



## wwPDB EM Validation Summary Report i

Nov 22, 2022 – 02:53 AM JST

PDB ID : 7DWX  
EMDB ID : EMD-30888  
Title : Conformation 1 of S-ACE2-B0AT1 ternary complex  
Authors : Yan, R.H.; Zhang, Y.Y.; Li, Y.N.; Ye, F.F.; Guo, Y.Y.; Xia, L.; Zhong, X.Y.; Chi, X.M.; Zhou, Q.  
Deposited on : 2021-01-18  
Resolution : 8.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

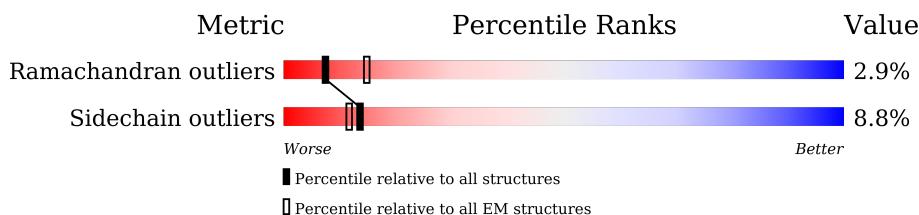
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
**ELECTRON MICROSCOPY**

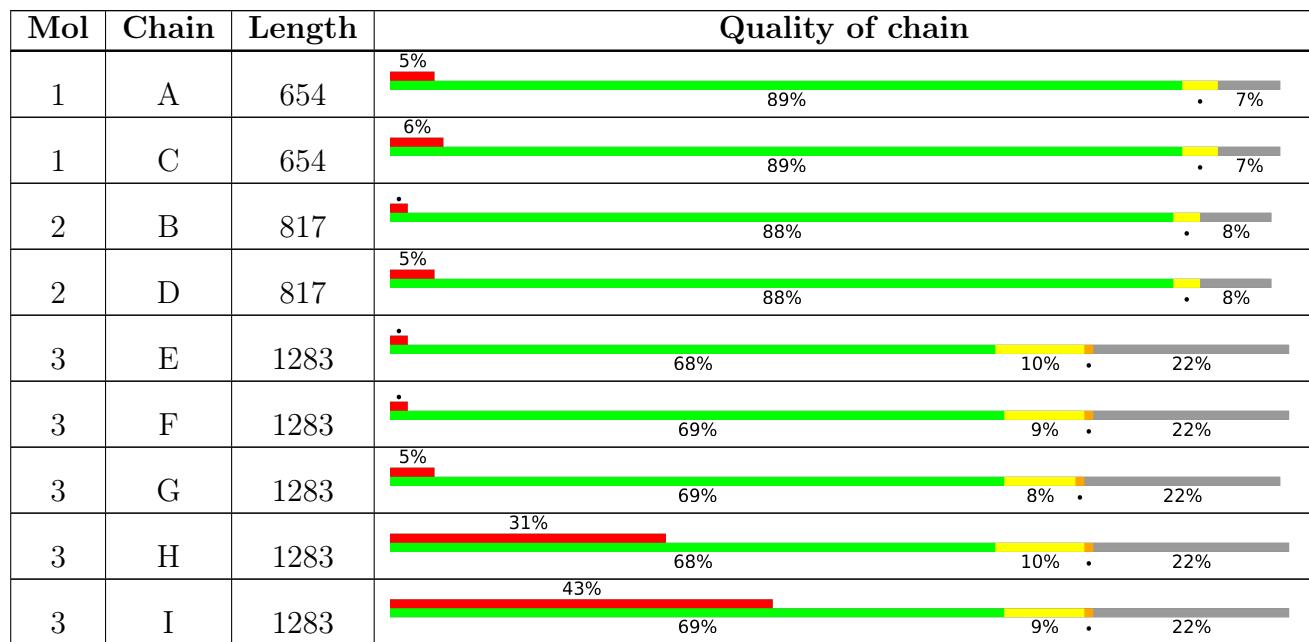
The reported resolution of this entry is 8.30 Å.

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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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.



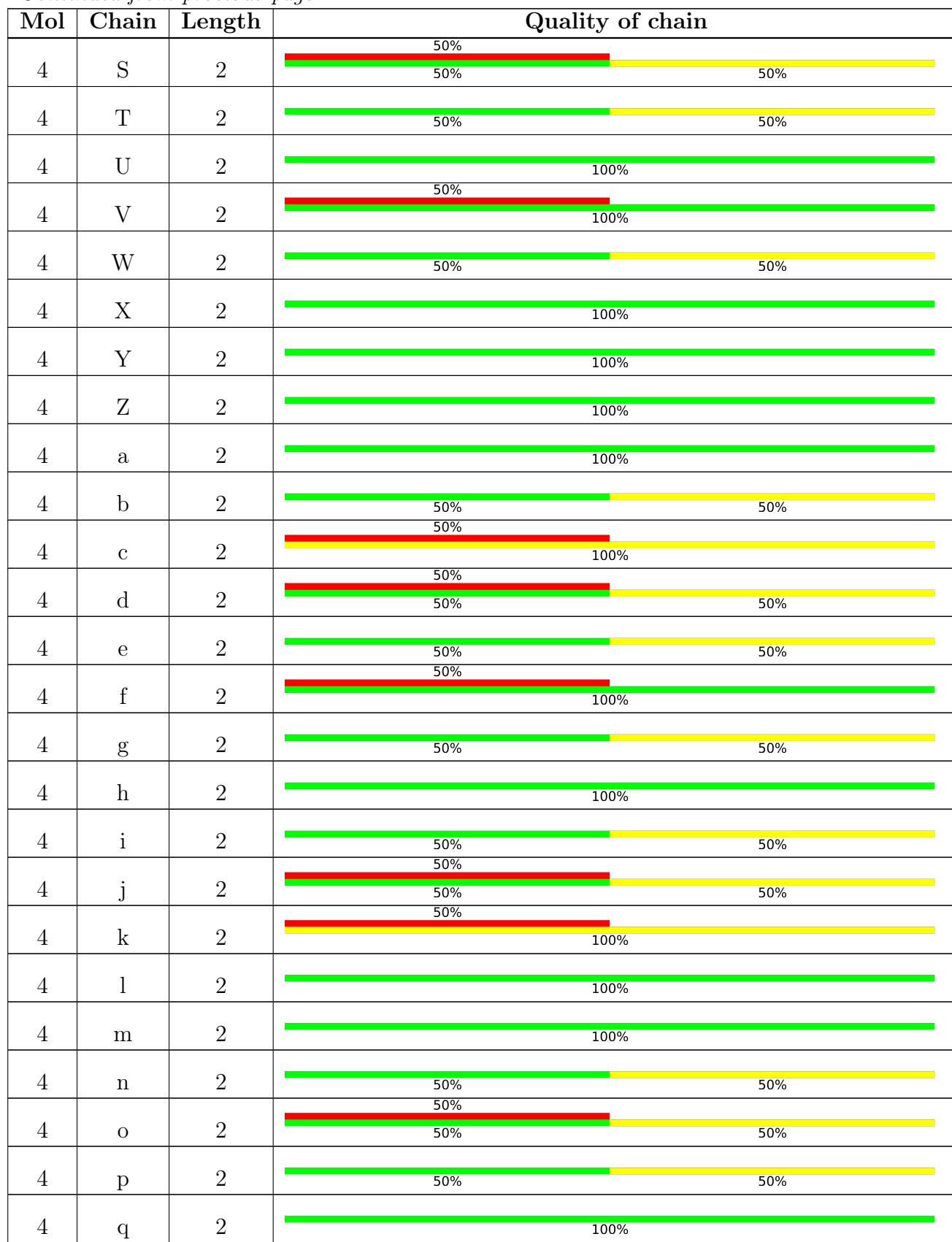
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Mol	Chain	Length	Quality of chain
3	J	1283	65% 69% 8% 22%
4	0	2	100% 50% 50%
4	1	2	100% 100% 100%
4	2	2	50% 100% 50%
4	3	2	100% 100% 100%
4	4	2	50% 100% 50%
4	5	2	50% 100% 50%
4	6	2	100% 100% 100%
4	7	2	100% 100% 100%
4	8	2	100% 100% 100%
4	9	2	50% 100% 50%
4	AA	2	50% 100% 50%
4	BA	2	50% 100% 50%
4	CA	2	100% 100% 100%
4	DA	2	50% 100% 50%
4	EA	2	100% 100% 100%
4	FA	2	100% 100% 100%
4	K	2	100% 100%
4	L	2	50% 100% 50%
4	M	2	50% 100% 50%
4	N	2	100% 100%
4	O	2	50% 100% 100%
4	P	2	50% 100% 50%
4	Q	2	100% 100%
4	R	2	100% 100%

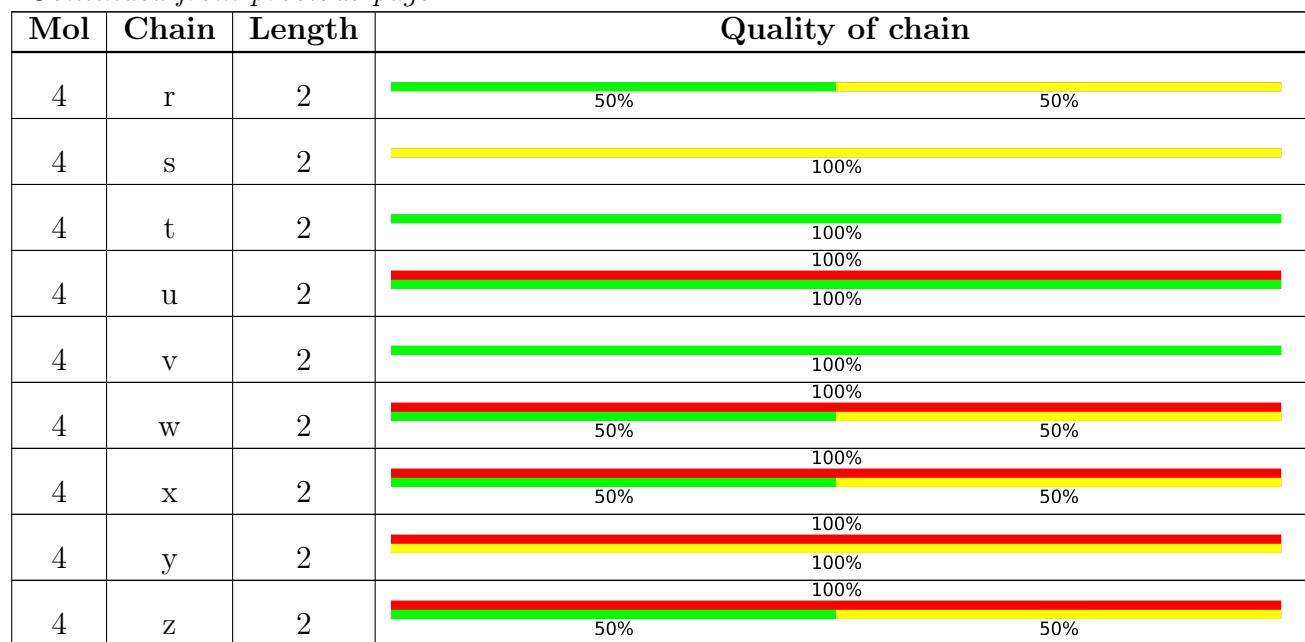
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## 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 71532 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 Sodium-dependent neutral amino acid transporter B(0)AT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	605	4799	3171	744	854	30	0	0
1	C	605	4799	3171	744	854	30	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q695T7
A	-18	ALA	-	expression tag	UNP Q695T7
A	-17	ASP	-	expression tag	UNP Q695T7
A	-16	TYR	-	expression tag	UNP Q695T7
A	-15	LYS	-	expression tag	UNP Q695T7
A	-14	ASP	-	expression tag	UNP Q695T7
A	-13	ASP	-	expression tag	UNP Q695T7
A	-12	ASP	-	expression tag	UNP Q695T7
A	-11	ASP	-	expression tag	UNP Q695T7
A	-10	LYS	-	expression tag	UNP Q695T7
A	-9	SER	-	expression tag	UNP Q695T7
A	-8	GLY	-	expression tag	UNP Q695T7
A	-7	PRO	-	expression tag	UNP Q695T7
A	-6	ASP	-	expression tag	UNP Q695T7
A	-5	GLU	-	expression tag	UNP Q695T7
A	-4	VAL	-	expression tag	UNP Q695T7
A	-3	ASP	-	expression tag	UNP Q695T7
A	-2	ALA	-	expression tag	UNP Q695T7
A	-1	SER	-	expression tag	UNP Q695T7
A	0	GLY	-	expression tag	UNP Q695T7
A	1	ARG	-	expression tag	UNP Q695T7
C	-19	MET	-	initiating methionine	UNP Q695T7
C	-18	ALA	-	expression tag	UNP Q695T7
C	-17	ASP	-	expression tag	UNP Q695T7
C	-16	TYR	-	expression tag	UNP Q695T7
C	-15	LYS	-	expression tag	UNP Q695T7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	ASP	-	expression tag	UNP Q695T7
C	-13	ASP	-	expression tag	UNP Q695T7
C	-12	ASP	-	expression tag	UNP Q695T7
C	-11	ASP	-	expression tag	UNP Q695T7
C	-10	LYS	-	expression tag	UNP Q695T7
C	-9	SER	-	expression tag	UNP Q695T7
C	-8	GLY	-	expression tag	UNP Q695T7
C	-7	PRO	-	expression tag	UNP Q695T7
C	-6	ASP	-	expression tag	UNP Q695T7
C	-5	GLU	-	expression tag	UNP Q695T7
C	-4	VAL	-	expression tag	UNP Q695T7
C	-3	ASP	-	expression tag	UNP Q695T7
C	-2	ALA	-	expression tag	UNP Q695T7
C	-1	SER	-	expression tag	UNP Q695T7
C	0	GLY	-	expression tag	UNP Q695T7
C	1	ARG	-	expression tag	UNP Q695T7

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	748	Total	C	N	O	S		
			6089	3906	1018	1131	34	0	0
2	D	748	Total	C	N	O	S		
			6089	3906	1018	1131	34	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	expression tag	UNP Q9BYF1
B	-10	ALA	-	expression tag	UNP Q9BYF1
B	-9	SER	-	expression tag	UNP Q9BYF1
B	-8	GLY	-	expression tag	UNP Q9BYF1
B	-7	ARG	-	expression tag	UNP Q9BYF1
B	10	TRP	-	insertion	UNP Q9BYF1
B	11	SER	-	insertion	UNP Q9BYF1
B	12	HIS	-	insertion	UNP Q9BYF1
B	13	PRO	-	insertion	UNP Q9BYF1
B	14	GLN	-	insertion	UNP Q9BYF1
B	15	PHE	-	insertion	UNP Q9BYF1
B	16	GLU	-	insertion	UNP Q9BYF1
B	17	LYS	-	insertion	UNP Q9BYF1
D	-11	MET	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	ALA	-	expression tag	UNP Q9BYF1
D	-9	SER	-	expression tag	UNP Q9BYF1
D	-8	GLY	-	expression tag	UNP Q9BYF1
D	-7	ARG	-	expression tag	UNP Q9BYF1
D	10	TRP	-	insertion	UNP Q9BYF1
D	11	SER	-	insertion	UNP Q9BYF1
D	12	HIS	-	insertion	UNP Q9BYF1
D	13	PRO	-	insertion	UNP Q9BYF1
D	14	GLN	-	insertion	UNP Q9BYF1
D	15	PHE	-	insertion	UNP Q9BYF1
D	16	GLU	-	insertion	UNP Q9BYF1
D	17	LYS	-	insertion	UNP Q9BYF1

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
3	E	1007	Total	C 7872	N 5025	O 1310	S 1501	36	0	0
3	F	1006	Total	C 7866	N 5022	O 1309	S 1499	36	0	0
3	G	1006	Total	C 7866	N 5022	O 1309	S 1499	36	0	0
3	H	1007	Total	C 7872	N 5025	O 1310	S 1501	36	0	0
3	I	1006	Total	C 7866	N 5022	O 1309	S 1499	36	0	0
3	J	1006	Total	C 7866	N 5022	O 1309	S 1499	36	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	986	PRO	LYS	engineered mutation	UNP P0DTC2
E	987	PRO	VAL	engineered mutation	UNP P0DTC2
E	1274	LEU	-	expression tag	UNP P0DTC2
E	1275	GLU	-	expression tag	UNP P0DTC2
E	1276	ASP	-	expression tag	UNP P0DTC2
E	1277	TYR	-	expression tag	UNP P0DTC2
E	1278	LYS	-	expression tag	UNP P0DTC2
E	1279	ASP	-	expression tag	UNP P0DTC2
E	1280	ASP	-	expression tag	UNP P0DTC2
E	1281	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1282	ASP	-	expression tag	UNP P0DTC2
E	1283	LYS	-	expression tag	UNP P0DTC2
F	986	PRO	LYS	engineered mutation	UNP P0DTC2
F	987	PRO	VAL	engineered mutation	UNP P0DTC2
F	1274	LEU	-	expression tag	UNP P0DTC2
F	1275	GLU	-	expression tag	UNP P0DTC2
F	1276	ASP	-	expression tag	UNP P0DTC2
F	1277	TYR	-	expression tag	UNP P0DTC2
F	1278	LYS	-	expression tag	UNP P0DTC2
F	1279	ASP	-	expression tag	UNP P0DTC2
F	1280	ASP	-	expression tag	UNP P0DTC2
F	1281	ASP	-	expression tag	UNP P0DTC2
F	1282	ASP	-	expression tag	UNP P0DTC2
F	1283	LYS	-	expression tag	UNP P0DTC2
G	986	PRO	LYS	engineered mutation	UNP P0DTC2
G	987	PRO	VAL	engineered mutation	UNP P0DTC2
G	1274	LEU	-	expression tag	UNP P0DTC2
G	1275	GLU	-	expression tag	UNP P0DTC2
G	1276	ASP	-	expression tag	UNP P0DTC2
G	1277	TYR	-	expression tag	UNP P0DTC2
G	1278	LYS	-	expression tag	UNP P0DTC2
G	1279	ASP	-	expression tag	UNP P0DTC2
G	1280	ASP	-	expression tag	UNP P0DTC2
G	1281	ASP	-	expression tag	UNP P0DTC2
G	1282	ASP	-	expression tag	UNP P0DTC2
G	1283	LYS	-	expression tag	UNP P0DTC2
H	986	PRO	LYS	engineered mutation	UNP P0DTC2
H	987	PRO	VAL	engineered mutation	UNP P0DTC2
H	1274	LEU	-	expression tag	UNP P0DTC2
H	1275	GLU	-	expression tag	UNP P0DTC2
H	1276	ASP	-	expression tag	UNP P0DTC2
H	1277	TYR	-	expression tag	UNP P0DTC2
H	1278	LYS	-	expression tag	UNP P0DTC2
H	1279	ASP	-	expression tag	UNP P0DTC2
H	1280	ASP	-	expression tag	UNP P0DTC2
H	1281	ASP	-	expression tag	UNP P0DTC2
H	1282	ASP	-	expression tag	UNP P0DTC2
H	1283	LYS	-	expression tag	UNP P0DTC2
I	986	PRO	LYS	engineered mutation	UNP P0DTC2
I	987	PRO	VAL	engineered mutation	UNP P0DTC2
I	1274	LEU	-	expression tag	UNP P0DTC2
I	1275	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	1276	ASP	-	expression tag	UNP P0DTC2
I	1277	TYR	-	expression tag	UNP P0DTC2
I	1278	LYS	-	expression tag	UNP P0DTC2
I	1279	ASP	-	expression tag	UNP P0DTC2
I	1280	ASP	-	expression tag	UNP P0DTC2
I	1281	ASP	-	expression tag	UNP P0DTC2
I	1282	ASP	-	expression tag	UNP P0DTC2
I	1283	LYS	-	expression tag	UNP P0DTC2
J	986	PRO	LYS	engineered mutation	UNP P0DTC2
J	987	PRO	VAL	engineered mutation	UNP P0DTC2
J	1274	LEU	-	expression tag	UNP P0DTC2
J	1275	GLU	-	expression tag	UNP P0DTC2
J	1276	ASP	-	expression tag	UNP P0DTC2
J	1277	TYR	-	expression tag	UNP P0DTC2
J	1278	LYS	-	expression tag	UNP P0DTC2
J	1279	ASP	-	expression tag	UNP P0DTC2
J	1280	ASP	-	expression tag	UNP P0DTC2
J	1281	ASP	-	expression tag	UNP P0DTC2
J	1282	ASP	-	expression tag	UNP P0DTC2
J	1283	LYS	-	expression tag	UNP P0DTC2

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		
4	c	2	Total	C	N	O	0	0
			28	16	2	10		
4	d	2	Total	C	N	O	0	0
			28	16	2	10		
4	e	2	Total	C	N	O	0	0
			28	16	2	10		
4	f	2	Total	C	N	O	0	0
			28	16	2	10		
4	g	2	Total	C	N	O	0	0
			28	16	2	10		
4	h	2	Total	C	N	O	0	0
			28	16	2	10		
4	i	2	Total	C	N	O	0	0
			28	16	2	10		
4	j	2	Total	C	N	O	0	0
			28	16	2	10		
4	k	2	Total	C	N	O	0	0
			28	16	2	10		

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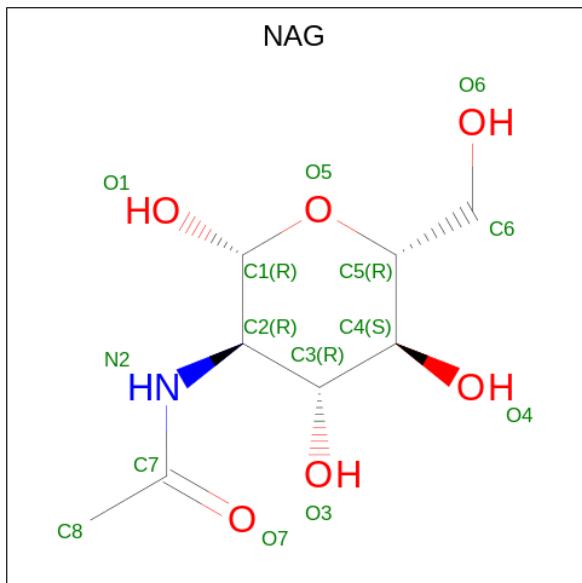
Mol	Chain	Residues	Atoms				AltConf	Trace
4	l	2	Total	C	N	O	0	0
			28	16	2	10		
4	m	2	Total	C	N	O	0	0
			28	16	2	10		
4	n	2	Total	C	N	O	0	0
			28	16	2	10		
4	o	2	Total	C	N	O	0	0
			28	16	2	10		
4	p	2	Total	C	N	O	0	0
			28	16	2	10		
4	q	2	Total	C	N	O	0	0
			28	16	2	10		
4	r	2	Total	C	N	O	0	0
			28	16	2	10		
4	s	2	Total	C	N	O	0	0
			28	16	2	10		
4	t	2	Total	C	N	O	0	0
			28	16	2	10		
4	u	2	Total	C	N	O	0	0
			28	16	2	10		
4	v	2	Total	C	N	O	0	0
			28	16	2	10		
4	w	2	Total	C	N	O	0	0
			28	16	2	10		
4	x	2	Total	C	N	O	0	0
			28	16	2	10		
4	y	2	Total	C	N	O	0	0
			28	16	2	10		
4	z	2	Total	C	N	O	0	0
			28	16	2	10		
4	0	2	Total	C	N	O	0	0
			28	16	2	10		
4	1	2	Total	C	N	O	0	0
			28	16	2	10		
4	2	2	Total	C	N	O	0	0
			28	16	2	10		
4	3	2	Total	C	N	O	0	0
			28	16	2	10		
4	4	2	Total	C	N	O	0	0
			28	16	2	10		
4	5	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	6	2	Total 28	C 16	N 2	O 10	0	0
4	7	2	Total 28	C 16	N 2	O 10	0	0
4	8	2	Total 28	C 16	N 2	O 10	0	0
4	9	2	Total 28	C 16	N 2	O 10	0	0
4	AA	2	Total 28	C 16	N 2	O 10	0	0
4	BA	2	Total 28	C 16	N 2	O 10	0	0
4	CA	2	Total 28	C 16	N 2	O 10	0	0
4	DA	2	Total 28	C 16	N 2	O 10	0	0
4	EA	2	Total 28	C 16	N 2	O 10	0	0
4	FA	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total 56	C 32	N 4	O 20	0

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Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			56	32	4	20	
5	A	1	Total	C	N	O	0
			56	32	4	20	
5	A	1	Total	C	N	O	0
			56	32	4	20	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			56	32	4	20	
5	C	1	Total	C	N	O	0
			56	32	4	20	
5	C	1	Total	C	N	O	0
			56	32	4	20	
5	C	1	Total	C	N	O	0
			56	32	4	20	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			126	72	9	45	
5	E	1	Total	C	N	O	0
			126	72	9	45	
5	E	1	Total	C	N	O	0
			126	72	9	45	
5	E	1	Total	C	N	O	0
			126	72	9	45	
5	E	1	Total	C	N	O	0
			126	72	9	45	
5	E	1	Total	C	N	O	0
			126	72	9	45	
5	E	1	Total	C	N	O	0
			126	72	9	45	
5	F	1	Total	C	N	O	0
			140	80	10	50	
5	F	1	Total	C	N	O	0
			140	80	10	50	
5	F	1	Total	C	N	O	0
			140	80	10	50	

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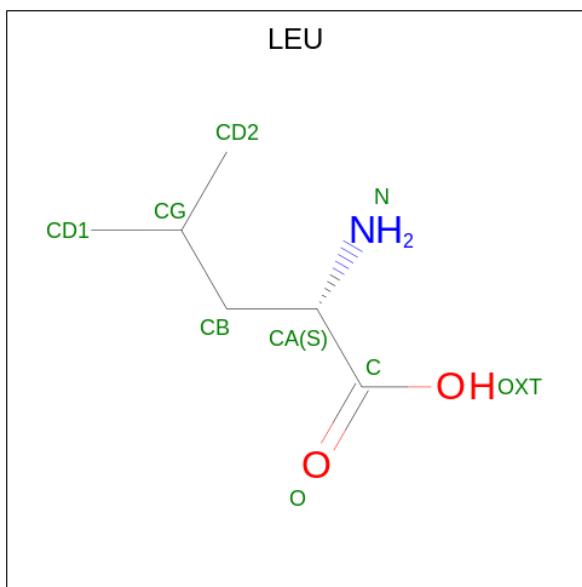
Mol	Chain	Residues	Atoms				AltConf
5	F	1	Total	C	N	O	0
			140	80	10	50	
5	F	1	Total	C	N	O	0
			140	80	10	50	
5	F	1	Total	C	N	O	0
			140	80	10	50	
5	F	1	Total	C	N	O	0
			140	80	10	50	
5	F	1	Total	C	N	O	0
			140	80	10	50	
5	F	1	Total	C	N	O	0
			140	80	10	50	
5	F	1	Total	C	N	O	0
			140	80	10	50	
5	G	1	Total	C	N	O	0
			112	64	8	40	
5	G	1	Total	C	N	O	0
			112	64	8	40	
5	G	1	Total	C	N	O	0
			112	64	8	40	
5	G	1	Total	C	N	O	0
			112	64	8	40	
5	G	1	Total	C	N	O	0
			112	64	8	40	
5	G	1	Total	C	N	O	0
			112	64	8	40	
5	G	1	Total	C	N	O	0
			112	64	8	40	
5	H	1	Total	C	N	O	0
			126	72	9	45	
5	H	1	Total	C	N	O	0
			126	72	9	45	
5	H	1	Total	C	N	O	0
			126	72	9	45	
5	H	1	Total	C	N	O	0
			126	72	9	45	
5	H	1	Total	C	N	O	0
			126	72	9	45	
5	H	1	Total	C	N	O	0
			126	72	9	45	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf
5	H	1	Total	C	N	O	0
			126	72	9	45	
5	H	1	Total	C	N	O	0
			126	72	9	45	
5	H	1	Total	C	N	O	0
			126	72	9	45	
5	I	1	Total	C	N	O	0
			140	80	10	50	
5	I	1	Total	C	N	O	0
			140	80	10	50	
5	I	1	Total	C	N	O	0
			140	80	10	50	
5	I	1	Total	C	N	O	0
			140	80	10	50	
5	I	1	Total	C	N	O	0
			140	80	10	50	
5	I	1	Total	C	N	O	0
			140	80	10	50	
5	I	1	Total	C	N	O	0
			140	80	10	50	
5	I	1	Total	C	N	O	0
			140	80	10	50	
5	J	1	Total	C	N	O	0
			112	64	8	40	
5	J	1	Total	C	N	O	0
			112	64	8	40	
5	J	1	Total	C	N	O	0
			112	64	8	40	
5	J	1	Total	C	N	O	0
			112	64	8	40	
5	J	1	Total	C	N	O	0
			112	64	8	40	
5	J	1	Total	C	N	O	0
			112	64	8	40	
5	J	1	Total	C	N	O	0
			112	64	8	40	
5	J	1	Total	C	N	O	0
			112	64	8	40	

- Molecule 6 is LEUCINE (three-letter code: LEU) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total    C    N    O 9    6    1    2	0
6	C	1	Total    C    N    O 9    6    1    2	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
7	B	1	Total    Zn 1    1	0
7	D	1	Total    Zn 1    1	0

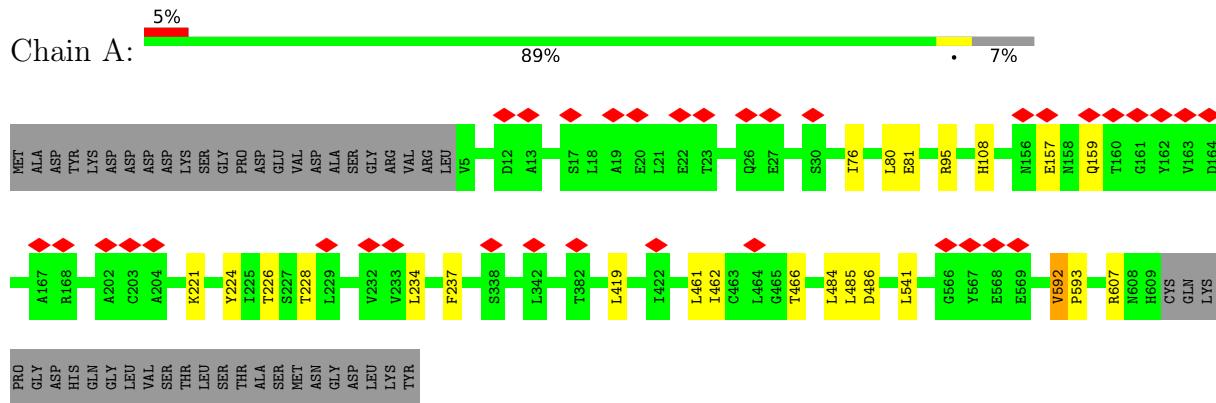
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	AltConf
8	B	4	Total    O 4    4	0
8	D	4	Total    O 4    4	0

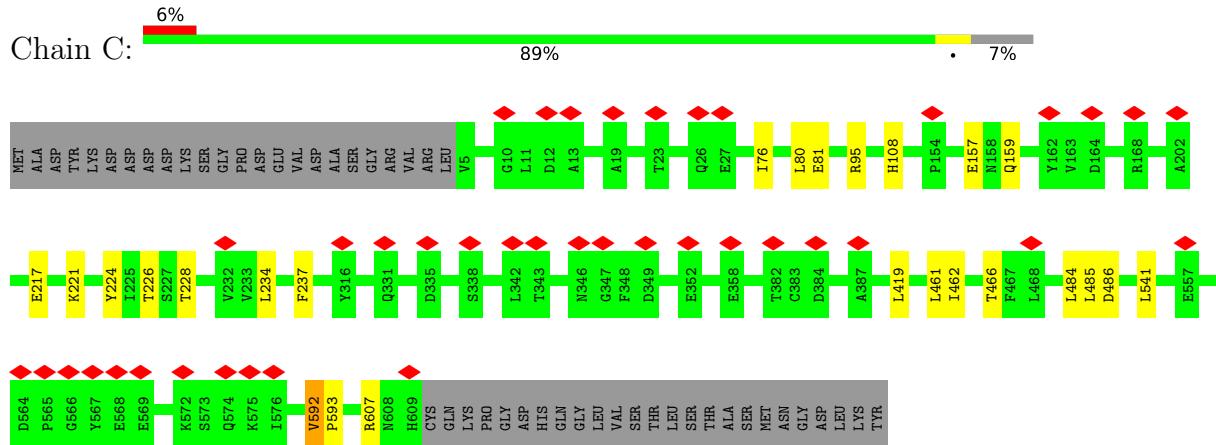
### 3 Residue-property plots

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.

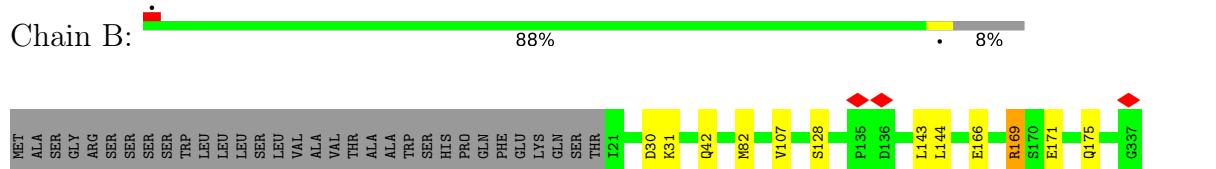
- Molecule 1: Sodium-dependent neutral amino acid transporter B(0)AT1



- Molecule 1: Sodium-dependent neutral amino acid transporter B(0)AT1

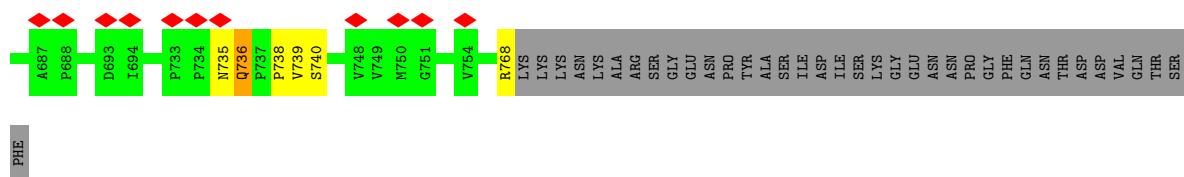
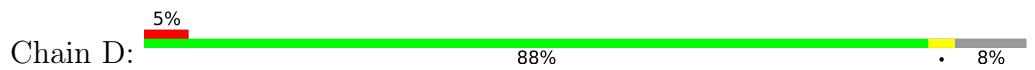


- Molecule 2: Angiotensin-converting enzyme 2

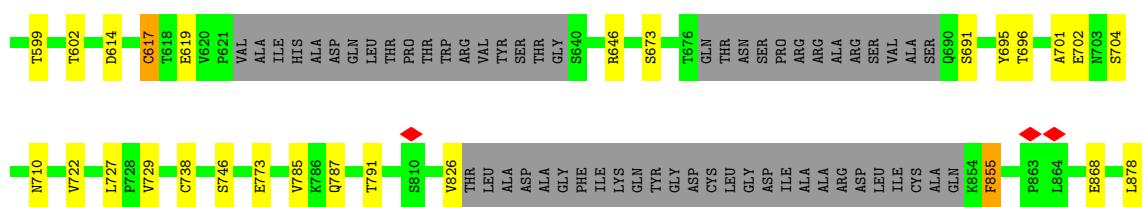
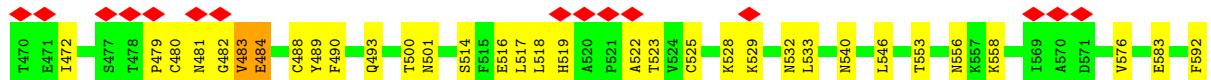


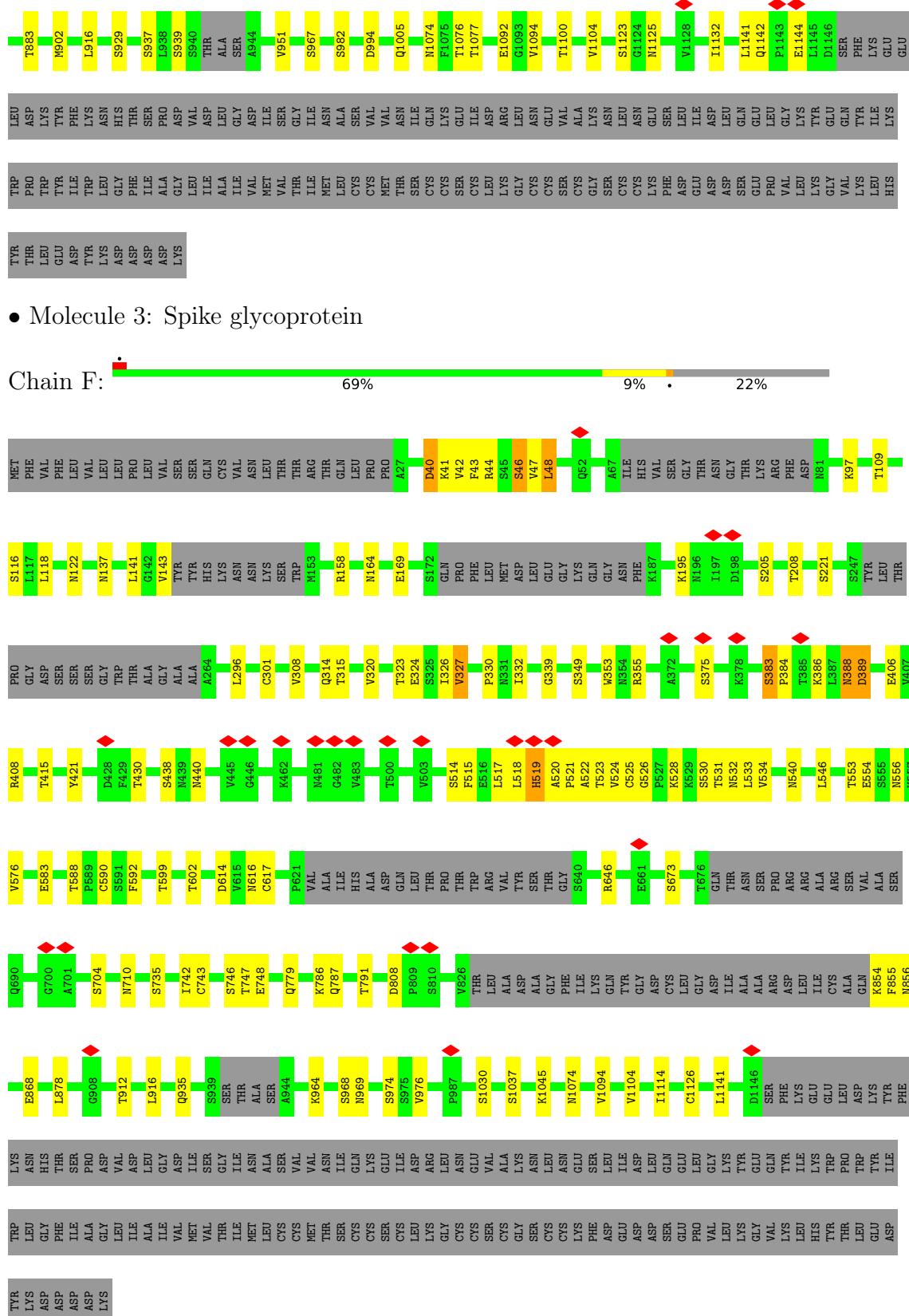


- Molecule 2: Angiotensin-converting enzyme 2

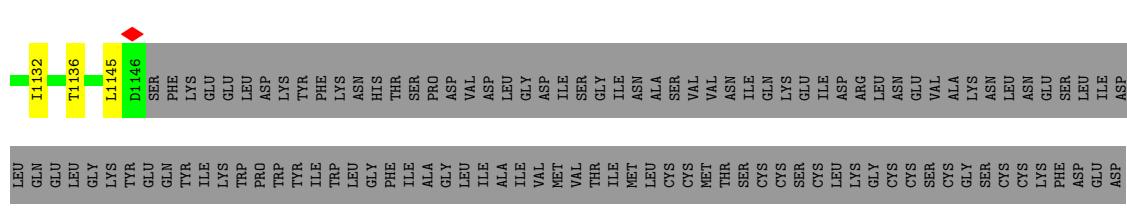
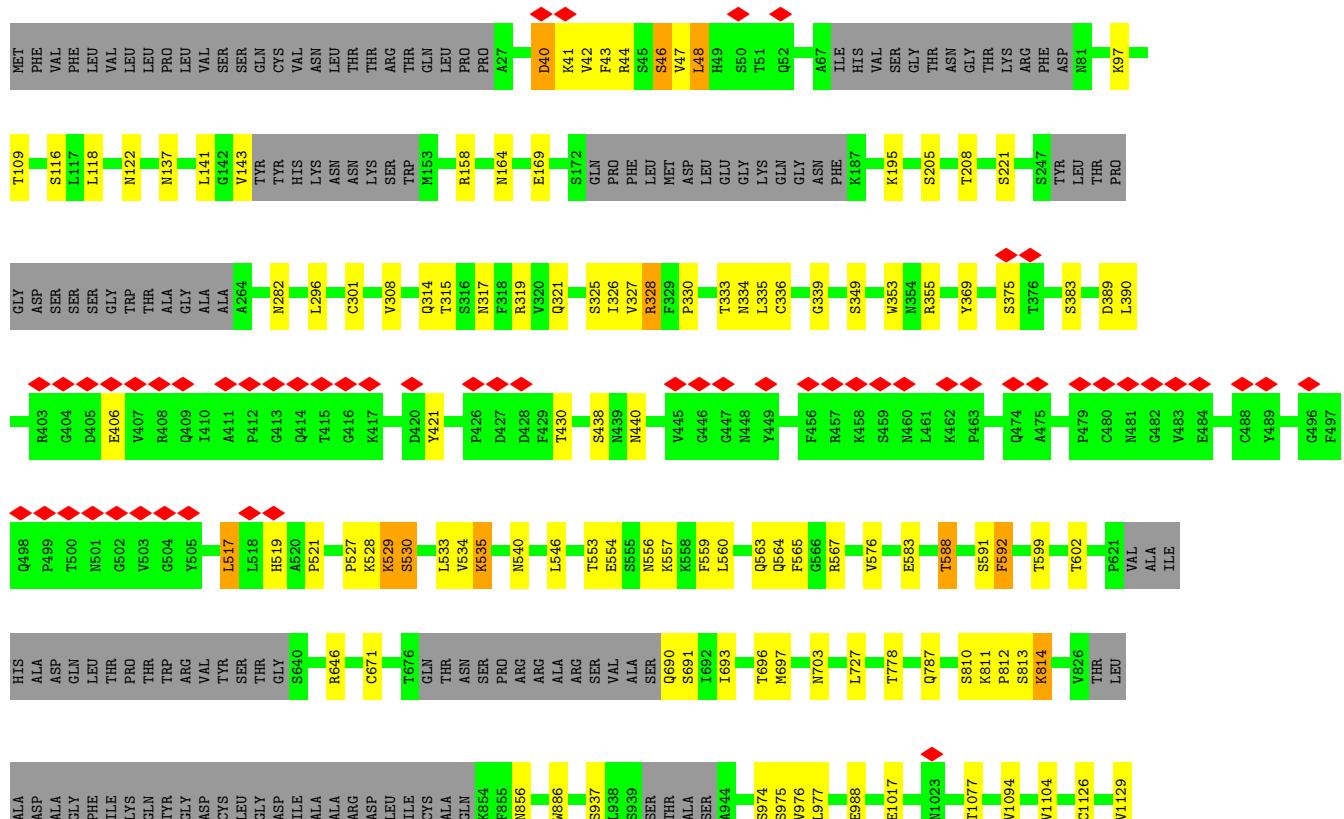


- Molecule 3: Spike glycoprotein

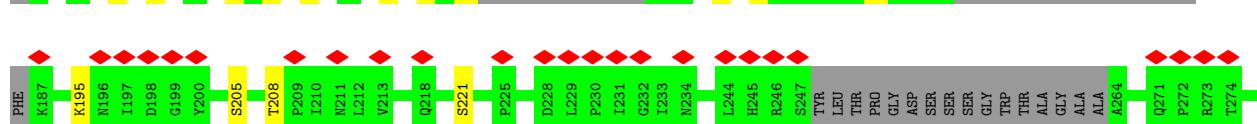


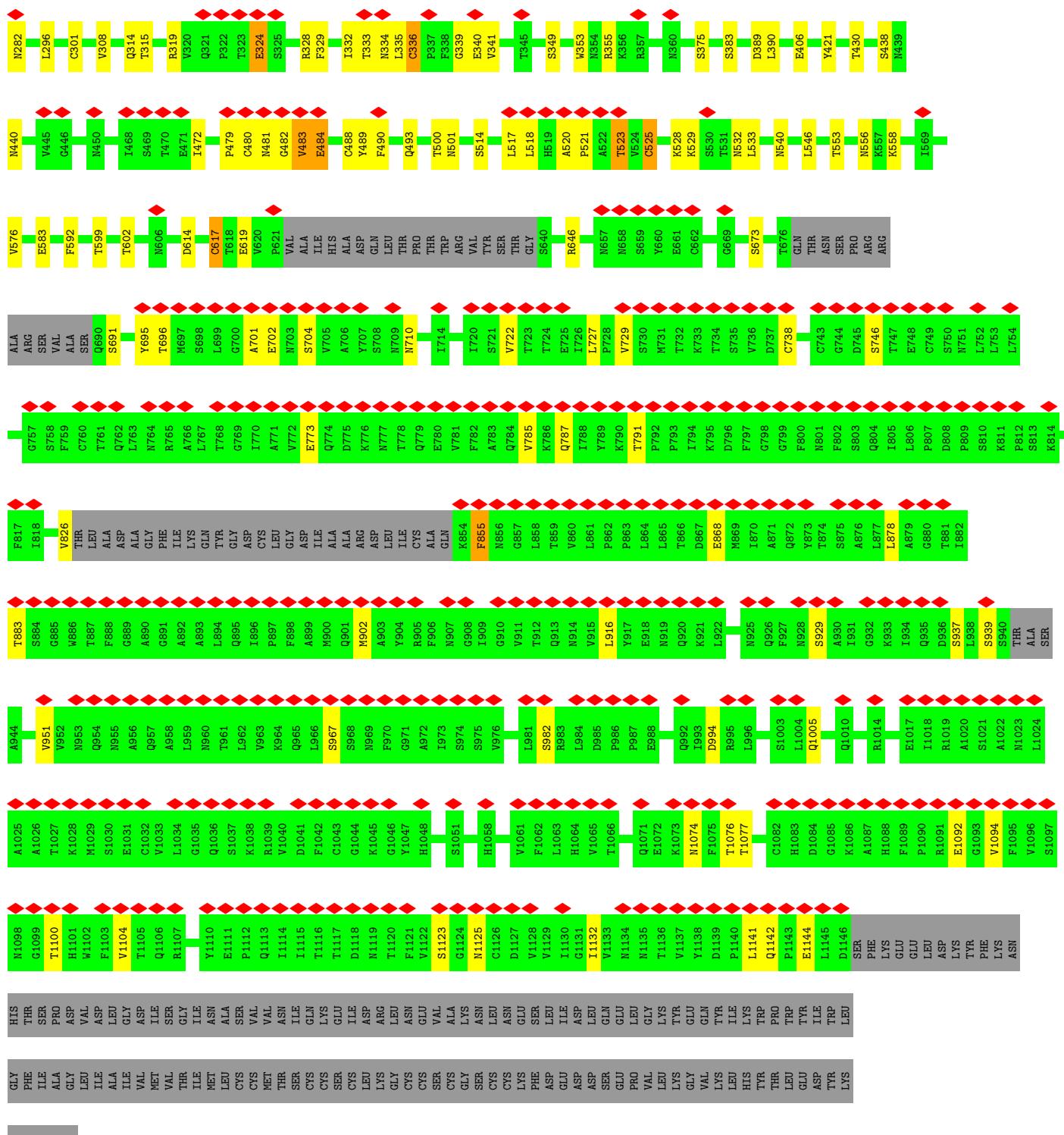


- Molecule 3: Spike glycoprotein

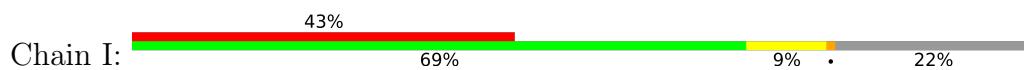


- Molecule 3: Spike glycoprotein



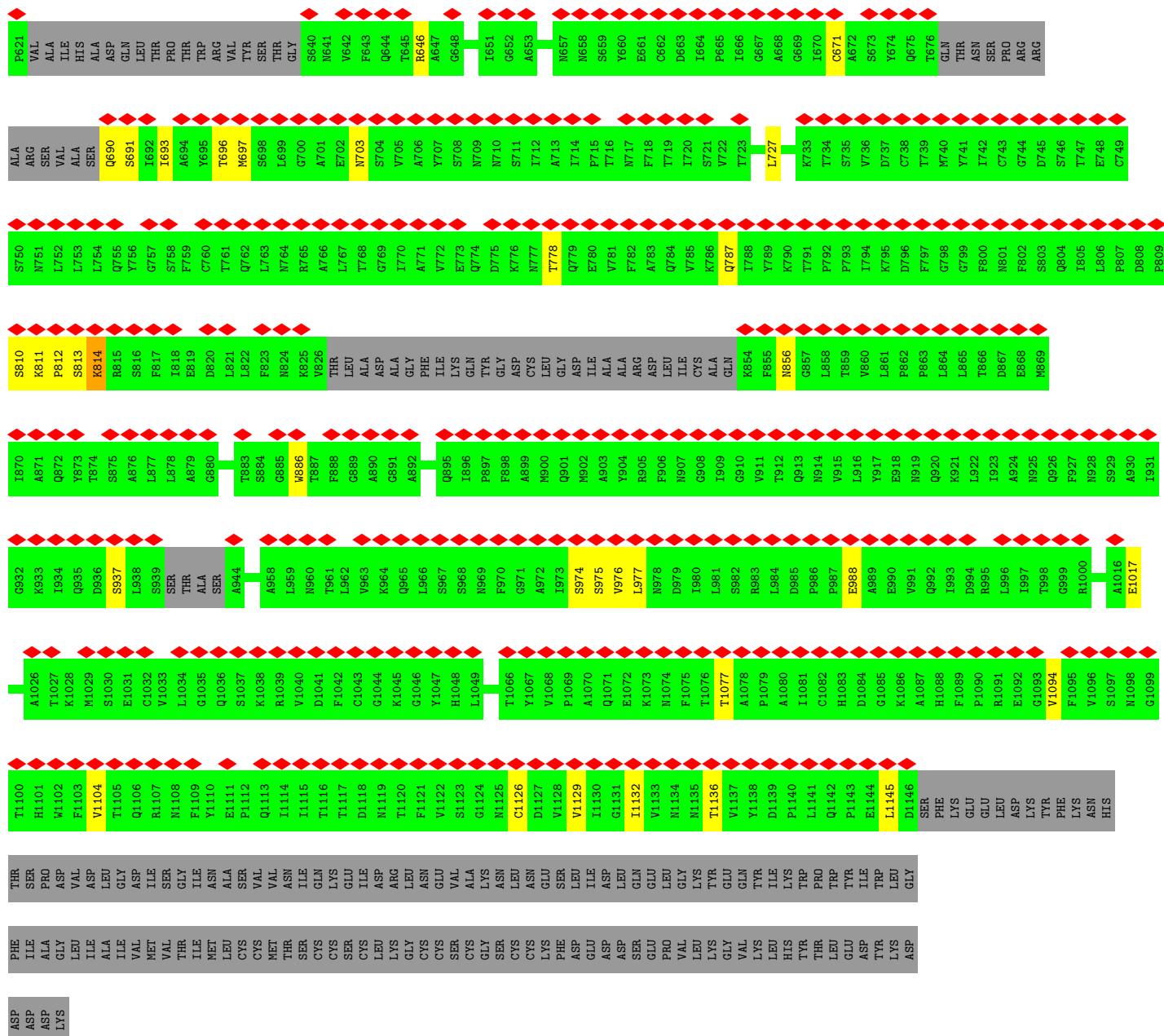


- Molecule 3: Spike glycoprotein









- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

**MAG1  
MAG2**

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 50% 50%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 50% 100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 50% 50%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



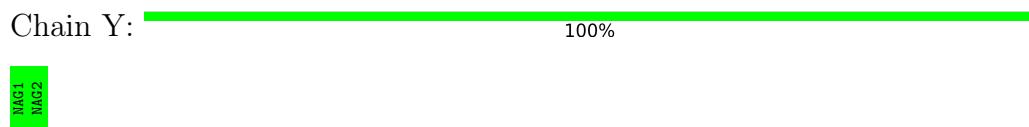
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



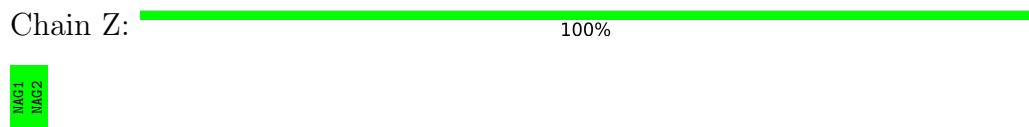
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



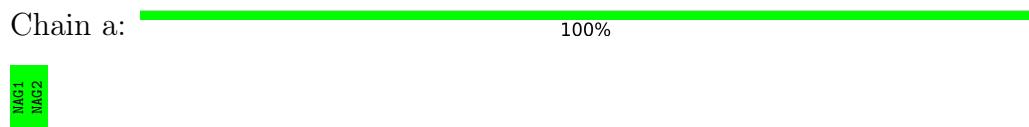
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



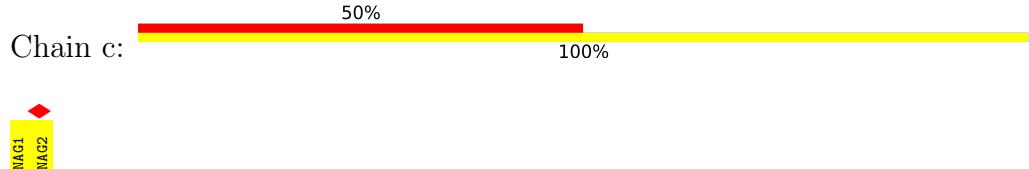
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



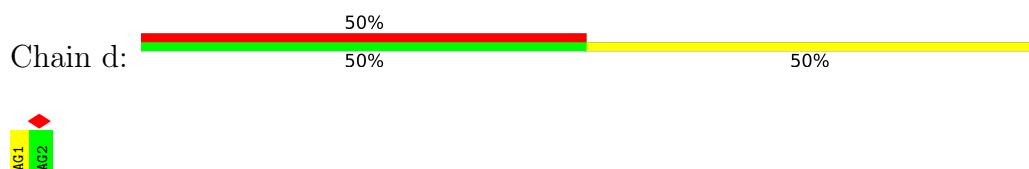
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l: 100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m: 100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n: 50% 50%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o: 50% 50%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p: 50% 50%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

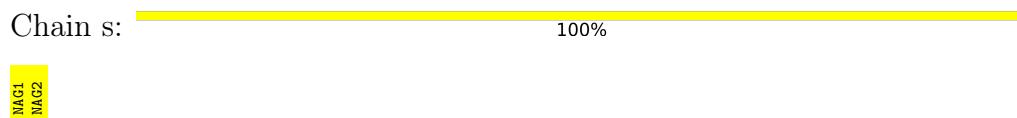
Chain q: 100%



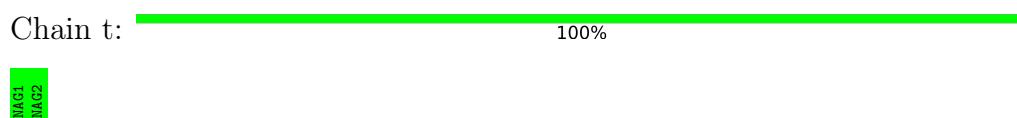
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



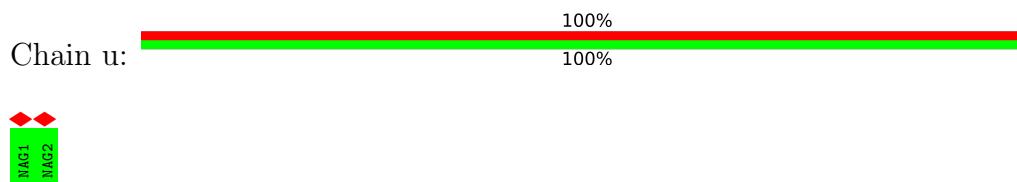
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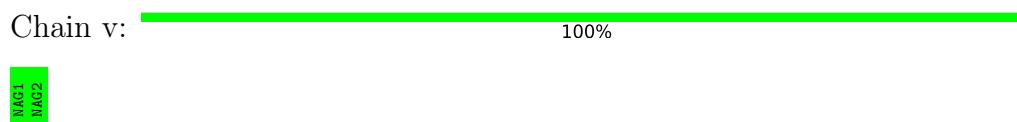
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



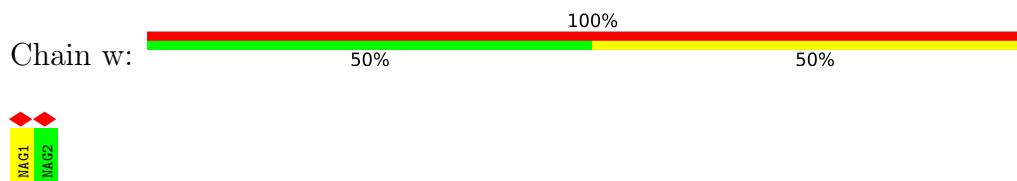
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



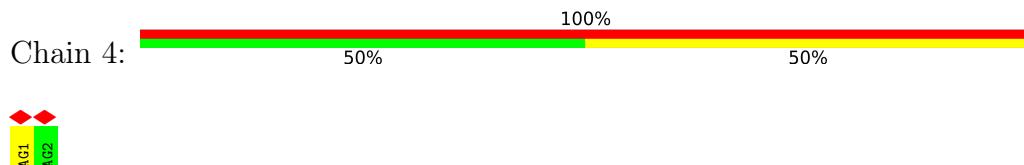
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



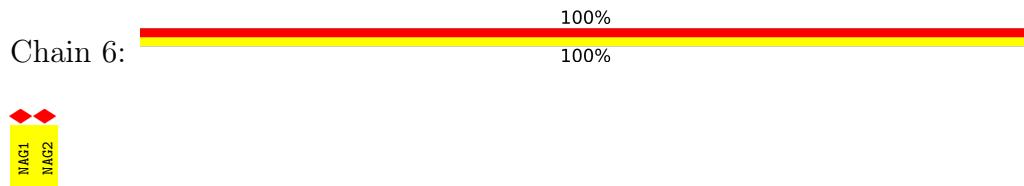
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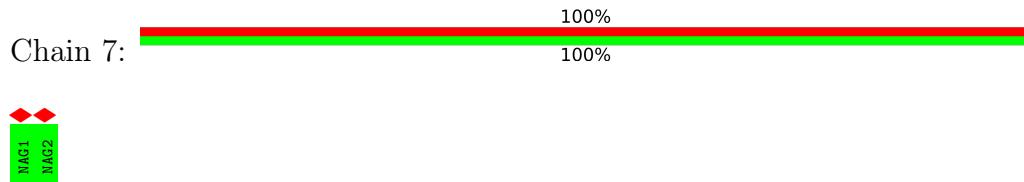
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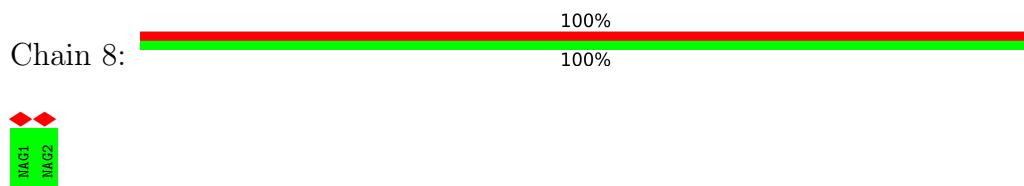
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FA: 100%



