	S	308	CLA	CBA-CGA-O2A-C1
26	b	601	CLA	CBA-CGA-O2A-C1
26	n	312	CLA	CBA-CGA-O2A-C1
26	s	301	CLA	CBA-CGA-O2A-C1
29	B	621	SQD	C24-C23-O48-C46
29	b	621	SQD	C24-C23-O48-C46
39	G	305	CHL	CBA-CGA-O2A-C1
39	G	309	CHL	CBA-CGA-O2A-C1
33	y	308	DGD	O1A-C1A-O1G-C1G
39	g	313	CHL	O1A-CGA-O2A-C1
29	W	202	SQD	C8-C7-O47-C45
29	w	202	SQD	C8-C7-O47-C45
26	B	611	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	C	504	CLA	CBD-CGD-O2D-CED
26	D	406	CLA	CBD-CGD-O2D-CED
26	G	317	CLA	CBD-CGD-O2D-CED
26	G	319	CLA	CBD-CGD-O2D-CED
26	b	606	CLA	CBD-CGD-O2D-CED
26	d	403	CLA	CBD-CGD-O2D-CED
26	g	308	CLA	CBD-CGD-O2D-CED
26	y	309	CLA	CBD-CGD-O2D-CED
26	N	312	CLA	O1D-CGD-O2D-CED
26	b	601	CLA	O1A-CGA-O2A-C1
36	d	406	LMT	O5B-C5B-C6B-O6B
26	S	303	CLA	O1D-CGD-O2D-CED
26	S	310	CLA	O1D-CGD-O2D-CED
33	c	519	DGD	C5B-C6B-C7B-C8B
39	Y	302	CHL	C15-C16-C17-C18
26	G	302	CLA	CBA-CGA-O2A-C1
26	N	308	CLA	CBA-CGA-O2A-C1
26	g	302	CLA	CBA-CGA-O2A-C1
34	C	518	LMG	C29-C28-O8-C9
34	c	509	LMG	C29-C28-O8-C9
39	G	301	CHL	CBA-CGA-O2A-C1
33	Y	303	DGD	O6E-C5E-C6E-O5E
36	D	402	LMT	O5B-C5B-C6B-O6B
29	a	403	SQD	C10-C11-C12-C13
39	s	313	CHL	O1A-CGA-O2A-C1
26	b	606	CLA	C2-C3-C5-C6
26	G	306	CLA	C2A-CAA-CBA-CGA
26	g	305	CLA	C2A-CAA-CBA-CGA
39	G	301	CHL	C2A-CAA-CBA-CGA
39	r	301	CHL	C2A-CAA-CBA-CGA
33	y	308	DGD	O6E-C5E-C6E-O5E
26	n	312	CLA	O1A-CGA-O2A-C1
34	c	509	LMG	O10-C28-O8-C9
39	R	301	CHL	O1A-CGA-O2A-C1
39	r	316	CHL	O1A-CGA-O2A-C1
39	y	303	CHL	C15-C16-C17-C18
26	N	306	CLA	CBA-CGA-O2A-C1
39	g	313	CHL	CBA-CGA-O2A-C1
39	g	314	CHL	CBA-CGA-O2A-C1
26	n	312	CLA	O1D-CGD-O2D-CED
26	s	310	CLA	O1D-CGD-O2D-CED
26	y	316	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	B	606	CLA	O1A-CGA-O2A-C1
26	N	308	CLA	O1A-CGA-O2A-C1
34	C	518	LMG	O10-C28-O8-C9
33	C	510	DGD	C5B-C6B-C7B-C8B
26	N	308	CLA	O1D-CGD-O2D-CED
26	b	607	CLA	O1D-CGD-O2D-CED
33	b	620	DGD	C6B-C7B-C8B-C9B
26	Y	312	CLA	O1D-CGD-O2D-CED
37	G	312	LHG	C1-C2-C3-O3
37	g	301	LHG	C1-C2-C3-O3
26	N	306	CLA	O1A-CGA-O2A-C1
33	B	620	DGD	C6B-C7B-C8B-C9B
26	c	503	CLA	C3-C5-C6-C7
26	n	315	CLA	CBA-CGA-O2A-C1
39	N	304	CHL	CBA-CGA-O2A-C1
39	R	301	CHL	CBA-CGA-O2A-C1
39	n	311	CHL	CBA-CGA-O2A-C1
39	r	316	CHL	CBA-CGA-O2A-C1
39	s	313	CHL	CBA-CGA-O2A-C1
26	Y	301	CLA	CBD-CGD-O2D-CED
26	c	518	CLA	CBD-CGD-O2D-CED
28	t	101	BCR	C15-C16-C17-C18
37	G	312	LHG	C23-C24-C25-C26
37	d	410	LHG	C7-C8-C9-C10
29	A	407	SQD	C10-C11-C12-C13
34	B	622	LMG	C34-C35-C36-C37
27	d	407	PHO	C15-C16-C17-C18
33	C	513	DGD	CAA-CBA-CCA-CDA
37	d	402	LHG	C29-C30-C31-C32
33	c	501	DGD	CAA-CBA-CCA-CDA
26	B	605	CLA	C13-C15-C16-C17
26	C	520	CLA	C8-C10-C11-C12
26	Y	312	CLA	C5-C6-C7-C8
26	b	608	CLA	C13-C15-C16-C17
26	c	506	CLA	C8-C10-C11-C12
26	y	309	CLA	C5-C6-C7-C8
26	y	310	CLA	C5-C6-C7-C8
37	d	402	LHG	C7-C8-C9-C10
29	B	621	SQD	C2-C1-O6-C44
29	W	202	SQD	C2-C1-O6-C44
26	s	304	CLA	CBA-CGA-O2A-C1
26	n	315	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	Y	303	DGD	C4E-C5E-C6E-O5E
33	y	308	DGD	C4E-C5E-C6E-O5E
26	b	601	CLA	C2-C3-C5-C6
26	g	317	CLA	C2-C3-C5-C6
39	Y	302	CHL	C2-C3-C5-C6
26	B	602	CLA	C11-C10-C8-C9
26	B	605	CLA	C14-C13-C15-C16
26	B	612	CLA	C14-C13-C15-C16
26	C	520	CLA	C14-C13-C15-C16
26	Y	301	CLA	C11-C12-C13-C14
26	Y	305	CLA	C14-C13-C15-C16
26	Y	308	CLA	C11-C10-C8-C9
26	Y	313	CLA	C6-C7-C8-C9
26	b	605	CLA	C11-C10-C8-C9
26	b	608	CLA	C14-C13-C15-C16
26	c	503	CLA	C6-C7-C8-C9
26	c	506	CLA	C14-C13-C15-C16
26	y	304	CLA	C11-C12-C13-C14
26	y	306	CLA	C11-C10-C8-C9
26	y	309	CLA	C14-C13-C15-C16
26	y	316	CLA	C6-C7-C8-C9
39	G	318	CHL	C11-C12-C13-C14
39	Y	302	CHL	C11-C10-C8-C9
39	Y	302	CHL	C14-C13-C15-C16
39	Y	307	CHL	C14-C13-C15-C16
39	y	303	CHL	C11-C10-C8-C9
39	y	303	CHL	C11-C12-C13-C14
39	y	303	CHL	C14-C13-C15-C16
39	y	314	CHL	C14-C13-C15-C16
26	B	601	CLA	O1D-CGD-O2D-CED
26	c	510	CLA	O1D-CGD-O2D-CED
26	s	301	CLA	O1D-CGD-O2D-CED
26	C	508	CLA	C13-C15-C16-C17
27	D	403	PHO	C15-C16-C17-C18
28	D	405	BCR	C37-C22-C23-C24
28	J	101	BCR	C7-C8-C9-C34
28	K	101	BCR	C7-C8-C9-C34
28	T	101	BCR	C11-C12-C13-C35
28	T	101	BCR	C36-C18-C19-C20
28	T	101	BCR	C37-C22-C23-C24
28	d	401	BCR	C37-C22-C23-C24
28	j	101	BCR	C7-C8-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	t	101	BCR	C11-C12-C13-C35
28	t	101	BCR	C36-C18-C19-C20
28	t	101	BCR	C37-C22-C23-C24
40	R	311	LUT	C11-C12-C13-C20
40	Y	309	LUT	C7-C8-C9-C19
40	Y	315	LUT	C27-C28-C29-C39
40	r	307	LUT	C11-C12-C13-C20
28	D	405	BCR	C21-C22-C23-C24
28	J	101	BCR	C7-C8-C9-C10
28	T	101	BCR	C17-C18-C19-C20
28	T	101	BCR	C21-C22-C23-C24
28	j	101	BCR	C7-C8-C9-C10
28	t	101	BCR	C17-C18-C19-C20
28	t	101	BCR	C21-C22-C23-C24
29	A	407	SQD	C8-C7-O47-C45
29	a	403	SQD	C8-C7-O47-C45
34	C	518	LMG	C11-C10-O7-C8
34	c	509	LMG	C11-C10-O7-C8
29	A	410	SQD	C12-C13-C14-C15
33	c	501	DGD	C3B-C4B-C5B-C6B
37	D	407	LHG	C29-C30-C31-C32
29	a	403	SQD	C23-C24-C25-C26
33	Y	303	DGD	C1B-C2B-C3B-C4B
37	D	410	LHG	C7-C8-C9-C10
37	g	301	LHG	C23-C24-C25-C26
39	N	304	CHL	O1A-CGA-O2A-C1
26	B	609	CLA	C15-C16-C17-C18
26	c	515	CLA	C13-C15-C16-C17
39	G	318	CHL	C15-C16-C17-C18
26	C	519	CLA	O1D-CGD-O2D-CED
26	B	605	CLA	CBA-CGA-O2A-C1
26	S	309	CLA	CBA-CGA-O2A-C1
26	S	311	CLA	CBA-CGA-O2A-C1
26	c	502	CLA	CBA-CGA-O2A-C1
26	C	506	CLA	C13-C15-C16-C17
26	C	507	CLA	C15-C16-C17-C18
26	C	512	CLA	C13-C15-C16-C17
26	C	516	CLA	C13-C15-C16-C17
26	c	505	CLA	C15-C16-C17-C18
26	c	508	CLA	C13-C15-C16-C17
39	g	311	CHL	C15-C16-C17-C18
29	A	407	SQD	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	C	518	LMG	C10-C11-C12-C13
33	C	513	DGD	C3B-C4B-C5B-C6B
26	B	605	CLA	C8-C10-C11-C12
26	Y	305	CLA	C5-C6-C7-C8
26	Y	312	CLA	C8-C10-C11-C12
26	b	608	CLA	C8-C10-C11-C12
26	b	618	CLA	C15-C16-C17-C18
26	c	516	CLA	C13-C15-C16-C17
26	y	310	CLA	C8-C10-C11-C12
26	S	308	CLA	O1D-CGD-O2D-CED
29	A	407	SQD	C7-C8-C9-C10
29	a	403	SQD	C7-C8-C9-C10
33	Y	303	DGD	C1A-C2A-C3A-C4A
33	y	308	DGD	C1A-C2A-C3A-C4A
34	c	509	LMG	C10-C11-C12-C13
37	D	407	LHG	C23-C24-C25-C26
37	d	402	LHG	C23-C24-C25-C26
26	B	606	CLA	C13-C15-C16-C17
26	B	609	CLA	C13-C15-C16-C17
26	b	601	CLA	C5-C6-C7-C8
26	b	601	CLA	C13-C15-C16-C17
26	b	608	CLA	CBA-CGA-O2A-C1
26	s	314	CLA	CBA-CGA-O2A-C1
26	b	604	CLA	O1D-CGD-O2D-CED
29	W	202	SQD	O49-C7-O47-C45
29	w	202	SQD	O49-C7-O47-C45
39	G	303	CHL	C2-C1-O2A-CGA
39	g	307	CHL	C2-C1-O2A-CGA
39	g	313	CHL	C2-C1-O2A-CGA
26	C	511	CLA	C15-C16-C17-C18
26	c	503	CLA	C15-C16-C17-C18
39	n	318	CHL	C10-C11-C12-C13
33	C	509	DGD	C1A-C2A-C3A-C4A
33	y	308	DGD	C1B-C2B-C3B-C4B
37	D	407	LHG	C7-C8-C9-C10
38	E	101	HEM	C3D-CAD-CBD-CGD
38	e	101	HEM	C3D-CAD-CBD-CGD
29	A	407	SQD	C17-C18-C19-C20
26	B	606	CLA	C5-C6-C7-C8
26	B	613	CLA	C15-C16-C17-C18
26	c	502	CLA	C10-C11-C12-C13
27	D	403	PHO	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	N	303	CHL	C5-C6-C7-C8
26	c	513	CLA	O1D-CGD-O2D-CED
26	B	602	CLA	C12-C13-C15-C16
26	C	506	CLA	C11-C12-C13-C15
26	C	507	CLA	C6-C7-C8-C10
26	Y	305	CLA	C11-C12-C13-C15
26	c	505	CLA	C6-C7-C8-C10
26	y	309	CLA	C11-C12-C13-C15
26	C	506	CLA	CBA-CGA-O2A-C1
26	N	319	CLA	C2A-CAA-CBA-CGA
26	S	304	CLA	C2A-CAA-CBA-CGA
26	s	305	CLA	C2A-CAA-CBA-CGA
39	N	303	CHL	C2A-CAA-CBA-CGA
39	S	316	CHL	C2A-CAA-CBA-CGA
39	n	318	CHL	C2A-CAA-CBA-CGA
26	B	613	CLA	O1D-CGD-O2D-CED
26	C	512	CLA	O1D-CGD-O2D-CED
26	C	517	CLA	O1D-CGD-O2D-CED
26	C	506	CLA	C10-C11-C12-C13
26	b	605	CLA	C15-C16-C17-C18
26	b	618	CLA	C13-C15-C16-C17
39	G	318	CHL	C10-C11-C12-C13
39	Y	302	CHL	C10-C11-C12-C13
39	g	311	CHL	C10-C11-C12-C13
39	S	312	CHL	O1A-CGA-O2A-C1
26	R	313	CLA	CBD-CGD-O2D-CED
26	B	607	CLA	C5-C6-C7-C8
26	B	607	CLA	C8-C10-C11-C12
26	b	613	CLA	C15-C16-C17-C18
39	y	303	CHL	C10-C11-C12-C13
30	A	408	PL9	C9-C11-C12-C13
30	a	407	PL9	C9-C11-C12-C13
33	c	517	DGD	C1A-C2A-C3A-C4A
26	B	618	CLA	C15-C16-C17-C18
26	b	616	CLA	C5-C6-C7-C8
26	b	616	CLA	C8-C10-C11-C12
39	N	303	CHL	C10-C11-C12-C13
39	y	314	CHL	C10-C11-C12-C13
29	A	410	SQD	C24-C23-O48-C46
29	a	413	SQD	C24-C23-O48-C46
26	c	502	CLA	O1A-CGA-O2A-C1
26	B	602	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	B	602	CLA	C15-C16-C17-C18
26	C	507	CLA	C5-C6-C7-C8
26	N	312	CLA	C5-C6-C7-C8
26	R	306	CLA	C5-C6-C7-C8
26	Y	313	CLA	C8-C10-C11-C12
26	b	605	CLA	C5-C6-C7-C8
26	b	610	CLA	C13-C15-C16-C17
26	c	502	CLA	C13-C15-C16-C17
26	c	505	CLA	C5-C6-C7-C8
26	c	506	CLA	C10-C11-C12-C13
39	Y	307	CHL	C10-C11-C12-C13
29	A	410	SQD	C18-C19-C20-C21
29	a	413	SQD	C18-C19-C20-C21
26	S	309	CLA	O1A-CGA-O2A-C1
26	S	311	CLA	O1A-CGA-O2A-C1
26	b	608	CLA	O1A-CGA-O2A-C1
26	s	304	CLA	O1A-CGA-O2A-C1
29	B	621	SQD	C25-C26-C27-C28
29	a	413	SQD	C12-C13-C14-C15
37	D	407	LHG	C27-C28-C29-C30
26	Y	305	CLA	O1D-CGD-O2D-CED
26	B	615	CLA	C5-C6-C7-C8
26	C	520	CLA	C10-C11-C12-C13
26	R	313	CLA	C10-C11-C12-C13
26	b	611	CLA	C5-C6-C7-C8
26	r	306	CLA	C5-C6-C7-C8
26	r	314	CLA	C10-C11-C12-C13
27	d	407	PHO	C13-C15-C16-C17
39	g	311	CHL	C13-C15-C16-C17
37	L	101	LHG	C3-O3-P-O6
37	Y	306	LHG	C4-O6-P-O3
37	d	409	LHG	C3-O3-P-O6
37	l	101	LHG	C3-O3-P-O6
37	y	301	LHG	C4-O6-P-O3
39	R	315	CHL	CBA-CGA-O2A-C1
26	g	304	CLA	CBD-CGD-O2D-CED
26	B	617	CLA	C10-C11-C12-C13
26	D	409	CLA	C13-C15-C16-C17
26	Y	313	CLA	C10-C11-C12-C13
26	y	316	CLA	C10-C11-C12-C13
26	B	605	CLA	O1A-CGA-O2A-C1
39	n	311	CHL	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	s	314	CLA	O1D-CGD-O2D-CED
37	d	409	LHG	C23-C24-C25-C26
37	s	309	LHG	C7-C8-C9-C10
37	Y	306	LHG	C1-C2-C3-O3
37	y	301	LHG	C1-C2-C3-O3
29	A	407	SQD	O49-C7-O47-C45
29	a	403	SQD	O49-C7-O47-C45
34	C	518	LMG	O9-C10-O7-C8
34	c	509	LMG	O9-C10-O7-C8
37	N	301	LHG	O9-C7-O7-C5
29	a	403	SQD	C17-C18-C19-C20
26	R	308	CLA	C2A-CAA-CBA-CGA
26	r	311	CLA	C2A-CAA-CBA-CGA
39	N	304	CHL	C2A-CAA-CBA-CGA
39	s	303	CHL	C2A-CAA-CBA-CGA
26	B	610	CLA	C16-C17-C18-C20
26	c	515	CLA	CBA-CGA-O2A-C1
39	S	312	CHL	CBA-CGA-O2A-C1
39	r	318	CHL	CBA-CGA-O2A-C1
26	B	616	CLA	C10-C11-C12-C13
34	b	622	LMG	C34-C35-C36-C37
37	R	303	LHG	C11-C12-C13-C14
28	T	101	BCR	C15-C16-C17-C18
34	B	622	LMG	C39-C40-C41-C42
34	c	509	LMG	C13-C14-C15-C16
37	g	301	LHG	C34-C35-C36-C37
26	S	311	CLA	O1D-CGD-O2D-CED
34	c	512	LMG	C11-C10-O7-C8
37	N	301	LHG	C8-C7-O7-C5
37	n	301	LHG	C8-C7-O7-C5
39	y	314	CHL	C8-C10-C11-C12
29	A	410	SQD	C26-C27-C28-C29
29	a	403	SQD	C15-C16-C17-C18
33	C	510	DGD	C7B-C8B-C9B-CAB
34	B	622	LMG	C35-C36-C37-C38
34	C	503	LMG	C17-C18-C19-C20
34	C	518	LMG	C13-C14-C15-C16
34	W	201	LMG	C29-C30-C31-C32
34	W	201	LMG	C39-C40-C41-C42
34	c	512	LMG	C17-C18-C19-C20
34	w	201	LMG	C29-C30-C31-C32
34	w	201	LMG	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	G	312	LHG	C34-C35-C36-C37
37	Y	306	LHG	C24-C25-C26-C27
37	y	301	LHG	C24-C25-C26-C27
26	a	411	CLA	C16-C17-C18-C19
26	b	617	CLA	C16-C17-C18-C20
27	A	404	PHO	C16-C17-C18-C20
27	a	410	PHO	C16-C17-C18-C20
26	C	512	CLA	CBA-CGA-O2A-C1
29	A	407	SQD	C15-C16-C17-C18
29	a	413	SQD	C25-C26-C27-C28
34	b	622	LMG	C38-C39-C40-C41
37	l	101	LHG	C16-C17-C18-C19
29	a	413	SQD	C46-C45-O47-C7
26	c	520	CLA	O1D-CGD-O2D-CED
26	n	303	CLA	O1D-CGD-O2D-CED
34	c	512	LMG	O9-C10-O7-C8
37	n	301	LHG	O9-C7-O7-C5
39	Y	307	CHL	C8-C10-C11-C12
39	n	318	CHL	C5-C6-C7-C8
34	C	518	LMG	C28-C29-C30-C31
33	c	519	DGD	C7B-C8B-C9B-CAB
34	B	622	LMG	C38-C39-C40-C41
34	D	404	LMG	C12-C13-C14-C15
34	D	404	LMG	C15-C16-C17-C18
37	L	101	LHG	C10-C11-C12-C13
26	C	506	CLA	O1A-CGA-O2A-C1
26	s	314	CLA	O1A-CGA-O2A-C1
33	C	510	DGD	C6B-C7B-C8B-C9B
33	C	513	DGD	CCB-CDB-CEB-CFB
34	D	404	LMG	C30-C31-C32-C33
34	d	405	LMG	C15-C16-C17-C18
37	D	407	LHG	C25-C26-C27-C28
37	d	402	LHG	C32-C33-C34-C35
33	c	501	DGD	CBB-CCB-CDB-CEB
34	B	622	LMG	C19-C20-C21-C22
34	d	405	LMG	C12-C13-C14-C15
34	c	509	LMG	C28-C29-C30-C31
37	n	301	LHG	C23-C24-C25-C26
26	y	313	CLA	O1D-CGD-O2D-CED
39	r	309	CHL	O1D-CGD-O2D-CED
29	b	621	SQD	C2-C1-O6-C44
33	C	510	DGD	C2E-C1E-O5D-C6D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	c	519	DGD	C2E-C1E-O5D-C6D
26	G	313	CLA	CBA-CGA-O2A-C1
26	g	315	CLA	CBA-CGA-O2A-C1
33	b	620	DGD	C7B-C8B-C9B-CAB
33	c	501	DGD	C7A-C8A-C9A-CAA
34	W	201	LMG	C12-C13-C14-C15
37	D	407	LHG	C32-C33-C34-C35
26	n	303	CLA	C8-C10-C11-C12
39	G	309	CHL	O1A-CGA-O2A-C1
26	A	403	CLA	C16-C17-C18-C19
26	Y	301	CLA	C16-C17-C18-C19
26	Y	310	CLA	O1D-CGD-O2D-CED
29	a	413	SQD	C26-C27-C28-C29
33	B	620	DGD	C7B-C8B-C9B-CAB
33	C	513	DGD	CBB-CCB-CDB-CEB
33	c	501	DGD	CCB-CDB-CEB-CFB
33	y	308	DGD	C3B-C4B-C5B-C6B
34	c	512	LMG	C11-C12-C13-C14
34	w	201	LMG	C12-C13-C14-C15
37	d	402	LHG	C33-C34-C35-C36
30	d	408	PL9	C13-C14-C16-C17
39	Y	307	CHL	C2-C3-C5-C6
39	y	314	CHL	C2-C3-C5-C6
26	Y	308	CLA	C6-C7-C8-C9
26	b	614	CLA	C14-C13-C15-C16
26	b	616	CLA	C11-C10-C8-C9
26	c	502	CLA	C11-C12-C13-C14
26	n	305	CLA	C14-C13-C15-C16
26	y	316	CLA	C11-C12-C13-C14
27	A	404	PHO	C11-C10-C8-C9
27	a	410	PHO	C11-C10-C8-C9
39	Y	302	CHL	C11-C12-C13-C14
39	g	311	CHL	C11-C12-C13-C14
29	A	407	SQD	C27-C28-C29-C30
29	A	410	SQD	C25-C26-C27-C28
29	a	403	SQD	C27-C28-C29-C30
33	C	513	DGD	C7A-C8A-C9A-CAA
33	Y	303	DGD	C3B-C4B-C5B-C6B
34	C	518	LMG	C31-C32-C33-C34
34	b	622	LMG	C35-C36-C37-C38
37	l	101	LHG	C10-C11-C12-C13
26	d	404	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	C	509	DGD	O6E-C5E-C6E-O5E
29	A	410	SQD	O10-C23-O48-C46
28	J	101	BCR	C37-C22-C23-C24
28	k	101	BCR	C7-C8-C9-C34
28	t	101	BCR	C7-C8-C9-C34
33	C	510	DGD	C9A-CAA-CBA-CCA
33	c	519	DGD	C9A-CAA-CBA-CCA
34	C	503	LMG	C11-C12-C13-C14
34	b	622	LMG	C39-C40-C41-C42
37	D	407	LHG	C28-C29-C30-C31
37	D	410	LHG	O1-C1-C2-C3
37	Y	306	LHG	O1-C1-C2-C3
37	d	410	LHG	O1-C1-C2-C3
37	y	301	LHG	O1-C1-C2-C3
28	J	101	BCR	C21-C22-C23-C24
28	K	101	BCR	C7-C8-C9-C10
28	d	401	BCR	C21-C22-C23-C24
28	j	101	BCR	C21-C22-C23-C24
28	k	101	BCR	C7-C8-C9-C10
28	t	101	BCR	C7-C8-C9-C10
34	C	503	LMG	O9-C10-O7-C8
33	Y	303	DGD	C2B-C1B-O2G-C2G
34	C	503	LMG	C11-C10-O7-C8
33	c	519	DGD	C6B-C7B-C8B-C9B
37	G	312	LHG	C25-C26-C27-C28
26	C	505	CLA	CBD-CGD-O2D-CED
37	N	301	LHG	C23-C24-C25-C26
33	B	620	DGD	CBB-CCB-CDB-CEB
34	d	405	LMG	C30-C31-C32-C33
37	D	407	LHG	C33-C34-C35-C36
37	d	402	LHG	C25-C26-C27-C28
37	d	402	LHG	C28-C29-C30-C31
37	g	301	LHG	C25-C26-C27-C28
33	c	517	DGD	O6E-C5E-C6E-O5E
26	G	313	CLA	C4B-C3B-CAB-CBB
26	G	319	CLA	C4B-C3B-CAB-CBB
26	N	309	CLA	C4B-C3B-CAB-CBB
26	R	302	CLA	C4B-C3B-CAB-CBB
26	R	309	CLA	C4B-C3B-CAB-CBB
26	R	314	CLA	C4B-C3B-CAB-CBB
26	Y	301	CLA	C4B-C3B-CAB-CBB
26	c	505	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	g	315	CLA	C4B-C3B-CAB-CBB
26	n	309	CLA	C4B-C3B-CAB-CBB
26	r	305	CLA	C4B-C3B-CAB-CBB
26	r	313	CLA	C4B-C3B-CAB-CBB
26	r	317	CLA	C4B-C3B-CAB-CBB
26	B	610	CLA	C16-C17-C18-C19
26	B	611	CLA	C16-C17-C18-C20
26	y	316	CLA	C8-C10-C11-C12
26	y	317	CLA	O1D-CGD-O2D-CED
29	A	407	SQD	C25-C26-C27-C28
29	b	621	SQD	C25-C26-C27-C28
33	c	501	DGD	C9B-CAB-CBB-CCB
34	b	622	LMG	C19-C20-C21-C22
26	C	521	CLA	CBD-CGD-O2D-CED
26	c	514	CLA	CBD-CGD-O2D-CED
33	B	620	DGD	CBA-CCA-CDA-CEA
33	C	513	DGD	C9B-CAB-CBB-CCB
33	b	620	DGD	CBB-CCB-CDB-CEB
34	C	518	LMG	C19-C20-C21-C22
34	c	512	LMG	C10-C11-C12-C13
26	b	605	CLA	C13-C15-C16-C17
39	g	314	CHL	O1A-CGA-O2A-C1
29	a	403	SQD	C25-C26-C27-C28
33	b	620	DGD	CBA-CCA-CDA-CEA
34	B	622	LMG	C37-C38-C39-C40
26	r	314	CLA	CBA-CGA-O2A-C1
29	B	621	SQD	C13-C14-C15-C16
34	c	509	LMG	C19-C20-C21-C22
34	c	509	LMG	C31-C32-C33-C34
34	w	201	LMG	C30-C31-C32-C33
26	B	615	CLA	C3A-C2A-CAA-CBA
26	G	302	CLA	C3A-C2A-CAA-CBA
26	G	307	CLA	C3A-C2A-CAA-CBA
26	G	317	CLA	C3A-C2A-CAA-CBA
26	N	306	CLA	C3A-C2A-CAA-CBA
26	R	302	CLA	C3A-C2A-CAA-CBA
26	R	308	CLA	C3A-C2A-CAA-CBA
26	S	309	CLA	C3A-C2A-CAA-CBA
26	Y	310	CLA	C3A-C2A-CAA-CBA
26	b	611	CLA	C3A-C2A-CAA-CBA
26	g	302	CLA	C3A-C2A-CAA-CBA
26	g	308	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	n	315	CLA	C3A-C2A-CAA-CBA
26	r	311	CLA	C3A-C2A-CAA-CBA
26	r	313	CLA	C3A-C2A-CAA-CBA
26	s	304	CLA	C3A-C2A-CAA-CBA
26	y	317	CLA	C3A-C2A-CAA-CBA
39	G	303	CHL	C3A-C2A-CAA-CBA
39	R	301	CHL	C3A-C2A-CAA-CBA
39	S	302	CHL	C3A-C2A-CAA-CBA
39	g	307	CHL	C3A-C2A-CAA-CBA
39	g	313	CHL	C3A-C2A-CAA-CBA
39	r	301	CHL	C3A-C2A-CAA-CBA
39	r	316	CHL	C3A-C2A-CAA-CBA
39	s	316	CHL	C3A-C2A-CAA-CBA
39	y	302	CHL	C3A-C2A-CAA-CBA
26	B	602	CLA	C13-C15-C16-C17
40	g	310	LUT	C29-C30-C31-C32
37	n	301	LHG	C12-C13-C14-C15
26	c	515	CLA	O1D-CGD-O2D-CED
26	D	409	CLA	C16-C17-C18-C20
26	b	606	CLA	C16-C17-C18-C20
26	b	617	CLA	C16-C17-C18-C19
29	a	413	SQD	C28-C29-C30-C31
33	C	513	DGD	C8A-C9A-CAA-CBA
33	C	513	DGD	CAB-CBB-CCB-CDB
33	c	501	DGD	C8A-C9A-CAA-CBA
34	W	201	LMG	C30-C31-C32-C33
34	b	622	LMG	C13-C14-C15-C16
37	L	101	LHG	C16-C17-C18-C19
37	N	301	LHG	C12-C13-C14-C15
37	Y	306	LHG	C18-C19-C20-C21
33	c	501	DGD	CAB-CBB-CCB-CDB
26	B	606	CLA	O2A-C1-C2-C3
26	y	309	CLA	O1D-CGD-O2D-CED
29	a	413	SQD	O10-C23-O48-C46
26	Y	312	CLA	C4-C3-C5-C6
26	y	310	CLA	C4-C3-C5-C6
30	D	411	PL9	C15-C14-C16-C17
39	n	318	CHL	C4-C3-C5-C6
36	d	406	LMT	C4B-C5B-C6B-O6B
26	G	307	CLA	C2-C3-C5-C6
26	Y	312	CLA	C2-C3-C5-C6
26	y	310	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	y	308	DGD	C2B-C1B-O2G-C2G
37	y	301	LHG	C34-C35-C36-C37
37	S	317	LHG	C10-C11-C12-C13
37	Y	306	LHG	C34-C35-C36-C37
37	s	309	LHG	C10-C11-C12-C13
37	y	301	LHG	C18-C19-C20-C21
26	Y	316	CLA	O1D-CGD-O2D-CED
26	c	515	CLA	O1A-CGA-O2A-C1
26	a	411	CLA	C16-C17-C18-C20
26	y	304	CLA	C16-C17-C18-C19
26	G	313	CLA	C2B-C3B-CAB-CBB
26	G	317	CLA	C2B-C3B-CAB-CBB
26	G	319	CLA	C2B-C3B-CAB-CBB
26	N	309	CLA	C2B-C3B-CAB-CBB
26	R	302	CLA	C2B-C3B-CAB-CBB
26	R	307	CLA	C2B-C3B-CAB-CBB
26	R	309	CLA	C2B-C3B-CAB-CBB
26	R	314	CLA	C2B-C3B-CAB-CBB
26	Y	301	CLA	C2B-C3B-CAB-CBB
26	Y	310	CLA	C2B-C3B-CAB-CBB
26	b	609	CLA	C2B-C3B-CAB-CBB
26	g	304	CLA	C2B-C3B-CAB-CBB
26	g	315	CLA	C2B-C3B-CAB-CBB
26	n	309	CLA	C2B-C3B-CAB-CBB
26	r	305	CLA	C2B-C3B-CAB-CBB
26	r	313	CLA	C2B-C3B-CAB-CBB
26	r	317	CLA	C2B-C3B-CAB-CBB
26	y	304	CLA	C2B-C3B-CAB-CBB
26	y	317	CLA	C2B-C3B-CAB-CBB
34	W	201	LMG	C38-C39-C40-C41
26	C	512	CLA	O1A-CGA-O2A-C1
34	B	622	LMG	C13-C14-C15-C16
34	b	622	LMG	C37-C38-C39-C40
33	Y	303	DGD	O1B-C1B-O2G-C2G
33	y	308	DGD	O1B-C1B-O2G-C2G
26	G	313	CLA	C2-C1-O2A-CGA
26	R	314	CLA	C2-C1-O2A-CGA
26	g	315	CLA	C2-C1-O2A-CGA
26	r	317	CLA	C2-C1-O2A-CGA
39	r	318	CHL	C2-C1-O2A-CGA
36	D	402	LMT	C4B-C5B-C6B-O6B
34	B	622	LMG	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	c	512	LMG	C21-C22-C23-C24
37	g	301	LHG	C17-C18-C19-C20
26	g	315	CLA	O1A-CGA-O2A-C1
33	c	519	DGD	C5A-C6A-C7A-C8A
34	d	405	LMG	C13-C14-C15-C16
37	y	301	LHG	C33-C34-C35-C36
27	A	404	PHO	C16-C17-C18-C19
27	a	410	PHO	C16-C17-C18-C19
34	b	622	LMG	C28-C29-C30-C31
26	r	314	CLA	CBD-CGD-O2D-CED
28	A	406	BCR	C23-C24-C25-C26
28	B	614	BCR	C1-C6-C7-C8
28	B	614	BCR	C23-C24-C25-C26
28	C	514	BCR	C1-C6-C7-C8
28	C	514	BCR	C5-C6-C7-C8
28	D	405	BCR	C1-C6-C7-C8
28	D	405	BCR	C23-C24-C25-C26
28	H	101	BCR	C23-C24-C25-C26
28	J	101	BCR	C23-C24-C25-C26
28	T	101	BCR	C5-C6-C7-C8
28	a	404	BCR	C23-C24-C25-C30
28	b	619	BCR	C1-C6-C7-C8
28	b	619	BCR	C23-C24-C25-C26
28	c	507	BCR	C5-C6-C7-C8
28	d	401	BCR	C1-C6-C7-C8
28	d	401	BCR	C23-C24-C25-C26
28	h	101	BCR	C23-C24-C25-C26
28	j	101	BCR	C23-C24-C25-C26
28	t	101	BCR	C5-C6-C7-C8
26	R	313	CLA	CBA-CGA-O2A-C1
39	G	311	CHL	CBA-CGA-O2A-C1
39	g	312	CHL	CBA-CGA-O2A-C1
26	b	604	CLA	C15-C16-C17-C18
26	n	303	CLA	C5-C6-C7-C8
39	G	318	CHL	C13-C15-C16-C17
37	L	101	LHG	C11-C10-C9-C8
37	S	317	LHG	C25-C26-C27-C28
37	r	312	LHG	C25-C26-C27-C28
26	G	313	CLA	O1A-CGA-O2A-C1
33	b	620	DGD	CAB-CBB-CCB-CDB
37	G	312	LHG	C17-C18-C19-C20
37	R	303	LHG	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	D	406	CLA	O1D-CGD-O2D-CED
33	C	510	DGD	C5A-C6A-C7A-C8A
37	Y	306	LHG	C33-C34-C35-C36
39	Y	307	CHL	C4-C3-C5-C6
26	B	610	CLA	O1D-CGD-O2D-CED
26	b	617	CLA	O1D-CGD-O2D-CED
26	B	618	CLA	C11-C12-C13-C15
26	Y	308	CLA	C6-C7-C8-C10
26	Y	308	CLA	C11-C10-C8-C7
26	Y	313	CLA	C11-C12-C13-C15
26	b	605	CLA	C12-C13-C15-C16
26	b	613	CLA	C11-C12-C13-C15
26	c	504	CLA	C11-C12-C13-C15
26	d	403	CLA	C11-C12-C13-C15
26	y	306	CLA	C6-C7-C8-C10
26	y	316	CLA	C11-C12-C13-C15
27	A	404	PHO	C11-C10-C8-C7
27	D	403	PHO	C11-C10-C8-C7
27	D	403	PHO	C11-C12-C13-C15
27	a	410	PHO	C11-C10-C8-C7
27	d	407	PHO	C11-C10-C8-C7
27	d	407	PHO	C11-C12-C13-C15
39	N	303	CHL	C2-C3-C5-C6
39	g	311	CHL	C12-C13-C15-C16
39	n	318	CHL	C2-C3-C5-C6
26	r	314	CLA	O1A-CGA-O2A-C1
33	B	620	DGD	CAB-CBB-CCB-CDB
34	D	404	LMG	C13-C14-C15-C16
34	w	201	LMG	C38-C39-C40-C41
26	B	617	CLA	C13-C15-C16-C17
26	b	609	CLA	C10-C11-C12-C13
28	H	101	BCR	C9-C10-C11-C12
28	T	101	BCR	C9-C10-C11-C12
28	t	101	BCR	C9-C10-C11-C12
26	A	403	CLA	C16-C17-C18-C20
26	C	507	CLA	C16-C17-C18-C20
26	Y	301	CLA	C16-C17-C18-C20
26	c	505	CLA	C16-C17-C18-C20
26	y	316	CLA	C16-C17-C18-C20
34	C	503	LMG	C10-C11-C12-C13
26	C	521	CLA	CBA-CGA-O2A-C1
26	D	406	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	c	514	CLA	CBA-CGA-O2A-C1
26	d	403	CLA	CBA-CGA-O2A-C1
29	A	410	SQD	C28-C29-C30-C31
37	s	309	LHG	C25-C26-C27-C28
37	y	301	LHG	C11-C10-C9-C8
26	B	615	CLA	C2A-CAA-CBA-CGA
26	b	611	CLA	C2A-CAA-CBA-CGA
26	n	310	CLA	C2A-CAA-CBA-CGA
39	N	311	CHL	C2A-CAA-CBA-CGA
39	n	307	CHL	C2A-CAA-CBA-CGA
26	G	314	CLA	C10-C11-C12-C13
26	c	508	CLA	C15-C16-C17-C18
34	w	201	LMG	C31-C32-C33-C34
26	d	403	CLA	O1D-CGD-O2D-CED
26	g	308	CLA	O1D-CGD-O2D-CED
37	G	312	LHG	C7-C8-C9-C10
26	G	317	CLA	O1D-CGD-O2D-CED
26	b	618	CLA	C10-C11-C12-C13
37	R	303	LHG	C25-C26-C27-C28
37	d	402	LHG	C10-C11-C12-C13
26	c	518	CLA	CBA-CGA-O2A-C1
26	r	303	CLA	CBA-CGA-O2A-C1
33	C	510	DGD	O6E-C1E-O5D-C6D
33	c	519	DGD	O6E-C1E-O5D-C6D
26	C	516	CLA	C15-C16-C17-C18
26	c	520	CLA	C15-C16-C17-C18
26	y	309	CLA	C15-C16-C17-C18
29	A	410	SQD	C24-C25-C26-C27
33	C	510	DGD	CCB-CDB-CEB-CFB
37	Y	306	LHG	C26-C27-C28-C29
37	y	301	LHG	C26-C27-C28-C29
33	c	517	DGD	C2B-C1B-O2G-C2G
37	Y	306	LHG	C8-C7-O7-C5
37	y	301	LHG	C8-C7-O7-C5
34	C	518	LMG	C30-C31-C32-C33
37	D	407	LHG	C10-C11-C12-C13
37	l	101	LHG	C11-C10-C9-C8
37	Y	306	LHG	O9-C7-O7-C5
37	y	301	LHG	O9-C7-O7-C5
33	Y	303	DGD	O2G-C2G-C3G-O3G
33	y	308	DGD	O2G-C2G-C3G-O3G
33	b	620	DGD	O6E-C5E-C6E-O5E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	R	303	LHG	C24-C23-O8-C6
29	A	407	SQD	C31-C32-C33-C34
29	b	621	SQD	C31-C32-C33-C34
34	c	509	LMG	C30-C31-C32-C33
26	Y	313	CLA	C16-C17-C18-C20
26	r	306	CLA	C16-C17-C18-C20
29	a	403	SQD	C31-C32-C33-C34
37	Y	306	LHG	C11-C10-C9-C8
34	D	404	LMG	O6-C5-C6-O5
34	d	405	LMG	O6-C5-C6-O5
26	A	403	CLA	C15-C16-C17-C18
26	a	411	CLA	C13-C15-C16-C17
26	G	319	CLA	O1D-CGD-O2D-CED
26	y	306	CLA	C4-C3-C5-C6
27	A	404	PHO	C4-C3-C5-C6
27	a	410	PHO	C4-C3-C5-C6
39	G	318	CHL	C4-C3-C5-C6
39	y	314	CHL	C4-C3-C5-C6
30	D	411	PL9	C13-C14-C16-C17
26	B	602	CLA	C14-C13-C15-C16
26	B	604	CLA	C14-C13-C15-C16
26	B	607	CLA	C6-C7-C8-C9
26	B	607	CLA	C11-C10-C8-C9
26	B	610	CLA	C14-C13-C15-C16
26	B	618	CLA	C11-C12-C13-C14
26	C	506	CLA	C11-C12-C13-C14
26	N	307	CLA	C14-C13-C15-C16
26	Y	313	CLA	C11-C12-C13-C14
26	b	605	CLA	C14-C13-C15-C16
26	b	613	CLA	C11-C12-C13-C14
26	b	616	CLA	C6-C7-C8-C9
26	b	617	CLA	C14-C13-C15-C16
26	g	317	CLA	C14-C13-C15-C16
26	y	306	CLA	C6-C7-C8-C9
27	D	403	PHO	C11-C10-C8-C9
27	d	407	PHO	C11-C10-C8-C9
39	G	318	CHL	C14-C13-C15-C16
39	g	311	CHL	C14-C13-C15-C16
26	D	406	CLA	C3-C5-C6-C7
26	R	307	CLA	C2A-CAA-CBA-CGA
26	R	309	CLA	C2A-CAA-CBA-CGA
26	r	305	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	r	318	CHL	C2A-CAA-CBA-CGA
29	B	621	SQD	C30-C31-C32-C33
34	C	518	LMG	C18-C19-C20-C21
33	B	620	DGD	O6E-C5E-C6E-O5E
28	T	101	BCR	C7-C8-C9-C34
28	j	101	BCR	C37-C22-C23-C24
26	N	312	CLA	C8-C10-C11-C12
26	a	411	CLA	C15-C16-C17-C18
29	a	413	SQD	C24-C25-C26-C27
28	T	101	BCR	C7-C8-C9-C10
40	S	306	LUT	C7-C8-C9-C10
26	R	313	CLA	O1A-CGA-O2A-C1
26	C	507	CLA	C1A-C2A-CAA-CBA
26	C	517	CLA	C1A-C2A-CAA-CBA
26	D	401	CLA	C1A-C2A-CAA-CBA
26	D	412	CLA	C1A-C2A-CAA-CBA
26	G	317	CLA	C1A-C2A-CAA-CBA
26	N	306	CLA	C1A-C2A-CAA-CBA
26	N	312	CLA	C1A-C2A-CAA-CBA
26	R	302	CLA	C1A-C2A-CAA-CBA
26	R	314	CLA	C1A-C2A-CAA-CBA
26	a	409	CLA	C1A-C2A-CAA-CBA
26	b	604	CLA	C1A-C2A-CAA-CBA
26	c	505	CLA	C1A-C2A-CAA-CBA
26	c	513	CLA	C1A-C2A-CAA-CBA
26	d	411	CLA	C1A-C2A-CAA-CBA
26	g	308	CLA	C1A-C2A-CAA-CBA
26	n	303	CLA	C1A-C2A-CAA-CBA
26	n	315	CLA	C1A-C2A-CAA-CBA
26	r	313	CLA	C1A-C2A-CAA-CBA
26	r	317	CLA	C1A-C2A-CAA-CBA
26	y	304	CLA	C16-C17-C18-C20
33	C	509	DGD	C2B-C1B-O2G-C2G
34	c	509	LMG	C18-C19-C20-C21
28	h	101	BCR	C9-C10-C11-C12
40	G	308	LUT	C29-C30-C31-C32
40	y	318	LUT	C29-C30-C31-C32
26	A	403	CLA	C13-C15-C16-C17
34	b	622	LMG	C16-C17-C18-C19
26	B	610	CLA	C3-C5-C6-C7
26	C	504	CLA	O1D-CGD-O2D-CED
26	B	616	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	N	307	CLA	C15-C16-C17-C18
26	b	609	CLA	C13-C15-C16-C17
37	S	317	LHG	O6-C4-C5-C6
26	B	611	CLA	O1D-CGD-O2D-CED
26	b	606	CLA	O1D-CGD-O2D-CED
37	G	312	LHG	C15-C16-C17-C18
26	b	610	CLA	C10-C11-C12-C13
29	B	621	SQD	C14-C15-C16-C17
34	c	509	LMG	C29-C30-C31-C32
39	g	311	CHL	C4-C3-C5-C6
29	b	621	SQD	C30-C31-C32-C33
34	C	518	LMG	C29-C30-C31-C32
34	C	518	LMG	C39-C40-C41-C42
26	C	521	CLA	O1A-CGA-O2A-C1
26	c	514	CLA	O1A-CGA-O2A-C1
26	d	403	CLA	O1A-CGA-O2A-C1
26	r	308	CLA	C2A-CAA-CBA-CGA
26	R	306	CLA	C16-C17-C18-C20
29	W	202	SQD	O6-C44-C45-C46
33	Y	303	DGD	C1G-C2G-C3G-O3G
34	W	201	LMG	C31-C32-C33-C34
37	s	309	LHG	C12-C13-C14-C15
36	d	406	LMT	C1-C2-C3-C4
33	c	517	DGD	CDB-CEB-CFB-CGB
26	D	406	CLA	O1A-CGA-O2A-C1
33	C	510	DGD	C2G-C3G-O3G-C1D
33	C	510	DGD	C5D-C6D-O5D-C1E
33	c	519	DGD	C2G-C3G-O3G-C1D
33	c	519	DGD	C5D-C6D-O5D-C1E
34	C	503	LMG	C8-C7-O1-C1
33	C	509	DGD	C2B-C3B-C4B-C5B
33	c	517	DGD	C2B-C3B-C4B-C5B
26	Y	305	CLA	C15-C16-C17-C18
29	b	621	SQD	C13-C14-C15-C16
34	c	509	LMG	C39-C40-C41-C42
37	d	402	LHG	C26-C27-C28-C29
33	B	620	DGD	O2G-C1B-C2B-C3B
33	C	513	DGD	O6E-C5E-C6E-O5E
37	Y	306	LHG	C7-C8-C9-C10
37	y	301	LHG	C7-C8-C9-C10
33	C	509	DGD	CDB-CEB-CFB-CGB
37	D	408	LHG	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	c	501	DGD	O6E-C5E-C6E-O5E
37	Y	306	LHG	O1-C1-C2-O2
37	y	301	LHG	O1-C1-C2-O2
33	B	620	DGD	CDB-CEB-CFB-CGB
33	c	519	DGD	CDB-CEB-CFB-CGB
37	d	410	LHG	C29-C30-C31-C32
26	r	303	CLA	O1A-CGA-O2A-C1
26	b	616	CLA	C4-C3-C5-C6
30	d	408	PL9	C15-C14-C16-C17
33	b	620	DGD	CDB-CEB-CFB-CGB
26	b	616	CLA	C2-C3-C5-C6
26	C	504	CLA	CBA-CGA-O2A-C1
26	Y	310	CLA	CBA-CGA-O2A-C1
37	r	312	LHG	C24-C23-O8-C6
39	N	317	CHL	CBA-CGA-O2A-C1
33	C	510	DGD	CDB-CEB-CFB-CGB
26	y	304	CLA	C15-C16-C17-C18
29	A	410	SQD	C46-C45-O47-C7
29	w	202	SQD	C46-C45-O47-C7
39	n	311	CHL	C2A-CAA-CBA-CGA
39	R	315	CHL	C2-C1-O2A-CGA
37	S	317	LHG	C12-C13-C14-C15
26	c	518	CLA	O1D-CGD-O2D-CED
37	D	410	LHG	C29-C30-C31-C32
26	B	609	CLA	C10-C11-C12-C13
26	Y	313	CLA	C15-C16-C17-C18
34	B	622	LMG	C22-C23-C24-C25
26	y	317	CLA	CBA-CGA-O2A-C1
26	c	518	CLA	O1A-CGA-O2A-C1
26	d	404	CLA	C16-C17-C18-C20
34	B	622	LMG	C30-C31-C32-C33
34	c	512	LMG	C16-C17-C18-C19
37	y	301	LHG	C12-C13-C14-C15
26	Y	301	CLA	O1D-CGD-O2D-CED
37	R	303	LHG	O10-C23-O8-C6
37	D	410	LHG	C11-C10-C9-C8
37	S	317	LHG	C7-C8-C9-C10
33	b	620	DGD	O2G-C1B-C2B-C3B
36	D	402	LMT	C1-C2-C3-C4
29	A	410	SQD	O6-C44-C45-O47
29	B	621	SQD	O47-C45-C46-O48
29	a	413	SQD	O6-C44-C45-O47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	b	621	SQD	O47-C45-C46-O48
29	B	621	SQD	C31-C32-C33-C34
26	Y	301	CLA	C15-C16-C17-C18
26	r	306	CLA	C16-C17-C18-C19
39	G	311	CHL	CHA-CBD-CGD-O1D
39	G	311	CHL	CHA-CBD-CGD-O2D
39	G	318	CHL	CHA-CBD-CGD-O1D
39	R	301	CHL	CHA-CBD-CGD-O1D
39	R	301	CHL	CHA-CBD-CGD-O2D
39	R	315	CHL	CHA-CBD-CGD-O2D
39	g	311	CHL	CHA-CBD-CGD-O1D
39	n	319	CHL	CHA-CBD-CGD-O2D
39	r	316	CHL	CHA-CBD-CGD-O1D
39	r	316	CHL	CHA-CBD-CGD-O2D
26	B	607	CLA	C4-C3-C5-C6
26	Y	308	CLA	C4-C3-C5-C6
26	A	405	CLA	C11-C10-C8-C7
26	B	601	CLA	C11-C12-C13-C15
26	B	605	CLA	C11-C12-C13-C15
26	B	605	CLA	C12-C13-C15-C16
26	B	610	CLA	C12-C13-C15-C16
26	B	615	CLA	C6-C7-C8-C10
26	C	515	CLA	C6-C7-C8-C10
26	C	515	CLA	C11-C12-C13-C15
26	D	406	CLA	C11-C12-C13-C15
26	G	307	CLA	C12-C13-C15-C16
26	G	314	CLA	C11-C10-C8-C7
26	N	312	CLA	C11-C10-C8-C7
26	Y	308	CLA	C11-C12-C13-C15
26	a	402	CLA	C11-C10-C8-C7
26	b	607	CLA	C11-C12-C13-C15
26	b	608	CLA	C11-C12-C13-C15
26	b	608	CLA	C12-C13-C15-C16
26	b	611	CLA	C6-C7-C8-C10
26	b	617	CLA	C12-C13-C15-C16
26	c	504	CLA	C6-C7-C8-C10
26	c	506	CLA	C11-C12-C13-C15
26	g	303	CLA	C11-C10-C8-C7
26	g	317	CLA	C12-C13-C15-C16
26	y	304	CLA	C11-C10-C8-C7
26	y	306	CLA	C2-C3-C5-C6
26	y	306	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	y	309	CLA	C12-C13-C15-C16
39	G	318	CHL	C12-C13-C15-C16
29	a	403	SQD	C13-C14-C15-C16
34	C	503	LMG	C16-C17-C18-C19
37	D	408	LHG	C9-C10-C11-C12
37	Y	306	LHG	C12-C13-C14-C15
26	A	405	CLA	C11-C10-C8-C9
26	B	601	CLA	C11-C10-C8-C9
26	B	605	CLA	C11-C12-C13-C14
26	B	611	CLA	C6-C7-C8-C9
26	C	515	CLA	C11-C12-C13-C14
26	D	406	CLA	C11-C12-C13-C14
26	D	406	CLA	C14-C13-C15-C16
26	G	307	CLA	C14-C13-C15-C16
26	G	314	CLA	C11-C10-C8-C9
26	Y	308	CLA	C11-C12-C13-C14
26	Y	313	CLA	C14-C13-C15-C16
26	a	402	CLA	C11-C10-C8-C9
26	b	605	CLA	C6-C7-C8-C9
26	b	606	CLA	C6-C7-C8-C9
26	b	607	CLA	C11-C10-C8-C9
26	b	608	CLA	C11-C12-C13-C14
26	c	504	CLA	C11-C12-C13-C14
26	d	403	CLA	C11-C12-C13-C14
26	d	403	CLA	C14-C13-C15-C16
26	g	303	CLA	C11-C10-C8-C9
26	r	314	CLA	C14-C13-C15-C16
26	y	306	CLA	C11-C12-C13-C14
40	Y	309	LUT	C29-C30-C31-C32
26	C	508	CLA	CBA-CGA-O2A-C1
39	n	319	CHL	CBA-CGA-O2A-C1
37	d	409	LHG	C32-C33-C34-C35
26	R	313	CLA	O1D-CGD-O2D-CED
26	C	504	CLA	O1A-CGA-O2A-C1
26	R	306	CLA	C16-C17-C18-C19
28	T	101	BCR	C11-C12-C13-C14
28	t	101	BCR	C11-C12-C13-C14
40	Y	315	LUT	C27-C28-C29-C30
37	g	301	LHG	C11-C10-C9-C8
37	S	317	LHG	C1-C2-C3-O3
33	c	517	DGD	O1B-C1B-O2G-C2G
26	B	615	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	b	622	LMG	C31-C32-C33-C34
26	R	316	CLA	CBA-CGA-O2A-C1
26	c	516	CLA	CBA-CGA-O2A-C1
37	s	309	LHG	C26-C27-C28-C29
26	b	611	CLA	C15-C16-C17-C18
26	B	616	CLA	C4B-C3B-CAB-CBB
26	B	618	CLA	C4B-C3B-CAB-CBB
26	C	511	CLA	C4B-C3B-CAB-CBB
26	R	306	CLA	C4B-C3B-CAB-CBB
26	S	307	CLA	C4B-C3B-CAB-CBB
26	S	308	CLA	C4B-C3B-CAB-CBB
26	Y	310	CLA	C4B-C3B-CAB-CBB
26	b	609	CLA	C4B-C3B-CAB-CBB
26	b	613	CLA	C4B-C3B-CAB-CBB
26	c	503	CLA	C4B-C3B-CAB-CBB
26	g	304	CLA	C4B-C3B-CAB-CBB
26	r	306	CLA	C4B-C3B-CAB-CBB
26	s	306	CLA	C4B-C3B-CAB-CBB
26	s	311	CLA	C4B-C3B-CAB-CBB
26	y	304	CLA	C4B-C3B-CAB-CBB
26	y	317	CLA	C4B-C3B-CAB-CBB
26	C	505	CLA	C15-C16-C17-C18
26	y	316	CLA	C15-C16-C17-C18
37	s	309	LHG	O6-C4-C5-C6
26	g	317	CLA	C5-C6-C7-C8
26	y	306	CLA	C10-C11-C12-C13
33	c	519	DGD	CCB-CDB-CEB-CFB
27	d	407	PHO	C4-C3-C5-C6
30	A	408	PL9	C12-C11-C9-C10
26	B	607	CLA	C2-C3-C5-C6
27	A	404	PHO	C2-C3-C5-C6
27	a	410	PHO	C2-C3-C5-C6
37	D	408	LHG	C7-C8-C9-C10
29	b	621	SQD	C12-C13-C14-C15
26	Y	308	CLA	C10-C11-C12-C13
33	C	509	DGD	O1B-C1B-O2G-C2G
26	B	615	CLA	CBA-CGA-O2A-C1
26	C	519	CLA	CBA-CGA-O2A-C1
33	C	509	DGD	O6D-C5D-C6D-O5D
33	c	517	DGD	O6D-C5D-C6D-O5D
34	B	622	LMG	C16-C17-C18-C19
37	d	410	LHG	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	l	101	LHG	C17-C18-C19-C20
37	Y	306	LHG	C5-C4-O6-P
37	y	301	LHG	C5-C4-O6-P
37	r	312	LHG	O10-C23-O8-C6
26	B	613	CLA	C3A-C2A-CAA-CBA
26	b	604	CLA	C3A-C2A-CAA-CBA
26	g	317	CLA	C3A-C2A-CAA-CBA
39	Y	307	CHL	C3A-C2A-CAA-CBA
39	Y	317	CHL	C3A-C2A-CAA-CBA
39	Y	318	CHL	C3A-C2A-CAA-CBA
39	y	303	CHL	C3A-C2A-CAA-CBA
39	y	305	CHL	C3A-C2A-CAA-CBA
34	C	503	LMG	C14-C15-C16-C17
37	S	317	LHG	C26-C27-C28-C29
40	N	305	LUT	C29-C30-C31-C32
40	n	317	LUT	C29-C30-C31-C32
33	c	517	DGD	C7B-C8B-C9B-CAB
37	D	407	LHG	C30-C31-C32-C33
37	D	407	LHG	C26-C27-C28-C29
26	S	310	CLA	CBA-CGA-O2A-C1
39	s	313	CHL	O2A-C1-C2-C3
26	B	616	CLA	C15-C16-C17-C18
26	g	303	CLA	C10-C11-C12-C13
29	w	202	SQD	O6-C44-C45-C46
33	y	308	DGD	C1G-C2G-C3G-O3G
29	B	621	SQD	C23-C24-C25-C26
29	b	621	SQD	C23-C24-C25-C26
26	Y	310	CLA	O1A-CGA-O2A-C1
26	c	506	CLA	C15-C16-C17-C18
26	C	521	CLA	O1D-CGD-O2D-CED
26	g	304	CLA	O1D-CGD-O2D-CED
29	A	407	SQD	C13-C14-C15-C16
30	a	407	PL9	C12-C11-C9-C10
37	G	312	LHG	C11-C10-C9-C8
29	B	621	SQD	C24-C25-C26-C27
34	d	405	LMG	C19-C20-C21-C22
37	g	301	LHG	C15-C16-C17-C18
37	r	312	LHG	C9-C10-C11-C12
26	c	514	CLA	O1D-CGD-O2D-CED
37	s	309	LHG	C4-O6-P-O3
39	G	309	CHL	C3C-C2C-CMC-OMC
39	N	310	CHL	C3C-C2C-CMC-OMC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	N	311	CHL	C3C-C2C-CMC-OMC
39	S	312	CHL	C3C-C2C-CMC-OMC
39	n	307	CHL	C3C-C2C-CMC-OMC
39	n	308	CHL	C3C-C2C-CMC-OMC
39	s	313	CHL	C3C-C2C-CMC-OMC
37	D	410	LHG	O1-C1-C2-O2
37	d	410	LHG	O1-C1-C2-O2
26	n	305	CLA	C13-C15-C16-C17
29	A	407	SQD	C9-C10-C11-C12
37	S	317	LHG	O6-C4-C5-O7
37	s	309	LHG	O6-C4-C5-O7
26	b	611	CLA	CBA-CGA-O2A-C1
26	c	510	CLA	CBA-CGA-O2A-C1
39	Y	314	CHL	CBA-CGA-O2A-C1
26	C	505	CLA	O1D-CGD-O2D-CED
39	r	318	CHL	O1A-CGA-O2A-C1
37	S	317	LHG	C23-C24-C25-C26
37	g	301	LHG	C9-C10-C11-C12
26	B	616	CLA	C2B-C3B-CAB-CBB
26	B	618	CLA	C2B-C3B-CAB-CBB
26	C	511	CLA	C2B-C3B-CAB-CBB
26	R	306	CLA	C2B-C3B-CAB-CBB
26	S	307	CLA	C2B-C3B-CAB-CBB
26	S	308	CLA	C2B-C3B-CAB-CBB
26	b	613	CLA	C2B-C3B-CAB-CBB
26	c	503	CLA	C2B-C3B-CAB-CBB
26	r	306	CLA	C2B-C3B-CAB-CBB
26	s	306	CLA	C2B-C3B-CAB-CBB
26	s	311	CLA	C2B-C3B-CAB-CBB
26	C	508	CLA	O1A-CGA-O2A-C1
26	y	317	CLA	O1A-CGA-O2A-C1
26	s	311	CLA	C2C-C3C-CAC-CBC
37	d	402	LHG	C30-C31-C32-C33
26	D	409	CLA	C16-C17-C18-C19
26	G	307	CLA	C5-C6-C7-C8
37	R	303	LHG	C1-C2-C3-O3
37	r	312	LHG	C1-C2-C3-O3
37	s	309	LHG	C1-C2-C3-O3
37	s	309	LHG	C16-C17-C18-C19
26	B	601	CLA	C2-C1-O2A-CGA
26	B	615	CLA	C2-C1-O2A-CGA
26	b	602	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	b	607	CLA	C2-C1-O2A-CGA
26	b	611	CLA	C2-C1-O2A-CGA
26	r	313	CLA	C2-C1-O2A-CGA
39	G	305	CHL	C2-C1-O2A-CGA
39	S	302	CHL	C2-C1-O2A-CGA
39	s	316	CHL	C2-C1-O2A-CGA
30	D	411	PL9	C43-C44-C46-C47
29	A	407	SQD	C30-C31-C32-C33
33	C	509	DGD	C7B-C8B-C9B-CAB
34	B	622	LMG	C14-C15-C16-C17
34	c	512	LMG	C14-C15-C16-C17
37	l	101	LHG	C27-C28-C29-C30
26	C	520	CLA	C15-C16-C17-C18
26	B	602	CLA	C6-C7-C8-C9
26	B	603	CLA	C6-C7-C8-C9
26	B	617	CLA	C11-C12-C13-C14
26	Y	305	CLA	C11-C12-C13-C14
26	b	602	CLA	C6-C7-C8-C9
26	b	611	CLA	C11-C10-C8-C9
26	c	515	CLA	C11-C12-C13-C14
26	y	309	CLA	C11-C12-C13-C14
26	r	314	CLA	O1D-CGD-O2D-CED
37	d	402	LHG	C27-C28-C29-C30
29	a	403	SQD	C30-C31-C32-C33
37	R	303	LHG	C30-C31-C32-C33
26	N	307	CLA	C13-C15-C16-C17
39	G	301	CHL	C1A-C2A-CAA-CBA
39	S	313	CHL	C1A-C2A-CAA-CBA
39	g	313	CHL	C1A-C2A-CAA-CBA
39	s	317	CHL	C1A-C2A-CAA-CBA
26	R	316	CLA	O1A-CGA-O2A-C1
26	C	505	CLA	C2A-CAA-CBA-CGA
26	c	520	CLA	C2A-CAA-CBA-CGA
39	G	305	CHL	C2A-CAA-CBA-CGA
39	g	314	CHL	C2A-CAA-CBA-CGA
26	B	611	CLA	C16-C17-C18-C19
26	Y	313	CLA	C16-C17-C18-C19
26	y	316	CLA	C16-C17-C18-C19
26	R	314	CLA	O2A-C1-C2-C3
26	S	303	CLA	O2A-C1-C2-C3
26	r	317	CLA	O2A-C1-C2-C3
26	s	307	CLA	O2A-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	B	608	BCR	C23-C24-C25-C26
28	T	101	BCR	C23-C24-C25-C26
28	a	404	BCR	C23-C24-C25-C26
28	b	615	BCR	C23-C24-C25-C26
40	R	311	LUT	C5-C6-C7-C8
40	r	307	LUT	C5-C6-C7-C8
40	R	311	LUT	C11-C12-C13-C14
40	Y	309	LUT	C7-C8-C9-C10
40	r	307	LUT	C11-C12-C13-C14
33	C	509	DGD	C4D-C5D-C6D-O5D
33	c	517	DGD	C4D-C5D-C6D-O5D
26	S	307	CLA	C2C-C3C-CAC-CBC
37	l	101	LHG	C29-C30-C31-C32
26	C	507	CLA	C16-C17-C18-C19
26	b	606	CLA	C16-C17-C18-C19
26	d	404	CLA	C16-C17-C18-C19
33	C	513	DGD	C1B-C2B-C3B-C4B
37	g	301	LHG	C7-C8-C9-C10
26	c	516	CLA	O1A-CGA-O2A-C1
39	R	315	CHL	O1A-CGA-O2A-C1
29	B	621	SQD	C11-C12-C13-C14
34	b	622	LMG	C33-C34-C35-C36
36	d	406	LMT	C9-C10-C11-C12
26	r	310	CLA	CBD-CGD-O2D-CED
33	C	513	DGD	CCA-CDA-CEA-CFA
26	B	602	CLA	C6-C7-C8-C10
26	B	611	CLA	C6-C7-C8-C10
26	B	611	CLA	C11-C10-C8-C7
26	B	615	CLA	C11-C10-C8-C7
26	B	617	CLA	C11-C12-C13-C15
26	C	508	CLA	C11-C12-C13-C15
26	C	515	CLA	C11-C10-C8-C7
26	C	516	CLA	C11-C10-C8-C7
26	C	520	CLA	C11-C12-C13-C15
26	D	406	CLA	C12-C13-C15-C16
26	Y	305	CLA	C12-C13-C15-C16
26	b	605	CLA	C6-C7-C8-C10
26	b	606	CLA	C6-C7-C8-C10
26	b	609	CLA	C12-C13-C15-C16
26	b	610	CLA	C11-C12-C13-C15
26	b	611	CLA	C11-C10-C8-C7
26	c	504	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	c	508	CLA	C11-C10-C8-C7
26	c	516	CLA	C11-C12-C13-C15
26	d	403	CLA	C12-C13-C15-C16
26	y	306	CLA	C11-C12-C13-C15
39	G	318	CHL	C11-C10-C8-C7
39	g	311	CHL	C11-C10-C8-C7
33	c	519	DGD	C4B-C5B-C6B-C7B
37	d	409	LHG	C9-C10-C11-C12
39	S	302	CHL	C1C-C2C-CMC-OMC
39	Y	317	CHL	C1C-C2C-CMC-OMC
39	s	316	CHL	C1C-C2C-CMC-OMC
39	y	305	CHL	C1C-C2C-CMC-OMC
28	C	502	BCR	C9-C10-C11-C12
28	c	511	BCR	C9-C10-C11-C12
26	c	505	CLA	C16-C17-C18-C19
26	c	516	CLA	C16-C17-C18-C20
33	c	501	DGD	CCA-CDA-CEA-CFA
30	a	407	PL9	C7-C8-C9-C11
33	C	510	DGD	C4B-C5B-C6B-C7B
26	B	616	CLA	C5-C6-C7-C8
26	b	609	CLA	C15-C16-C17-C18
29	b	621	SQD	C15-C16-C17-C18
29	b	621	SQD	C14-C15-C16-C17
26	b	617	CLA	C3-C5-C6-C7
26	C	508	CLA	C16-C17-C18-C20
26	G	319	CLA	CBA-CGA-O2A-C1
26	N	318	CLA	CBA-CGA-O2A-C1
26	g	304	CLA	CBA-CGA-O2A-C1
26	n	302	CLA	CBA-CGA-O2A-C1
39	y	312	CHL	CBA-CGA-O2A-C1
37	r	312	LHG	C14-C15-C16-C17
39	g	313	CHL	O1D-CGD-O2D-CED
37	L	101	LHG	C14-C15-C16-C17
37	S	317	LHG	C16-C17-C18-C19
26	D	406	CLA	C8-C10-C11-C12
34	b	622	LMG	C14-C15-C16-C17
26	B	609	CLA	CAD-CBD-CGD-O2D
26	C	511	CLA	CAD-CBD-CGD-O2D
26	C	520	CLA	CAD-CBD-CGD-O2D
26	N	312	CLA	CAD-CBD-CGD-O2D
26	R	306	CLA	CAD-CBD-CGD-O2D
26	R	309	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	R	317	CLA	CAD-CBD-CGD-O2D
26	S	304	CLA	CAD-CBD-CGD-O2D
26	S	311	CLA	CAD-CBD-CGD-O2D
26	Y	311	CLA	CAD-CBD-CGD-O2D
26	b	618	CLA	CAD-CBD-CGD-O2D
26	c	503	CLA	CAD-CBD-CGD-O2D
26	c	506	CLA	CAD-CBD-CGD-O2D
26	n	303	CLA	CAD-CBD-CGD-O2D
26	n	315	CLA	CAD-CBD-CGD-O2D
26	s	305	CLA	CAD-CBD-CGD-O2D
26	s	314	CLA	CAD-CBD-CGD-O2D
26	y	315	CLA	CAD-CBD-CGD-O2D
27	A	404	PHO	CAD-CBD-CGD-O2D
27	a	410	PHO	CAD-CBD-CGD-O2D
29	W	202	SQD	C46-C45-O47-C7
29	b	621	SQD	C46-C45-O47-C7
34	C	503	LMG	C9-C8-O7-C10
34	c	512	LMG	C9-C8-O7-C10
39	G	301	CHL	CAD-CBD-CGD-O2D
39	g	313	CHL	CAD-CBD-CGD-O2D
39	g	314	CHL	CAD-CBD-CGD-O2D
29	B	621	SQD	C15-C16-C17-C18
37	D	407	LHG	C9-C10-C11-C12
26	B	601	CLA	C10-C11-C12-C13
26	b	610	CLA	C15-C16-C17-C18
26	b	617	CLA	C10-C11-C12-C13
26	n	305	CLA	C15-C16-C17-C18
26	r	314	CLA	C13-C15-C16-C17
29	b	621	SQD	C24-C25-C26-C27
33	c	501	DGD	C1B-C2B-C3B-C4B
29	B	621	SQD	C44-C45-C46-O48
29	W	202	SQD	C44-C45-C46-O48
29	b	621	SQD	C44-C45-C46-O48
34	W	201	LMG	C7-C8-C9-O8
34	w	201	LMG	C7-C8-C9-O8
37	D	410	LHG	C2-C3-O3-P
37	d	410	LHG	C2-C3-O3-P
26	B	615	CLA	O1A-CGA-O2A-C1
26	C	511	CLA	C13-C15-C16-C17
26	b	607	CLA	C10-C11-C12-C13
26	c	503	CLA	C13-C15-C16-C17
26	G	302	CLA	O2A-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	g	302	CLA	O2A-C1-C2-C3
26	r	313	CLA	O2A-C1-C2-C3
26	s	314	CLA	O2A-C1-C2-C3
37	S	317	LHG	C33-C34-C35-C36
38	E	101	HEM	C4C-C3C-CAC-CBC
38	e	101	HEM	C4C-C3C-CAC-CBC
26	y	315	CLA	CBA-CGA-O2A-C1
29	a	413	SQD	C30-C31-C32-C33
26	C	520	CLA	NC-C1C-CHC-C4B
26	c	506	CLA	NC-C1C-CHC-C4B
26	B	611	CLA	CHA-CBD-CGD-O1D
26	B	611	CLA	CHA-CBD-CGD-O2D
26	B	613	CLA	CHA-CBD-CGD-O2D
26	B	618	CLA	CHA-CBD-CGD-O1D
26	C	505	CLA	CHA-CBD-CGD-O1D
26	C	505	CLA	CHA-CBD-CGD-O2D
26	C	506	CLA	CHA-CBD-CGD-O1D
26	C	512	CLA	CHA-CBD-CGD-O2D
26	G	319	CLA	CHA-CBD-CGD-O1D
26	G	319	CLA	CHA-CBD-CGD-O2D
26	R	308	CLA	CHA-CBD-CGD-O1D
26	R	308	CLA	CHA-CBD-CGD-O2D
26	R	310	CLA	CHA-CBD-CGD-O1D
26	R	313	CLA	CHA-CBD-CGD-O1D
26	R	313	CLA	CHA-CBD-CGD-O2D
26	b	604	CLA	CHA-CBD-CGD-O2D
26	b	606	CLA	CHA-CBD-CGD-O1D
26	b	606	CLA	CHA-CBD-CGD-O2D
26	b	611	CLA	CHA-CBD-CGD-O1D
26	b	613	CLA	CHA-CBD-CGD-O1D
26	c	502	CLA	CHA-CBD-CGD-O1D
26	c	520	CLA	CHA-CBD-CGD-O1D
26	c	520	CLA	CHA-CBD-CGD-O2D
26	g	304	CLA	CHA-CBD-CGD-O1D
26	g	304	CLA	CHA-CBD-CGD-O2D
26	r	311	CLA	CHA-CBD-CGD-O1D
26	r	314	CLA	CHA-CBD-CGD-O1D
26	s	310	CLA	CHA-CBD-CGD-O2D
26	r	314	CLA	C8-C10-C11-C12
26	C	521	CLA	C3-C5-C6-C7
26	C	519	CLA	O1A-CGA-O2A-C1
39	N	310	CHL	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	n	308	CHL	O1A-CGA-O2A-C1
37	Y	306	LHG	C35-C36-C37-C38
29	A	407	SQD	O6-C44-C45-O47
29	W	202	SQD	O6-C44-C45-O47
29	a	403	SQD	O6-C44-C45-O47
34	C	518	LMG	O7-C8-C9-O8
34	W	201	LMG	O7-C8-C9-O8
34	c	509	LMG	O7-C8-C9-O8
34	w	201	LMG	O7-C8-C9-O8
26	G	319	CLA	O1A-CGA-O2A-C1
39	G	303	CHL	O1A-CGA-O2A-C1
39	g	307	CHL	O1A-CGA-O2A-C1
37	y	301	LHG	C35-C36-C37-C38
26	S	310	CLA	O1A-CGA-O2A-C1
26	c	510	CLA	O1A-CGA-O2A-C1
33	C	513	DGD	C1A-C2A-C3A-C4A
26	Y	308	CLA	C2-C3-C5-C6
26	B	615	CLA	C11-C10-C8-C9
26	C	507	CLA	C6-C7-C8-C9
26	C	515	CLA	C11-C10-C8-C9
26	Y	312	CLA	C11-C12-C13-C14
26	b	609	CLA	C14-C13-C15-C16
26	b	610	CLA	C11-C12-C13-C14
26	c	504	CLA	C11-C10-C8-C9
26	n	303	CLA	C11-C10-C8-C9
26	y	310	CLA	C11-C12-C13-C14
37	D	408	LHG	C26-C27-C28-C29
26	n	302	CLA	O1A-CGA-O2A-C1
34	D	404	LMG	C19-C20-C21-C22
26	B	601	CLA	C2A-CAA-CBA-CGA
26	c	502	CLA	C2A-CAA-CBA-CGA
39	G	309	CHL	C2A-CAA-CBA-CGA
39	Y	314	CHL	C2A-CAA-CBA-CGA
26	b	609	CLA	C5-C6-C7-C8
29	A	410	SQD	C31-C32-C33-C34
26	g	304	CLA	O1A-CGA-O2A-C1
40	y	318	LUT	C7-C8-C9-C19
37	n	301	LHG	C9-C10-C11-C12
37	r	312	LHG	C28-C29-C30-C31
26	B	617	CLA	C1A-C2A-CAA-CBA
26	S	314	CLA	C1A-C2A-CAA-CBA
26	b	610	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	n	312	CLA	C1A-C2A-CAA-CBA
26	s	315	CLA	C1A-C2A-CAA-CBA
37	s	309	LHG	C23-C24-C25-C26
26	Y	311	CLA	CBA-CGA-O2A-C1
37	d	409	LHG	C11-C12-C13-C14
37	r	312	LHG	C15-C16-C17-C18
26	R	313	CLA	C8-C10-C11-C12
37	S	317	LHG	C4-O6-P-O3
33	C	509	DGD	C9B-CAB-CBB-CCB
34	d	405	LMG	C32-C33-C34-C35
27	D	403	PHO	C4-C3-C5-C6
29	A	407	SQD	C12-C13-C14-C15
33	B	620	DGD	CAA-CBA-CCA-CDA
26	N	318	CLA	O1A-CGA-O2A-C1
26	b	611	CLA	O1A-CGA-O2A-C1
26	B	605	CLA	C4B-C3B-CAB-CBB
26	B	612	CLA	C4B-C3B-CAB-CBB
26	b	608	CLA	C4B-C3B-CAB-CBB
26	b	614	CLA	C4B-C3B-CAB-CBB
26	s	301	CLA	C4B-C3B-CAB-CBB
26	s	314	CLA	C4B-C3B-CAB-CBB
37	D	408	LHG	C3-O3-P-O4
37	L	101	LHG	C3-O3-P-O5
37	N	301	LHG	C4-O6-P-O4
37	S	317	LHG	C3-O3-P-O4
37	d	409	LHG	C3-O3-P-O4
37	l	101	LHG	C3-O3-P-O5
37	r	312	LHG	C3-O3-P-O5
37	s	309	LHG	C3-O3-P-O4
37	N	301	LHG	C32-C33-C34-C35
26	G	304	CLA	O2A-C1-C2-C3
26	S	309	CLA	O2A-C1-C2-C3
26	S	311	CLA	O2A-C1-C2-C3
26	g	318	CLA	O2A-C1-C2-C3
26	s	304	CLA	O2A-C1-C2-C3
27	a	410	PHO	C15-C16-C17-C18
26	b	607	CLA	C2A-CAA-CBA-CGA
26	n	305	CLA	C2A-CAA-CBA-CGA
26	C	508	CLA	C3-C5-C6-C7
26	c	514	CLA	C3-C5-C6-C7
26	c	516	CLA	C3-C5-C6-C7
37	d	409	LHG	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	C	505	CLA	C16-C17-C18-C20
33	y	308	DGD	C3A-C4A-C5A-C6A
34	B	622	LMG	C33-C34-C35-C36
34	b	622	LMG	C22-C23-C24-C25
26	B	605	CLA	CAD-CBD-CGD-O1D
26	B	611	CLA	CAD-CBD-CGD-O1D
26	B	613	CLA	CAD-CBD-CGD-O1D
26	B	615	CLA	CAD-CBD-CGD-O1D
26	B	618	CLA	CAD-CBD-CGD-O1D
26	C	505	CLA	CAD-CBD-CGD-O1D
26	C	512	CLA	CAD-CBD-CGD-O1D
26	D	412	CLA	CAD-CBD-CGD-O1D
26	G	304	CLA	CAD-CBD-CGD-O1D
26	N	319	CLA	CAD-CBD-CGD-O1D
26	S	310	CLA	CAD-CBD-CGD-O1D
26	Y	316	CLA	CAD-CBD-CGD-O1D
26	b	604	CLA	CAD-CBD-CGD-O1D
26	b	606	CLA	CAD-CBD-CGD-O1D
26	b	608	CLA	CAD-CBD-CGD-O1D
26	b	613	CLA	CAD-CBD-CGD-O1D
26	c	520	CLA	CAD-CBD-CGD-O1D
26	d	411	CLA	CAD-CBD-CGD-O1D
26	g	318	CLA	CAD-CBD-CGD-O1D
26	n	310	CLA	CAD-CBD-CGD-O1D
26	s	310	CLA	CAD-CBD-CGD-O1D
26	y	313	CLA	CAD-CBD-CGD-O1D
29	A	407	SQD	C5-C6-S-O7
29	a	403	SQD	C5-C6-S-O7
34	B	622	LMG	C28-C29-C30-C31
34	C	503	LMG	C33-C34-C35-C36
26	C	511	CLA	C3-C5-C6-C7
27	A	404	PHO	C15-C16-C17-C18
26	R	310	CLA	CBD-CGD-O2D-CED
33	c	501	DGD	C1A-C2A-C3A-C4A
34	c	512	LMG	C33-C34-C35-C36
26	b	618	CLA	CBA-CGA-O2A-C1
39	r	309	CHL	CBA-CGA-O2A-C1
36	D	402	LMT	C9-C10-C11-C12
26	D	406	CLA	C4-C3-C5-C6
26	B	602	CLA	C11-C10-C8-C7
26	B	606	CLA	C11-C10-C8-C7
26	B	616	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	C	506	CLA	C12-C13-C15-C16
26	C	511	CLA	C11-C12-C13-C15
26	D	409	CLA	C12-C13-C15-C16
26	Y	312	CLA	C6-C7-C8-C10
26	Y	312	CLA	C11-C12-C13-C15
26	b	601	CLA	C11-C10-C8-C7
26	b	605	CLA	C11-C10-C8-C7
26	b	606	CLA	C11-C10-C8-C7
26	c	502	CLA	C12-C13-C15-C16
26	c	503	CLA	C11-C12-C13-C15
26	d	404	CLA	C12-C13-C15-C16
26	n	303	CLA	C11-C10-C8-C7
26	y	310	CLA	C6-C7-C8-C10
26	y	310	CLA	C11-C12-C13-C15
30	d	408	PL9	C43-C44-C46-C47
39	Y	302	CHL	C12-C13-C15-C16
39	y	303	CHL	C12-C13-C15-C16
26	R	313	CLA	C13-C15-C16-C17
29	A	407	SQD	C19-C20-C21-C22
26	y	315	CLA	O1A-CGA-O2A-C1
37	S	317	LHG	O2-C2-C3-O3
34	w	201	LMG	C16-C17-C18-C19
39	R	315	CHL	C2A-CAA-CBA-CGA
39	g	319	CHL	C2A-CAA-CBA-CGA
39	Y	314	CHL	C2C-C3C-CAC-CBC
39	y	312	CHL	C2C-C3C-CAC-CBC
29	A	407	SQD	O6-C44-C45-C46
29	a	403	SQD	O6-C44-C45-C46
29	a	413	SQD	O6-C44-C45-C46
33	C	509	DGD	C4B-C5B-C6B-C7B
33	c	519	DGD	CBA-CCA-CDA-CEA
33	c	519	DGD	C8B-C9B-CAB-CBB
34	C	518	LMG	C7-C8-C9-O8
34	c	509	LMG	C7-C8-C9-O8
37	L	101	LHG	C27-C28-C29-C30
37	S	317	LHG	C4-C5-C6-O8
37	s	309	LHG	C4-C5-C6-O8
29	w	202	SQD	O6-C44-C45-O47
37	S	317	LHG	O7-C5-C6-O8
37	s	309	LHG	O7-C5-C6-O8
26	b	611	CLA	C16-C17-C18-C20
37	d	410	LHG	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	r	312	LHG	C2-C3-O3-P
26	Y	311	CLA	O1A-CGA-O2A-C1
26	c	504	CLA	C8-C10-C11-C12
39	R	312	CHL	CBA-CGA-O2A-C1
29	B	621	SQD	C33-C34-C35-C36
26	R	302	CLA	O2A-C1-C2-C3
26	B	601	CLA	C11-C12-C13-C14
26	B	611	CLA	C11-C10-C8-C9
26	B	616	CLA	C14-C13-C15-C16
26	C	508	CLA	C11-C12-C13-C14
26	C	511	CLA	C11-C12-C13-C14
26	C	512	CLA	C11-C12-C13-C14
26	C	516	CLA	C11-C10-C8-C9
26	b	606	CLA	C11-C10-C8-C9
26	b	607	CLA	C11-C12-C13-C14
26	b	609	CLA	C11-C10-C8-C9
26	c	508	CLA	C11-C10-C8-C9
26	c	516	CLA	C11-C12-C13-C14
26	y	316	CLA	C14-C13-C15-C16
39	G	311	CHL	C2C-C3C-CAC-CBC
34	W	201	LMG	C16-C17-C18-C19
26	d	403	CLA	C3-C5-C6-C7
26	d	403	CLA	C8-C10-C11-C12
39	N	317	CHL	C2C-C3C-CAC-CBC
39	S	302	CHL	C2C-C3C-CAC-CBC
39	g	312	CHL	C2C-C3C-CAC-CBC
37	D	408	LHG	C24-C25-C26-C27
28	T	101	BCR	C18-C19-C20-C21
28	t	101	BCR	C18-C19-C20-C21
40	R	311	LUT	C10-C11-C12-C13
40	r	307	LUT	C10-C11-C12-C13
41	G	320	XAT	C10-C11-C12-C13
41	g	320	XAT	C10-C11-C12-C13
42	S	305	NEX	C30-C31-C32-C33
42	s	302	NEX	C30-C31-C32-C33
33	C	509	DGD	C2A-C3A-C4A-C5A
26	C	517	CLA	C16-C17-C18-C20
26	c	513	CLA	C16-C17-C18-C20
26	c	520	CLA	C16-C17-C18-C20
37	d	409	LHG	C12-C13-C14-C15
26	B	605	CLA	C2B-C3B-CAB-CBB
26	B	606	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	B	613	CLA	C2B-C3B-CAB-CBB
26	N	318	CLA	C2B-C3B-CAB-CBB
26	Y	305	CLA	C2B-C3B-CAB-CBB
26	b	604	CLA	C2B-C3B-CAB-CBB
26	b	608	CLA	C2B-C3B-CAB-CBB
26	c	520	CLA	C2B-C3B-CAB-CBB
26	n	302	CLA	C2B-C3B-CAB-CBB
26	s	301	CLA	C2B-C3B-CAB-CBB
33	c	517	DGD	C4B-C5B-C6B-C7B
37	D	408	LHG	C11-C12-C13-C14
37	D	408	LHG	C19-C20-C21-C22
26	a	411	CLA	C3-C5-C6-C7
37	d	402	LHG	C9-C10-C11-C12
26	C	515	CLA	C8-C10-C11-C12
26	C	519	CLA	C1-C2-C3-C4
26	D	412	CLA	C1-C2-C3-C4
26	G	302	CLA	C1-C2-C3-C4
26	G	304	CLA	C1-C2-C3-C4
26	G	306	CLA	C1-C2-C3-C4
26	G	313	CLA	C1-C2-C3-C4
26	G	317	CLA	C1-C2-C3-C4
26	G	319	CLA	C1-C2-C3-C4
26	N	306	CLA	C1-C2-C3-C4
26	N	308	CLA	C1-C2-C3-C4
26	N	309	CLA	C1-C2-C3-C4
26	N	313	CLA	C1-C2-C3-C4
26	N	318	CLA	C1-C2-C3-C4
26	N	319	CLA	C1-C2-C3-C4
26	R	307	CLA	C1-C2-C3-C4
26	R	308	CLA	C1-C2-C3-C4
26	R	309	CLA	C1-C2-C3-C4
26	R	310	CLA	C1-C2-C3-C4
26	R	314	CLA	C1-C2-C3-C4
26	R	316	CLA	C1-C2-C3-C4
26	R	317	CLA	C1-C2-C3-C4
26	S	303	CLA	C1-C2-C3-C4
26	S	304	CLA	C1-C2-C3-C4
26	S	307	CLA	C1-C2-C3-C4
26	S	308	CLA	C1-C2-C3-C4
26	S	309	CLA	C1-C2-C3-C4
26	S	310	CLA	C1-C2-C3-C4
26	S	311	CLA	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	S	314	CLA	C1-C2-C3-C4
26	S	315	CLA	C1-C2-C3-C4
26	Y	310	CLA	C1-C2-C3-C4
26	Y	311	CLA	C1-C2-C3-C4
26	Y	316	CLA	C1-C2-C3-C4
26	c	510	CLA	C1-C2-C3-C4
26	d	411	CLA	C1-C2-C3-C4
26	g	302	CLA	C1-C2-C3-C4
26	g	304	CLA	C1-C2-C3-C4
26	g	305	CLA	C1-C2-C3-C4
26	g	308	CLA	C1-C2-C3-C4
26	g	315	CLA	C1-C2-C3-C4
26	g	318	CLA	C1-C2-C3-C4
26	n	302	CLA	C1-C2-C3-C4
26	n	304	CLA	C1-C2-C3-C4
26	n	309	CLA	C1-C2-C3-C4
26	n	310	CLA	C1-C2-C3-C4
26	n	312	CLA	C1-C2-C3-C4
26	n	315	CLA	C1-C2-C3-C4
26	r	303	CLA	C1-C2-C3-C4
26	r	305	CLA	C1-C2-C3-C4
26	r	308	CLA	C1-C2-C3-C4
26	r	310	CLA	C1-C2-C3-C4
26	r	311	CLA	C1-C2-C3-C4
26	r	315	CLA	C1-C2-C3-C4
26	r	317	CLA	C1-C2-C3-C4
26	s	301	CLA	C1-C2-C3-C4
26	s	304	CLA	C1-C2-C3-C4
26	s	305	CLA	C1-C2-C3-C4
26	s	306	CLA	C1-C2-C3-C4
26	s	307	CLA	C1-C2-C3-C4
26	s	310	CLA	C1-C2-C3-C4
26	s	311	CLA	C1-C2-C3-C4
26	s	314	CLA	C1-C2-C3-C4
26	s	315	CLA	C1-C2-C3-C4
26	y	313	CLA	C1-C2-C3-C4
26	y	315	CLA	C1-C2-C3-C4
26	y	317	CLA	C1-C2-C3-C4
39	G	301	CHL	C1-C2-C3-C4
39	G	303	CHL	C1-C2-C3-C4
39	G	305	CHL	C1-C2-C3-C4
39	G	311	CHL	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	N	304	CHL	C1-C2-C3-C4
39	N	311	CHL	C1-C2-C3-C4
39	N	316	CHL	C1-C2-C3-C4
39	N	317	CHL	C1-C2-C3-C4
39	R	301	CHL	C1-C2-C3-C4
39	R	312	CHL	C1-C2-C3-C4
39	R	315	CHL	C1-C2-C3-C4
39	S	302	CHL	C1-C2-C3-C4
39	Y	314	CHL	C1-C2-C3-C4
39	Y	317	CHL	C1-C2-C3-C4
39	Y	318	CHL	C1-C2-C3-C4
39	g	307	CHL	C1-C2-C3-C4
39	g	312	CHL	C1-C2-C3-C4
39	g	313	CHL	C1-C2-C3-C4
39	g	319	CHL	C1-C2-C3-C4
39	n	306	CHL	C1-C2-C3-C4
39	n	307	CHL	C1-C2-C3-C4
39	n	311	CHL	C1-C2-C3-C4
39	n	319	CHL	C1-C2-C3-C4
39	r	309	CHL	C1-C2-C3-C4
39	r	316	CHL	C1-C2-C3-C4
39	r	318	CHL	C1-C2-C3-C4
39	s	316	CHL	C1-C2-C3-C4
39	y	302	CHL	C1-C2-C3-C4
39	y	305	CHL	C1-C2-C3-C4
39	y	312	CHL	C1-C2-C3-C4
39	R	312	CHL	O1D-CGD-O2D-CED
33	C	513	DGD	CBA-CCA-CDA-CEA
33	Y	303	DGD	C3A-C4A-C5A-C6A
37	y	301	LHG	C25-C26-C27-C28
29	A	407	SQD	C46-C45-O47-C7
29	B	621	SQD	C46-C45-O47-C7
29	a	403	SQD	C46-C45-O47-C7
34	C	518	LMG	C7-C8-O7-C10
34	c	509	LMG	C7-C8-O7-C10
37	N	301	LHG	C6-C5-O7-C7
37	n	301	LHG	C6-C5-O7-C7
26	C	506	CLA	C2A-CAA-CBA-CGA
26	N	307	CLA	C2A-CAA-CBA-CGA
26	N	318	CLA	C2A-CAA-CBA-CGA
26	n	302	CLA	C2A-CAA-CBA-CGA
26	r	314	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	y	310	CLA	C2A-CAA-CBA-CGA
39	y	312	CHL	C2A-CAA-CBA-CGA
26	A	403	CLA	C2-C1-O2A-CGA
26	B	603	CLA	C2-C1-O2A-CGA
26	D	409	CLA	C2-C1-O2A-CGA
26	R	302	CLA	C2-C1-O2A-CGA
26	a	411	CLA	C2-C1-O2A-CGA
26	d	404	CLA	C2-C1-O2A-CGA
26	n	304	CLA	C2-C1-O2A-CGA
26	r	305	CLA	C2-C1-O2A-CGA
39	N	303	CHL	C2-C1-O2A-CGA
39	S	313	CHL	C2-C1-O2A-CGA
39	Y	317	CHL	C2-C1-O2A-CGA
39	n	318	CHL	C2-C1-O2A-CGA
39	y	305	CHL	C2-C1-O2A-CGA
37	d	409	LHG	C7-C8-C9-C10
29	A	410	SQD	C29-C30-C31-C32
29	b	621	SQD	C33-C34-C35-C36
37	R	303	LHG	C2-C3-O3-P
26	b	618	CLA	O1A-CGA-O2A-C1
26	c	502	CLA	C5-C6-C7-C8
26	y	309	CLA	C8-C10-C11-C12
26	r	308	CLA	O2A-C1-C2-C3
39	N	303	CHL	C4-C3-C5-C6
33	b	620	DGD	CAA-CBA-CCA-CDA
28	J	101	BCR	C23-C24-C25-C30
28	c	507	BCR	C23-C24-C25-C26
26	C	515	CLA	C13-C15-C16-C17
26	B	609	CLA	CBA-CGA-O2A-C1
26	D	409	CLA	C2C-C3C-CAC-CBC
26	s	311	CLA	C4C-C3C-CAC-CBC
34	b	622	LMG	C30-C31-C32-C33
37	N	301	LHG	C9-C10-C11-C12
37	s	309	LHG	C24-C25-C26-C27
26	B	615	CLA	C16-C17-C18-C20
29	a	403	SQD	C19-C20-C21-C22
33	C	513	DGD	C5B-C6B-C7B-C8B
37	D	408	LHG	C12-C13-C14-C15
26	r	311	CLA	CBA-CGA-O2A-C1
26	s	310	CLA	CBA-CGA-O2A-C1
37	N	301	LHG	C3-O3-P-O6
37	n	301	LHG	C3-O3-P-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	b	621	SQD	C19-C20-C21-C22
33	C	509	DGD	C3A-C4A-C5A-C6A
39	Y	307	CHL	C2C-C3C-CAC-CBC
26	b	602	CLA	C16-C17-C18-C20
39	G	303	CHL	CHA-CBD-CGD-O2D
39	G	318	CHL	CHA-CBD-CGD-O2D
39	N	303	CHL	CHA-CBD-CGD-O2D
39	N	316	CHL	CHA-CBD-CGD-O1D
39	N	316	CHL	CHA-CBD-CGD-O2D
39	N	317	CHL	CHA-CBD-CGD-O2D
39	Y	302	CHL	CHA-CBD-CGD-O1D
39	g	307	CHL	CHA-CBD-CGD-O2D
39	n	306	CHL	CHA-CBD-CGD-O1D
39	n	306	CHL	CHA-CBD-CGD-O2D
39	n	318	CHL	CHA-CBD-CGD-O2D
39	y	303	CHL	CHA-CBD-CGD-O1D
33	c	517	DGD	C2A-C3A-C4A-C5A
37	R	303	LHG	C18-C19-C20-C21
29	A	410	SQD	O6-C44-C45-C46
29	w	202	SQD	C44-C45-C46-O48
29	B	621	SQD	C19-C20-C21-C22
37	Y	306	LHG	C25-C26-C27-C28
26	C	506	CLA	C5-C6-C7-C8
26	B	607	CLA	C6-C7-C8-C10
26	G	314	CLA	C11-C12-C13-C15
26	c	515	CLA	C11-C12-C13-C15
39	n	319	CHL	C2C-C3C-CAC-CBC
34	d	405	LMG	C14-C15-C16-C17
26	B	606	CLA	C11-C10-C8-C9
26	C	511	CLA	C11-C10-C8-C9
26	N	312	CLA	C11-C10-C8-C9
26	Y	312	CLA	C6-C7-C8-C9
26	b	601	CLA	C11-C10-C8-C9
26	b	602	CLA	C11-C12-C13-C14
26	c	503	CLA	C11-C12-C13-C14
26	d	404	CLA	C14-C13-C15-C16
26	y	310	CLA	C6-C7-C8-C9
26	b	612	CLA	C5-C6-C7-C8
26	B	603	CLA	C16-C17-C18-C20
26	S	307	CLA	C4C-C3C-CAC-CBC
26	B	610	CLA	C10-C11-C12-C13
29	b	621	SQD	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	C	513	DGD	C7B-C8B-C9B-CAB
33	B	620	DGD	O1B-C1B-C2B-C3B
39	S	312	CHL	O2A-C1-C2-C3
39	G	318	CHL	C2A-CAA-CBA-CGA
26	C	504	CLA	C16-C17-C18-C20
37	G	312	LHG	C5-C4-O6-P
37	g	301	LHG	C5-C4-O6-P
40	y	318	LUT	C7-C8-C9-C10
33	c	501	DGD	C5B-C6B-C7B-C8B
37	D	407	LHG	C31-C32-C33-C34
37	L	101	LHG	C31-C32-C33-C34
33	c	501	DGD	CDA-CEA-CFA-CGA
26	c	503	CLA	C10-C11-C12-C13
30	A	408	PL9	C7-C8-C9-C11
37	n	301	LHG	C32-C33-C34-C35
26	C	504	CLA	C16-C17-C18-C19
26	b	608	CLA	C16-C17-C18-C20
26	C	511	CLA	CBA-CGA-O2A-C1
26	a	402	CLA	CBA-CGA-O2A-C1
26	c	503	CLA	CBA-CGA-O2A-C1
37	g	301	LHG	C33-C34-C35-C36
34	C	503	LMG	C21-C22-C23-C24
37	S	317	LHG	C15-C16-C17-C18
26	r	311	CLA	O1A-CGA-O2A-C1
26	y	304	CLA	CBD-CGD-O2D-CED
26	R	308	CLA	CBA-CGA-O2A-C1
34	C	503	LMG	C15-C16-C17-C18
26	N	318	CLA	C4B-C3B-CAB-CBB
26	R	308	CLA	C4B-C3B-CAB-CBB
26	S	315	CLA	C4B-C3B-CAB-CBB
26	Y	305	CLA	C4B-C3B-CAB-CBB
26	b	604	CLA	C4B-C3B-CAB-CBB
26	b	606	CLA	C4B-C3B-CAB-CBB
26	b	611	CLA	C4B-C3B-CAB-CBB
26	b	617	CLA	C4B-C3B-CAB-CBB
26	c	520	CLA	C4B-C3B-CAB-CBB
26	n	302	CLA	C4B-C3B-CAB-CBB
26	r	311	CLA	C4B-C3B-CAB-CBB
26	S	314	CLA	C2A-CAA-CBA-CGA
26	s	315	CLA	C2A-CAA-CBA-CGA
33	c	517	DGD	C6B-C7B-C8B-C9B
37	S	317	LHG	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	B	609	CLA	O1A-CGA-O2A-C1
26	a	402	CLA	O1A-CGA-O2A-C1
37	G	312	LHG	C9-C10-C11-C12
34	C	503	LMG	C28-C29-C30-C31
33	Y	303	DGD	C2B-C3B-C4B-C5B
26	s	310	CLA	O1A-CGA-O2A-C1
34	D	404	LMG	C16-C17-C18-C19
26	B	605	CLA	C16-C17-C18-C20
39	r	301	CHL	CAA-CBA-CGA-O2A
37	S	317	LHG	C24-C25-C26-C27
26	d	403	CLA	C4-C3-C5-C6
33	C	510	DGD	C8B-C9B-CAB-CBB
33	c	501	DGD	CBA-CCA-CDA-CEA
37	s	309	LHG	C33-C34-C35-C36
26	C	511	CLA	O1A-CGA-O2A-C1
26	R	308	CLA	O1A-CGA-O2A-C1
26	c	503	CLA	O1A-CGA-O2A-C1
37	d	410	LHG	C31-C32-C33-C34
26	B	607	CLA	C10-C11-C12-C13
26	C	511	CLA	C10-C11-C12-C13
27	A	404	PHO	C10-C11-C12-C13
33	c	501	DGD	C7B-C8B-C9B-CAB
37	D	410	LHG	C9-C10-C11-C12
37	g	301	LHG	C14-C15-C16-C17
26	C	512	CLA	C2-C1-O2A-CGA
26	R	309	CLA	C2-C1-O2A-CGA
26	Y	301	CLA	C2-C1-O2A-CGA
26	c	503	CLA	C2-C1-O2A-CGA
26	c	515	CLA	C2-C1-O2A-CGA
26	y	304	CLA	C2-C1-O2A-CGA
39	Y	307	CHL	C2-C1-O2A-CGA
39	g	311	CHL	C2-C1-O2A-CGA
39	y	314	CHL	C2-C1-O2A-CGA
26	d	404	CLA	C2C-C3C-CAC-CBC
26	n	303	CLA	C16-C17-C18-C20
26	r	314	CLA	C16-C17-C18-C20
33	c	517	DGD	C2E-C1E-O5D-C6D
34	w	201	LMG	C40-C41-C42-C43
37	D	410	LHG	C31-C32-C33-C34
26	R	313	CLA	C2A-CAA-CBA-CGA
26	S	307	CLA	C2A-CAA-CBA-CGA
26	Y	312	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	g	303	CLA	C2A-CAA-CBA-CGA
33	C	513	DGD	CDA-CEA-CFA-CGA
37	n	301	LHG	C30-C31-C32-C33
33	c	517	DGD	C3A-C4A-C5A-C6A
34	w	201	LMG	C15-C16-C17-C18
26	R	309	CLA	C3A-C2A-CAA-CBA
26	s	314	CLA	C3A-C2A-CAA-CBA
39	N	304	CHL	C3A-C2A-CAA-CBA
39	Y	302	CHL	C3A-C2A-CAA-CBA
39	n	311	CHL	C3A-C2A-CAA-CBA
26	R	316	CLA	O2A-C1-C2-C3
39	N	311	CHL	O2A-C1-C2-C3
39	R	312	CHL	O2A-C1-C2-C3
39	r	309	CHL	O2A-C1-C2-C3
41	G	320	XAT	C29-C30-C31-C32
39	y	314	CHL	C2C-C3C-CAC-CBC
33	C	509	DGD	C6B-C7B-C8B-C9B
29	B	621	SQD	C9-C10-C11-C12
34	B	622	LMG	C4-C5-C6-O5
26	B	603	CLA	C11-C12-C13-C14
26	B	616	CLA	C6-C7-C8-C9
26	C	507	CLA	C11-C10-C8-C9
26	C	521	CLA	C6-C7-C8-C9
26	R	313	CLA	C14-C13-C15-C16
26	b	609	CLA	C6-C7-C8-C9
26	b	612	CLA	C14-C13-C15-C16
26	c	505	CLA	C6-C7-C8-C9
26	c	505	CLA	C11-C10-C8-C9
26	c	514	CLA	C6-C7-C8-C9
39	n	318	CHL	C11-C10-C8-C9
26	Y	305	CLA	C8-C10-C11-C12
33	c	517	DGD	C9B-CAB-CBB-CCB
34	b	622	LMG	C12-C13-C14-C15
28	C	514	BCR	C35-C13-C14-C15
28	c	507	BCR	C35-C13-C14-C15
40	R	311	LUT	C11-C10-C9-C19
40	R	311	LUT	C40-C33-C34-C35
40	S	301	LUT	C20-C13-C14-C15
40	r	307	LUT	C11-C10-C9-C19
40	r	307	LUT	C40-C33-C34-C35
40	s	308	LUT	C20-C13-C14-C15
41	G	320	XAT	C11-C10-C9-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
41	g	320	XAT	C11-C10-C9-C19
42	G	315	NEX	C39-C29-C30-C31
42	N	302	NEX	C39-C29-C30-C31
42	R	305	NEX	C39-C29-C30-C31
42	S	305	NEX	C20-C13-C14-C15
42	Y	304	NEX	C39-C29-C30-C31
42	g	306	NEX	C39-C29-C30-C31
42	n	313	NEX	C39-C29-C30-C31
42	r	302	NEX	C39-C29-C30-C31
42	s	302	NEX	C20-C13-C14-C15
42	y	307	NEX	C39-C29-C30-C31
27	A	404	PHO	C2A-CAA-CBA-CGA
27	a	410	PHO	C2A-CAA-CBA-CGA
39	y	303	CHL	O1A-CGA-O2A-C1
34	W	201	LMG	C40-C41-C42-C43
26	b	611	CLA	C16-C17-C18-C19
37	s	309	LHG	O2-C2-C3-O3
33	C	509	DGD	O6E-C1E-O5D-C6D
33	c	517	DGD	O6E-C1E-O5D-C6D
39	G	301	CHL	O1D-CGD-O2D-CED
37	Y	306	LHG	C17-C18-C19-C20
26	r	310	CLA	O1D-CGD-O2D-CED
34	W	201	LMG	C15-C16-C17-C18
26	C	511	CLA	C1A-C2A-CAA-CBA
26	N	308	CLA	C1A-C2A-CAA-CBA
26	c	503	CLA	C1A-C2A-CAA-CBA
26	g	303	CLA	C1A-C2A-CAA-CBA
26	g	303	CLA	C16-C17-C18-C20
26	B	609	CLA	C11-C10-C8-C7
26	C	504	CLA	C12-C13-C15-C16
26	C	508	CLA	C6-C7-C8-C10
26	C	512	CLA	C11-C12-C13-C15
26	Y	301	CLA	C11-C10-C8-C7
26	b	616	CLA	C6-C7-C8-C10
26	b	618	CLA	C11-C10-C8-C7
26	c	516	CLA	C6-C7-C8-C10
27	d	407	PHO	C2-C3-C5-C6
39	N	303	CHL	C11-C12-C13-C15
39	n	318	CHL	C11-C12-C13-C15
26	c	504	CLA	C13-C15-C16-C17
39	s	316	CHL	C2C-C3C-CAC-CBC
28	D	405	BCR	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	c	512	LMG	C15-C16-C17-C18
39	Y	314	CHL	C3C-C2C-CMC-OMC
27	D	403	PHO	C2A-CAA-CBA-CGA
27	d	407	PHO	C2A-CAA-CBA-CGA
39	S	302	CHL	C2A-CAA-CBA-CGA
39	R	318	CHL	CAA-CBA-CGA-O2A
37	y	301	LHG	C17-C18-C19-C20
37	y	301	LHG	C28-C29-C30-C31
26	G	306	CLA	O2A-C1-C2-C3
26	S	307	CLA	O2A-C1-C2-C3
26	s	311	CLA	O2A-C1-C2-C3
34	b	622	LMG	C4-C5-C6-O5
27	a	410	PHO	C10-C11-C12-C13
34	c	512	LMG	C12-C13-C14-C15
37	N	301	LHG	C30-C31-C32-C33
27	d	407	PHO	C8-C10-C11-C12
26	B	611	CLA	C2B-C3B-CAB-CBB
26	B	612	CLA	C2B-C3B-CAB-CBB
26	C	505	CLA	C2B-C3B-CAB-CBB
26	R	308	CLA	C2B-C3B-CAB-CBB
26	S	315	CLA	C2B-C3B-CAB-CBB
26	b	606	CLA	C2B-C3B-CAB-CBB
26	b	611	CLA	C2B-C3B-CAB-CBB
26	b	614	CLA	C2B-C3B-CAB-CBB
26	g	305	CLA	C2B-C3B-CAB-CBB
26	r	311	CLA	C2B-C3B-CAB-CBB
26	s	314	CLA	C2B-C3B-CAB-CBB
26	y	309	CLA	C2B-C3B-CAB-CBB
37	R	303	LHG	C9-C10-C11-C12
28	C	514	BCR	C12-C13-C14-C15
28	c	507	BCR	C12-C13-C14-C15
33	C	509	DGD	C2E-C1E-O5D-C6D
40	R	311	LUT	C11-C10-C9-C8
40	R	311	LUT	C32-C33-C34-C35
40	S	301	LUT	C12-C13-C14-C15
40	r	307	LUT	C11-C10-C9-C8
40	r	307	LUT	C32-C33-C34-C35
40	s	308	LUT	C12-C13-C14-C15
41	G	320	XAT	C11-C10-C9-C8
41	g	320	XAT	C11-C10-C9-C8
42	G	315	NEX	C28-C29-C30-C31
42	N	302	NEX	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
42	R	305	NEX	C28-C29-C30-C31
42	S	305	NEX	C12-C13-C14-C15
42	Y	304	NEX	C28-C29-C30-C31
42	g	306	NEX	C28-C29-C30-C31
42	n	313	NEX	C28-C29-C30-C31
42	r	302	NEX	C28-C29-C30-C31
42	s	302	NEX	C12-C13-C14-C15
42	y	307	NEX	C28-C29-C30-C31
37	Y	306	LHG	C28-C29-C30-C31
28	c	511	BCR	C19-C20-C21-C22
42	n	313	NEX	C29-C30-C31-C32
37	s	309	LHG	C15-C16-C17-C18
33	C	509	DGD	CCB-CDB-CEB-CFB
34	D	404	LMG	C14-C15-C16-C17
33	b	620	DGD	O1B-C1B-C2B-C3B
26	B	603	CLA	C15-C16-C17-C18
39	Y	307	CHL	C5-C6-C7-C8
39	n	308	CHL	CAA-CBA-CGA-O2A
39	r	309	CHL	O1A-CGA-O2A-C1
29	B	621	SQD	C29-C30-C31-C32
39	G	309	CHL	C2-C1-O2A-CGA
30	D	411	PL9	C45-C44-C46-C47
34	B	622	LMG	C12-C13-C14-C15
26	N	313	CLA	C2-C1-O2A-CGA
39	R	312	CHL	C2-C1-O2A-CGA
39	r	309	CHL	C2-C1-O2A-CGA
39	g	314	CHL	C2-C1-O2A-CGA
26	s	304	CLA	CAA-CBA-CGA-O2A
39	g	314	CHL	CAA-CBA-CGA-O2A
37	G	312	LHG	C33-C34-C35-C36
37	n	301	LHG	C11-C12-C13-C14
39	G	311	CHL	C1A-C2A-CAA-CBA
39	N	317	CHL	C1A-C2A-CAA-CBA
39	g	312	CHL	C1A-C2A-CAA-CBA
39	n	319	CHL	C1A-C2A-CAA-CBA
39	s	303	CHL	C4-C3-C5-C6
39	y	303	CHL	C1A-C2A-CAA-CBA
26	G	314	CLA	C2A-CAA-CBA-CGA
26	G	314	CLA	C16-C17-C18-C20
26	c	516	CLA	C16-C17-C18-C19
27	D	403	PHO	C16-C17-C18-C20
26	R	307	CLA	O2A-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	g	305	CLA	O2A-C1-C2-C3
26	r	303	CLA	O2A-C1-C2-C3
39	n	307	CHL	O2A-C1-C2-C3
37	y	301	LHG	C11-C12-C13-C14
39	R	312	CHL	O1A-CGA-O2A-C1
39	g	312	CHL	O1A-CGA-O2A-C1
28	J	101	BCR	C1-C6-C7-C8
28	c	511	BCR	C23-C24-C25-C30
28	j	101	BCR	C1-C6-C7-C8
28	j	101	BCR	C23-C24-C25-C30
28	t	101	BCR	C23-C24-C25-C26
40	S	301	LUT	C5-C6-C7-C8
26	Y	311	CLA	O1D-CGD-O2D-CED
26	S	309	CLA	CAA-CBA-CGA-O2A
39	G	309	CHL	CAA-CBA-CGA-O2A
39	N	310	CHL	CAA-CBA-CGA-O2A
37	d	409	LHG	C4-C5-C6-O8
37	D	408	LHG	C23-C24-C25-C26
26	b	616	CLA	C10-C11-C12-C13
37	R	303	LHG	C15-C16-C17-C18
40	s	308	LUT	C9-C10-C11-C12
41	R	304	XAT	C29-C30-C31-C32
41	r	304	XAT	C29-C30-C31-C32
26	b	608	CLA	C16-C17-C18-C19
26	n	303	CLA	C16-C17-C18-C19
33	b	620	DGD	C6A-C7A-C8A-C9A
29	B	621	SQD	C45-C44-O6-C1
29	b	621	SQD	C45-C44-O6-C1
34	D	404	LMG	C8-C7-O1-C1
37	s	309	LHG	C9-C10-C11-C12
39	g	307	CHL	C2A-CAA-CBA-CGA
39	g	311	CHL	C2C-C3C-CAC-CBC
36	d	406	LMT	C6-C7-C8-C9
34	C	518	LMG	C17-C18-C19-C20
26	B	606	CLA	C4B-C3B-CAB-CBB
26	B	610	CLA	C4B-C3B-CAB-CBB
26	B	611	CLA	C4B-C3B-CAB-CBB
26	B	613	CLA	C4B-C3B-CAB-CBB
26	C	505	CLA	C4B-C3B-CAB-CBB
26	D	409	CLA	C4B-C3B-CAB-CBB
26	G	302	CLA	C4B-C3B-CAB-CBB
26	G	306	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	b	601	CLA	C4B-C3B-CAB-CBB
26	d	404	CLA	C4B-C3B-CAB-CBB
26	g	302	CLA	C4B-C3B-CAB-CBB
26	g	305	CLA	C4B-C3B-CAB-CBB
26	y	309	CLA	C4B-C3B-CAB-CBB
33	c	519	DGD	C4A-C5A-C6A-C7A
26	d	404	CLA	C10-C11-C12-C13
29	b	621	SQD	C17-C18-C19-C20
37	Y	306	LHG	O6-C4-C5-C6
37	y	301	LHG	O6-C4-C5-C6
26	R	310	CLA	O1D-CGD-O2D-CED
37	D	408	LHG	C33-C34-C35-C36
26	B	603	CLA	C11-C12-C13-C15
26	B	618	CLA	C11-C10-C8-C7
26	C	511	CLA	C11-C10-C8-C7
26	b	602	CLA	C11-C12-C13-C15
26	c	503	CLA	C6-C7-C8-C10
27	D	403	PHO	C8-C10-C11-C12
34	C	503	LMG	C12-C13-C14-C15
37	N	301	LHG	C11-C12-C13-C14
37	l	101	LHG	C14-C15-C16-C17
37	d	409	LHG	O7-C5-C6-O8
26	N	313	CLA	O2A-C1-C2-C3
26	R	310	CLA	O2A-C1-C2-C3
26	S	315	CLA	O2A-C1-C2-C3
26	Y	310	CLA	O2A-C1-C2-C3
26	n	304	CLA	O2A-C1-C2-C3
26	n	310	CLA	O2A-C1-C2-C3
26	n	315	CLA	O2A-C1-C2-C3
26	r	310	CLA	O2A-C1-C2-C3
26	y	317	CLA	O2A-C1-C2-C3
26	B	603	CLA	CAA-CBA-CGA-O2A
26	B	609	CLA	CAA-CBA-CGA-O2A
26	S	315	CLA	CAA-CBA-CGA-O2A
37	d	402	LHG	C31-C32-C33-C34
26	C	516	CLA	C2A-CAA-CBA-CGA
26	C	520	CLA	O1D-CGD-O2D-CED
26	B	605	CLA	C15-C16-C17-C18
26	b	602	CLA	C15-C16-C17-C18
26	G	307	CLA	C13-C15-C16-C17
33	c	519	DGD	CBB-CCB-CDB-CEB
26	b	618	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	Y	313	CLA	C4-C3-C5-C6
26	y	316	CLA	C4-C3-C5-C6
30	d	408	PL9	C45-C44-C46-C47
26	B	604	CLA	C5-C6-C7-C8
26	c	514	CLA	C5-C6-C7-C8
26	D	406	CLA	C2-C3-C5-C6
27	D	403	PHO	C2-C3-C5-C6
39	G	318	CHL	C2C-C3C-CAC-CBC
34	D	404	LMG	C32-C33-C34-C35
26	B	615	CLA	C16-C17-C18-C19
26	c	518	CLA	C16-C17-C18-C19
26	g	303	CLA	C16-C17-C18-C19
26	b	602	CLA	CAA-CBA-CGA-O2A
39	G	305	CHL	CAA-CBA-CGA-O2A
39	g	319	CHL	CAA-CBA-CGA-O2A
26	B	616	CLA	C11-C10-C8-C9
26	B	617	CLA	C14-C13-C15-C16
26	D	409	CLA	C14-C13-C15-C16
26	b	608	CLA	C11-C10-C8-C9
26	c	502	CLA	C14-C13-C15-C16
26	c	506	CLA	C11-C12-C13-C14
26	c	515	CLA	C6-C7-C8-C9
27	D	403	PHO	C11-C12-C13-C14
29	B	621	SQD	C28-C29-C30-C31
26	S	311	CLA	C3A-C2A-CAA-CBA
26	b	618	CLA	C3A-C2A-CAA-CBA
26	r	305	CLA	C3A-C2A-CAA-CBA
39	S	316	CHL	C3A-C2A-CAA-CBA
39	s	303	CHL	C3A-C2A-CAA-CBA
34	C	518	LMG	C15-C16-C17-C18
39	G	311	CHL	O1A-CGA-O2A-C1
26	s	310	CLA	CAA-CBA-CGA-O2A
39	y	312	CHL	CAA-CBA-CGA-O2A
26	C	520	CLA	CBD-CGD-O2D-CED
26	B	603	CLA	CAD-CBD-CGD-O2D
26	B	612	CLA	CAD-CBD-CGD-O2D
26	C	508	CLA	CAD-CBD-CGD-O2D
26	G	307	CLA	CAD-CBD-CGD-O2D
26	N	306	CLA	CAD-CBD-CGD-O2D
26	N	318	CLA	CAD-CBD-CGD-O2D
26	S	308	CLA	CAD-CBD-CGD-O2D
26	S	314	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	b	602	CLA	CAD-CBD-CGD-O2D
26	b	614	CLA	CAD-CBD-CGD-O2D
26	c	516	CLA	CAD-CBD-CGD-O2D
26	g	317	CLA	CAD-CBD-CGD-O2D
26	n	302	CLA	CAD-CBD-CGD-O2D
26	r	305	CLA	CAD-CBD-CGD-O2D
26	r	306	CLA	CAD-CBD-CGD-O2D
26	r	315	CLA	CAD-CBD-CGD-O2D
26	s	301	CLA	CAD-CBD-CGD-O2D
26	s	311	CLA	CAD-CBD-CGD-O2D
26	s	315	CLA	CAD-CBD-CGD-O2D
37	Y	306	LHG	C4-C5-O7-C7
37	y	301	LHG	C4-C5-O7-C7
39	S	312	CHL	CAD-CBD-CGD-O2D
39	s	313	CHL	CAD-CBD-CGD-O2D
26	B	605	CLA	C16-C17-C18-C19
26	c	518	CLA	C16-C17-C18-C20
26	r	314	CLA	C16-C17-C18-C19
37	D	408	LHG	C31-C32-C33-C34
26	y	304	CLA	O1D-CGD-O2D-CED
26	B	617	CLA	C15-C16-C17-C18
39	s	316	CHL	C2A-CAA-CBA-CGA
29	B	621	SQD	C16-C17-C18-C19
39	G	318	CHL	C2-C1-O2A-CGA
39	g	319	CHL	C2-C1-O2A-CGA
26	R	302	CLA	CAA-CBA-CGA-O2A
26	s	301	CLA	CAA-CBA-CGA-O2A
39	Y	314	CHL	CAA-CBA-CGA-O2A
39	g	313	CHL	CAA-CBA-CGA-O2A
39	n	318	CHL	CAA-CBA-CGA-O2A
29	b	621	SQD	C11-C12-C13-C14
39	G	303	CHL	O1D-CGD-O2D-CED
26	C	508	CLA	C16-C17-C18-C19
39	G	318	CHL	C16-C17-C18-C20
26	s	306	CLA	CAA-CBA-CGA-O2A
34	C	503	LMG	O8-C28-C29-C30
33	b	620	DGD	C5B-C6B-C7B-C8B
39	Y	314	CHL	O1A-CGA-O2A-C1
37	g	301	LHG	C16-C17-C18-C19
42	S	305	NEX	O24-C26-C27-C28
34	d	405	LMG	C16-C17-C18-C19
39	Y	302	CHL	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	b	620	DGD	CCA-CDA-CEA-CFA
26	S	308	CLA	CAA-CBA-CGA-O2A
34	C	518	LMG	O7-C10-C11-C12
34	c	509	LMG	O7-C10-C11-C12
39	N	303	CHL	CAA-CBA-CGA-O2A
26	N	306	CLA	O2A-C1-C2-C3
26	s	306	CLA	O2A-C1-C2-C3
39	Y	318	CHL	O2A-C1-C2-C3
39	y	302	CHL	O2A-C1-C2-C3
36	D	402	LMT	C6-C7-C8-C9
26	B	605	CLA	O2A-C1-C2-C3
26	D	409	CLA	O2A-C1-C2-C3
26	Y	301	CLA	O2A-C1-C2-C3
26	Y	313	CLA	O2A-C1-C2-C3
26	b	608	CLA	O2A-C1-C2-C3
26	d	404	CLA	O2A-C1-C2-C3
26	y	304	CLA	O2A-C1-C2-C3
26	y	316	CLA	O2A-C1-C2-C3
39	n	318	CHL	O2A-C1-C2-C3
29	a	403	SQD	C9-C10-C11-C12
26	c	508	CLA	C2A-CAA-CBA-CGA
26	r	315	CLA	C2A-CAA-CBA-CGA
26	s	311	CLA	C2A-CAA-CBA-CGA
26	g	308	CLA	CAA-CBA-CGA-O2A
26	y	315	CLA	O1D-CGD-O2D-CED
26	B	606	CLA	CHA-CBD-CGD-O1D
26	B	606	CLA	CHA-CBD-CGD-O2D
26	B	618	CLA	CHA-CBD-CGD-O2D
26	C	506	CLA	CHA-CBD-CGD-O2D
26	C	507	CLA	CHA-CBD-CGD-O1D
26	C	516	CLA	CHA-CBD-CGD-O1D
26	C	516	CLA	CHA-CBD-CGD-O2D
26	C	521	CLA	CHA-CBD-CGD-O1D
26	G	302	CLA	CHA-CBD-CGD-O1D
26	N	307	CLA	CHA-CBD-CGD-O2D
26	N	309	CLA	CHA-CBD-CGD-O1D
26	N	309	CLA	CHA-CBD-CGD-O2D
26	R	310	CLA	CHA-CBD-CGD-O2D
26	S	308	CLA	CHA-CBD-CGD-O1D
26	Y	313	CLA	CHA-CBD-CGD-O1D
26	Y	313	CLA	CHA-CBD-CGD-O2D
26	b	601	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	b	601	CLA	CHA-CBD-CGD-O2D
26	b	611	CLA	CHA-CBD-CGD-O2D
26	b	613	CLA	CHA-CBD-CGD-O2D
26	c	502	CLA	CHA-CBD-CGD-O2D
26	c	503	CLA	CHA-CBD-CGD-O2D
26	c	505	CLA	CHA-CBD-CGD-O1D
26	c	506	CLA	CHA-CBD-CGD-O2D
26	c	508	CLA	CHA-CBD-CGD-O1D
26	c	508	CLA	CHA-CBD-CGD-O2D
26	c	514	CLA	CHA-CBD-CGD-O1D
26	g	302	CLA	CHA-CBD-CGD-O1D
26	n	309	CLA	CHA-CBD-CGD-O1D
26	n	309	CLA	CHA-CBD-CGD-O2D
26	r	310	CLA	CHA-CBD-CGD-O1D
26	r	310	CLA	CHA-CBD-CGD-O2D
26	r	311	CLA	CHA-CBD-CGD-O2D
26	s	301	CLA	CHA-CBD-CGD-O1D
26	y	316	CLA	CHA-CBD-CGD-O1D
26	n	309	CLA	CAA-CBA-CGA-O2A
26	r	313	CLA	CAA-CBA-CGA-O2A
33	b	620	DGD	C9A-CAA-CBA-CCA
26	C	520	CLA	CAA-CBA-CGA-O2A
26	G	317	CLA	CAA-CBA-CGA-O2A
39	n	311	CHL	CAA-CBA-CGA-O2A
33	y	308	DGD	C2B-C3B-C4B-C5B
26	A	405	CLA	O1A-CGA-O2A-C1
26	C	521	CLA	C5-C6-C7-C8
26	D	409	CLA	C10-C11-C12-C13
37	d	409	LHG	C31-C32-C33-C34
26	B	602	CLA	CAA-CBA-CGA-O2A
26	G	306	CLA	CAA-CBA-CGA-O2A
26	G	319	CLA	CAA-CBA-CGA-O2A
26	N	309	CLA	CAA-CBA-CGA-O2A
26	S	310	CLA	CAA-CBA-CGA-O2A
26	c	506	CLA	CAA-CBA-CGA-O2A
26	g	304	CLA	CAA-CBA-CGA-O2A
26	g	305	CLA	CAA-CBA-CGA-O2A
26	n	315	CLA	CAA-CBA-CGA-O2A
39	G	301	CHL	CAA-CBA-CGA-O2A
39	G	303	CHL	C2A-CAA-CBA-CGA
39	g	311	CHL	C2A-CAA-CBA-CGA
27	d	407	PHO	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	A	404	PHO	CHA-CBD-CGD-O2D
27	D	403	PHO	CHA-CBD-CGD-O1D
27	d	407	PHO	CHA-CBD-CGD-O1D
39	S	312	CHL	CHA-CBD-CGD-O1D
39	Y	307	CHL	CHA-CBD-CGD-O2D
39	y	314	CHL	CHA-CBD-CGD-O2D
29	a	413	SQD	C15-C16-C17-C18
26	B	606	CLA	C12-C13-C15-C16
26	Y	301	CLA	C11-C12-C13-C15
26	G	314	CLA	C16-C17-C18-C19
26	N	306	CLA	CAA-CBA-CGA-O2A
34	c	512	LMG	O8-C28-C29-C30
39	N	304	CHL	CAA-CBA-CGA-O2A
29	a	413	SQD	C31-C32-C33-C34
37	l	101	LHG	C34-C35-C36-C37
26	B	609	CLA	C11-C10-C8-C9
26	C	504	CLA	C14-C13-C15-C16
26	C	506	CLA	C14-C13-C15-C16
26	C	508	CLA	C6-C7-C8-C9
26	b	618	CLA	C11-C10-C8-C9
27	d	407	PHO	C11-C12-C13-C14
28	d	401	BCR	C9-C10-C11-C12
29	b	621	SQD	C27-C28-C29-C30
26	b	601	CLA	C2B-C3B-CAB-CBB
26	r	305	CLA	O2A-C1-C2-C3
34	c	512	LMG	C28-C29-C30-C31
33	B	620	DGD	CCA-CDA-CEA-CFA
33	c	517	DGD	CCB-CDB-CEB-CFB
29	A	407	SQD	C4-C5-C6-S
29	W	202	SQD	C4-C5-C6-S
29	a	403	SQD	C4-C5-C6-S
29	w	202	SQD	C4-C5-C6-S
29	b	621	SQD	C29-C30-C31-C32
26	R	317	CLA	C2A-CAA-CBA-CGA
39	n	306	CHL	C2A-CAA-CBA-CGA
33	y	308	DGD	C4B-C5B-C6B-C7B
37	g	301	LHG	C10-C11-C12-C13
26	b	605	CLA	CAA-CBA-CGA-O2A
37	d	409	LHG	C30-C31-C32-C33
34	c	512	LMG	C30-C31-C32-C33
27	D	403	PHO	C16-C17-C18-C19
26	Y	305	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	G	312	LHG	C31-C32-C33-C34
39	N	303	CHL	CAA-CBA-CGA-O1A
39	S	313	CHL	CAA-CBA-CGA-O1A
40	n	314	LUT	C11-C12-C13-C14
26	A	405	CLA	CBA-CGA-O2A-C1
37	G	312	LHG	C32-C33-C34-C35
26	B	609	CLA	C1A-C2A-CAA-CBA
26	C	520	CLA	C2B-C3B-CAB-CBB
26	R	309	CLA	C1A-C2A-CAA-CBA
26	S	304	CLA	C1A-C2A-CAA-CBA
26	b	618	CLA	C1A-C2A-CAA-CBA
26	c	506	CLA	C2B-C3B-CAB-CBB
26	r	305	CLA	C1A-C2A-CAA-CBA
26	s	314	CLA	C1A-C2A-CAA-CBA
26	b	618	CLA	CAA-CBA-CGA-O1A
39	G	305	CHL	CAA-CBA-CGA-O1A
39	N	317	CHL	C2-C1-O2A-CGA
39	Y	302	CHL	C2-C1-O2A-CGA
26	B	609	CLA	CAA-CBA-CGA-O1A
34	c	512	LMG	O10-C28-C29-C30
39	N	304	CHL	CAA-CBA-CGA-O1A
39	n	318	CHL	CAA-CBA-CGA-O1A
39	s	317	CHL	CAA-CBA-CGA-O1A
26	B	604	CLA	C2A-CAA-CBA-CGA
26	Y	308	CLA	C2A-CAA-CBA-CGA
26	b	612	CLA	C2A-CAA-CBA-CGA
26	b	614	CLA	C2A-CAA-CBA-CGA
26	y	306	CLA	C2A-CAA-CBA-CGA
34	c	509	LMG	C17-C18-C19-C20
26	S	315	CLA	CAA-CBA-CGA-O1A
26	b	602	CLA	CAA-CBA-CGA-O1A
26	s	306	CLA	CAA-CBA-CGA-O1A
34	C	503	LMG	O10-C28-C29-C30
26	b	610	CLA	C8-C10-C11-C12
37	l	101	LHG	O7-C7-C8-C9
37	D	408	LHG	O9-C7-O7-C5
26	A	403	CLA	C3-C5-C6-C7
26	B	602	CLA	CAA-CBA-CGA-O1A
26	b	605	CLA	CAA-CBA-CGA-O1A
26	g	304	CLA	CAA-CBA-CGA-O1A
26	s	310	CLA	CAA-CBA-CGA-O1A
39	g	319	CHL	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	Y	306	LHG	C11-C12-C13-C14
26	C	516	CLA	C5-C6-C7-C8
37	n	301	LHG	C4-O6-P-O4
26	B	603	CLA	CAA-CBA-CGA-O1A
26	G	317	CLA	CAA-CBA-CGA-O1A
26	G	319	CLA	CAA-CBA-CGA-O1A
26	n	309	CLA	CAA-CBA-CGA-O1A
26	N	318	CLA	O2A-C1-C2-C3
26	R	309	CLA	O2A-C1-C2-C3
26	n	302	CLA	O2A-C1-C2-C3
26	n	312	CLA	O2A-C1-C2-C3
26	s	305	CLA	O2A-C1-C2-C3
39	S	313	CHL	CAA-CBA-CGA-O2A
37	S	317	LHG	C11-C12-C13-C14
28	j	101	BCR	C5-C6-C7-C8
40	s	308	LUT	C5-C6-C7-C8
26	N	312	CLA	C13-C15-C16-C17
26	N	306	CLA	CAA-CBA-CGA-O1A
26	R	302	CLA	CAA-CBA-CGA-O1A
26	r	313	CLA	CAA-CBA-CGA-O1A
39	Y	314	CHL	CAA-CBA-CGA-O1A
26	S	308	CLA	CAA-CBA-CGA-O1A
26	n	315	CLA	CAA-CBA-CGA-O1A
26	s	301	CLA	CAA-CBA-CGA-O1A
26	c	508	CLA	C5-C6-C7-C8
34	C	503	LMG	C30-C31-C32-C33
29	A	410	SQD	C15-C16-C17-C18
26	b	608	CLA	CAA-CBA-CGA-O2A
39	S	312	CHL	CAA-CBA-CGA-O2A
26	g	308	CLA	CAA-CBA-CGA-O1A
39	y	312	CHL	CAA-CBA-CGA-O1A
33	c	519	DGD	C4E-C5E-C6E-O5E
26	C	506	CLA	CAD-CBD-CGD-O1D
26	C	507	CLA	CAD-CBD-CGD-O1D
26	C	521	CLA	CAD-CBD-CGD-O1D
26	G	302	CLA	CAD-CBD-CGD-O1D
26	R	310	CLA	CAD-CBD-CGD-O1D
26	b	611	CLA	CAD-CBD-CGD-O1D
26	c	502	CLA	CAD-CBD-CGD-O1D
26	c	505	CLA	CAD-CBD-CGD-O1D
26	c	514	CLA	CAD-CBD-CGD-O1D
26	g	302	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	r	310	CLA	CAD-CBD-CGD-O1D
29	W	202	SQD	O5-C5-C6-S
29	w	202	SQD	O5-C5-C6-S
37	r	312	LHG	C6-C5-O7-C7
39	y	312	CHL	O1A-CGA-O2A-C1
26	c	506	CLA	CAA-CBA-CGA-O1A
37	D	410	LHG	C27-C28-C29-C30
29	A	407	SQD	O48-C23-C24-C25
33	c	501	DGD	O2G-C1B-C2B-C3B
37	y	301	LHG	O8-C23-C24-C25
39	s	317	CHL	CAA-CBA-CGA-O2A
26	B	617	CLA	C8-C10-C11-C12
26	b	608	CLA	C15-C16-C17-C18
37	R	303	LHG	O2-C2-C3-O3
26	B	606	CLA	C6-C7-C8-C9
26	C	512	CLA	C6-C7-C8-C9
26	C	520	CLA	C11-C12-C13-C14
26	b	601	CLA	C6-C7-C8-C9
26	b	612	CLA	C11-C10-C8-C9
26	c	516	CLA	C6-C7-C8-C9
26	c	518	CLA	C11-C10-C8-C9
26	N	309	CLA	CAA-CBA-CGA-O1A
26	S	310	CLA	CAA-CBA-CGA-O1A
26	g	305	CLA	CAA-CBA-CGA-O1A
34	c	509	LMG	C34-C35-C36-C37
34	B	622	LMG	C15-C16-C17-C18
37	d	410	LHG	C27-C28-C29-C30
37	s	309	LHG	C28-C29-C30-C31
26	G	306	CLA	CAA-CBA-CGA-O1A
39	R	318	CHL	C2C-C3C-CAC-CBC
26	b	602	CLA	C13-C15-C16-C17
26	B	612	CLA	C2A-CAA-CBA-CGA
33	C	513	DGD	O2G-C1B-C2B-C3B
37	g	301	LHG	O8-C23-C24-C25
39	s	313	CHL	CAA-CBA-CGA-O2A
26	B	603	CLA	C13-C15-C16-C17
30	d	408	PL9	C30-C29-C31-C32
34	w	201	LMG	C13-C14-C15-C16
26	C	505	CLA	C11-C12-C13-C15
26	Y	313	CLA	C11-C10-C8-C7
26	b	601	CLA	C3A-C2A-CAA-CBA
26	b	601	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	d	403	CLA	C2-C3-C5-C6
26	g	303	CLA	C11-C12-C13-C15
26	n	305	CLA	C6-C7-C8-C10
26	y	304	CLA	C11-C12-C13-C15
39	R	315	CHL	C3A-C2A-CAA-CBA
39	Y	307	CHL	C12-C13-C15-C16
39	y	314	CHL	C12-C13-C15-C16
33	c	501	DGD	O1B-C1B-C2B-C3B
37	l	101	LHG	O9-C7-C8-C9
26	r	310	CLA	CAA-CBA-CGA-O2A
26	r	315	CLA	CAA-CBA-CGA-O2A
29	a	403	SQD	O48-C23-C24-C25
37	L	101	LHG	O7-C7-C8-C9
39	S	302	CHL	CAA-CBA-CGA-O2A
39	s	316	CHL	CAA-CBA-CGA-O2A
26	N	308	CLA	O2A-C1-C2-C3
26	N	319	CLA	O2A-C1-C2-C3
26	S	304	CLA	O2A-C1-C2-C3
28	B	614	BCR	C21-C22-C23-C24
28	b	619	BCR	C21-C22-C23-C24
40	N	314	LUT	C11-C12-C13-C14
40	g	310	LUT	C7-C8-C9-C10
39	R	301	CHL	CAA-CBA-CGA-O1A
39	n	311	CHL	CAA-CBA-CGA-O1A
39	s	316	CHL	CAA-CBA-CGA-O1A
28	b	619	BCR	C13-C14-C15-C16
40	g	316	LUT	C29-C30-C31-C32
37	g	301	LHG	C19-C20-C21-C22
27	d	407	PHO	C16-C17-C18-C19
37	G	312	LHG	O8-C23-C24-C25
37	Y	306	LHG	O8-C23-C24-C25
37	r	312	LHG	O7-C7-C8-C9
33	C	510	DGD	CBB-CCB-CDB-CEB
26	C	520	CLA	CAA-CBA-CGA-O1A
37	L	101	LHG	O9-C7-C8-C9
39	S	302	CHL	CAA-CBA-CGA-O1A
37	Y	306	LHG	C24-C23-O8-C6
37	r	312	LHG	O2-C2-C3-O3
26	R	317	CLA	CAA-CBA-CGA-O2A
37	S	317	LHG	O8-C23-C24-C25
26	B	618	CLA	C2A-CAA-CBA-CGA
26	C	519	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	Y	316	CLA	C2A-CAA-CBA-CGA
26	b	613	CLA	C2A-CAA-CBA-CGA
26	c	510	CLA	C2A-CAA-CBA-CGA
30	D	411	PL9	C7-C8-C9-C10
37	g	301	LHG	O10-C23-C24-C25
30	D	411	PL9	C30-C29-C31-C32
33	c	519	DGD	CCA-CDA-CEA-CFA
37	R	303	LHG	C33-C34-C35-C36
26	B	605	CLA	CAA-CBA-CGA-O2A
26	R	310	CLA	CAA-CBA-CGA-O2A
37	d	410	LHG	O8-C23-C24-C25
37	s	309	LHG	O8-C23-C24-C25

There are no ring outliers.

304 monomers are involved in 836 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	S	308	CLA	3	0
26	c	518	CLA	8	0
42	G	315	NEX	4	0
26	R	317	CLA	2	0
26	G	314	CLA	4	0
26	c	515	CLA	4	0
26	Y	305	CLA	8	0
26	b	605	CLA	7	0
26	B	605	CLA	7	0
26	b	610	CLA	4	0
37	g	301	LHG	8	0
40	Y	315	LUT	7	0
28	b	619	BCR	5	0
39	n	311	CHL	1	0
40	g	310	LUT	4	0
39	S	316	CHL	1	0
26	D	401	CLA	3	0
26	C	505	CLA	3	0
39	Y	307	CHL	3	0
39	r	316	CHL	1	0
33	C	509	DGD	4	0
37	N	301	LHG	5	0
28	t	101	BCR	6	0
26	g	315	CLA	2	0
39	Y	318	CHL	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	y	304	CLA	3	0
26	R	313	CLA	2	0
27	d	407	PHO	8	0
40	n	317	LUT	3	0
28	b	615	BCR	3	0
26	b	608	CLA	6	0
27	D	403	PHO	7	0
33	b	620	DGD	3	0
26	c	516	CLA	2	0
26	s	305	CLA	1	0
28	j	101	BCR	4	0
26	D	406	CLA	1	0
39	R	318	CHL	1	0
42	Y	304	NEX	3	0
37	D	410	LHG	2	0
26	S	314	CLA	4	0
26	B	609	CLA	4	0
37	l	101	LHG	3	0
26	G	304	CLA	1	0
35	a	408	OEX	3	0
30	A	408	PL9	3	0
34	D	404	LMG	1	0
39	y	314	CHL	3	0
26	B	601	CLA	5	0
26	y	316	CLA	4	0
41	G	320	XAT	4	0
26	G	307	CLA	5	0
26	G	319	CLA	2	0
37	D	407	LHG	3	0
34	W	201	LMG	3	0
26	B	615	CLA	4	0
40	Y	309	LUT	5	0
26	c	508	CLA	3	0
42	r	302	NEX	4	0
39	G	311	CHL	3	0
34	b	622	LMG	3	0
30	a	407	PL9	4	0
39	n	307	CHL	4	0
28	J	101	BCR	4	0
26	C	508	CLA	1	0
26	d	403	CLA	4	0
28	b	603	BCR	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	g	306	NEX	4	0
26	S	310	CLA	4	0
26	C	506	CLA	3	0
37	s	309	LHG	2	0
33	C	510	DGD	3	0
37	n	301	LHG	5	0
26	C	515	CLA	5	0
26	s	311	CLA	4	0
26	r	315	CLA	1	0
26	C	521	CLA	4	0
39	N	310	CHL	2	0
26	B	611	CLA	3	0
26	s	314	CLA	2	0
26	s	304	CLA	2	0
29	A	410	SQD	2	0
39	n	306	CHL	6	0
26	r	311	CLA	4	0
39	Y	314	CHL	1	0
35	C	501	OEX	2	0
29	a	403	SQD	5	0
26	B	606	CLA	6	0
42	n	313	NEX	1	0
29	a	413	SQD	3	0
26	S	303	CLA	2	0
26	B	612	CLA	2	0
26	y	309	CLA	7	0
26	b	609	CLA	7	0
39	n	319	CHL	2	0
26	r	305	CLA	1	0
33	Y	303	DGD	3	0
26	d	411	CLA	3	0
33	C	513	DGD	3	0
28	C	514	BCR	2	0
39	N	316	CHL	5	0
26	C	504	CLA	7	0
26	n	303	CLA	3	0
39	s	316	CHL	6	0
26	s	307	CLA	2	0
28	a	404	BCR	1	0
39	Y	302	CHL	7	0
26	C	520	CLA	5	0
39	g	311	CHL	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	Y	317	CHL	3	0
29	A	407	SQD	5	0
26	s	315	CLA	2	0
28	A	406	BCR	1	0
29	b	621	SQD	3	0
26	r	303	CLA	1	0
33	c	501	DGD	3	0
39	S	312	CHL	5	0
26	a	402	CLA	1	0
26	N	307	CLA	4	0
26	s	301	CLA	3	0
40	S	306	LUT	3	0
37	r	312	LHG	2	0
26	s	310	CLA	4	0
30	d	408	PL9	2	0
26	Y	310	CLA	1	0
39	N	311	CHL	4	0
33	c	519	DGD	3	0
34	C	503	LMG	2	0
37	G	312	LHG	6	0
26	N	312	CLA	3	0
26	g	308	CLA	3	0
26	R	307	CLA	1	0
28	h	101	BCR	3	0
39	N	303	CHL	3	0
40	N	314	LUT	4	0
26	c	504	CLA	5	0
26	d	404	CLA	9	0
41	g	320	XAT	6	0
26	S	304	CLA	1	0
39	G	301	CHL	5	0
26	B	607	CLA	3	0
40	n	314	LUT	4	0
40	R	311	LUT	5	0
26	b	602	CLA	4	0
28	B	608	BCR	3	0
26	B	617	CLA	2	0
26	Y	316	CLA	3	0
26	C	512	CLA	5	0
26	N	313	CLA	2	0
26	S	315	CLA	1	0
26	G	313	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	g	316	LUT	3	0
26	r	306	CLA	5	0
28	H	101	BCR	2	0
26	b	601	CLA	6	0
39	R	315	CHL	1	0
26	B	610	CLA	7	0
28	K	101	BCR	5	0
26	R	309	CLA	2	0
26	C	519	CLA	1	0
37	D	408	LHG	6	0
26	C	516	CLA	4	0
37	d	409	LHG	4	0
39	G	303	CHL	3	0
26	b	614	CLA	3	0
39	S	302	CHL	6	0
37	S	317	LHG	2	0
42	S	305	NEX	7	0
40	r	307	LUT	6	0
40	G	316	LUT	1	0
26	y	313	CLA	2	0
26	b	613	CLA	7	0
33	y	308	DGD	2	0
26	b	618	CLA	3	0
40	N	305	LUT	3	0
26	S	311	CLA	2	0
26	C	517	CLA	3	0
26	Y	312	CLA	5	0
41	g	309	XAT	4	0
26	N	318	CLA	3	0
34	c	512	LMG	2	0
33	c	517	DGD	2	0
26	A	403	CLA	1	0
39	G	305	CHL	3	0
26	c	514	CLA	5	0
41	n	316	XAT	4	0
40	y	318	LUT	5	0
26	r	317	CLA	1	0
26	n	305	CLA	2	0
42	N	302	NEX	2	0
39	g	312	CHL	4	0
26	n	304	CLA	2	0
26	G	302	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	N	317	CHL	2	0
26	Y	308	CLA	4	0
39	y	303	CHL	6	0
26	c	506	CLA	5	0
39	G	309	CHL	4	0
26	R	302	CLA	6	0
26	g	302	CLA	2	0
39	s	317	CHL	3	0
26	R	316	CLA	1	0
39	r	301	CHL	2	0
37	Y	306	LHG	4	0
33	B	620	DGD	3	0
42	R	305	NEX	3	0
26	g	317	CLA	6	0
39	n	318	CHL	5	0
26	N	319	CLA	3	0
39	y	305	CHL	3	0
34	B	622	LMG	2	0
26	r	313	CLA	7	0
40	S	301	LUT	3	0
28	k	101	BCR	5	0
26	b	611	CLA	6	0
26	S	309	CLA	2	0
26	a	409	CLA	2	0
26	B	603	CLA	4	0
26	b	607	CLA	5	0
38	e	101	HEM	4	0
26	B	602	CLA	7	0
26	r	314	CLA	3	0
30	D	411	PL9	3	0
39	y	302	CHL	2	0
39	S	313	CHL	3	0
39	N	304	CHL	1	0
39	s	313	CHL	6	0
26	c	520	CLA	3	0
26	a	411	CLA	3	0
26	G	317	CLA	3	0
28	T	101	BCR	6	0
39	g	314	CHL	4	0
34	C	518	LMG	1	0
39	r	318	CHL	2	0
28	B	614	BCR	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	n	315	CLA	2	0
26	c	503	CLA	5	0
41	R	304	XAT	1	0
39	R	301	CHL	2	0
26	N	306	CLA	1	0
39	n	308	CHL	1	0
26	R	308	CLA	4	0
39	s	303	CHL	1	0
26	g	303	CLA	3	0
26	C	511	CLA	4	0
37	d	410	LHG	2	0
26	A	405	CLA	2	0
26	b	606	CLA	3	0
28	c	511	BCR	4	0
26	n	310	CLA	3	0
26	g	305	CLA	1	0
26	B	616	CLA	6	0
28	C	502	BCR	4	0
27	A	404	PHO	2	0
26	c	510	CLA	2	0
41	N	315	XAT	6	0
26	C	507	CLA	5	0
26	b	616	CLA	1	0
27	a	410	PHO	1	0
37	y	301	LHG	4	0
38	E	101	HEM	5	0
26	B	618	CLA	7	0
26	y	317	CLA	1	0
26	c	502	CLA	4	0
26	D	412	CLA	3	0
39	G	318	CHL	7	0
26	Y	311	CLA	1	0
26	b	612	CLA	2	0
26	c	513	CLA	3	0
37	d	402	LHG	4	0
39	g	313	CHL	5	0
40	s	312	LUT	3	0
26	R	306	CLA	4	0
34	d	405	LMG	2	0
26	r	308	CLA	1	0
26	S	307	CLA	3	0
26	Y	313	CLA	3	0

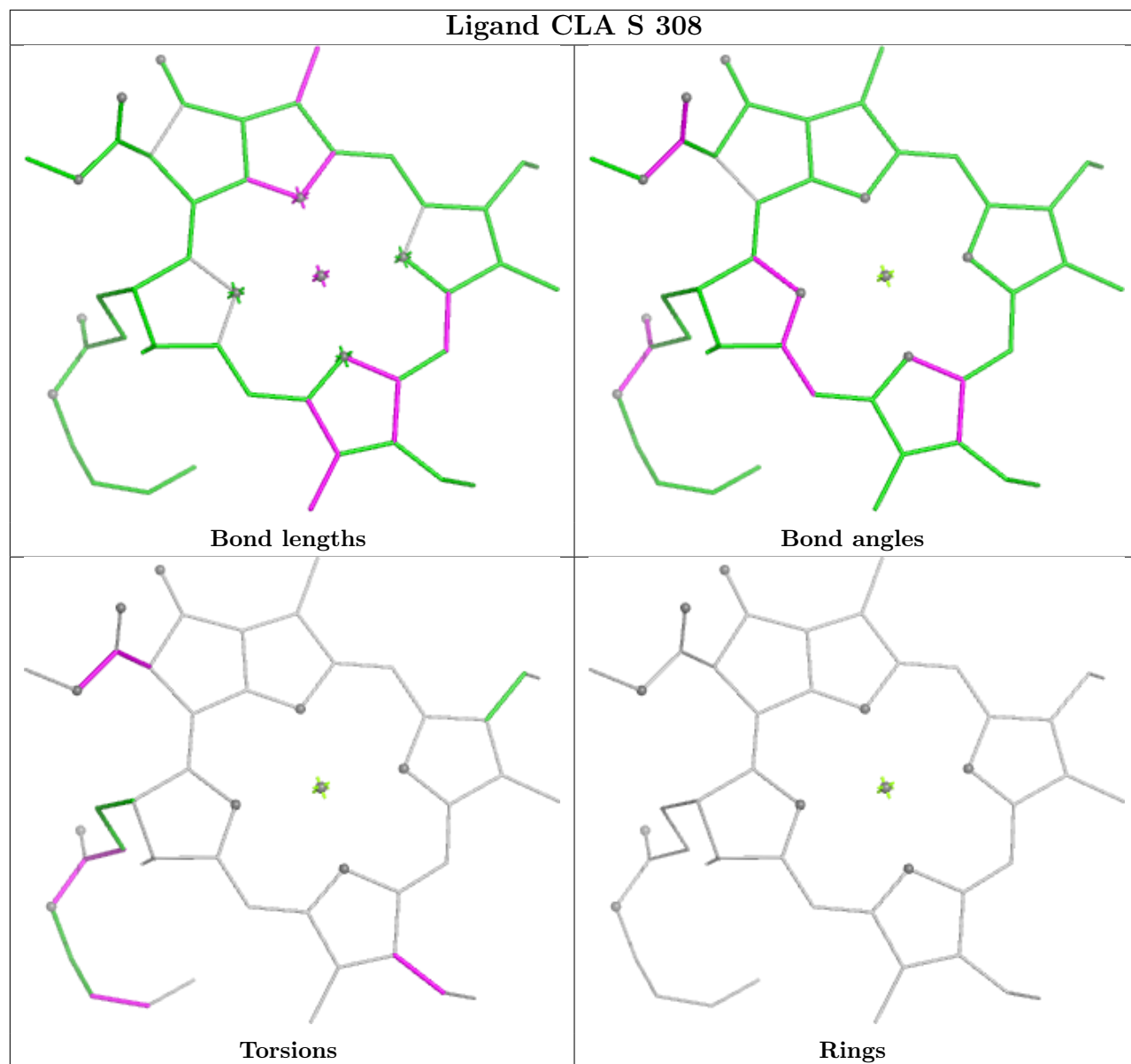
Continued on next page...

