



wwPDB EM Validation Summary Report ⓘ

Nov 11, 2024 – 06:40 PM JST

PDB ID : 7V7I
EMDB ID : EMD-31772
Title : Cryo-EM structure of SARS-CoV-2 S-Kappa variant (B.1.617.1), dimer of S trimer conformation 2
Authors : Yang, T.J.; Yu, P.Y.; Chang, Y.C.; Hsu, S.T.D.
Deposited on : 2021-08-21
Resolution : 3.30 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

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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

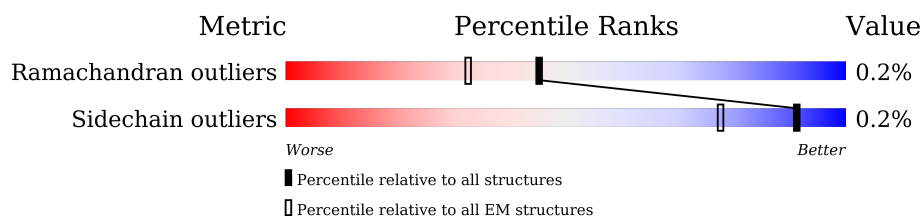
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.









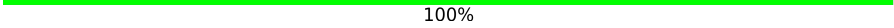
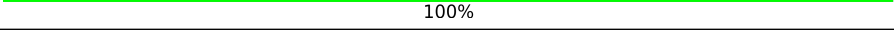
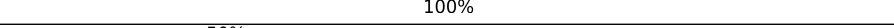
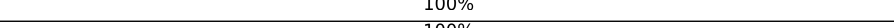
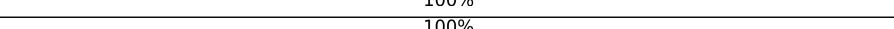

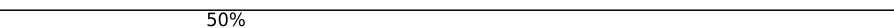
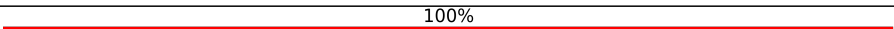











Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1283	
1	B	1283	
1	C	1283	
1	D	1283	
1	E	1283	
1	F	1283	
2	0	2	
2	1	2	
2	2	2	

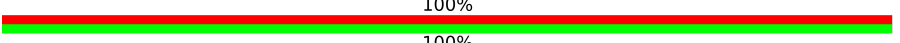

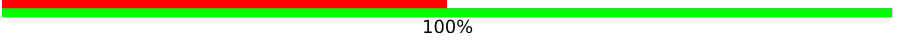
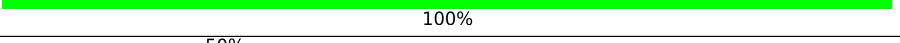
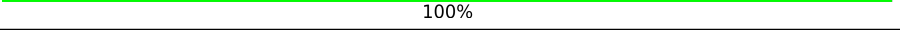
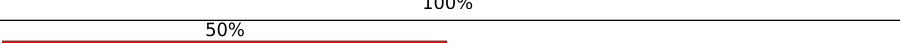

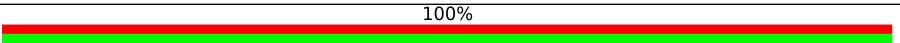



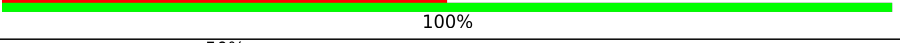
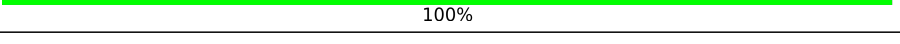
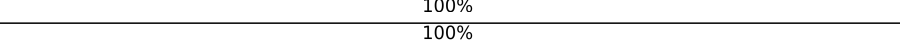

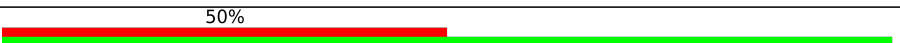

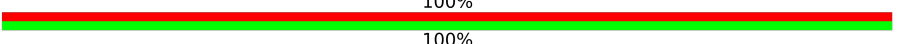

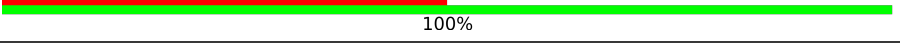
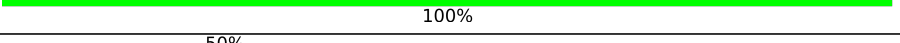
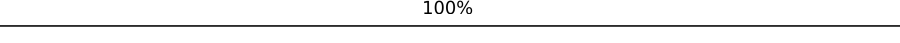
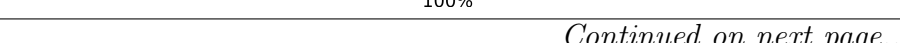


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	3	2	100% 
2	4	2	100% 
2	5	2	50%  100%
2	7	2	50%  100%
2	8	2	100%  100%
2	9	2	50%  100%
2	AA	2	50%  100%
2	BA	2	100%  100%
2	CA	2	50%  100%
2	DA	2	50%  100%
2	EA	2	100%  100%
2	FA	2	100%  50% 50%
2	G	2	50%  100%
2	GA	2	50%  100%
2	H	2	100%  100%
2	HA	2	50%  100%
2	I	2	50%  100%
2	J	2	50%  100%
2	JA	2	50%  100%
2	KA	2	50%  100%
2	L	2	50%  100%
2	LA	2	50%  100%
2	M	2	50%  100%
2	MA	2	50%  100%
2	N	2	100% 

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	NA	2	100% 
2	O	2	50%  100%
2	OA	2	50%  100%
2	P	2	50%  100%
2	PA	2	50%  100%
2	Q	2	 100%
2	R	2	50%  100%
2	S	2	50%  100%
2	T	2	100%  100%
2	U	2	50%  100%
2	V	2	50%  100%
2	X	2	50%  100%
2	Y	2	50%  100%
2	Z	2	50%  100%
2	a	2	 100%
2	b	2	50%  50%
2	c	2	50%  100%
2	d	2	50%  100%
2	e	2	50%  100%
2	f	2	100%  100%
2	g	2	50%  100%
2	h	2	50%  100%
2	j	2	50%  100%
2	k	2	50%  100%
2	l	2	 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	m	2	<div> <div>50%</div> <div>100%</div> </div>
2	n	2	<div> <div>50%</div> <div>100%</div> </div>
2	o	2	<div> <div>50%</div> <div>100%</div> </div>
2	p	2	<div> <div>50%</div> <div>100%</div> </div>
2	q	2	<div> <div>50%</div> <div>100%</div> </div>
2	r	2	<div> <div>50%</div> <div>100%</div> <div>50%</div> </div>
2	s	2	<div> <div>100%</div> <div>100%</div> </div>
2	t	2	<div> <div>50%</div> <div>100%</div> </div>
2	v	2	<div> <div>50%</div> <div>100%</div> </div>
2	w	2	<div> <div>100%</div> <div>100%</div> </div>
2	x	2	<div> <div>50%</div> <div>100%</div> </div>
2	y	2	<div> <div>50%</div> <div>100%</div> </div>
2	z	2	<div> <div>100%</div> <div>50%</div> </div>
3	6	3	<div> <div>33%</div> <div>100%</div> </div>
3	IA	3	<div> <div>33%</div> <div>100%</div> </div>
3	K	3	<div> <div>33%</div> <div>100%</div> </div>
3	W	3	<div> <div>33%</div> <div>100%</div> </div>
3	i	3	<div> <div>33%</div> <div>100%</div> </div>
3	u	3	<div> <div>33%</div> <div>100%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 51072 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1038	Total	C	N	O	S	0	0
			8109	5177	1351	1544	37		
1	B	1038	Total	C	N	O	S	0	0
			8109	5177	1351	1544	37		
1	C	1038	Total	C	N	O	S	0	0
			8109	5177	1351	1544	37		
1	D	1038	Total	C	N	O	S	0	0
			8109	5177	1351	1544	37		
1	E	1038	Total	C	N	O	S	0	0
			8109	5177	1351	1544	37		
1	F	1038	Total	C	N	O	S	0	0
			8109	5177	1351	1544	37		