## 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53141	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.786	Depositor
Minimum map value	-0.869	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	521.76, 521.76, 521.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

## 5 Model quality [\(i\)](#)

### 5.1 Standard geometry [\(i\)](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAG

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	0.34	0/4940	0.56	0/6748
1	C	0.34	0/4940	0.56	0/6748
2	B	0.36	0/6252	0.52	0/8488
2	D	0.36	0/6252	0.52	0/8488
3	E	0.58	0/8048	0.56	0/10947
3	F	0.57	0/8042	0.55	0/10939
3	G	0.58	0/8042	0.54	0/10939
3	H	0.58	0/8048	0.56	0/10947
3	I	0.57	0/8042	0.55	0/10939
3	J	0.58	0/8042	0.54	0/10939
All	All	0.51	0/70648	0.54	0/96122

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [\(i\)](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

### 5.3 Torsion angles [\(i\)](#)

#### 5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	603/654 (92%)	540 (90%)	59 (10%)	4 (1%)	22 63
1	C	603/654 (92%)	540 (90%)	59 (10%)	4 (1%)	22 63
2	B	746/817 (91%)	685 (92%)	51 (7%)	10 (1%)	12 48
2	D	746/817 (91%)	684 (92%)	52 (7%)	10 (1%)	12 48
3	E	989/1283 (77%)	841 (85%)	113 (11%)	35 (4%)	3 25
3	F	988/1283 (77%)	855 (86%)	96 (10%)	37 (4%)	3 24
3	G	988/1283 (77%)	842 (85%)	106 (11%)	40 (4%)	3 23
3	H	989/1283 (77%)	841 (85%)	112 (11%)	36 (4%)	3 25
3	I	988/1283 (77%)	855 (86%)	96 (10%)	37 (4%)	3 24
3	J	988/1283 (77%)	842 (85%)	106 (11%)	40 (4%)	3 23
All	All	8628/10640 (81%)	7525 (87%)	850 (10%)	253 (3%)	7 29

5 of 253 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	144	LEU
2	B	631	LYS
2	B	736	GLN
2	D	144	LEU
2	D	631	LYS

### 5.3.2 Protein sidechains [\(i\)](#)

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	531/572 (93%)	510 (96%)	21 (4%)	31 55
1	C	531/572 (93%)	509 (96%)	22 (4%)	30 55
2	B	662/721 (92%)	638 (96%)	24 (4%)	35 59
2	D	662/721 (92%)	638 (96%)	24 (4%)	35 59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	E	882/1122 (79%)	771 (87%)	111 (13%)	4 19
3	F	881/1122 (78%)	787 (89%)	94 (11%)	6 23
3	G	881/1122 (78%)	793 (90%)	88 (10%)	7 26
3	H	882/1122 (79%)	770 (87%)	112 (13%)	4 18
3	I	881/1122 (78%)	786 (89%)	95 (11%)	6 23
3	J	881/1122 (78%)	793 (90%)	88 (10%)	7 26
All	All	7674/9318 (82%)	6995 (91%)	679 (9%)	13 31

5 of 679 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	746	SER
3	I	878	LEU
3	H	937	SER
3	H	738	CYS
3	I	323	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 217 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	703	ASN
3	H	644	GLN
3	J	556	ASN
3	G	907	ASN
3	H	137	ASN

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

116 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	0	1	4,3	14,14,15	0.26	0	17,19,21	0.68	1 (5%)
4	NAG	0	2	4	14,14,15	0.15	0	17,19,21	0.49	0
4	NAG	1	1	4,3	14,14,15	0.28	0	17,19,21	0.62	0
4	NAG	1	2	4	14,14,15	0.24	0	17,19,21	0.58	0
4	NAG	2	1	4,3	14,14,15	0.61	1 (7%)	17,19,21	0.57	0
4	NAG	2	2	4	14,14,15	0.32	0	17,19,21	0.46	0
4	NAG	3	1	4,3	14,14,15	0.31	0	17,19,21	0.41	0
4	NAG	3	2	4	14,14,15	0.40	0	17,19,21	0.37	0
4	NAG	4	1	4,3	14,14,15	0.35	0	17,19,21	1.13	1 (5%)
4	NAG	4	2	4	14,14,15	0.29	0	17,19,21	0.48	0
4	NAG	5	1	4,3	14,14,15	0.32	0	17,19,21	0.71	1 (5%)
4	NAG	5	2	4	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	6	1	4,3	14,14,15	0.77	1 (7%)	17,19,21	0.90	1 (5%)
4	NAG	6	2	4	14,14,15	0.31	0	17,19,21	0.70	1 (5%)
4	NAG	7	1	4,3	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	7	2	4	14,14,15	0.26	0	17,19,21	0.36	0
4	NAG	8	1	4,3	14,14,15	0.55	0	17,19,21	0.49	0
4	NAG	8	2	4	14,14,15	0.25	0	17,19,21	0.56	0
4	NAG	9	1	4,3	14,14,15	0.58	1 (7%)	17,19,21	0.56	0
4	NAG	9	2	4	14,14,15	0.30	0	17,19,21	0.47	0
4	NAG	AA	1	4,3	14,14,15	0.23	0	17,19,21	1.37	1 (5%)
4	NAG	AA	2	4	14,14,15	0.19	0	17,19,21	0.50	0
4	NAG	BA	1	4,3	14,14,15	0.54	0	17,19,21	0.71	1 (5%)
4	NAG	BA	2	4	14,14,15	0.40	0	17,19,21	0.46	0
4	NAG	CA	1	4,3	14,14,15	0.36	0	17,19,21	0.40	0
4	NAG	CA	2	4	14,14,15	0.20	0	17,19,21	0.74	0
4	NAG	DA	1	4,3	14,14,15	0.36	0	17,19,21	0.48	0
4	NAG	DA	2	4	14,14,15	0.56	0	17,19,21	1.31	1 (5%)
4	NAG	EA	1	4,3	14,14,15	0.65	1 (7%)	17,19,21	0.42	0
4	NAG	EA	2	4	14,14,15	0.32	0	17,19,21	1.36	2 (11%)
4	NAG	FA	1	4,3	14,14,15	0.40	0	17,19,21	0.45	0
4	NAG	FA	2	4	14,14,15	0.24	0	17,19,21	0.50	0
4	NAG	K	1	4,1	14,14,15	0.32	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	K	2	4	14,14,15	0.32	0	17,19,21	0.49	0
4	NAG	L	1	4,2	14,14,15	0.61	1 (7%)	17,19,21	0.73	0
4	NAG	L	2	4	14,14,15	0.53	0	17,19,21	0.36	0
4	NAG	M	1	4,2	14,14,15	0.42	0	17,19,21	0.64	0
4	NAG	M	2	4	14,14,15	0.28	0	17,19,21	0.69	1 (5%)
4	NAG	N	1	4,2	14,14,15	0.29	0	17,19,21	0.63	0
4	NAG	N	2	4	14,14,15	0.30	0	17,19,21	0.61	0
4	NAG	O	1	4,2	14,14,15	0.30	0	17,19,21	0.51	0
4	NAG	O	2	4	14,14,15	0.37	0	17,19,21	0.47	0
4	NAG	P	1	4,2	14,14,15	0.24	0	17,19,21	0.62	0
4	NAG	P	2	4	14,14,15	0.31	0	17,19,21	0.60	1 (5%)
4	NAG	Q	1	4,2	14,14,15	0.25	0	17,19,21	0.56	0
4	NAG	Q	2	4	14,14,15	0.22	0	17,19,21	0.57	0
4	NAG	R	1	4,1	14,14,15	0.33	0	17,19,21	0.51	0
4	NAG	R	2	4	14,14,15	0.32	0	17,19,21	0.47	0
4	NAG	S	1	4,2	14,14,15	0.60	1 (7%)	17,19,21	0.73	0
4	NAG	S	2	4	14,14,15	0.53	0	17,19,21	0.36	0
4	NAG	T	1	4,2	14,14,15	0.40	0	17,19,21	0.64	0
4	NAG	T	2	4	14,14,15	0.27	0	17,19,21	0.69	1 (5%)
4	NAG	U	1	4,2	14,14,15	0.29	0	17,19,21	0.62	0
4	NAG	U	2	4	14,14,15	0.30	0	17,19,21	0.61	0
4	NAG	V	1	4,2	14,14,15	0.32	0	17,19,21	0.52	0
4	NAG	V	2	4	14,14,15	0.34	0	17,19,21	0.46	0
4	NAG	W	1	4,2	14,14,15	0.23	0	17,19,21	0.62	0
4	NAG	W	2	4	14,14,15	0.32	0	17,19,21	0.59	1 (5%)
4	NAG	X	1	4,2	14,14,15	0.26	0	17,19,21	0.56	0
4	NAG	X	2	4	14,14,15	0.22	0	17,19,21	0.57	0
4	NAG	Y	1	4,3	14,14,15	0.54	0	17,19,21	0.50	0
4	NAG	Y	2	4	14,14,15	0.25	0	17,19,21	0.58	0
4	NAG	Z	1	4,3	14,14,15	0.28	0	17,19,21	0.62	0
4	NAG	Z	2	4	14,14,15	0.29	0	17,19,21	0.62	0
4	NAG	a	1	4,3	14,14,15	0.32	0	17,19,21	0.62	0
4	NAG	a	2	4	14,14,15	0.51	0	17,19,21	0.47	0
4	NAG	b	1	4,3	14,14,15	0.37	0	17,19,21	0.73	0
4	NAG	b	2	4	14,14,15	0.30	0	17,19,21	1.32	2 (11%)
4	NAG	c	1	4,3	14,14,15	0.71	1 (7%)	17,19,21	0.70	0
4	NAG	c	2	4	14,14,15	0.38	0	17,19,21	1.41	3 (17%)
4	NAG	d	1	4,3	14,14,15	0.70	1 (7%)	17,19,21	0.66	0
4	NAG	d	2	4	14,14,15	0.30	0	17,19,21	0.63	0
4	NAG	e	1	4,3	14,14,15	0.25	0	17,19,21	0.69	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	e	2	4	14,14,15	0.18	0	17,19,21	0.48	0
4	NAG	f	1	4,3	14,14,15	0.30	0	17,19,21	0.62	0
4	NAG	f	2	4	14,14,15	0.24	0	17,19,21	0.58	0
4	NAG	g	1	4,3	14,14,15	0.58	1 (7%)	17,19,21	0.57	0
4	NAG	g	2	4	14,14,15	0.31	0	17,19,21	0.46	0
4	NAG	h	1	4,3	14,14,15	0.32	0	17,19,21	0.39	0
4	NAG	h	2	4	14,14,15	0.39	0	17,19,21	0.37	0
4	NAG	i	1	4,3	14,14,15	0.35	0	17,19,21	1.13	1 (5%)
4	NAG	i	2	4	14,14,15	0.25	0	17,19,21	0.47	0
4	NAG	j	1	4,3	14,14,15	0.32	0	17,19,21	0.70	1 (5%)
4	NAG	j	2	4	14,14,15	0.22	0	17,19,21	0.40	0
4	NAG	k	1	4,3	14,14,15	0.77	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	k	2	4	14,14,15	0.31	0	17,19,21	0.70	1 (5%)
4	NAG	l	1	4,3	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	l	2	4	14,14,15	0.28	0	17,19,21	0.38	0
4	NAG	m	1	4,3	14,14,15	0.55	0	17,19,21	0.49	0
4	NAG	m	2	4	14,14,15	0.24	0	17,19,21	0.57	0
4	NAG	n	1	4,3	14,14,15	0.59	1 (7%)	17,19,21	0.57	0
4	NAG	n	2	4	14,14,15	0.30	0	17,19,21	0.46	0
4	NAG	o	1	4,3	14,14,15	0.22	0	17,19,21	1.37	1 (5%)
4	NAG	o	2	4	14,14,15	0.20	0	17,19,21	0.51	0
4	NAG	p	1	4,3	14,14,15	0.55	0	17,19,21	0.72	1 (5%)
4	NAG	p	2	4	14,14,15	0.39	0	17,19,21	0.46	0
4	NAG	q	1	4,3	14,14,15	0.36	0	17,19,21	0.39	0
4	NAG	q	2	4	14,14,15	0.20	0	17,19,21	0.74	0
4	NAG	r	1	4,3	14,14,15	0.36	0	17,19,21	0.47	0
4	NAG	r	2	4	14,14,15	0.56	0	17,19,21	1.31	1 (5%)
4	NAG	s	1	4,3	14,14,15	0.65	1 (7%)	17,19,21	0.43	0
4	NAG	s	2	4	14,14,15	0.32	0	17,19,21	1.36	2 (11%)
4	NAG	t	1	4,3	14,14,15	0.39	0	17,19,21	0.46	0
4	NAG	t	2	4	14,14,15	0.23	0	17,19,21	0.50	0
4	NAG	u	1	4,3	14,14,15	0.53	0	17,19,21	0.49	0
4	NAG	u	2	4	14,14,15	0.24	0	17,19,21	0.59	0
4	NAG	v	1	4,3	14,14,15	0.28	0	17,19,21	0.63	0
4	NAG	v	2	4	14,14,15	0.29	0	17,19,21	0.61	0
4	NAG	w	1	4,3	14,14,15	0.33	0	17,19,21	0.63	1 (5%)
4	NAG	w	2	4	14,14,15	0.52	0	17,19,21	0.47	0
4	NAG	x	1	4,3	14,14,15	0.38	0	17,19,21	0.73	0
4	NAG	x	2	4	14,14,15	0.31	0	17,19,21	1.32	2 (11%)
4	NAG	y	1	4,3	14,14,15	0.71	1 (7%)	17,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	y	2	4	14,14,15	0.38	0	17,19,21	1.40	3 (17%)
4	NAG	z	1	4,3	14,14,15	0.70	1 (7%)	17,19,21	0.67	0
4	NAG	z	2	4	14,14,15	0.28	0	17,19,21	0.63	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
4	NAG	0	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	0	2	4	-	0/6/23/26	0/1/1/1
4	NAG	1	1	4,3	-	3/6/23/26	0/1/1/1
4	NAG	1	2	4	-	2/6/23/26	0/1/1/1
4	NAG	2	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	2	2	4	-	4/6/23/26	0/1/1/1
4	NAG	3	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	3	2	4	-	1/6/23/26	0/1/1/1
4	NAG	4	1	4,3	-	1/6/23/26	0/1/1/1
4	NAG	4	2	4	-	0/6/23/26	0/1/1/1
4	NAG	5	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	5	2	4	-	3/6/23/26	0/1/1/1
4	NAG	6	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	6	2	4	-	3/6/23/26	0/1/1/1
4	NAG	7	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	7	2	4	-	2/6/23/26	0/1/1/1
4	NAG	8	1	4,3	-	1/6/23/26	0/1/1/1
4	NAG	8	2	4	-	2/6/23/26	0/1/1/1
4	NAG	9	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	9	2	4	-	4/6/23/26	0/1/1/1
4	NAG	AA	1	4,3	-	6/6/23/26	0/1/1/1
4	NAG	AA	2	4	-	2/6/23/26	0/1/1/1
4	NAG	BA	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	BA	2	4	-	2/6/23/26	0/1/1/1
4	NAG	CA	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	CA	2	4	-	1/6/23/26	0/1/1/1
4	NAG	DA	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	DA	2	4	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	EA	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	EA	2	4	-	4/6/23/26	0/1/1/1
4	NAG	FA	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	FA	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	L	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	NAG	M	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	4/6/23/26	0/1/1/1
4	NAG	O	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	NAG	P	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	NAG	S	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	NAG	T	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	NAG	U	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	4/6/23/26	0/1/1/1
4	NAG	V	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	NAG	W	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Y	1	4,3	-	1/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Z	1	4,3	-	4/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	4/6/23/26	0/1/1/1
4	NAG	a	1	4,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	a	2	4	-	2/6/23/26	0/1/1/1
4	NAG	b	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	b	2	4	-	3/6/23/26	0/1/1/1
4	NAG	c	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	c	2	4	-	5/6/23/26	0/1/1/1
4	NAG	d	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	d	2	4	-	3/6/23/26	0/1/1/1
4	NAG	e	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	e	2	4	-	0/6/23/26	0/1/1/1
4	NAG	f	1	4,3	-	3/6/23/26	0/1/1/1
4	NAG	f	2	4	-	2/6/23/26	0/1/1/1
4	NAG	g	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	g	2	4	-	4/6/23/26	0/1/1/1
4	NAG	h	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	h	2	4	-	1/6/23/26	0/1/1/1
4	NAG	i	1	4,3	-	1/6/23/26	0/1/1/1
4	NAG	i	2	4	-	0/6/23/26	0/1/1/1
4	NAG	j	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	j	2	4	-	3/6/23/26	0/1/1/1
4	NAG	k	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	k	2	4	-	3/6/23/26	0/1/1/1
4	NAG	l	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	l	2	4	-	2/6/23/26	0/1/1/1
4	NAG	m	1	4,3	-	1/6/23/26	0/1/1/1
4	NAG	m	2	4	-	2/6/23/26	0/1/1/1
4	NAG	n	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	n	2	4	-	4/6/23/26	0/1/1/1
4	NAG	o	1	4,3	-	6/6/23/26	0/1/1/1
4	NAG	o	2	4	-	2/6/23/26	0/1/1/1
4	NAG	p	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	p	2	4	-	2/6/23/26	0/1/1/1
4	NAG	q	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	q	2	4	-	1/6/23/26	0/1/1/1
4	NAG	r	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	r	2	4	-	5/6/23/26	0/1/1/1
4	NAG	s	1	4,3	-	2/6/23/26	0/1/1/1

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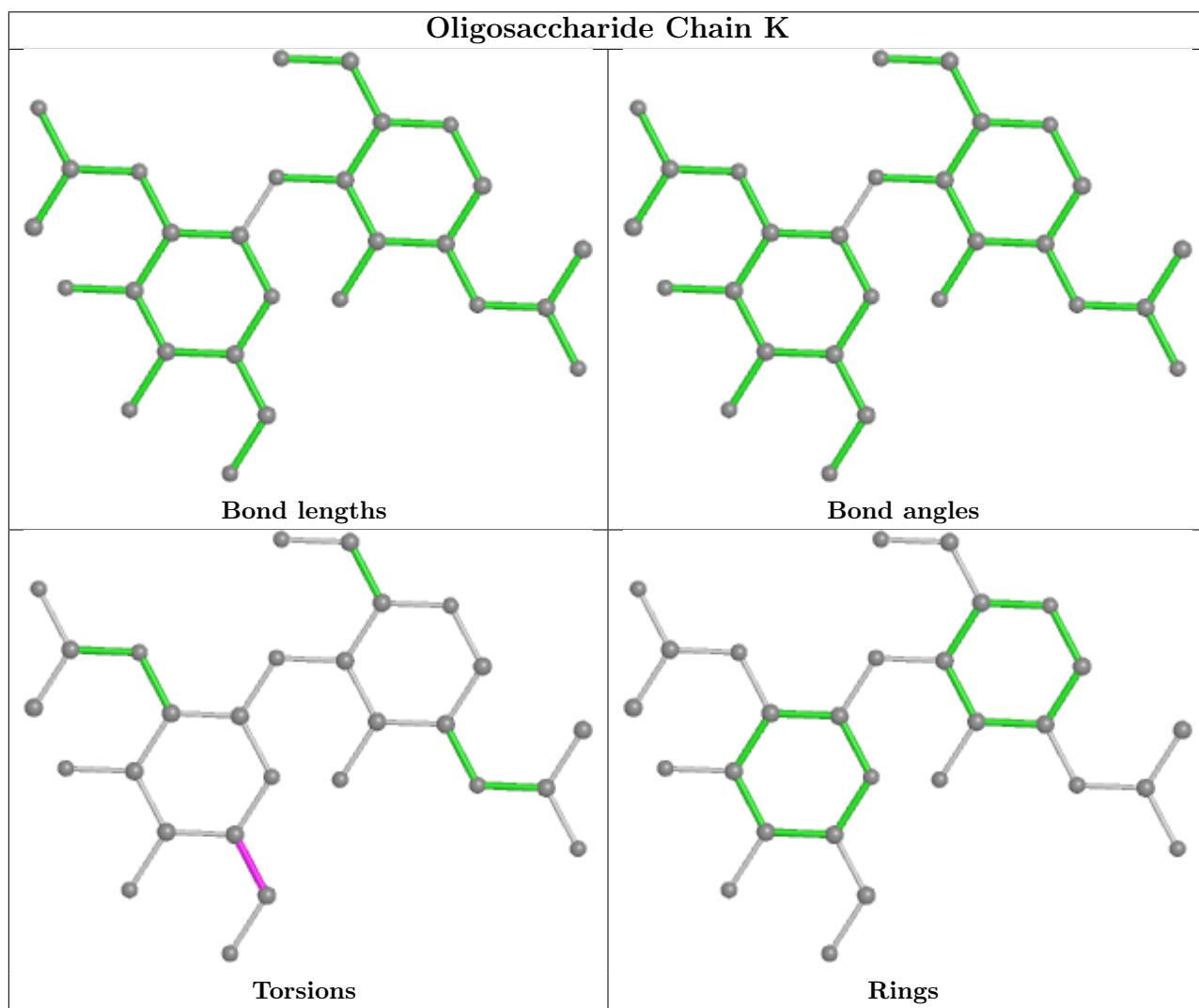
*Continued from previous page...*

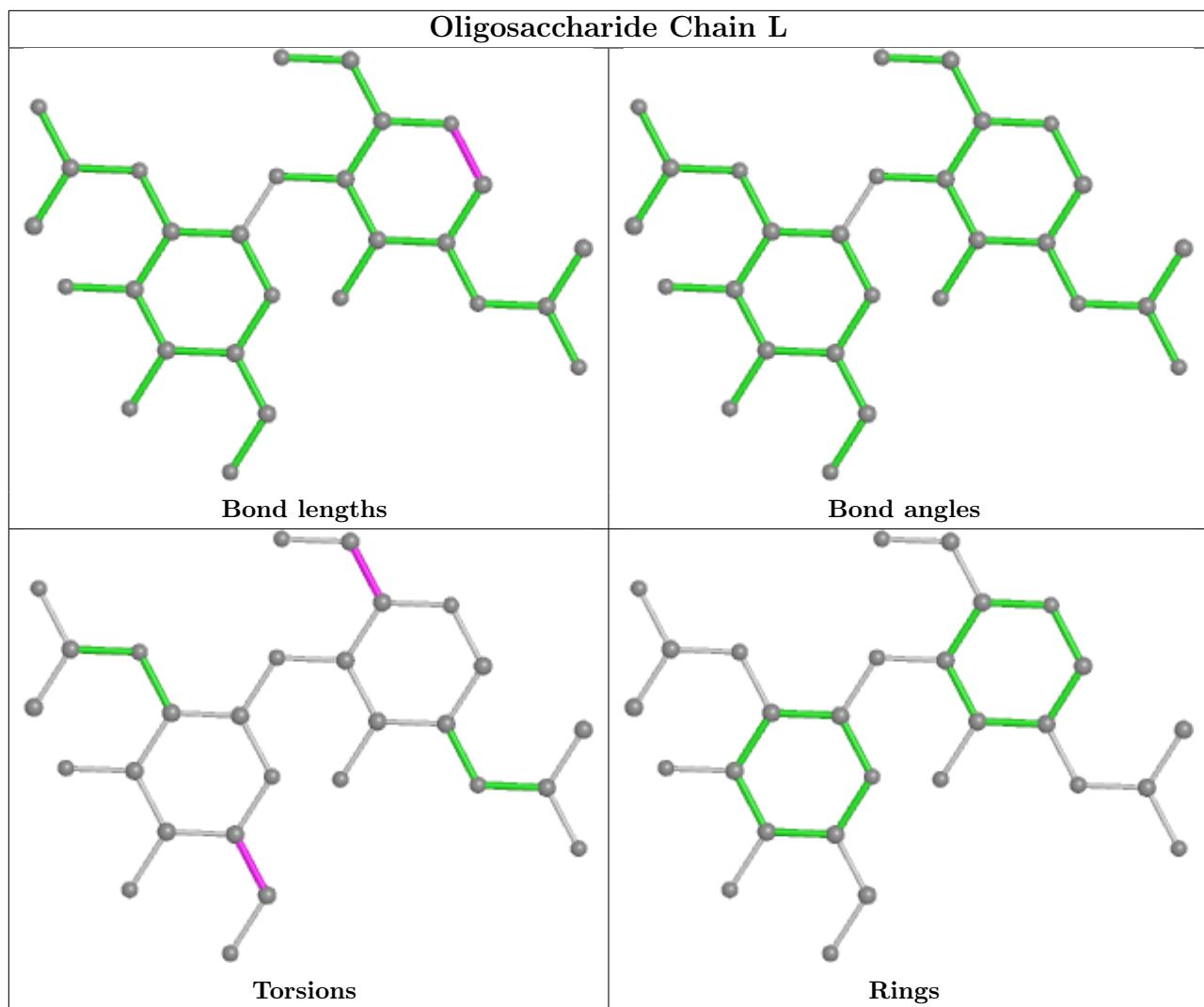
Mol	Chain	Res	Type	Atoms
4	N	2	NAG	C3-C2-N2-C7
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	U	1	NAG	O7-C7-N2-C2

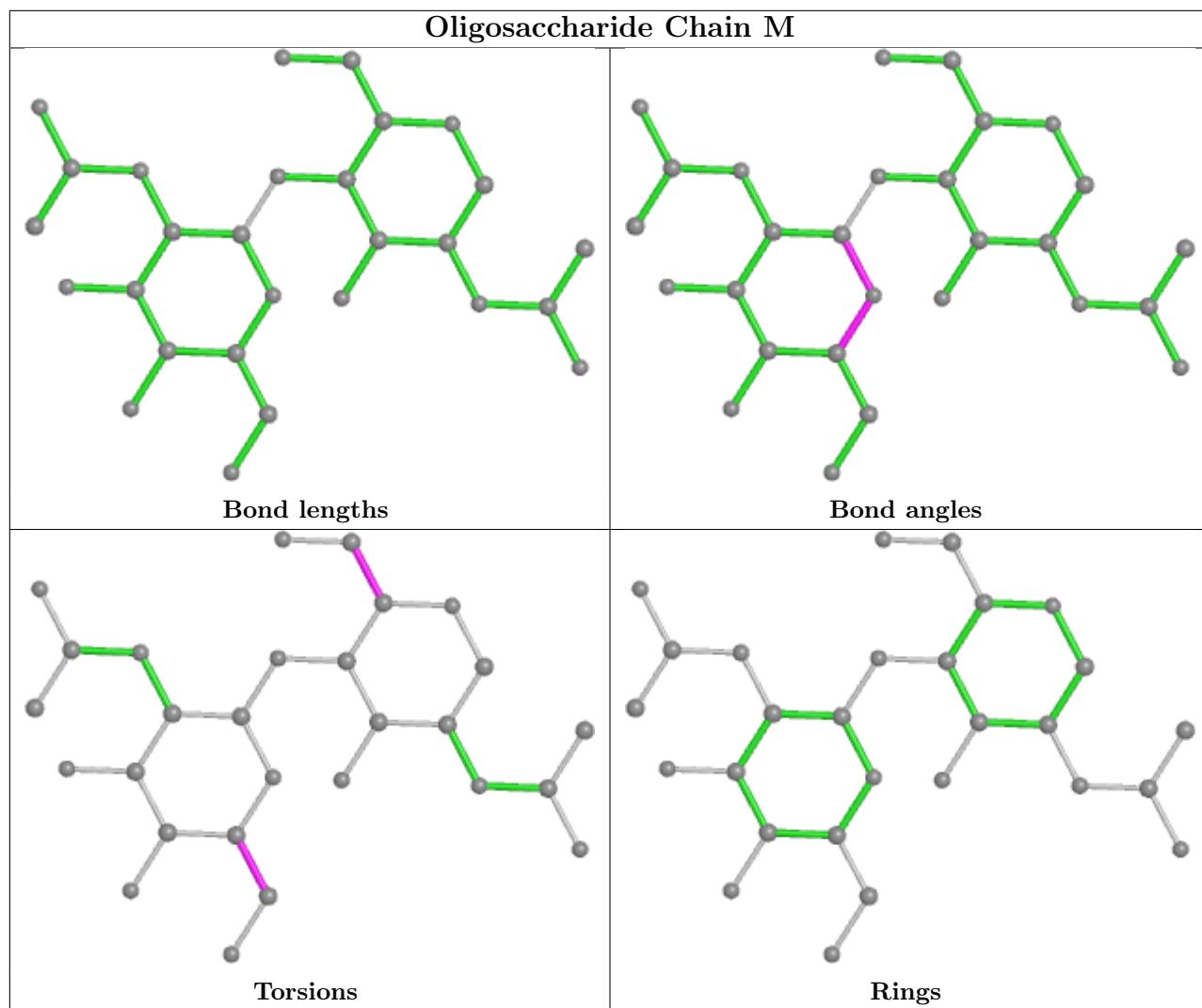
There are no ring outliers.

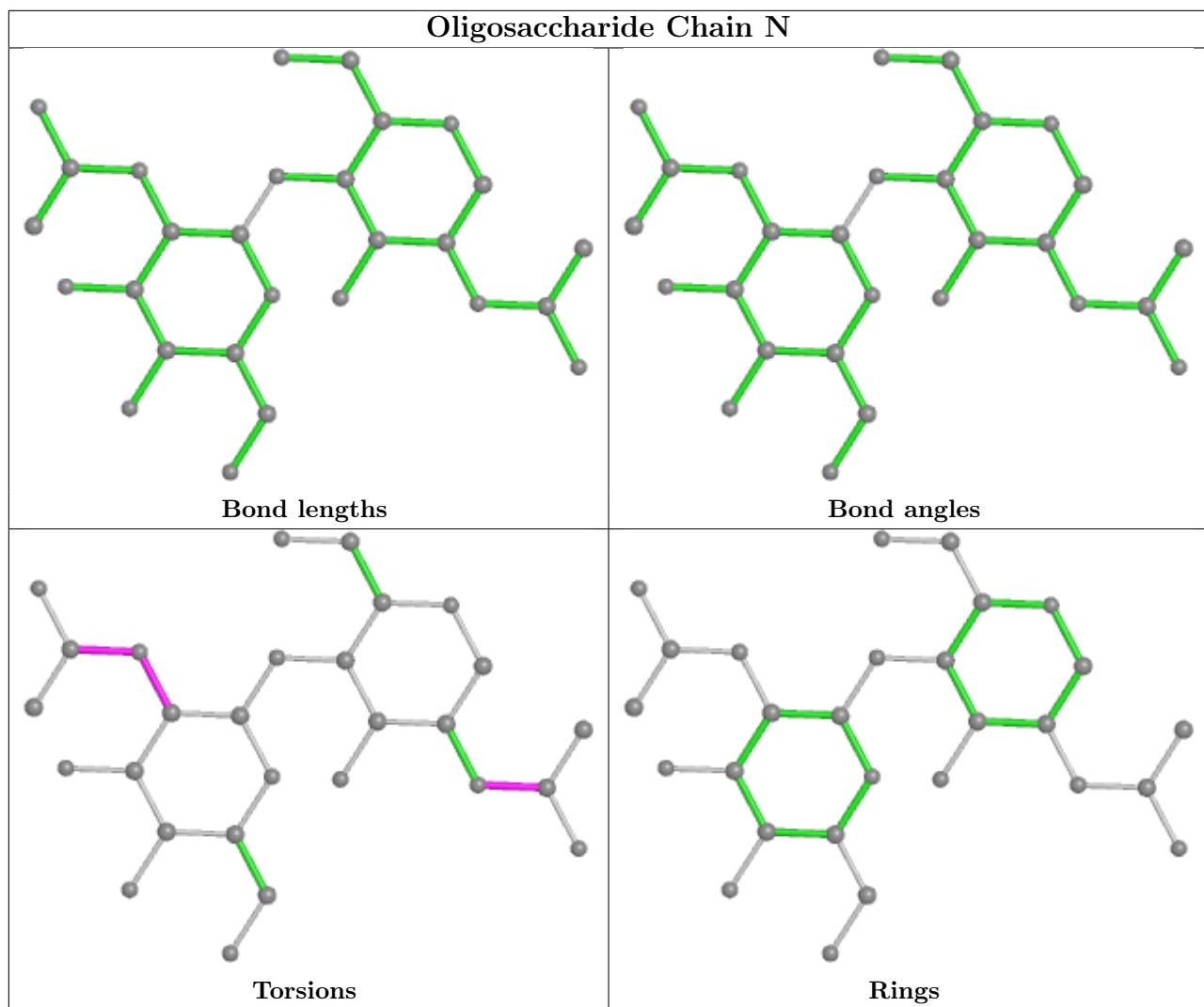
No monomer is involved in short contacts.

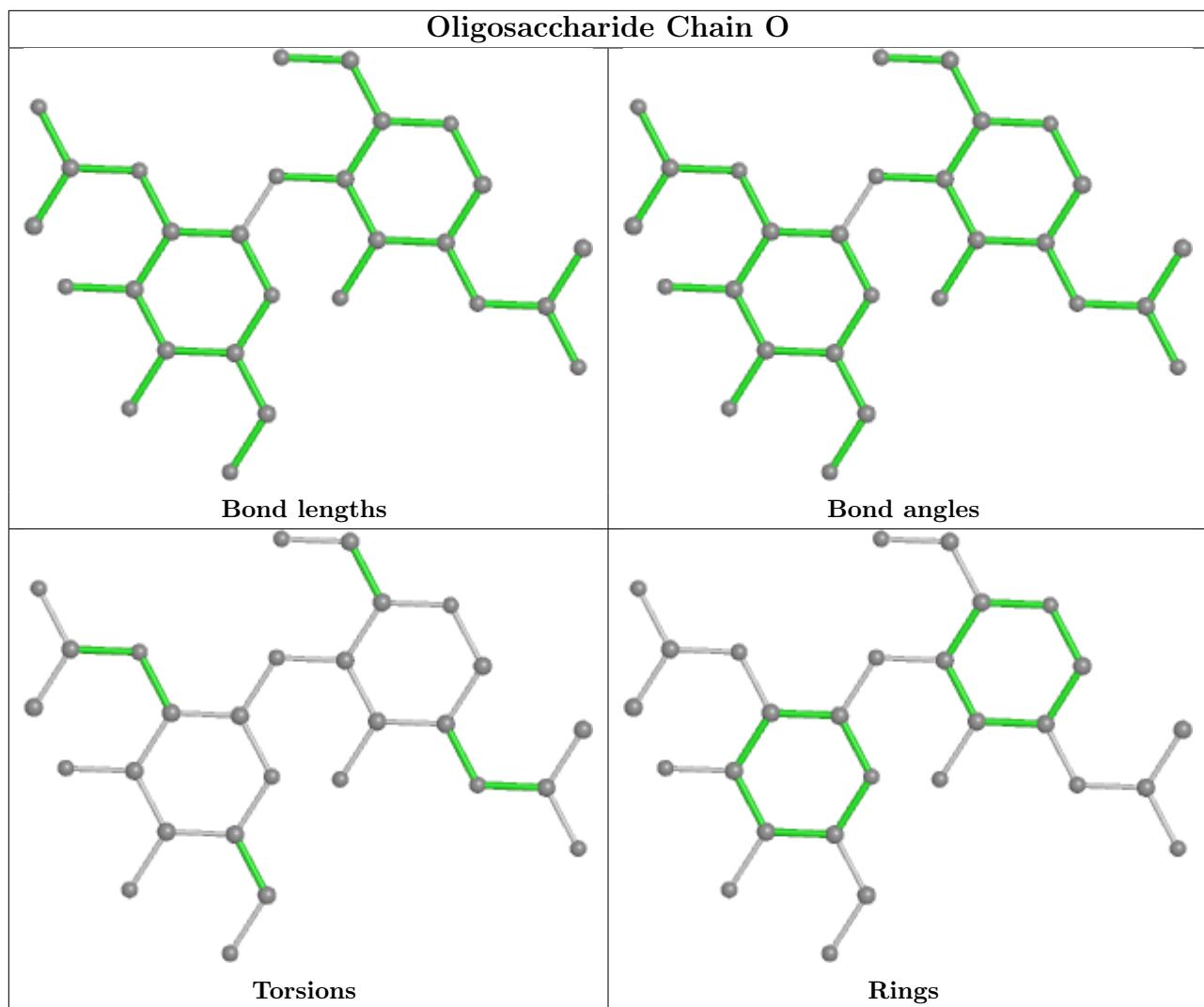
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