Continued from previous page...

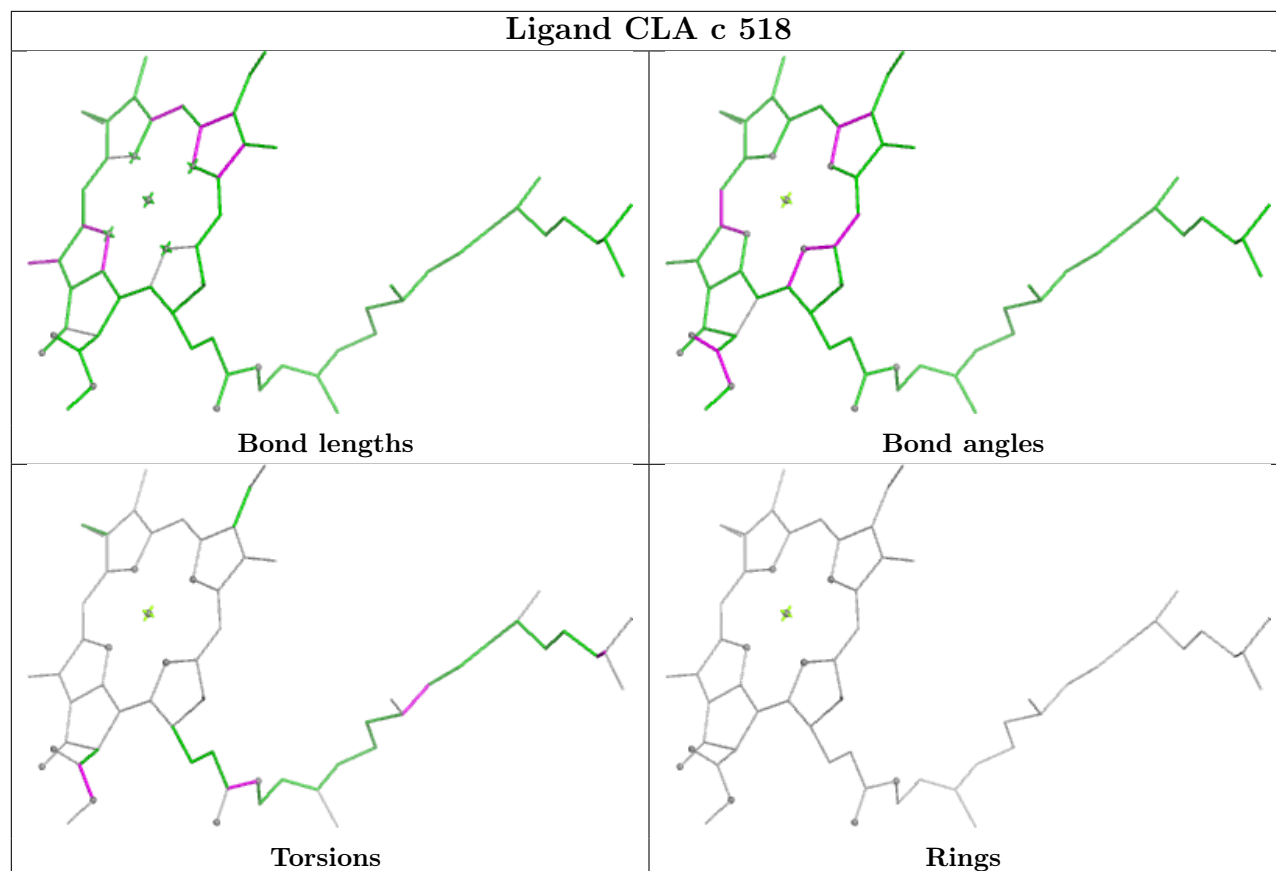
Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	r	304	XAT	2	0
39	r	309	CHL	3	0
29	B	621	SQD	2	0
42	y	307	NEX	3	0
26	D	409	CLA	9	0
40	G	308	LUT	4	0
42	s	302	NEX	6	0
26	Y	301	CLA	3	0
26	y	315	CLA	2	0
26	y	310	CLA	6	0
26	n	302	CLA	2	0
26	c	505	CLA	6	0
26	y	306	CLA	3	0
26	g	304	CLA	1	0
37	L	101	LHG	2	0
40	s	308	LUT	2	0
39	g	307	CHL	4	0
39	g	319	CHL	3	0
28	c	507	BCR	3	0
39	y	312	CHL	2	0
41	G	310	XAT	6	0
39	R	312	CHL	3	0
26	B	604	CLA	2	0
34	w	201	LMG	2	0
40	y	311	LUT	6	0
26	b	617	CLA	6	0
28	B	619	BCR	5	0

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

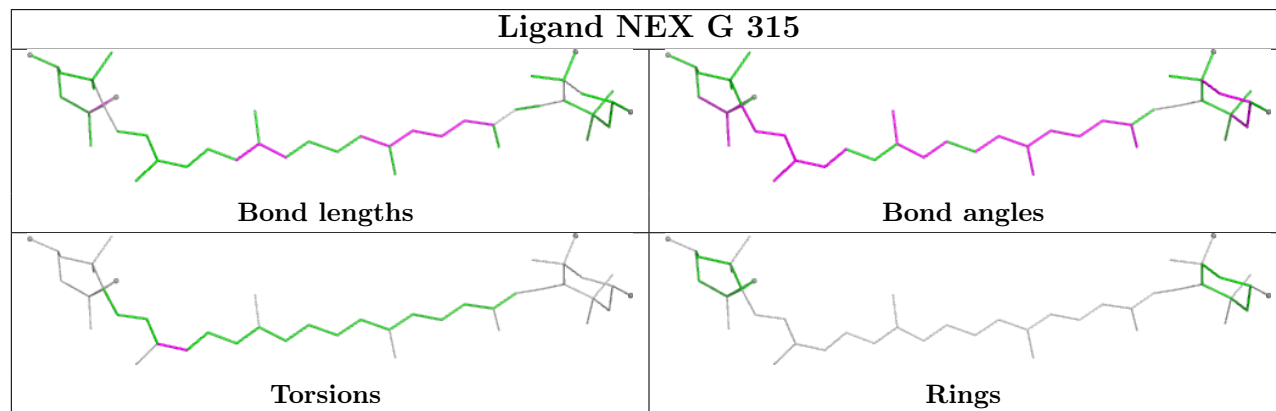
Ligand CLA S 308



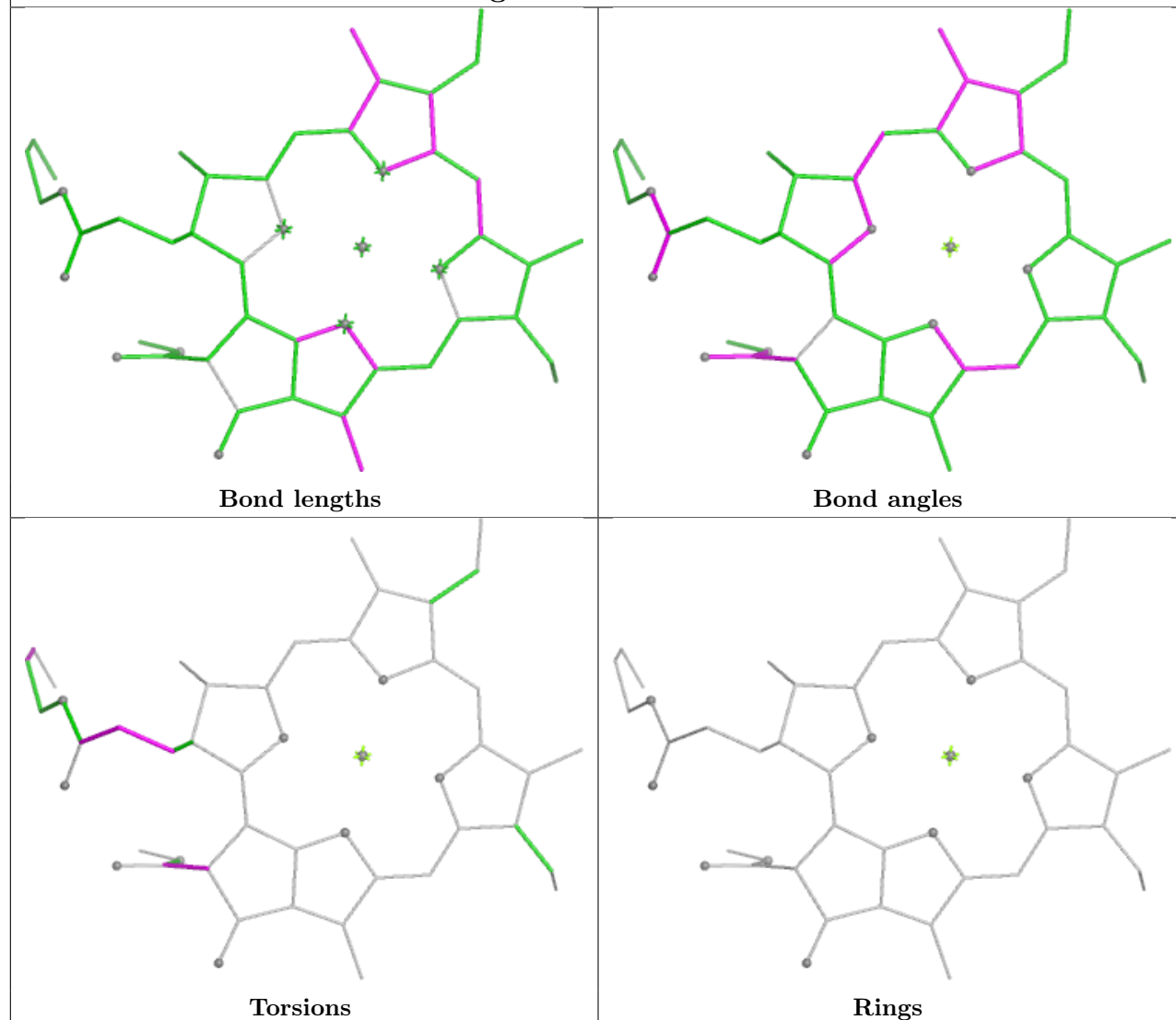
Ligand CLA c 518



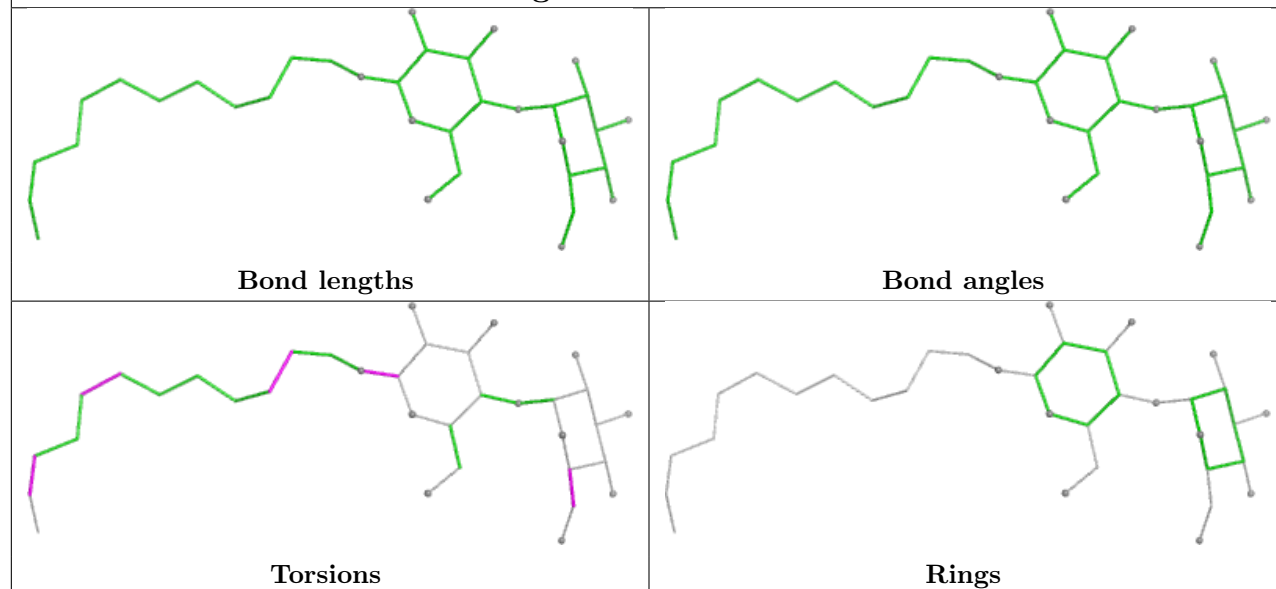
Ligand NEX G 315

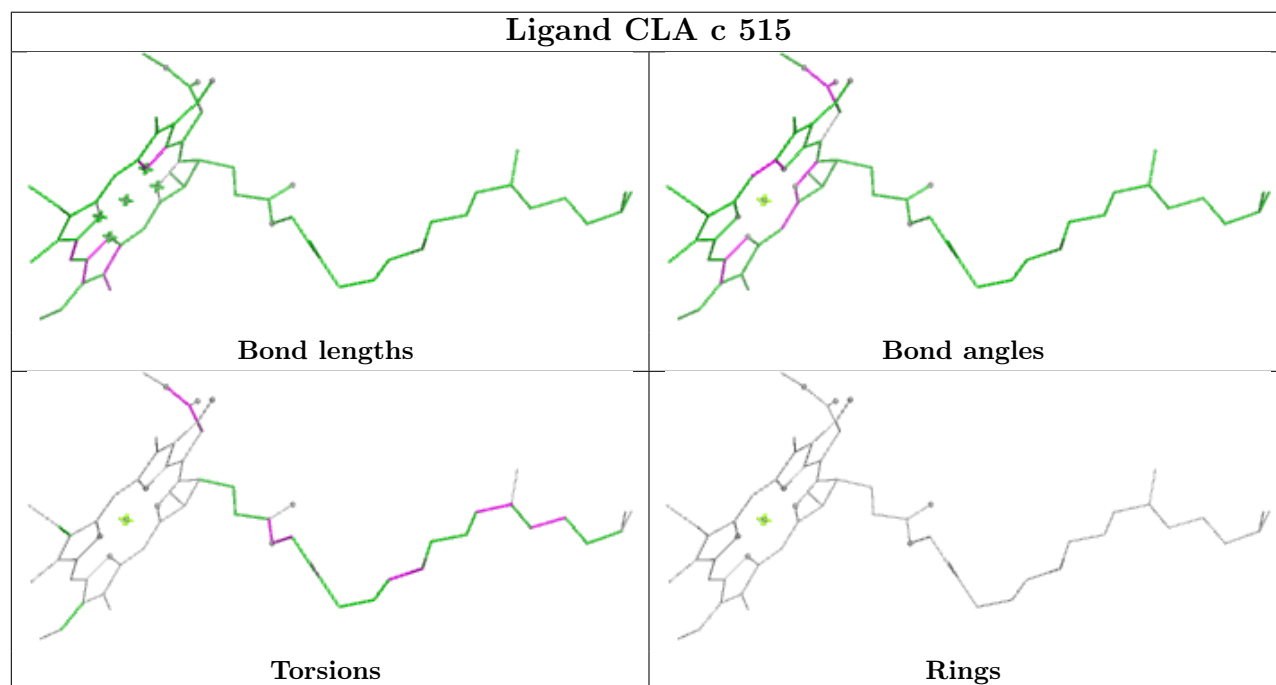
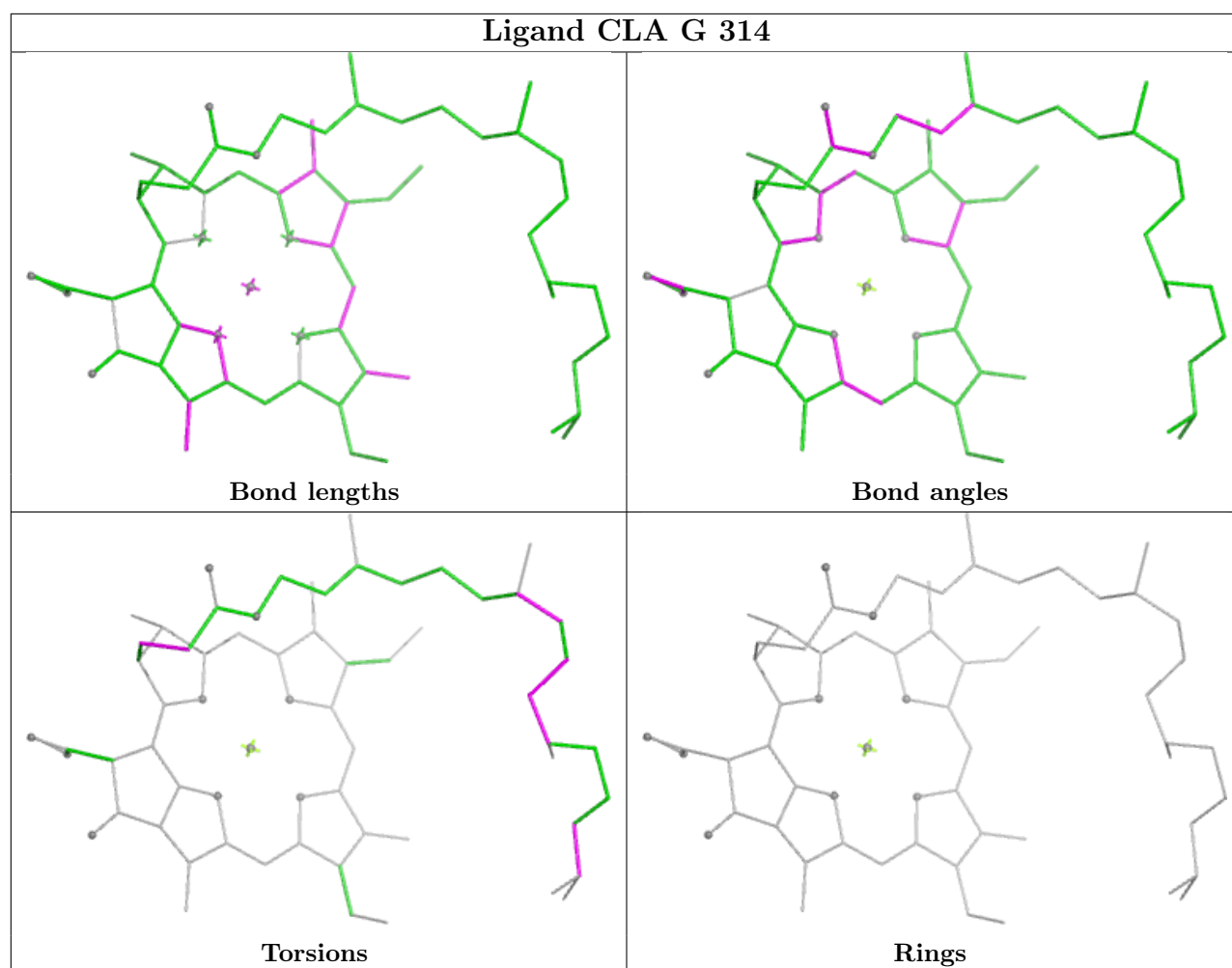


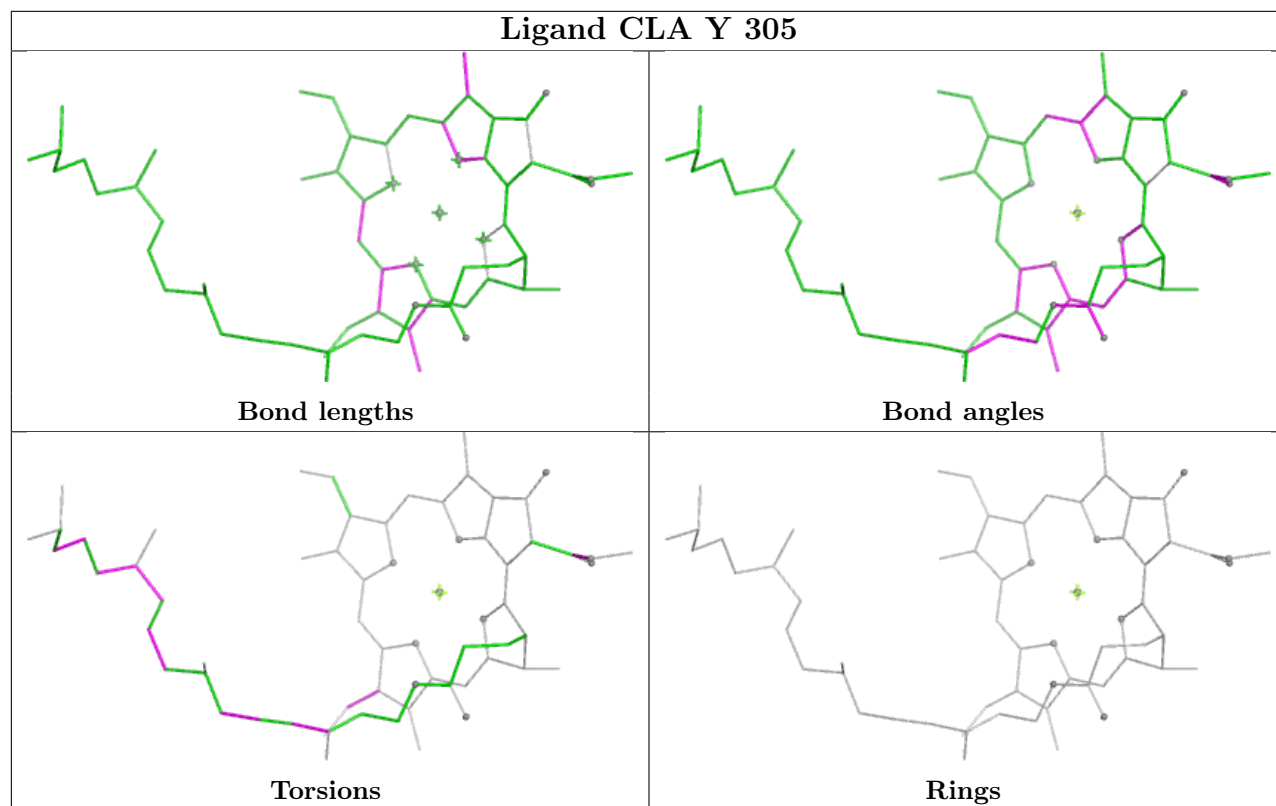
Ligand CLA R 317

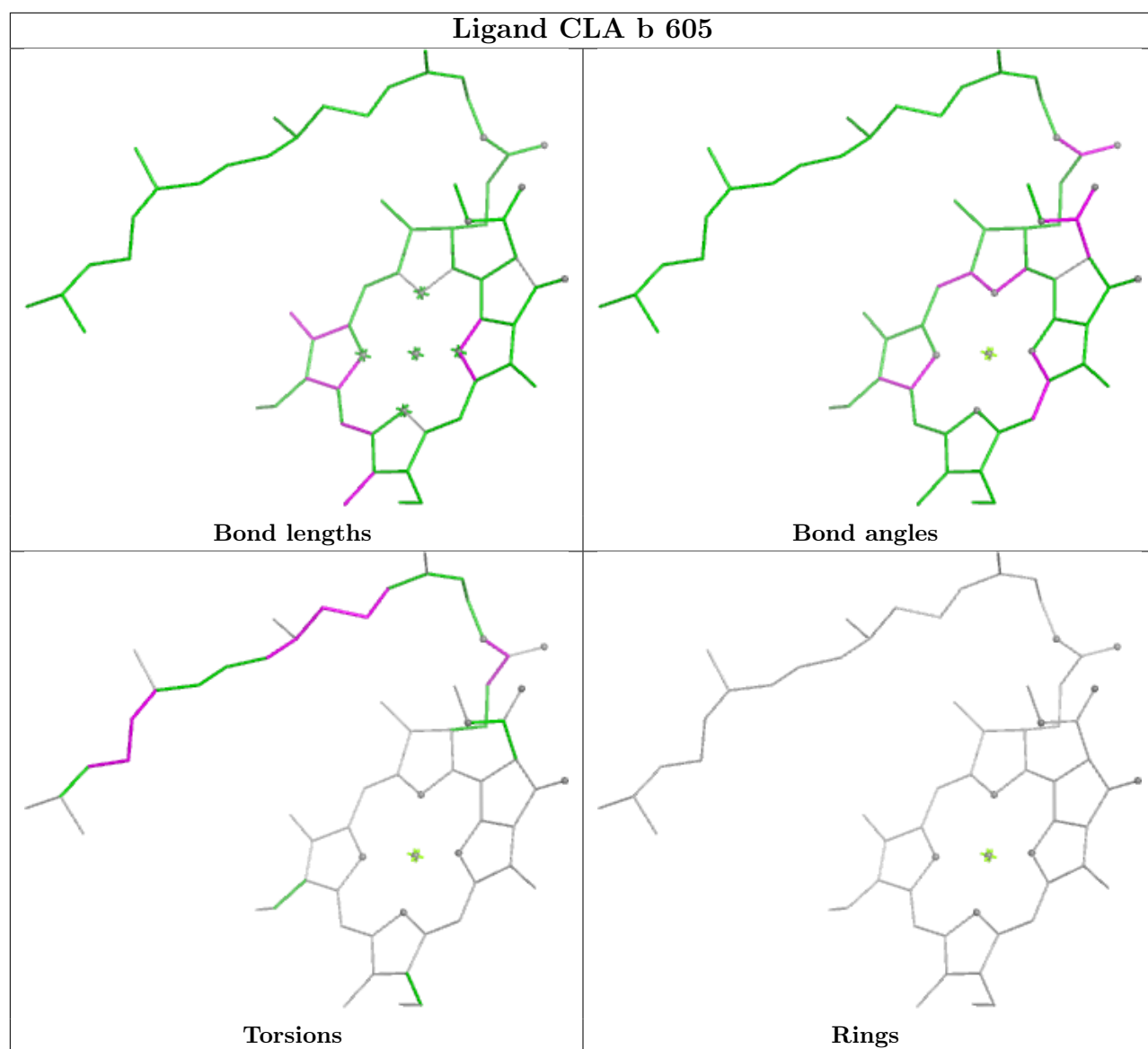


Ligand LMT d 406

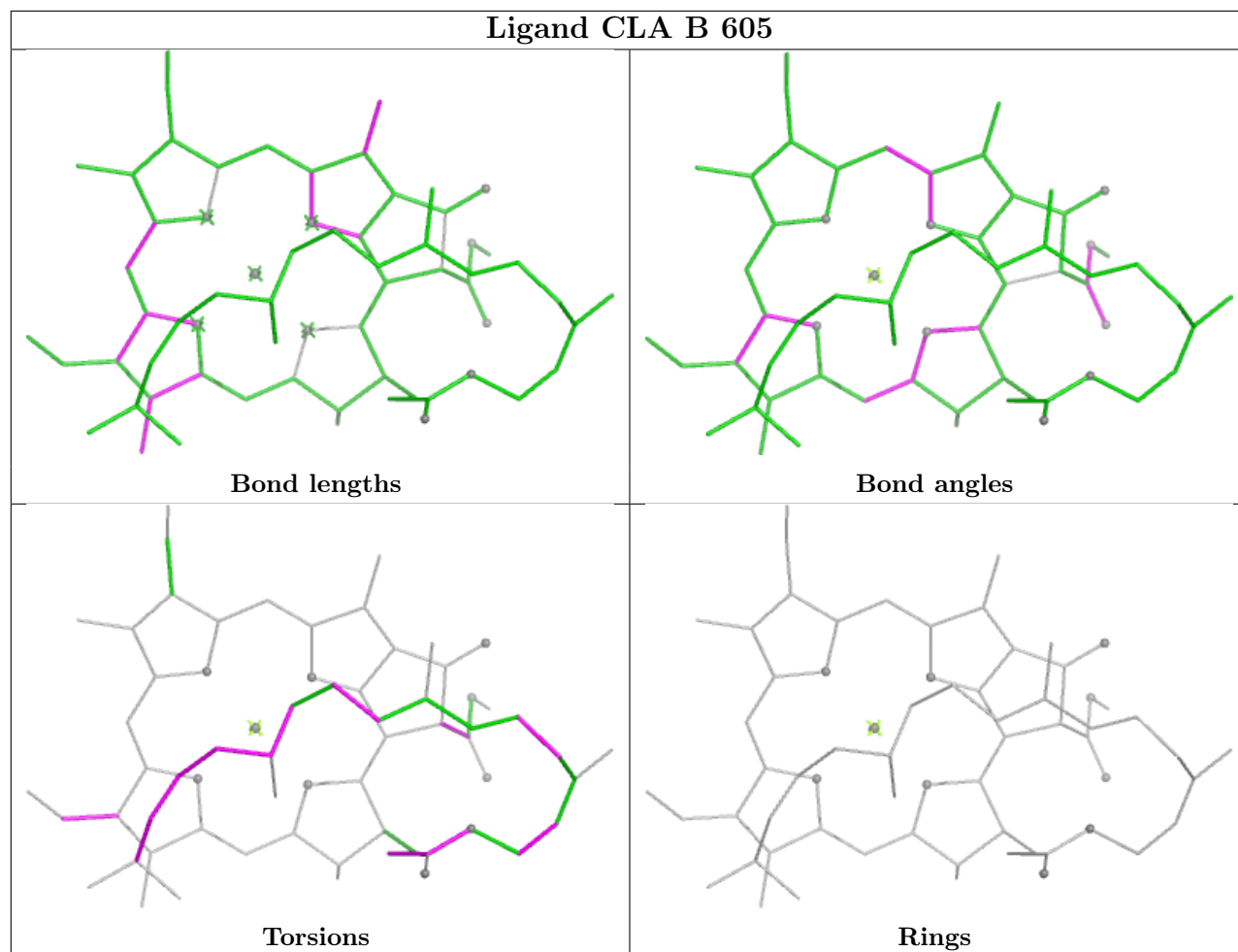


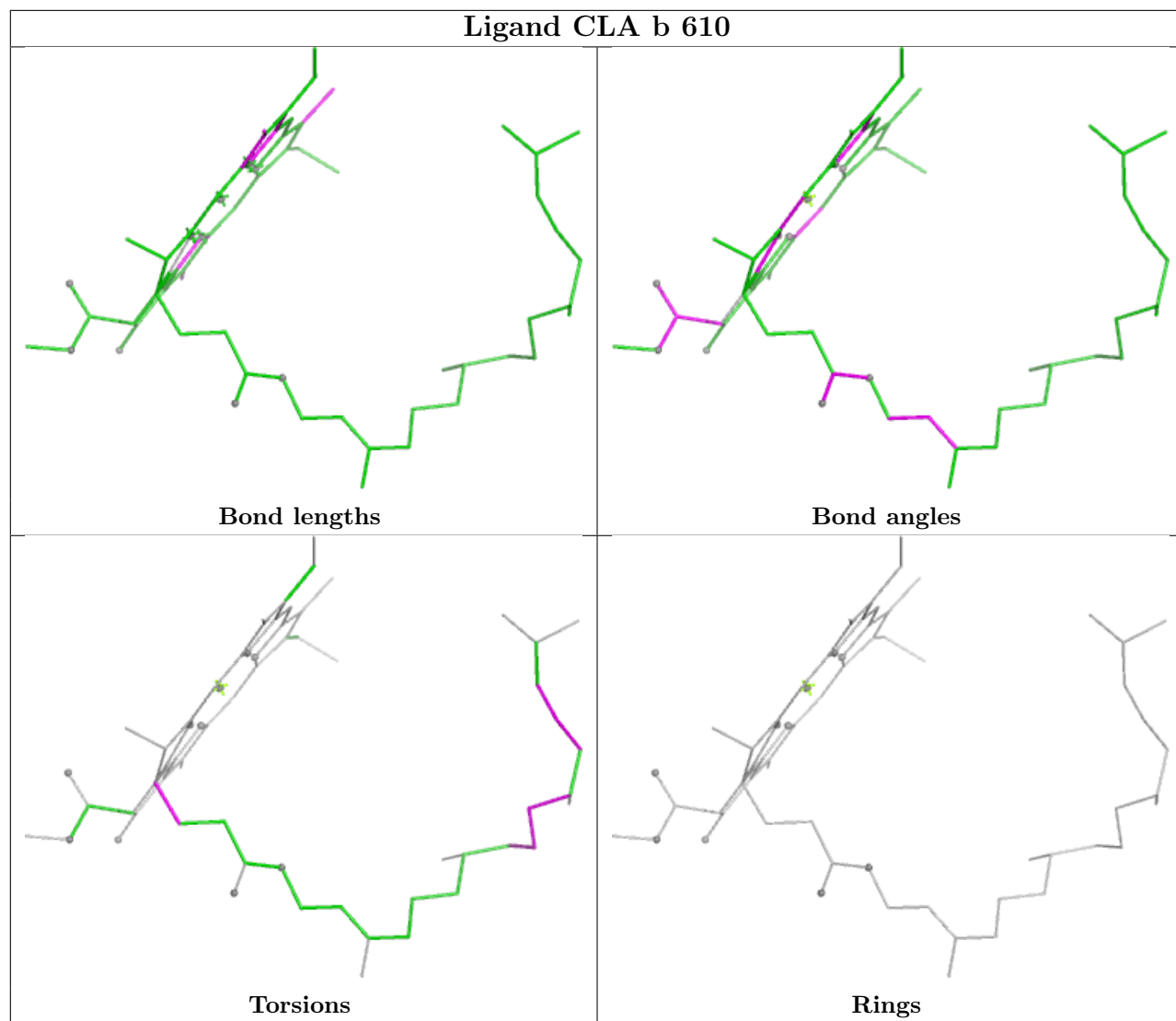


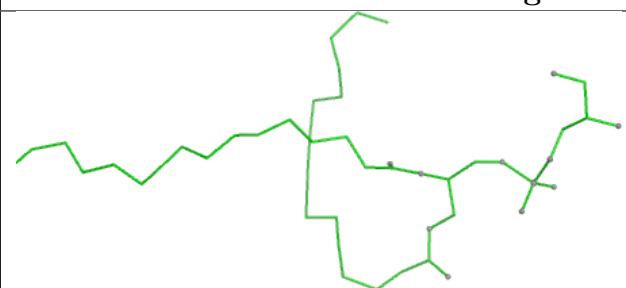
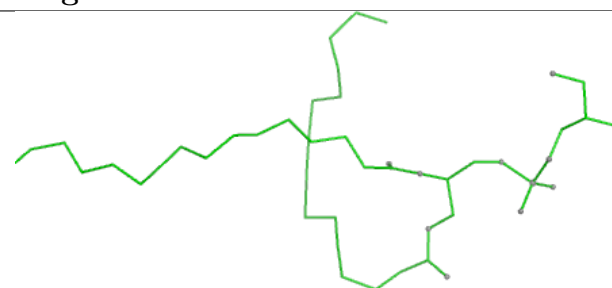
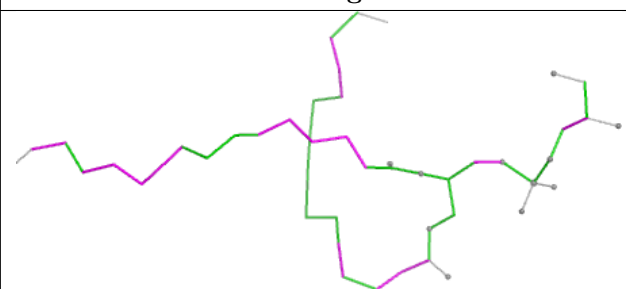
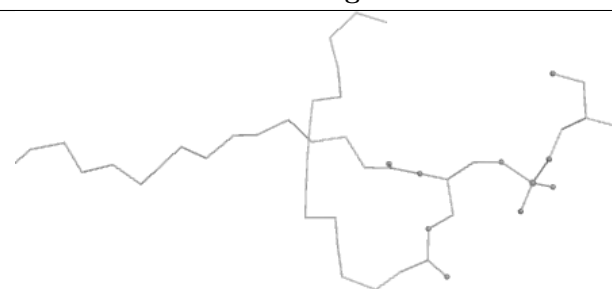


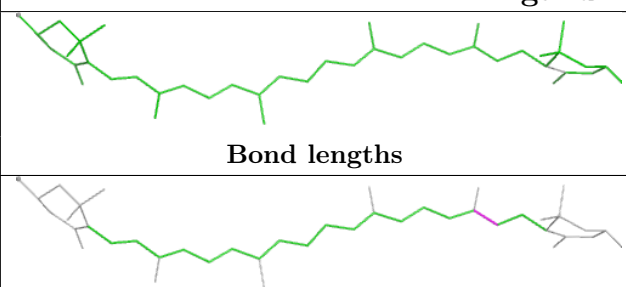
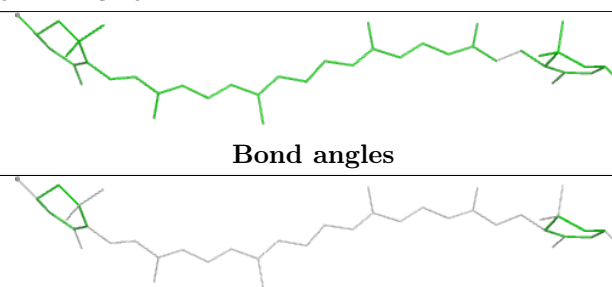
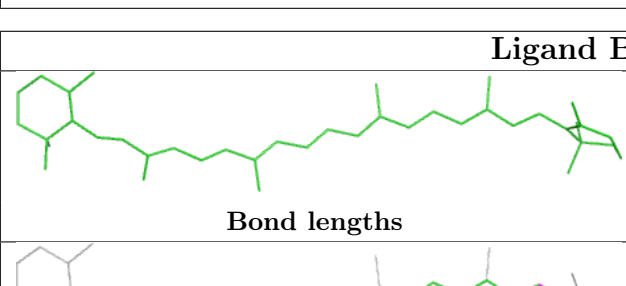
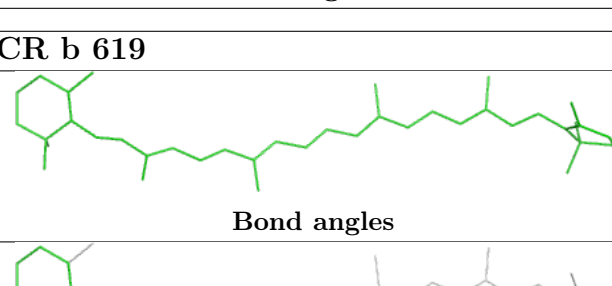


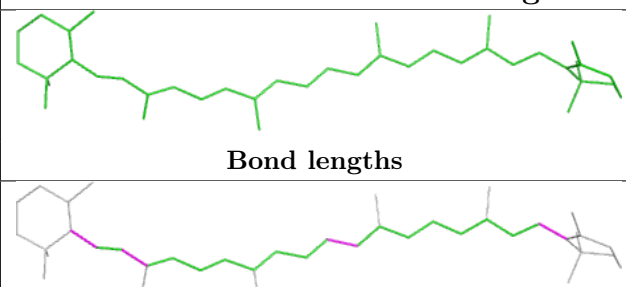
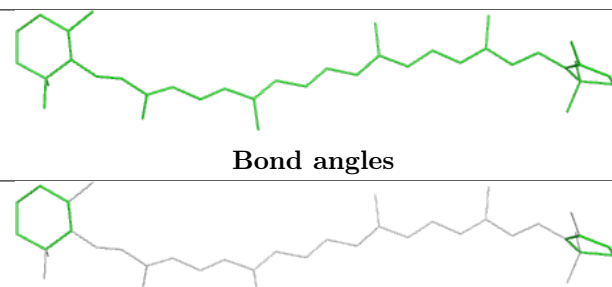
Ligand CLA B 605

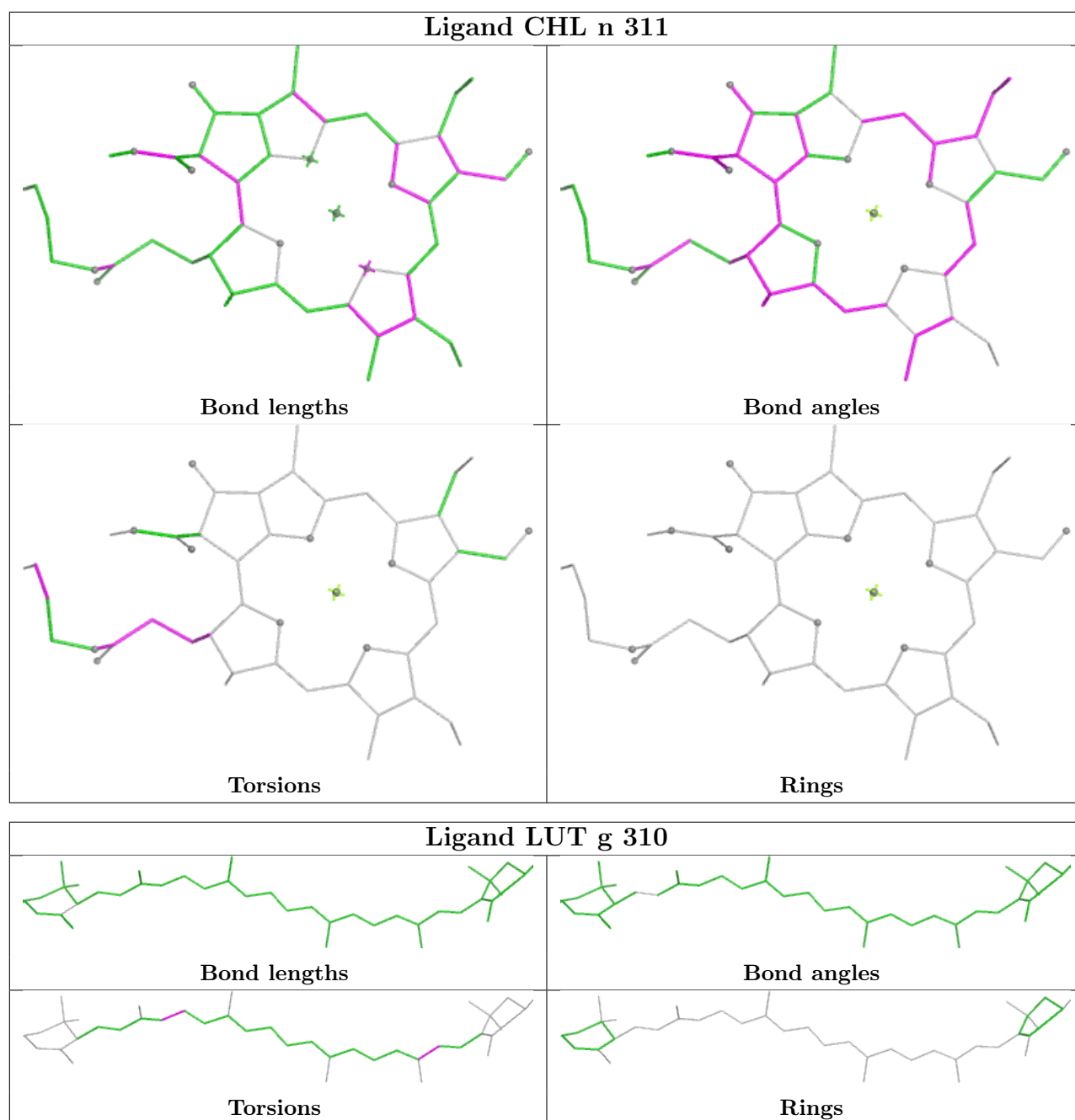




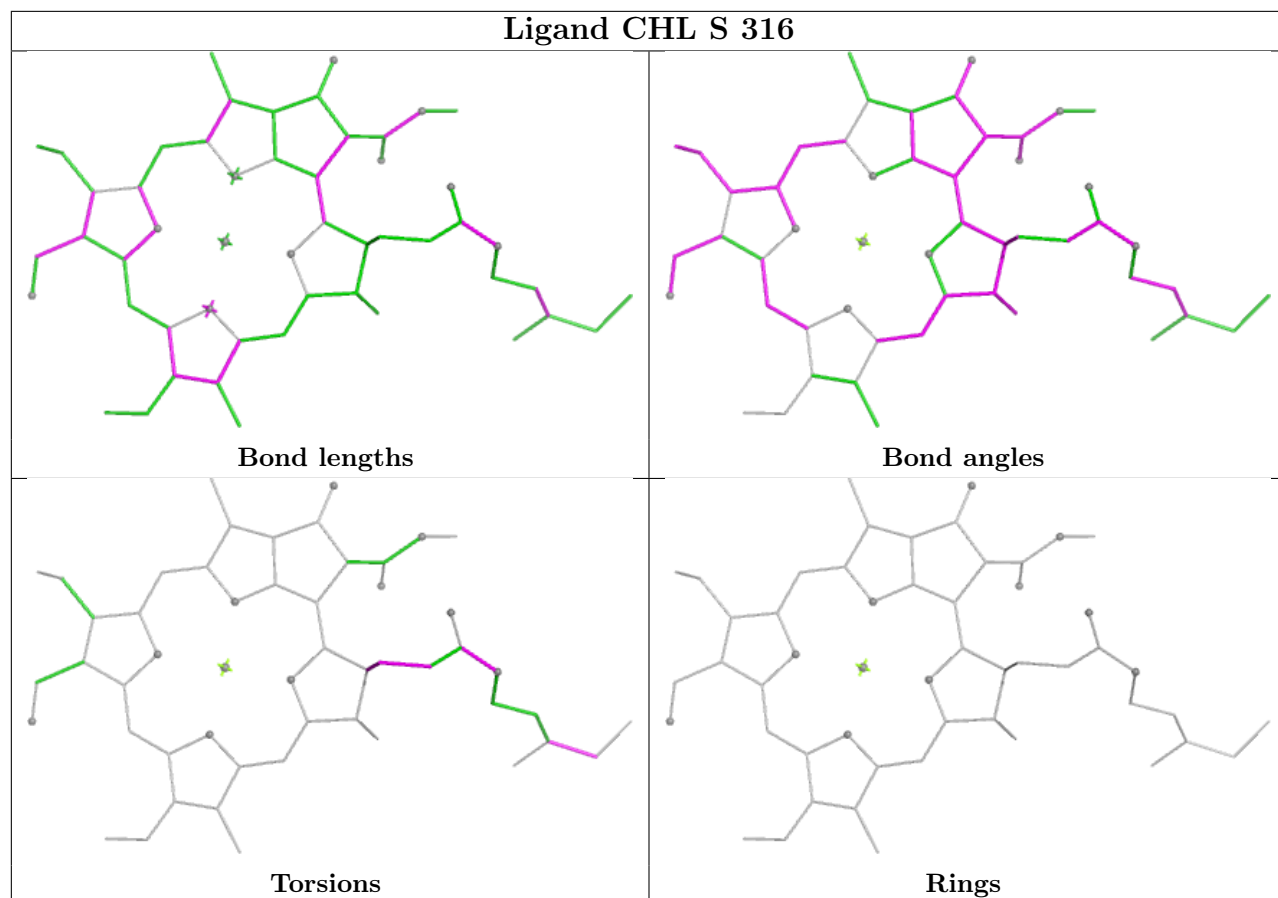
Ligand LHG g 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT Y 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

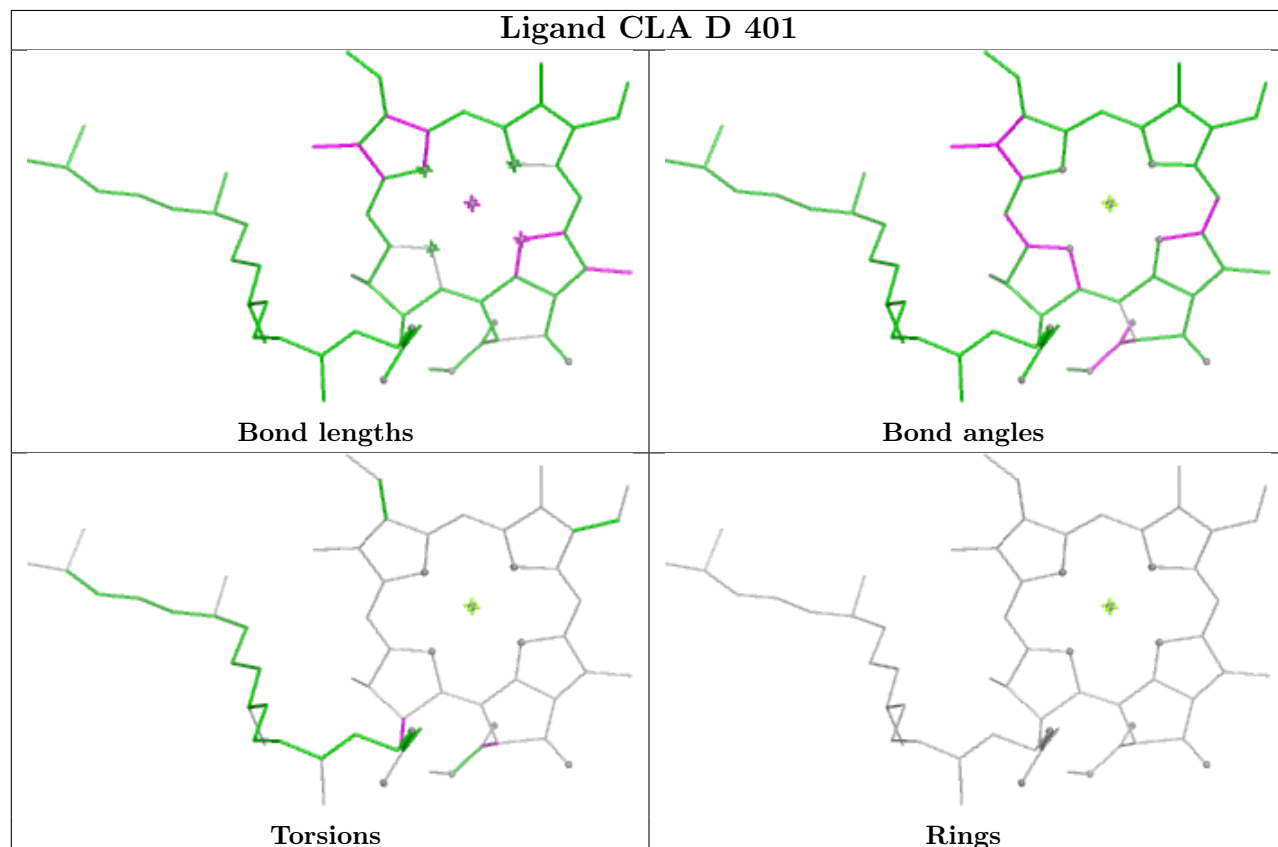
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

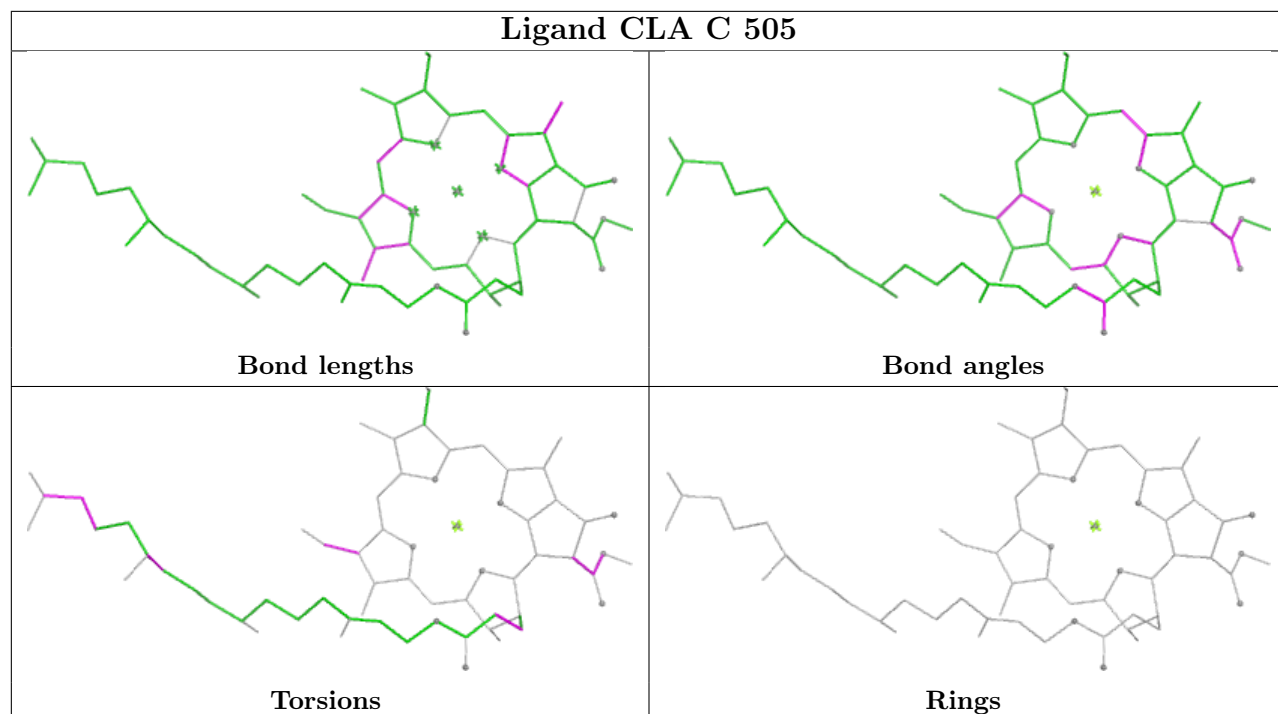
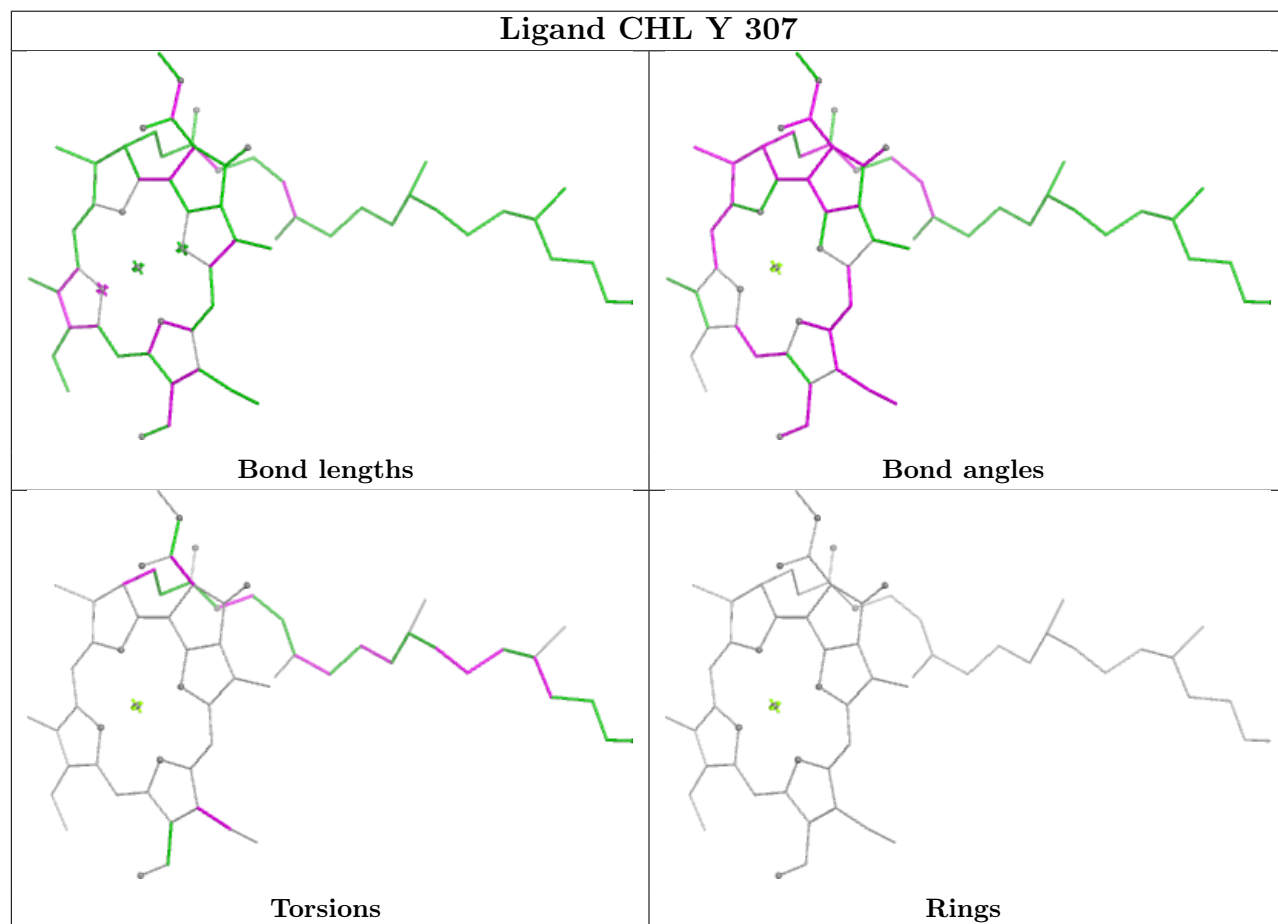


Ligand CHL S 316

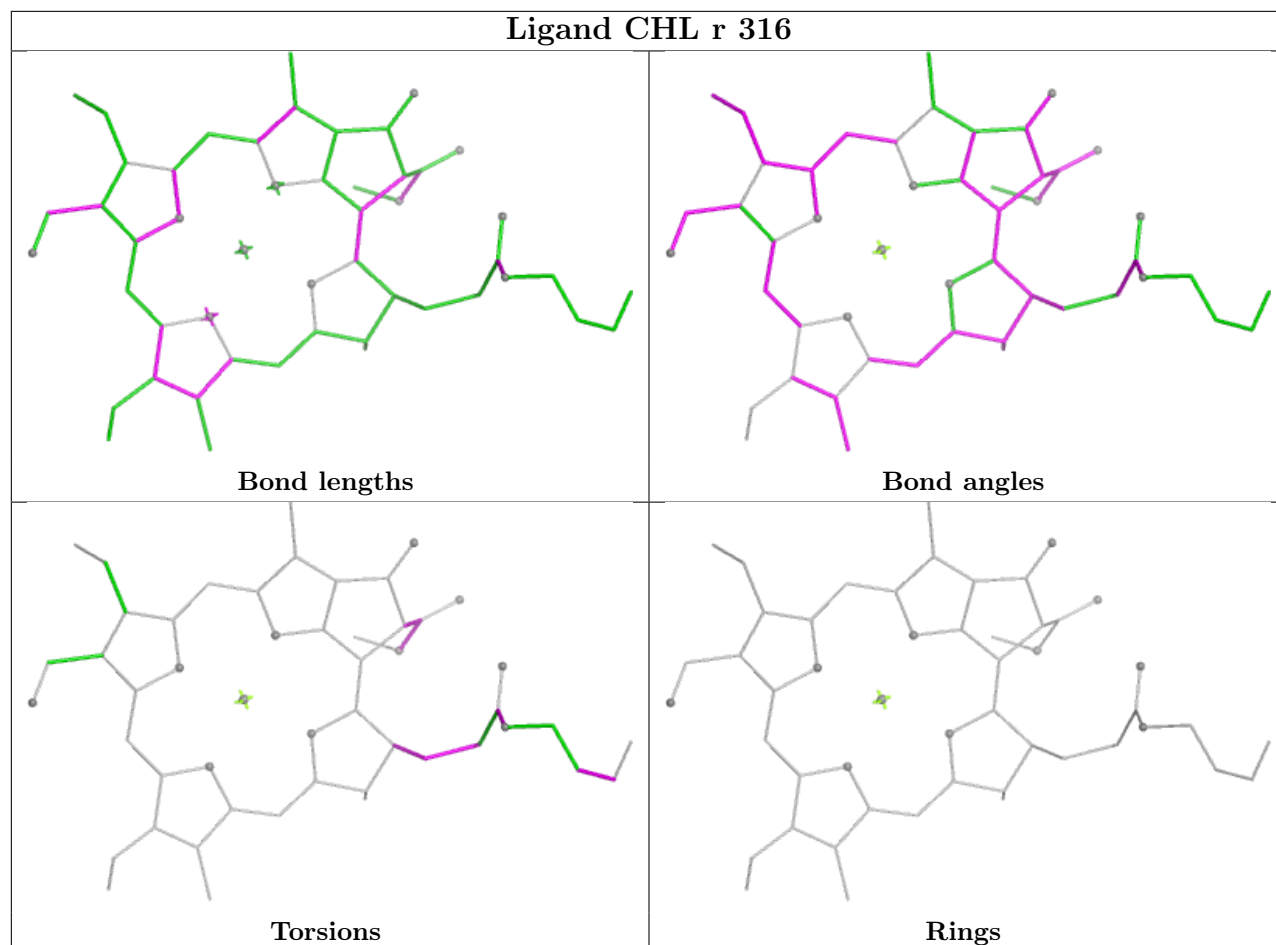


Ligand CLA D 401

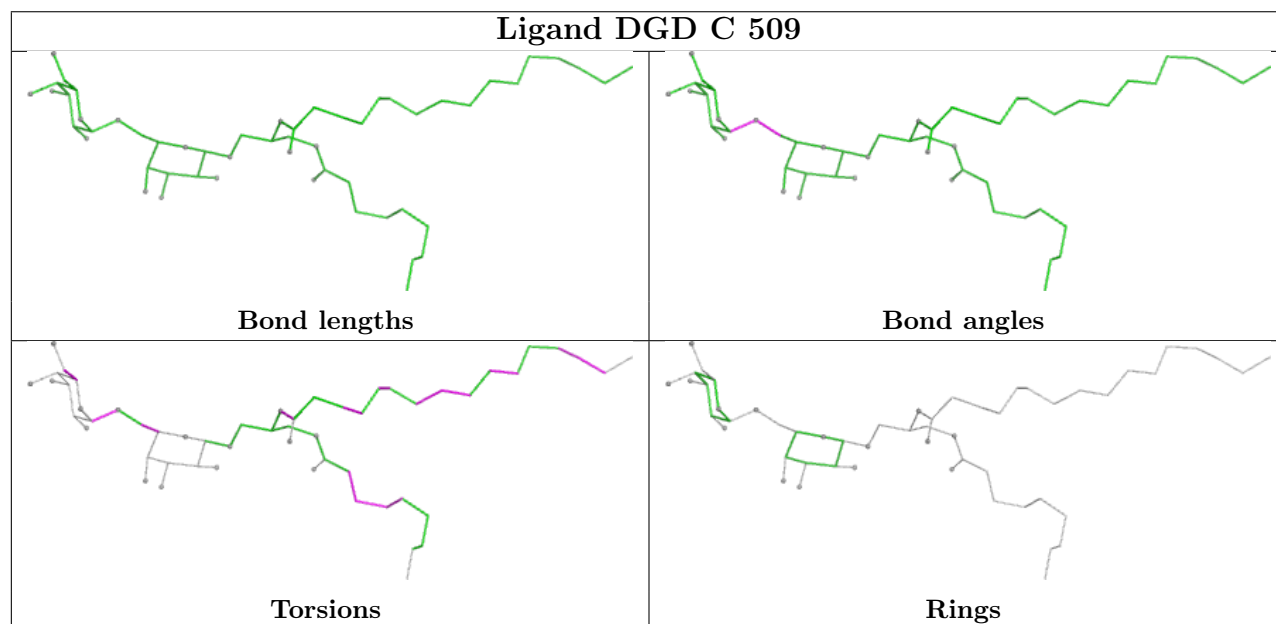


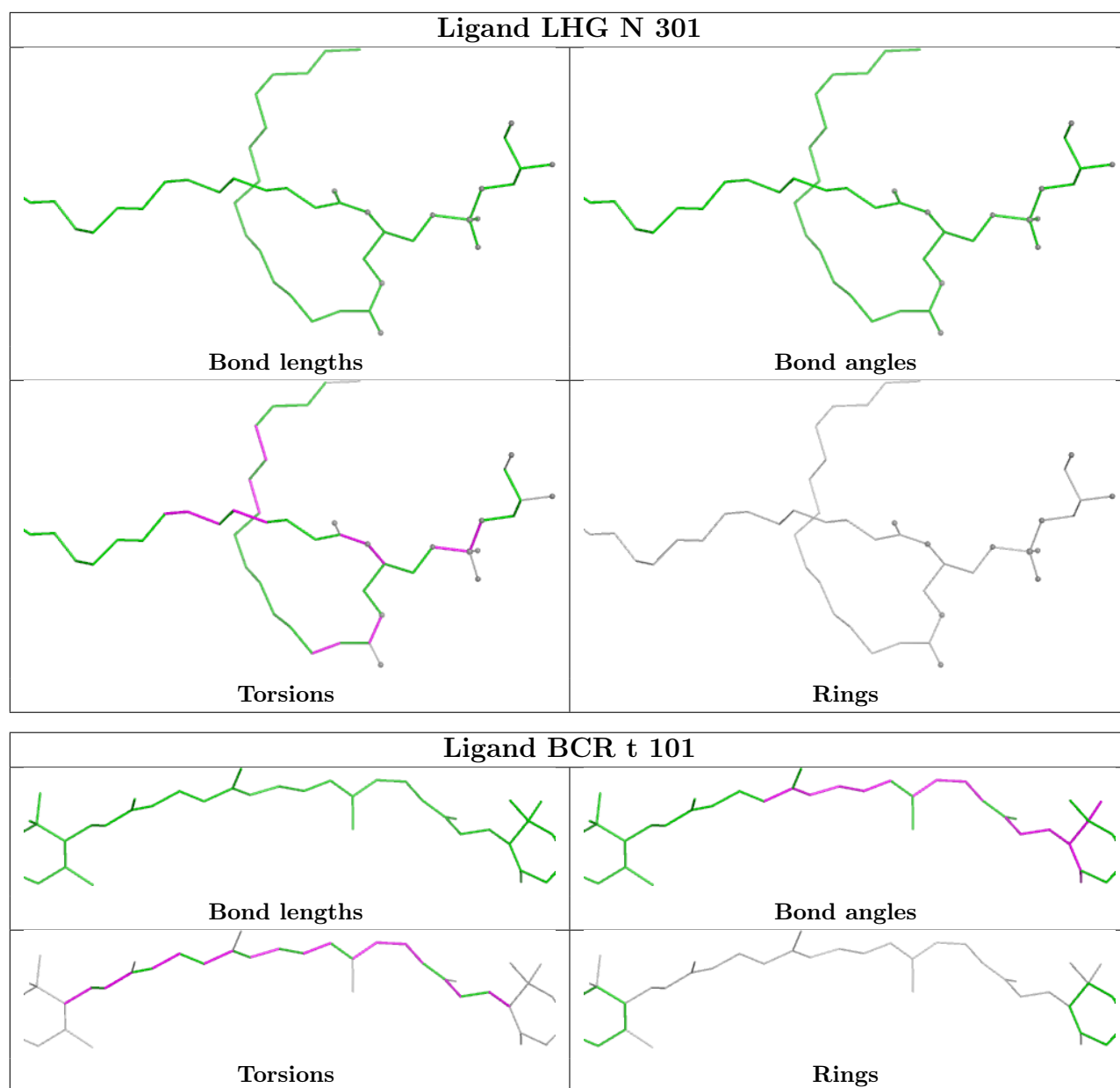
Ligand CLA C 505**Ligand CHL Y 307**

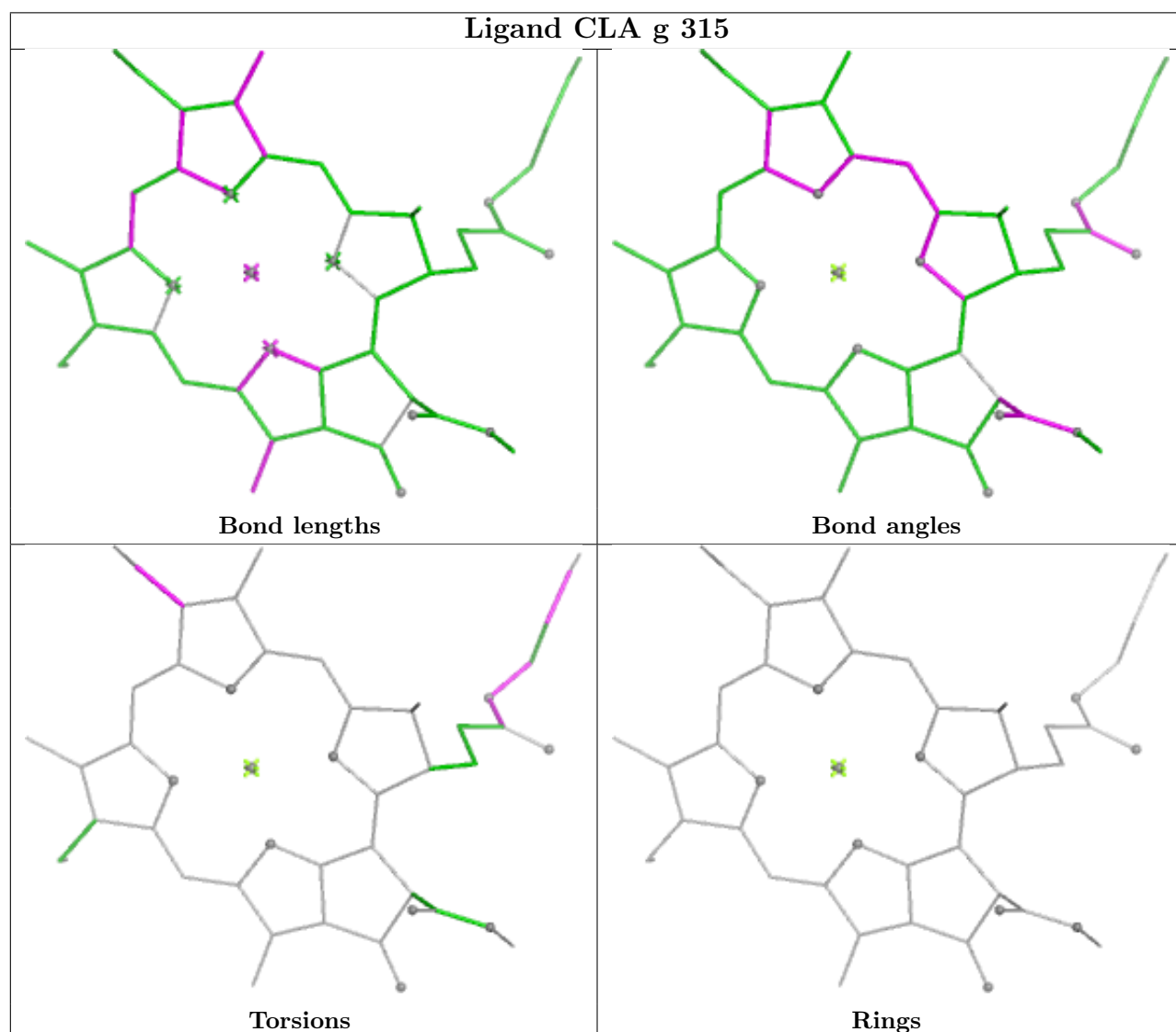
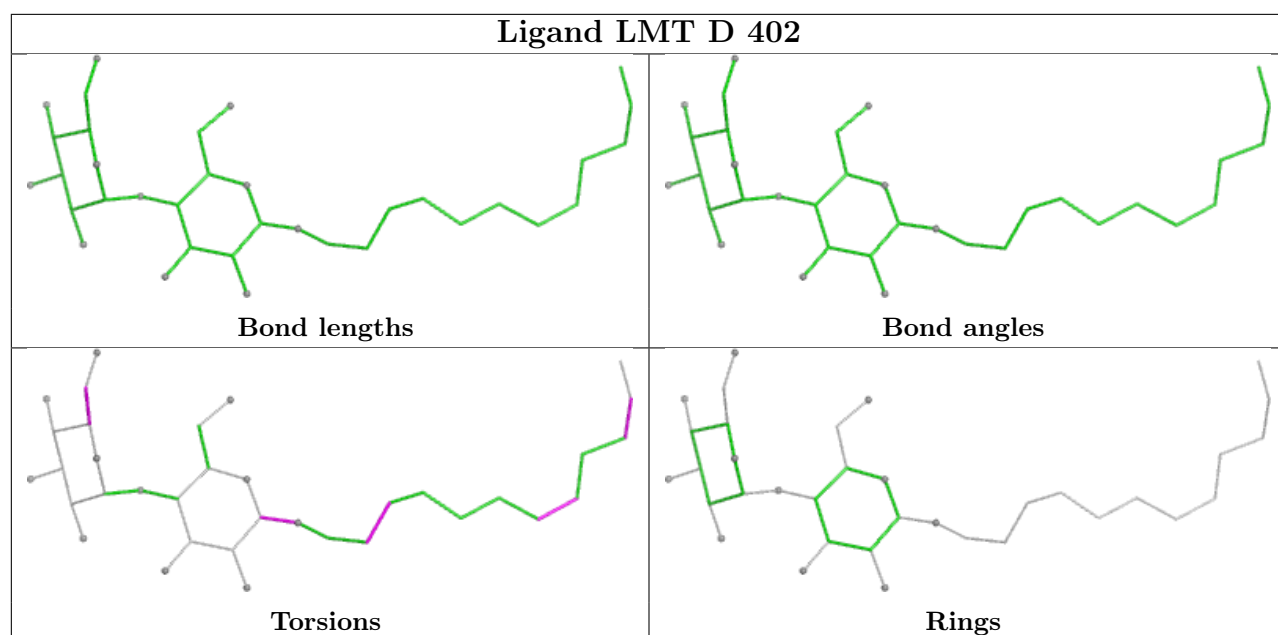
Ligand CHL r 316

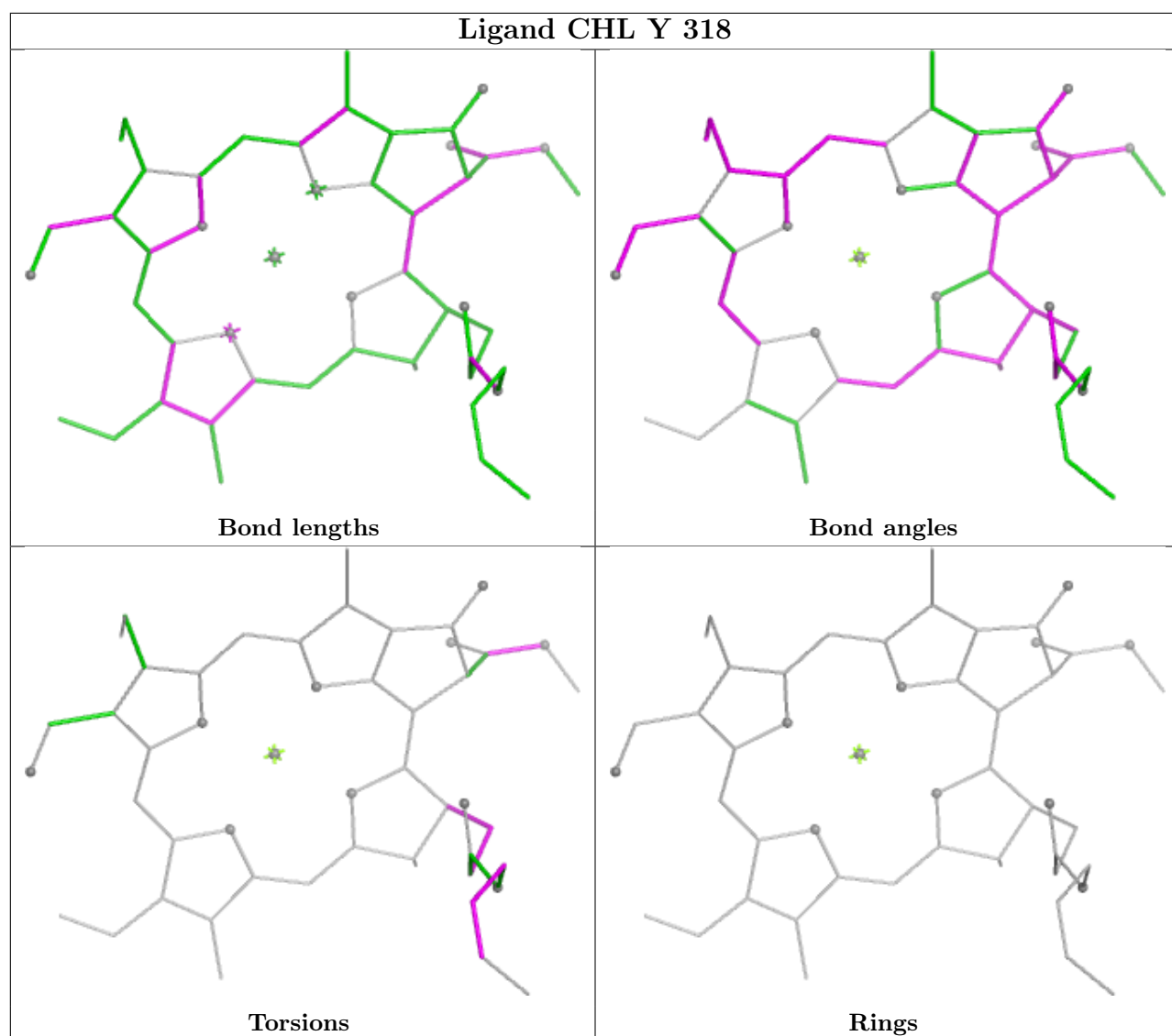


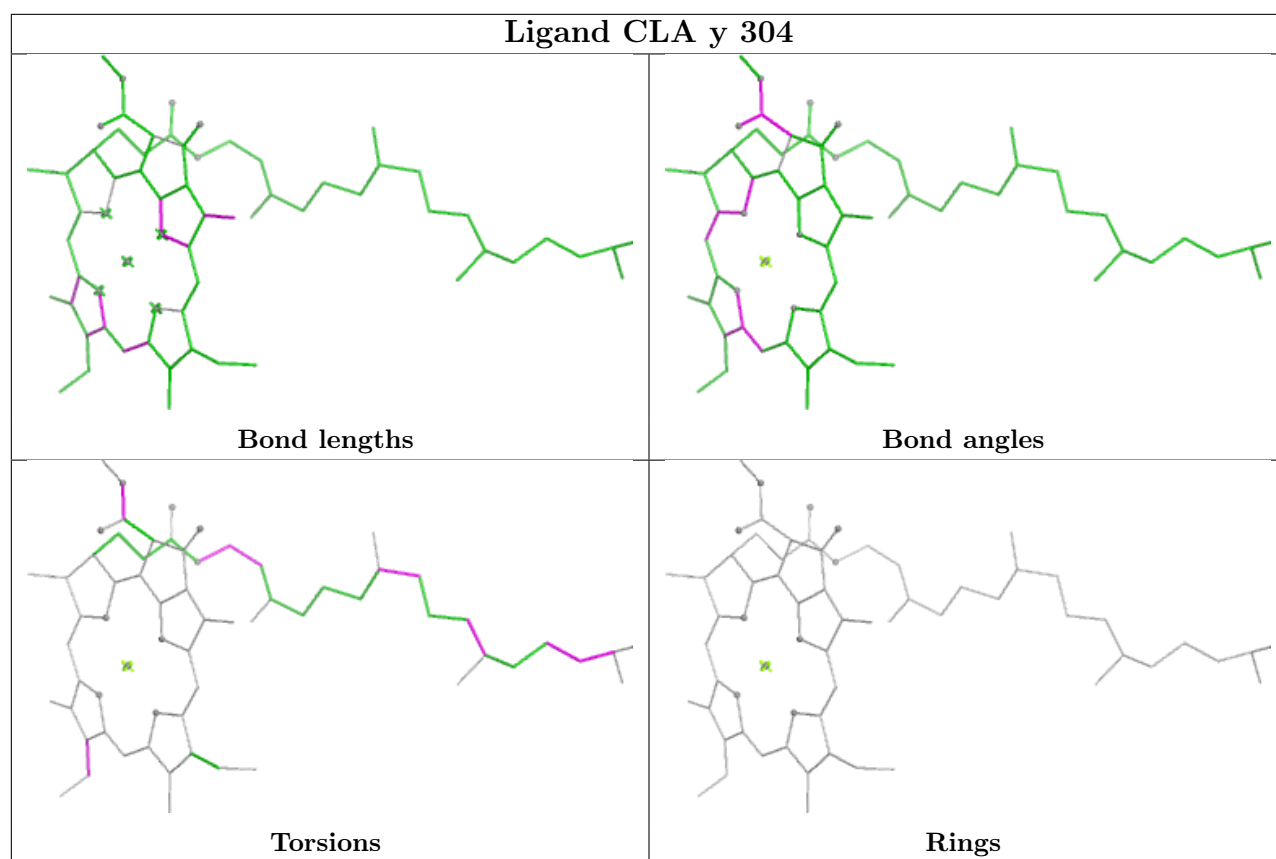
Ligand DGD C 509

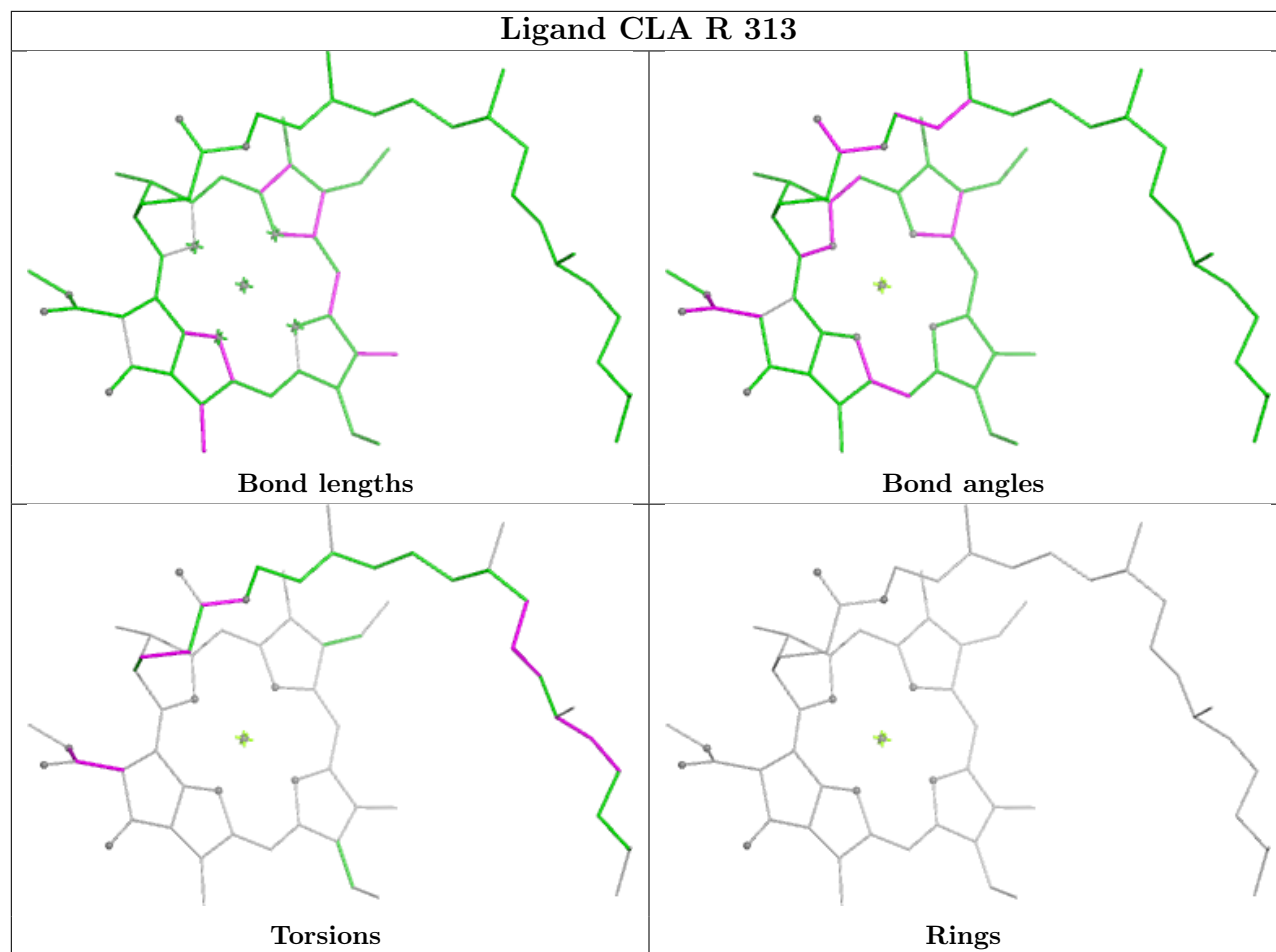
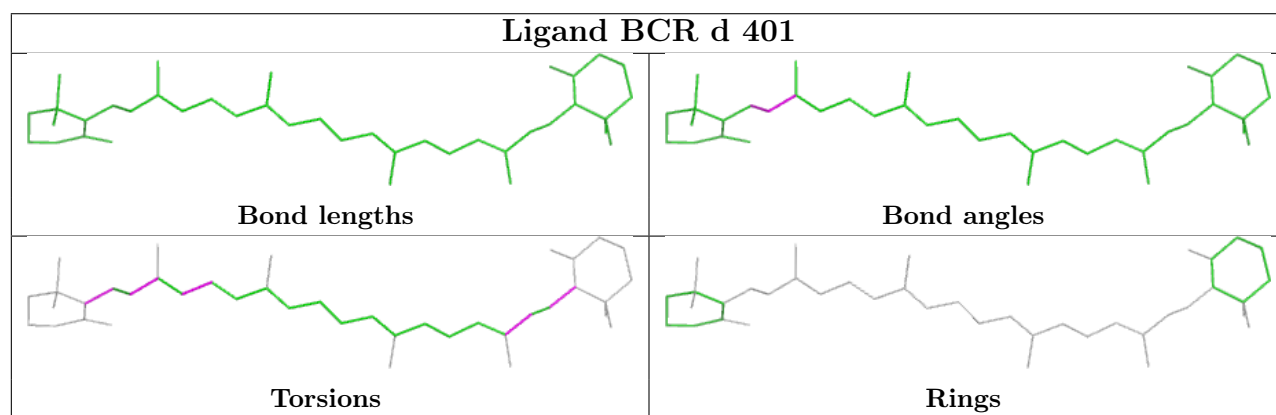


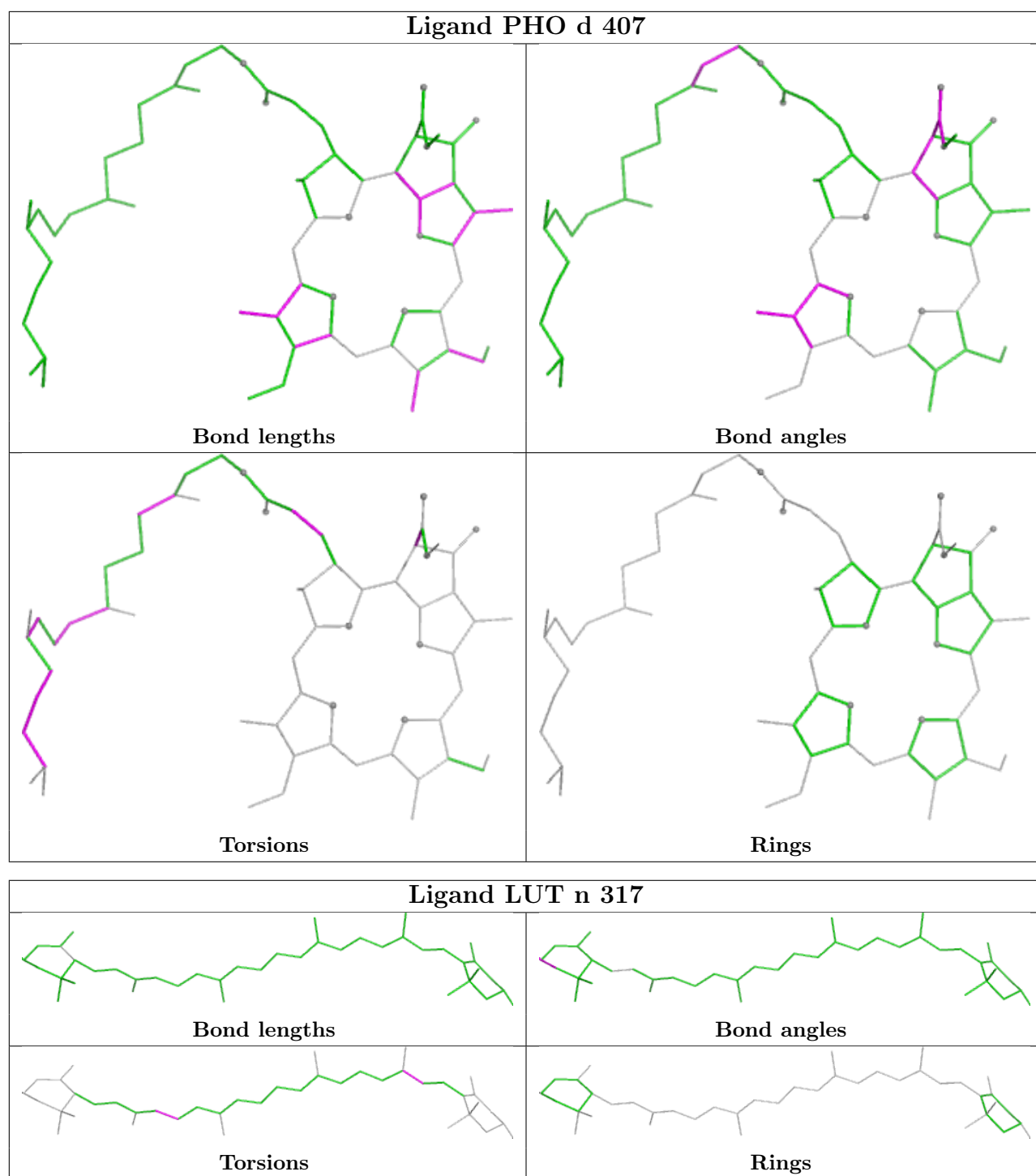


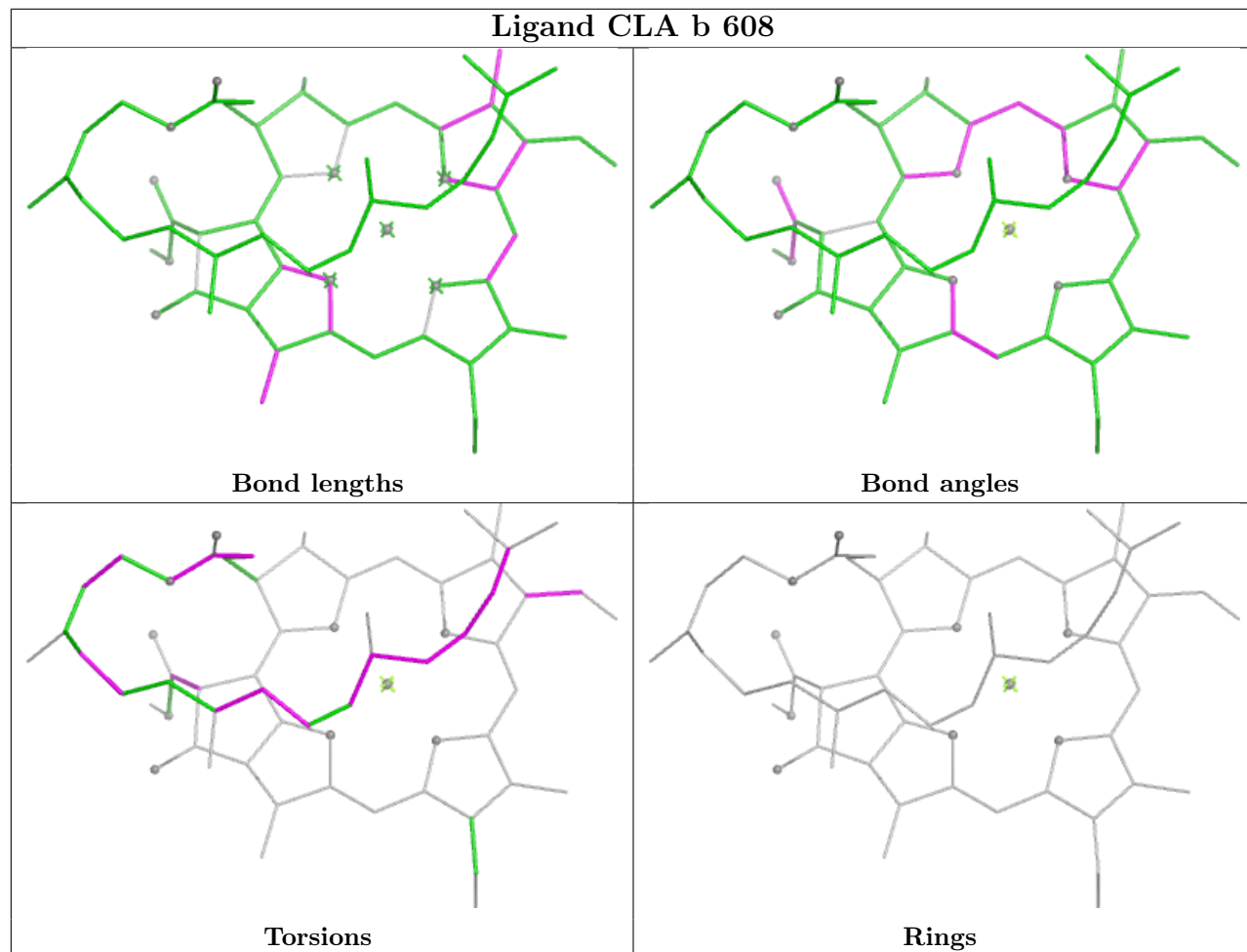
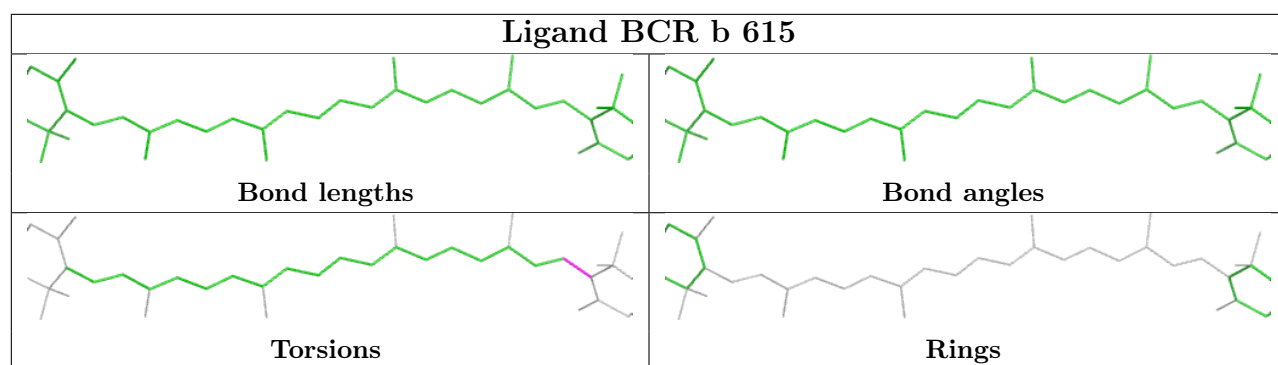


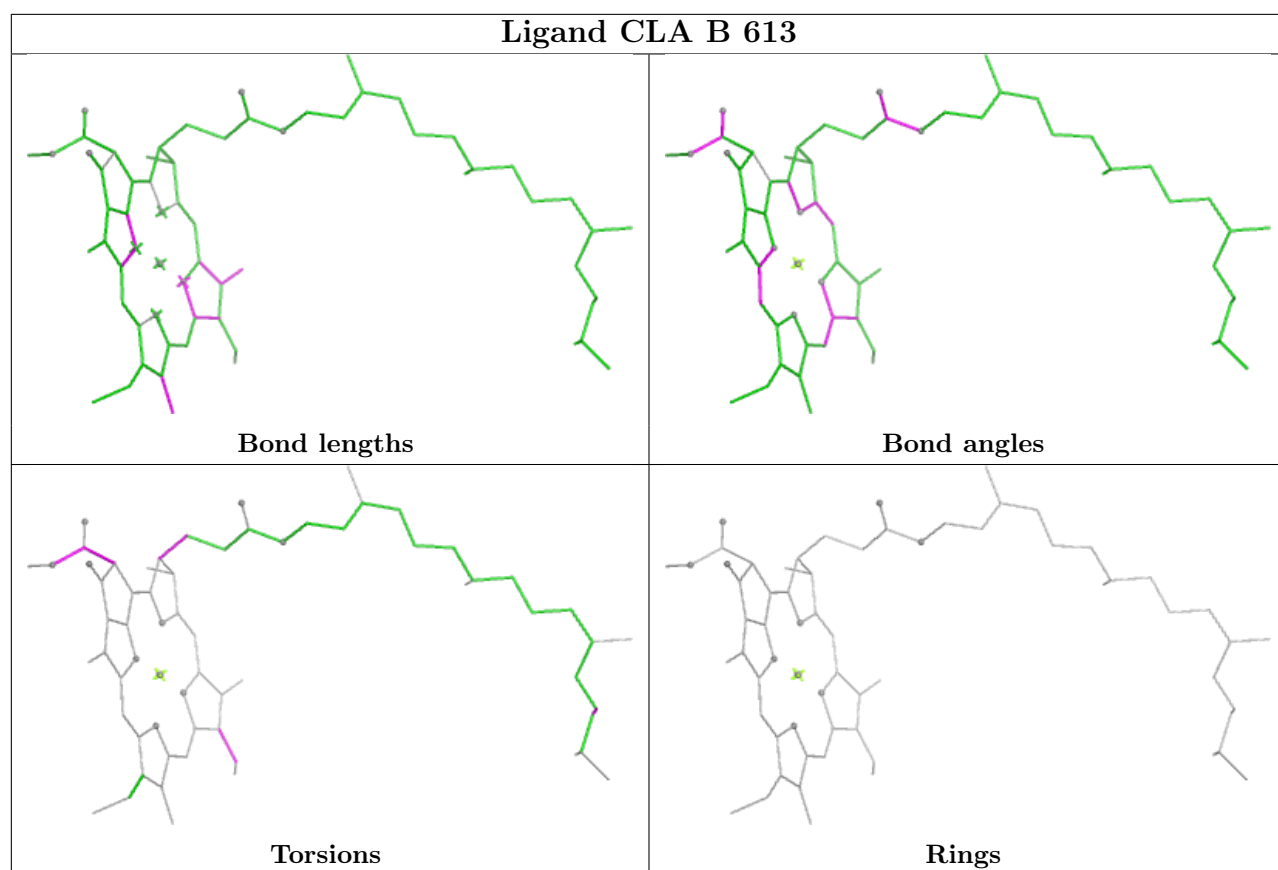




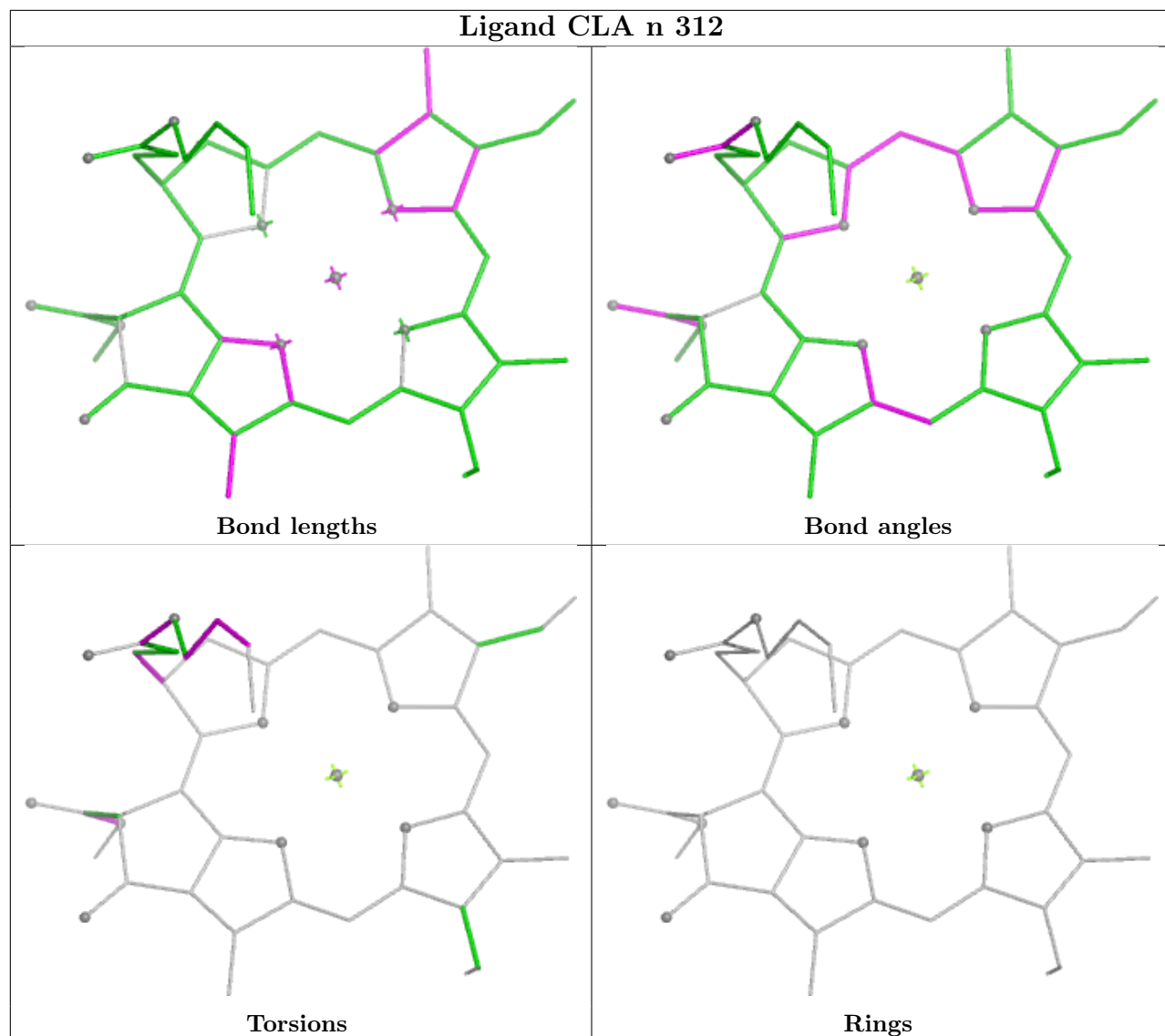
Ligand CLA R 313**Ligand BCR d 401**

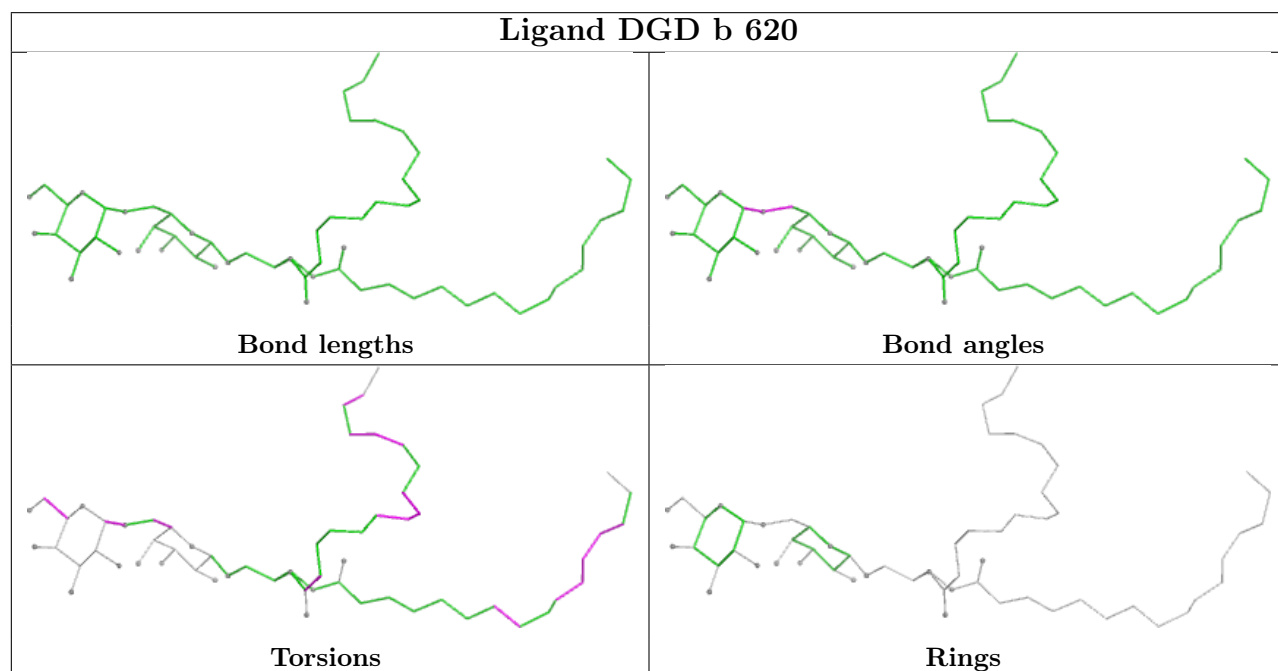
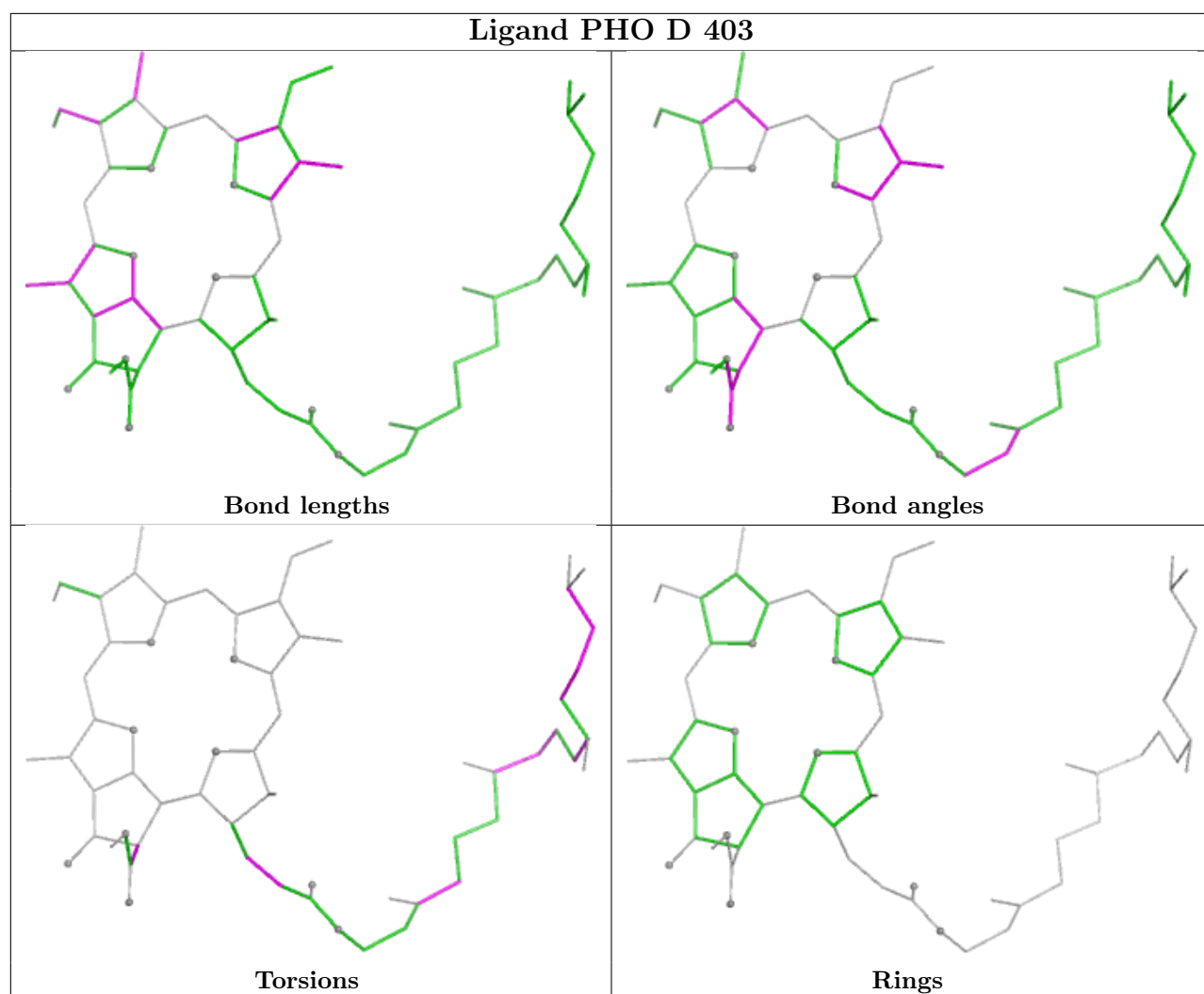


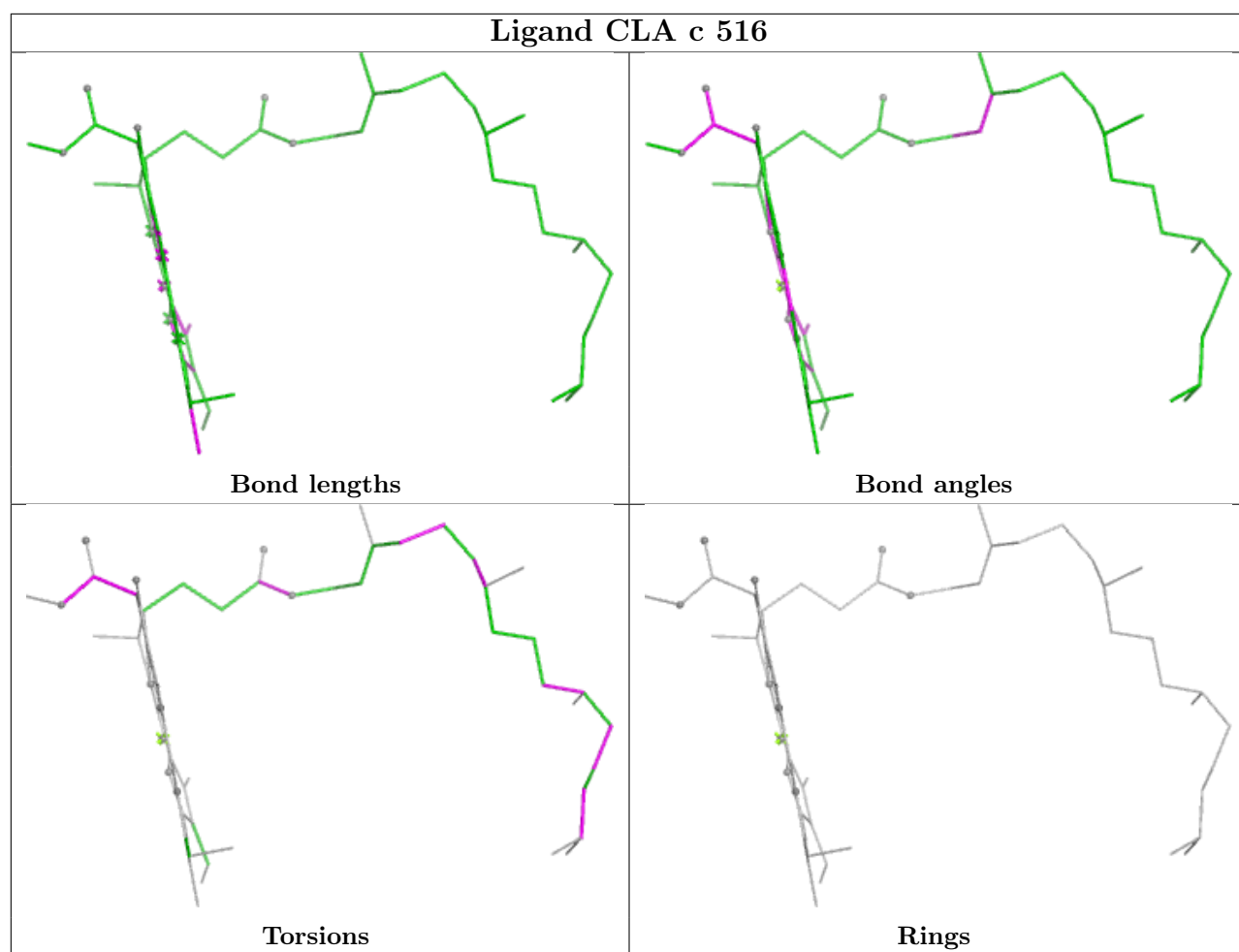




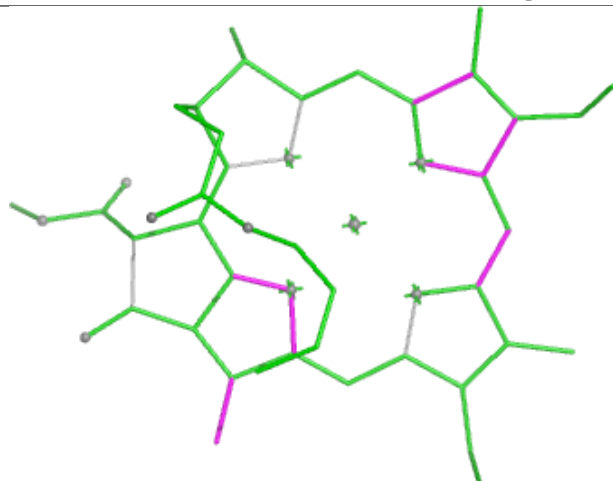
Ligand CLA n 312



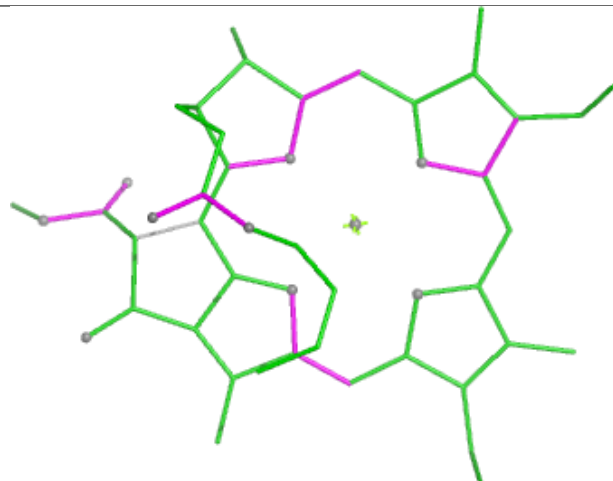




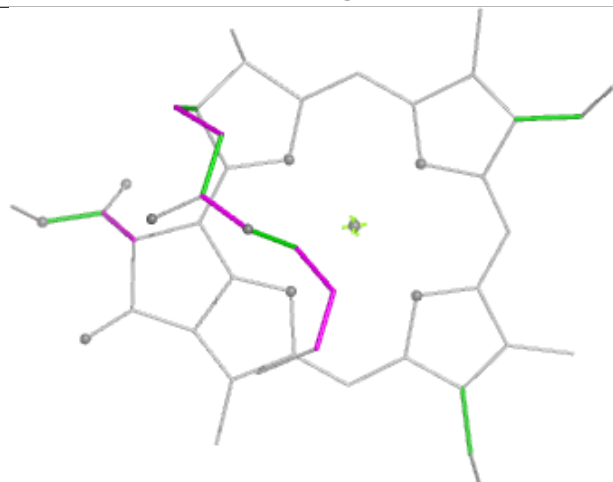
Ligand CLA s 305



Bond lengths



Bond angles



Torsions



Rings

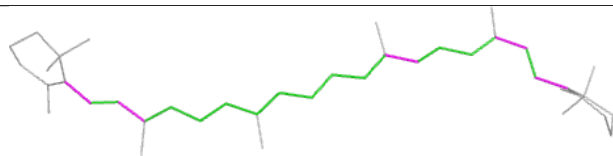
Ligand BCR j 101



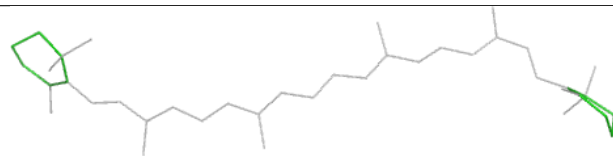
Bond lengths



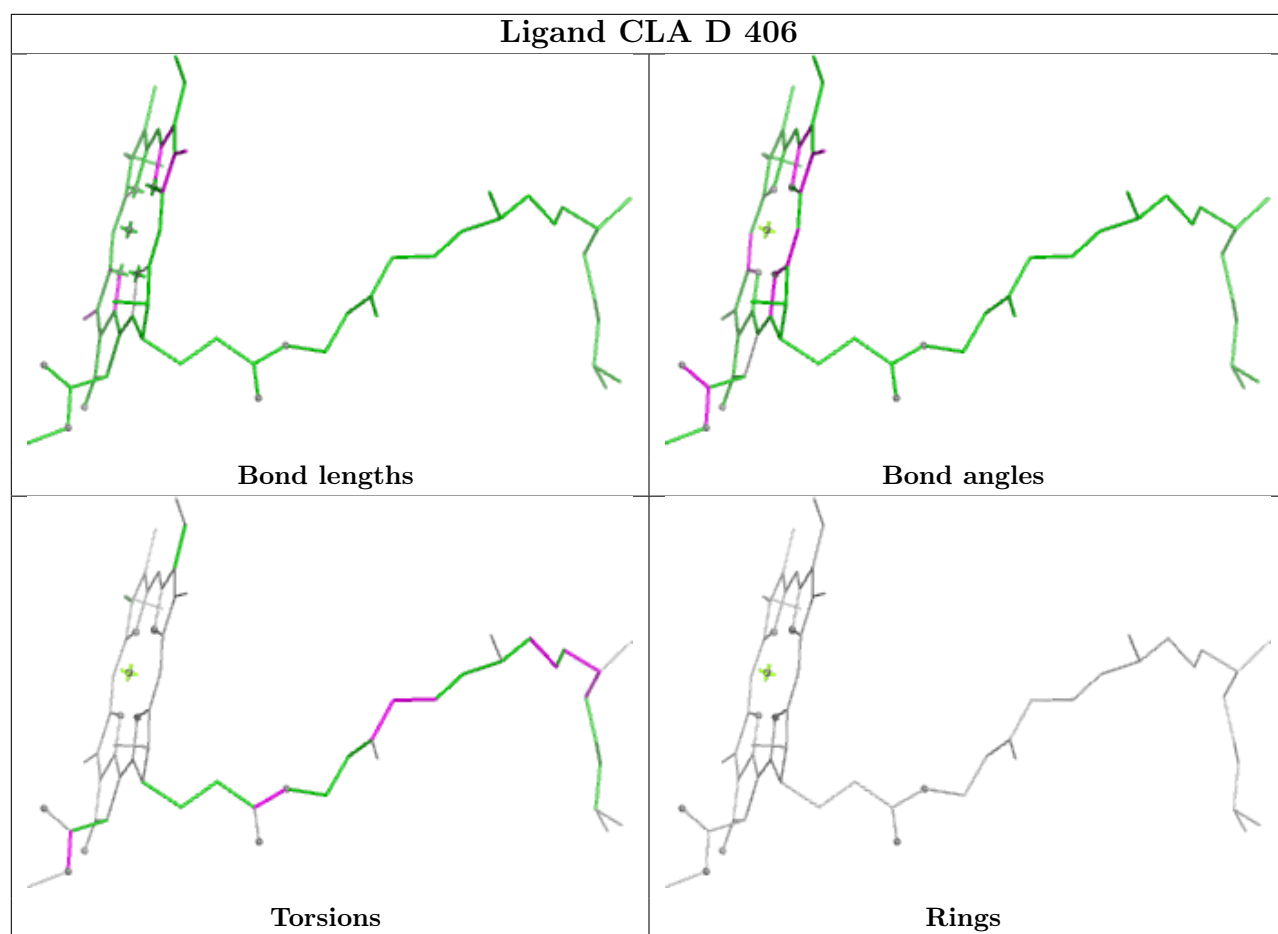
Bond angles



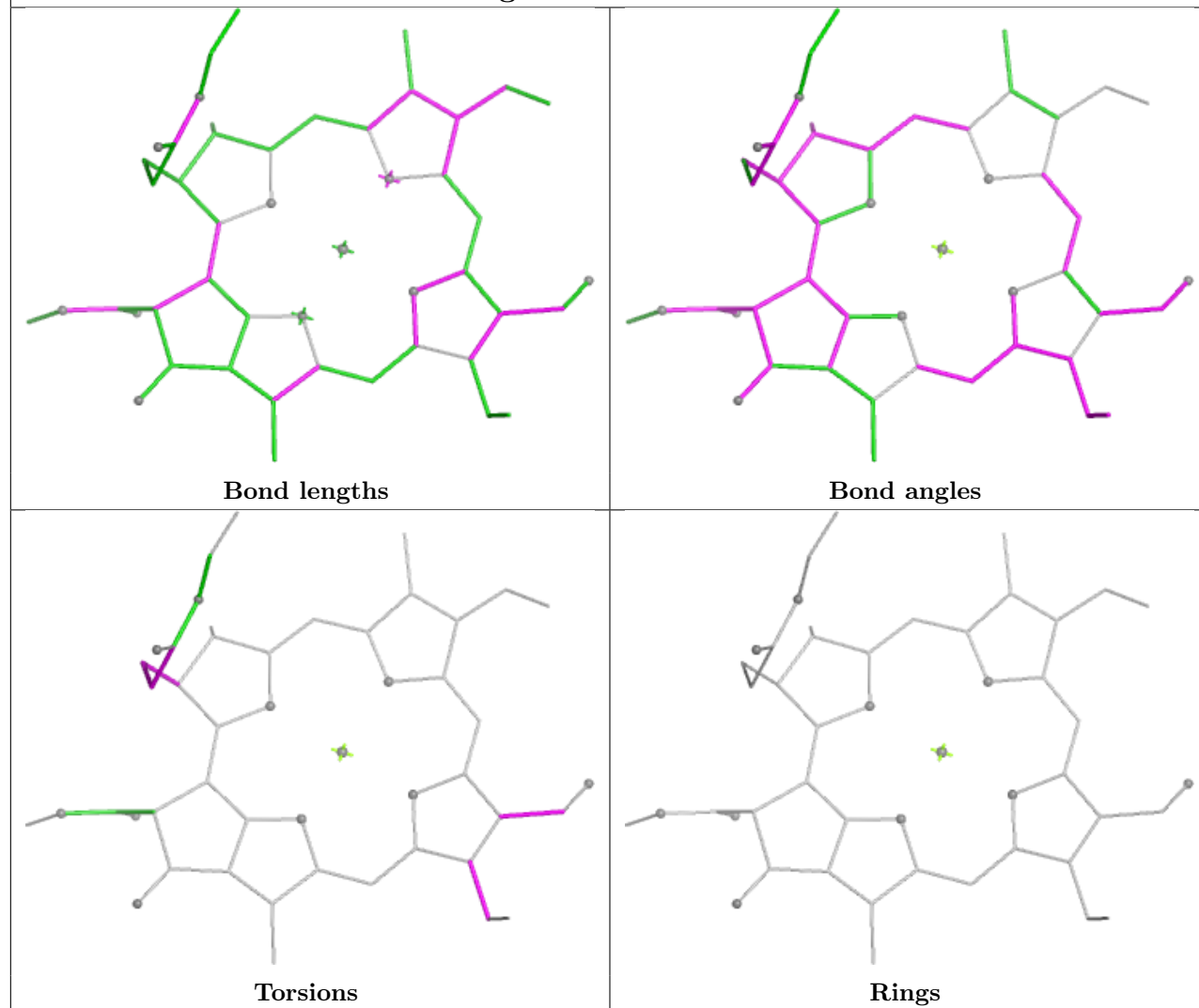
Torsions



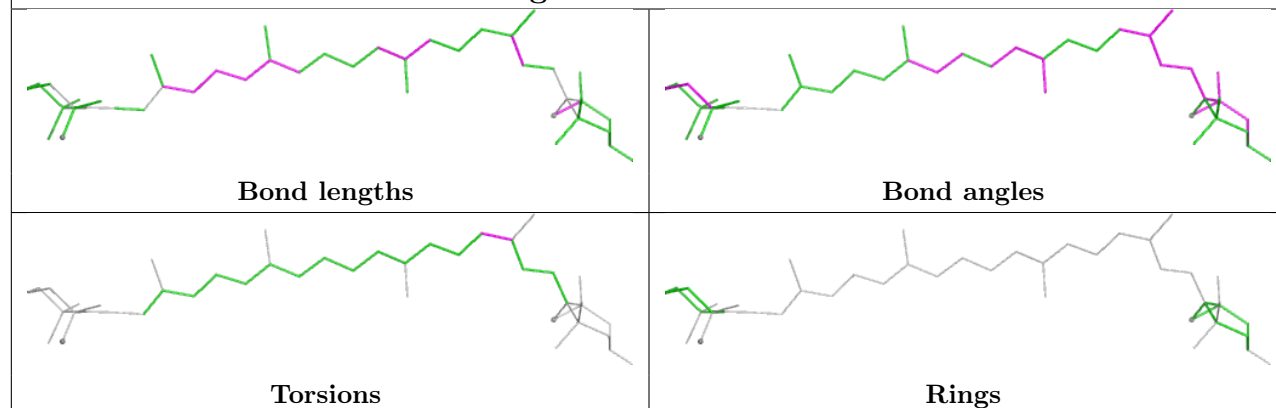
Rings

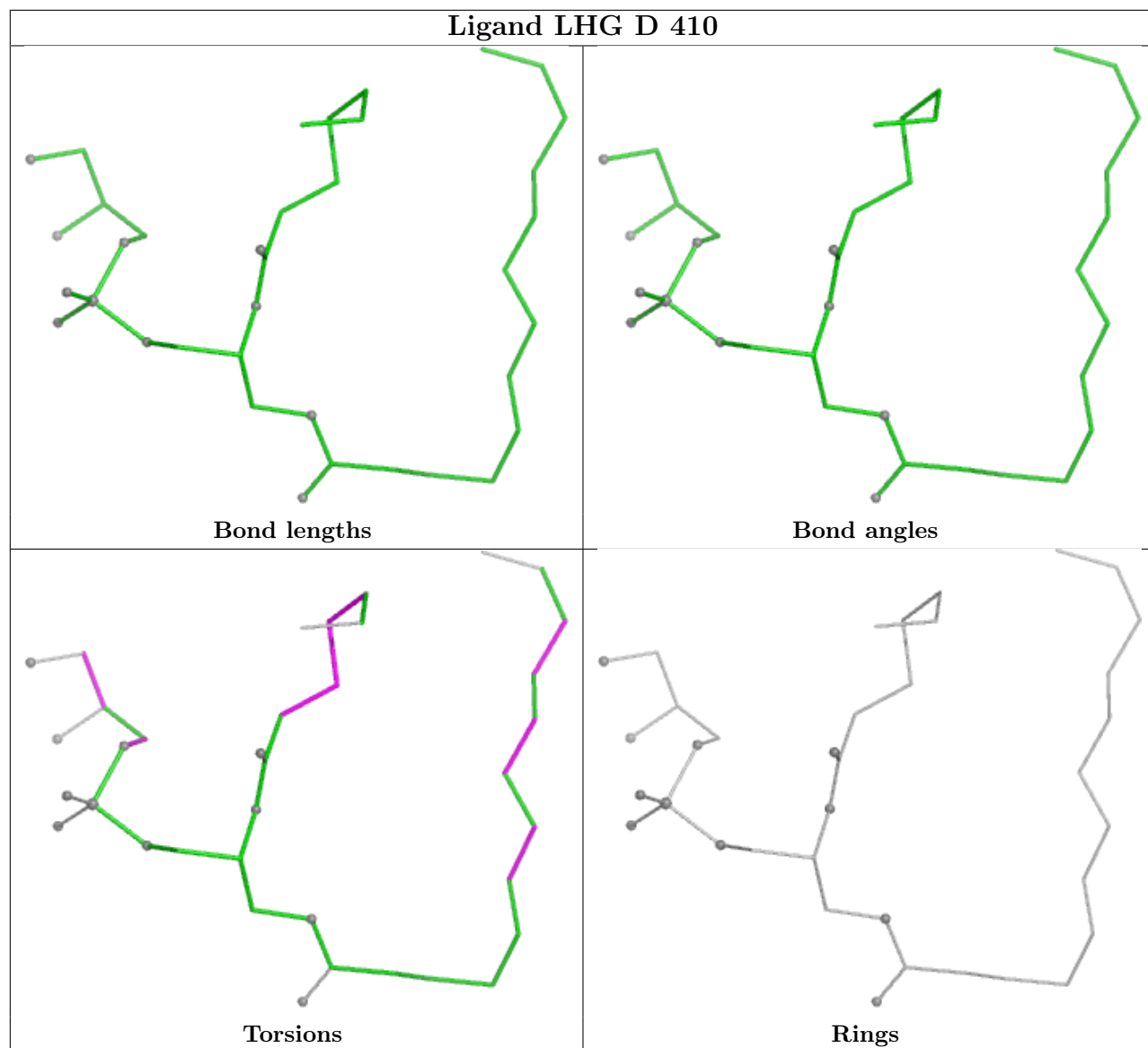


Ligand CHL R 318

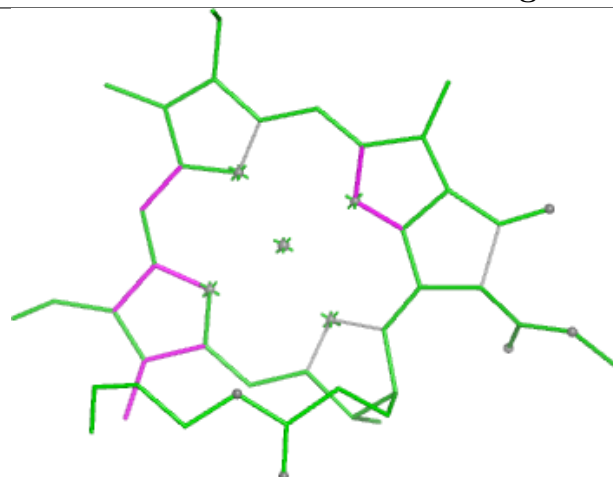


Ligand NEX Y 304

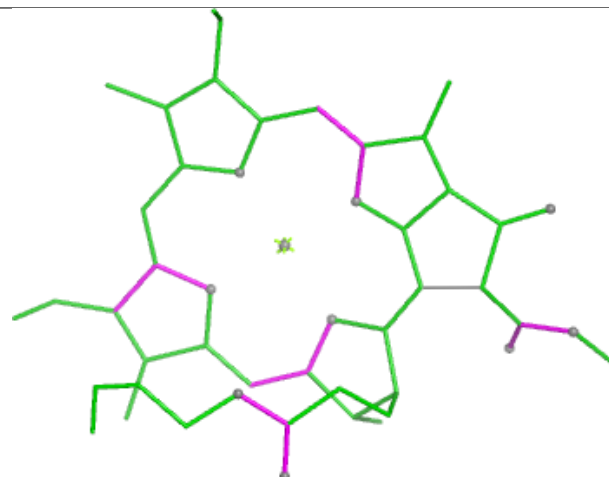




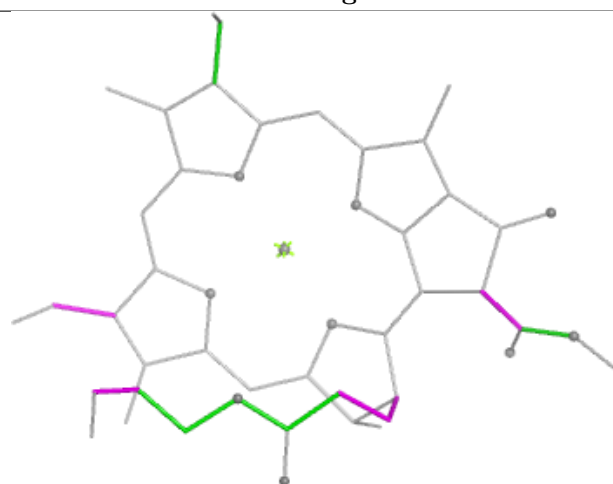
Ligand CLA S 314



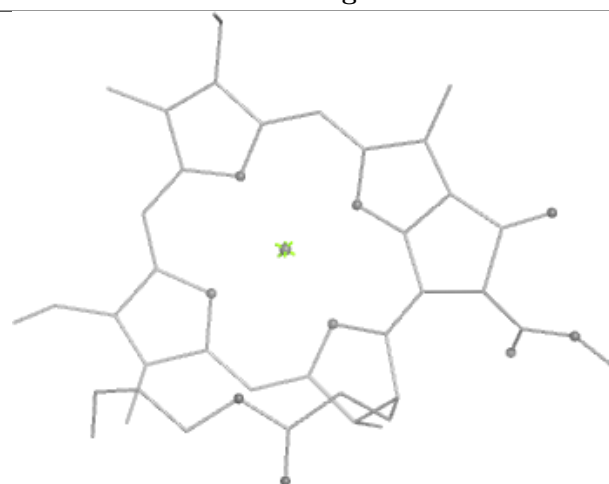
Bond lengths



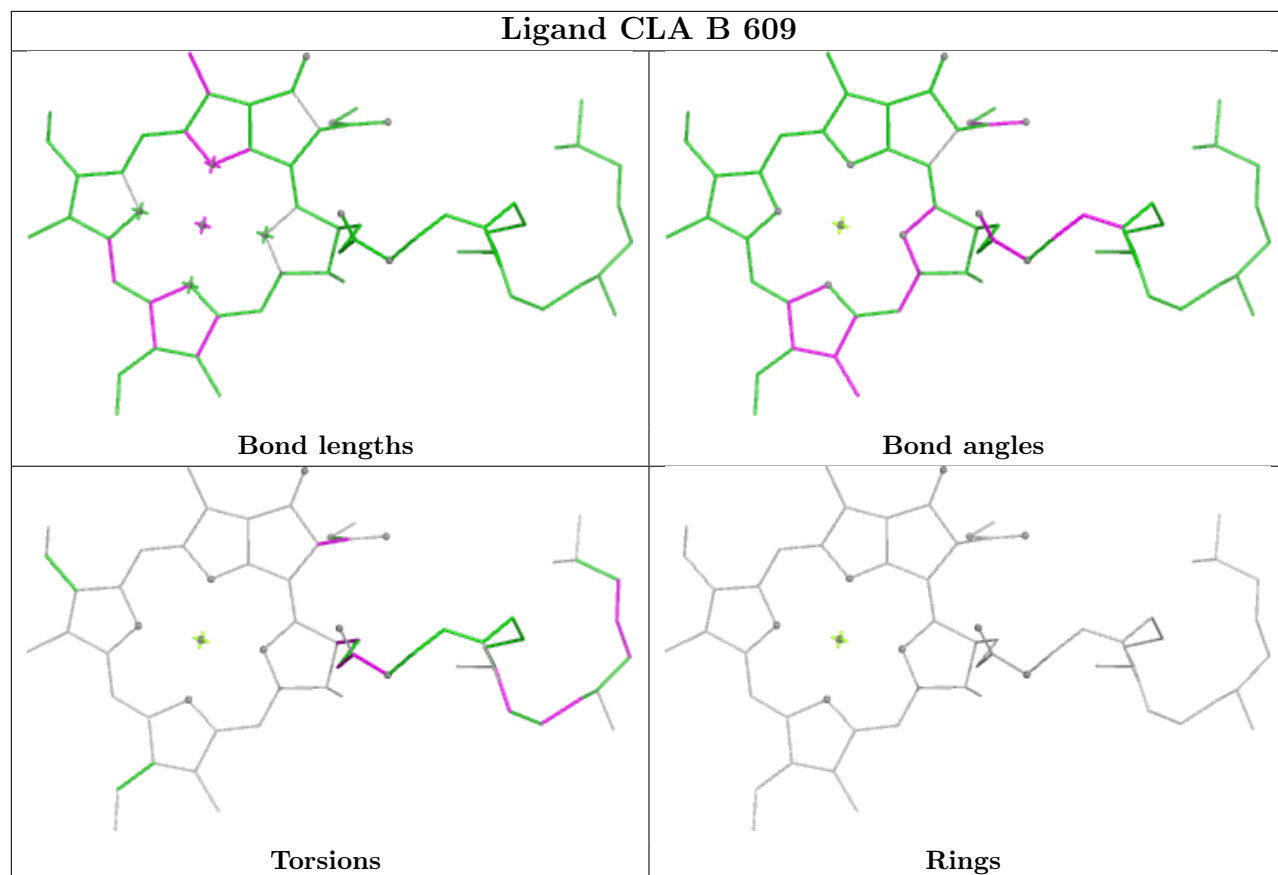
Bond angles

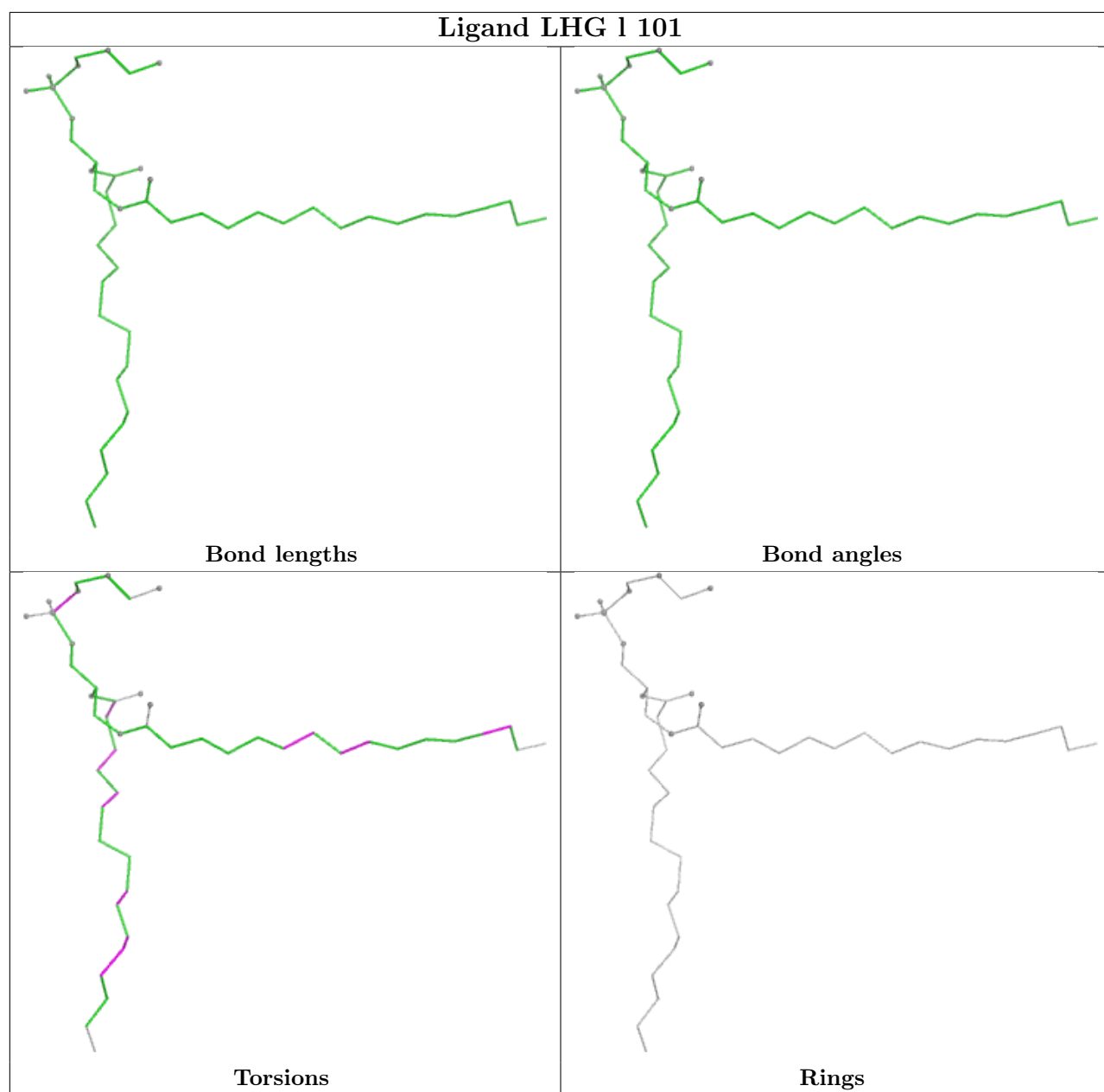


Torsions

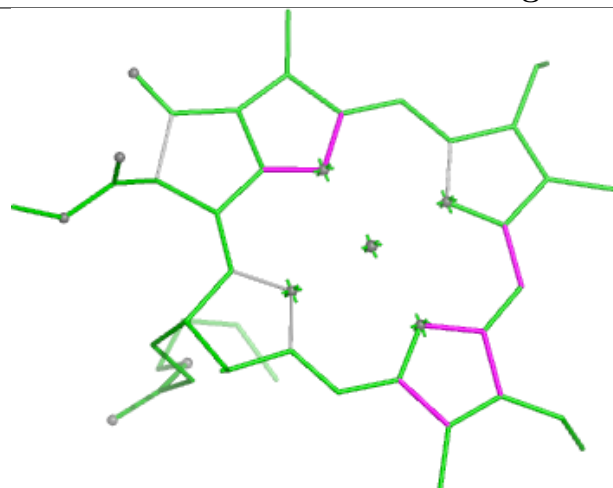


Rings

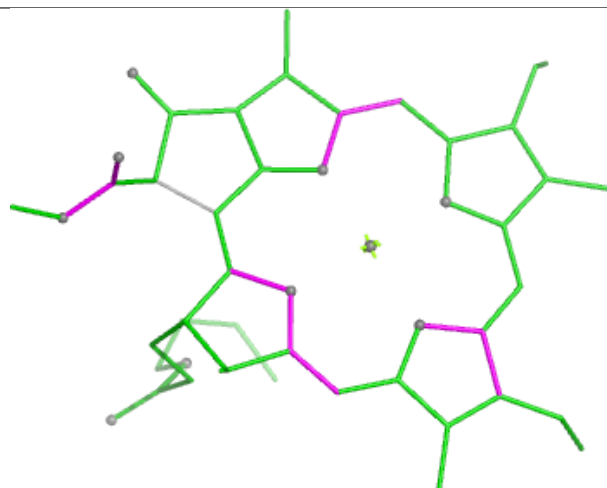




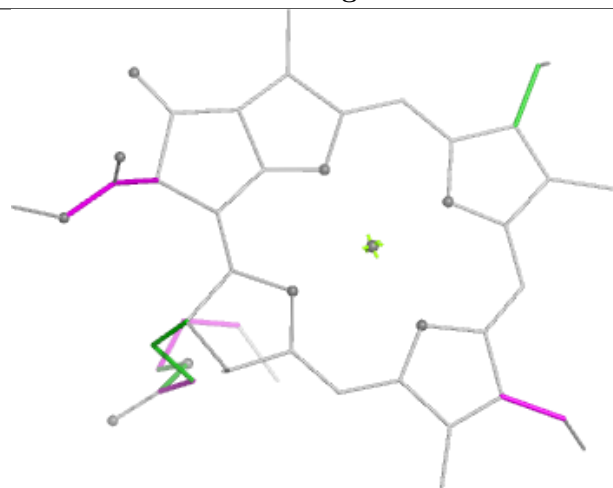
Ligand CLA r 310



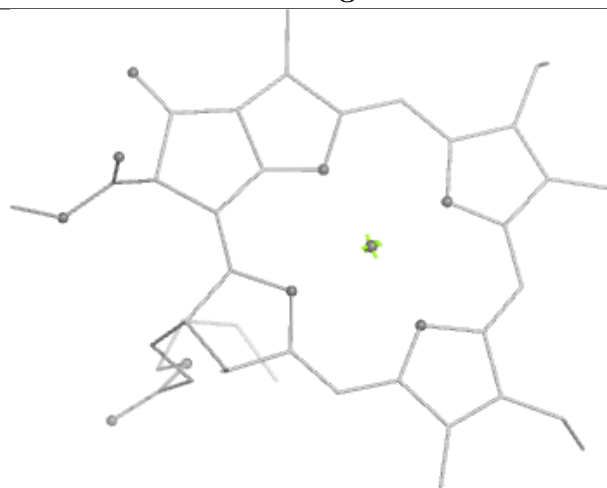
Bond lengths



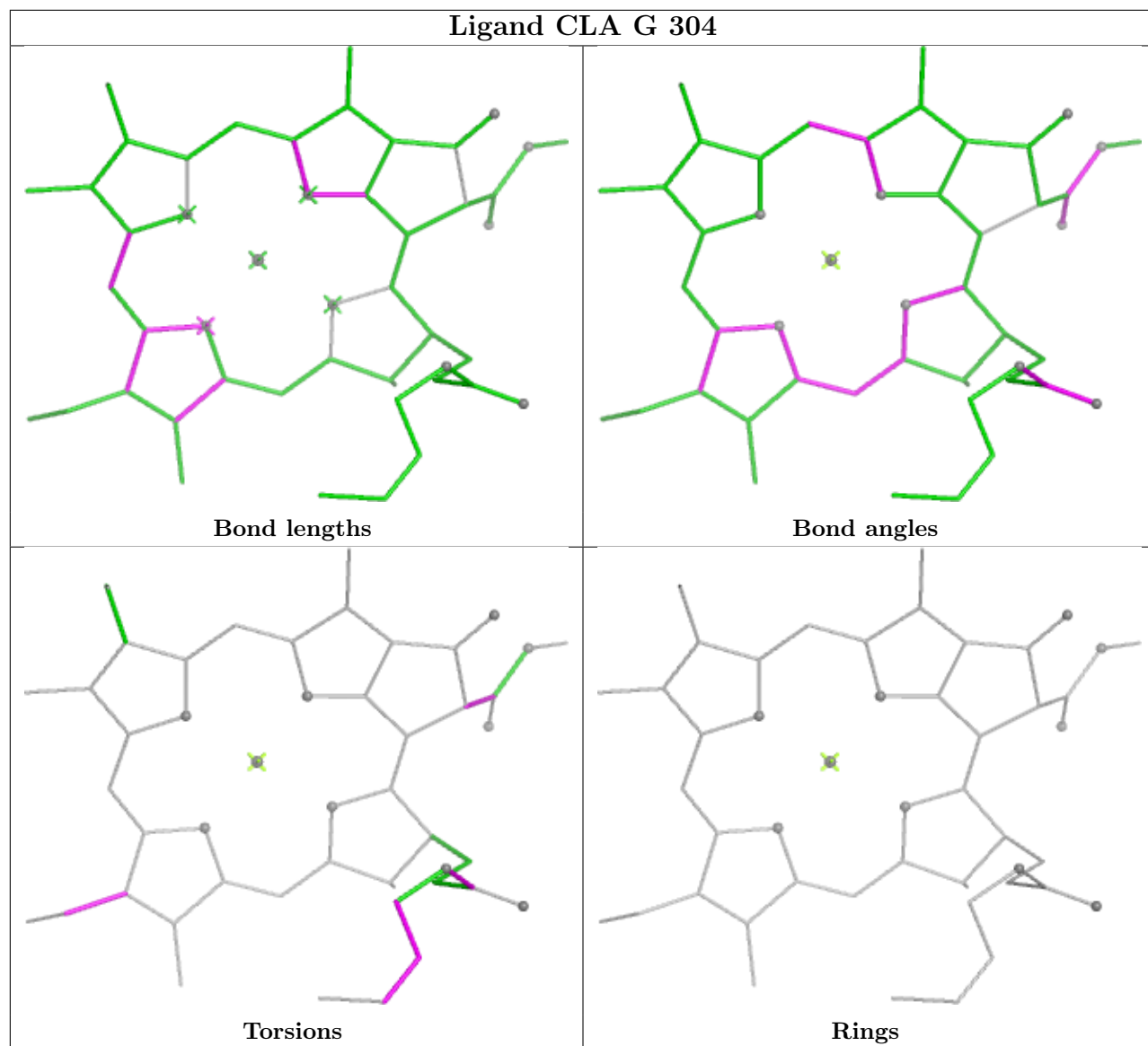
Bond angles

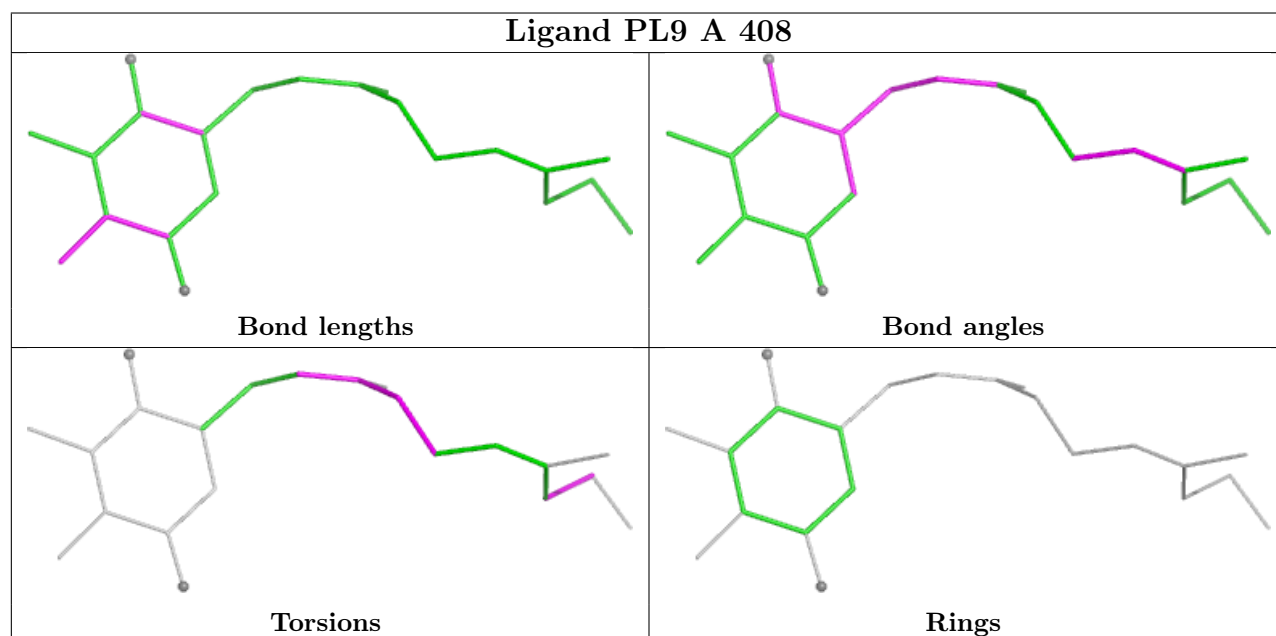
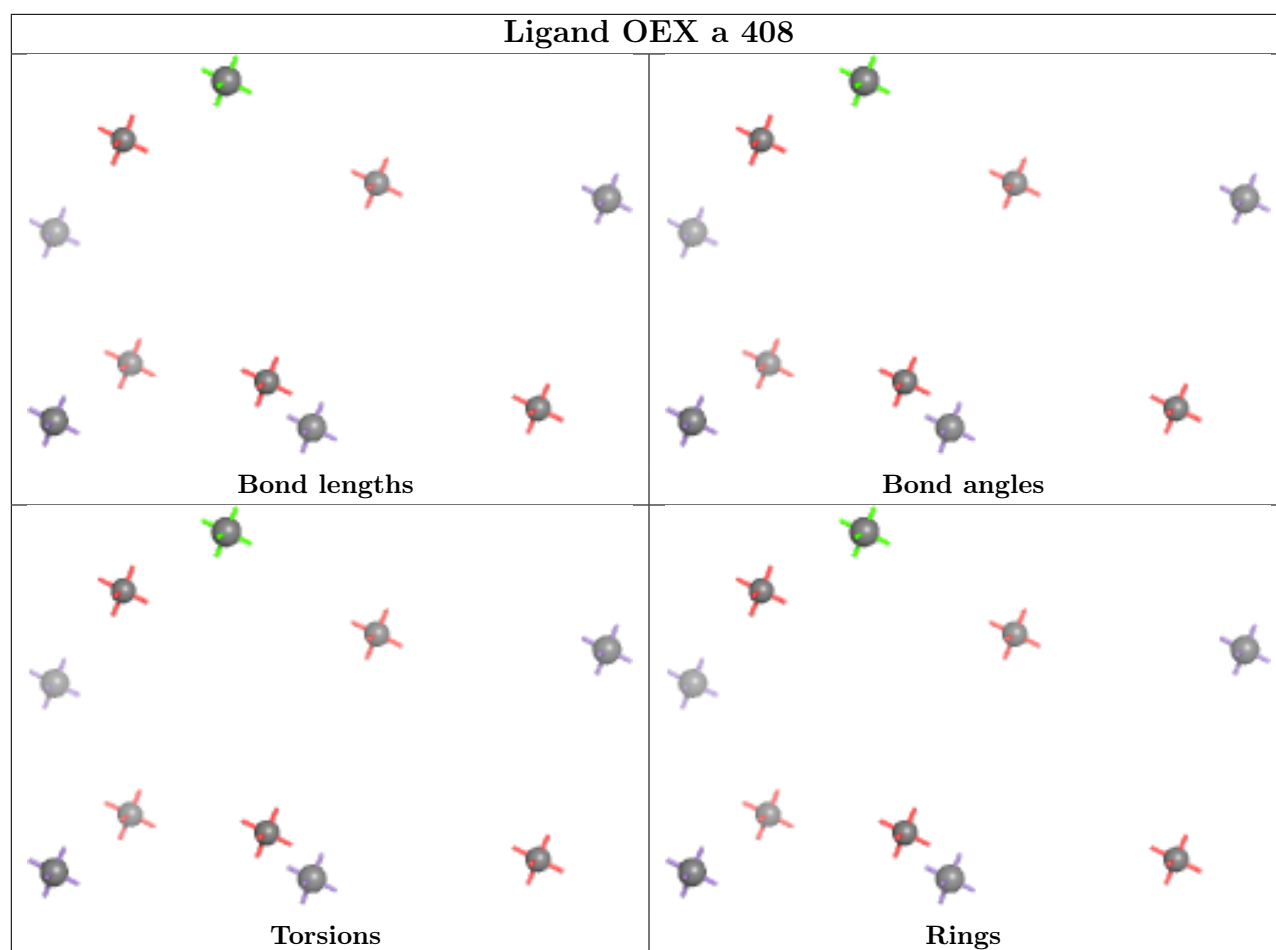