There are 522 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	ASP	GLY	engineered mutation	UNP P0DTC2
A	154	LYS	GLU	engineered mutation	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	484	GLN	GLU	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1071	HIS	GLN	engineered mutation	UNP P0DTC2
A	1101	ASP	HIS	engineered mutation	UNP P0DTC2
A	1209	GLU	-	expression tag	UNP P0DTC2
A	1210	PHE	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	SER	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1215	TYR	-	expression tag	UNP P0DTC2
A	1216	ILE	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	GLU	-	expression tag	UNP P0DTC2
A	1219	ALA	-	expression tag	UNP P0DTC2
A	1220	PRO	-	expression tag	UNP P0DTC2
A	1221	ARG	-	expression tag	UNP P0DTC2
A	1222	ASP	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLN	-	expression tag	UNP P0DTC2
A	1225	ALA	-	expression tag	UNP P0DTC2
A	1226	TYR	-	expression tag	UNP P0DTC2
A	1227	VAL	-	expression tag	UNP P0DTC2
A	1228	ARG	-	expression tag	UNP P0DTC2
A	1229	LYS	-	expression tag	UNP P0DTC2
A	1230	ASP	-	expression tag	UNP P0DTC2
A	1231	GLY	-	expression tag	UNP P0DTC2
A	1232	GLU	-	expression tag	UNP P0DTC2
A	1233	TRP	-	expression tag	UNP P0DTC2
A	1234	VAL	-	expression tag	UNP P0DTC2
A	1235	LEU	-	expression tag	UNP P0DTC2
A	1236	LEU	-	expression tag	UNP P0DTC2
A	1237	SER	-	expression tag	UNP P0DTC2
A	1238	THR	-	expression tag	UNP P0DTC2
A	1239	PHE	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	LYS	-	expression tag	UNP P0DTC2
A	1242	GLY	-	expression tag	UNP P0DTC2
A	1243	GLN	-	expression tag	UNP P0DTC2
A	1244	ASP	-	expression tag	UNP P0DTC2
A	1245	ASN	-	expression tag	UNP P0DTC2
A	1246	SER	-	expression tag	UNP P0DTC2
A	1247	ALA	-	expression tag	UNP P0DTC2
A	1248	ASP	-	expression tag	UNP P0DTC2
A	1249	ILE	-	expression tag	UNP P0DTC2
A	1250	GLN	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	SER	-	expression tag	UNP P0DTC2
A	1253	GLY	-	expression tag	UNP P0DTC2
A	1254	ARG	-	expression tag	UNP P0DTC2
A	1255	PRO	-	expression tag	UNP P0DTC2
A	1256	LEU	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1257	GLU	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ARG	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	PRO	-	expression tag	UNP P0DTC2
A	1262	PHE	-	expression tag	UNP P0DTC2
A	1263	GLU	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	LYS	-	expression tag	UNP P0DTC2
A	1266	LEU	-	expression tag	UNP P0DTC2
A	1267	ILE	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	GLU	-	expression tag	UNP P0DTC2
A	1270	GLU	-	expression tag	UNP P0DTC2
A	1271	ASP	-	expression tag	UNP P0DTC2
A	1272	LEU	-	expression tag	UNP P0DTC2
A	1273	ASN	-	expression tag	UNP P0DTC2
A	1274	MET	-	expression tag	UNP P0DTC2
A	1275	HIS	-	expression tag	UNP P0DTC2
A	1276	THR	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	HIS	-	expression tag	UNP P0DTC2
A	1279	HIS	-	expression tag	UNP P0DTC2
A	1280	HIS	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
B	142	ASP	GLY	engineered mutation	UNP P0DTC2
B	154	LYS	GLU	engineered mutation	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	484	GLN	GLU	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1071	HIS	GLN	engineered mutation	UNP P0DTC2
B	1101	ASP	HIS	engineered mutation	UNP P0DTC2
B	1209	GLU	-	expression tag	UNP P0DTC2
B	1210	PHE	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1212	SER	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	TYR	-	expression tag	UNP P0DTC2
B	1216	ILE	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	GLU	-	expression tag	UNP P0DTC2
B	1219	ALA	-	expression tag	UNP P0DTC2
B	1220	PRO	-	expression tag	UNP P0DTC2
B	1221	ARG	-	expression tag	UNP P0DTC2
B	1222	ASP	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLN	-	expression tag	UNP P0DTC2
B	1225	ALA	-	expression tag	UNP P0DTC2
B	1226	TYR	-	expression tag	UNP P0DTC2
B	1227	VAL	-	expression tag	UNP P0DTC2
B	1228	ARG	-	expression tag	UNP P0DTC2
B	1229	LYS	-	expression tag	UNP P0DTC2
B	1230	ASP	-	expression tag	UNP P0DTC2
B	1231	GLY	-	expression tag	UNP P0DTC2
B	1232	GLU	-	expression tag	UNP P0DTC2
B	1233	TRP	-	expression tag	UNP P0DTC2
B	1234	VAL	-	expression tag	UNP P0DTC2
B	1235	LEU	-	expression tag	UNP P0DTC2
B	1236	LEU	-	expression tag	UNP P0DTC2
B	1237	SER	-	expression tag	UNP P0DTC2
B	1238	THR	-	expression tag	UNP P0DTC2
B	1239	PHE	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	LYS	-	expression tag	UNP P0DTC2
B	1242	GLY	-	expression tag	UNP P0DTC2
B	1243	GLN	-	expression tag	UNP P0DTC2
B	1244	ASP	-	expression tag	UNP P0DTC2
B	1245	ASN	-	expression tag	UNP P0DTC2
B	1246	SER	-	expression tag	UNP P0DTC2
B	1247	ALA	-	expression tag	UNP P0DTC2
B	1248	ASP	-	expression tag	UNP P0DTC2
B	1249	ILE	-	expression tag	UNP P0DTC2
B	1250	GLN	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	SER	-	expression tag	UNP P0DTC2
B	1253	GLY	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1254	ARG	-	expression tag	UNP P0DTC2
B	1255	PRO	-	expression tag	UNP P0DTC2
B	1256	LEU	-	expression tag	UNP P0DTC2
B	1257	GLU	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ARG	-	expression tag	UNP P0DTC2
B	1260	GLY	-	expression tag	UNP P0DTC2
B	1261	PRO	-	expression tag	UNP P0DTC2
B	1262	PHE	-	expression tag	UNP P0DTC2
B	1263	GLU	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	LYS	-	expression tag	UNP P0DTC2
B	1266	LEU	-	expression tag	UNP P0DTC2
B	1267	ILE	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	GLU	-	expression tag	UNP P0DTC2
B	1270	GLU	-	expression tag	UNP P0DTC2
B	1271	ASP	-	expression tag	UNP P0DTC2
B	1272	LEU	-	expression tag	UNP P0DTC2
B	1273	ASN	-	expression tag	UNP P0DTC2
B	1274	MET	-	expression tag	UNP P0DTC2
B	1275	HIS	-	expression tag	UNP P0DTC2
B	1276	THR	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	HIS	-	expression tag	UNP P0DTC2
B	1279	HIS	-	expression tag	UNP P0DTC2
B	1280	HIS	-	expression tag	UNP P0DTC2
B	1281	HIS	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
C	142	ASP	GLY	engineered mutation	UNP P0DTC2
C	154	LYS	GLU	engineered mutation	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	484	GLN	GLU	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1071	HIS	GLN	engineered mutation	UNP P0DTC2
C	1101	ASP	HIS	engineered mutation	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1209	GLU	-	expression tag	UNP P0DTC2
C	1210	PHE	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	SER	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2
C	1215	TYR	-	expression tag	UNP P0DTC2
C	1216	ILE	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	GLU	-	expression tag	UNP P0DTC2
C	1219	ALA	-	expression tag	UNP P0DTC2
C	1220	PRO	-	expression tag	UNP P0DTC2
C	1221	ARG	-	expression tag	UNP P0DTC2
C	1222	ASP	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	GLN	-	expression tag	UNP P0DTC2
C	1225	ALA	-	expression tag	UNP P0DTC2
C	1226	TYR	-	expression tag	UNP P0DTC2
C	1227	VAL	-	expression tag	UNP P0DTC2
C	1228	ARG	-	expression tag	UNP P0DTC2
C	1229	LYS	-	expression tag	UNP P0DTC2
C	1230	ASP	-	expression tag	UNP P0DTC2
C	1231	GLY	-	expression tag	UNP P0DTC2
C	1232	GLU	-	expression tag	UNP P0DTC2
C	1233	TRP	-	expression tag	UNP P0DTC2
C	1234	VAL	-	expression tag	UNP P0DTC2
C	1235	LEU	-	expression tag	UNP P0DTC2
C	1236	LEU	-	expression tag	UNP P0DTC2
C	1237	SER	-	expression tag	UNP P0DTC2
C	1238	THR	-	expression tag	UNP P0DTC2
C	1239	PHE	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	LYS	-	expression tag	UNP P0DTC2
C	1242	GLY	-	expression tag	UNP P0DTC2
C	1243	GLN	-	expression tag	UNP P0DTC2
C	1244	ASP	-	expression tag	UNP P0DTC2
C	1245	ASN	-	expression tag	UNP P0DTC2
C	1246	SER	-	expression tag	UNP P0DTC2
C	1247	ALA	-	expression tag	UNP P0DTC2
C	1248	ASP	-	expression tag	UNP P0DTC2
C	1249	ILE	-	expression tag	UNP P0DTC2
C	1250	GLN	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	SER	-	expression tag	UNP P0DTC2
C	1253	GLY	-	expression tag	UNP P0DTC2
C	1254	ARG	-	expression tag	UNP P0DTC2
C	1255	PRO	-	expression tag	UNP P0DTC2
C	1256	LEU	-	expression tag	UNP P0DTC2
C	1257	GLU	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ARG	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2
C	1261	PRO	-	expression tag	UNP P0DTC2
C	1262	PHE	-	expression tag	UNP P0DTC2
C	1263	GLU	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	LYS	-	expression tag	UNP P0DTC2
C	1266	LEU	-	expression tag	UNP P0DTC2
C	1267	ILE	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	GLU	-	expression tag	UNP P0DTC2
C	1270	GLU	-	expression tag	UNP P0DTC2
C	1271	ASP	-	expression tag	UNP P0DTC2
C	1272	LEU	-	expression tag	UNP P0DTC2
C	1273	ASN	-	expression tag	UNP P0DTC2
C	1274	MET	-	expression tag	UNP P0DTC2
C	1275	HIS	-	expression tag	UNP P0DTC2
C	1276	THR	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	HIS	-	expression tag	UNP P0DTC2
C	1279	HIS	-	expression tag	UNP P0DTC2
C	1280	HIS	-	expression tag	UNP P0DTC2
C	1281	HIS	-	expression tag	UNP P0DTC2
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
D	142	ASP	GLY	engineered mutation	UNP P0DTC2
D	154	LYS	GLU	engineered mutation	UNP P0DTC2
D	452	ARG	LEU	variant	UNP P0DTC2
D	484	GLN	GLU	variant	UNP P0DTC2
D	614	GLY	ASP	variant	UNP P0DTC2
D	682	GLY	ARG	engineered mutation	UNP P0DTC2
D	683	SER	ARG	engineered mutation	UNP P0DTC2
D	685	SER	ARG	engineered mutation	UNP P0DTC2
D	986	PRO	LYS	engineered mutation	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	987	PRO	VAL	engineered mutation	UNP P0DTC2
D	1071	HIS	GLN	engineered mutation	UNP P0DTC2
D	1101	ASP	HIS	engineered mutation	UNP P0DTC2
D	1209	GLU	-	expression tag	UNP P0DTC2
D	1210	PHE	-	expression tag	UNP P0DTC2
D	1211	GLY	-	expression tag	UNP P0DTC2
D	1212	SER	-	expression tag	UNP P0DTC2
D	1213	GLY	-	expression tag	UNP P0DTC2
D	1214	GLY	-	expression tag	UNP P0DTC2
D	1215	TYR	-	expression tag	UNP P0DTC2
D	1216	ILE	-	expression tag	UNP P0DTC2
D	1217	PRO	-	expression tag	UNP P0DTC2
D	1218	GLU	-	expression tag	UNP P0DTC2
D	1219	ALA	-	expression tag	UNP P0DTC2
D	1220	PRO	-	expression tag	UNP P0DTC2
D	1221	ARG	-	expression tag	UNP P0DTC2
D	1222	ASP	-	expression tag	UNP P0DTC2
D	1223	GLY	-	expression tag	UNP P0DTC2
D	1224	GLN	-	expression tag	UNP P0DTC2
D	1225	ALA	-	expression tag	UNP P0DTC2
D	1226	TYR	-	expression tag	UNP P0DTC2
D	1227	VAL	-	expression tag	UNP P0DTC2
D	1228	ARG	-	expression tag	UNP P0DTC2
D	1229	LYS	-	expression tag	UNP P0DTC2
D	1230	ASP	-	expression tag	UNP P0DTC2
D	1231	GLY	-	expression tag	UNP P0DTC2
D	1232	GLU	-	expression tag	UNP P0DTC2
D	1233	TRP	-	expression tag	UNP P0DTC2
D	1234	VAL	-	expression tag	UNP P0DTC2
D	1235	LEU	-	expression tag	UNP P0DTC2
D	1236	LEU	-	expression tag	UNP P0DTC2
D	1237	SER	-	expression tag	UNP P0DTC2
D	1238	THR	-	expression tag	UNP P0DTC2
D	1239	PHE	-	expression tag	UNP P0DTC2
D	1240	LEU	-	expression tag	UNP P0DTC2
D	1241	LYS	-	expression tag	UNP P0DTC2
D	1242	GLY	-	expression tag	UNP P0DTC2
D	1243	GLN	-	expression tag	UNP P0DTC2
D	1244	ASP	-	expression tag	UNP P0DTC2
D	1245	ASN	-	expression tag	UNP P0DTC2
D	1246	SER	-	expression tag	UNP P0DTC2
D	1247	ALA	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1248	ASP	-	expression tag	UNP P0DTC2
D	1249	ILE	-	expression tag	UNP P0DTC2
D	1250	GLN	-	expression tag	UNP P0DTC2
D	1251	HIS	-	expression tag	UNP P0DTC2
D	1252	SER	-	expression tag	UNP P0DTC2
D	1253	GLY	-	expression tag	UNP P0DTC2
D	1254	ARG	-	expression tag	UNP P0DTC2
D	1255	PRO	-	expression tag	UNP P0DTC2
D	1256	LEU	-	expression tag	UNP P0DTC2
D	1257	GLU	-	expression tag	UNP P0DTC2
D	1258	SER	-	expression tag	UNP P0DTC2
D	1259	ARG	-	expression tag	UNP P0DTC2
D	1260	GLY	-	expression tag	UNP P0DTC2
D	1261	PRO	-	expression tag	UNP P0DTC2
D	1262	PHE	-	expression tag	UNP P0DTC2
D	1263	GLU	-	expression tag	UNP P0DTC2
D	1264	GLN	-	expression tag	UNP P0DTC2
D	1265	LYS	-	expression tag	UNP P0DTC2
D	1266	LEU	-	expression tag	UNP P0DTC2
D	1267	ILE	-	expression tag	UNP P0DTC2
D	1268	SER	-	expression tag	UNP P0DTC2
D	1269	GLU	-	expression tag	UNP P0DTC2
D	1270	GLU	-	expression tag	UNP P0DTC2
D	1271	ASP	-	expression tag	UNP P0DTC2
D	1272	LEU	-	expression tag	UNP P0DTC2
D	1273	ASN	-	expression tag	UNP P0DTC2
D	1274	MET	-	expression tag	UNP P0DTC2
D	1275	HIS	-	expression tag	UNP P0DTC2
D	1276	THR	-	expression tag	UNP P0DTC2
D	1277	GLY	-	expression tag	UNP P0DTC2
D	1278	HIS	-	expression tag	UNP P0DTC2
D	1279	HIS	-	expression tag	UNP P0DTC2
D	1280	HIS	-	expression tag	UNP P0DTC2
D	1281	HIS	-	expression tag	UNP P0DTC2
D	1282	HIS	-	expression tag	UNP P0DTC2
D	1283	HIS	-	expression tag	UNP P0DTC2
E	142	ASP	GLY	engineered mutation	UNP P0DTC2
E	154	LYS	GLU	engineered mutation	UNP P0DTC2
E	452	ARG	LEU	variant	UNP P0DTC2
E	484	GLN	GLU	variant	UNP P0DTC2
E	614	GLY	ASP	variant	UNP P0DTC2
E	682	GLY	ARG	engineered mutation	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	683	SER	ARG	engineered mutation	UNP P0DTC2
E	685	SER	ARG	engineered mutation	UNP P0DTC2
E	986	PRO	LYS	engineered mutation	UNP P0DTC2
E	987	PRO	VAL	engineered mutation	UNP P0DTC2
E	1071	HIS	GLN	engineered mutation	UNP P0DTC2
E	1101	ASP	HIS	engineered mutation	UNP P0DTC2
E	1209	GLU	-	expression tag	UNP P0DTC2
E	1210	PHE	-	expression tag	UNP P0DTC2
E	1211	GLY	-	expression tag	UNP P0DTC2
E	1212	SER	-	expression tag	UNP P0DTC2
E	1213	GLY	-	expression tag	UNP P0DTC2
E	1214	GLY	-	expression tag	UNP P0DTC2
E	1215	TYR	-	expression tag	UNP P0DTC2
E	1216	ILE	-	expression tag	UNP P0DTC2
E	1217	PRO	-	expression tag	UNP P0DTC2
E	1218	GLU	-	expression tag	UNP P0DTC2
E	1219	ALA	-	expression tag	UNP P0DTC2
E	1220	PRO	-	expression tag	UNP P0DTC2
E	1221	ARG	-	expression tag	UNP P0DTC2
E	1222	ASP	-	expression tag	UNP P0DTC2
E	1223	GLY	-	expression tag	UNP P0DTC2
E	1224	GLN	-	expression tag	UNP P0DTC2
E	1225	ALA	-	expression tag	UNP P0DTC2
E	1226	TYR	-	expression tag	UNP P0DTC2
E	1227	VAL	-	expression tag	UNP P0DTC2
E	1228	ARG	-	expression tag	UNP P0DTC2
E	1229	LYS	-	expression tag	UNP P0DTC2
E	1230	ASP	-	expression tag	UNP P0DTC2
E	1231	GLY	-	expression tag	UNP P0DTC2
E	1232	GLU	-	expression tag	UNP P0DTC2
E	1233	TRP	-	expression tag	UNP P0DTC2
E	1234	VAL	-	expression tag	UNP P0DTC2
E	1235	LEU	-	expression tag	UNP P0DTC2
E	1236	LEU	-	expression tag	UNP P0DTC2
E	1237	SER	-	expression tag	UNP P0DTC2
E	1238	THR	-	expression tag	UNP P0DTC2
E	1239	PHE	-	expression tag	UNP P0DTC2
E	1240	LEU	-	expression tag	UNP P0DTC2
E	1241	LYS	-	expression tag	UNP P0DTC2
E	1242	GLY	-	expression tag	UNP P0DTC2
E	1243	GLN	-	expression tag	UNP P0DTC2
E	1244	ASP	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	1245	ASN	-	expression tag	UNP P0DTC2
E	1246	SER	-	expression tag	UNP P0DTC2
E	1247	ALA	-	expression tag	UNP P0DTC2
E	1248	ASP	-	expression tag	UNP P0DTC2
E	1249	ILE	-	expression tag	UNP P0DTC2
E	1250	GLN	-	expression tag	UNP P0DTC2
E	1251	HIS	-	expression tag	UNP P0DTC2
E	1252	SER	-	expression tag	UNP P0DTC2
E	1253	GLY	-	expression tag	UNP P0DTC2
E	1254	ARG	-	expression tag	UNP P0DTC2
E	1255	PRO	-	expression tag	UNP P0DTC2
E	1256	LEU	-	expression tag	UNP P0DTC2
E	1257	GLU	-	expression tag	UNP P0DTC2
E	1258	SER	-	expression tag	UNP P0DTC2
E	1259	ARG	-	expression tag	UNP P0DTC2
E	1260	GLY	-	expression tag	UNP P0DTC2
E	1261	PRO	-	expression tag	UNP P0DTC2
E	1262	PHE	-	expression tag	UNP P0DTC2
E	1263	GLU	-	expression tag	UNP P0DTC2
E	1264	GLN	-	expression tag	UNP P0DTC2
E	1265	LYS	-	expression tag	UNP P0DTC2
E	1266	LEU	-	expression tag	UNP P0DTC2
E	1267	ILE	-	expression tag	UNP P0DTC2
E	1268	SER	-	expression tag	UNP P0DTC2
E	1269	GLU	-	expression tag	UNP P0DTC2
E	1270	GLU	-	expression tag	UNP P0DTC2
E	1271	ASP	-	expression tag	UNP P0DTC2
E	1272	LEU	-	expression tag	UNP P0DTC2
E	1273	ASN	-	expression tag	UNP P0DTC2
E	1274	MET	-	expression tag	UNP P0DTC2
E	1275	HIS	-	expression tag	UNP P0DTC2
E	1276	THR	-	expression tag	UNP P0DTC2
E	1277	GLY	-	expression tag	UNP P0DTC2
E	1278	HIS	-	expression tag	UNP P0DTC2
E	1279	HIS	-	expression tag	UNP P0DTC2
E	1280	HIS	-	expression tag	UNP P0DTC2
E	1281	HIS	-	expression tag	UNP P0DTC2
E	1282	HIS	-	expression tag	UNP P0DTC2
E	1283	HIS	-	expression tag	UNP P0DTC2
F	142	ASP	GLY	engineered mutation	UNP P0DTC2
F	154	LYS	GLU	engineered mutation	UNP P0DTC2
F	452	ARG	LEU	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	484	GLN	GLU	variant	UNP P0DTC2
F	614	GLY	ASP	variant	UNP P0DTC2
F	682	GLY	ARG	engineered mutation	UNP P0DTC2
F	683	SER	ARG	engineered mutation	UNP P0DTC2
F	685	SER	ARG	engineered mutation	UNP P0DTC2
F	986	PRO	LYS	engineered mutation	UNP P0DTC2
F	987	PRO	VAL	engineered mutation	UNP P0DTC2
F	1071	HIS	GLN	engineered mutation	UNP P0DTC2
F	1101	ASP	HIS	engineered mutation	UNP P0DTC2
F	1209	GLU	-	expression tag	UNP P0DTC2
F	1210	PHE	-	expression tag	UNP P0DTC2
F	1211	GLY	-	expression tag	UNP P0DTC2
F	1212	SER	-	expression tag	UNP P0DTC2
F	1213	GLY	-	expression tag	UNP P0DTC2
F	1214	GLY	-	expression tag	UNP P0DTC2
F	1215	TYR	-	expression tag	UNP P0DTC2
F	1216	ILE	-	expression tag	UNP P0DTC2
F	1217	PRO	-	expression tag	UNP P0DTC2
F	1218	GLU	-	expression tag	UNP P0DTC2
F	1219	ALA	-	expression tag	UNP P0DTC2
F	1220	PRO	-	expression tag	UNP P0DTC2
F	1221	ARG	-	expression tag	UNP P0DTC2
F	1222	ASP	-	expression tag	UNP P0DTC2
F	1223	GLY	-	expression tag	UNP P0DTC2
F	1224	GLN	-	expression tag	UNP P0DTC2
F	1225	ALA	-	expression tag	UNP P0DTC2
F	1226	TYR	-	expression tag	UNP P0DTC2
F	1227	VAL	-	expression tag	UNP P0DTC2
F	1228	ARG	-	expression tag	UNP P0DTC2
F	1229	LYS	-	expression tag	UNP P0DTC2
F	1230	ASP	-	expression tag	UNP P0DTC2
F	1231	GLY	-	expression tag	UNP P0DTC2
F	1232	GLU	-	expression tag	UNP P0DTC2
F	1233	TRP	-	expression tag	UNP P0DTC2
F	1234	VAL	-	expression tag	UNP P0DTC2
F	1235	LEU	-	expression tag	UNP P0DTC2
F	1236	LEU	-	expression tag	UNP P0DTC2
F	1237	SER	-	expression tag	UNP P0DTC2
F	1238	THR	-	expression tag	UNP P0DTC2
F	1239	PHE	-	expression tag	UNP P0DTC2
F	1240	LEU	-	expression tag	UNP P0DTC2
F	1241	LYS	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	1242	GLY	-	expression tag	UNP P0DTC2
F	1243	GLN	-	expression tag	UNP P0DTC2
F	1244	ASP	-	expression tag	UNP P0DTC2
F	1245	ASN	-	expression tag	UNP P0DTC2
F	1246	SER	-	expression tag	UNP P0DTC2
F	1247	ALA	-	expression tag	UNP P0DTC2
F	1248	ASP	-	expression tag	UNP P0DTC2
F	1249	ILE	-	expression tag	UNP P0DTC2
F	1250	GLN	-	expression tag	UNP P0DTC2
F	1251	HIS	-	expression tag	UNP P0DTC2
F	1252	SER	-	expression tag	UNP P0DTC2
F	1253	GLY	-	expression tag	UNP P0DTC2
F	1254	ARG	-	expression tag	UNP P0DTC2
F	1255	PRO	-	expression tag	UNP P0DTC2
F	1256	LEU	-	expression tag	UNP P0DTC2
F	1257	GLU	-	expression tag	UNP P0DTC2
F	1258	SER	-	expression tag	UNP P0DTC2
F	1259	ARG	-	expression tag	UNP P0DTC2
F	1260	GLY	-	expression tag	UNP P0DTC2
F	1261	PRO	-	expression tag	UNP P0DTC2
F	1262	PHE	-	expression tag	UNP P0DTC2
F	1263	GLU	-	expression tag	UNP P0DTC2
F	1264	GLN	-	expression tag	UNP P0DTC2
F	1265	LYS	-	expression tag	UNP P0DTC2
F	1266	LEU	-	expression tag	UNP P0DTC2
F	1267	ILE	-	expression tag	UNP P0DTC2
F	1268	SER	-	expression tag	UNP P0DTC2
F	1269	GLU	-	expression tag	UNP P0DTC2
F	1270	GLU	-	expression tag	UNP P0DTC2
F	1271	ASP	-	expression tag	UNP P0DTC2
F	1272	LEU	-	expression tag	UNP P0DTC2
F	1273	ASN	-	expression tag	UNP P0DTC2
F	1274	MET	-	expression tag	UNP P0DTC2
F	1275	HIS	-	expression tag	UNP P0DTC2
F	1276	THR	-	expression tag	UNP P0DTC2
F	1277	GLY	-	expression tag	UNP P0DTC2
F	1278	HIS	-	expression tag	UNP P0DTC2
F	1279	HIS	-	expression tag	UNP P0DTC2
F	1280	HIS	-	expression tag	UNP P0DTC2
F	1281	HIS	-	expression tag	UNP P0DTC2
F	1282	HIS	-	expression tag	UNP P0DTC2
F	1283	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 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
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		
2	U	2	Total	C	N	O	0	0
			28	16	2	10		
2	V	2	Total	C	N	O	0	0
			28	16	2	10		
2	X	2	Total	C	N	O	0	0
			28	16	2	10		
2	Y	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
2	a	2	Total	C	N	O	0	0
			28	16	2	10		
2	b	2	Total	C	N	O	0	0
			28	16	2	10		
2	c	2	Total	C	N	O	0	0
			28	16	2	10		
2	d	2	Total	C	N	O	0	0
			28	16	2	10		
2	e	2	Total	C	N	O	0	0
			28	16	2	10		
2	f	2	Total	C	N	O	0	0
			28	16	2	10		
2	g	2	Total	C	N	O	0	0
			28	16	2	10		
2	h	2	Total	C	N	O	0	0
			28	16	2	10		
2	j	2	Total	C	N	O	0	0
			28	16	2	10		
2	k	2	Total	C	N	O	0	0
			28	16	2	10		
2	l	2	Total	C	N	O	0	0
			28	16	2	10		
2	m	2	Total	C	N	O	0	0
			28	16	2	10		
2	n	2	Total	C	N	O	0	0
			28	16	2	10		
2	o	2	Total	C	N	O	0	0
			28	16	2	10		
2	p	2	Total	C	N	O	0	0
			28	16	2	10		
2	q	2	Total	C	N	O	0	0
			28	16	2	10		
2	r	2	Total	C	N	O	0	0
			28	16	2	10		
2	s	2	Total	C	N	O	0	0
			28	16	2	10		
2	t	2	Total	C	N	O	0	0
			28	16	2	10		
2	v	2	Total	C	N	O	0	0
			28	16	2	10		
2	w	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
2	x	2	Total	C	N	O	0	0
			28	16	2	10		
2	y	2	Total	C	N	O	0	0
			28	16	2	10		
2	z	2	Total	C	N	O	0	0
			28	16	2	10		
2	0	2	Total	C	N	O	0	0
			28	16	2	10		
2	1	2	Total	C	N	O	0	0
			28	16	2	10		
2	2	2	Total	C	N	O	0	0
			28	16	2	10		
2	3	2	Total	C	N	O	0	0
			28	16	2	10		
2	4	2	Total	C	N	O	0	0
			28	16	2	10		
2	5	2	Total	C	N	O	0	0
			28	16	2	10		
2	7	2	Total	C	N	O	0	0
			28	16	2	10		
2	8	2	Total	C	N	O	0	0
			28	16	2	10		
2	9	2	Total	C	N	O	0	0
			28	16	2	10		
2	AA	2	Total	C	N	O	0	0
			28	16	2	10		
2	BA	2	Total	C	N	O	0	0
			28	16	2	10		
2	CA	2	Total	C	N	O	0	0
			28	16	2	10		
2	DA	2	Total	C	N	O	0	0
			28	16	2	10		
2	EA	2	Total	C	N	O	0	0
			28	16	2	10		
2	FA	2	Total	C	N	O	0	0
			28	16	2	10		
2	GA	2	Total	C	N	O	0	0
			28	16	2	10		
2	HA	2	Total	C	N	O	0	0
			28	16	2	10		
2	JA	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
2	KA	2	Total	C	N	O	0	0
			28	16	2	10		
2	LA	2	Total	C	N	O	0	0
			28	16	2	10		
2	MA	2	Total	C	N	O	0	0
			28	16	2	10		
2	NA	2	Total	C	N	O	0	0
			28	16	2	10		
2	OA	2	Total	C	N	O	0	0
			28	16	2	10		
2	PA	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	W	3	Total	C	N	O	0	0
			39	22	2	15		
3	i	3	Total	C	N	O	0	0
			39	22	2	15		
3	u	3	Total	C	N	O	0	0
			39	22	2	15		
3	6	3	Total	C	N	O	0	0
			39	22	2	15		
3	IA	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