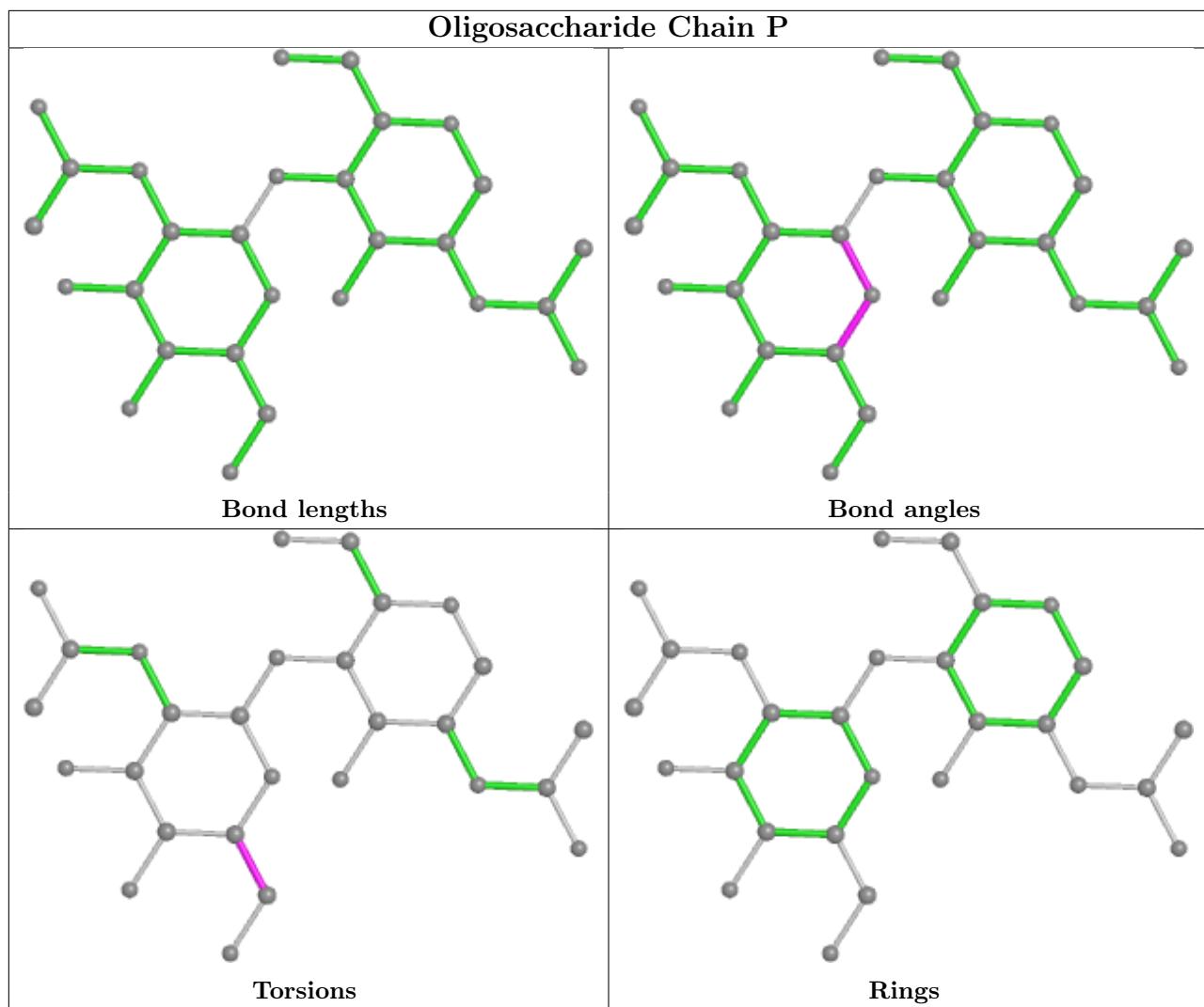


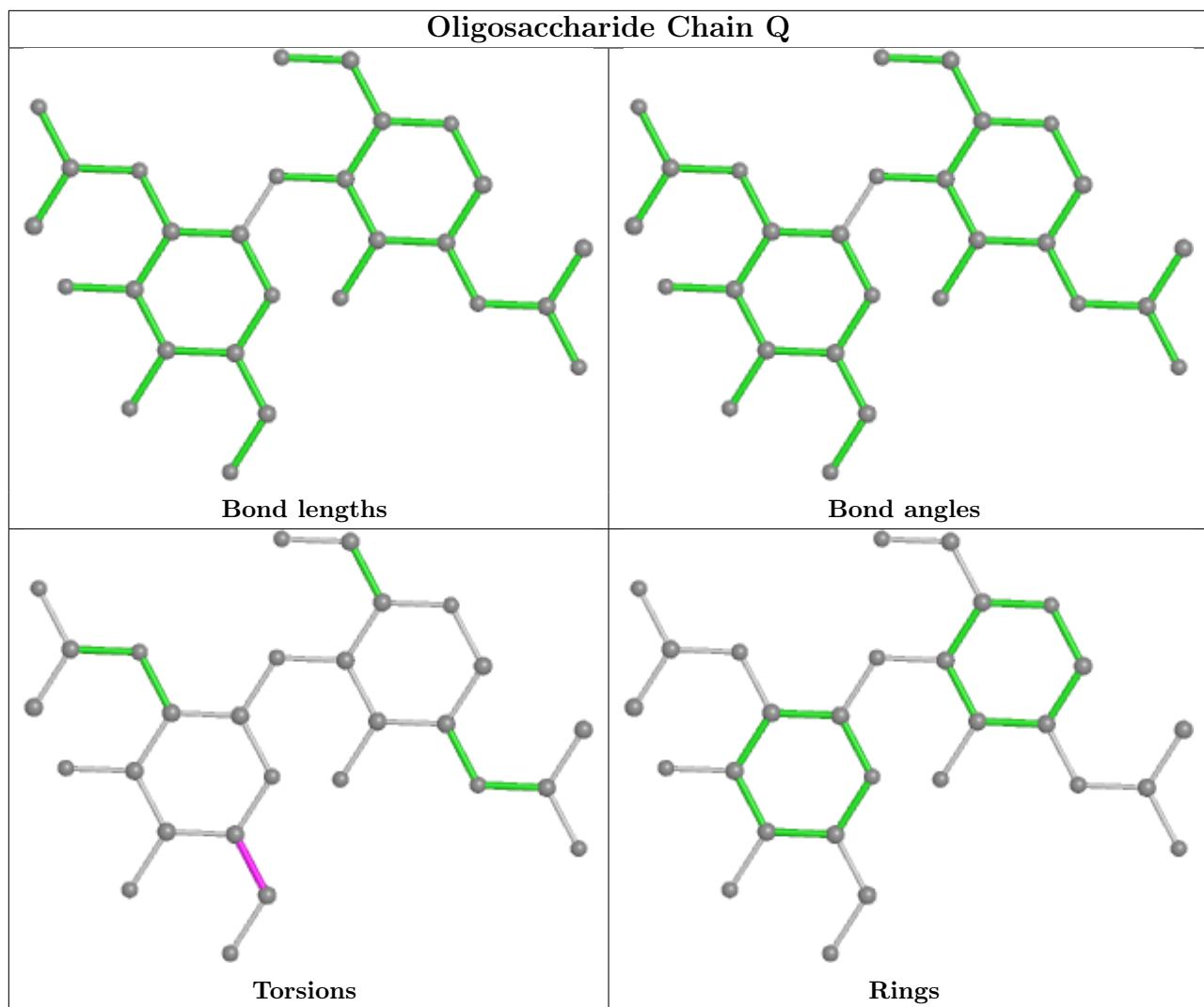


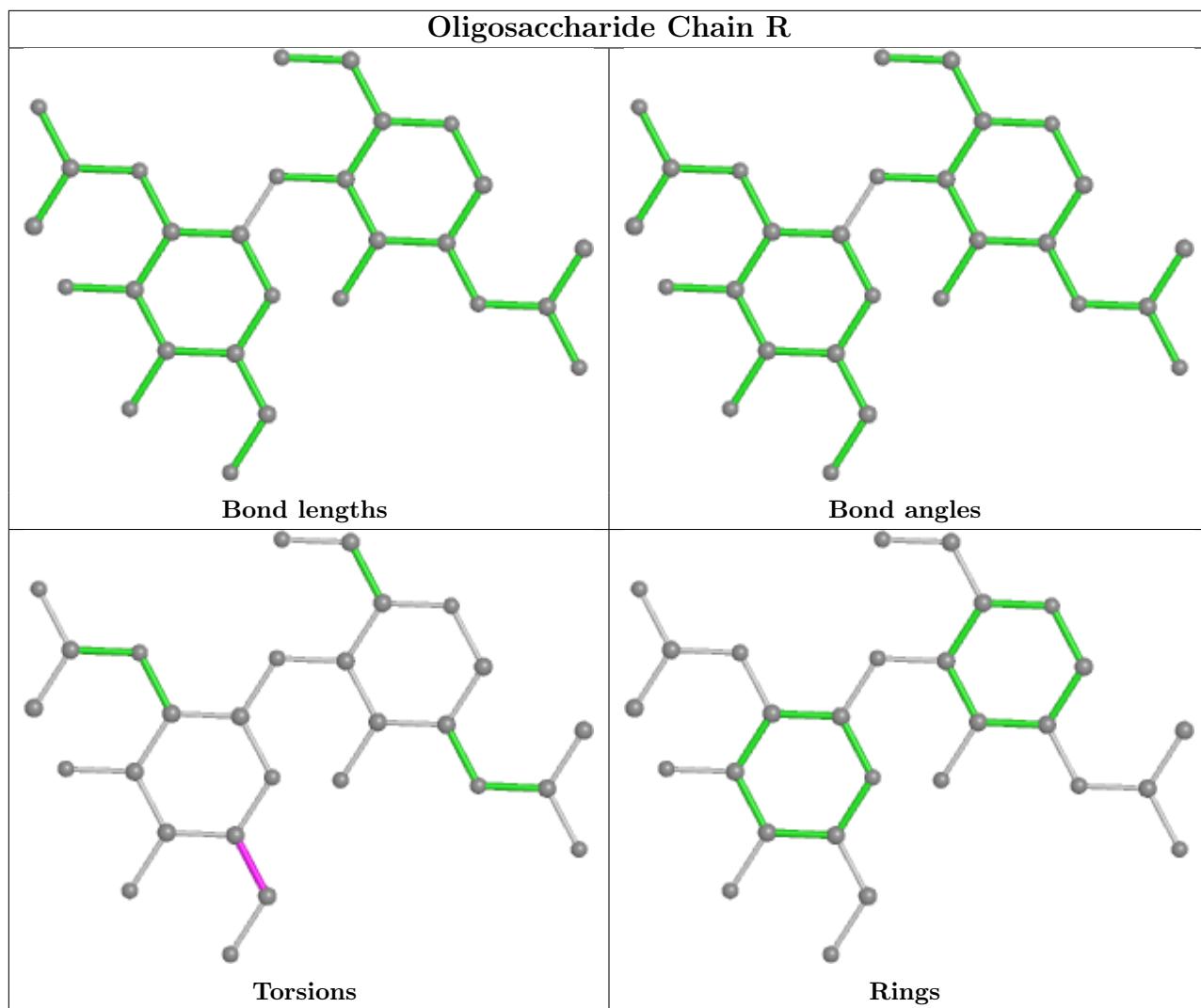


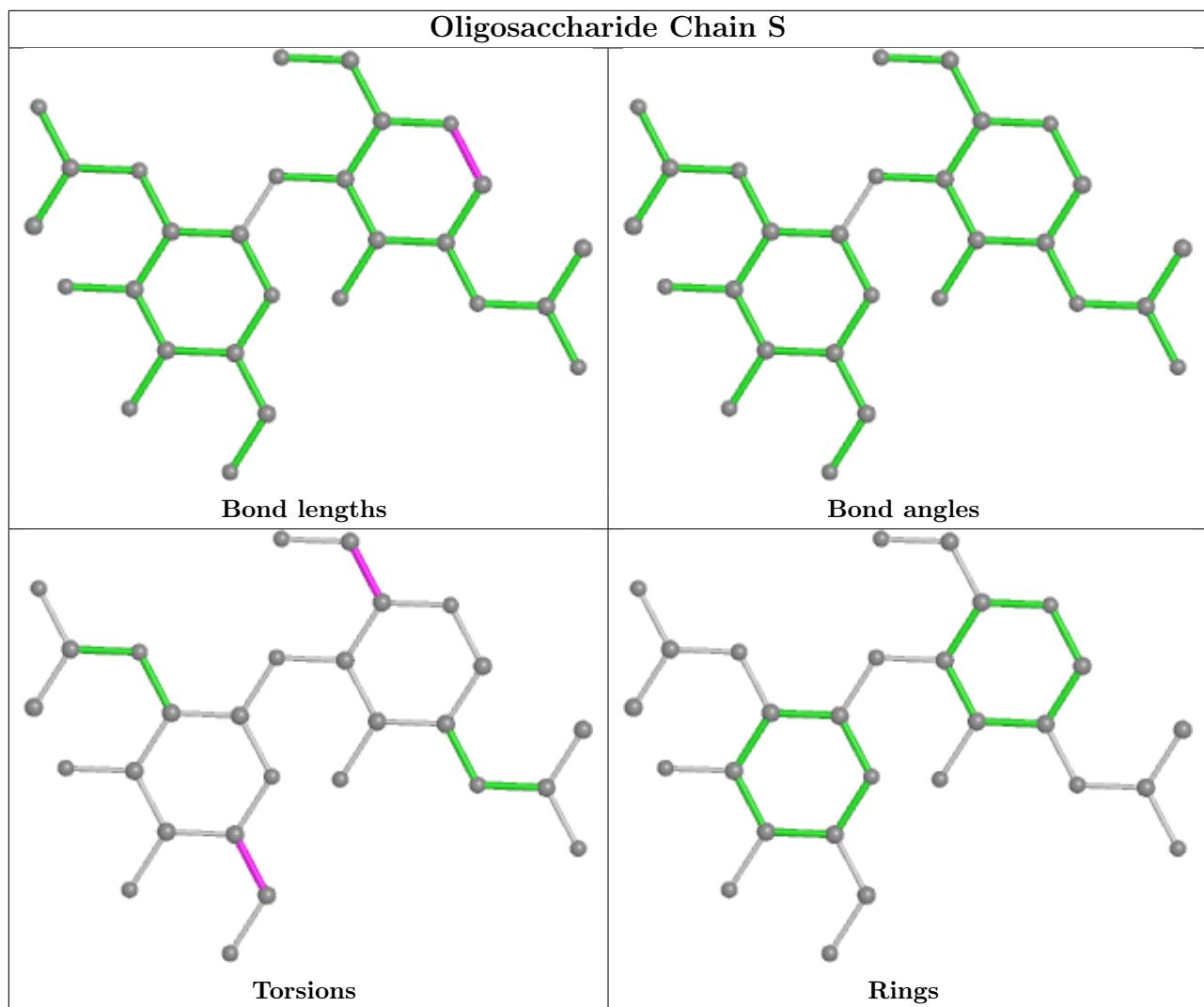


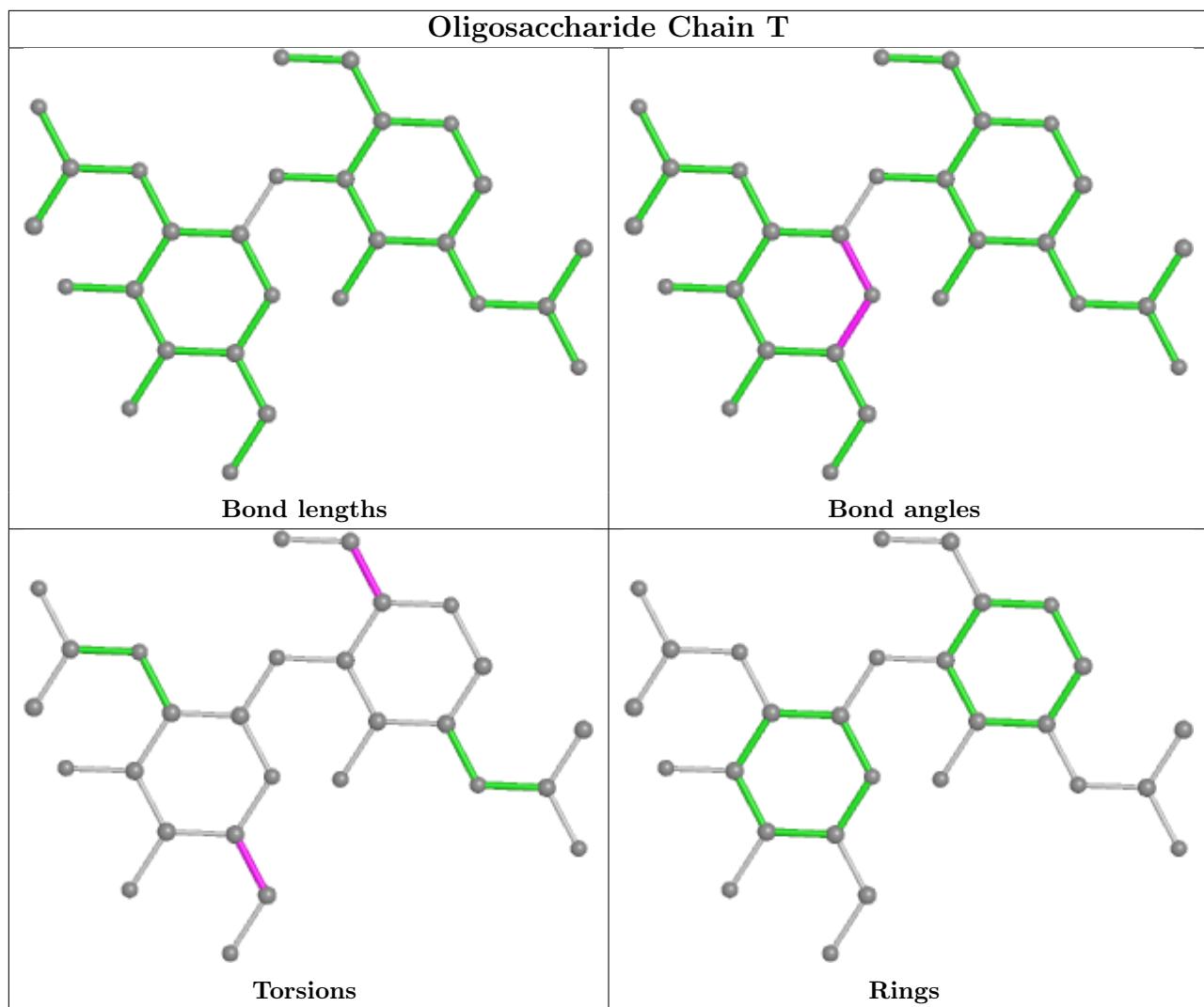


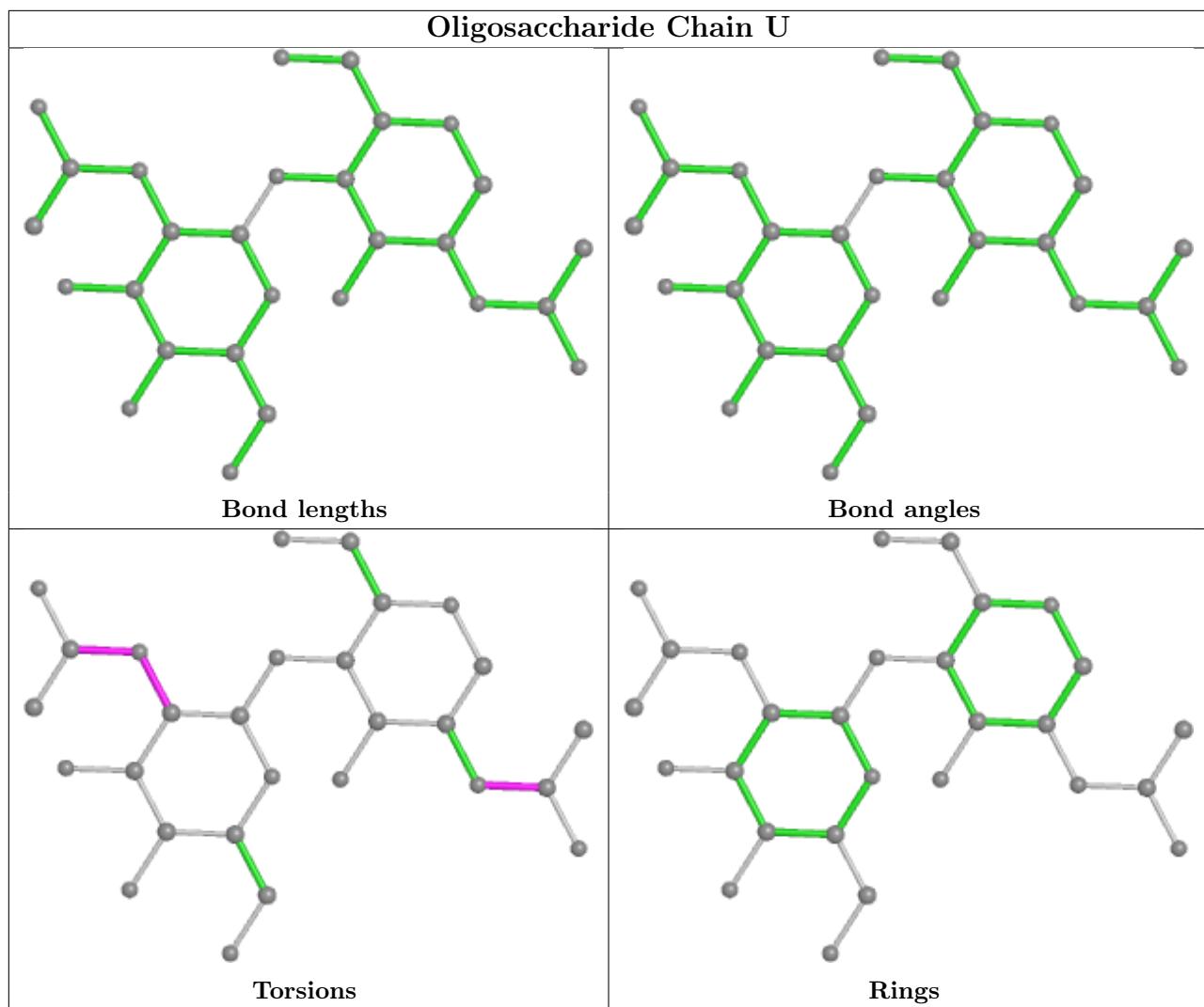


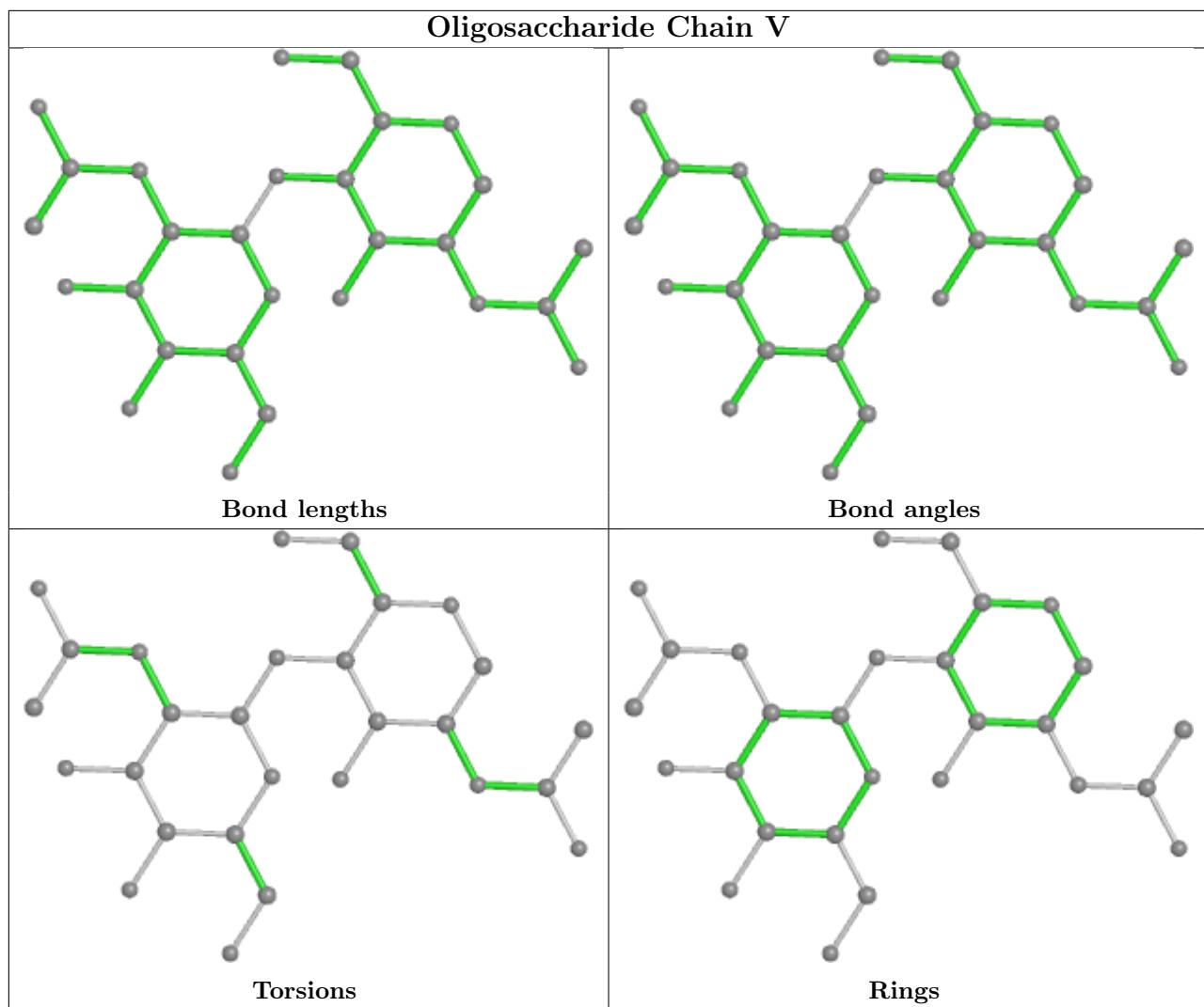


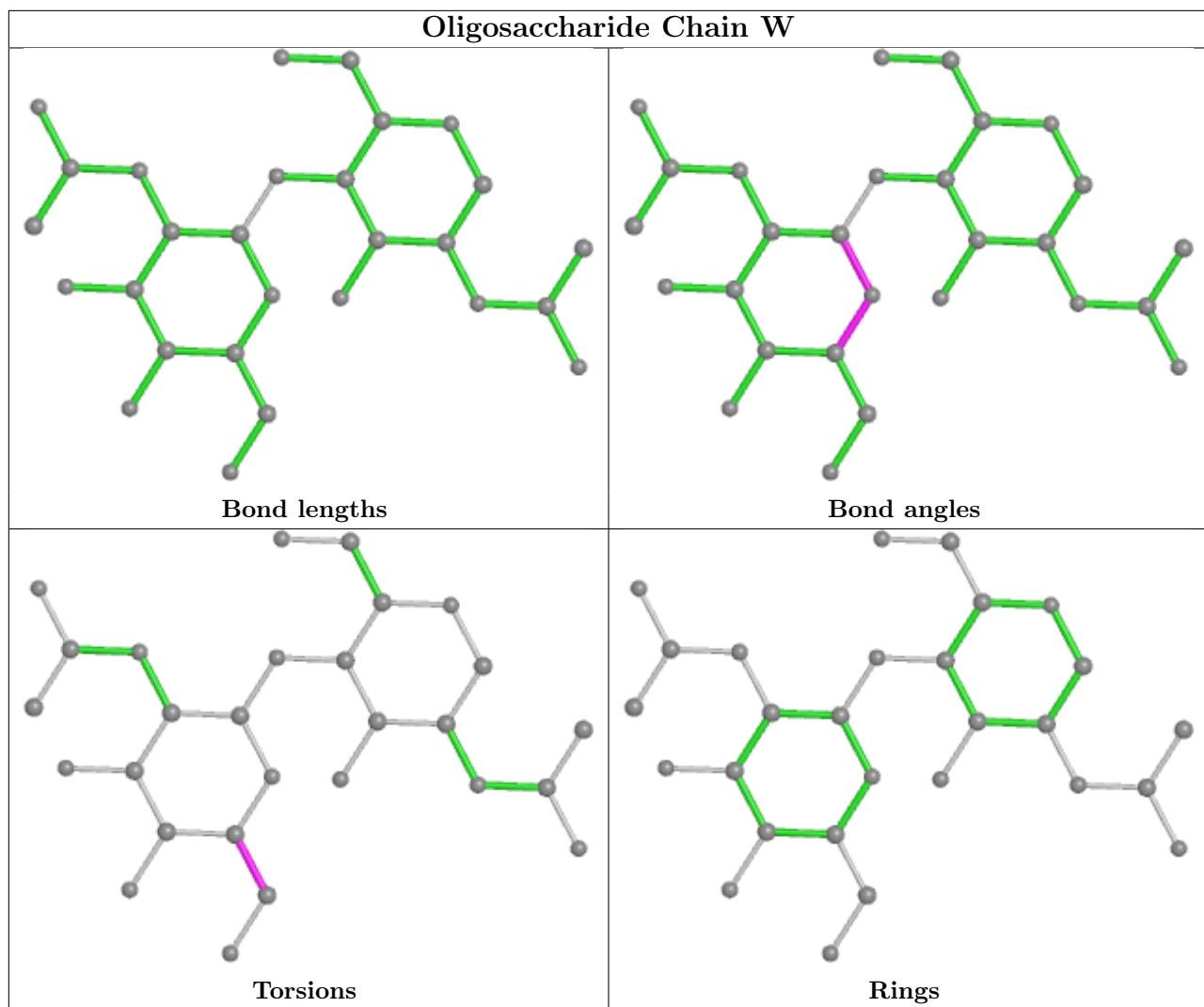


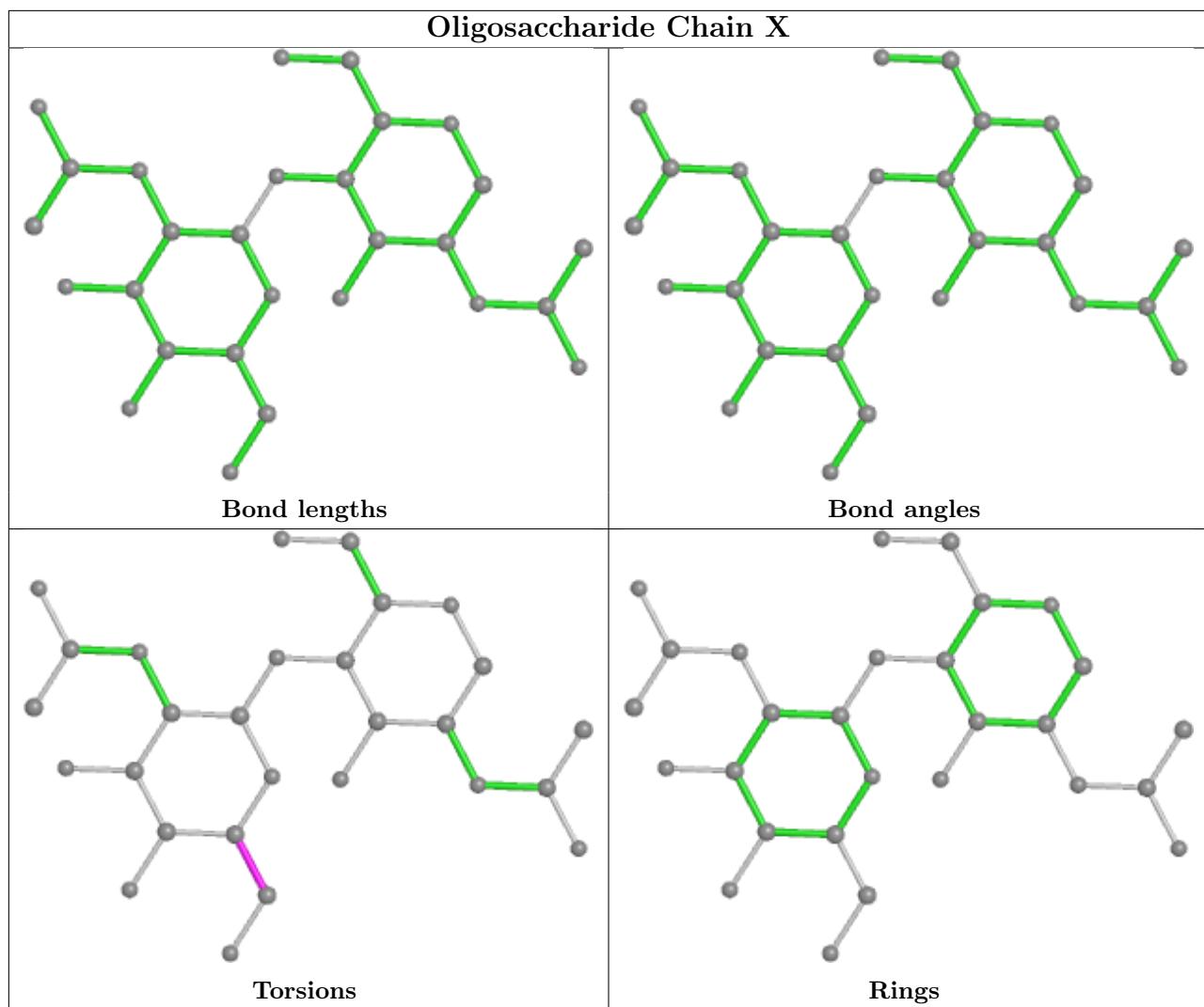


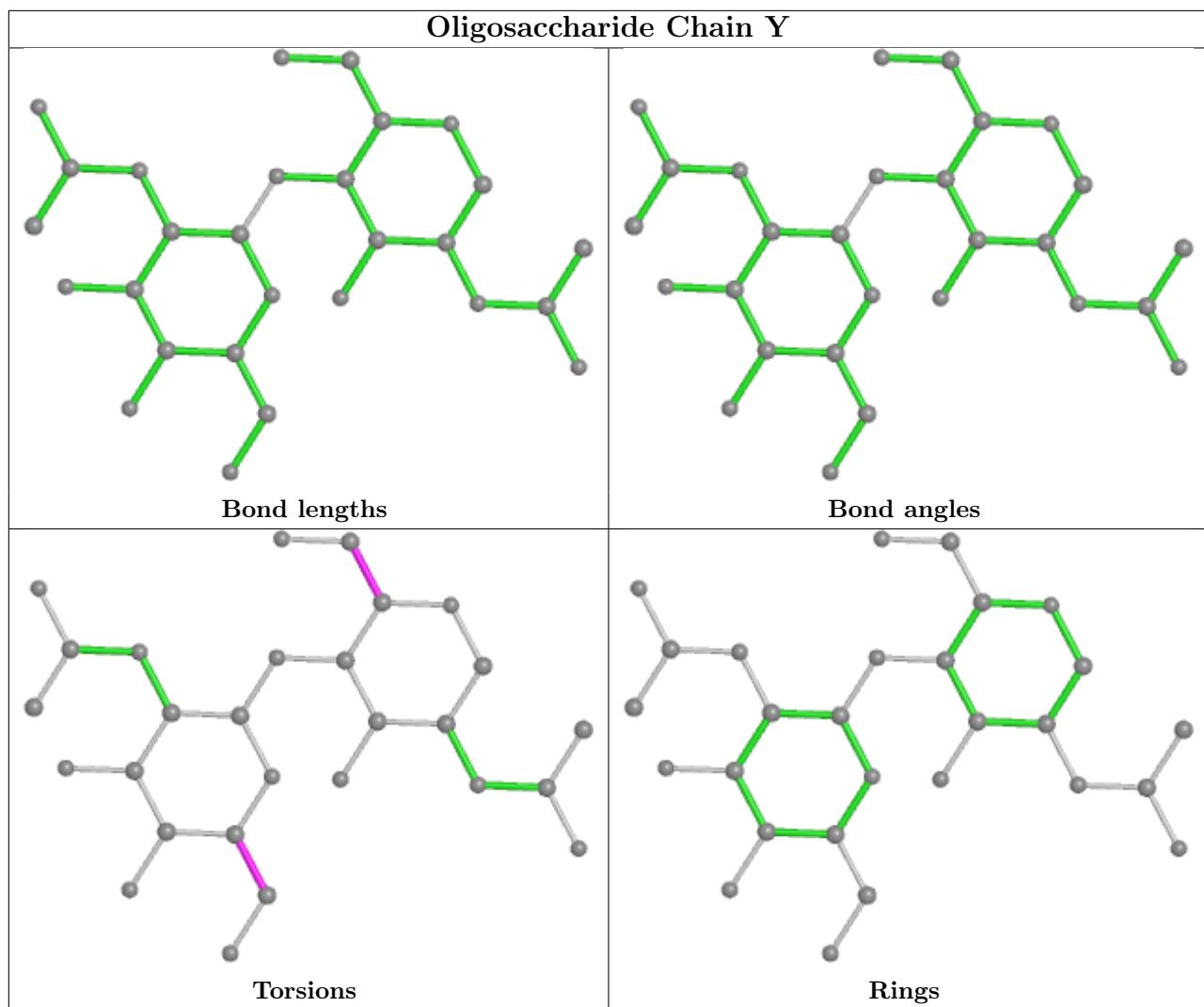


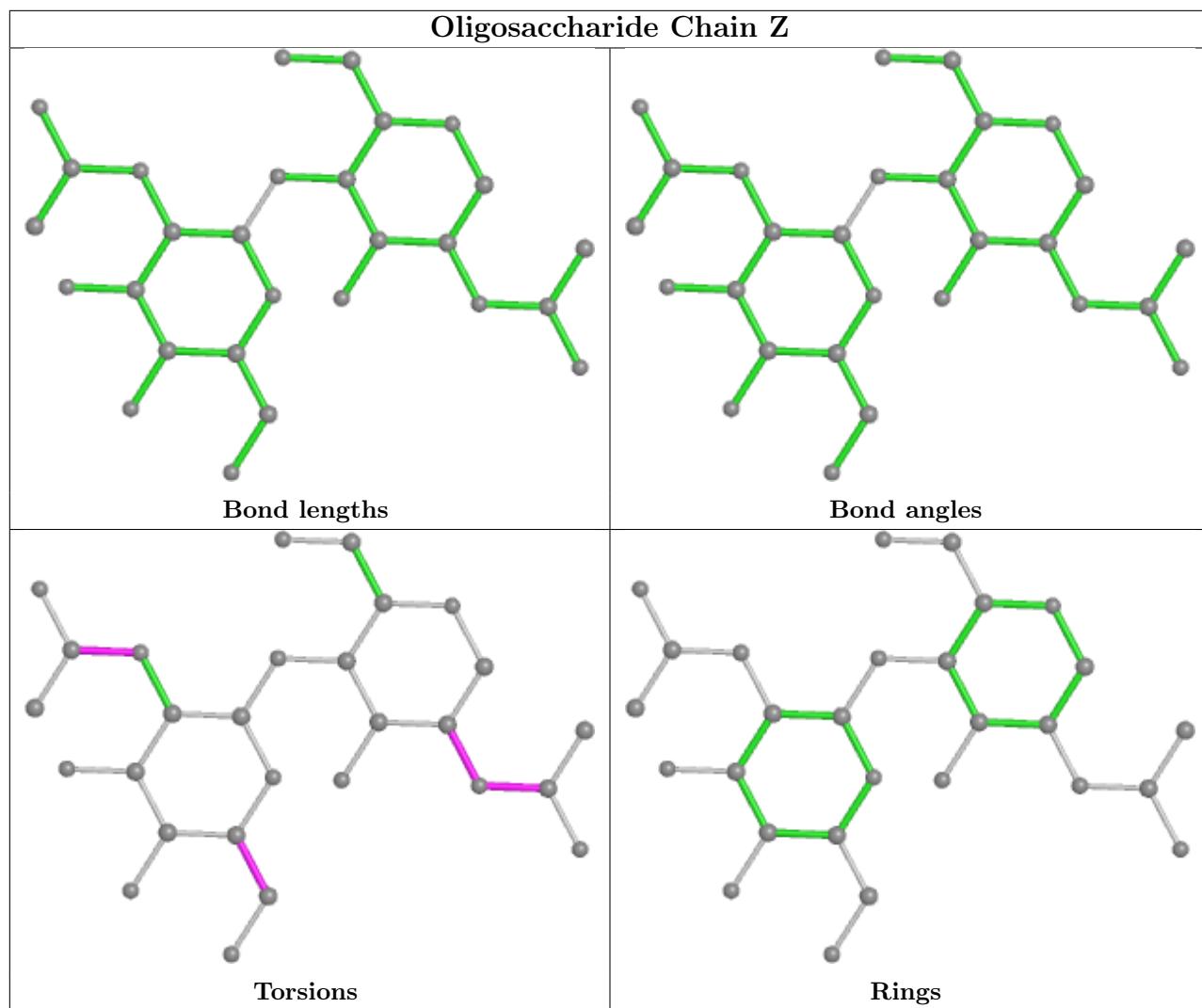


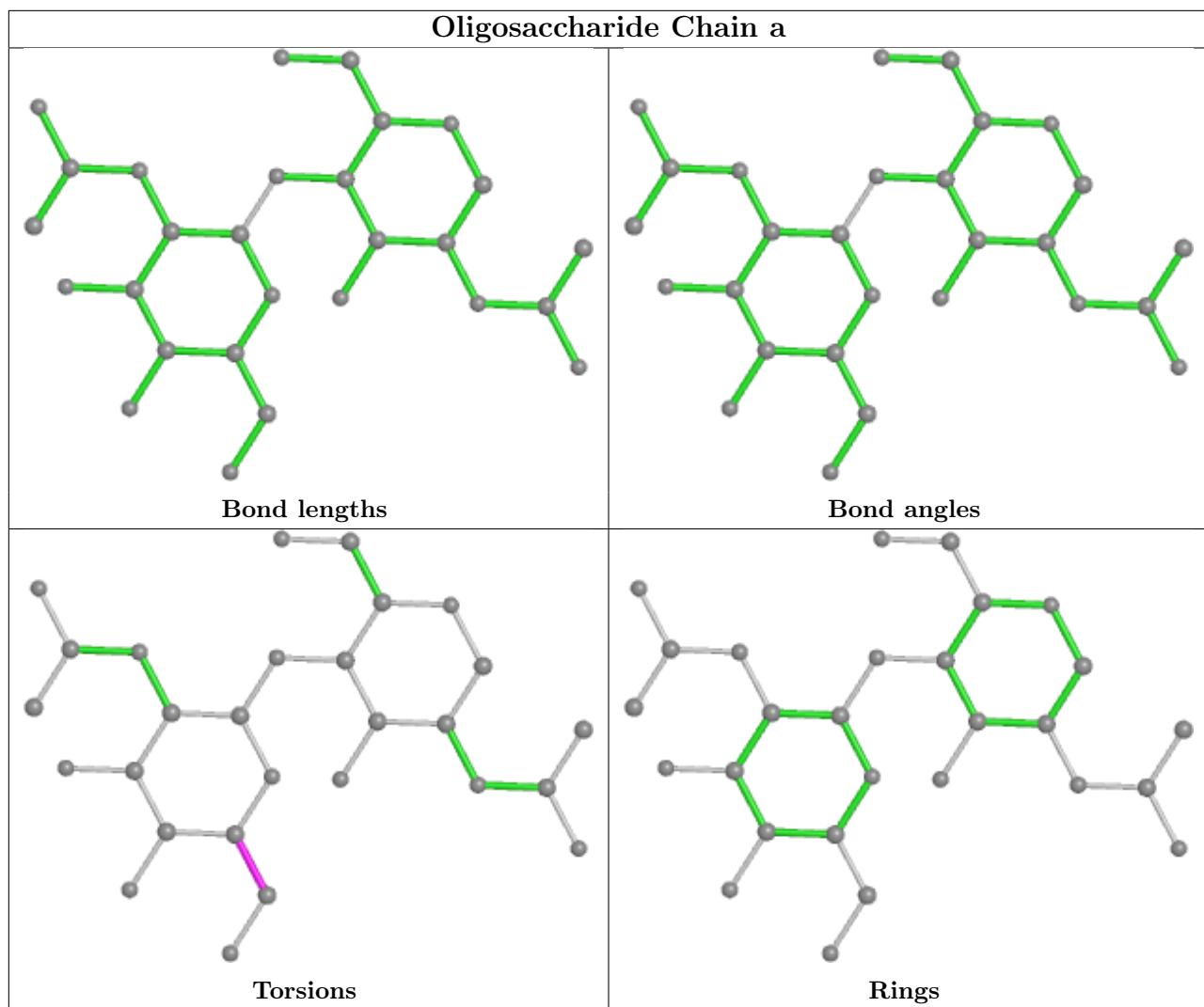


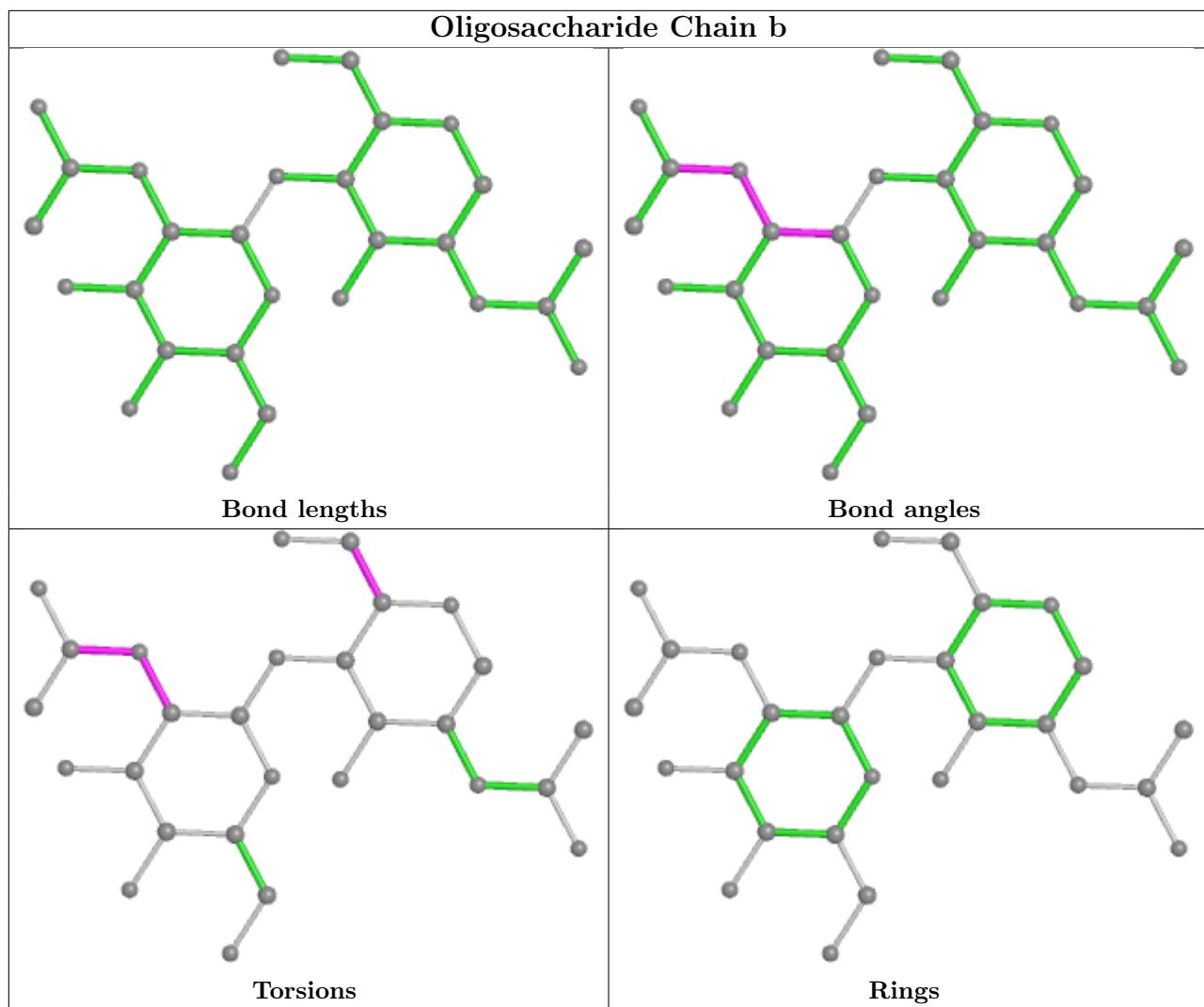


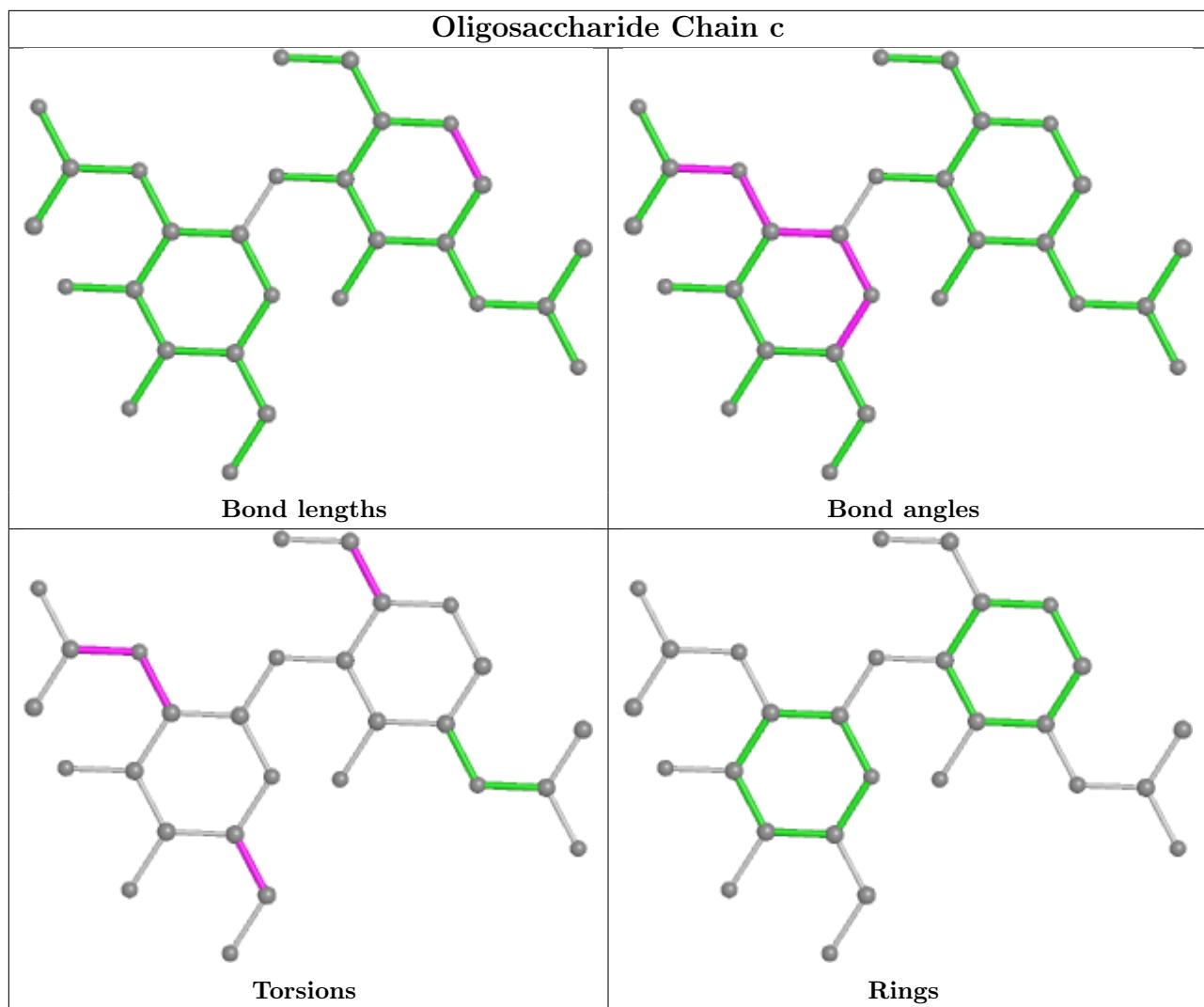


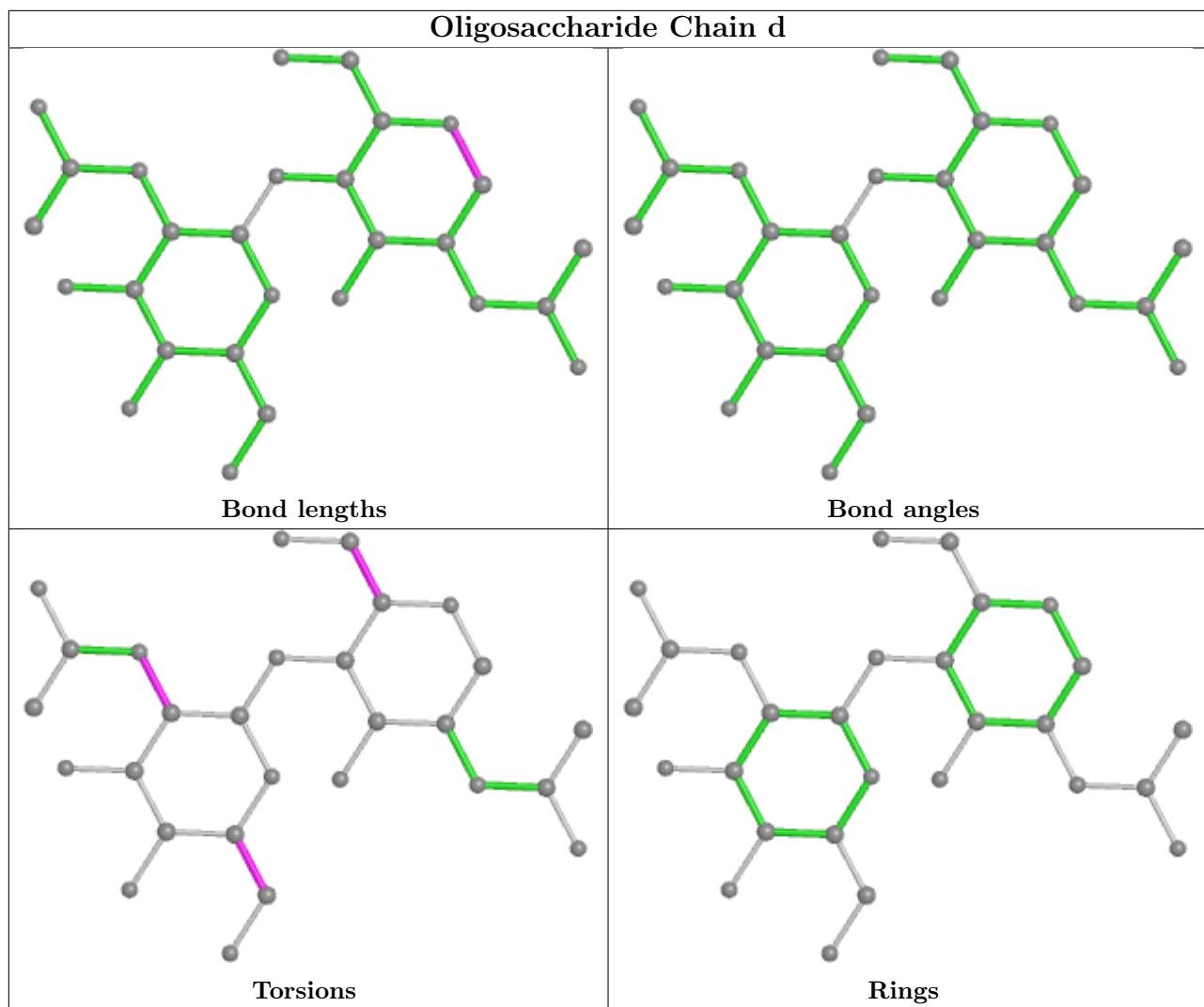


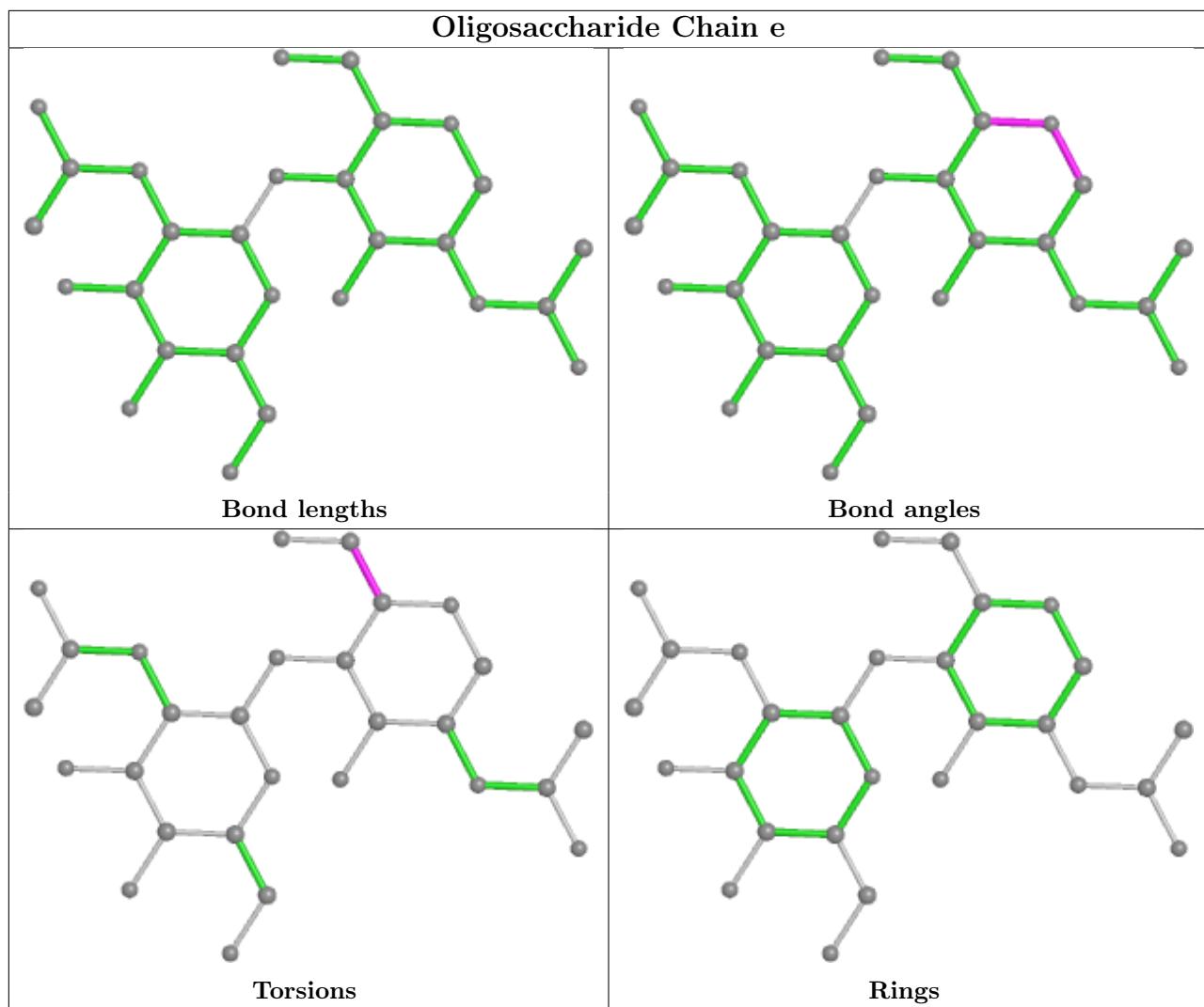


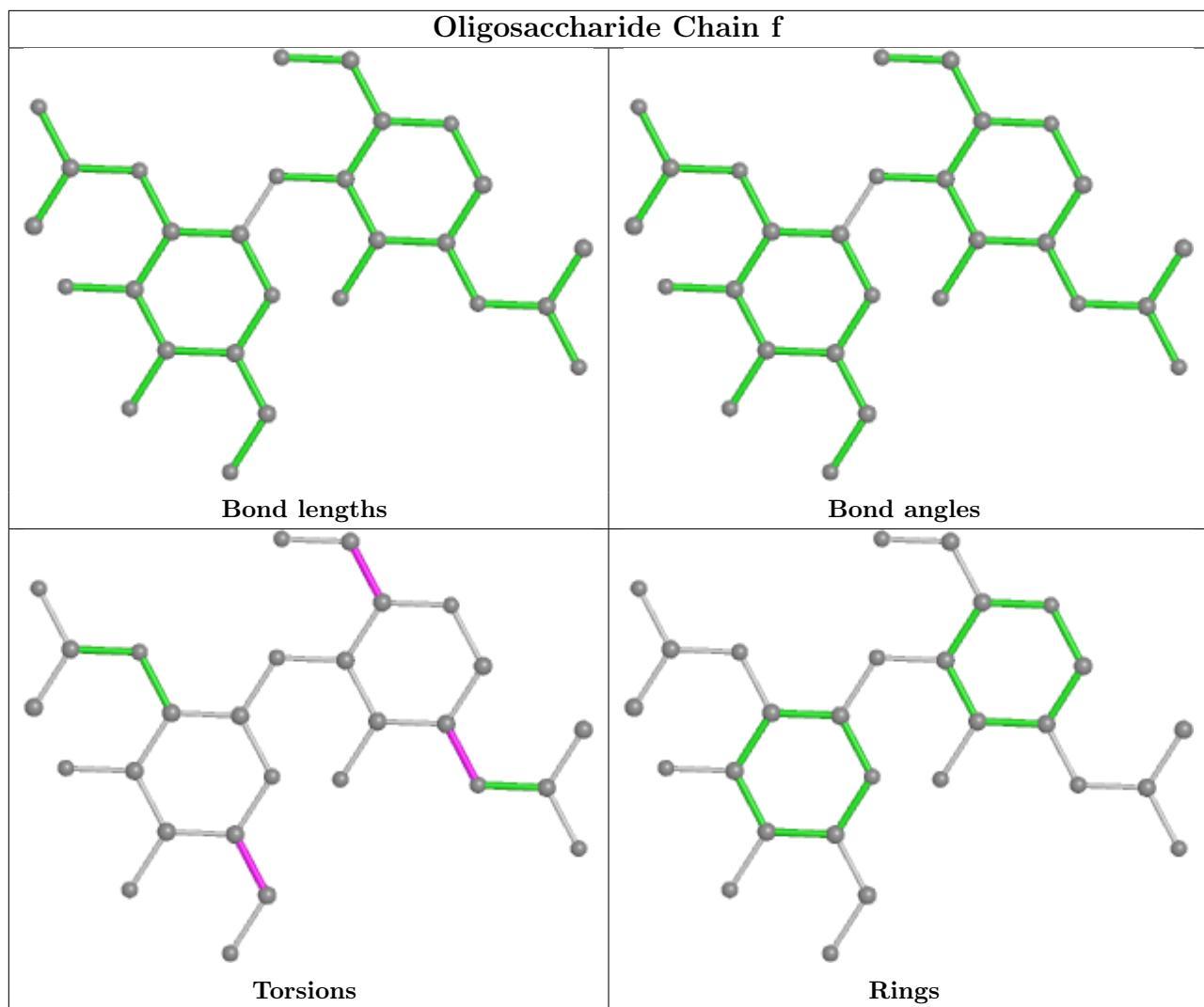


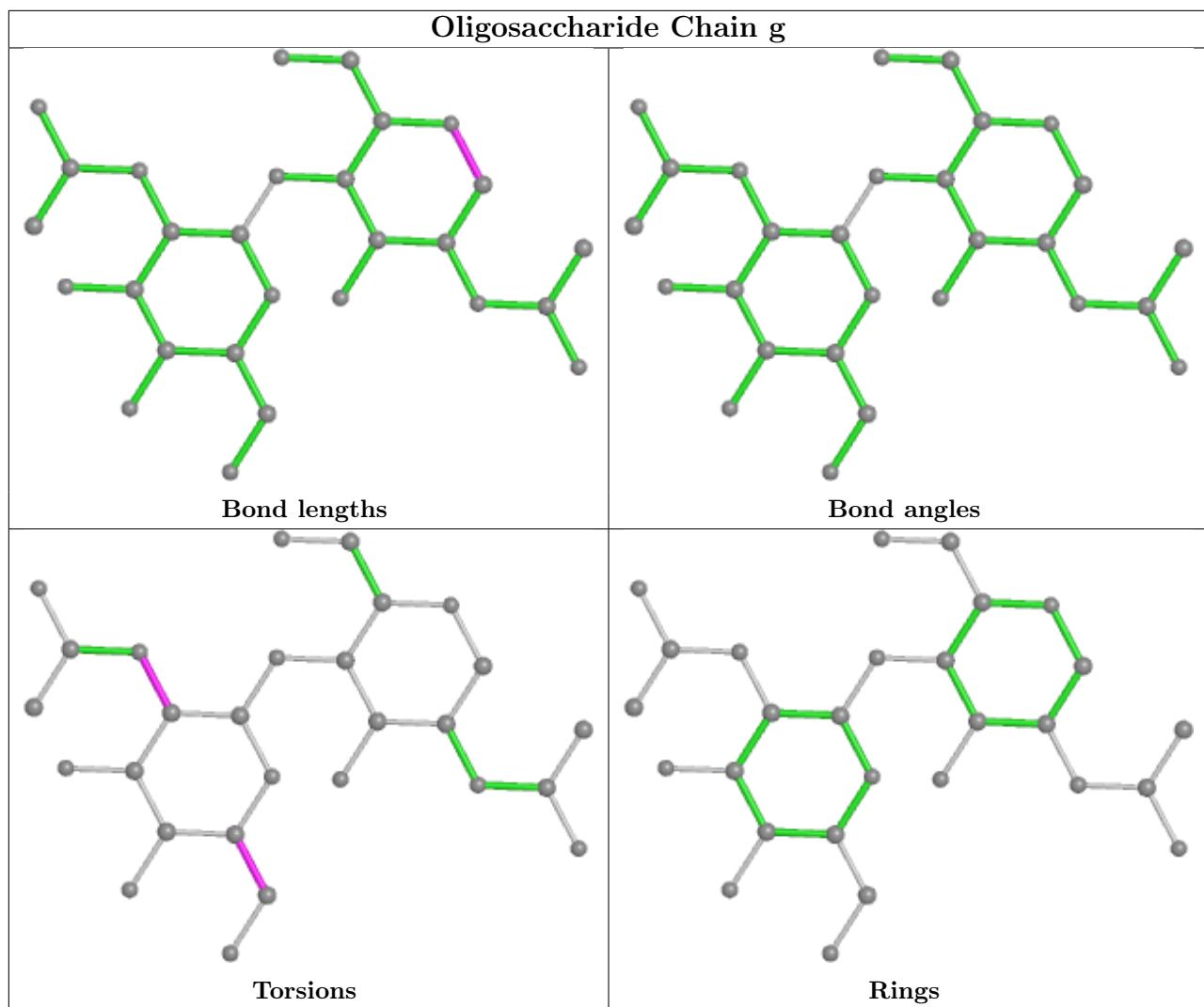


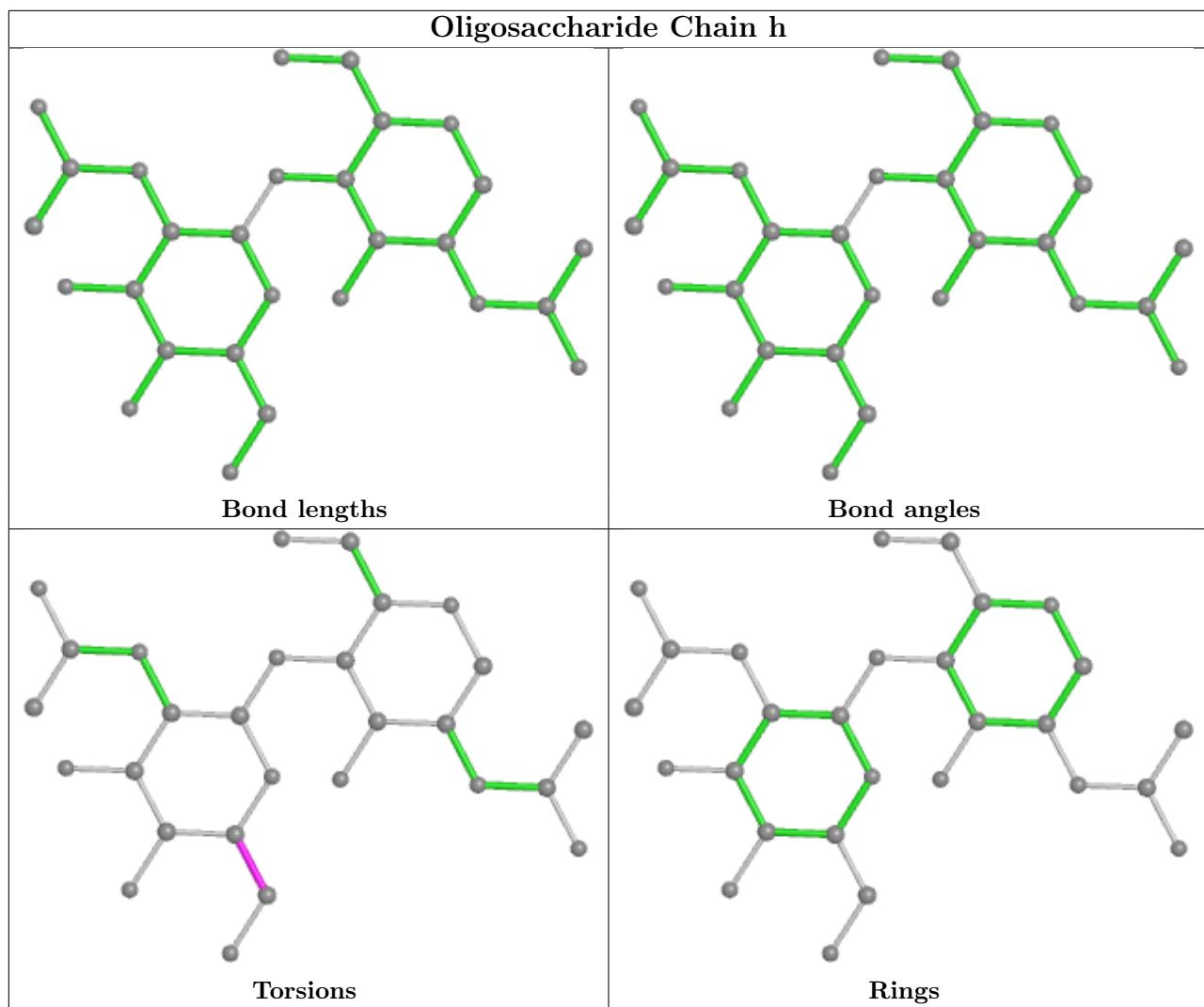


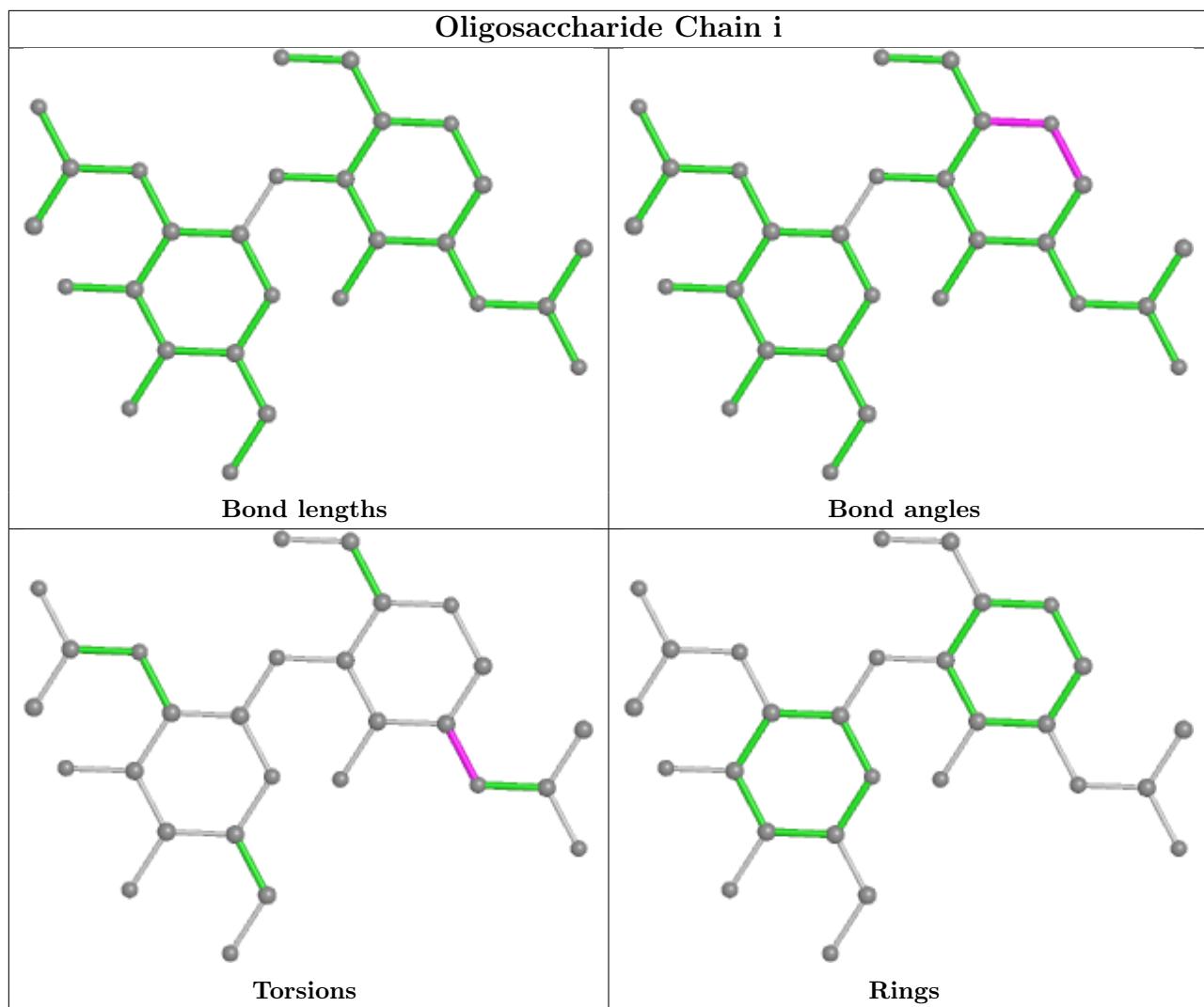


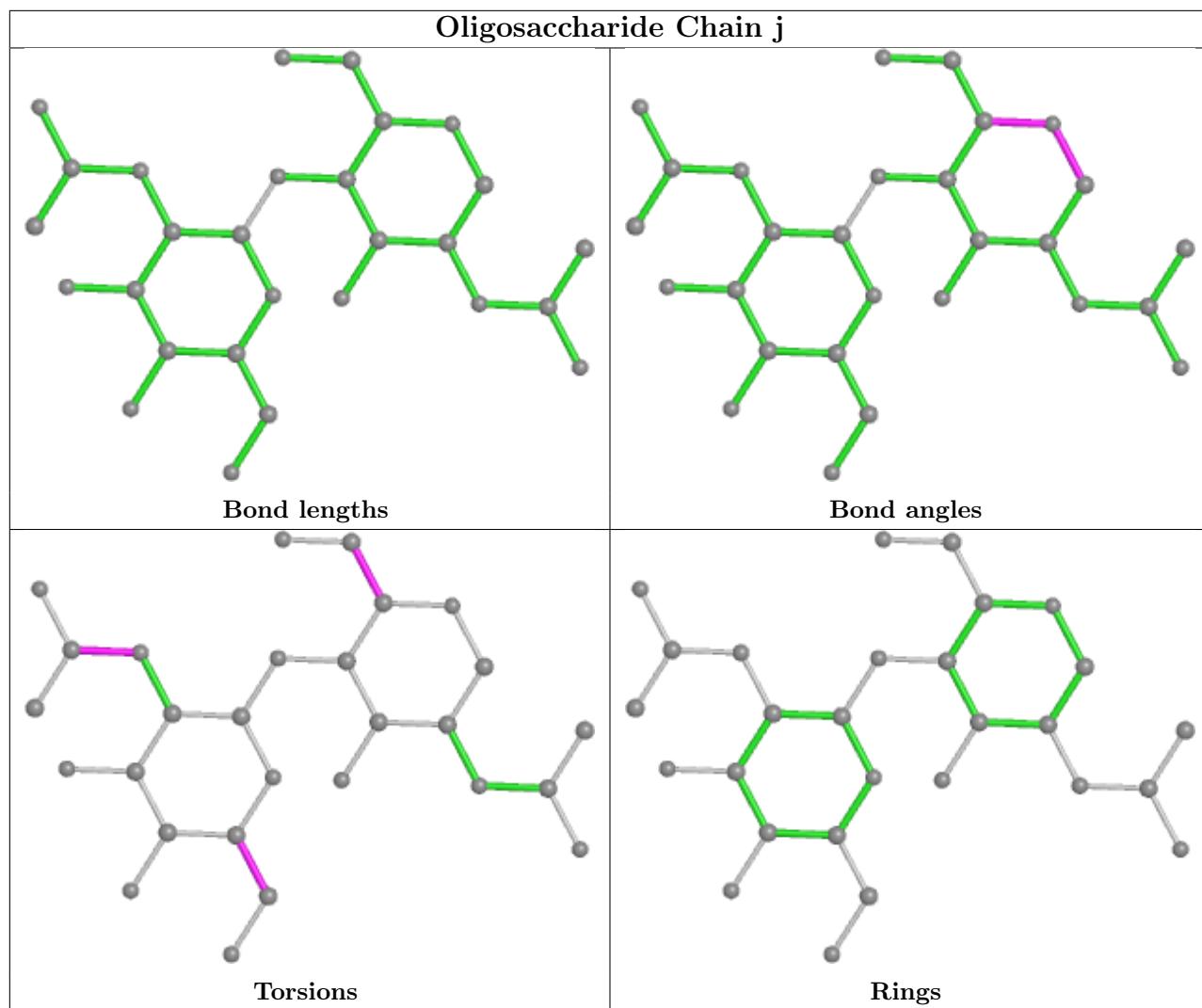


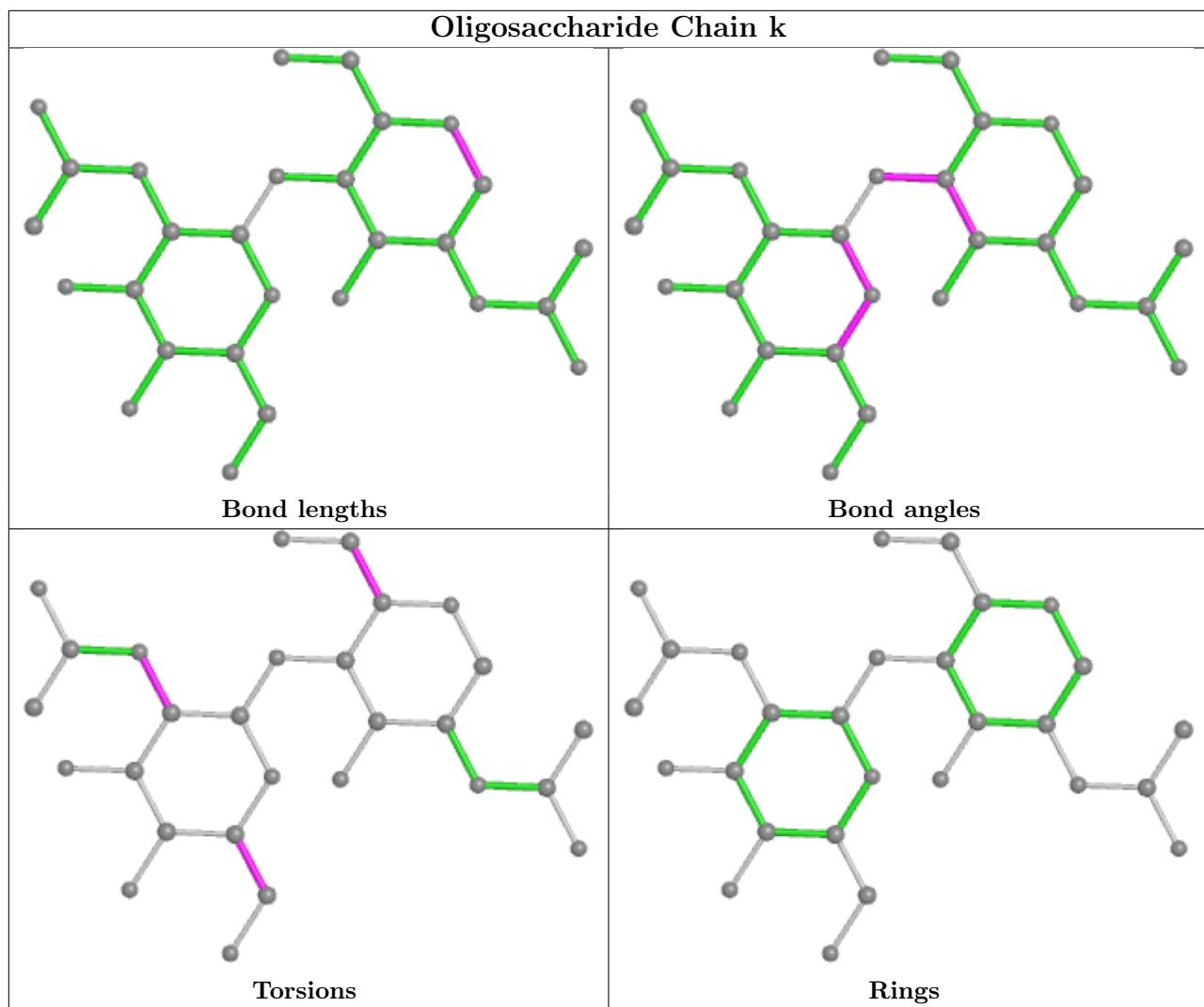


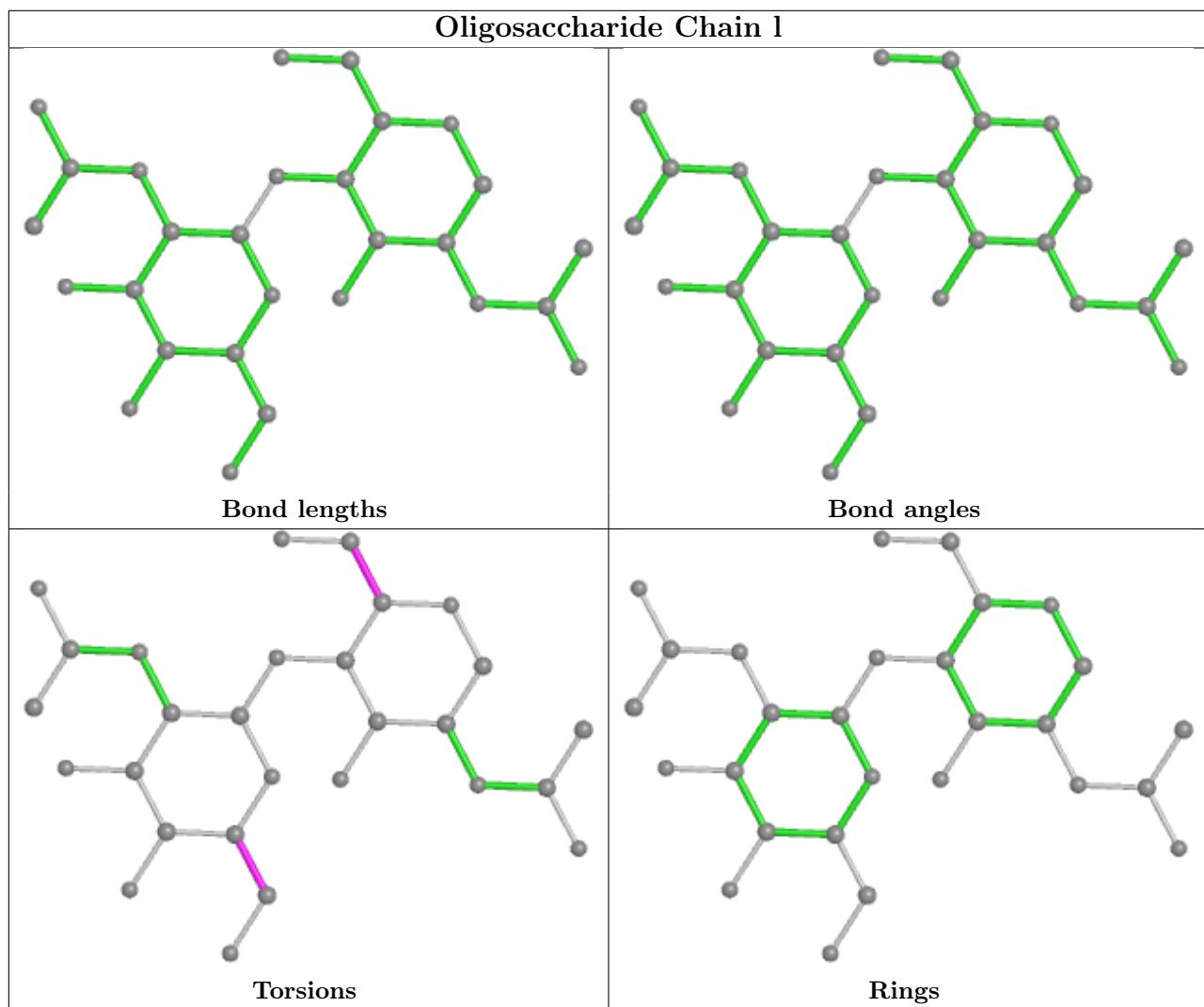


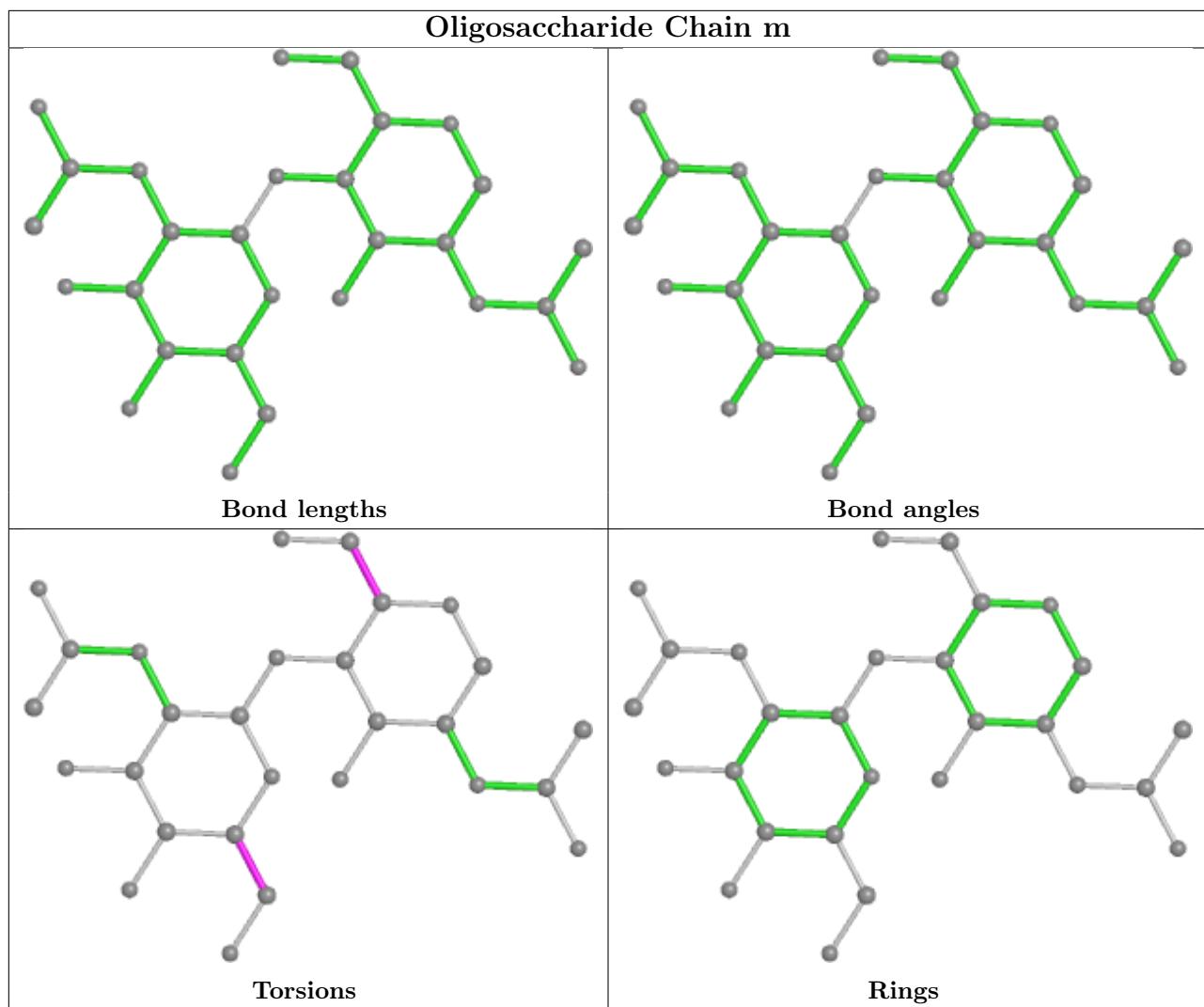


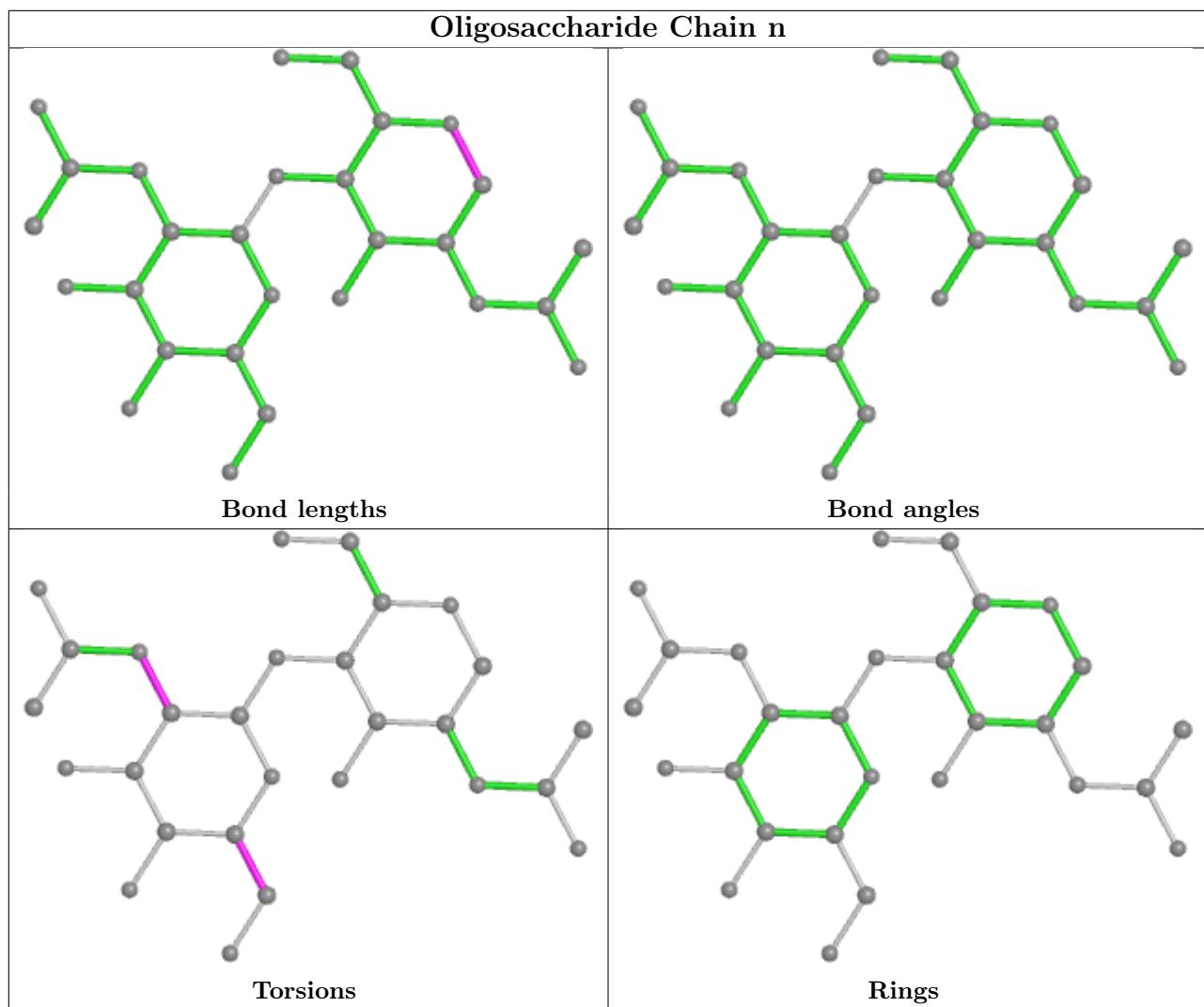


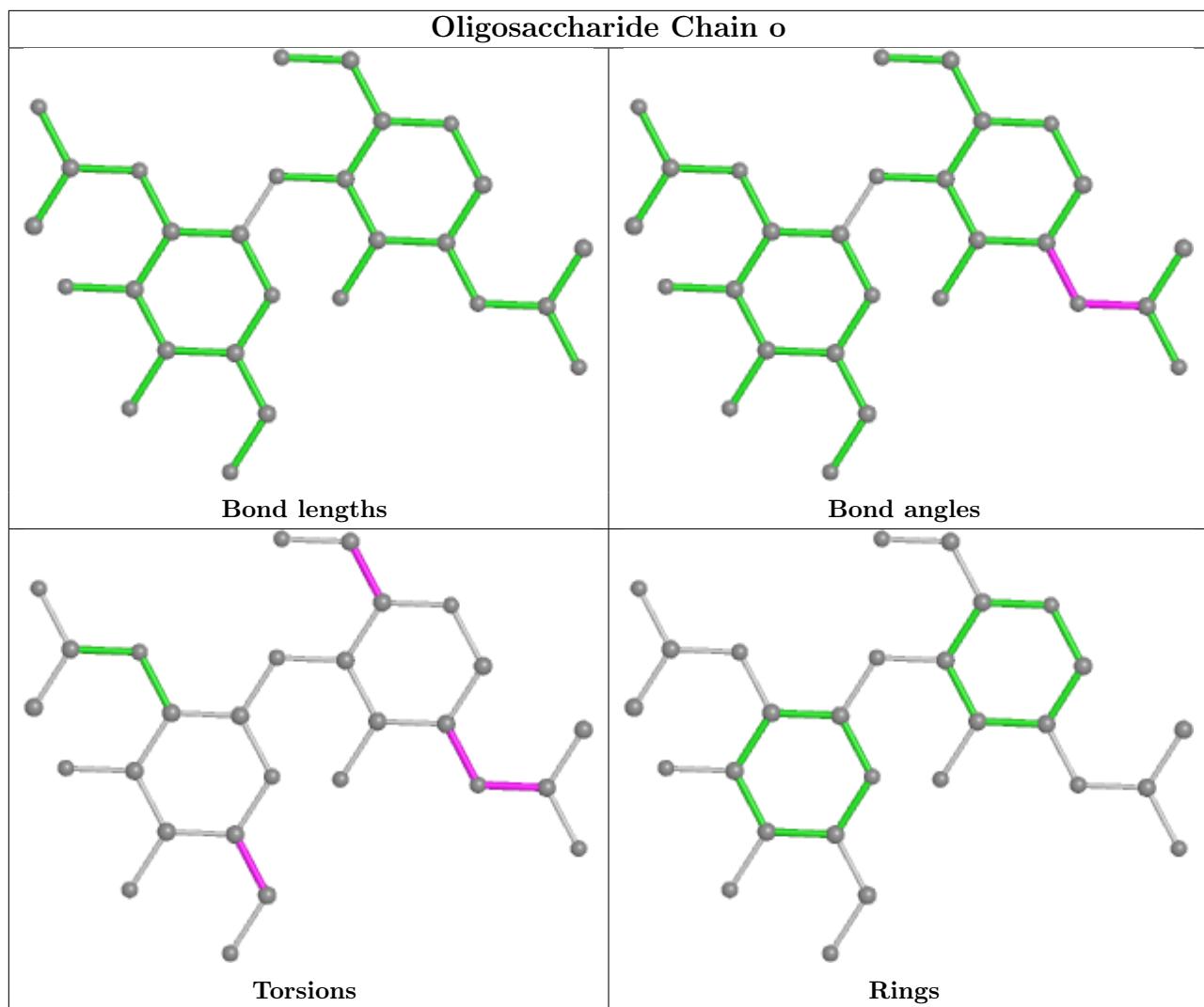


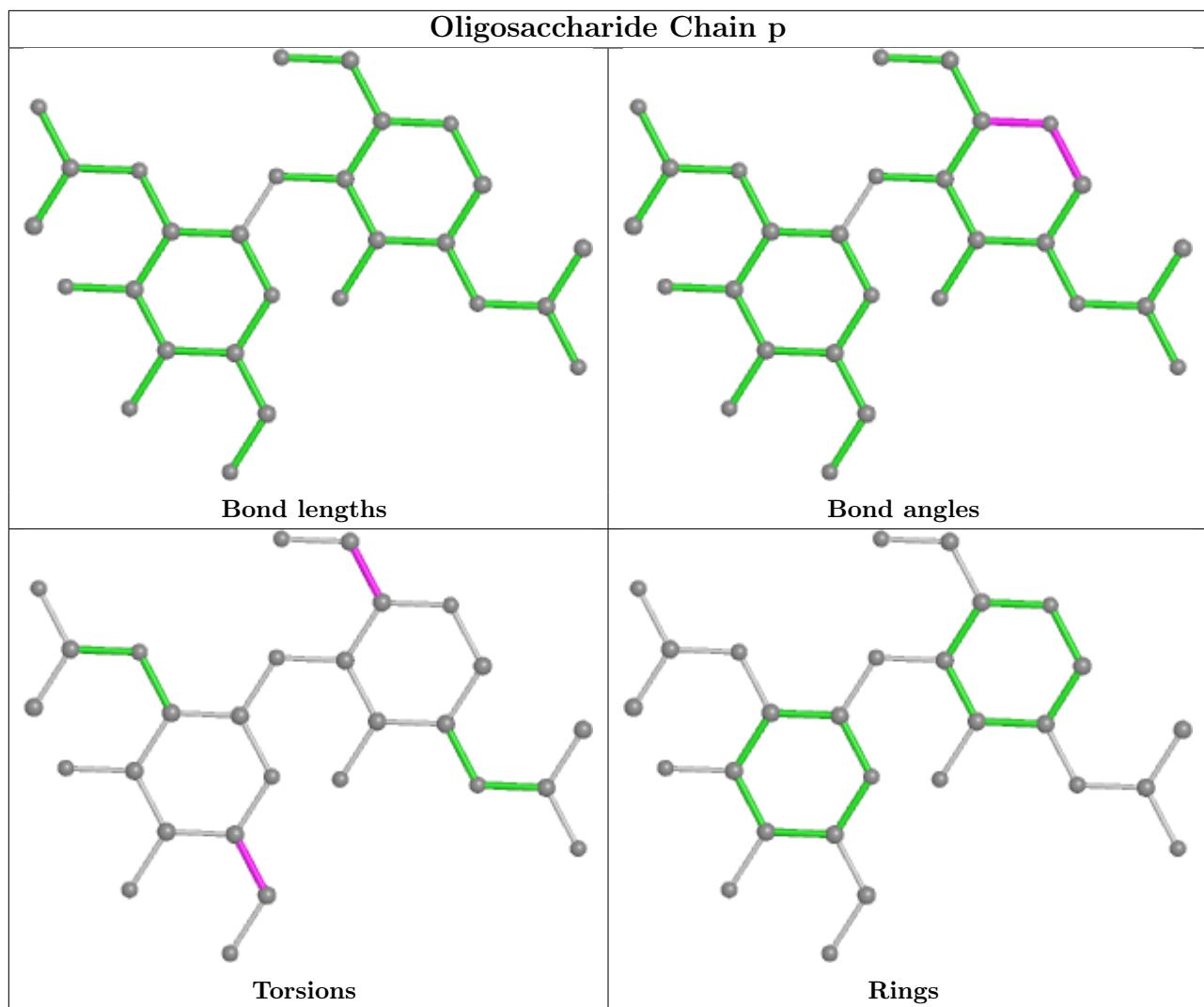


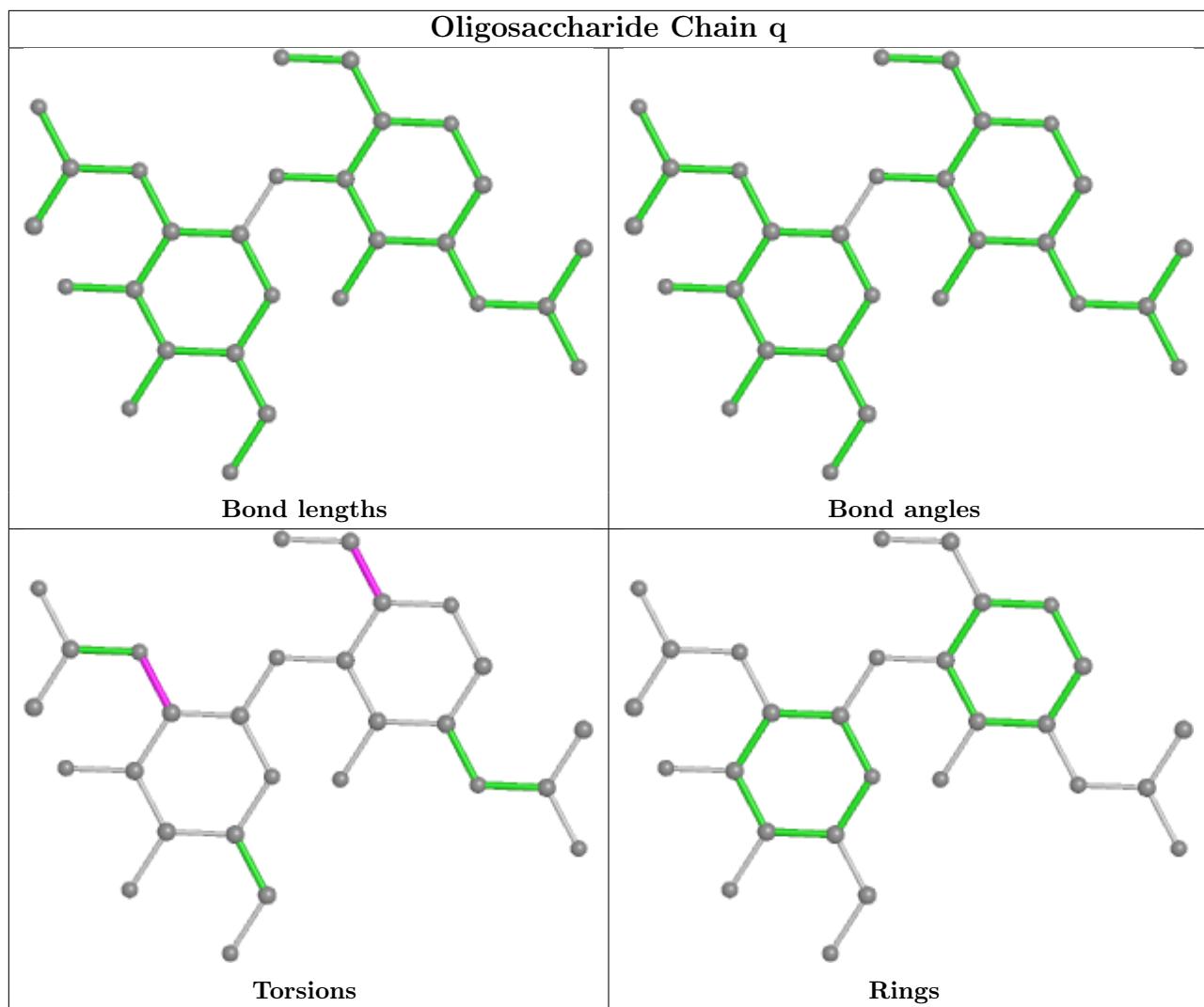


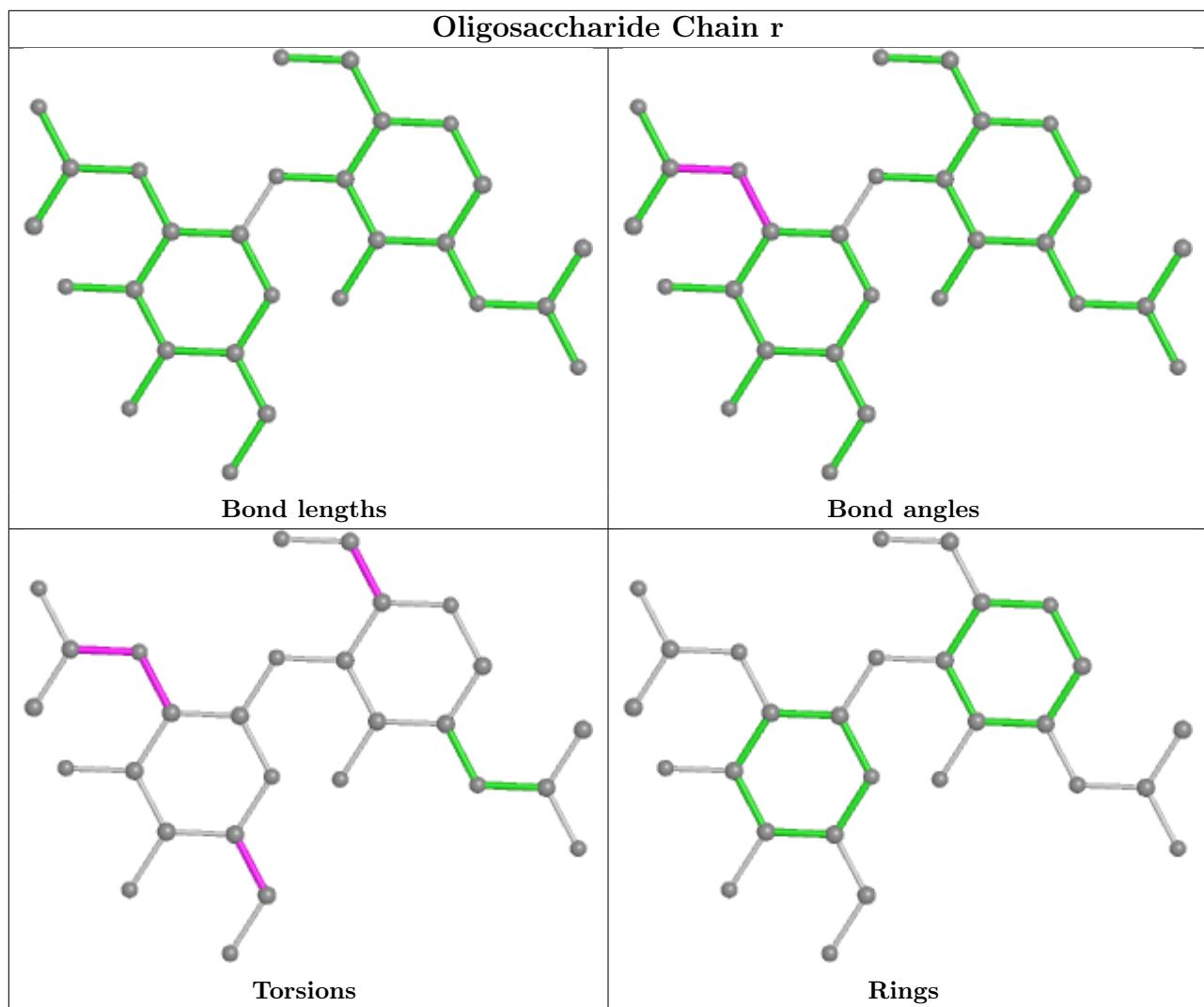


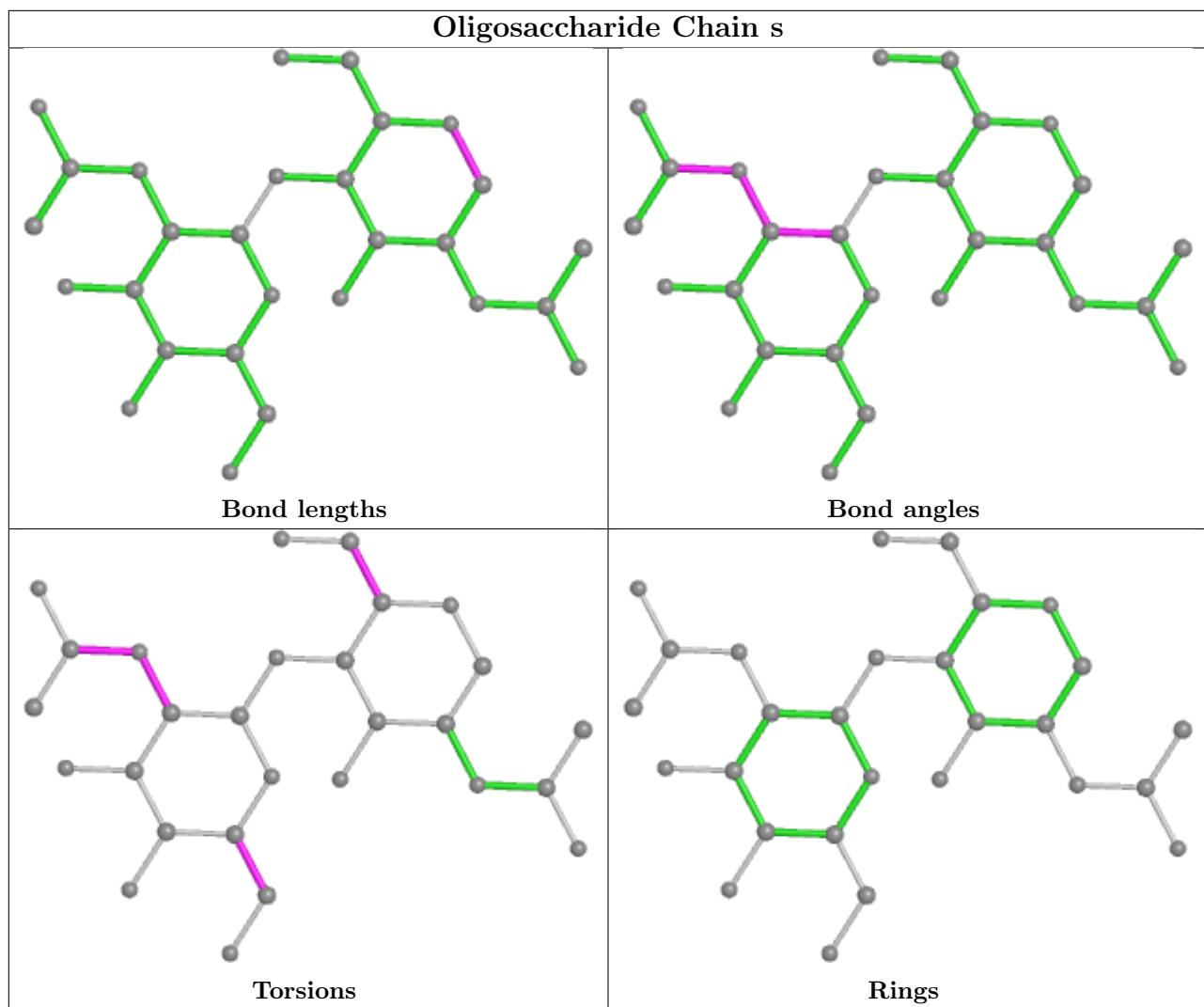


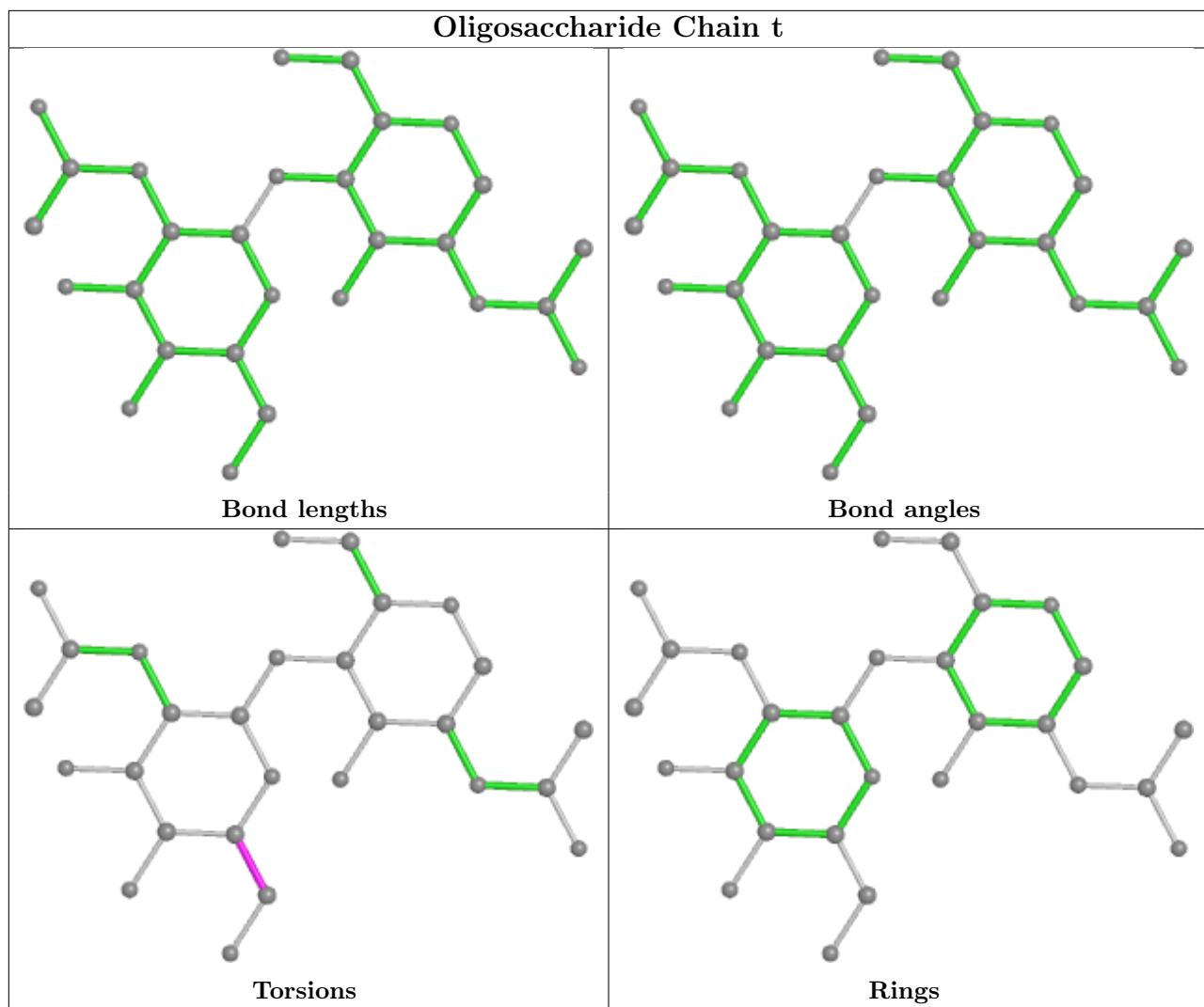


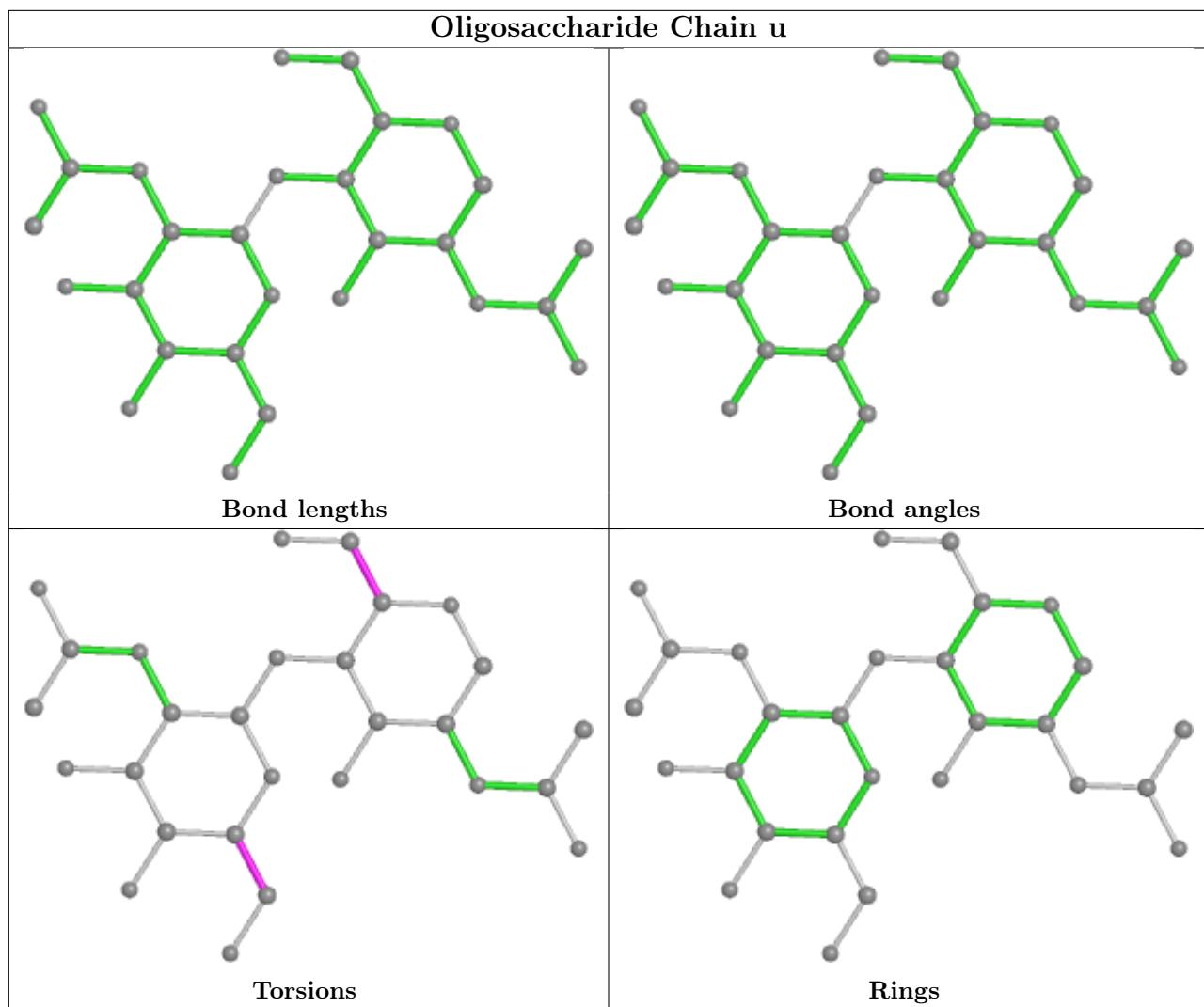


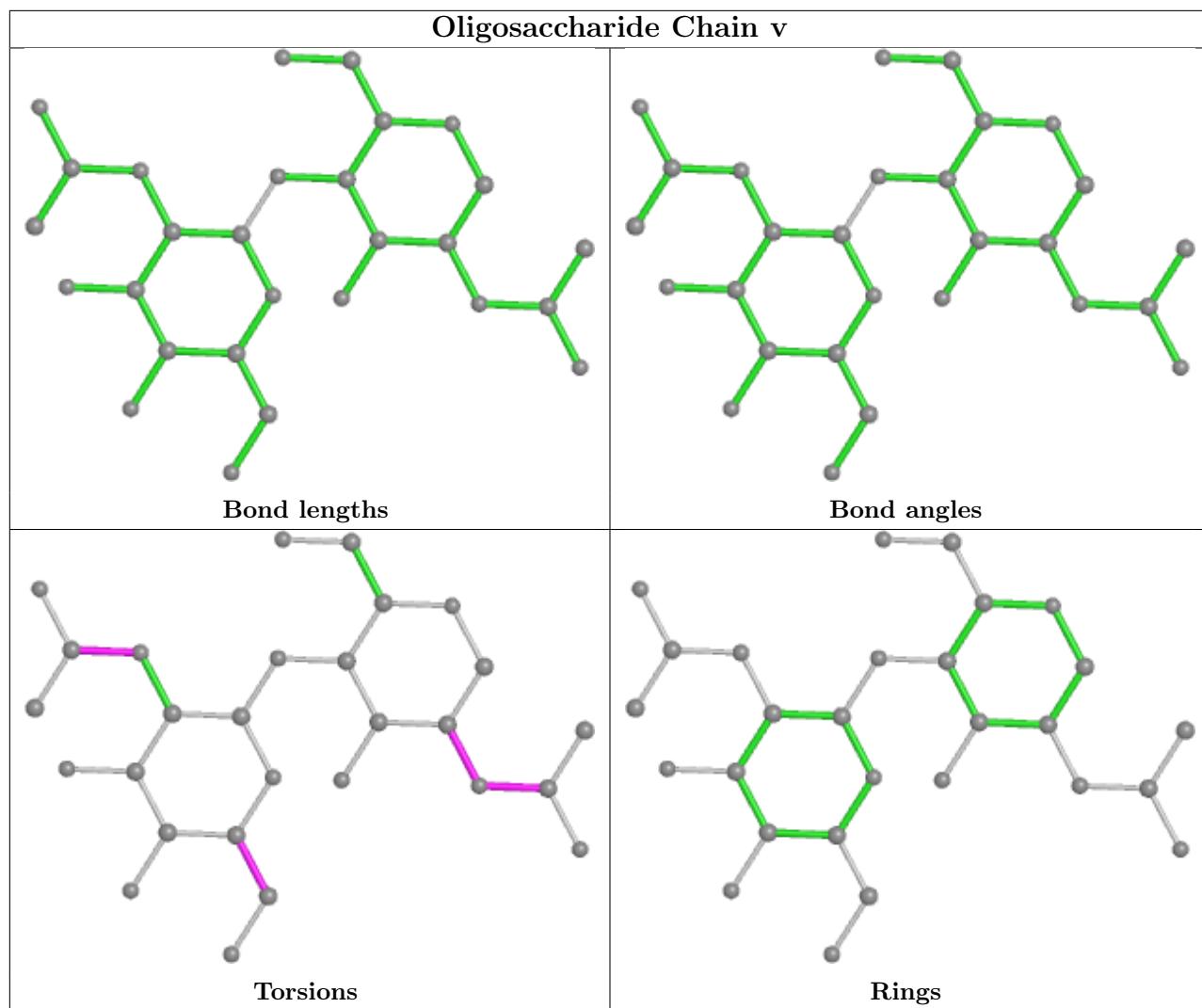


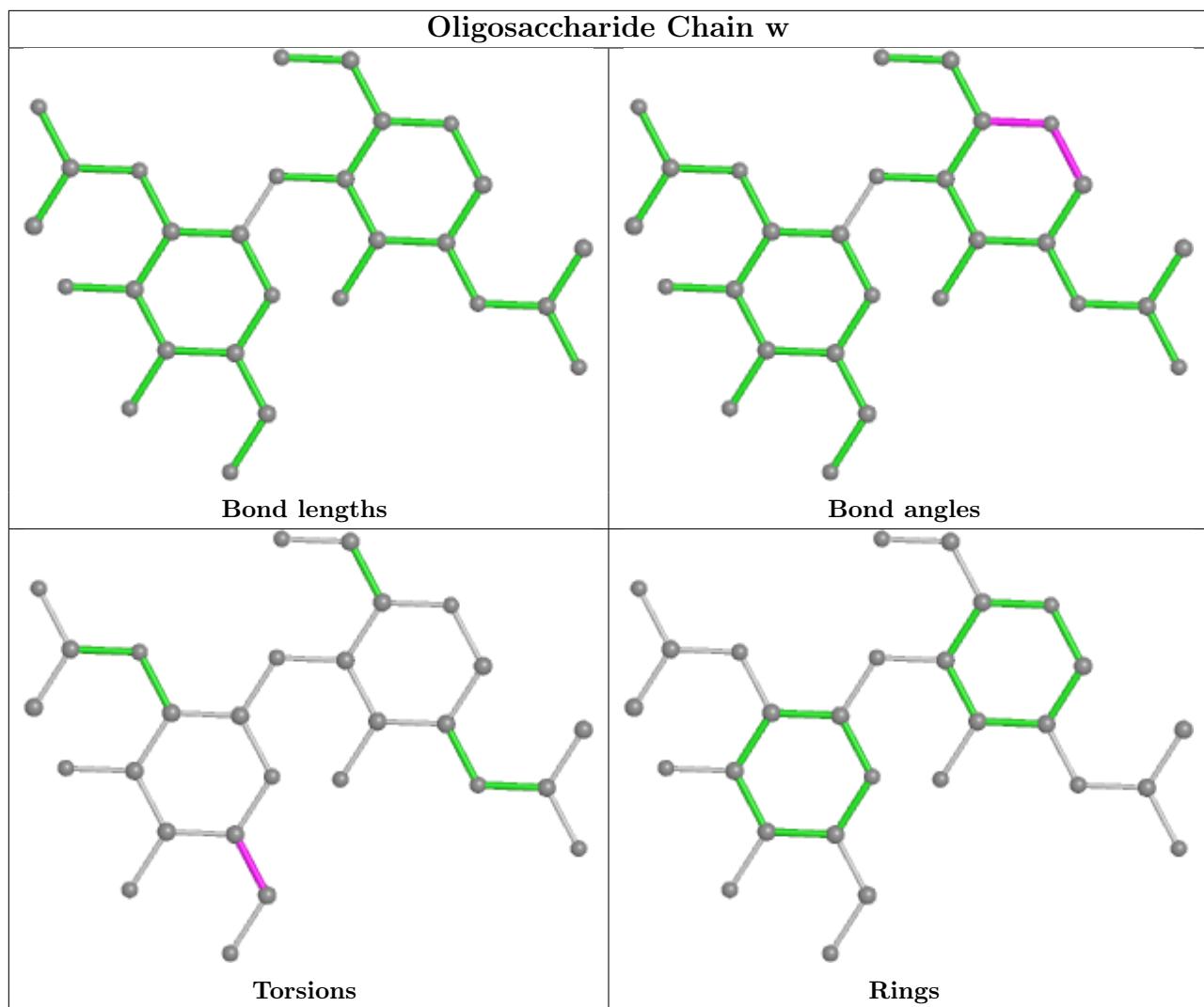


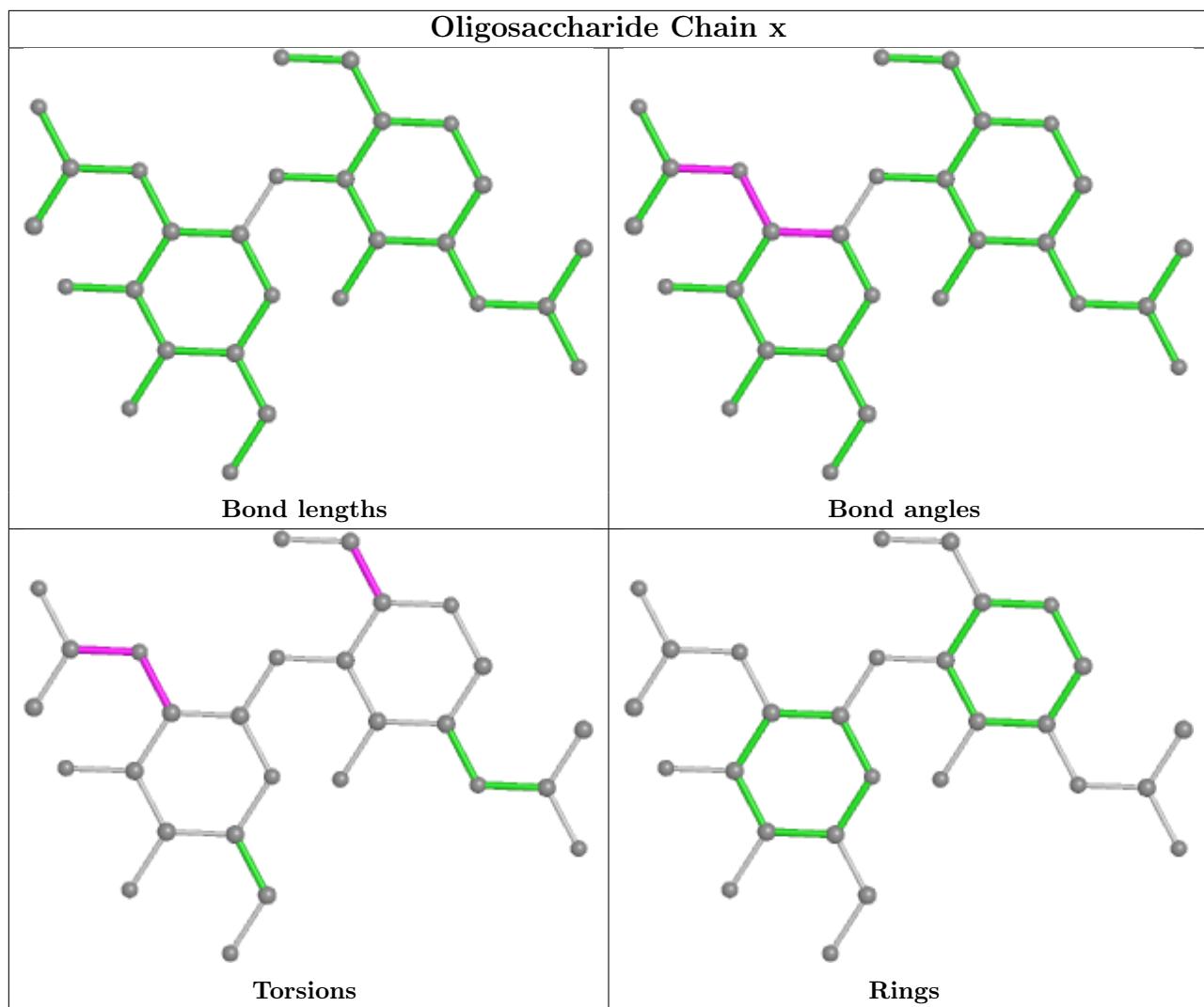


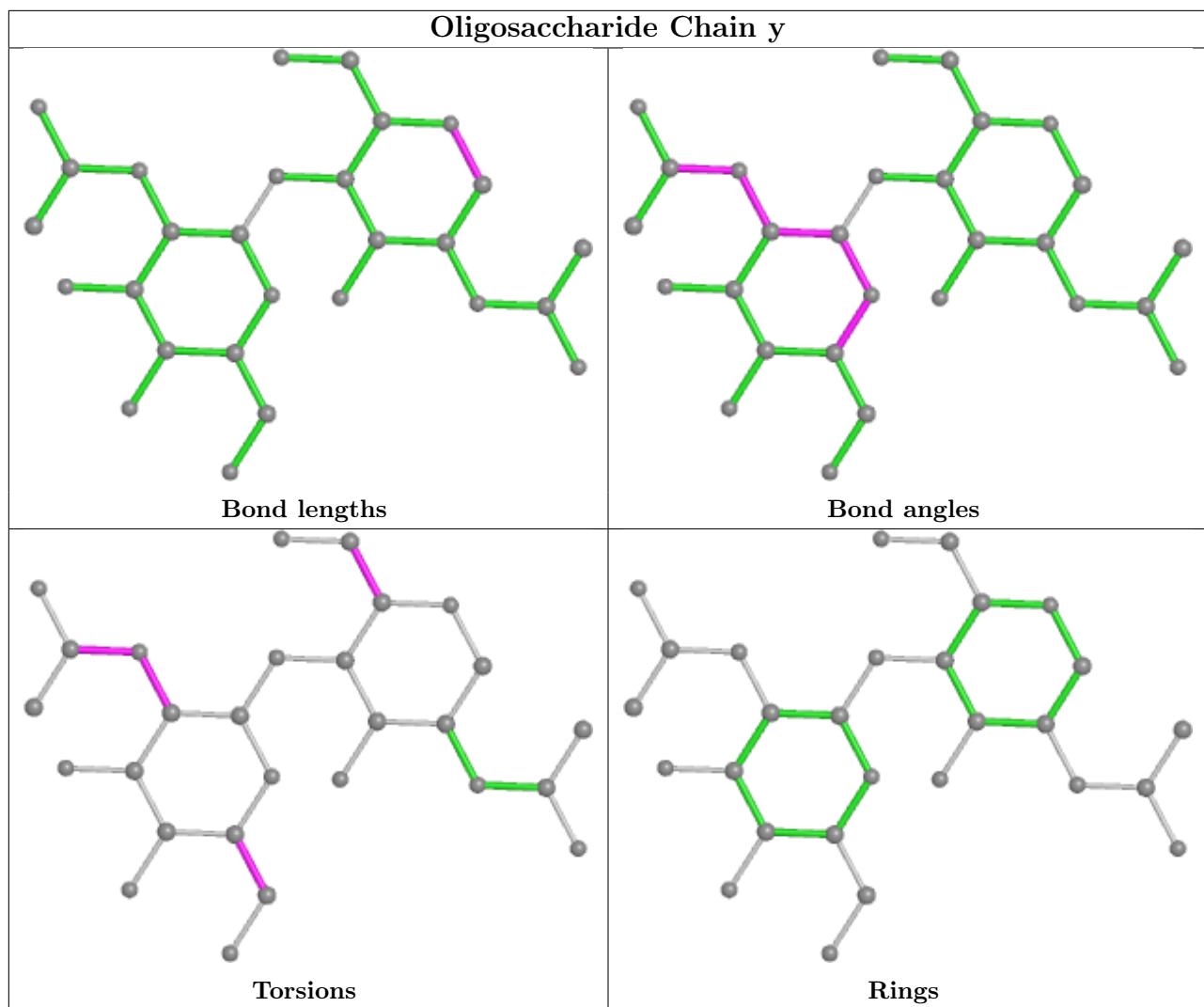


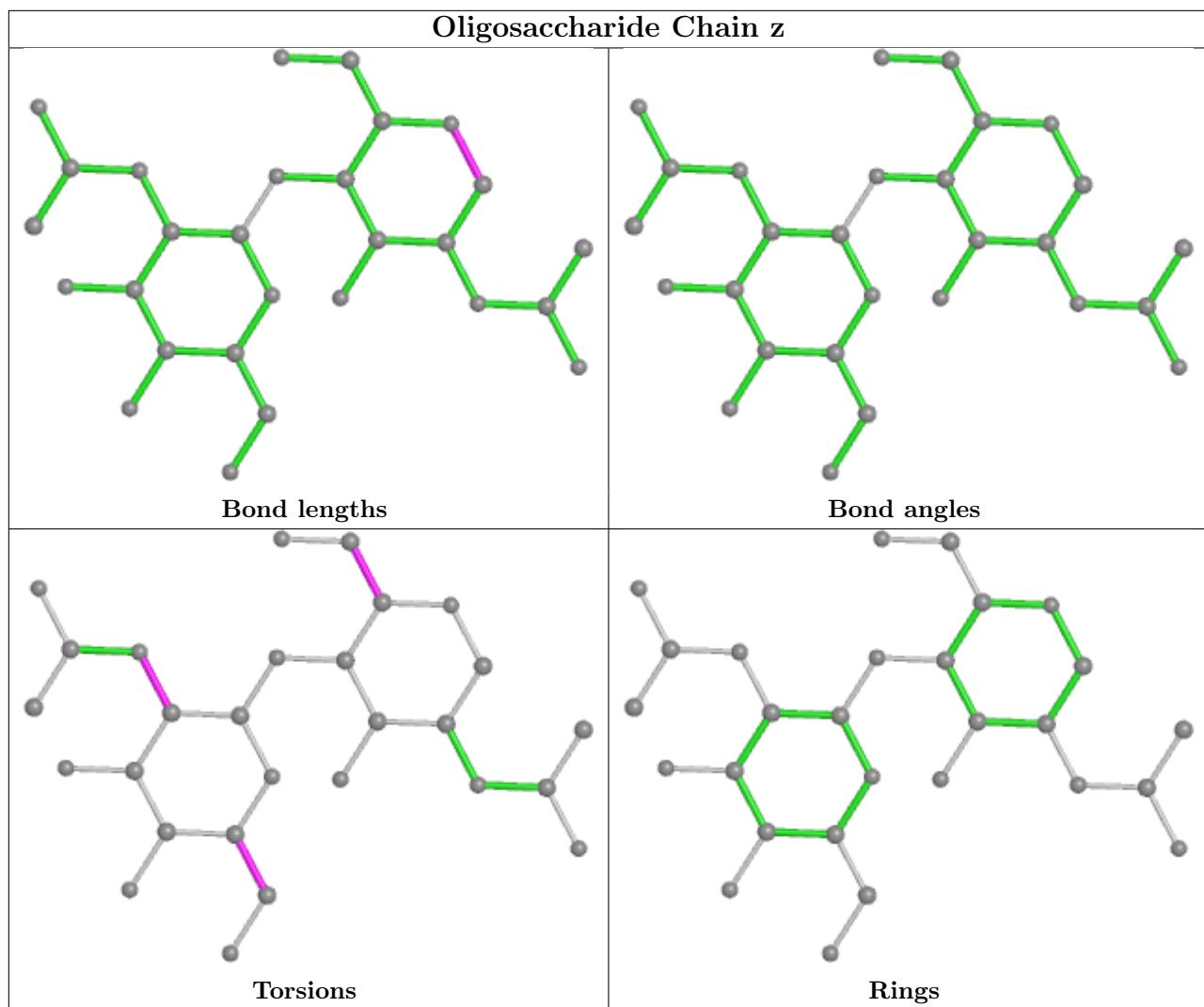


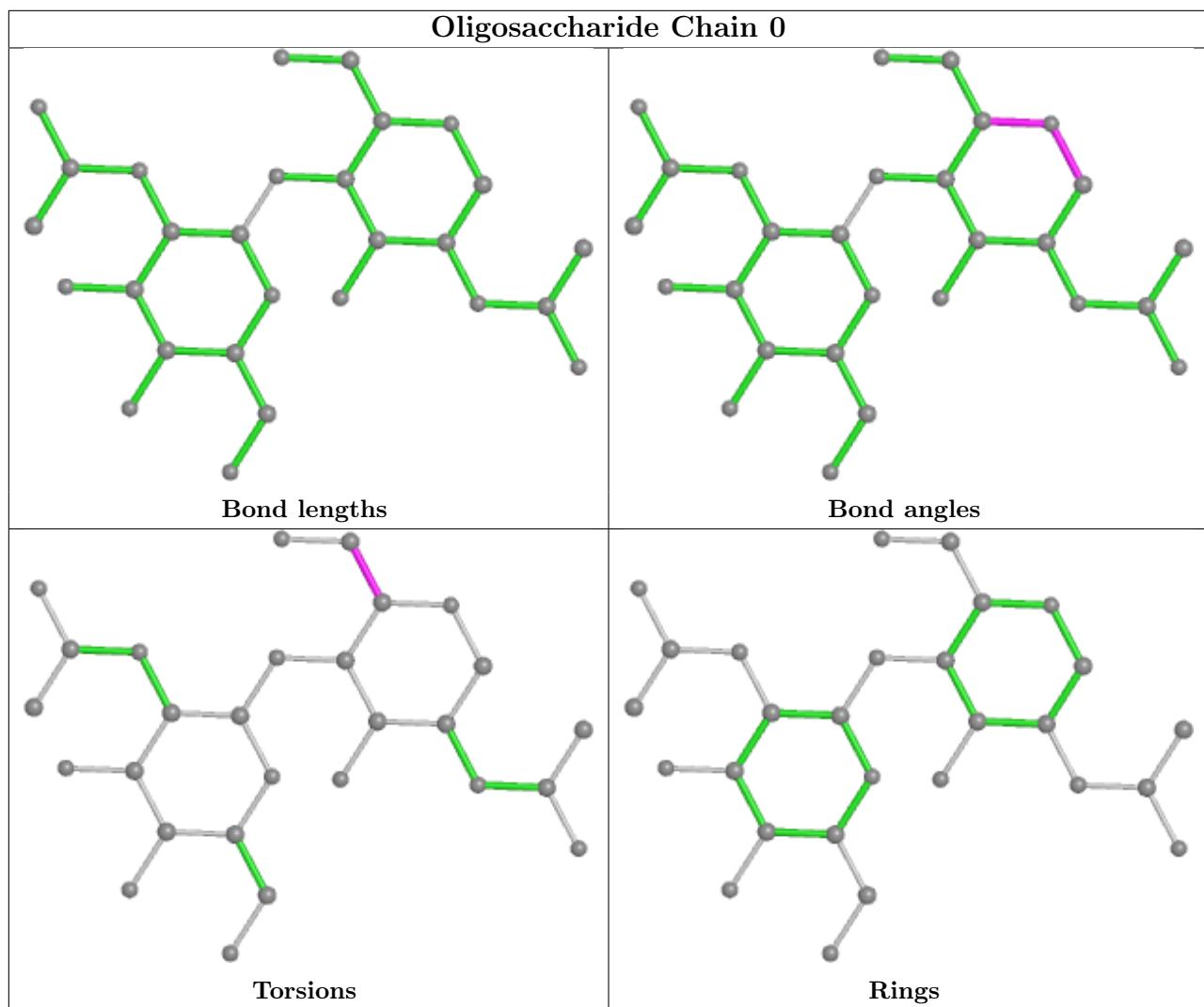


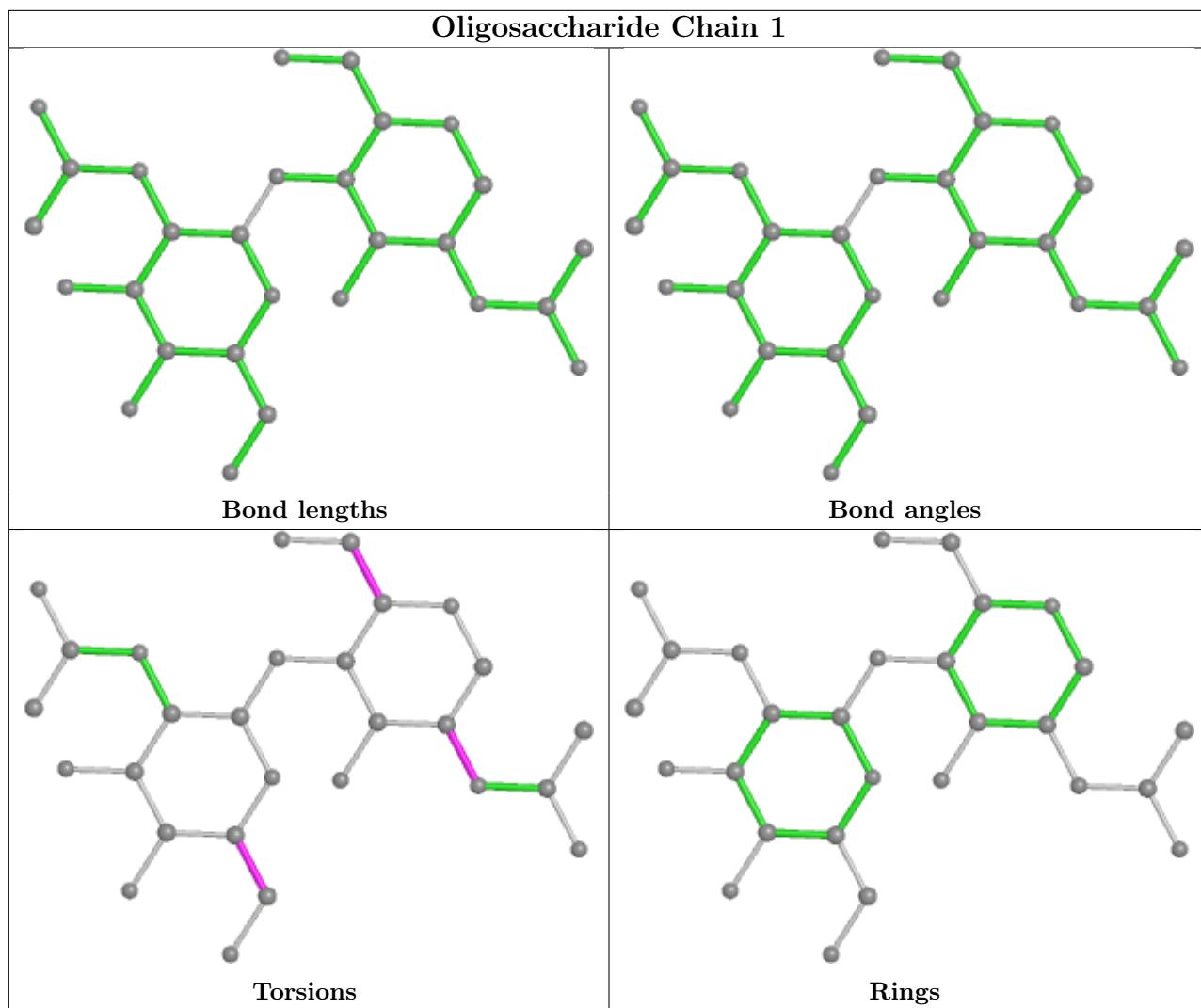


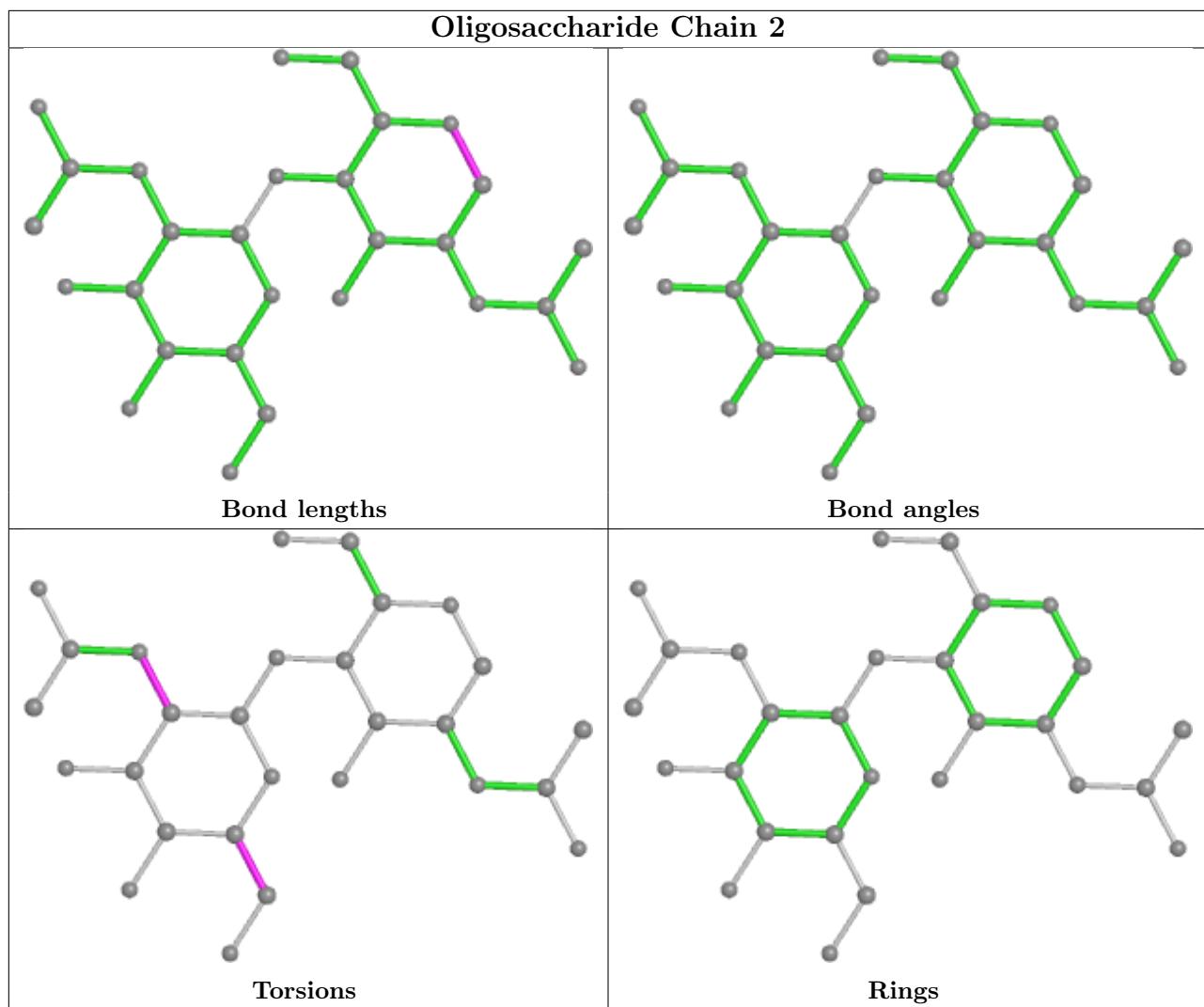


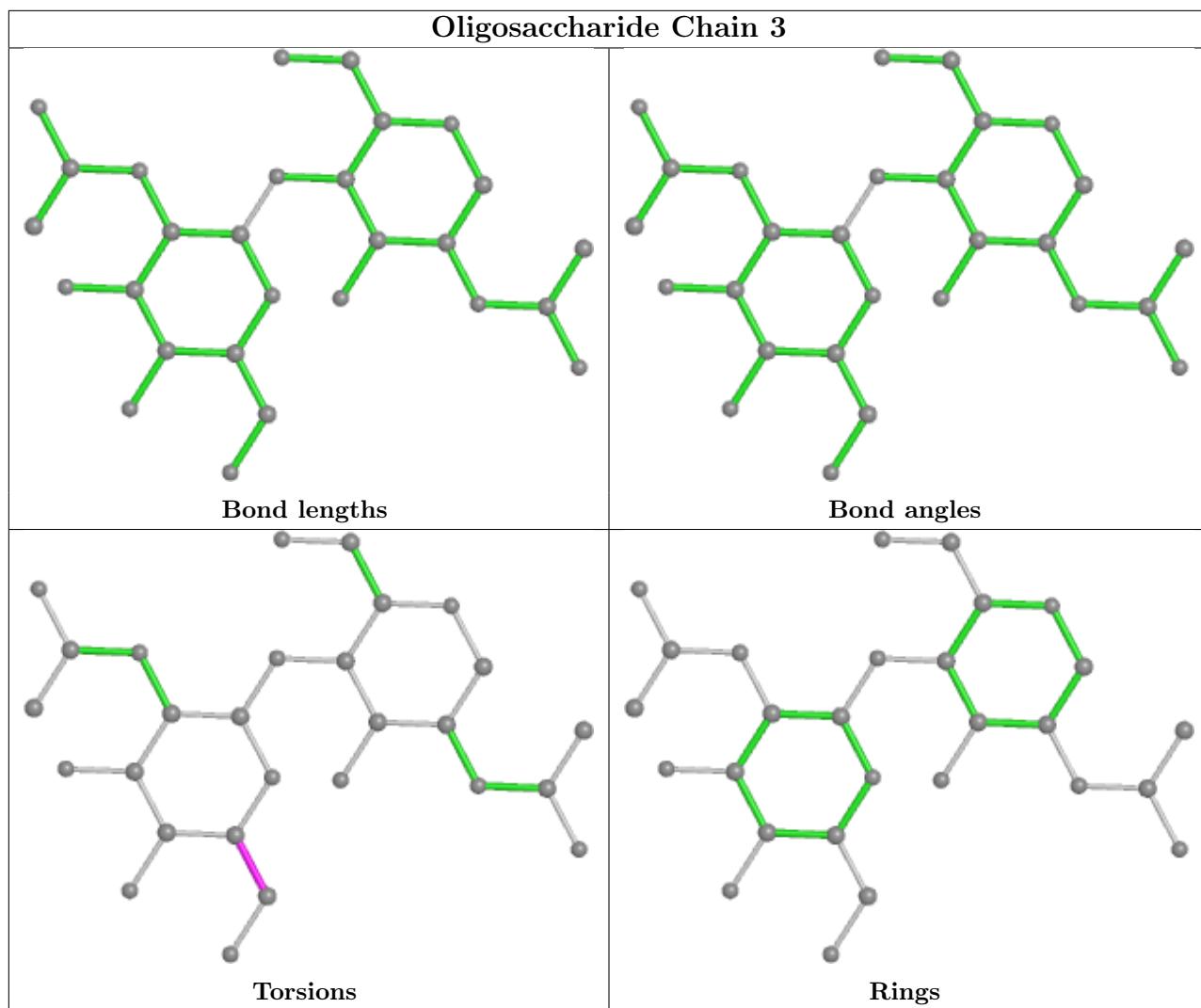


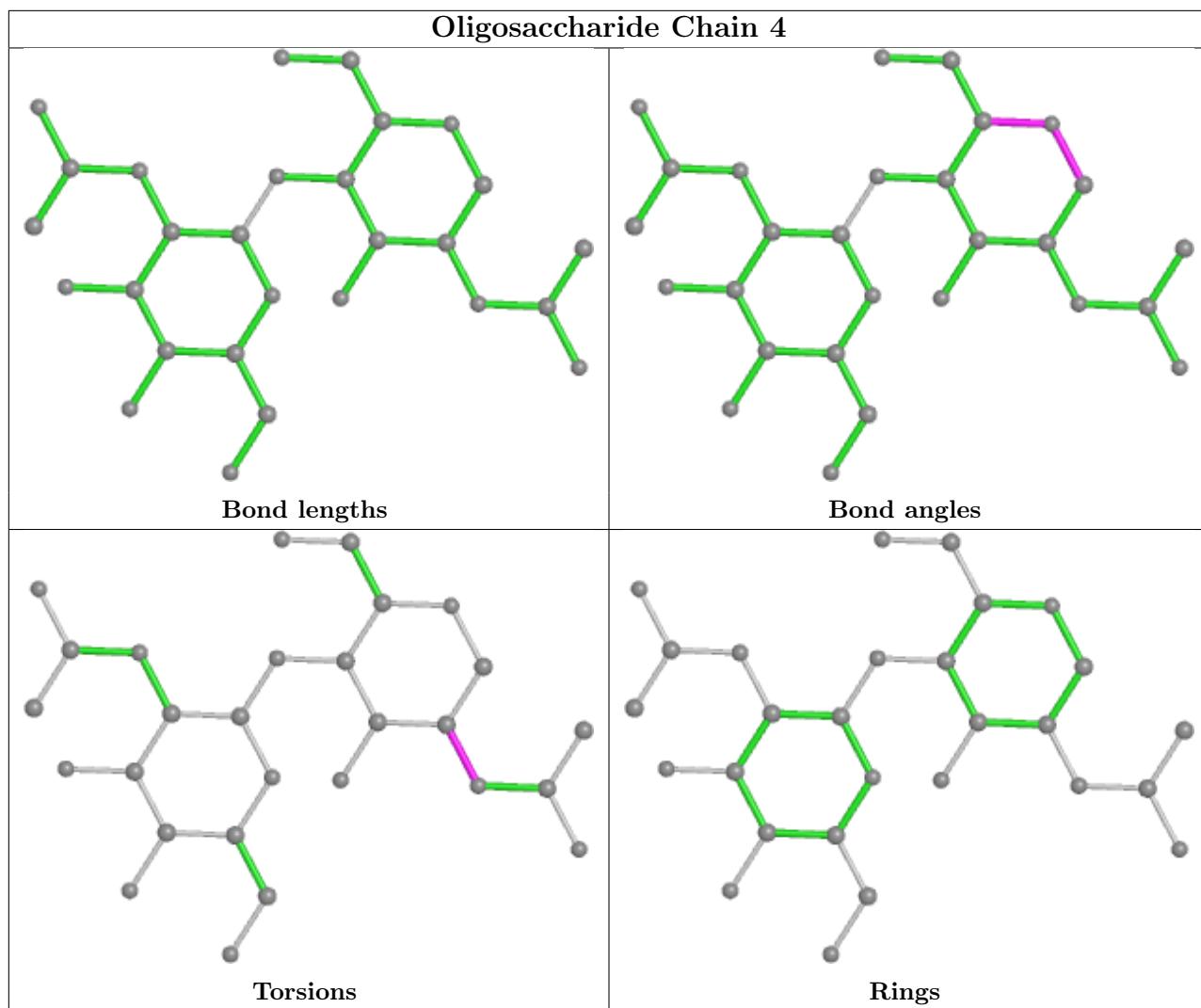


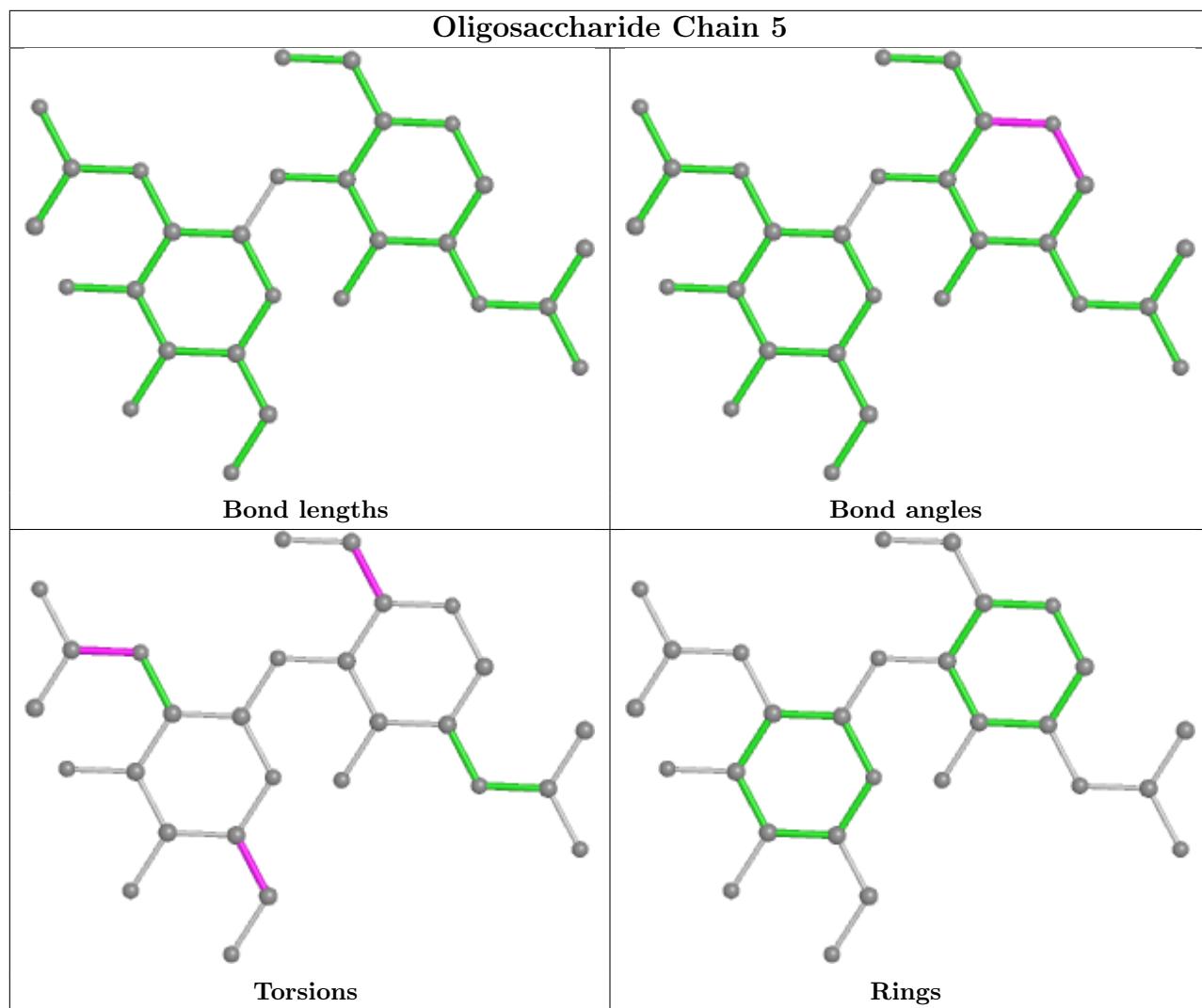


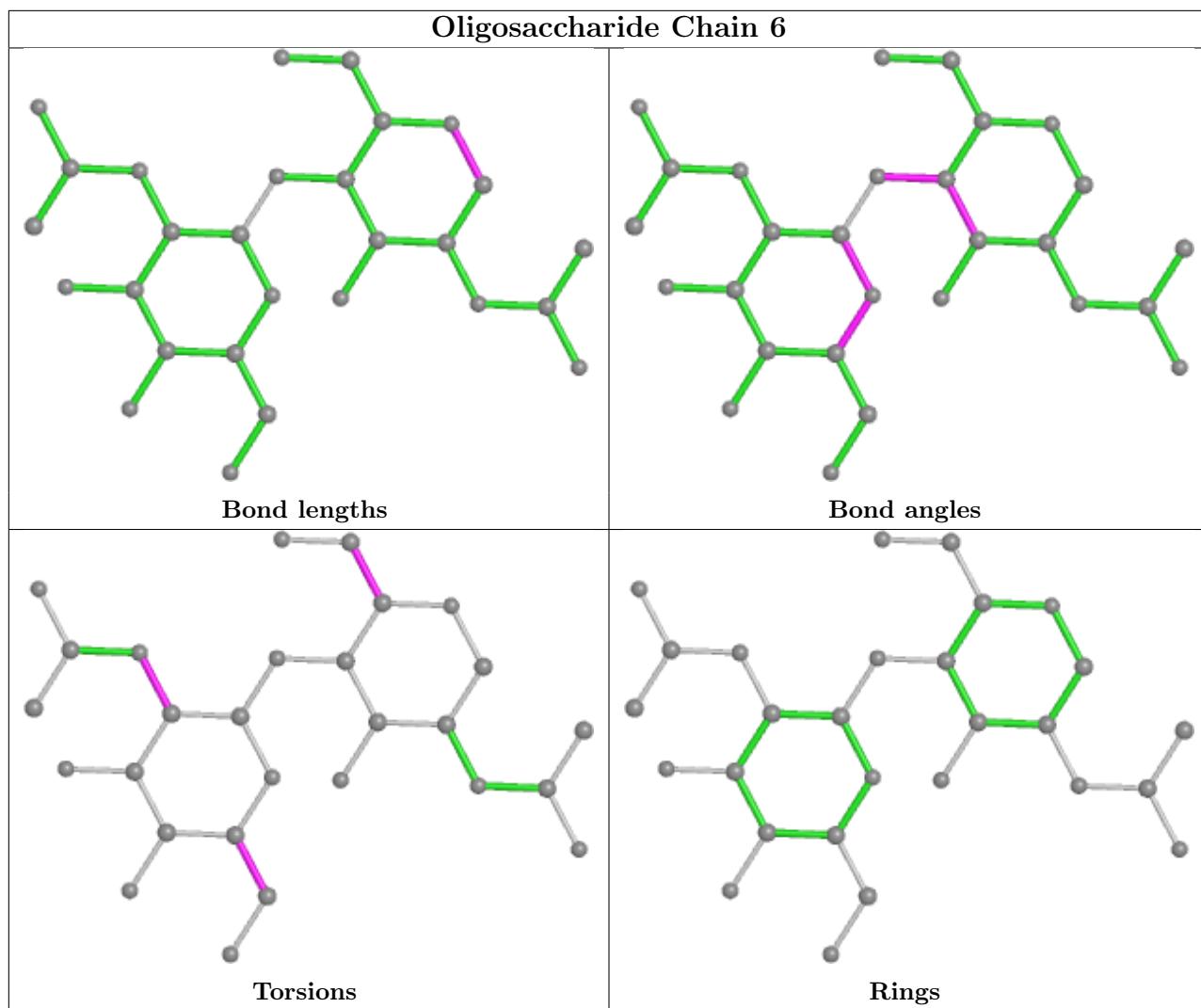


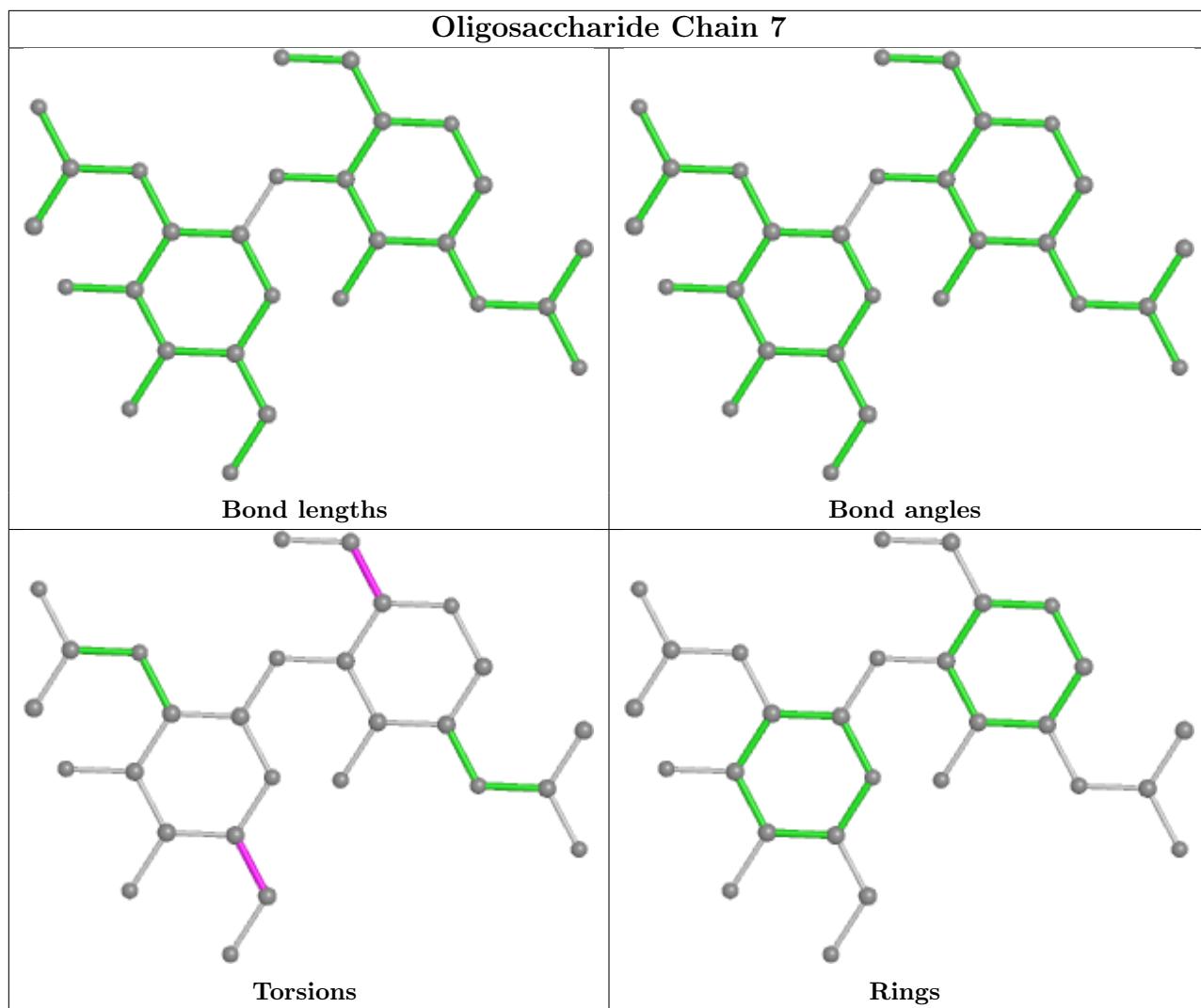


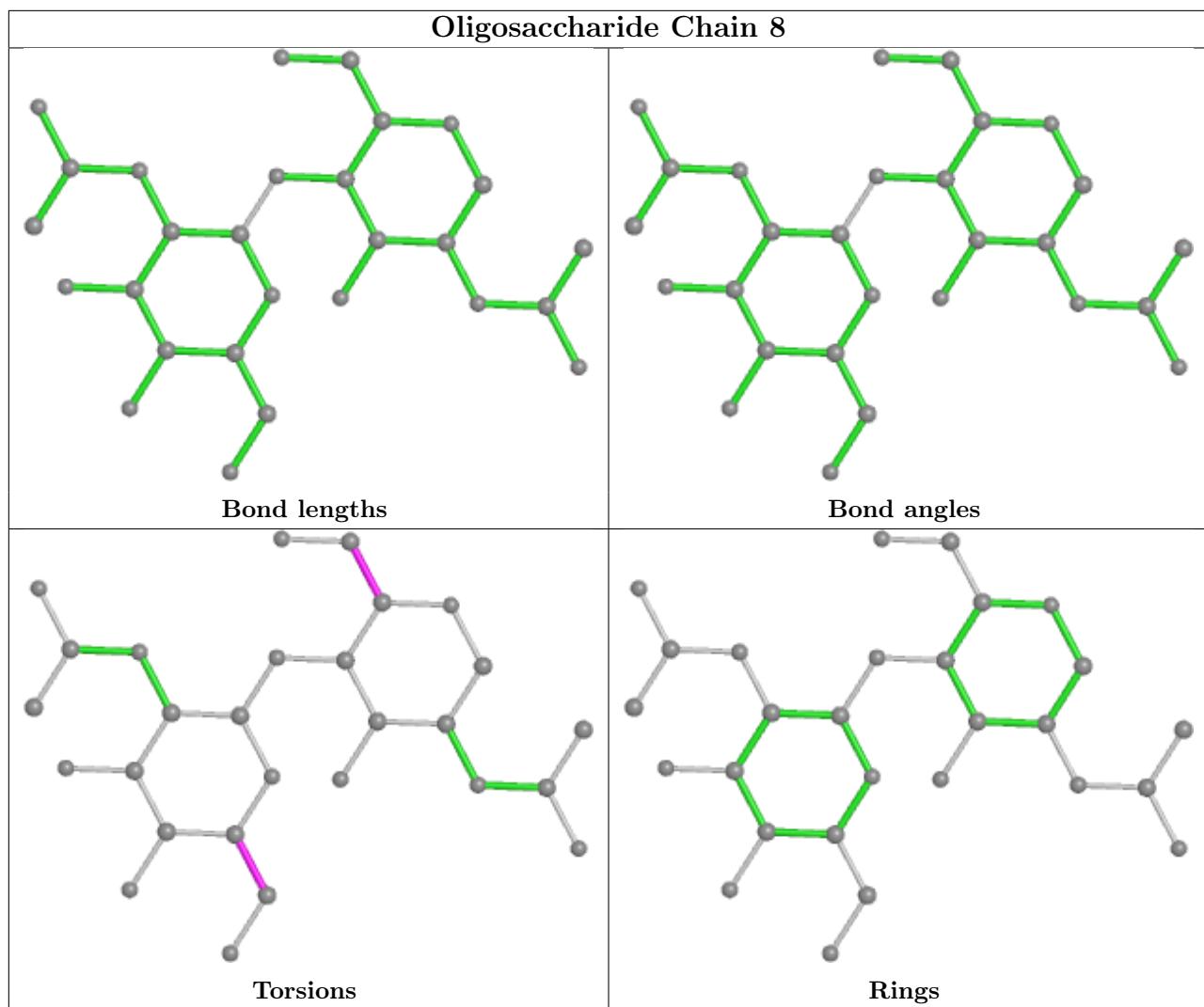


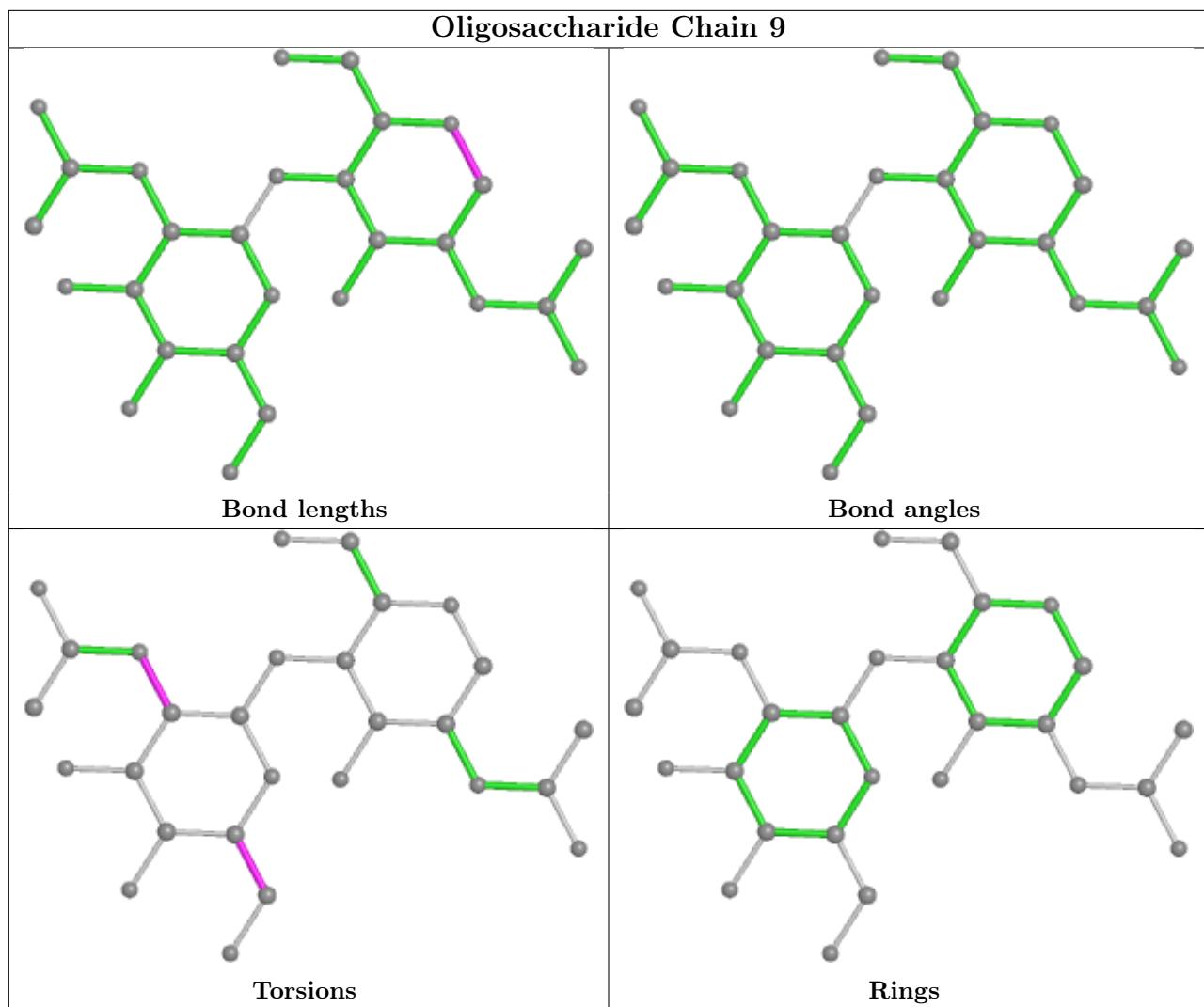


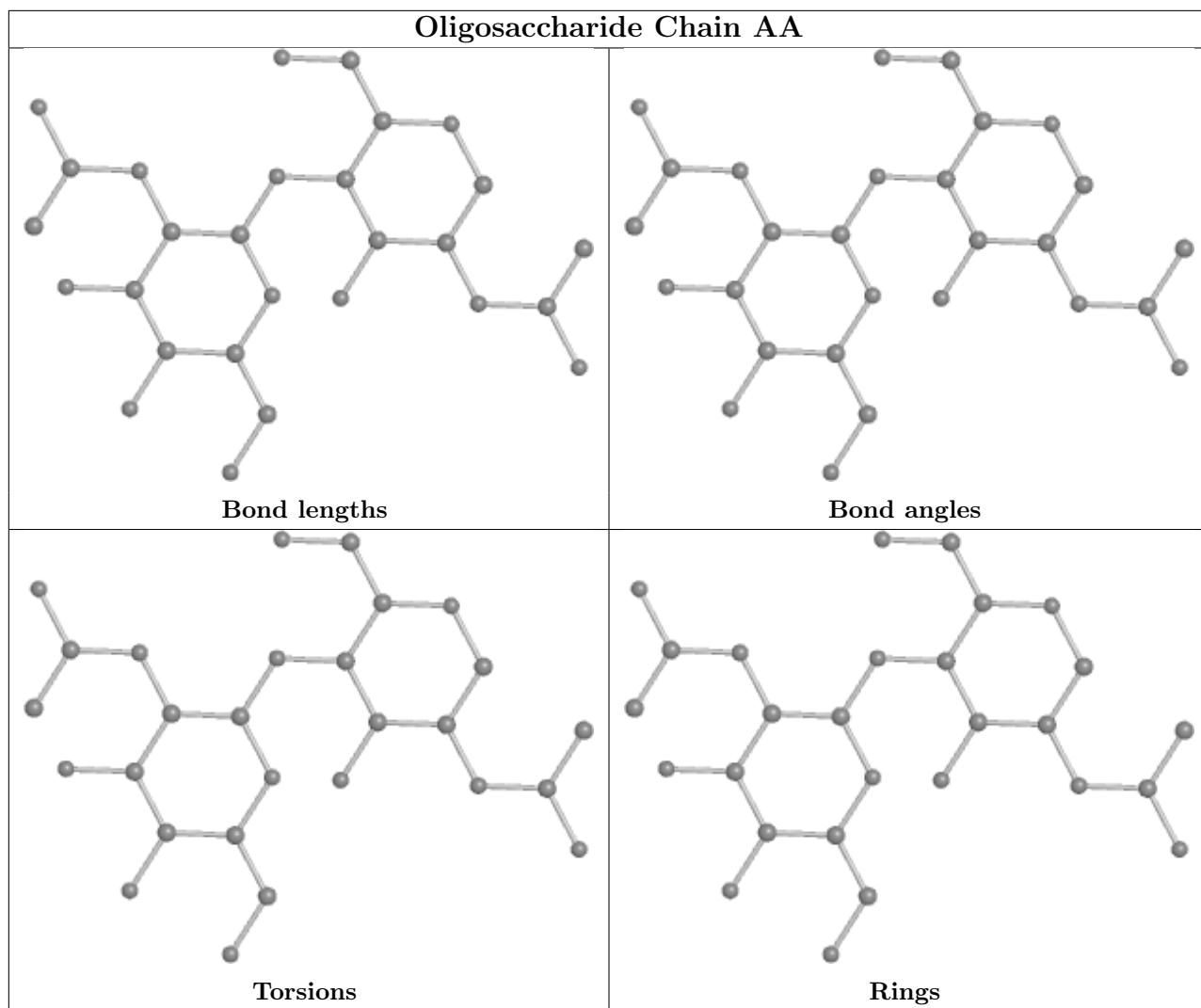


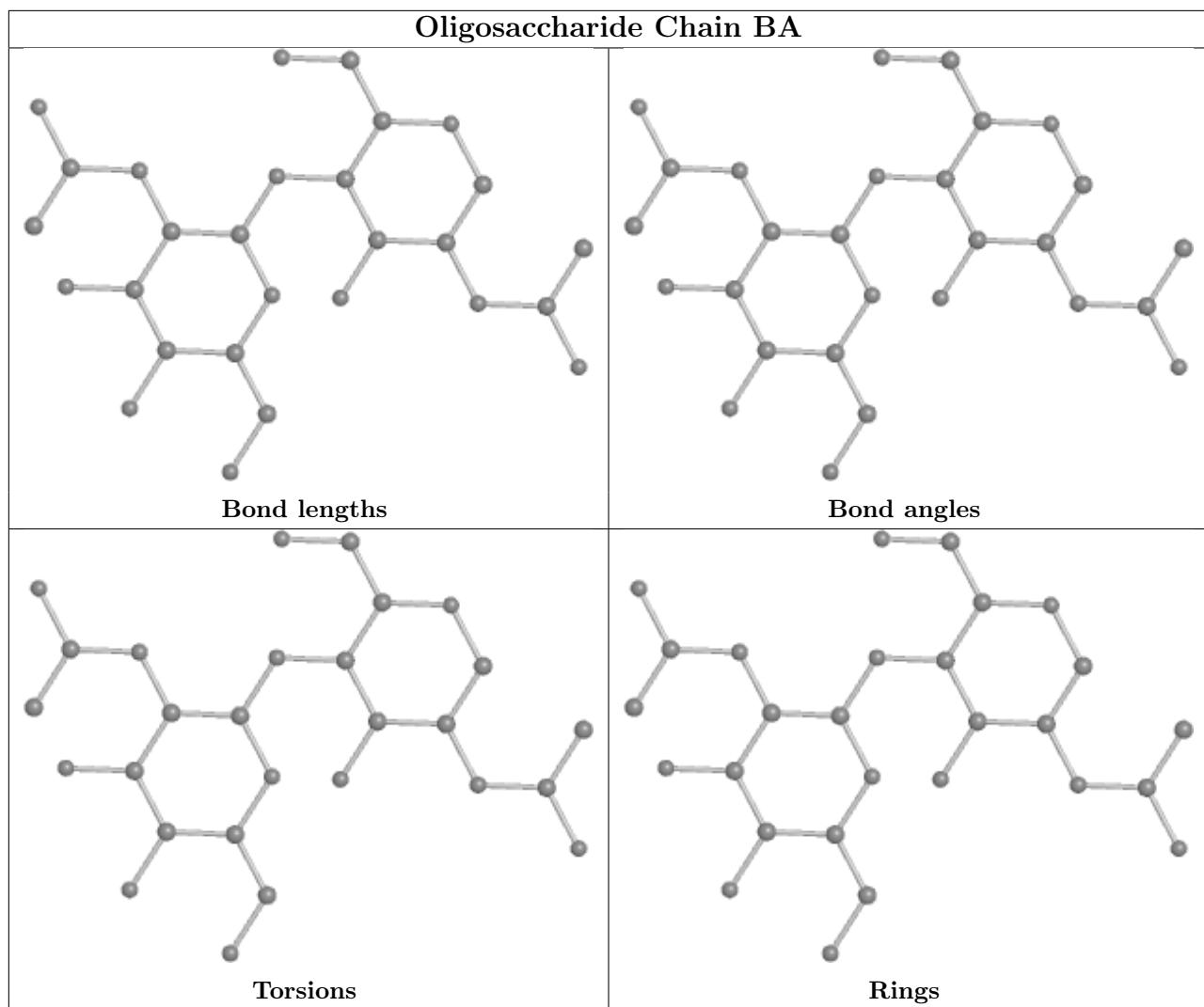


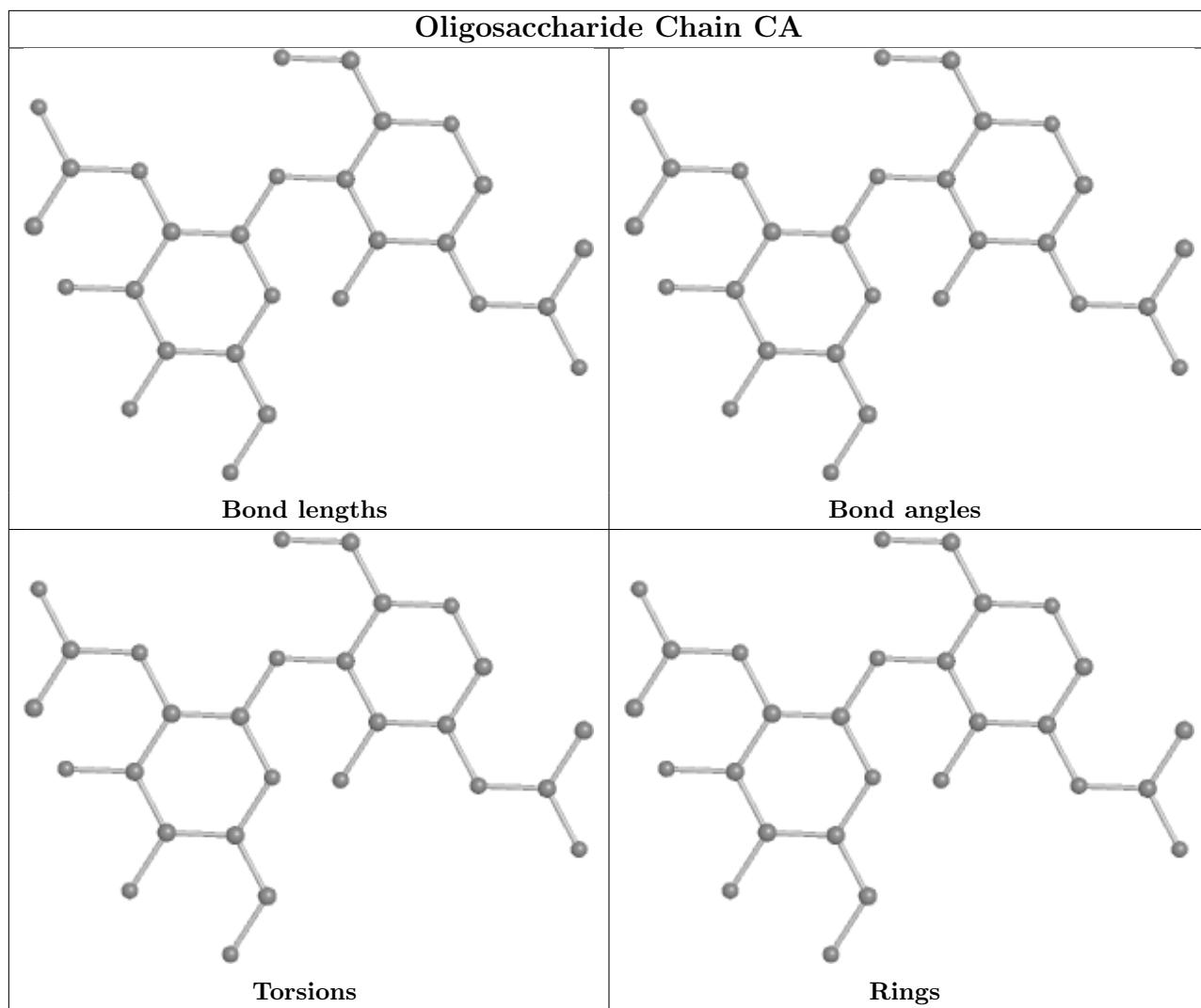


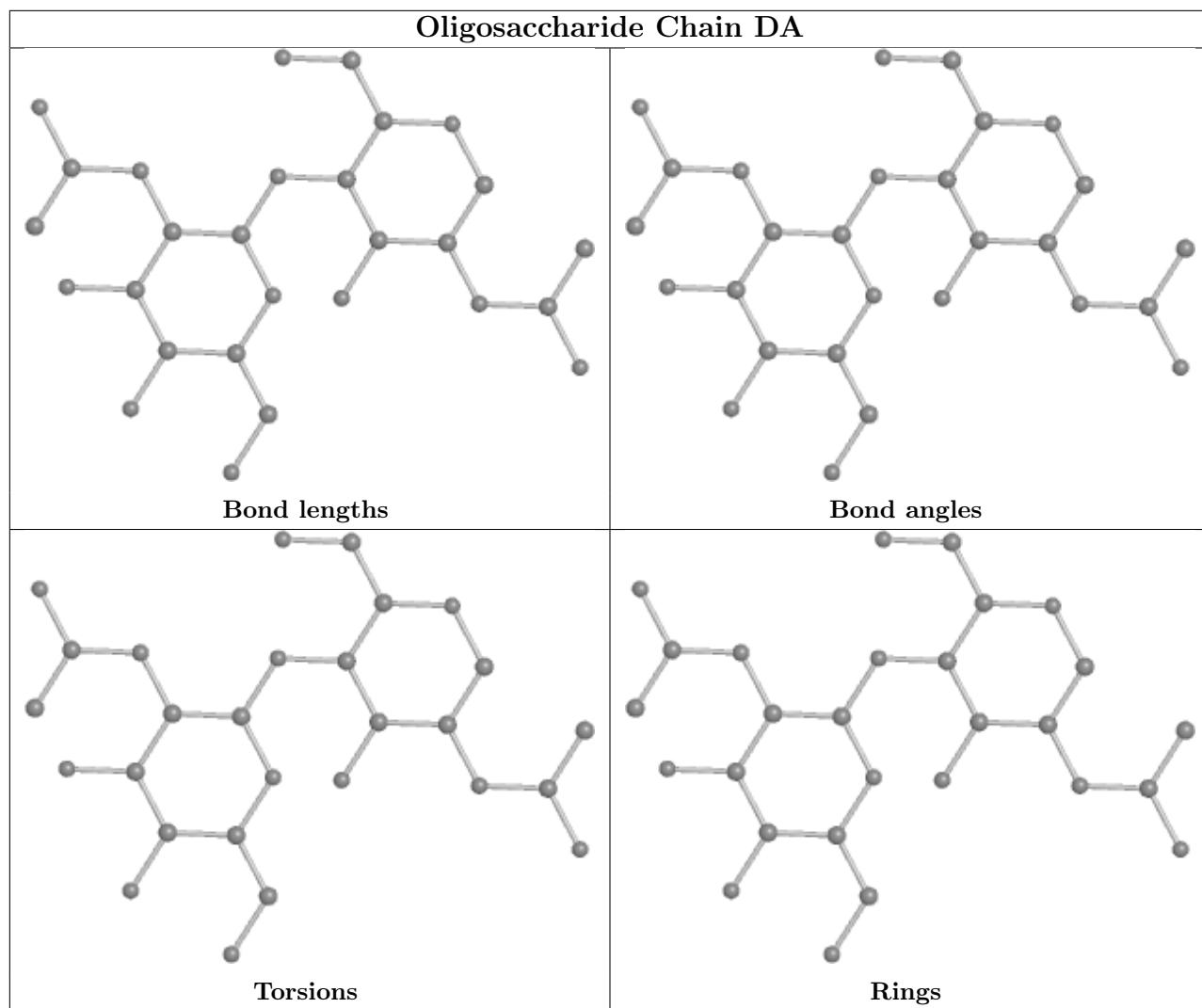