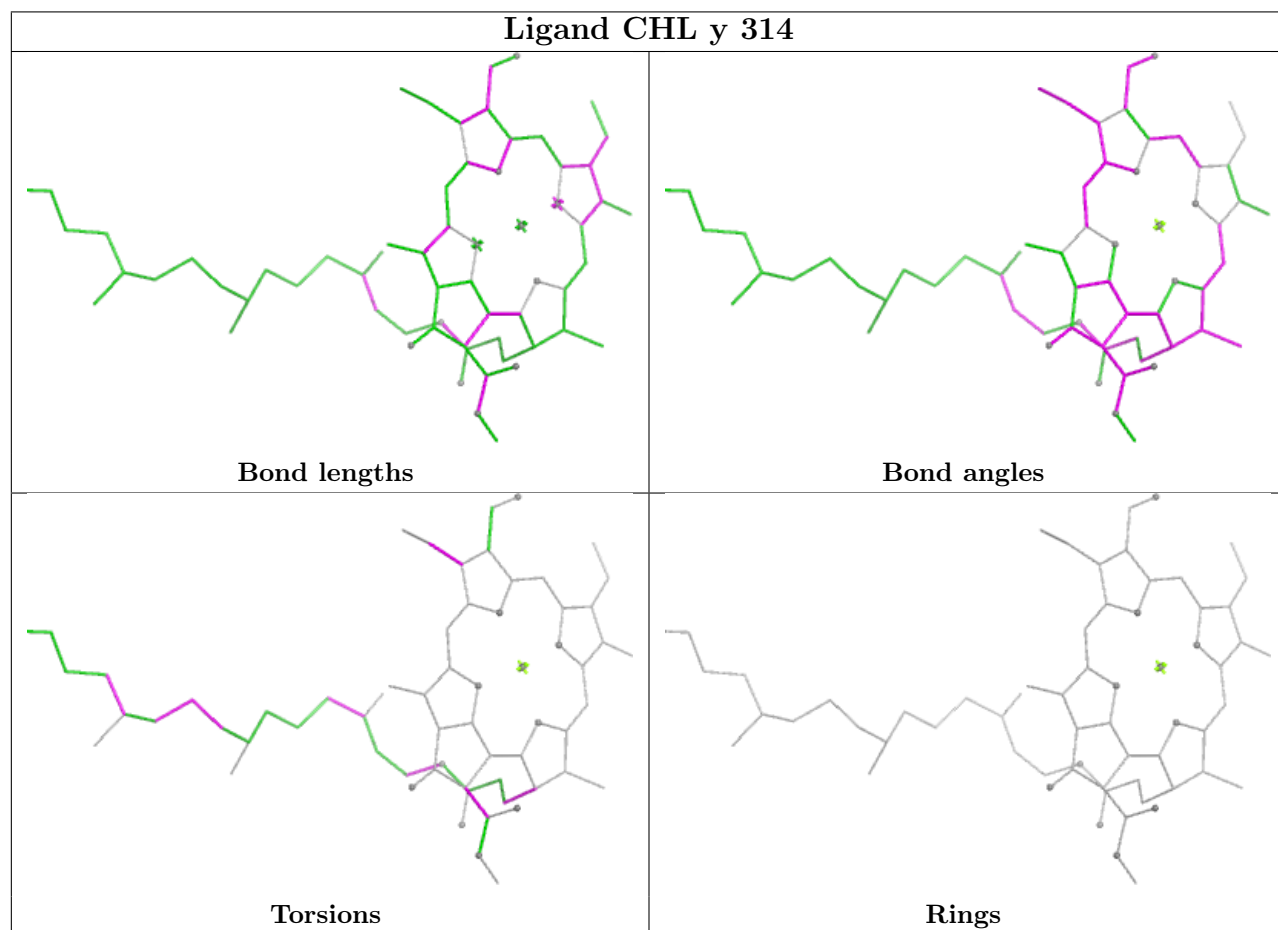
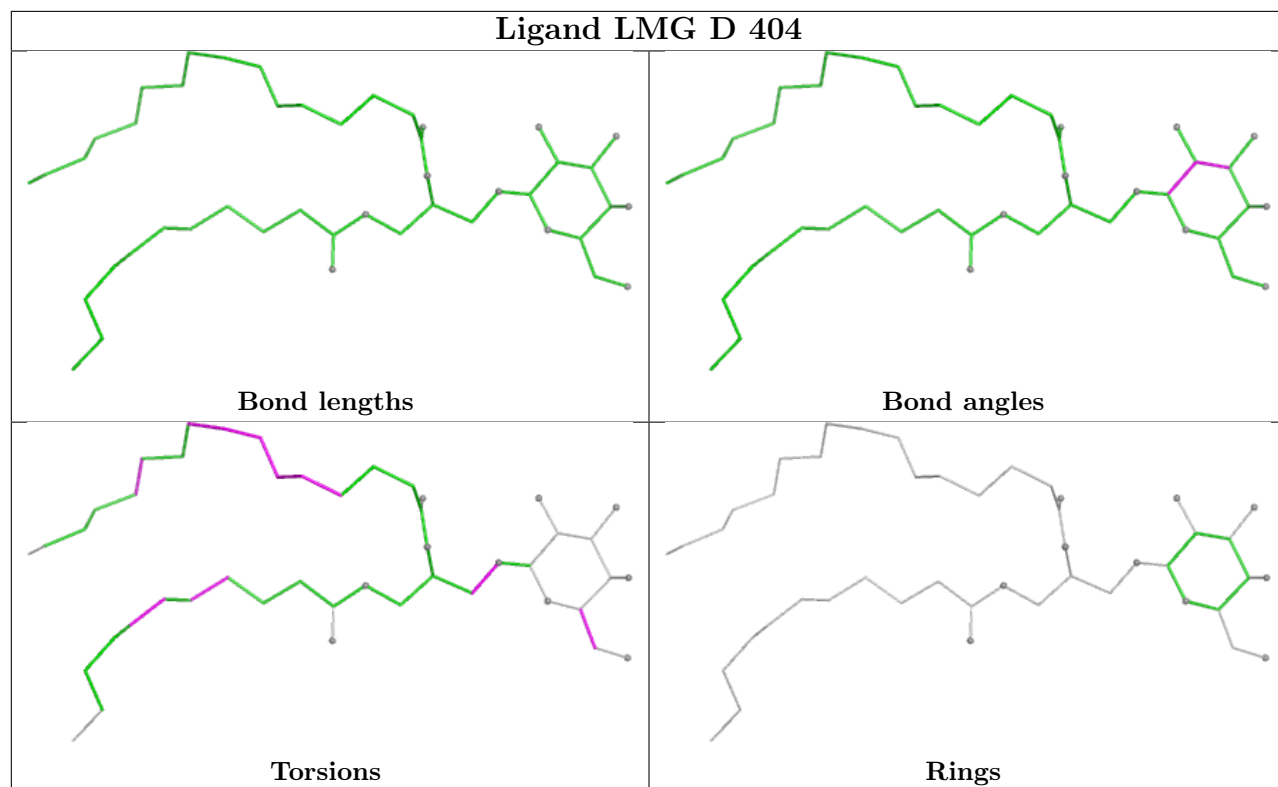
Torsions

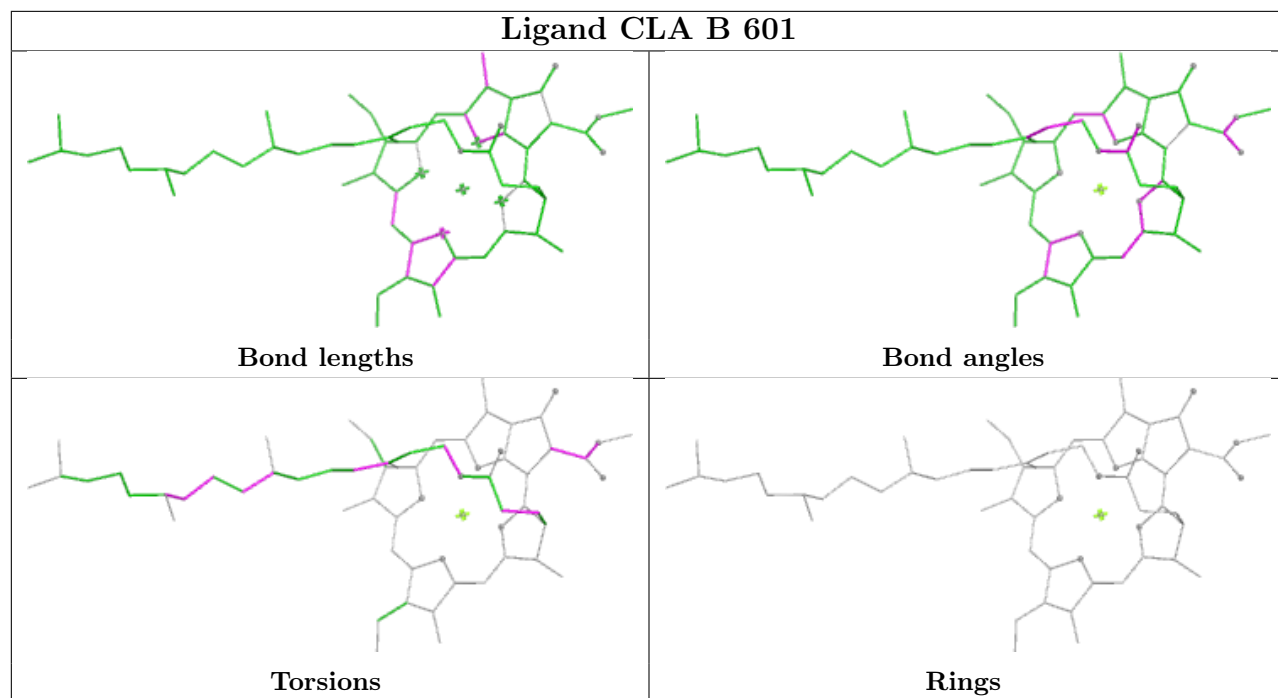


Rings

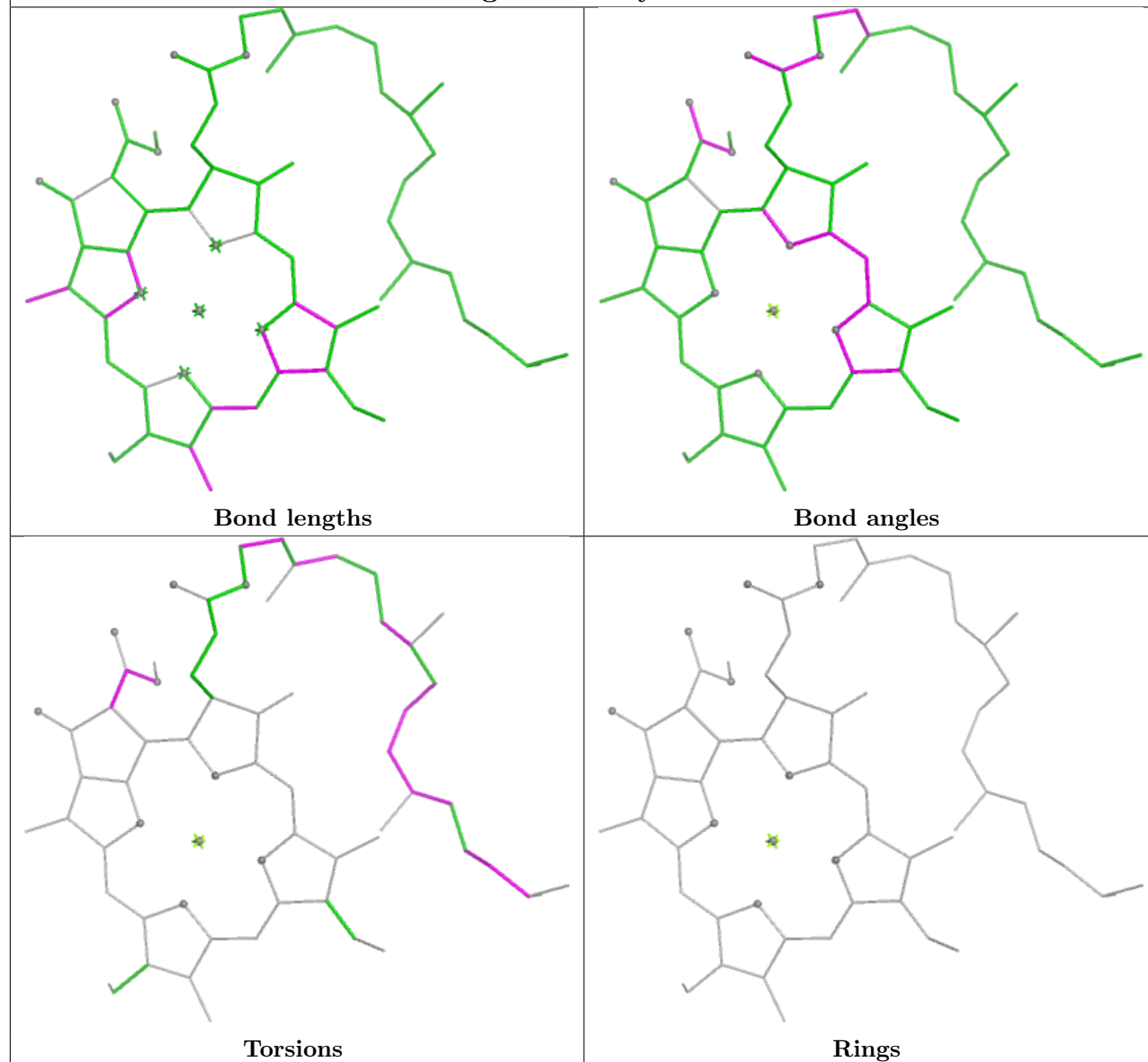




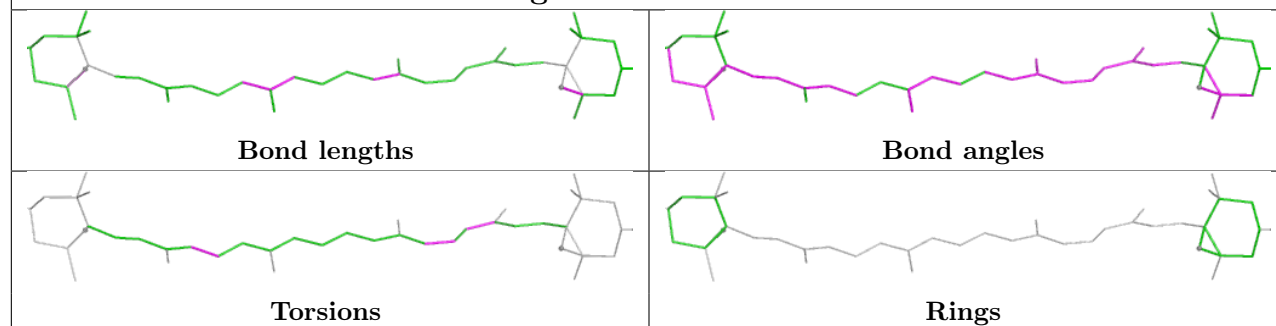


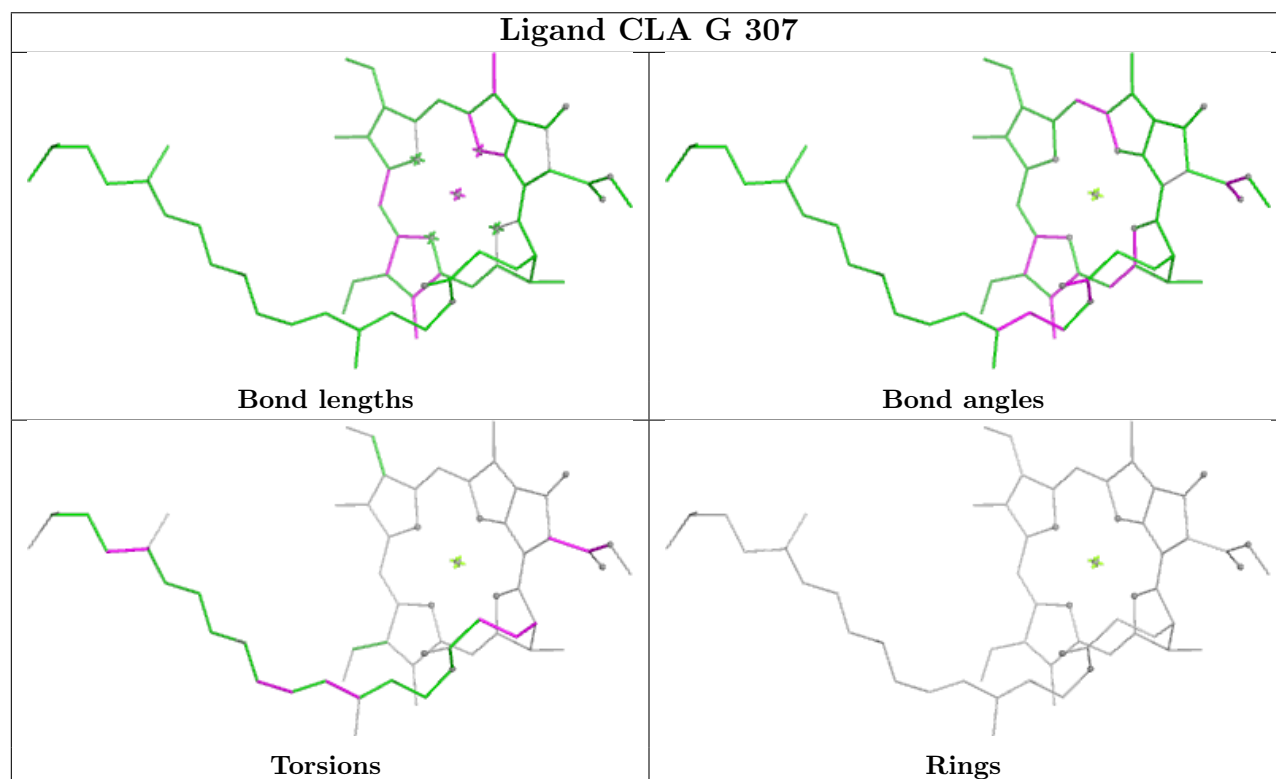
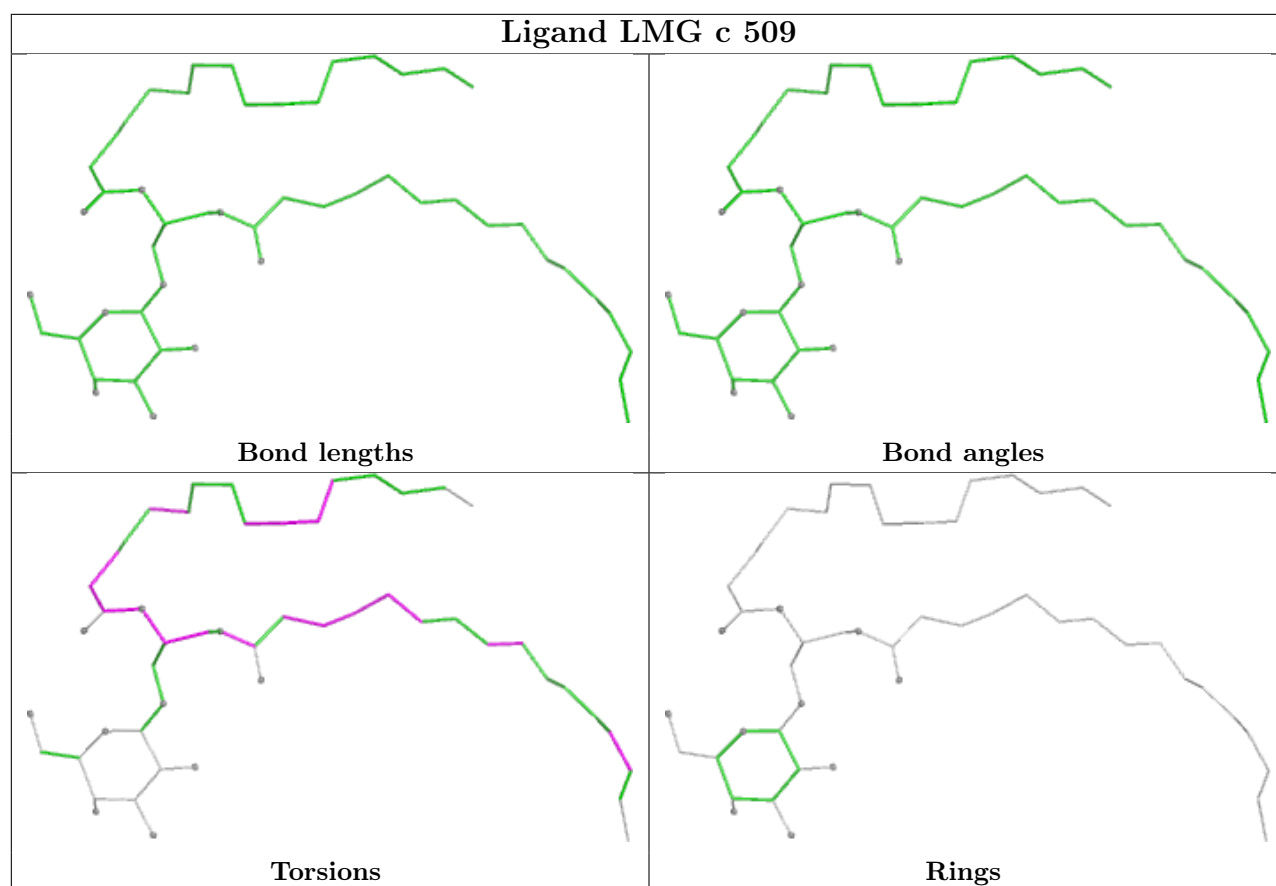


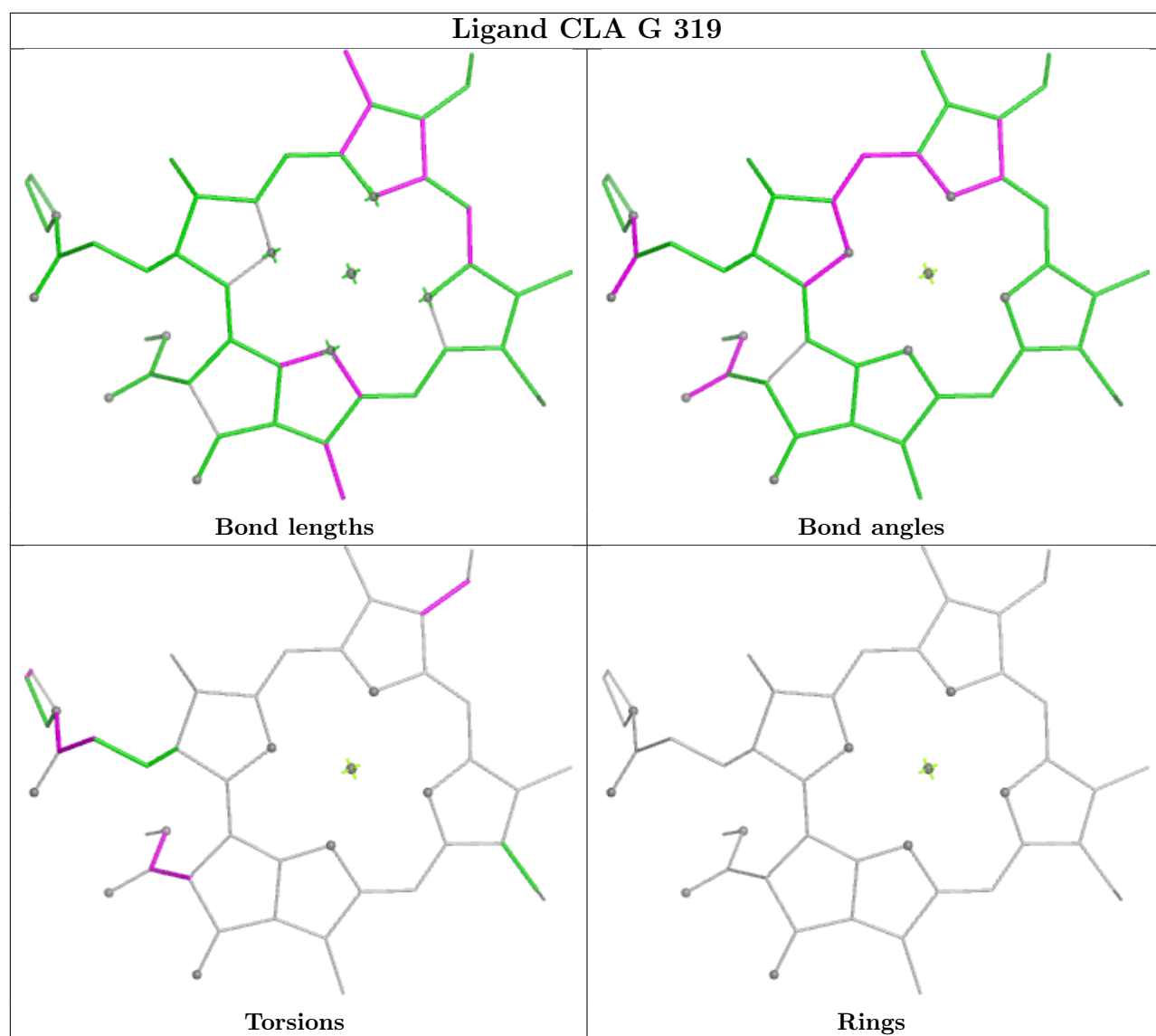
Ligand CLA y 316

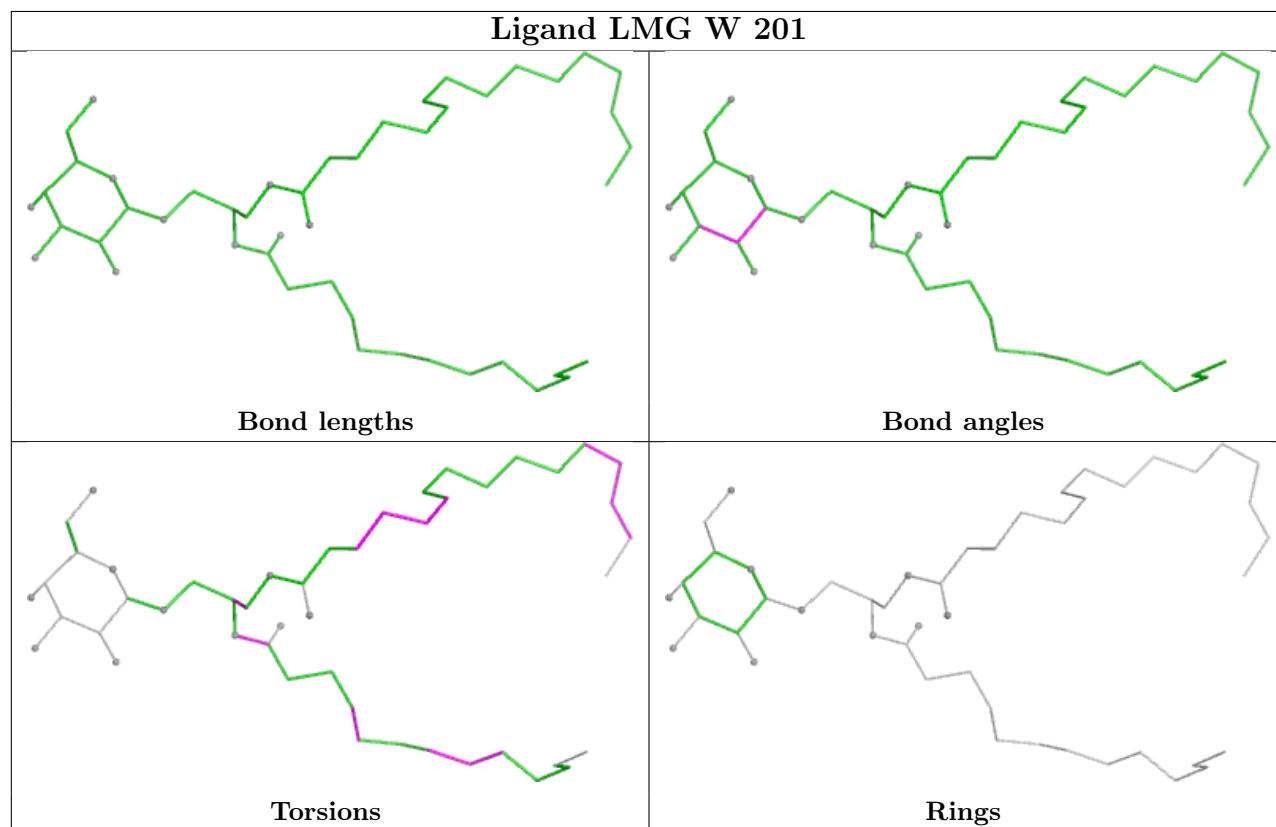
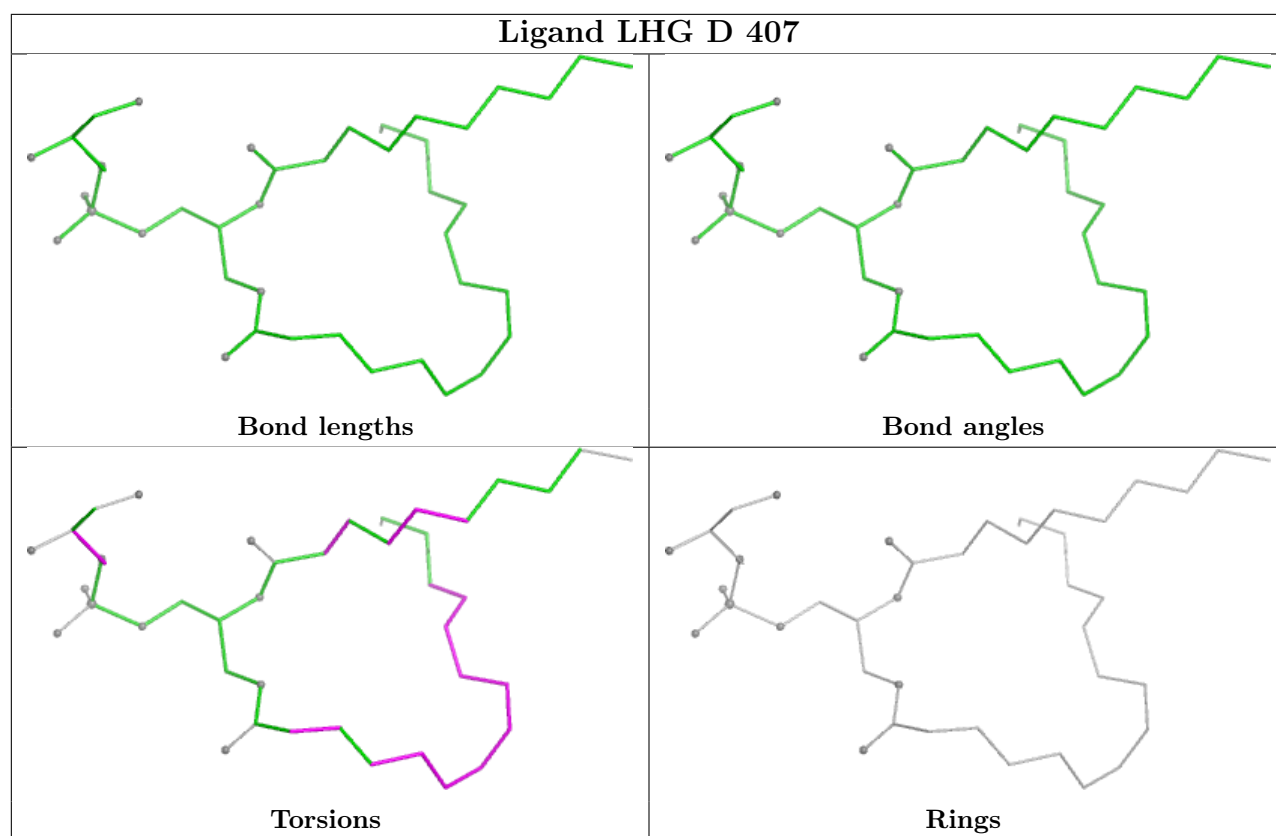


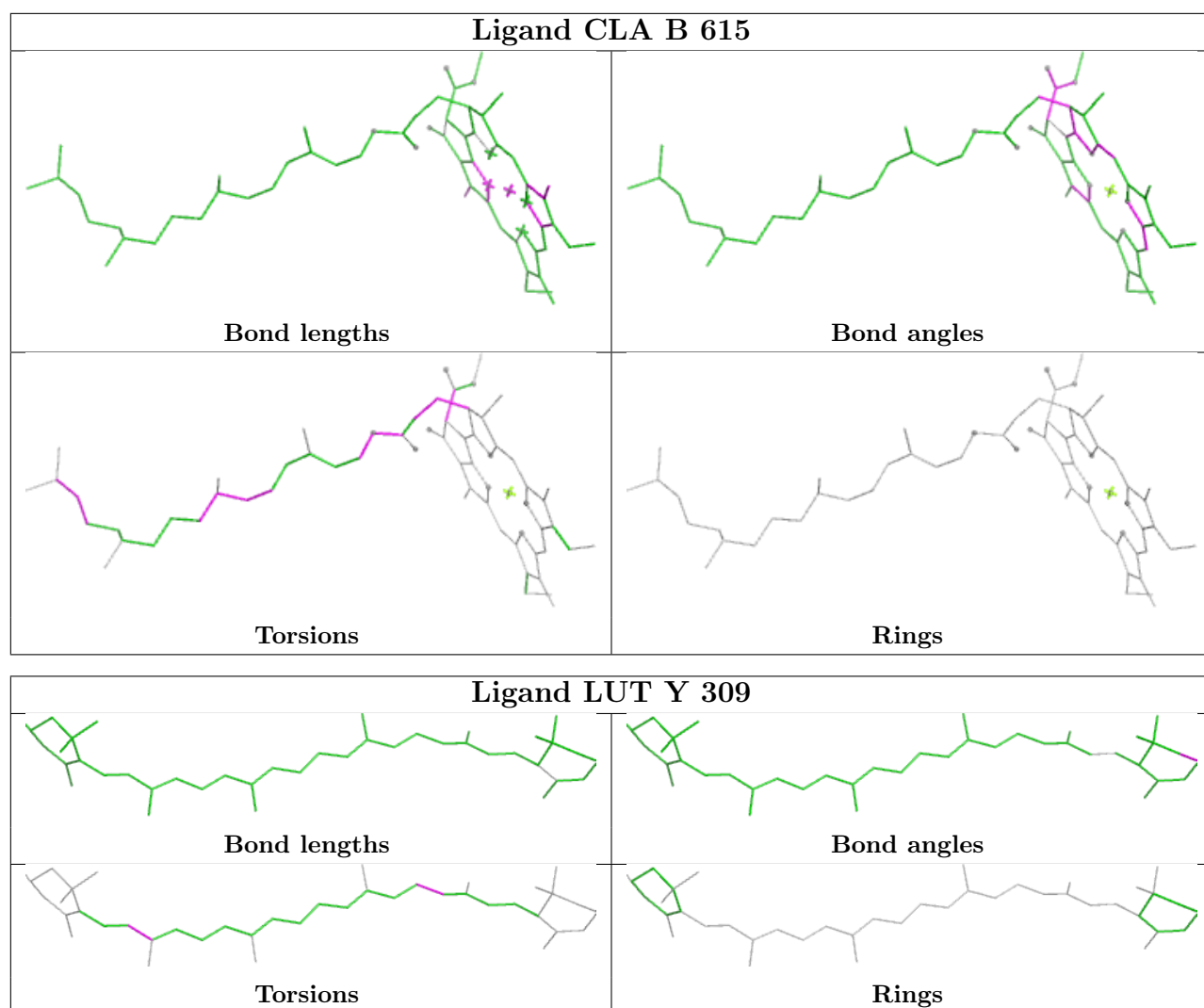
Ligand XAT G 320



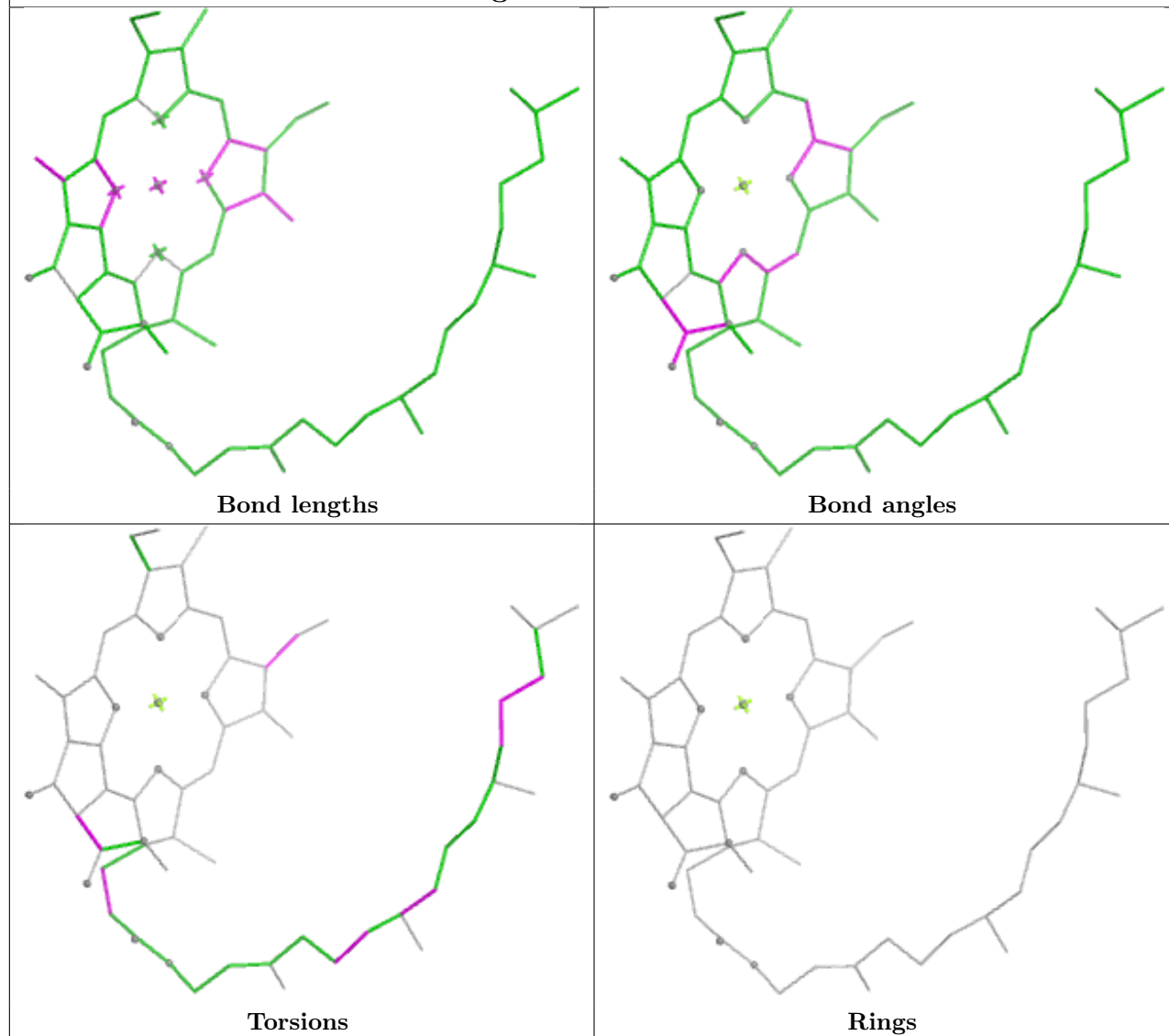




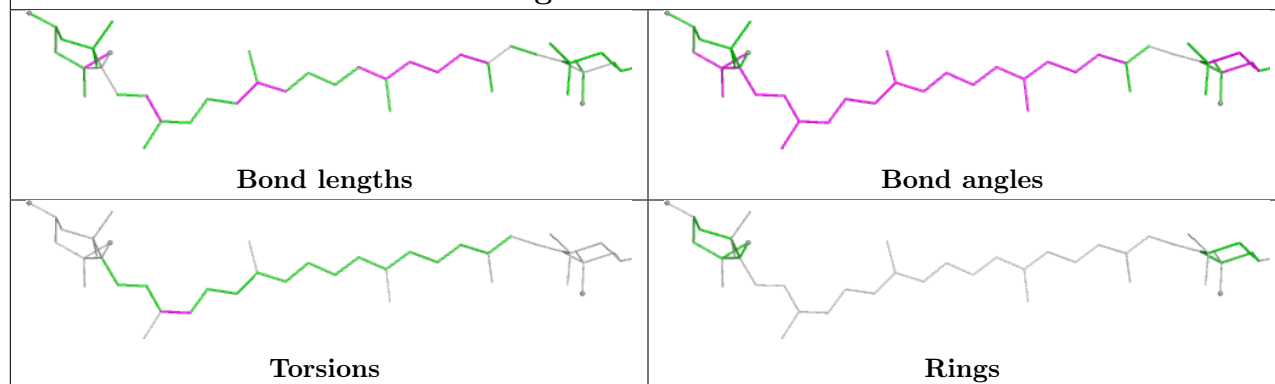


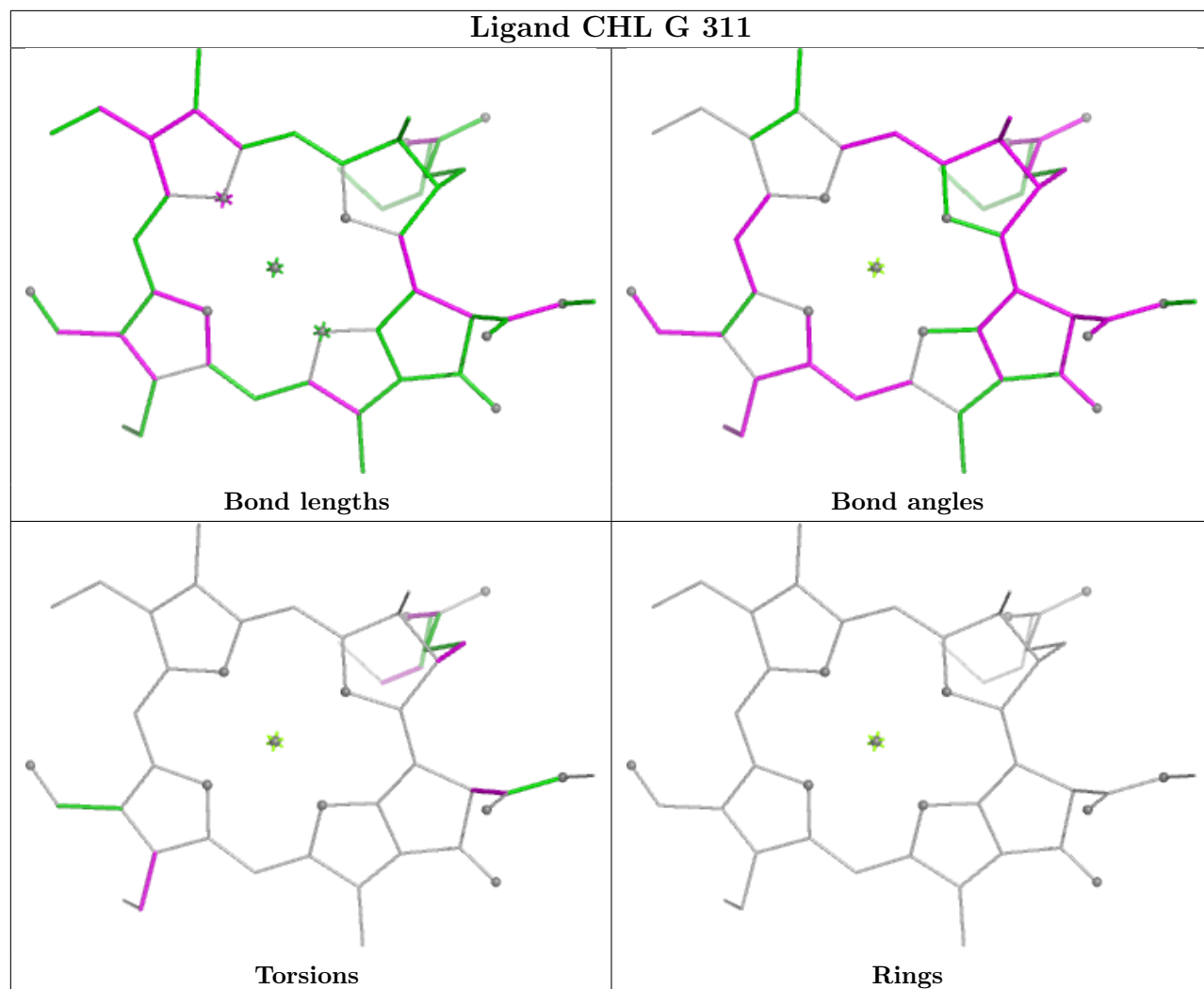


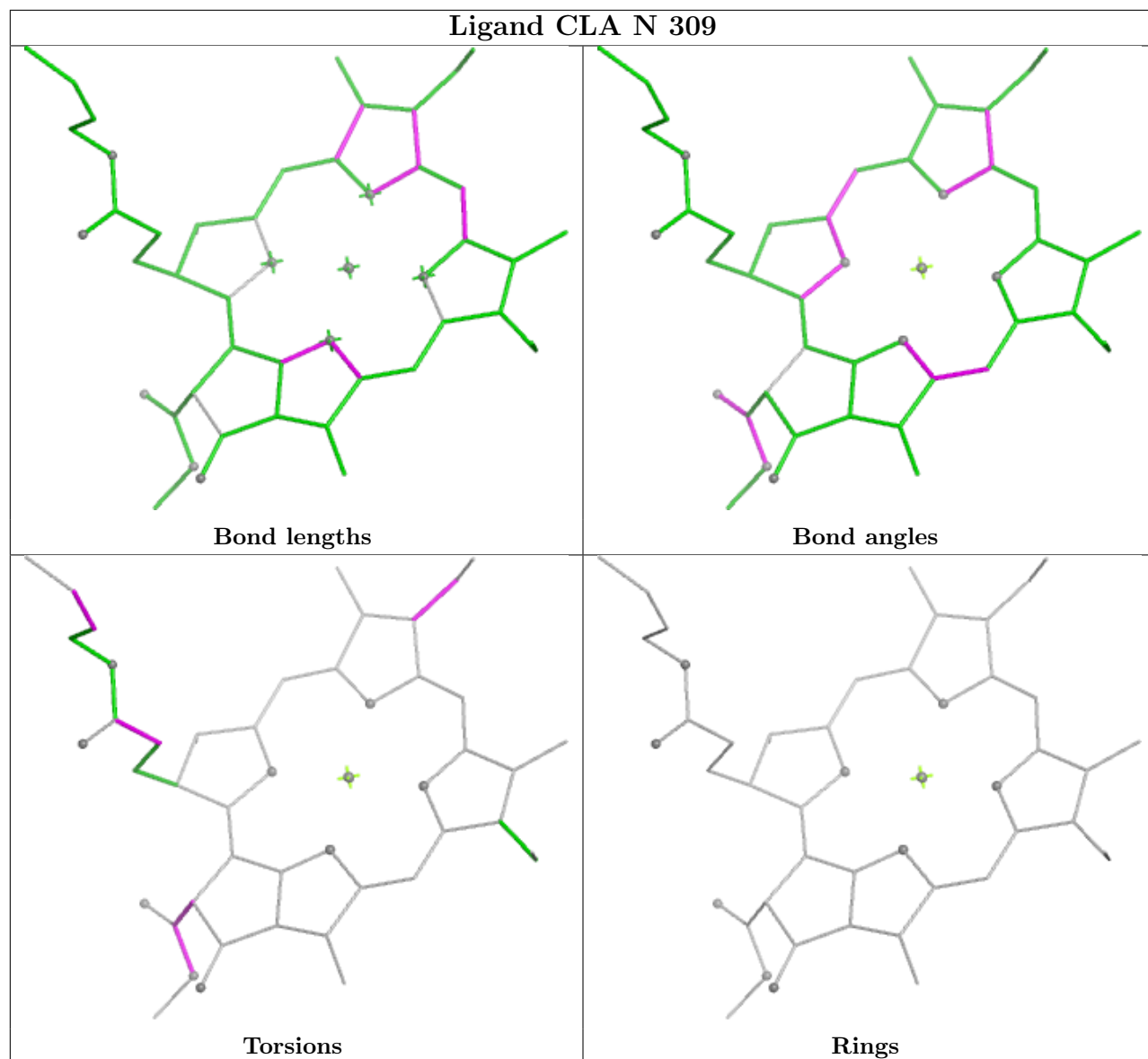
Ligand CLA c 508

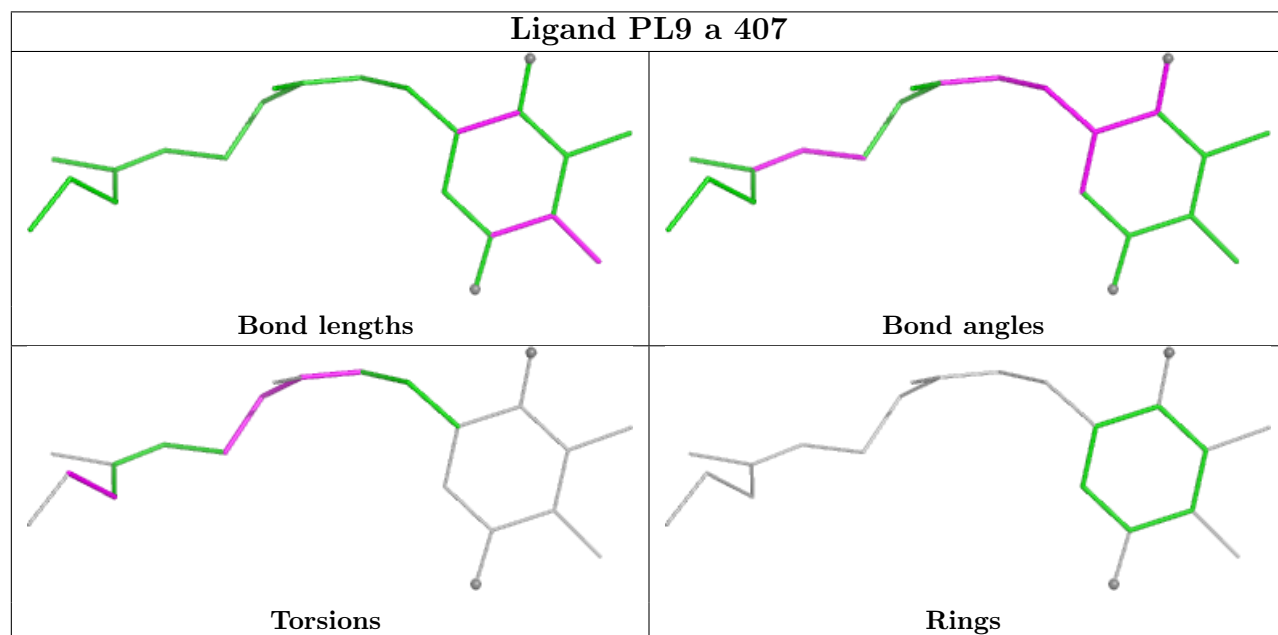
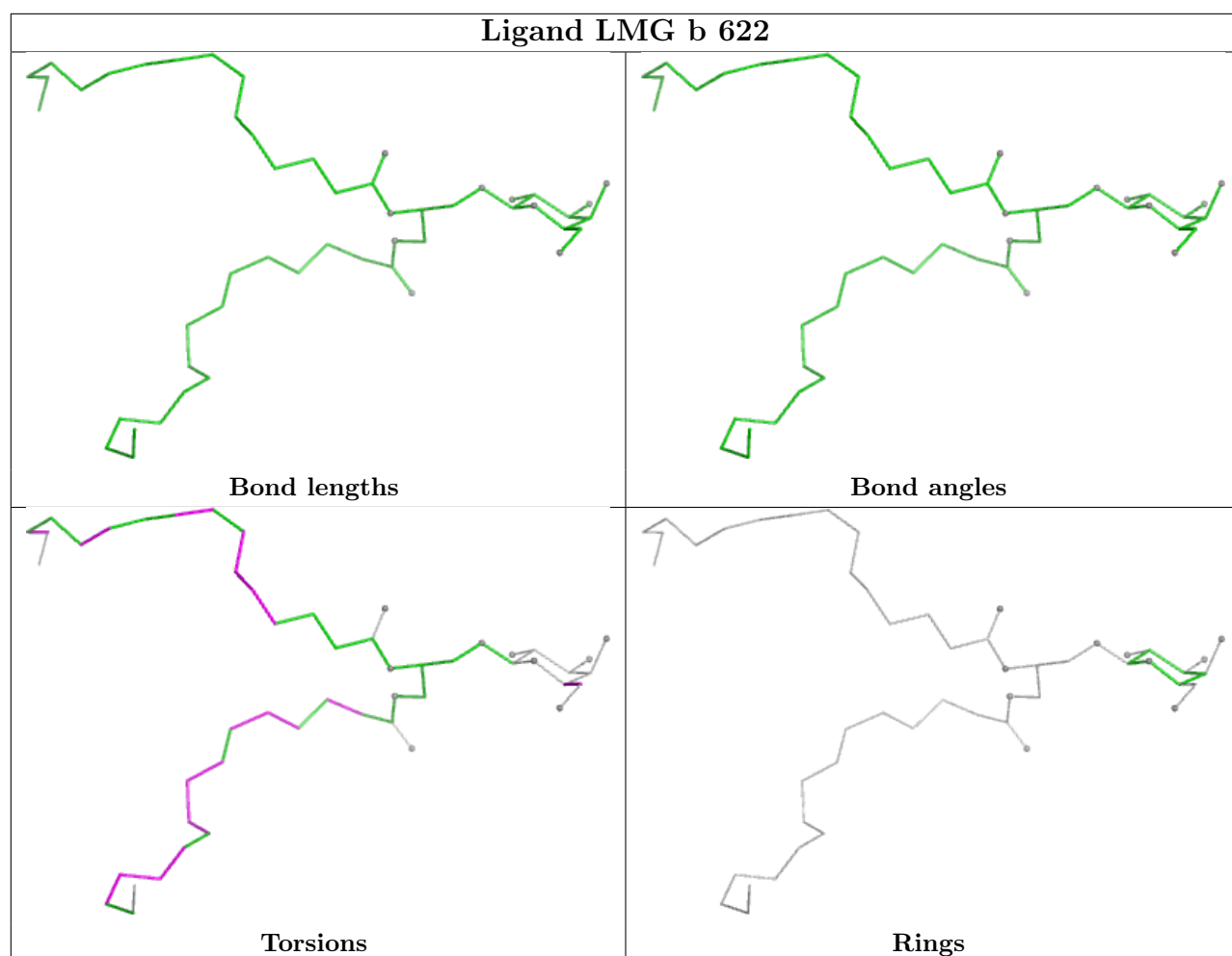


Ligand NEX r 302

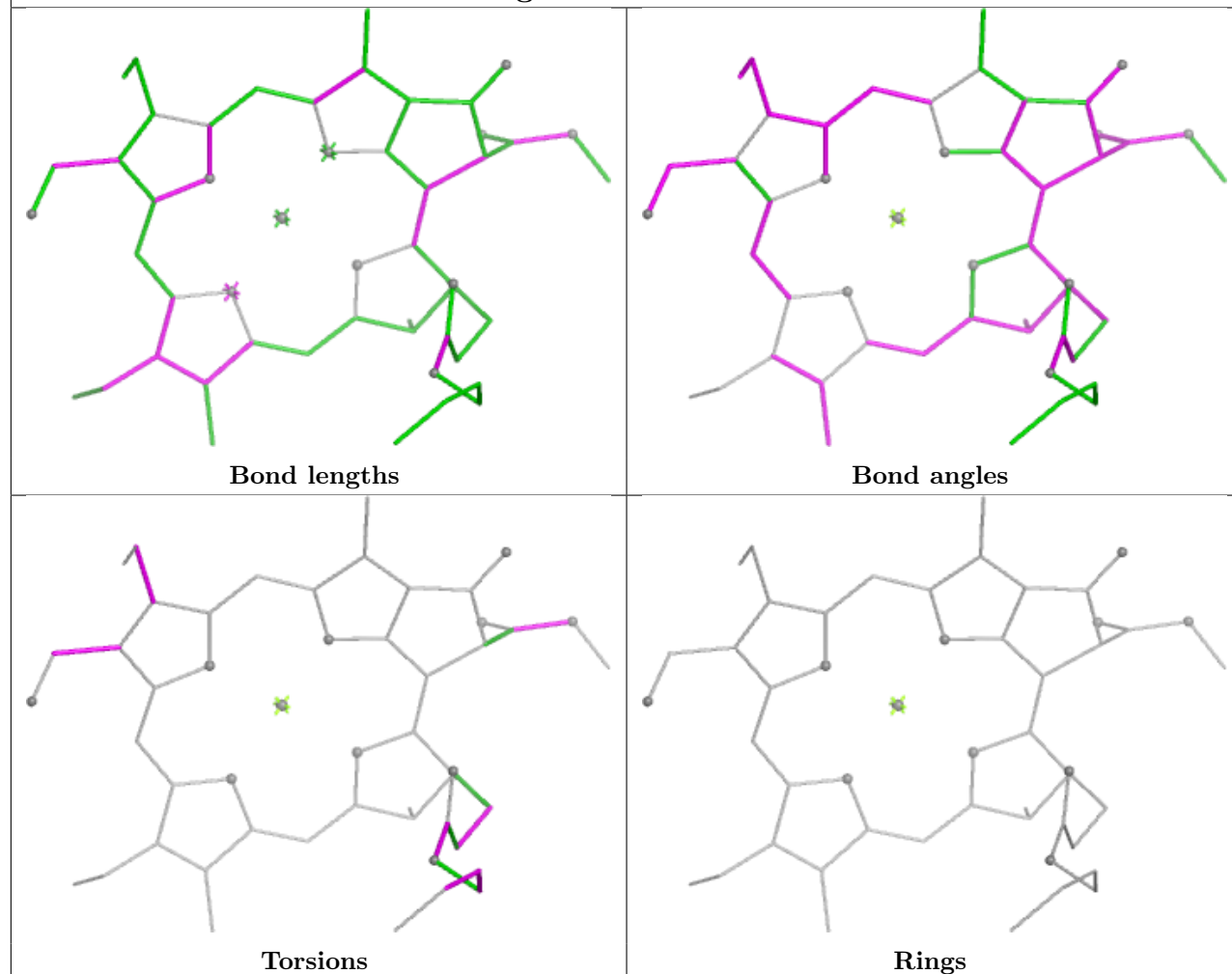




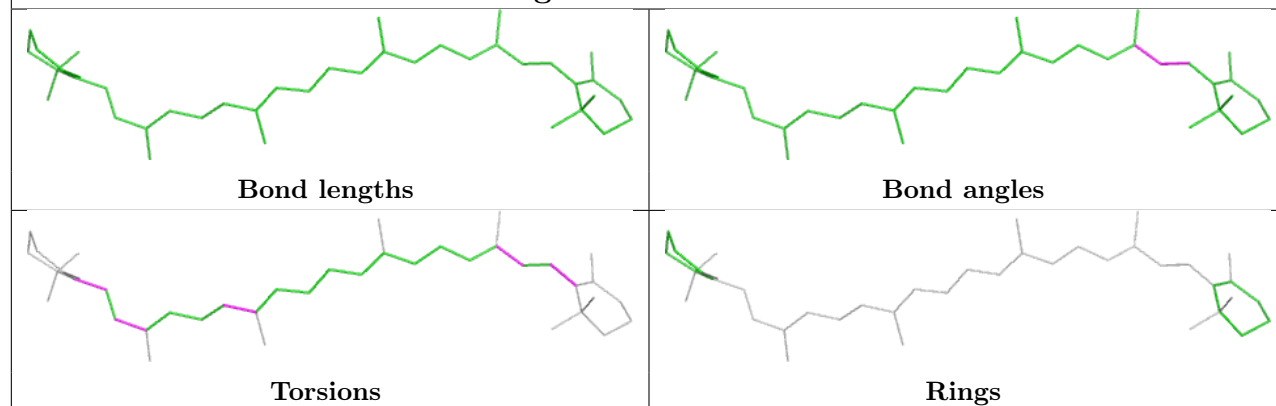


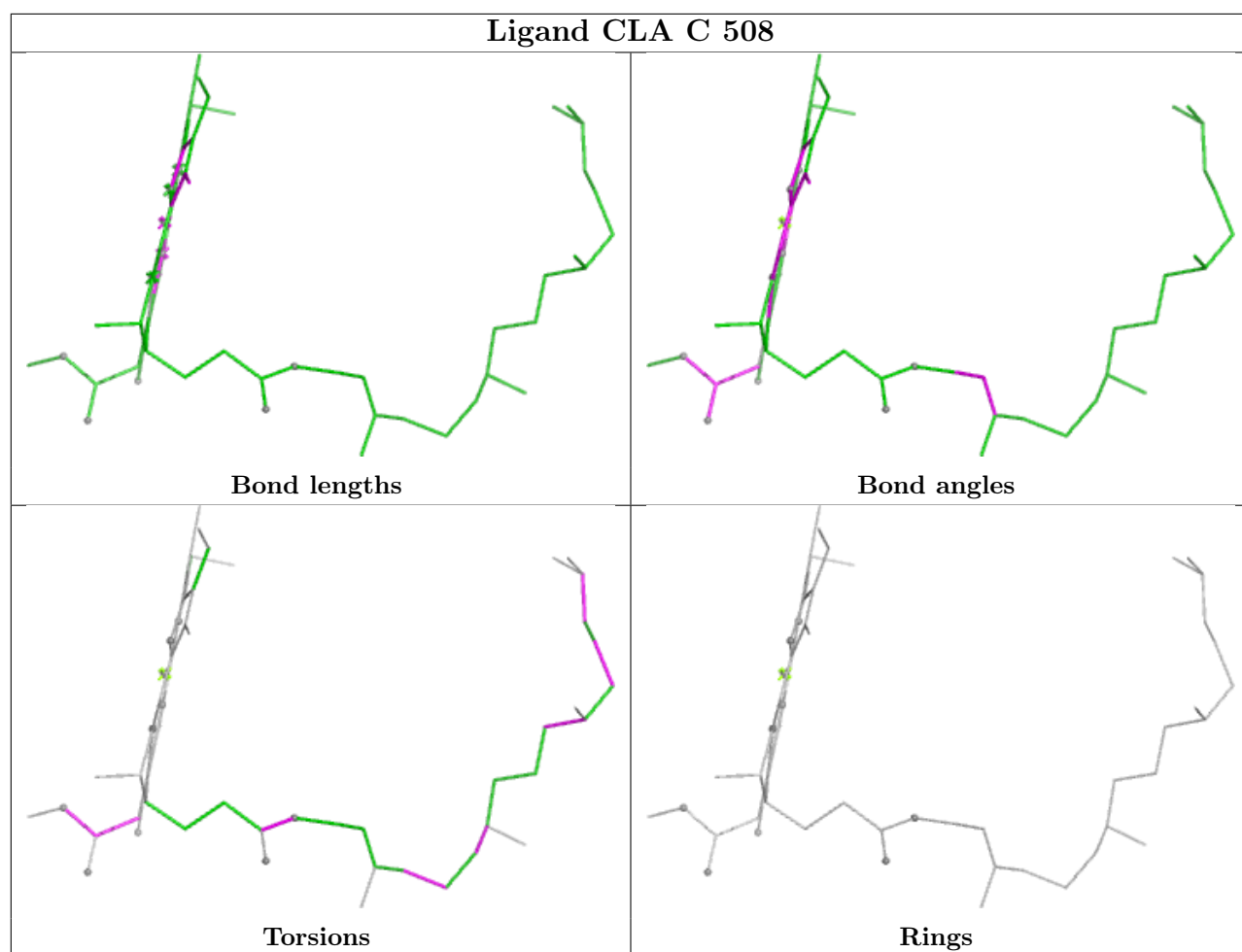


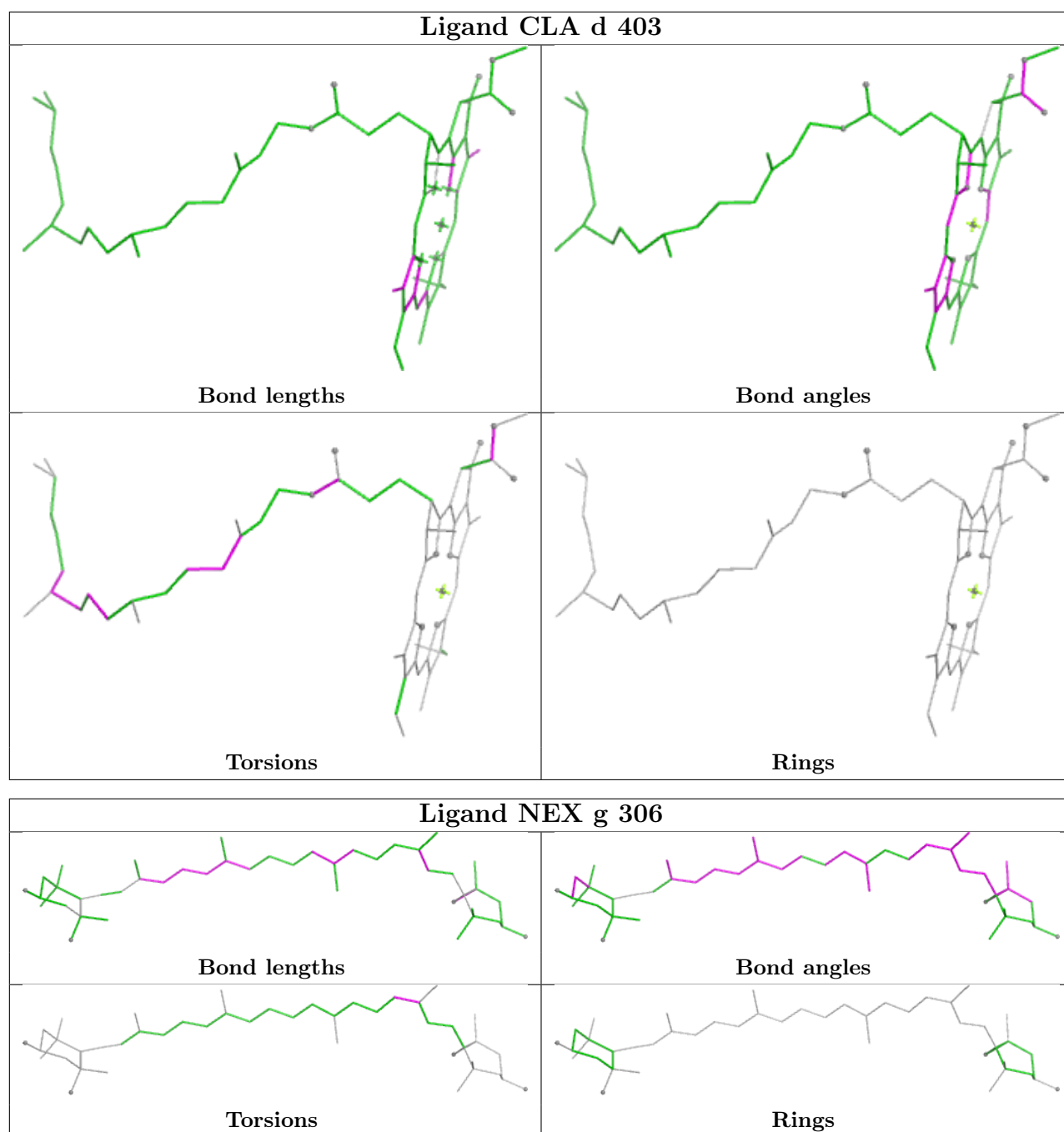
Ligand CHL n 307



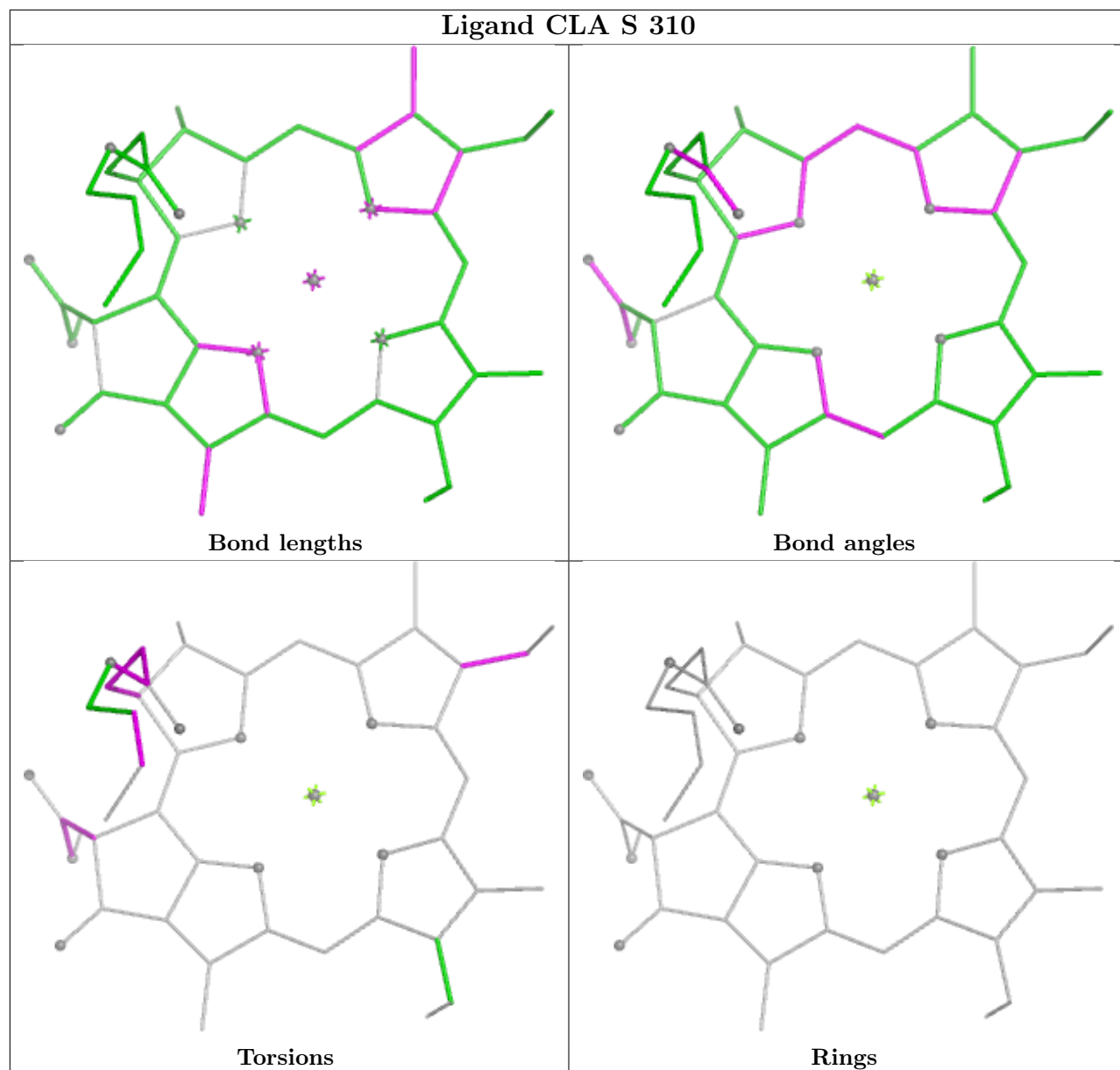
Ligand BCR J 101

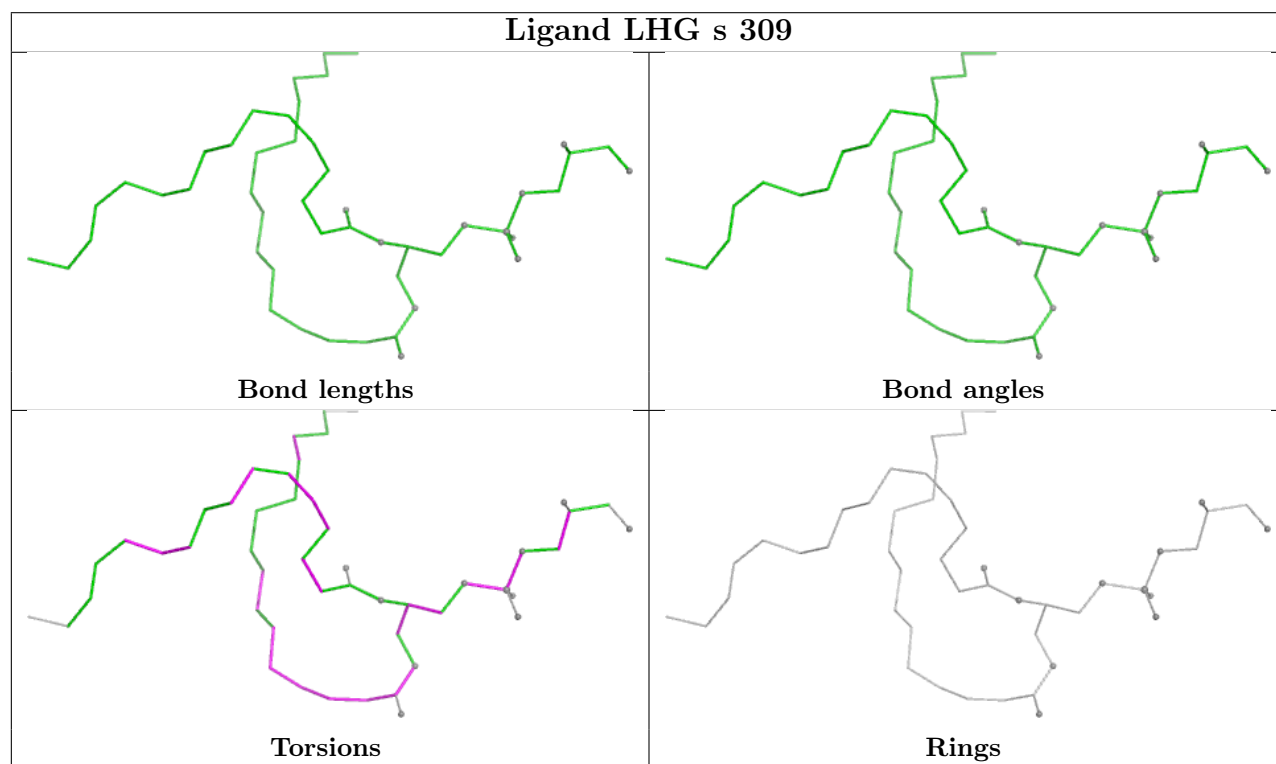
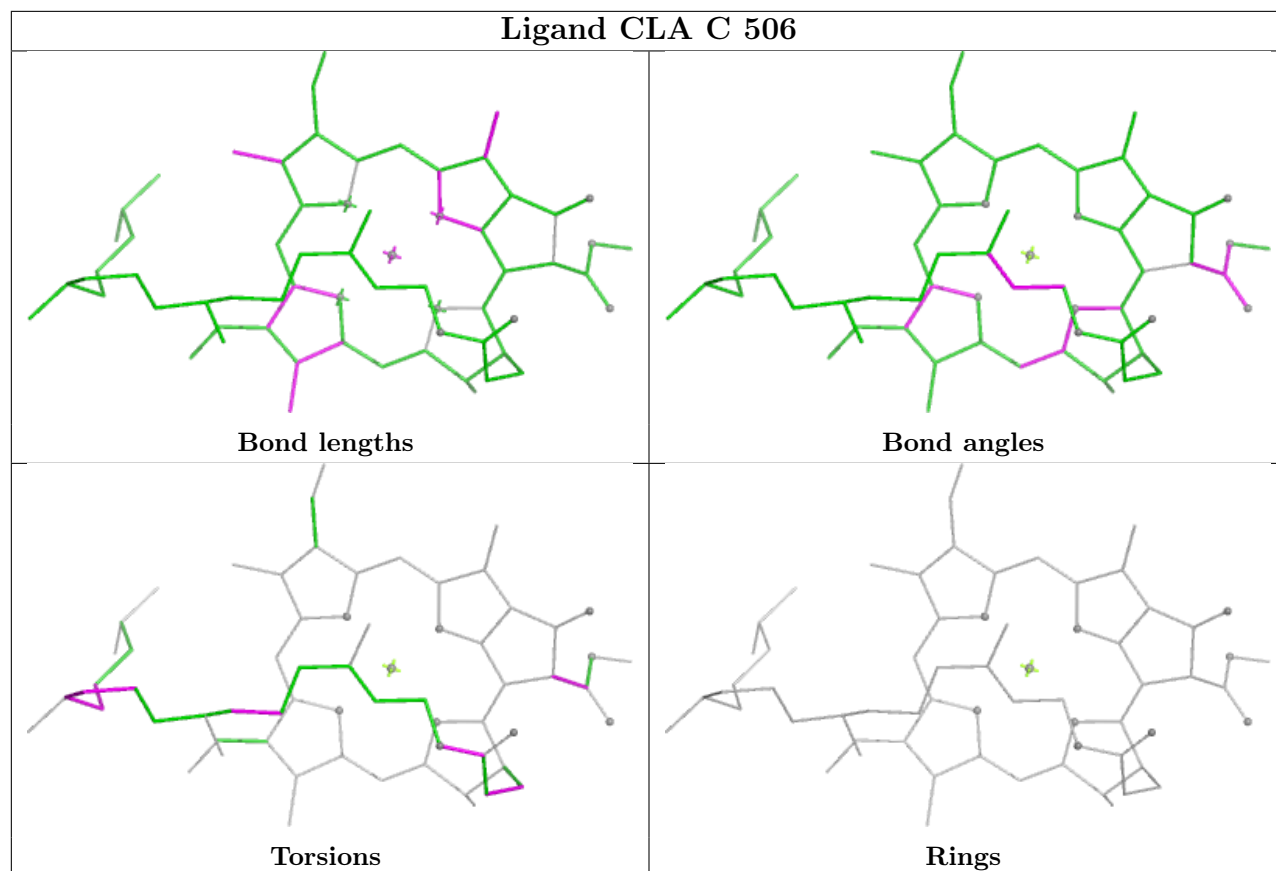


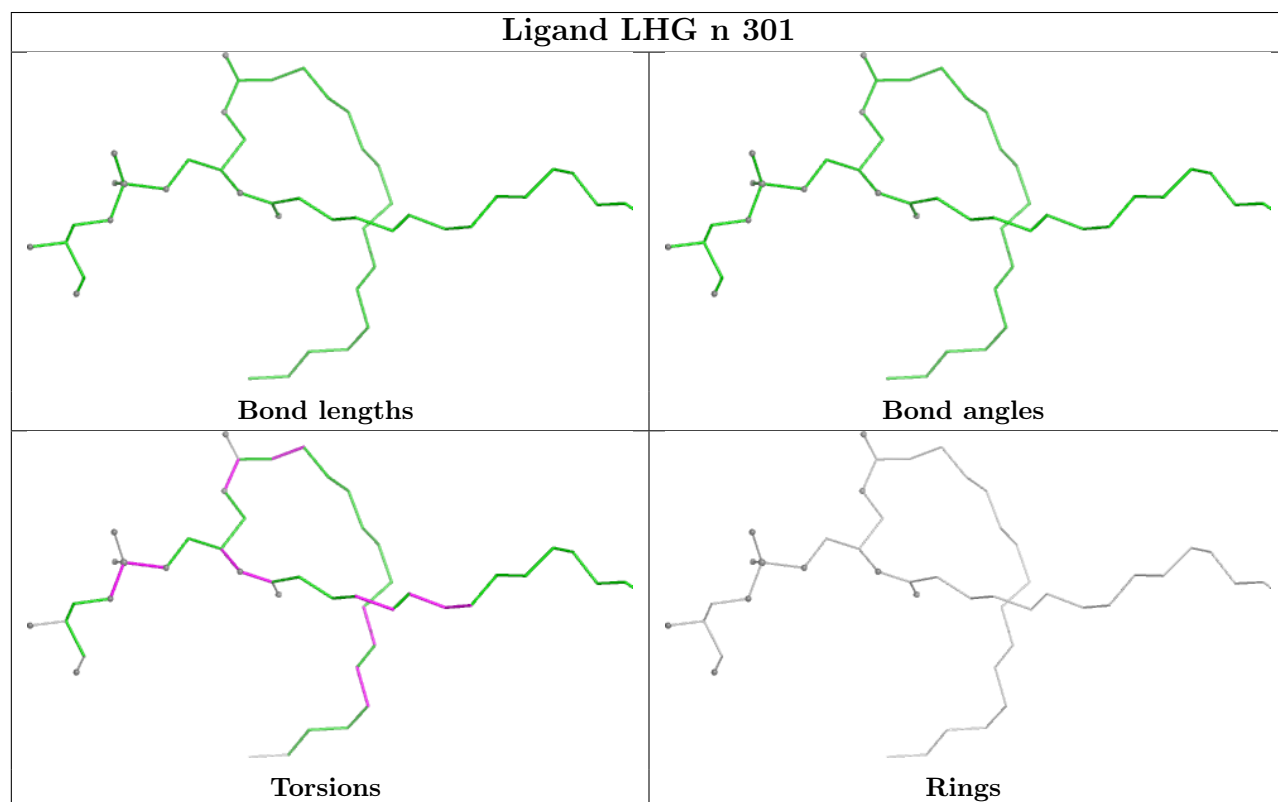
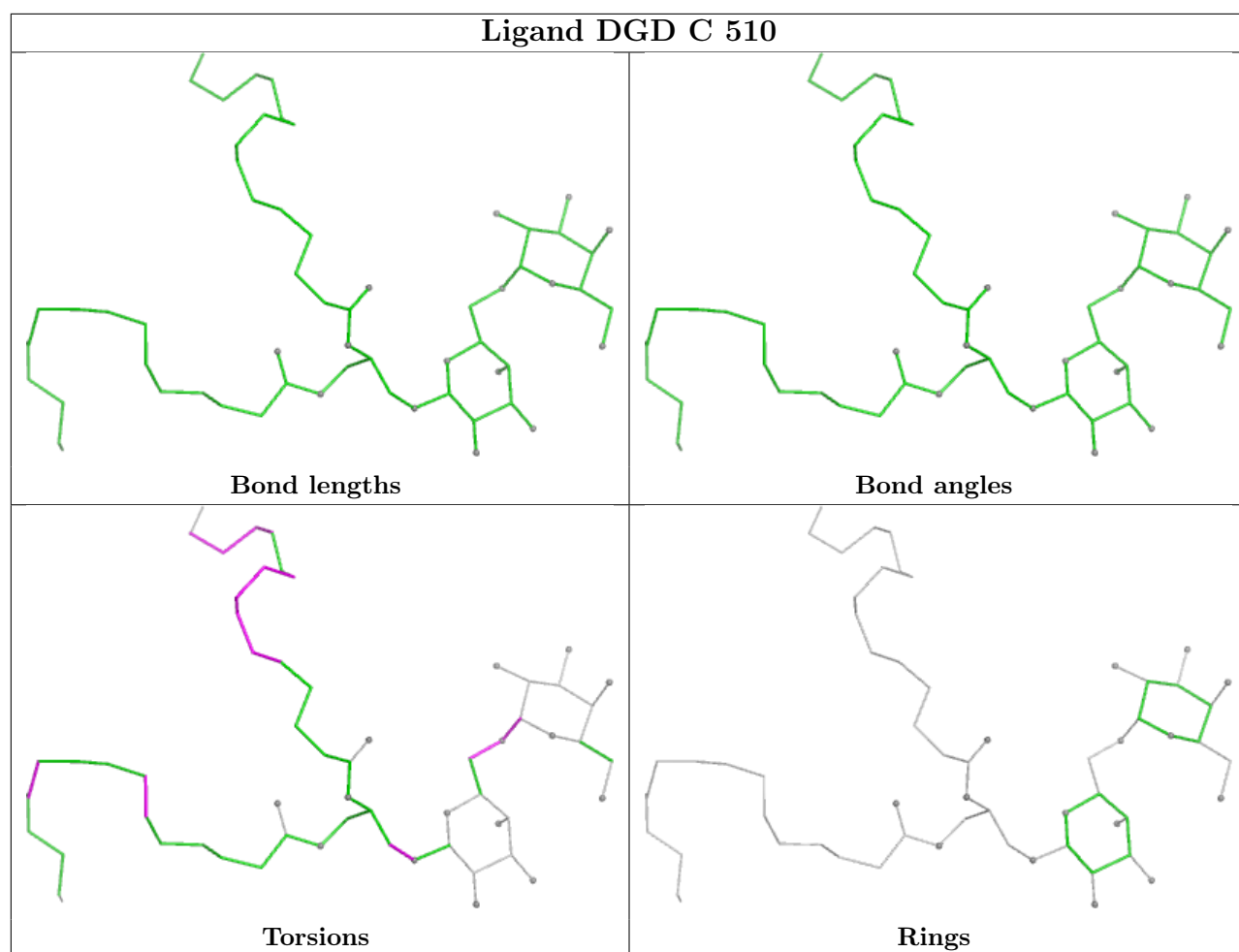


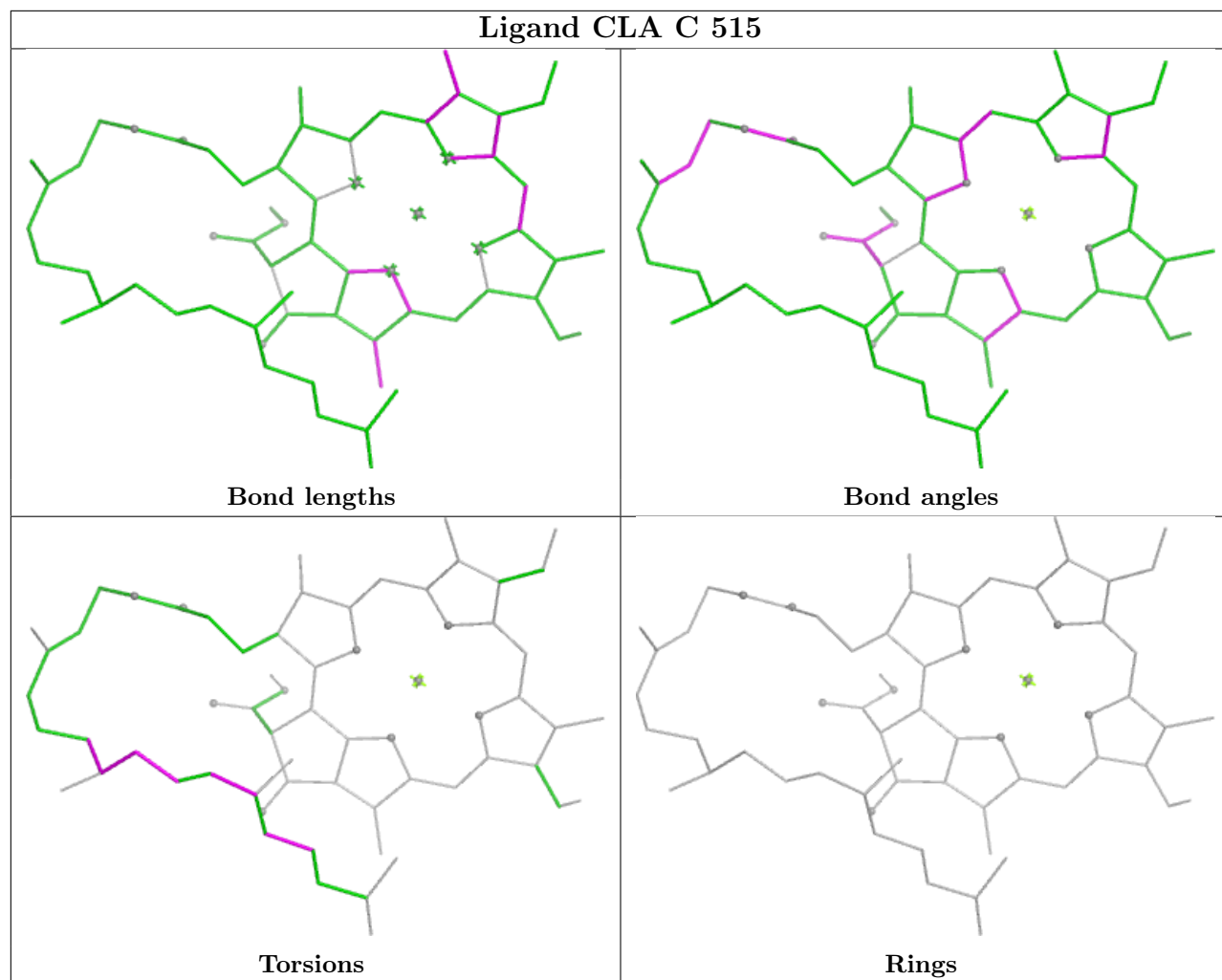


Ligand CLA S 310

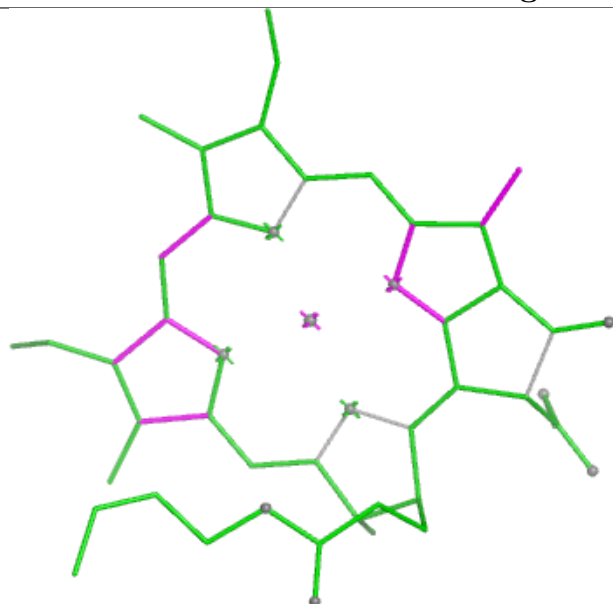




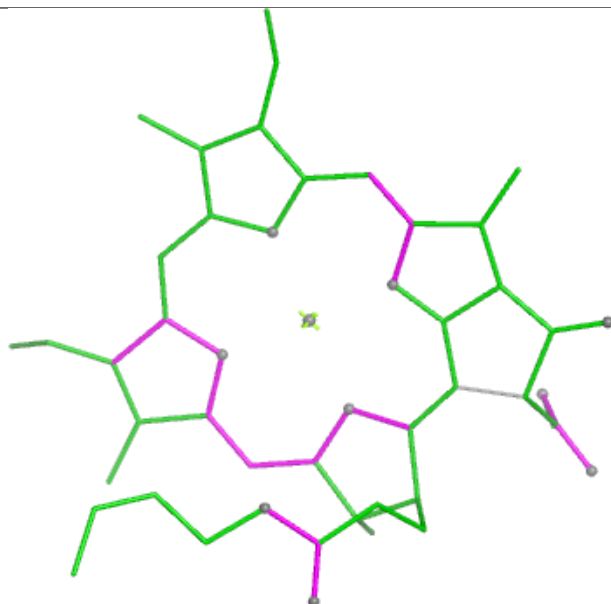




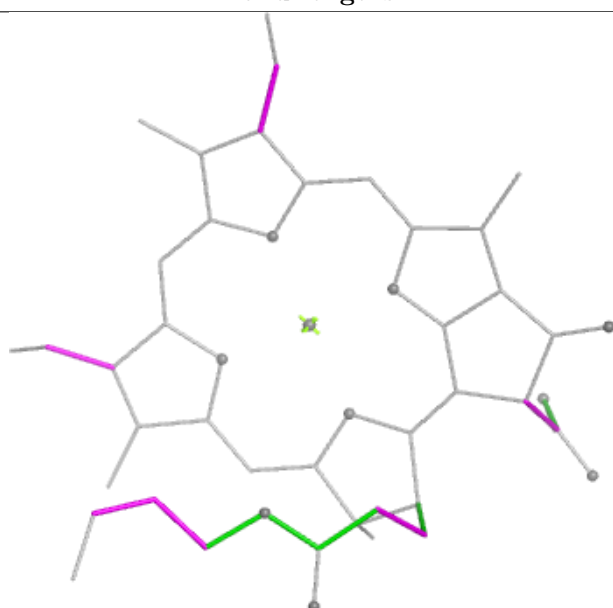
Ligand CLA s 311



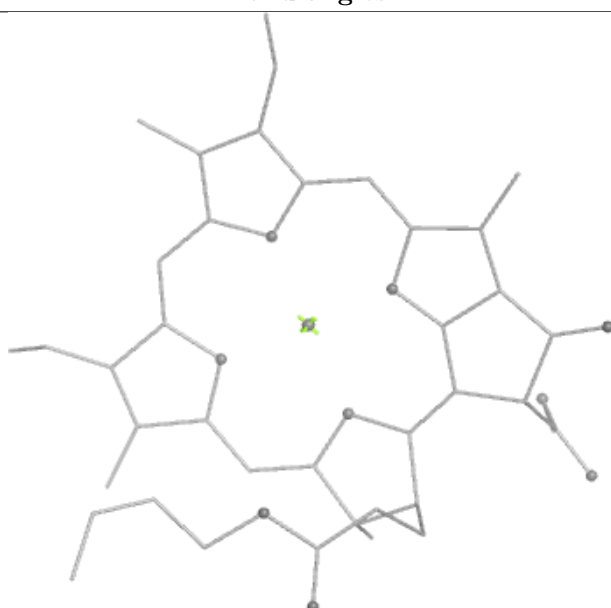
Bond lengths



Bond angles

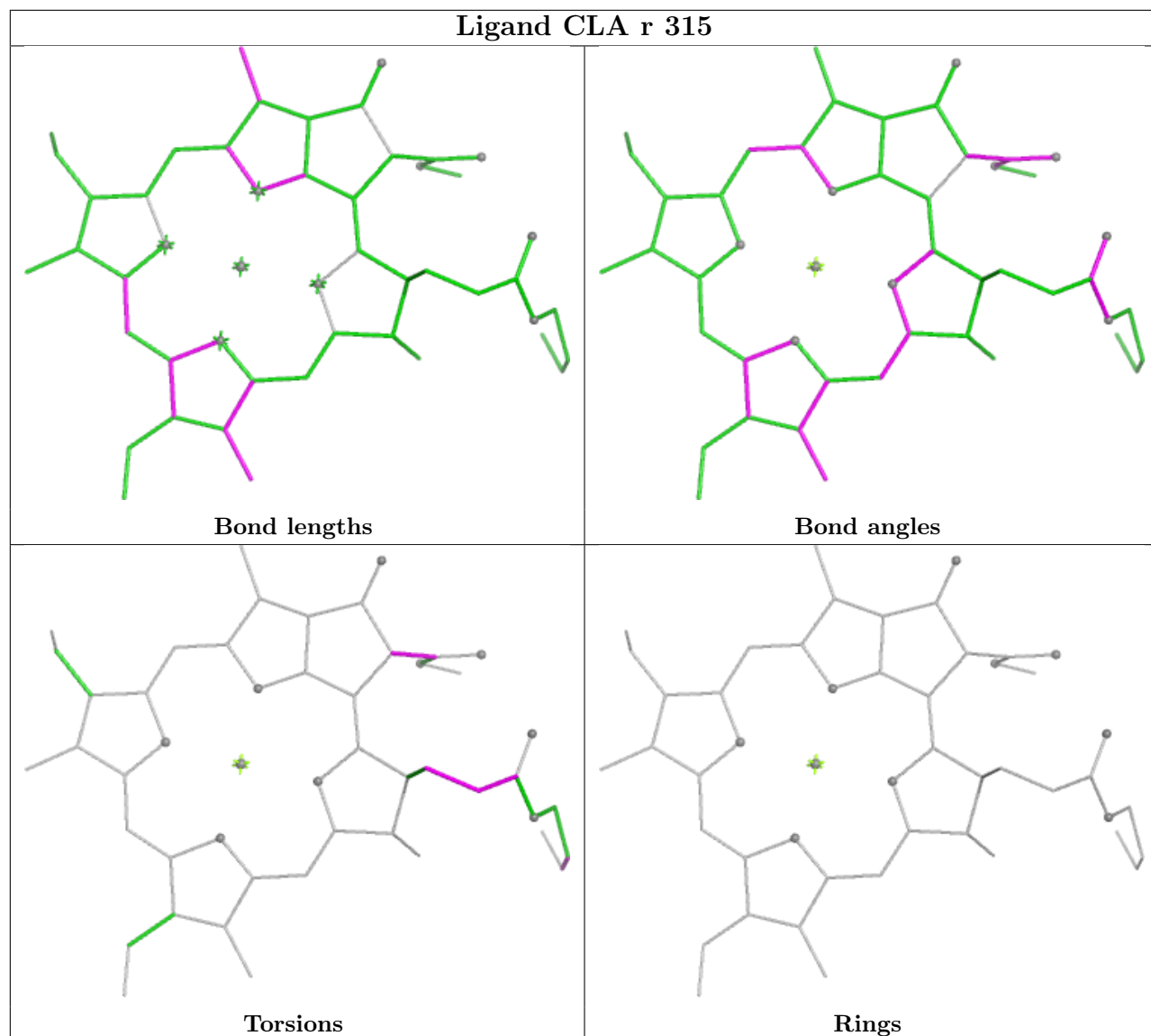


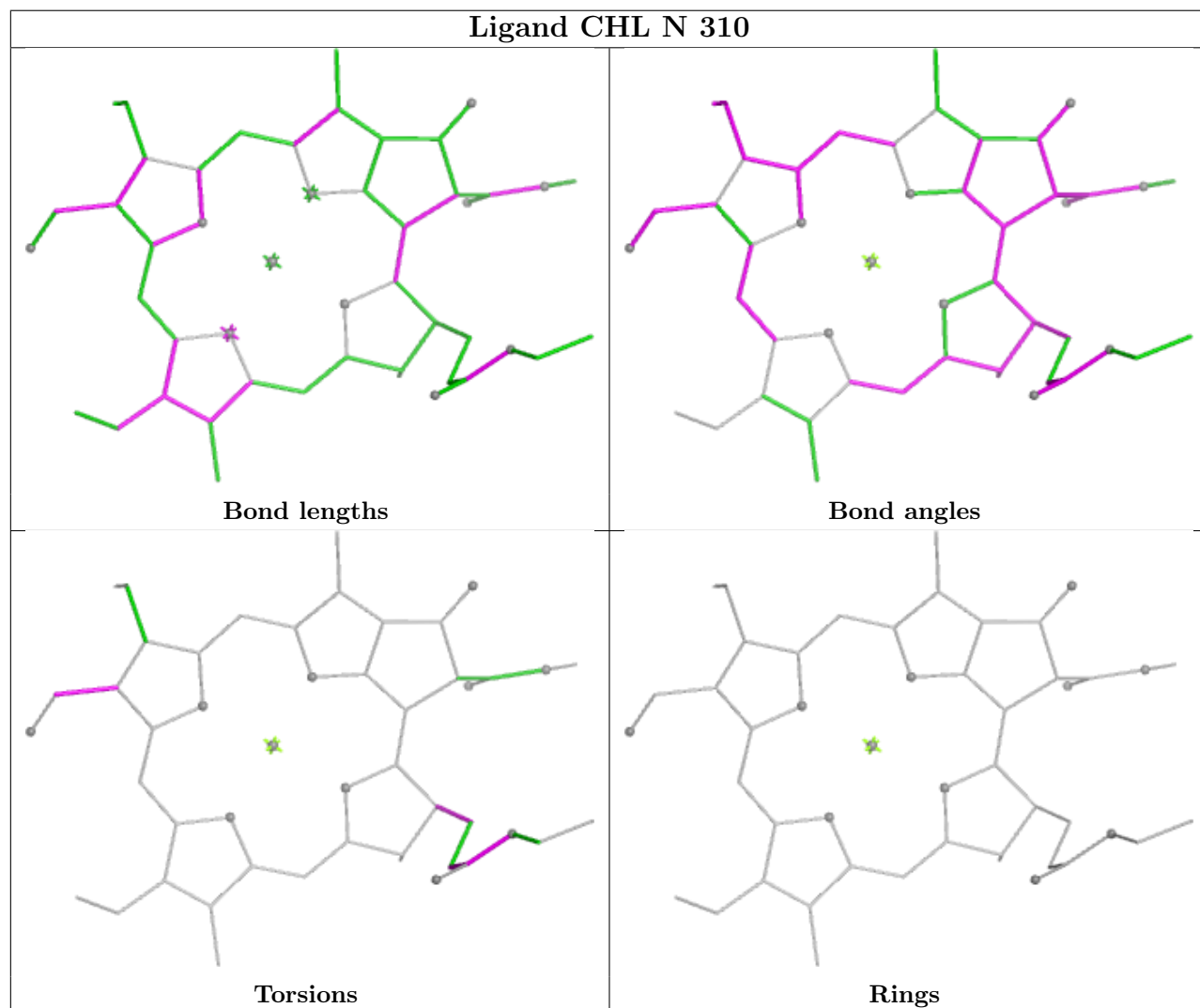
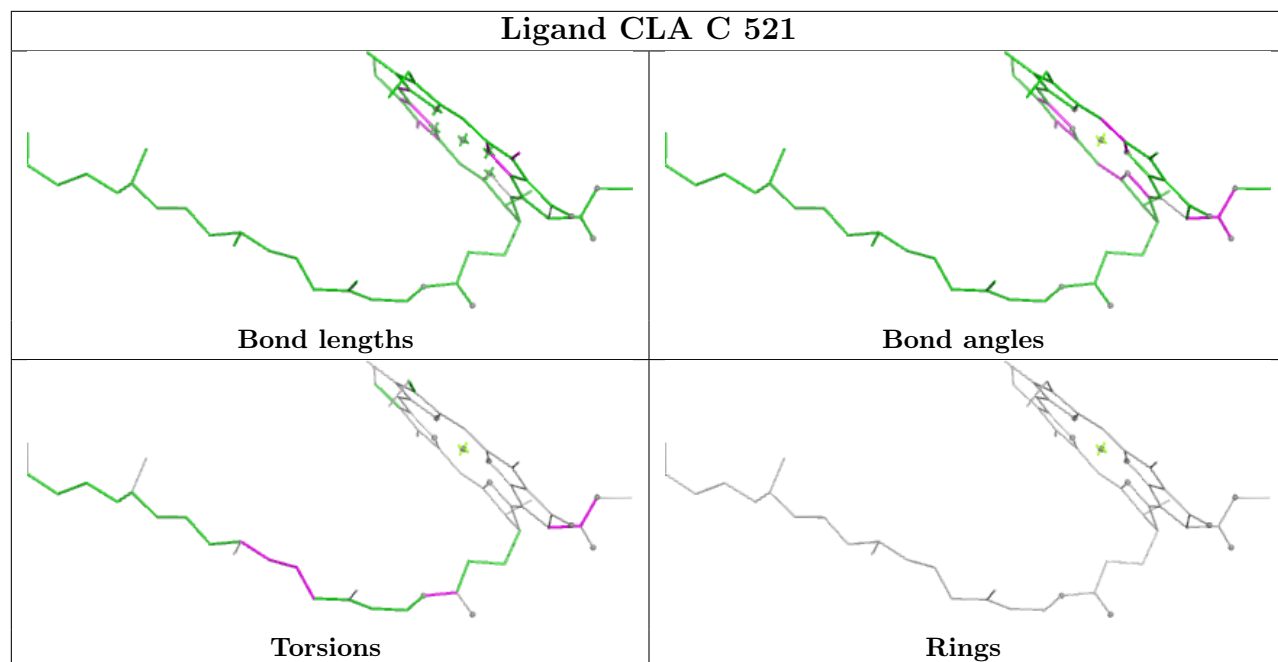
Torsions

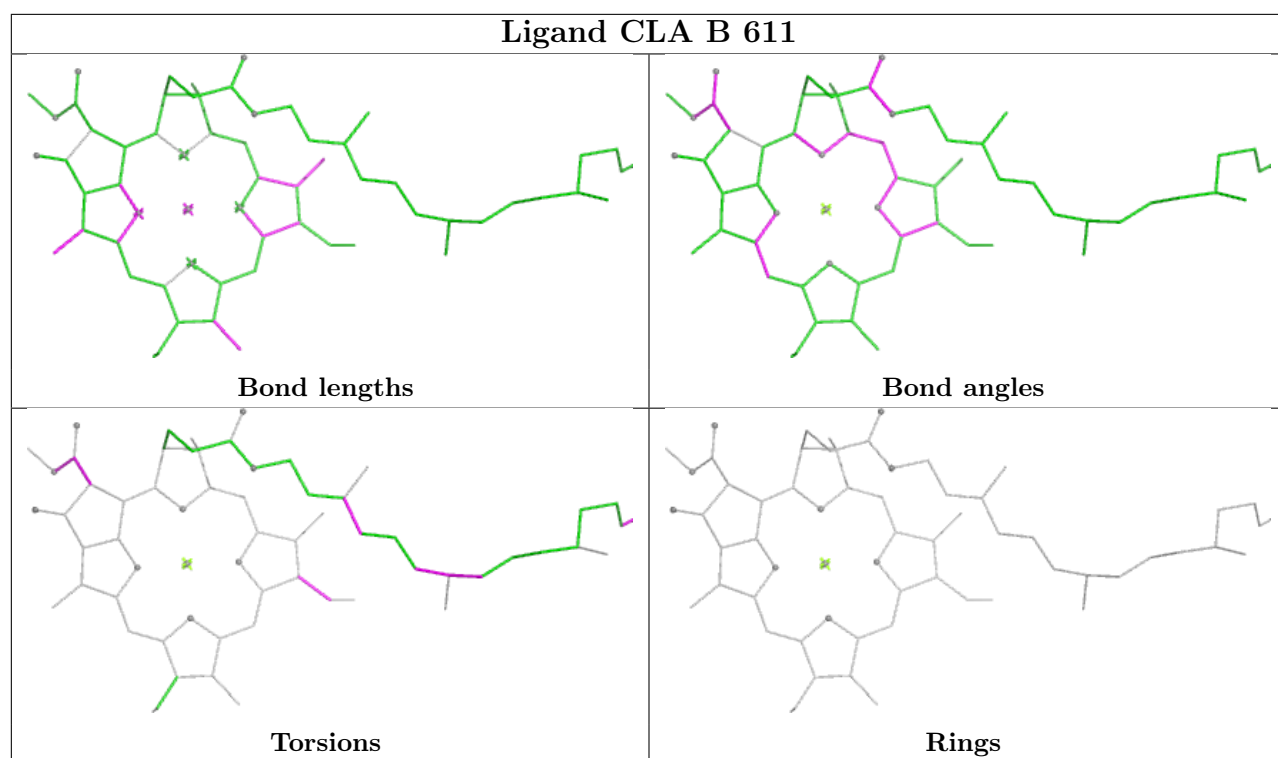


Rings

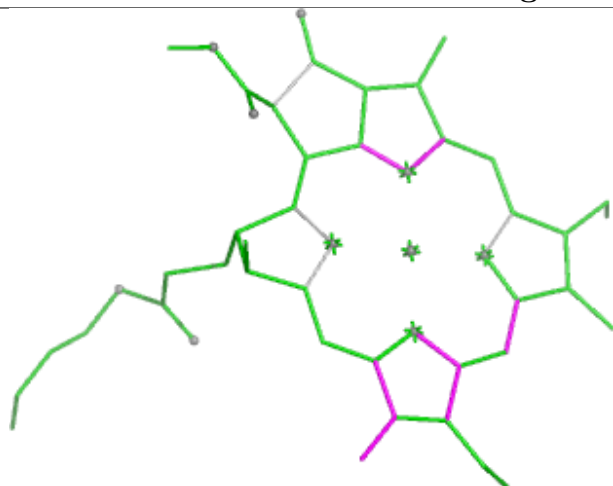
Ligand CLA r 315



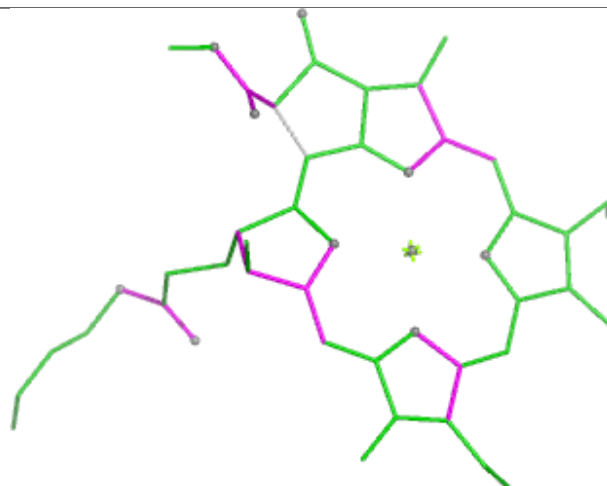




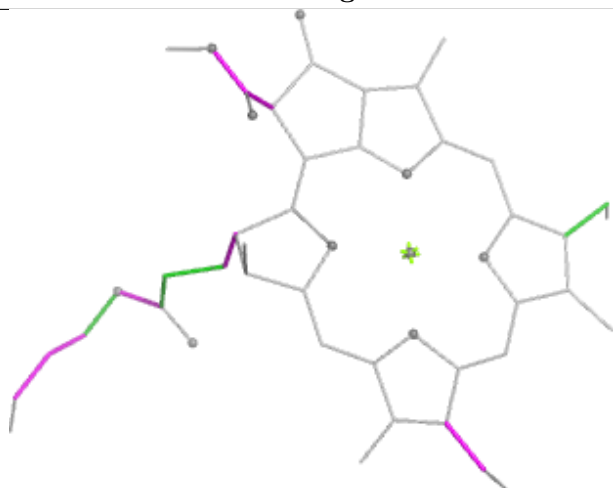
Ligand CLA s 314



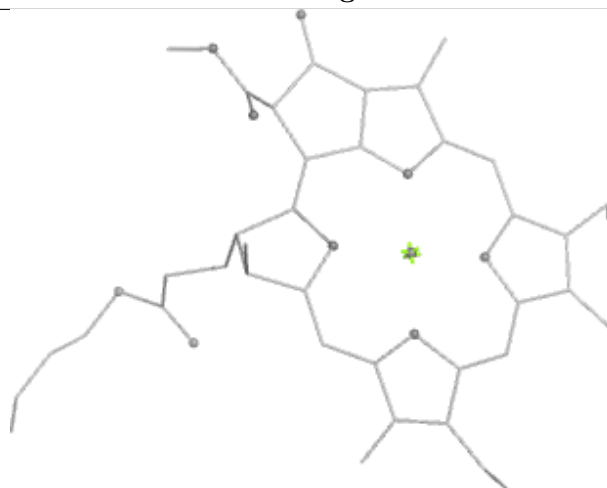
Bond lengths



Bond angles

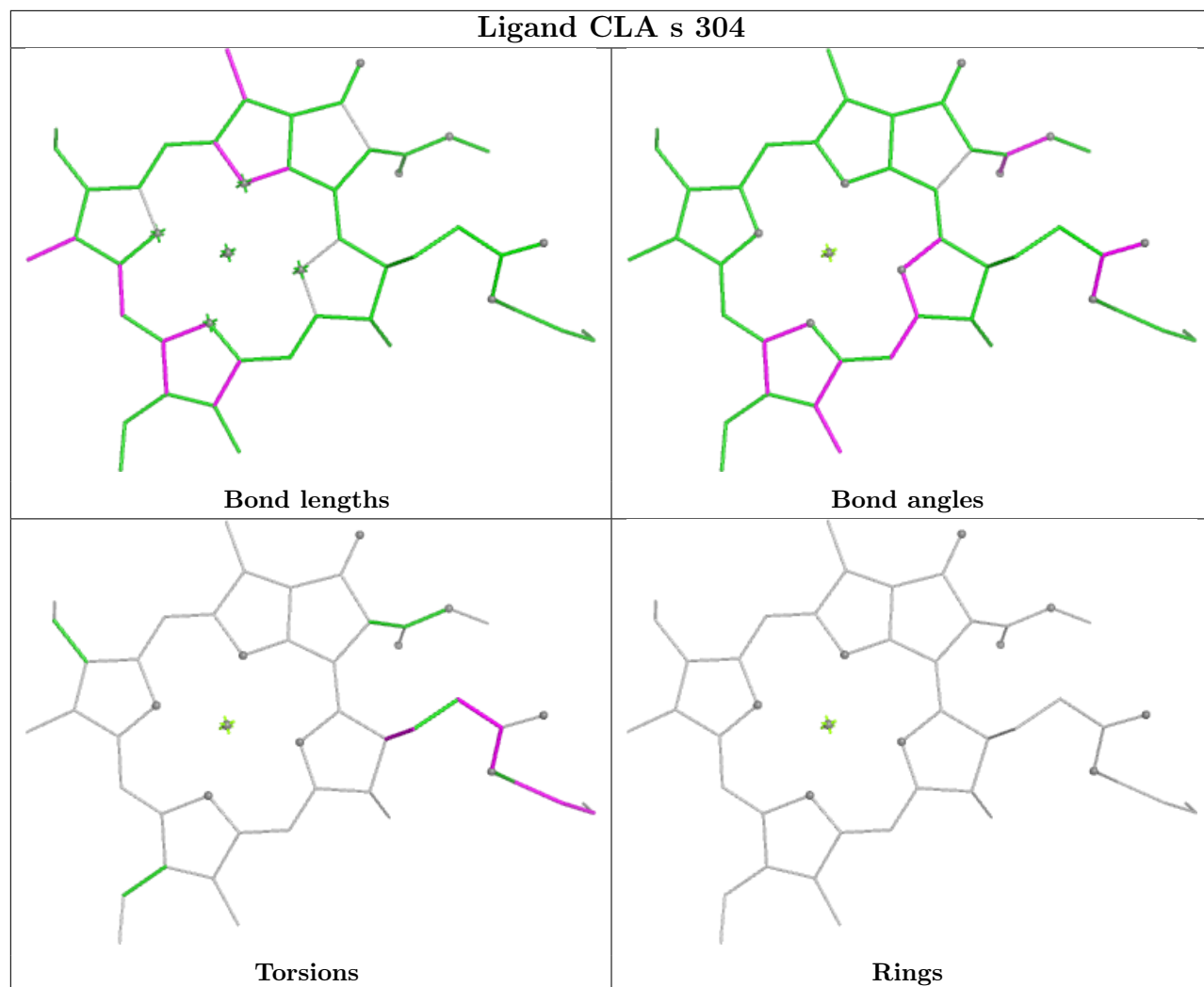


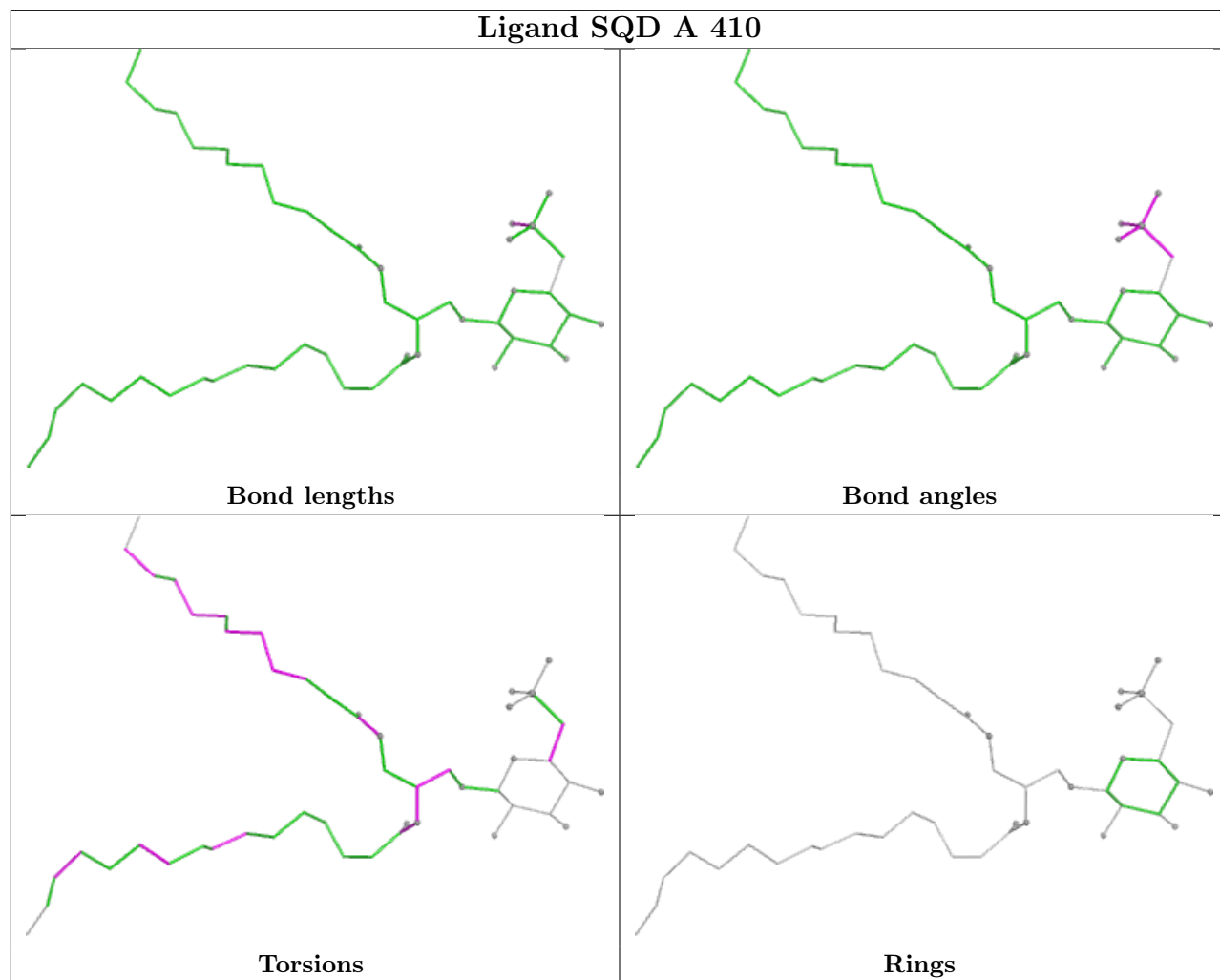
Torsions

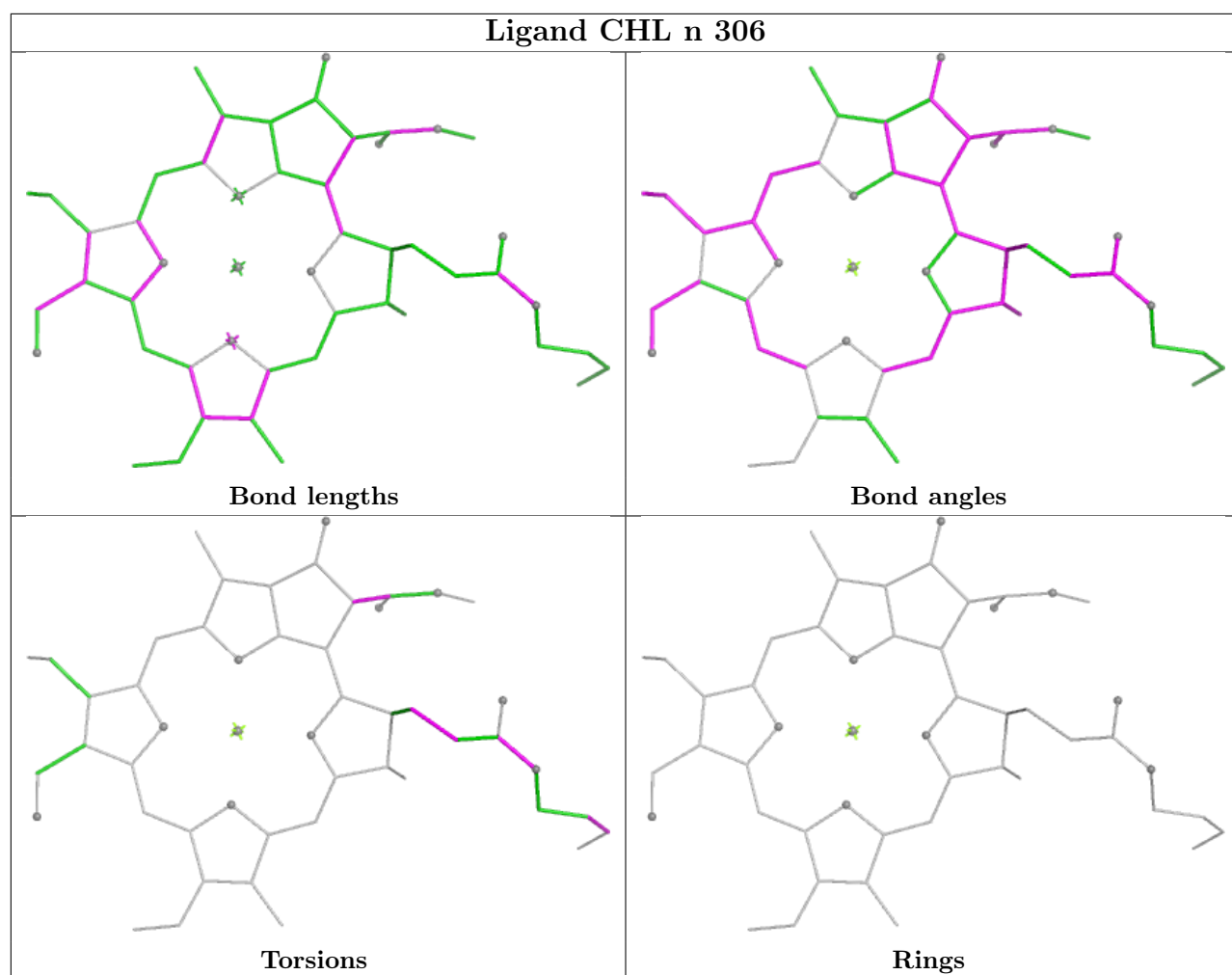


Rings

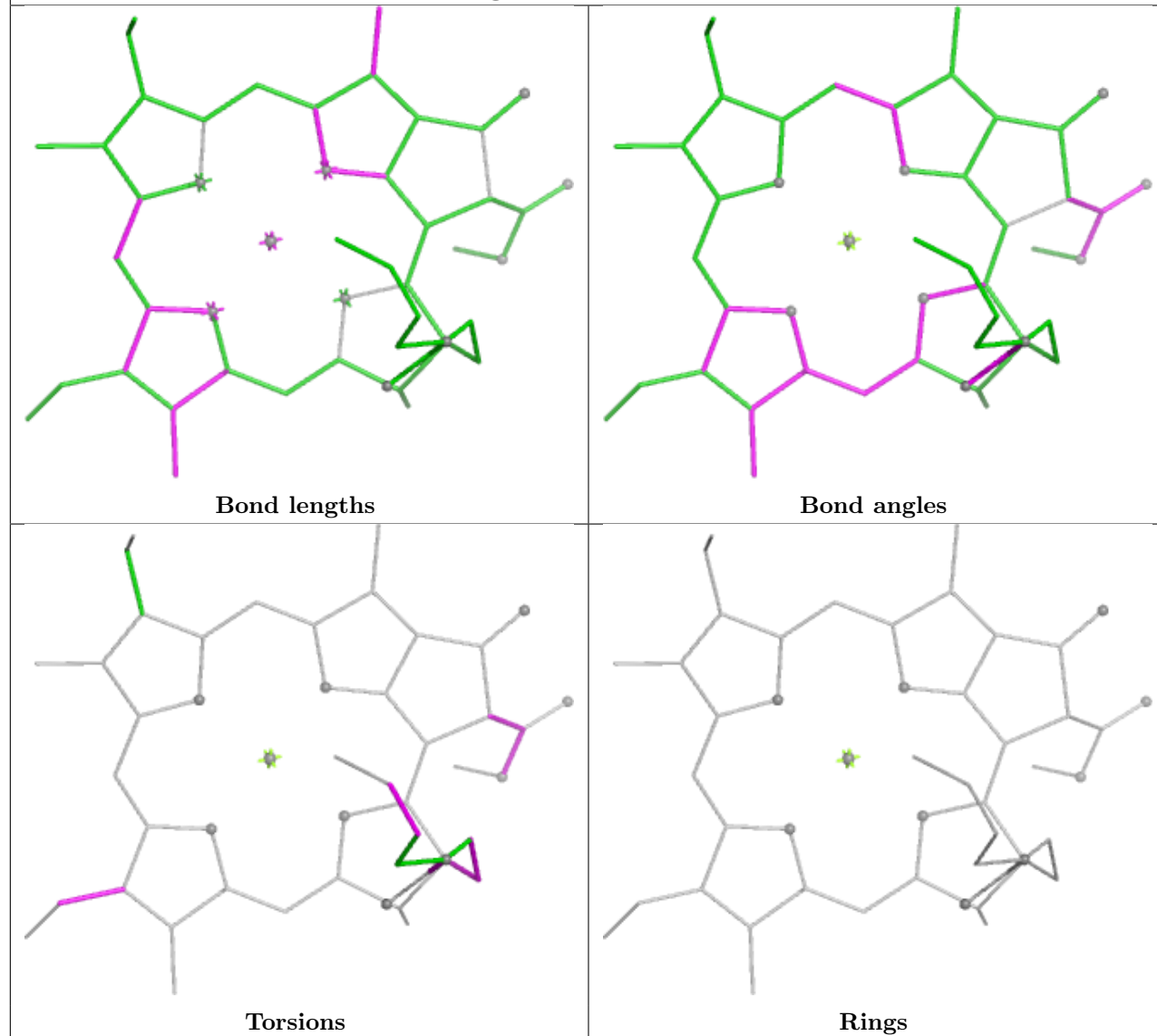
Ligand CLA s 304

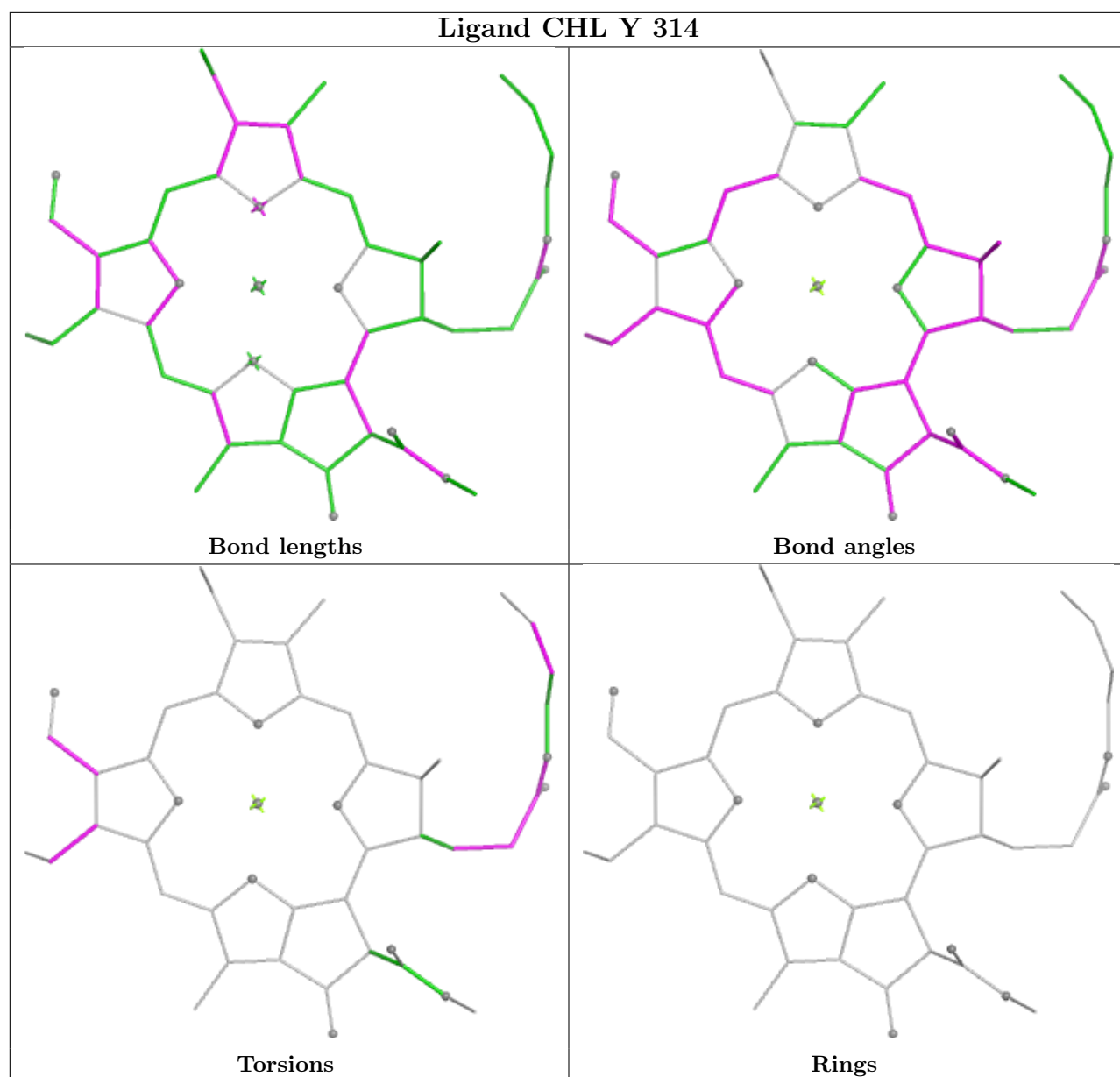


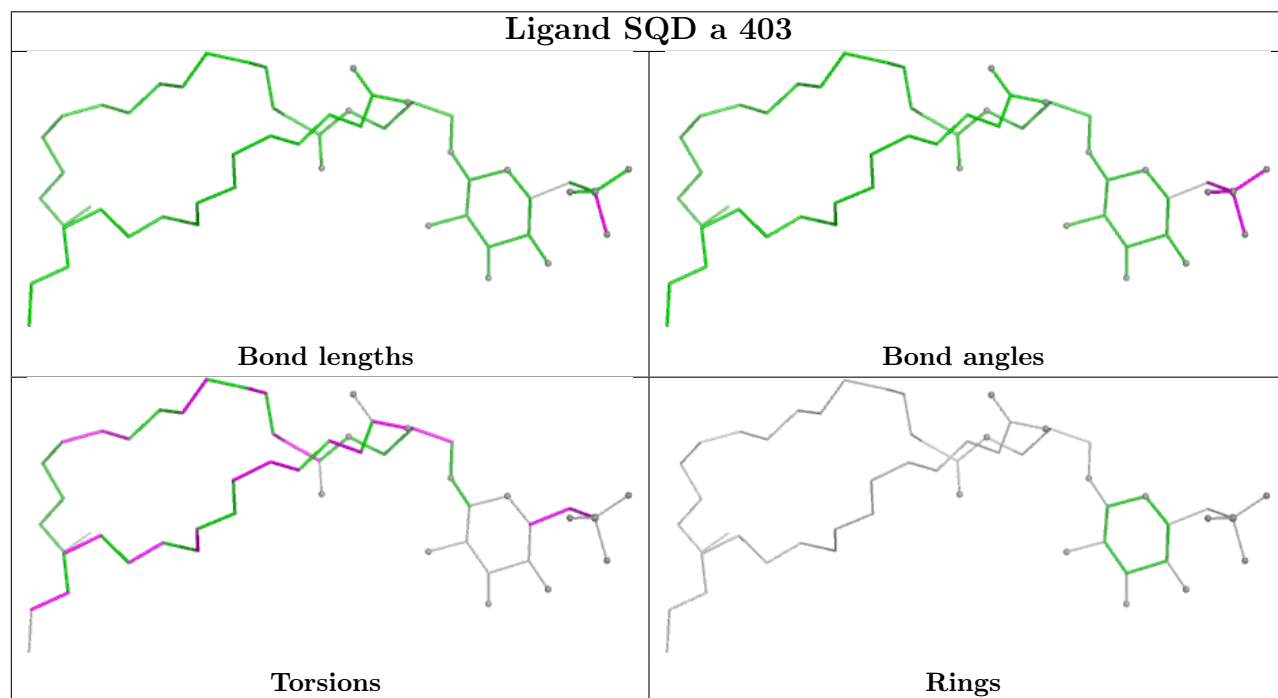
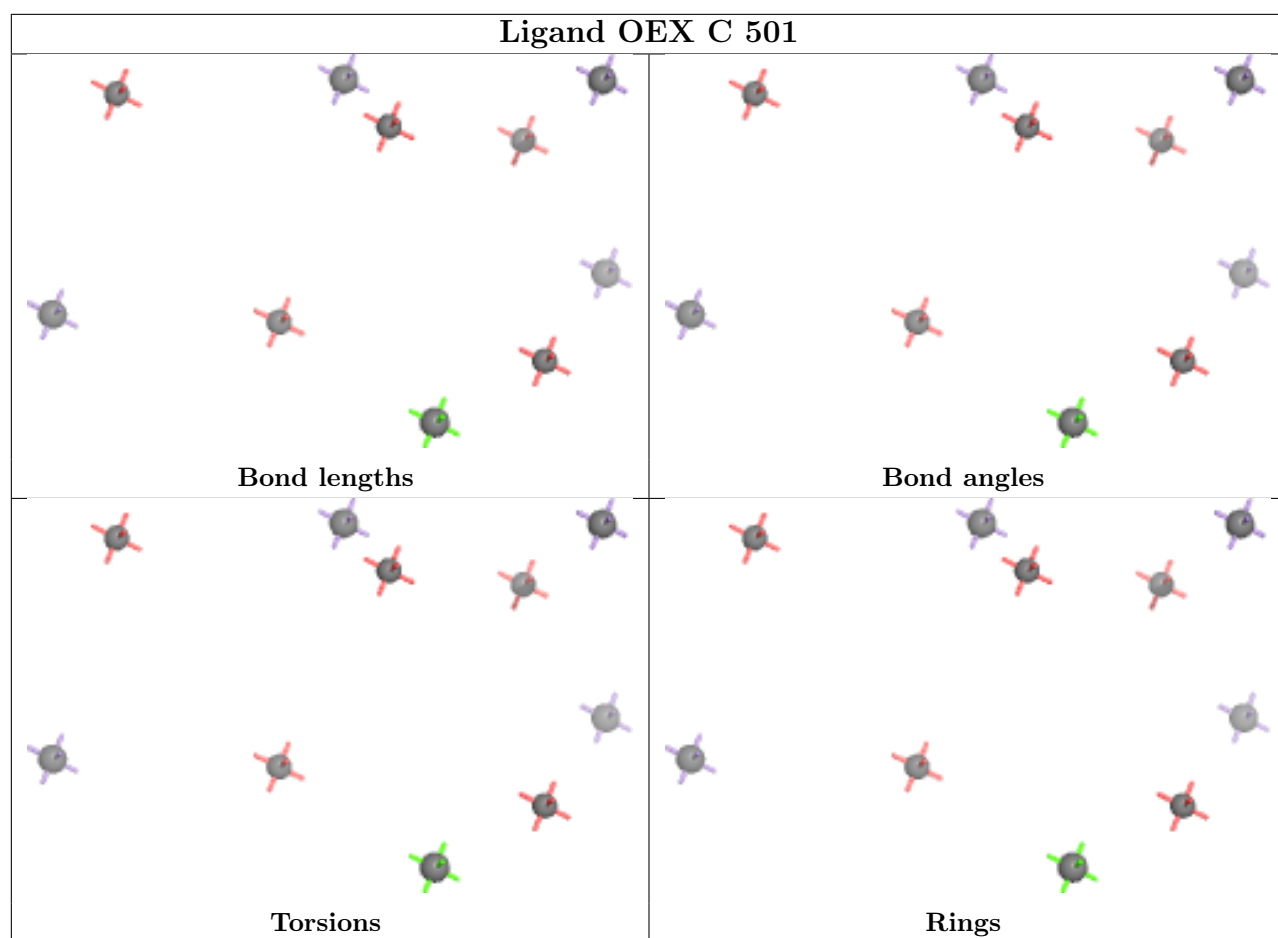