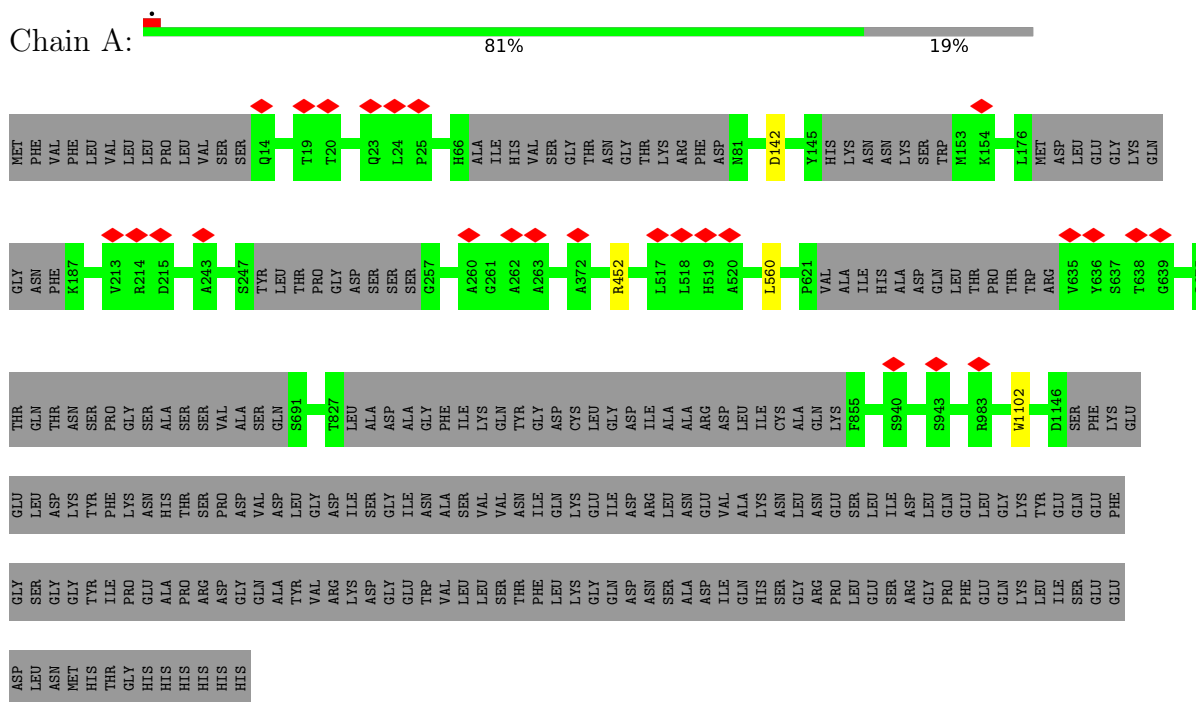
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	