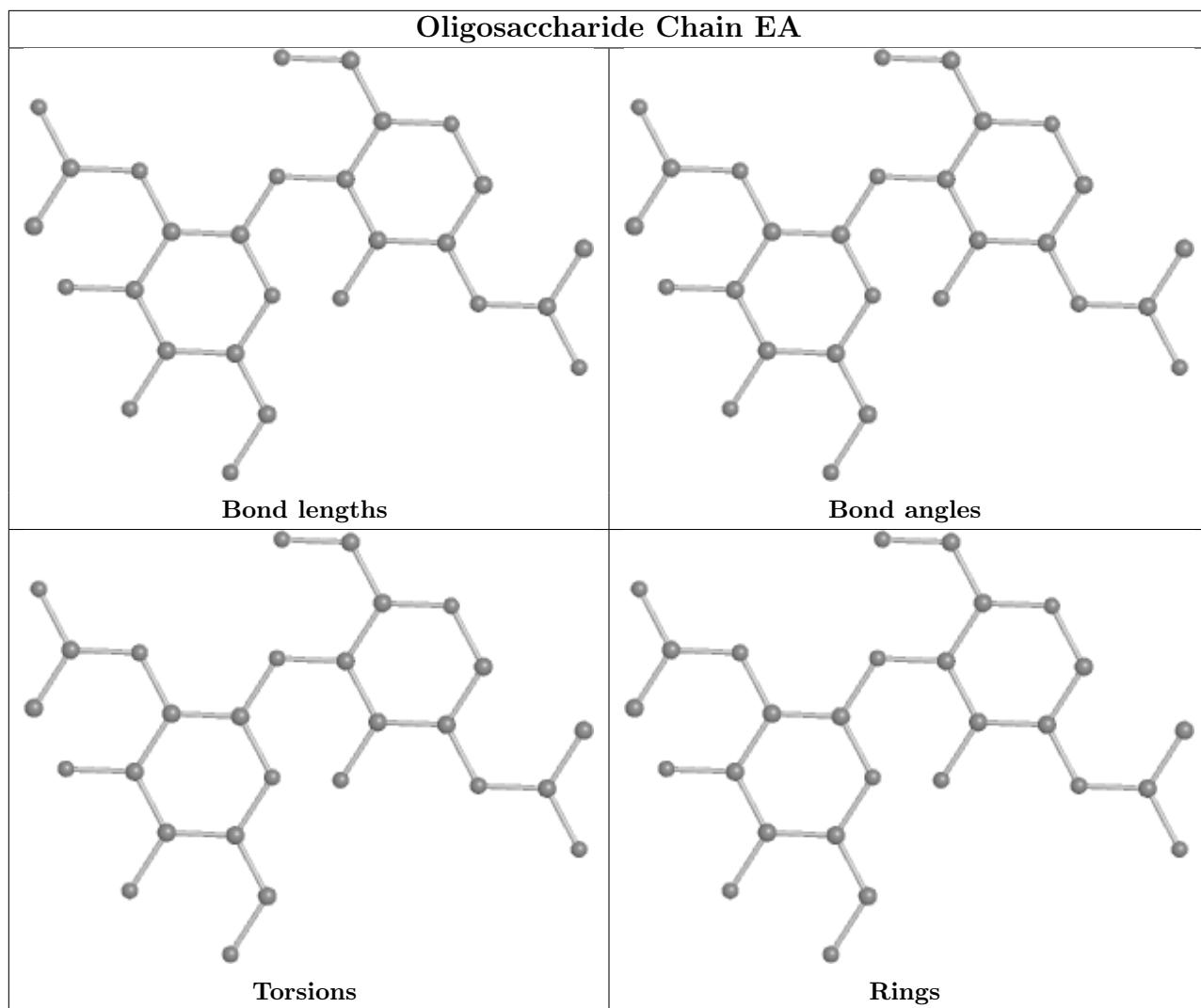


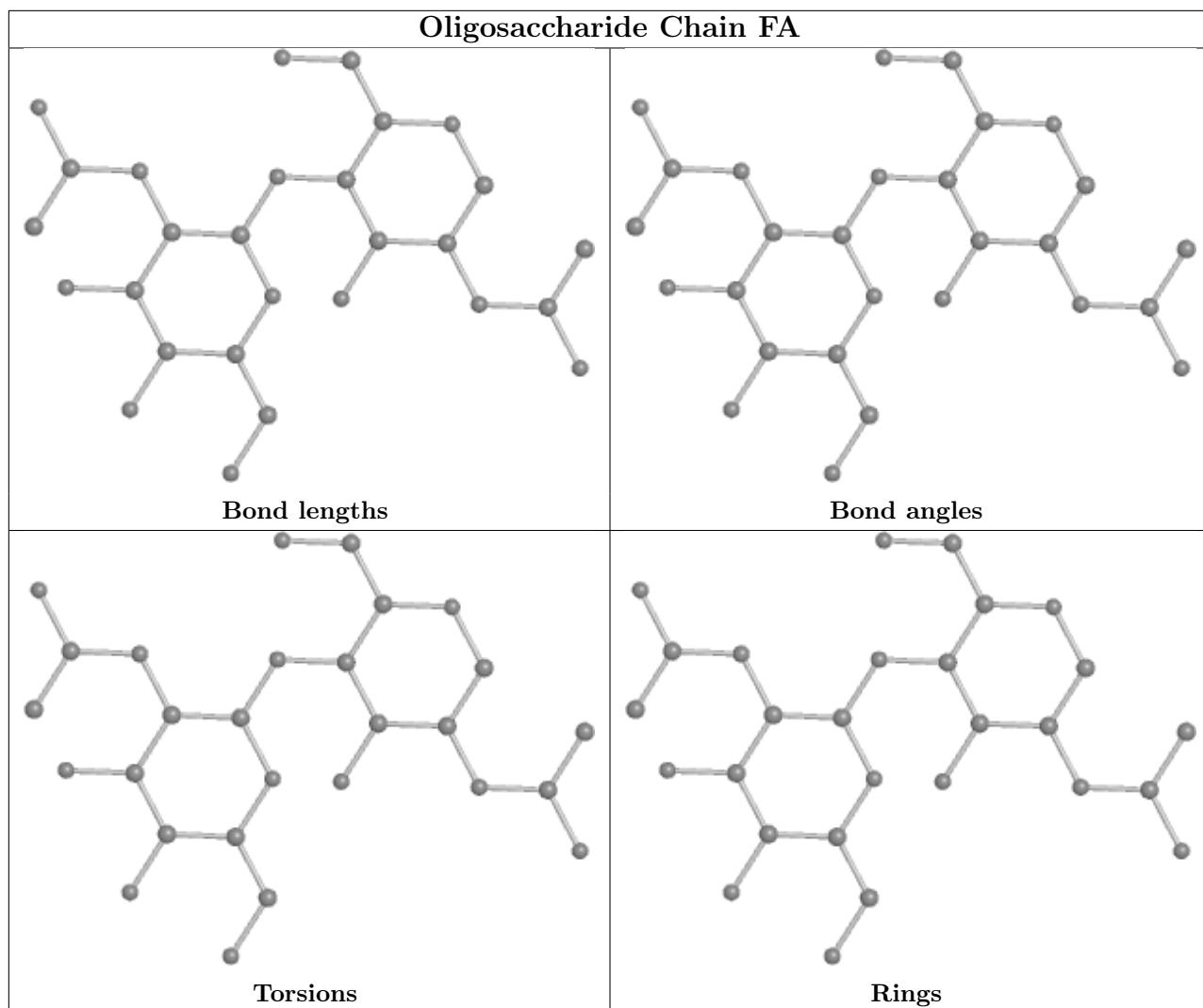












## 5.6 Ligand geometry (i)

Of 68 ligands modelled in this entry, 2 are monoatomic - leaving 66 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
5	NAG	I	1405	3	14,14,15	0.57	0	17,19,21	1.27	1 (5%)
5	NAG	F	1410	-	14,14,15	0.37	0	17,19,21	0.42	0
5	NAG	I	1402	3	14,14,15	0.21	0	17,19,21	0.63	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	J	1403	3	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	E	1401	3	14,14,15	0.30	0	17,19,21	0.34	0
5	NAG	C	703	1	14,14,15	0.39	0	17,19,21	0.64	0
5	NAG	E	1409	3	14,14,15	0.49	0	17,19,21	0.36	0
5	NAG	G	1404	3	14,14,15	0.47	0	17,19,21	0.53	0
5	NAG	G	1401	3	14,14,15	0.29	0	17,19,21	0.33	0
6	LEU	C	705	-	7,8,8	0.91	1 (14%)	9,10,10	1.19	2 (22%)
5	NAG	D	901	2	14,14,15	0.39	0	17,19,21	0.59	1 (5%)
5	NAG	I	1410	-	14,14,15	0.36	0	17,19,21	0.42	0
5	NAG	E	1405	3	14,14,15	0.57	0	17,19,21	1.27	1 (5%)
5	NAG	F	1407	3	14,14,15	0.25	0	17,19,21	0.50	0
5	NAG	J	1408	3	14,14,15	0.32	0	17,19,21	0.39	0
5	NAG	F	1404	3	14,14,15	0.48	0	17,19,21	0.54	0
5	NAG	J	1407	3	14,14,15	0.23	0	17,19,21	0.49	0
5	NAG	A	704	1	14,14,15	0.38	0	17,19,21	0.55	0
5	NAG	I	1403	3	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	F	1402	3	14,14,15	0.21	0	17,19,21	0.63	0
5	NAG	I	1409	3	14,14,15	0.42	0	17,19,21	1.15	2 (11%)
5	NAG	H	1409	3	14,14,15	0.50	0	17,19,21	0.36	0
5	NAG	A	703	1	14,14,15	0.40	0	17,19,21	0.65	1 (5%)
5	NAG	C	704	1	14,14,15	0.37	0	17,19,21	0.55	0
5	NAG	F	1408	3	14,14,15	0.31	0	17,19,21	0.39	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
5	NAG	I	1405	3	-	5/6/23/26	0/1/1/1
5	NAG	F	1410	-	-	0/6/23/26	0/1/1/1
5	NAG	I	1402	3	-	2/6/23/26	0/1/1/1
5	NAG	F	1409	3	-	0/6/23/26	0/1/1/1
5	NAG	J	1406	3	-	2/6/23/26	0/1/1/1
5	NAG	C	702	1	-	2/6/23/26	0/1/1/1
5	NAG	I	1408	3	-	2/6/23/26	0/1/1/1
6	LEU	A	705	-	-	1/8/8/8	-
5	NAG	G	1403	3	-	2/6/23/26	0/1/1/1
5	NAG	I	1407	3	-	1/6/23/26	0/1/1/1
5	NAG	J	1404	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	1408	3	-	2/6/23/26	0/1/1/1
5	NAG	F	1405	3	-	5/6/23/26	0/1/1/1
5	NAG	B	901	2	-	2/6/23/26	0/1/1/1
5	NAG	G	1402	3	-	2/6/23/26	0/1/1/1
5	NAG	H	1404	3	-	2/6/23/26	0/1/1/1
5	NAG	H	1403	3	-	2/6/23/26	0/1/1/1
5	NAG	I	1404	3	-	2/6/23/26	0/1/1/1