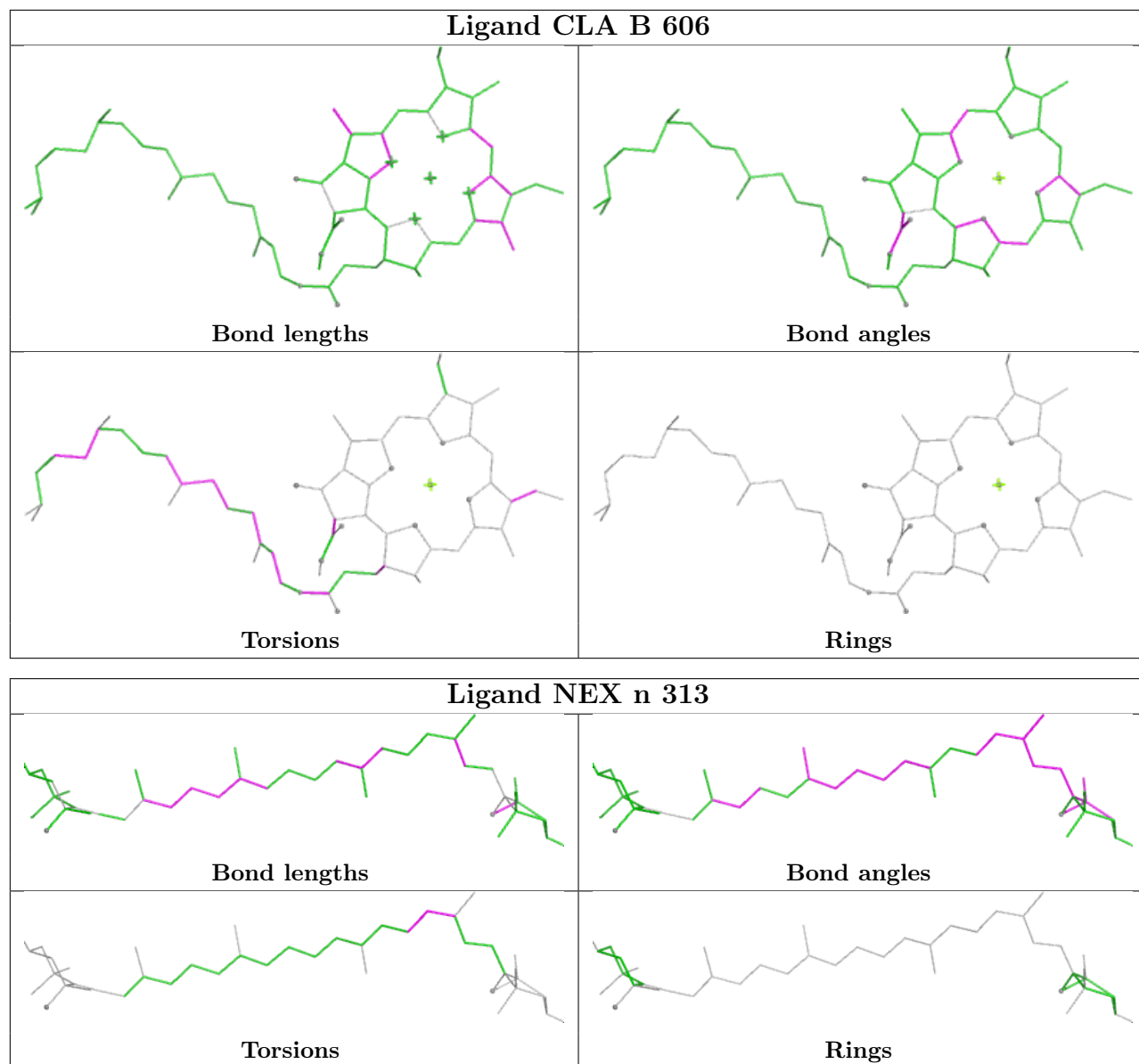


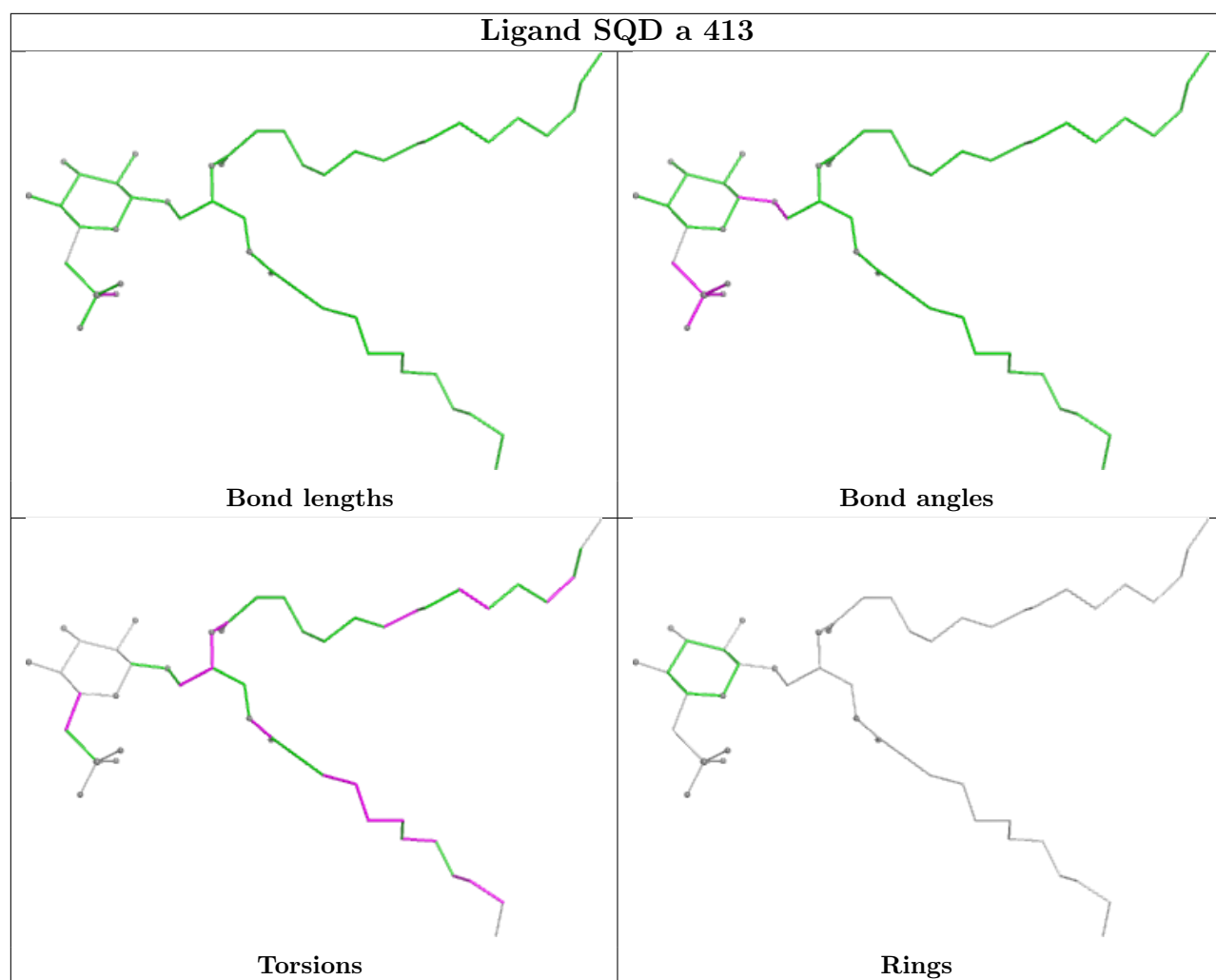
Ligand CLA r 311



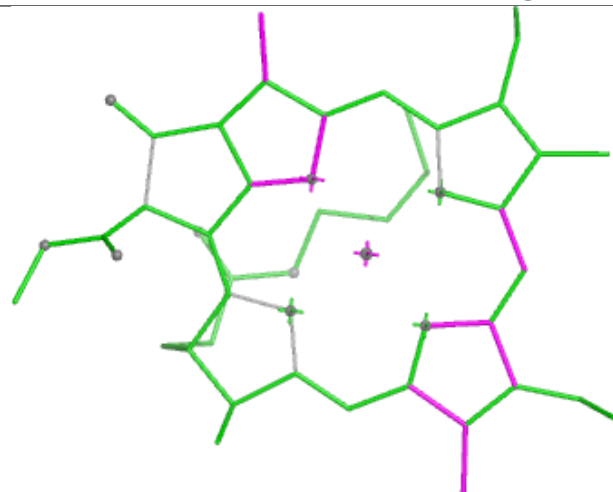




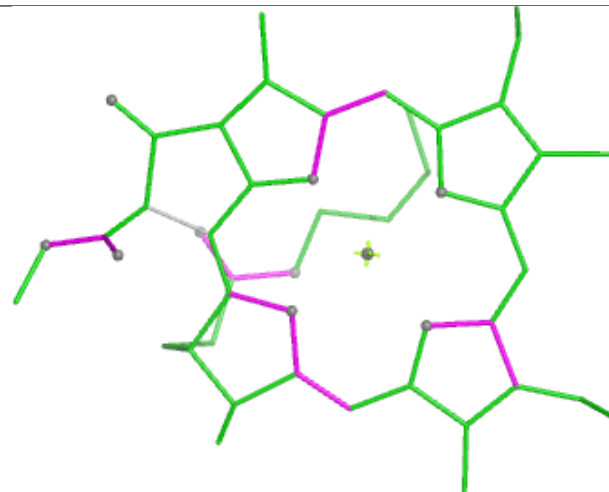




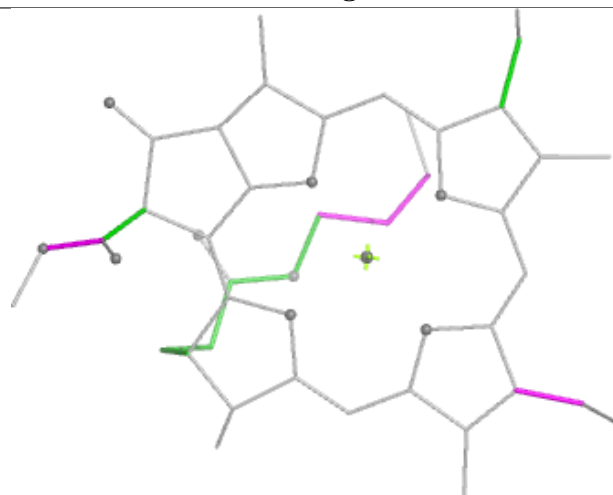
Ligand CLA S 303



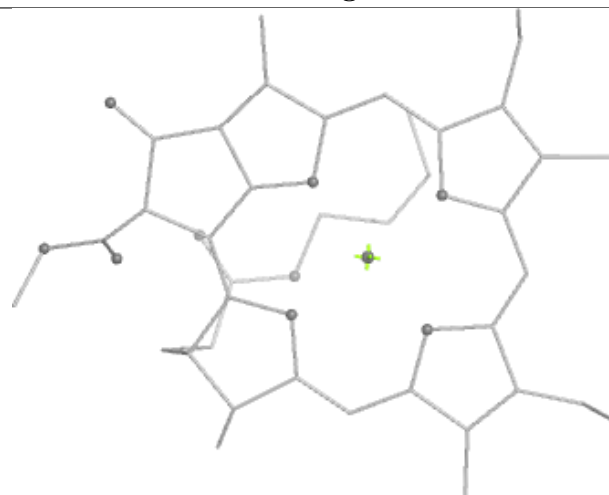
Bond lengths



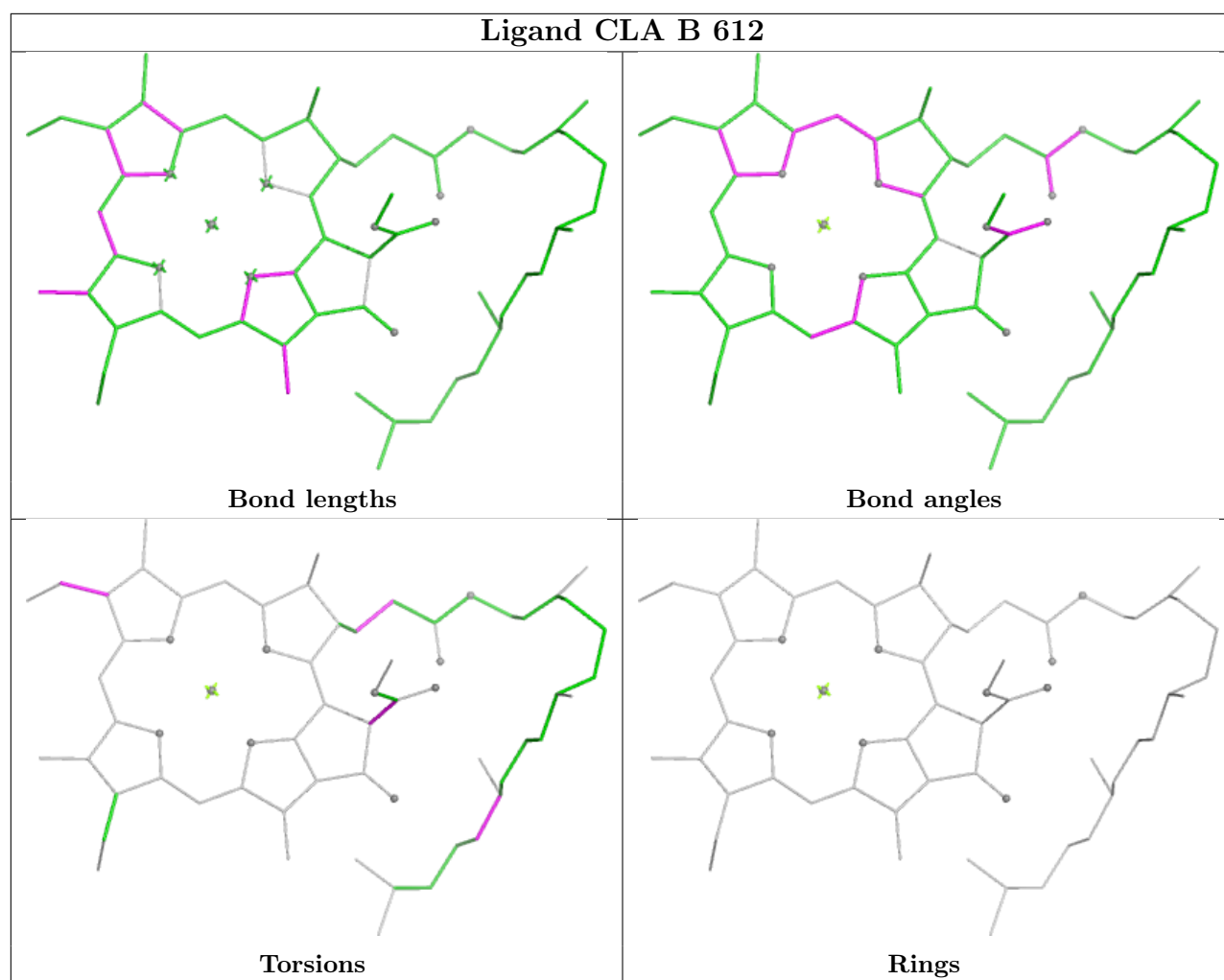
Bond angles

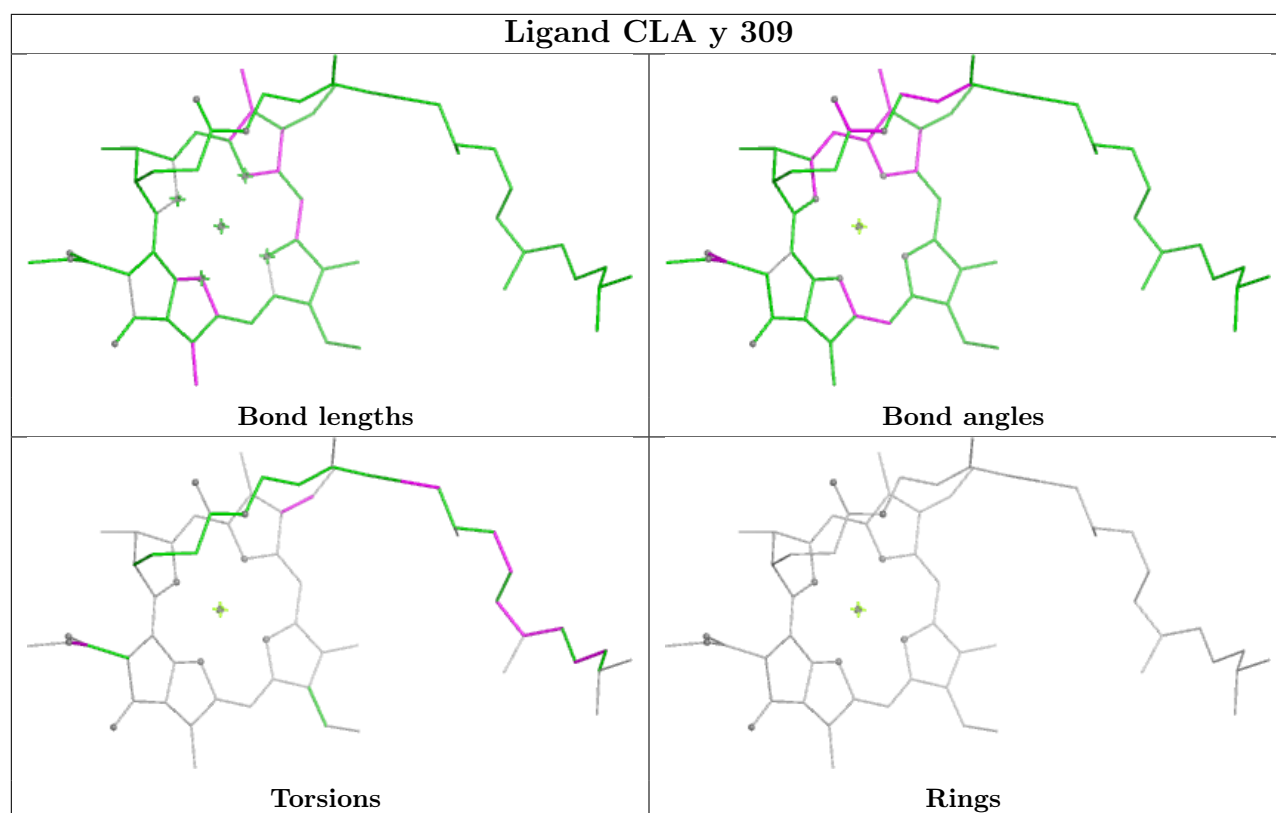


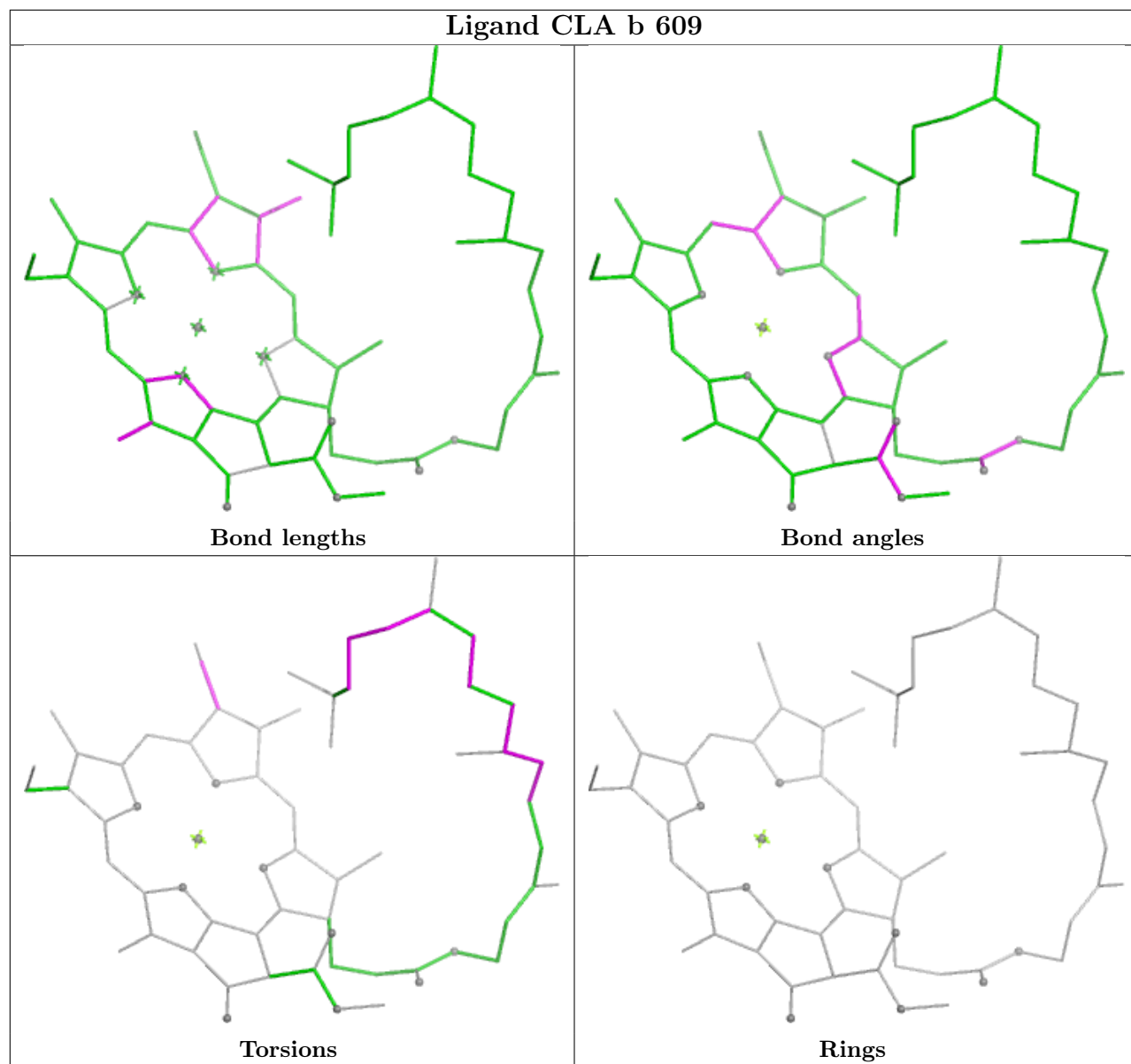
Torsions



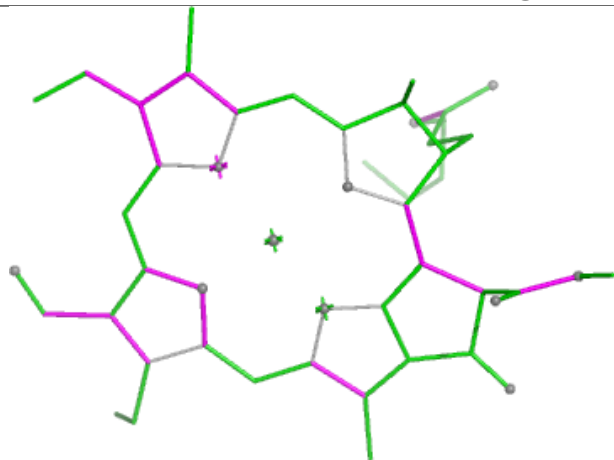
Rings



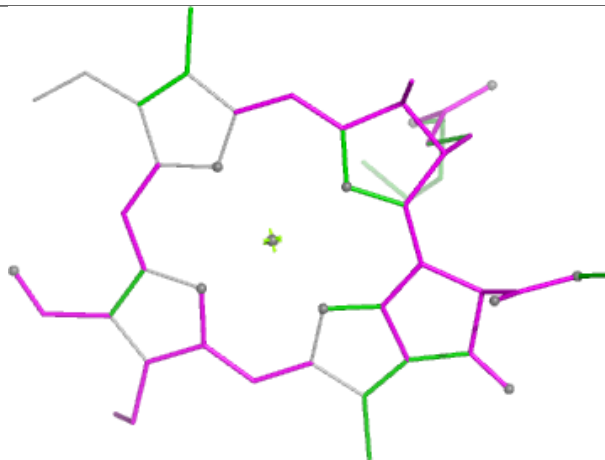




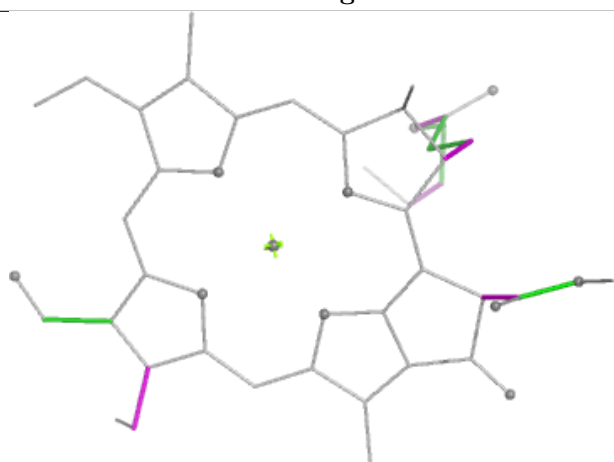
Ligand CHL n 319



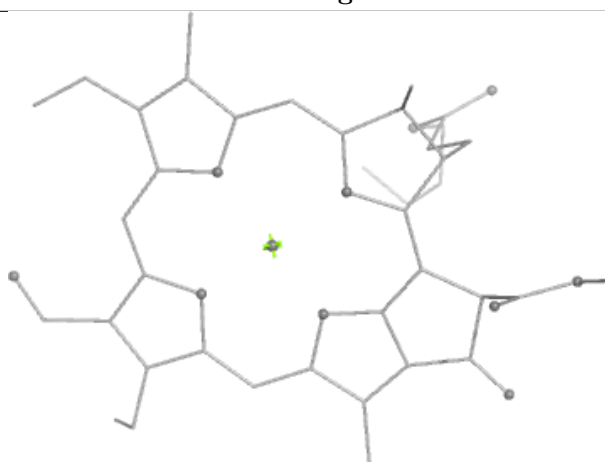
Bond lengths



Bond angles

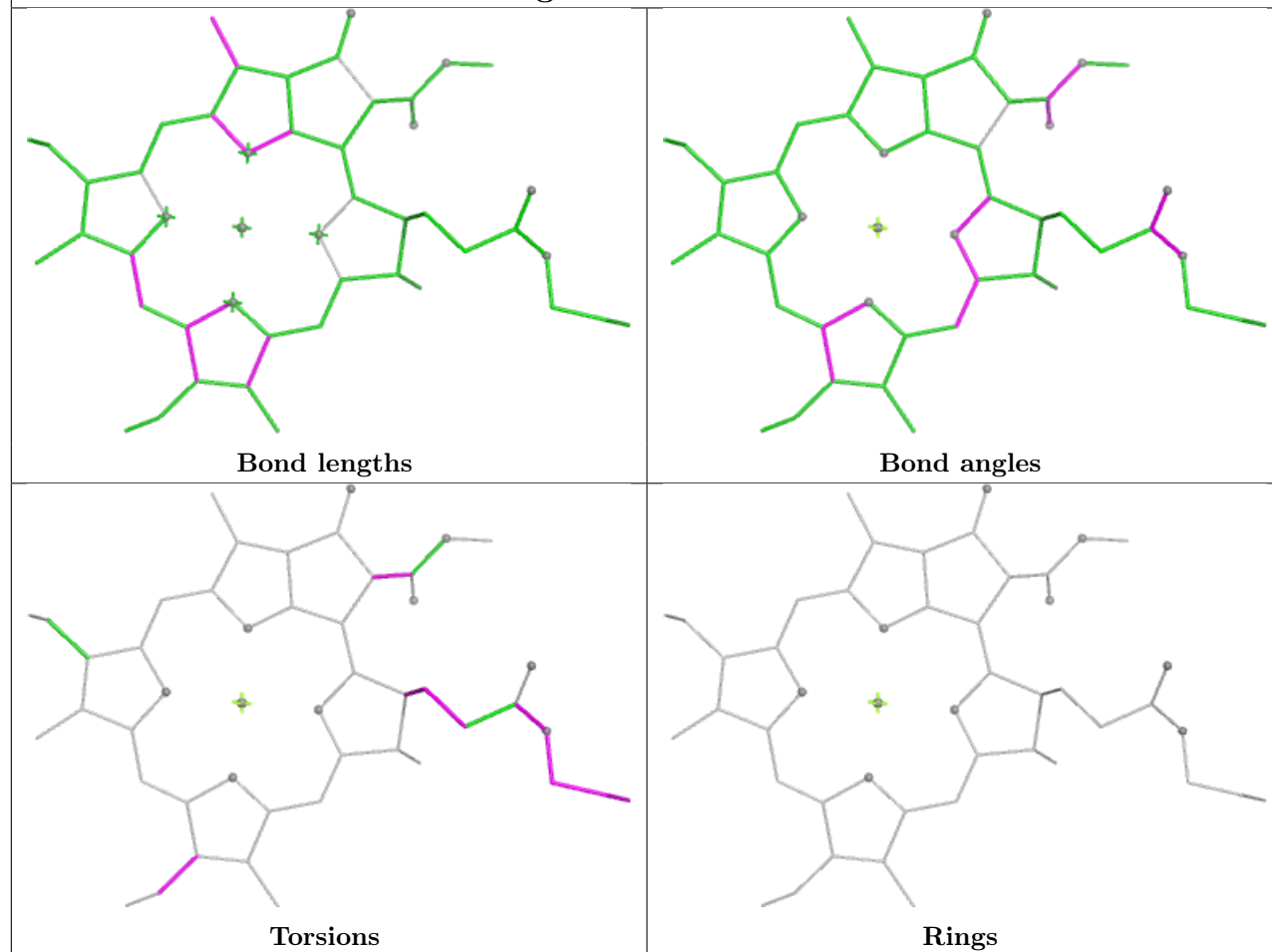


Torsions

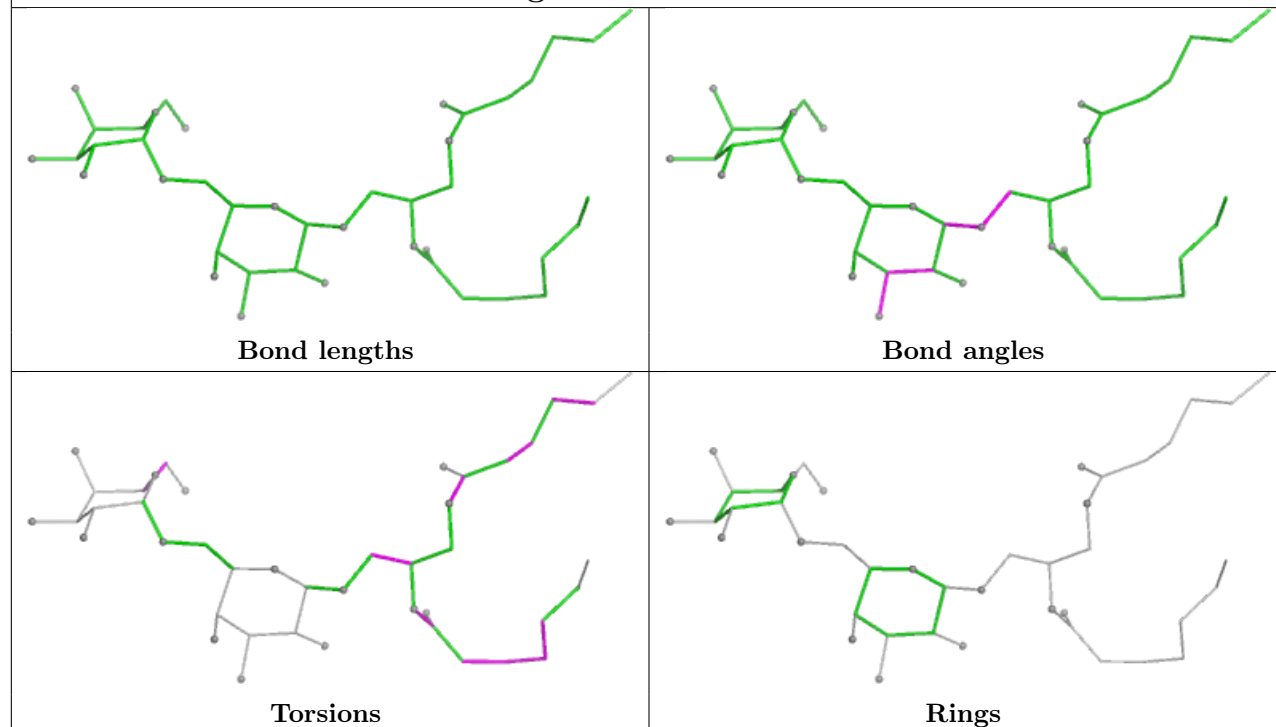


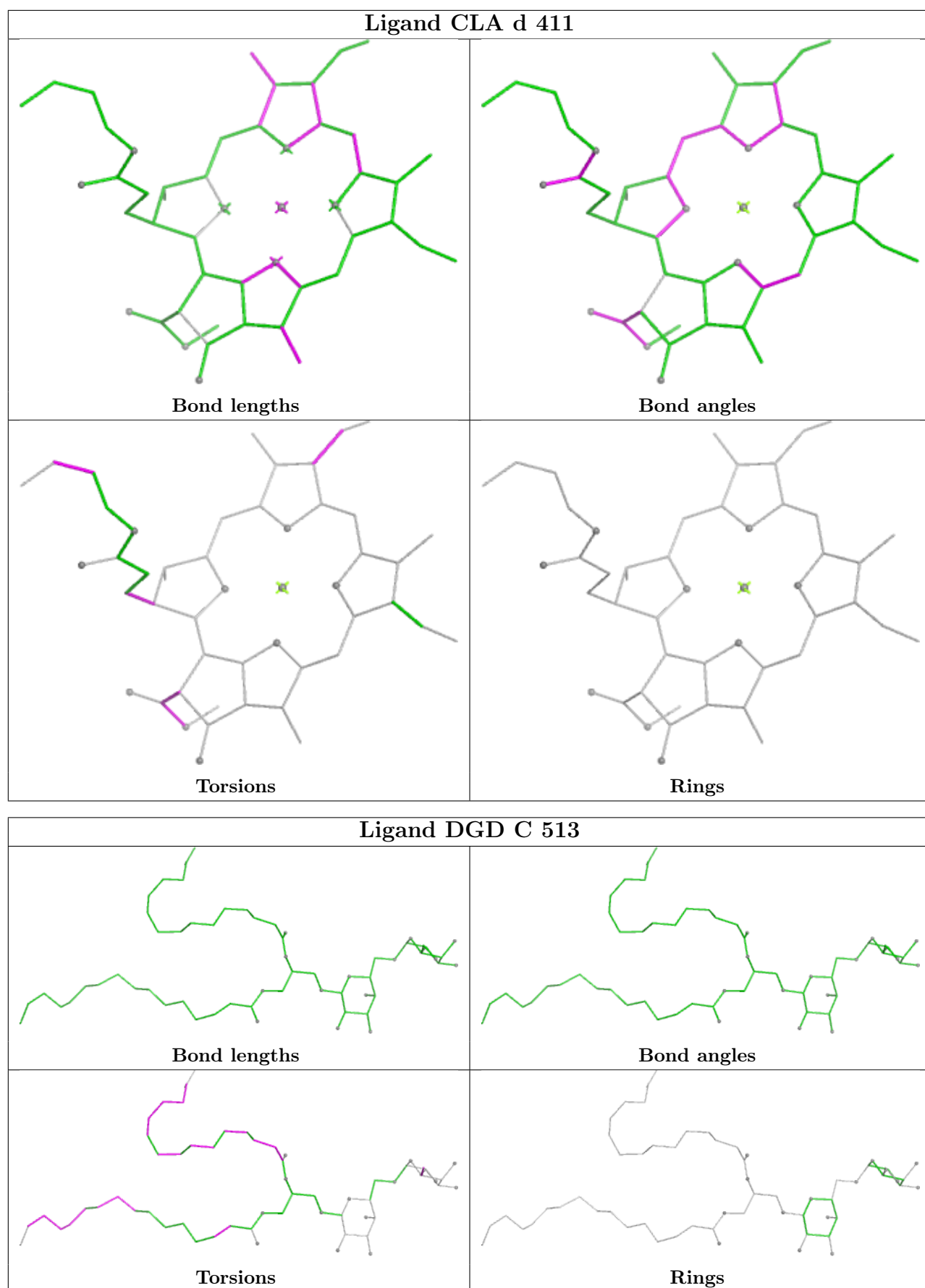
Rings

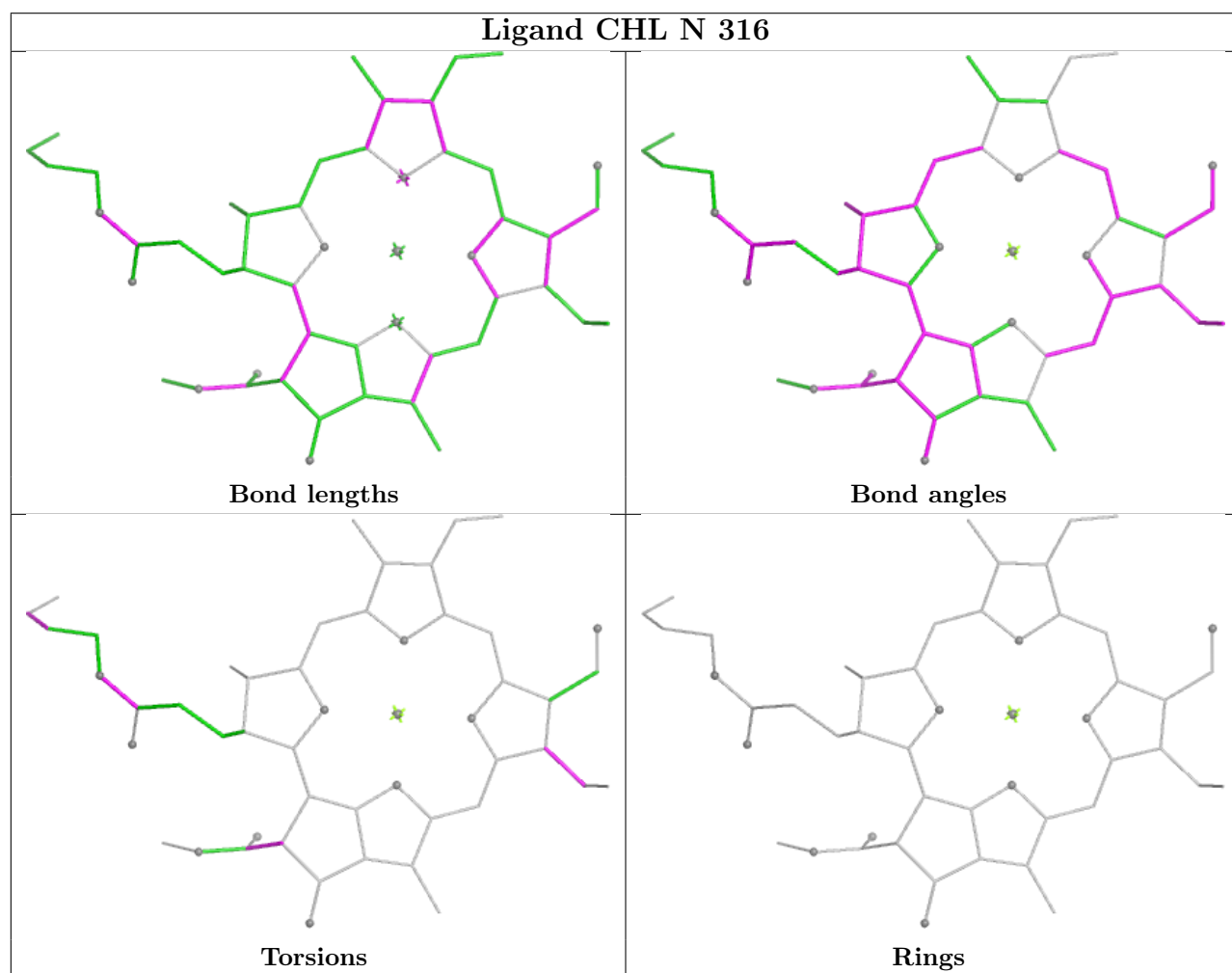
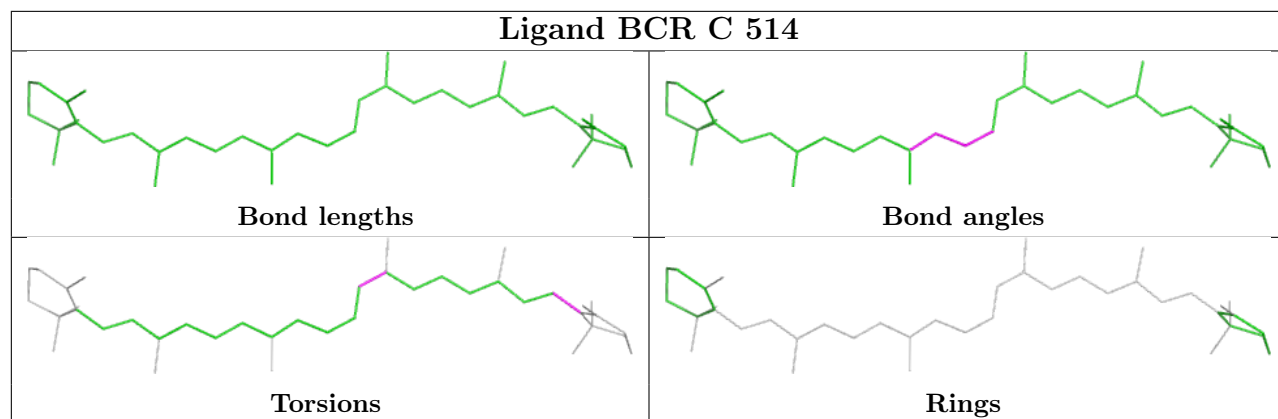
Ligand CLA r 305

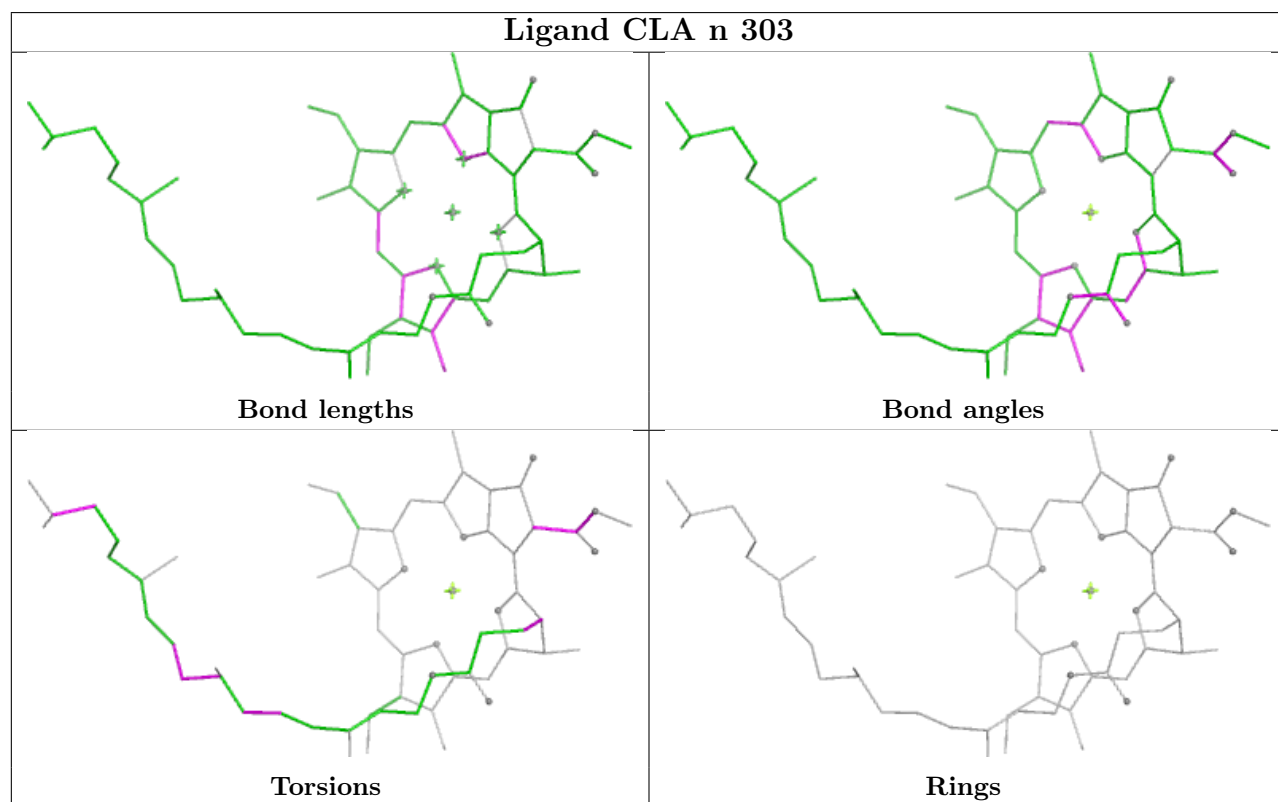
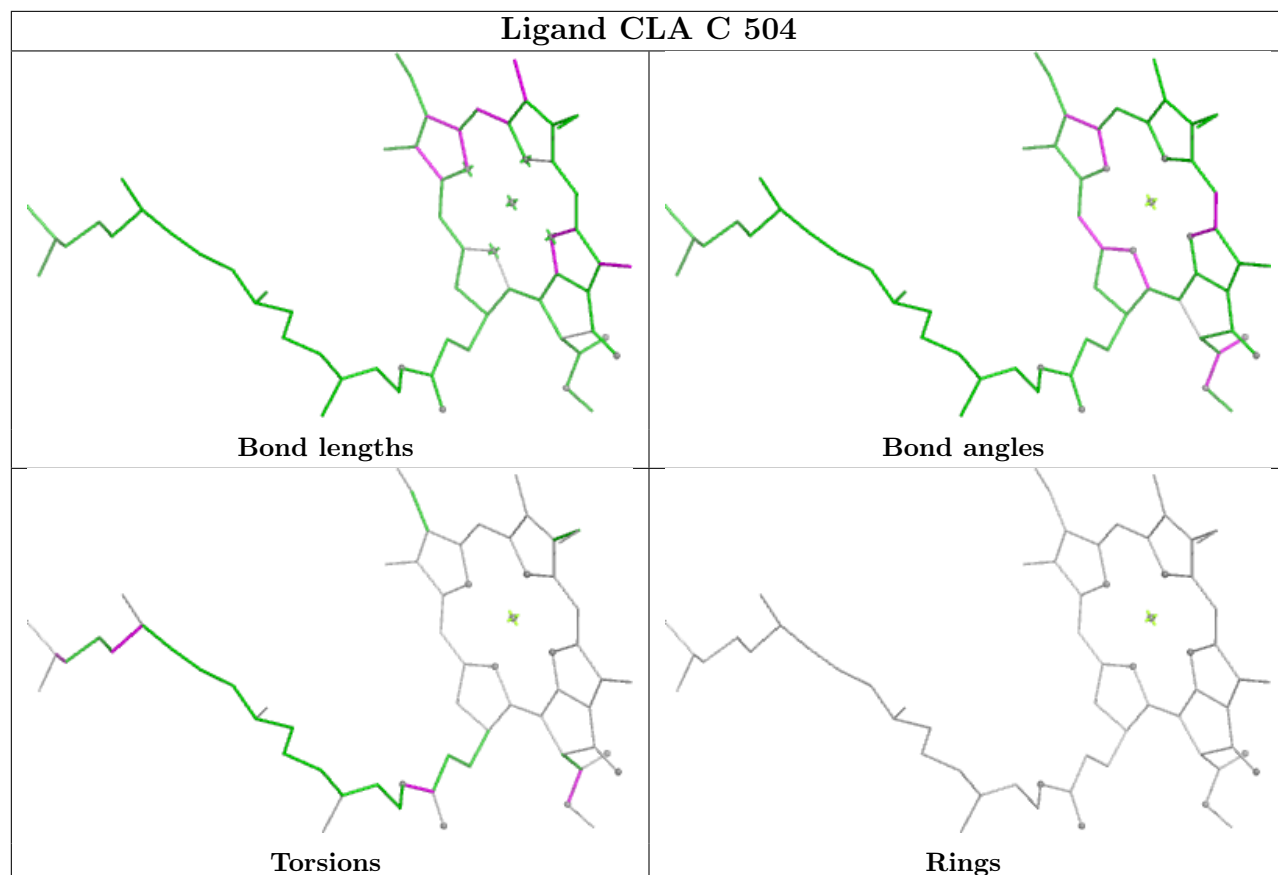


Ligand DGD Y 303

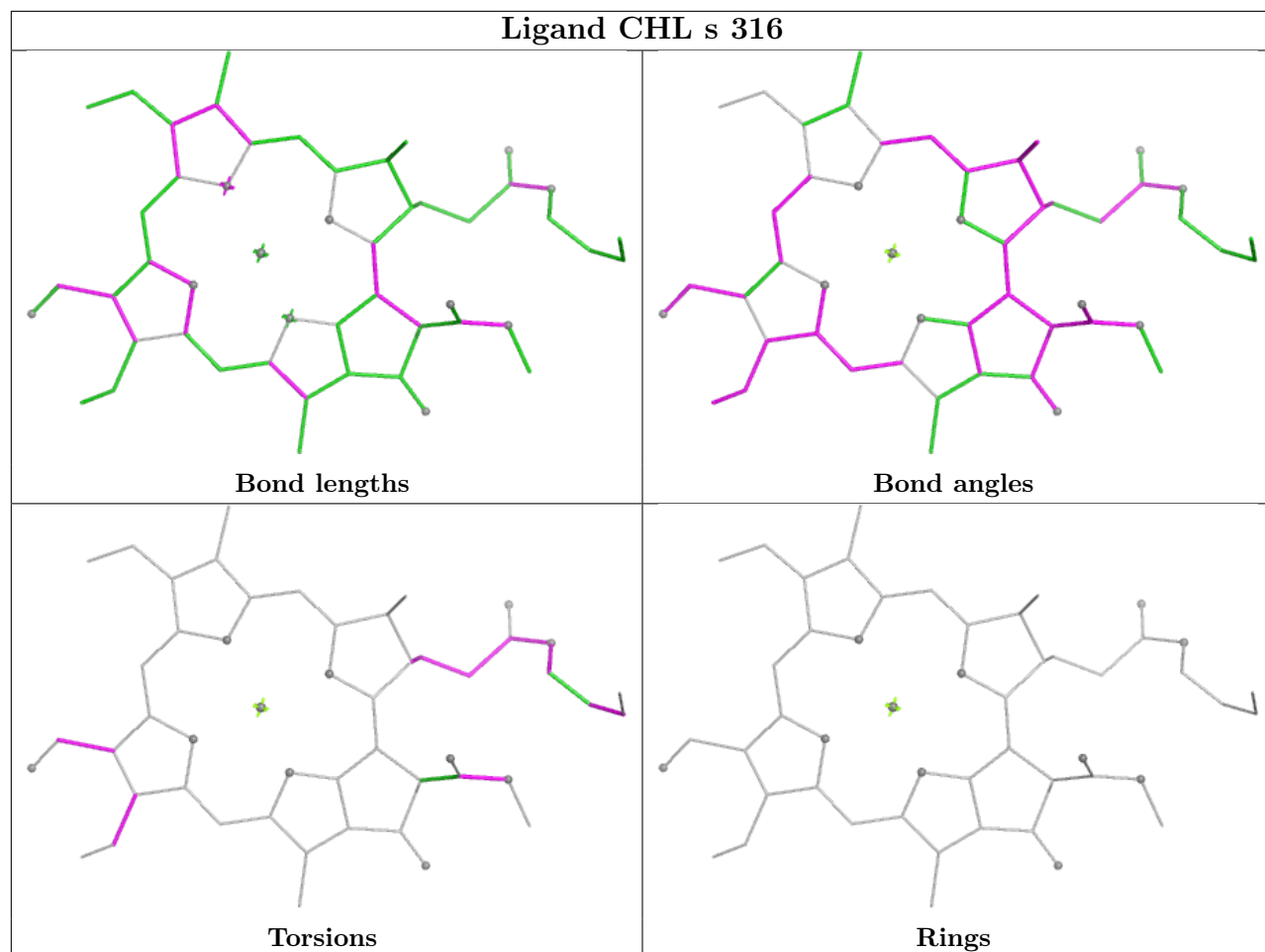


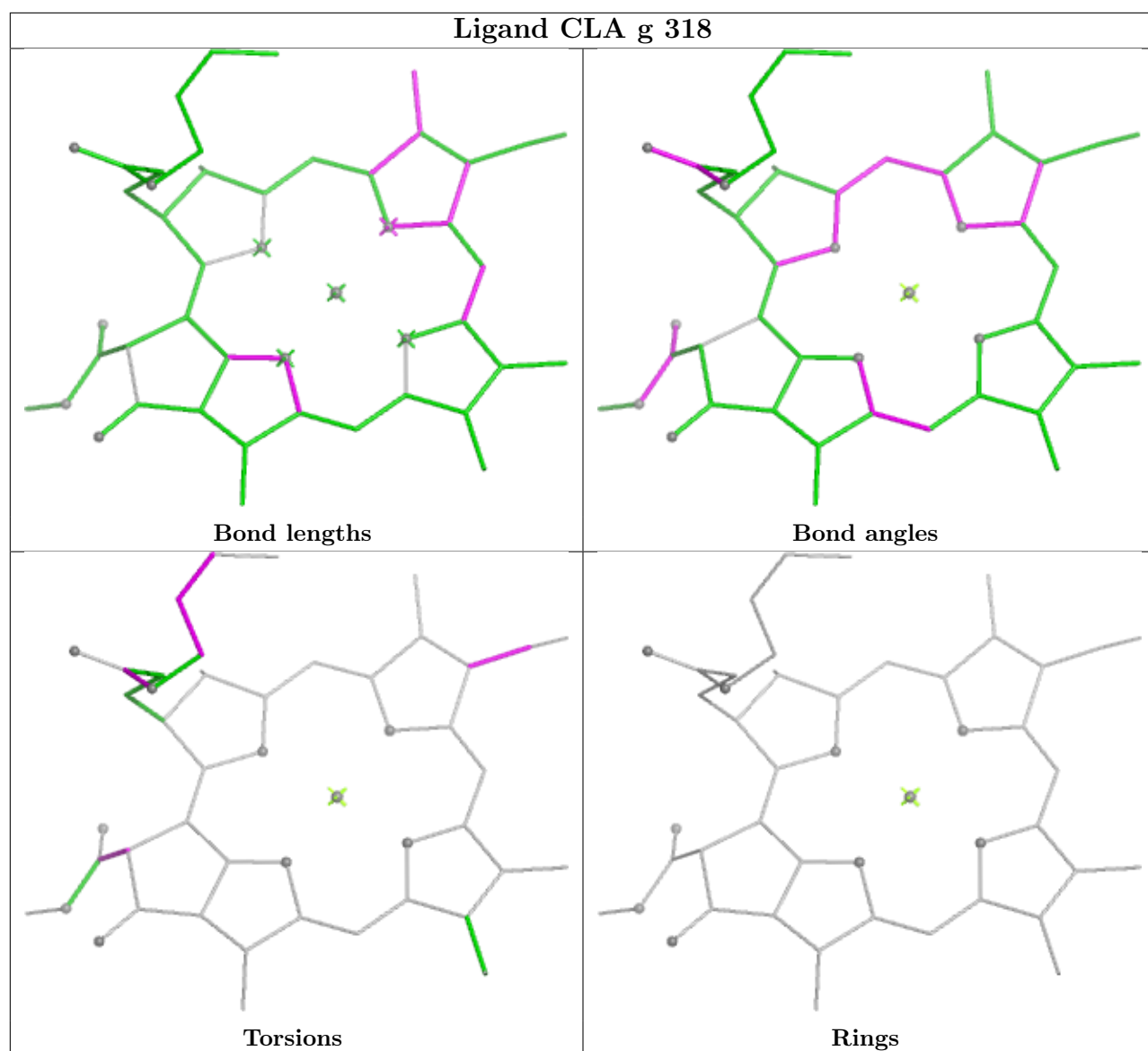




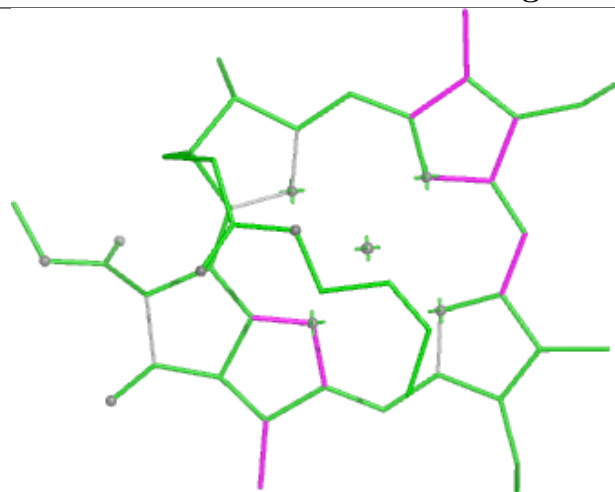


Ligand CHL s 316

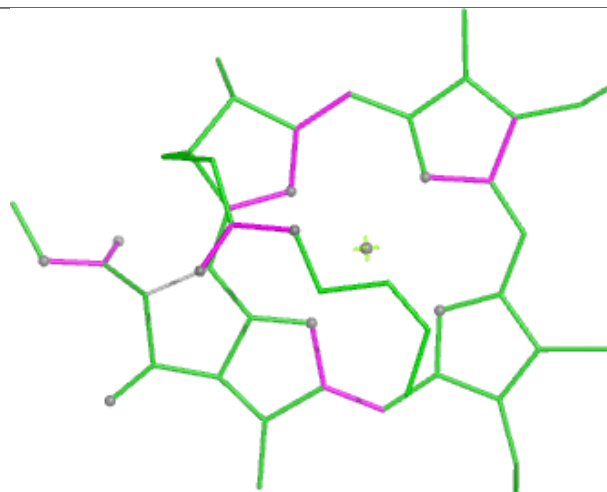




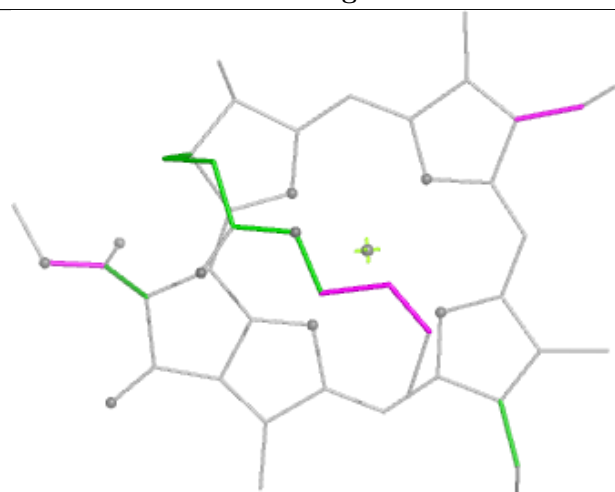
Ligand CLA s 307



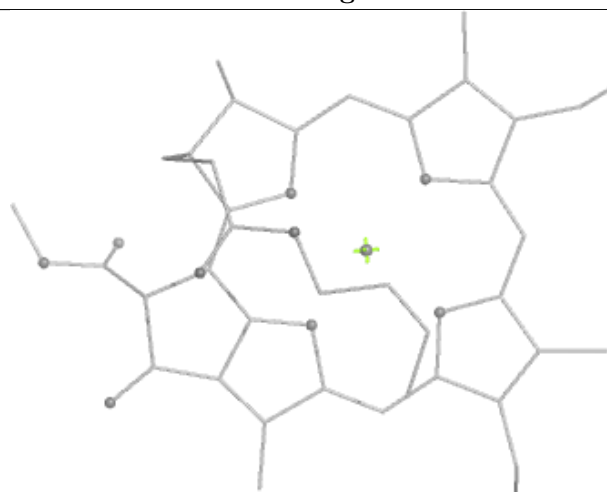
Bond lengths



Bond angles



Torsions



Rings

Ligand BCR a 404



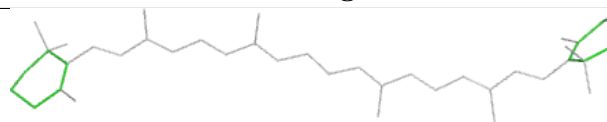
Bond lengths



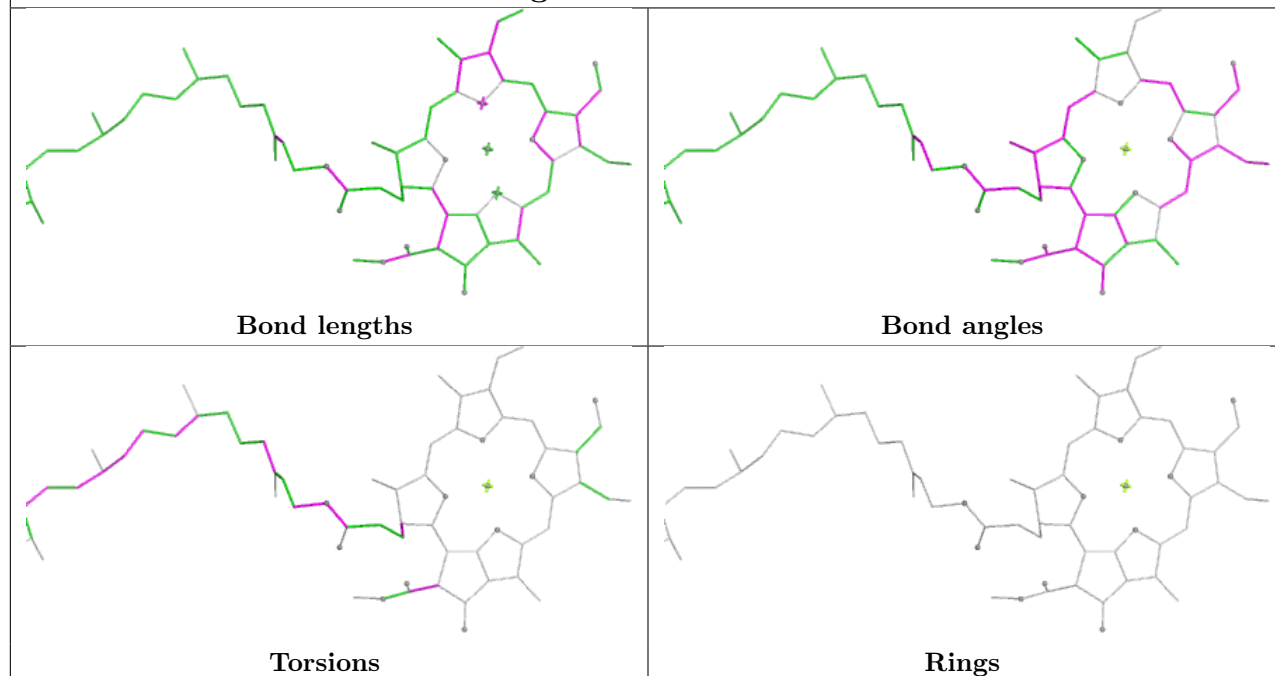
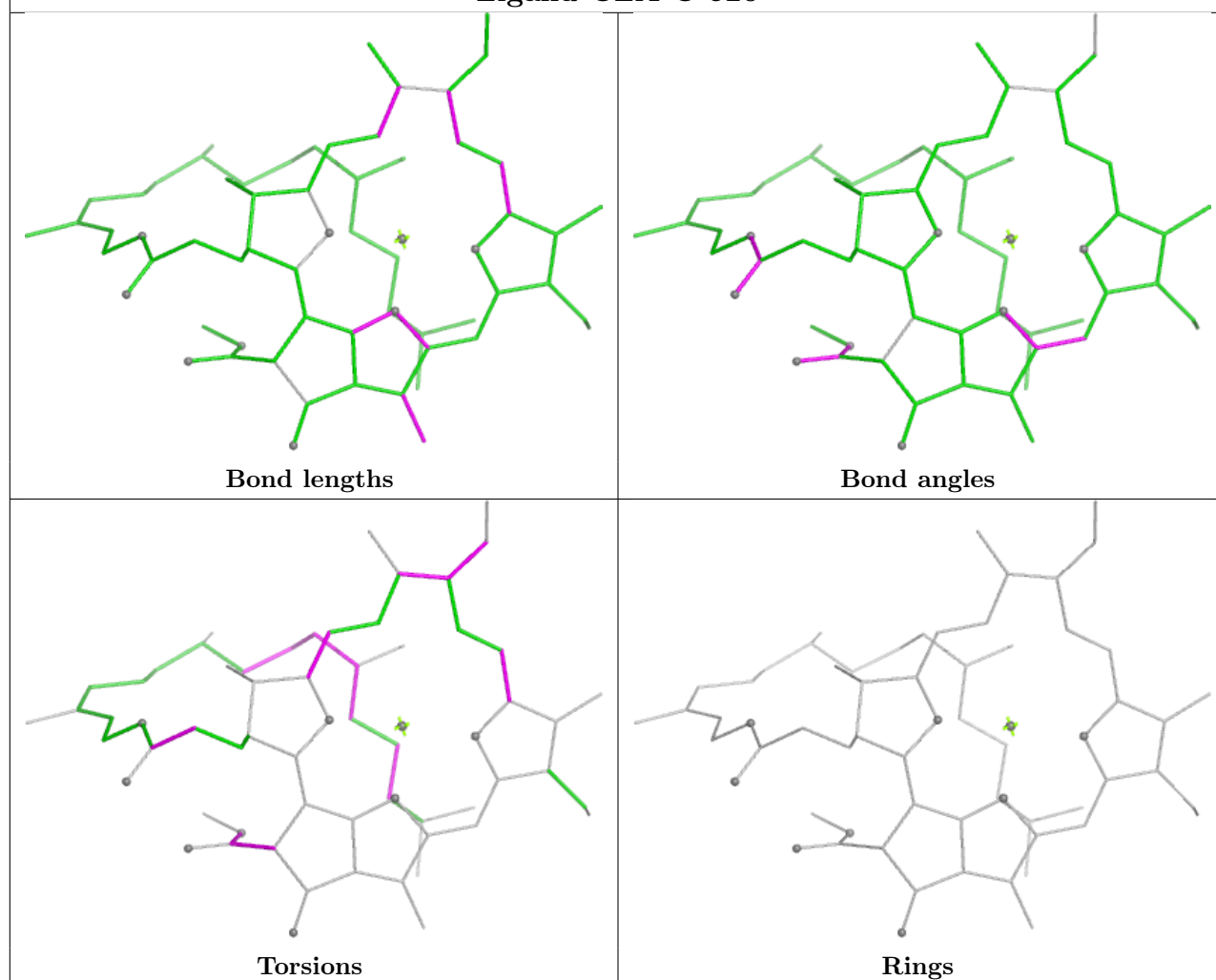
Bond angles

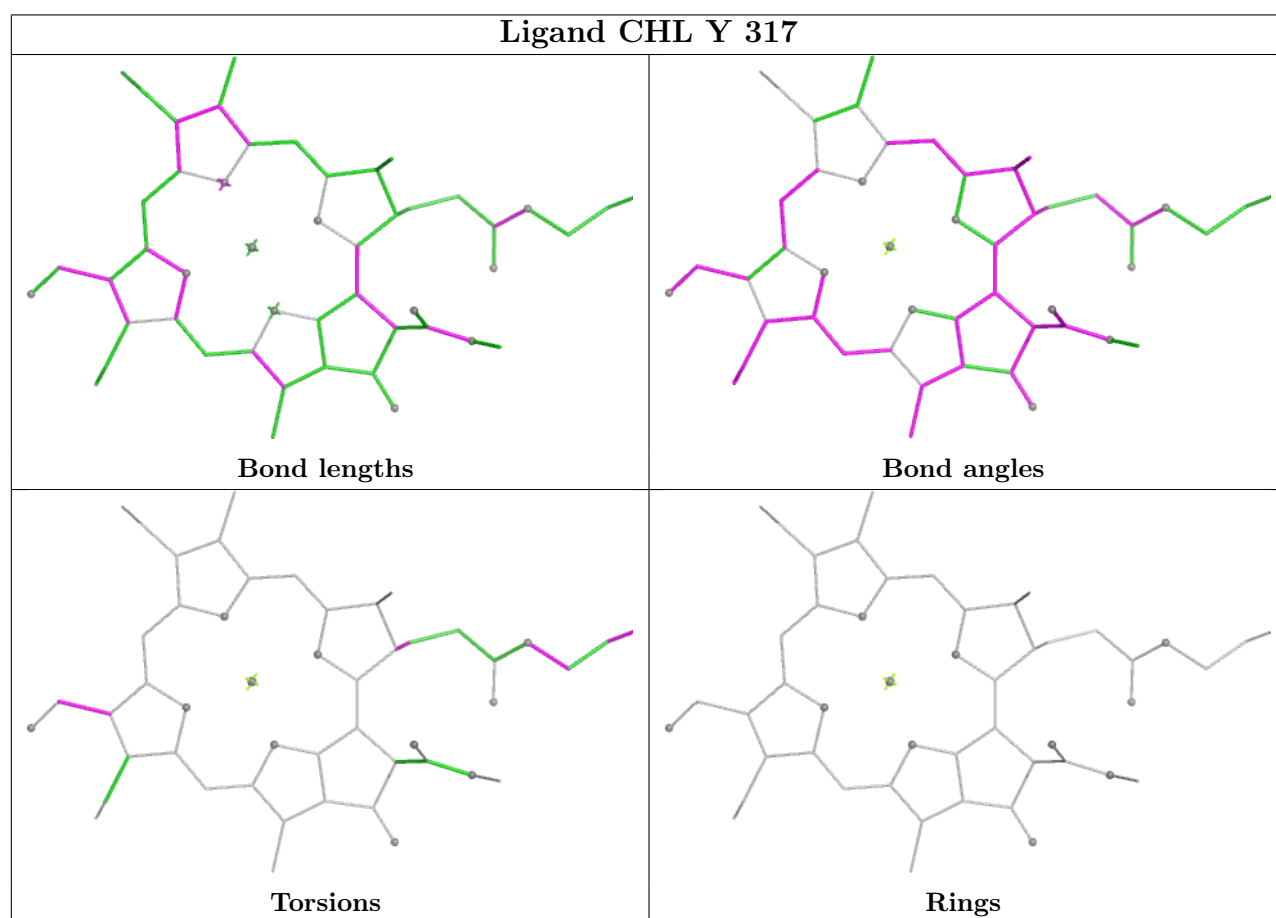
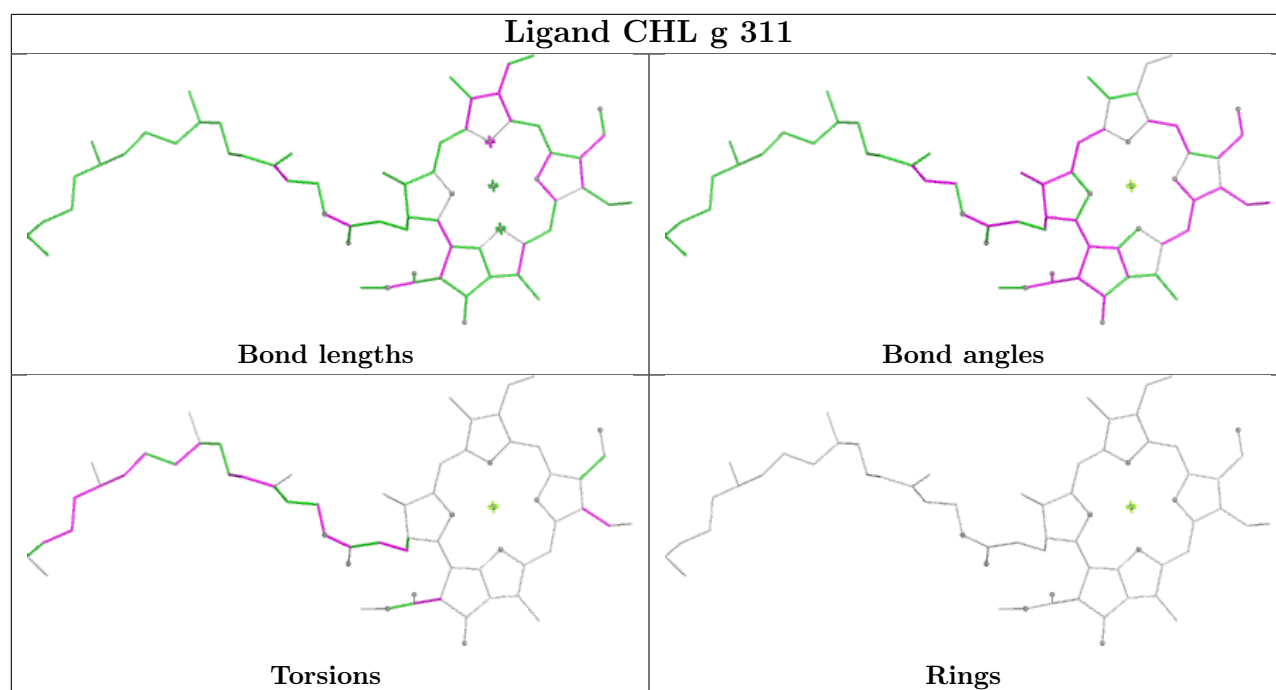


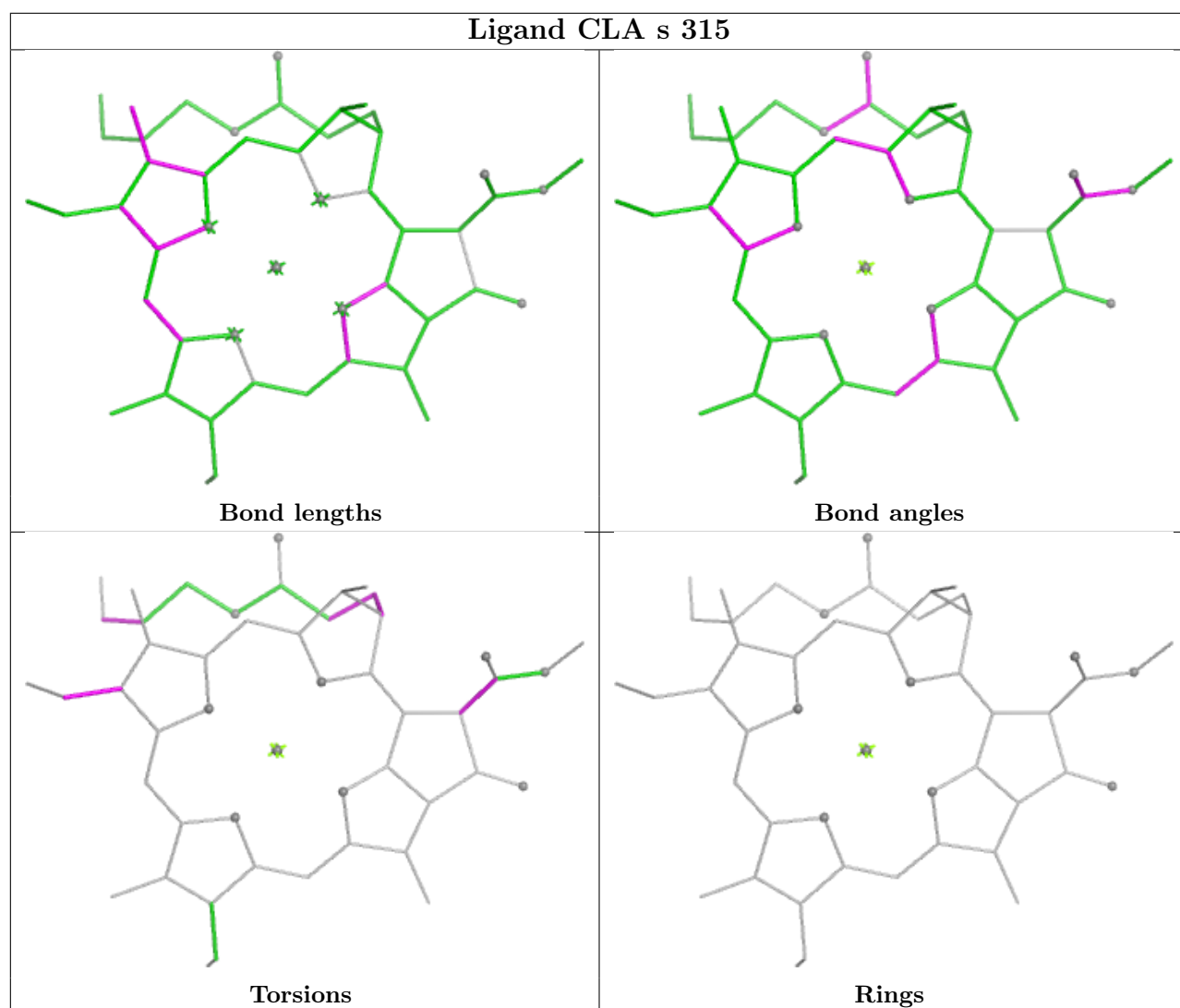
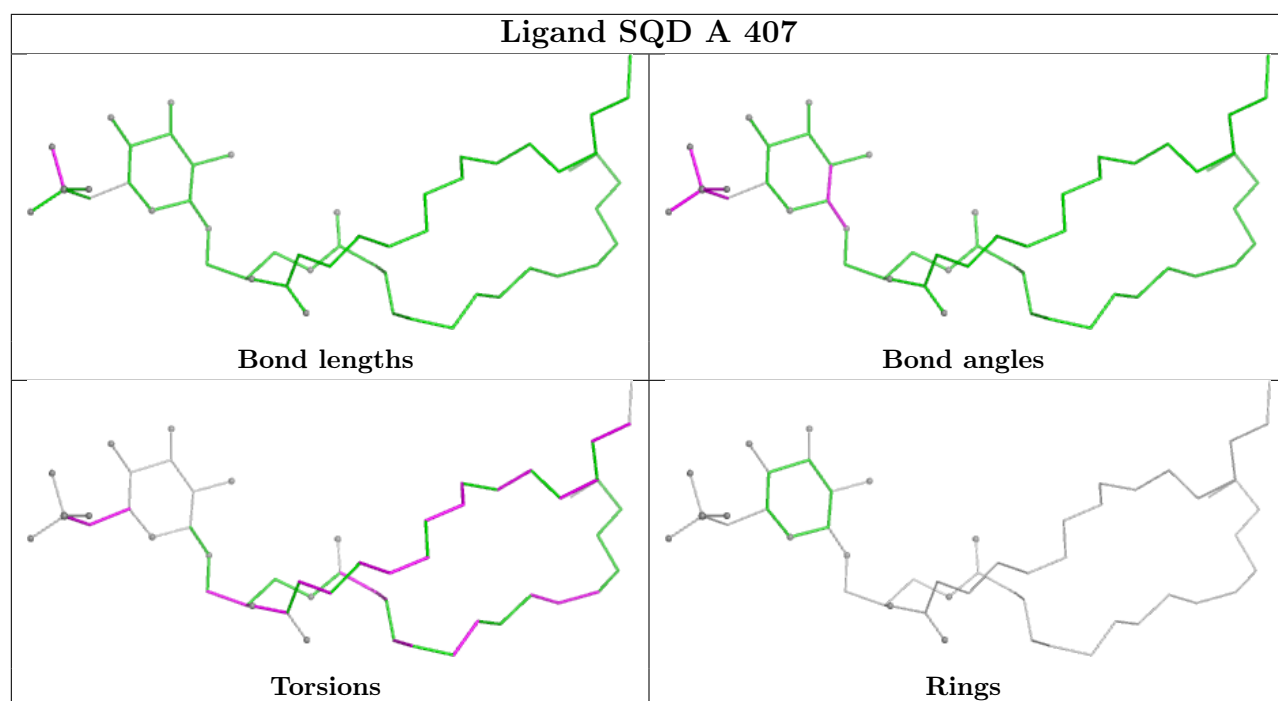
Torsions

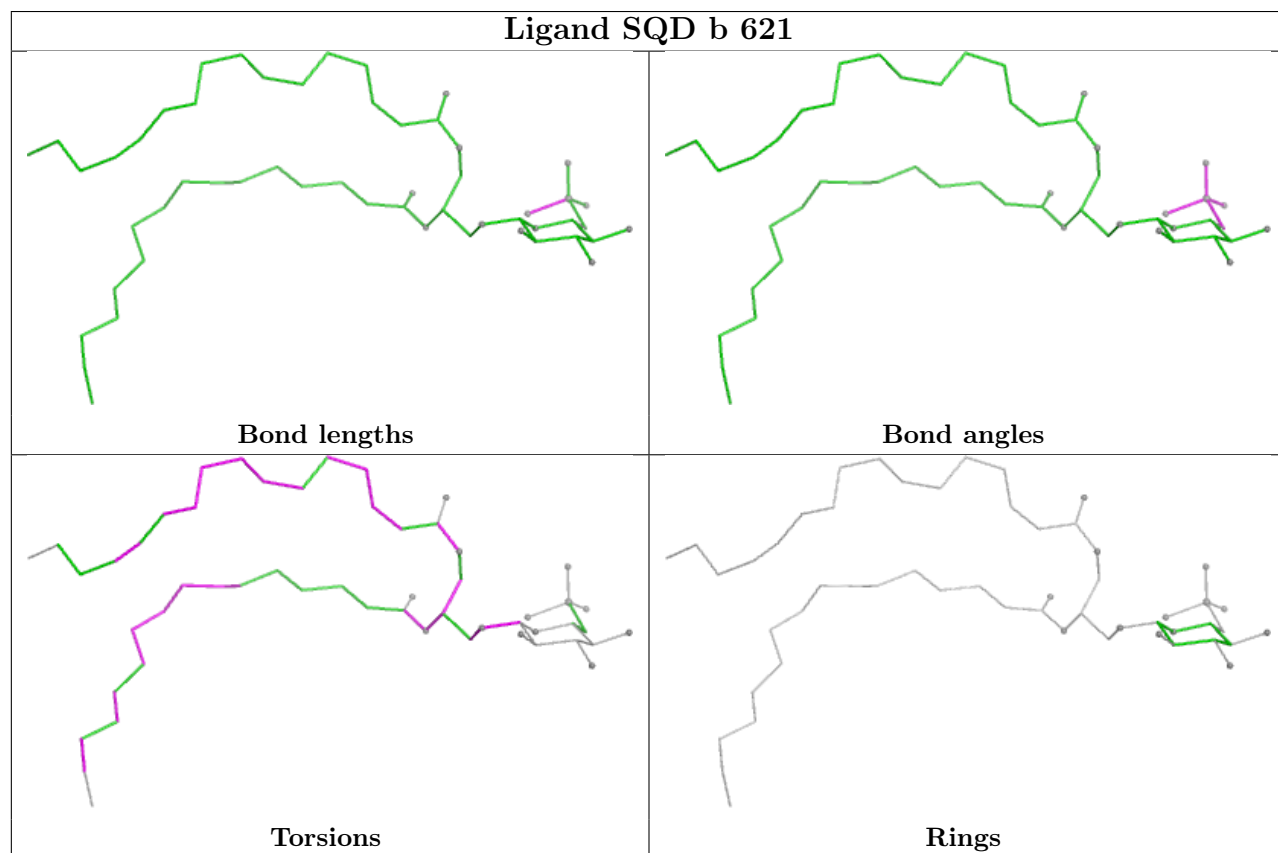
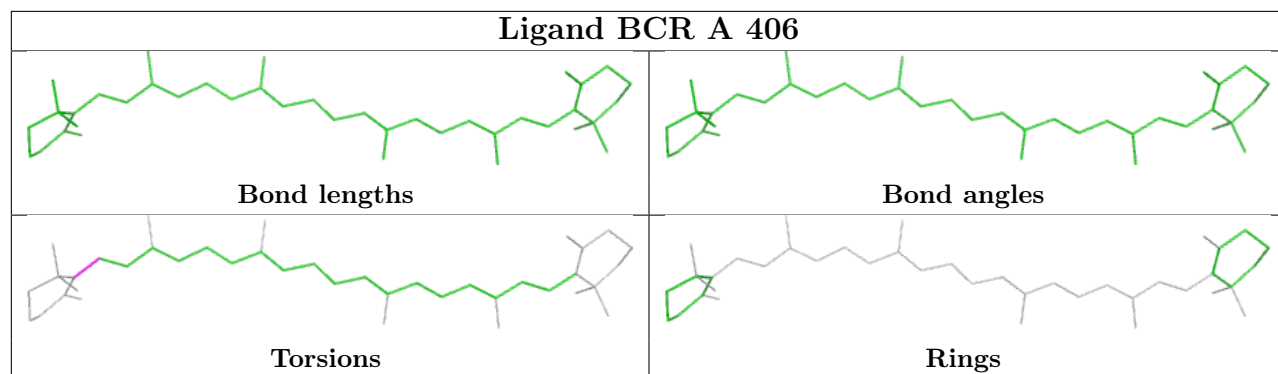


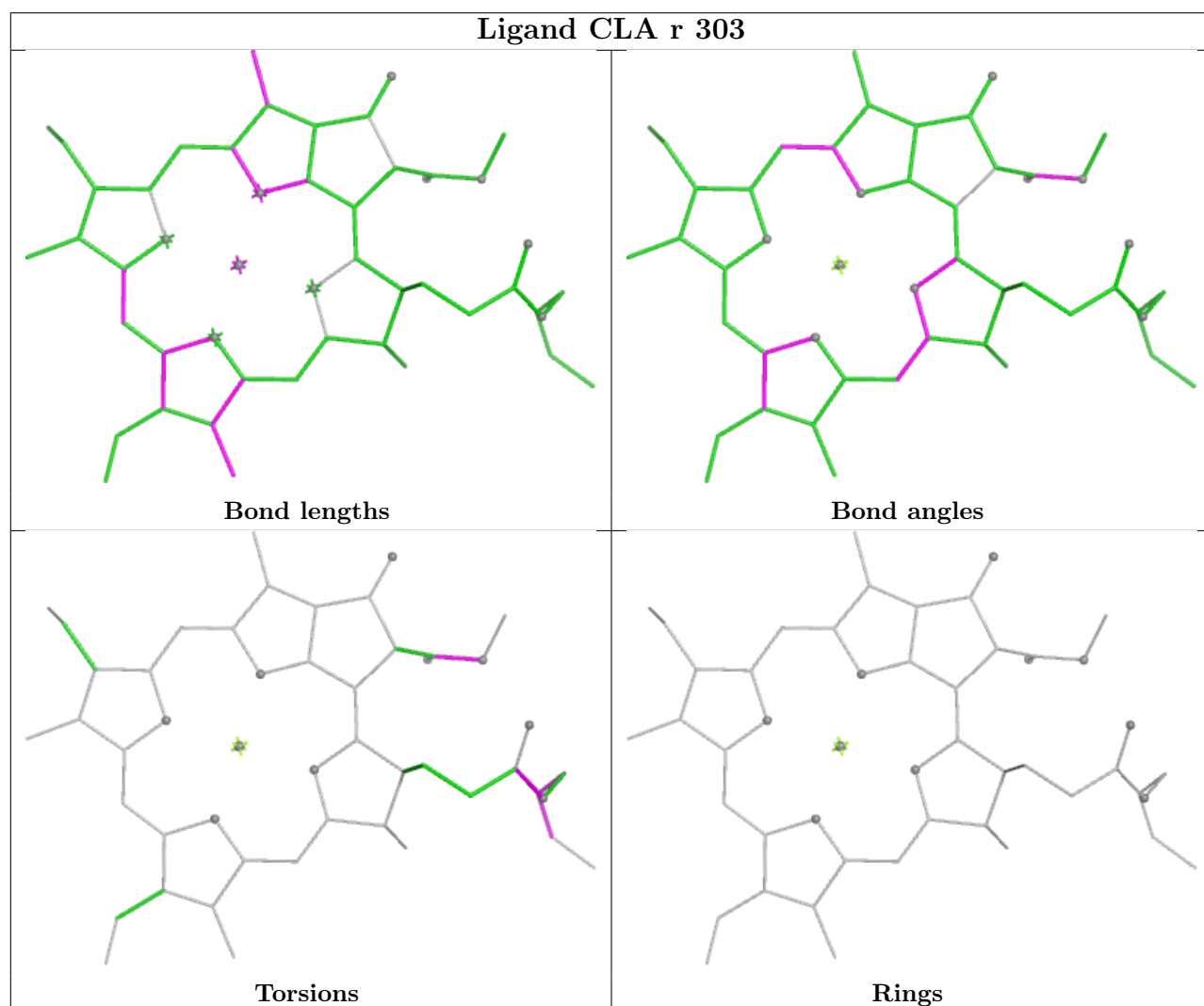
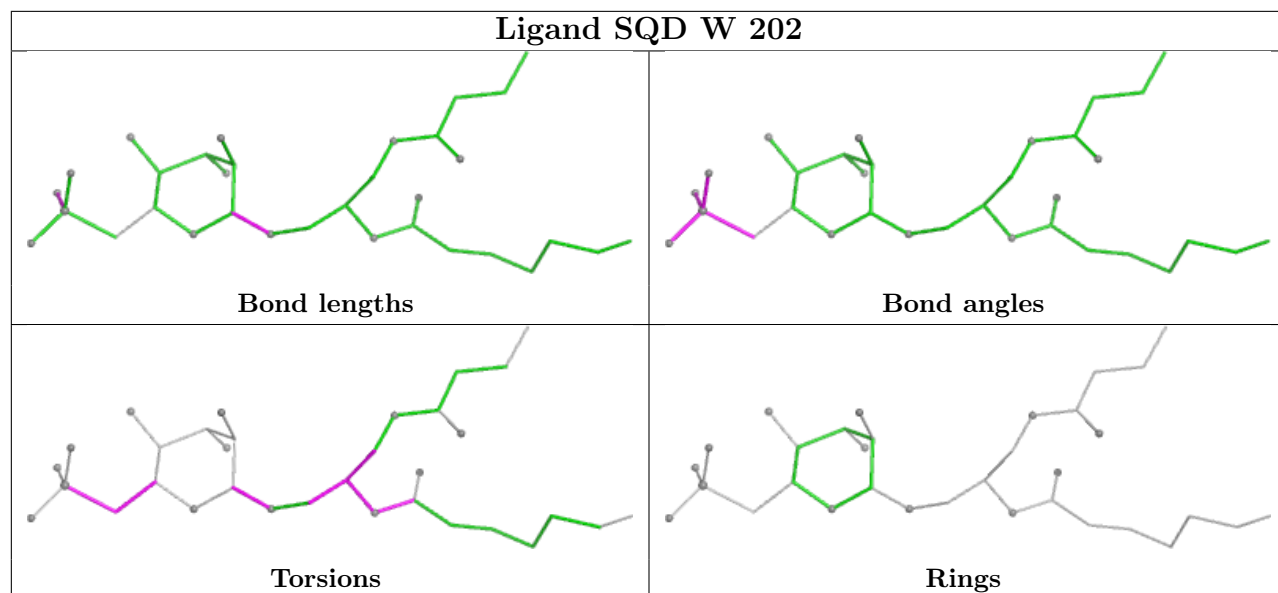
Rings

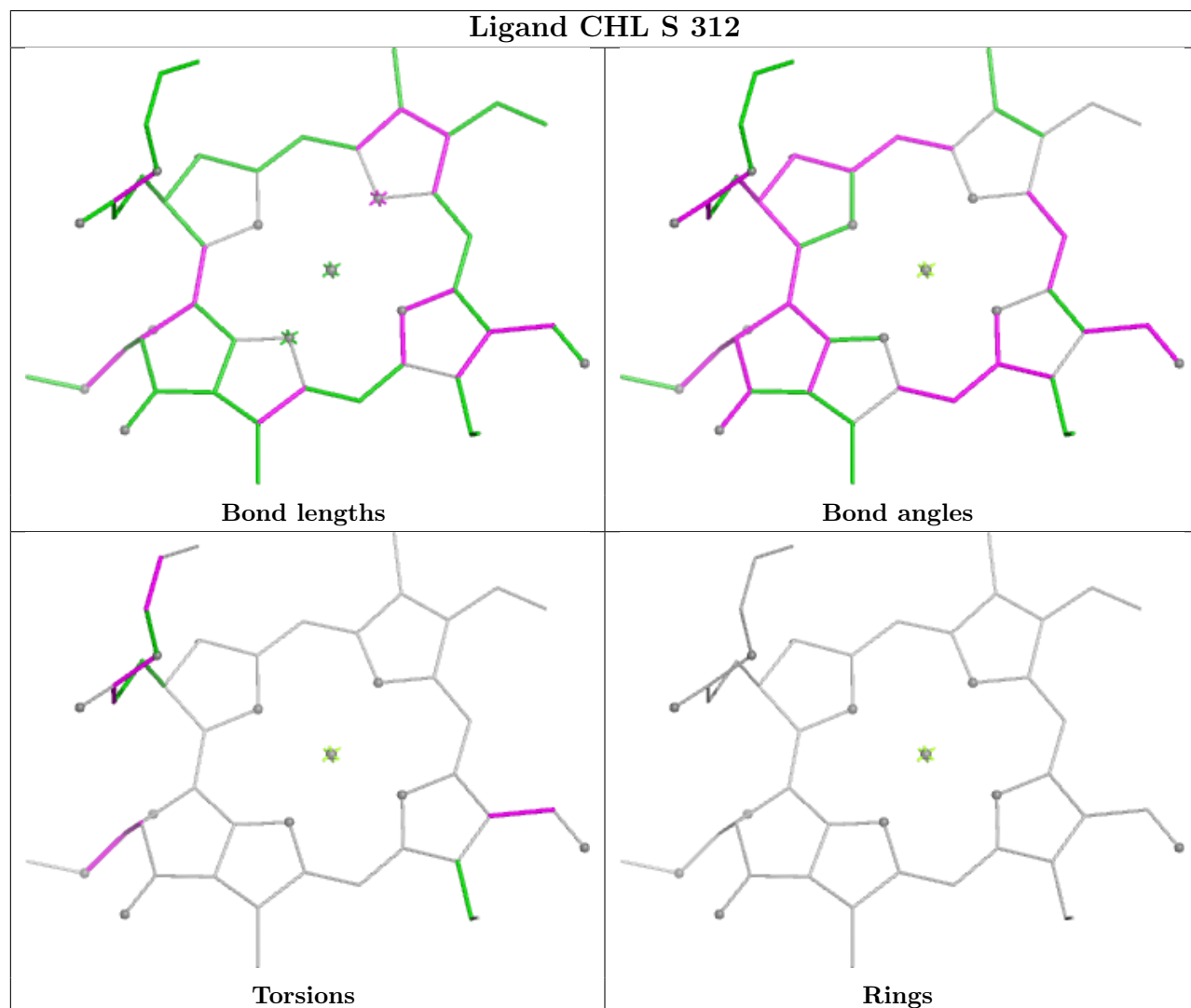
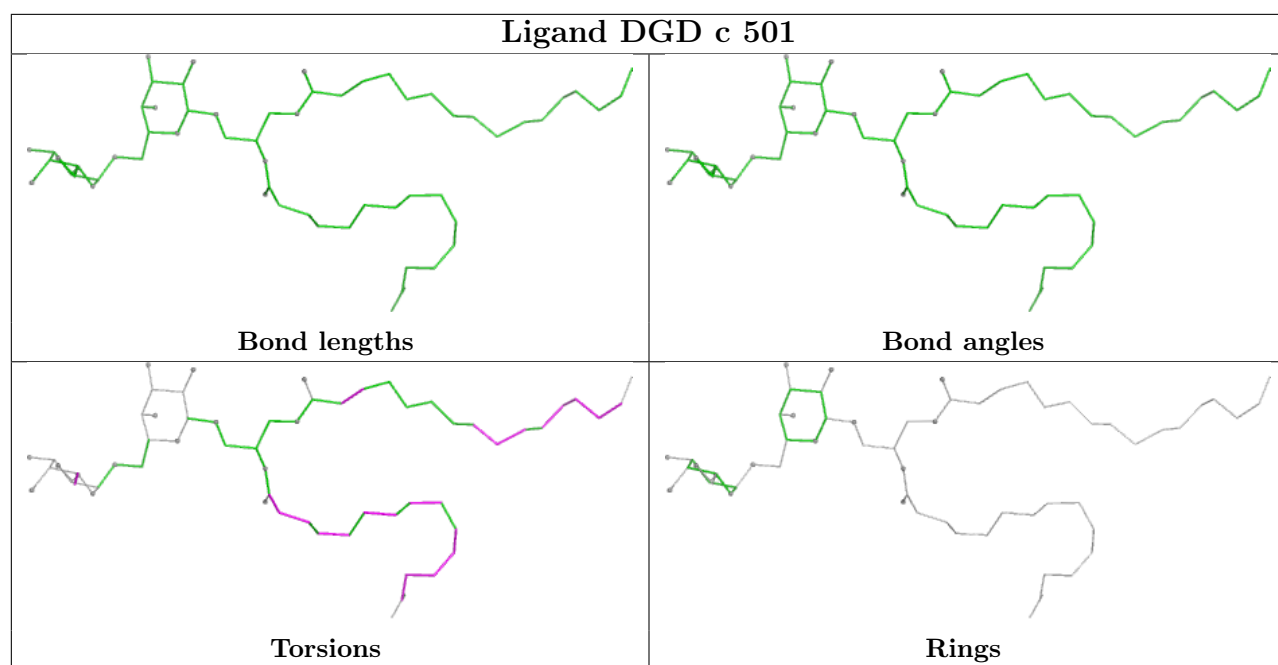
Ligand CHL Y 302**Ligand CLA C 520**



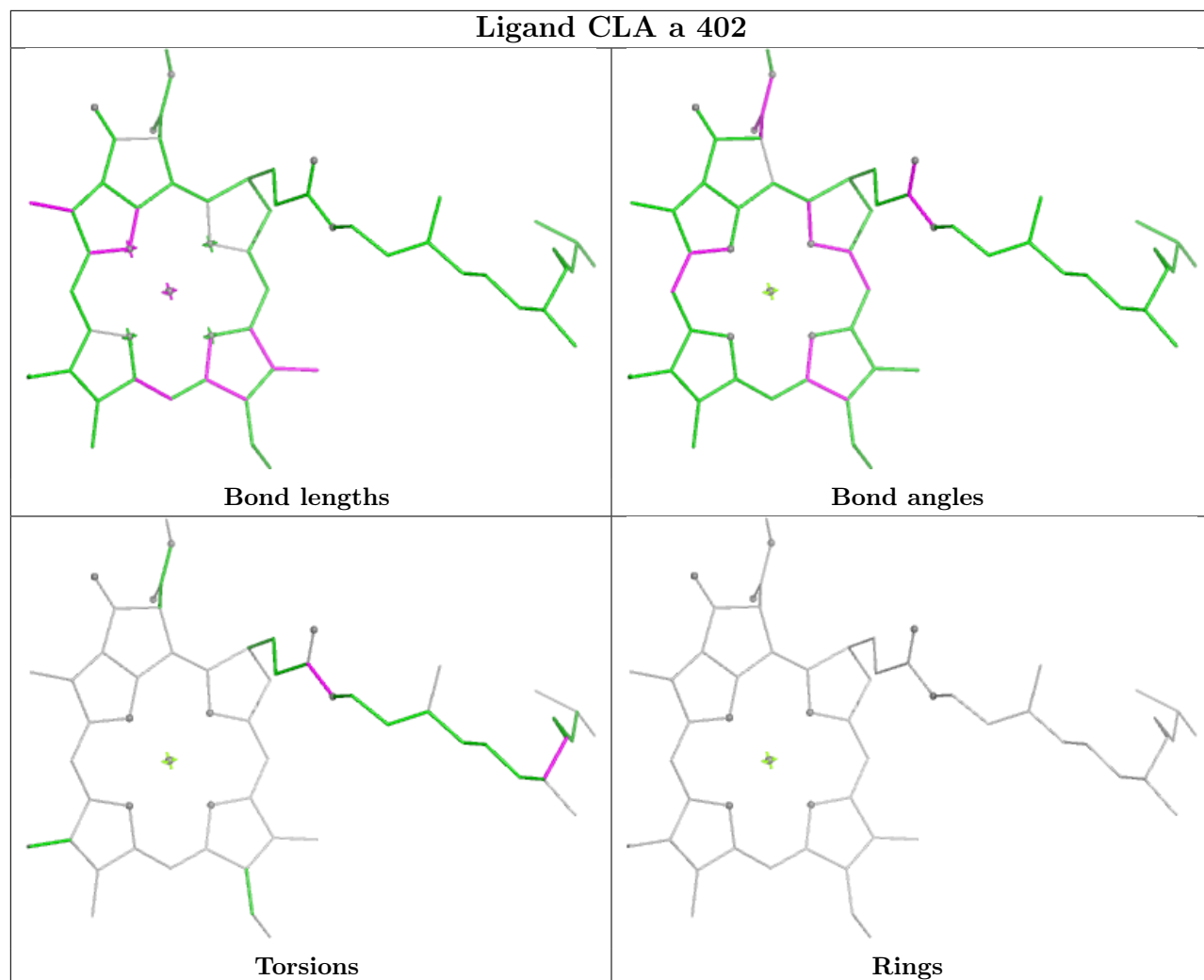


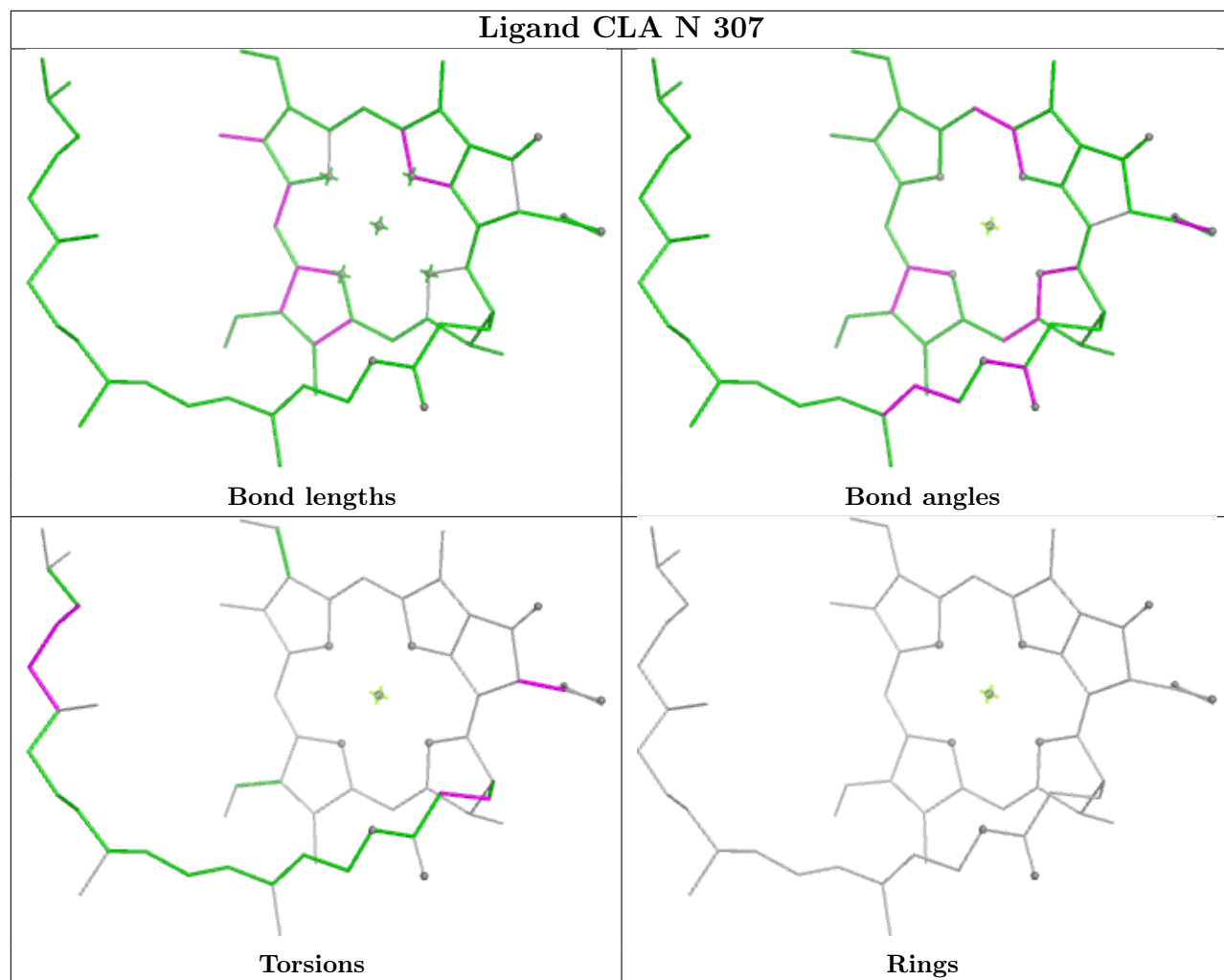




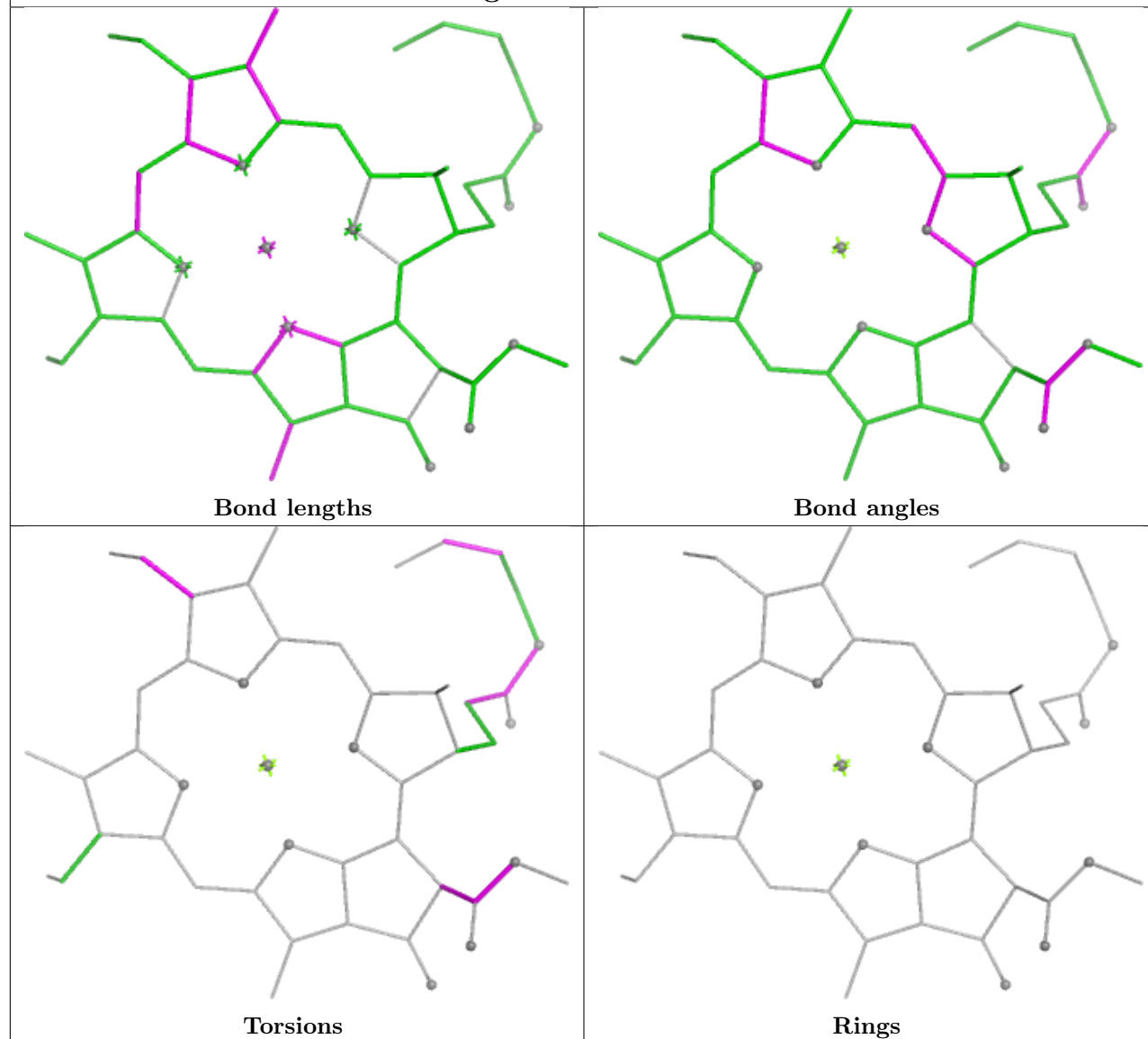


Ligand CLA a 402

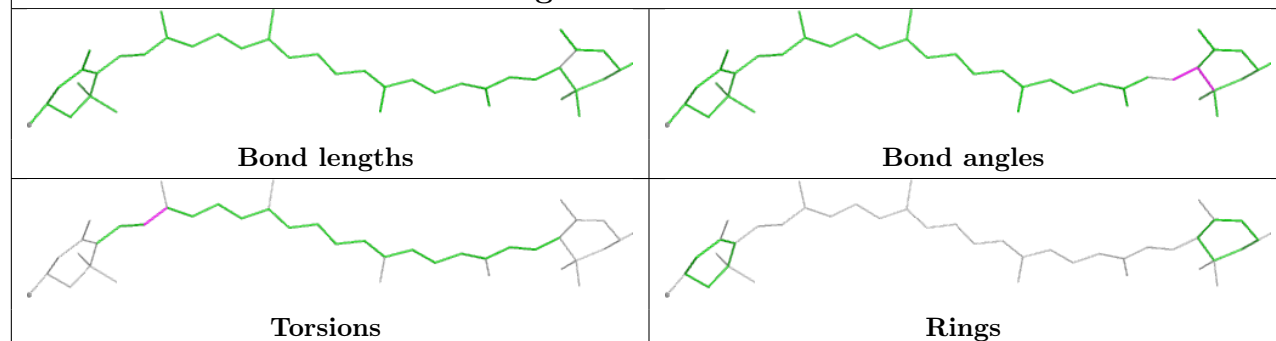


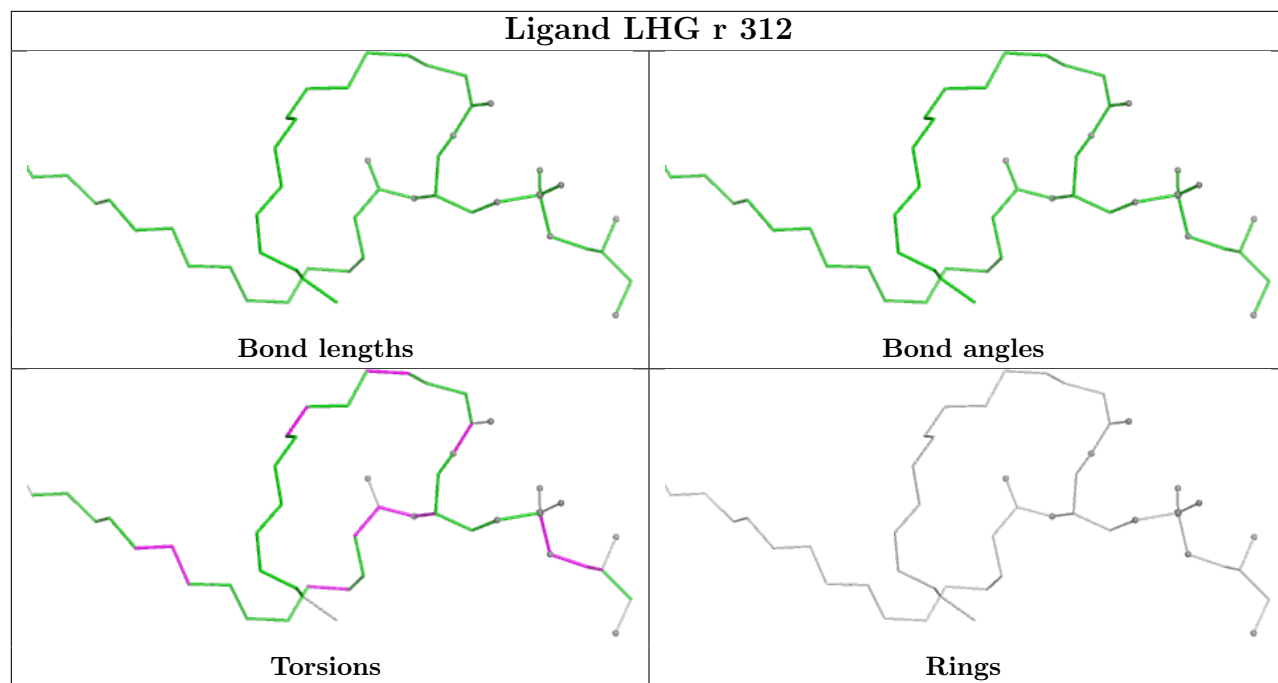


Ligand CLA s 301

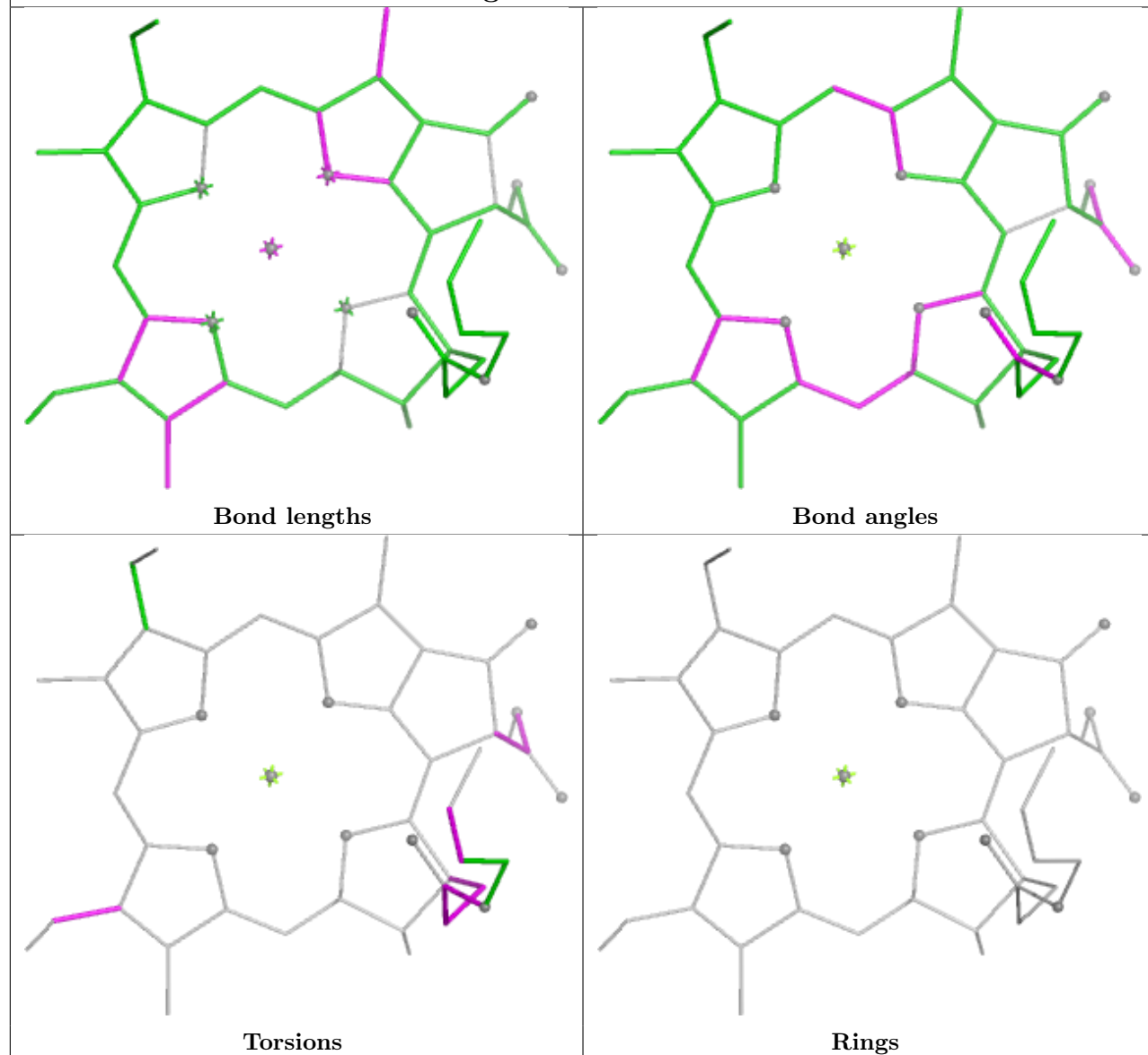


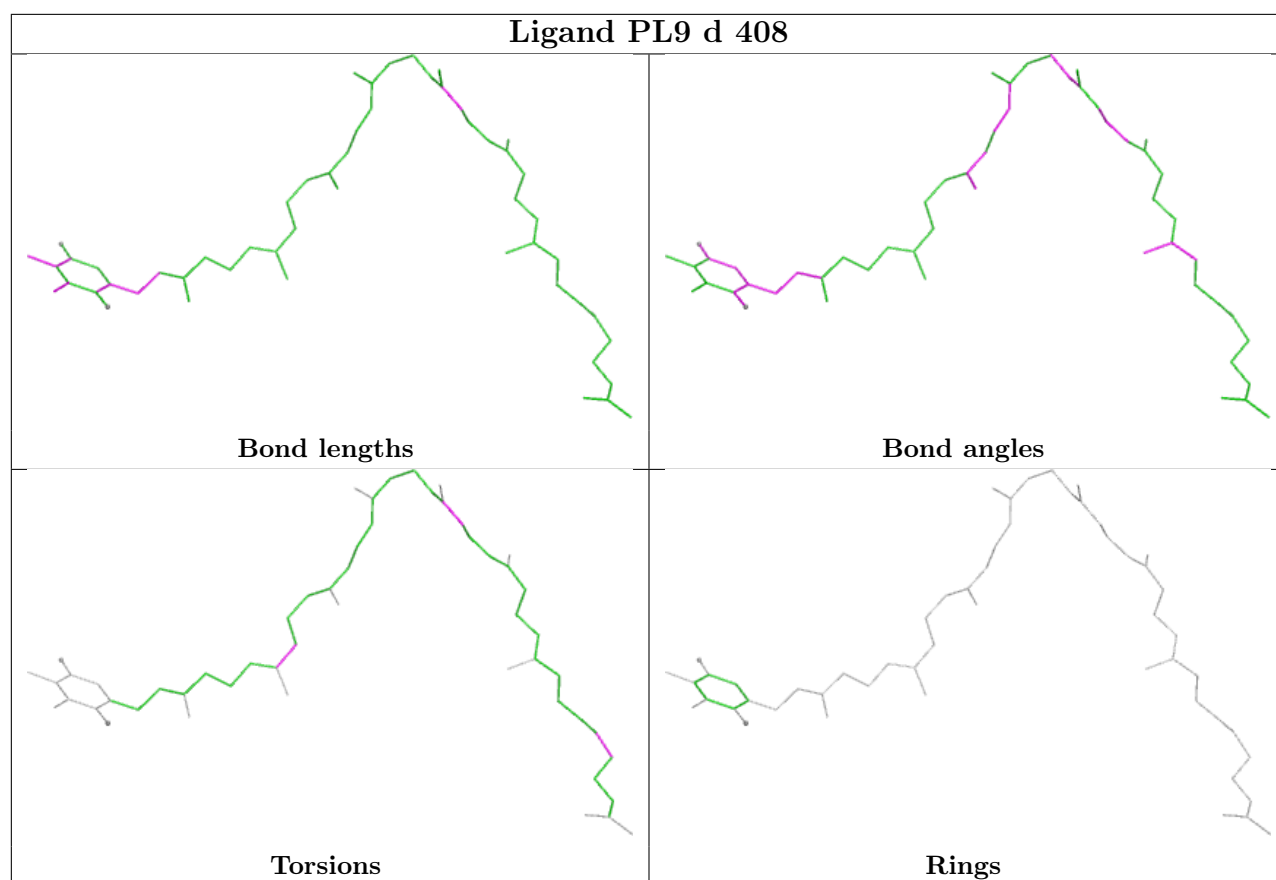
Ligand LUT S 306



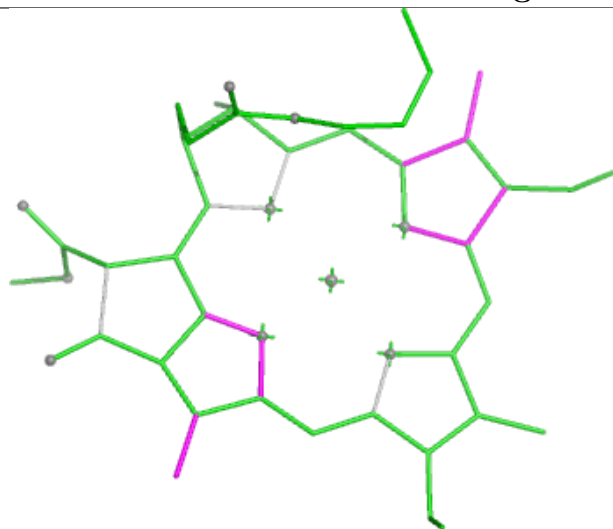


Ligand CLA s 310

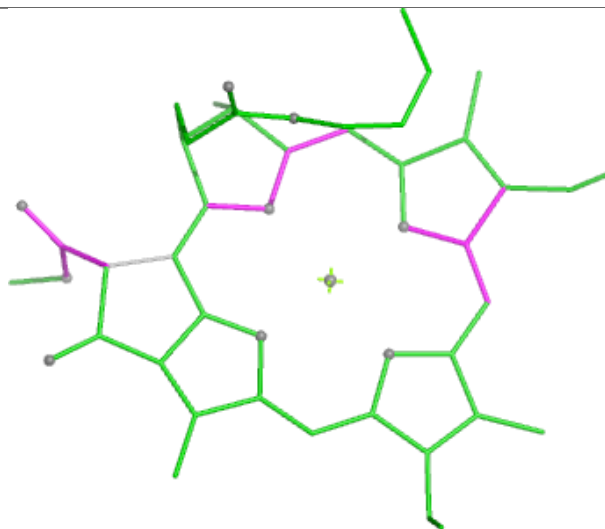




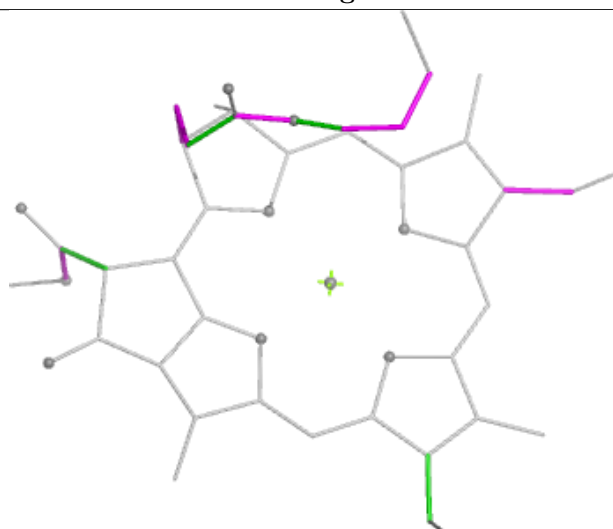
Ligand CLA Y 310



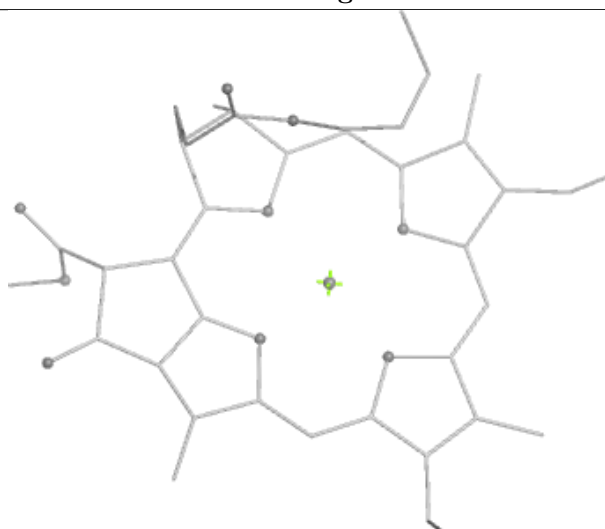
Bond lengths



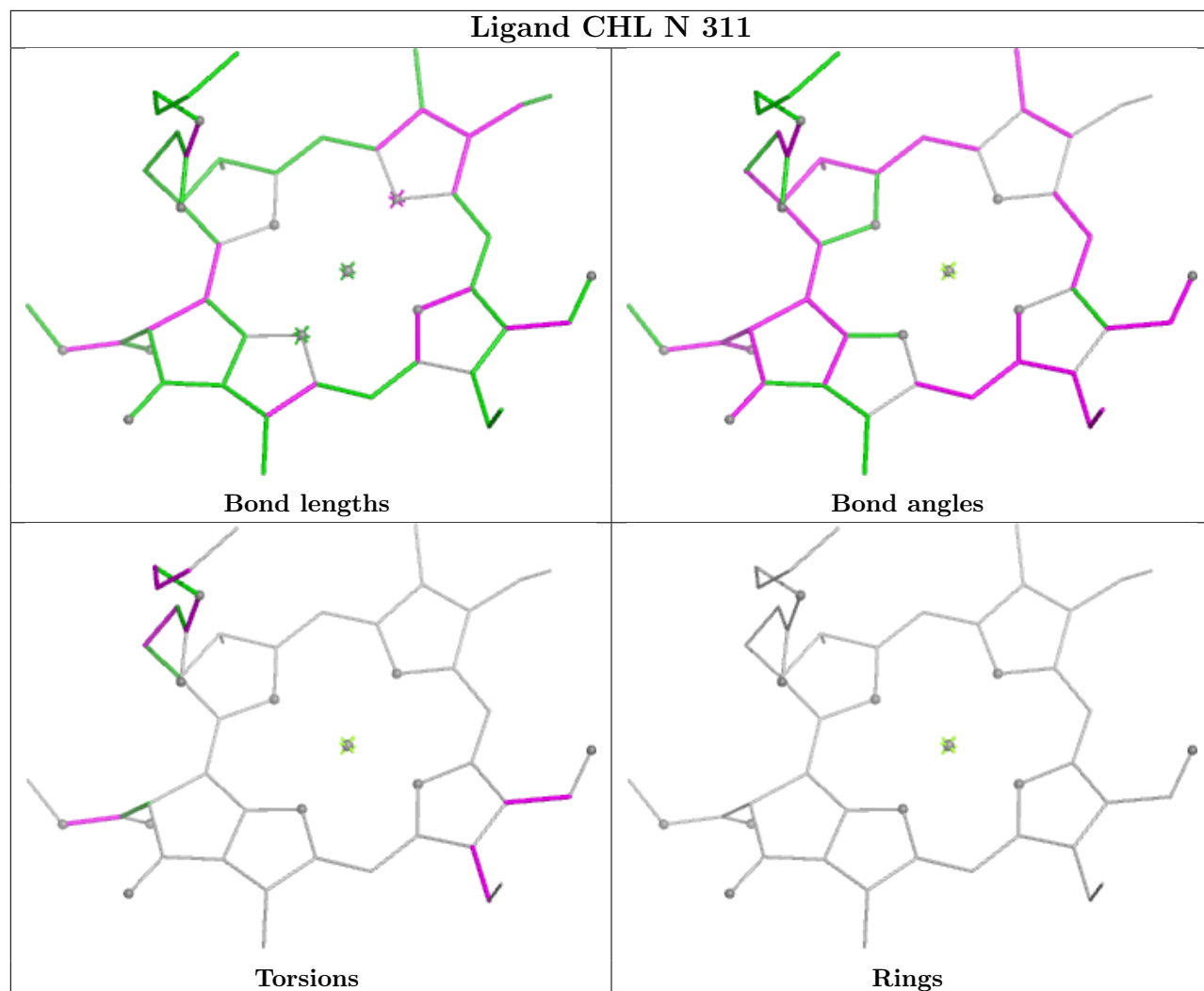
Bond angles

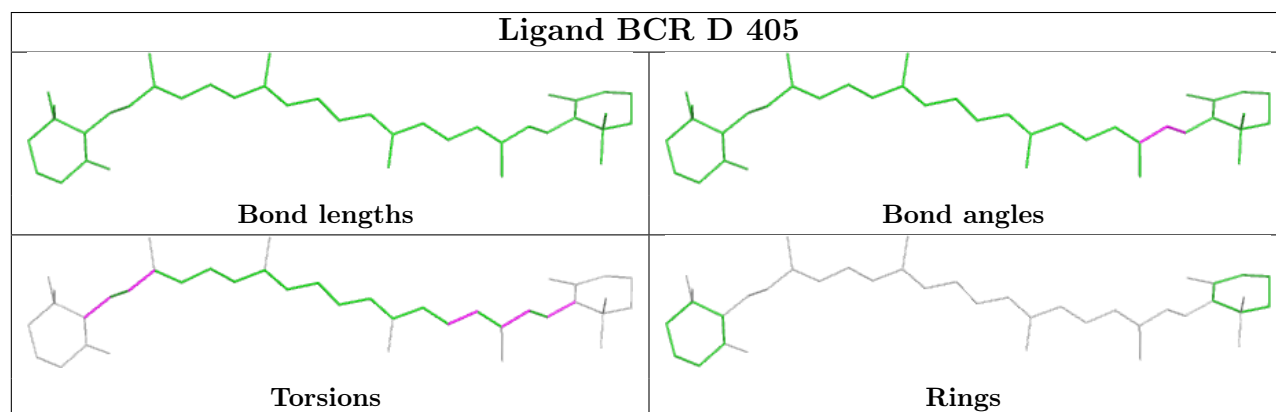
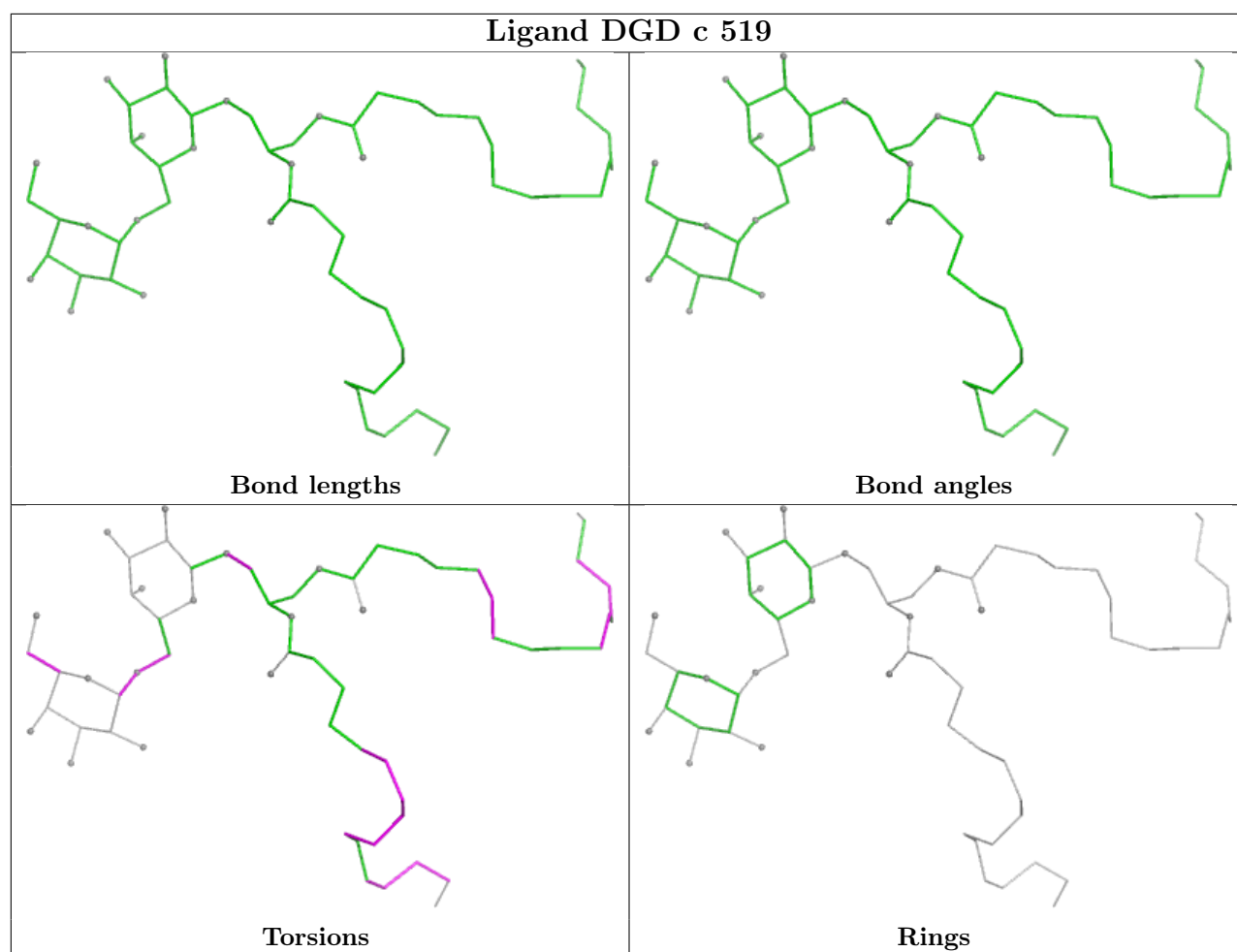


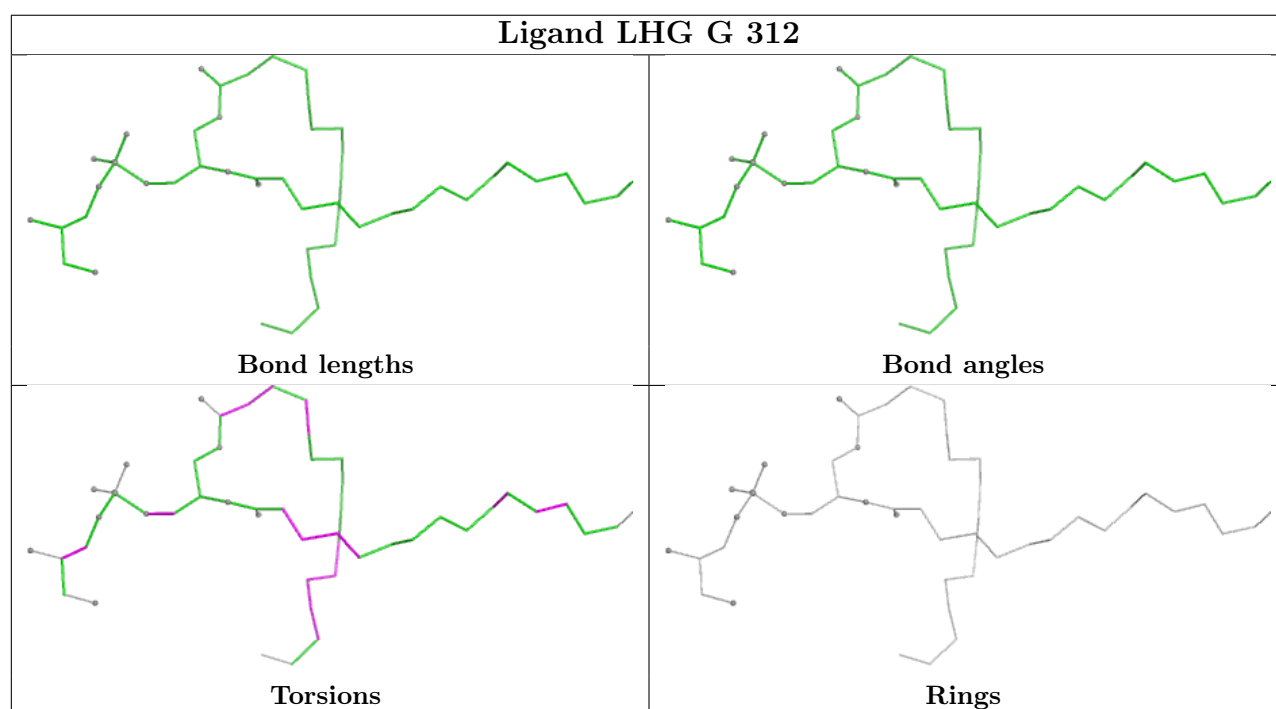
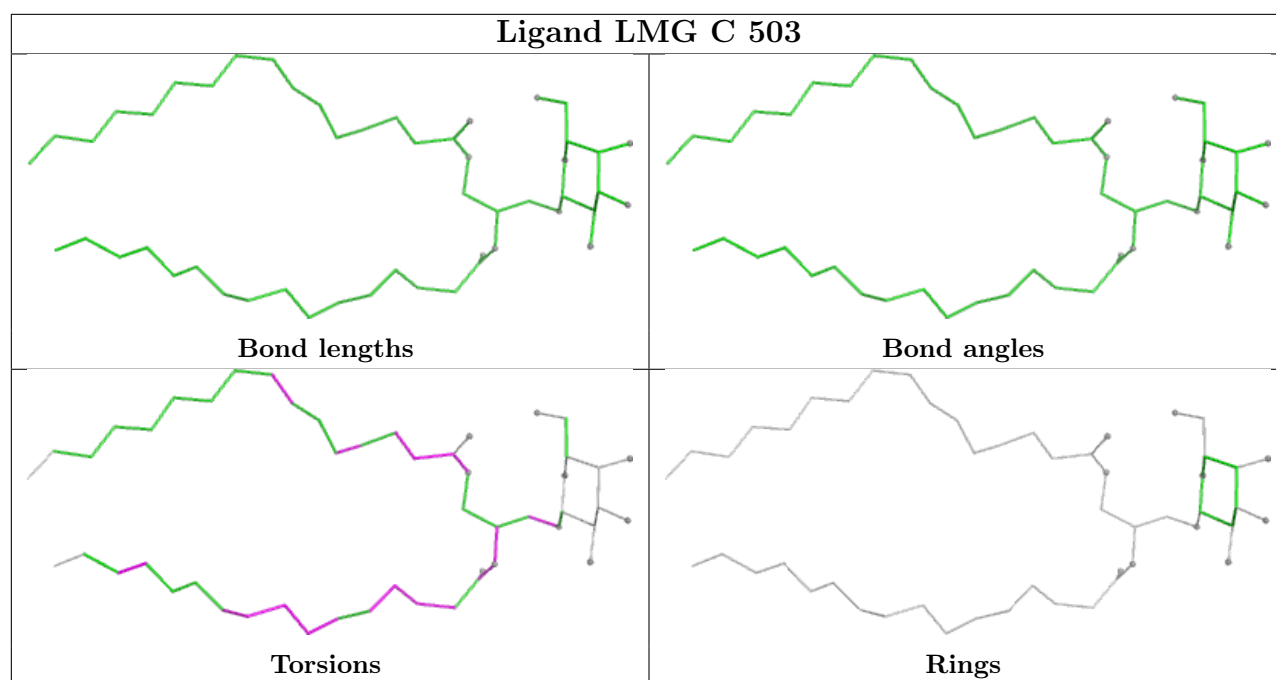
Torsions