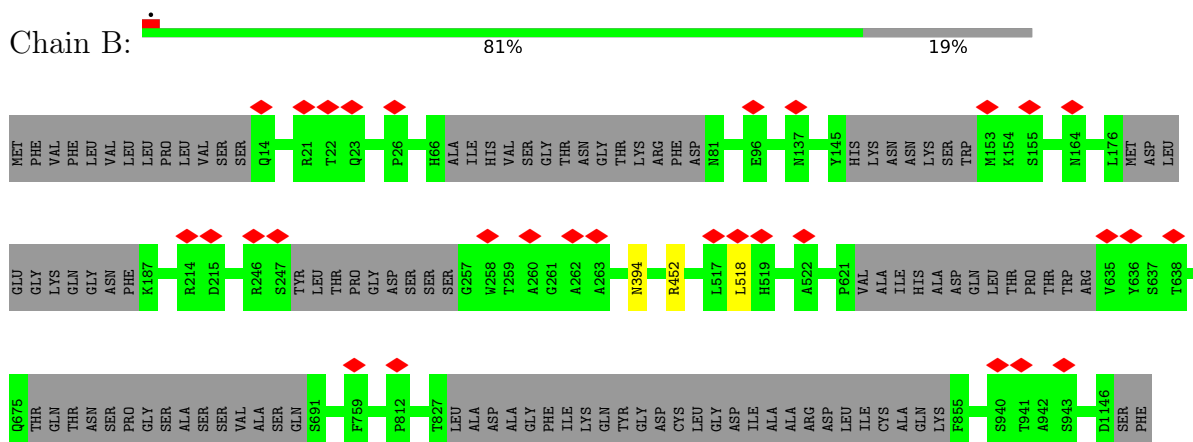
3 Residue-property plots [i](#)