5	NAG	J	1401	3	-	2/6/23/26	0/1/1/1
5	NAG	E	1402	3	-	2/6/23/26	0/1/1/1
5	NAG	E	1403	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1408	3	-	2/6/23/26	0/1/1/1
5	NAG	A	701	1	-	2/6/23/26	0/1/1/1
5	NAG	F	1406	3	-	2/6/23/26	0/1/1/1
5	NAG	E	1407	3	-	1/6/23/26	0/1/1/1
5	NAG	H	1401	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1407	3	-	1/6/23/26	0/1/1/1
5	NAG	I	1401	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1405	3	-	5/6/23/26	0/1/1/1
5	NAG	I	1406	3	-	2/6/23/26	0/1/1/1
5	NAG	J	1402	3	-	2/6/23/26	0/1/1/1
5	NAG	J	1405	3	-	5/6/23/26	0/1/1/1
5	NAG	H	1405	3	-	5/6/23/26	0/1/1/1
5	NAG	F	1401	3	-	2/6/23/26	0/1/1/1
5	NAG	F	1403	3	-	2/6/23/26	0/1/1/1
5	NAG	H	1402	3	-	2/6/23/26	0/1/1/1
5	NAG	C	701	1	-	2/6/23/26	0/1/1/1
5	NAG	H	1408	3	-	2/6/23/26	0/1/1/1
5	NAG	E	1406	3	-	2/6/23/26	0/1/1/1
5	NAG	H	1407	3	-	1/6/23/26	0/1/1/1
5	NAG	H	1406	3	-	2/6/23/26	0/1/1/1
5	NAG	A	702	1	-	2/6/23/26	0/1/1/1
5	NAG	E	1404	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1406	3	-	2/6/23/26	0/1/1/1
5	NAG	J	1403	3	-	2/6/23/26	0/1/1/1
5	NAG	E	1401	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	703	1	-	2/6/23/26	0/1/1/1
5	NAG	E	1409	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1404	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1401	3	-	2/6/23/26	0/1/1/1
6	LEU	C	705	-	-	1/8/8/8	-
5	NAG	D	901	2	-	2/6/23/26	0/1/1/1
5	NAG	I	1410	-	-	0/6/23/26	0/1/1/1
5	NAG	E	1405	3	-	5/6/23/26	0/1/1/1
5	NAG	F	1407	3	-	1/6/23/26	0/1/1/1
5	NAG	J	1408	3	-	2/6/23/26	0/1/1/1
5	NAG	F	1404	3	-	2/6/23/26	0/1/1/1
5	NAG	J	1407	3	-	1/6/23/26	0/1/1/1
5	NAG	A	704	1	-	0/6/23/26	0/1/1/1
5	NAG	I	1403	3	-	2/6/23/26	0/1/1/1
5	NAG	F	1402	3	-	2/6/23/26	0/1/1/1
5	NAG	I	1409	3	-	0/6/23/26	0/1/1/1
5	NAG	H	1409	3	-	2/6/23/26	0/1/1/1
5	NAG	A	703	1	-	2/6/23/26	0/1/1/1
5	NAG	C	704	1	-	0/6/23/26	0/1/1/1
5	NAG	F	1408	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	705	LEU	OXT-C	-2.31	1.23	1.30
6	C	705	LEU	OXT-C	-2.28	1.23	1.30

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1405	NAG	C2-N2-C7	4.35	129.09	122.90
5	I	1405	NAG	C2-N2-C7	4.34	129.08	122.90
5	H	1405	NAG	C2-N2-C7	4.33	129.07	122.90
5	G	1405	NAG	C2-N2-C7	4.31	129.05	122.90
5	F	1405	NAG	C2-N2-C7	4.31	129.04	122.90

There are no chirality outliers.