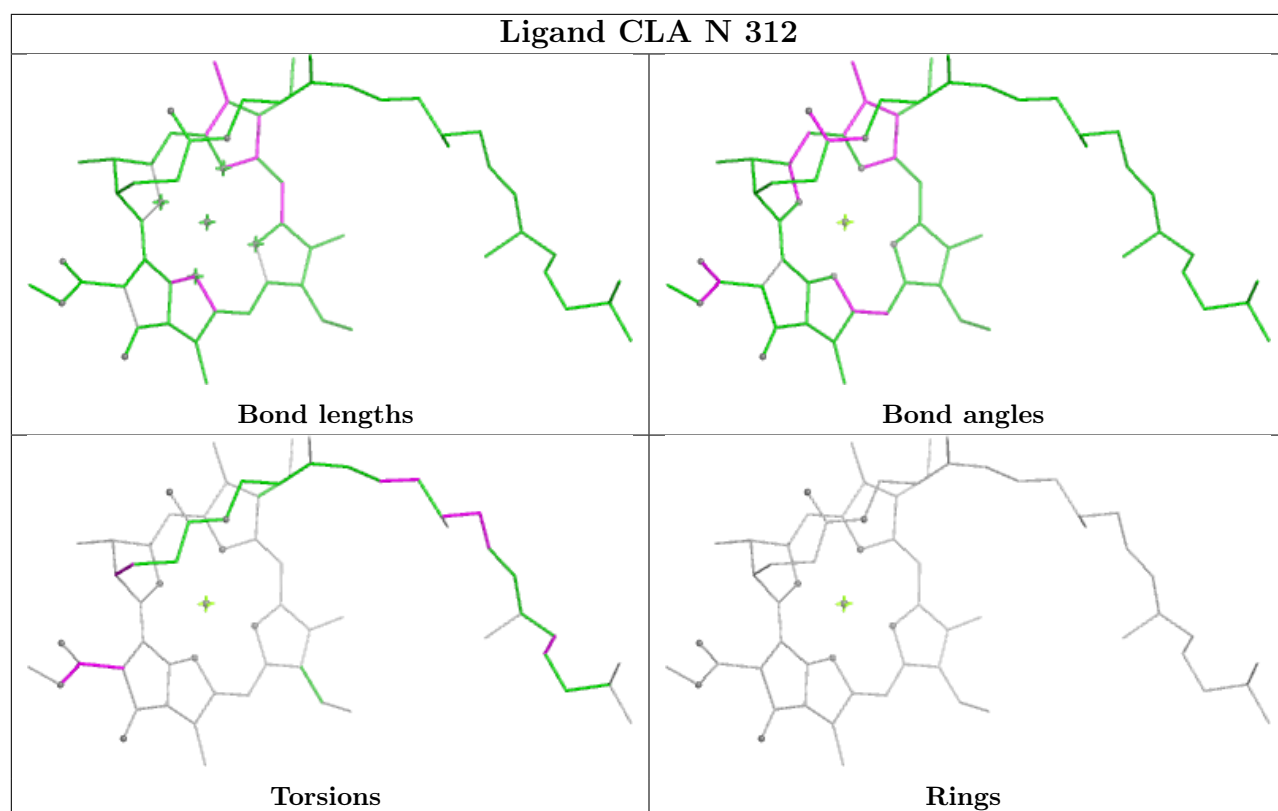


Rings

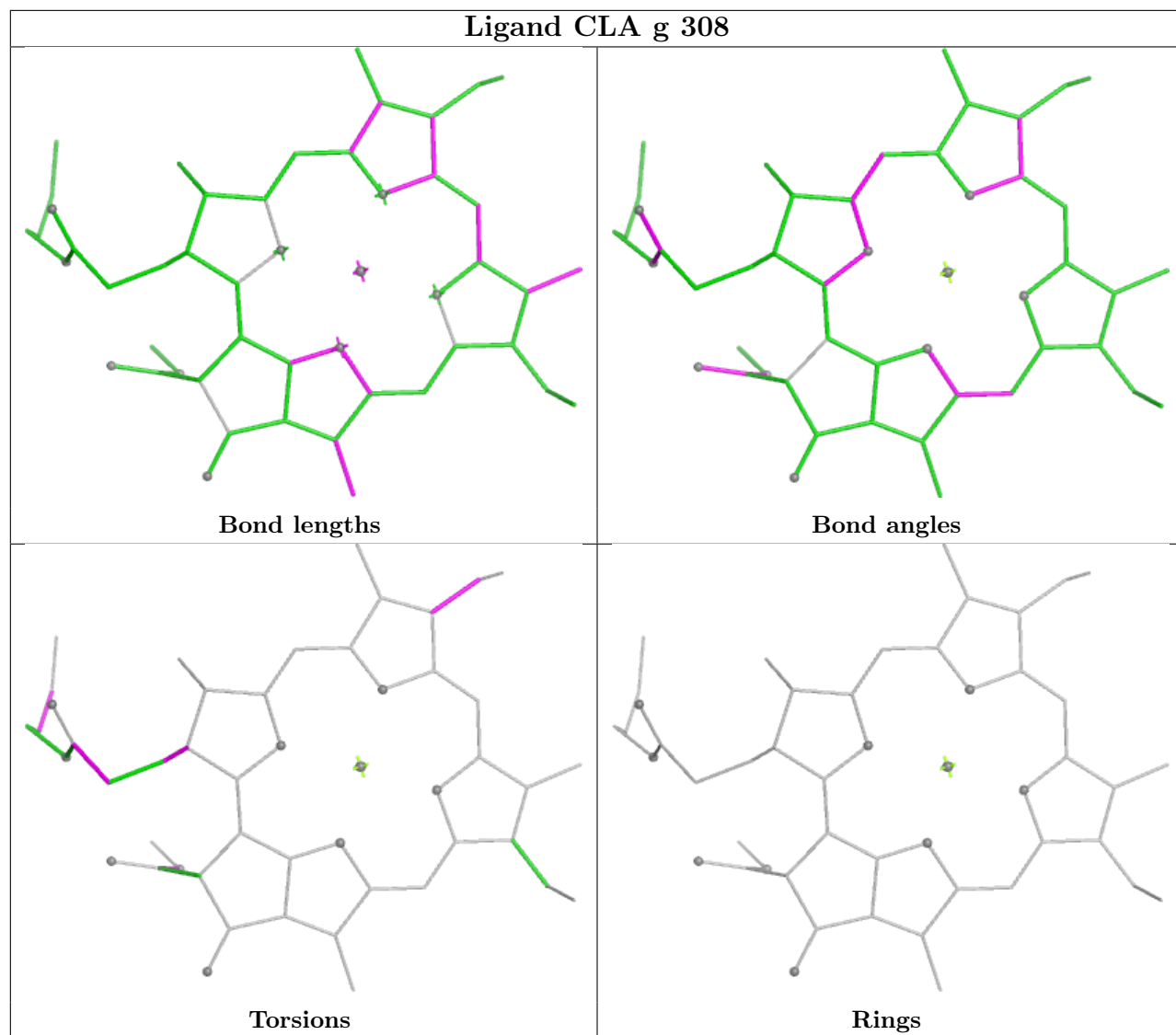




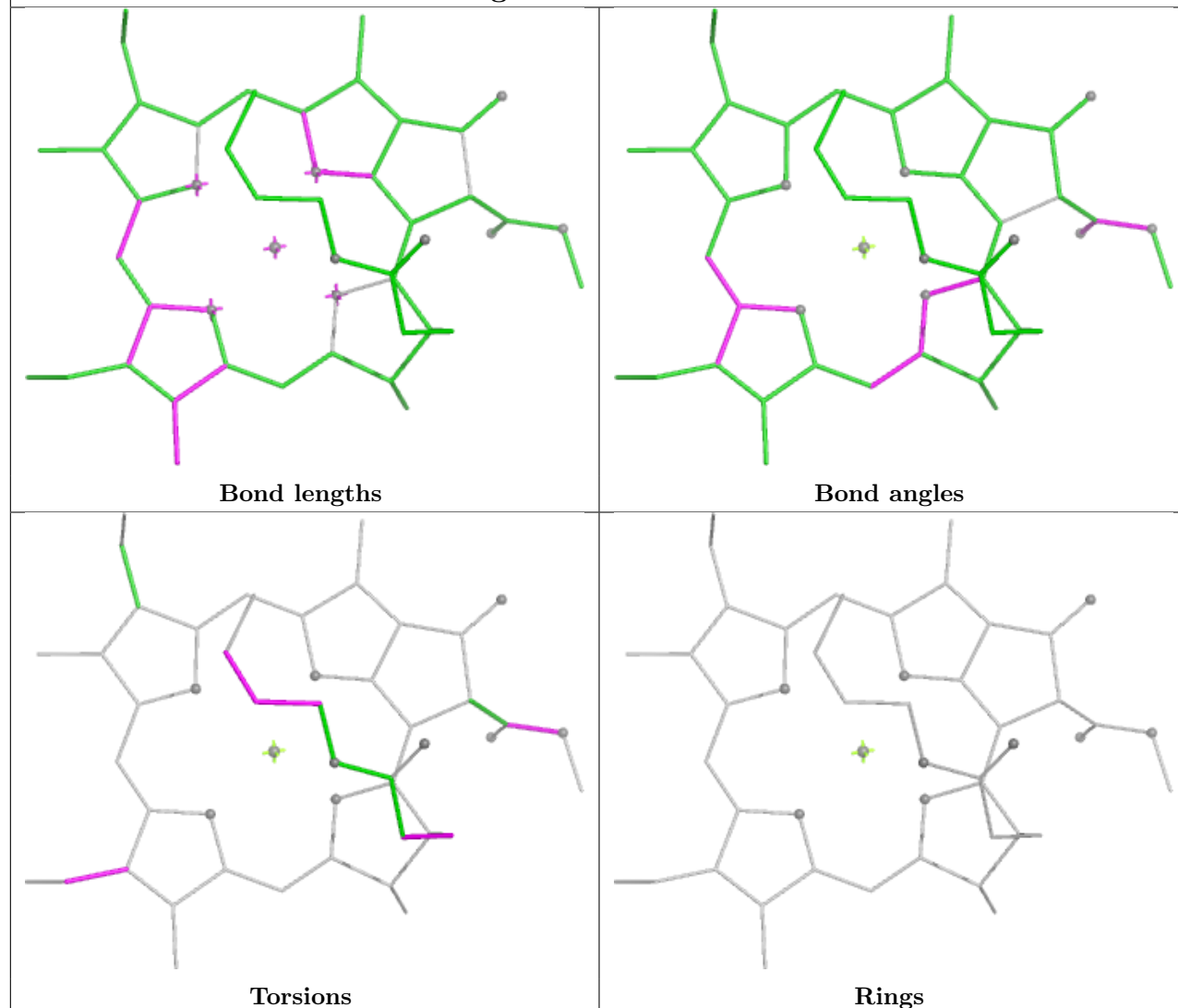




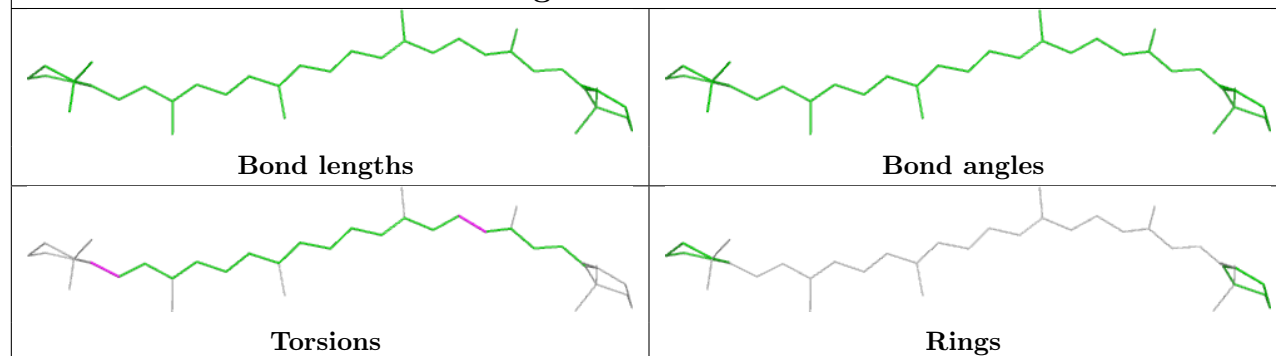
Ligand CLA g 308

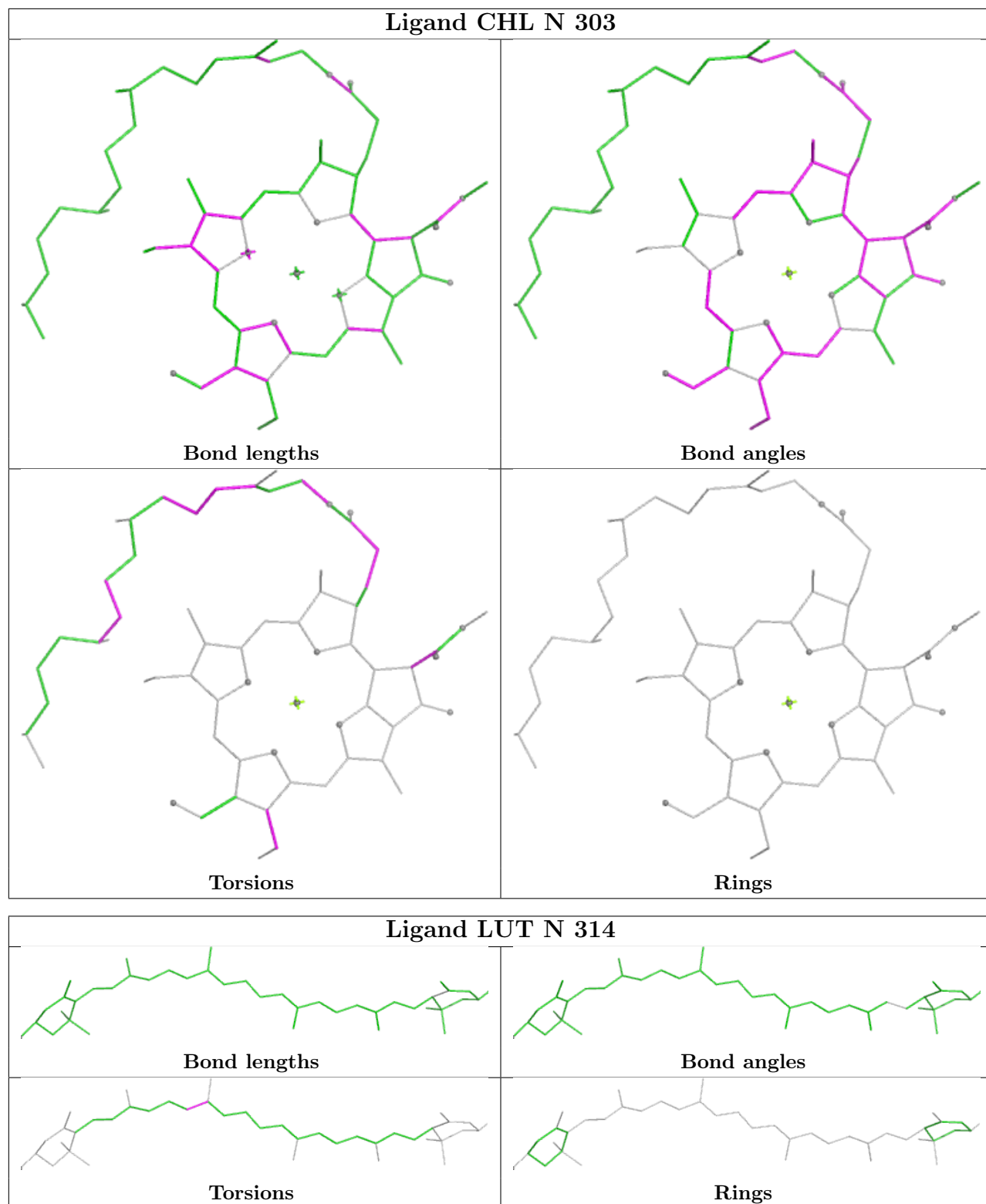


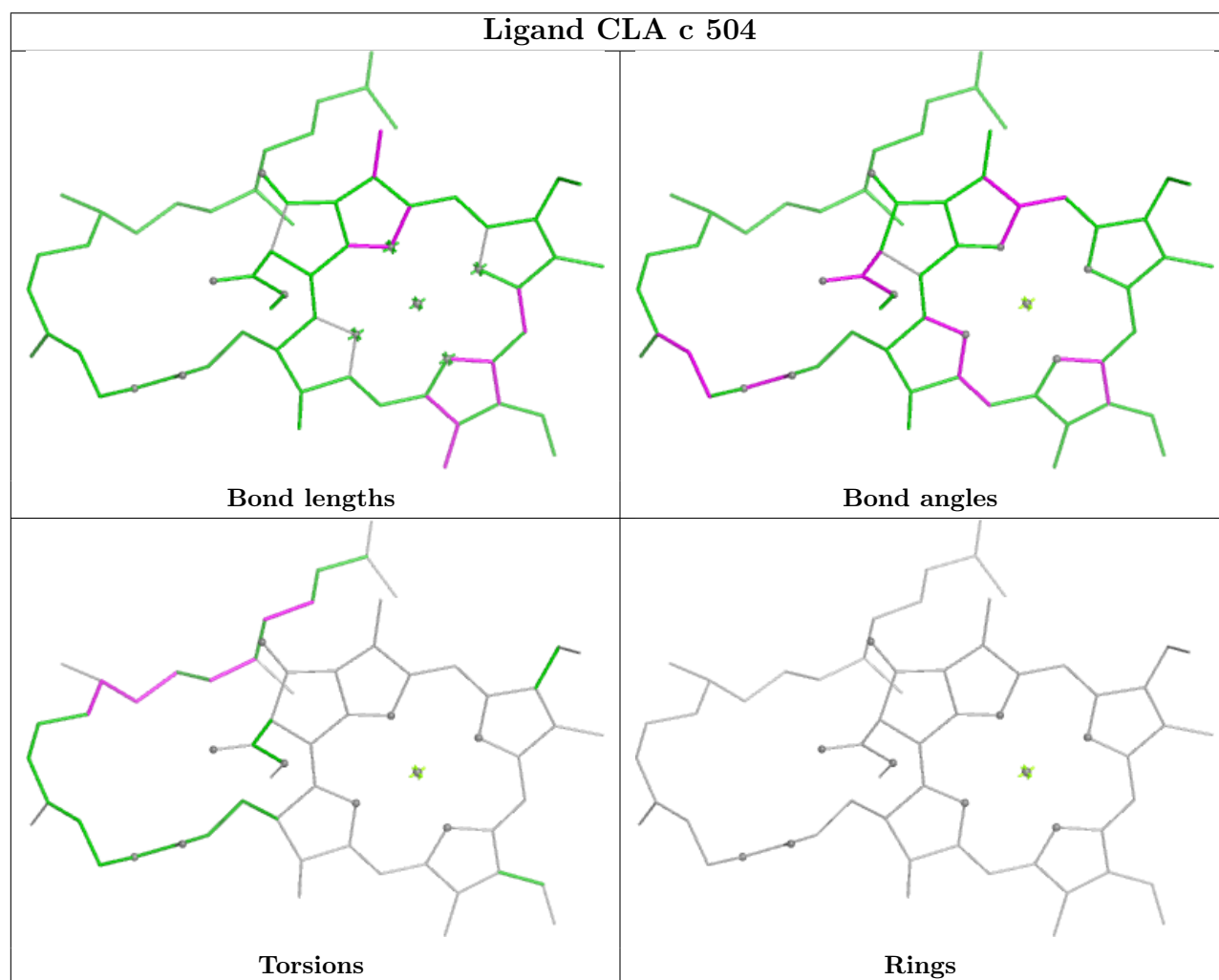
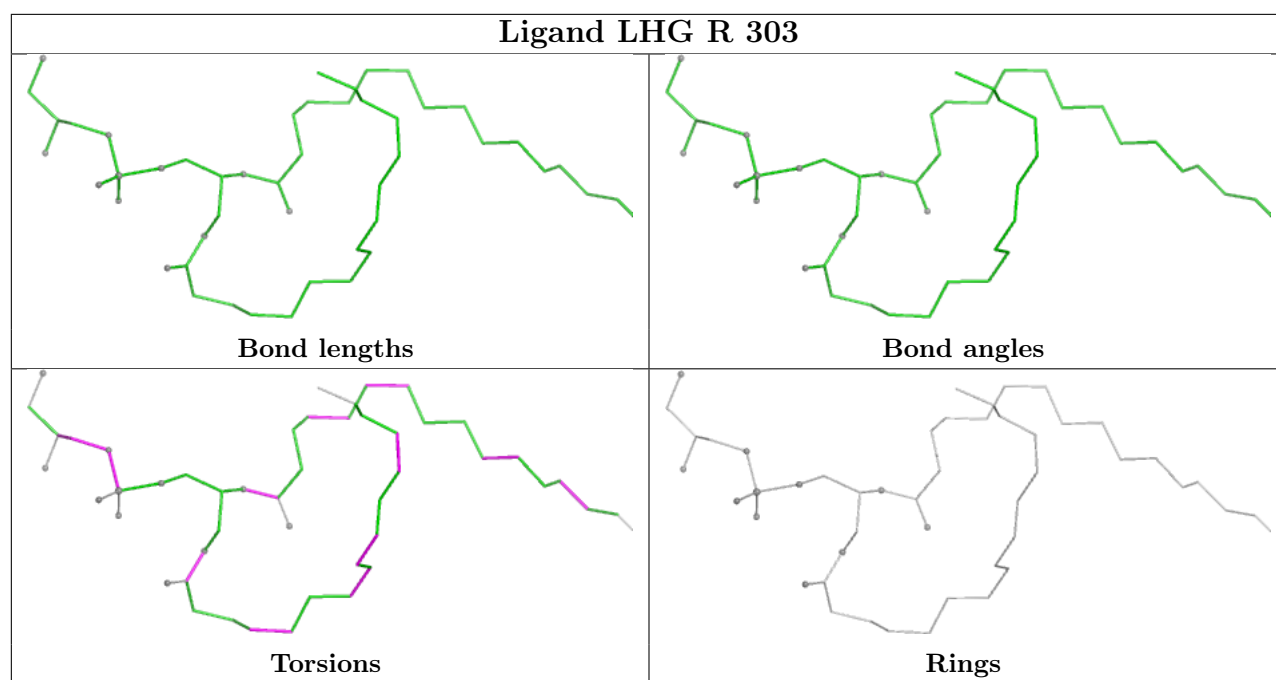
Ligand CLA R 307

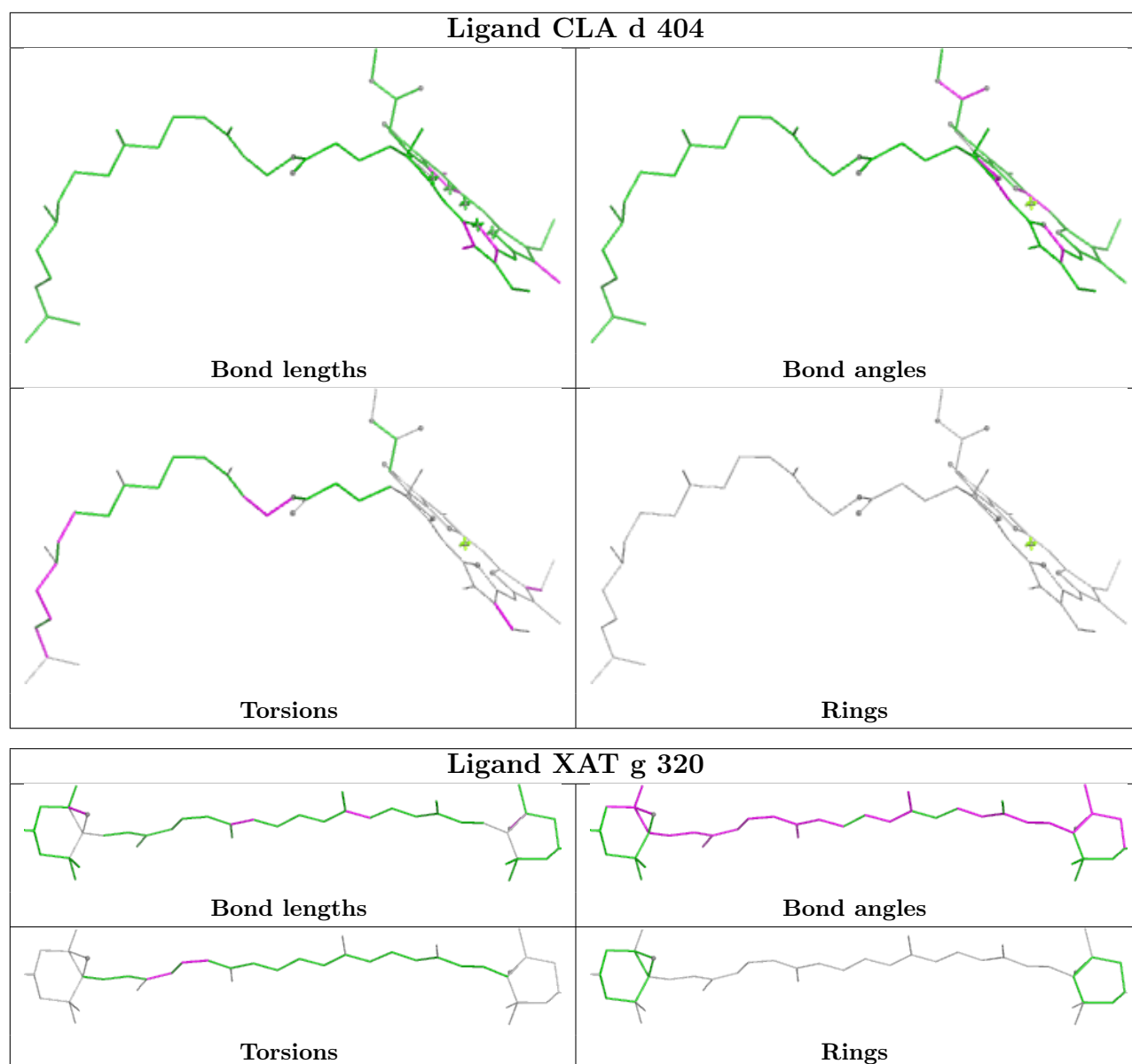


Ligand BCR h 101

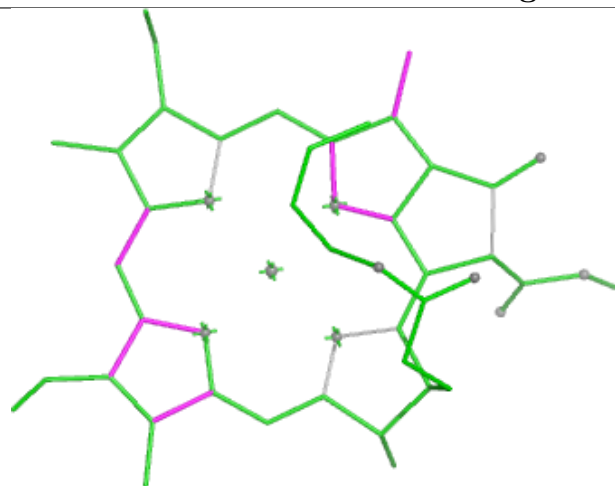




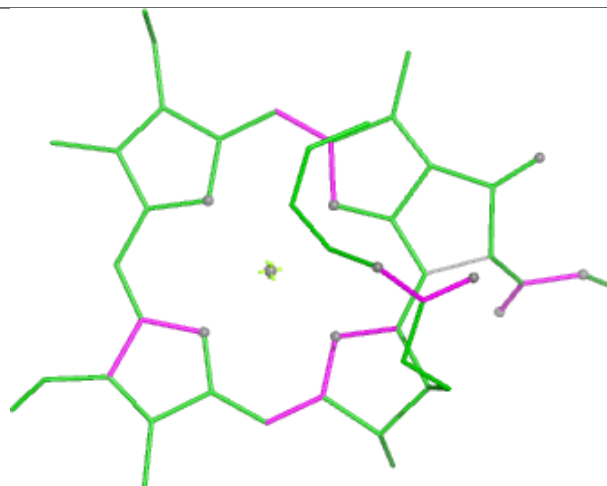




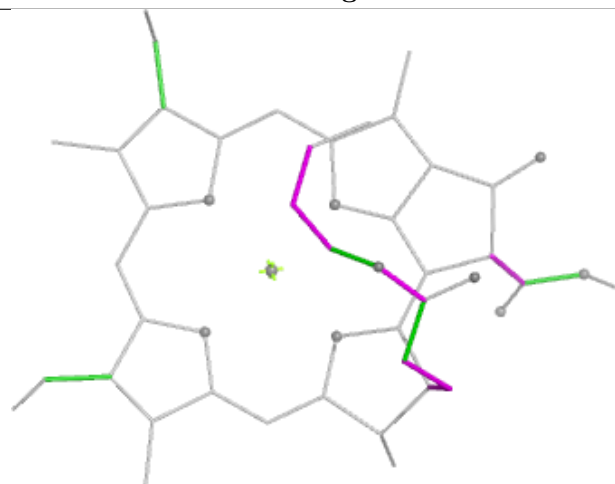
Ligand CLA S 304



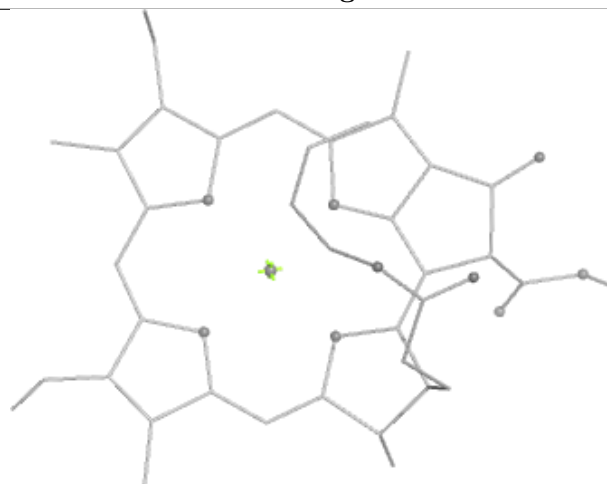
Bond lengths



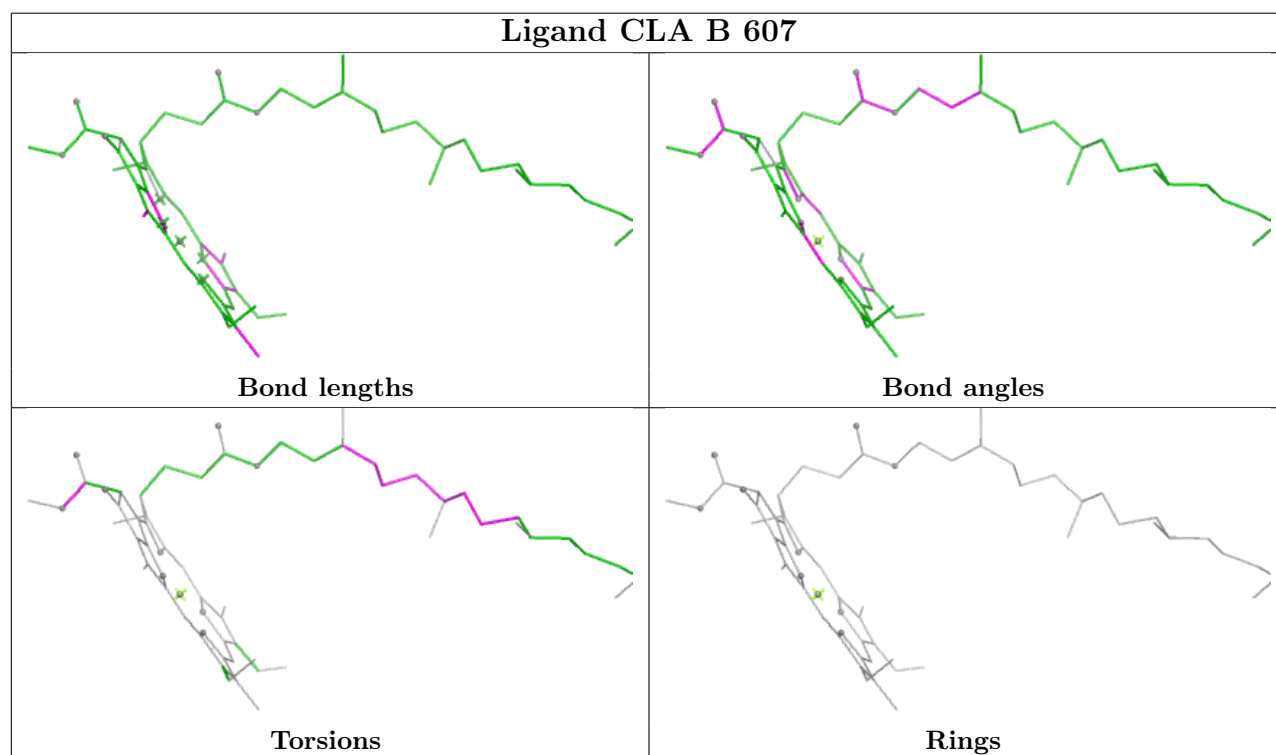
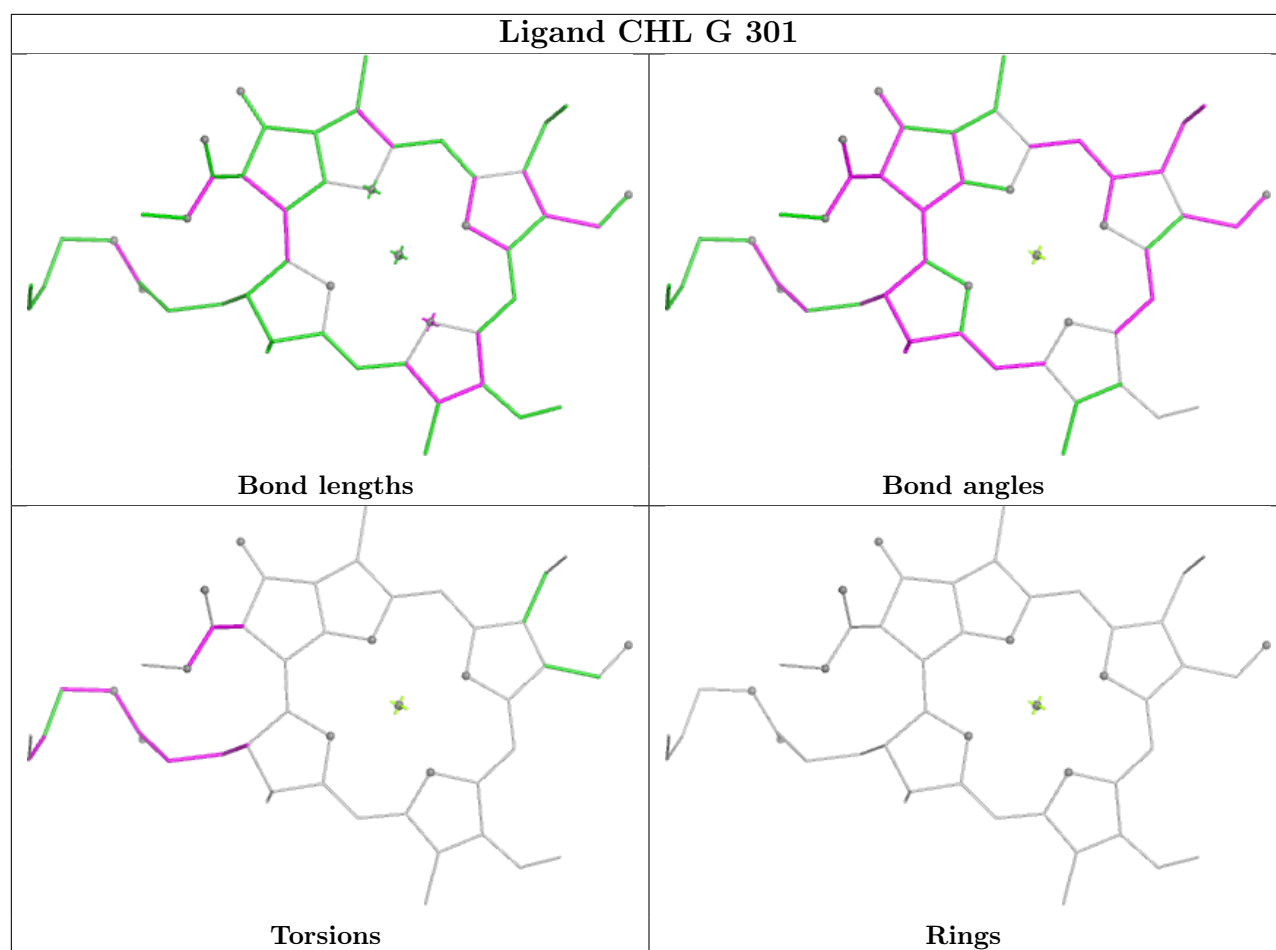
Bond angles

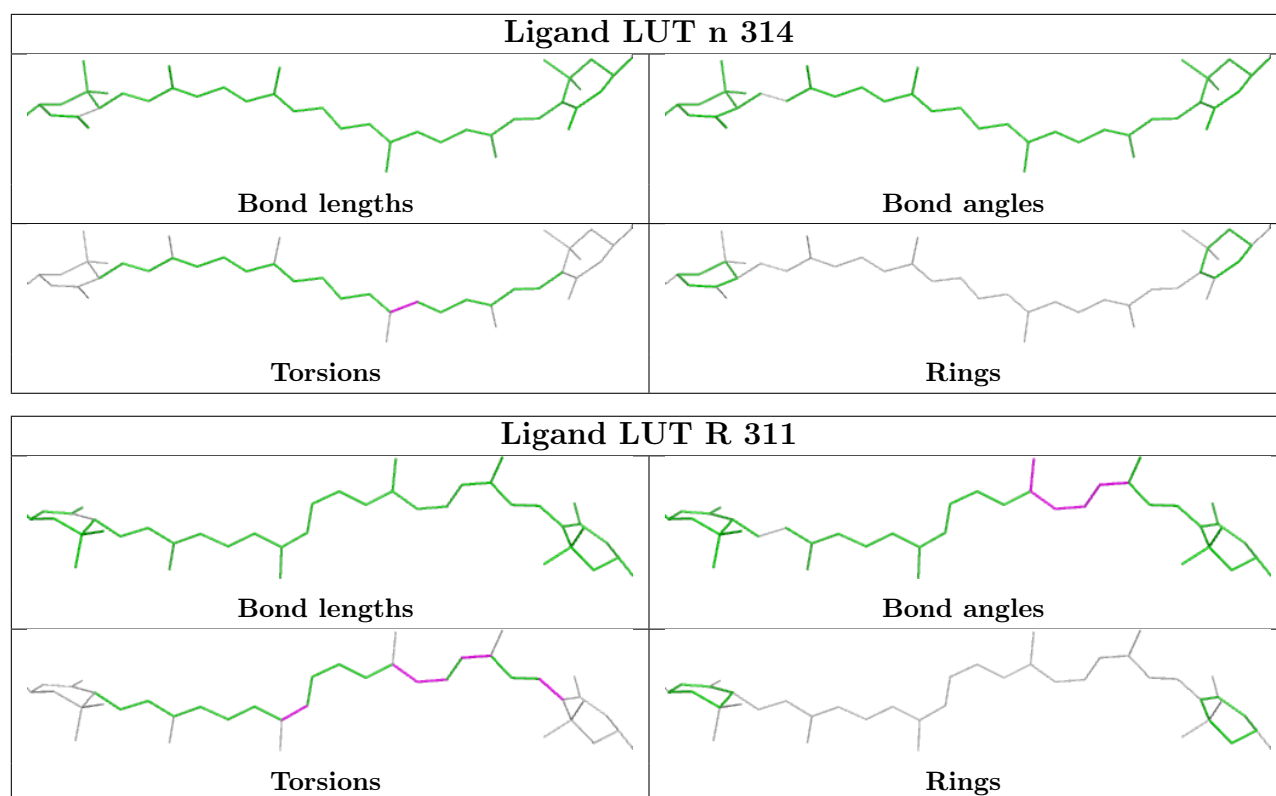


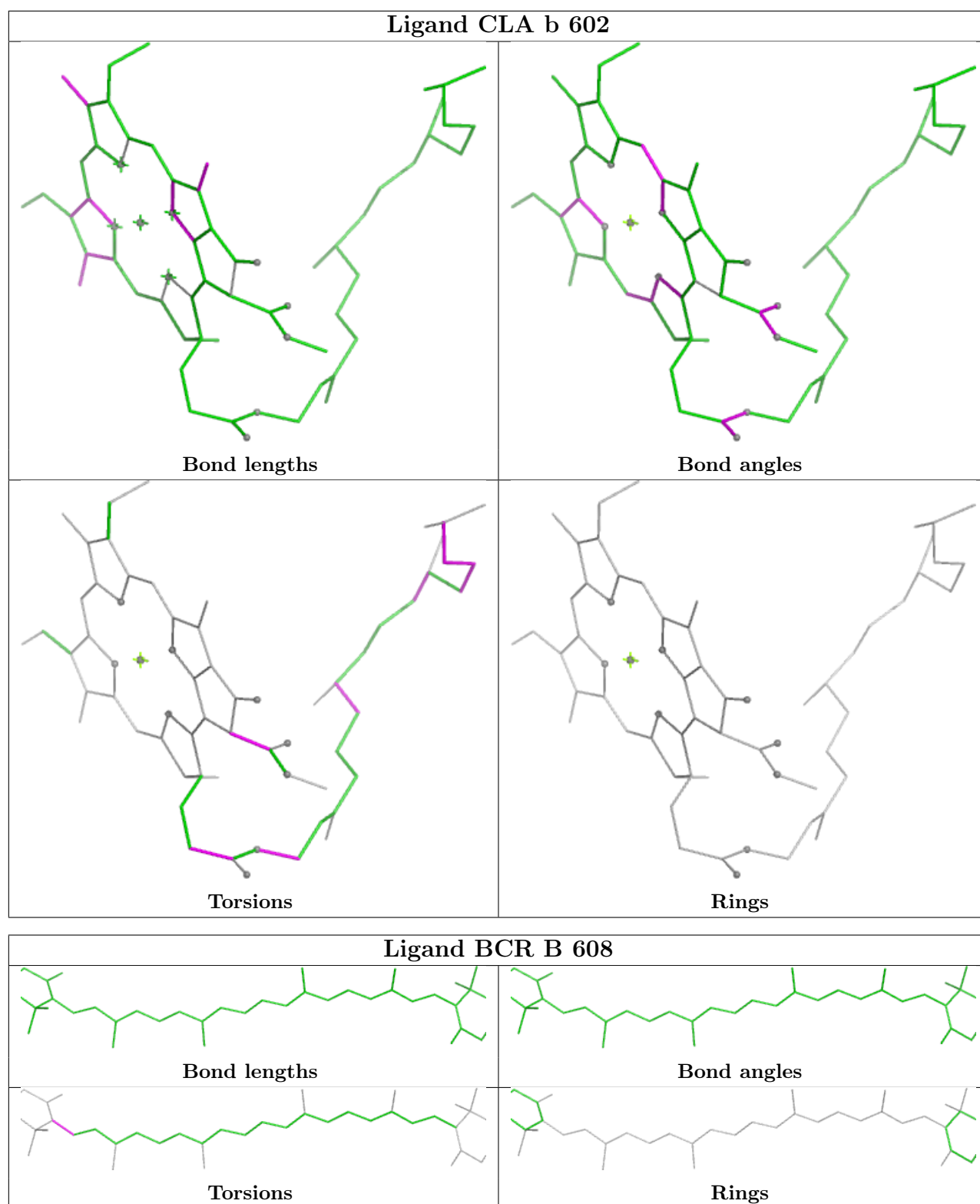
Torsions

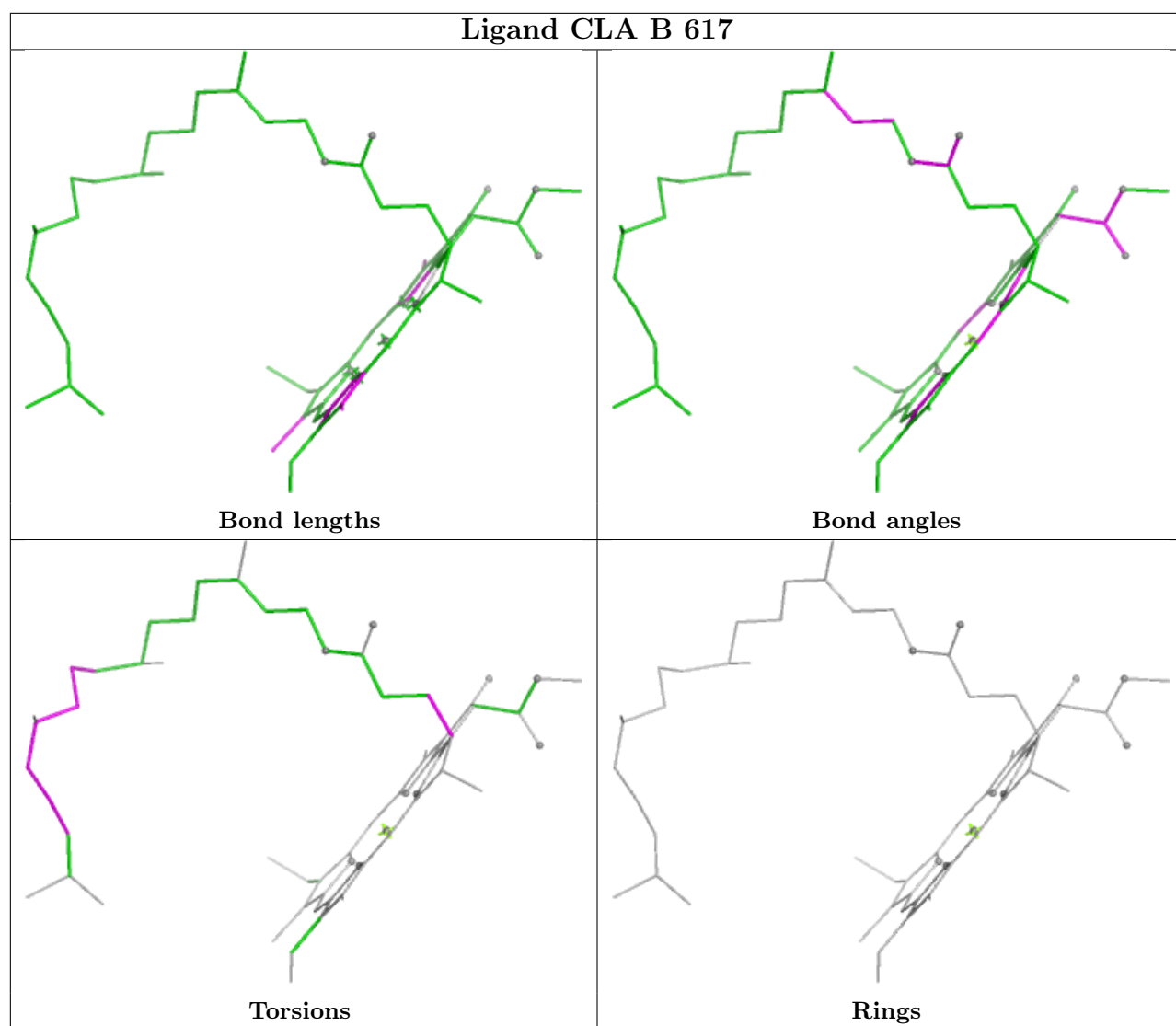


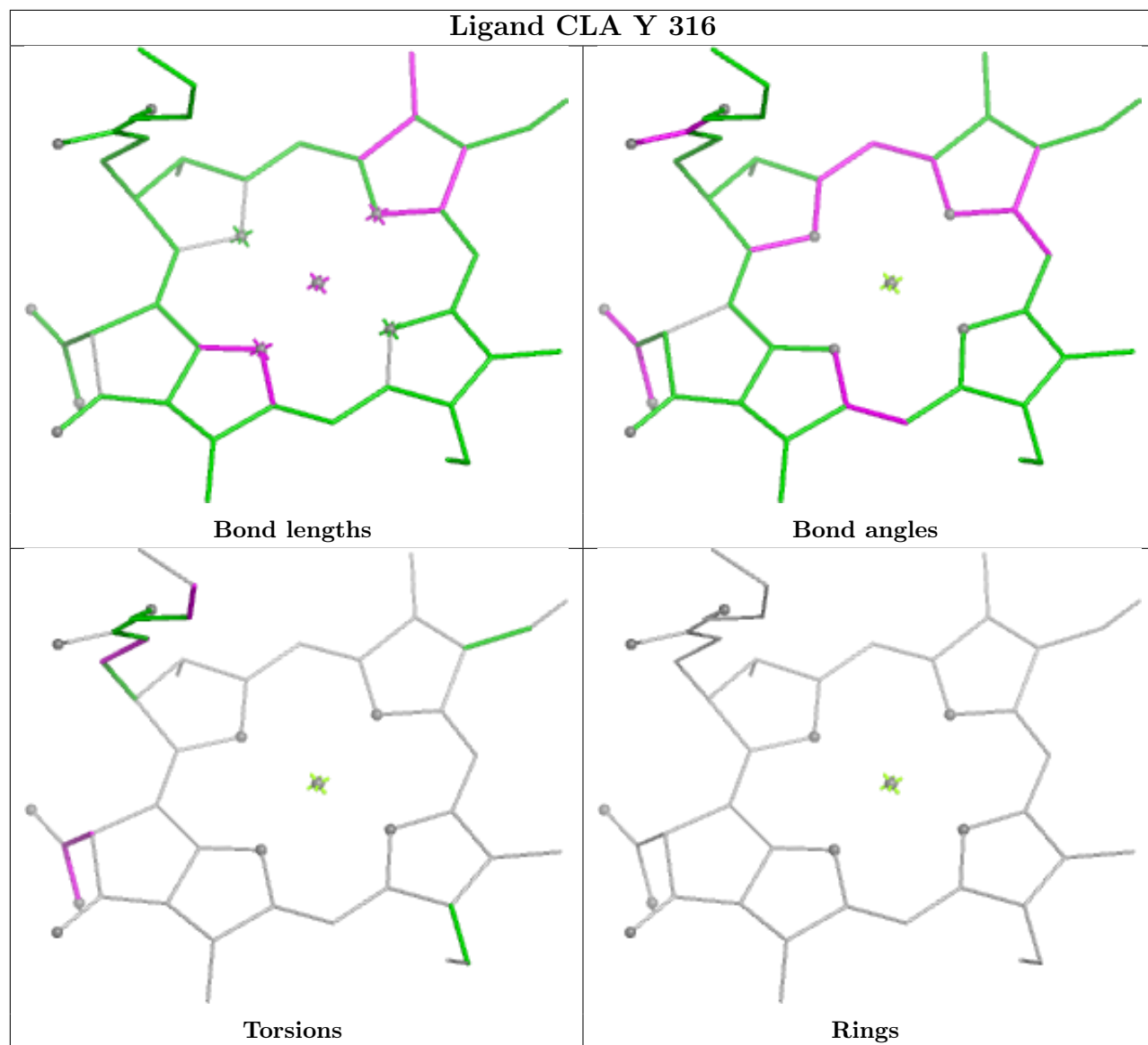
Rings



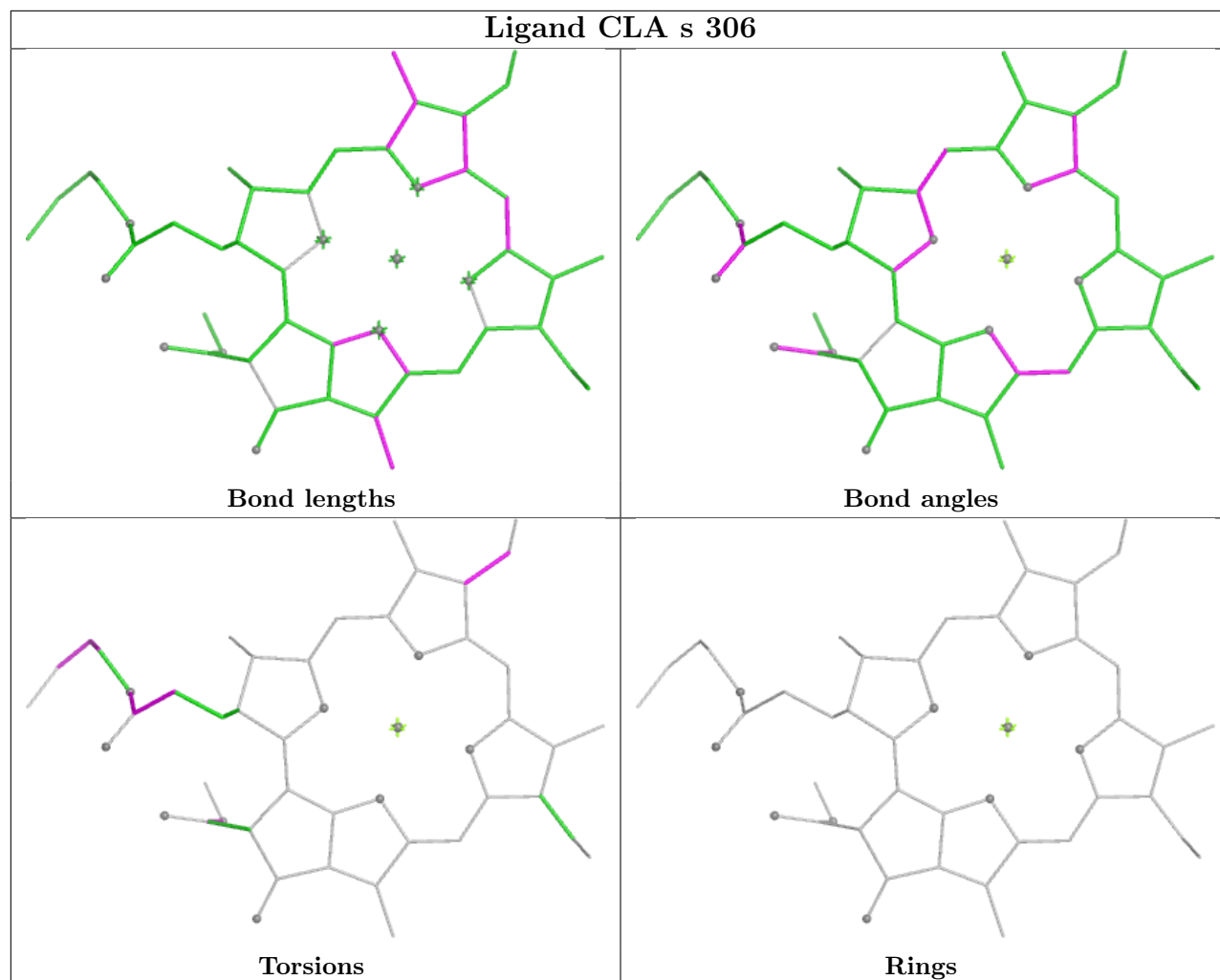




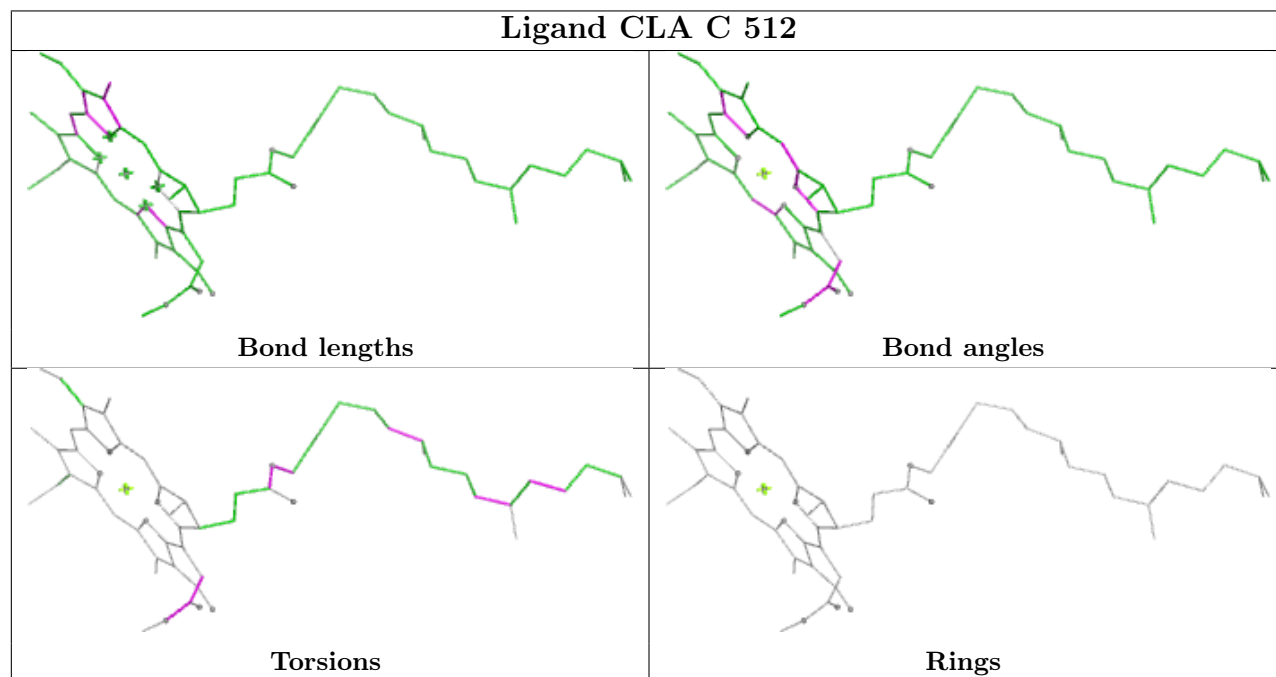


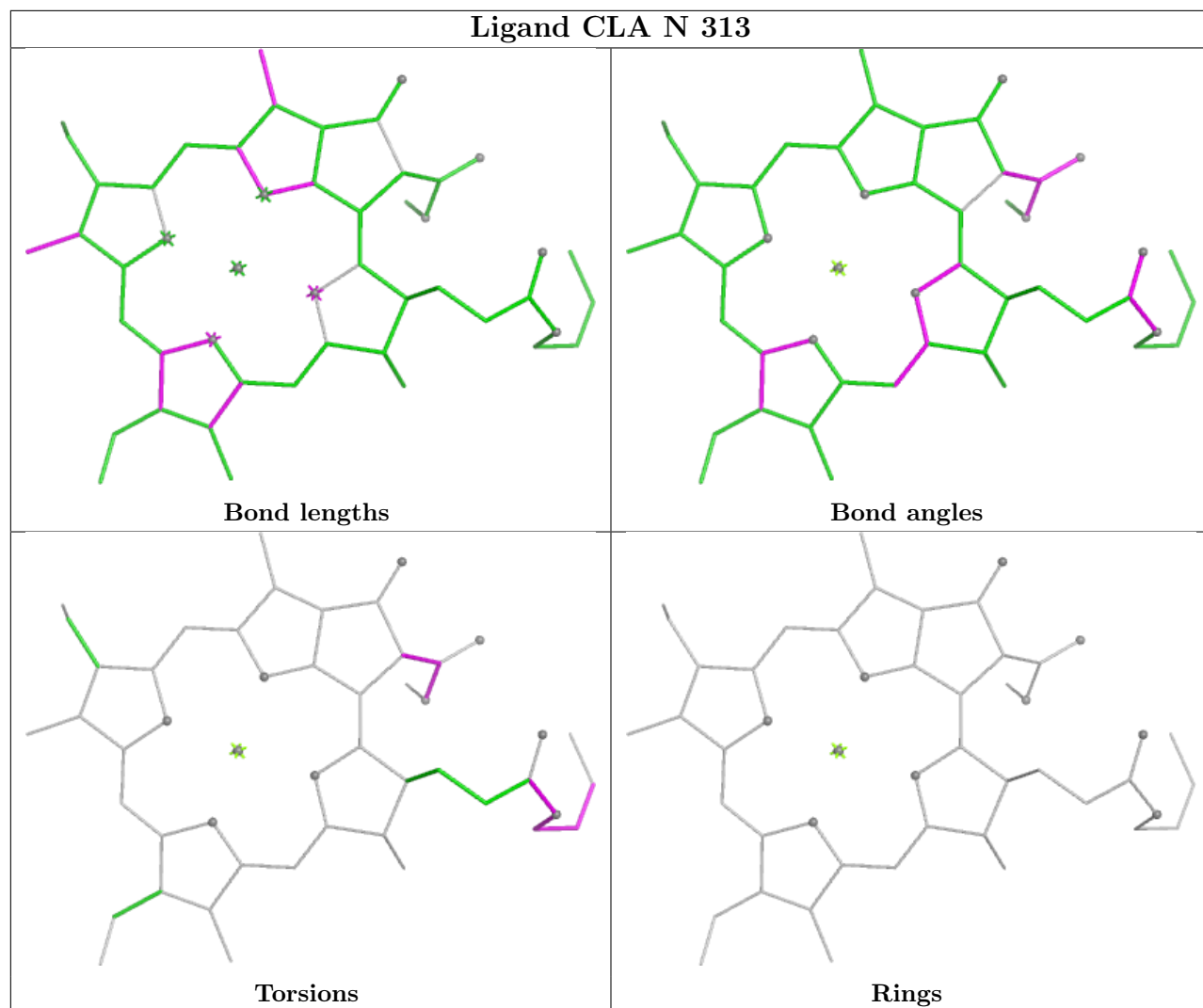


Ligand CLA s 306

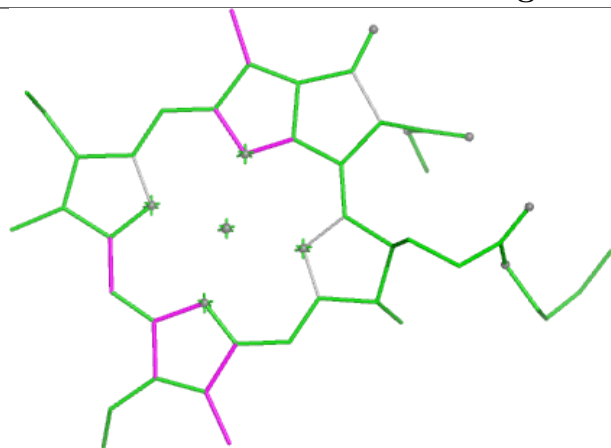


Ligand CLA C 512

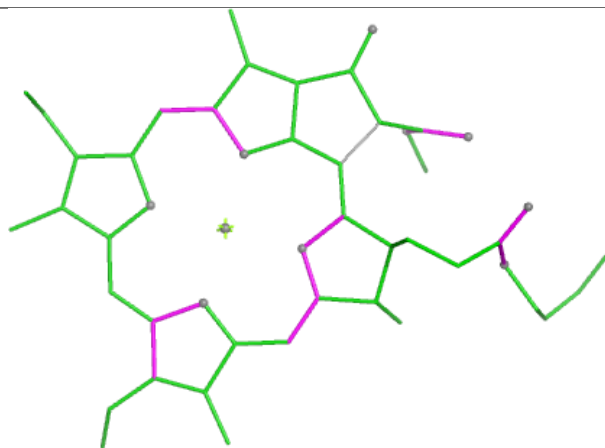




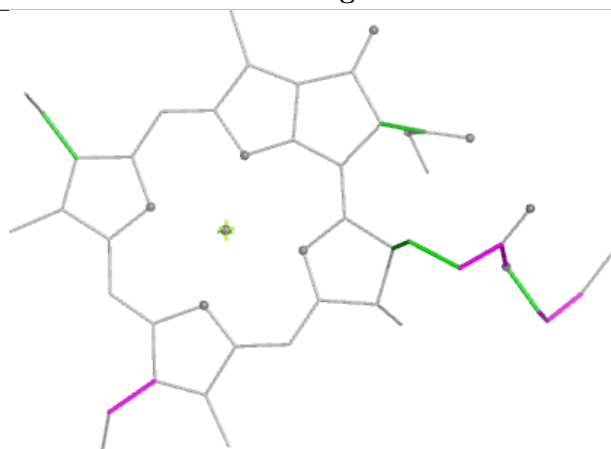
Ligand CLA S 315



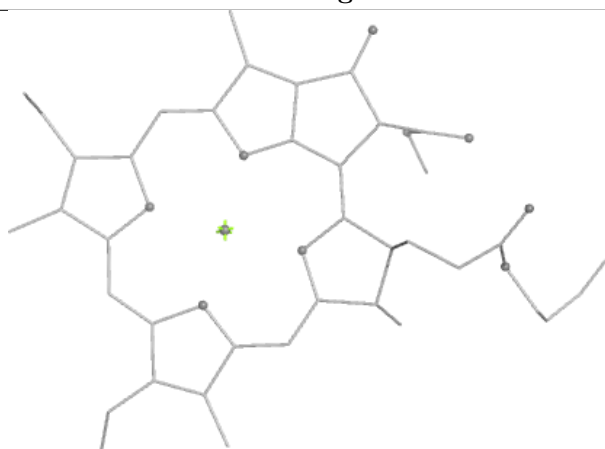
Bond lengths



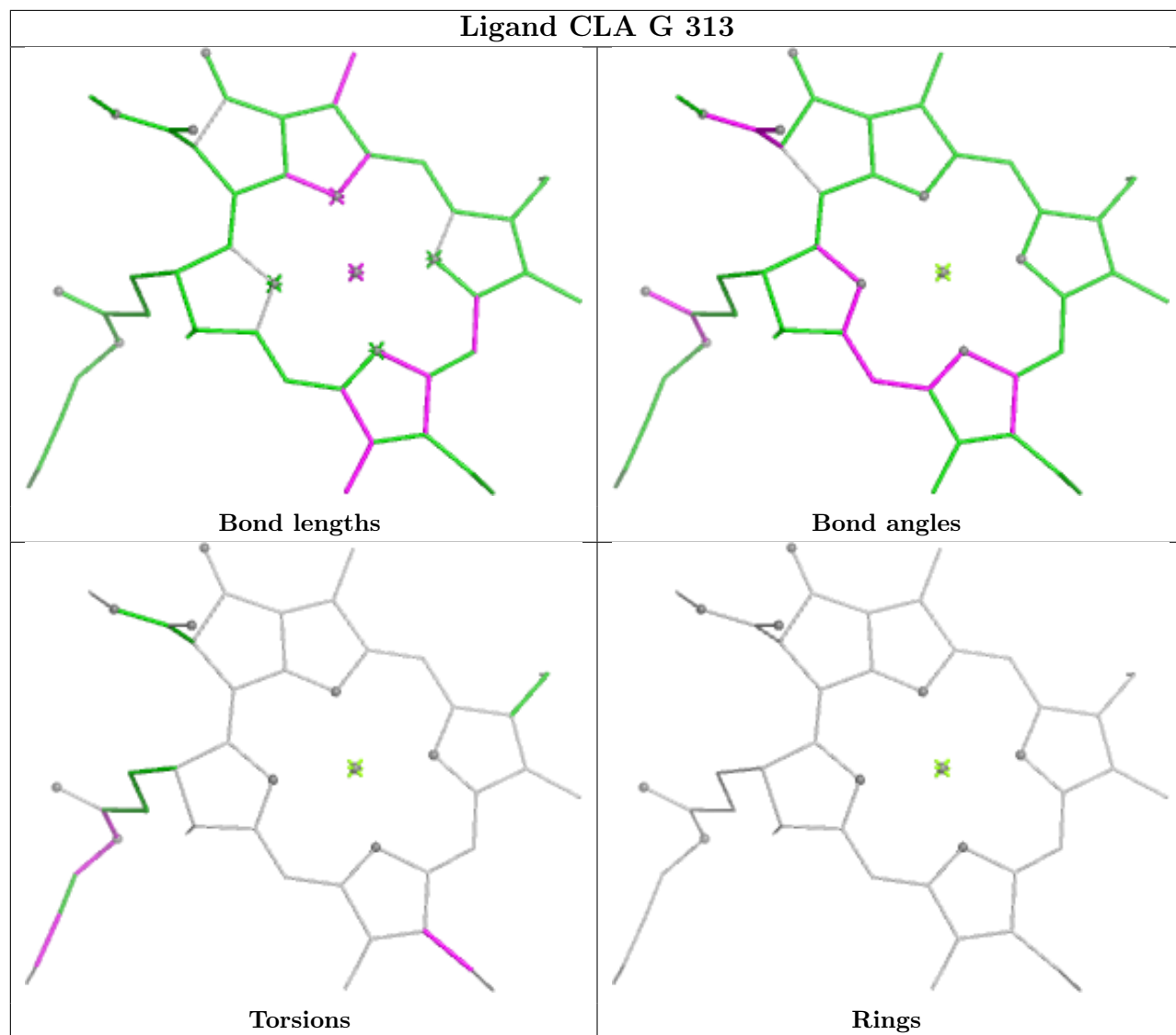
Bond angles

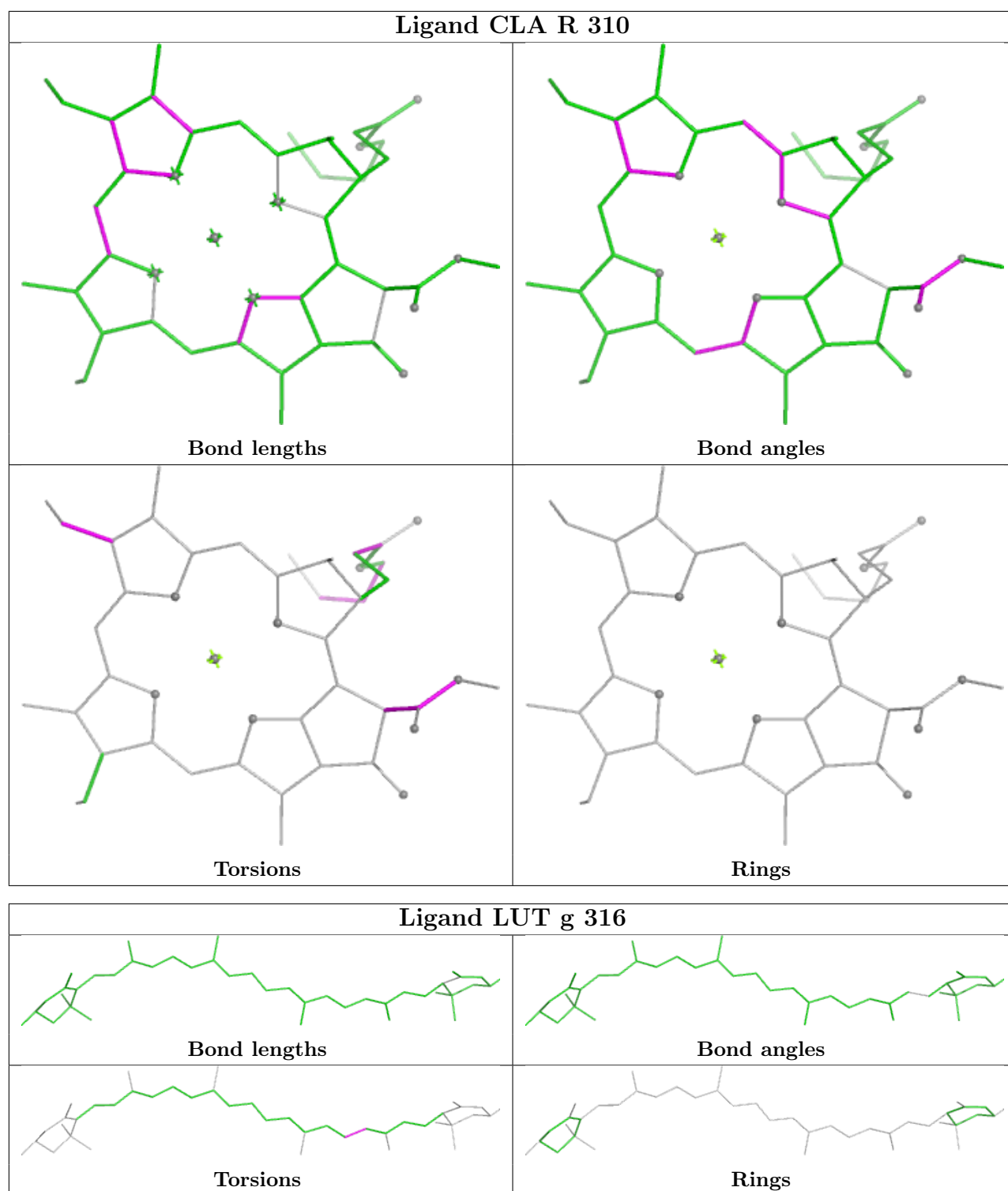


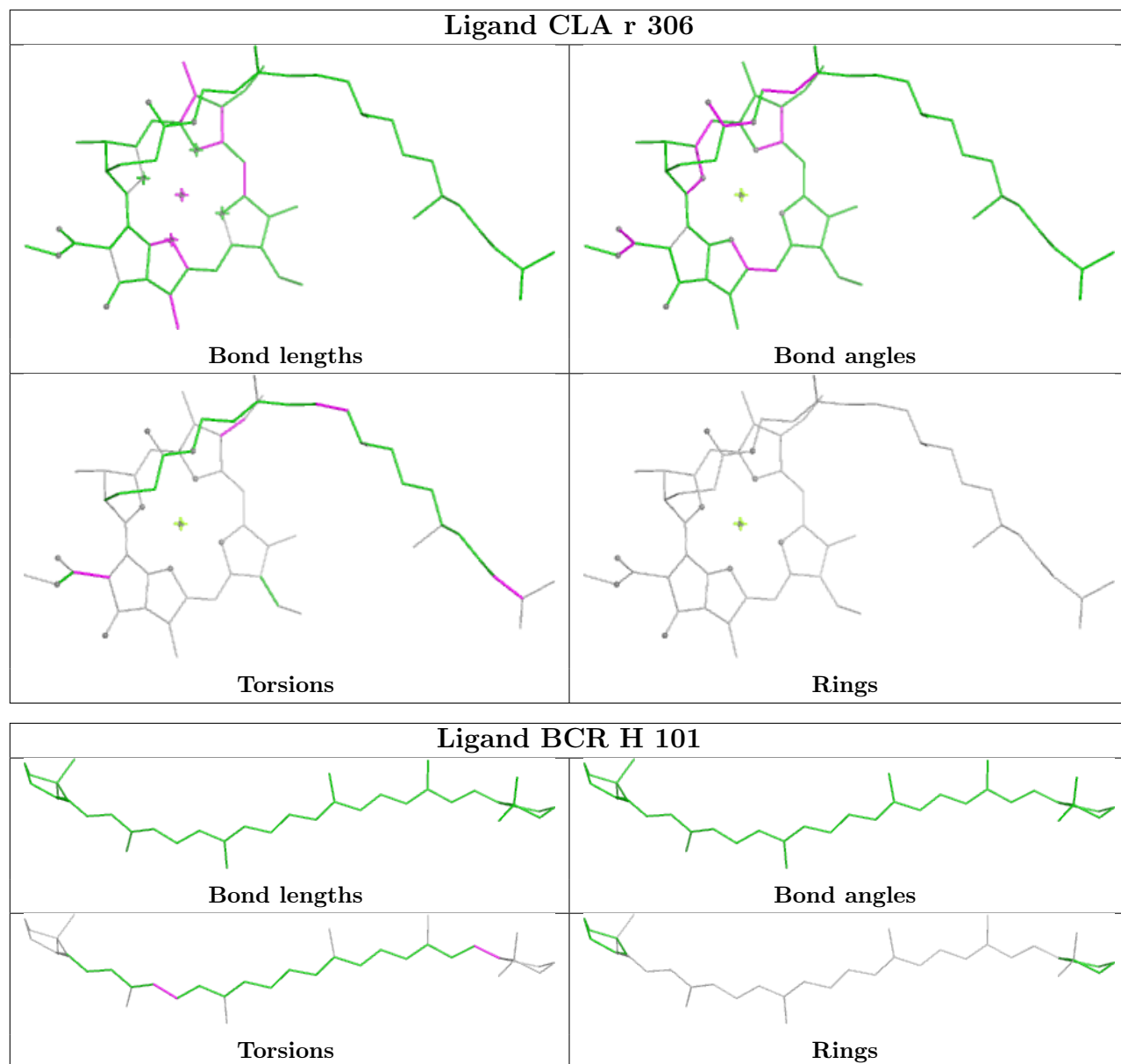
Torsions



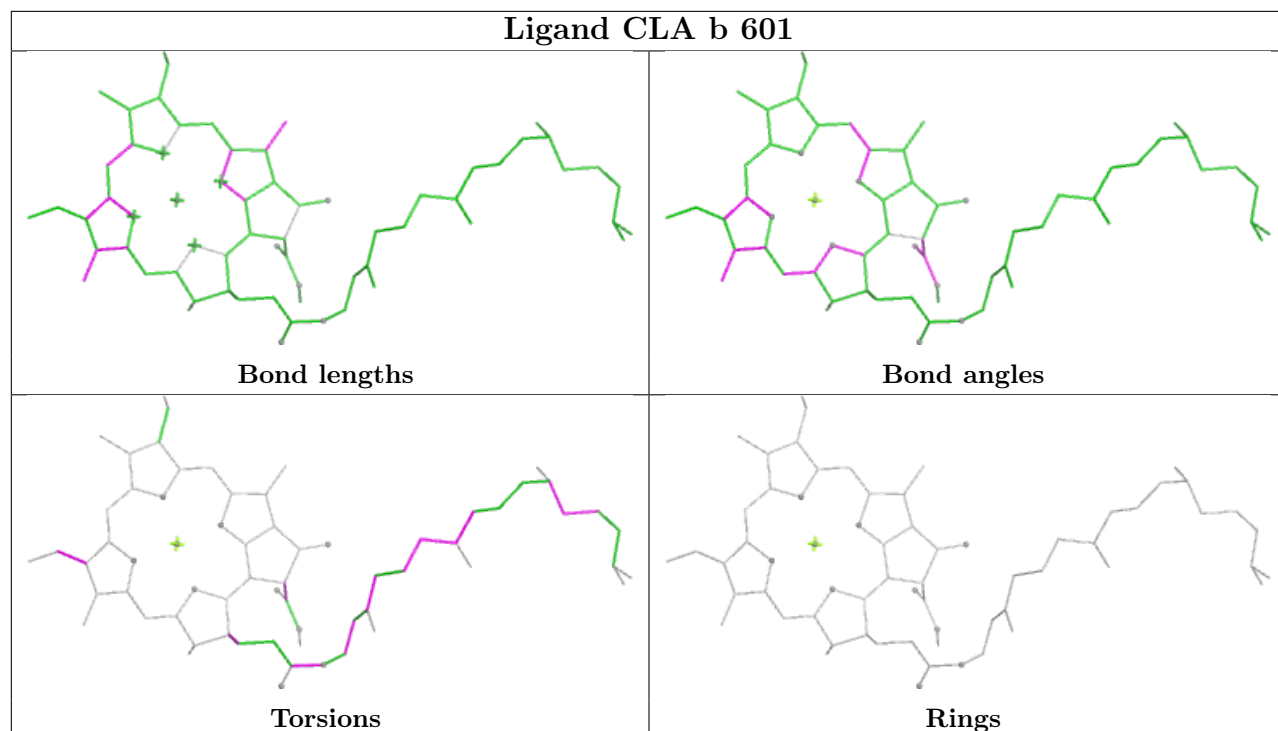
Rings



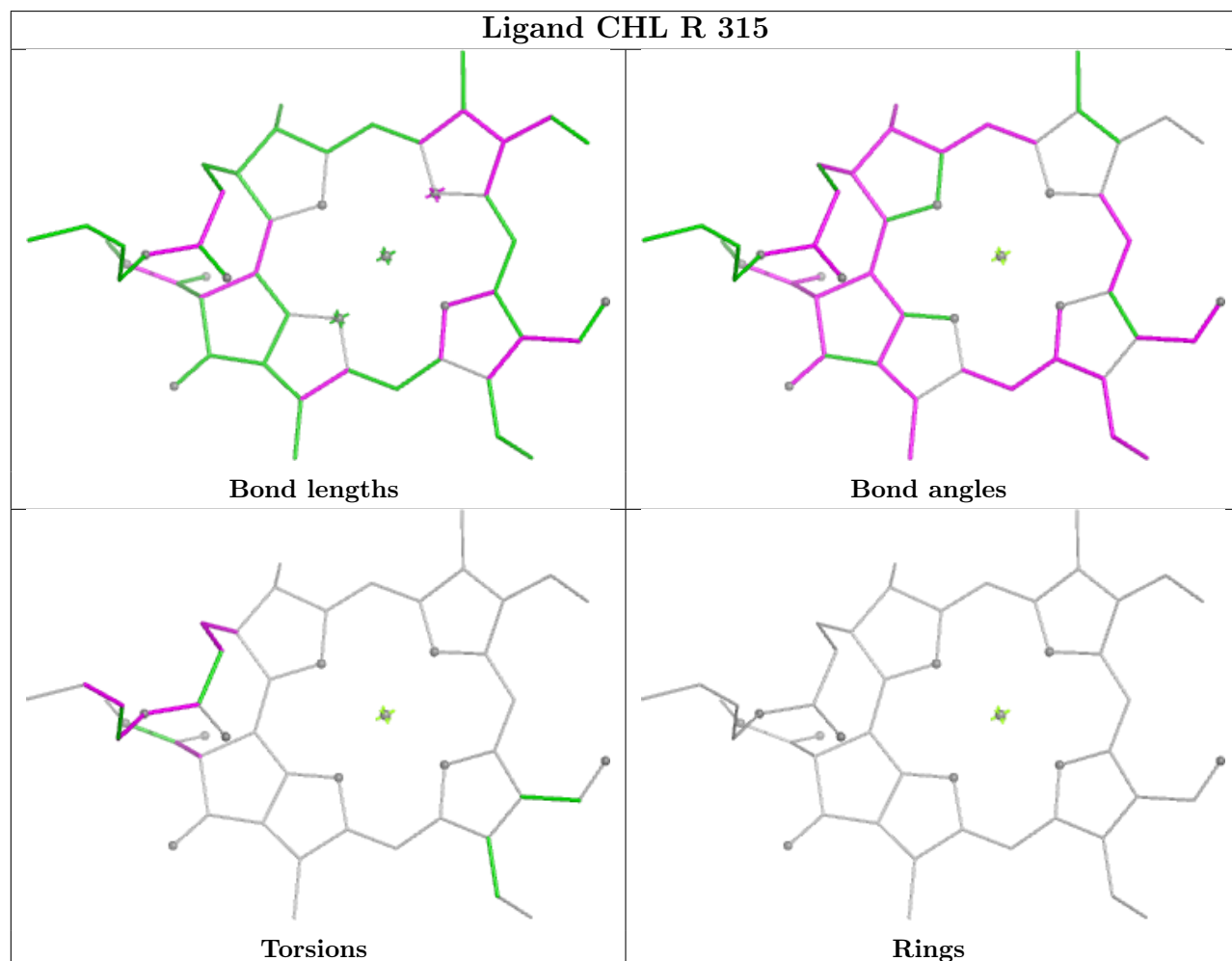


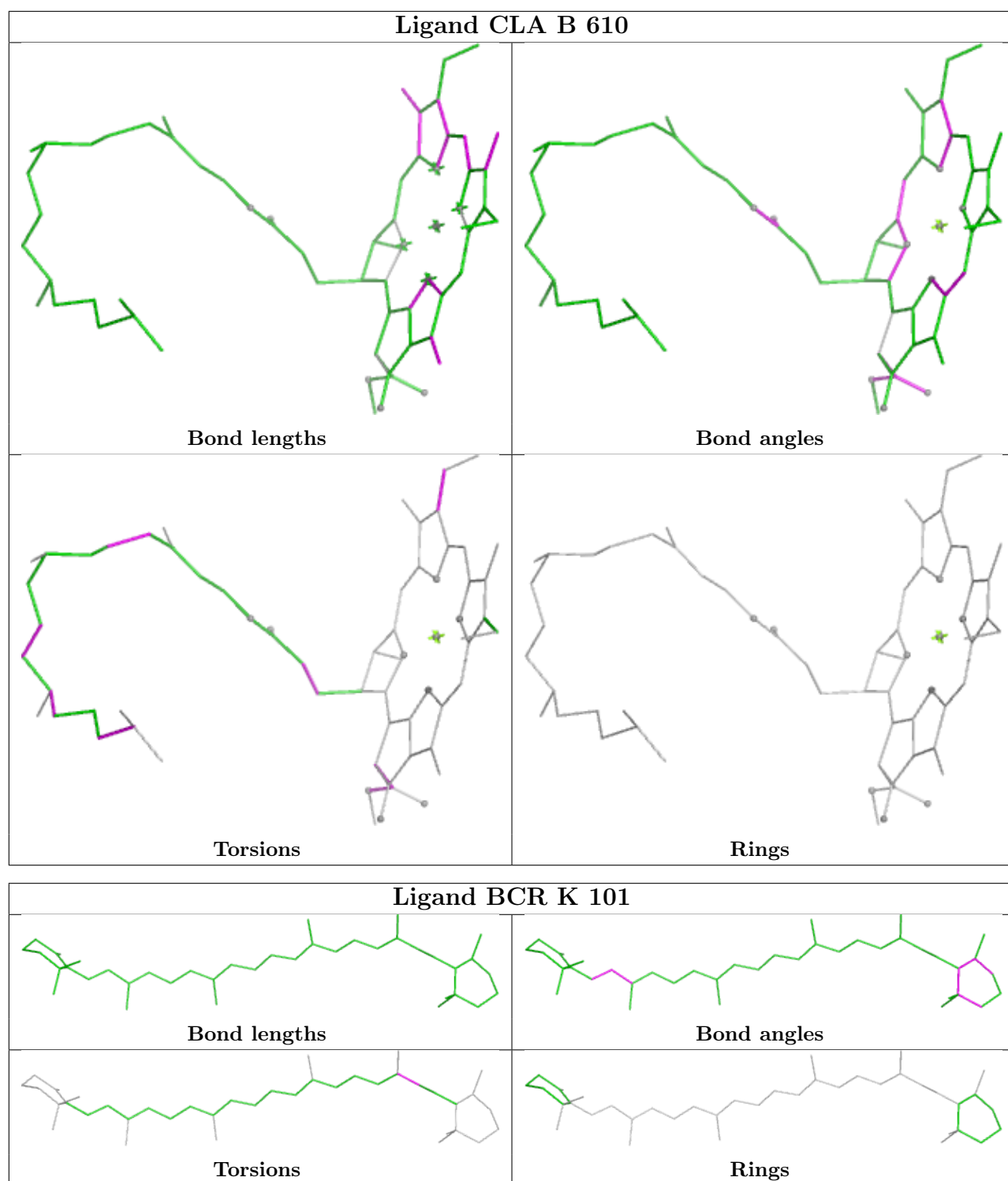


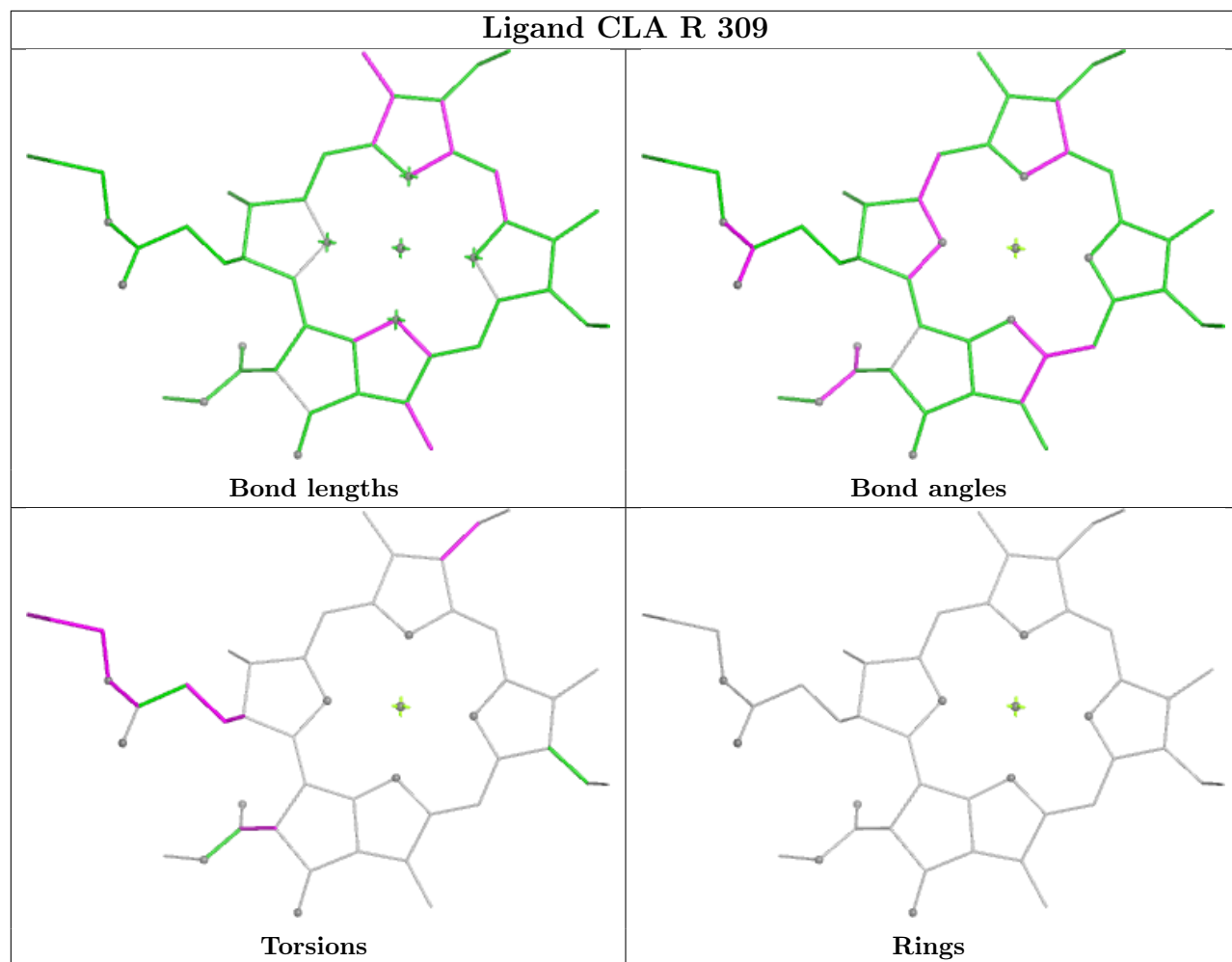
Ligand CLA b 601

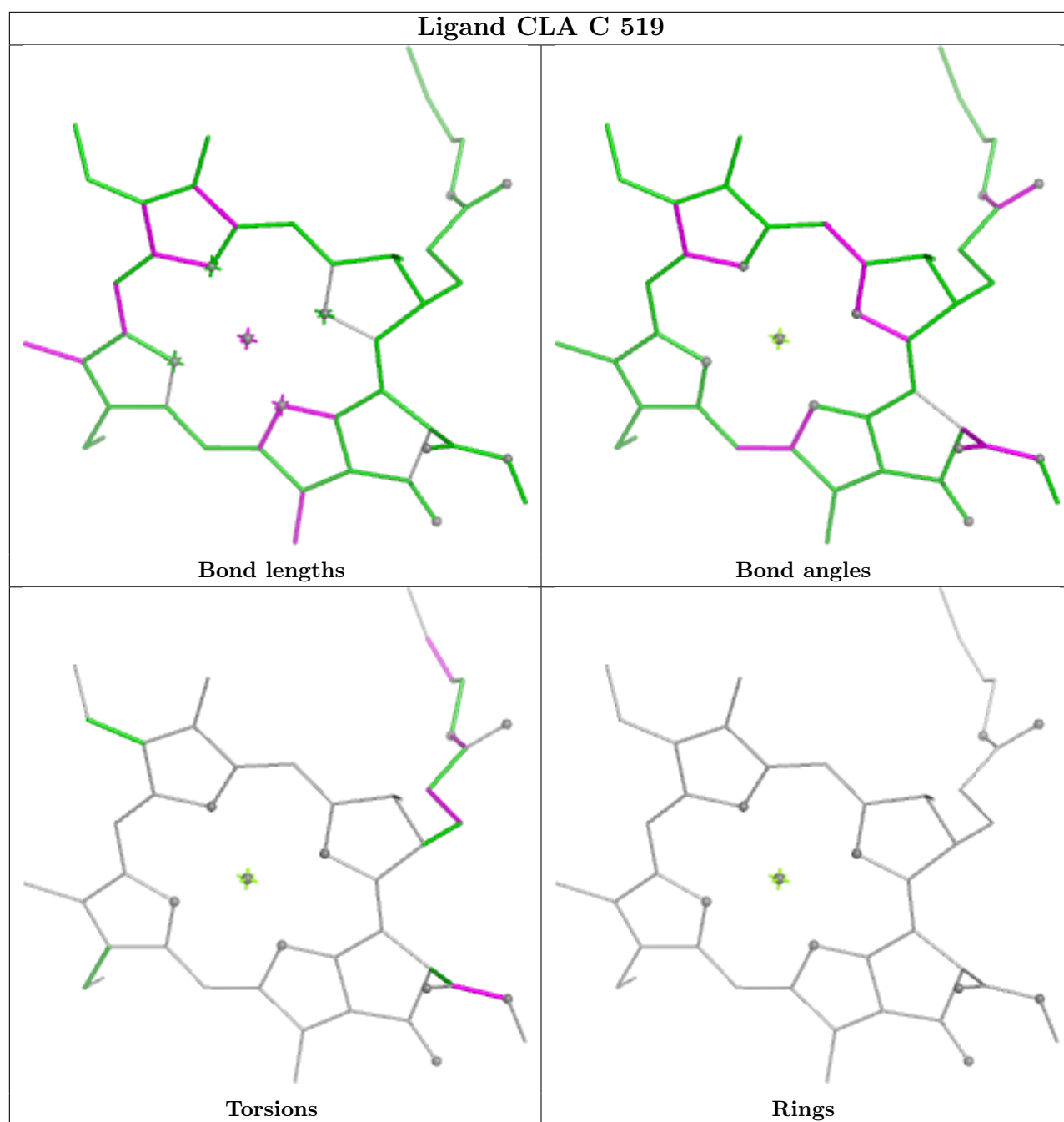


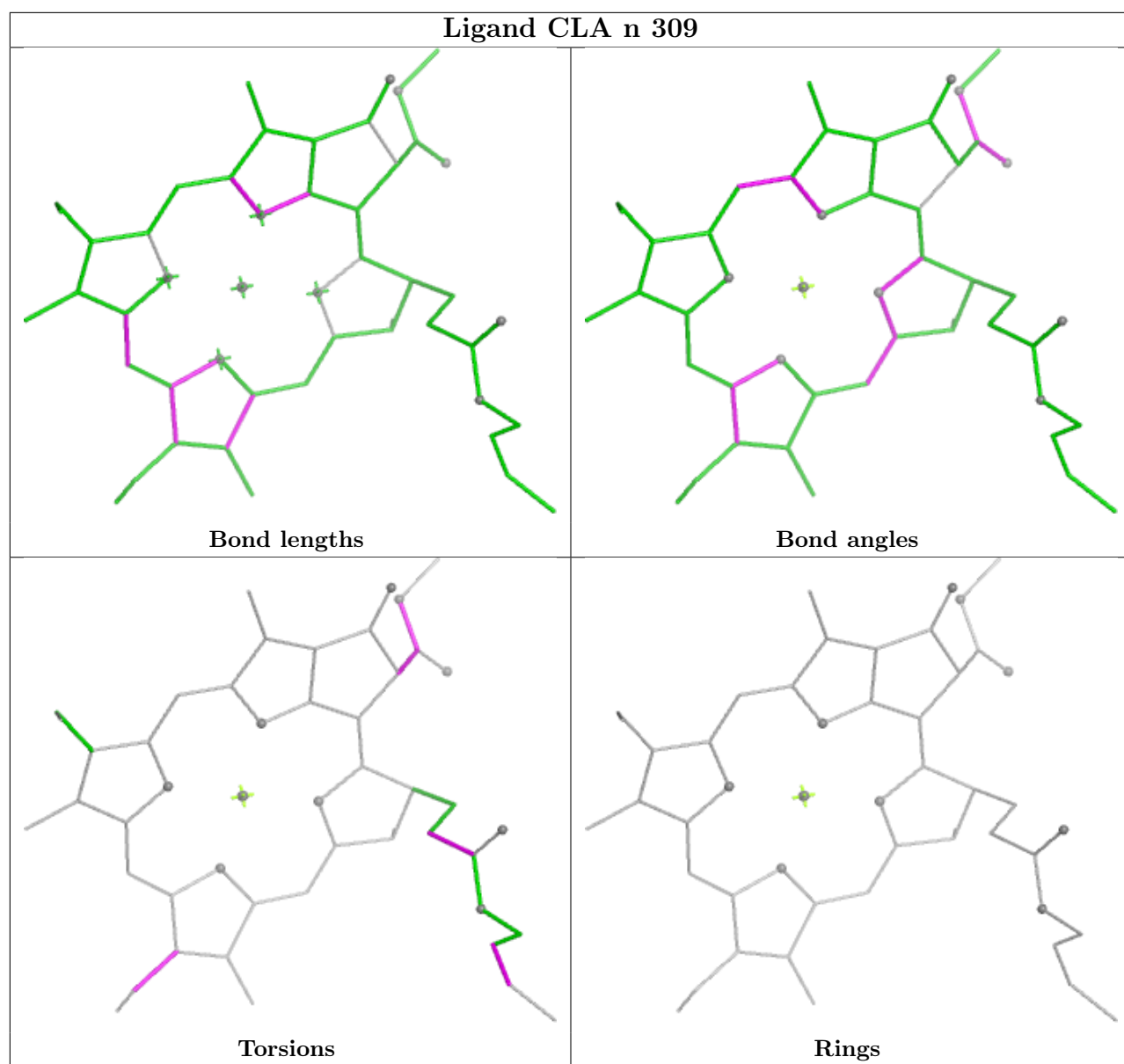
Ligand CHL R 315

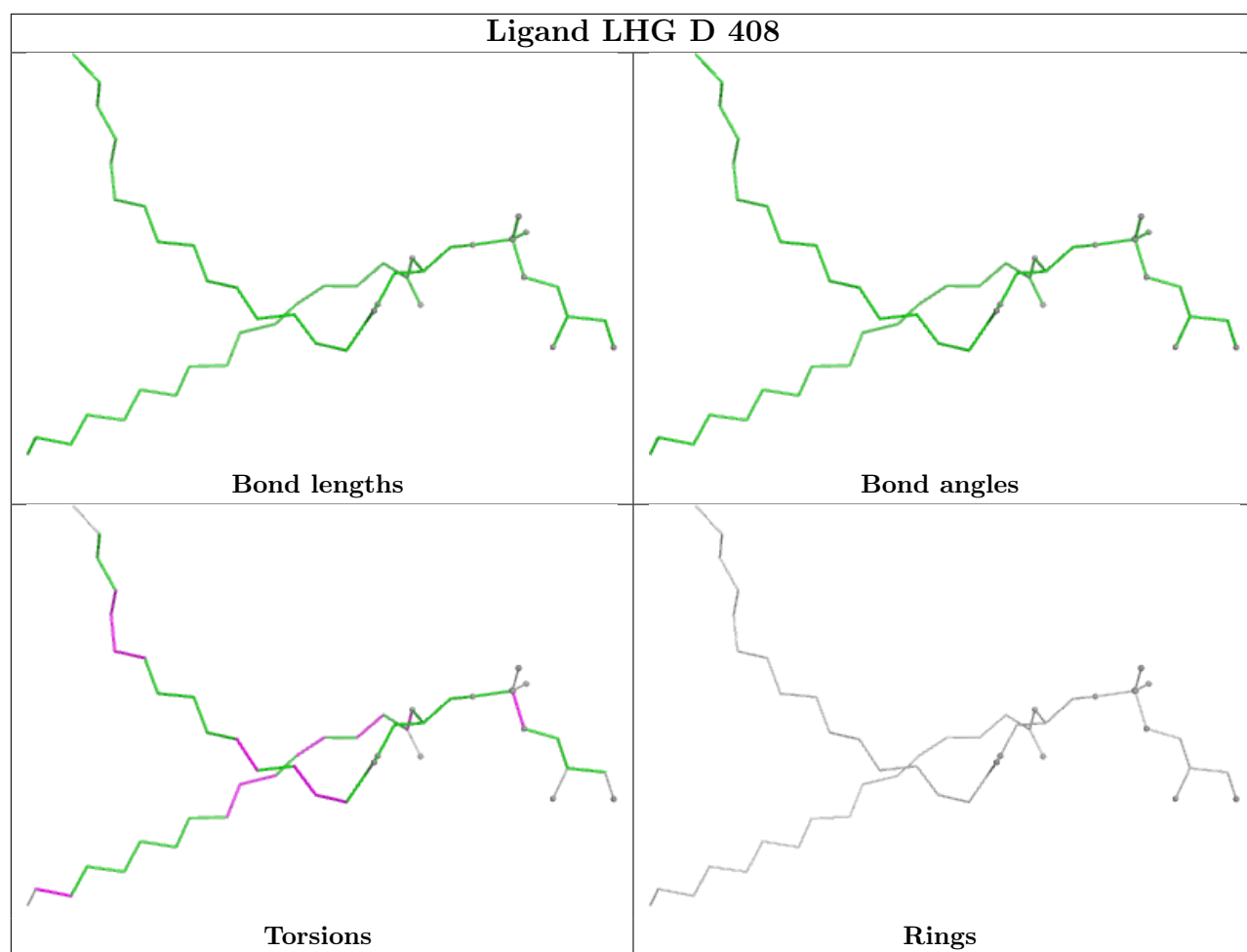


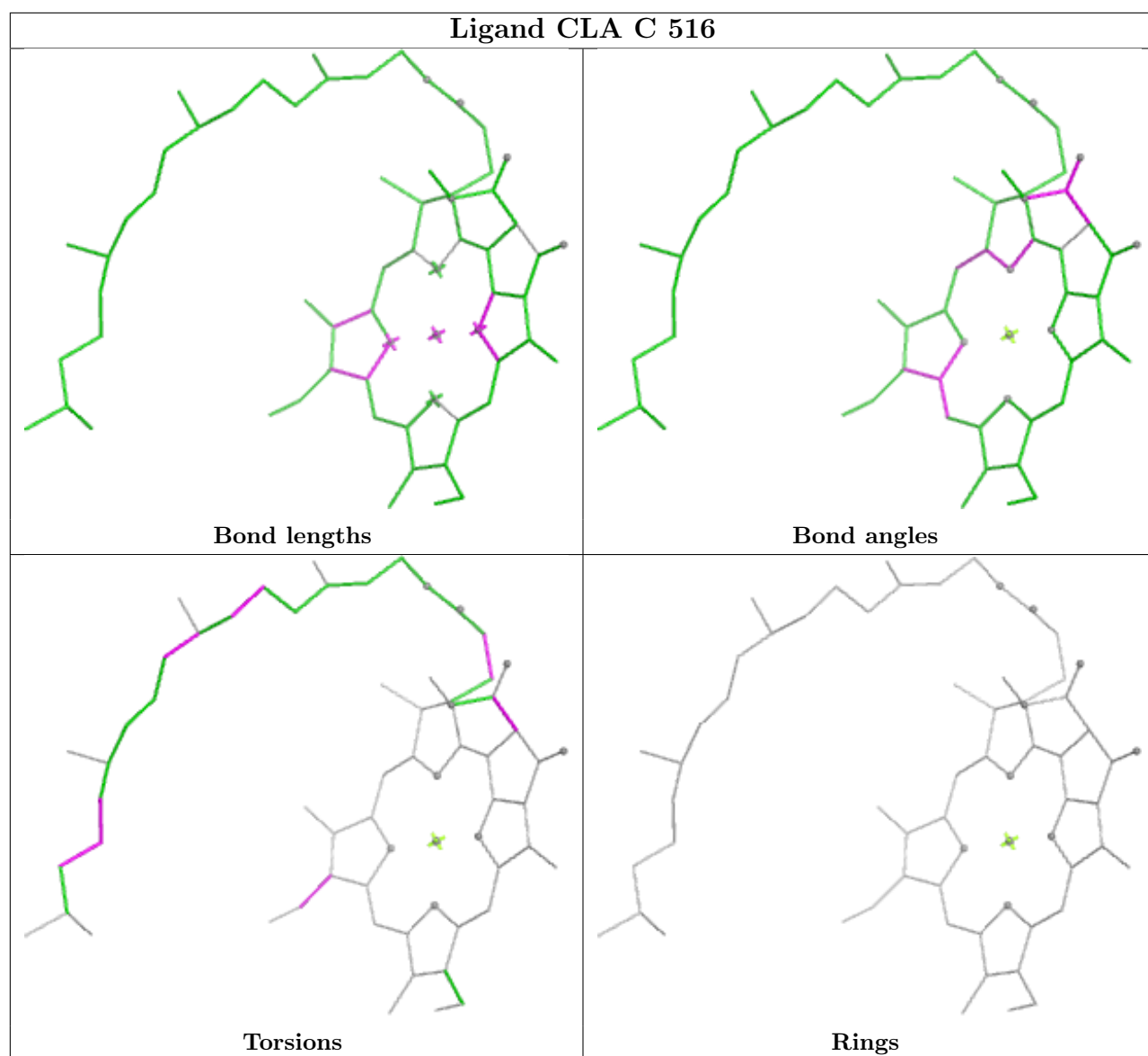


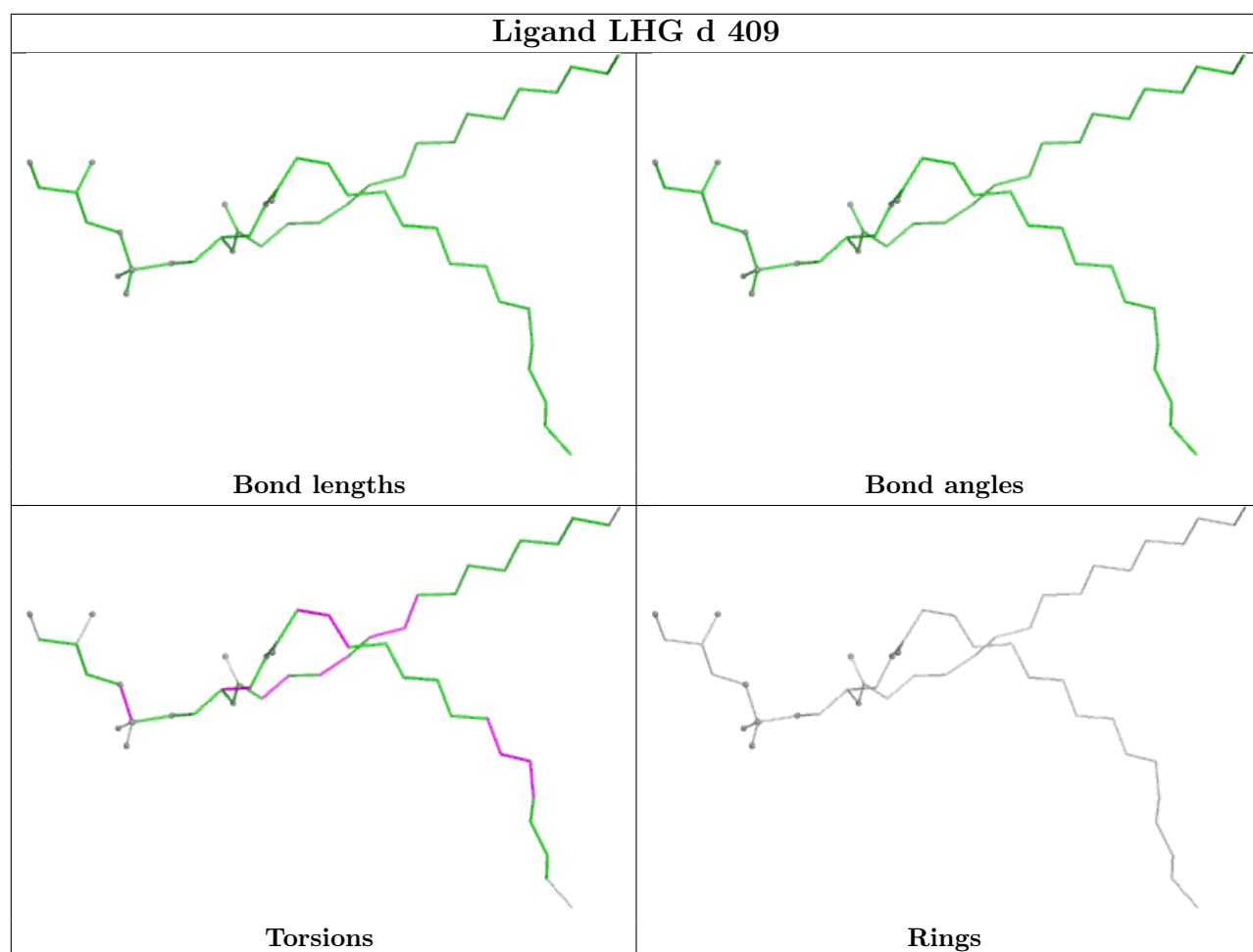


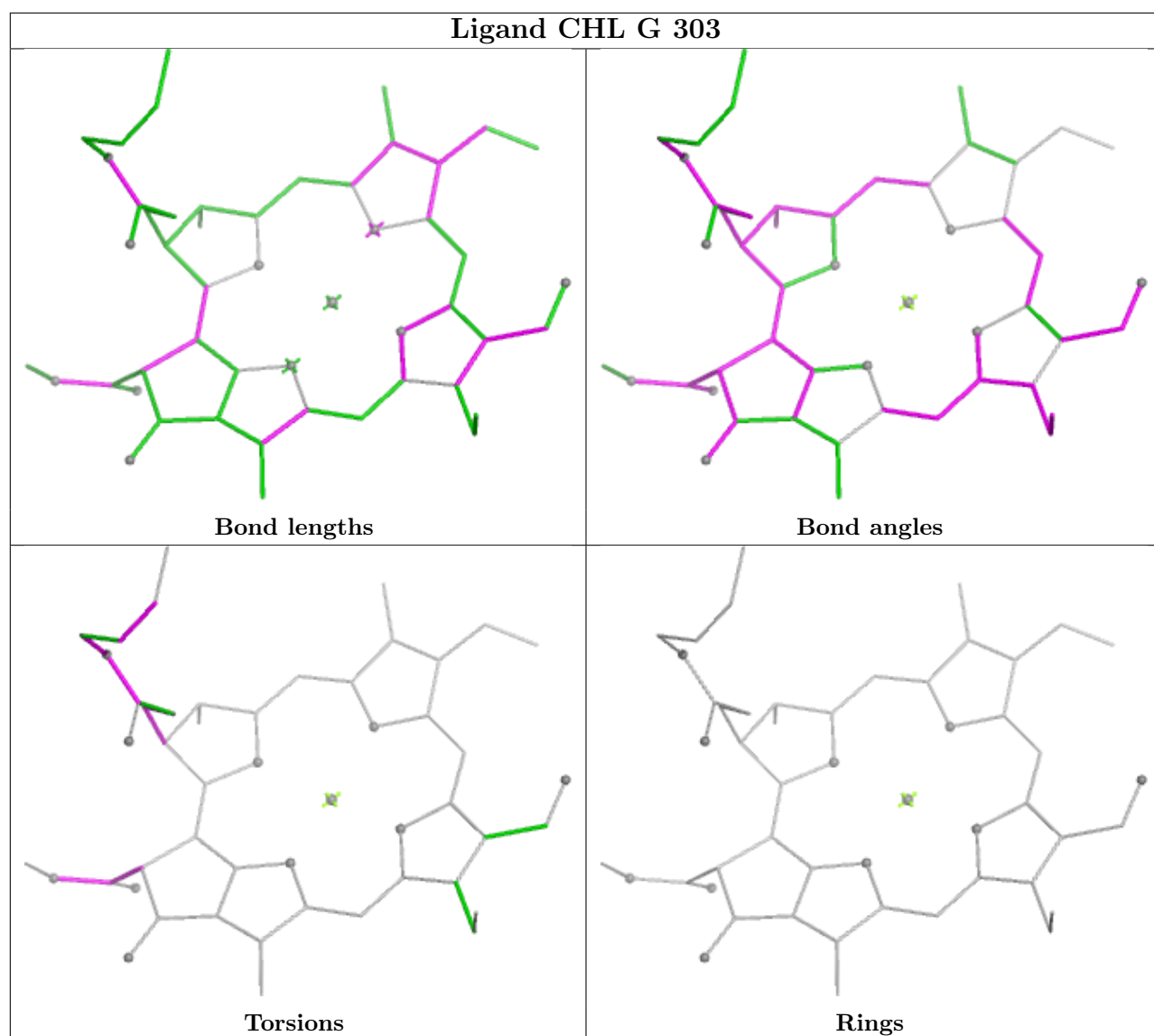


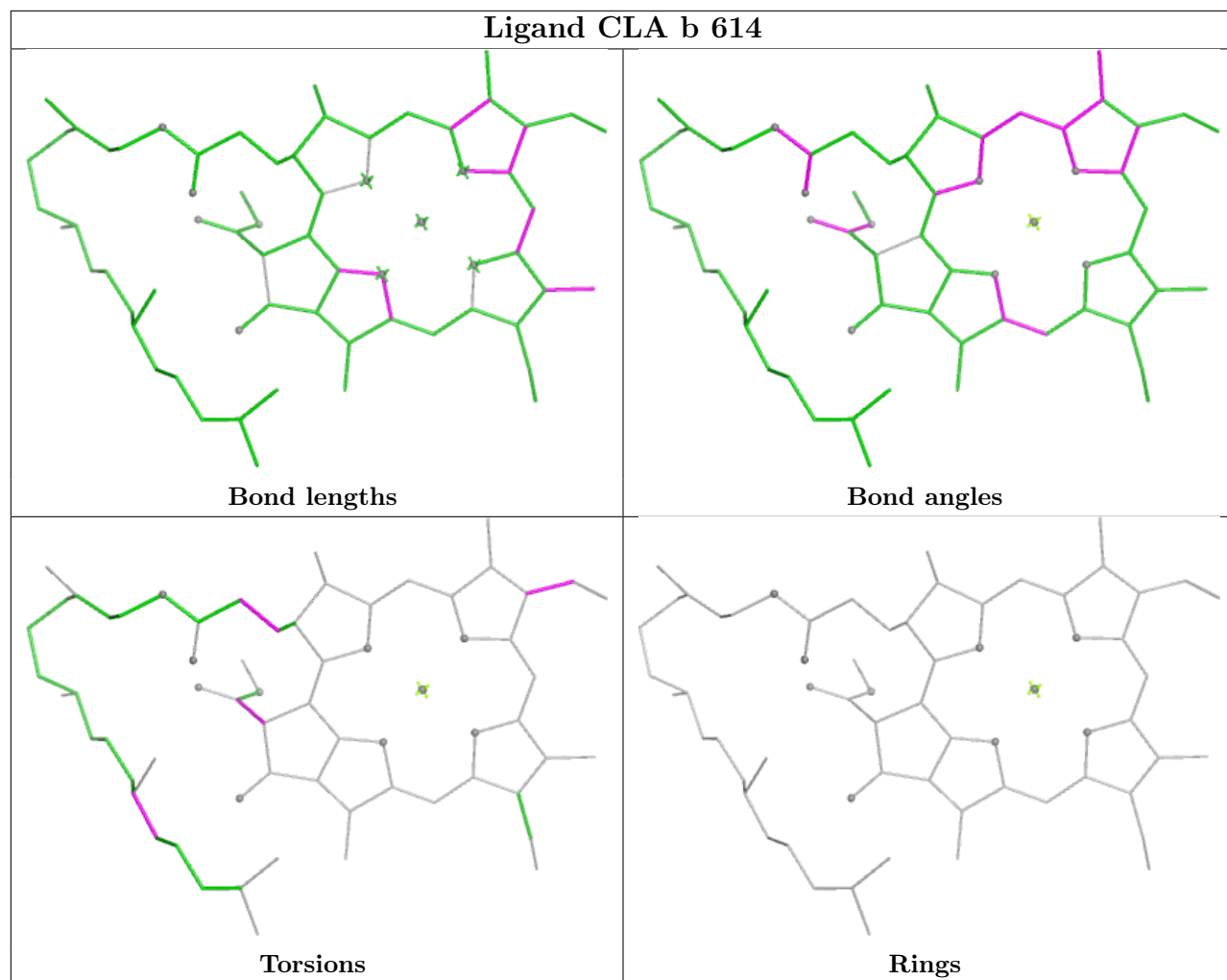




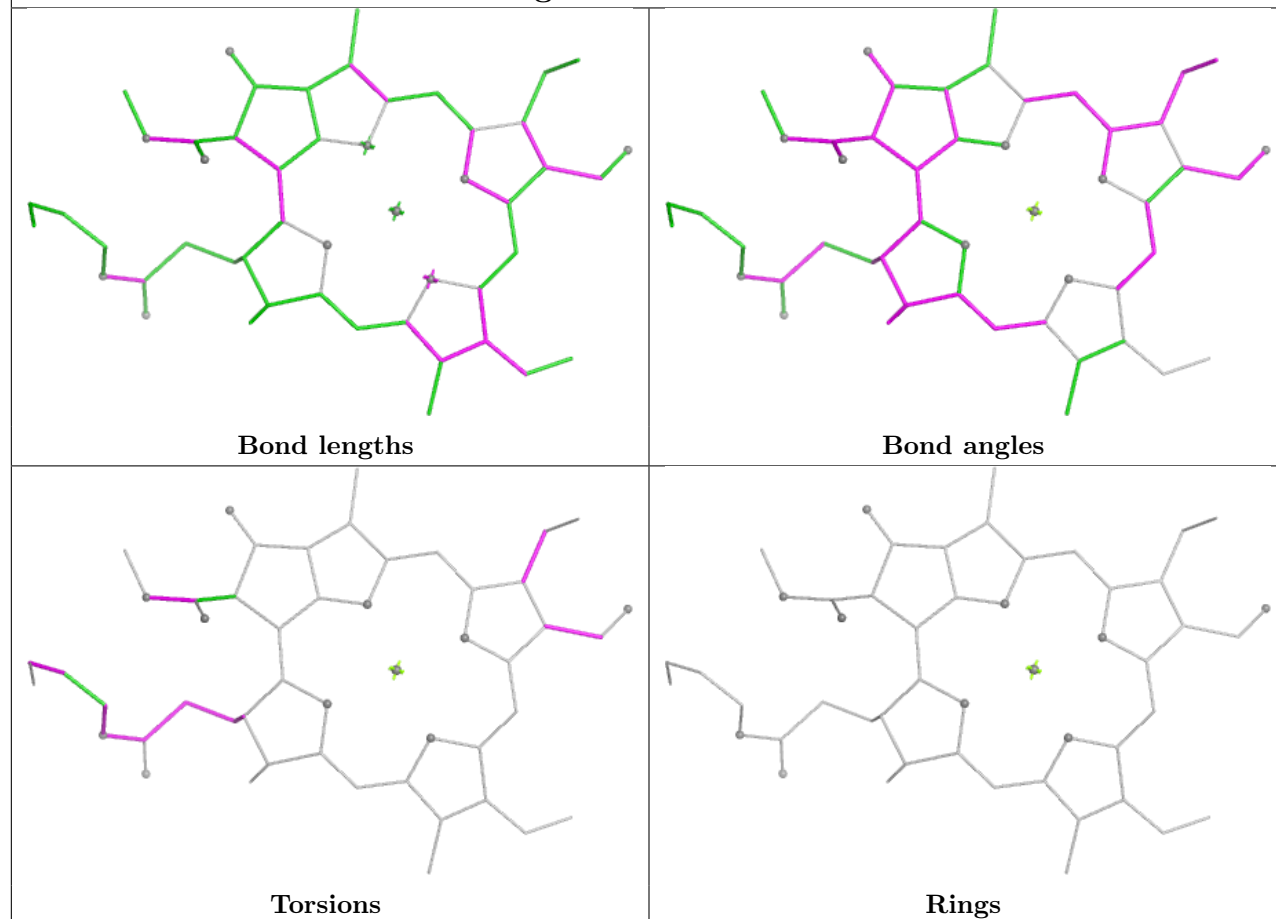




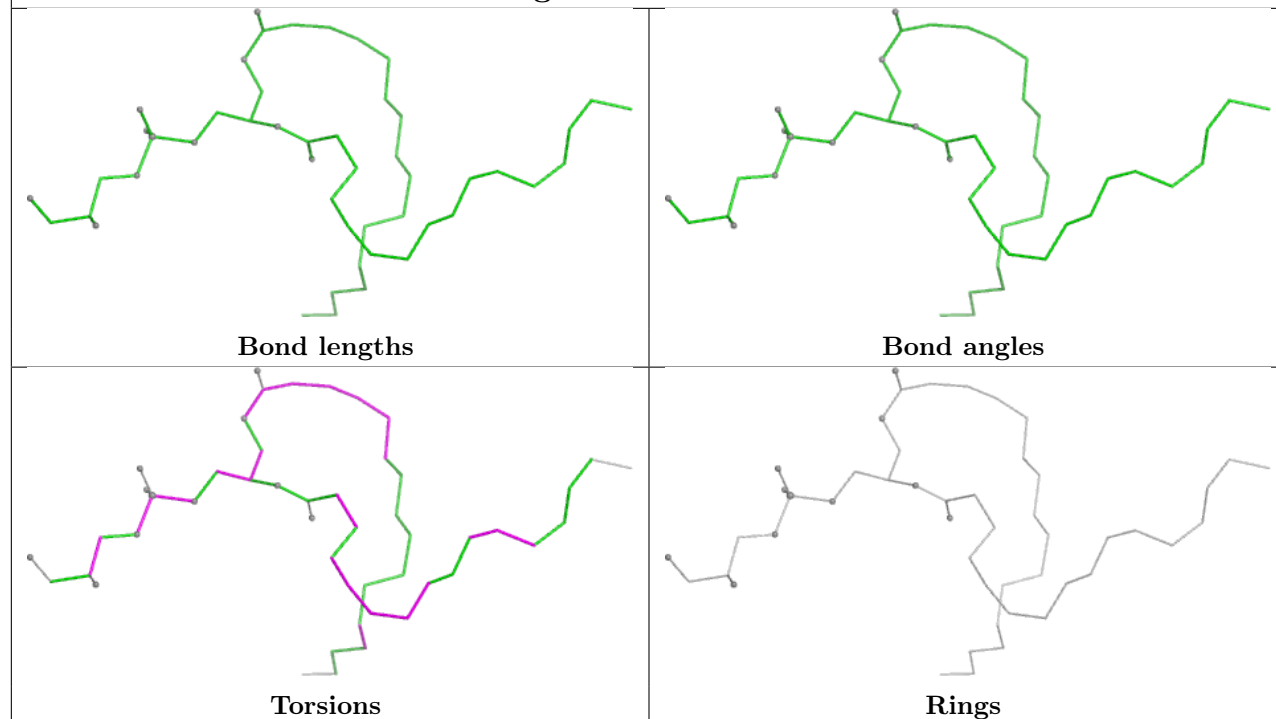


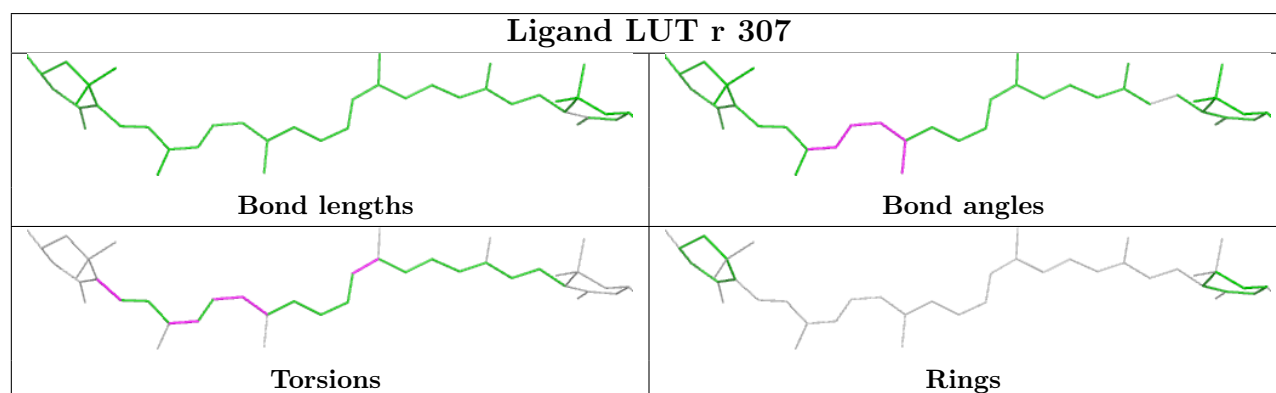
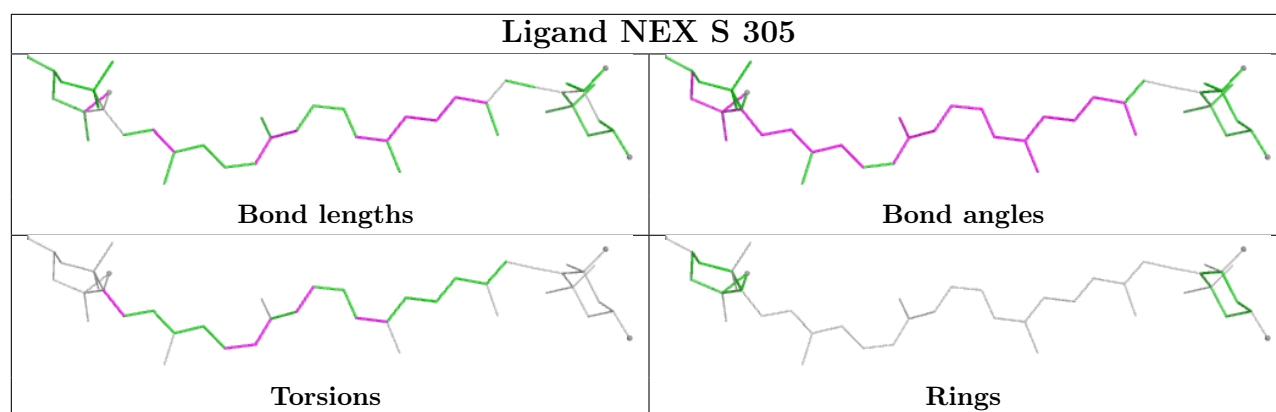


Ligand CHL S 302

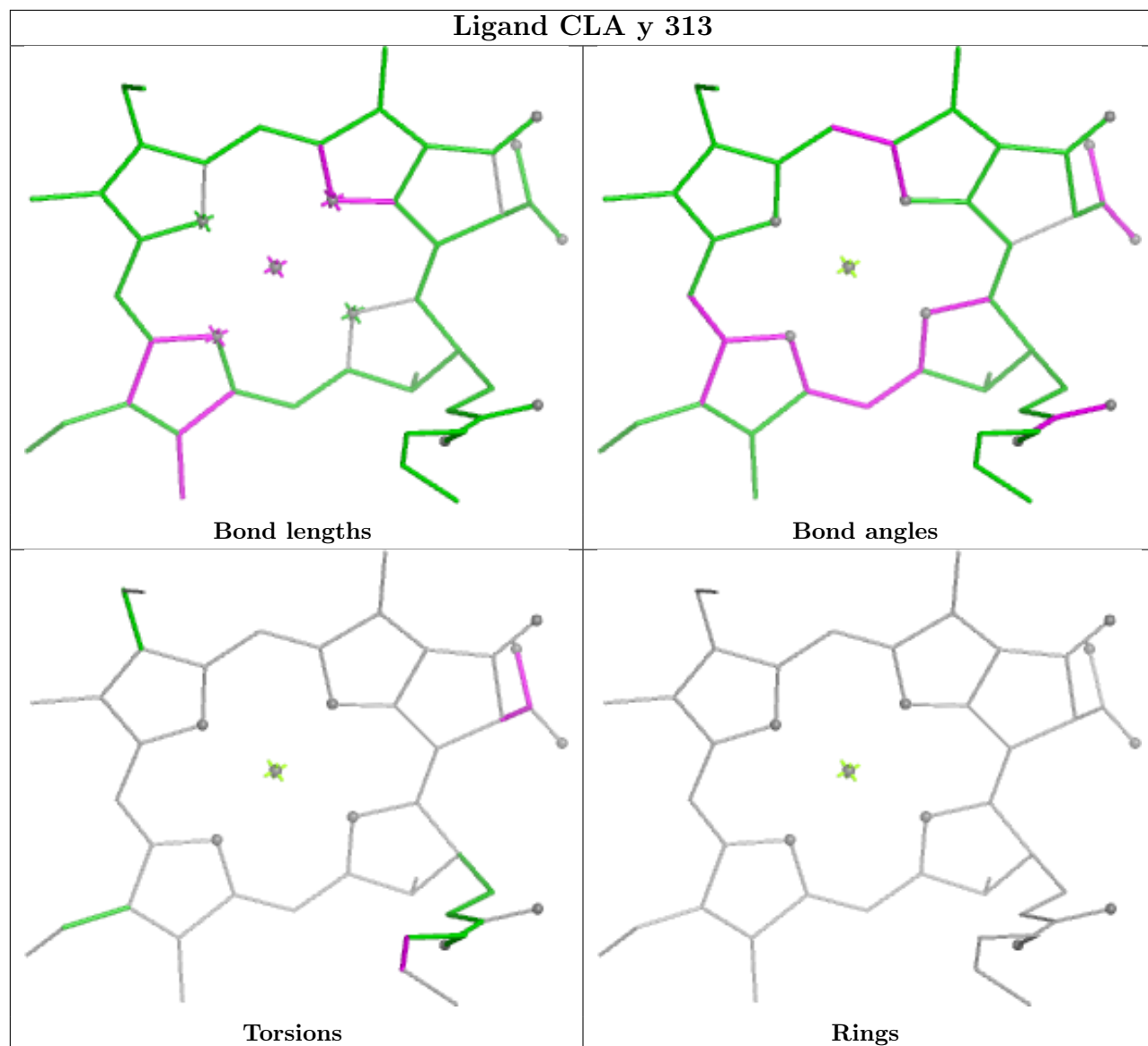


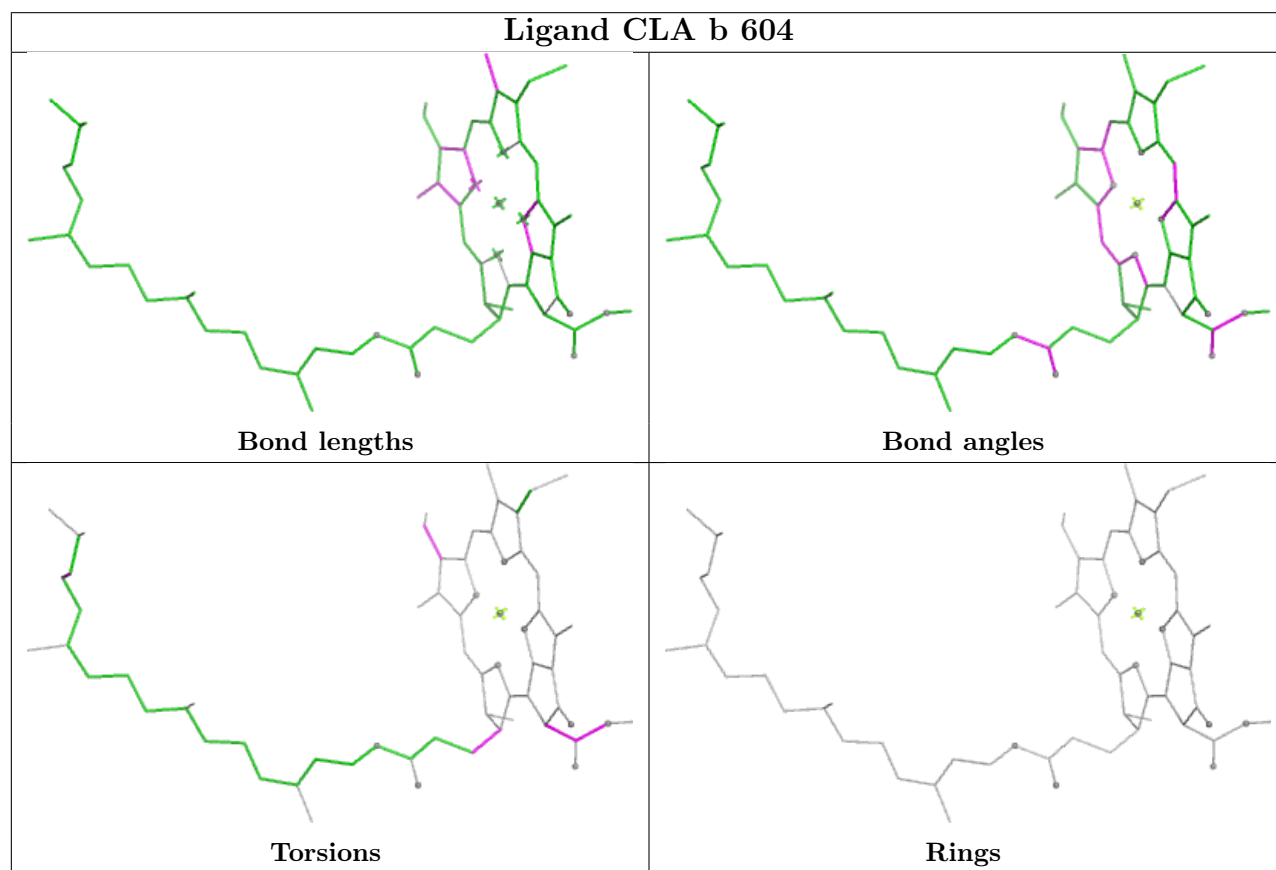
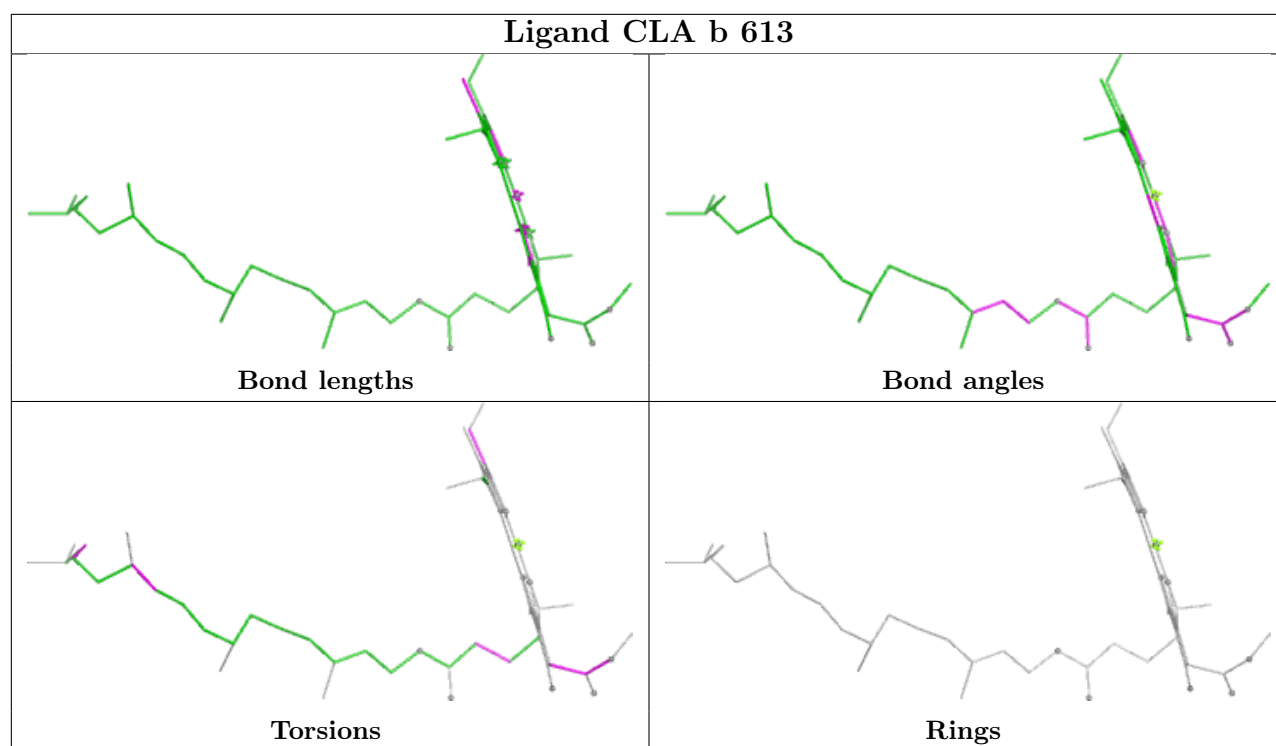
Ligand LHG S 317

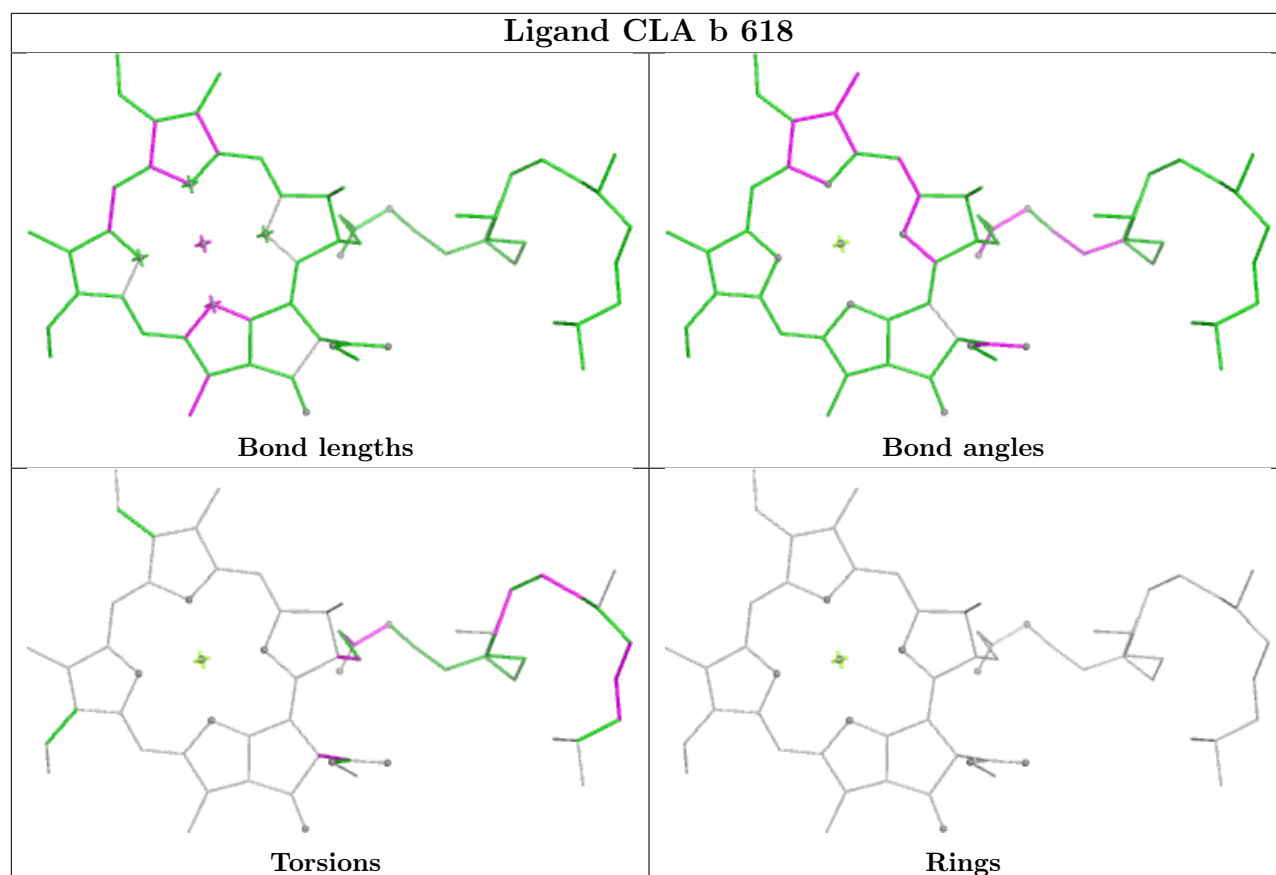
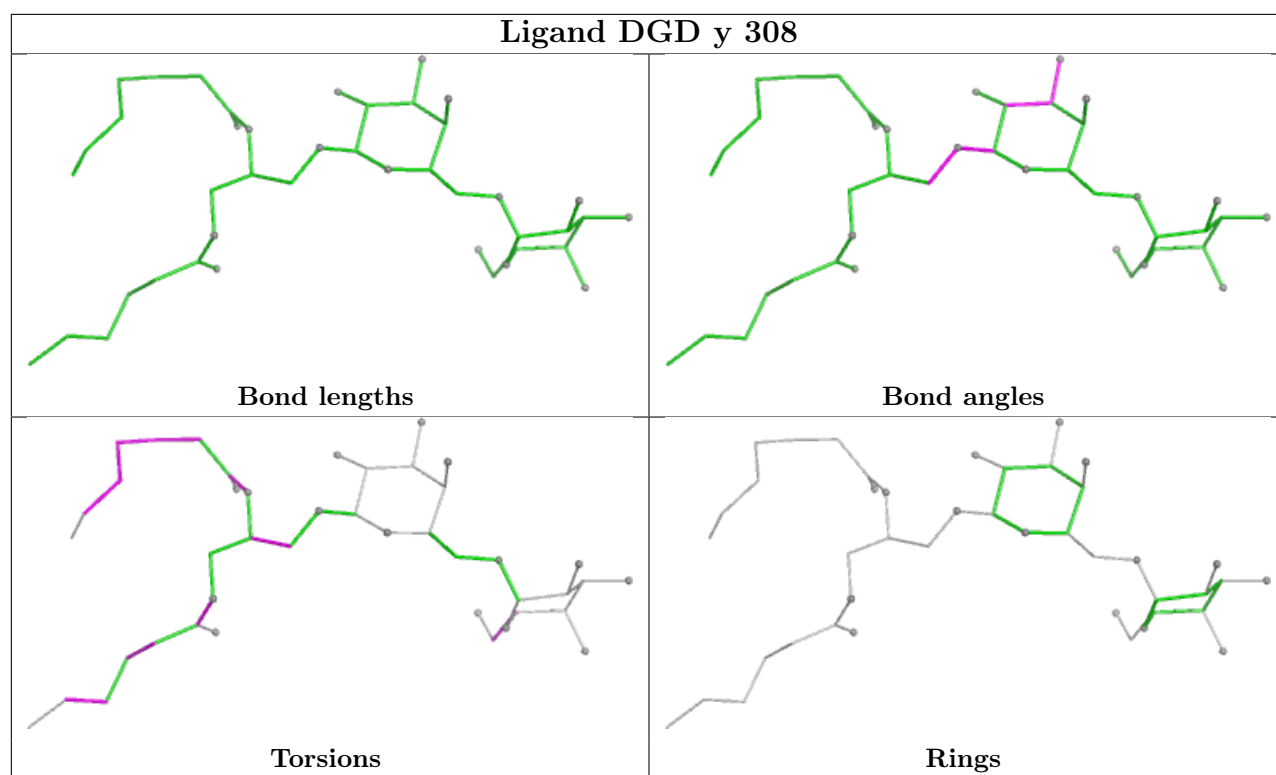


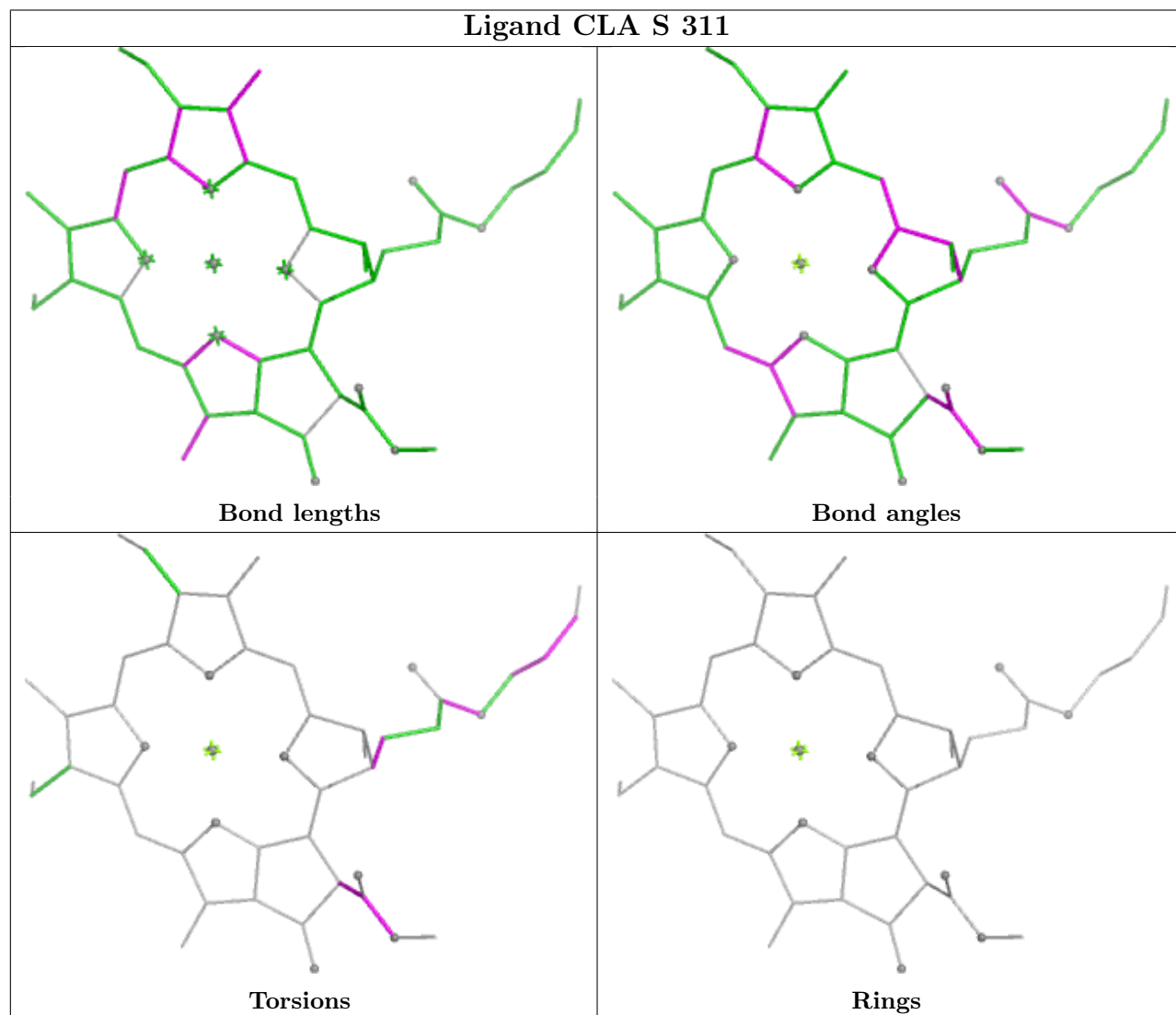
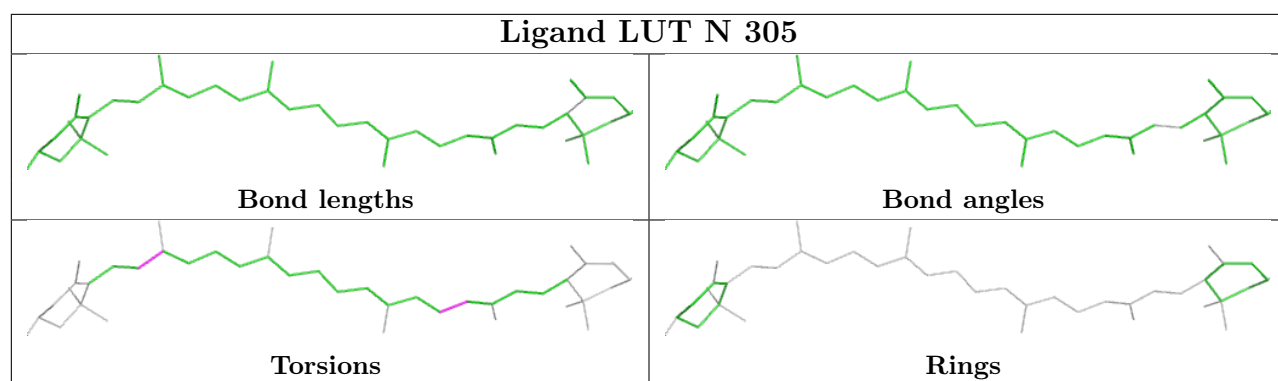