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

• Molecule 1: Spike glycoprotein



• Molecule 1: Spike glycoprotein



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



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



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



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



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



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





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

Chain N:  100%



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

Chain O:  50%
100%



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

Chain P:  50%
100%



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

Chain Q:  100%



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

Chain R:  50%
100%



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

Chain S:  50%
100%



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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

Chain s: 



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

Chain t: 



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

Chain v: 



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

Chain w: 



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

Chain x: 



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

Chain y: 



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



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



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



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



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



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



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



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



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



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



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



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

Chain BA: 



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

Chain CA: 



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

Chain DA: 



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

Chain EA: 



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

Chain FA: 



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

Chain GA: 



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



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



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



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



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



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

Chain NA: 



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

Chain OA: 



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

Chain PA: 



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i: 



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:  33% 100%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6:  33% 100%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain IA:  33% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114129	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 ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.873	Depositor
Minimum map value	-0.722	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.35	Depositor
Map size (\AA)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.33	0/8295	0.50	1/11291 (0.0%)
1	B	0.33	0/8295	0.50	0/11291
1	C	0.34	0/8295	0.49	0/11291
1	D	0.31	0/8295	0.49	1/11291 (0.0%)
1	E	0.31	0/8295	0.49	0/11291
1	F	0.32	0/8295	0.49	1/11291 (0.0%)
All	All	0.32	0/49770	0.49	3/67746 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	517	LEU	CA-CB-CG	6.02	129.15	115.30
1	A	560	LEU	CA-CB-CG	5.52	127.99	115.30
1	D	560	LEU	CA-CB-CG	5.08	127.00	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1022/1283 (80%)	972 (95%)	48 (5%)	2 (0%)	44	71
1	B	1022/1283 (80%)	966 (94%)	55 (5%)	1 (0%)	48	76
1	C	1022/1283 (80%)	964 (94%)	57 (6%)	1 (0%)	48	76
1	D	1022/1283 (80%)	961 (94%)	60 (6%)	1 (0%)	48	76
1	E	1022/1283 (80%)	967 (95%)	54 (5%)	1 (0%)	48	76
1	F	1022/1283 (80%)	963 (94%)	55 (5%)	4 (0%)	30	61
All	All	6132/7698 (80%)	5793 (94%)	329 (5%)	10 (0%)	45	71

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	517	LEU
1	E	943	SER
1	A	142	ASP
1	B	518	LEU
1	D	142	ASP

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	907/1116 (81%)	906 (100%)	1 (0%)	92	96
1	B	907/1116 (81%)	905 (100%)	2 (0%)	92	95
1	C	907/1116 (81%)	907 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	907/1116 (81%)	903 (100%)	4 (0%)	89	93
1	E	907/1116 (81%)	906 (100%)	1 (0%)	92	96
1	F	907/1116 (81%)	906 (100%)	1 (0%)	92	96
All	All	5442/6696 (81%)	5433 (100%)	9 (0%)	91	95

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	214	ARG
1	F	452	ARG
1	D	137	ASN
1	D	319	ARG
1	D	452	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	121	ASN
1	E	440	ASN
1	D	955	ASN
1	C	440	ASN
1	E	121	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](#)