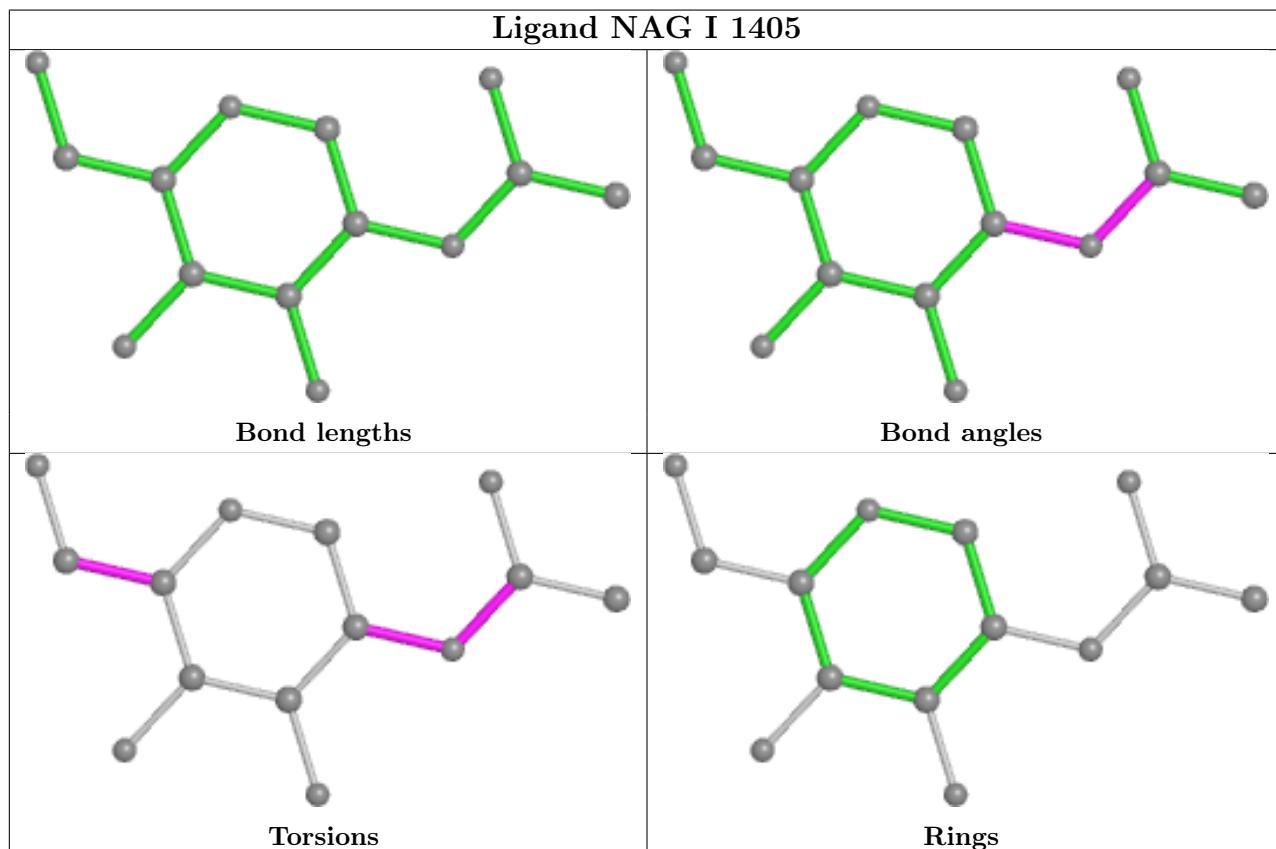
5 of 130 torsion outliers are listed below:

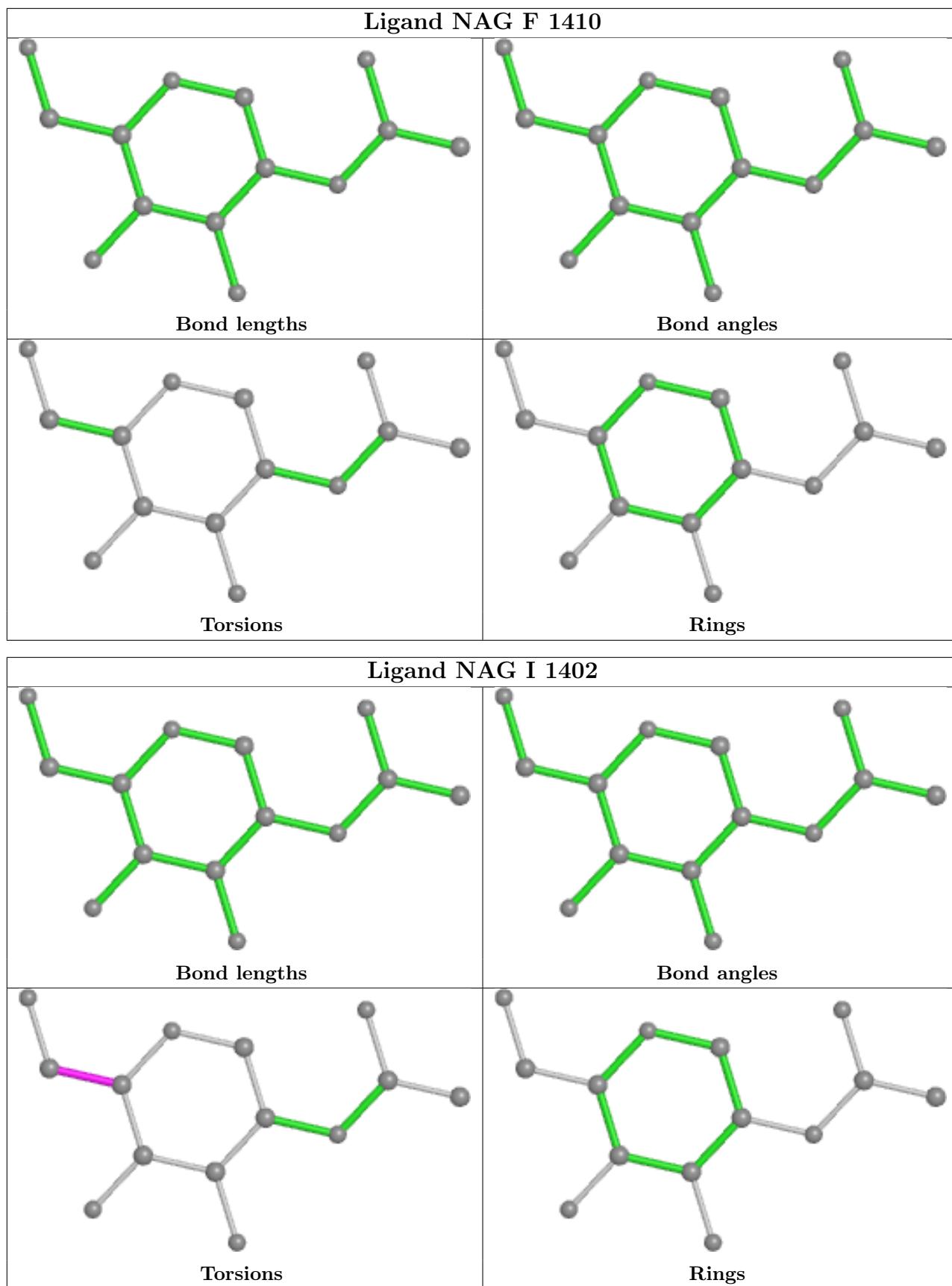
Mol	Chain	Res	Type	Atoms
6	A	705	LEU	N-CA-CB-CG
6	C	705	LEU	N-CA-CB-CG
5	A	701	NAG	O5-C5-C6-O6
5	C	701	NAG	O5-C5-C6-O6
5	A	701	NAG	C4-C5-C6-O6

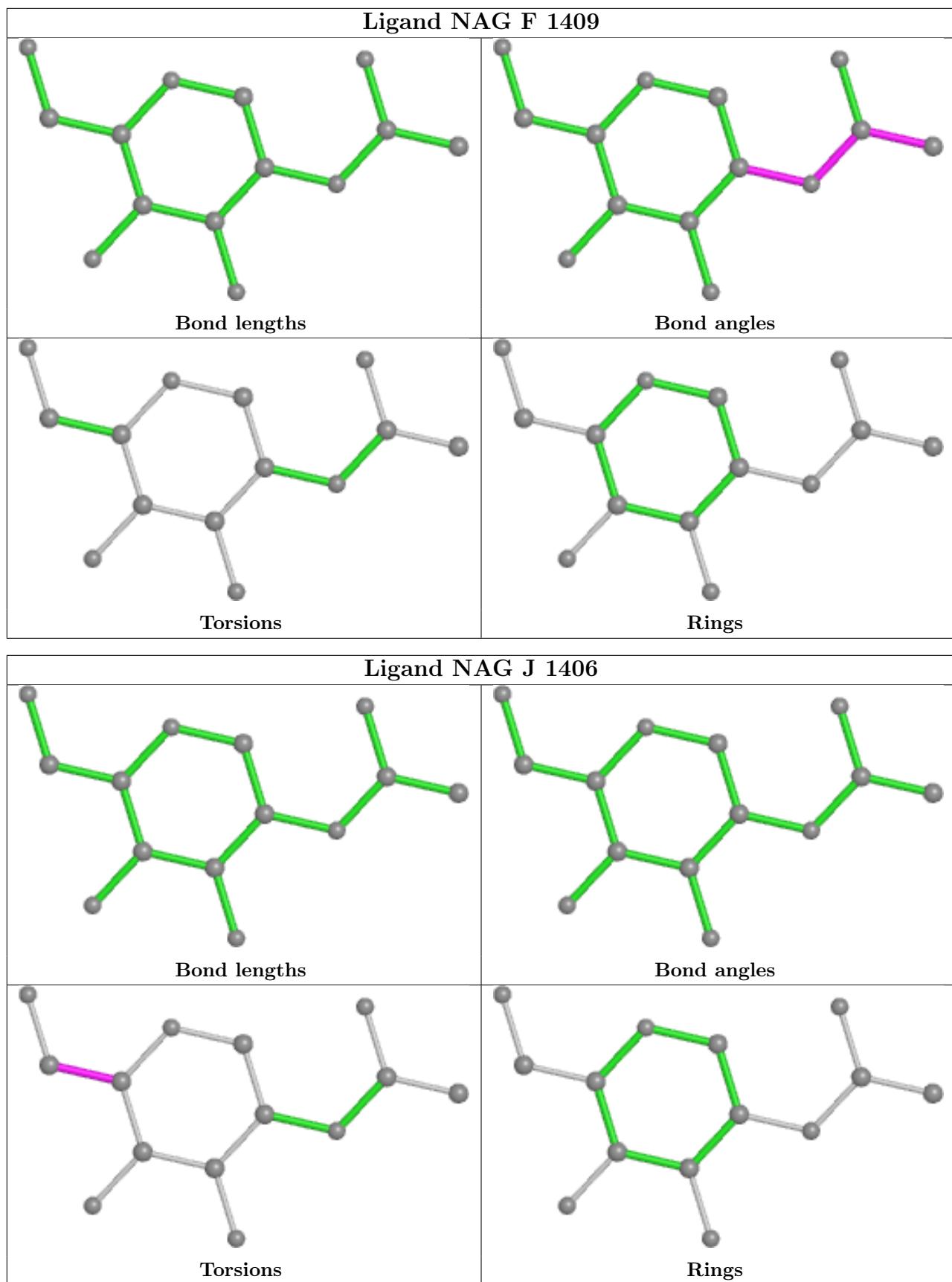
There are no ring outliers.

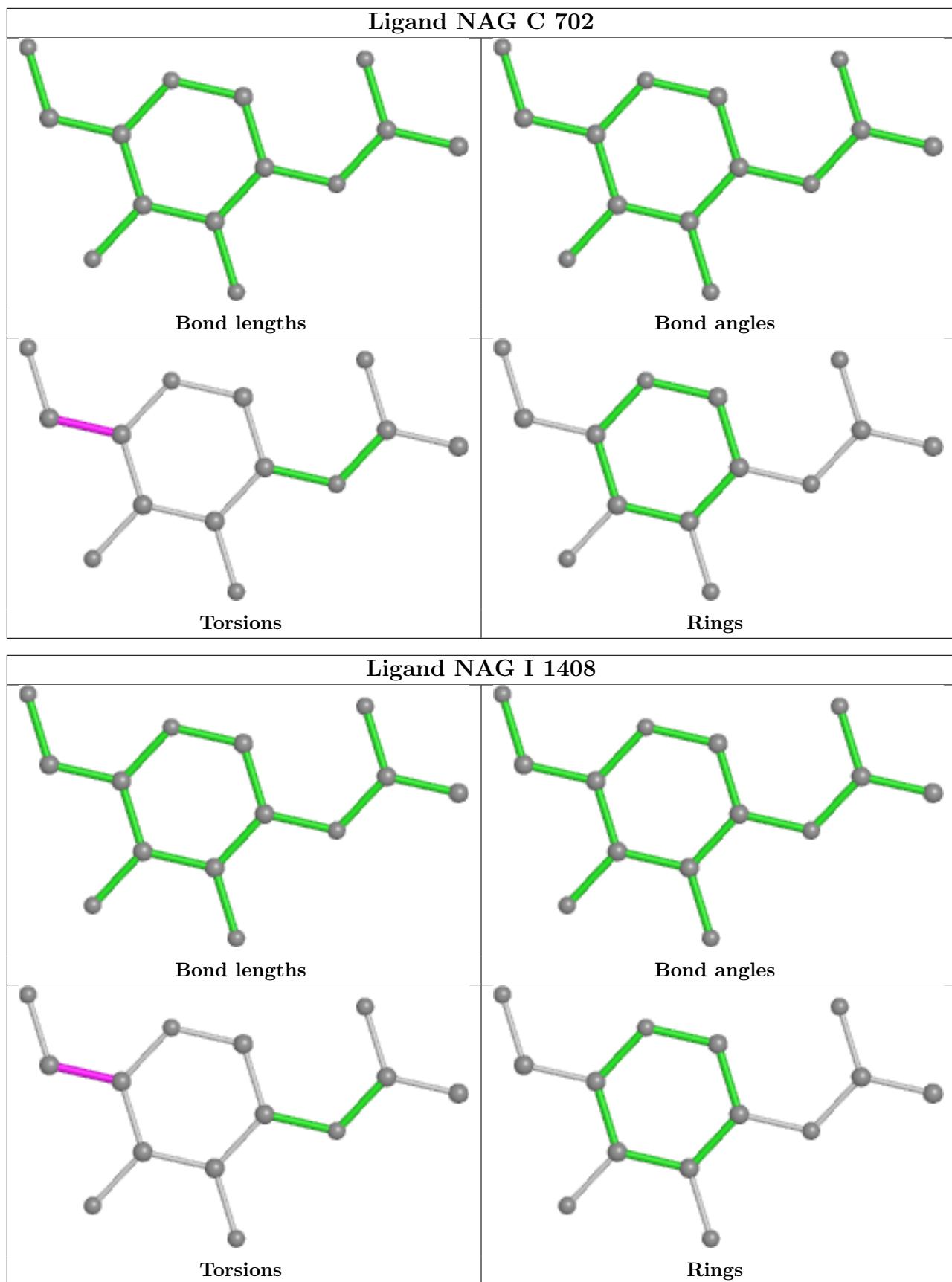
No monomer is involved in short contacts.

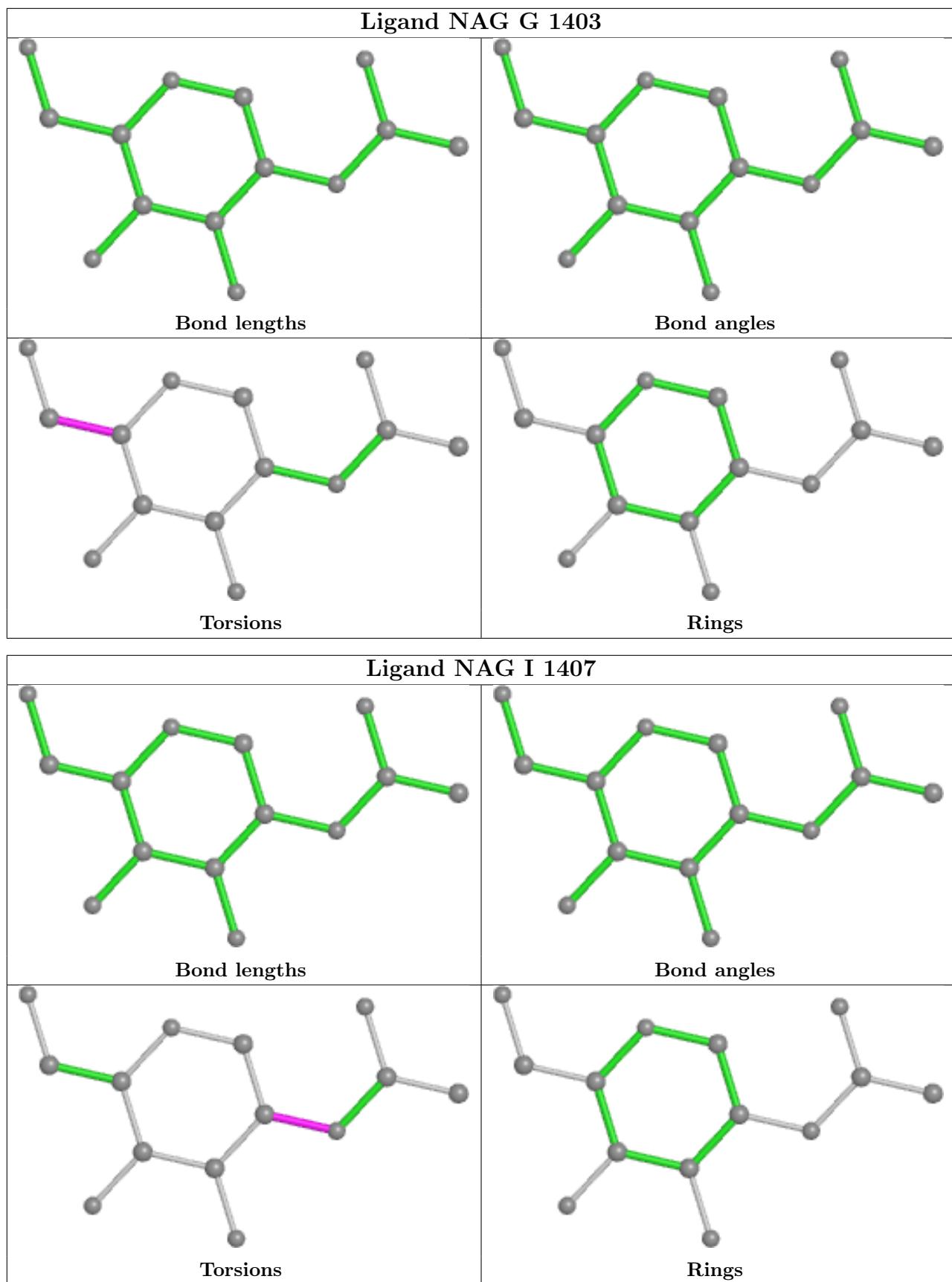
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

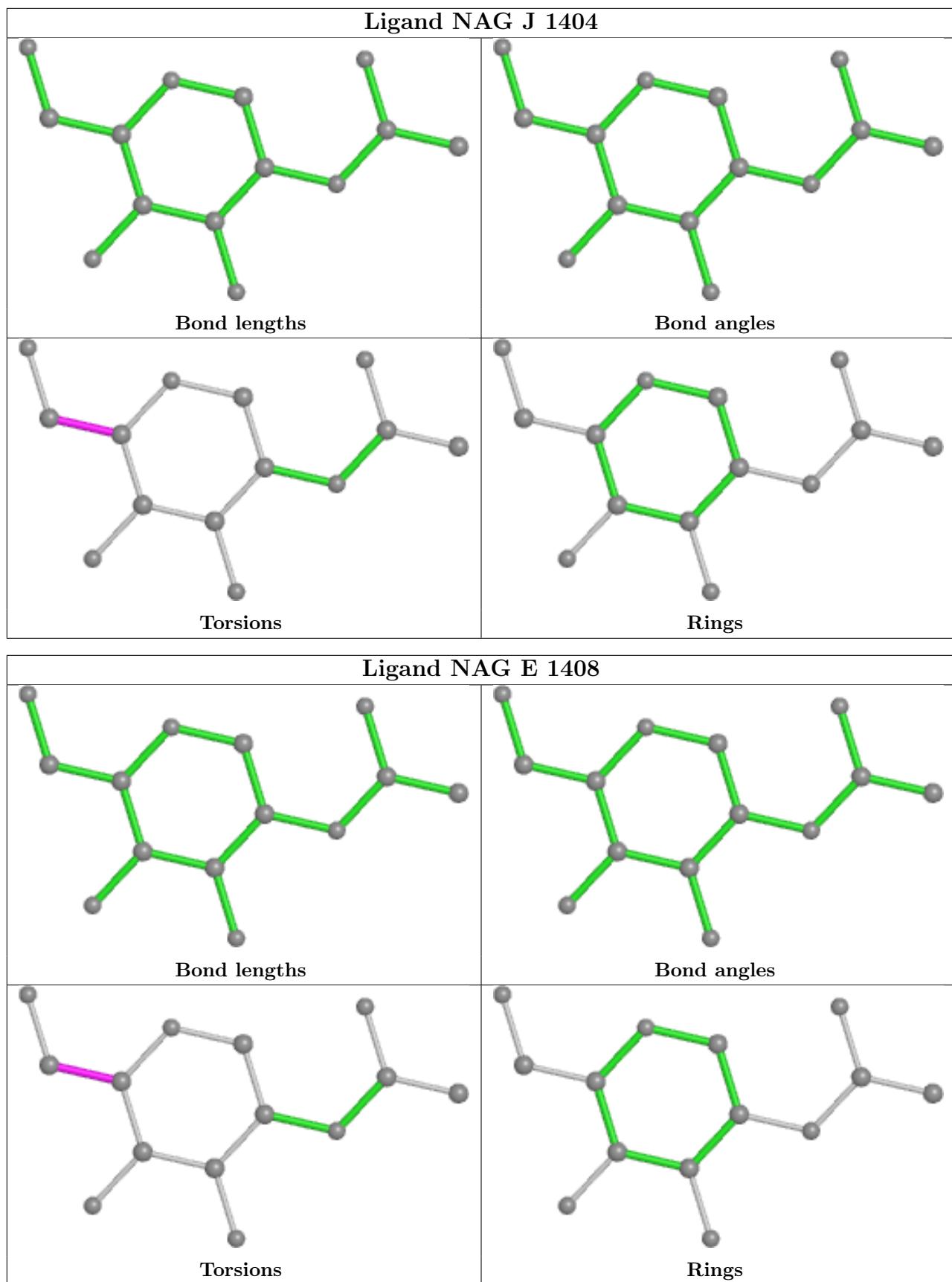


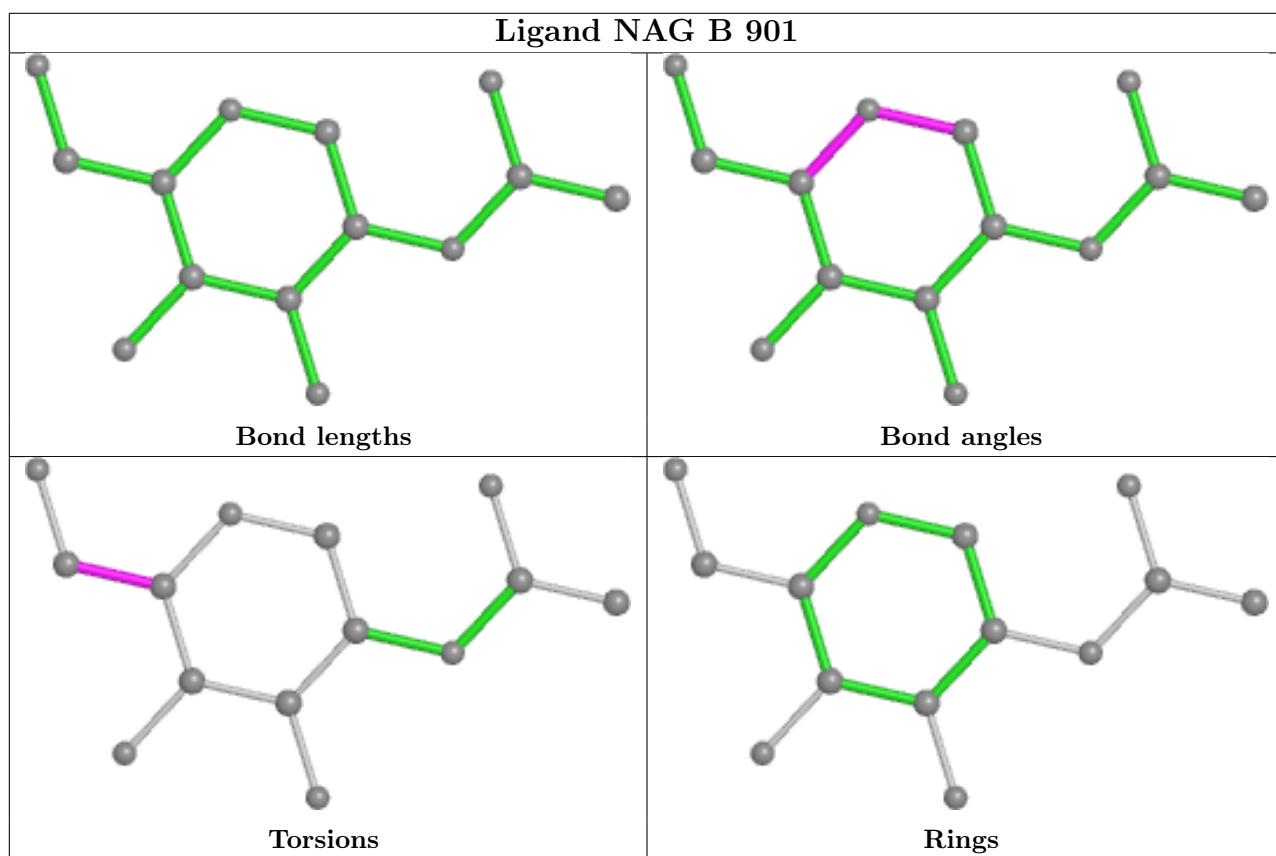
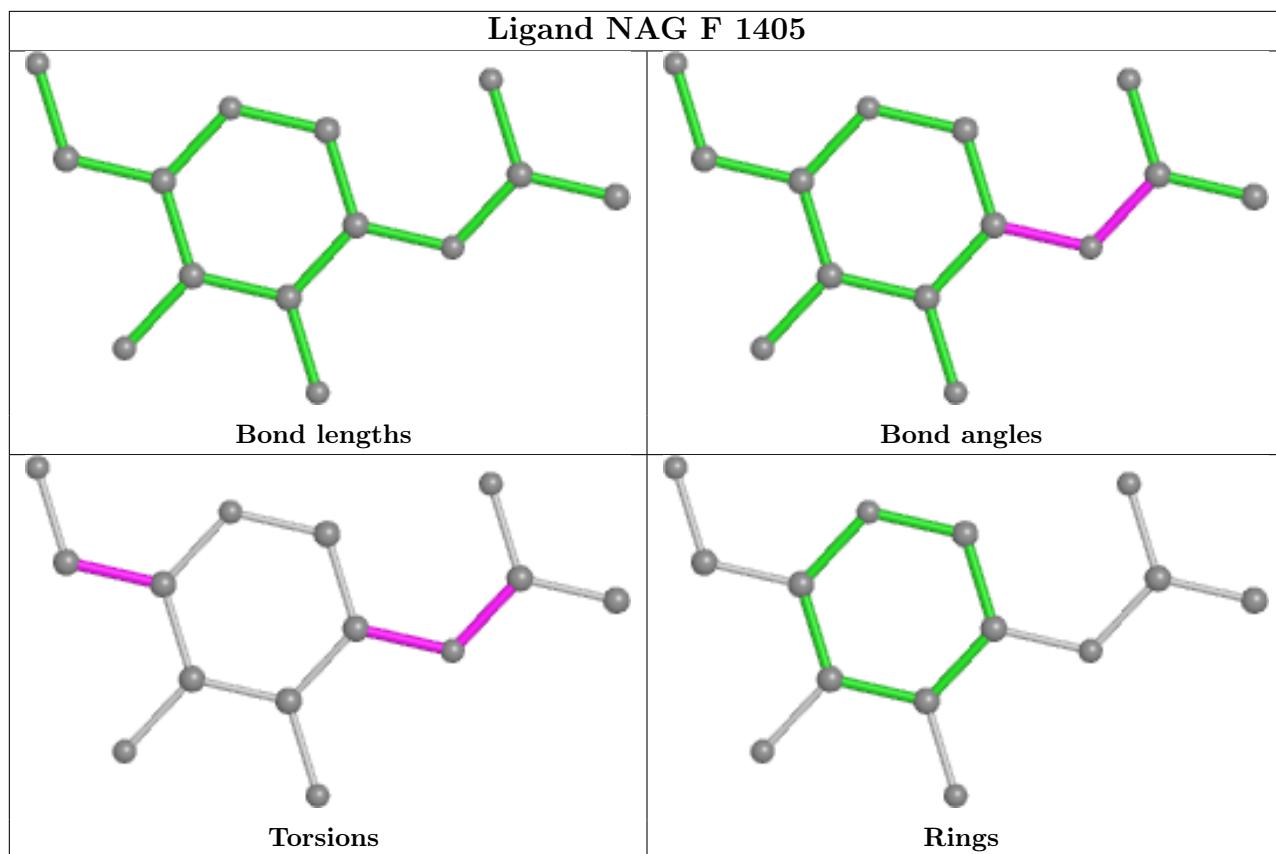


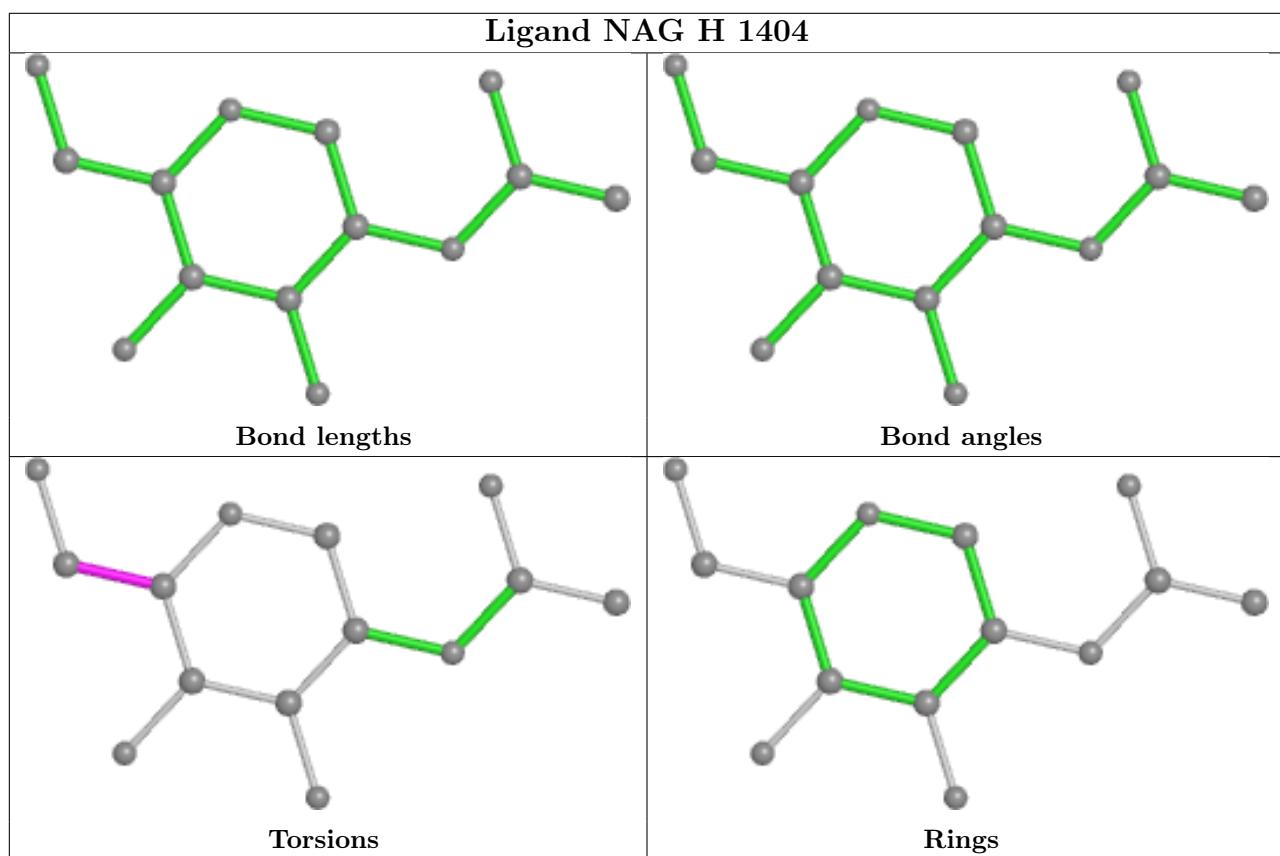
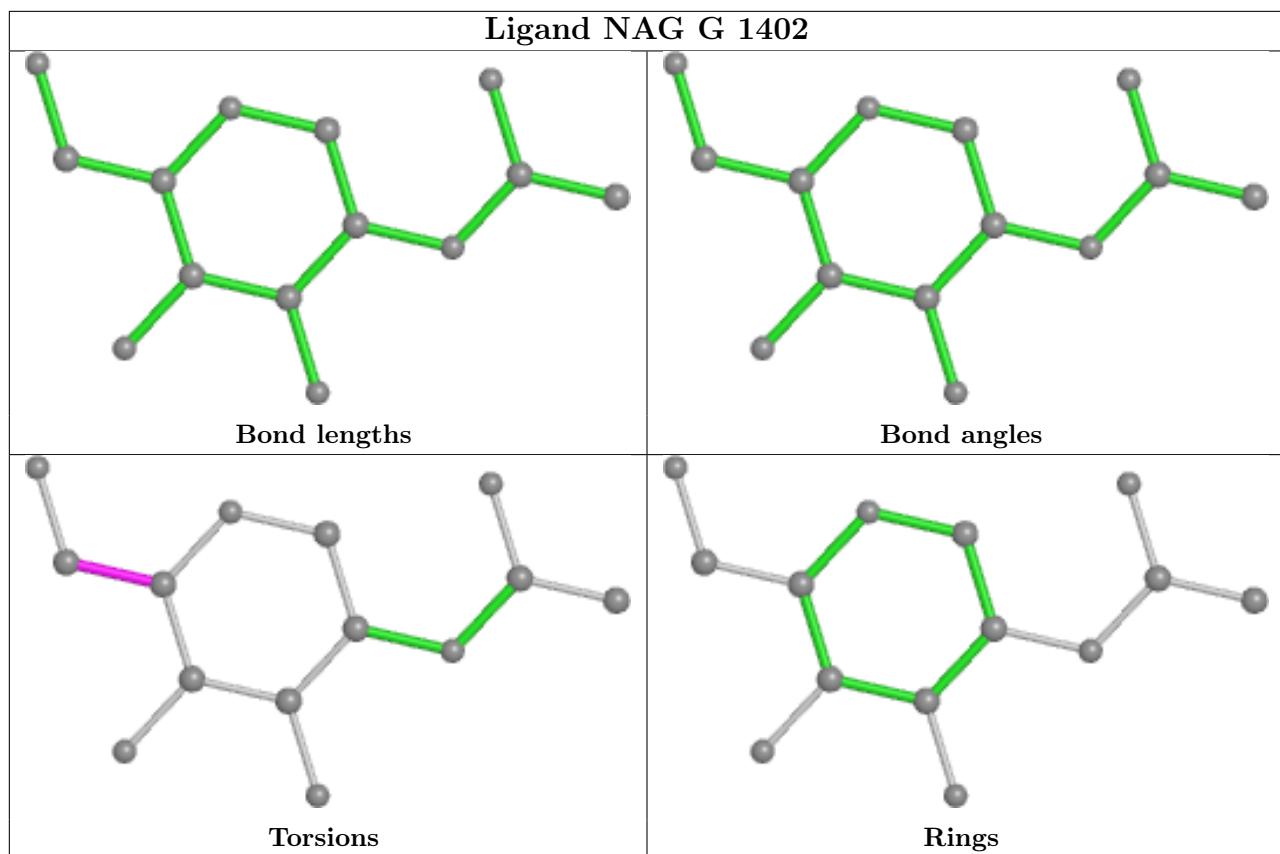