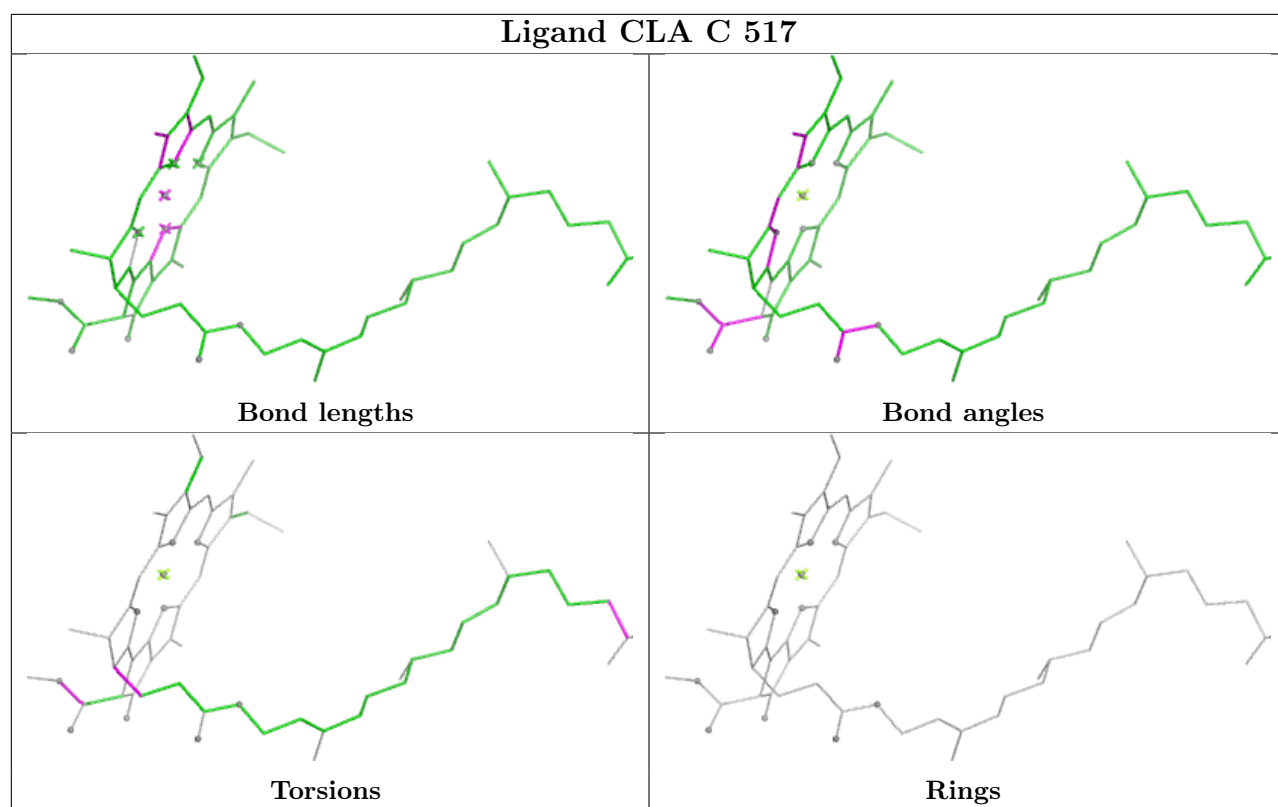
Ligand CLA y 313

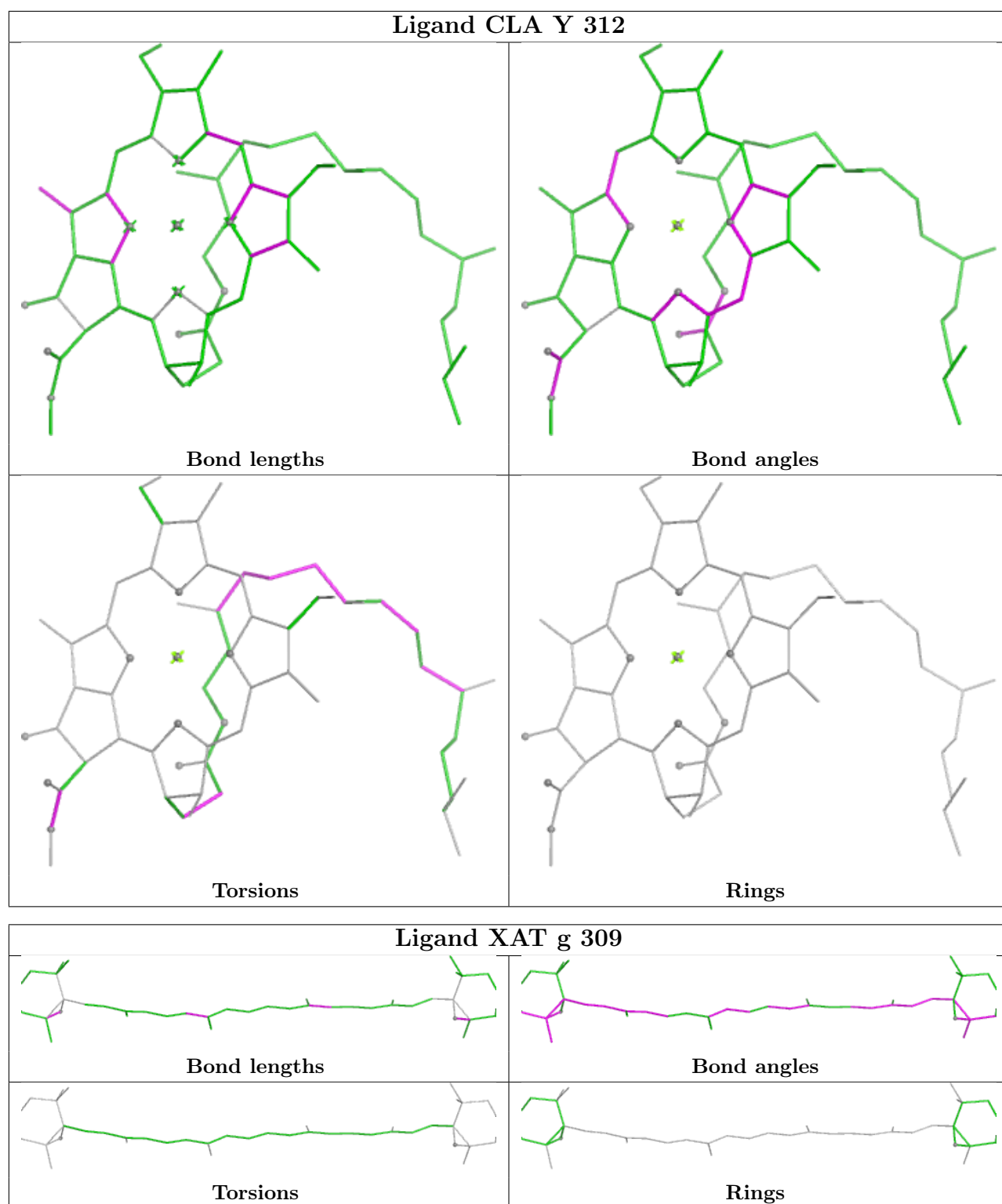


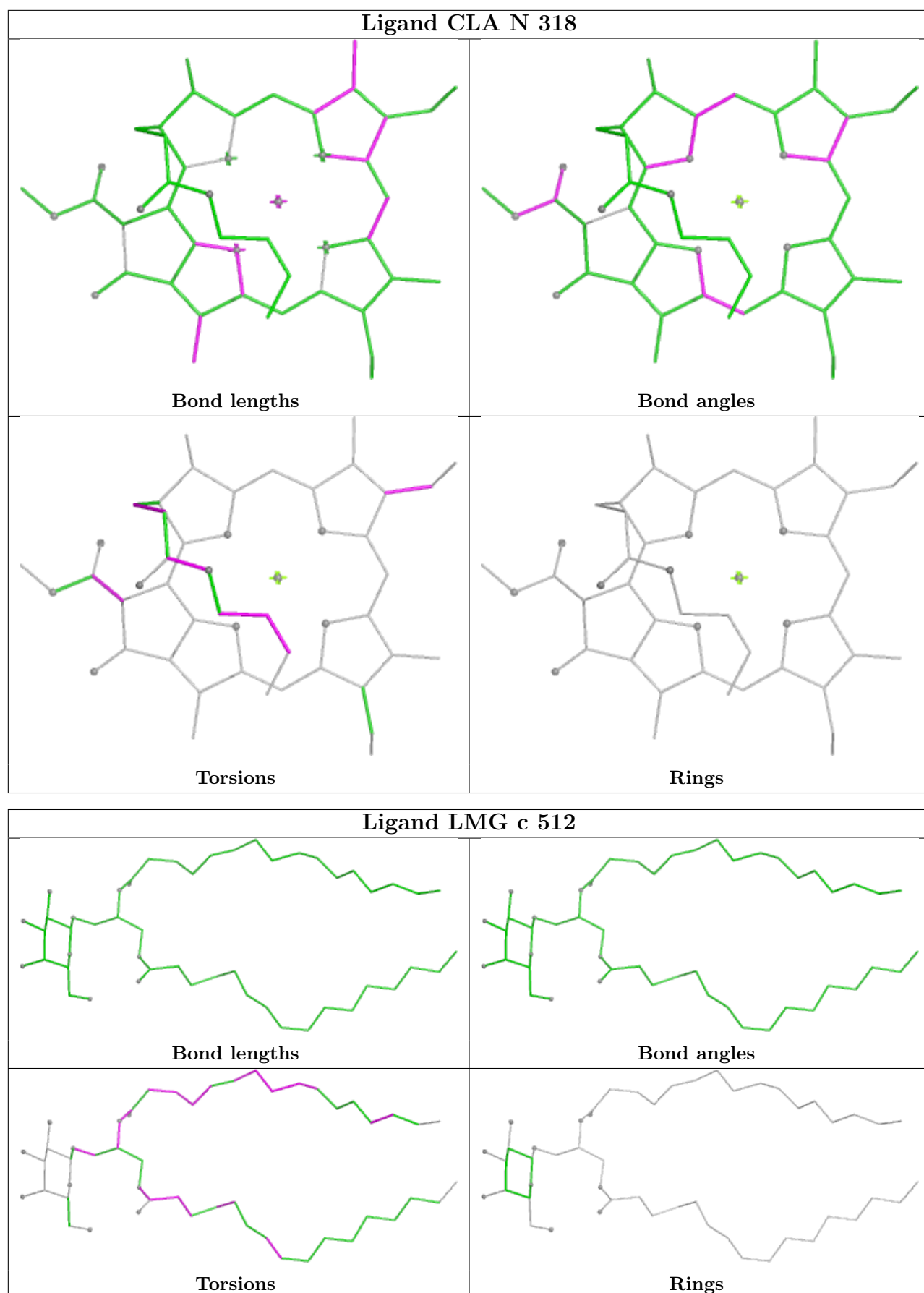


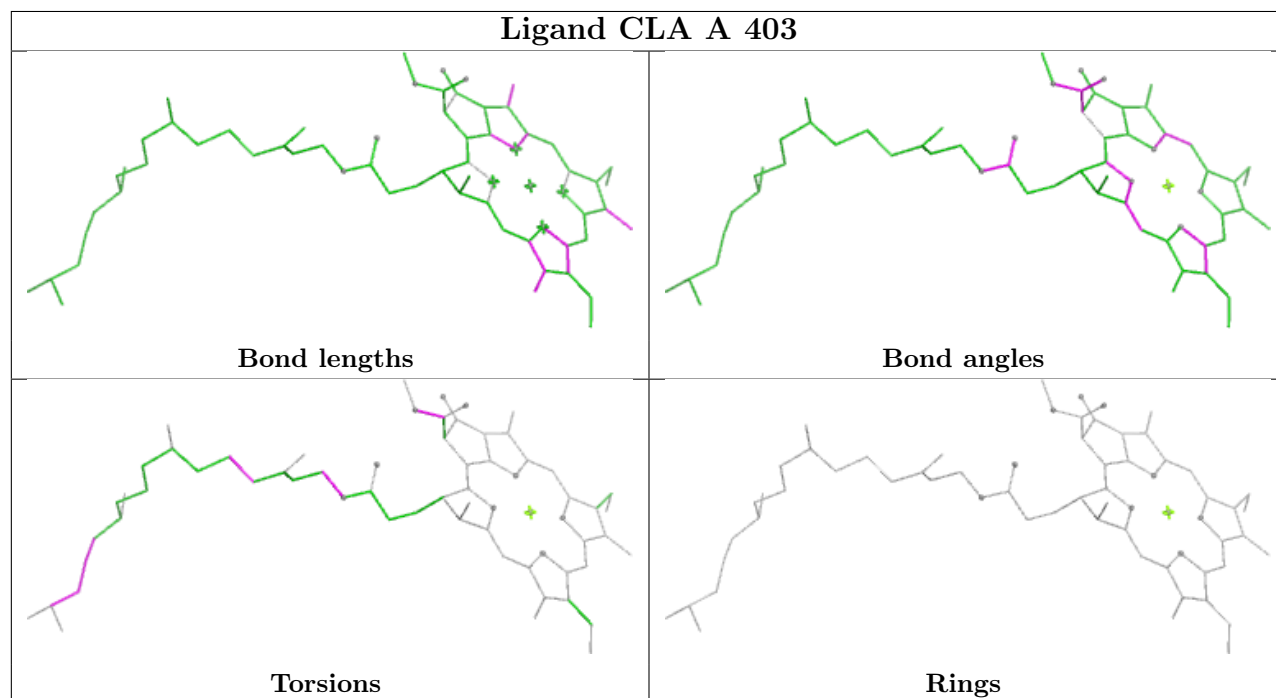
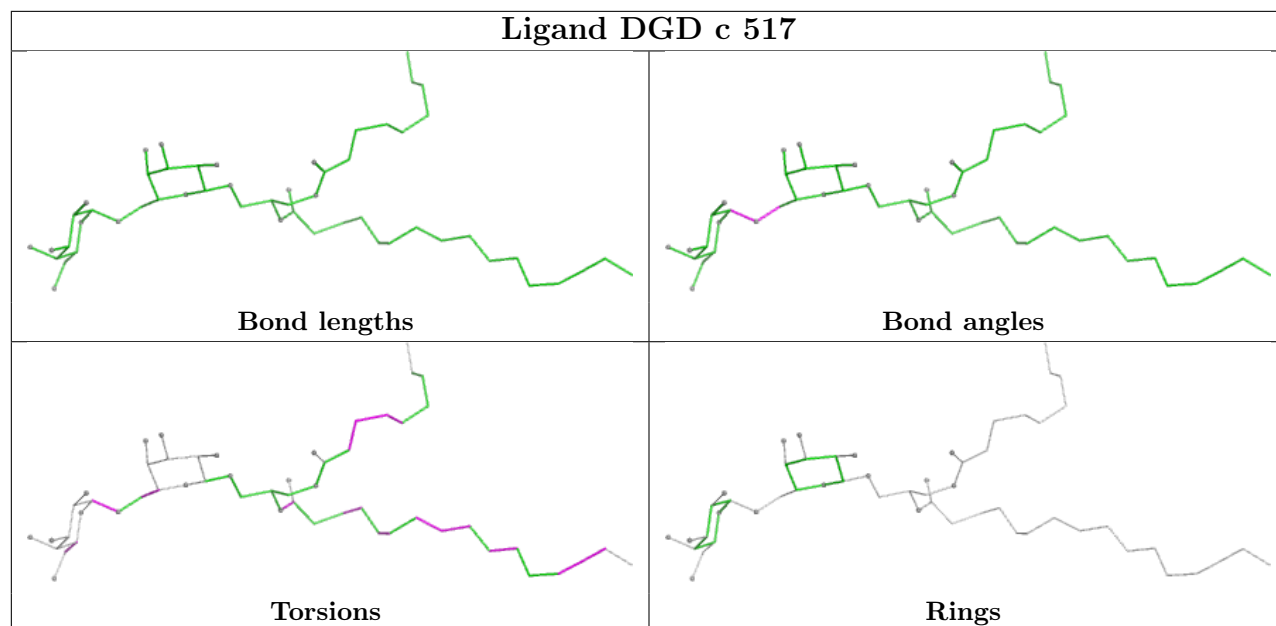


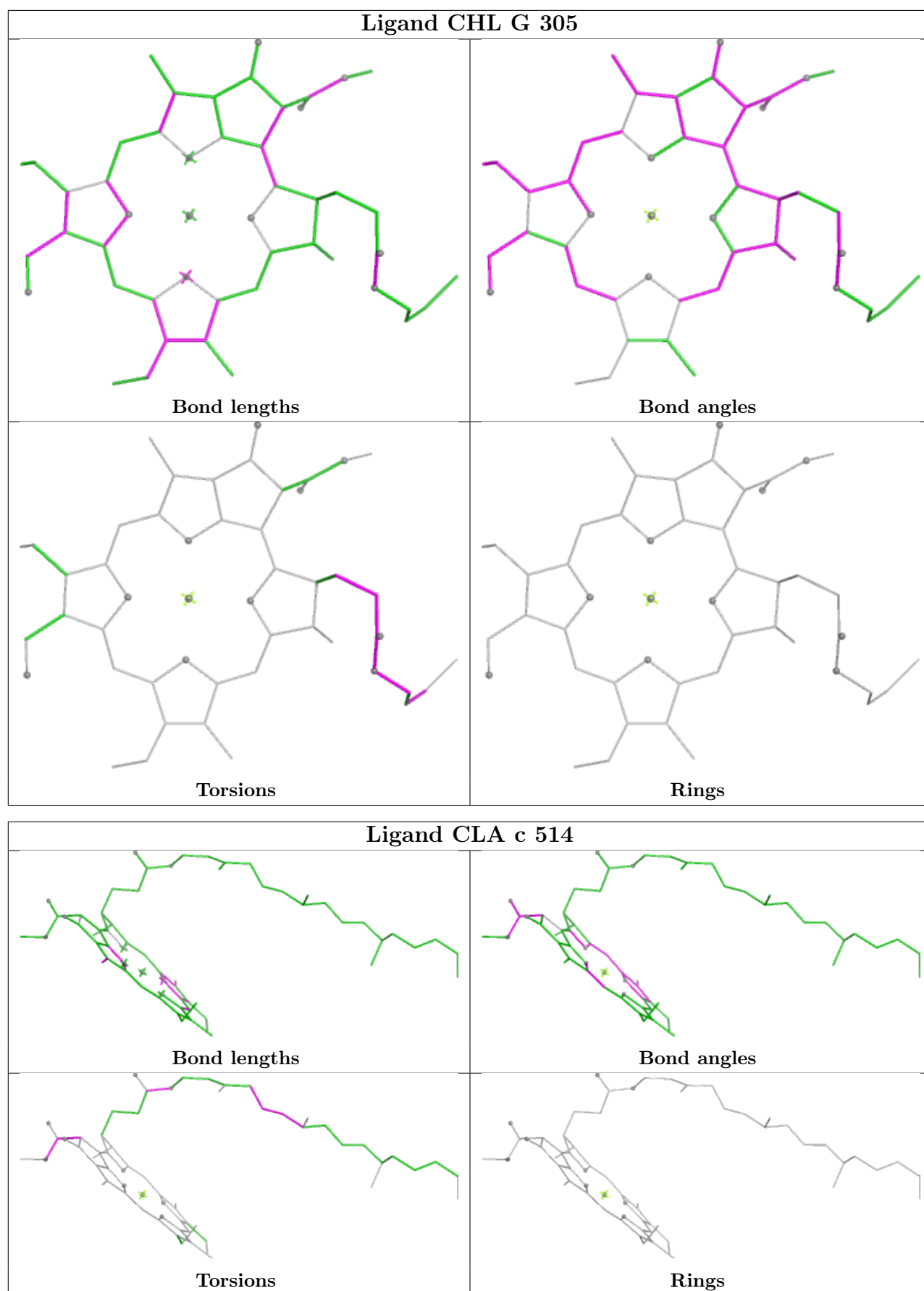


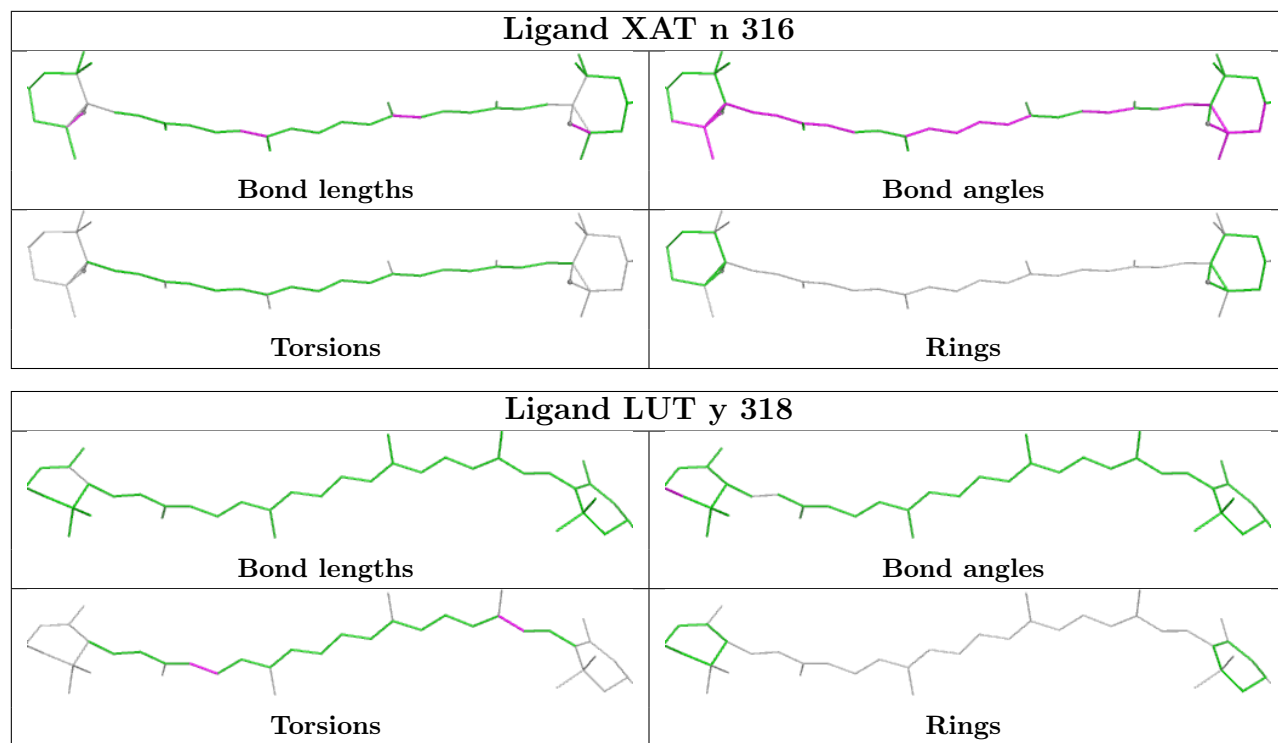


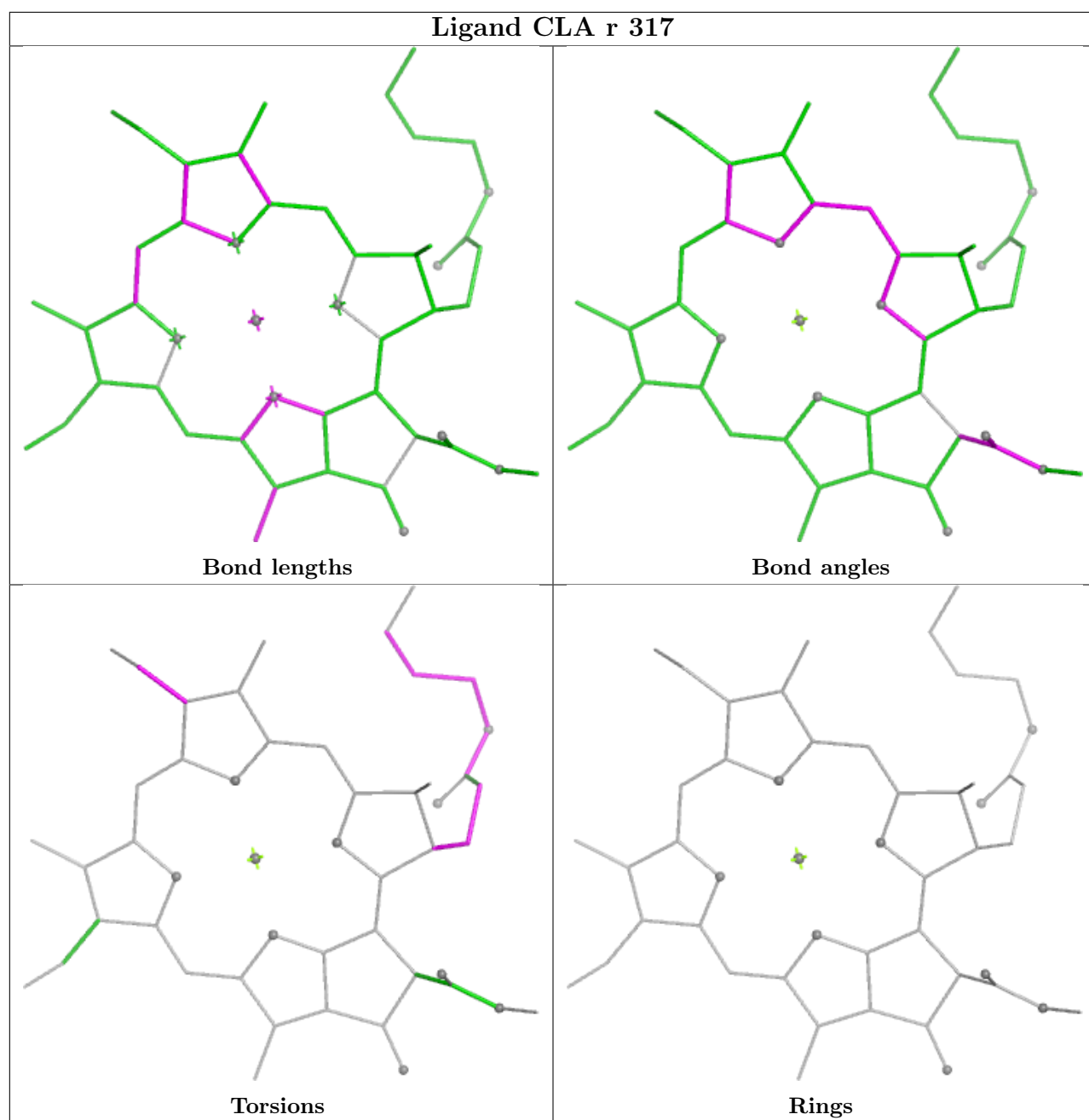




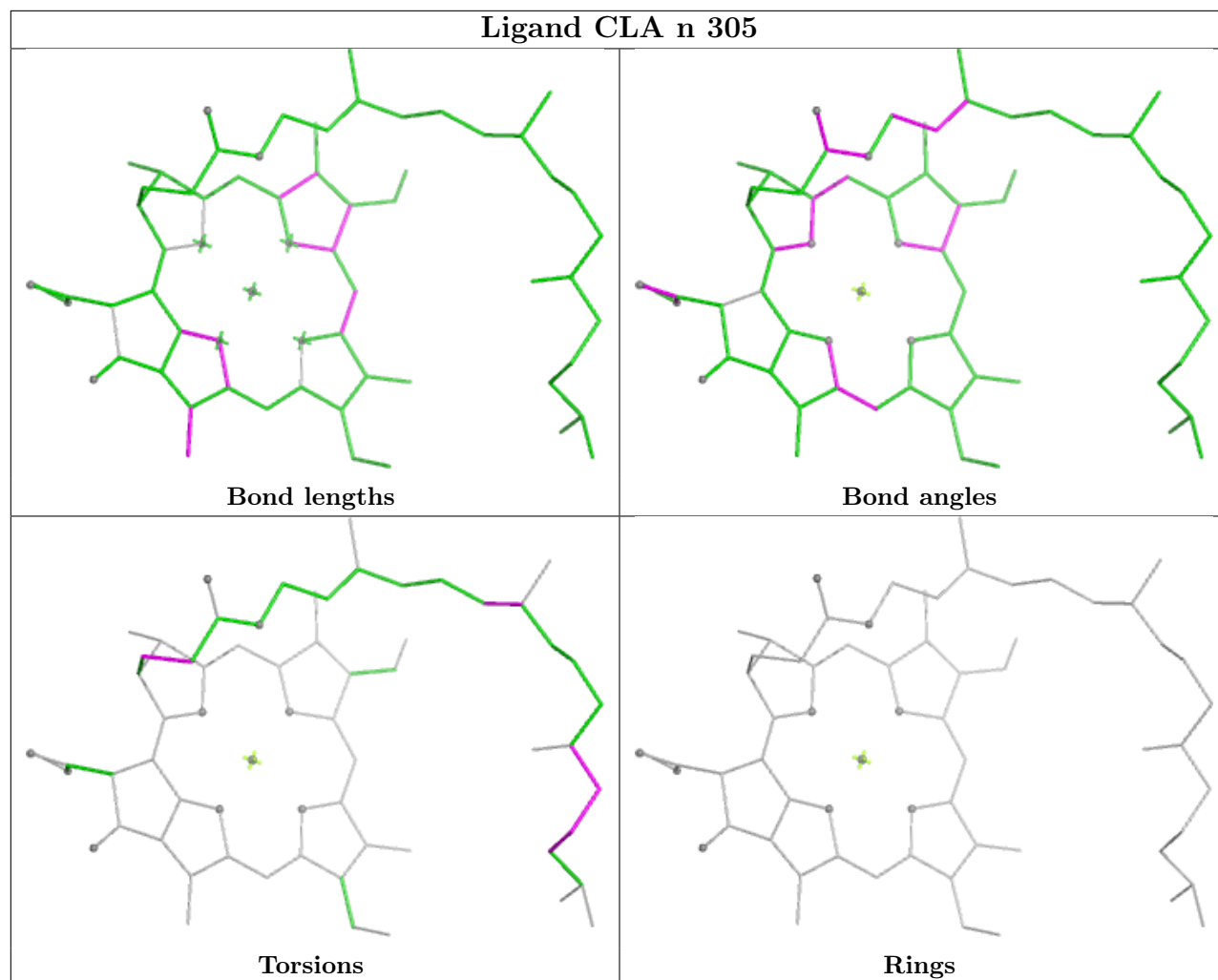




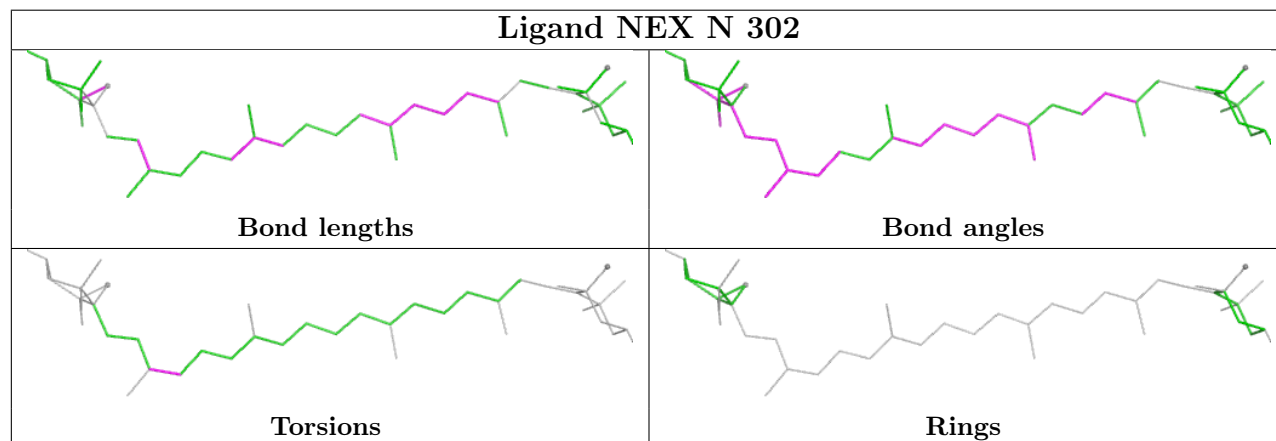




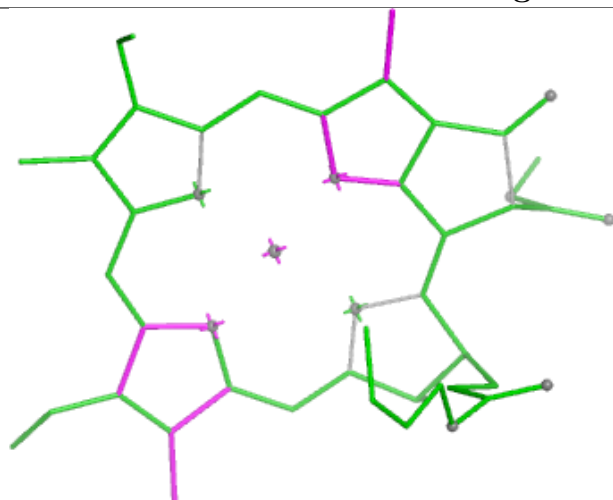
Ligand CLA n 305



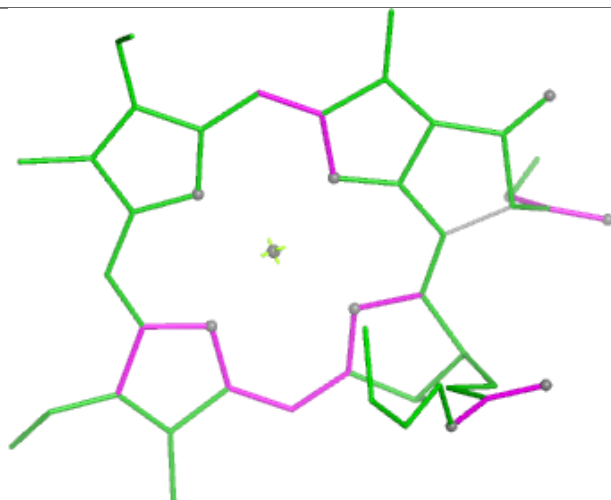
Ligand NEX N 302



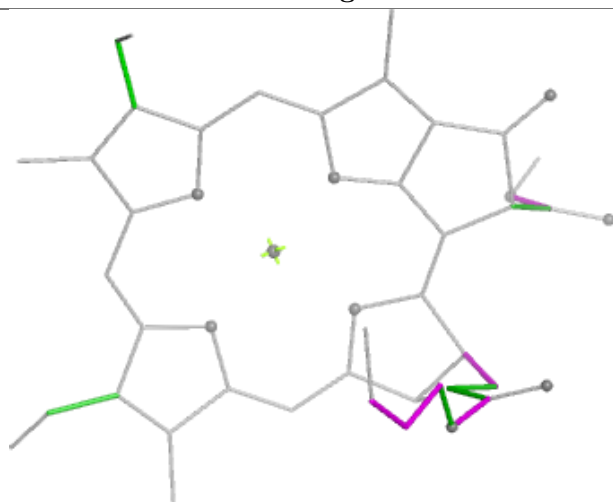
Ligand CLA N 308



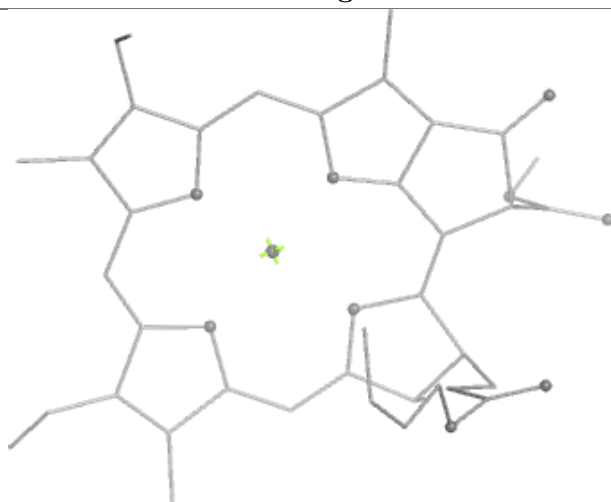
Bond lengths



Bond angles

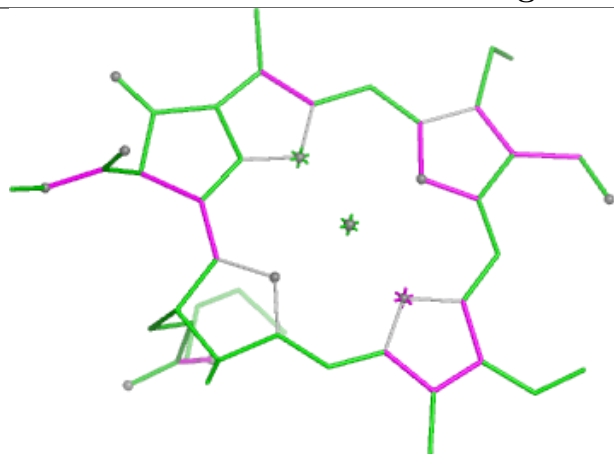


Torsions

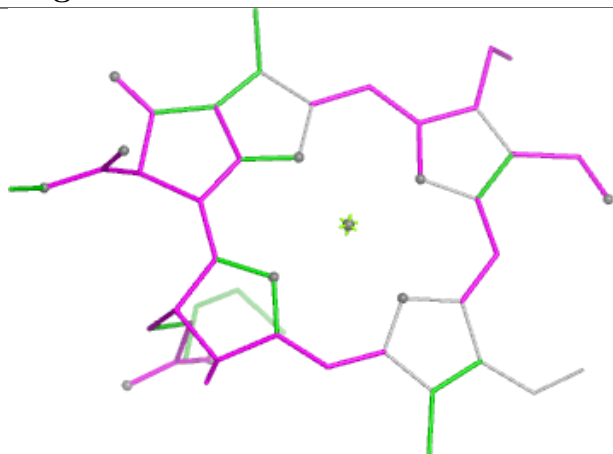


Rings

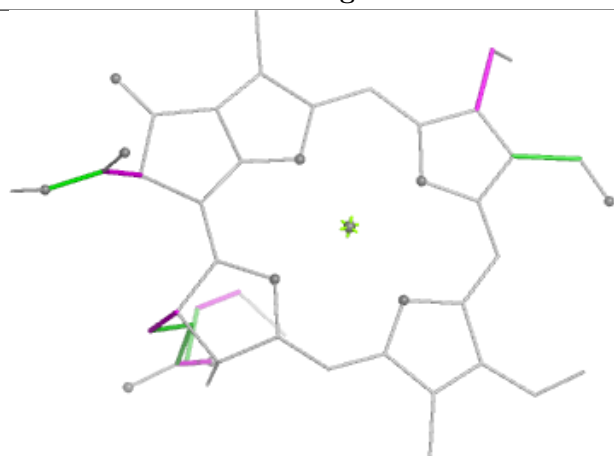
Ligand CHL g 312



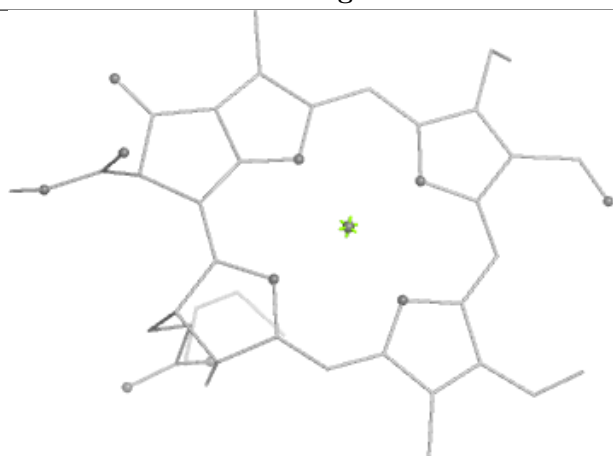
Bond lengths



Bond angles

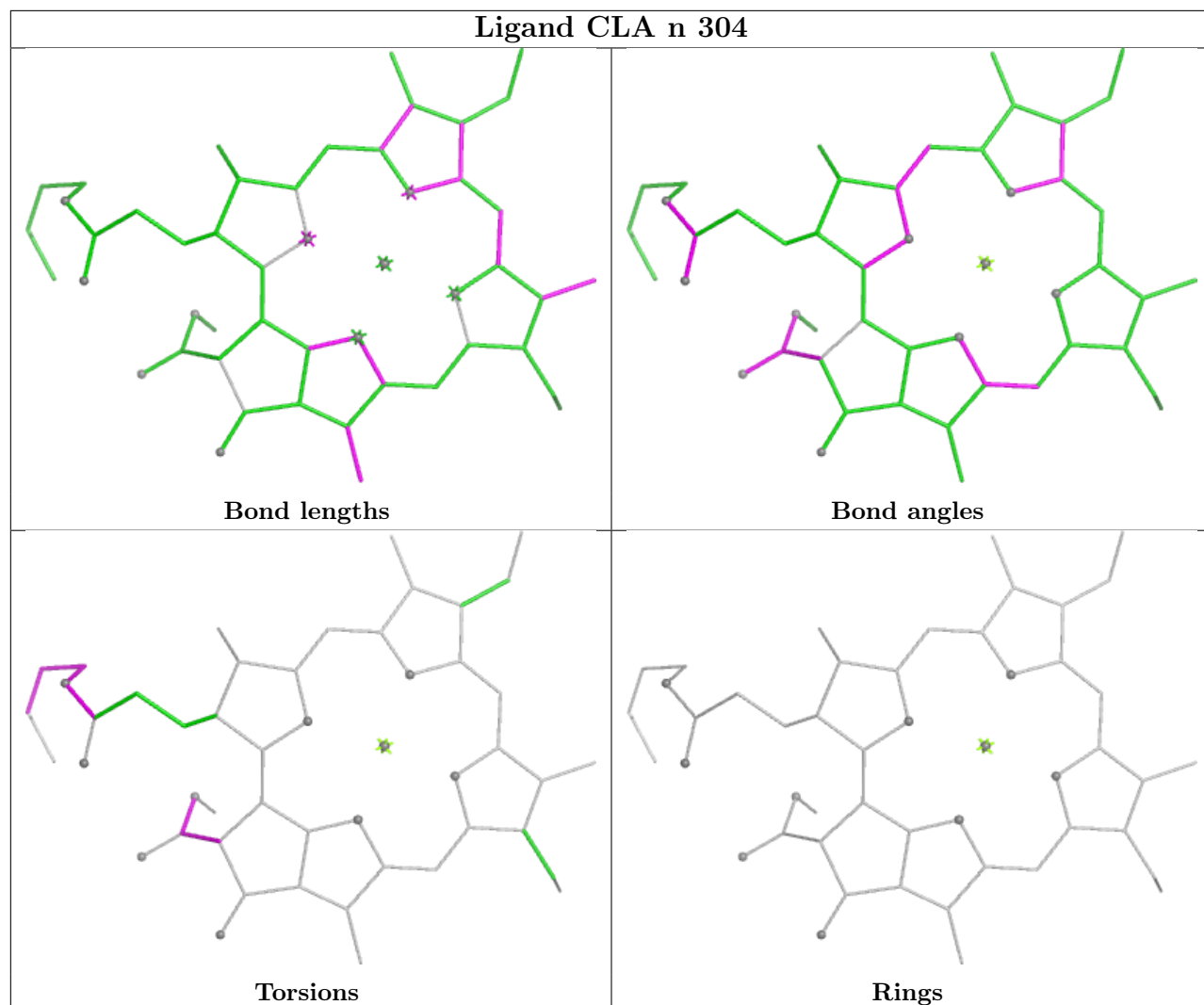


Torsions

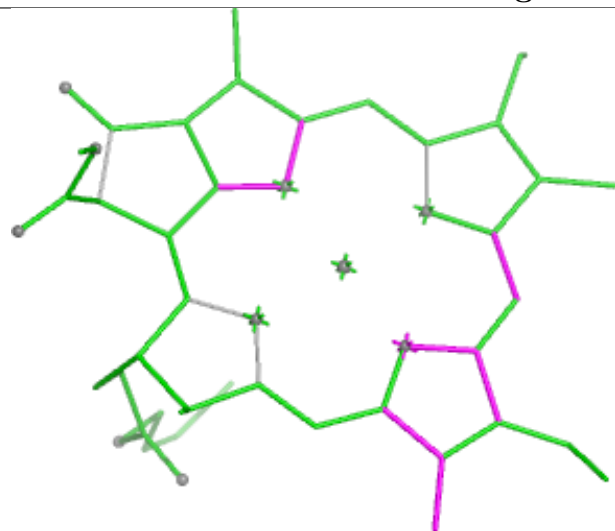


Rings

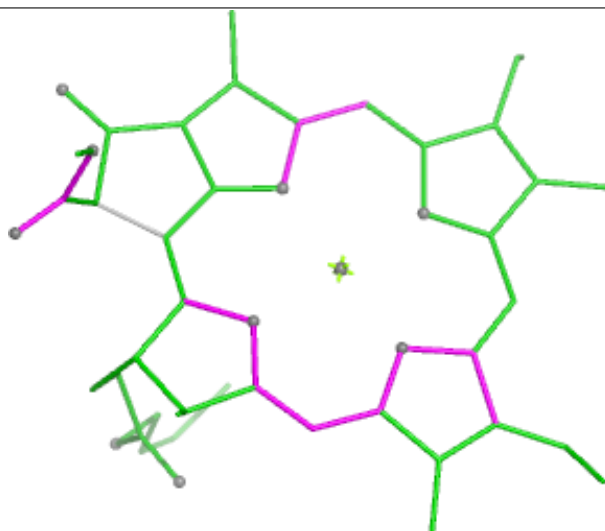
Ligand CLA n 304



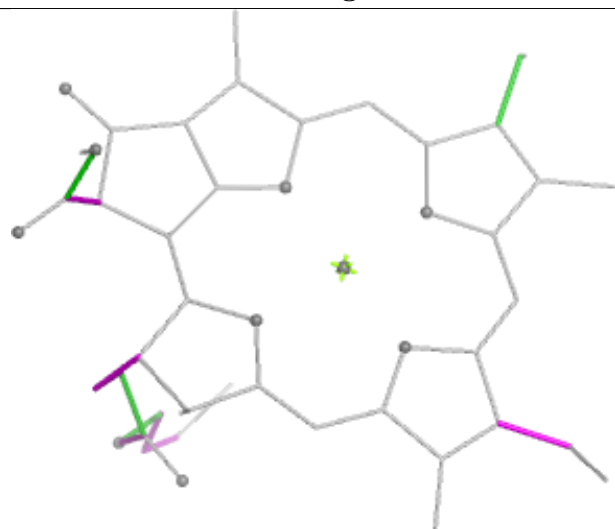
Ligand CLA G 302



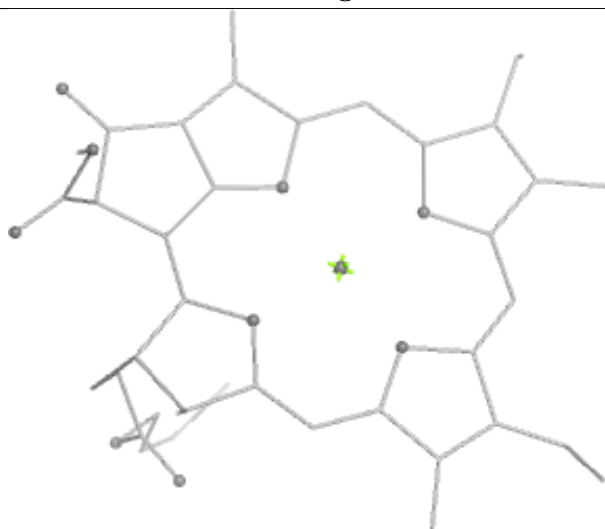
Bond lengths



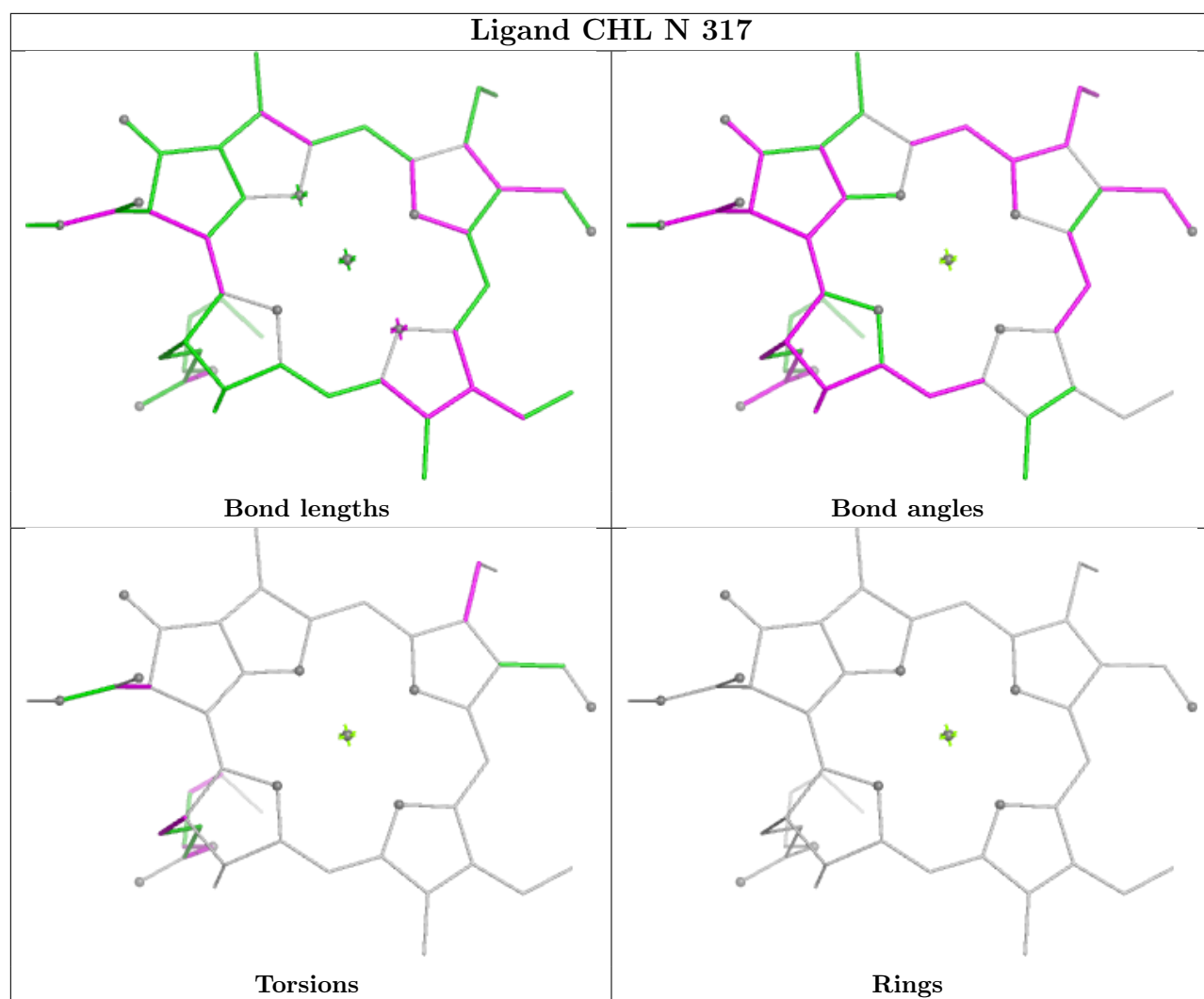
Bond angles



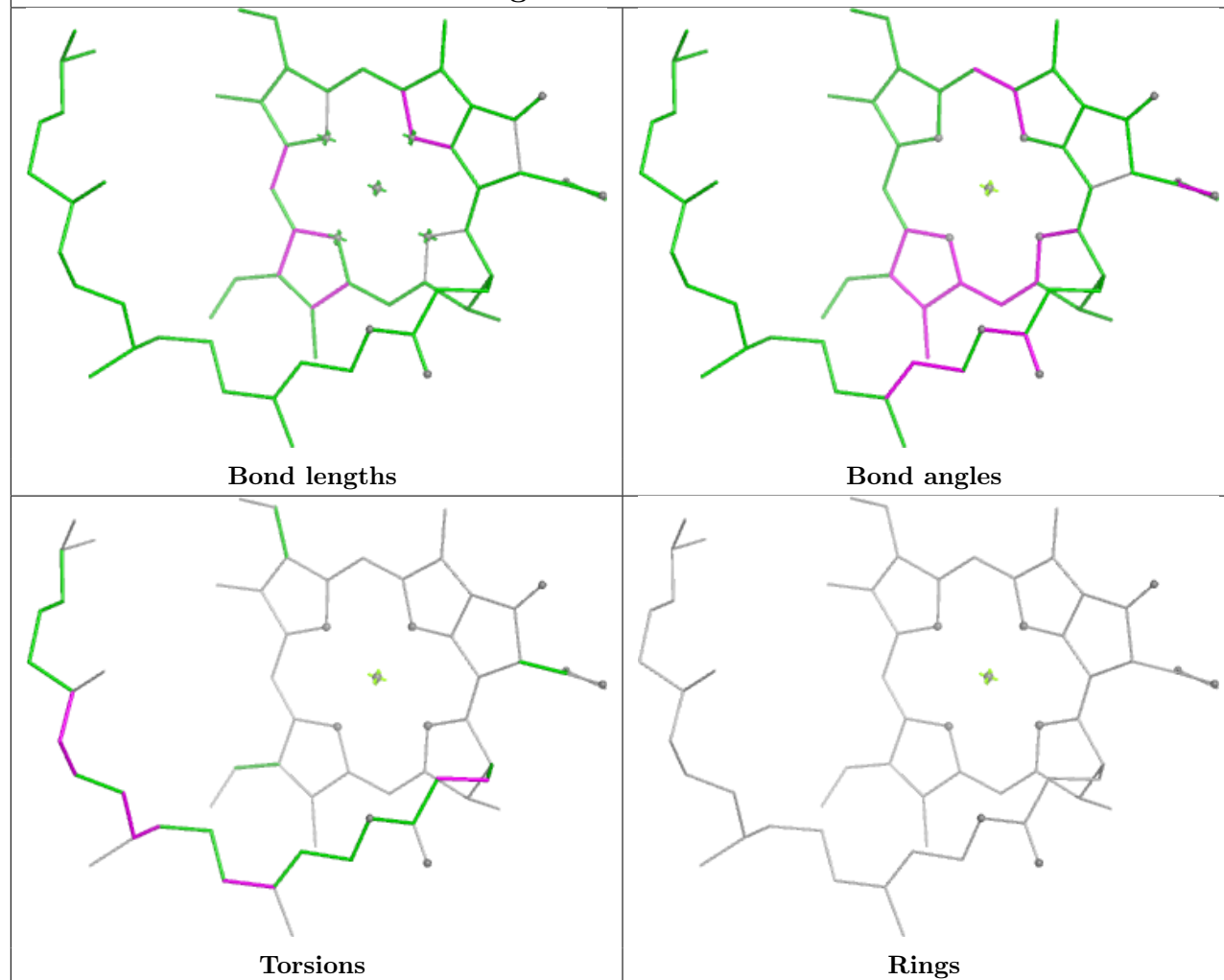
Torsions



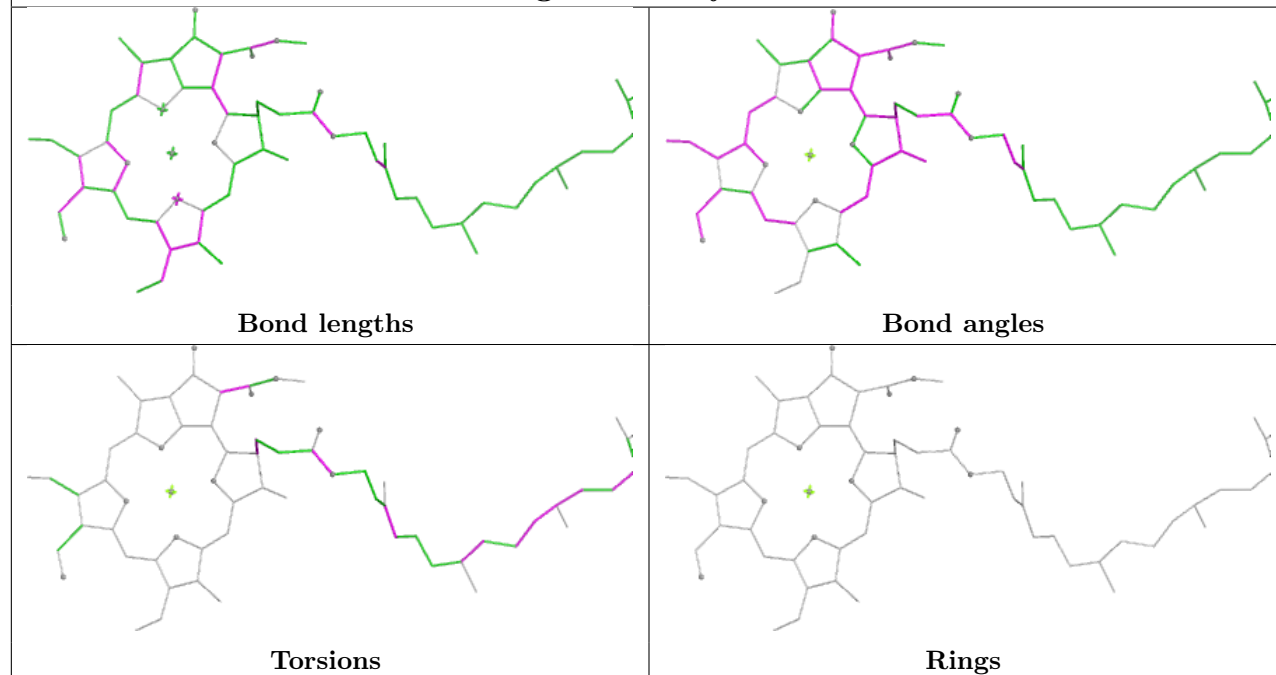
Rings



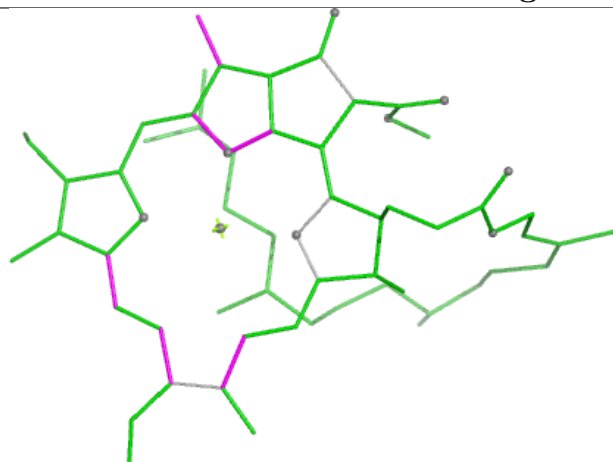
Ligand CLA Y 308



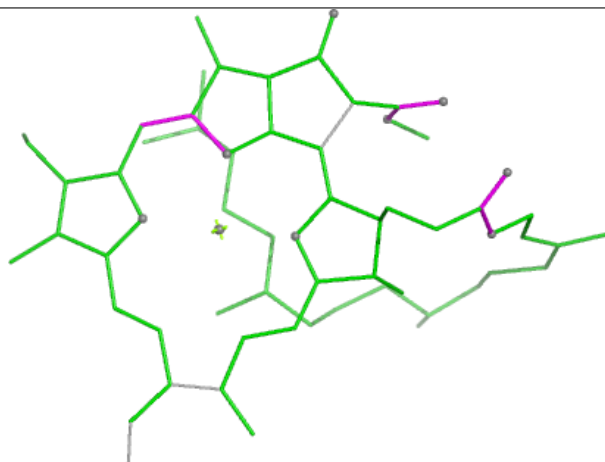
Ligand CHL y 303



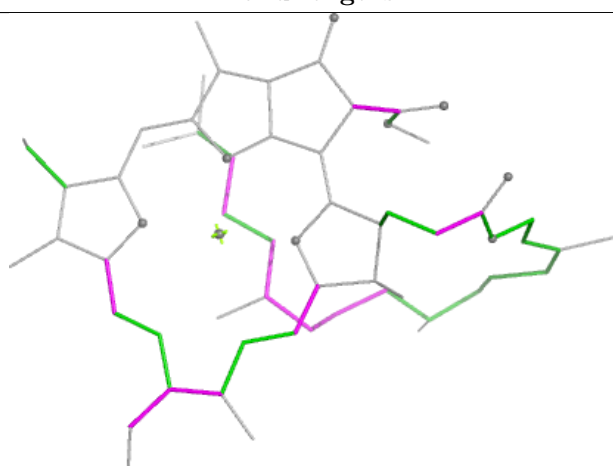
Ligand CLA c 506



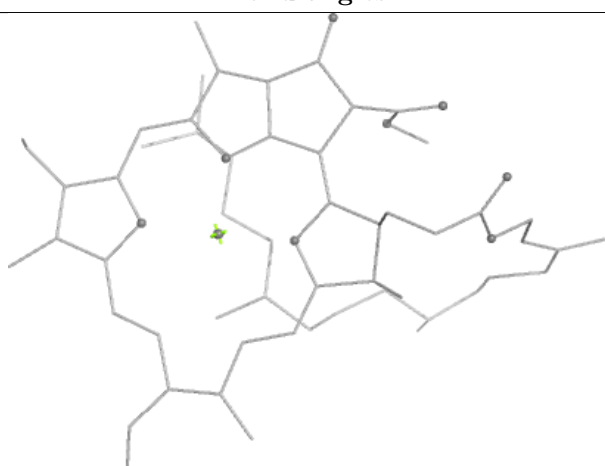
Bond lengths



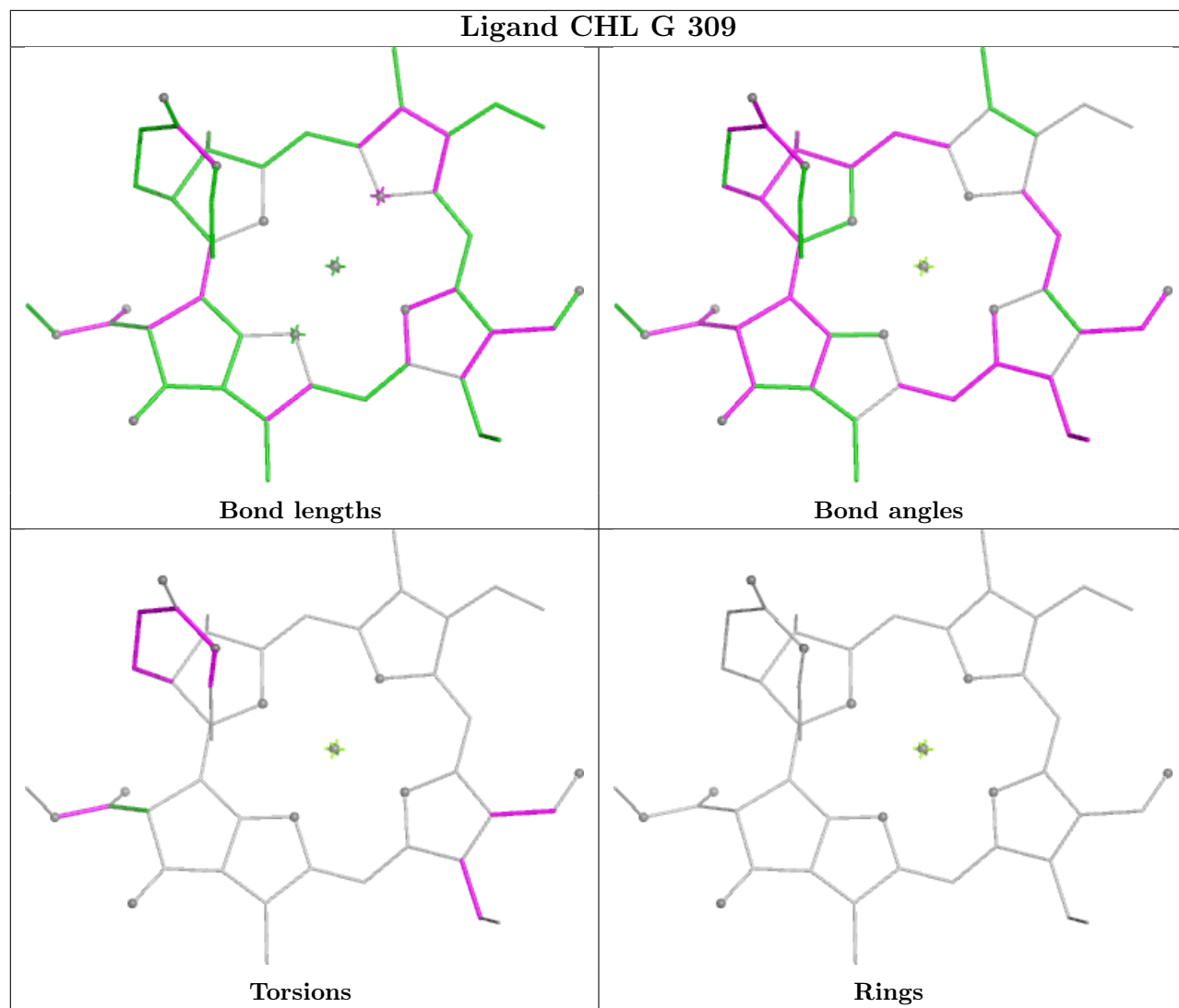
Bond angles

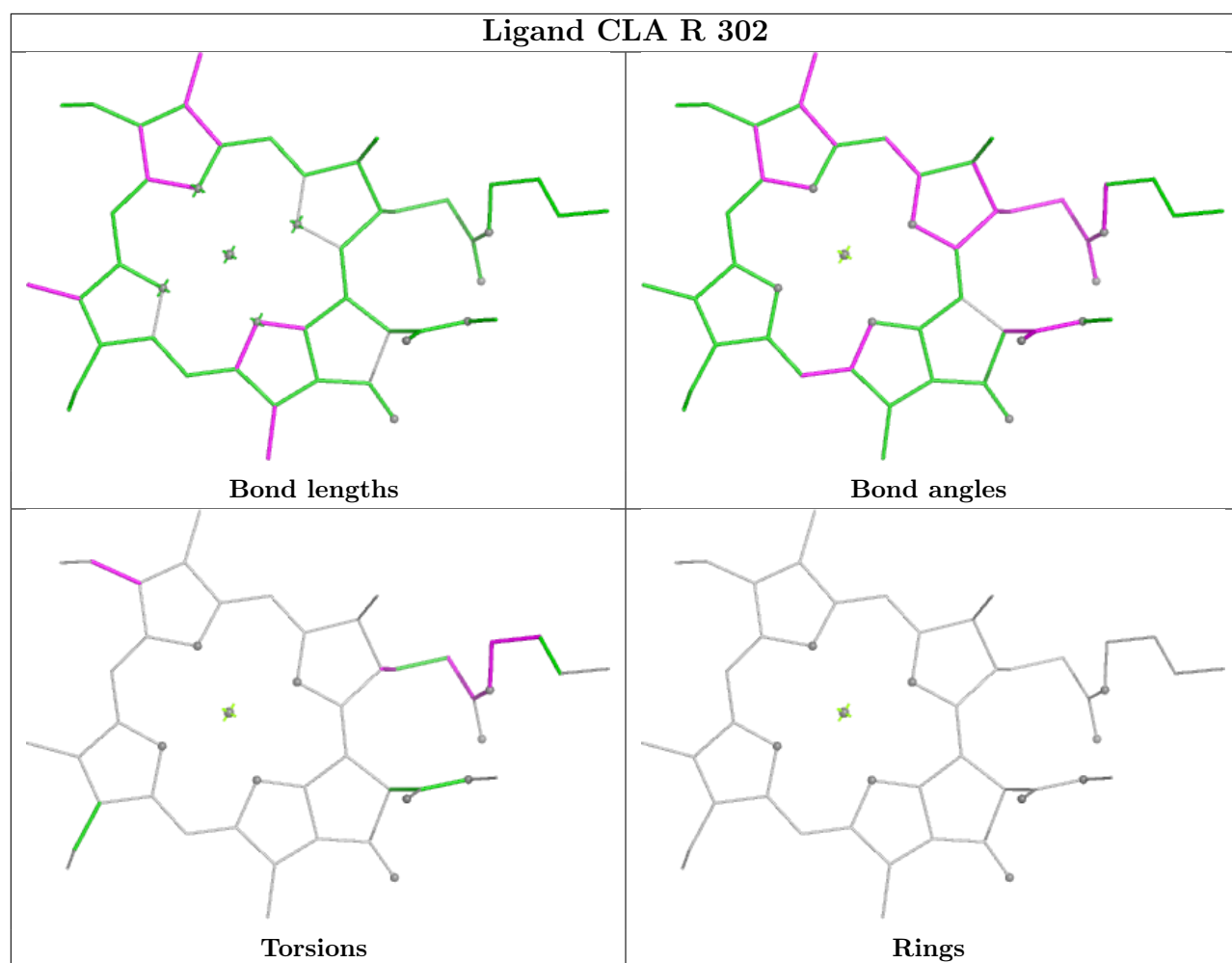


Torsions

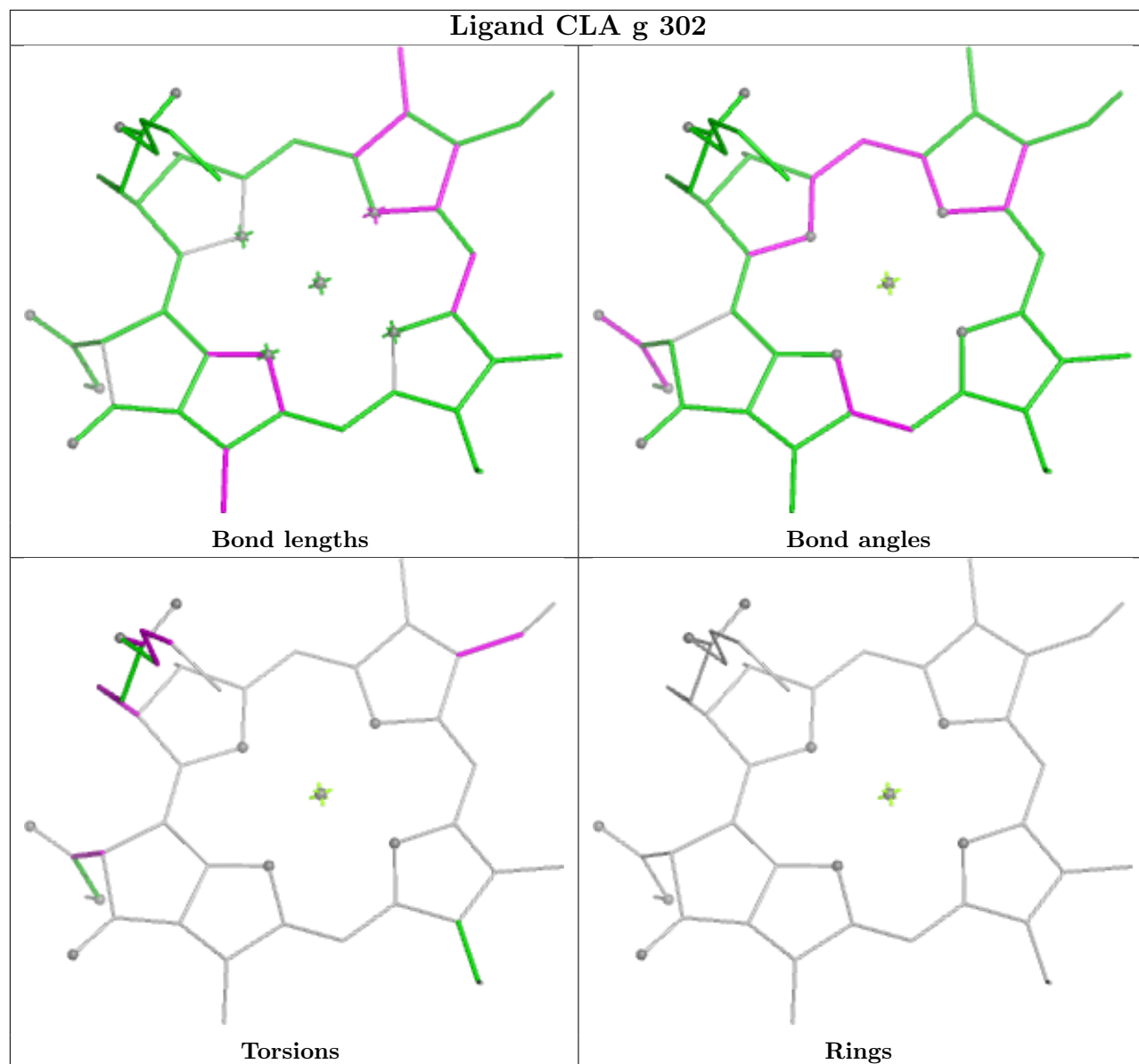


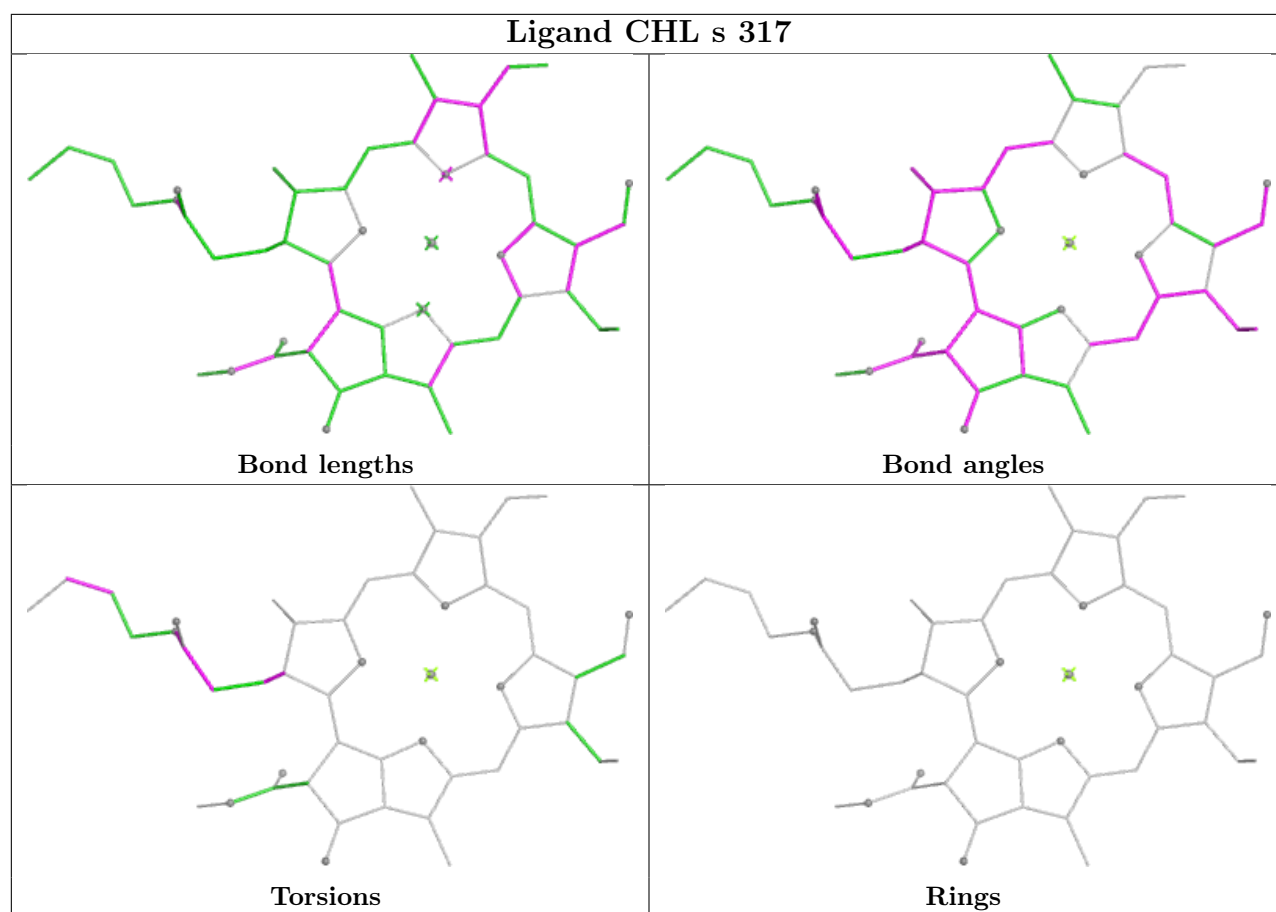
Rings

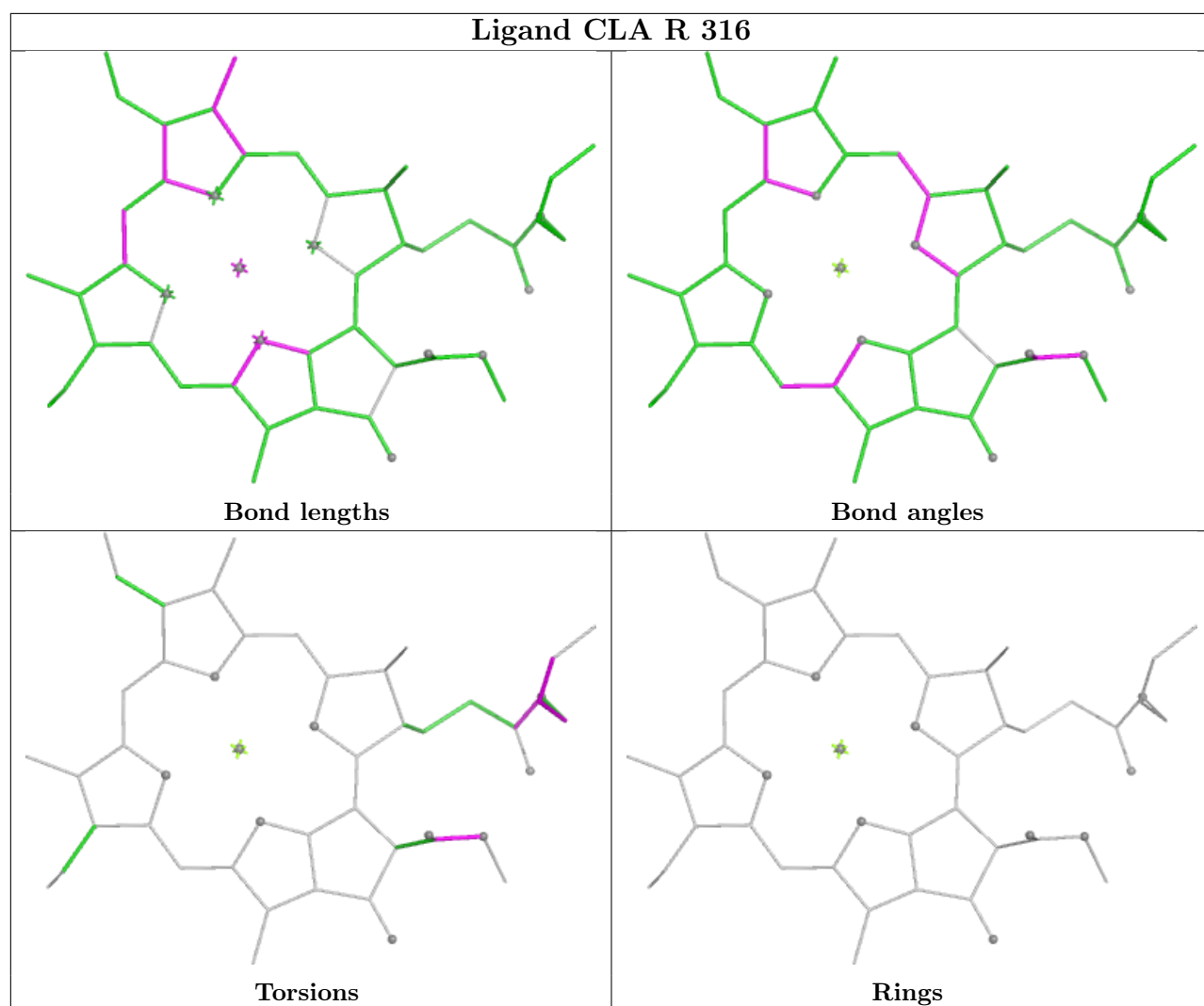




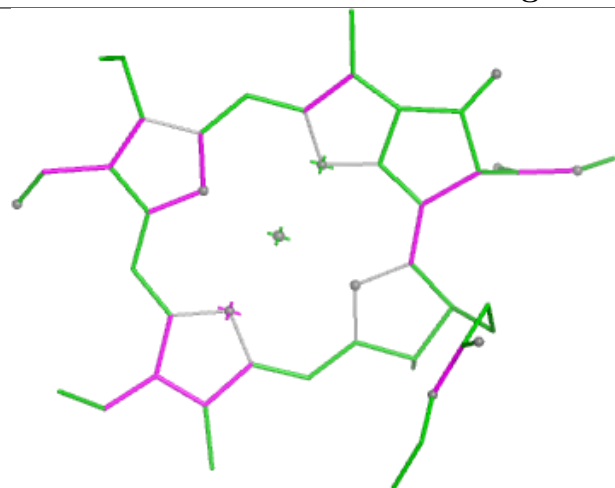
Ligand CLA g 302



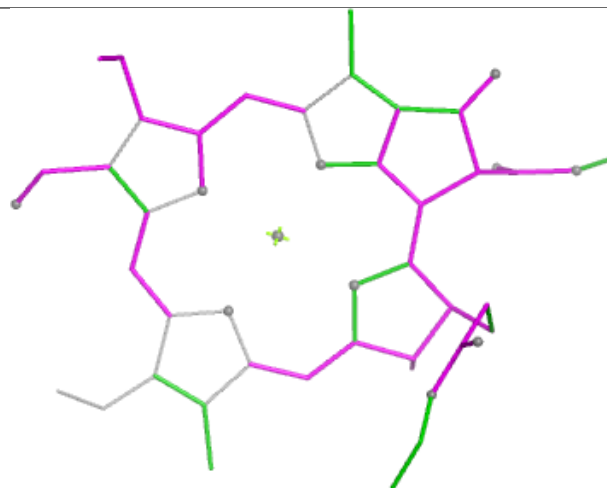




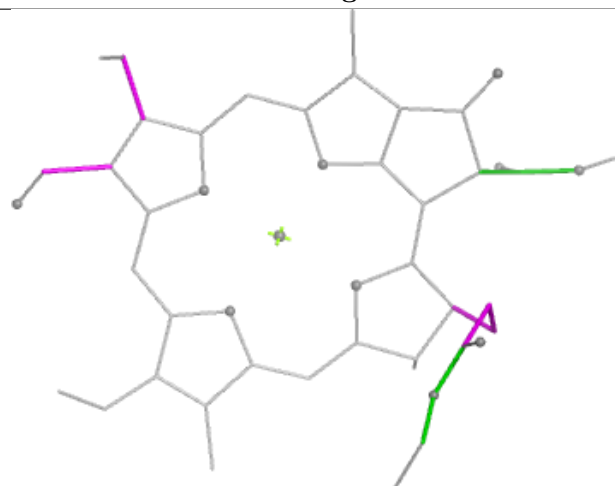
Ligand CHL r 301



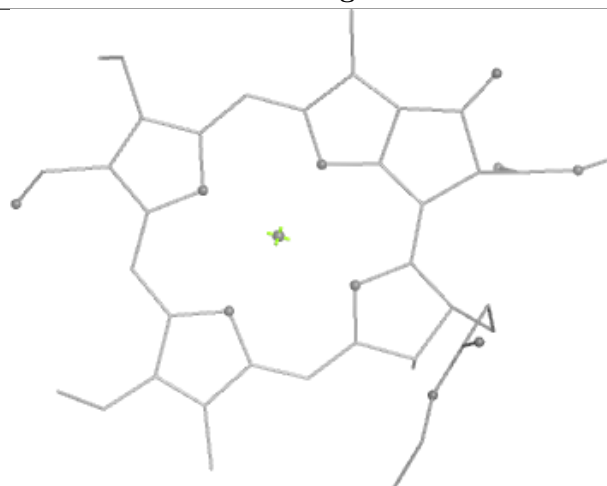
Bond lengths



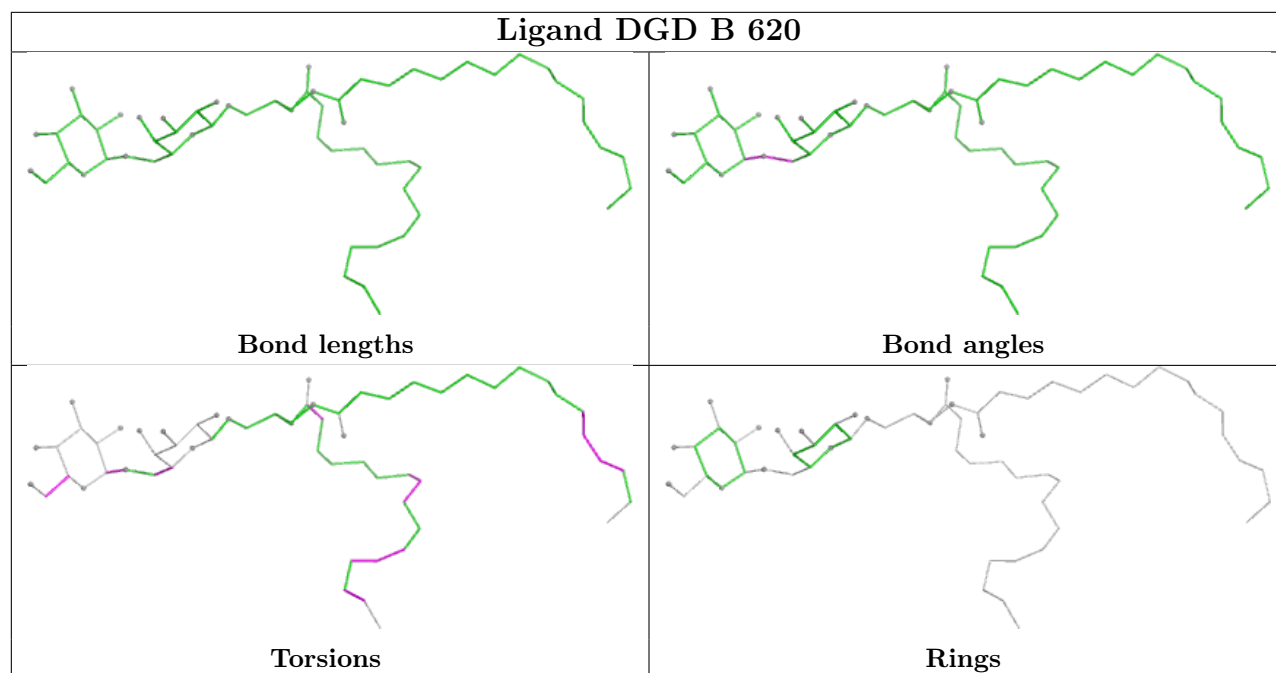
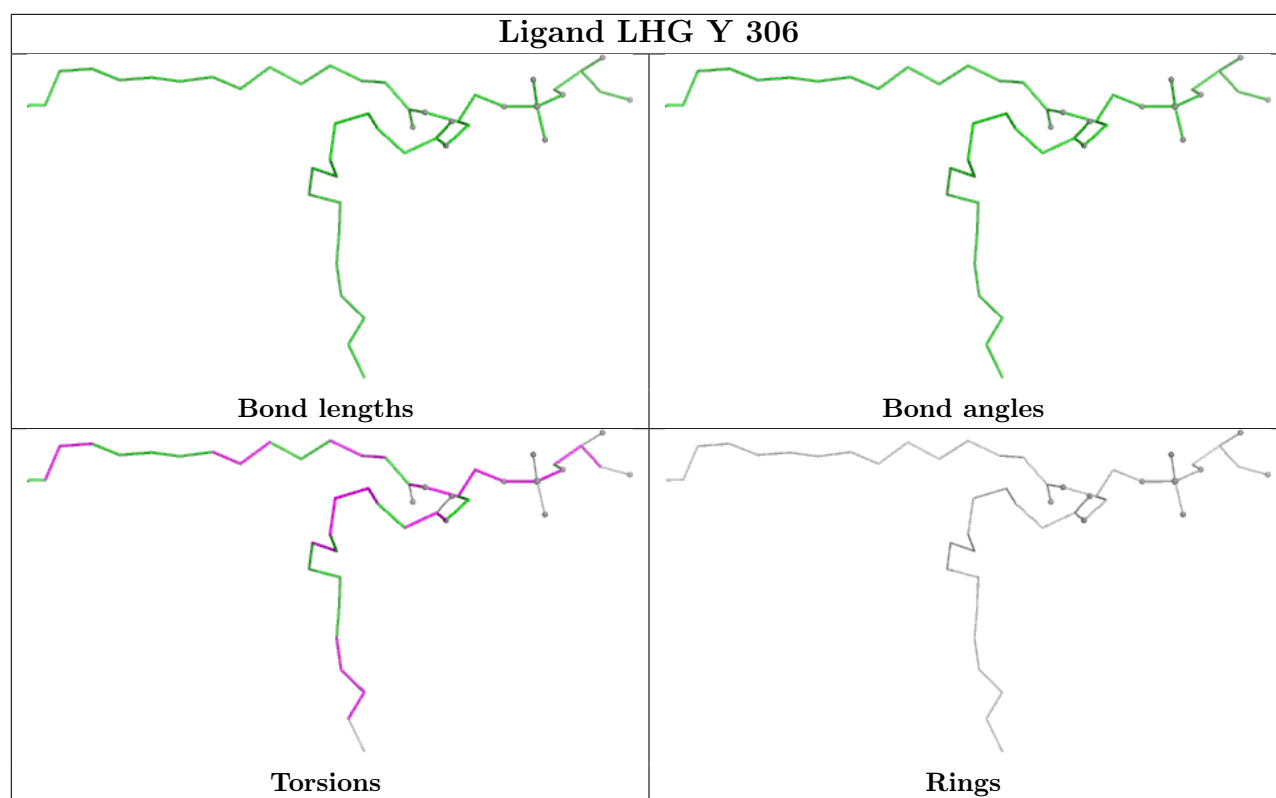
Bond angles

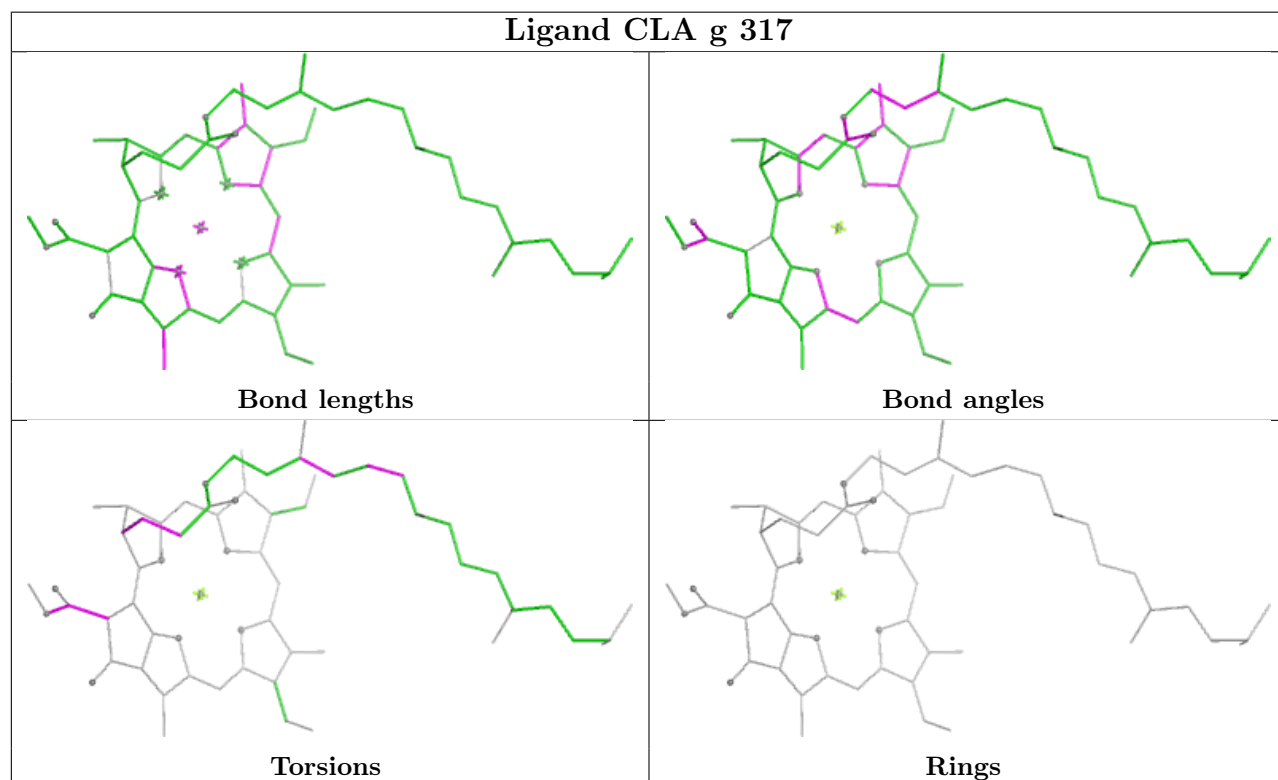
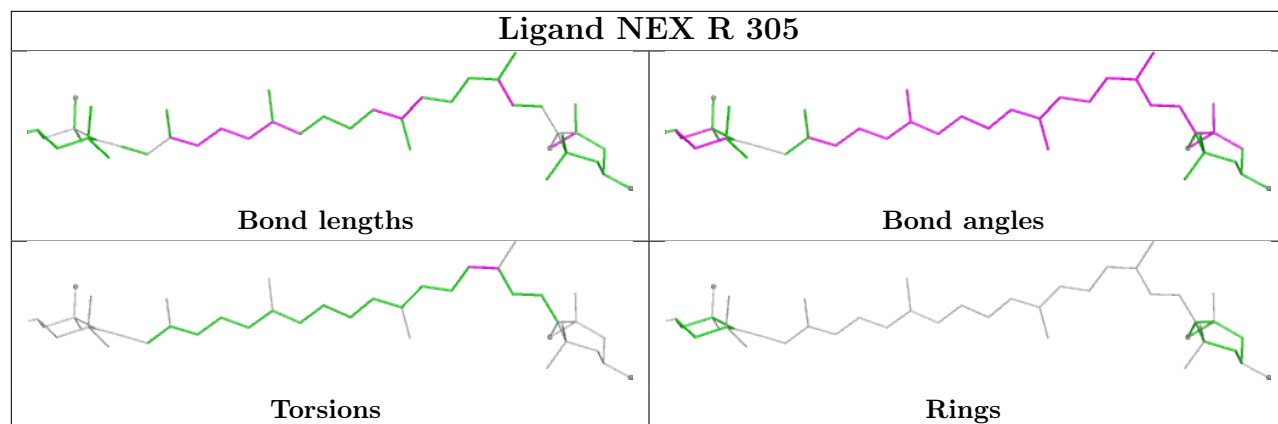


Torsions

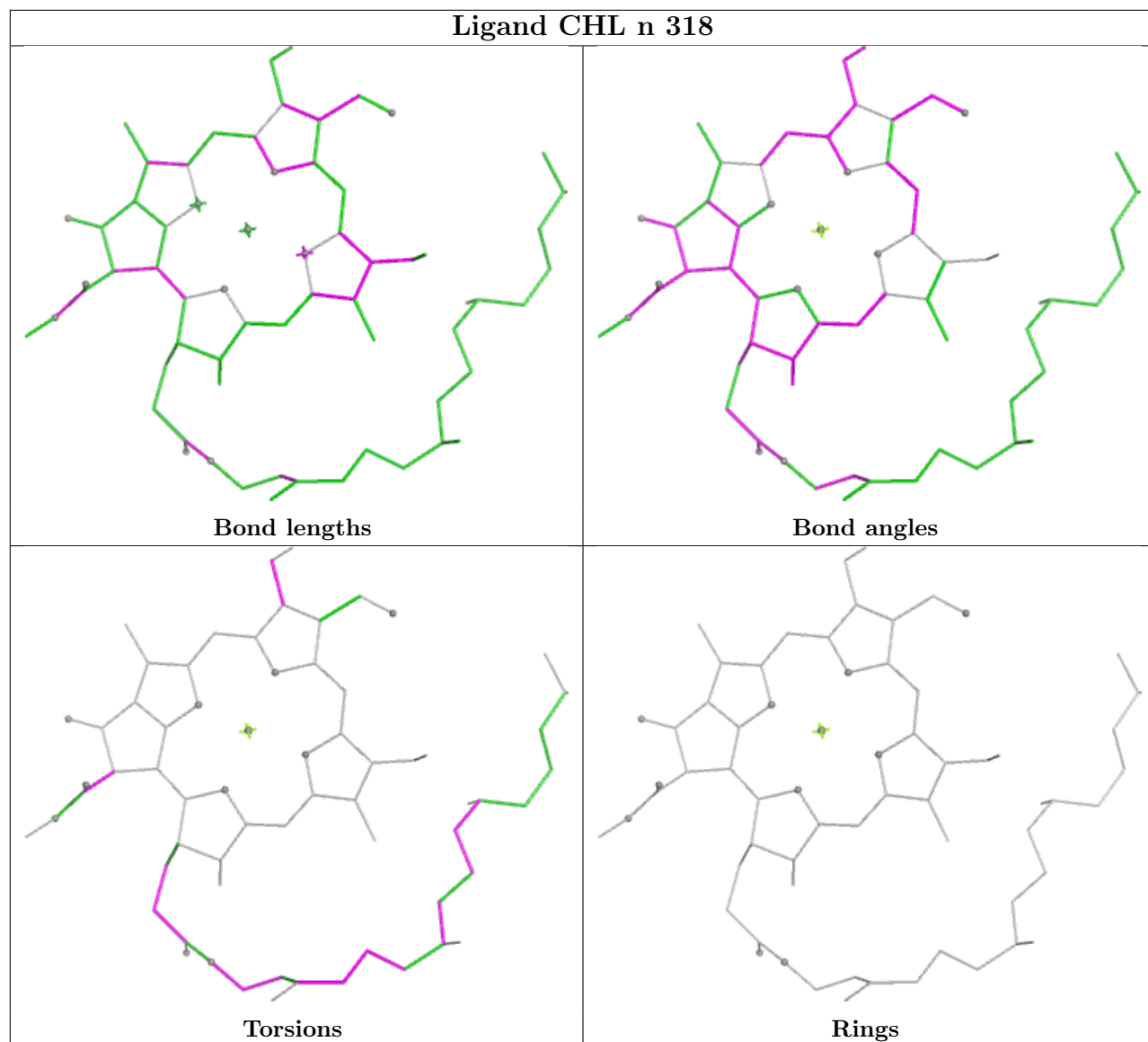


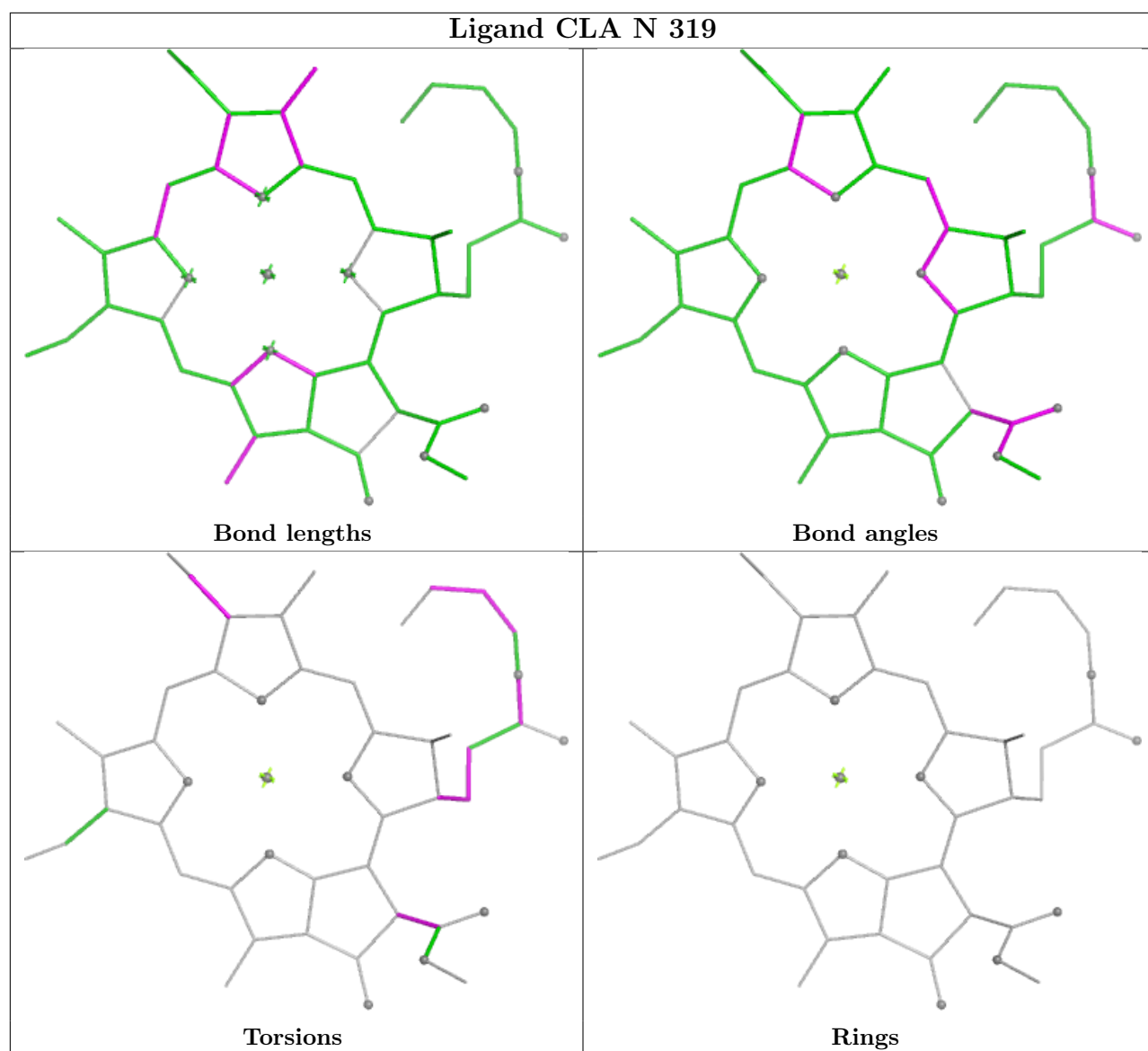
Rings

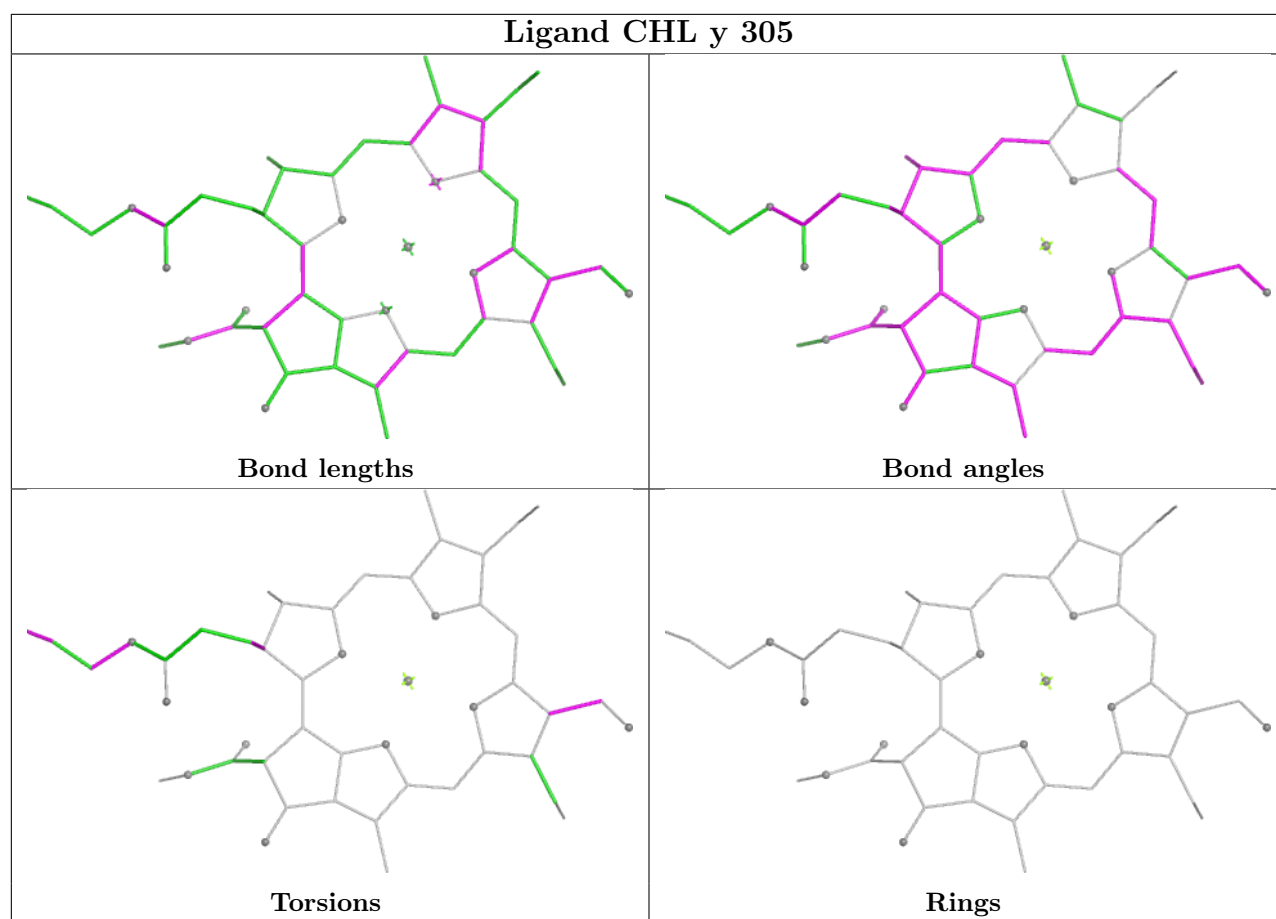


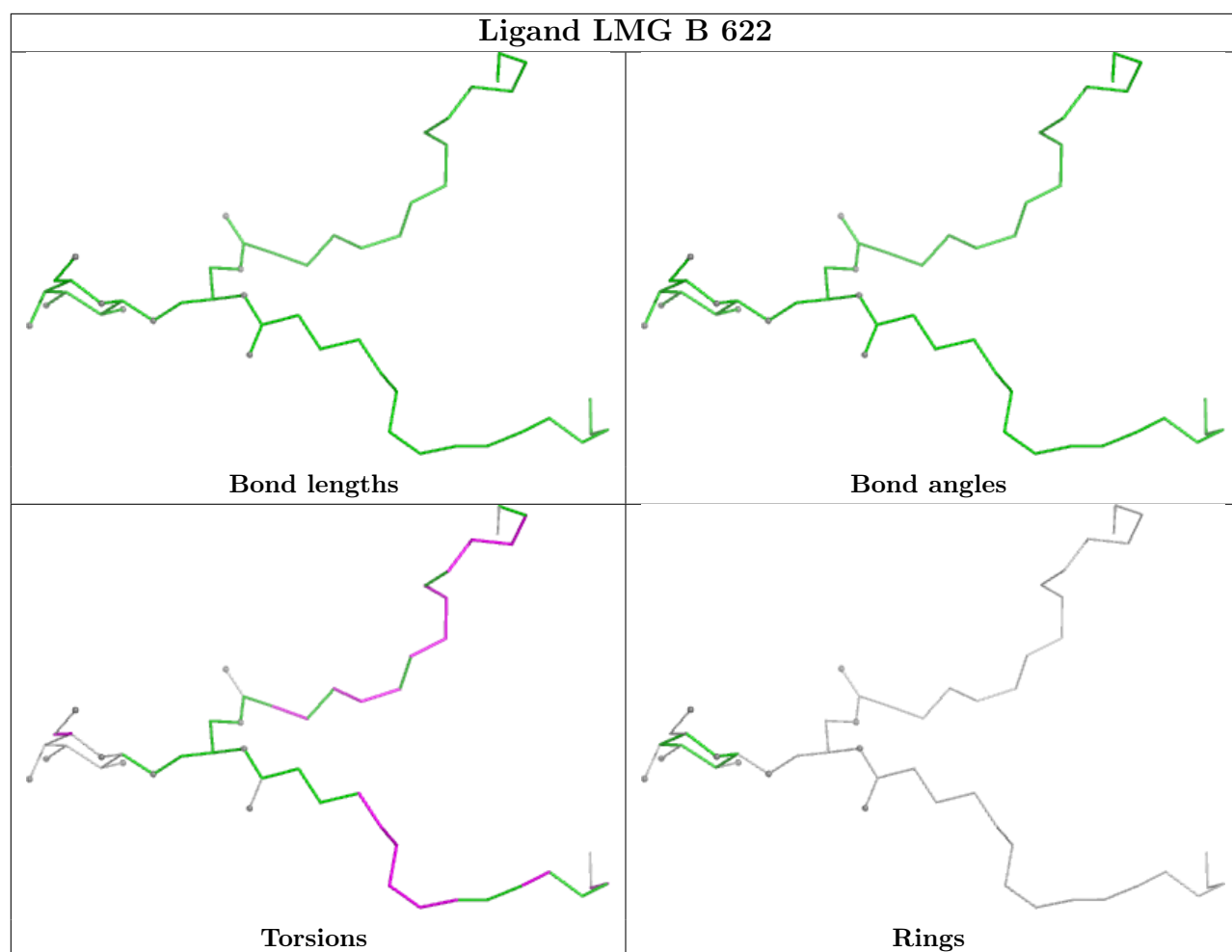


Ligand CHL n 318

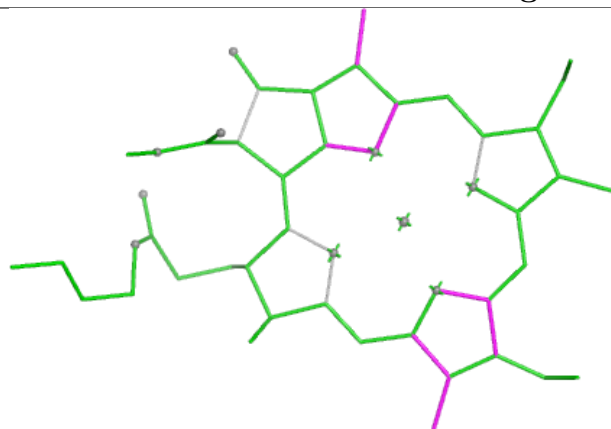




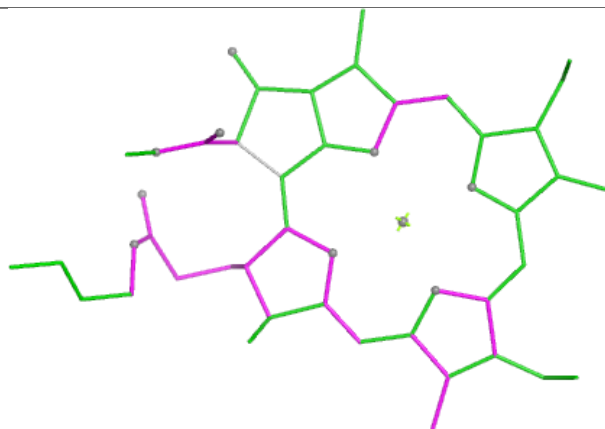




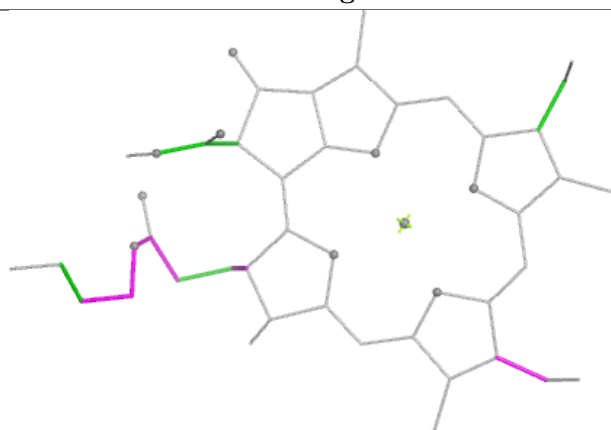
Ligand CLA r 313



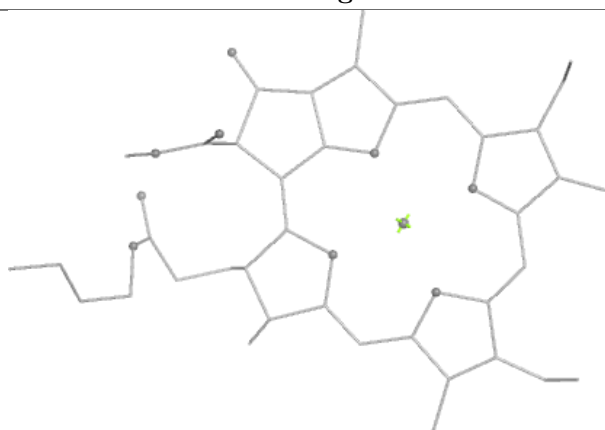
Bond lengths



Bond angles

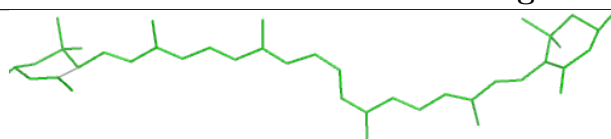


Torsions

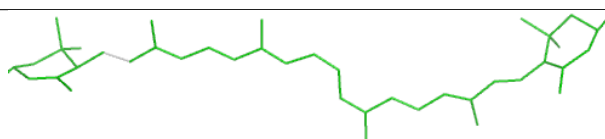


Rings

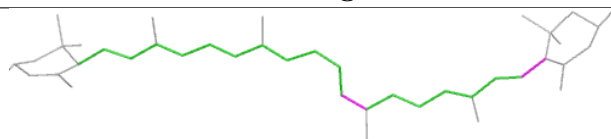
Ligand LUT S 301



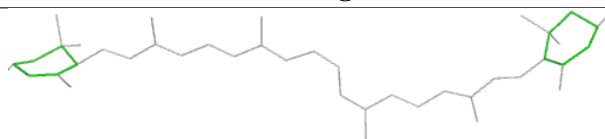
Bond lengths



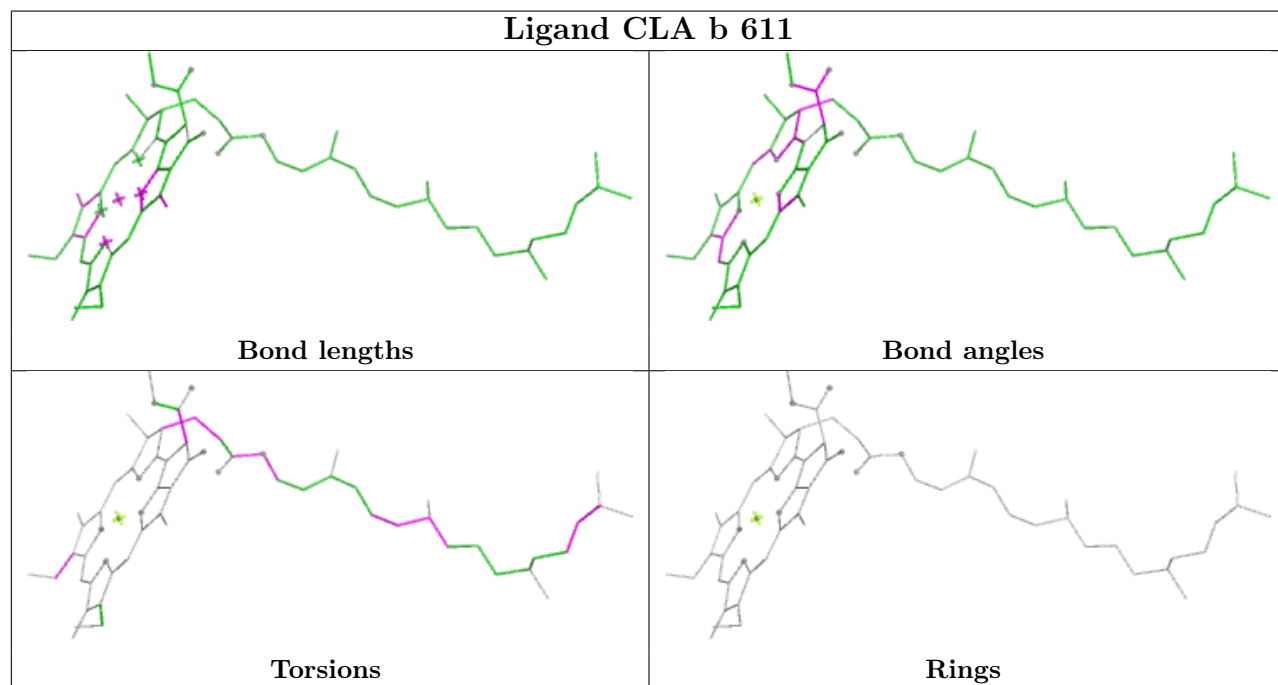
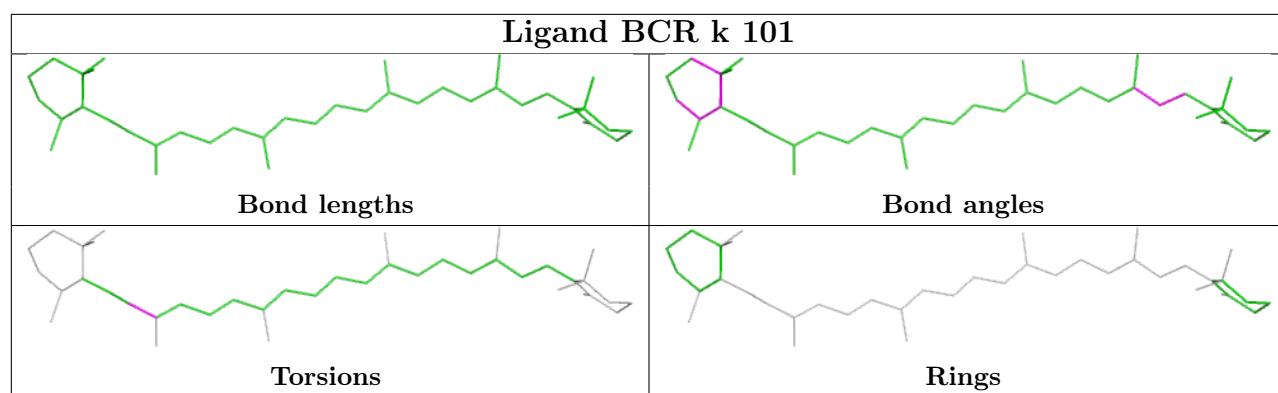
Bond angles