150 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	$\# Z > 2$
2	NAG	0	1	2,1	14,14,15	0.26	0	17,19,21	0.40	0
2	NAG	0	2	2	14,14,15	0.21	0	17,19,21	0.41	0
2	NAG	1	1	2,1	14,14,15	0.21	0	17,19,21	0.46	0
2	NAG	1	2	2	14,14,15	0.21	0	17,19,21	0.44	0
2	NAG	2	1	2,1	14,14,15	0.35	0	17,19,21	0.58	0
2	NAG	2	2	2	14,14,15	0.33	0	17,19,21	0.36	0
2	NAG	3	1	2,1	14,14,15	0.29	0	17,19,21	0.39	0
2	NAG	3	2	2	14,14,15	0.20	0	17,19,21	0.46	0
2	NAG	4	1	2,1	14,14,15	0.23	0	17,19,21	0.44	0
2	NAG	4	2	2	14,14,15	0.20	0	17,19,21	0.47	0
2	NAG	5	1	2,1	14,14,15	0.33	0	17,19,21	0.50	0
2	NAG	5	2	2	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	6	1	3,1	14,14,15	0.31	0	17,19,21	0.53	0
3	NAG	6	2	3	14,14,15	0.20	0	17,19,21	0.40	0
3	BMA	6	3	3	11,11,12	0.54	0	15,15,17	0.79	0
2	NAG	7	1	2,1	14,14,15	0.20	0	17,19,21	0.47	0
2	NAG	7	2	2	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	8	1	2,1	14,14,15	0.31	0	17,19,21	0.39	0
2	NAG	8	2	2	14,14,15	0.22	0	17,19,21	0.40	0
2	NAG	9	1	2,1	14,14,15	0.23	0	17,19,21	0.47	0
2	NAG	9	2	2	14,14,15	0.21	0	17,19,21	0.41	0
2	NAG	AA	1	2,1	14,14,15	0.38	0	17,19,21	0.40	0
2	NAG	AA	2	2	14,14,15	0.22	0	17,19,21	0.45	0
2	NAG	BA	1	2,1	14,14,15	0.40	0	17,19,21	0.57	0
2	NAG	BA	2	2	14,14,15	0.23	0	17,19,21	0.54	0
2	NAG	CA	1	2,1	14,14,15	0.28	0	17,19,21	0.43	0
2	NAG	CA	2	2	14,14,15	0.23	0	17,19,21	0.42	0
2	NAG	DA	1	2,1	14,14,15	0.22	0	17,19,21	0.45	0
2	NAG	DA	2	2	14,14,15	0.22	0	17,19,21	0.38	0
2	NAG	EA	1	2,1	14,14,15	0.20	0	17,19,21	0.55	0
2	NAG	EA	2	2	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	FA	1	2,1	14,14,15	0.59	0	17,19,21	1.25	1 (5%)
2	NAG	FA	2	2	14,14,15	0.25	0	17,19,21	0.43	0
2	NAG	G	1	2,1	14,14,15	0.52	0	17,19,21	0.67	0
2	NAG	G	2	2	14,14,15	0.26	0	17,19,21	0.57	0
2	NAG	GA	1	2,1	14,14,15	0.25	0	17,19,21	0.45	0
2	NAG	GA	2	2	14,14,15	0.20	0	17,19,21	0.43	0
2	NAG	H	1	2,1	14,14,15	0.35	0	17,19,21	0.41	0
2	NAG	H	2	2	14,14,15	0.33	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	HA	1	2,1	14,14,15	0.28	0	17,19,21	0.49	0
2	NAG	HA	2	2	14,14,15	0.18	0	17,19,21	0.41	0
2	NAG	I	1	2,1	14,14,15	0.25	0	17,19,21	0.41	0
2	NAG	I	2	2	14,14,15	0.21	0	17,19,21	0.47	0
3	NAG	IA	1	3,1	14,14,15	0.49	0	17,19,21	0.58	0
3	NAG	IA	2	3	14,14,15	0.24	0	17,19,21	0.60	0
3	BMA	IA	3	3	11,11,12	0.77	0	15,15,17	0.78	0
2	NAG	J	1	2,1	14,14,15	0.29	0	17,19,21	0.48	0
2	NAG	J	2	2	14,14,15	0.20	0	17,19,21	0.43	0
2	NAG	JA	1	2,1	14,14,15	0.19	0	17,19,21	0.46	0
2	NAG	JA	2	2	14,14,15	0.18	0	17,19,21	0.40	0
3	NAG	K	1	3,1	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	K	2	3	14,14,15	0.24	0	17,19,21	0.42	0
3	BMA	K	3	3	11,11,12	0.53	0	15,15,17	0.75	0
2	NAG	KA	1	2,1	14,14,15	0.26	0	17,19,21	0.48	0
2	NAG	KA	2	2	14,14,15	0.16	0	17,19,21	0.46	0
2	NAG	L	1	2,1	14,14,15	0.23	0	17,19,21	0.46	0
2	NAG	L	2	2	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	LA	1	2,1	14,14,15	0.23	0	17,19,21	0.49	0
2	NAG	LA	2	2	14,14,15	0.24	0	17,19,21	0.37	0
2	NAG	M	1	2,1	14,14,15	0.25	0	17,19,21	0.51	0
2	NAG	M	2	2	14,14,15	0.24	0	17,19,21	0.45	0
2	NAG	MA	1	2,1	14,14,15	0.24	0	17,19,21	0.45	0
2	NAG	MA	2	2	14,14,15	0.18	0	17,19,21	0.41	0
2	NAG	N	1	2,1	14,14,15	0.32	0	17,19,21	0.46	0
2	NAG	N	2	2	14,14,15	0.19	0	17,19,21	0.40	0
2	NAG	NA	1	2,1	14,14,15	0.37	0	17,19,21	0.52	0
2	NAG	NA	2	2	14,14,15	0.29	0	17,19,21	0.55	0
2	NAG	O	1	2,1	14,14,15	0.30	0	17,19,21	0.42	0
2	NAG	O	2	2	14,14,15	0.17	0	17,19,21	0.43	0
2	NAG	OA	1	2,1	14,14,15	0.25	0	17,19,21	0.38	0
2	NAG	OA	2	2	14,14,15	0.23	0	17,19,21	0.40	0
2	NAG	P	1	2,1	14,14,15	0.34	0	17,19,21	0.52	0
2	NAG	P	2	2	14,14,15	0.23	0	17,19,21	0.56	0
2	NAG	PA	1	2,1	14,14,15	0.28	0	17,19,21	0.39	0
2	NAG	PA	2	2	14,14,15	0.23	0	17,19,21	0.41	0
2	NAG	Q	1	2,1	14,14,15	0.36	0	17,19,21	0.43	0
2	NAG	Q	2	2	14,14,15	0.23	0	17,19,21	0.38	0
2	NAG	R	1	2,1	14,14,15	0.25	0	17,19,21	0.38	0
2	NAG	R	2	2	14,14,15	0.21	0	17,19,21	0.44	0
2	NAG	S	1	2,1	14,14,15	0.23	0	17,19,21	0.37	0
2	NAG	S	2	2	14,14,15	0.21	0	17,19,21	0.40	0
2	NAG	T	1	2,1	14,14,15	0.17	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	T	2	2	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	U	1	2,1	14,14,15	0.22	0	17,19,21	0.61	0
2	NAG	U	2	2	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	V	1	2,1	14,14,15	0.24	0	17,19,21	0.48	0
2	NAG	V	2	2	14,14,15	0.19	0	17,19,21	0.46	0
3	NAG	W	1	3,1	14,14,15	0.26	0	17,19,21	0.52	0
3	NAG	W	2	3	14,14,15	0.17	0	17,19,21	0.45	0
3	BMA	W	3	3	11,11,12	0.51	0	15,15,17	0.73	0
2	NAG	X	1	2,1	14,14,15	0.21	0	17,19,21	0.52	0
2	NAG	X	2	2	14,14,15	0.19	0	17,19,21	0.42	0
2	NAG	Y	1	2,1	14,14,15	0.25	0	17,19,21	0.36	0
2	NAG	Y	2	2	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	Z	1	2,1	14,14,15	0.25	0	17,19,21	0.50	0
2	NAG	Z	2	2	14,14,15	0.19	0	17,19,21	0.40	0
2	NAG	a	1	2,1	14,14,15	0.44	0	17,19,21	0.44	0
2	NAG	a	2	2	14,14,15	0.18	0	17,19,21	0.38	0
2	NAG	b	1	2,1	14,14,15	0.51	0	17,19,21	0.94	1 (5%)
2	NAG	b	2	2	14,14,15	0.25	0	17,19,21	0.53	0
2	NAG	c	1	2,1	14,14,15	0.28	0	17,19,21	0.41	0
2	NAG	c	2	2	14,14,15	0.25	0	17,19,21	0.37	0
2	NAG	d	1	2,1	14,14,15	0.18	0	17,19,21	0.48	0
2	NAG	d	2	2	14,14,15	0.18	0	17,19,21	0.41	0
2	NAG	e	1	2,1	14,14,15	0.46	0	17,19,21	0.61	0
2	NAG	e	2	2	14,14,15	0.23	0	17,19,21	0.44	0
2	NAG	f	1	2,1	14,14,15	0.18	0	17,19,21	0.48	0
2	NAG	f	2	2	14,14,15	0.21	0	17,19,21	0.43	0
2	NAG	g	1	2,1	14,14,15	0.34	0	17,19,21	0.40	0
2	NAG	g	2	2	14,14,15	0.21	0	17,19,21	0.45	0
2	NAG	h	1	2,1	14,14,15	0.25	0	17,19,21	0.48	0
2	NAG	h	2	2	14,14,15	0.27	0	17,19,21	0.46	0
3	NAG	i	1	3,1	14,14,15	0.32	0	17,19,21	0.54	0
3	NAG	i	2	3	14,14,15	0.21	0	17,19,21	0.52	0
3	BMA	i	3	3	11,11,12	0.56	0	15,15,17	0.70	0
2	NAG	j	1	2,1	14,14,15	0.19	0	17,19,21	0.46	0
2	NAG	j	2	2	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	k	1	2,1	14,14,15	0.23	0	17,19,21	0.34	0
2	NAG	k	2	2	14,14,15	0.20	0	17,19,21	0.44	0
2	NAG	l	1	2,1	14,14,15	0.24	0	17,19,21	0.45	0
2	NAG	l	2	2	14,14,15	0.20	0	17,19,21	0.42	0
2	NAG	m	1	2,1	14,14,15	0.26	0	17,19,21	0.39	0
2	NAG	m	2	2	14,14,15	0.19	0	17,19,21	0.44	0
2	NAG	n	1	2,1	14,14,15	0.26	0	17,19,21	0.52	0
2	NAG	n	2	2	14,14,15	0.20	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	o	1	2,1	14,14,15	0.26	0	17,19,21	0.41	0
2	NAG	o	2	2	14,14,15	0.20	0	17,19,21	0.43	0
2	NAG	p	1	2,1	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	p	2	2	14,14,15	0.17	0	17,19,21	0.41	0
2	NAG	q	1	2,1	14,14,15	0.23	0	17,19,21	0.45	0
2	NAG	q	2	2	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	r	1	2,1	14,14,15	0.46	0	17,19,21	1.49	2 (11%)
2	NAG	r	2	2	14,14,15	0.23	0	17,19,21	0.51	0
2	NAG	s	1	2,1	14,14,15	0.23	0	17,19,21	0.56	0
2	NAG	s	2	2	14,14,15	0.19	0	17,19,21	0.44	0
2	NAG	t	1	2,1	14,14,15	0.20	0	17,19,21	0.55	0
2	NAG	t	2	2	14,14,15	0.19	0	17,19,21	0.44	0
3	NAG	u	1	3,1	14,14,15	0.36	0	17,19,21	0.54	0
3	NAG	u	2	3	14,14,15	0.19	0	17,19,21	0.51	0
3	BMA	u	3	3	11,11,12	0.50	0	15,15,17	0.84	0
2	NAG	v	1	2,1	14,14,15	0.18	0	17,19,21	0.40	0
2	NAG	v	2	2	14,14,15	0.23	0	17,19,21	0.41	0
2	NAG	w	1	2,1	14,14,15	0.21	0	17,19,21	0.40	0
2	NAG	w	2	2	14,14,15	0.19	0	17,19,21	0.42	0
2	NAG	x	1	2,1	14,14,15	0.23	0	17,19,21	0.49	0
2	NAG	x	2	2	14,14,15	0.19	0	17,19,21	0.41	0
2	NAG	y	1	2,1	14,14,15	0.24	0	17,19,21	0.41	0
2	NAG	y	2	2	14,14,15	0.21	0	17,19,21	0.45	0
2	NAG	z	1	2,1	14,14,15	0.39	0	17,19,21	0.90	1 (5%)
2	NAG	z	2	2	14,14,15	0.21	0	17,19,21	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	0	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	0	2	2	-	0/6/23/26	0/1/1/1
2	NAG	1	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	1	2	2	-	0/6/23/26	0/1/1/1
2	NAG	2	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	2	2	2	-	2/6/23/26	0/1/1/1
2	NAG	3	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	3	2	2	-	2/6/23/26	0/1/1/1
2	NAG	4	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	4	2	2	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	5	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	5	2	2	-	4/6/23/26	0/1/1/1
3	NAG	6	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	6	2	3	-	1/6/23/26	0/1/1/1
3	BMA	6	3	3	-	1/2/19/22	0/1/1/1
2	NAG	7	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	7	2	2	-	0/6/23/26	0/1/1/1
2	NAG	8	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	8	2	2	-	4/6/23/26	0/1/1/1
2	NAG	9	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	9	2	2	-	1/6/23/26	0/1/1/1
2	NAG	AA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	AA	2	2	-	2/6/23/26	0/1/1/1
2	NAG	BA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	BA	2	2	-	4/6/23/26	0/1/1/1
2	NAG	CA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	CA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	DA	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	DA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	EA	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	EA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	FA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	FA	2	2	-	1/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
2	NAG	GA	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	GA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	HA	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	HA	2	2	-	3/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
3	NAG	IA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	IA	2	3	-	1/6/23/26	0/1/1/1
3	BMA	IA	3	3	-	1/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	JA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	JA	2	2	-	0/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
2	NAG	KA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	KA	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	NAG	LA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	LA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	MA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	MA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	NA	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	NA	2	2	-	4/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	NAG	OA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	OA	2	2	-	2/6/23/26	0/1/1/1
2	NAG	P	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1
2	NAG	PA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	PA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	R	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
2	NAG	S	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	1/6/23/26	0/1/1/1
2	NAG	T	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	1/6/23/26	0/1/1/1
2	NAG	U	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	U	2	2	-	0/6/23/26	0/1/1/1
2	NAG	V	1	2,1	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	V	2	2	-	2/6/23/26	0/1/1/1
3	NAG	W	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	W	2	3	-	3/6/23/26	0/1/1/1
3	BMA	W	3	3	-	0/2/19/22	0/1/1/1
2	NAG	X	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	X	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Y	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Z	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	2/6/23/26	0/1/1/1
2	NAG	a	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	a	2	2	-	0/6/23/26	0/1/1/1
2	NAG	b	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	b	2	2	-	0/6/23/26	0/1/1/1
2	NAG	c	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	c	2	2	-	0/6/23/26	0/1/1/1
2	NAG	d	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	d	2	2	-	2/6/23/26	0/1/1/1
2	NAG	e	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	e	2	2	-	2/6/23/26	0/1/1/1
2	NAG	f	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	f	2	2	-	1/6/23/26	0/1/1/1
2	NAG	g	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	g	2	2	-	0/6/23/26	0/1/1/1
2	NAG	h	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	h	2	2	-	4/6/23/26	0/1/1/1
3	NAG	i	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	i	2	3	-	2/6/23/26	0/1/1/1
3	BMA	i	3	3	-	0/2/19/22	0/1/1/1
2	NAG	j	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	j	2	2	-	2/6/23/26	0/1/1/1
2	NAG	k	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	k	2	2	-	1/6/23/26	0/1/1/1
2	NAG	l	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	l	2	2	-	2/6/23/26	0/1/1/1
2	NAG	m	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	m	2	2	-	2/6/23/26	0/1/1/1
2	NAG	n	1	2,1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	n	2	2	-	3/6/23/26	0/1/1/1
2	NAG	o	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	o	2	2	-	2/6/23/26	0/1/1/1
2	NAG	p	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	p	2	2	-	0/6/23/26	0/1/1/1
2	NAG	q	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	r	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	r	2	2	-	1/6/23/26	0/1/1/1
2	NAG	s	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	s	2	2	-	2/6/23/26	0/1/1/1
2	NAG	t	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	t	2	2	-	2/6/23/26	0/1/1/1
3	NAG	u	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	u	2	3	-	1/6/23/26	0/1/1/1
3	BMA	u	3	3	-	0/2/19/22	0/1/1/1
2	NAG	v	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	v	2	2	-	0/6/23/26	0/1/1/1
2	NAG	w	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	w	2	2	-	2/6/23/26	0/1/1/1
2	NAG	x	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	x	2	2	-	0/6/23/26	0/1/1/1
2	NAG	y	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	y	2	2	-	2/6/23/26	0/1/1/1
2	NAG	z	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	z	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	FA	1	NAG	C1-O5-C5	4.91	118.84	112.19
2	r	1	NAG	C2-N2-C7	4.25	128.95	122.90
2	r	1	NAG	C1-O5-C5	3.18	116.50	112.19
2	b	1	NAG	C1-O5-C5	2.75	115.92	112.19
2	z	1	NAG	C1-O5-C5	2.56	115.66	112.19