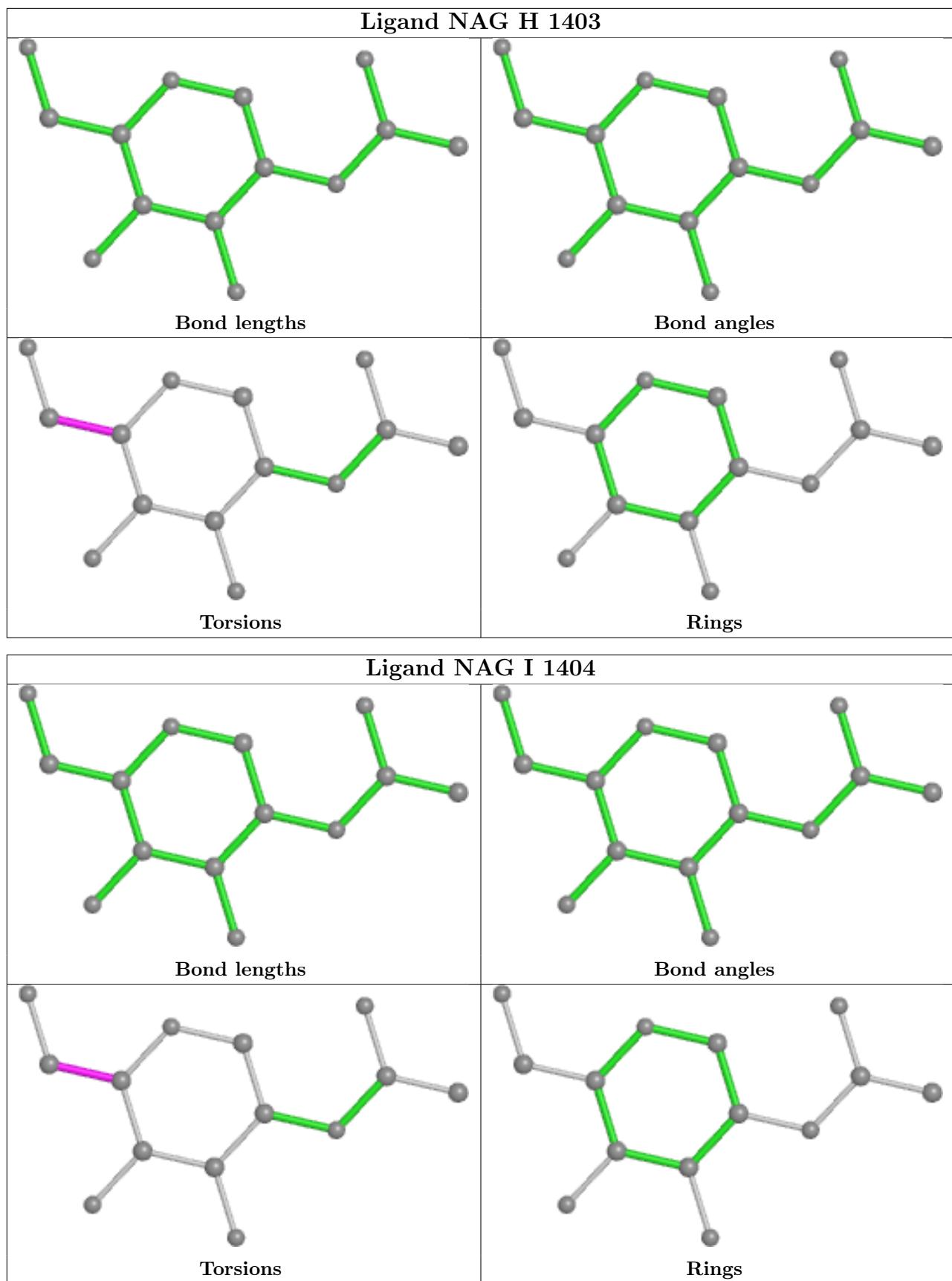


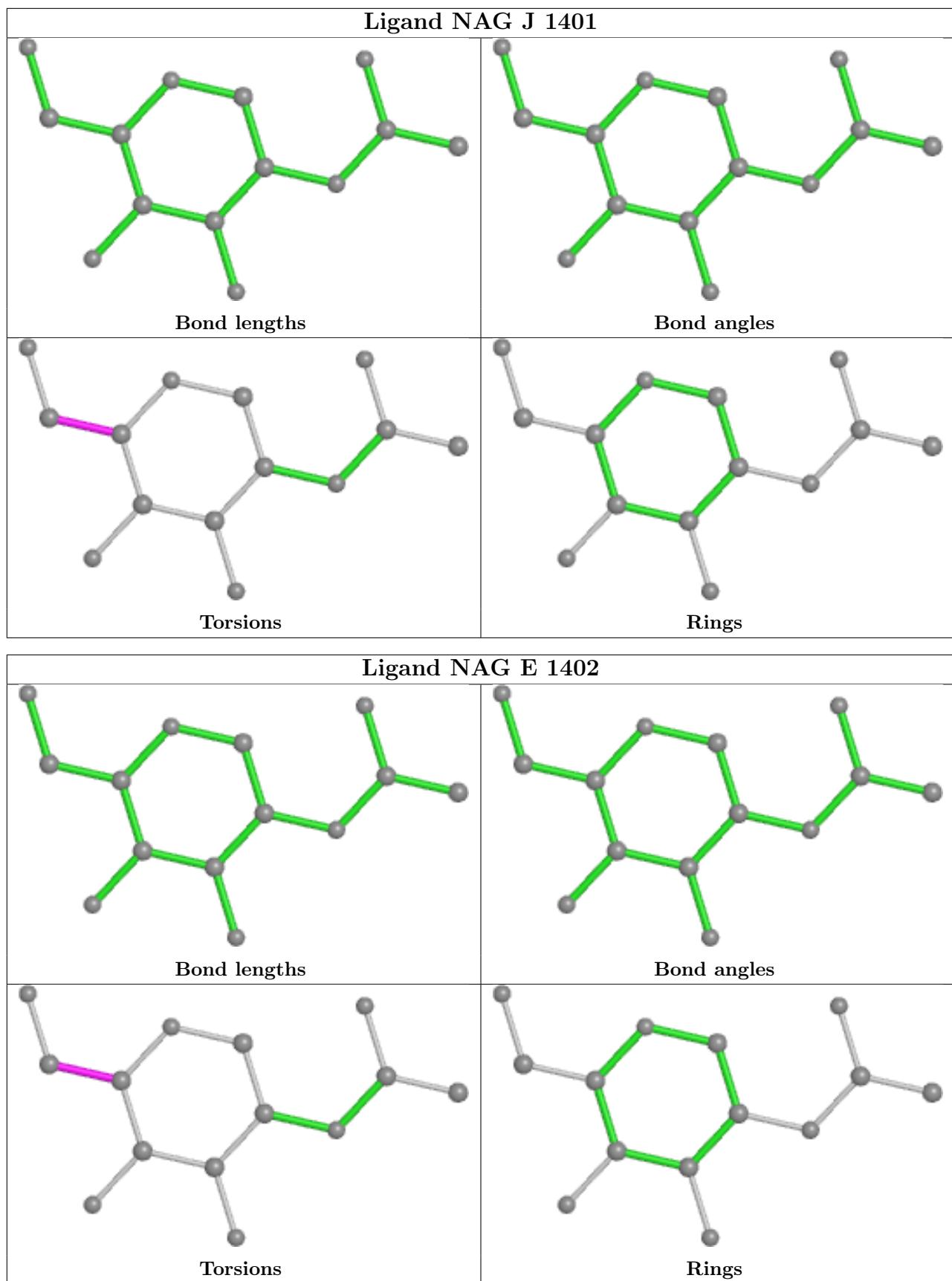


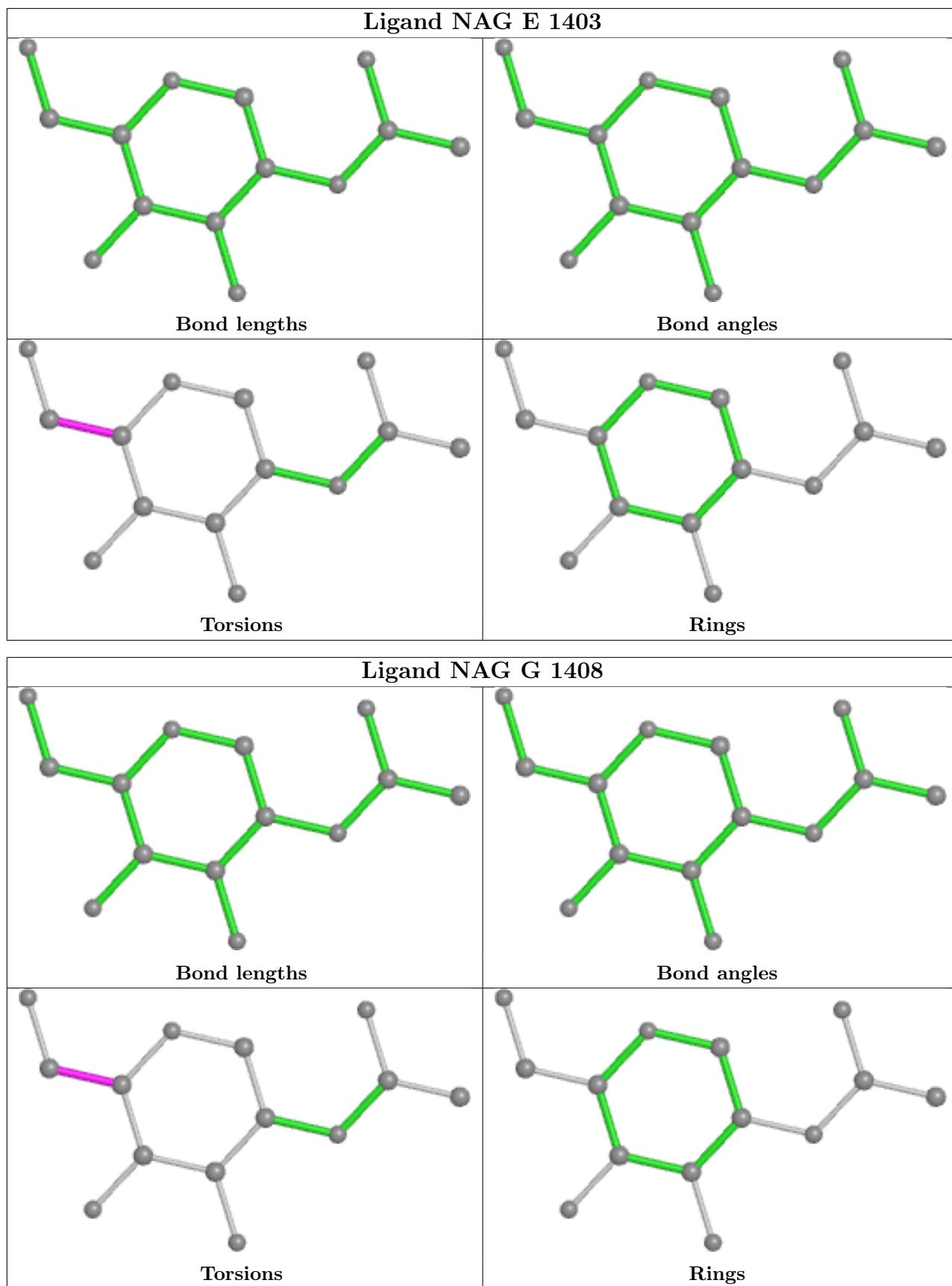


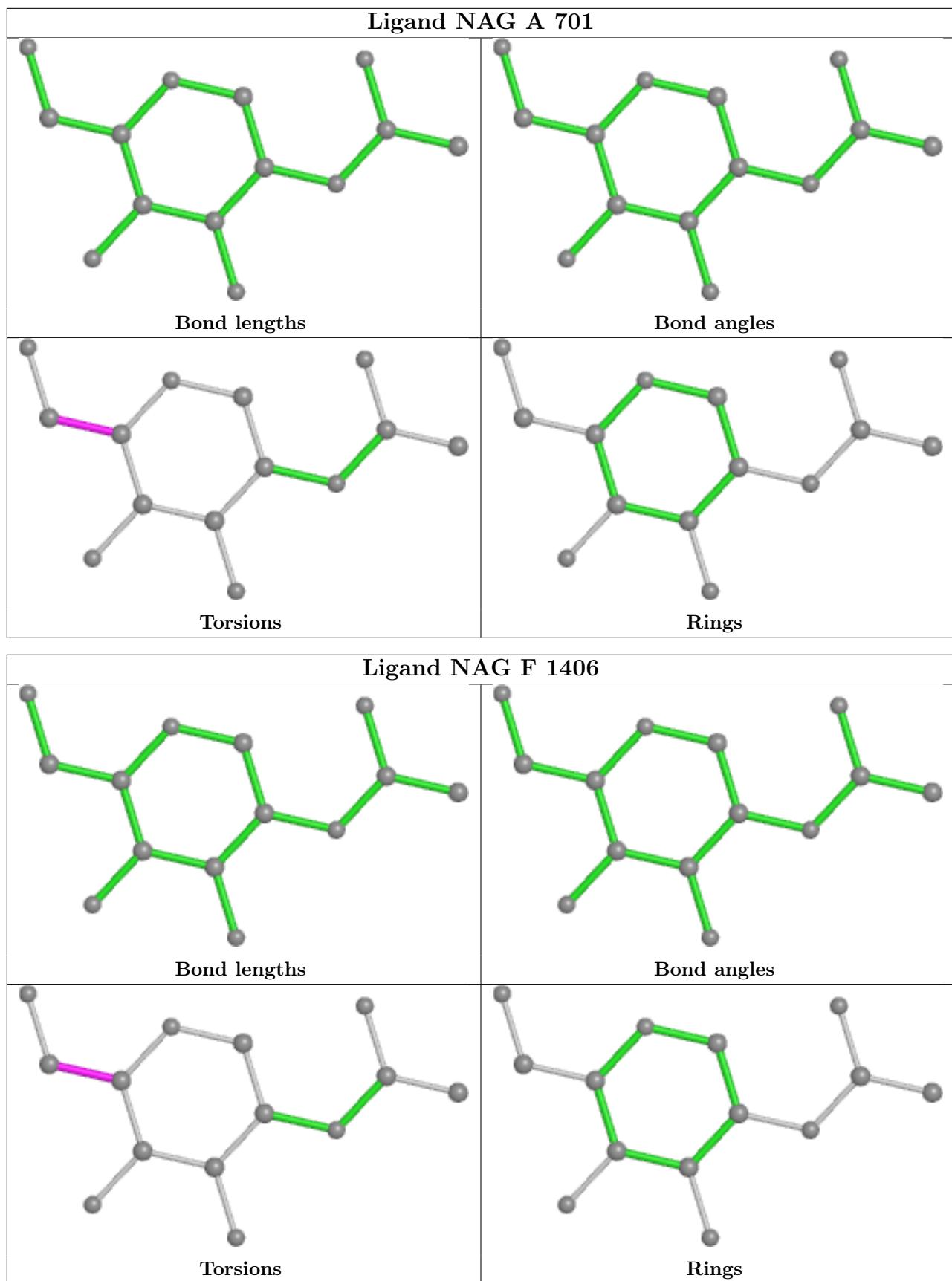


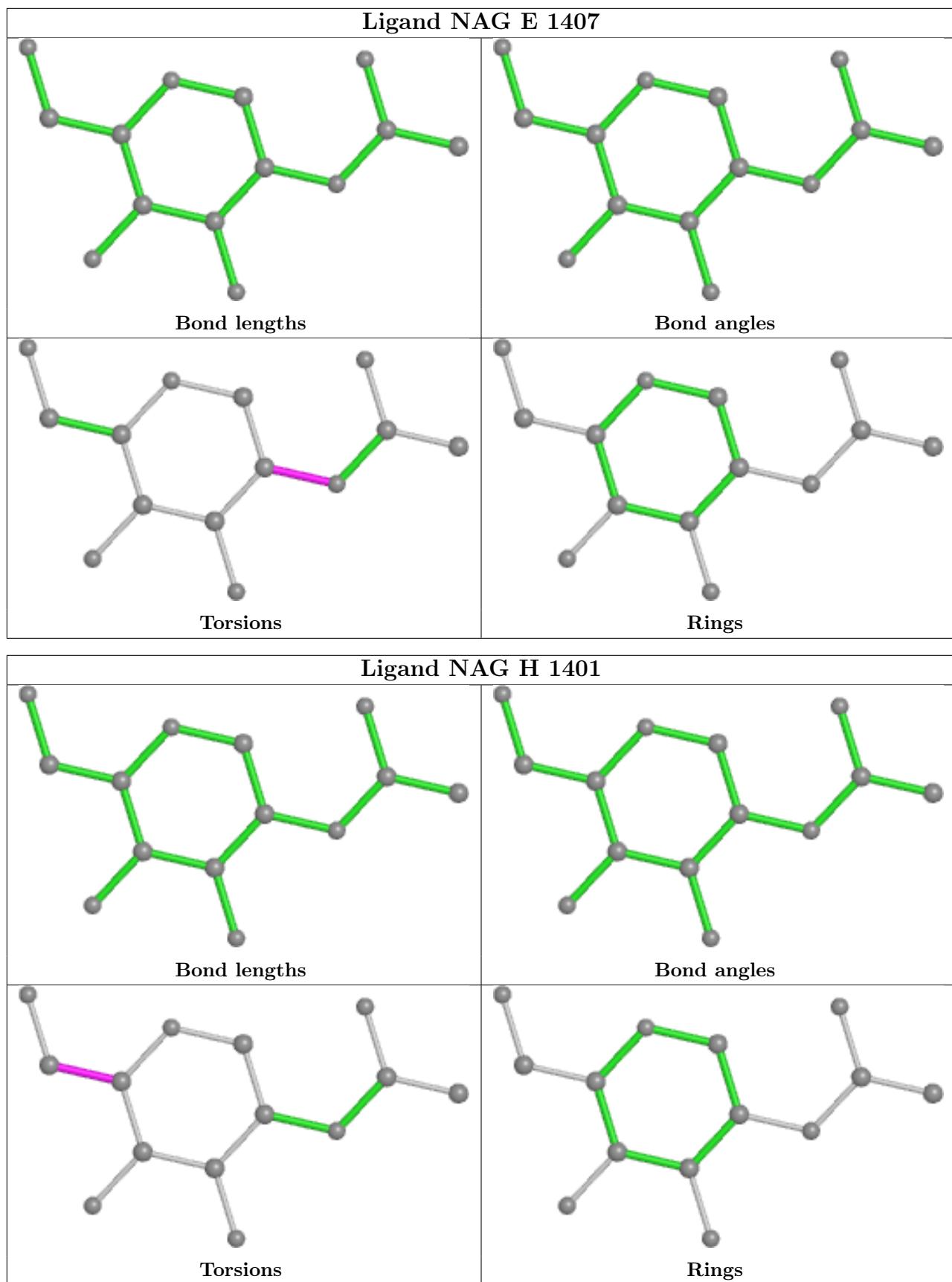


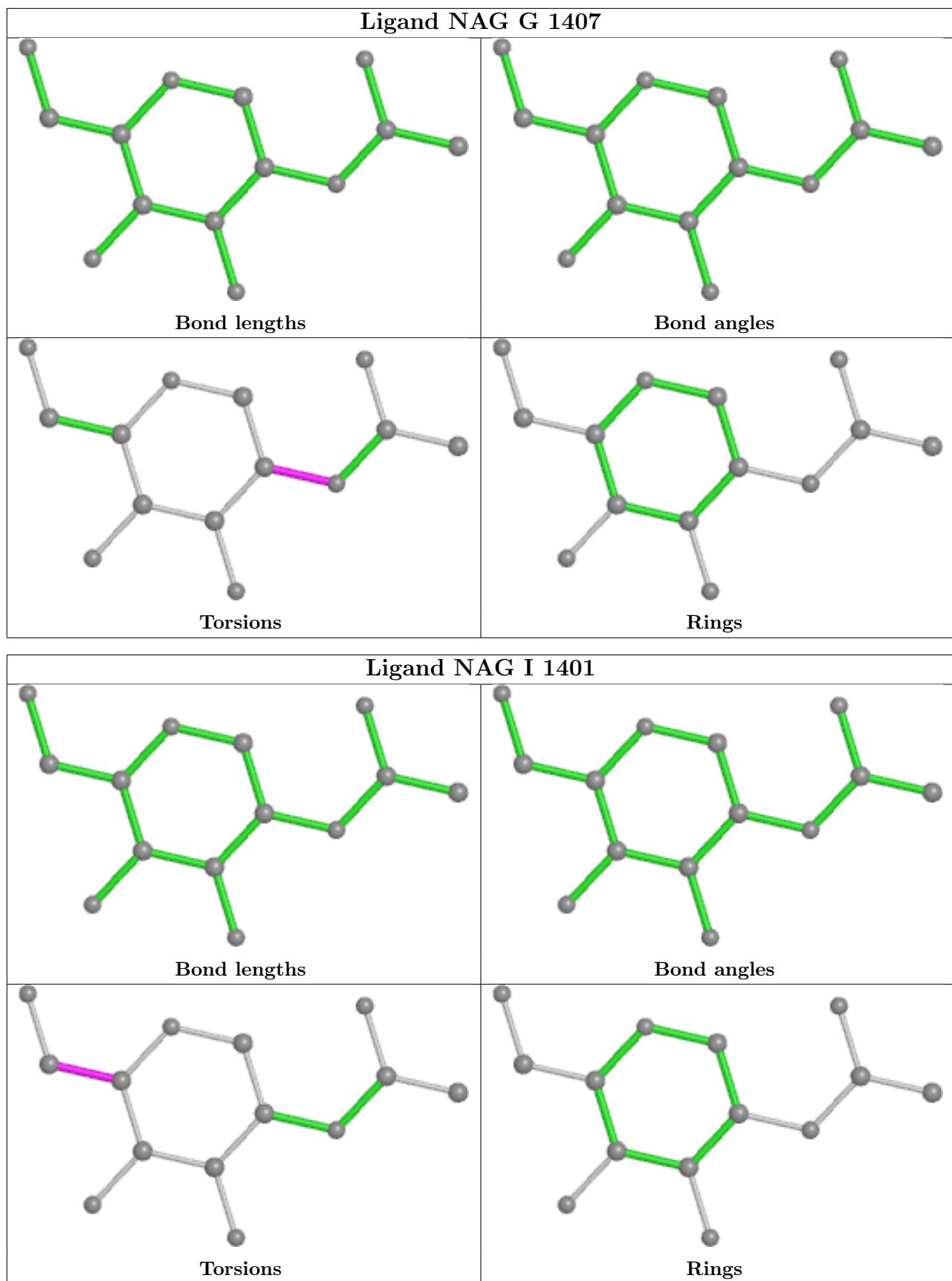


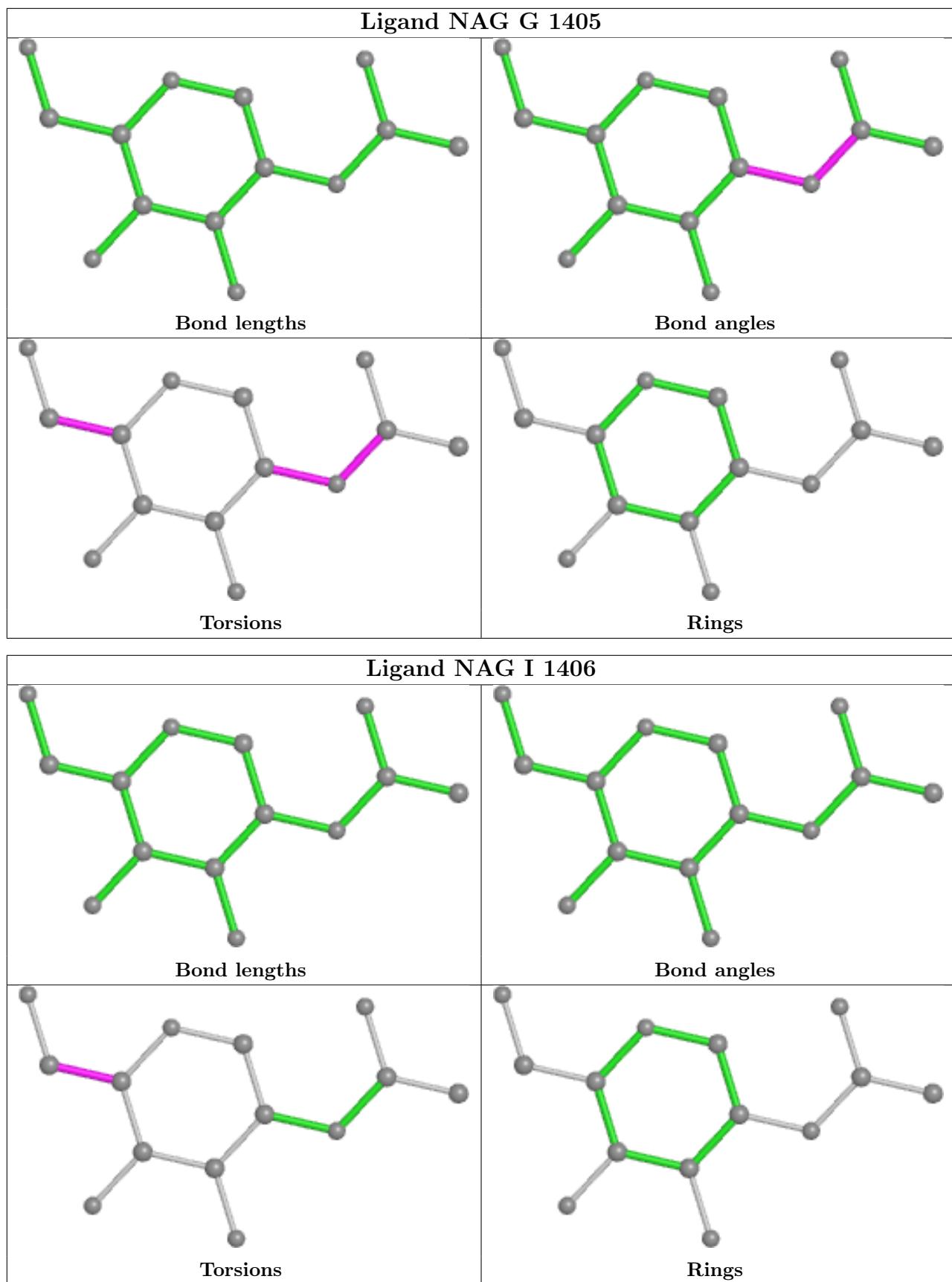


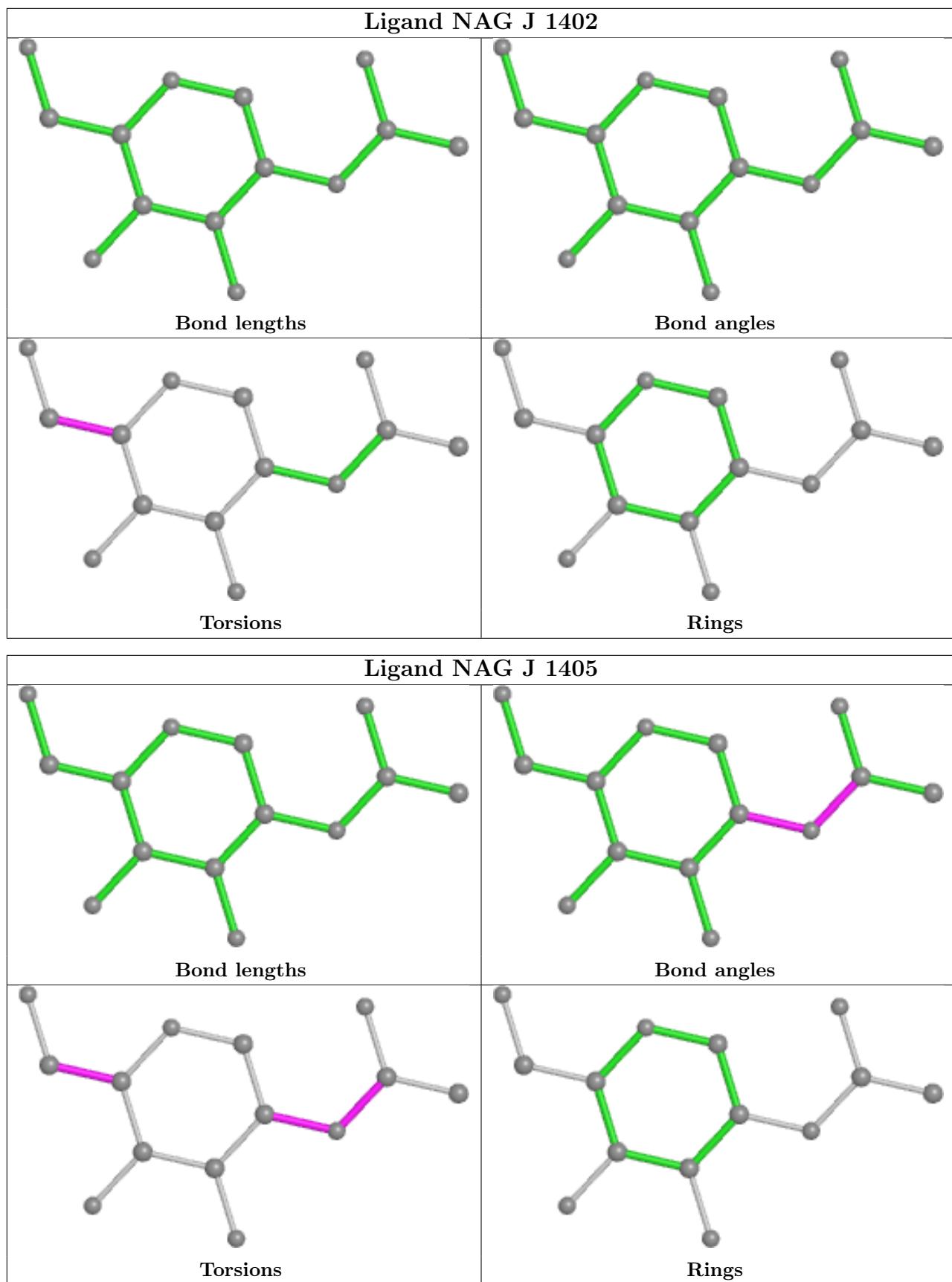


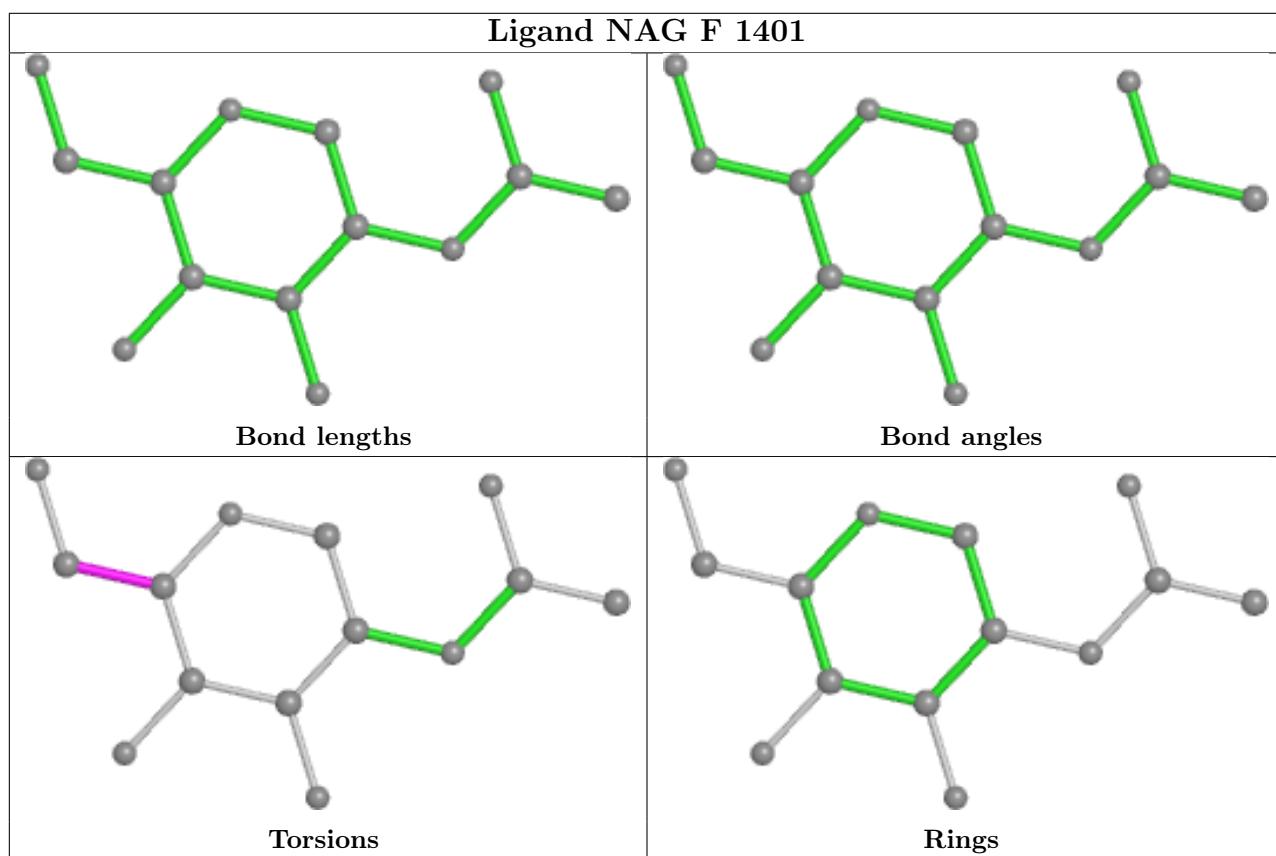
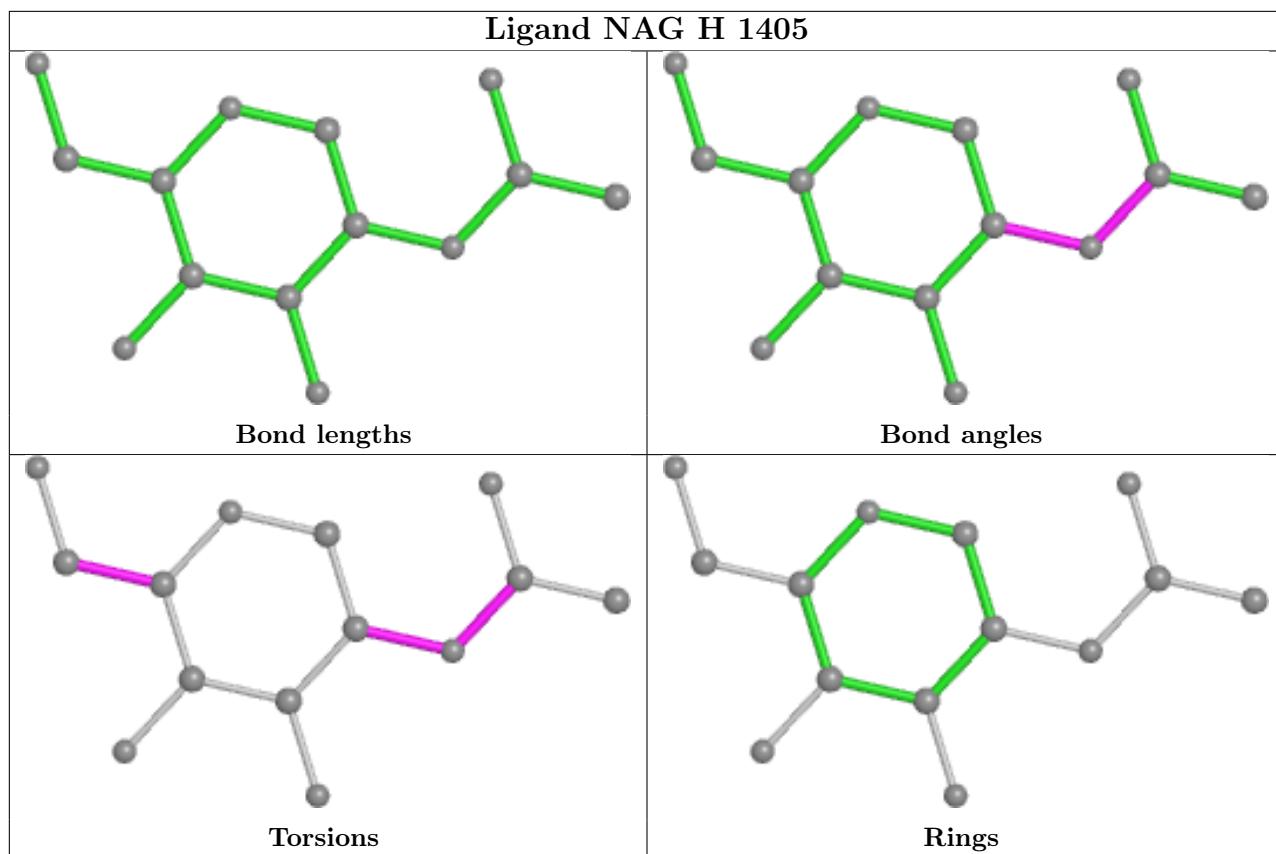


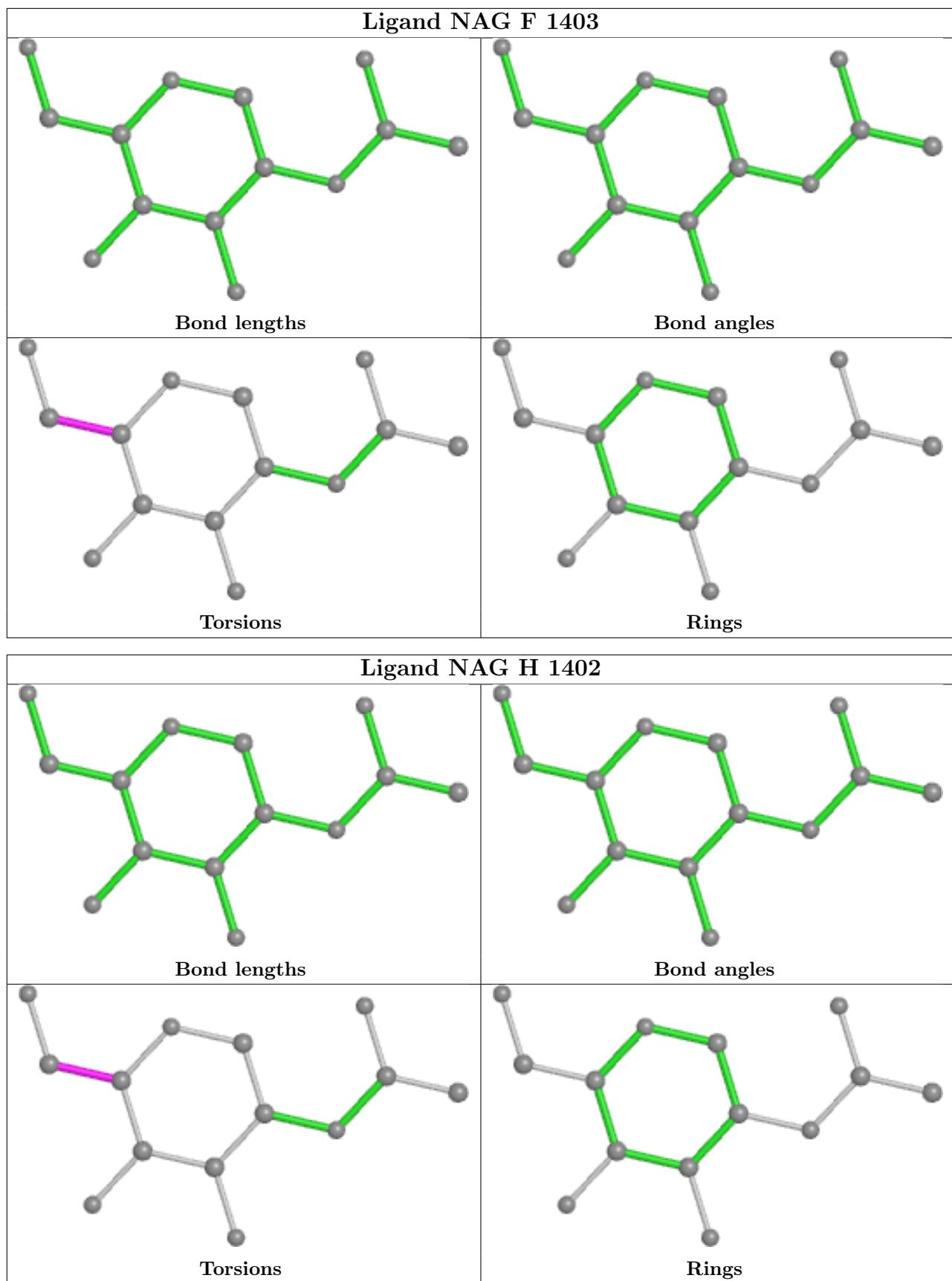


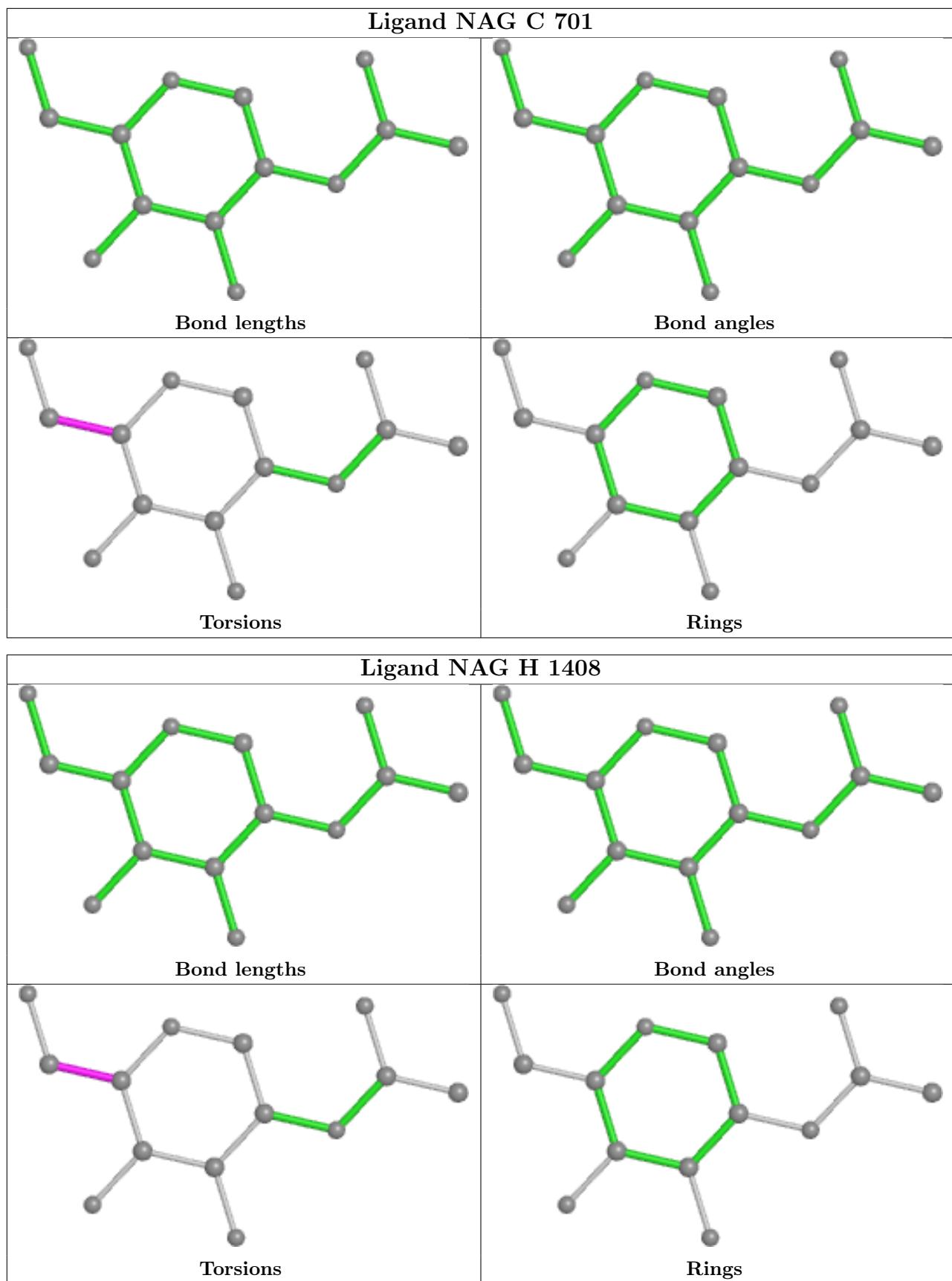


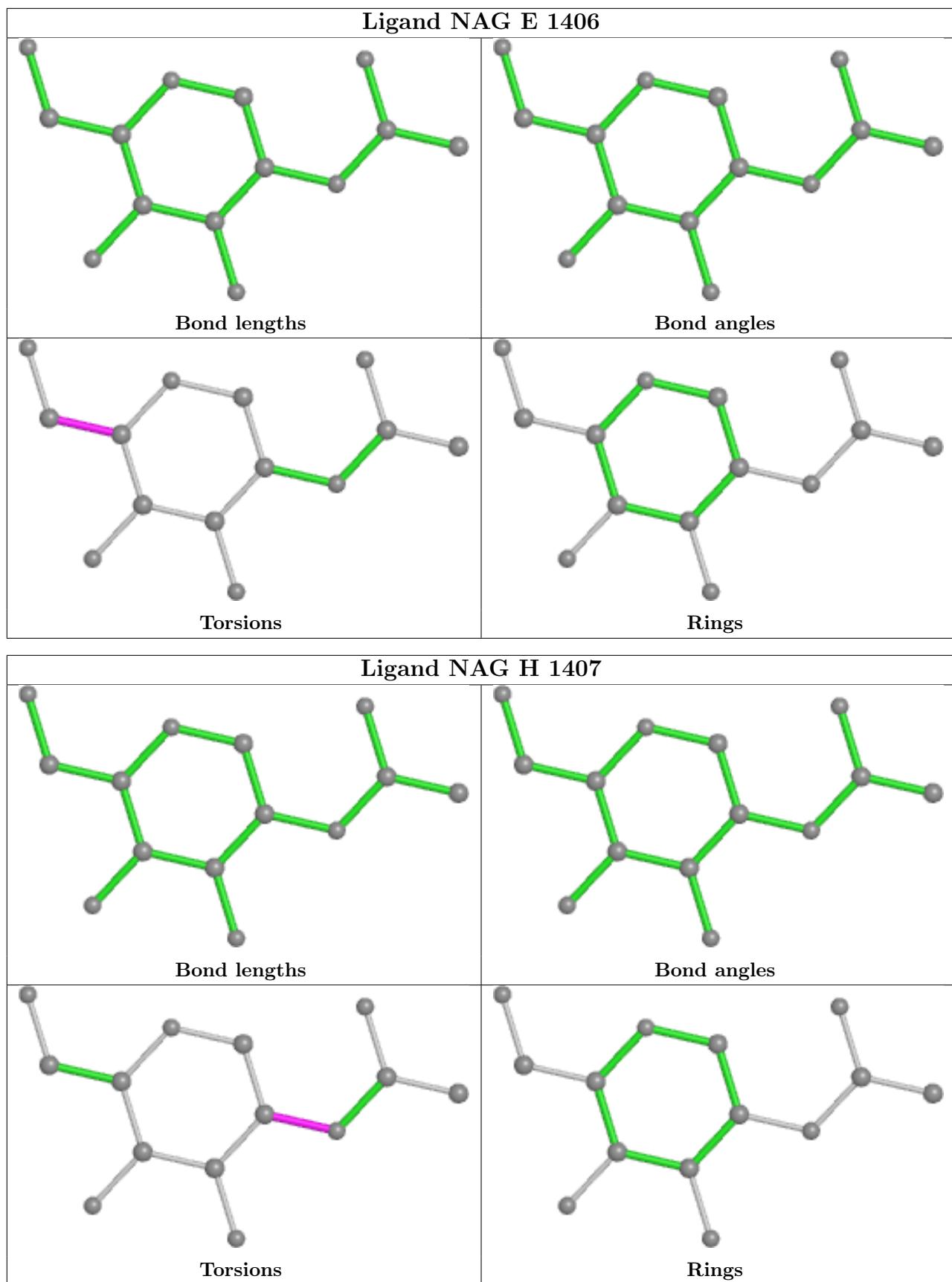


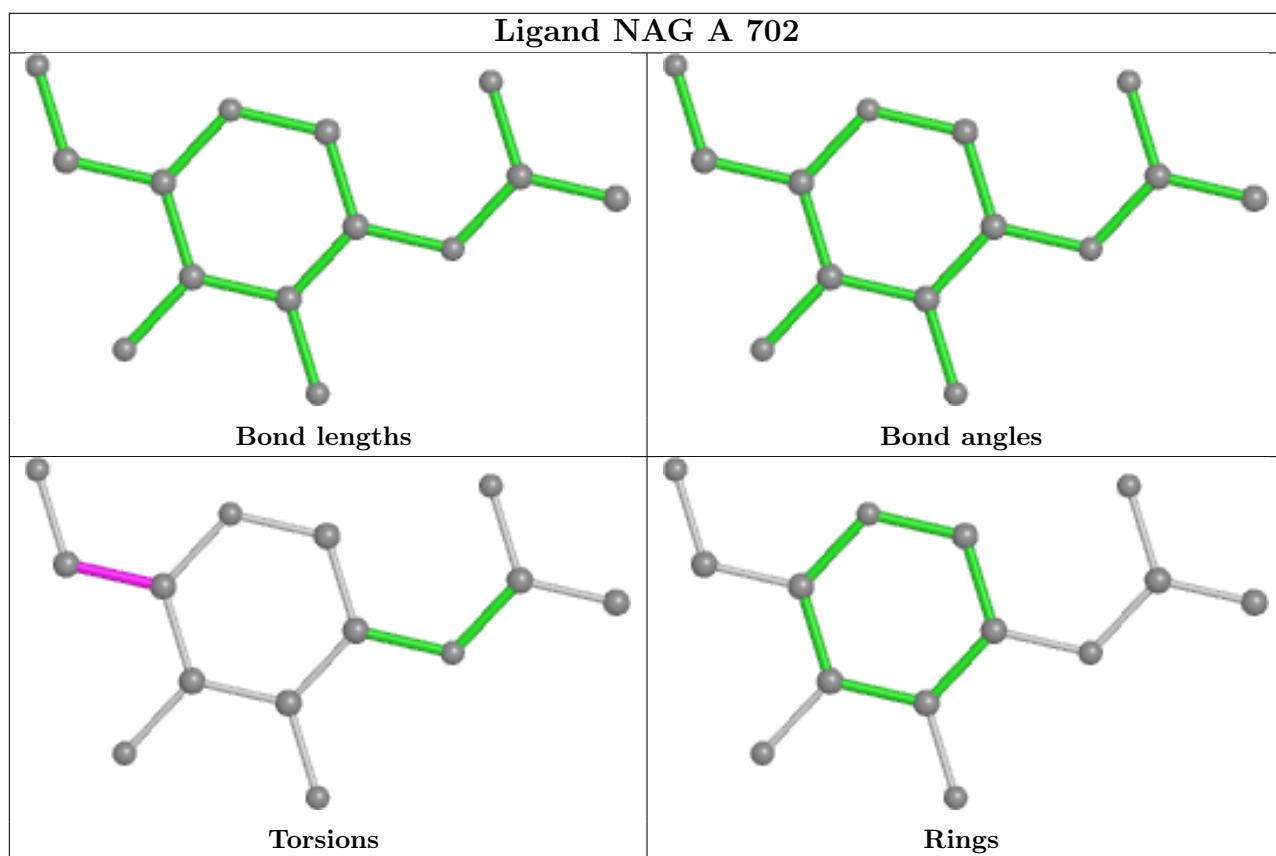
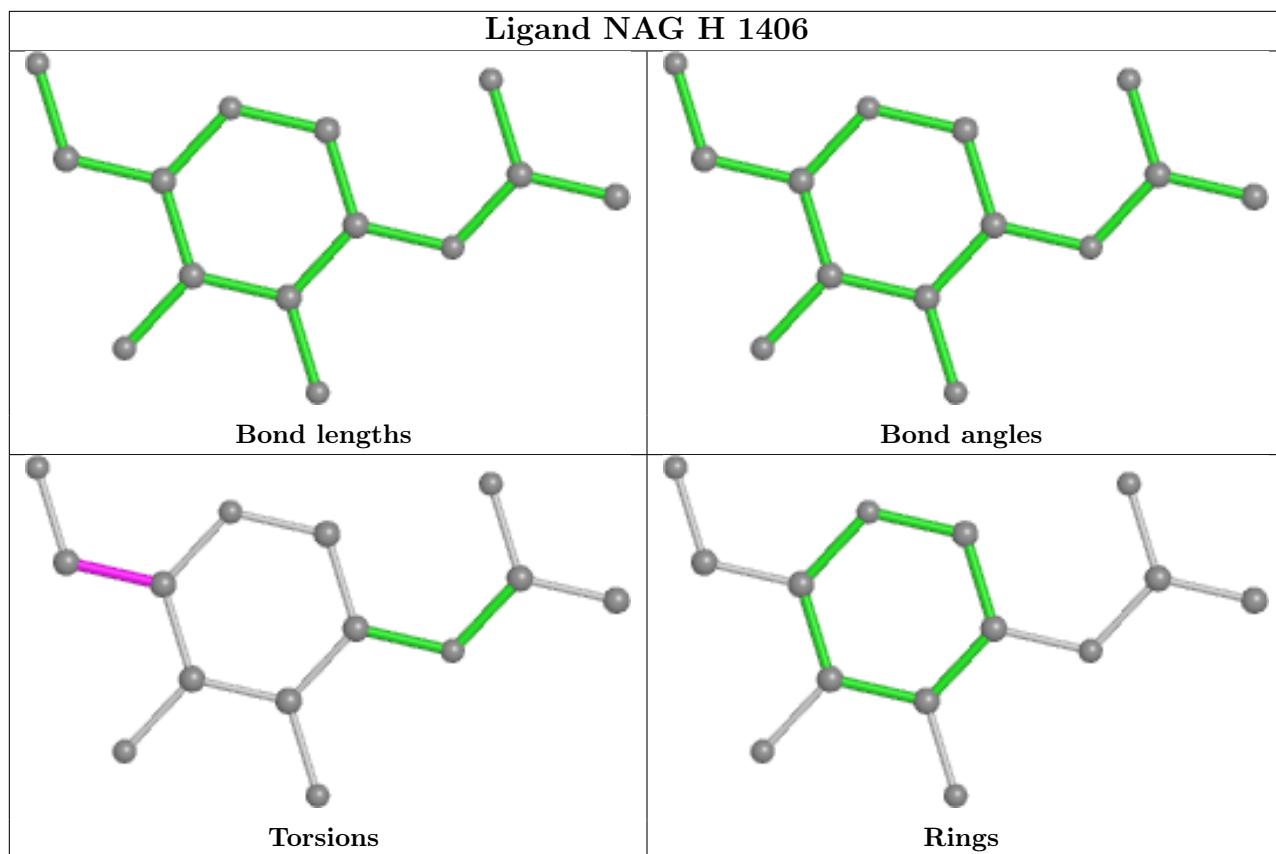


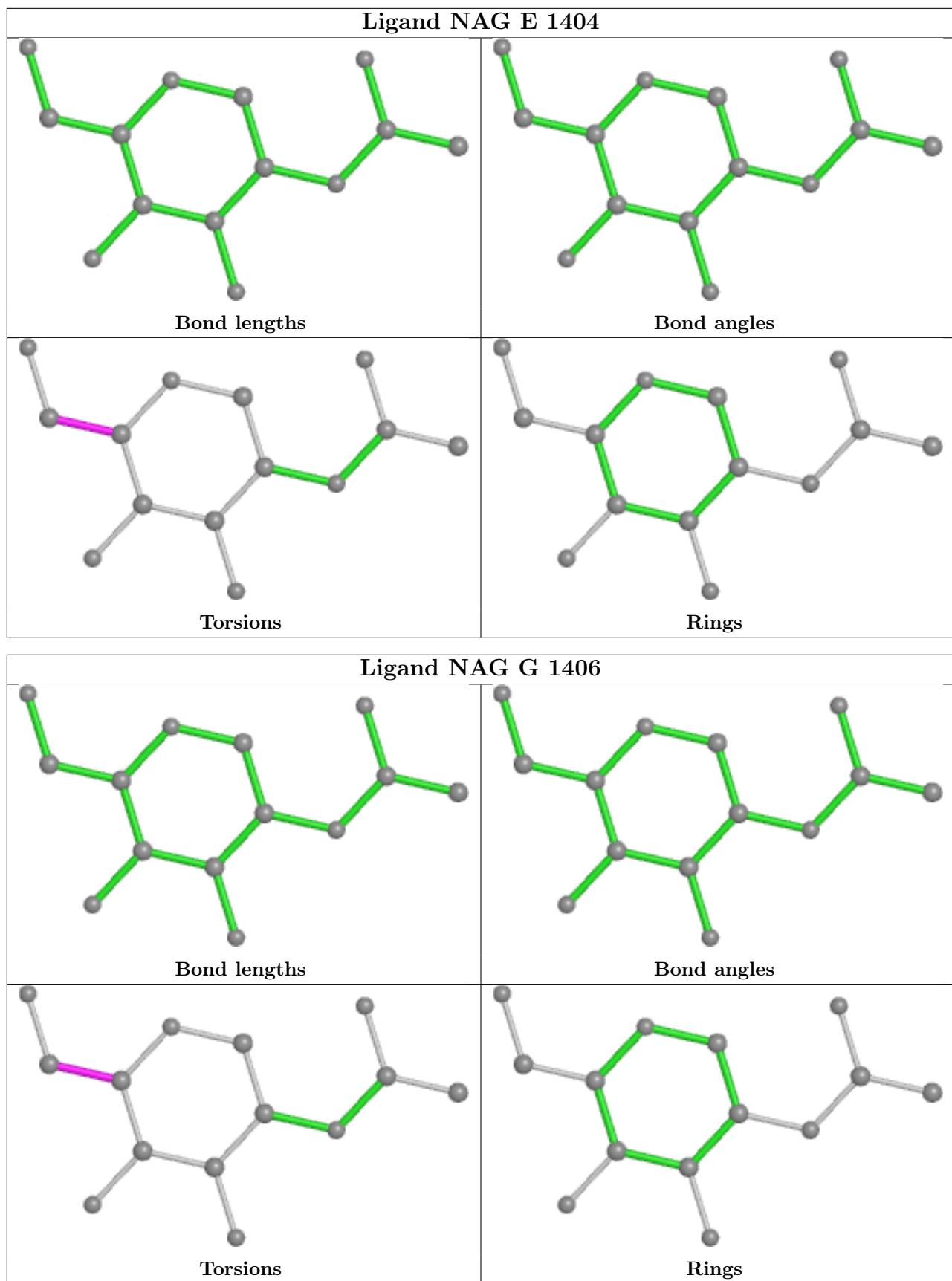


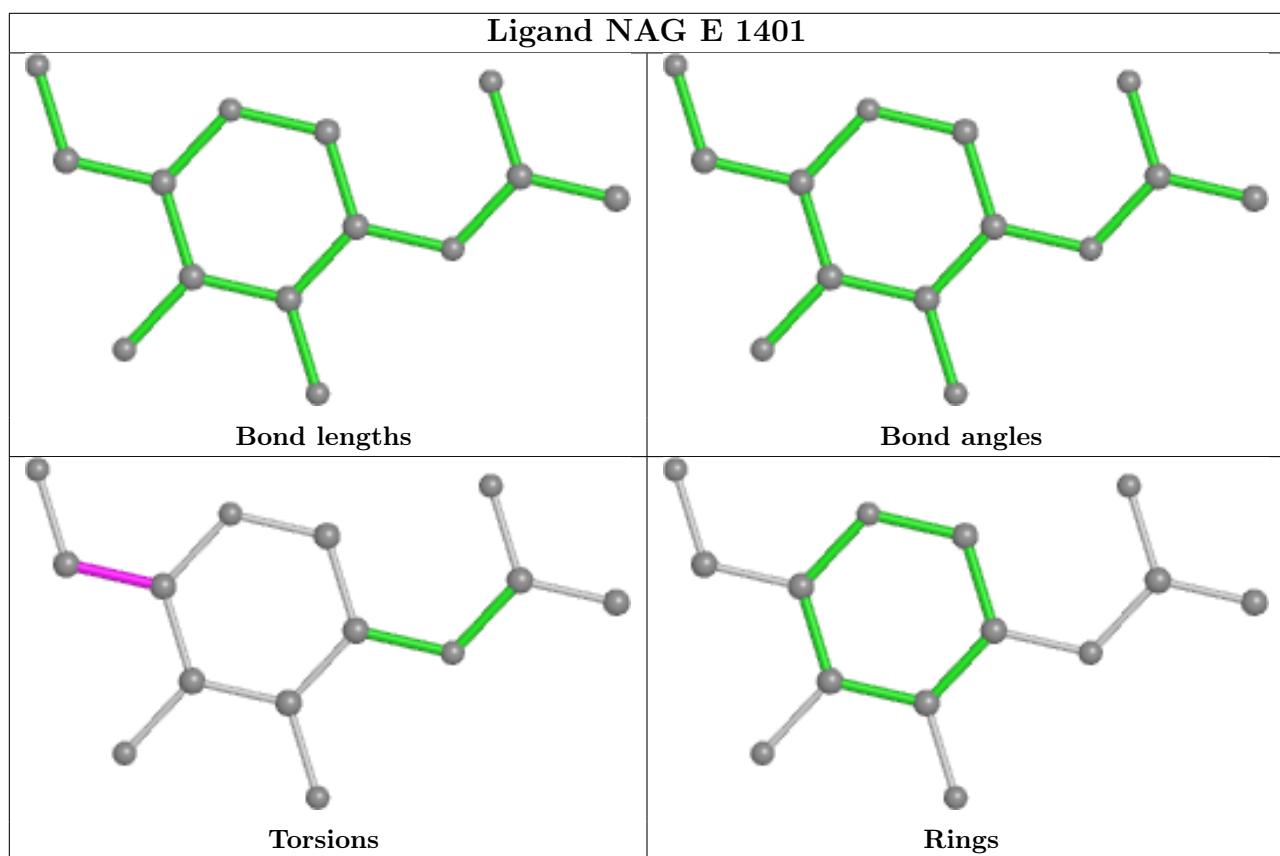
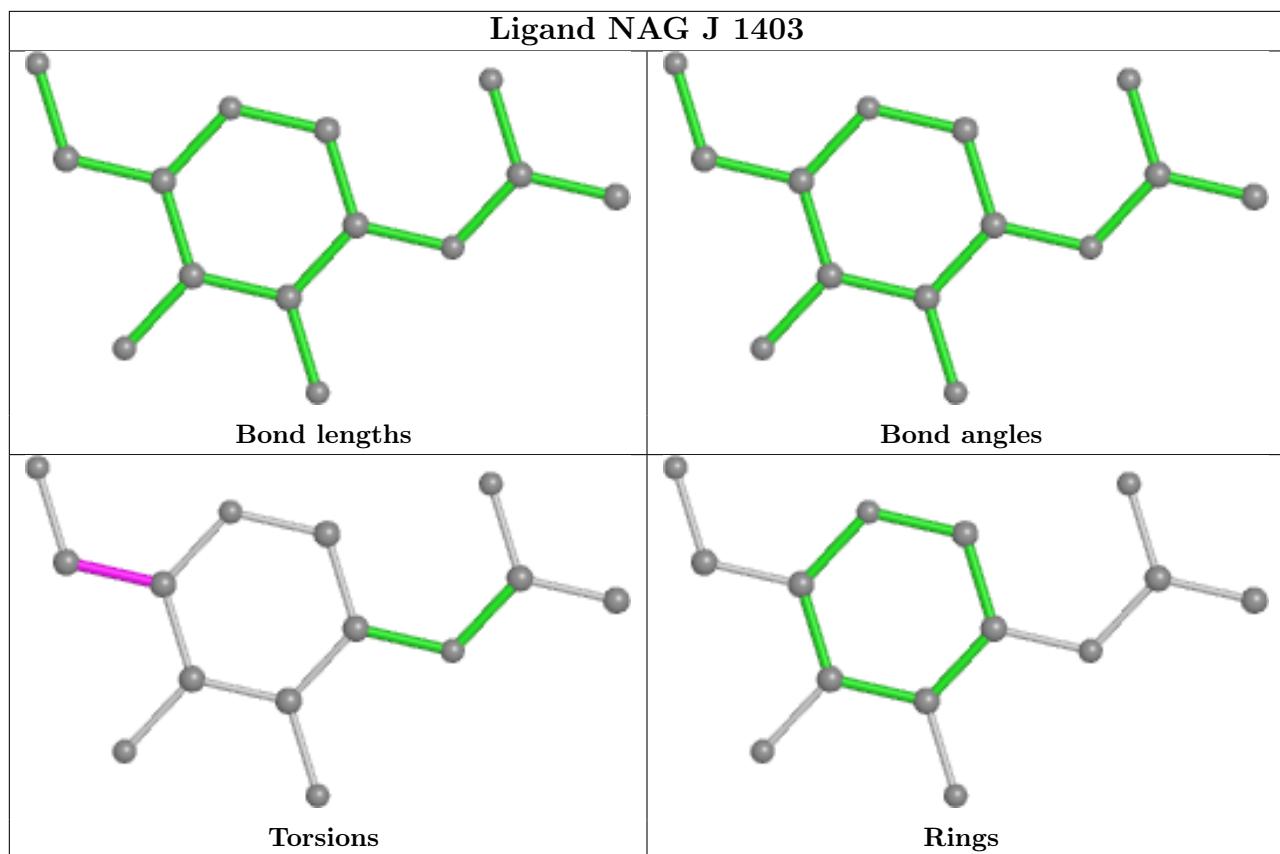


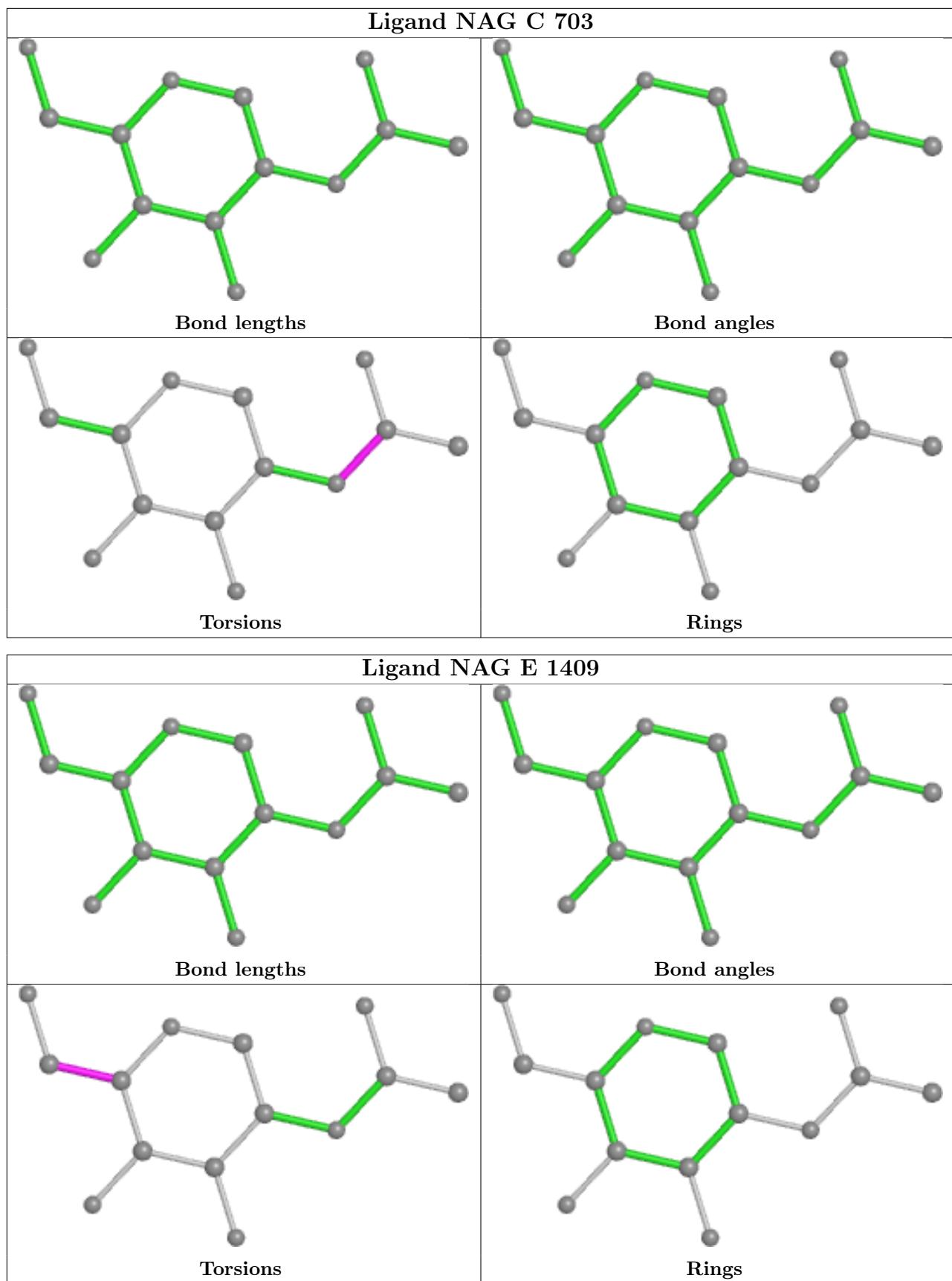


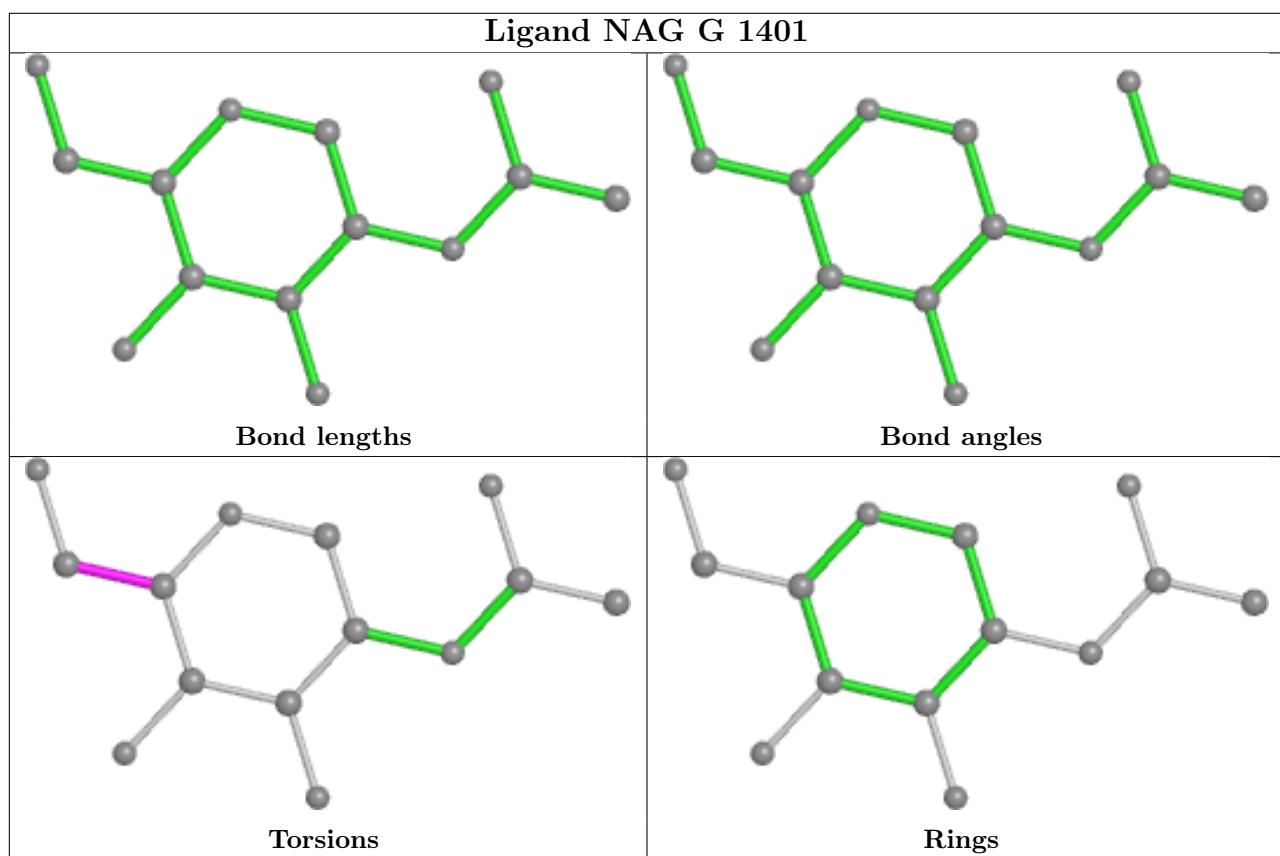
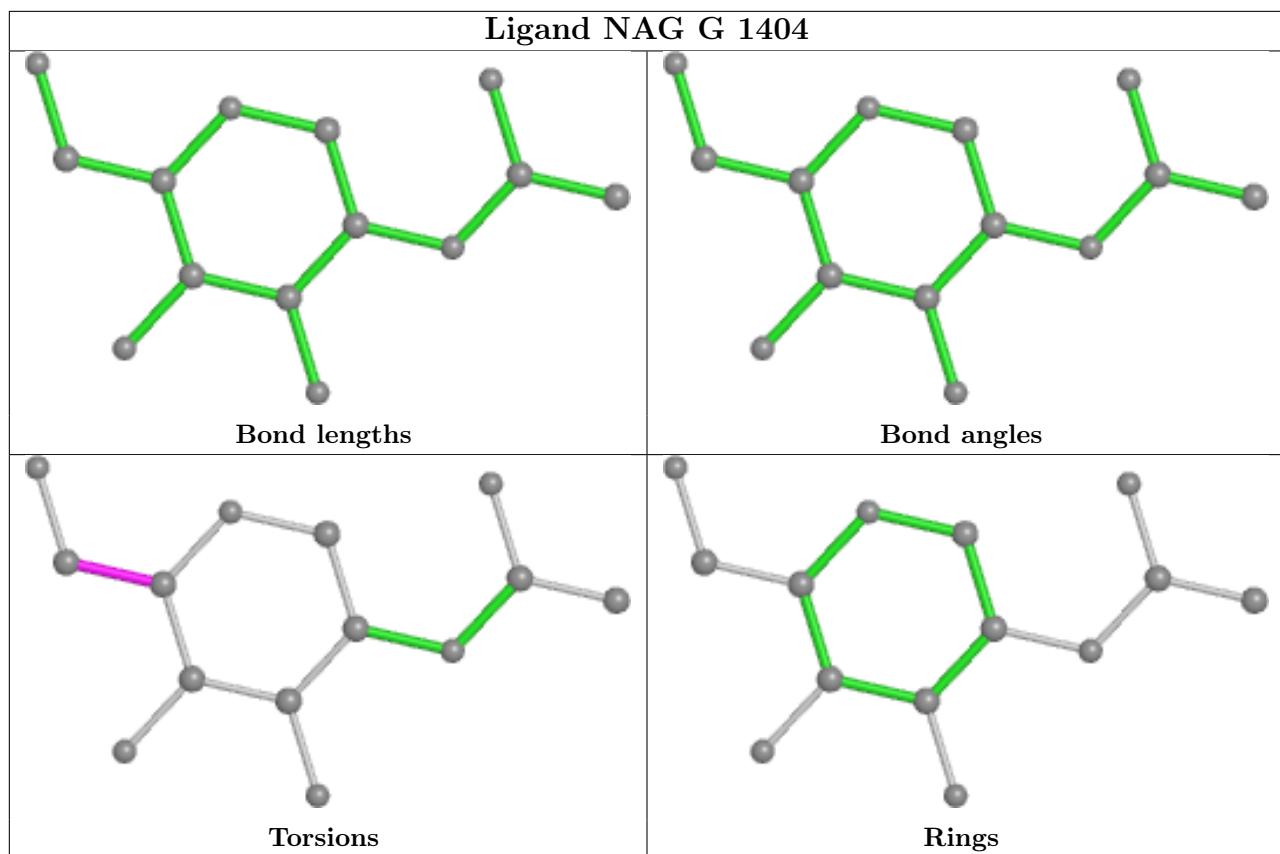