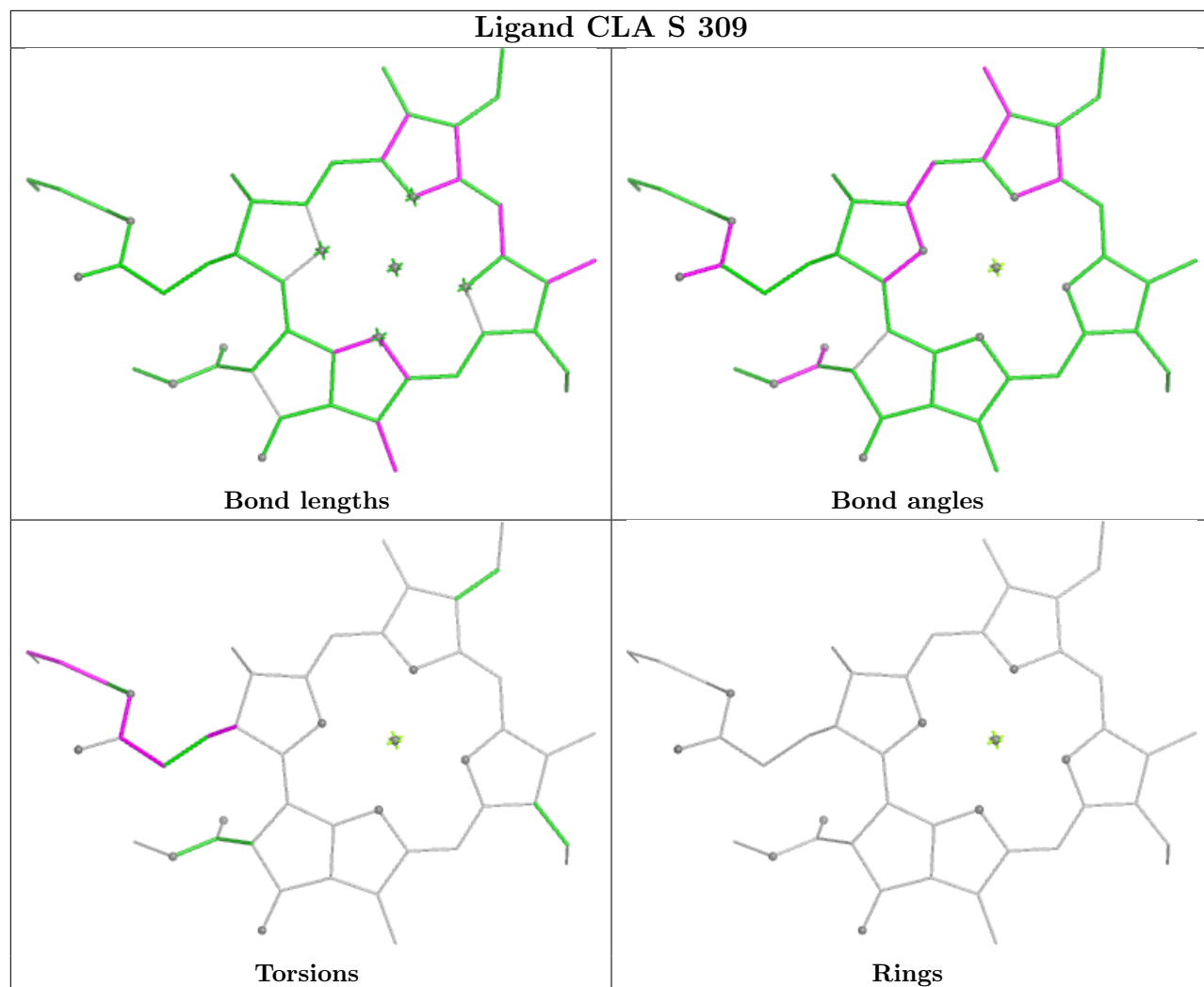
Torsions

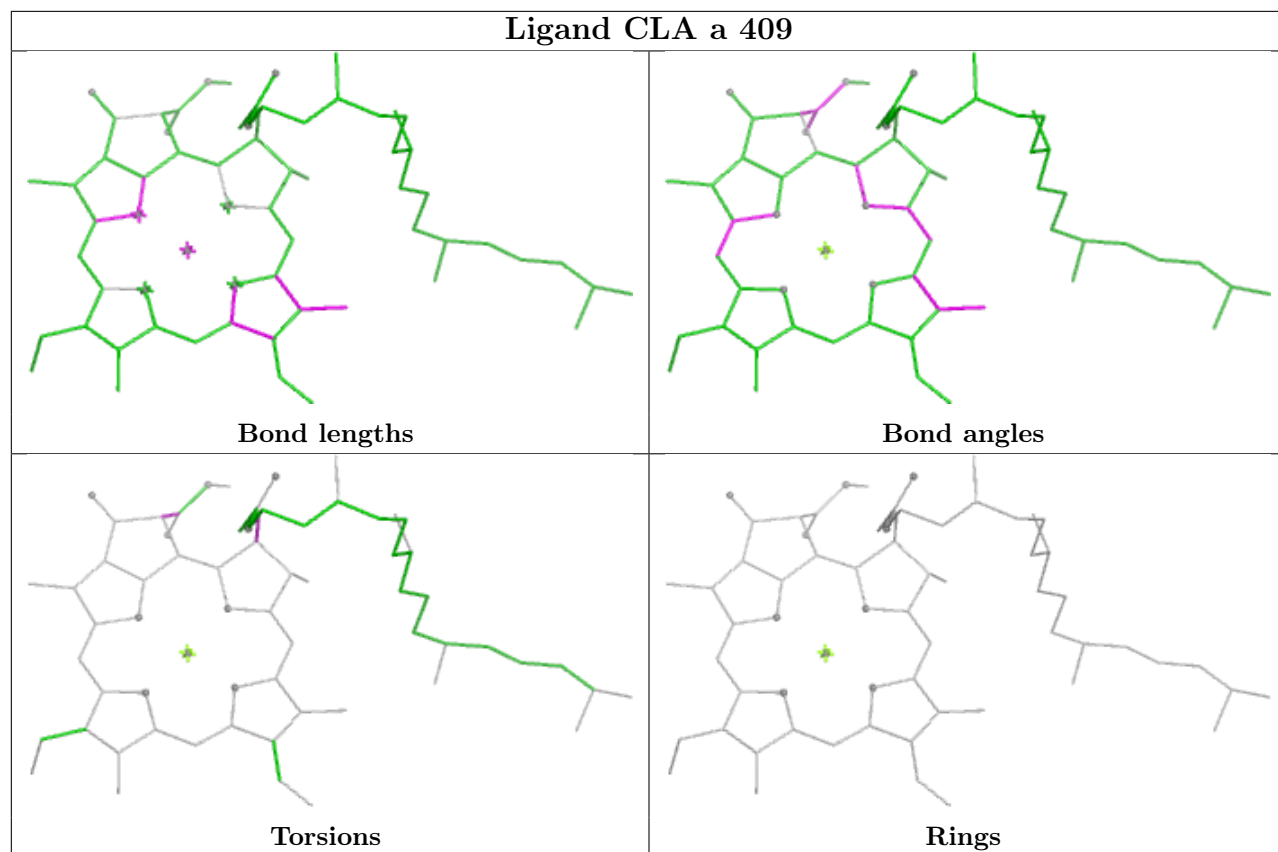


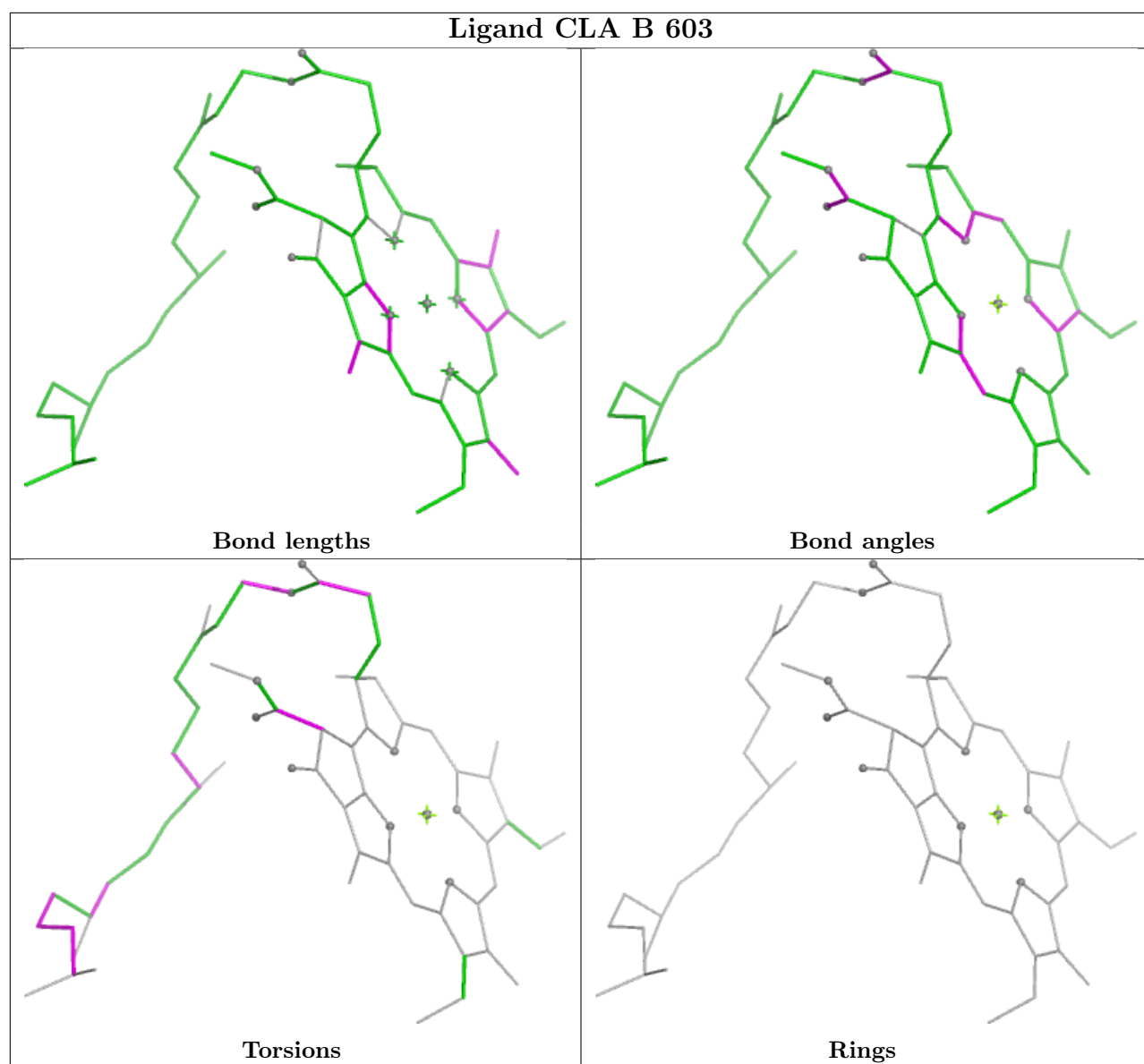
Rings

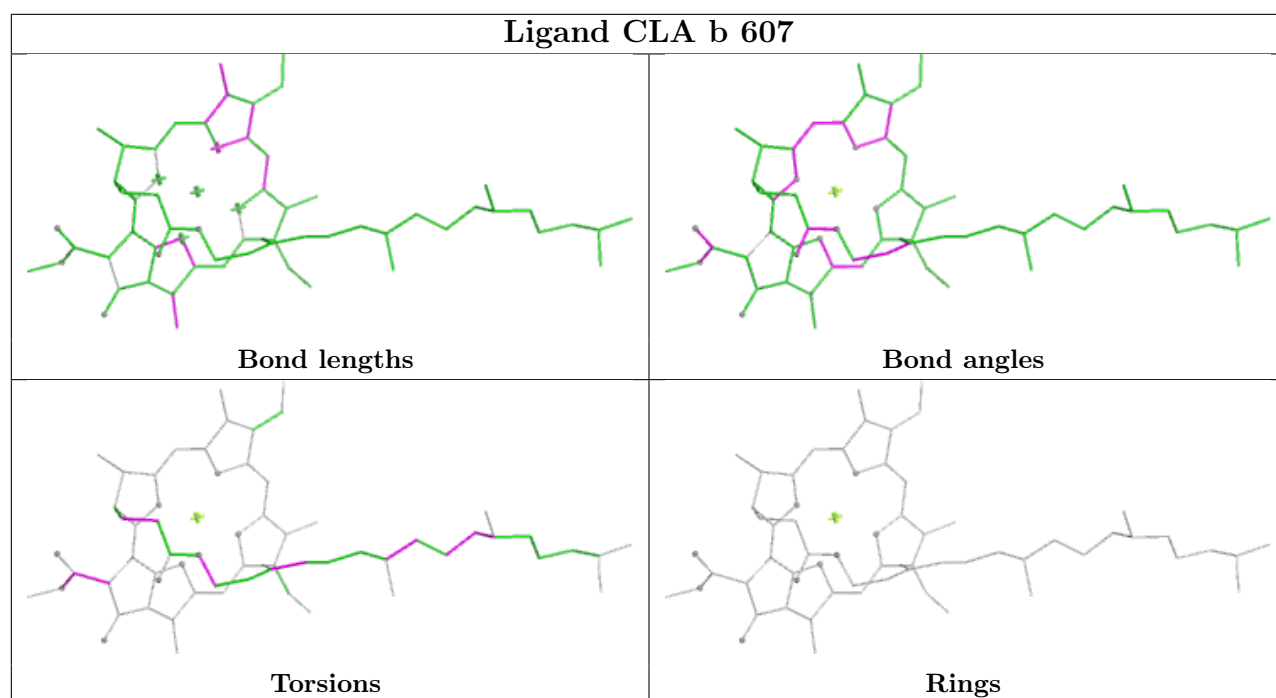


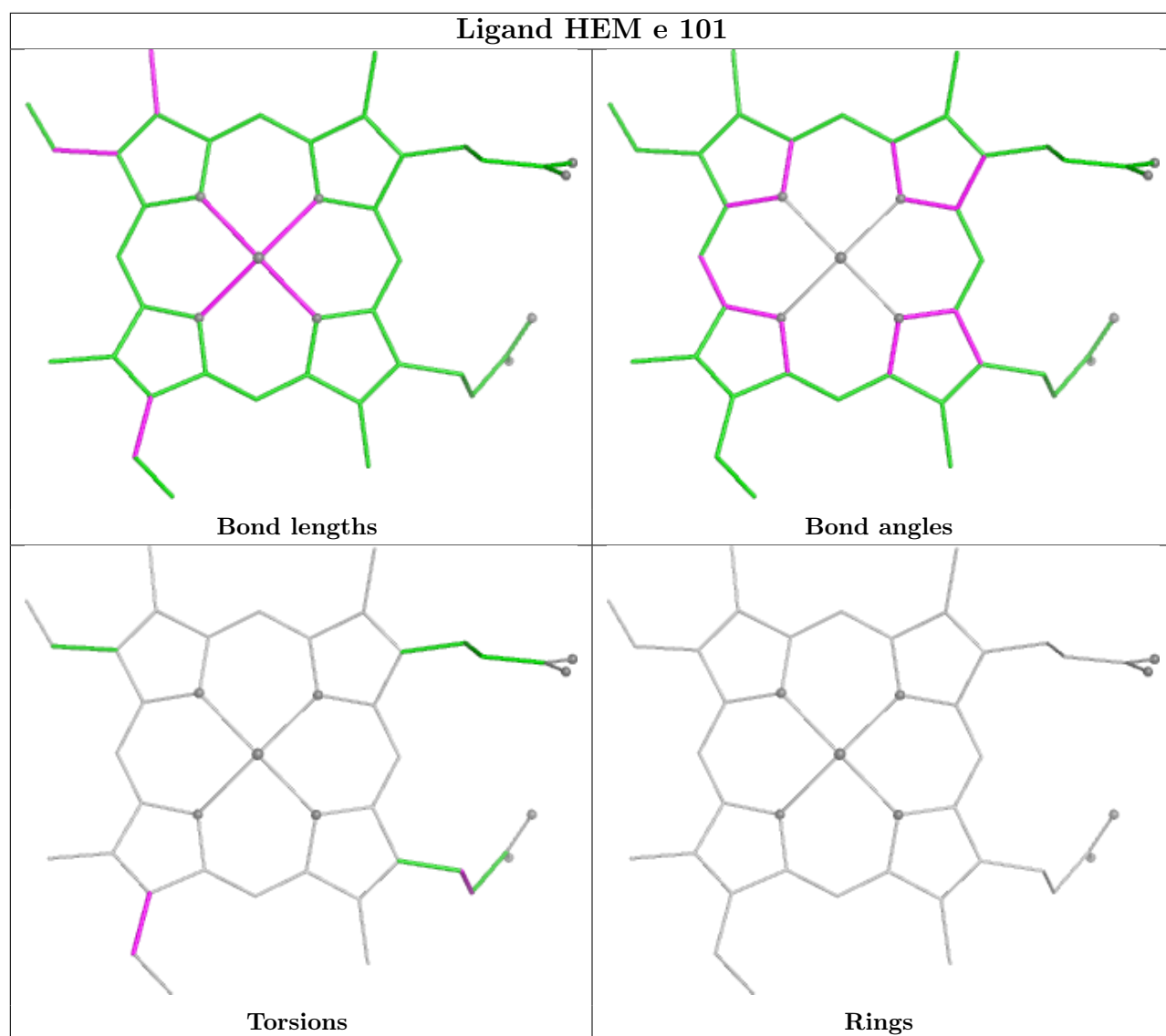
Ligand CLA S 309

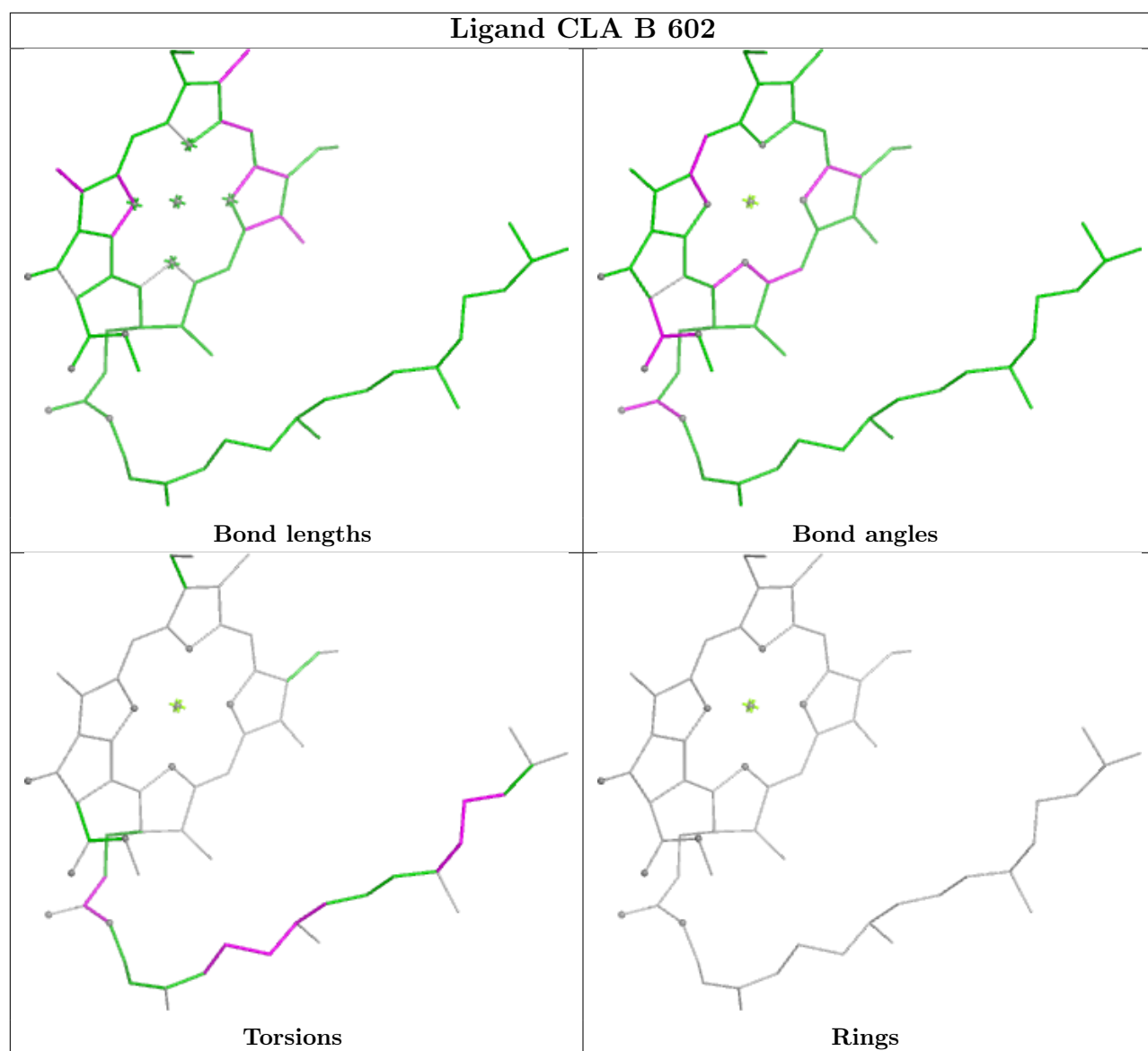


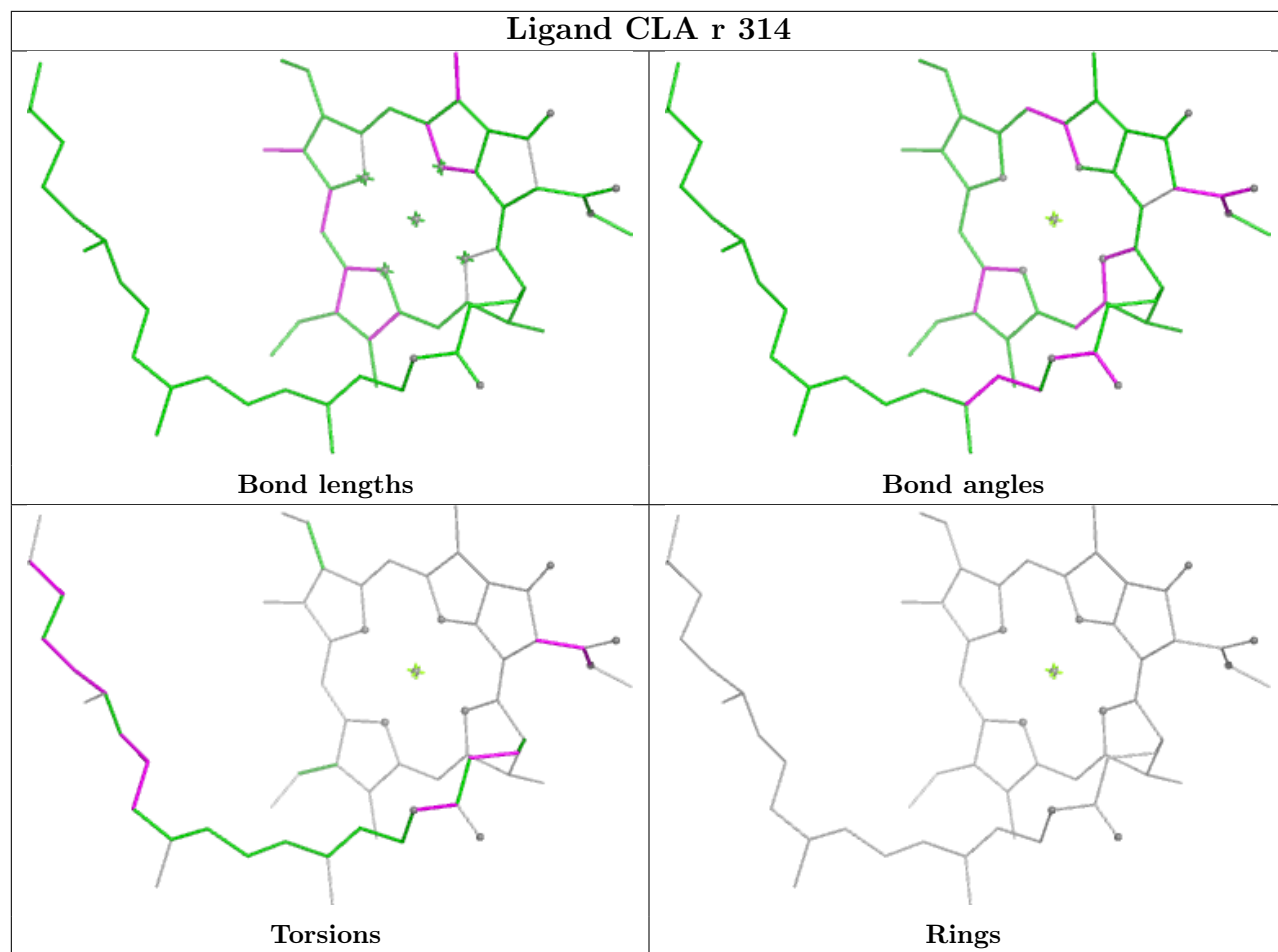


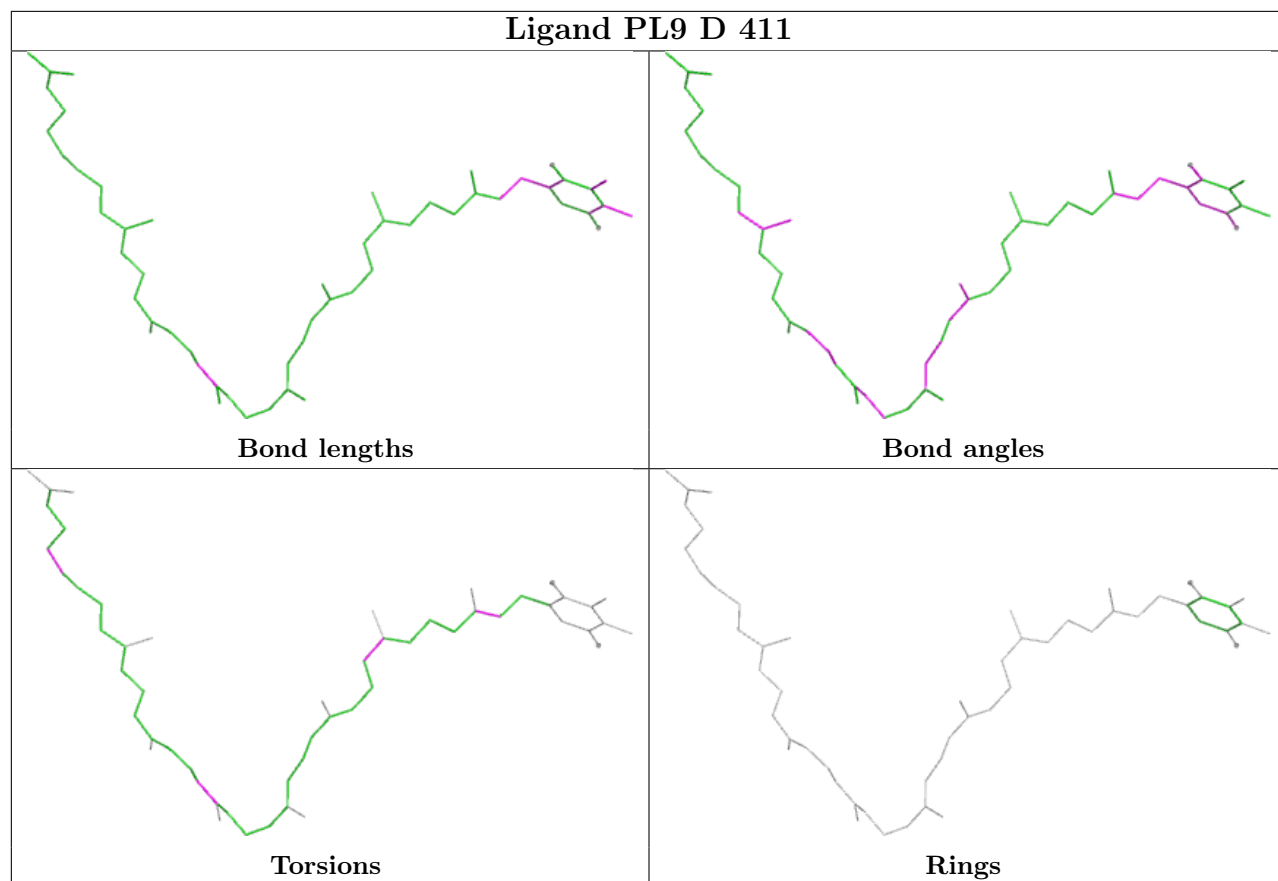


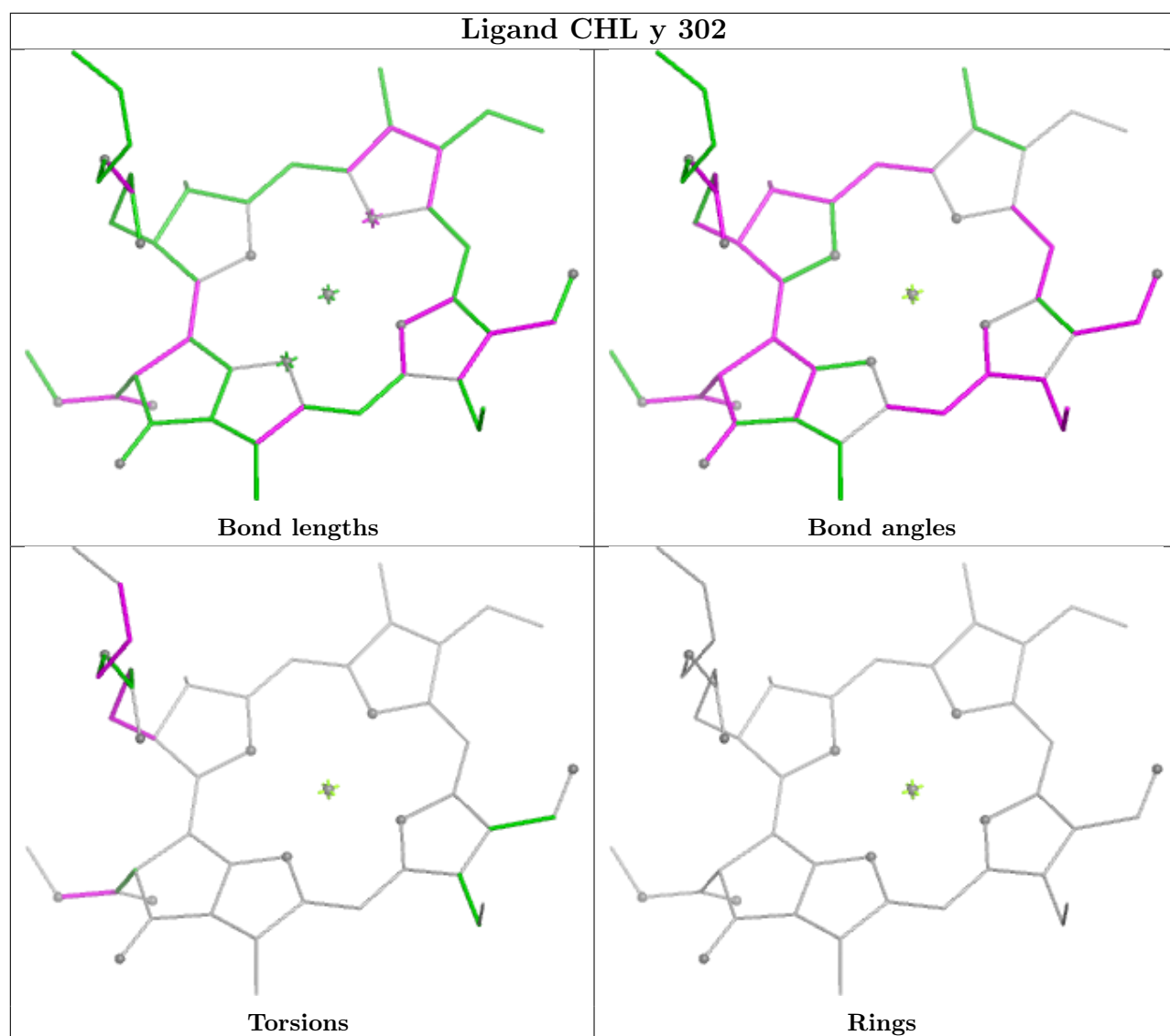


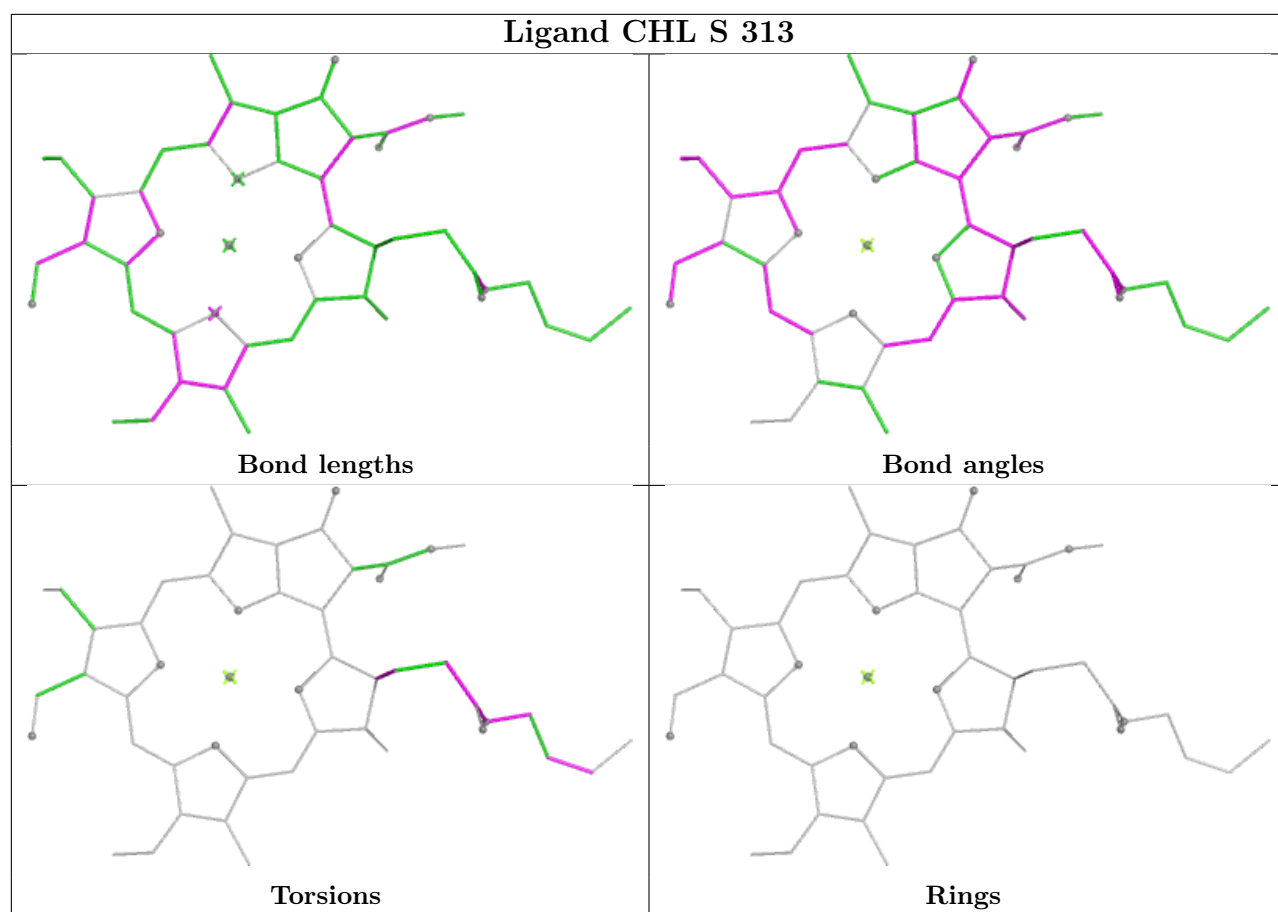


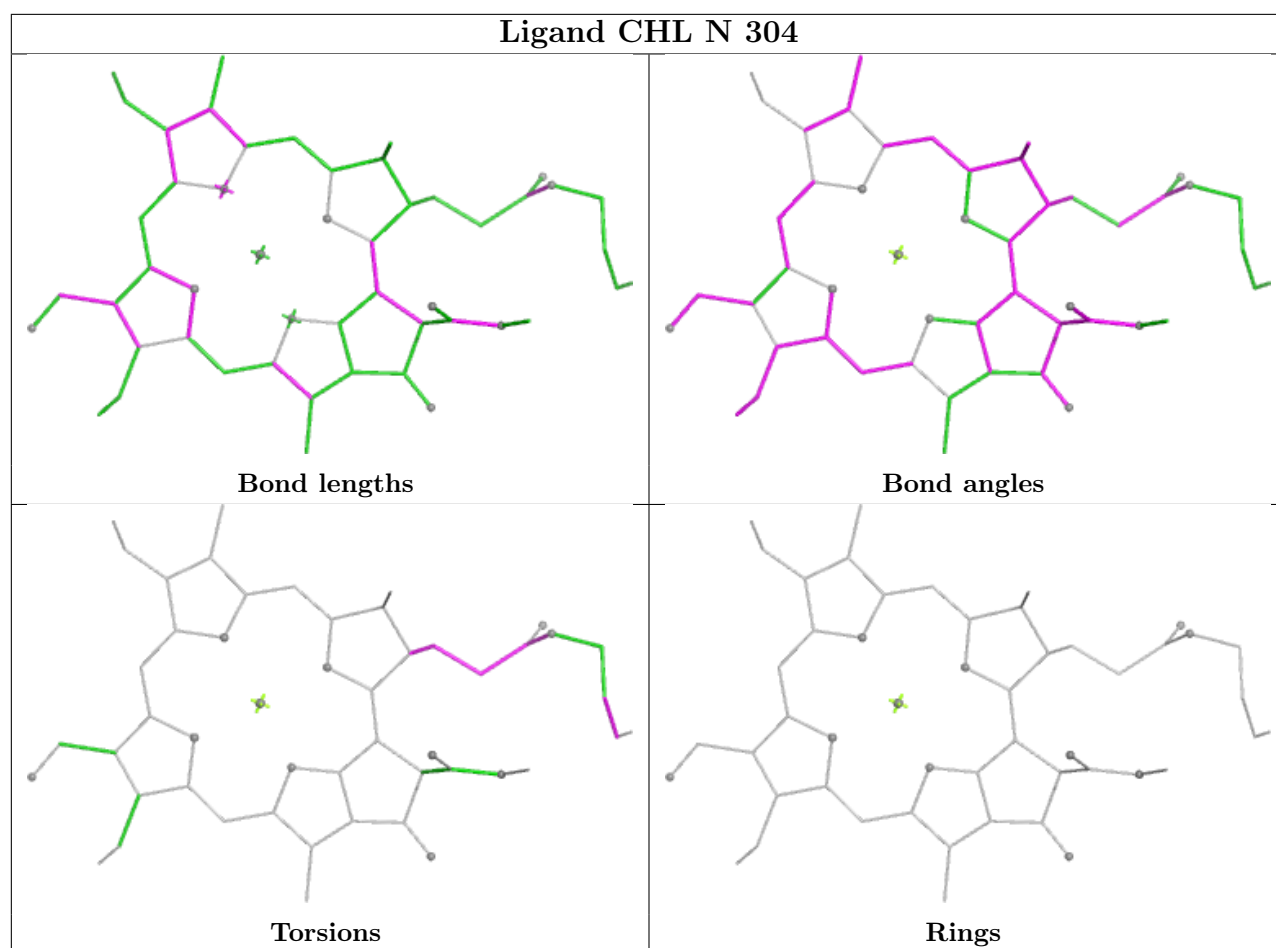




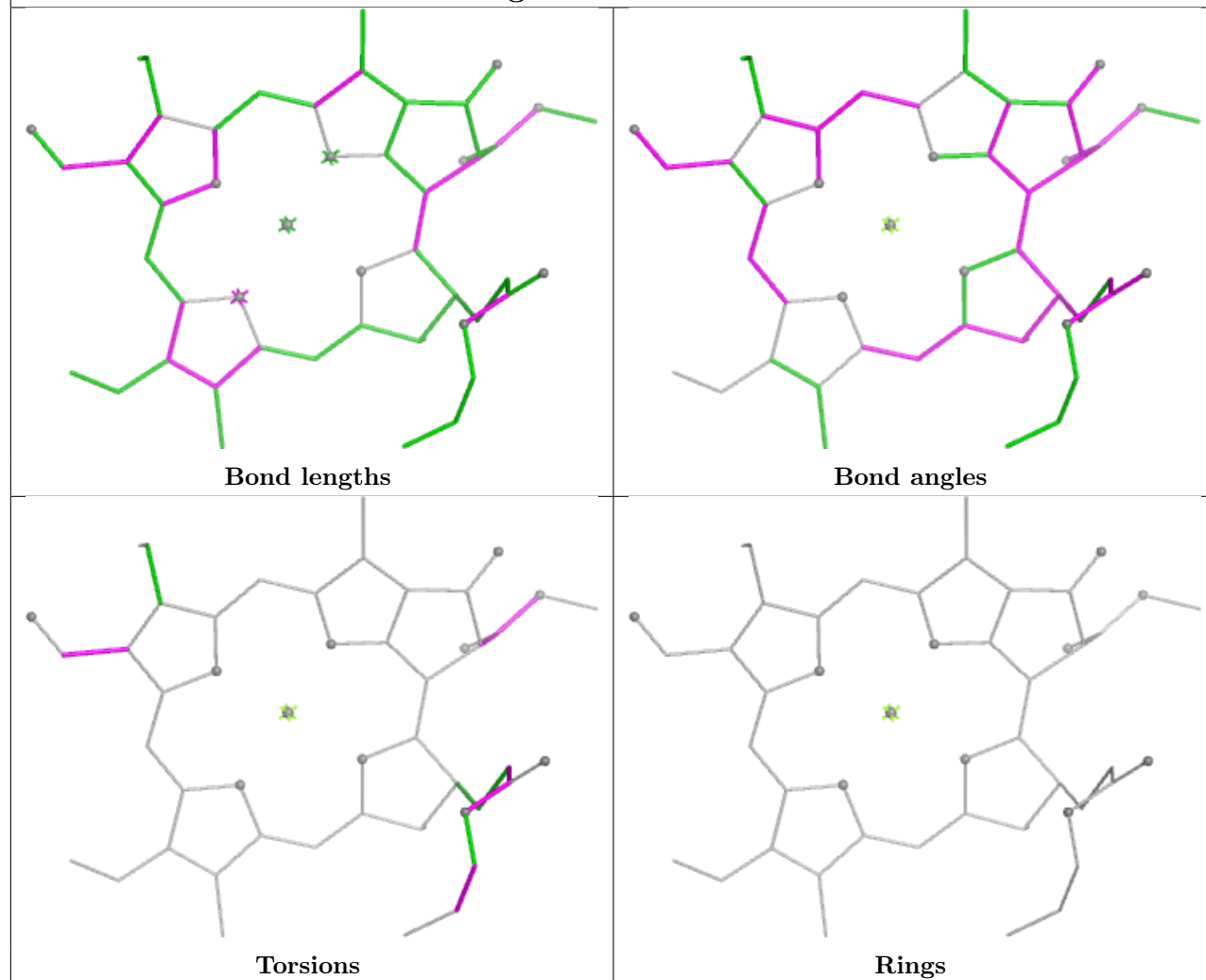




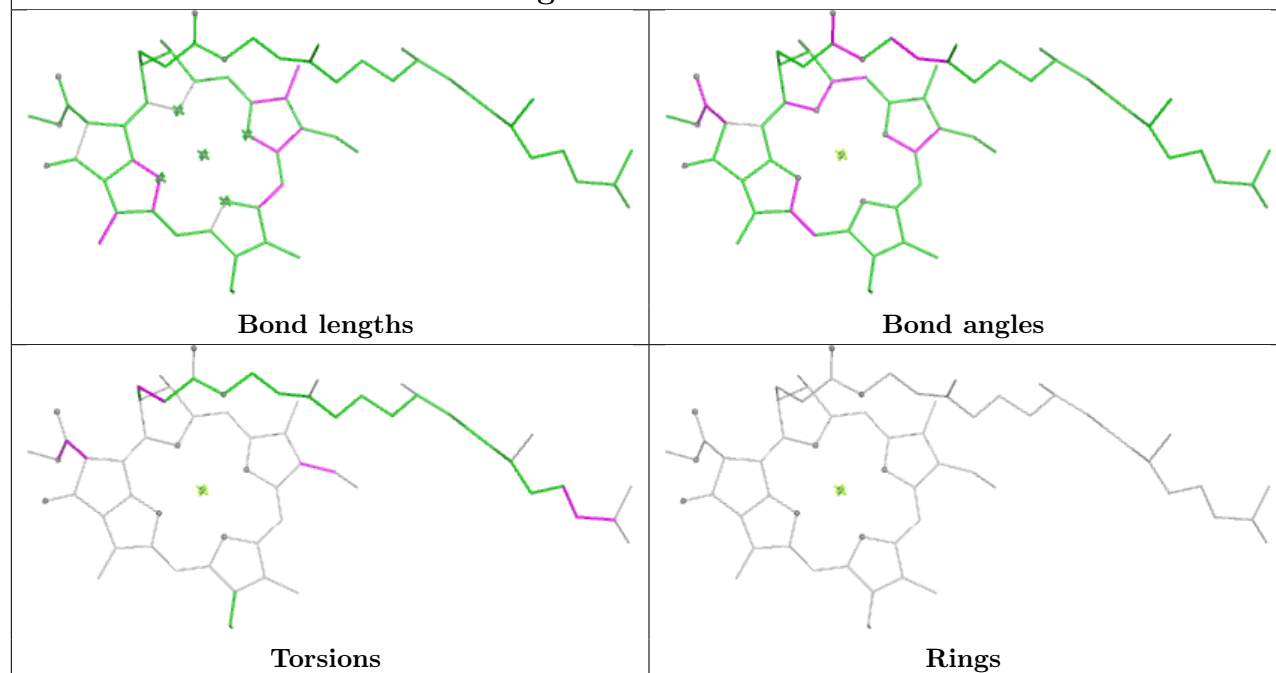


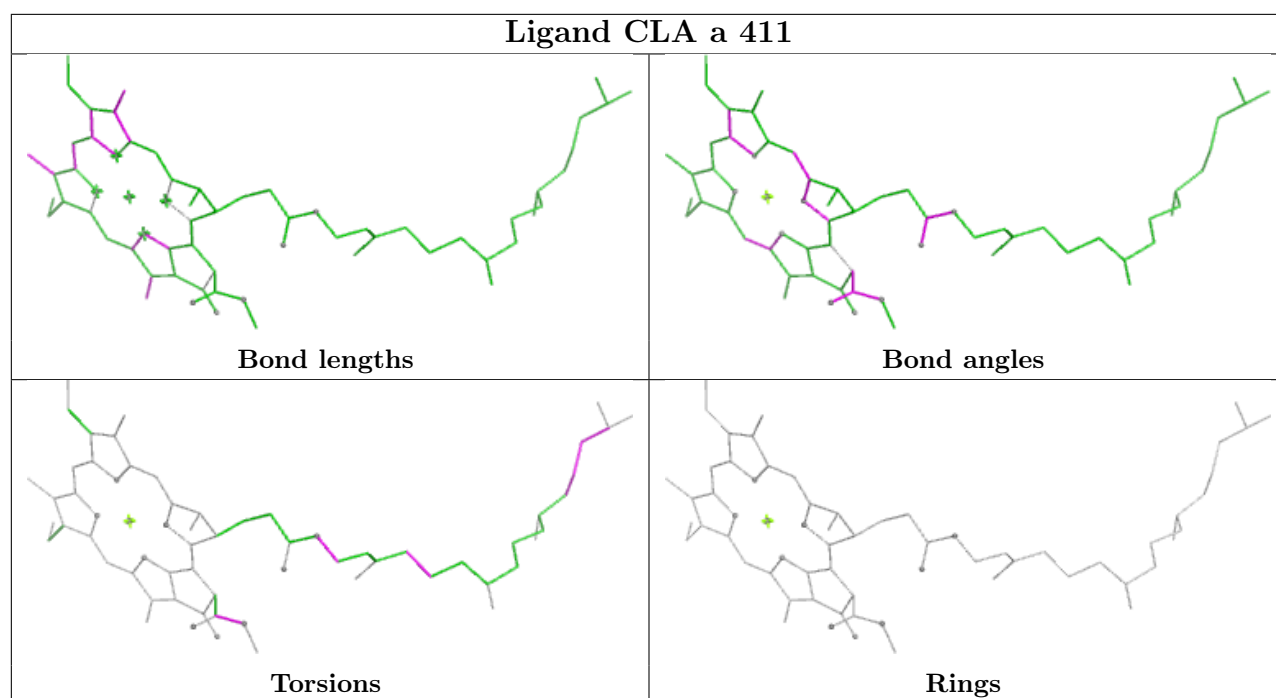


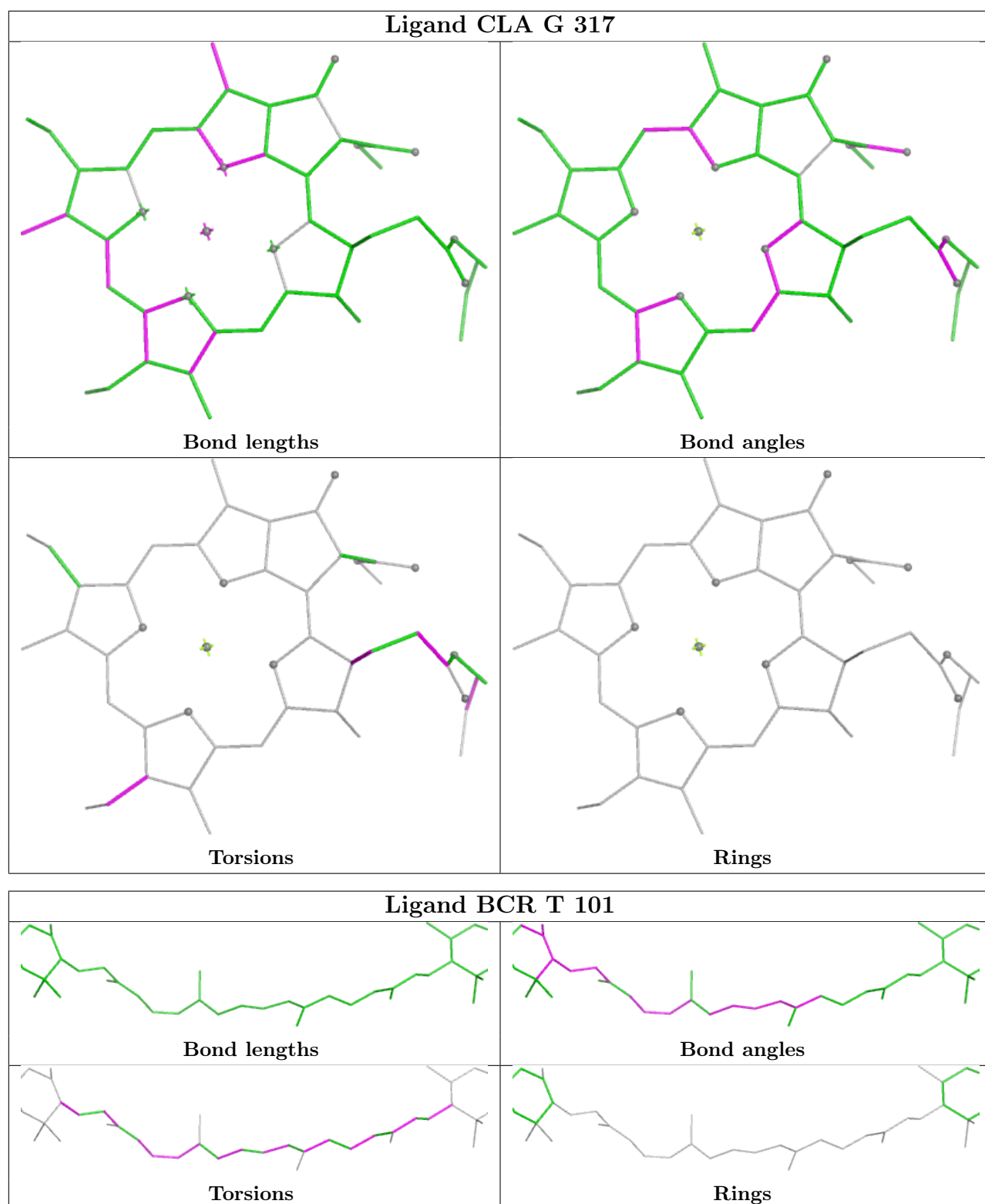
Ligand CHL s 313



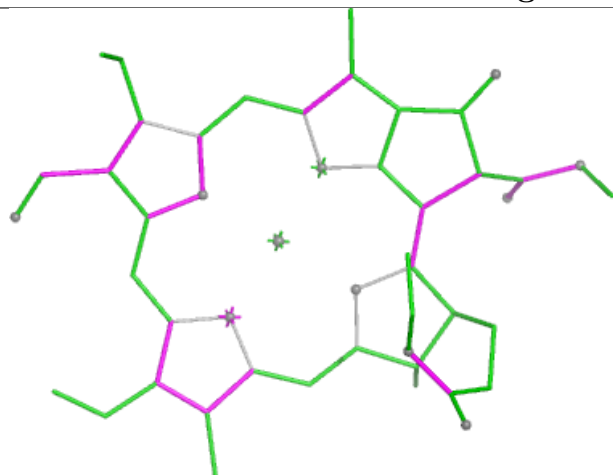
Ligand CLA c 520



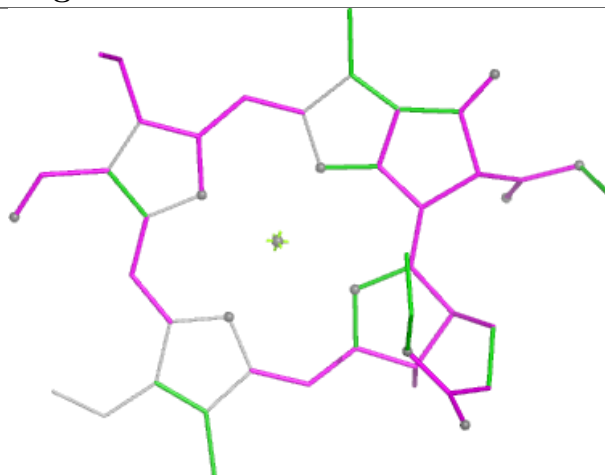




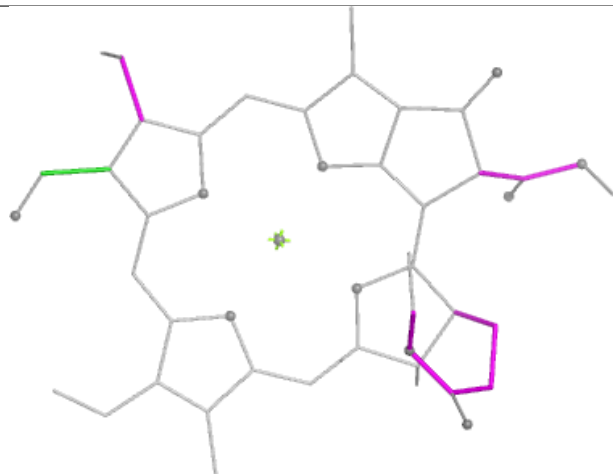
Ligand CHL g 314



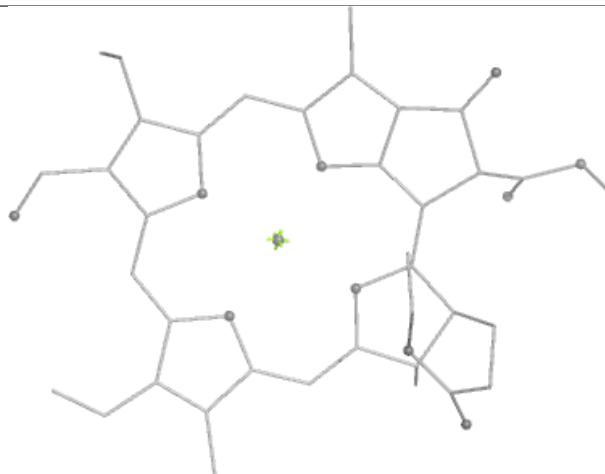
Bond lengths



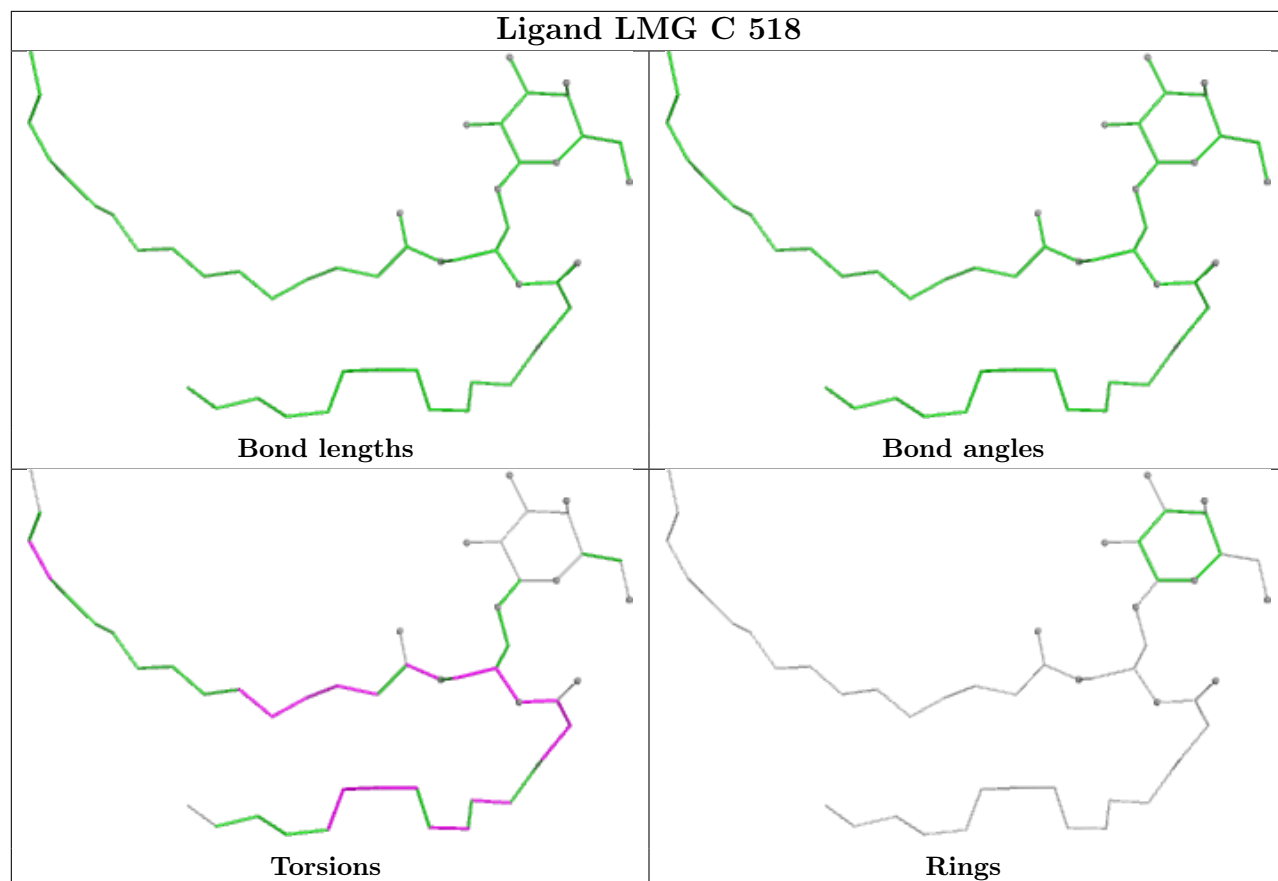
Bond angles

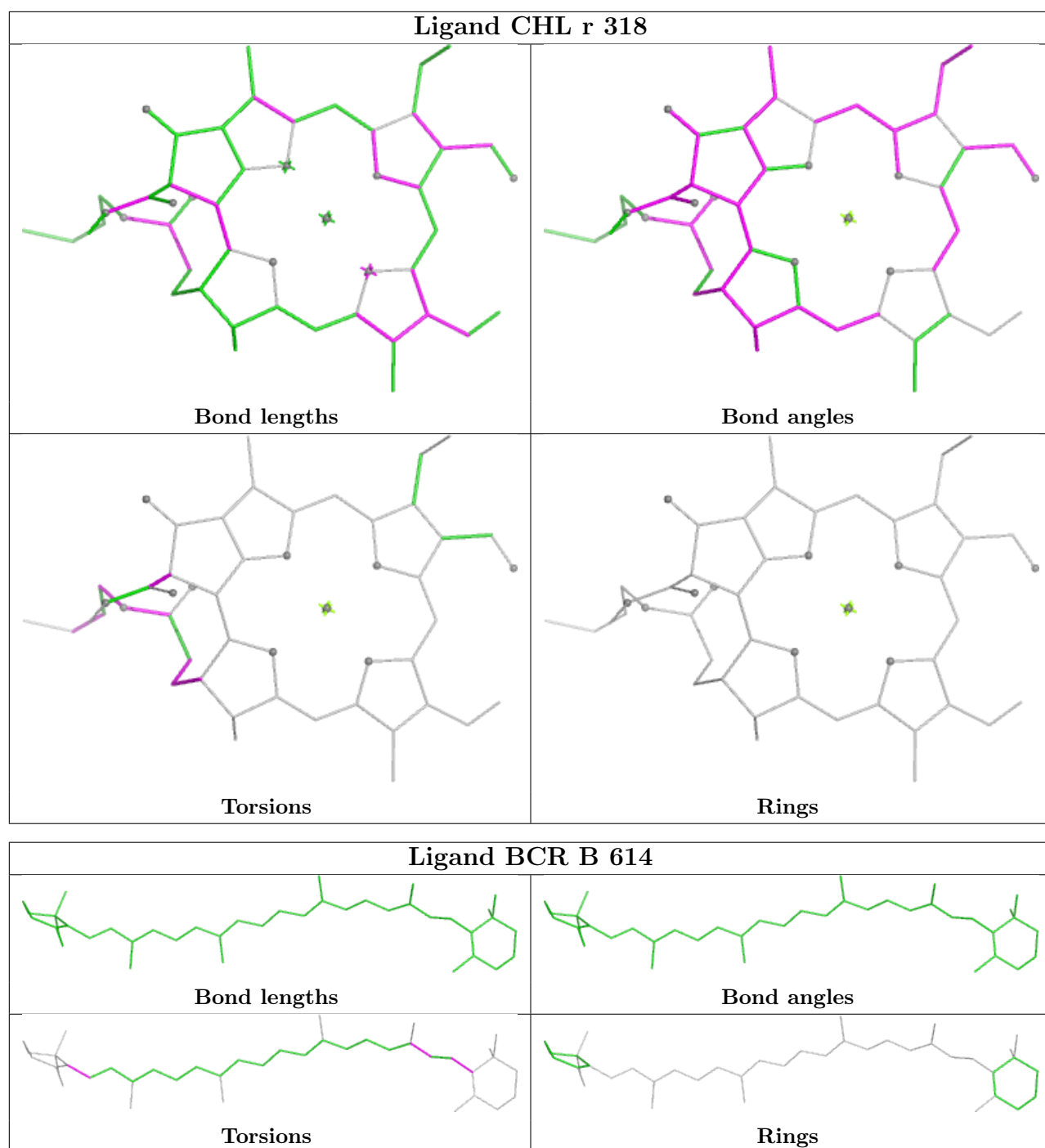


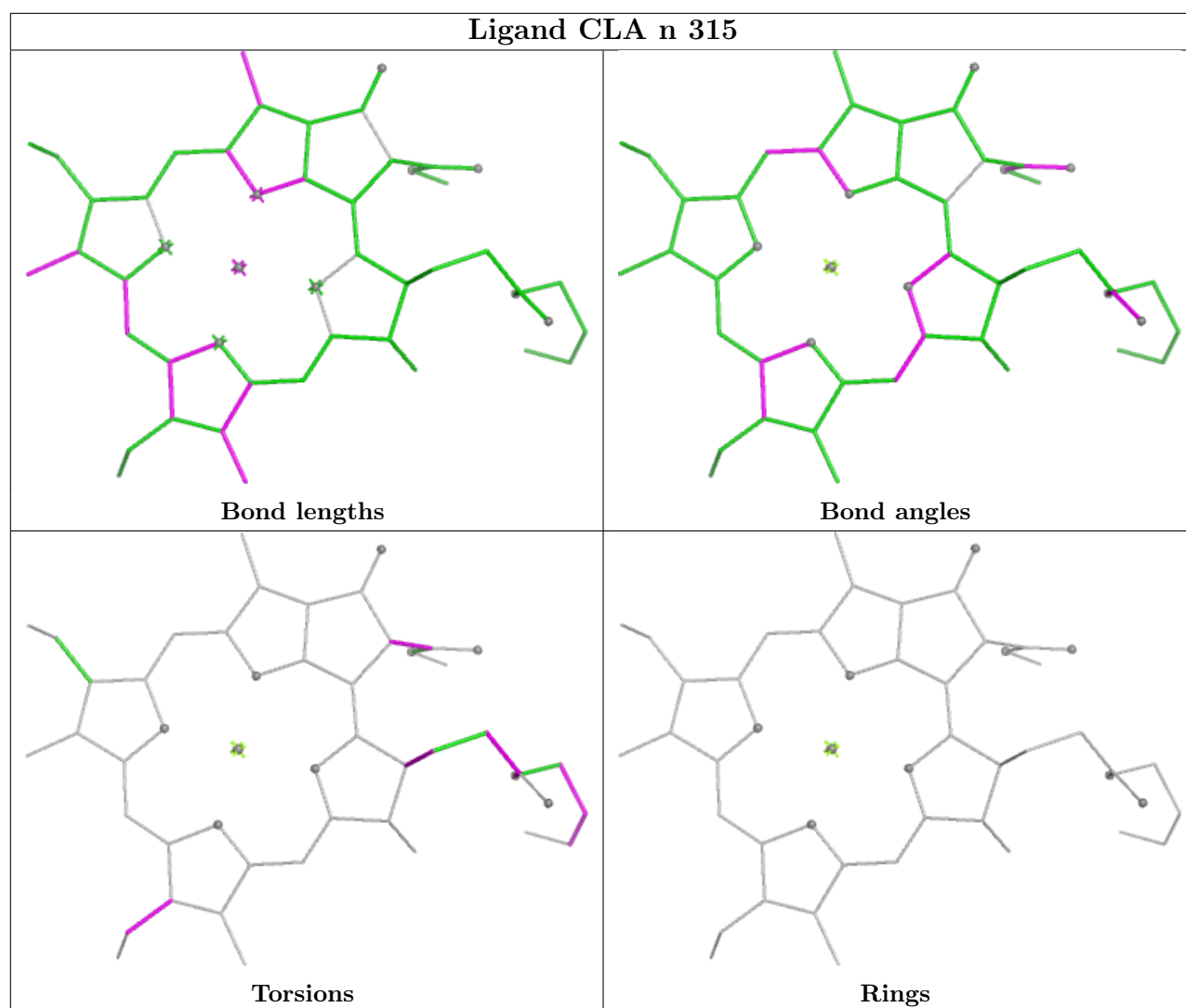
Torsions



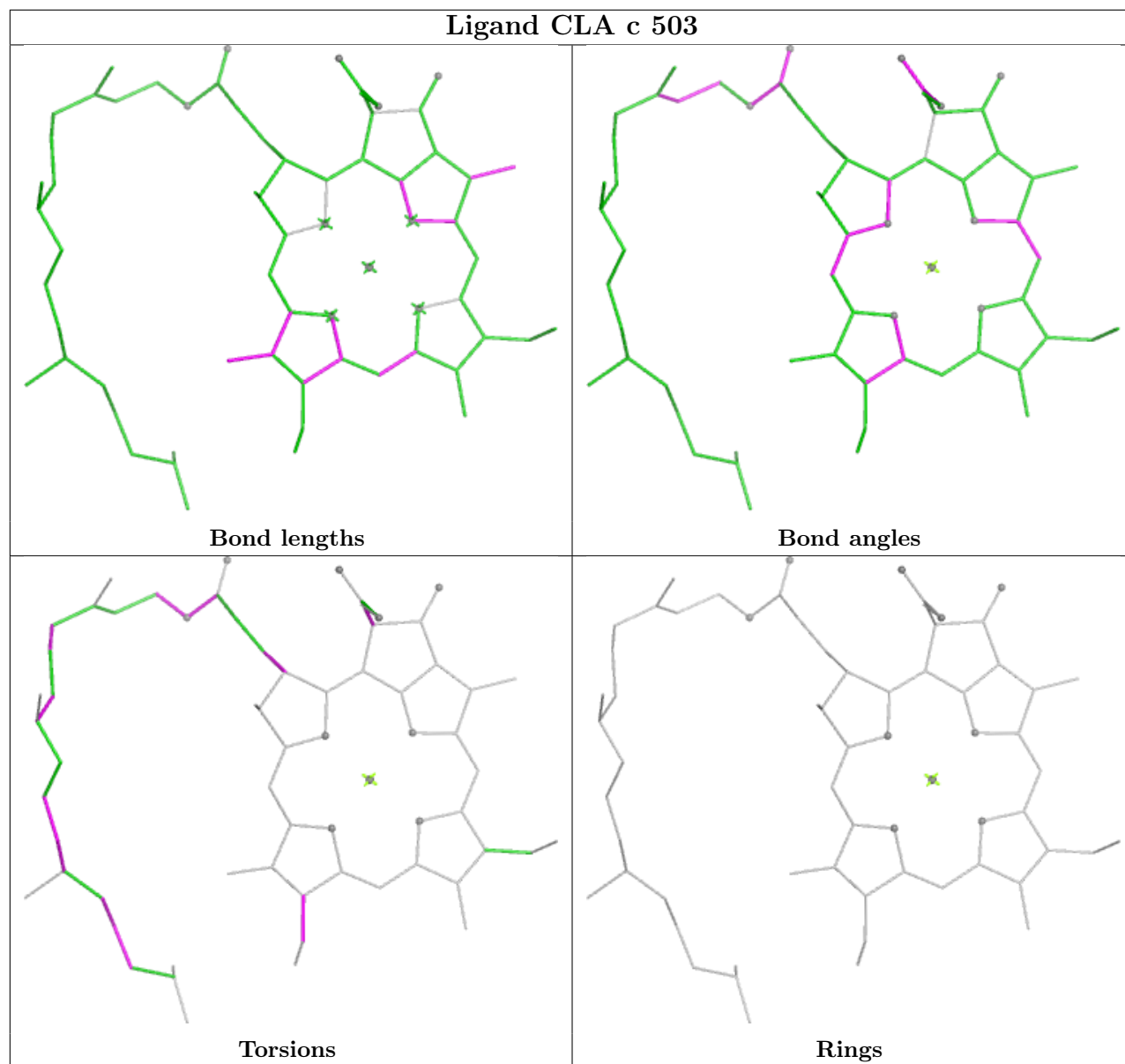
Rings



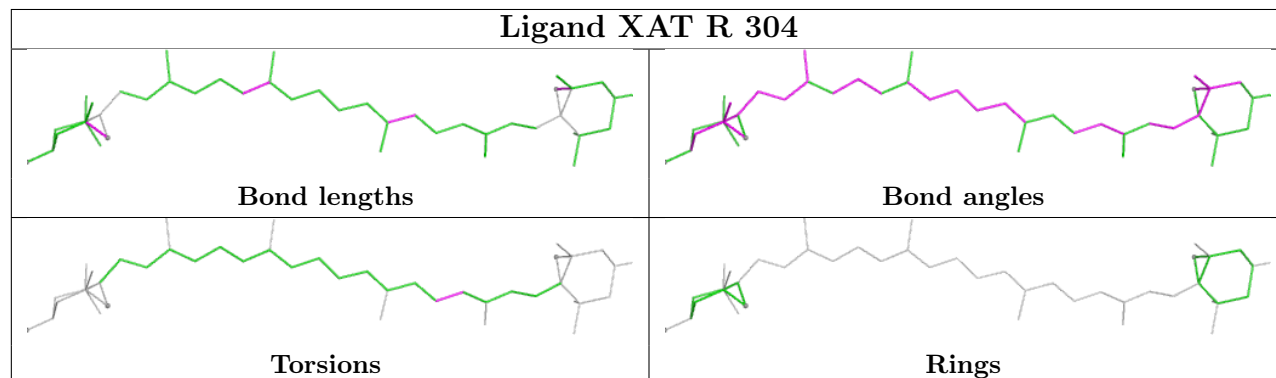


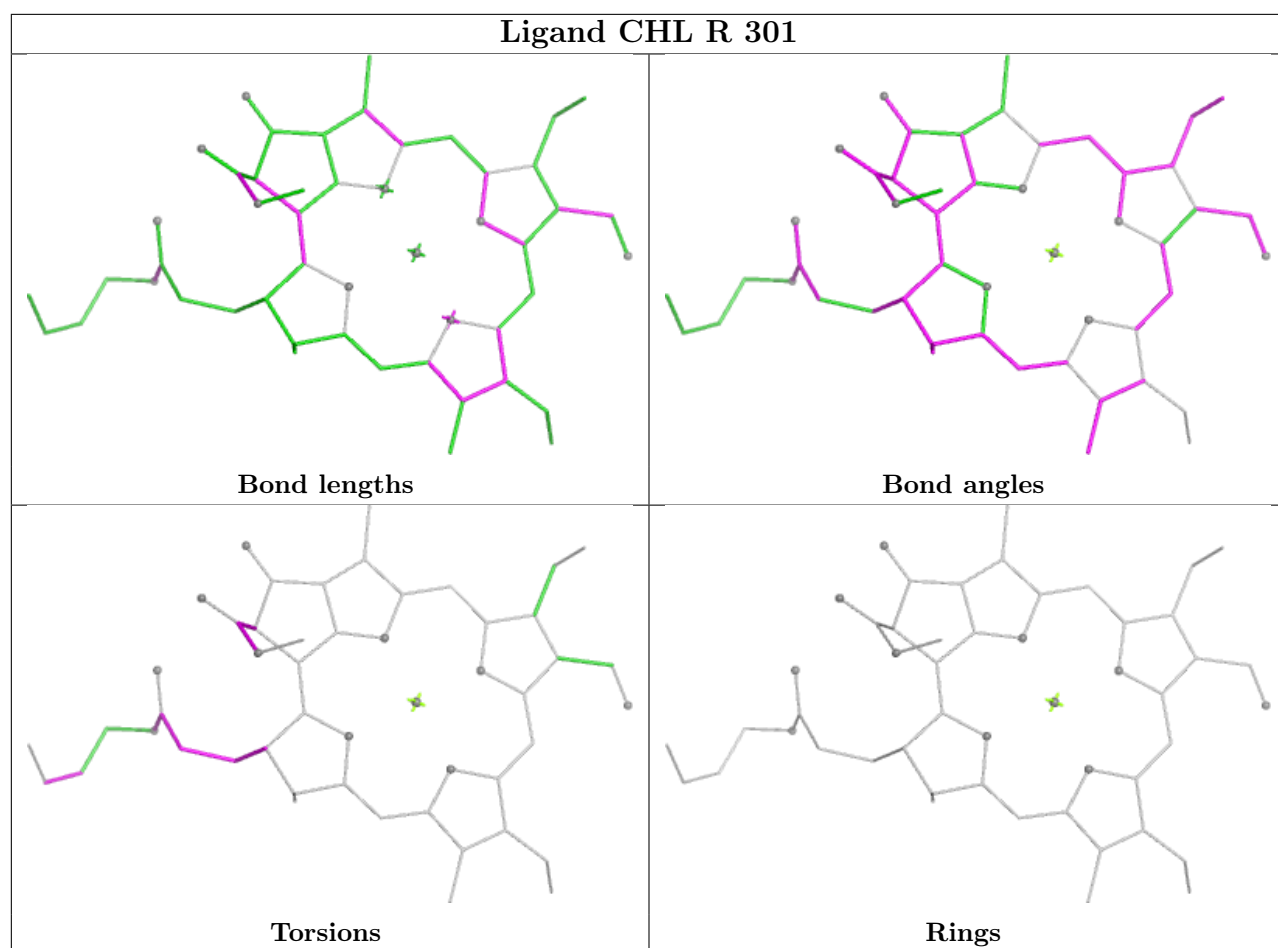


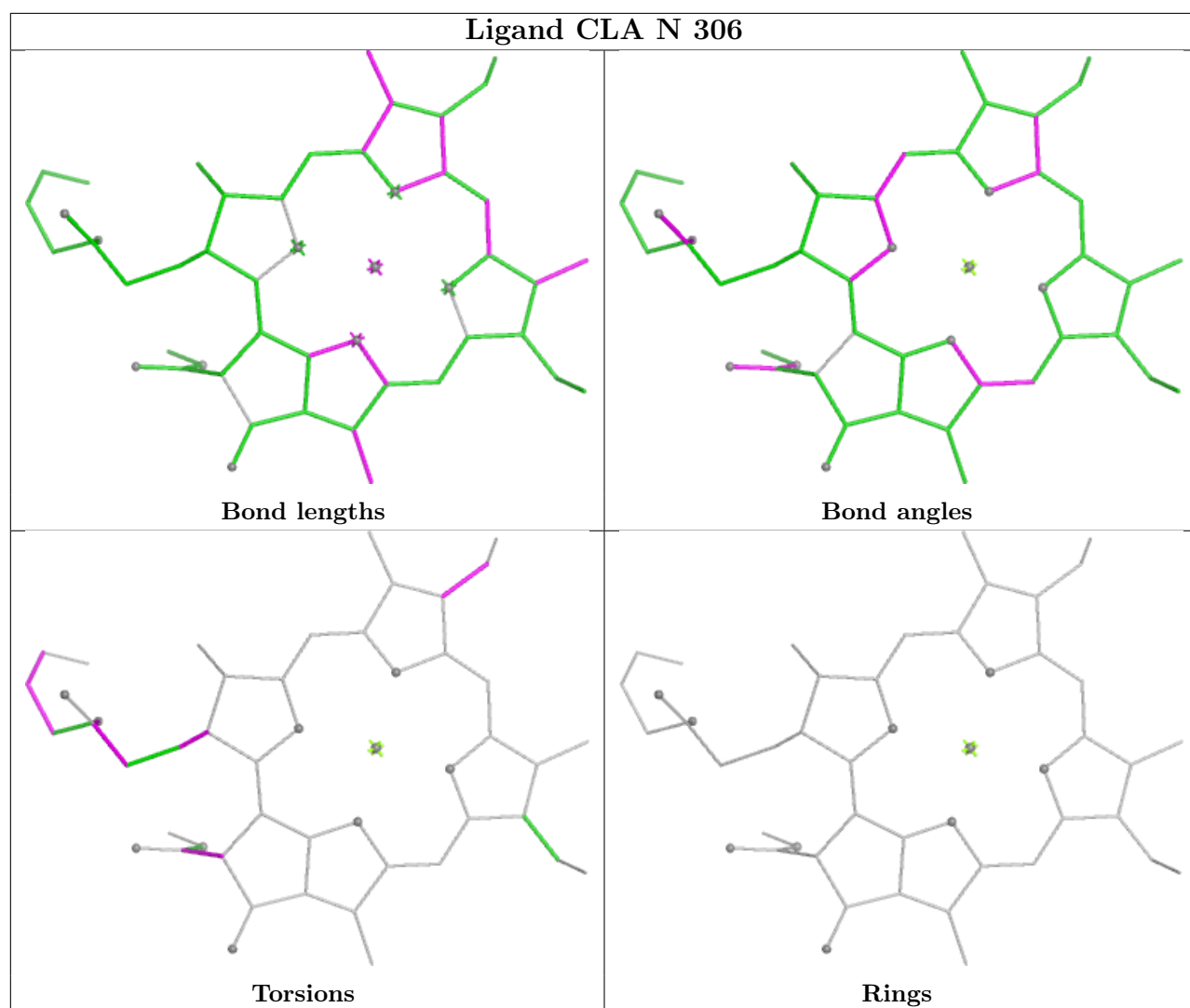
Ligand CLA c 503



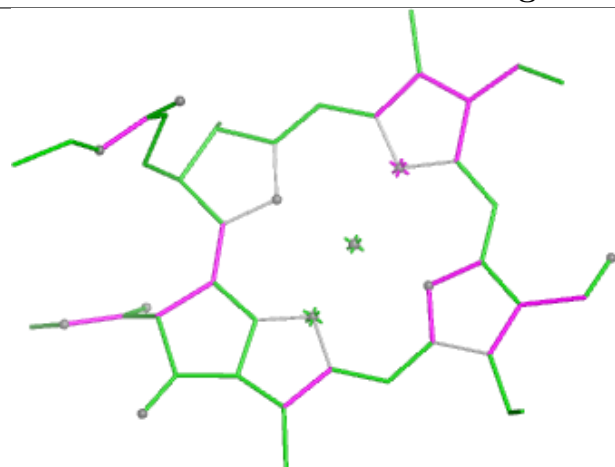
Ligand XAT R 304



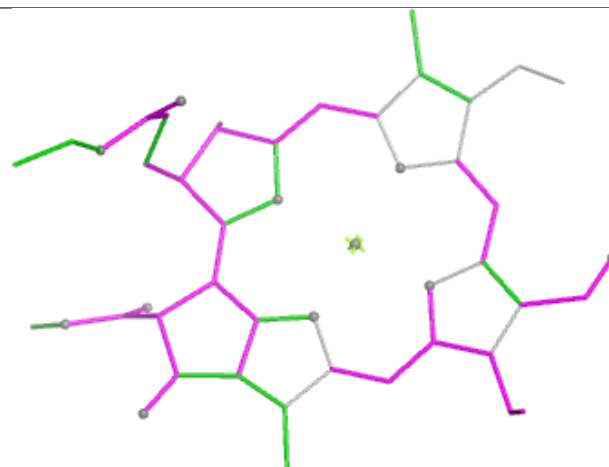




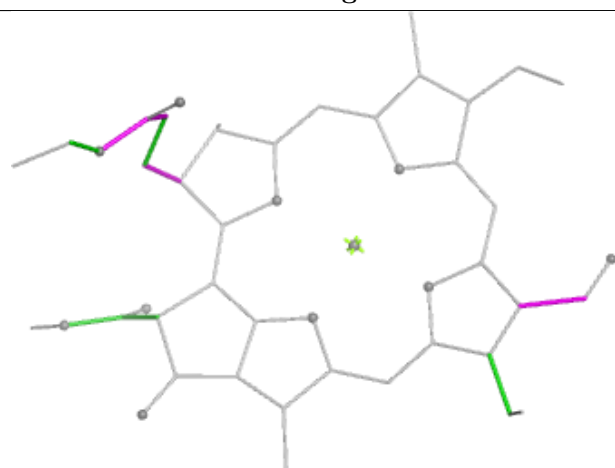
Ligand CHL n 308



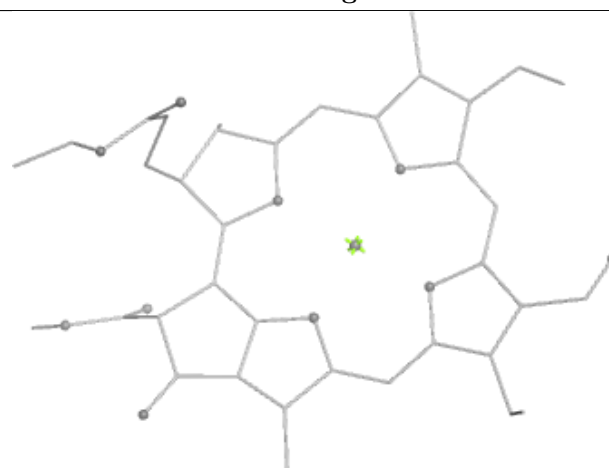
Bond lengths



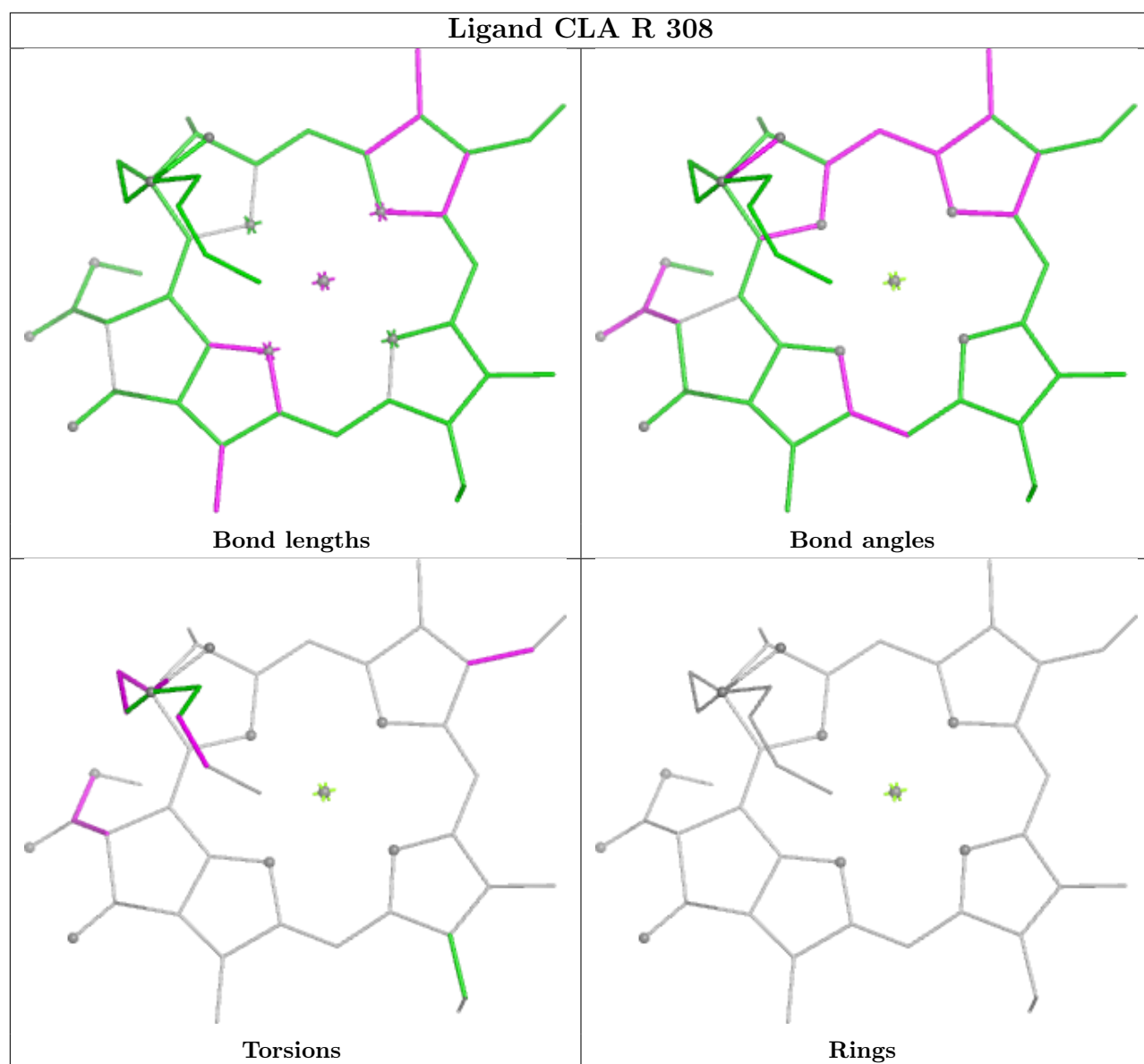
Bond angles

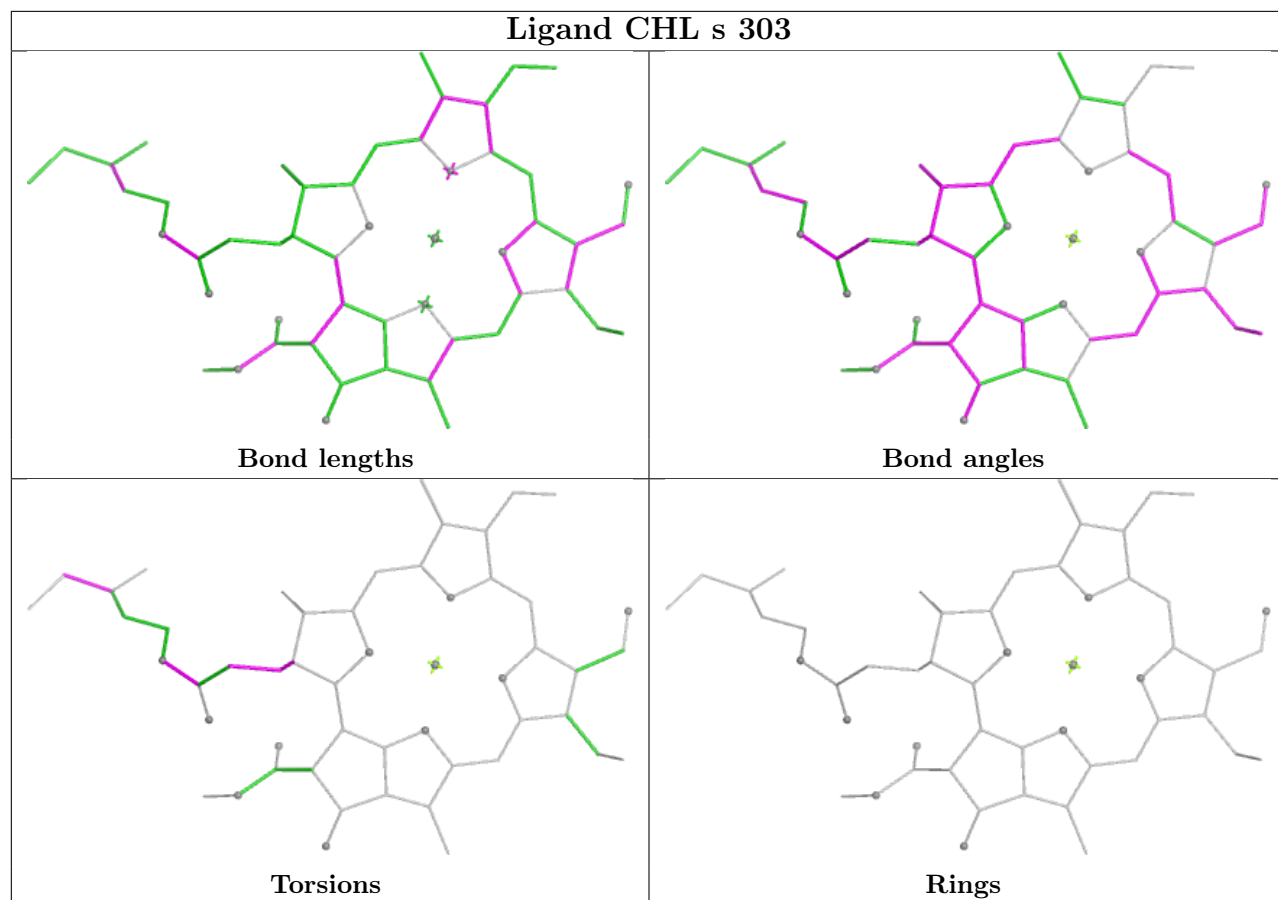


Torsions

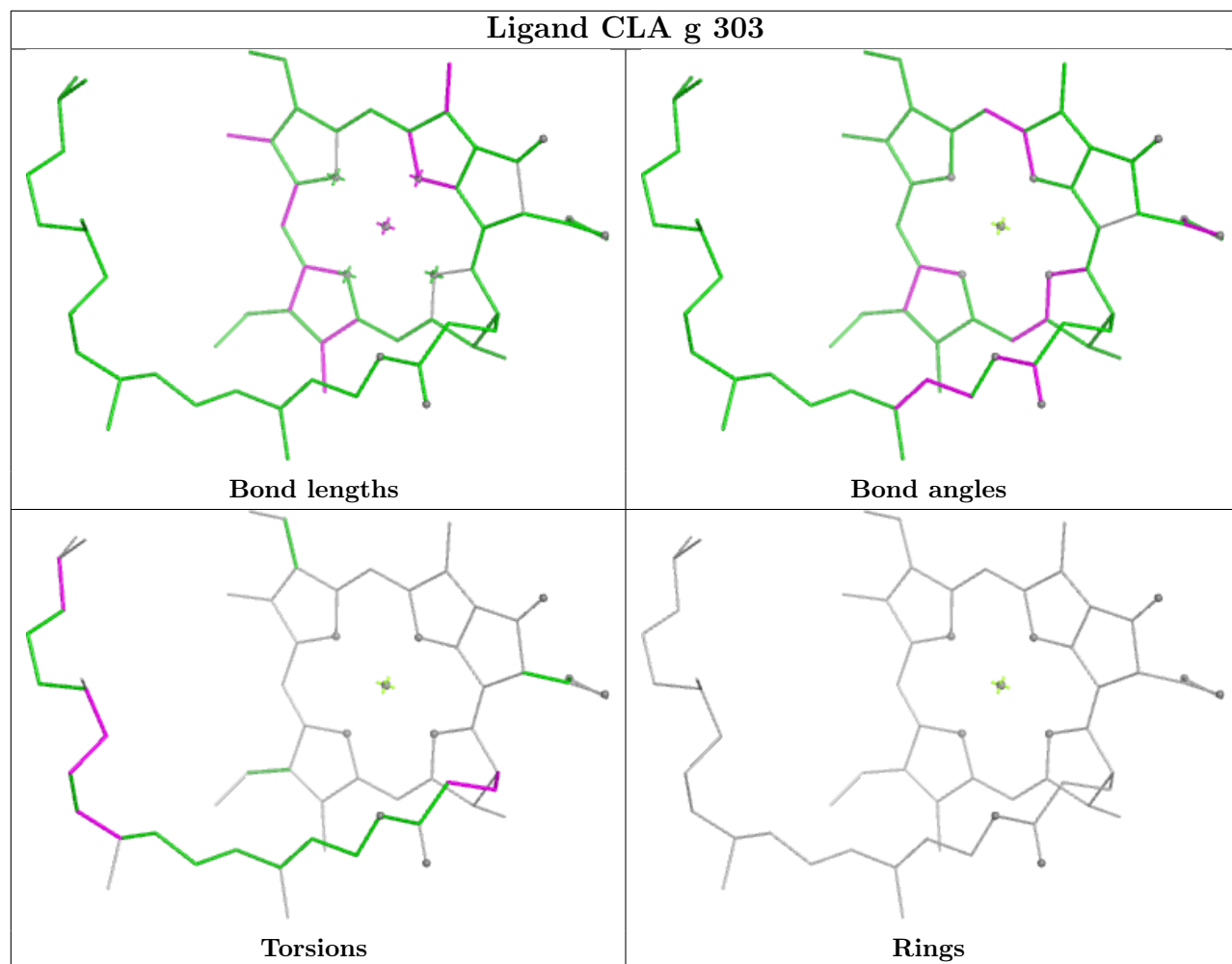


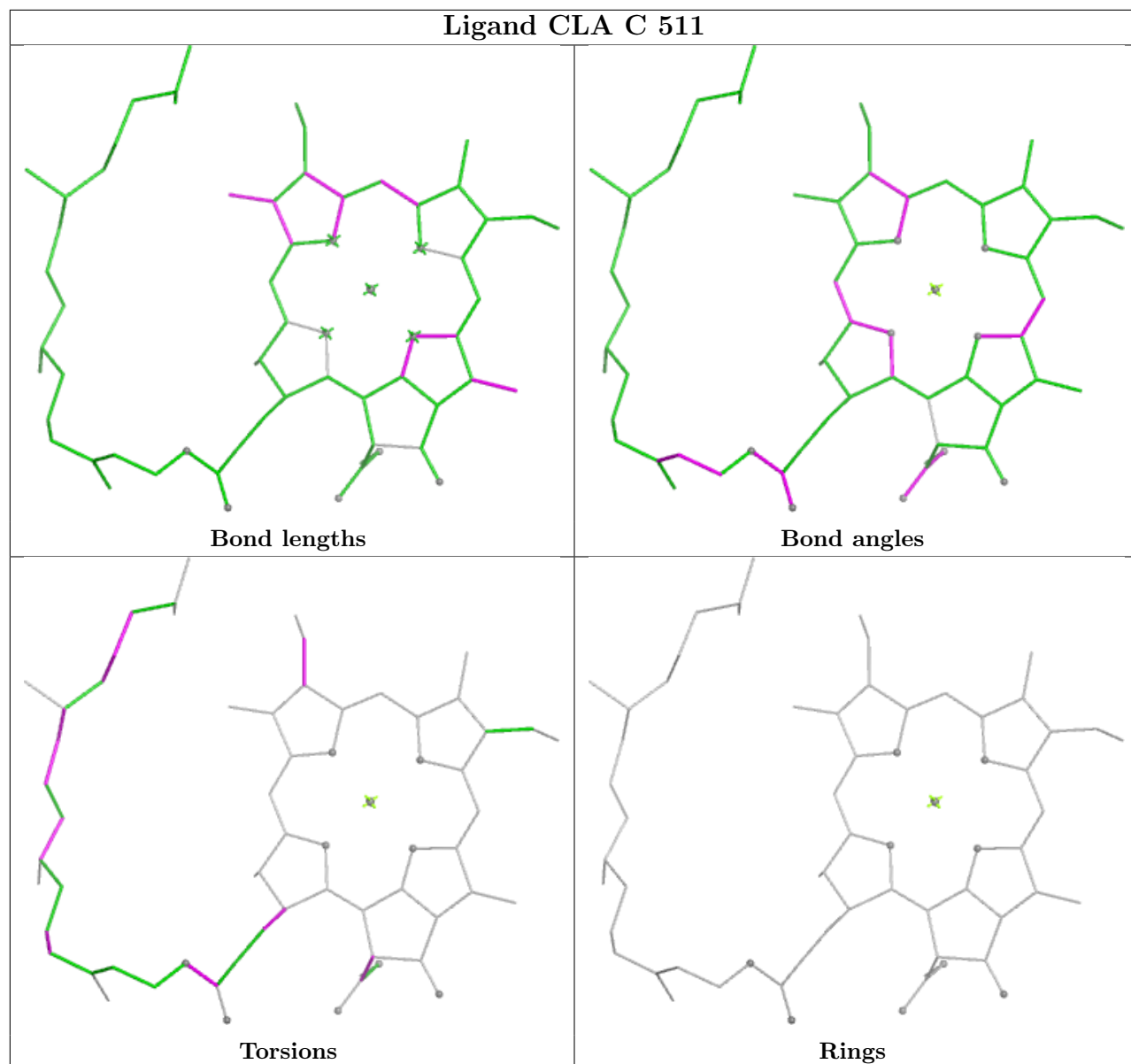
Rings

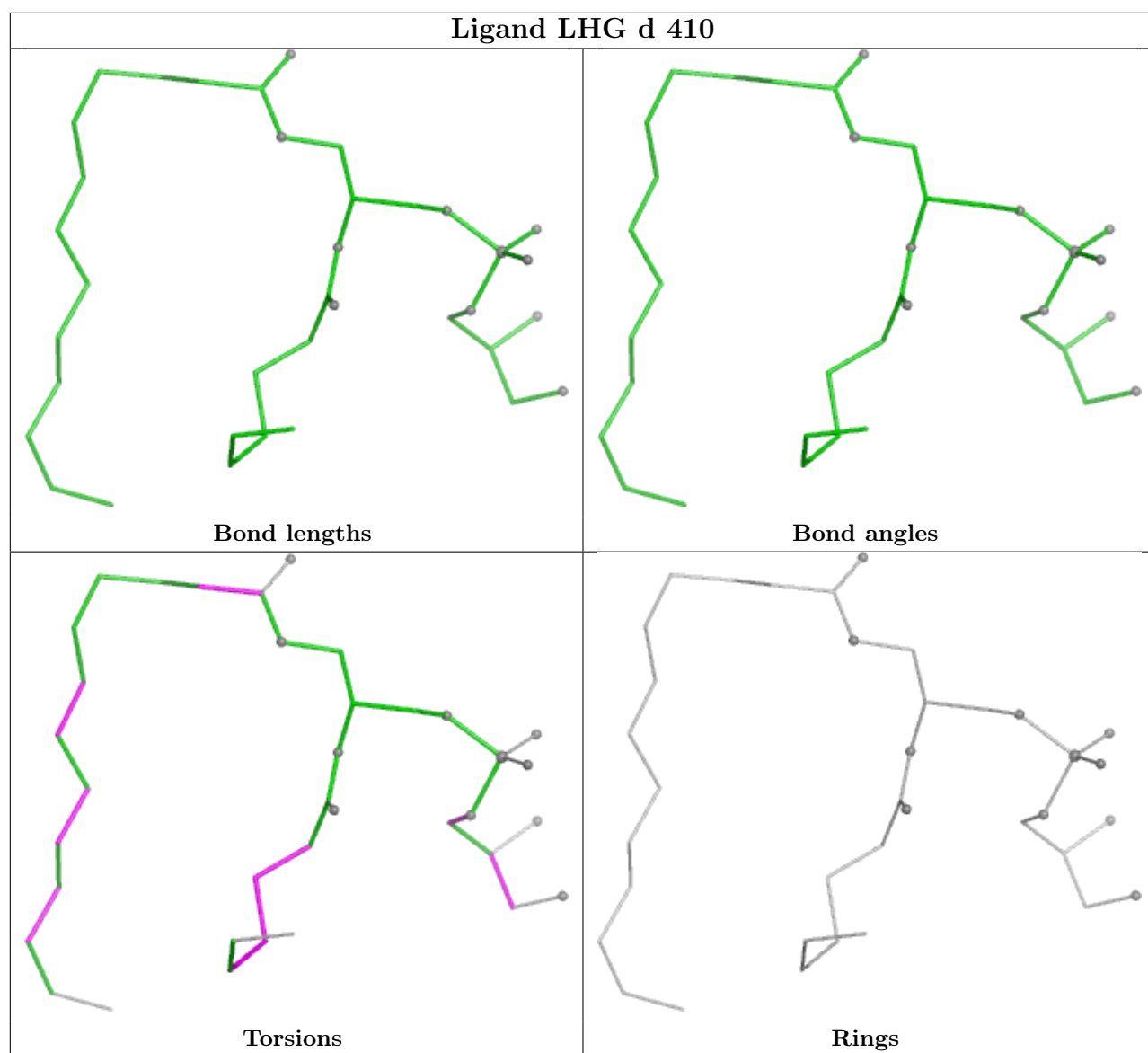


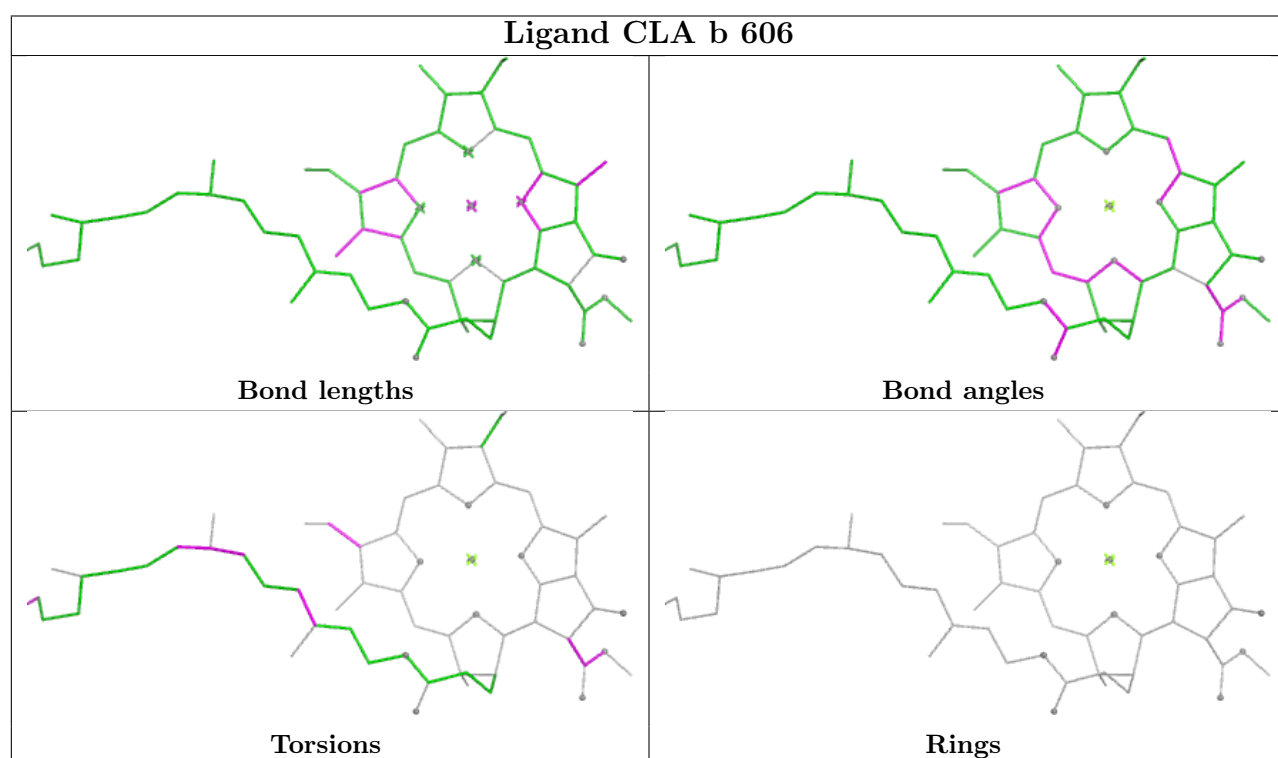
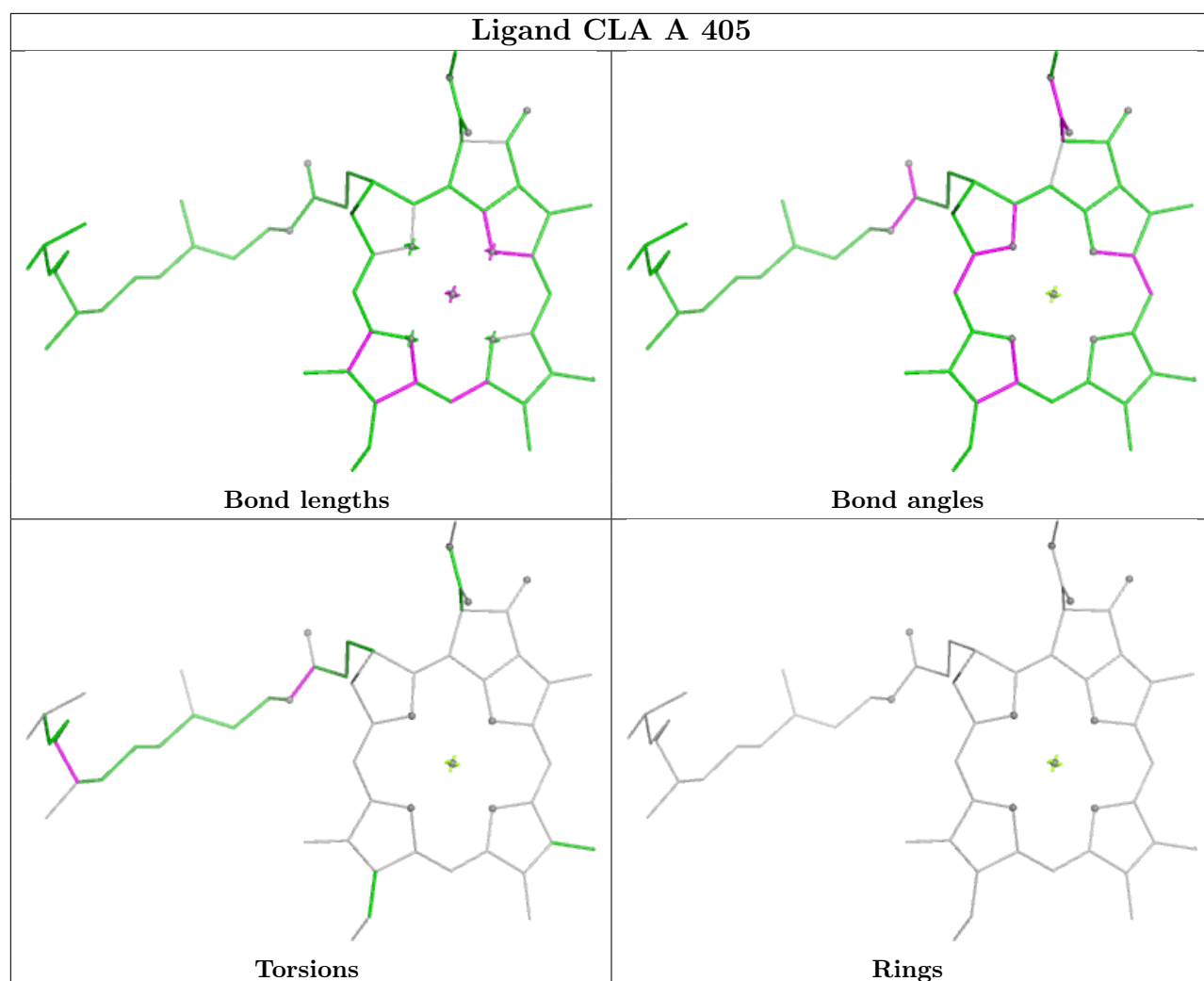


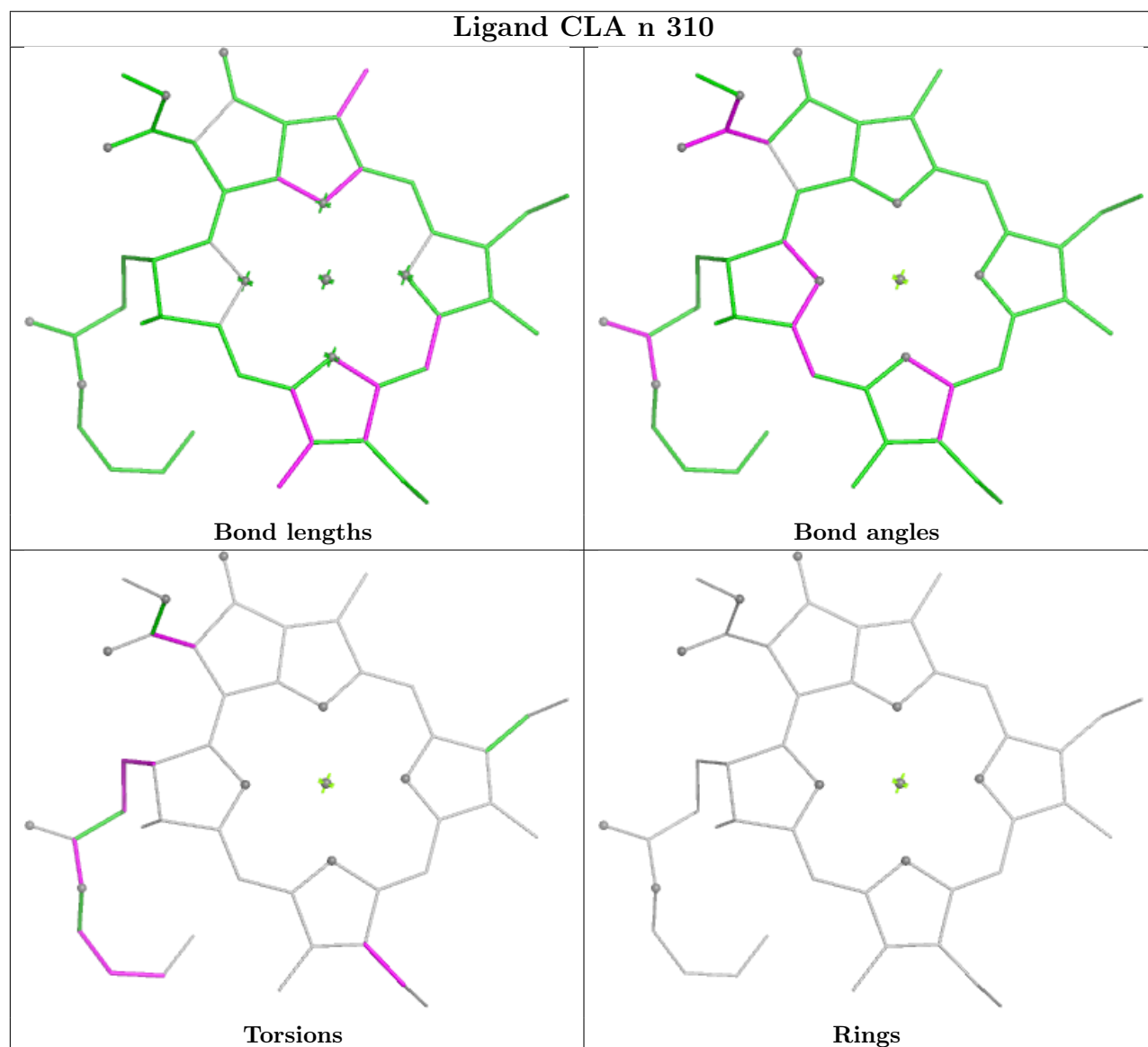
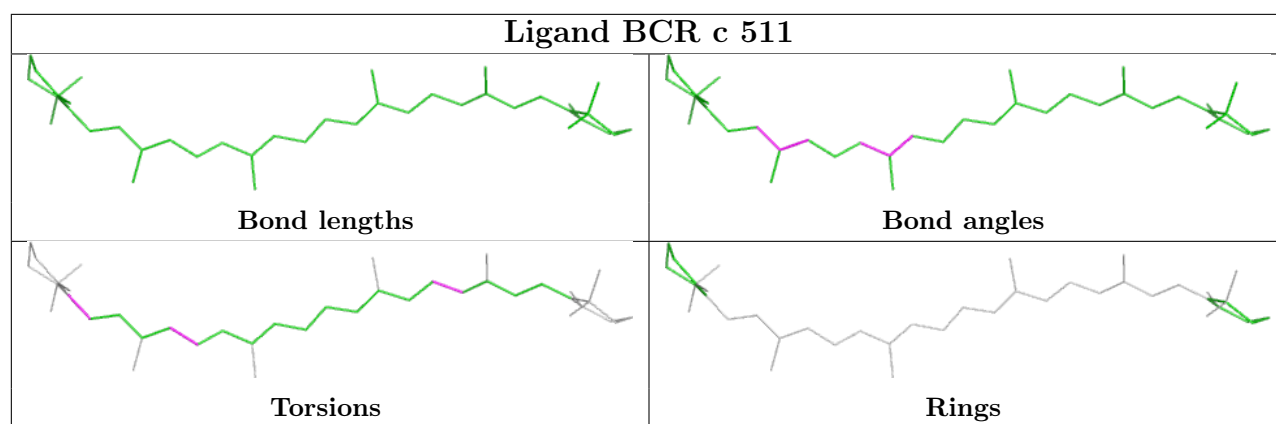
Ligand CLA g 303



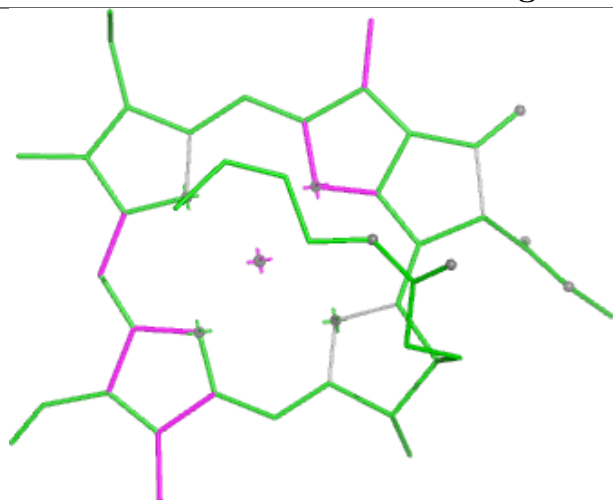




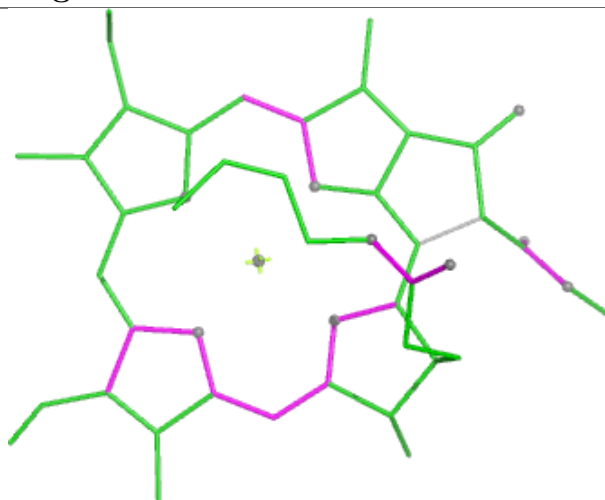




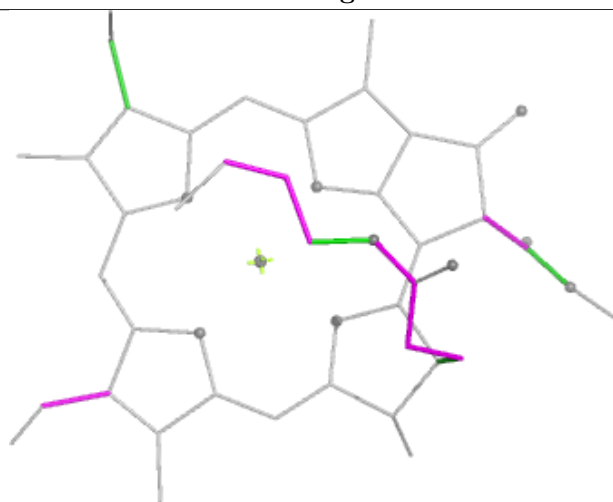
Ligand CLA g 305



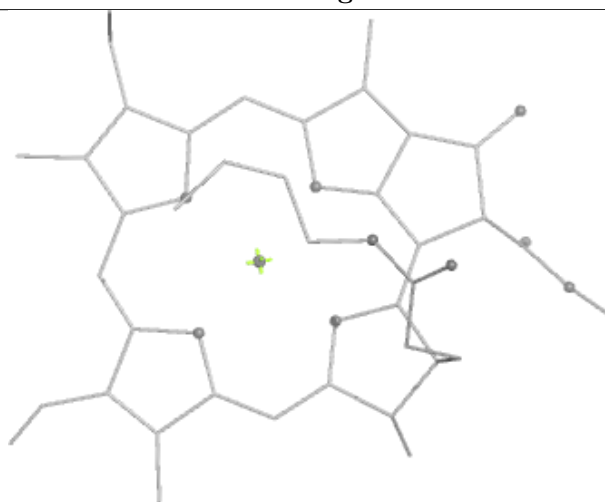
Bond lengths



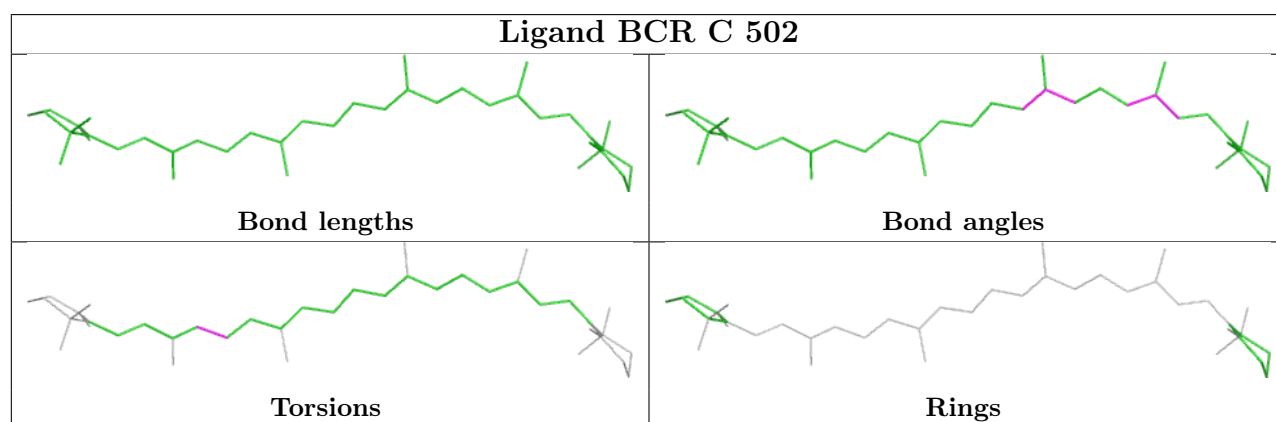
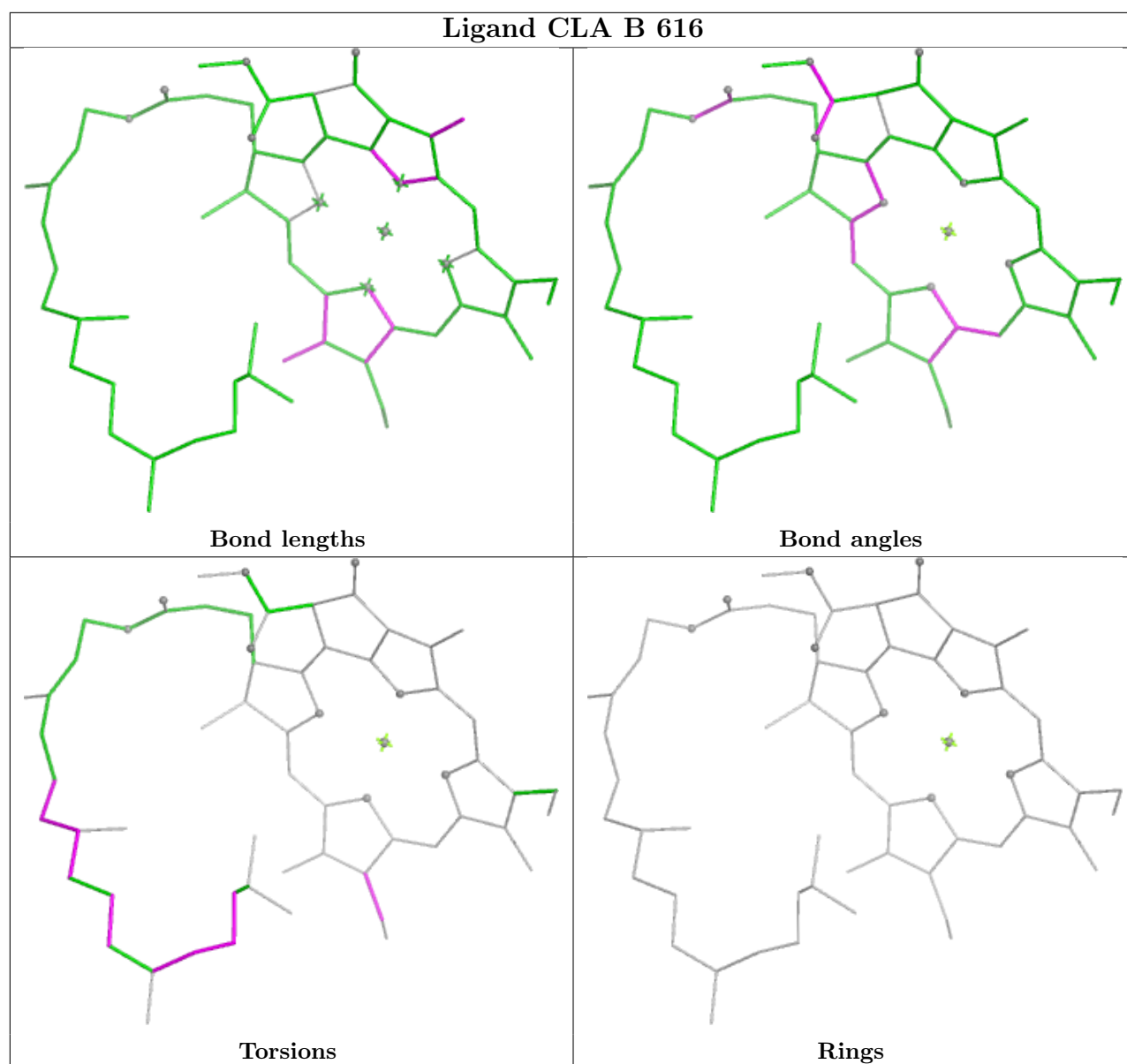
Bond angles

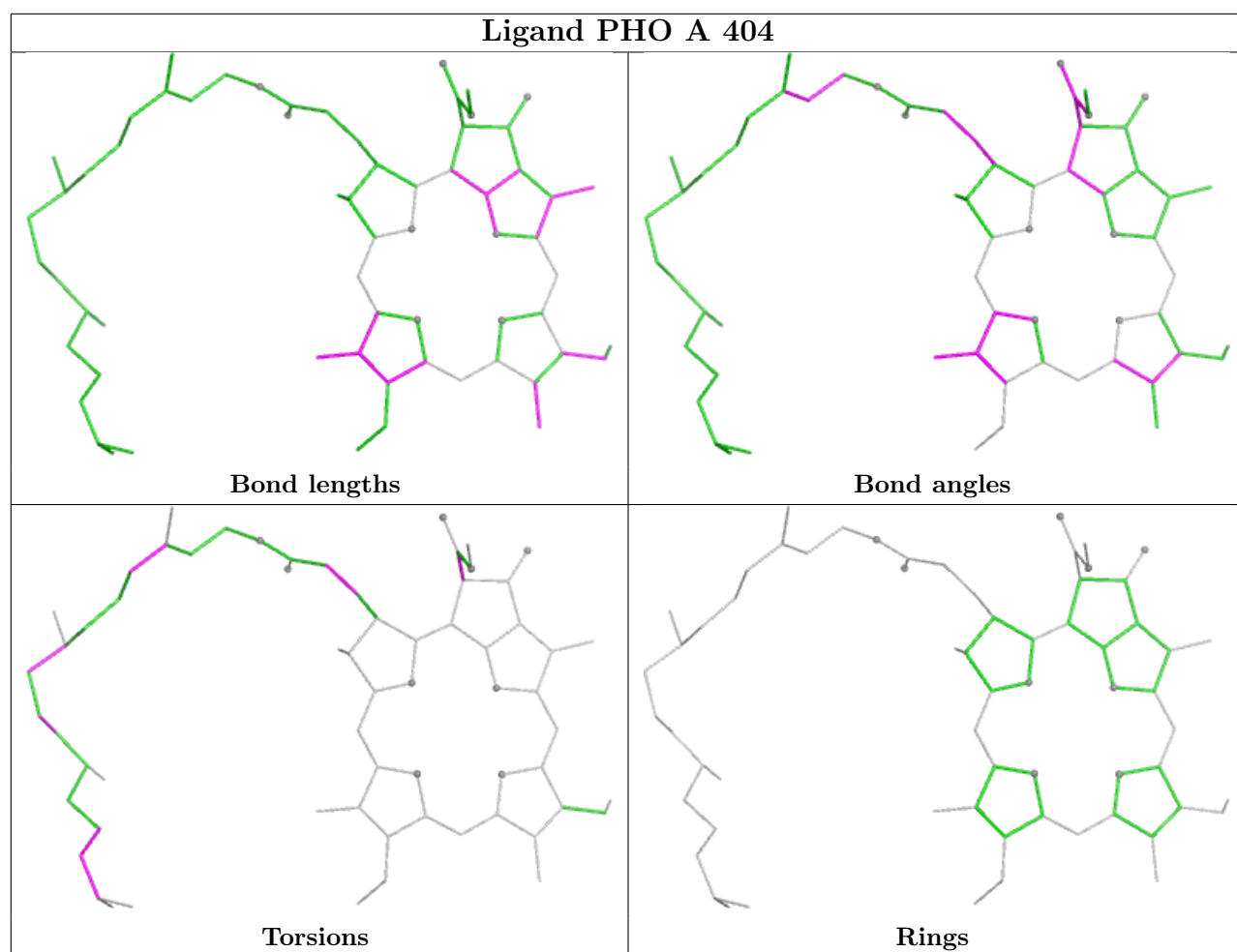


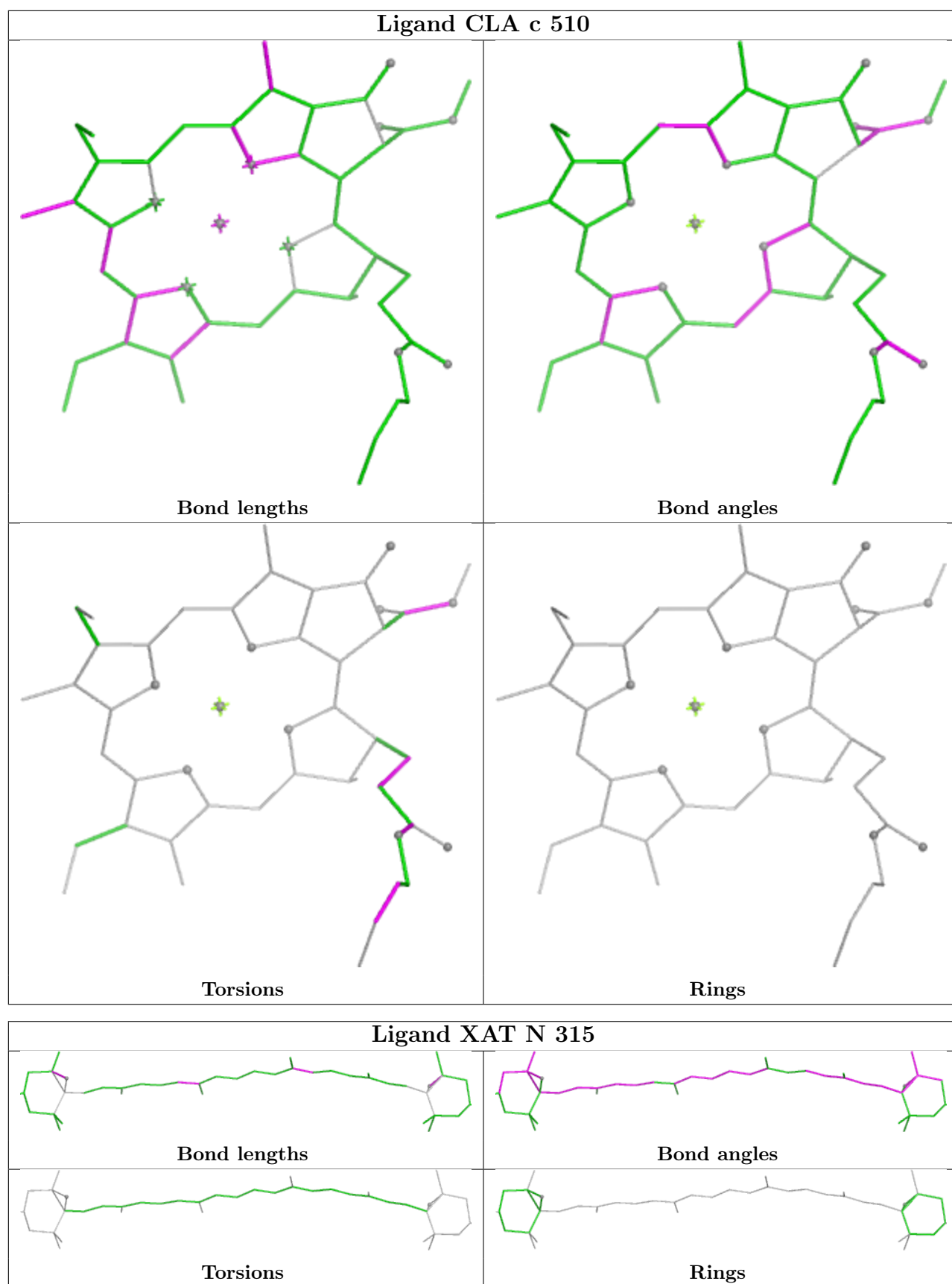
Torsions

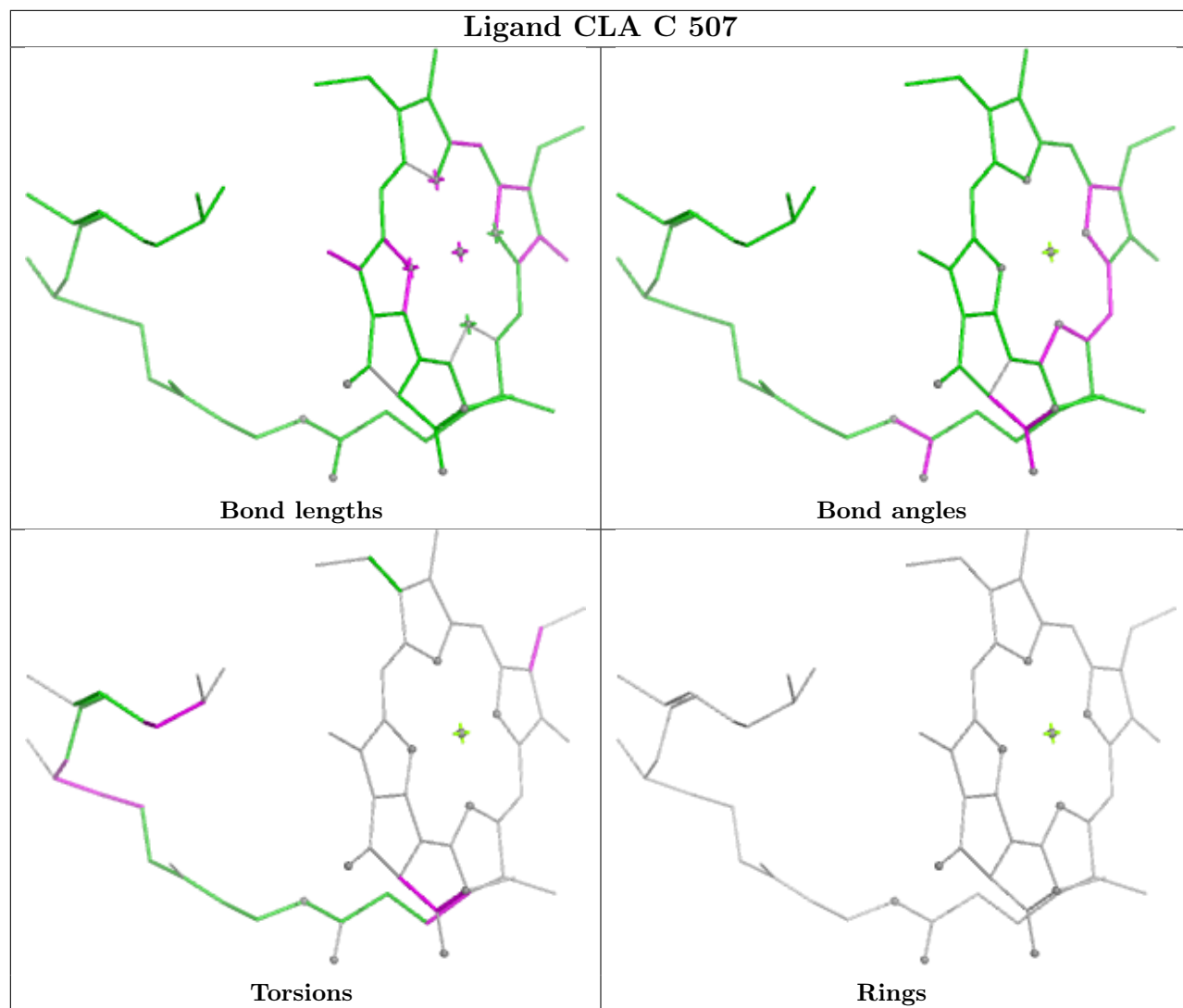


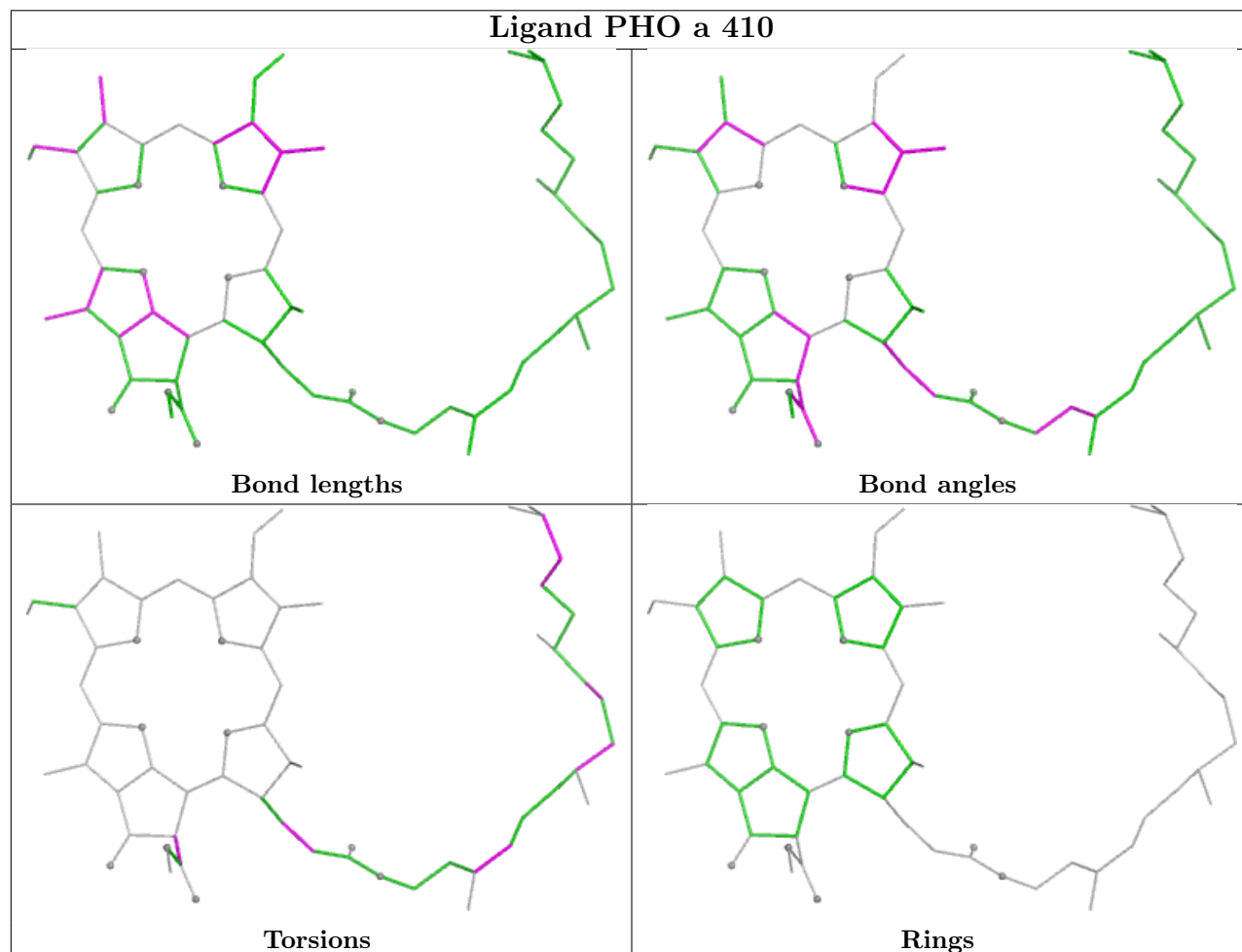
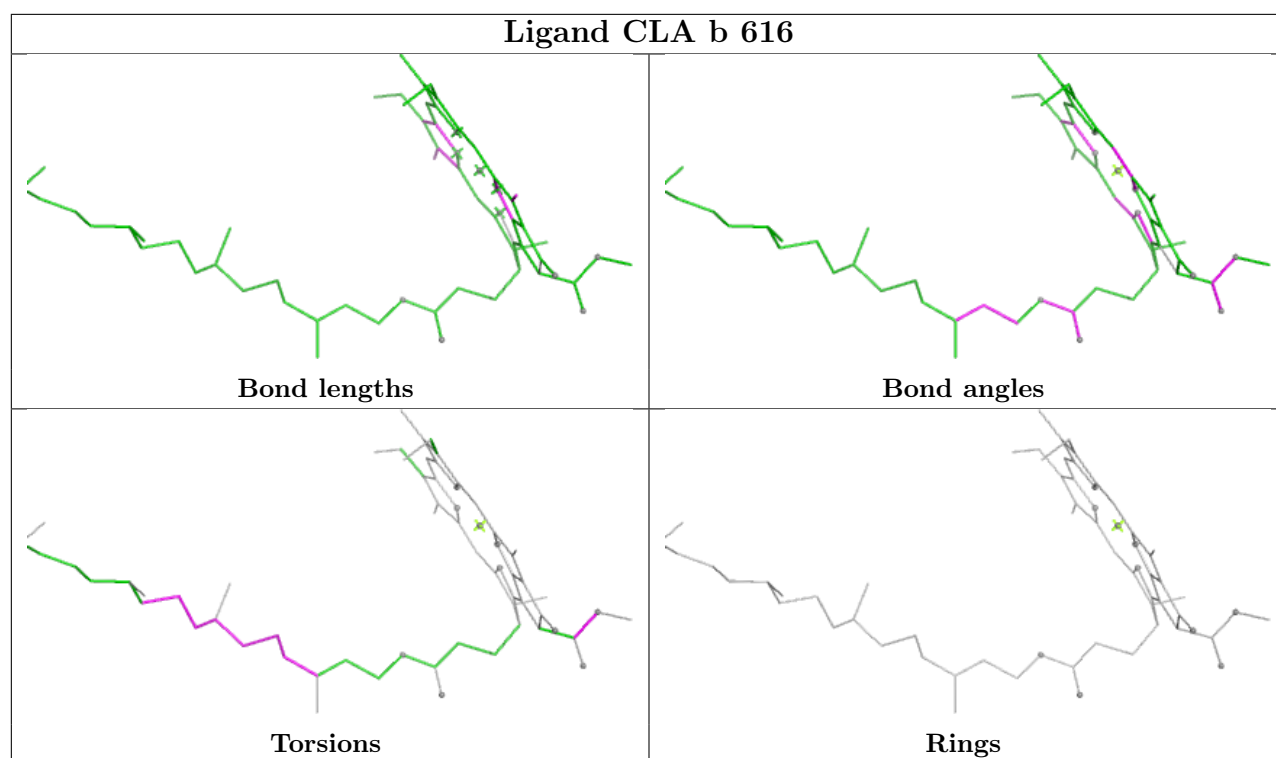
Rings

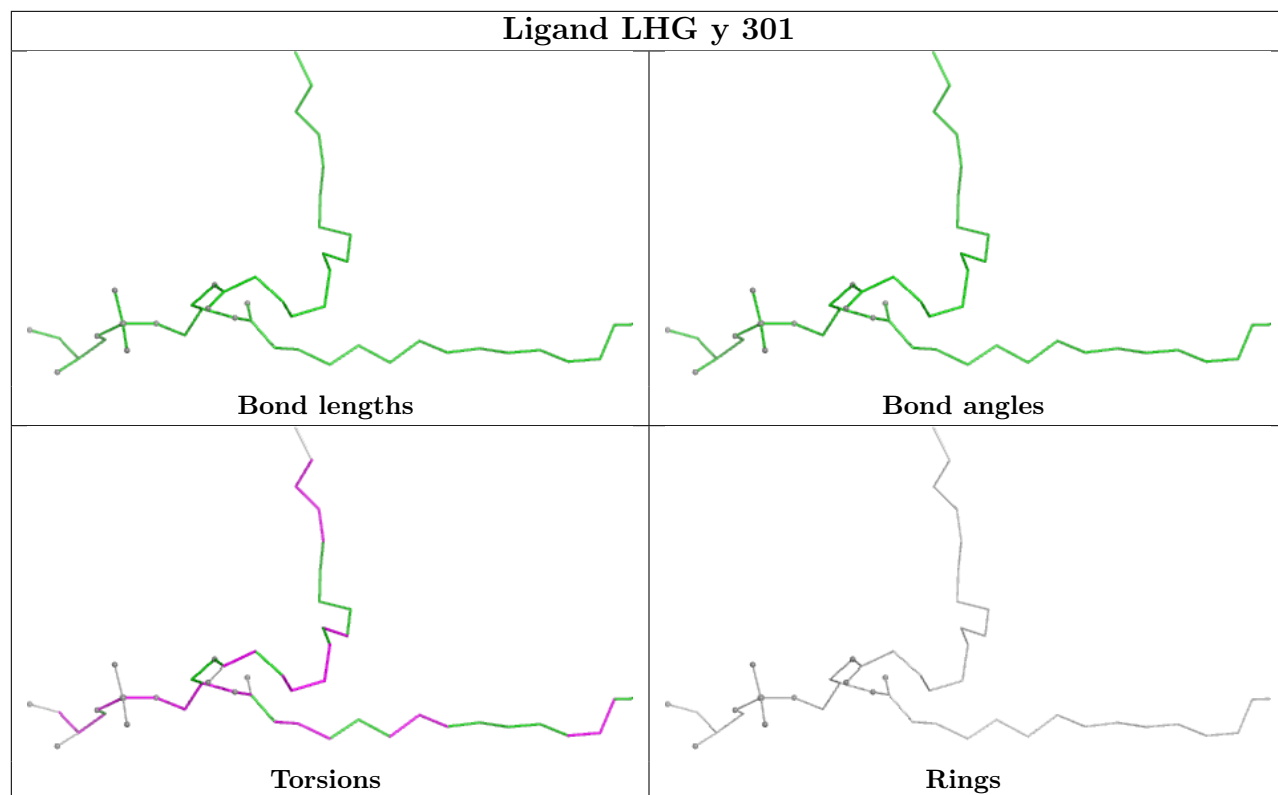


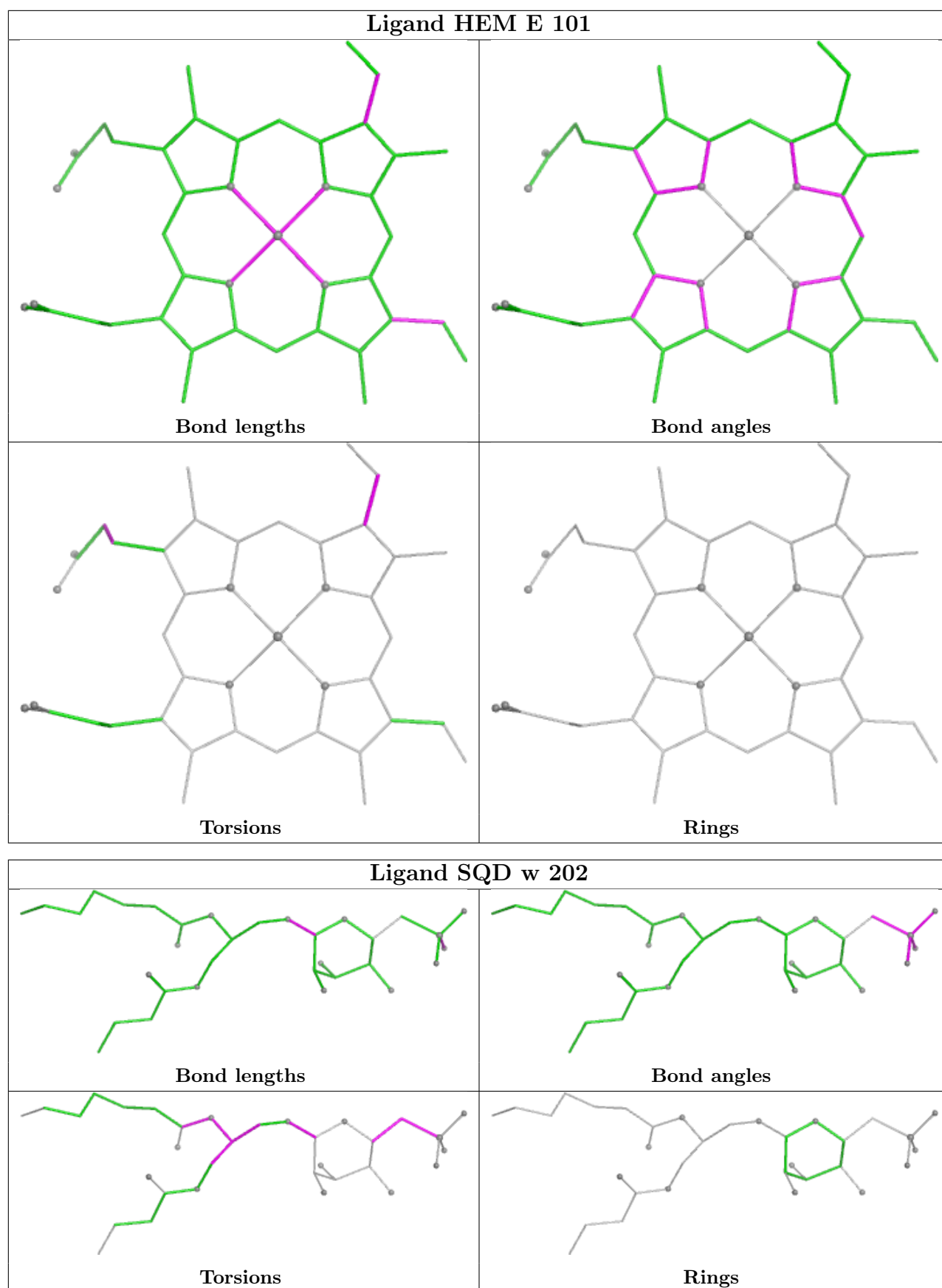


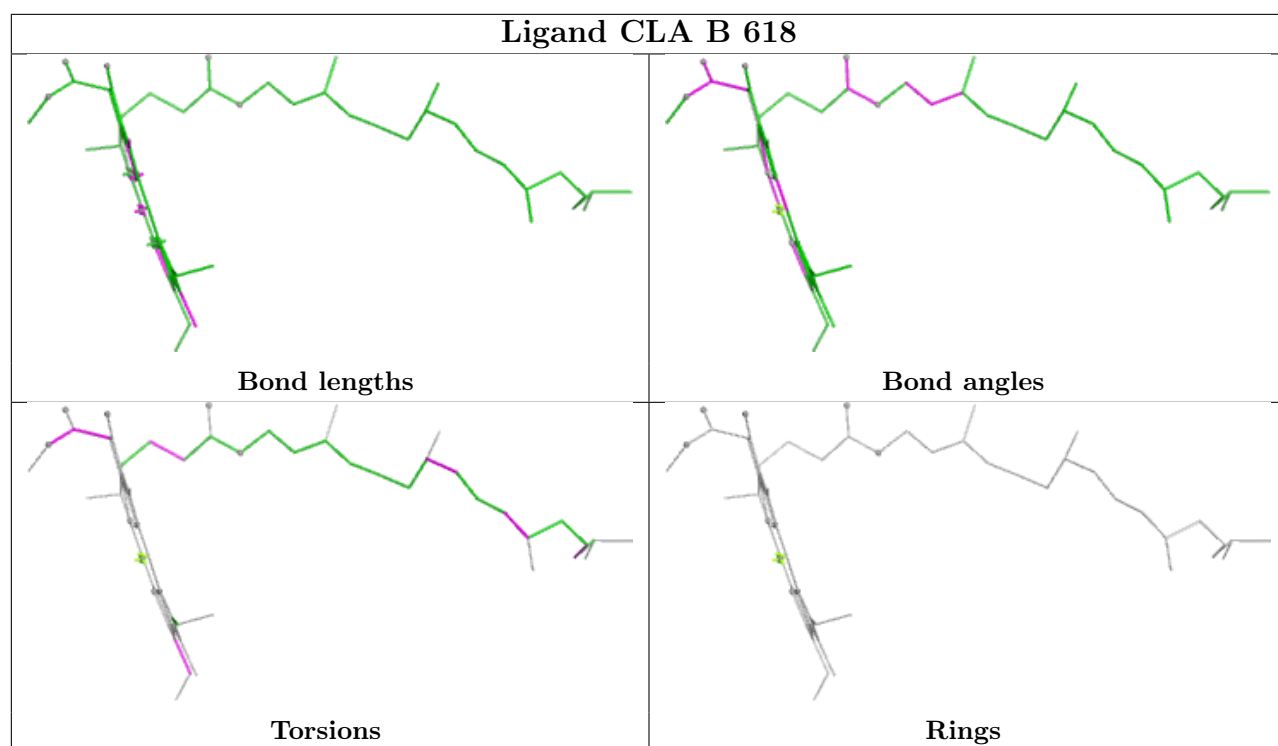




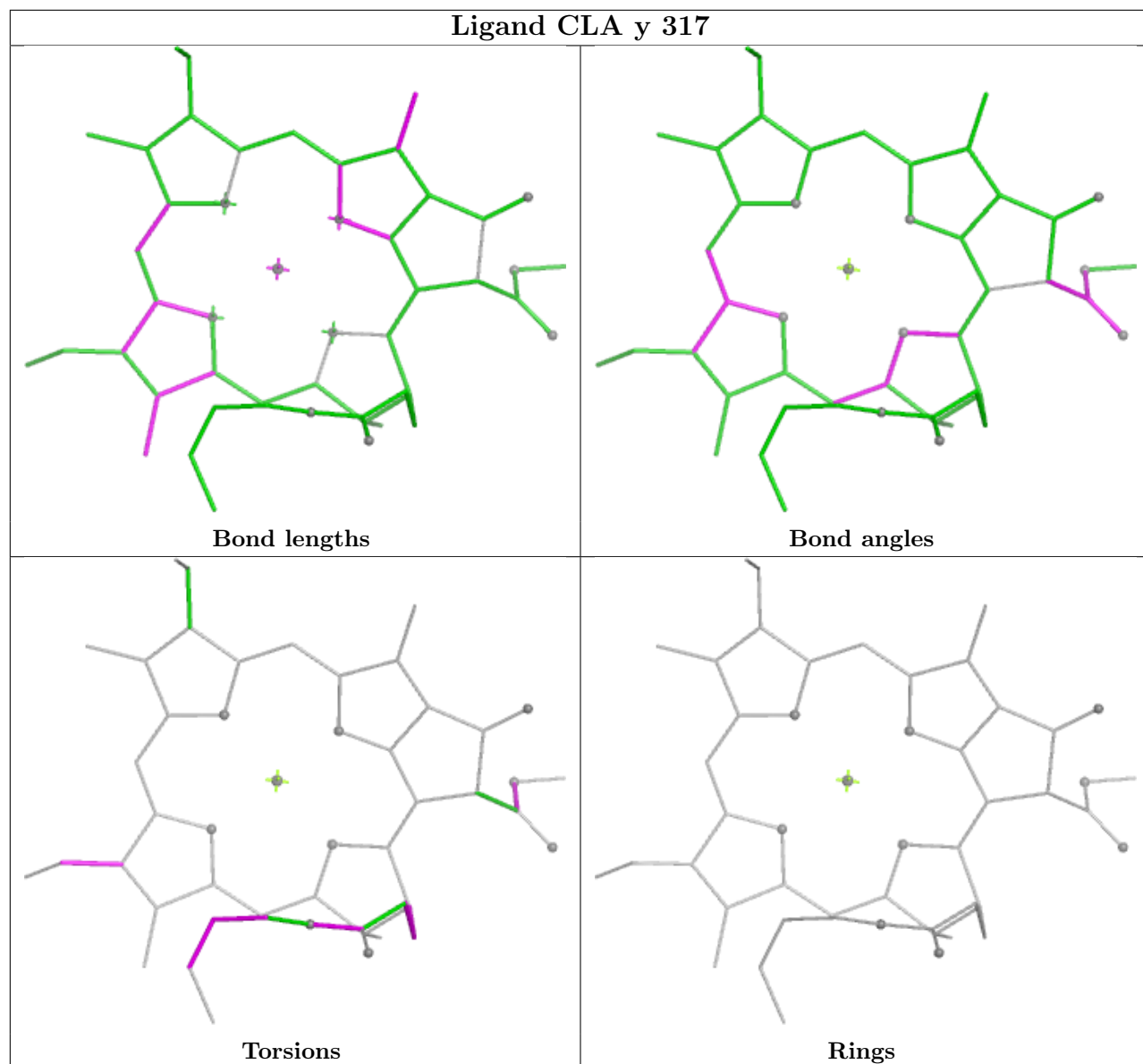


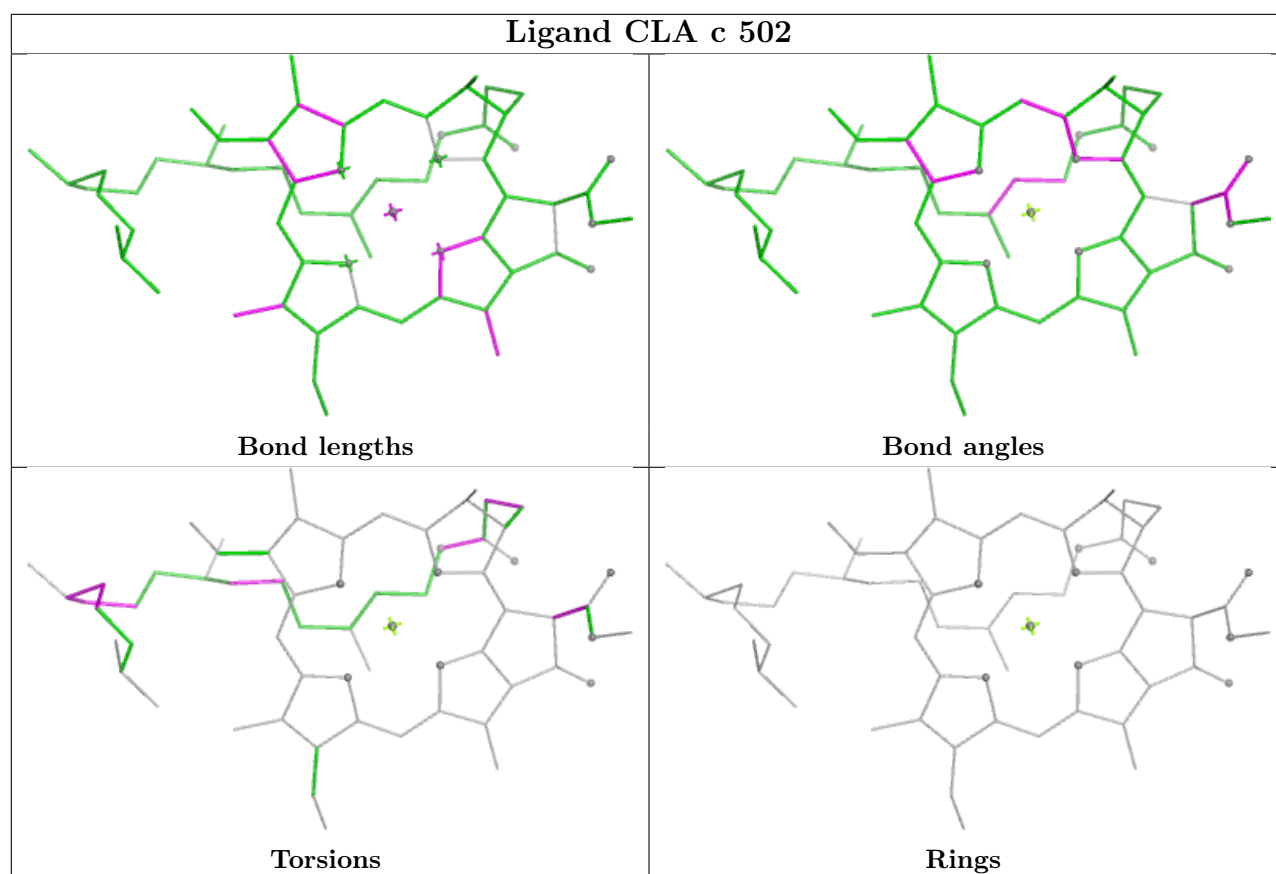




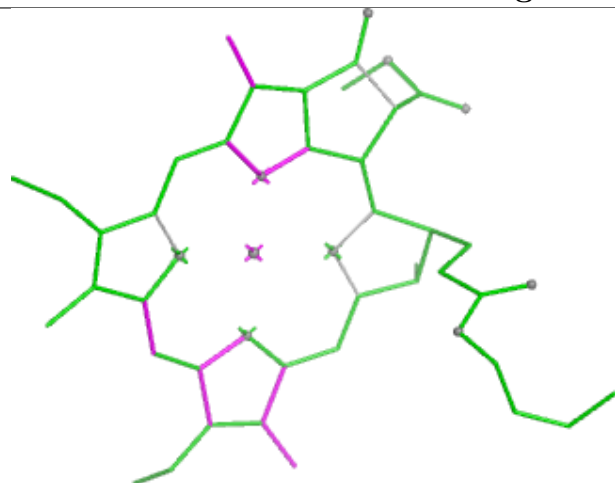


Ligand CLA y 317

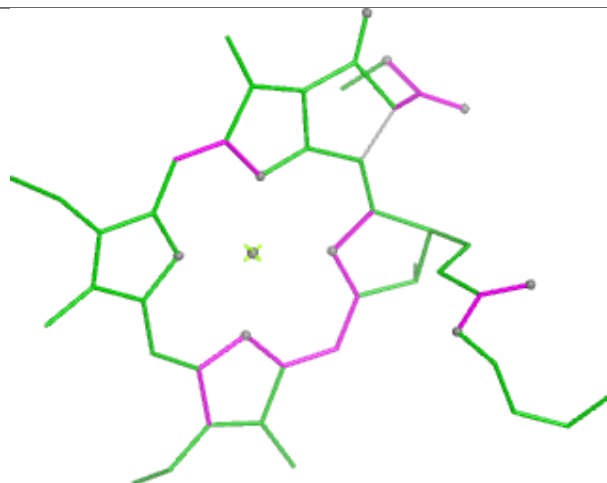




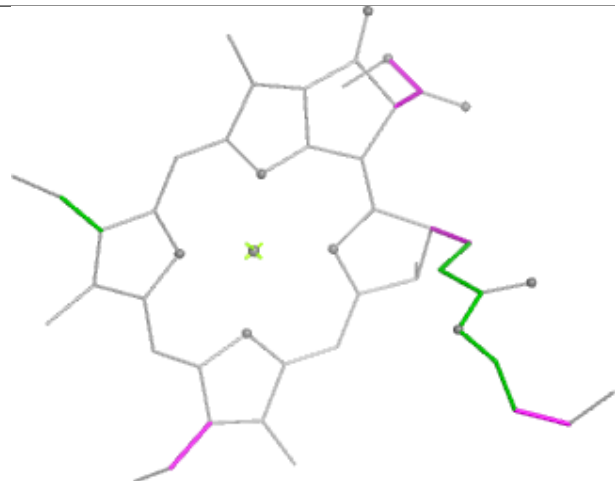
Ligand CLA D 412



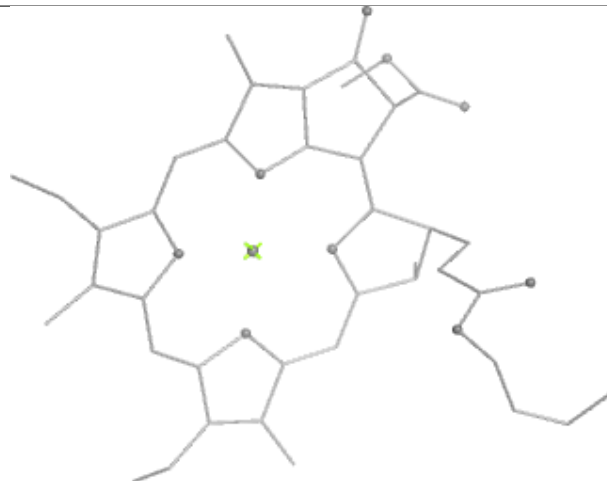
Bond lengths



Bond angles

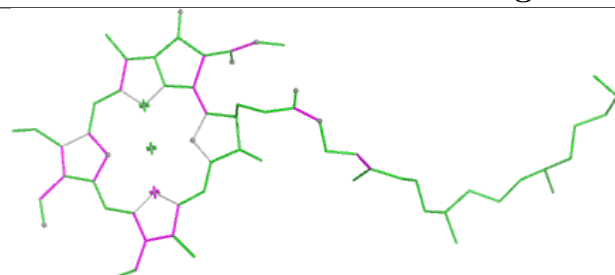


Torsions

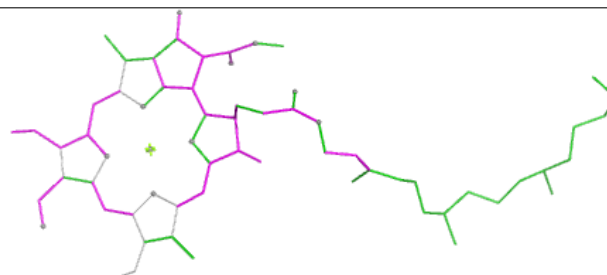


Rings

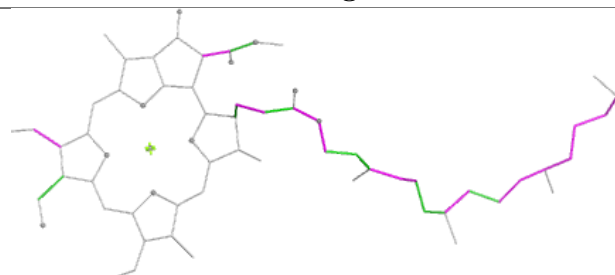
Ligand CHL G 318



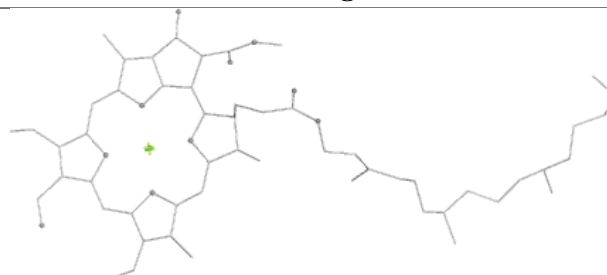
Bond lengths



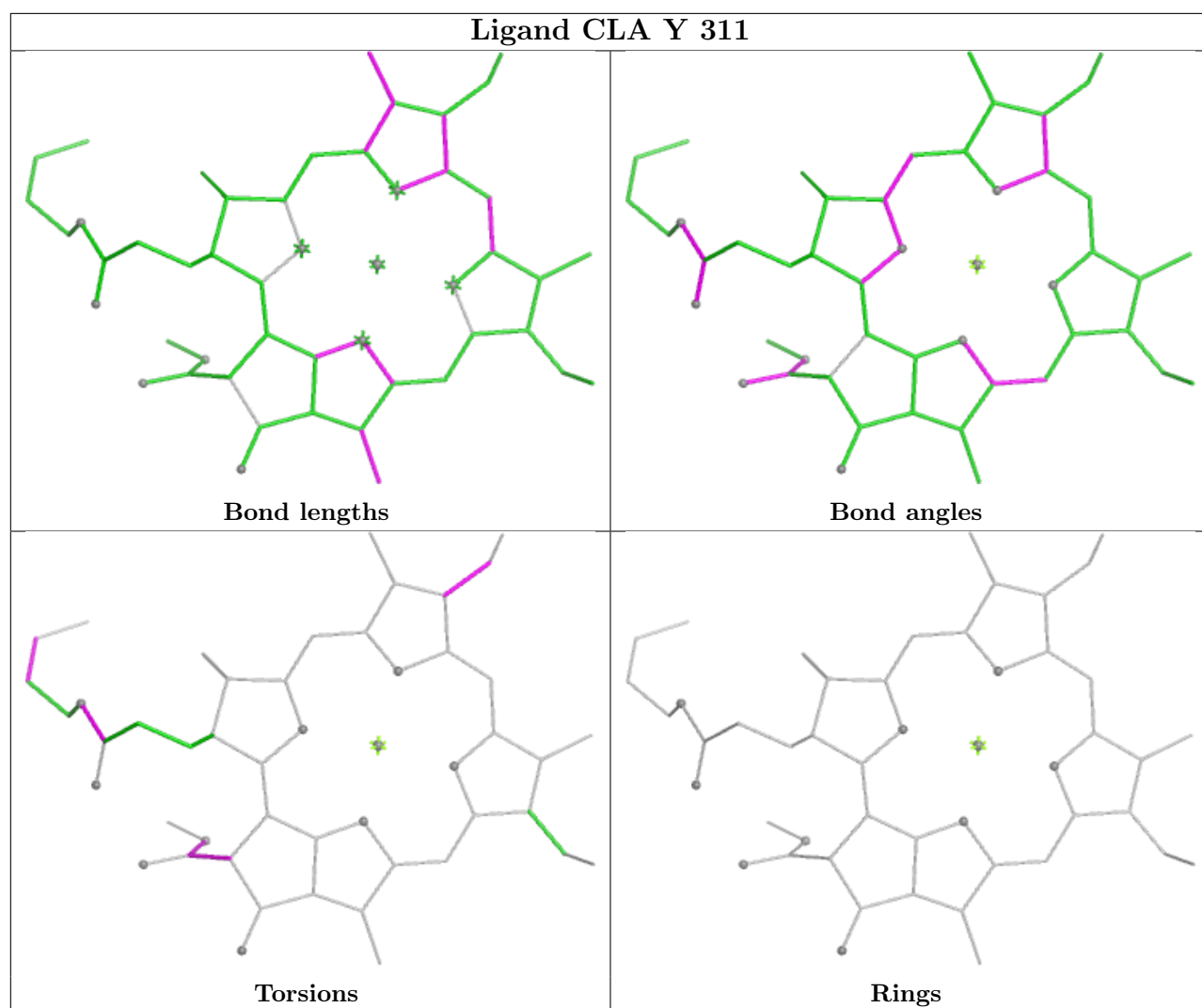
Bond angles

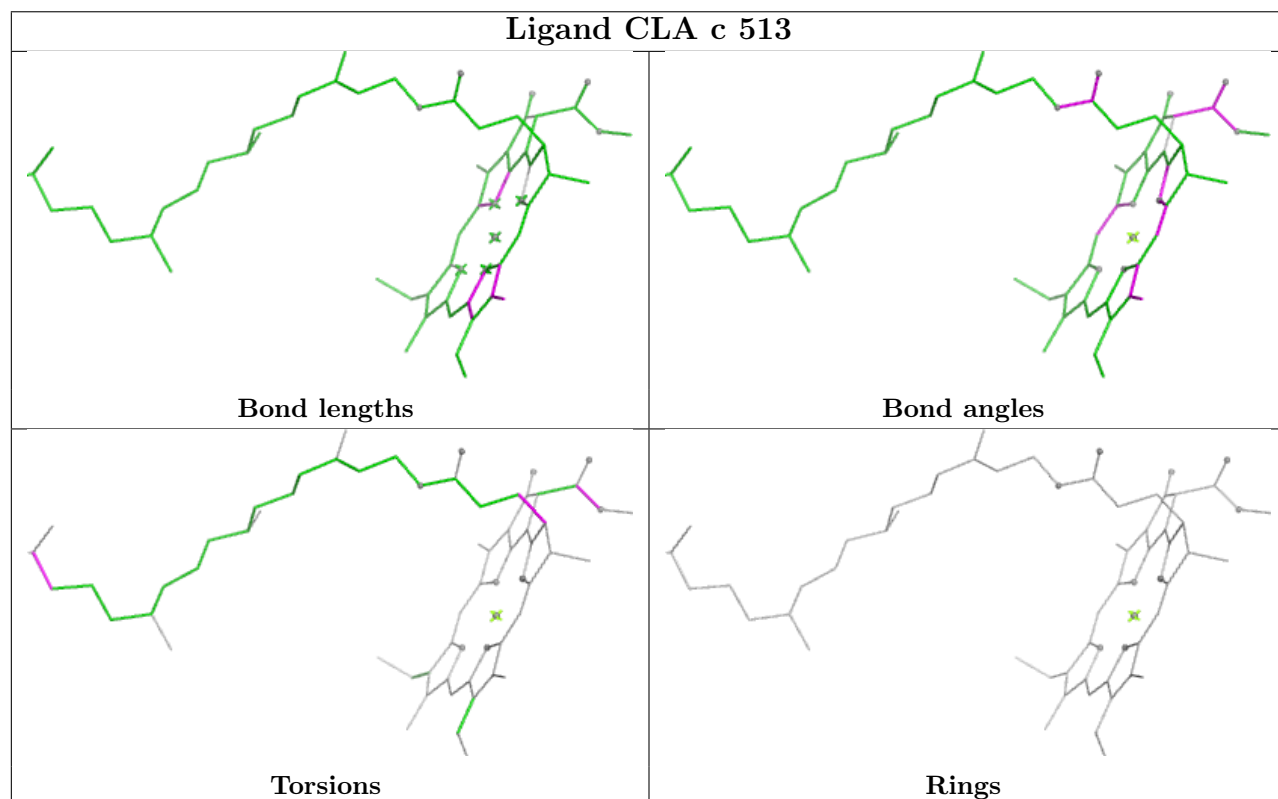
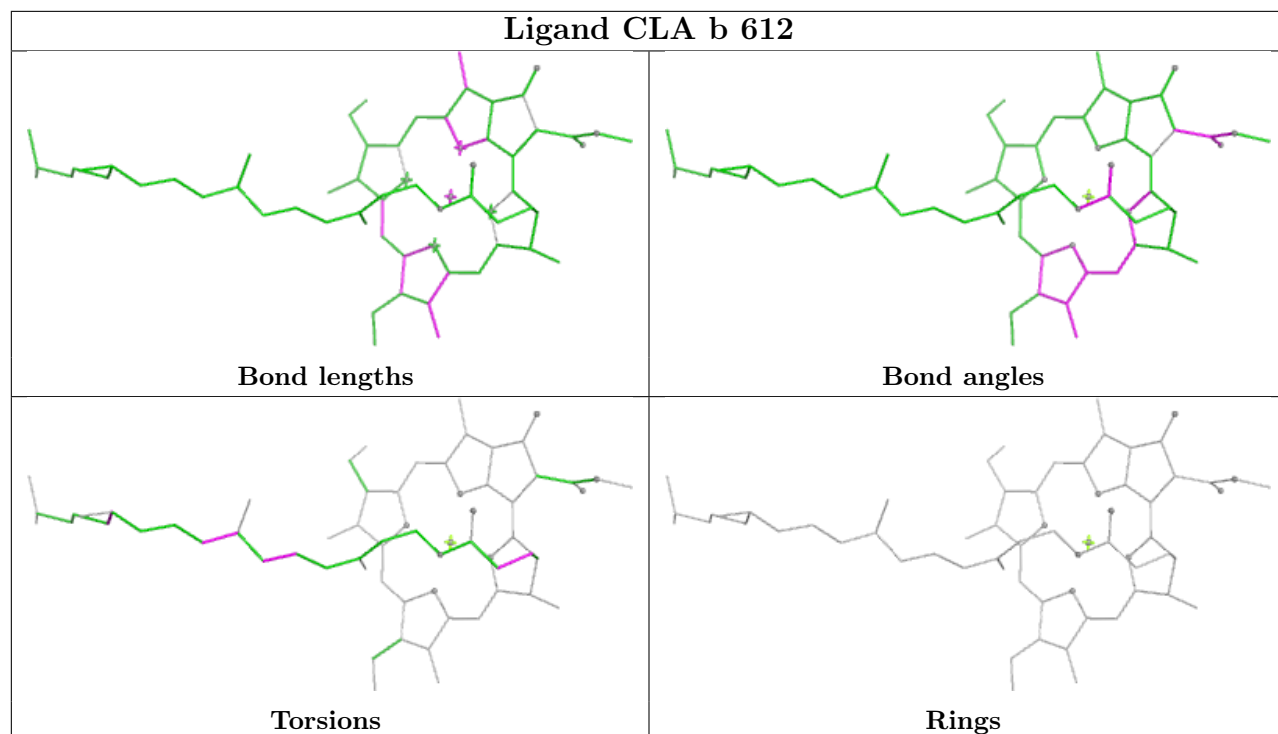