There are no chirality outliers.

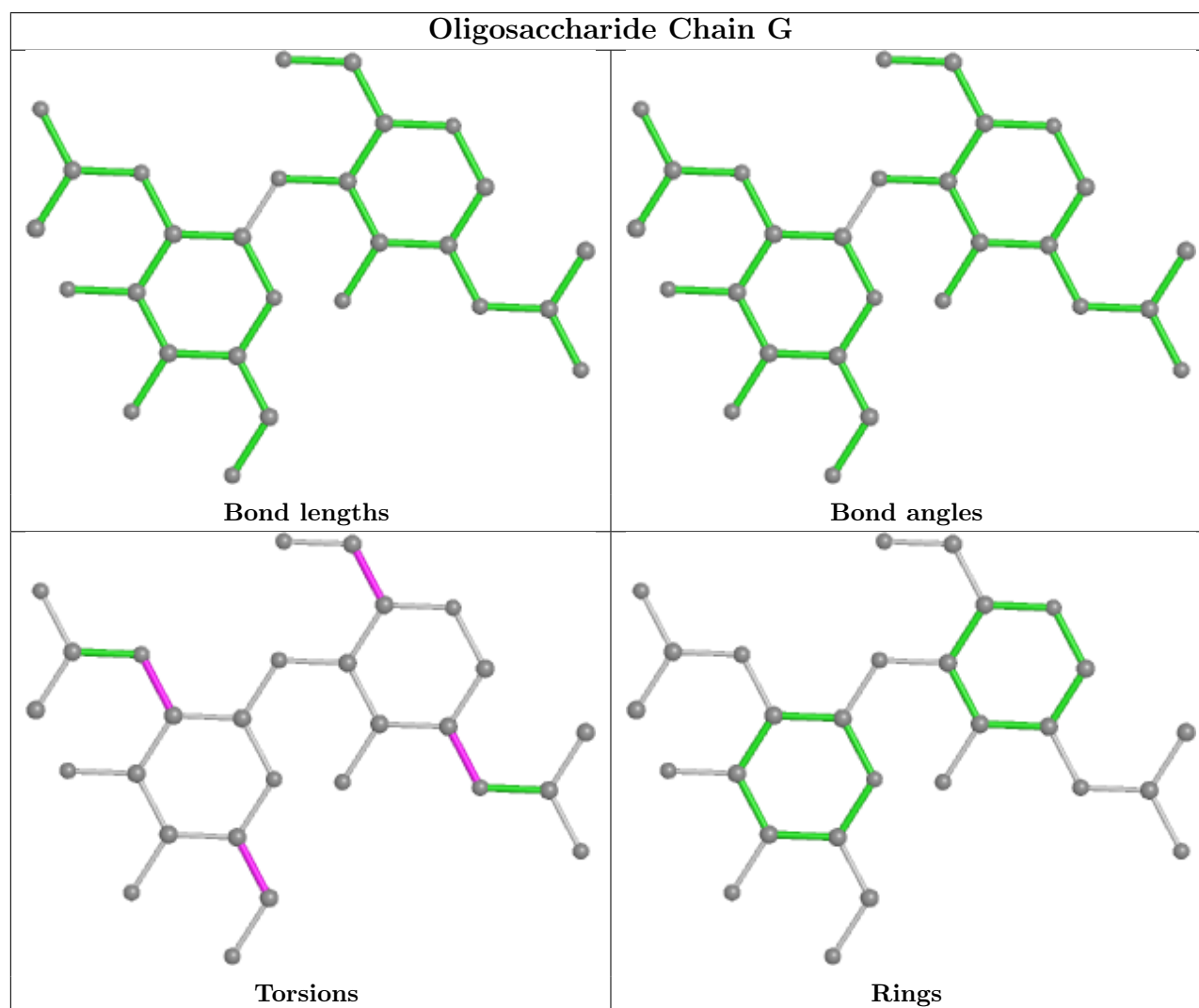
5 of 202 torsion outliers are listed below:

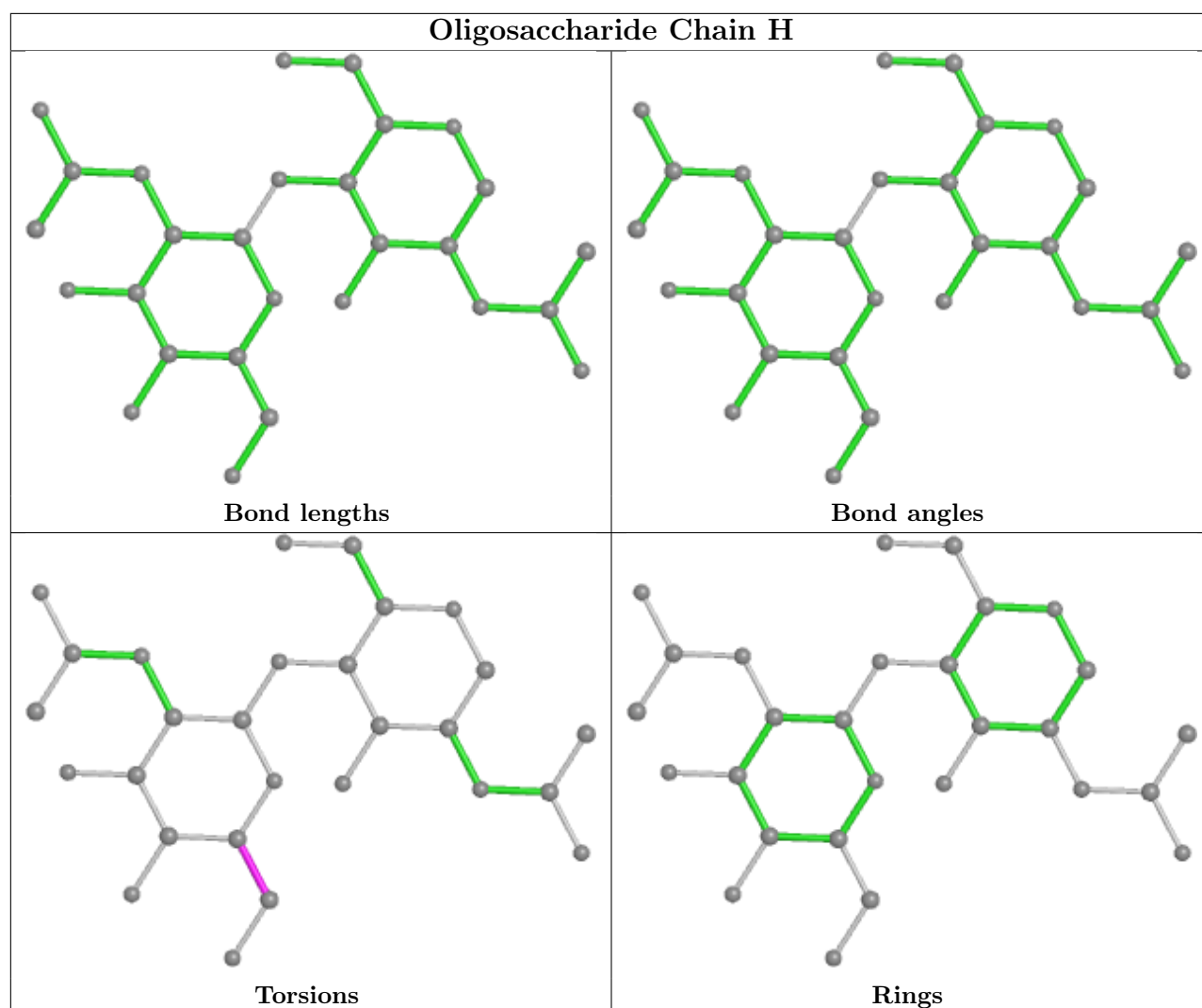
Mol	Chain	Res	Type	Atoms
2	M	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
2	s	1	NAG	O5-C5-C6-O6
2	t	2	NAG	C4-C5-C6-O6