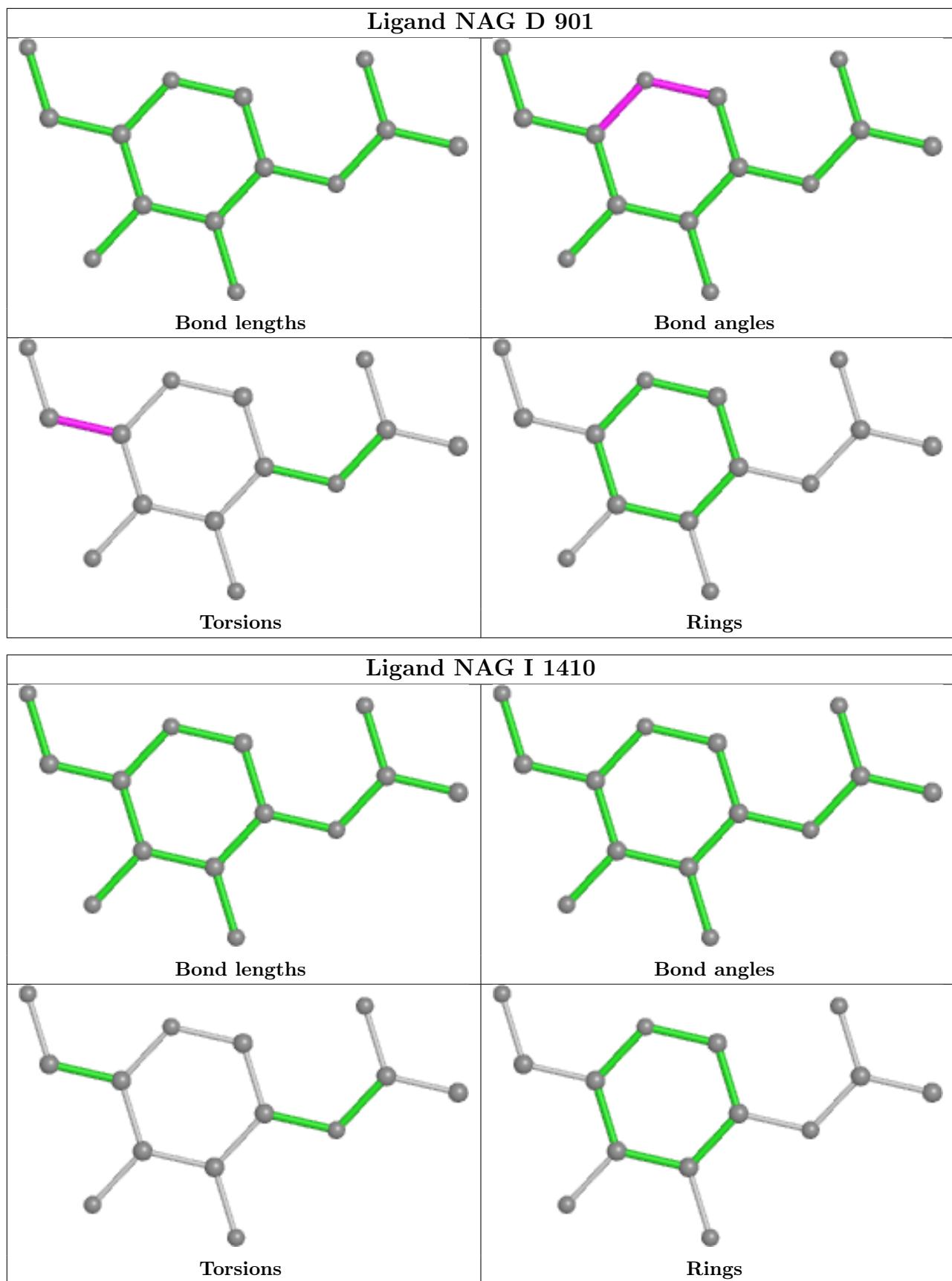


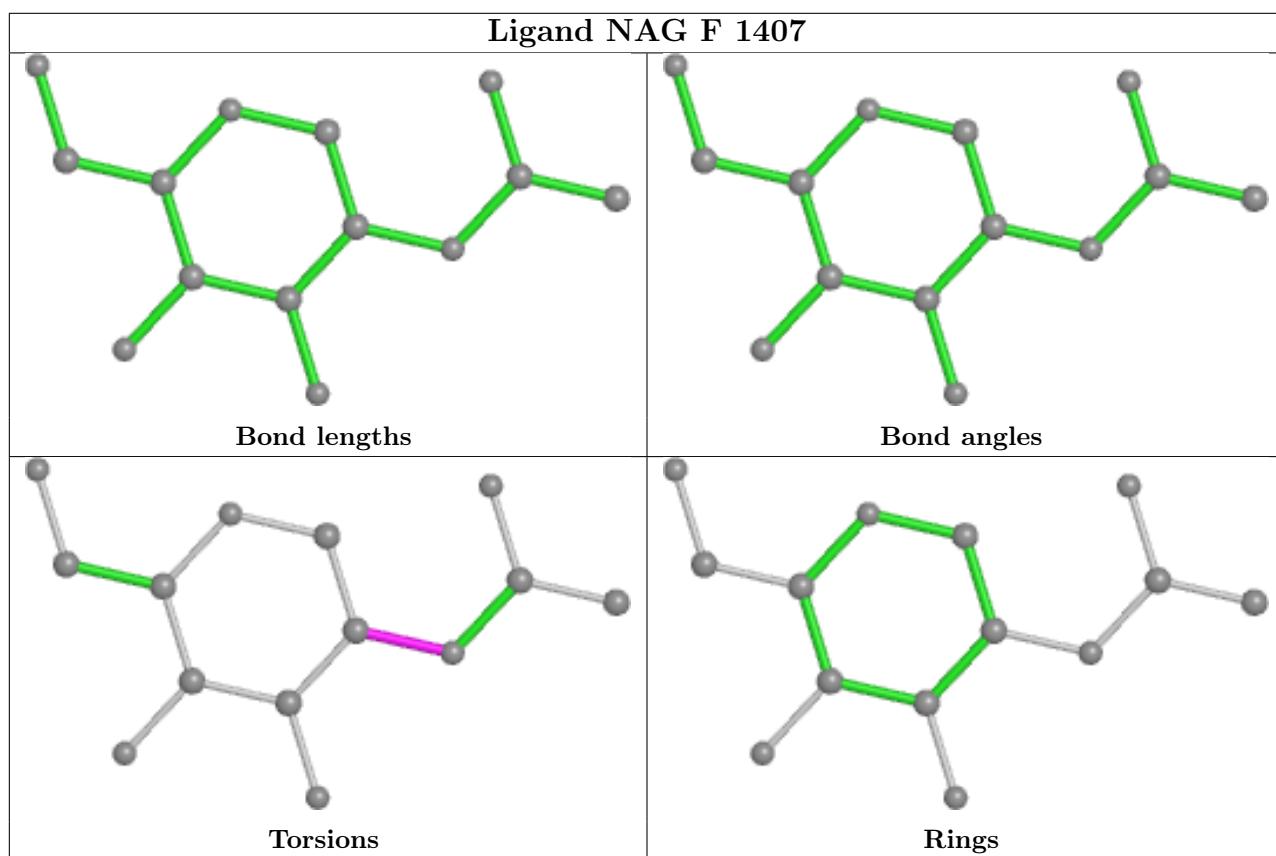
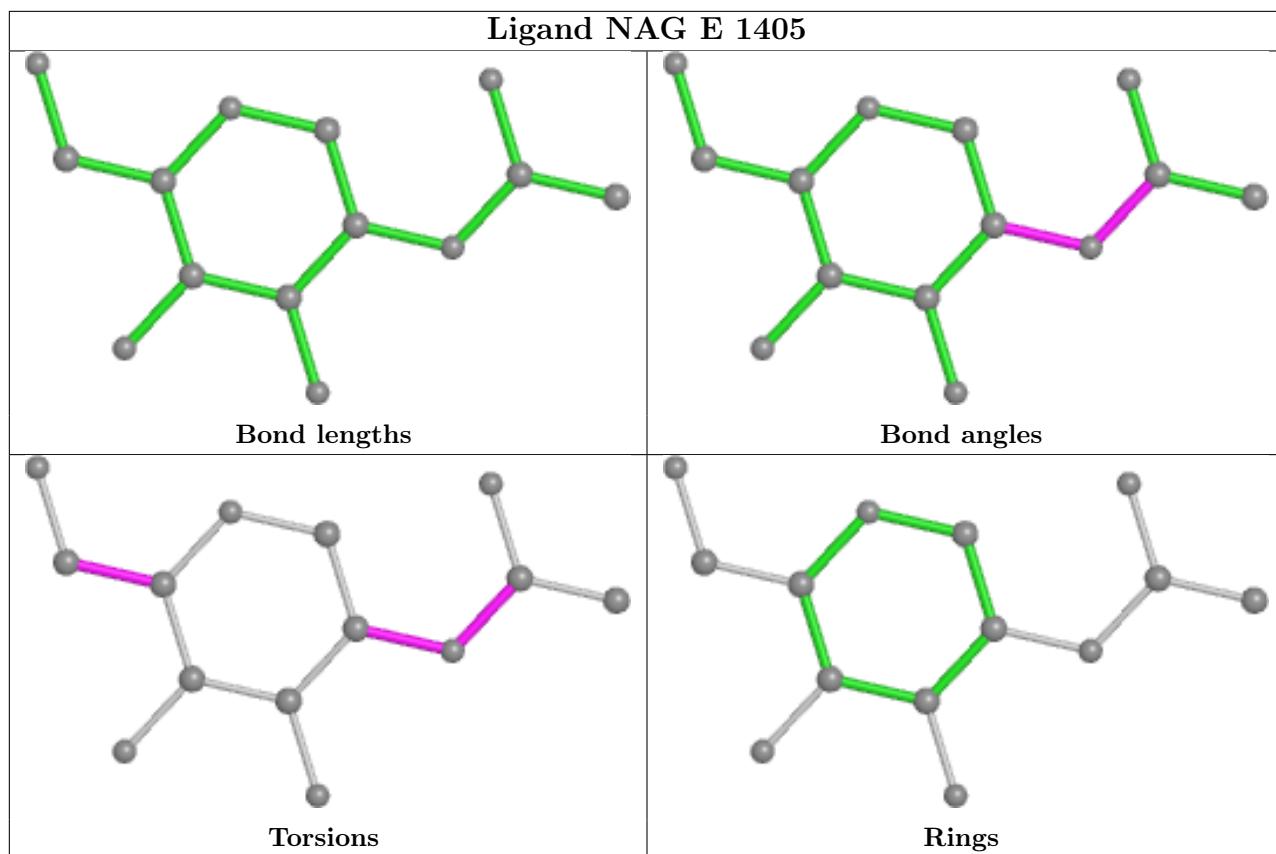


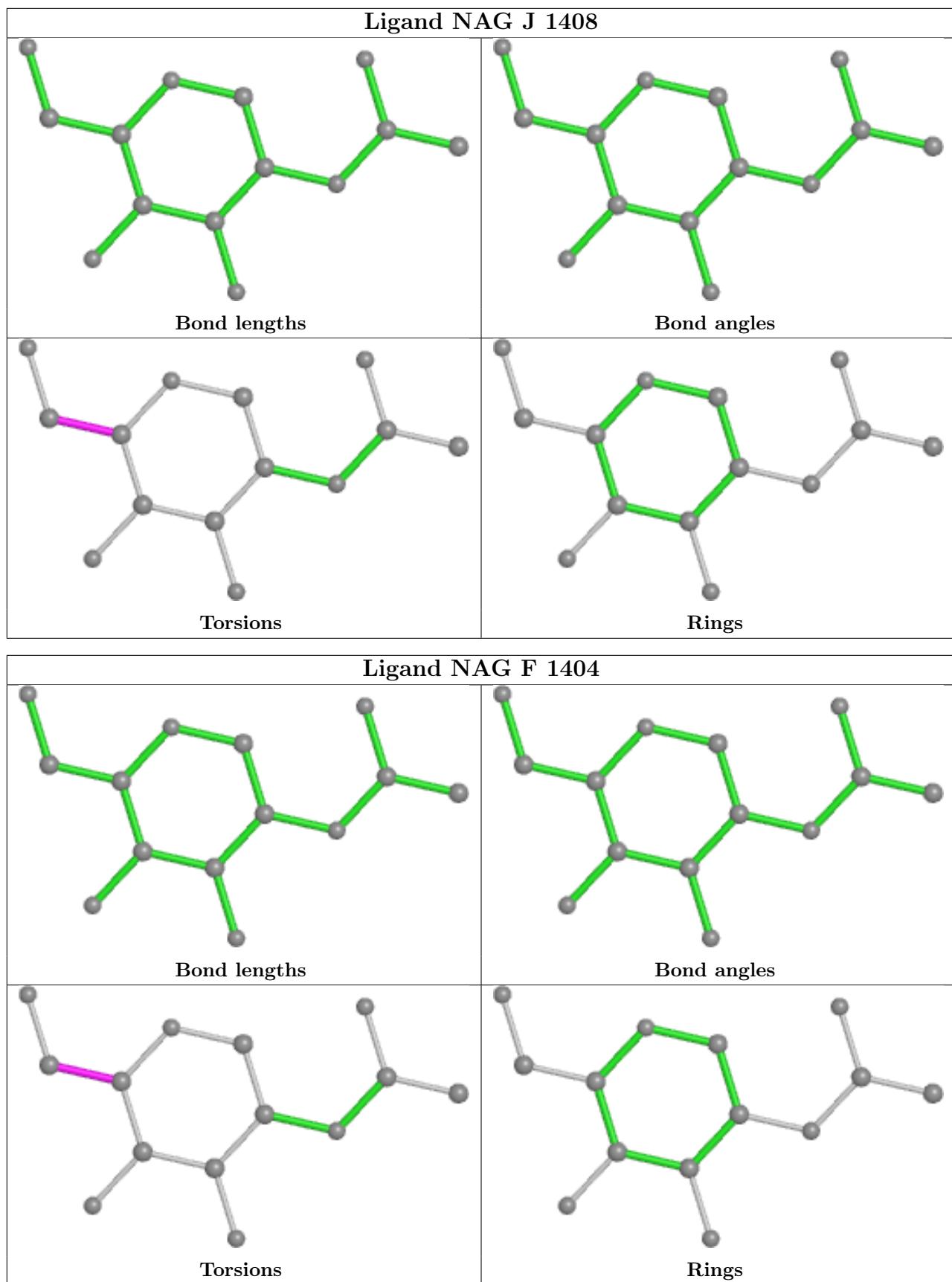


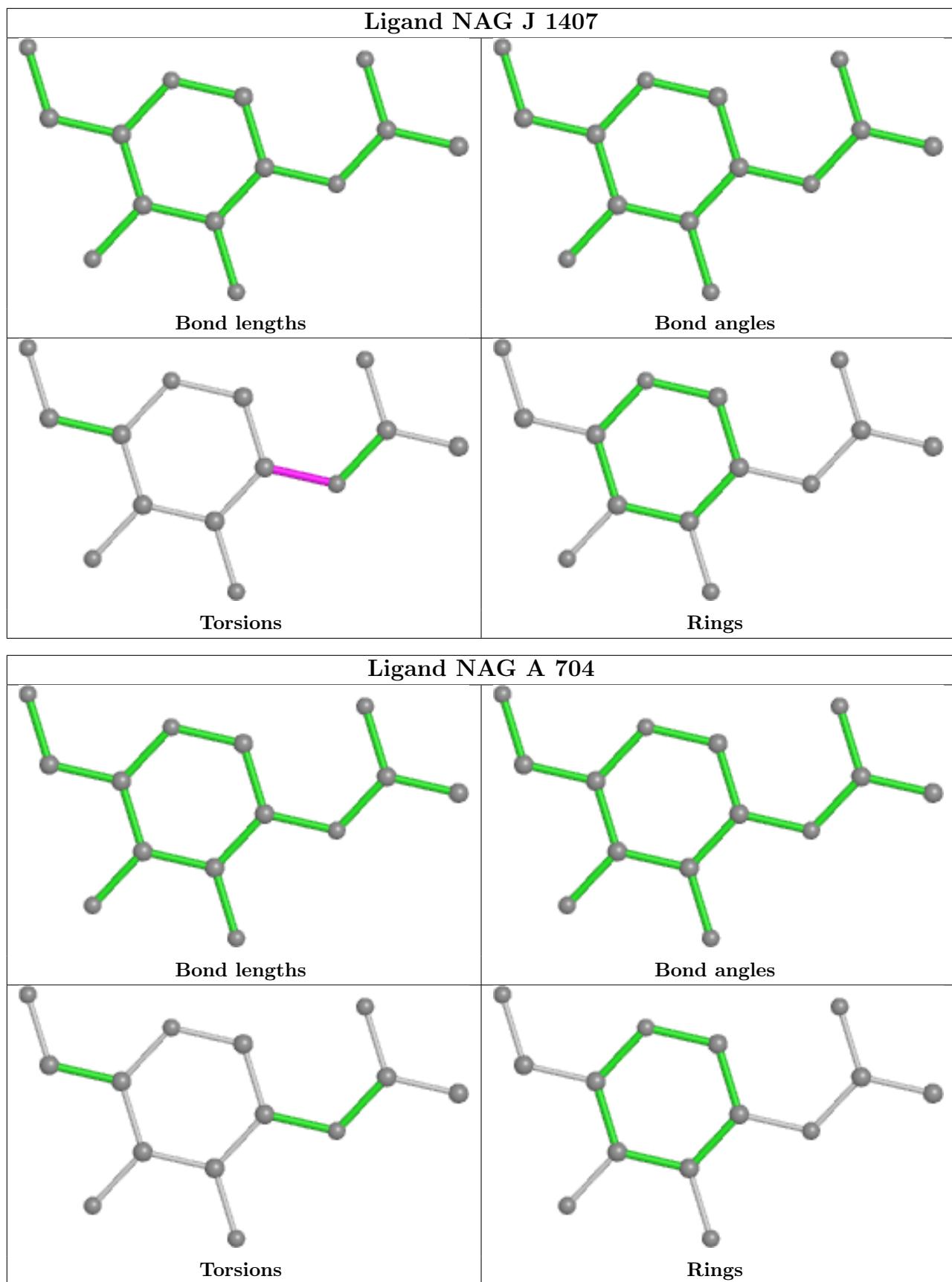


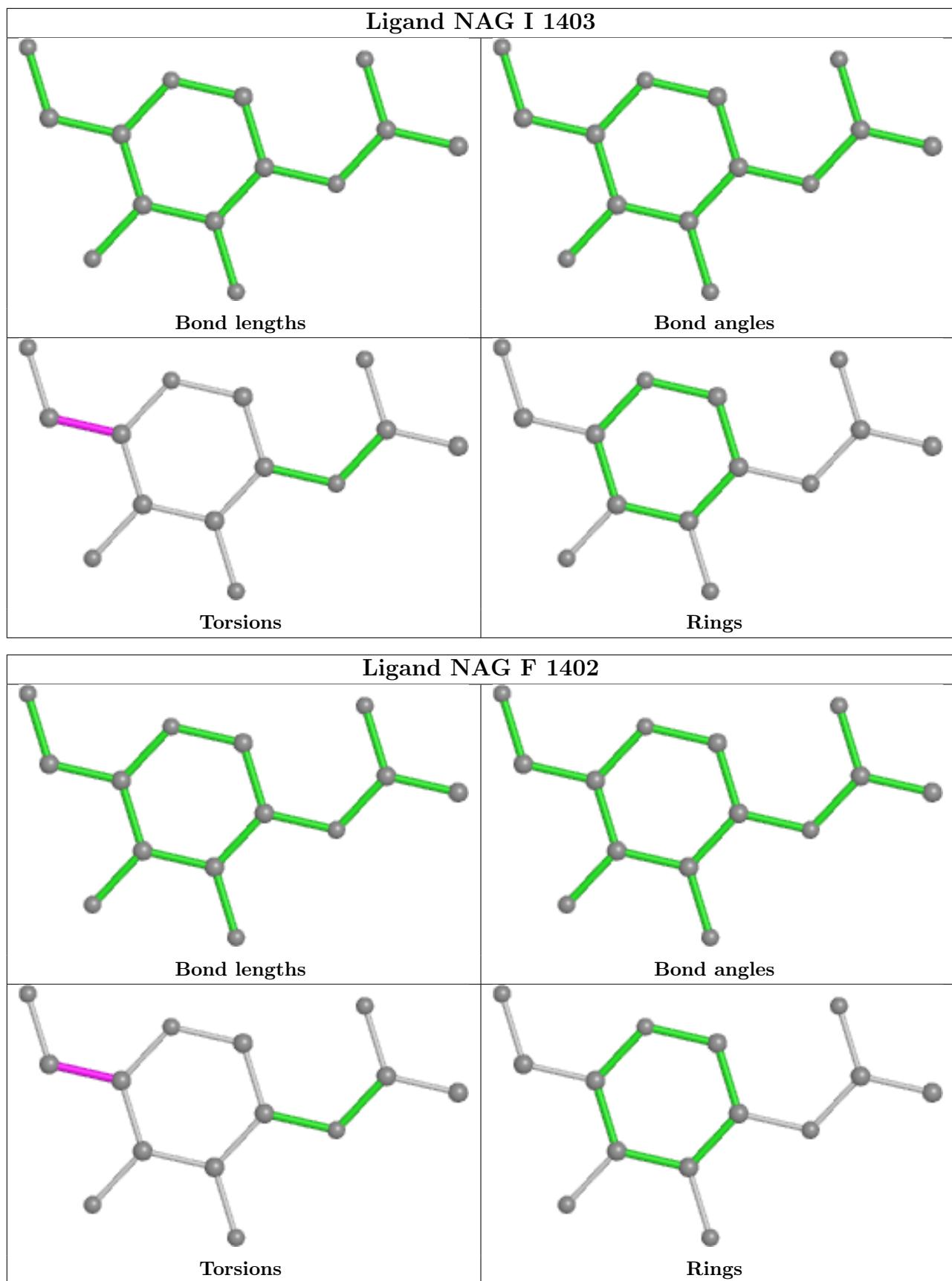


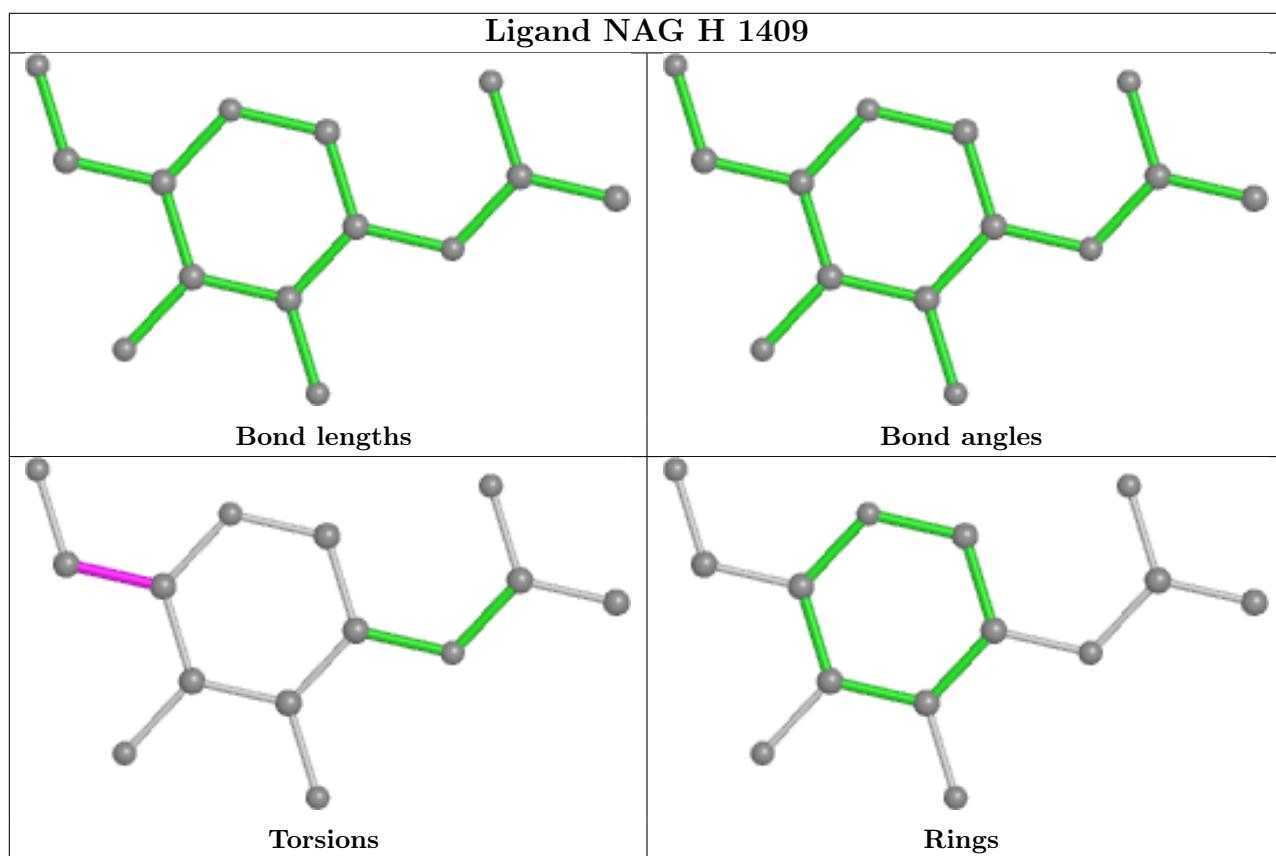
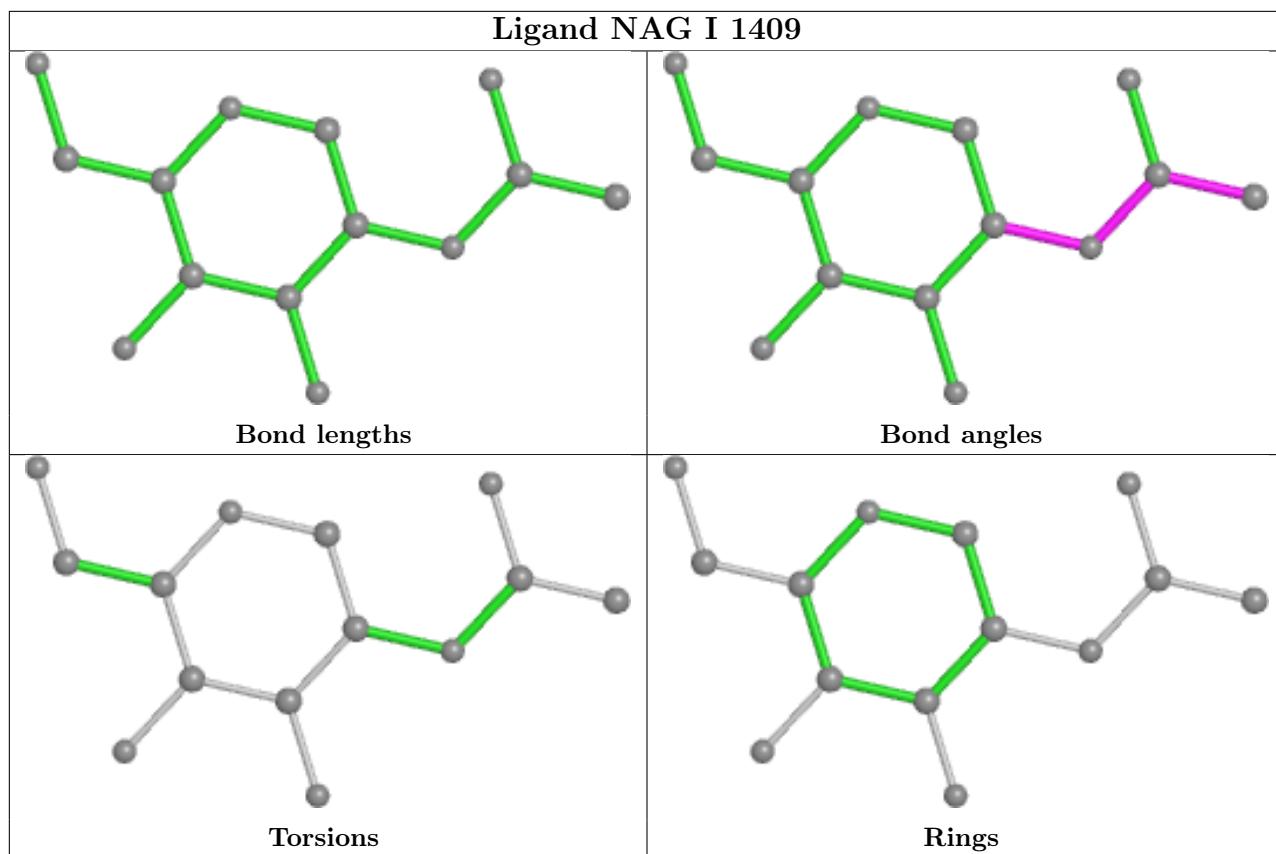


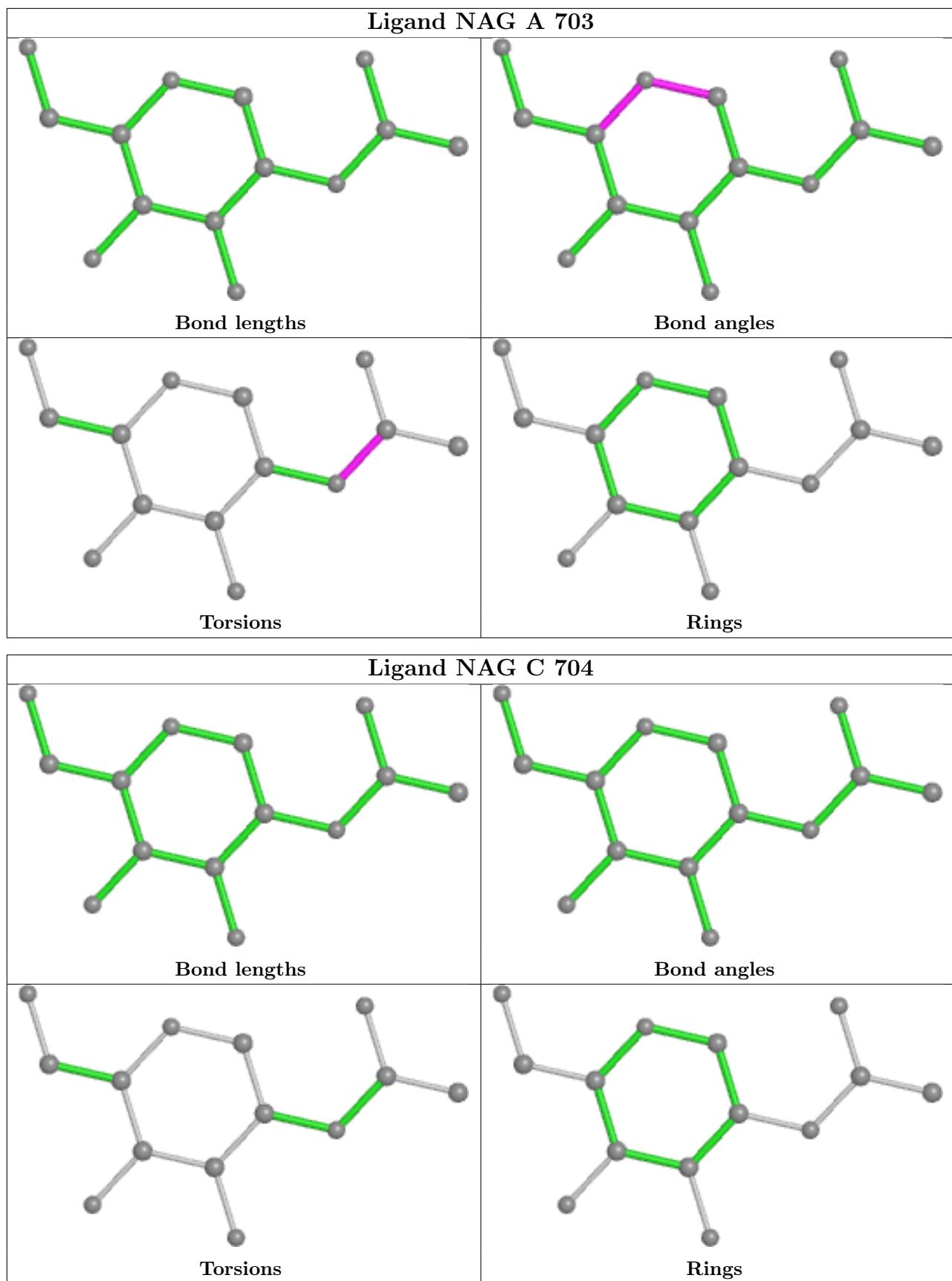


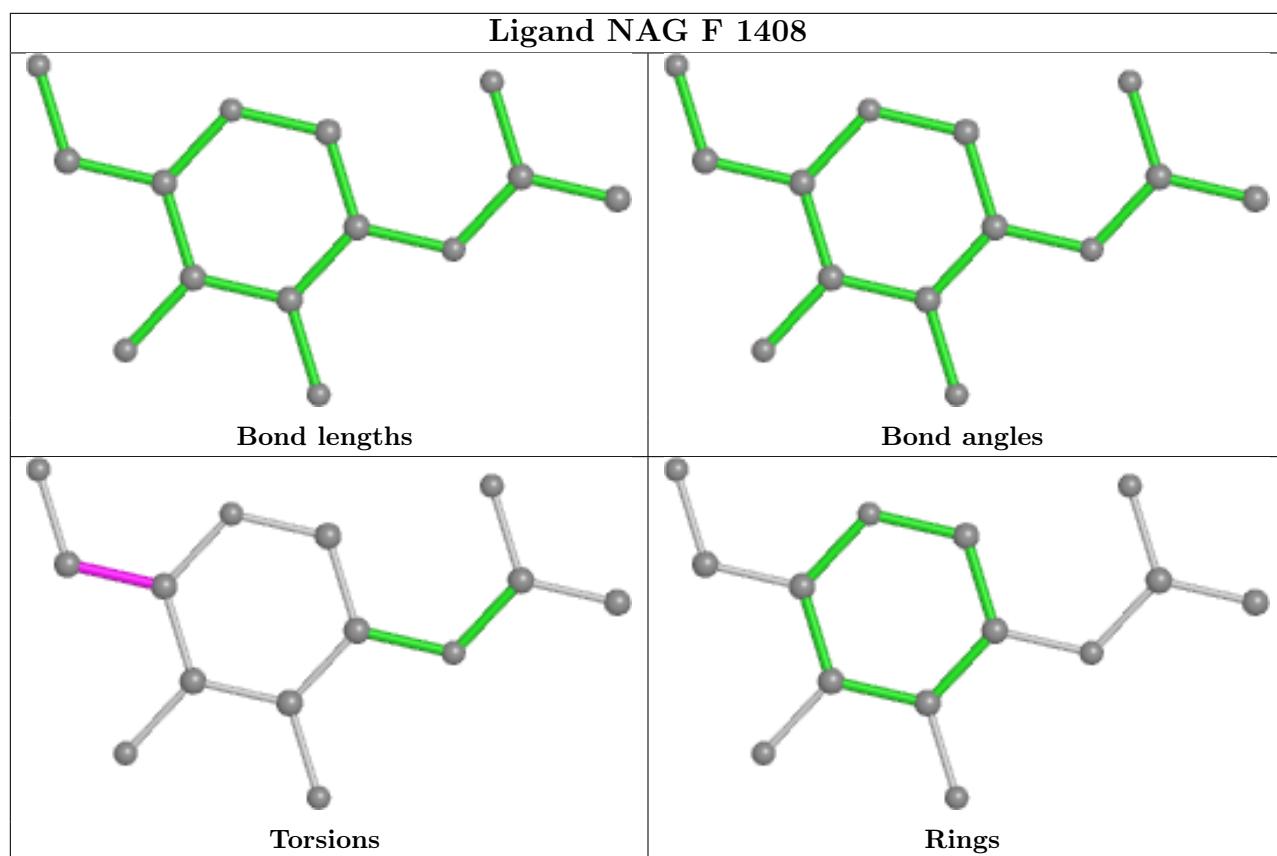












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

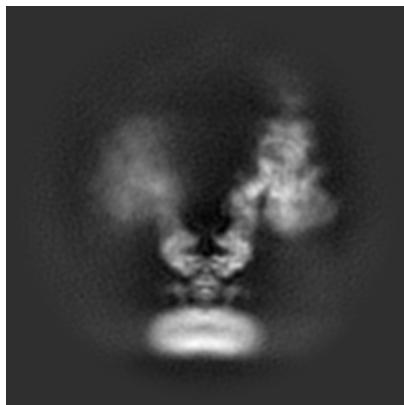
## 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30888. These allow visual inspection of the internal detail of the map and identification of artifacts.

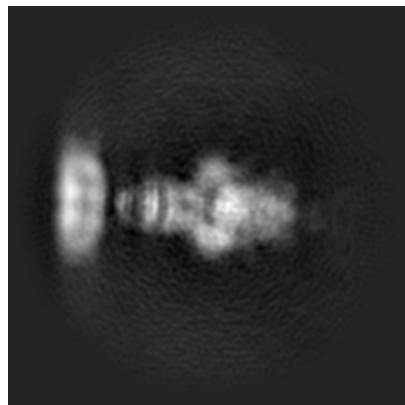
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections (i)

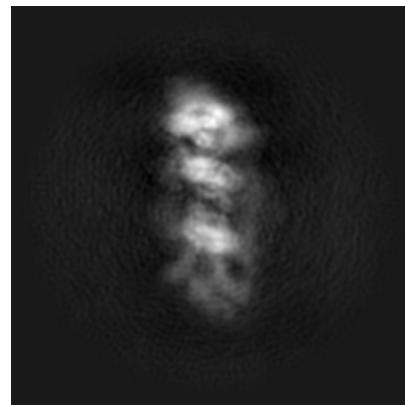
#### 6.1.1 Primary map



X



Y

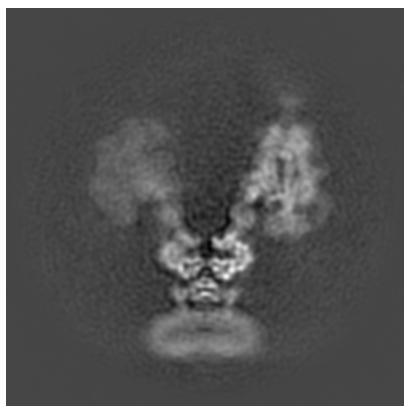


Z

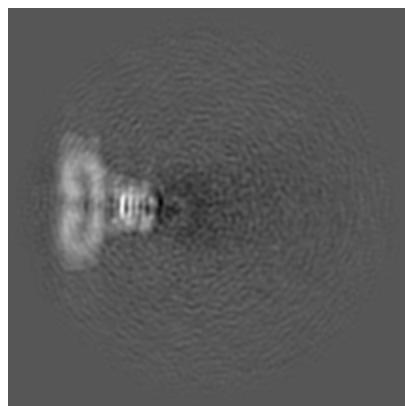
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices (i)

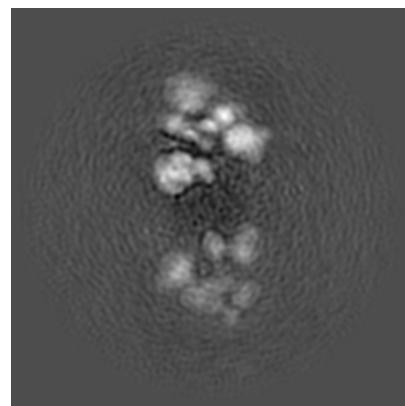
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

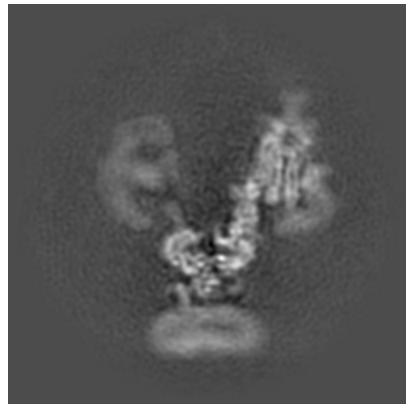


Z Index: 240

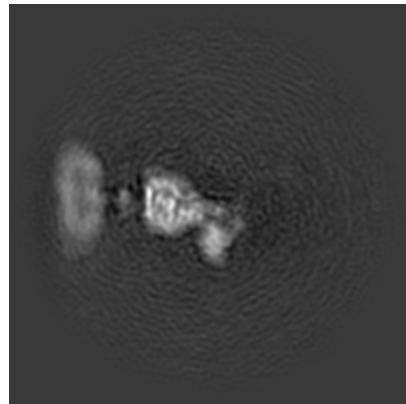
The images above show central slices of the map in three orthogonal directions.

### 6.3 Largest variance slices [\(i\)](#)

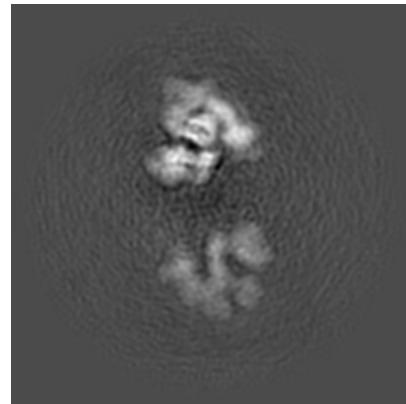
#### 6.3.1 Primary map



X Index: 231



Y Index: 279



Z Index: 253

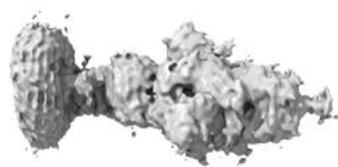
The images above show the largest variance slices of the map in three orthogonal directions.

### 6.4 Orthogonal surface views [\(i\)](#)

#### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

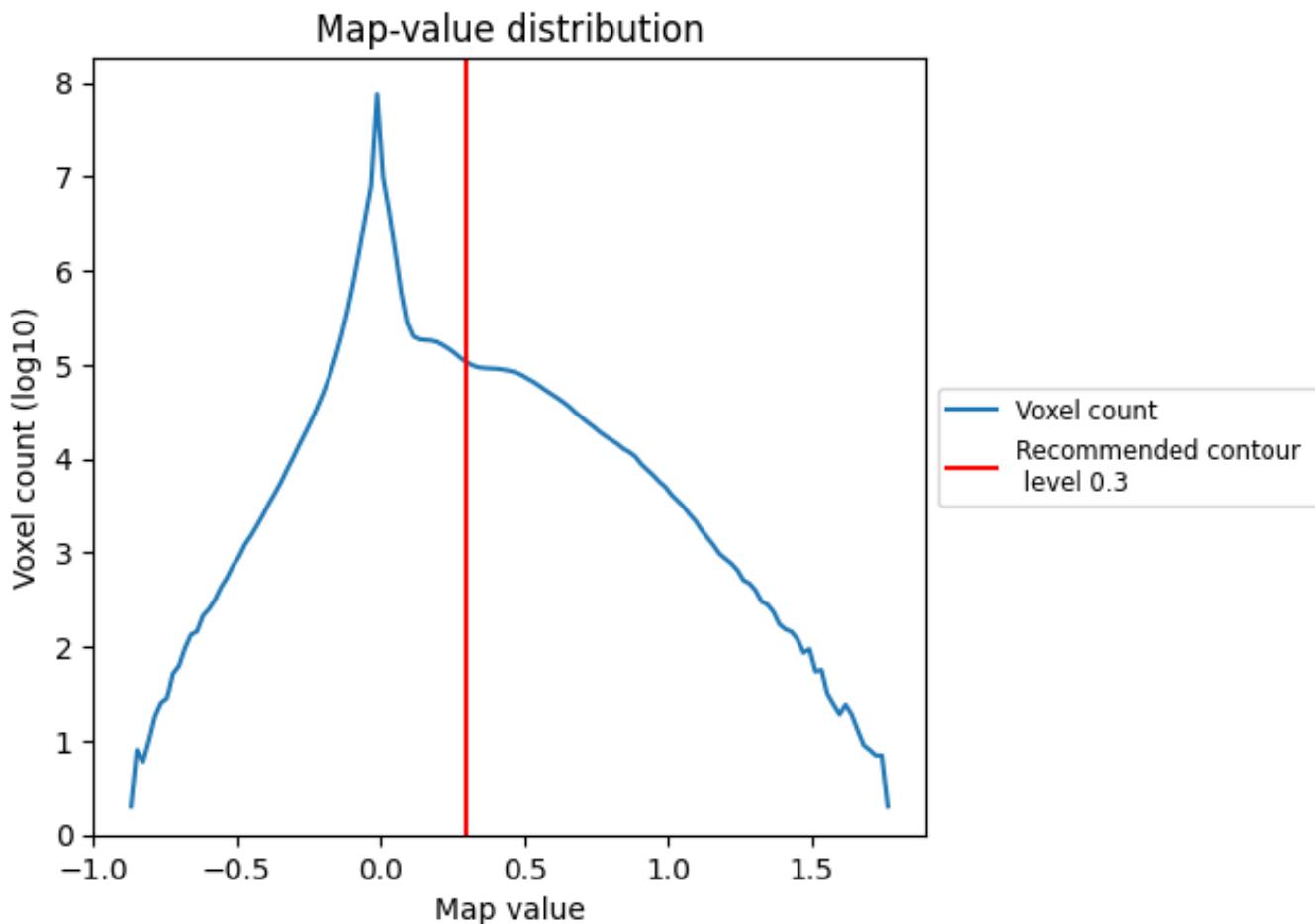
## 6.5 Mask visualisation

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

## 7 Map analysis (i)

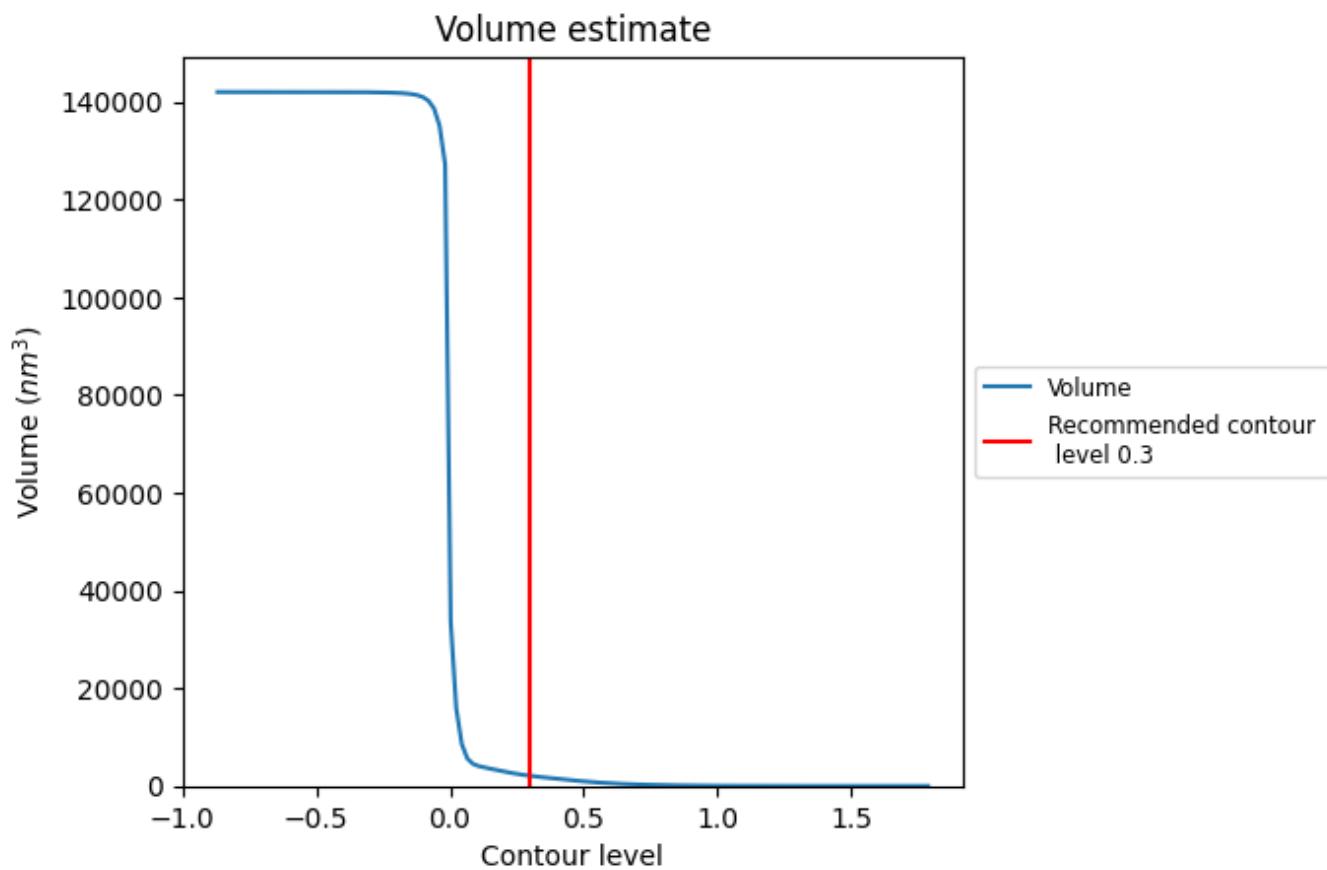
This section contains the results of statistical analysis of the map.

### 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.

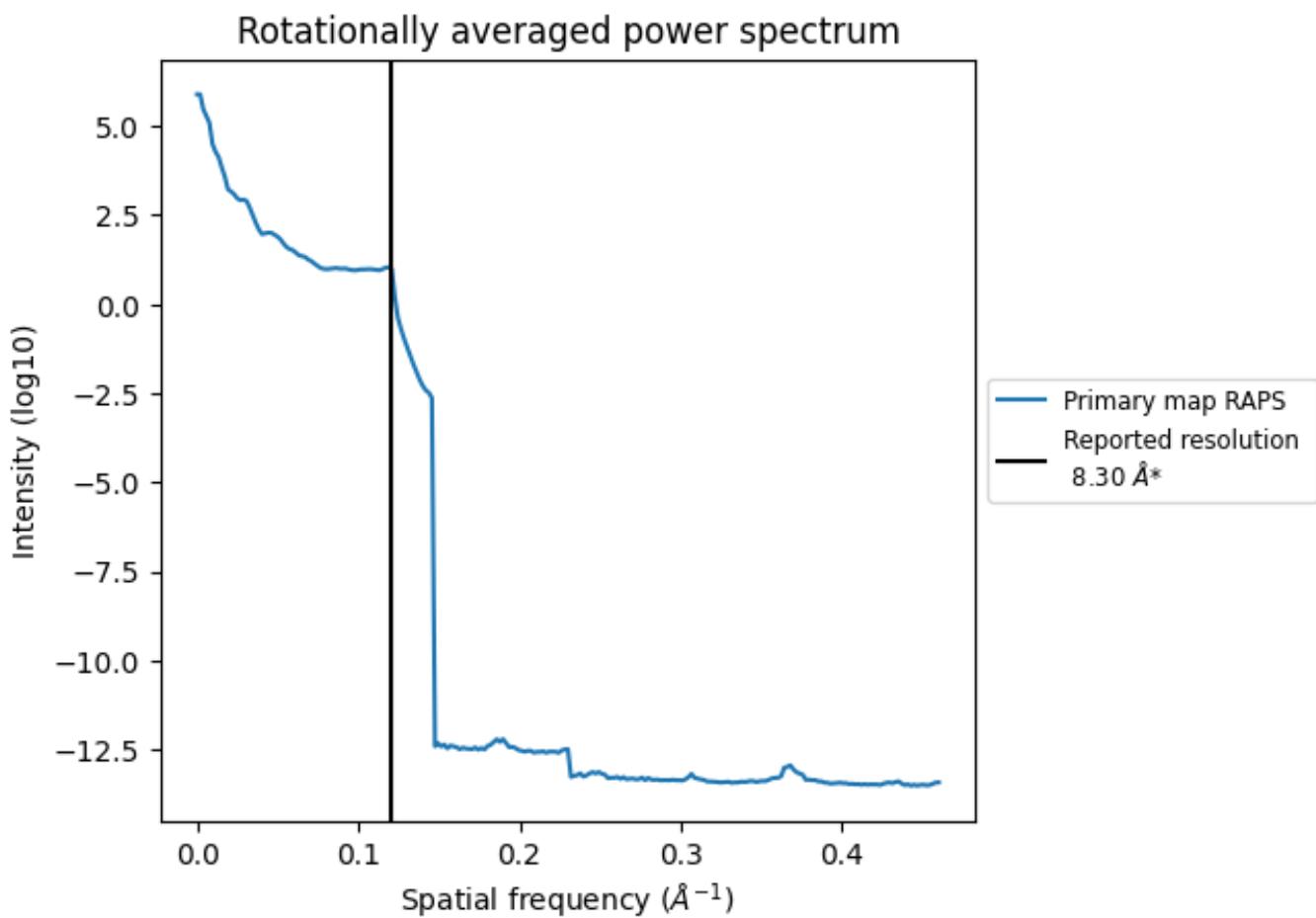
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is  $2071 \text{ nm}^3$ ; this corresponds to an approximate mass of  $1871 \text{ kDa}$ .

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 [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of  $0.120 \text{ \AA}^{-1}$

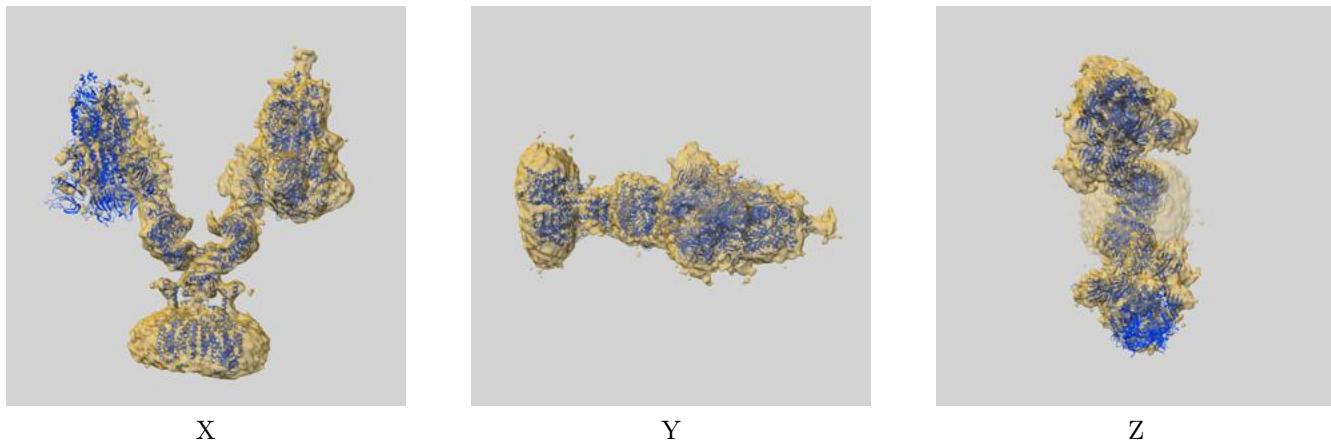
## 8 Fourier-Shell correlation [i](#)

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

## 9 Map-model fit (i)

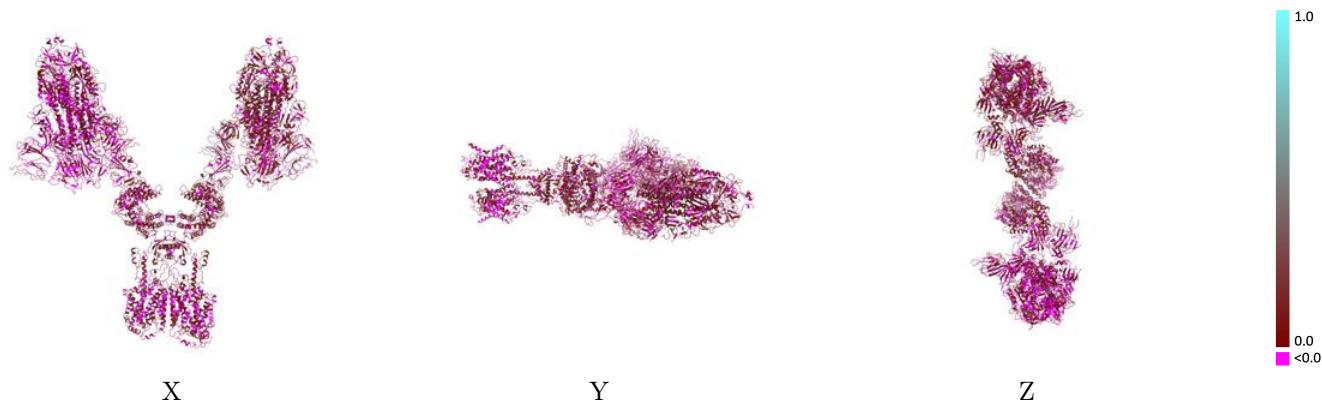
This section contains information regarding the fit between EMDB map EMD-30888 and PDB model 7DWX. Per-residue inclusion information can be found in section [3](#) on page [18](#).

### 9.1 Map-model overlay (i)



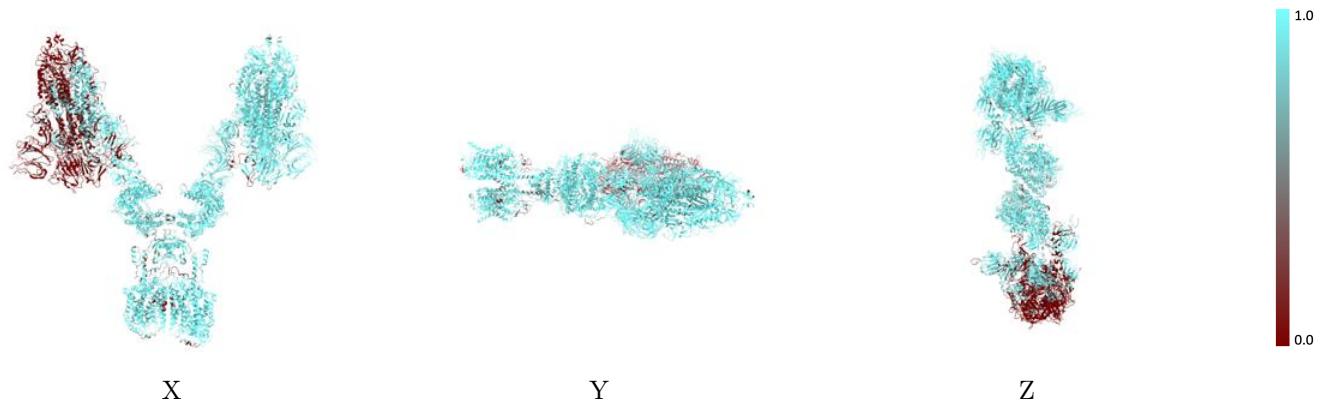
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



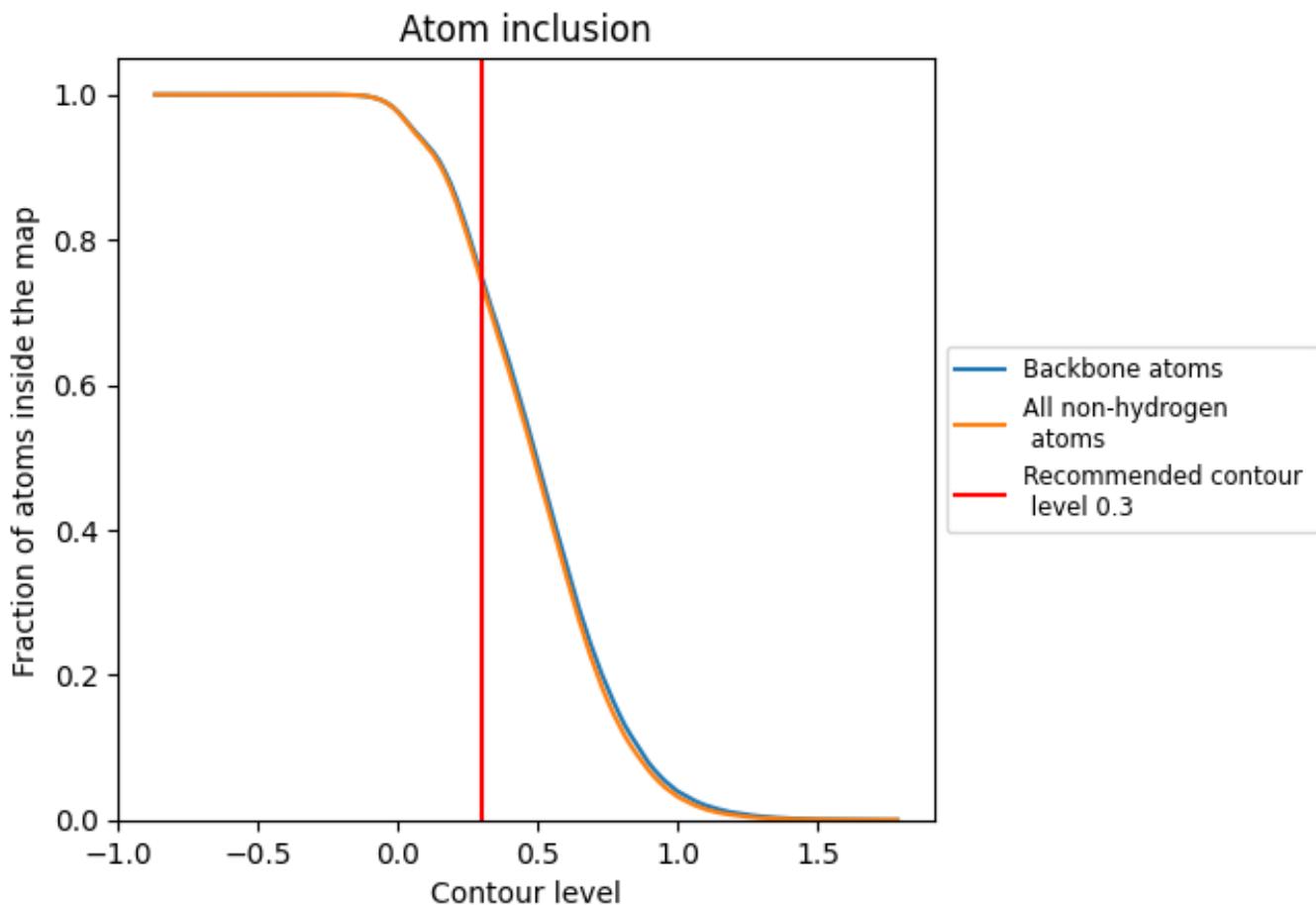
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

## 9.4 Atom inclusion [\(i\)](#)



At the recommended contour level, 75% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7381	0.0590
0	0.0000	<0.0
1	0.0000	0.2380
2	0.0000	-0.0390
3	0.0000	0.0190
4	0.0357	0.2120
5	0.6071	0.0500
6	0.0000	0.0020
7	0.0000	-0.2070
8	0.1071	-0.0560
9	0.0357	-0.0570
A	0.9273	0.0490
AA	0.0000	-0.0820
B	0.9439	0.1070
BA	0.0000	-0.0660
C	0.9087	0.0470
CA	0.0000	0.1510
D	0.9068	0.0910
DA	0.0000	-0.0150
E	0.9640	0.0800
EA	0.0000	-0.0910
F	0.9468	0.0870
FA	0.0000	-0.0470
G	0.9252	0.0690
H	0.5642	0.0340
I	0.4232	0.0240
J	0.1580	0.0150
K	0.5357	0.0770
L	0.7143	0.0810
M	0.8214	0.0720
N	1.0000	0.0400
O	0.2143	-0.0370
P	0.8214	0.0760
Q	0.8214	0.0990
R	0.5357	0.0400



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Chain	Atom inclusion	Q-score
S	0.2857	0.1170
T	0.7857	0.0600
U	0.7857	0.0600
V	0.2500	0.0480
W	0.9286	0.0700
X	1.0000	0.2210
Y	1.0000	0.2510
Z	1.0000	0.1410
a	0.8929	0.0060
b	0.8214	0.0300
c	0.5714	0.0880
d	0.4643	-0.0740
e	0.5714	0.1110
f	0.3929	0.0910
g	0.8214	-0.0920
h	0.9286	0.0370
i	0.8214	0.1070
j	0.5714	0.0380
k	0.4286	-0.0010
l	0.7857	0.0880
m	0.9643	0.1240
n	1.0000	0.1630
o	0.5000	-0.0350
p	1.0000	0.1070
q	1.0000	0.1420
r	0.7500	0.0740
s	0.6786	0.0080
t	0.7500	0.0860
u	0.2500	0.0420
v	0.6429	0.0270
w	0.1429	-0.0040
x	0.0000	0.1240
y	0.0000	-0.1520
z	0.0000	-0.1580