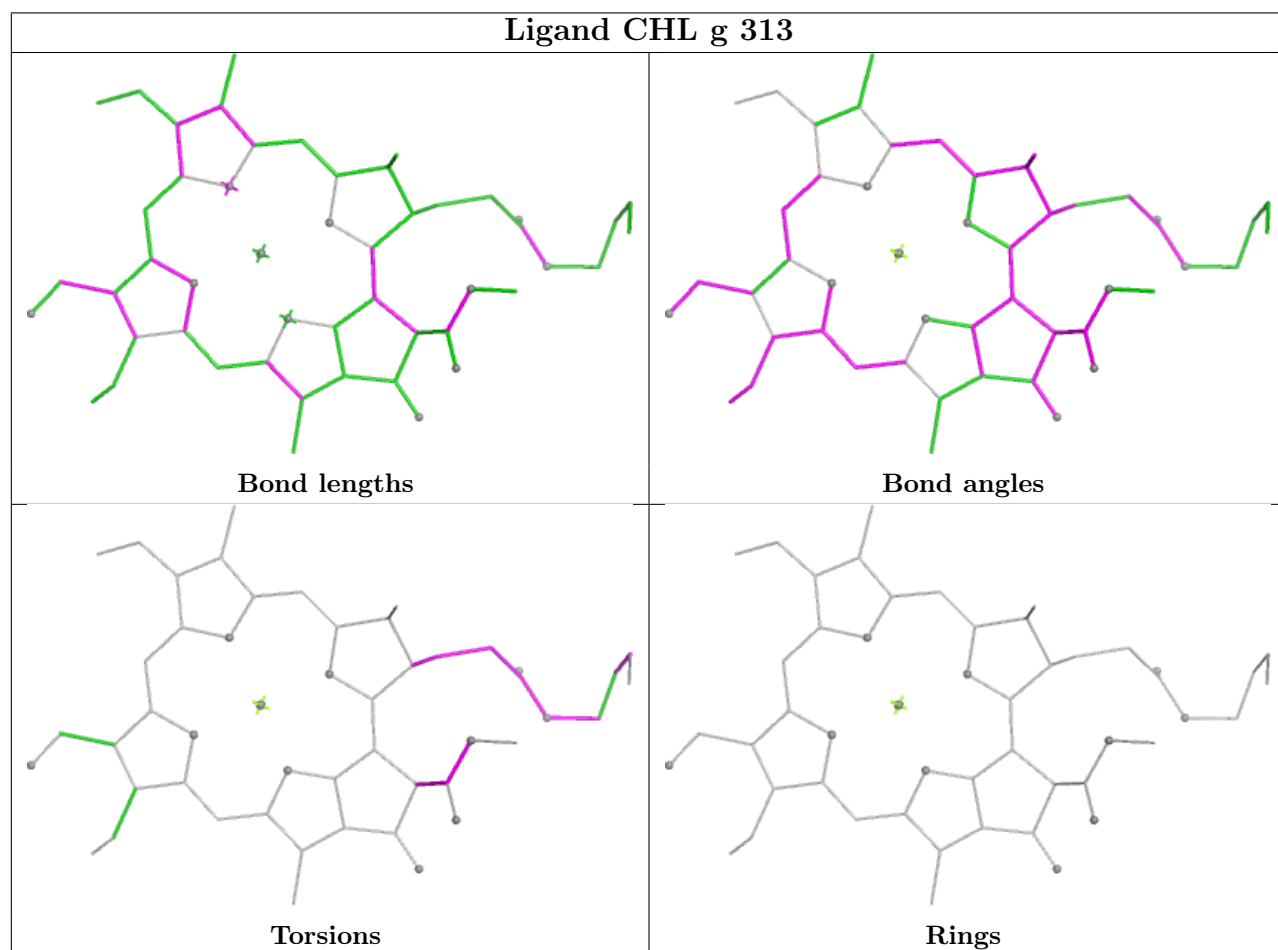
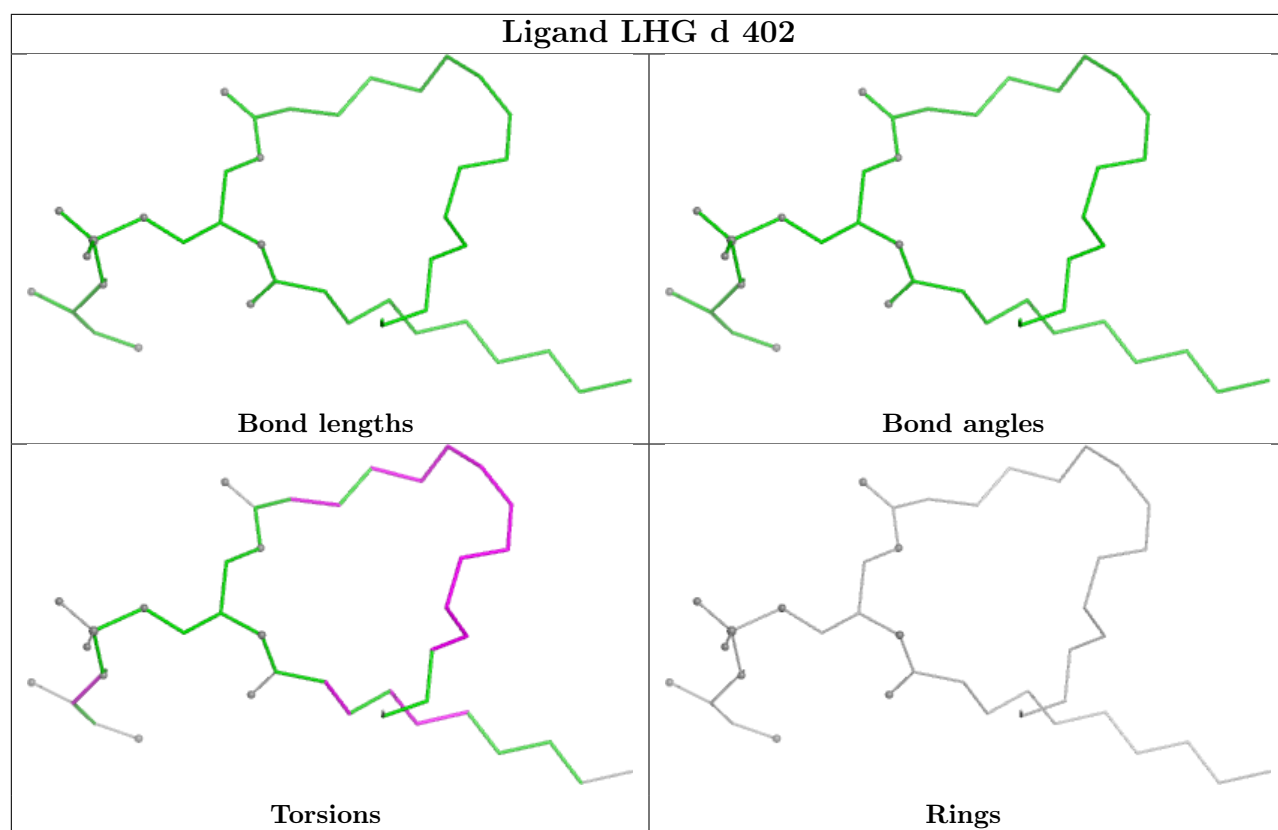
Torsions

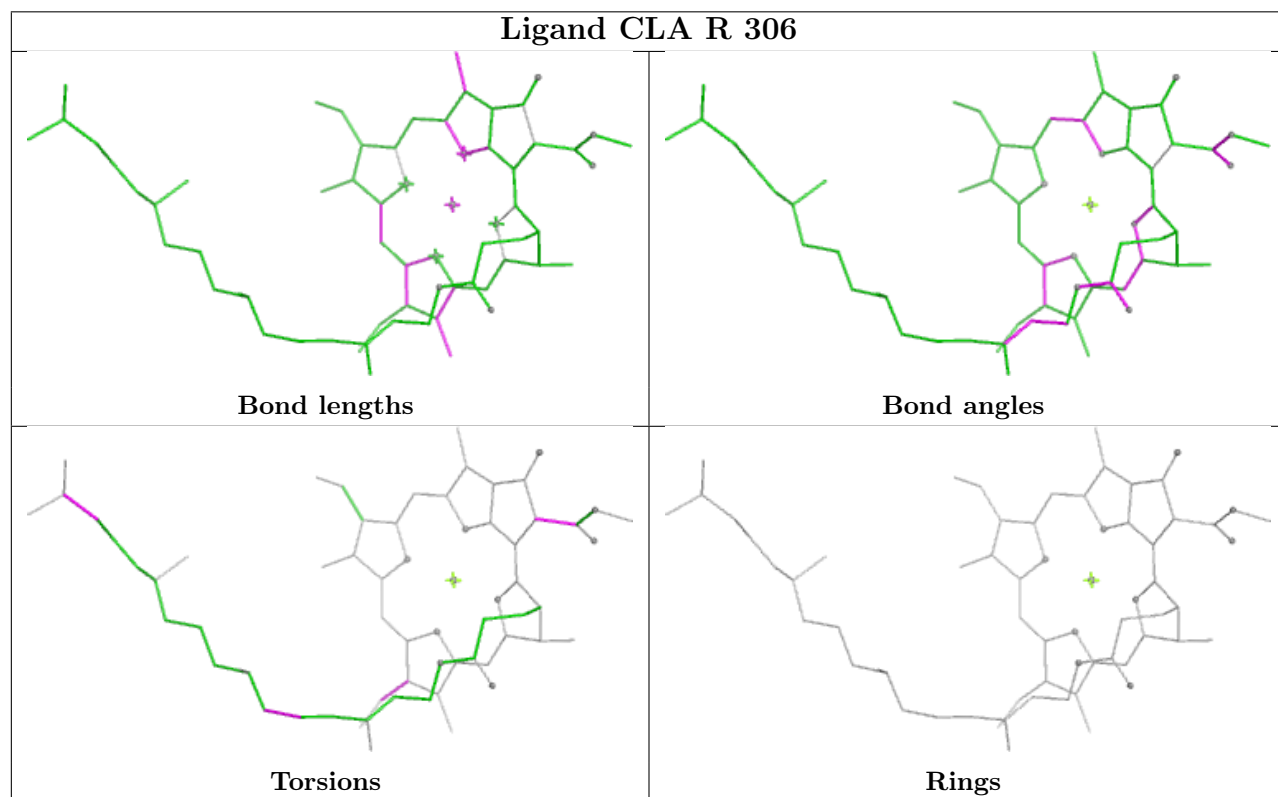
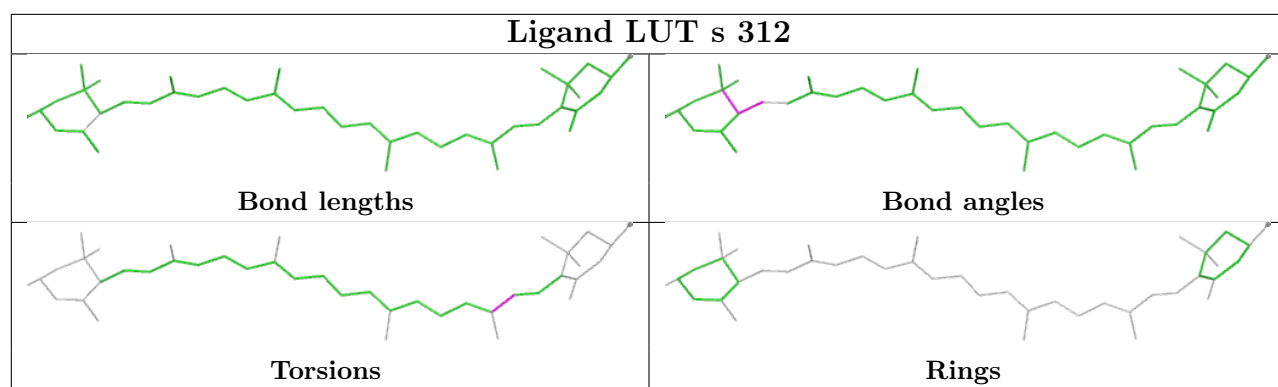


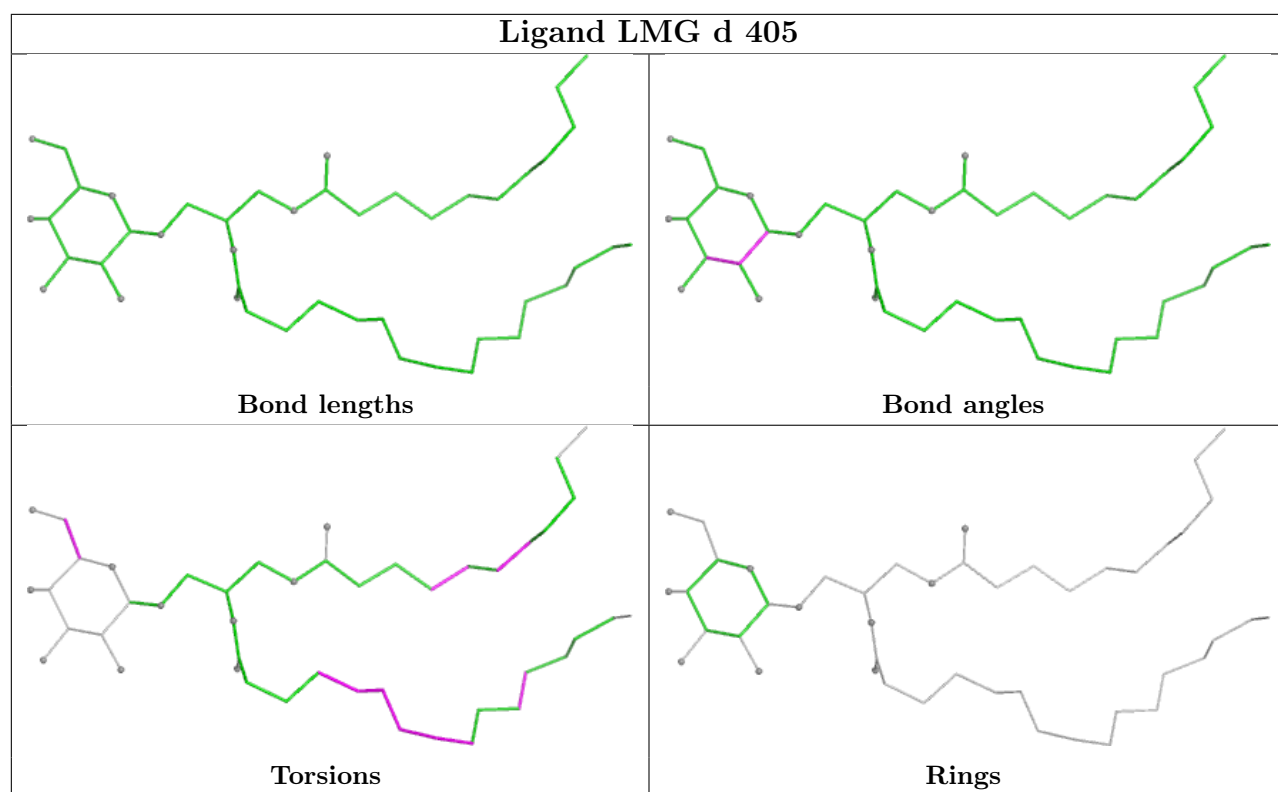
Rings



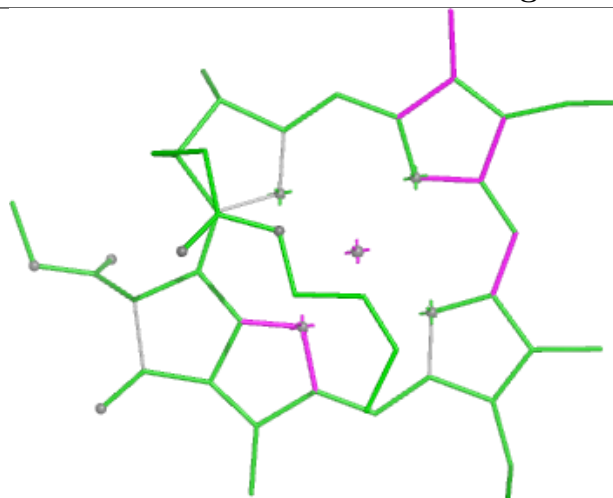




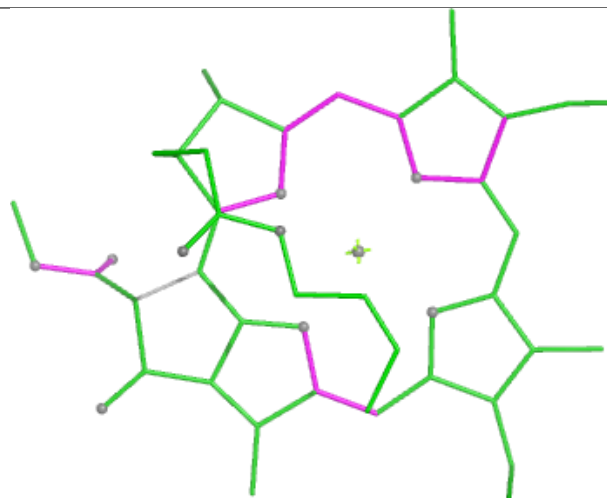




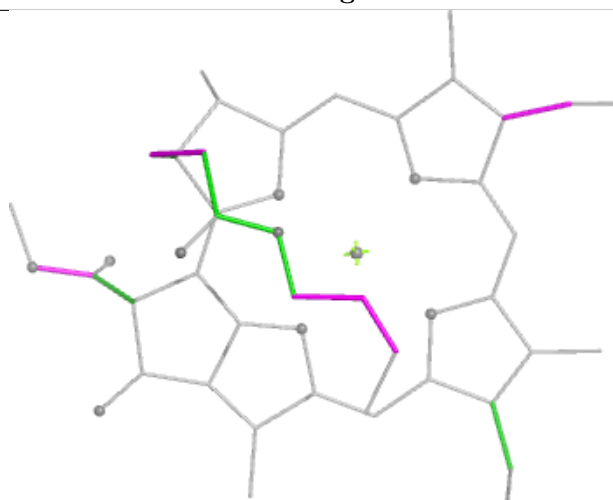
Ligand CLA r 308



Bond lengths



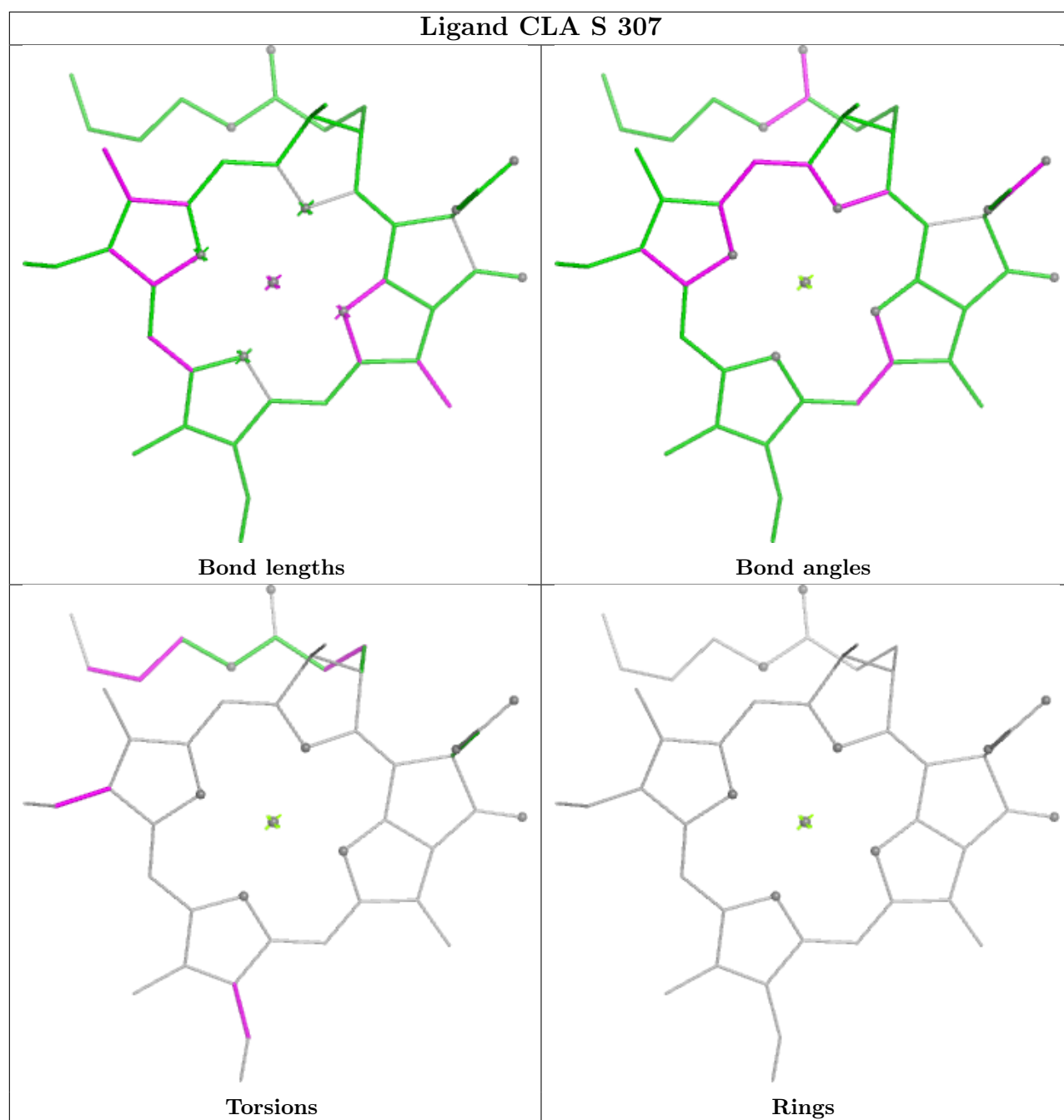
Bond angles

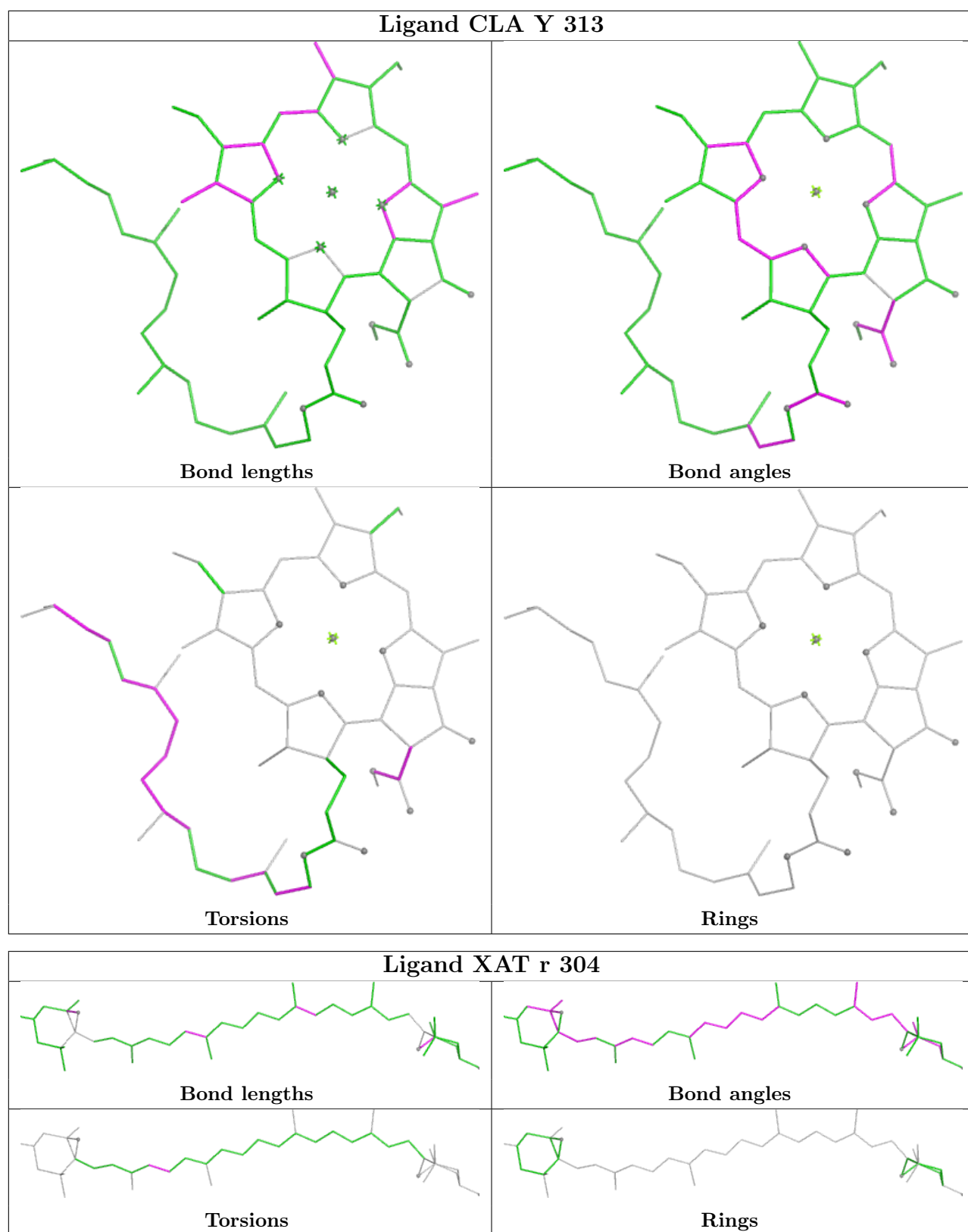


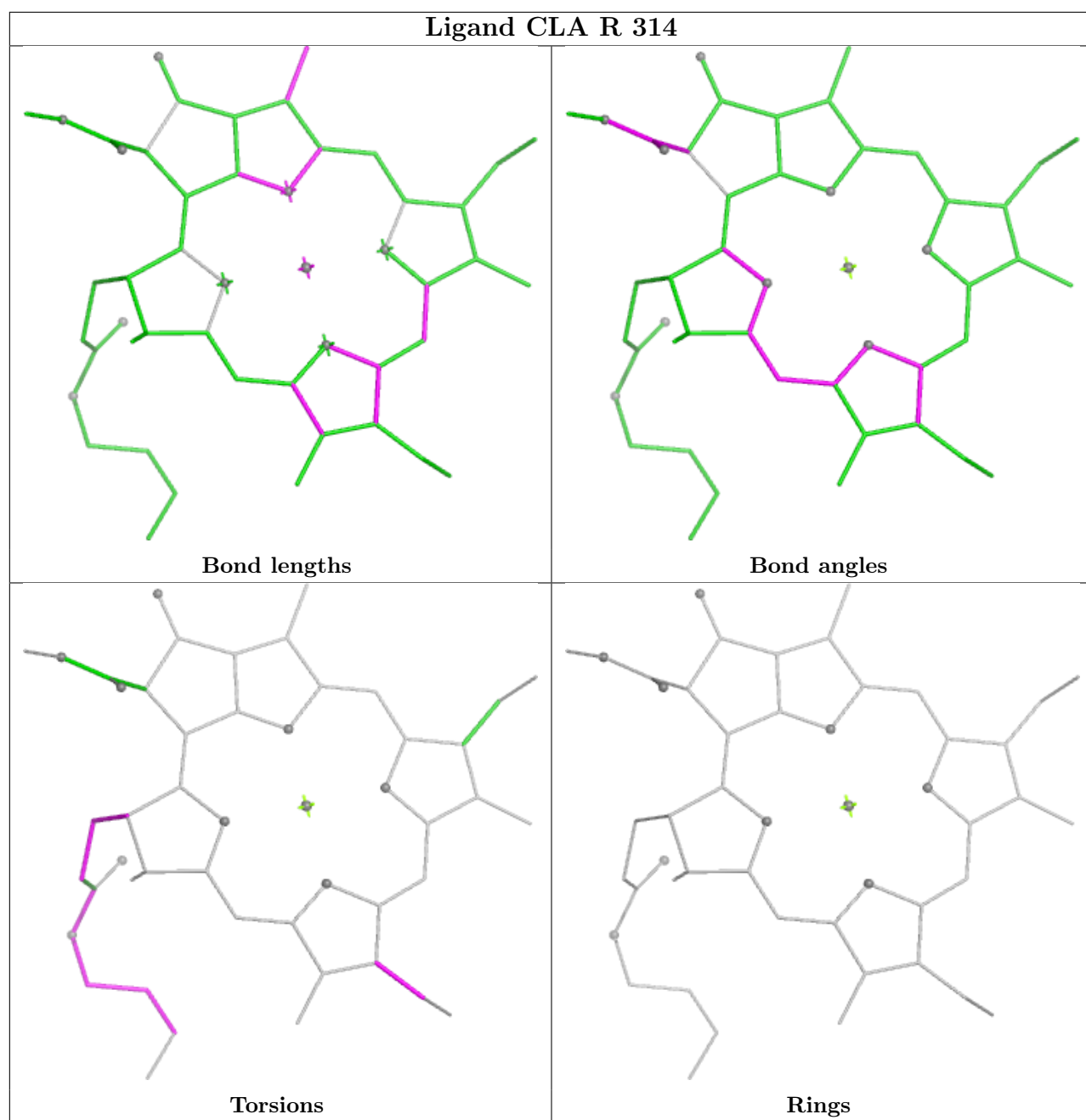
Torsions



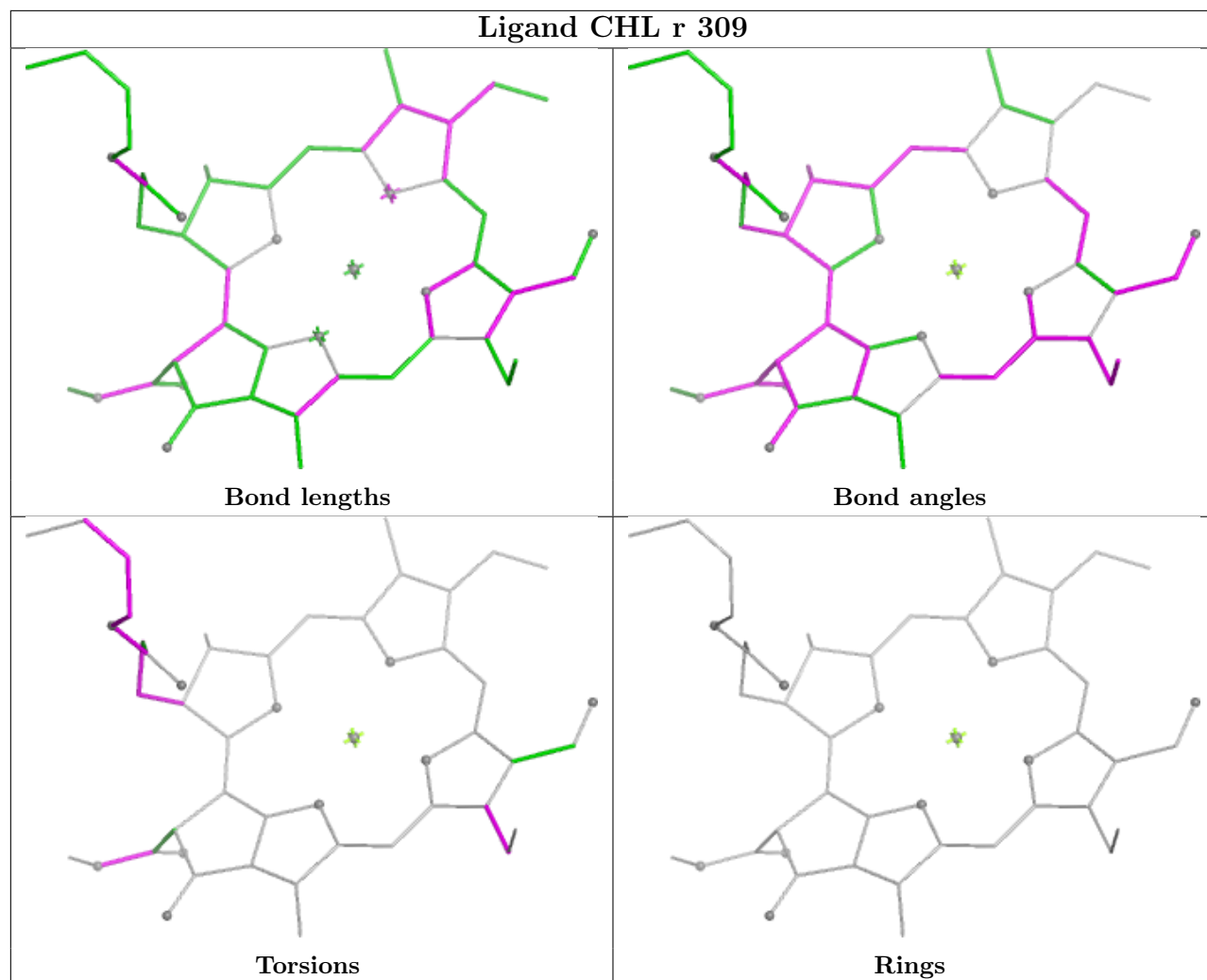
Rings

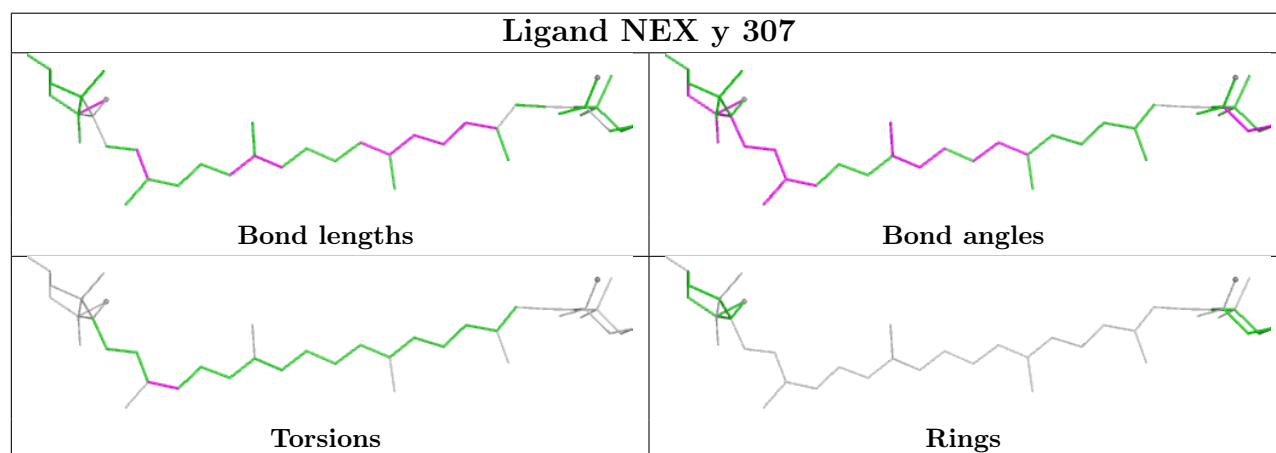
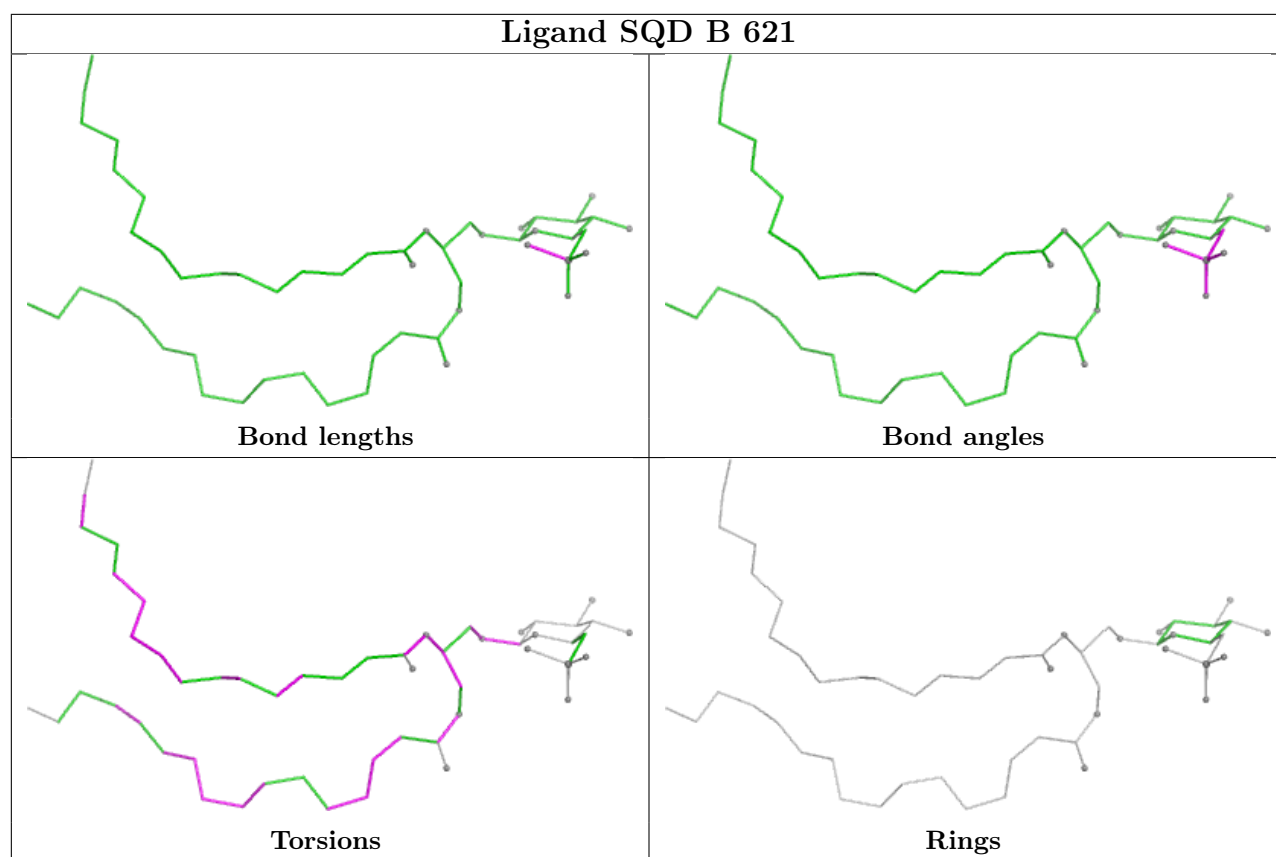


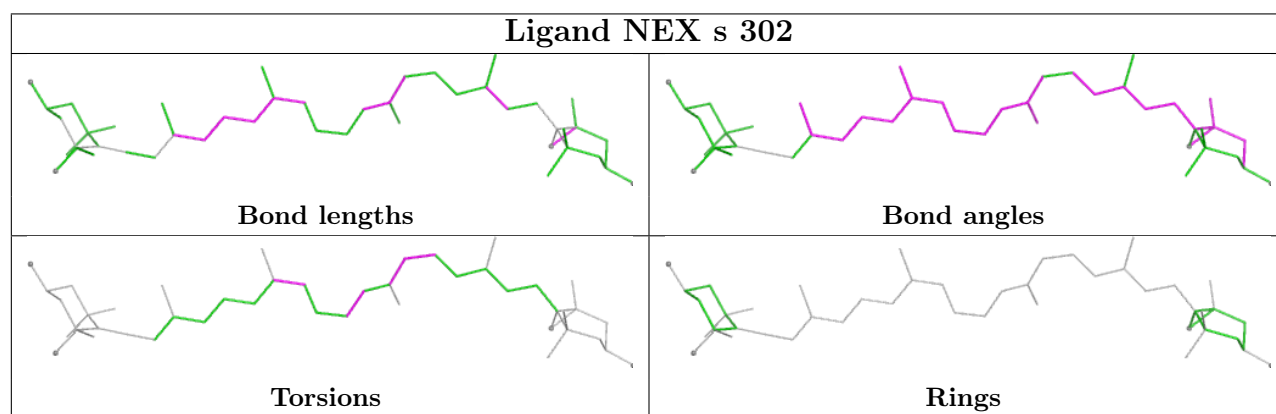
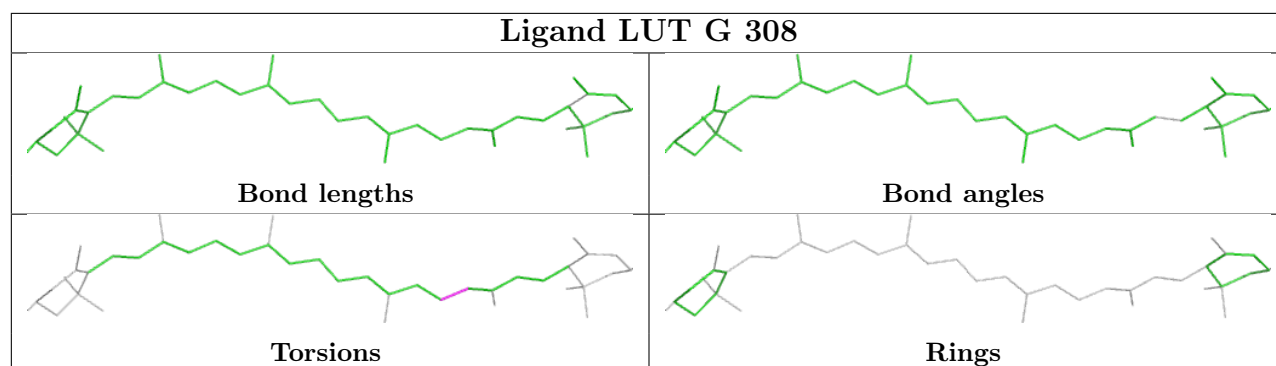
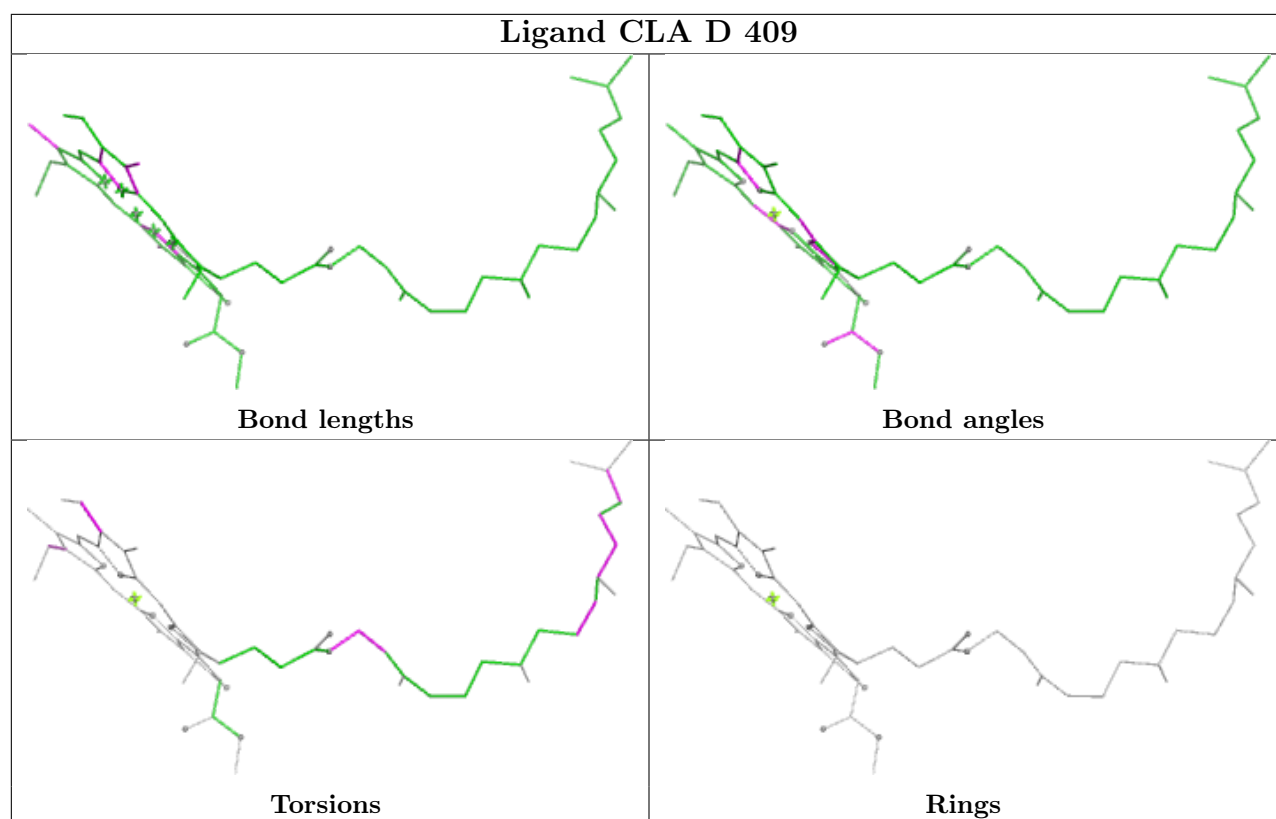


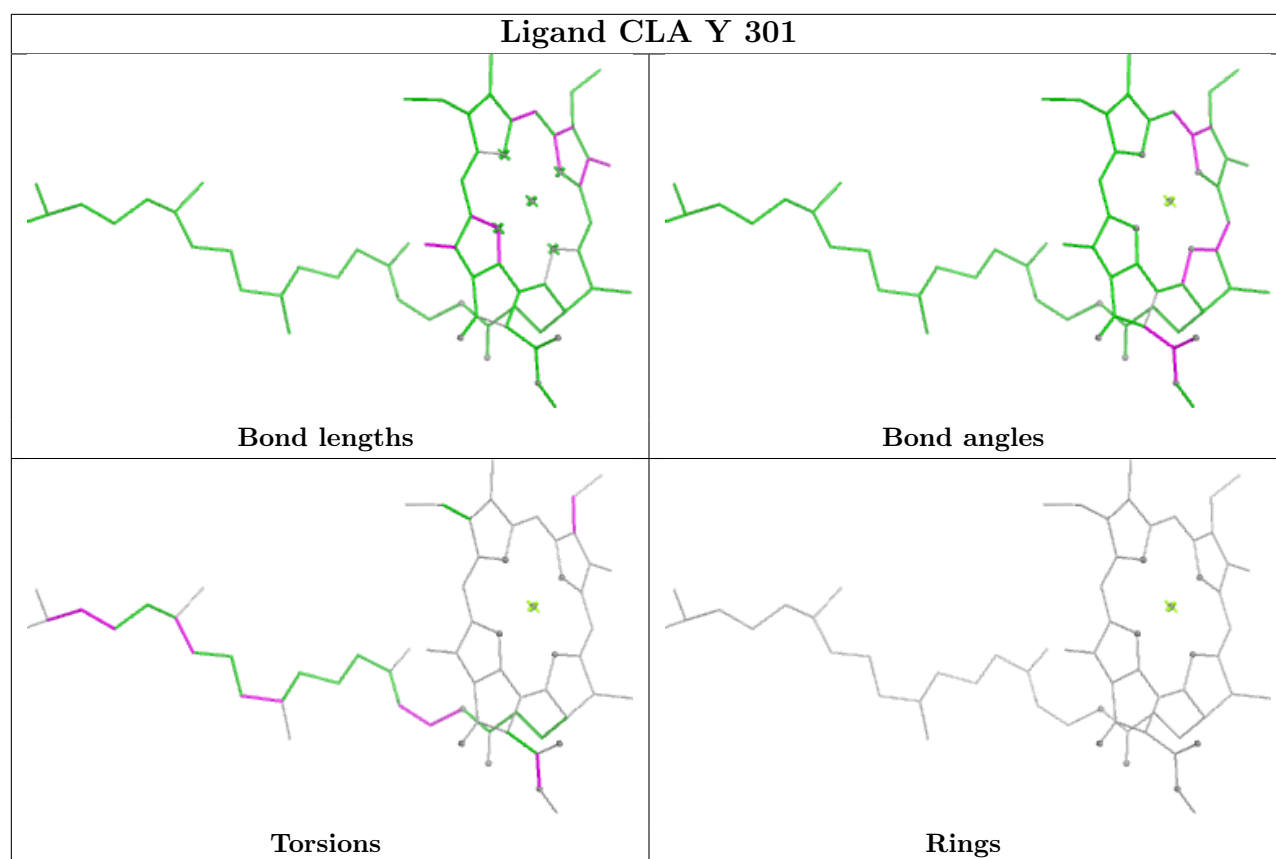


Ligand CHL r 309

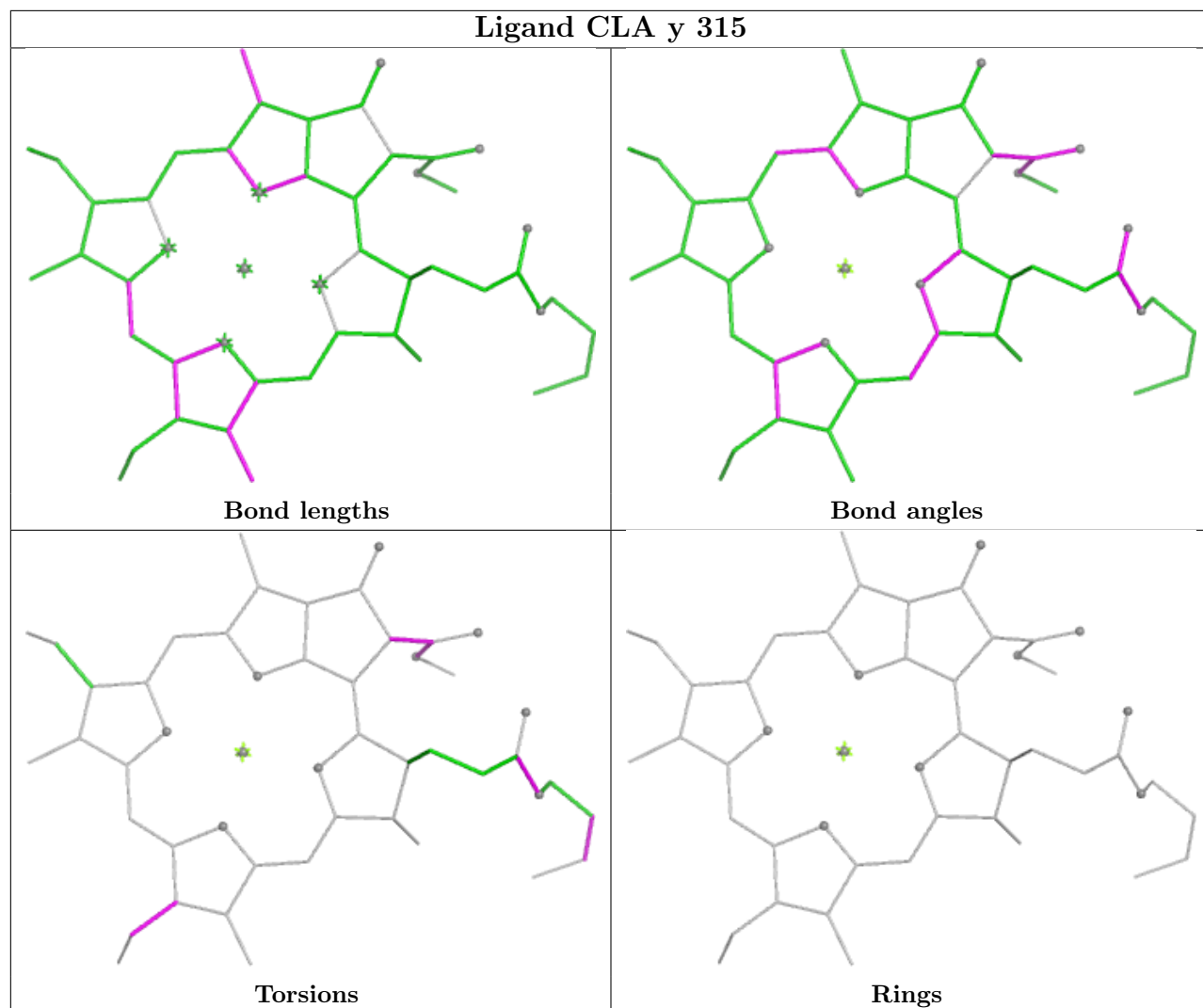


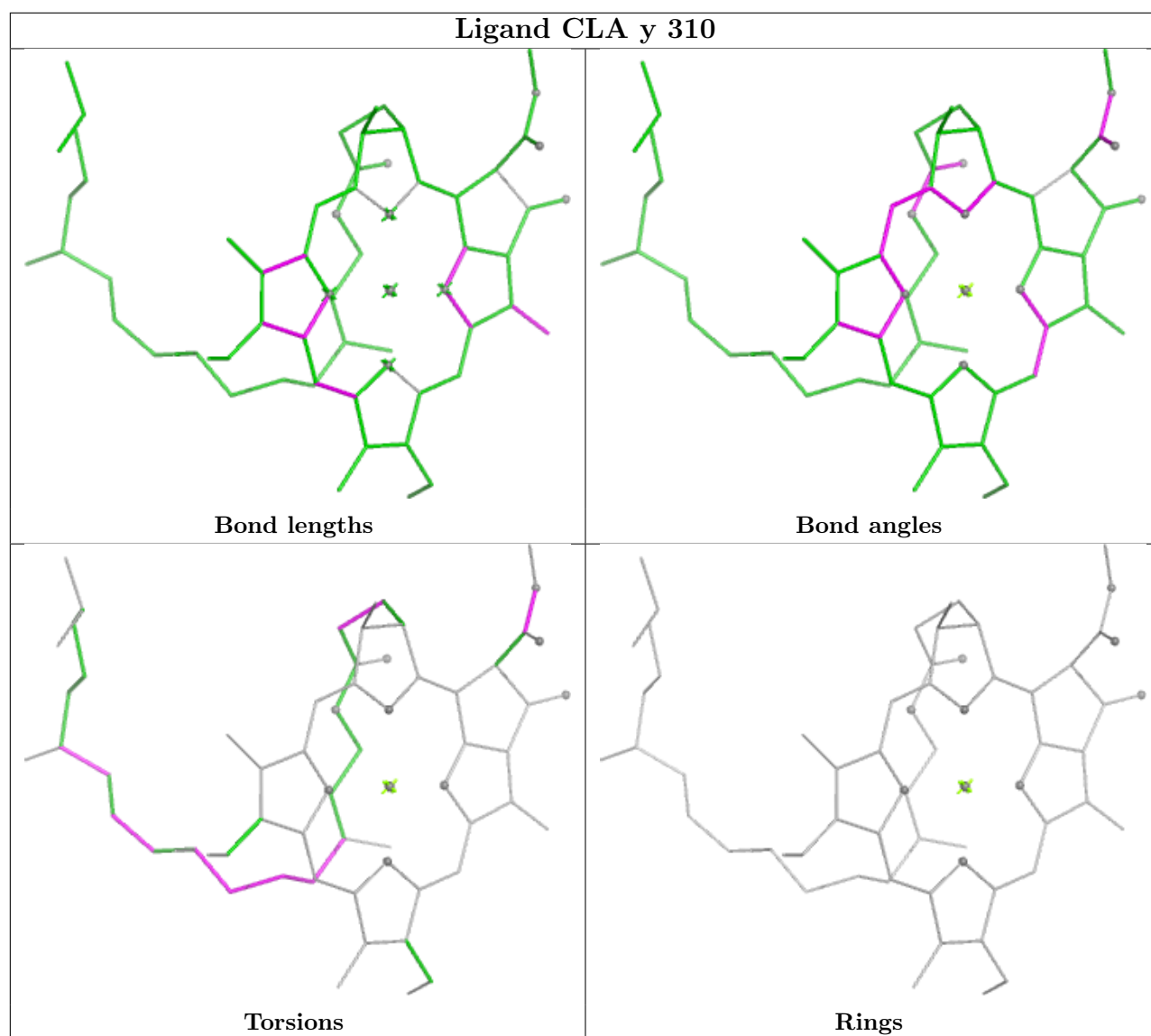


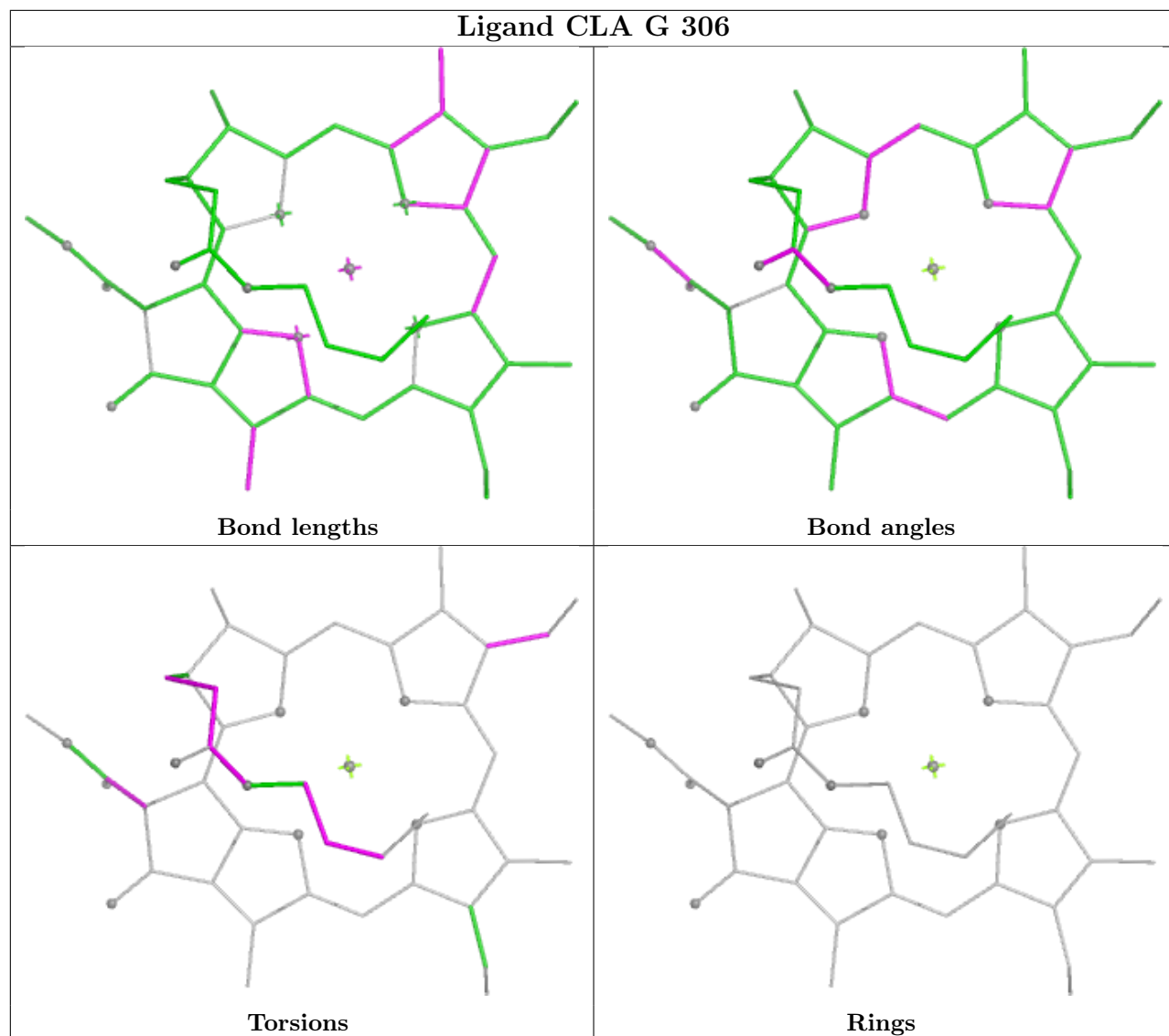




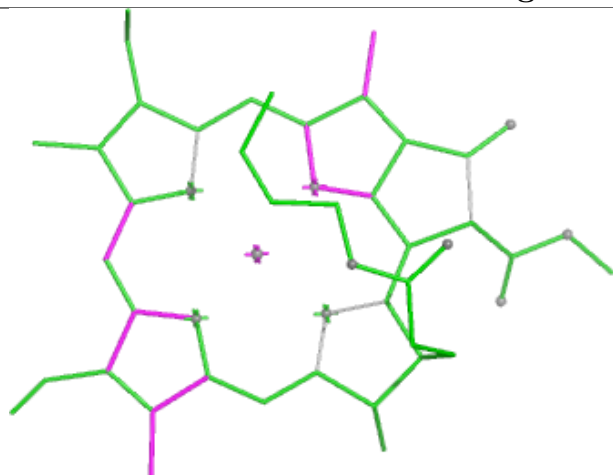
Ligand CLA y 315



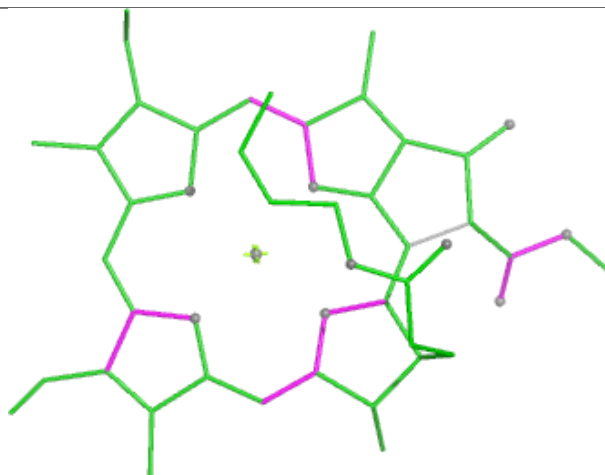




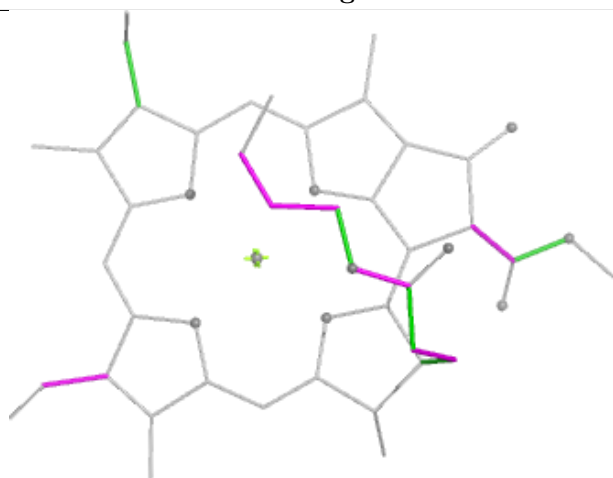
Ligand CLA n 302



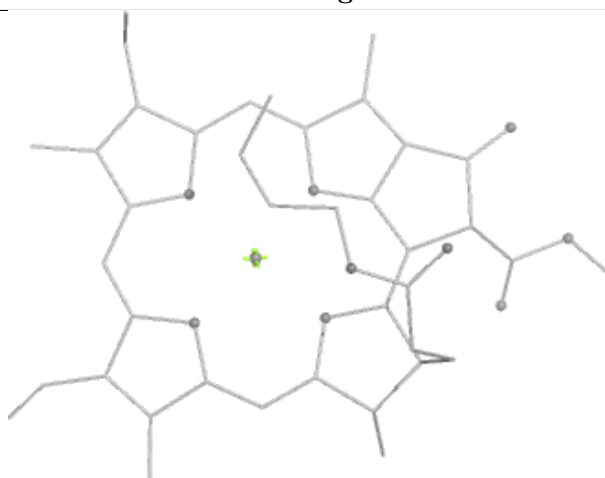
Bond lengths



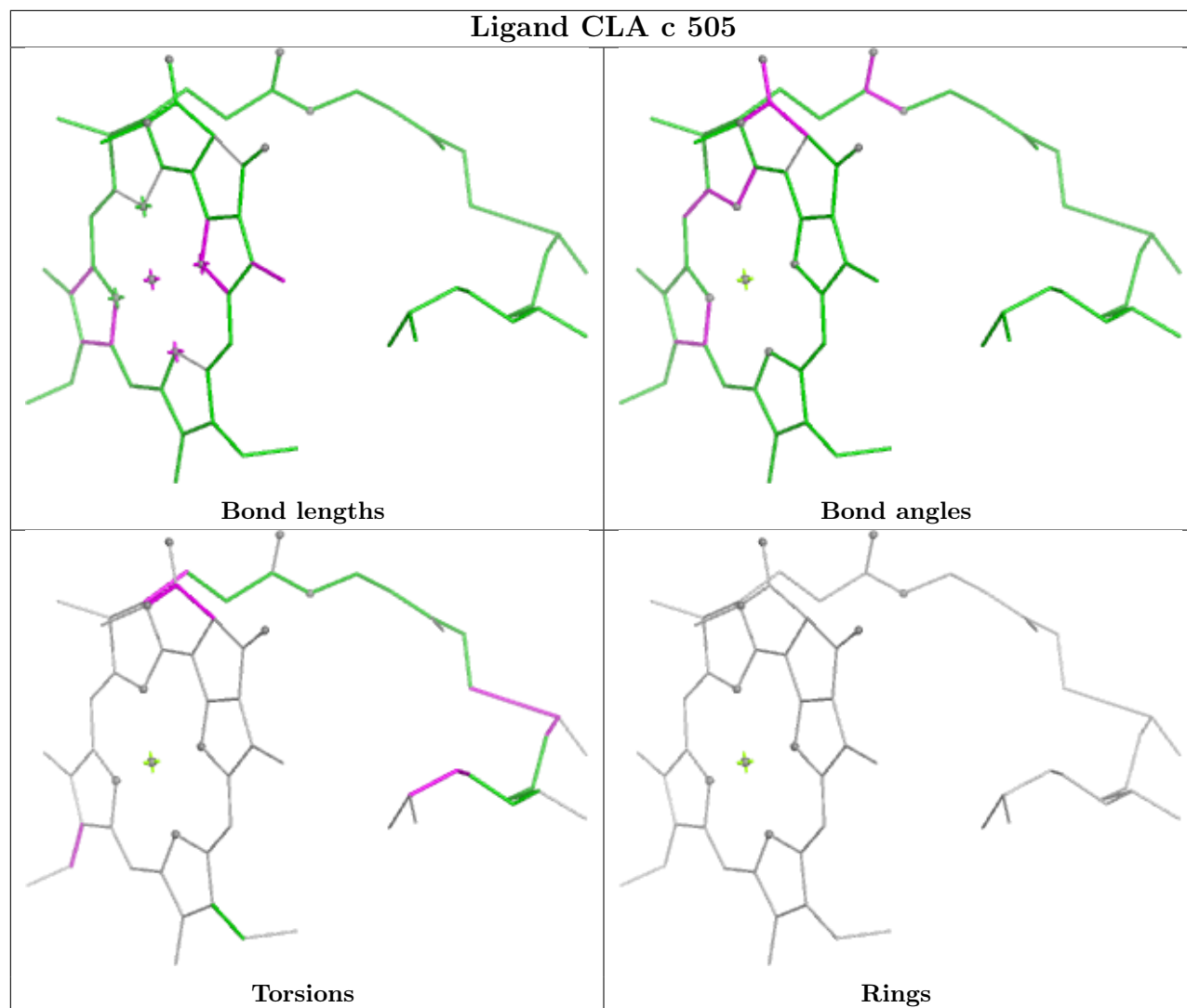
Bond angles



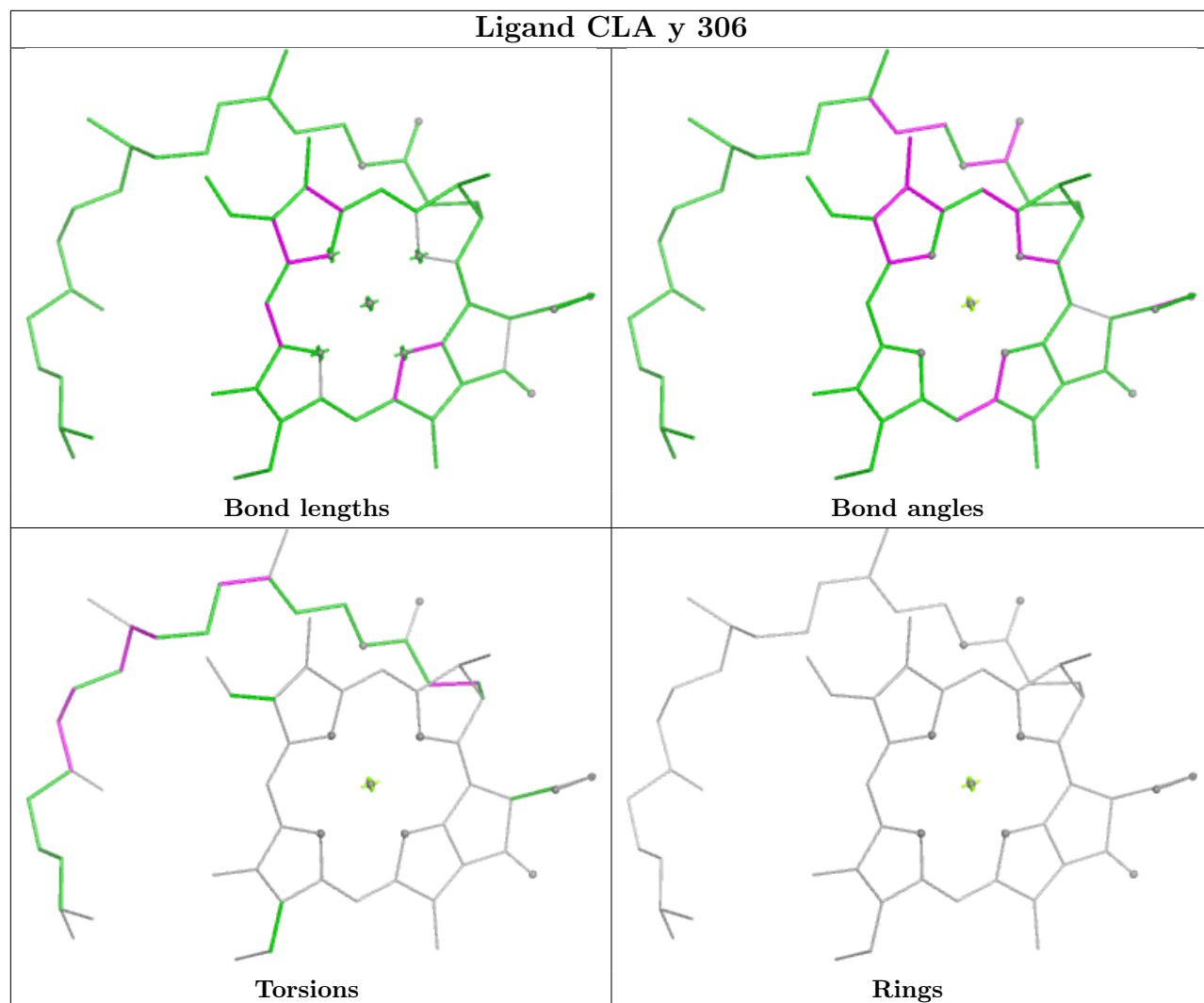
Torsions



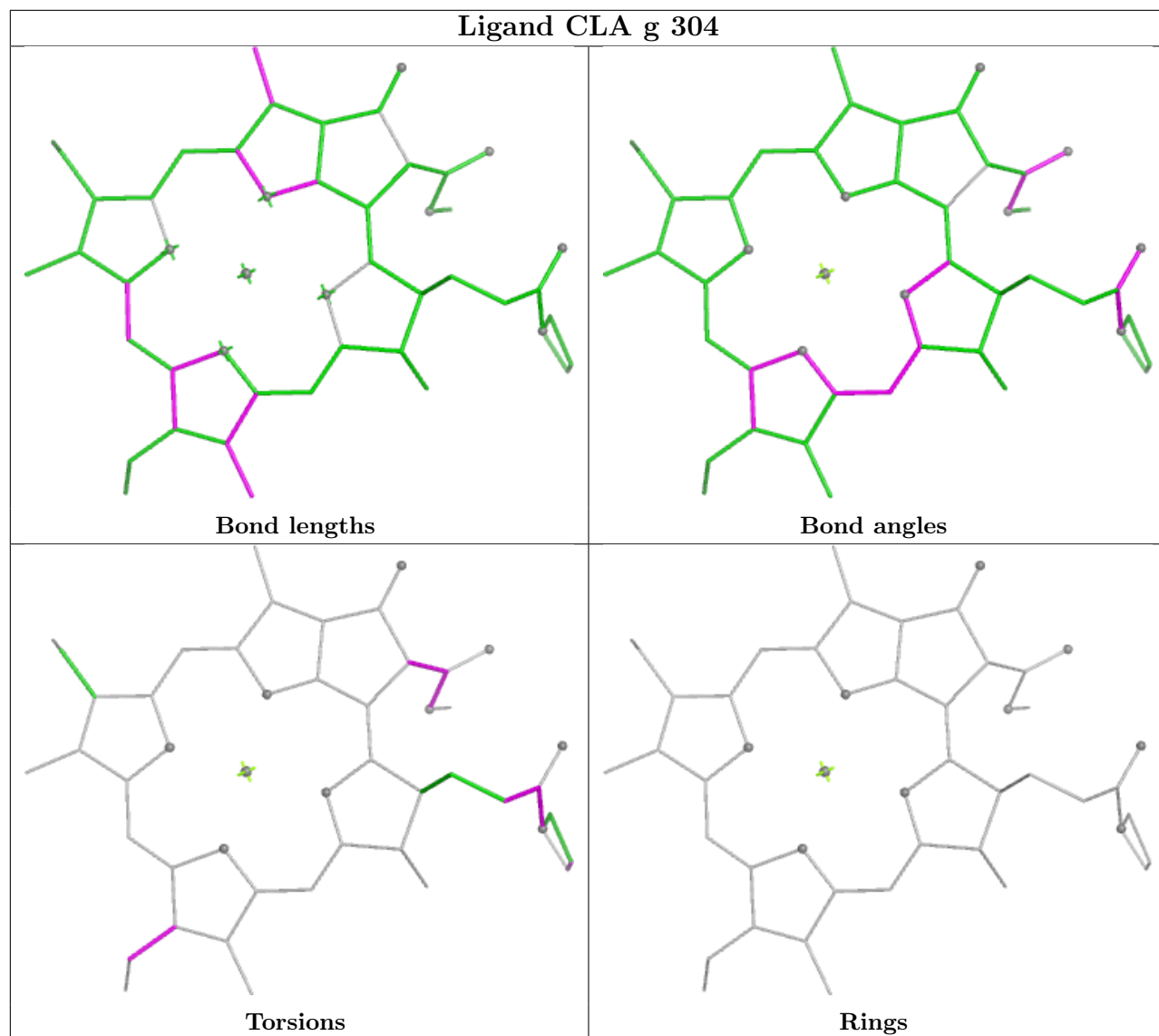
Rings

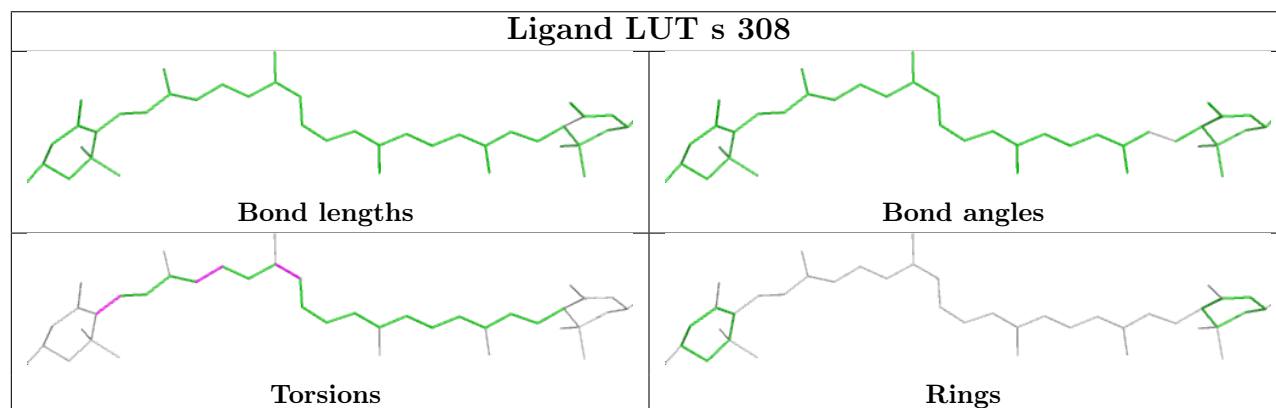
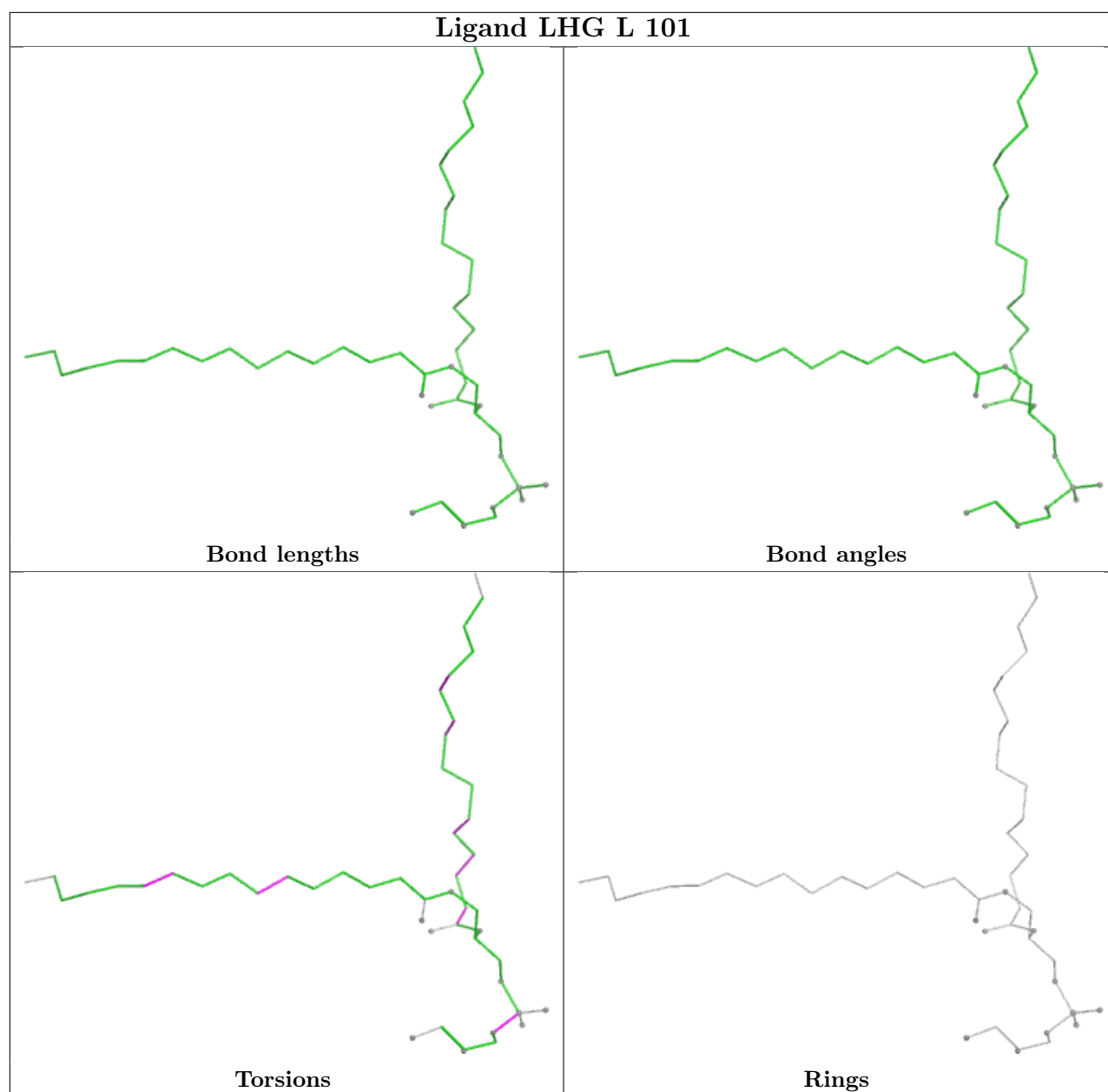


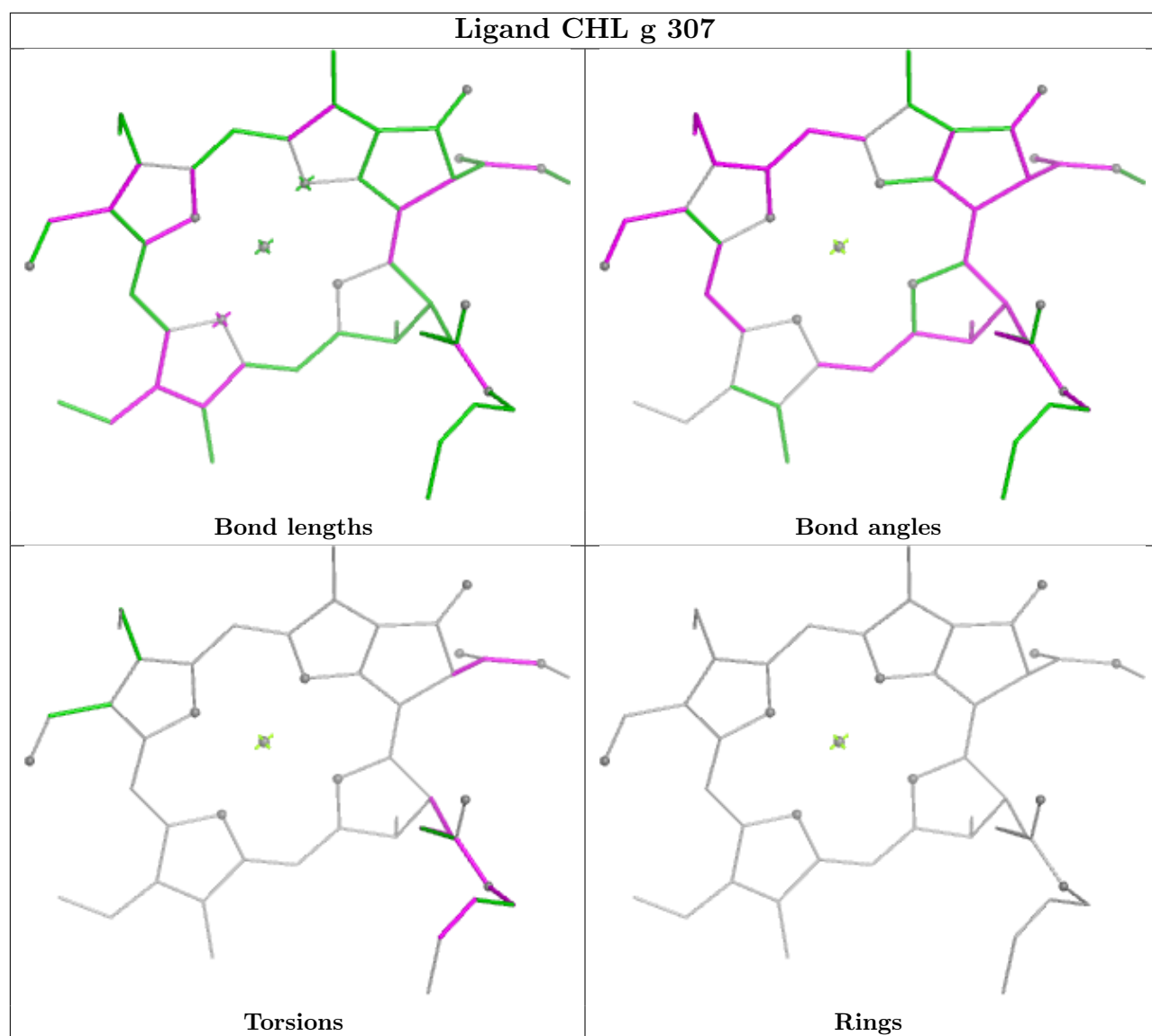
Ligand CLA y 306



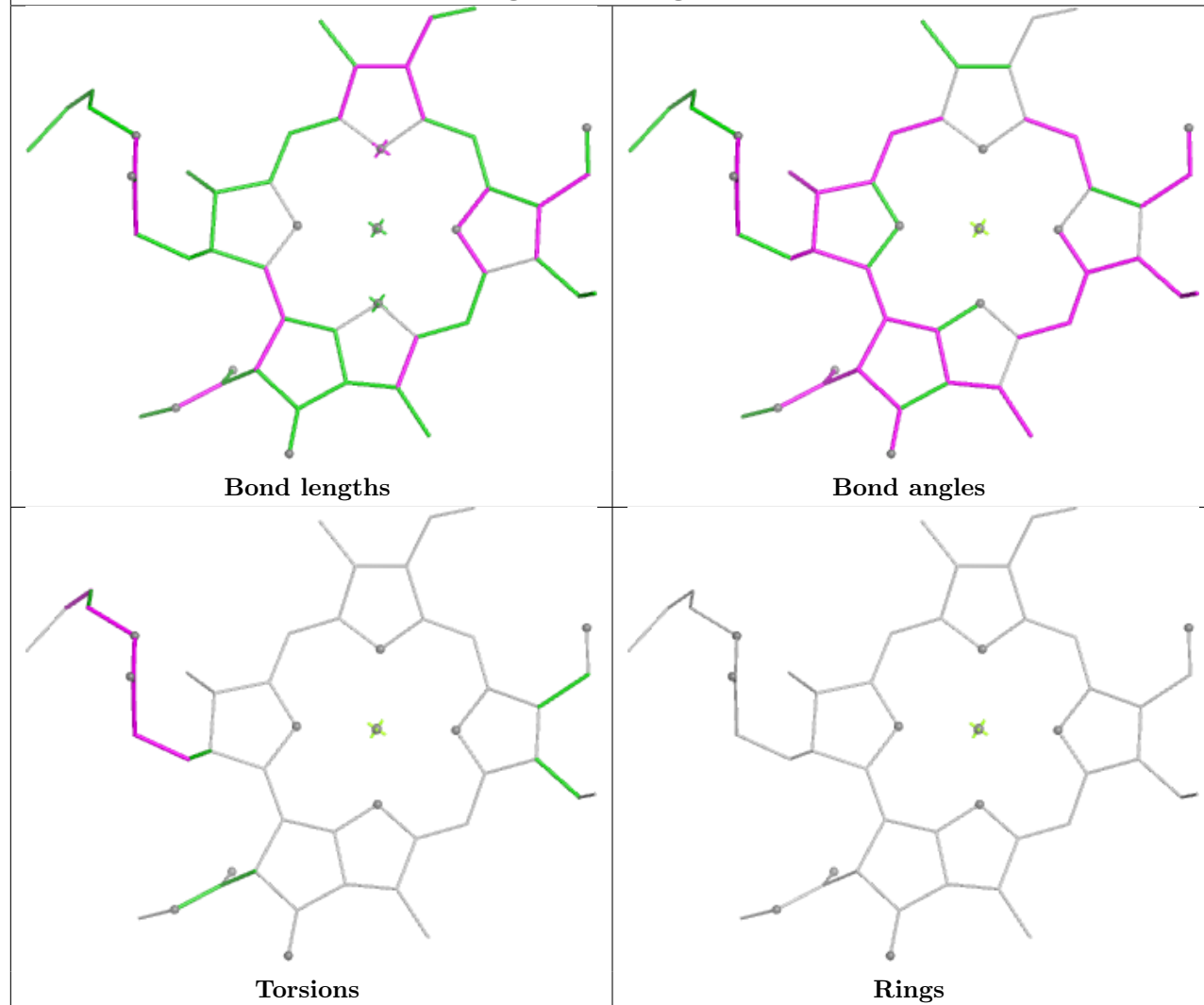
Ligand CLA g 304



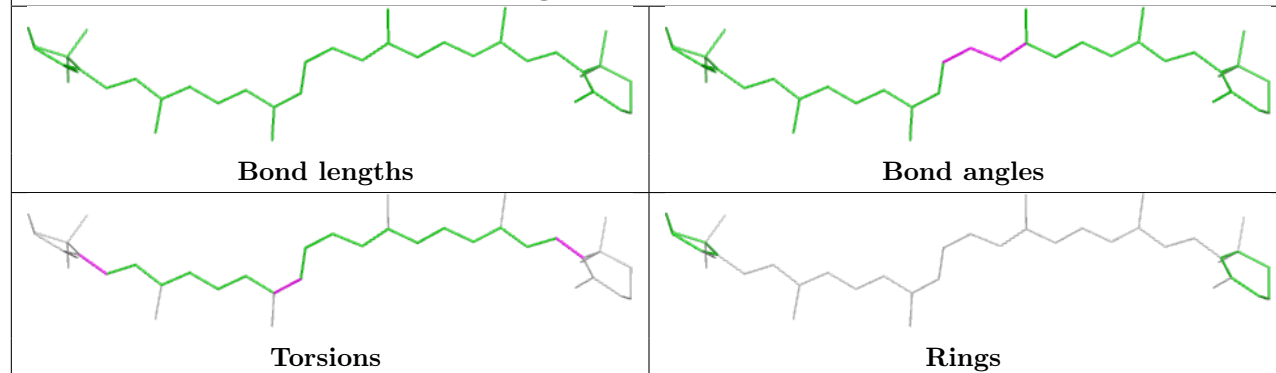


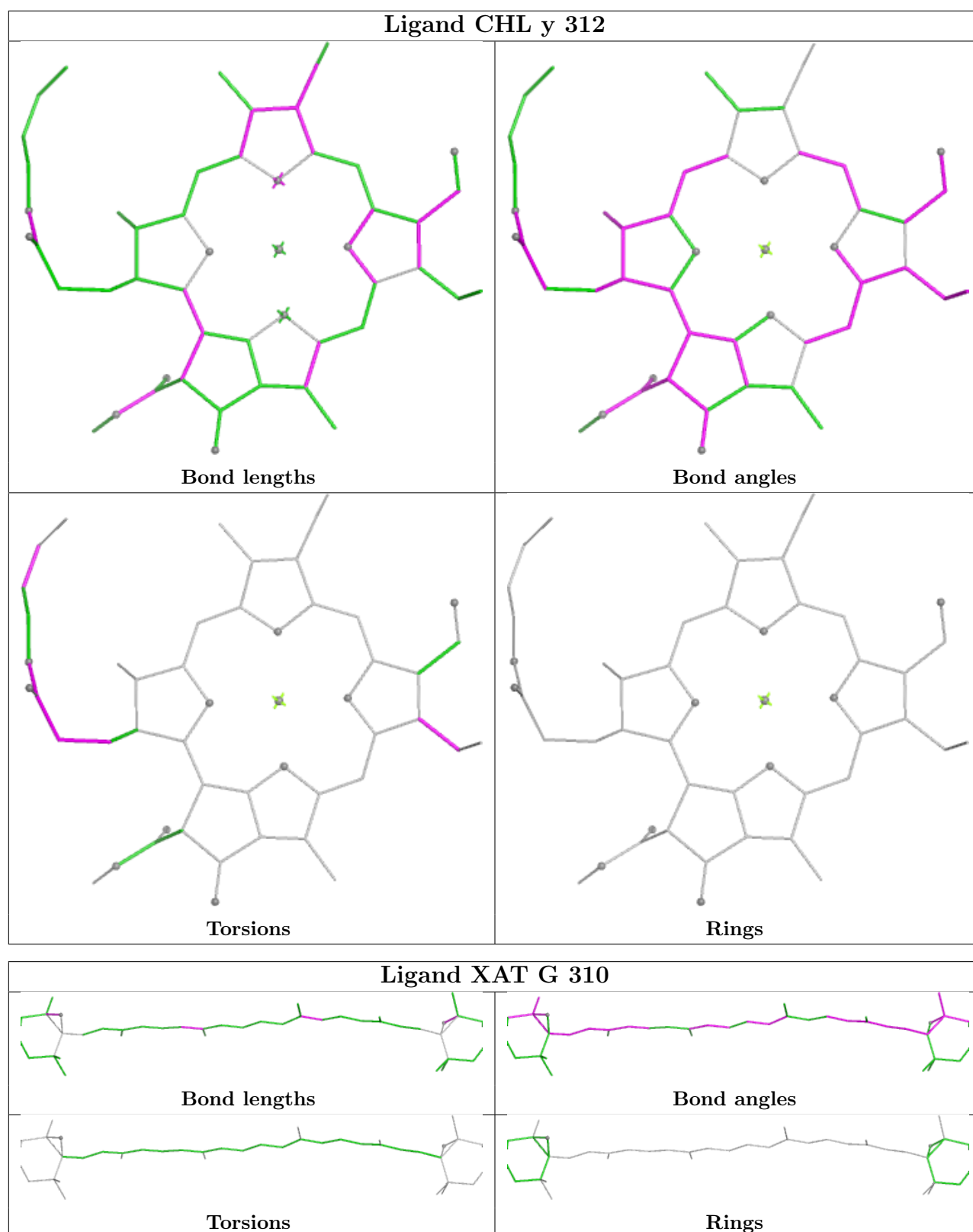


Ligand CHL g 319

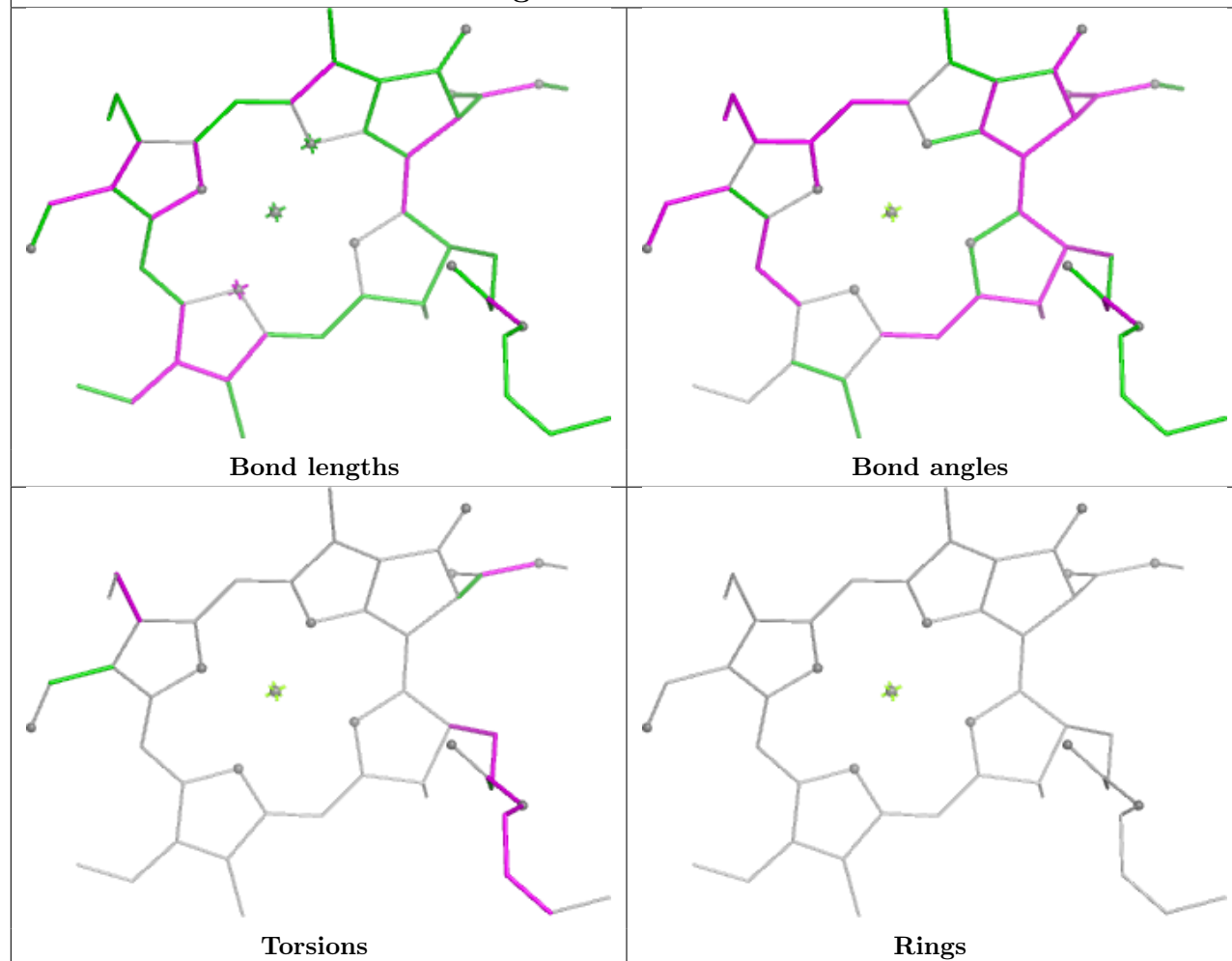


Ligand BCR c 507

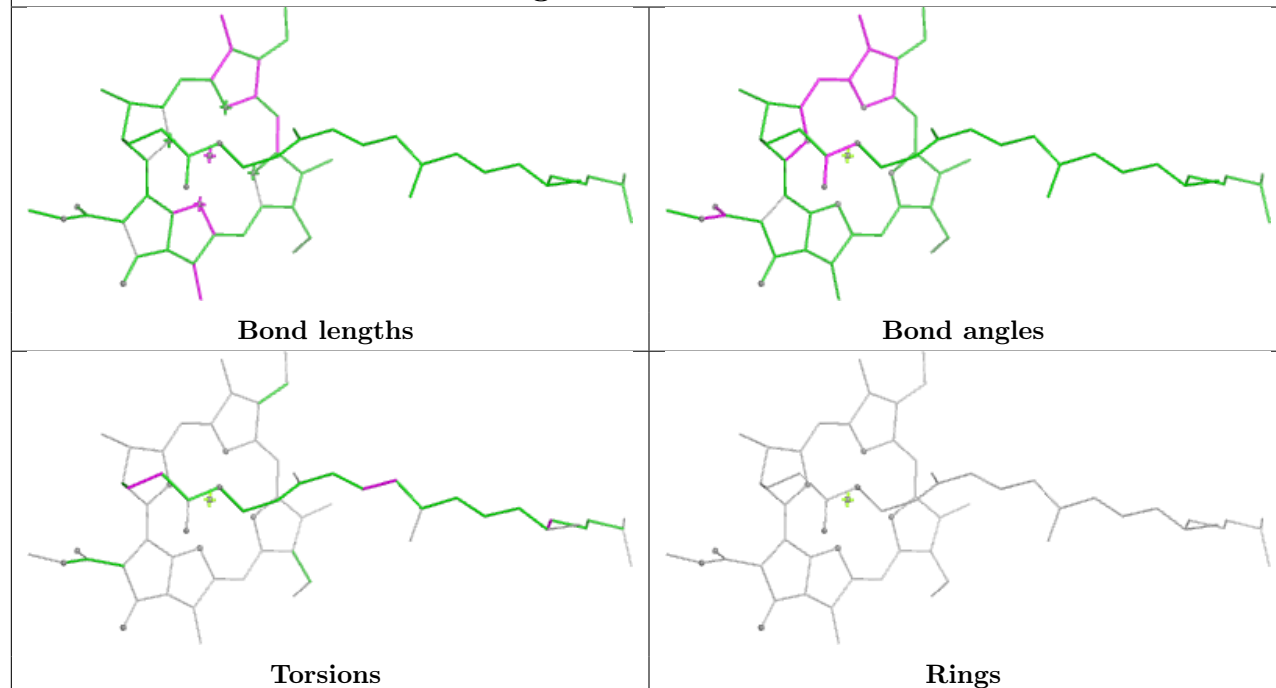


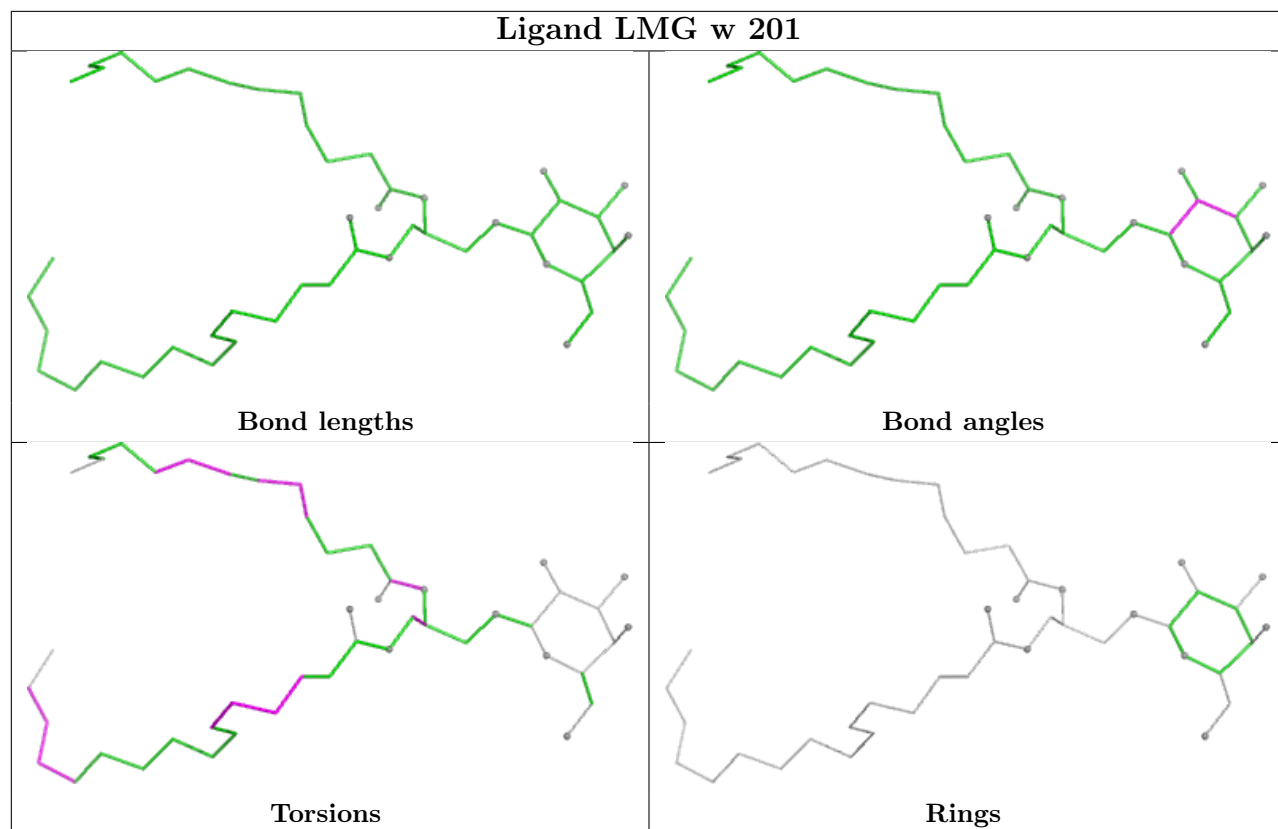


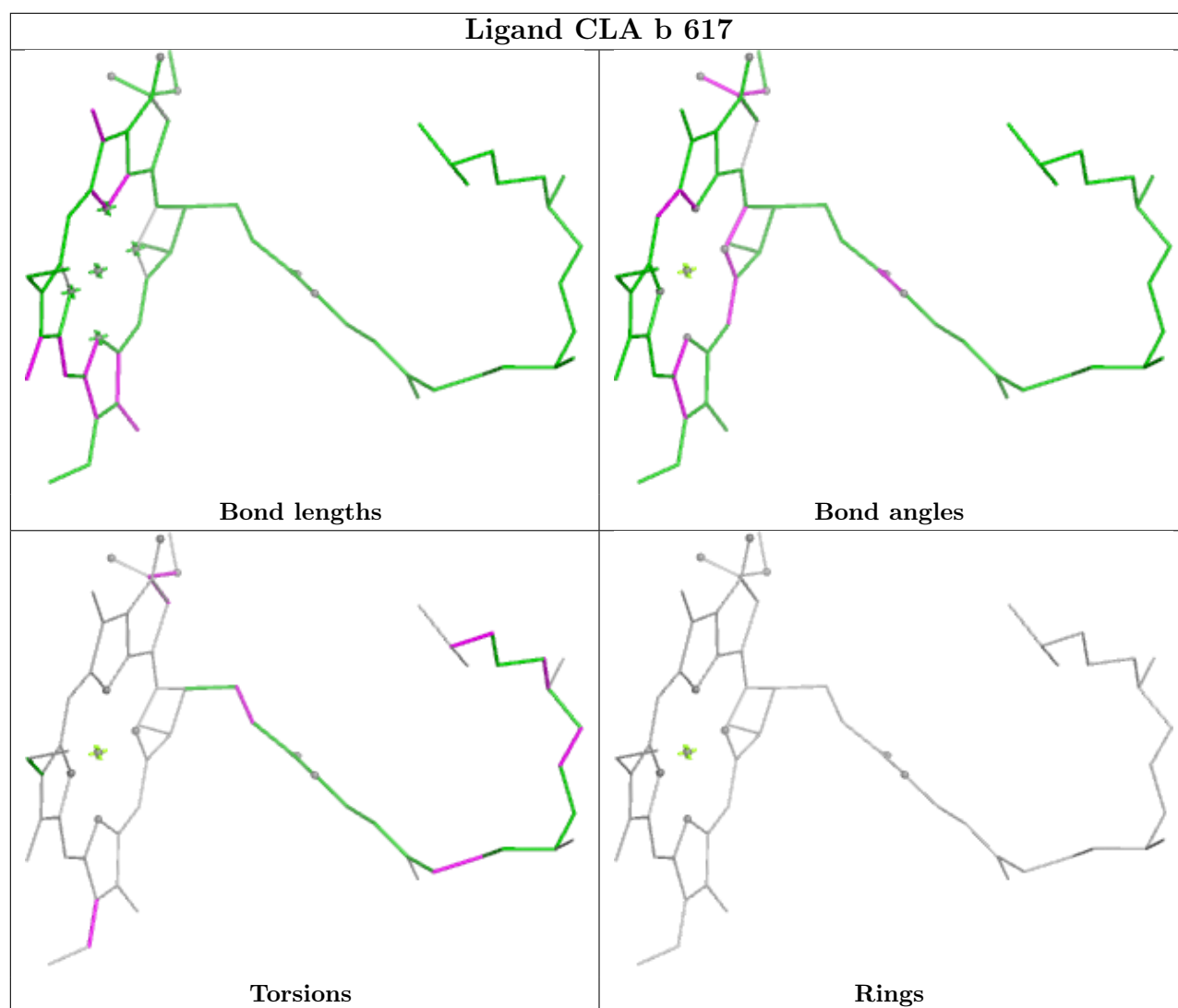
Ligand CHL R 312



Ligand CLA B 604







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

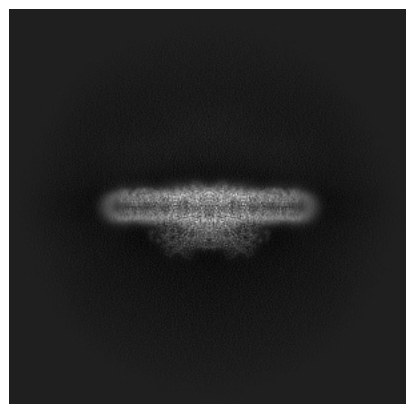
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52620. These allow visual inspection of the internal detail of the map and identification of artifacts.

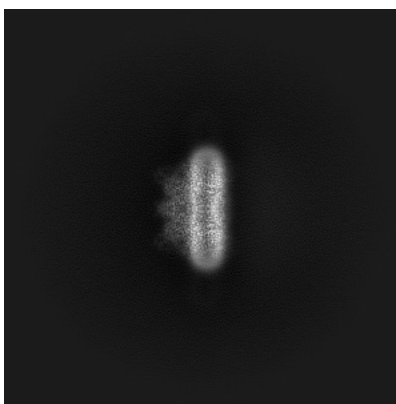
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

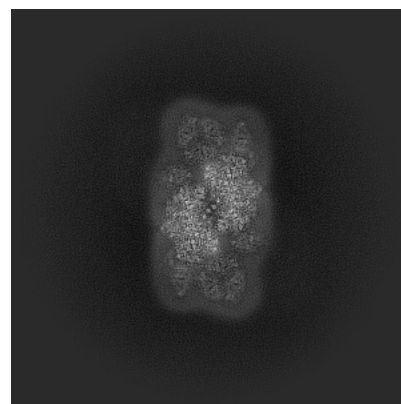
6.1.1 Primary map



X

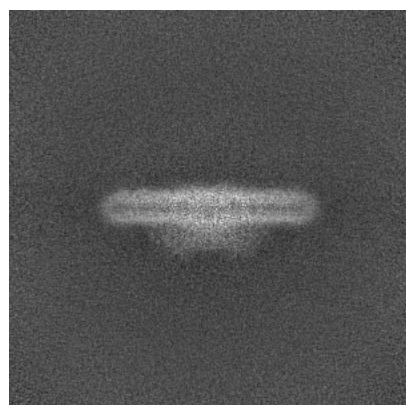


Y

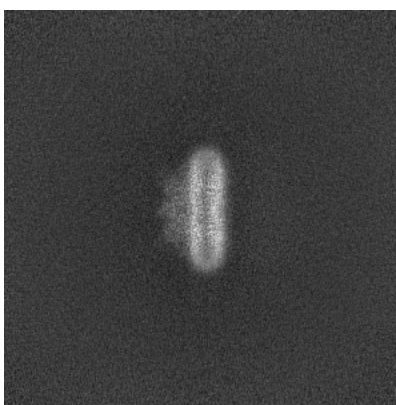


Z

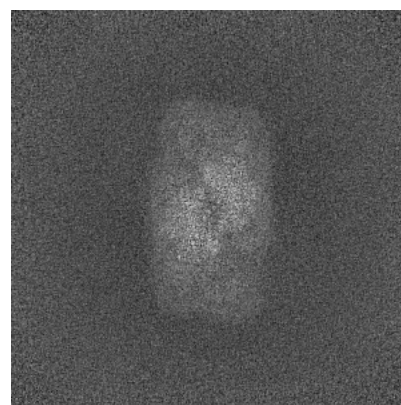
6.1.2 Raw map



X



Y

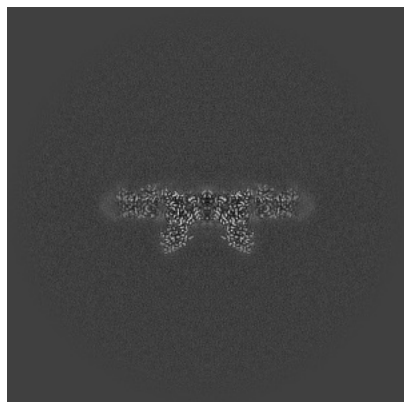


Z

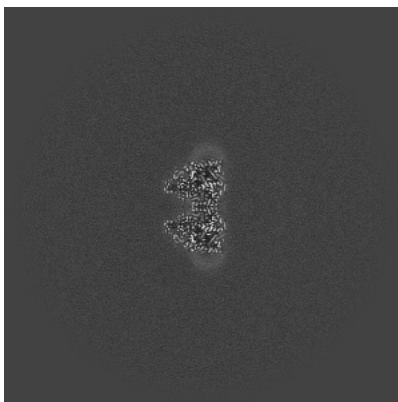
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

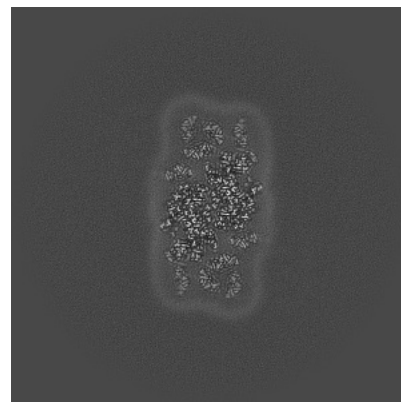
6.2.1 Primary map



X Index: 392

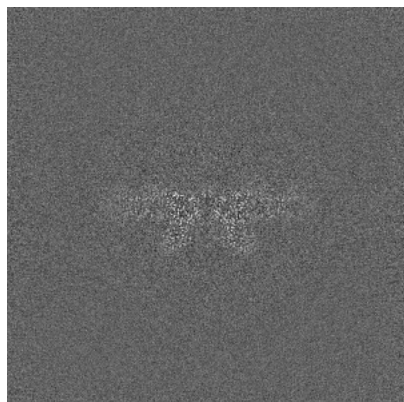


Y Index: 392

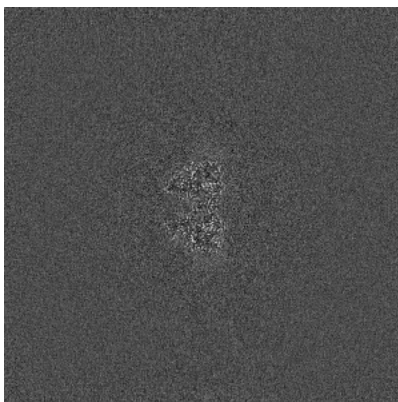


Z Index: 392

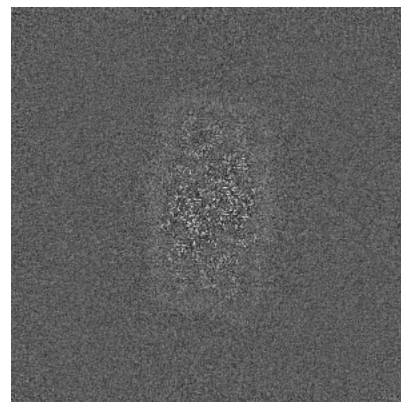
6.2.2 Raw map



X Index: 392



Y Index: 392

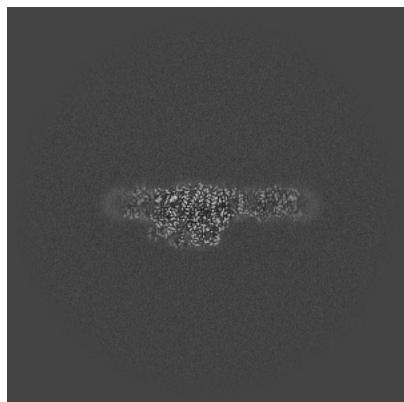


Z Index: 392

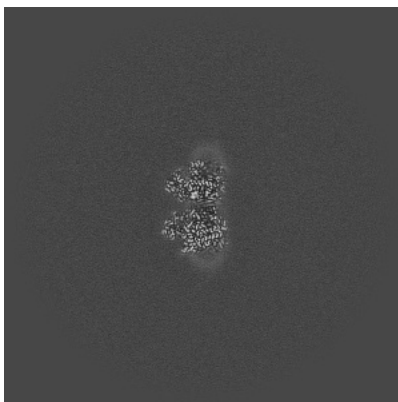
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

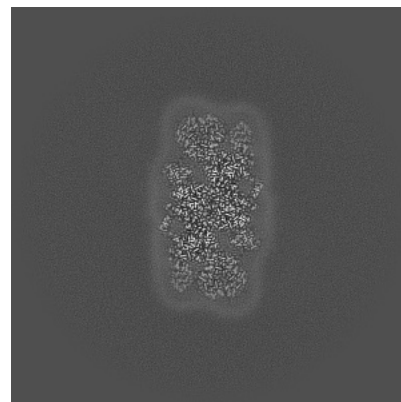
6.3.1 Primary map



X Index: 348

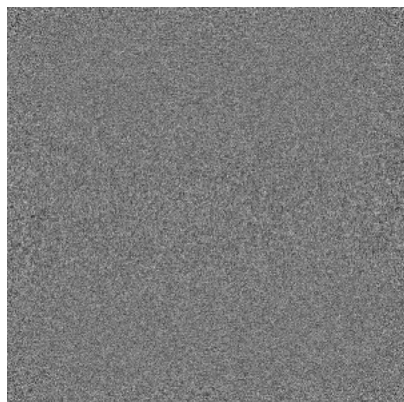


Y Index: 381

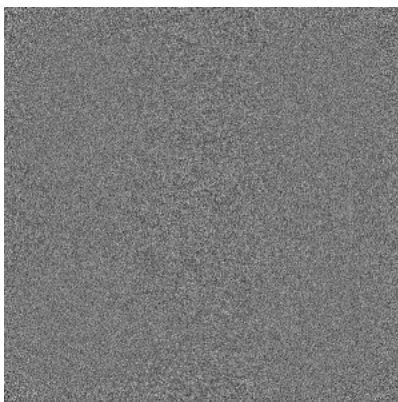


Z Index: 408

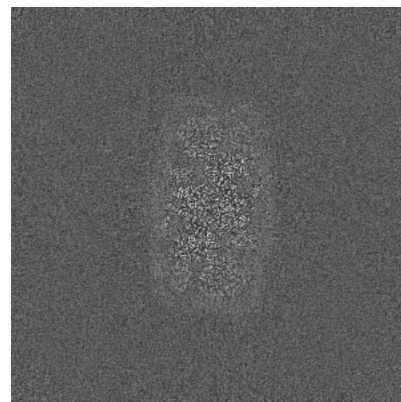
6.3.2 Raw map



X Index: 0



Y Index: 0

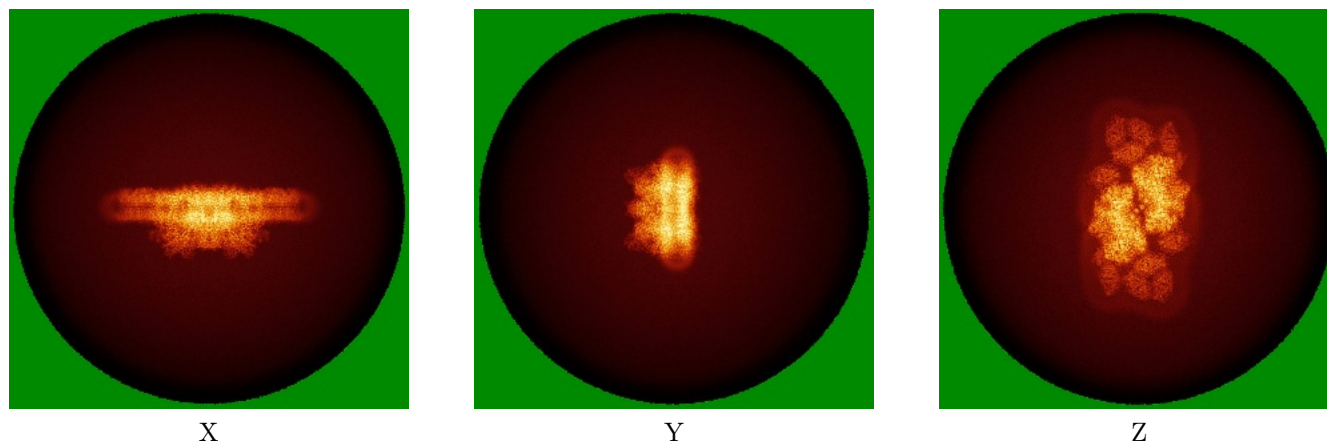


Z Index: 408

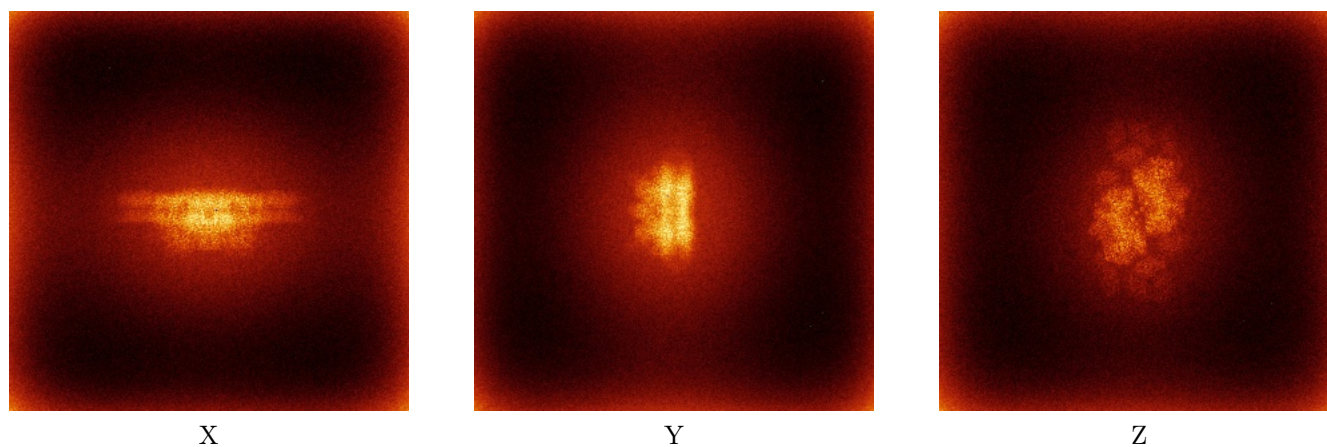
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



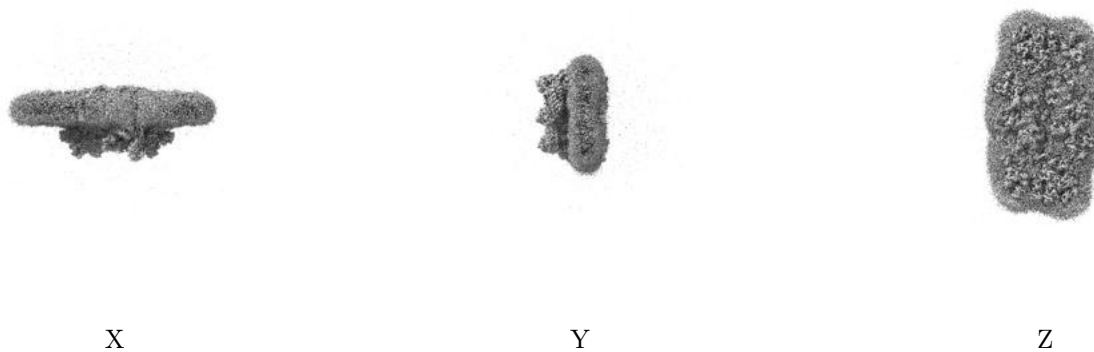
6.4.2 Raw map



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

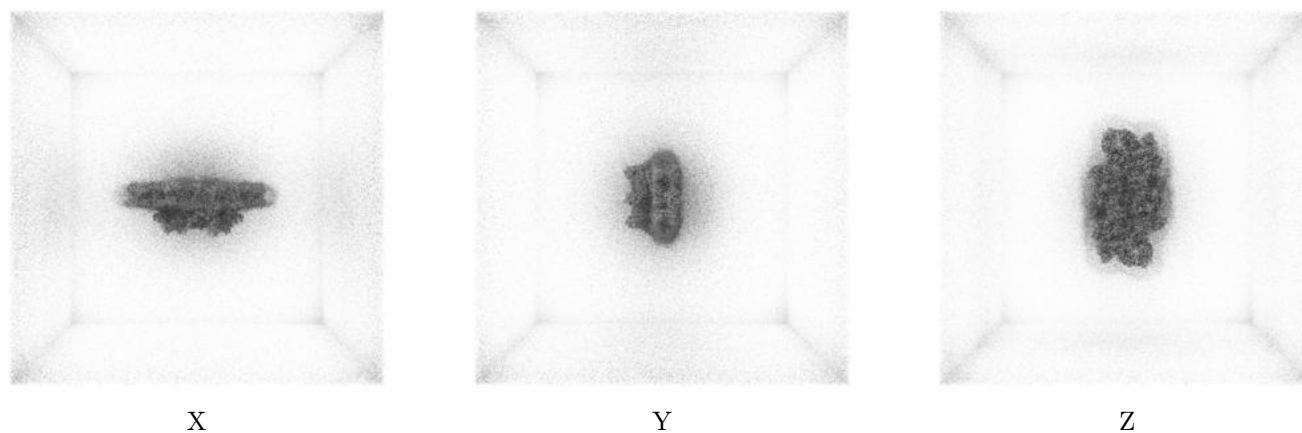
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.149. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

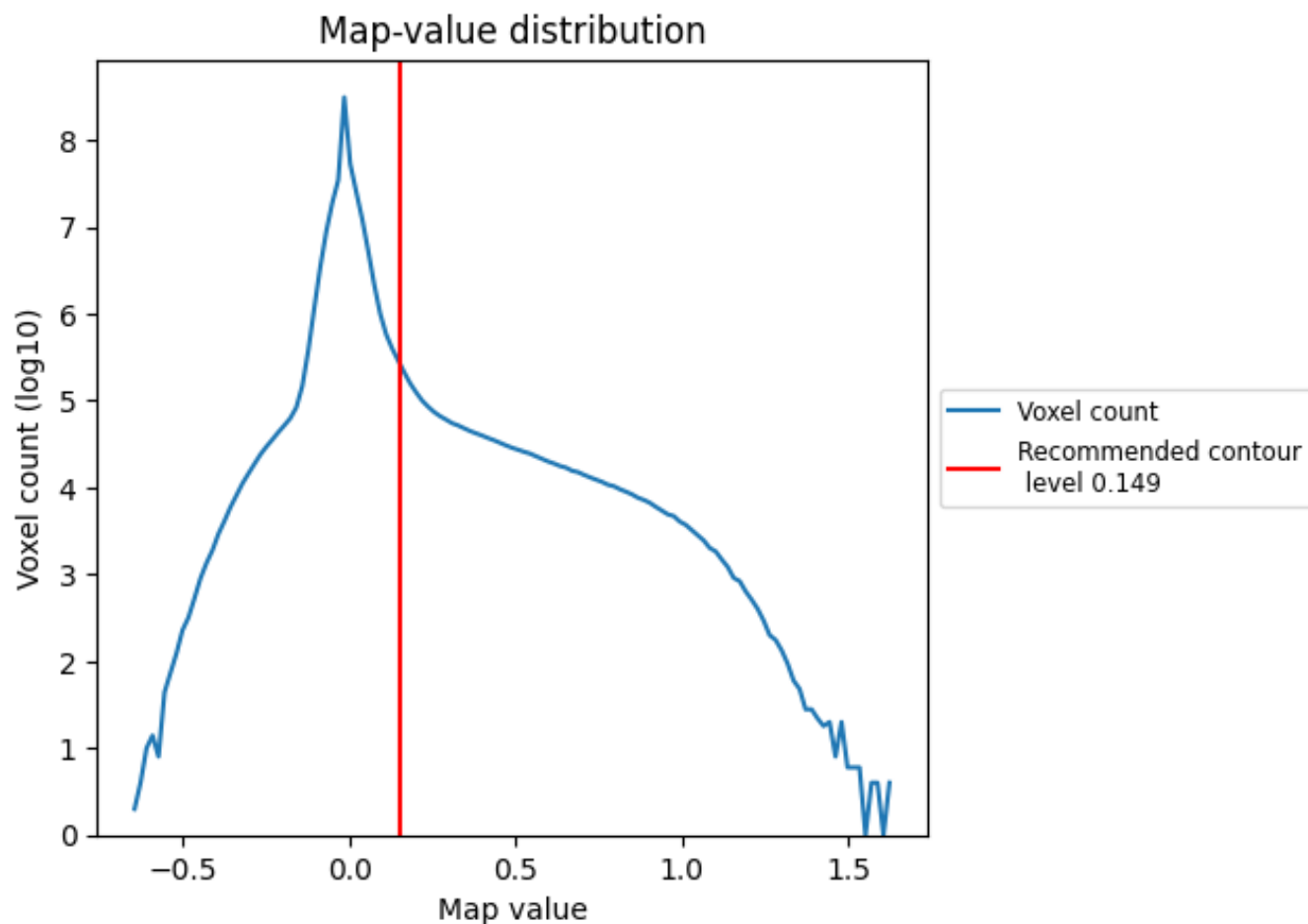
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

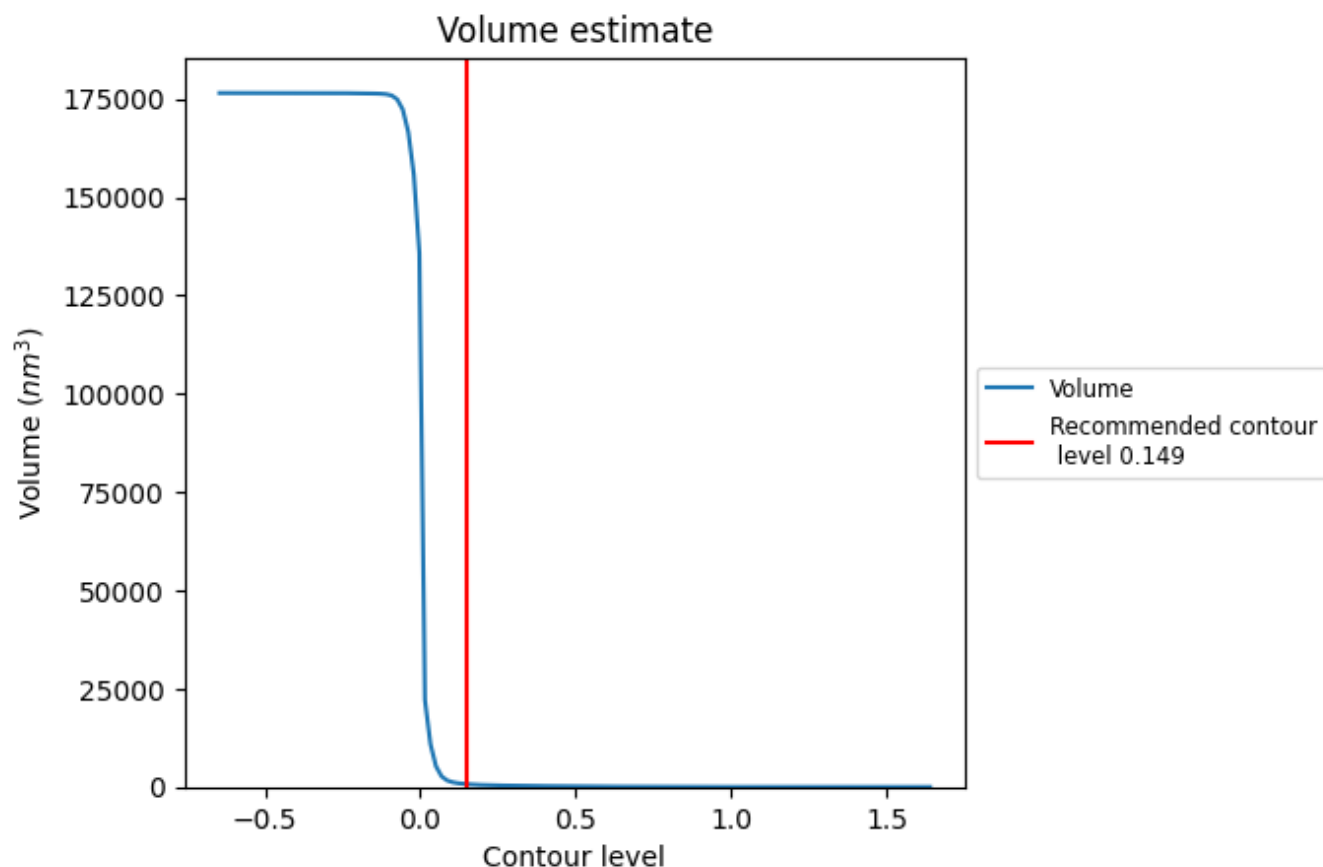
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

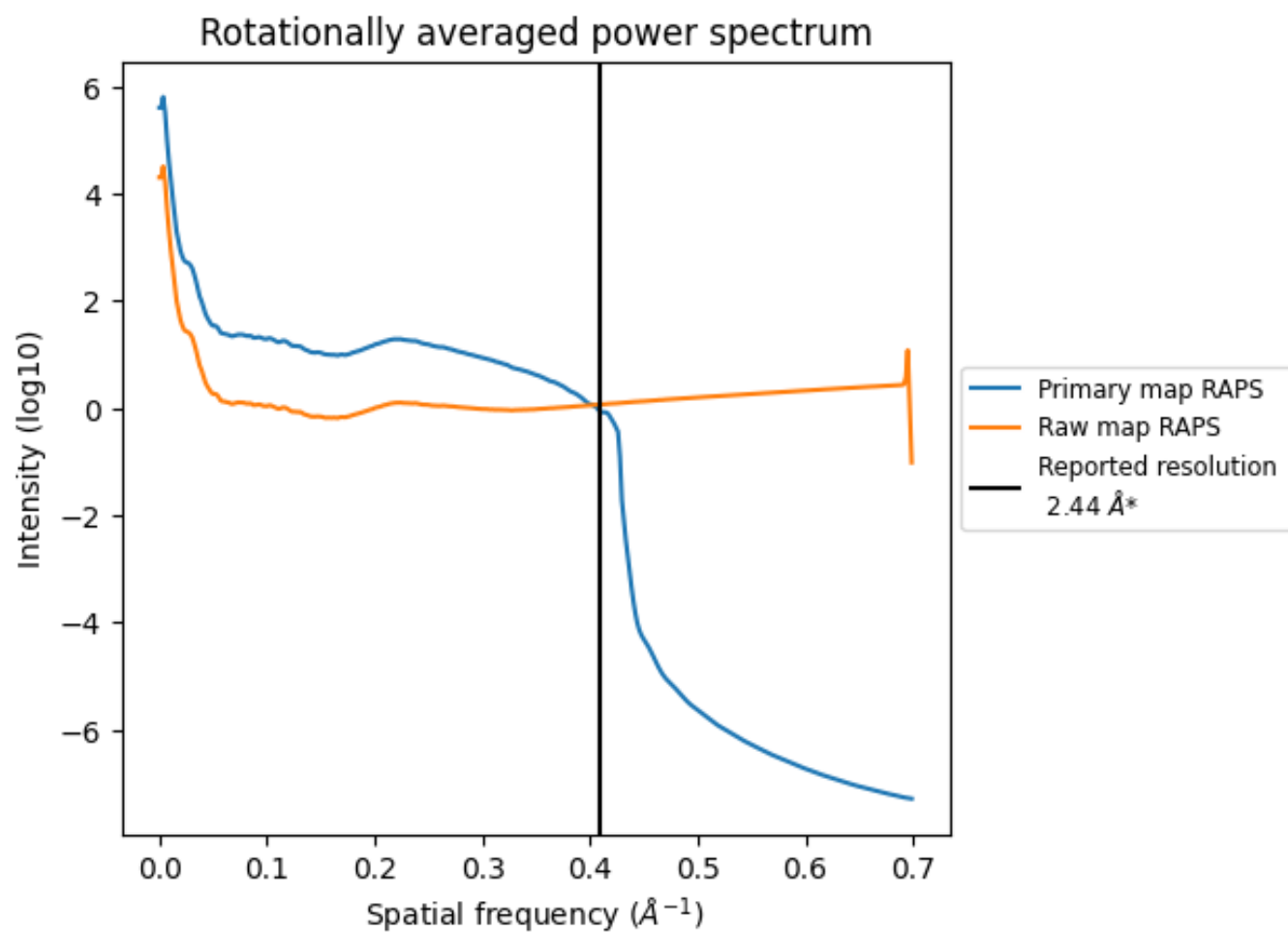
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 724 nm^3 ; this corresponds to an approximate mass of 654 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 ⓘ

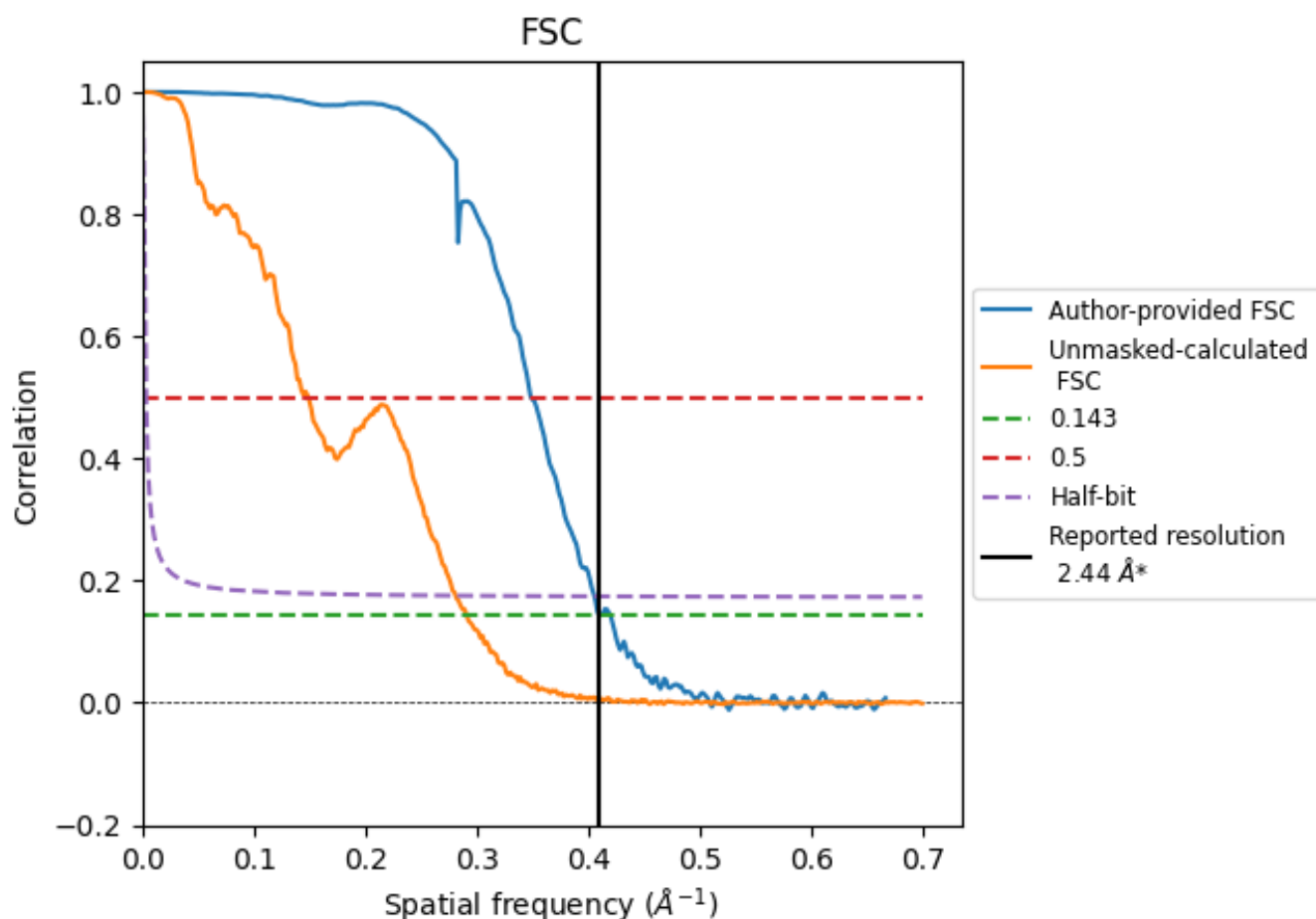


*Reported resolution corresponds to spatial frequency of 0.410 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.410 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

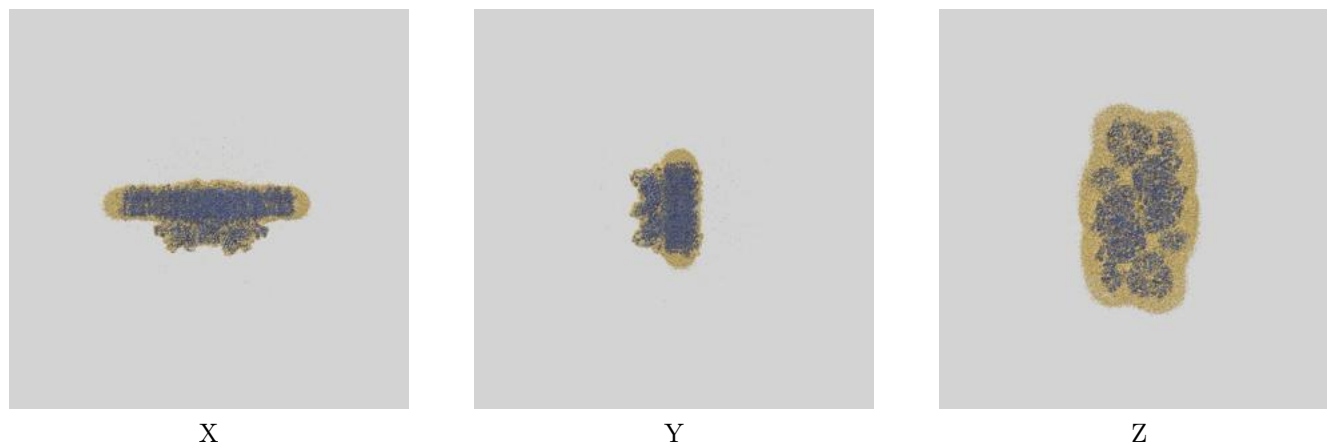
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	2.44	2.87	2.47
Unmasked-calculated*	3.44	6.72	3.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.44 differs from the reported value 2.44 by more than 10 %

9 Map-model fit [i](#)

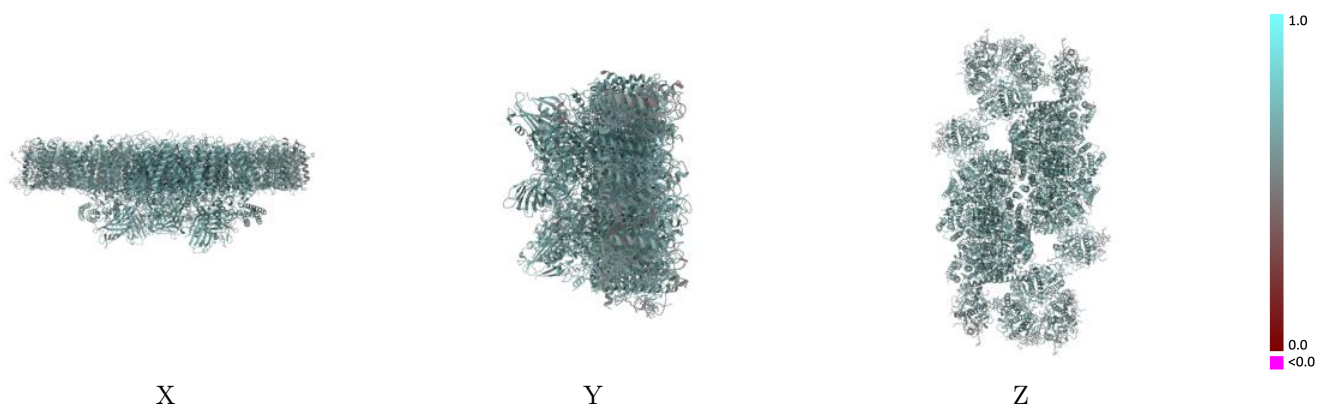
This section contains information regarding the fit between EMDB map EMD-52620 and PDB model 9I4T. Per-residue inclusion information can be found in section 3 on page 37.

9.1 Map-model overlay [i](#)



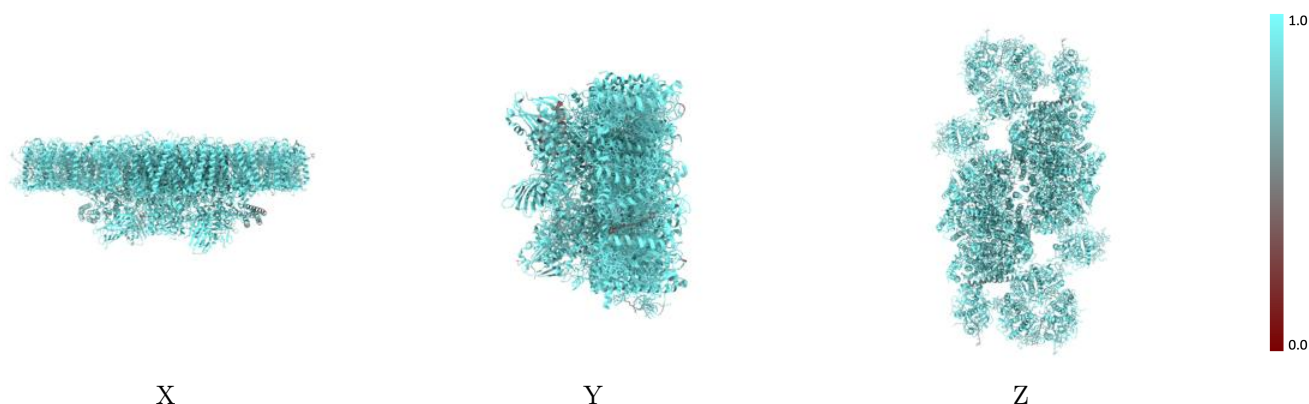
The images above show the 3D surface view of the map at the recommended contour level 0.149 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



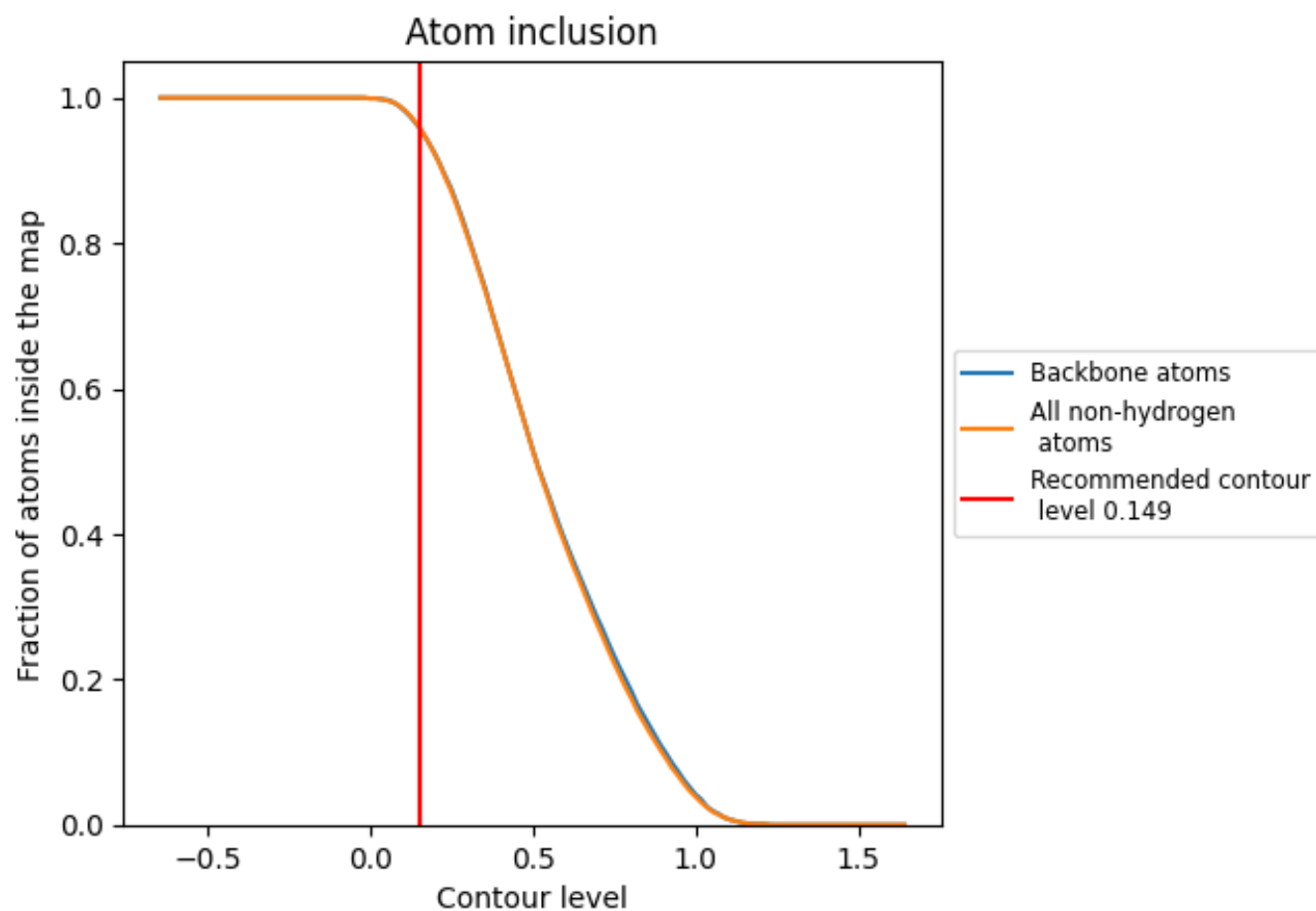
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.149).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.149) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9600	 0.6330
A	 0.9940	 0.6680
B	 0.9920	 0.6650
C	 0.9830	 0.6550
D	 0.9910	 0.6720
E	 0.9900	 0.6360
F	 0.9830	 0.6340
G	 0.8890	 0.5710
H	 0.9960	 0.6570
I	 1.0000	 0.6690
J	 0.9900	 0.6260
K	 0.9820	 0.6380
L	 0.9970	 0.6720
M	 0.9880	 0.6430
N	 0.9390	 0.5990
O	 0.9570	 0.6270
P	 0.9530	 0.6390
Q	 0.7890	 0.5870
R	 0.9490	 0.6090
S	 0.9120	 0.5660
T	 0.9530	 0.6360
U	 0.9480	 0.6290
W	 0.9600	 0.6250
X	 0.9780	 0.6270
Y	 0.9720	 0.6380
Z	 0.9630	 0.5960
a	 0.9940	 0.6680
b	 0.9910	 0.6640
c	 0.9830	 0.6540
d	 0.9910	 0.6710
e	 0.9890	 0.6340
f	 0.9790	 0.6330
g	 0.8900	 0.5700
h	 0.9940	 0.6580
i	 1.0000	 0.6700



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
j	 0.9830	 0.6240
k	 0.9820	 0.6360
l	 0.9970	 0.6680
m	 0.9880	 0.6440
n	 0.9400	 0.5990
o	 0.9550	 0.6260
p	 0.9520	 0.6360
q	 0.7920	 0.5870
r	 0.9480	 0.6090
s	 0.9110	 0.5670
t	 0.9560	 0.6300
u	 0.9480	 0.6300
w	 0.9620	 0.6220
x	 0.9780	 0.6220
y	 0.9720	 0.6370
z	 0.9600	 0.5930