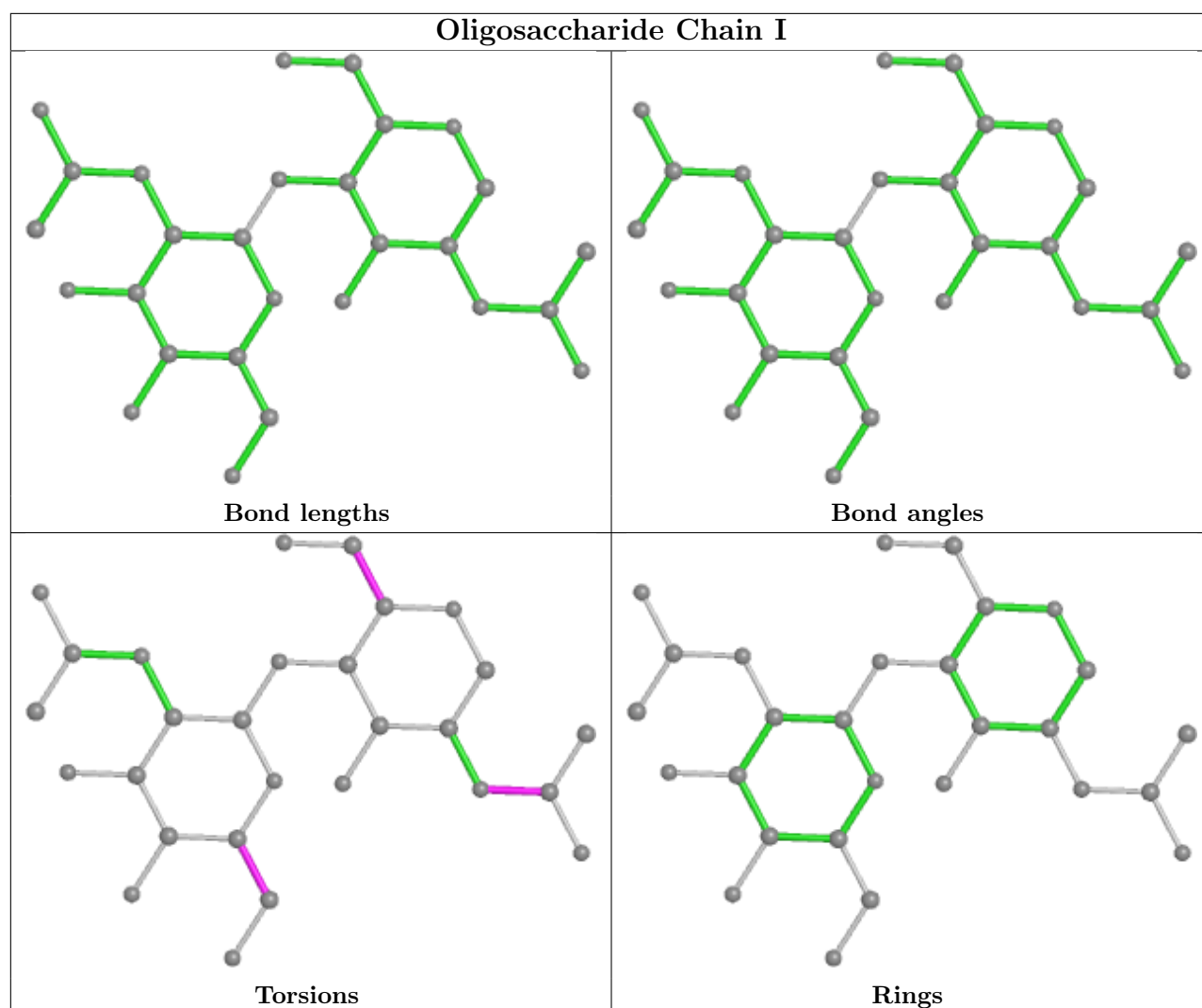
There are no ring outliers.

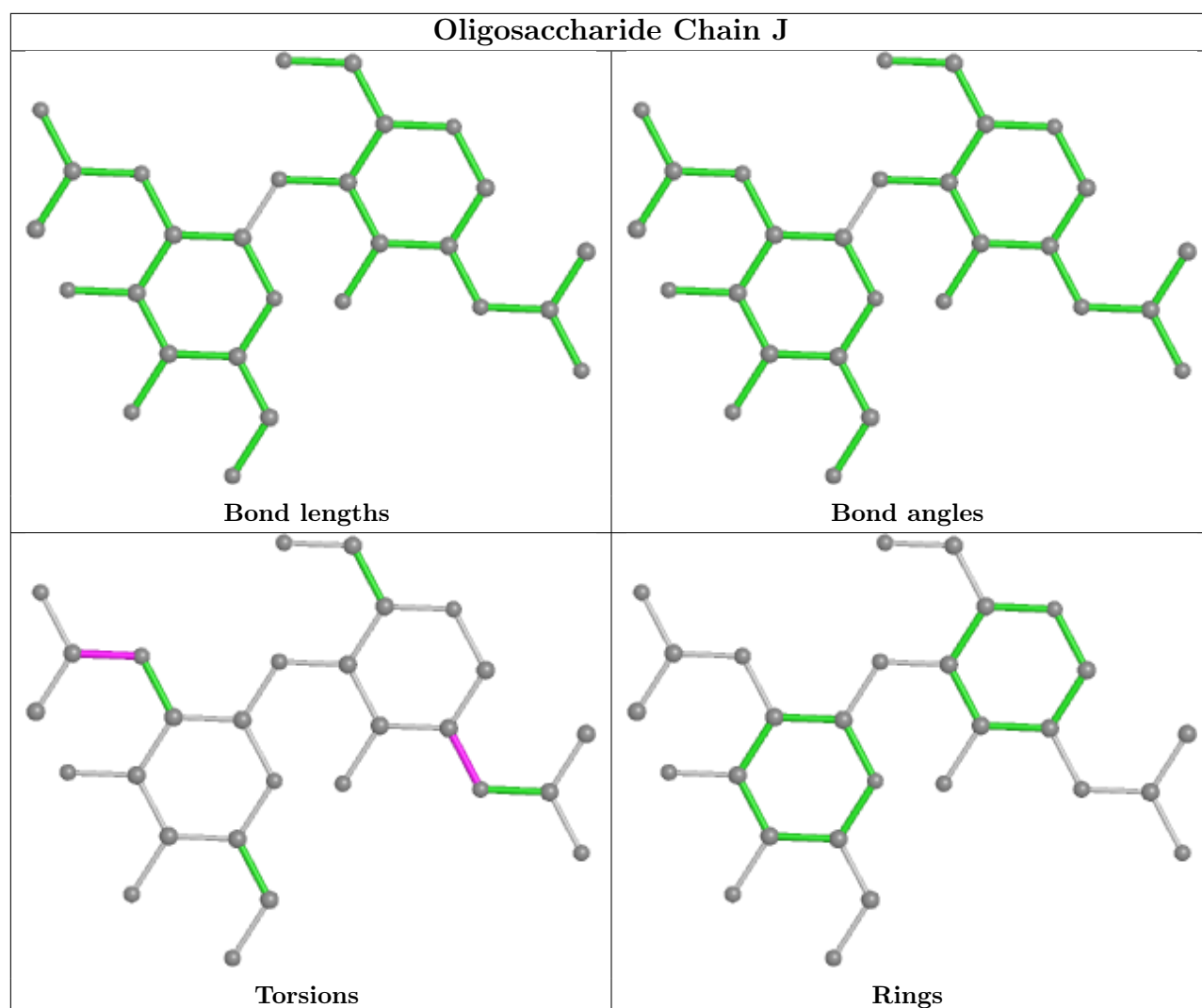
No monomer is involved in short contacts.

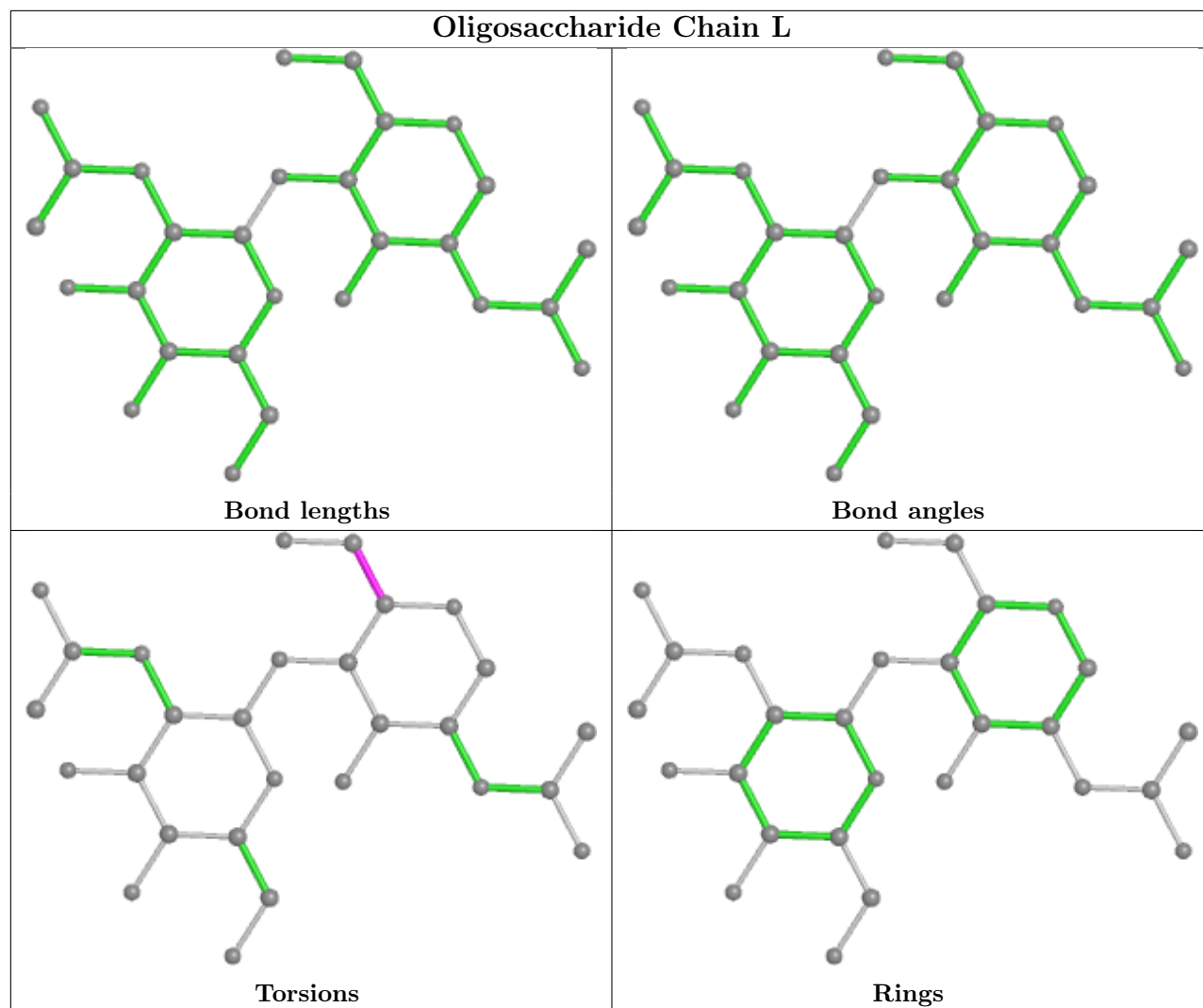
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

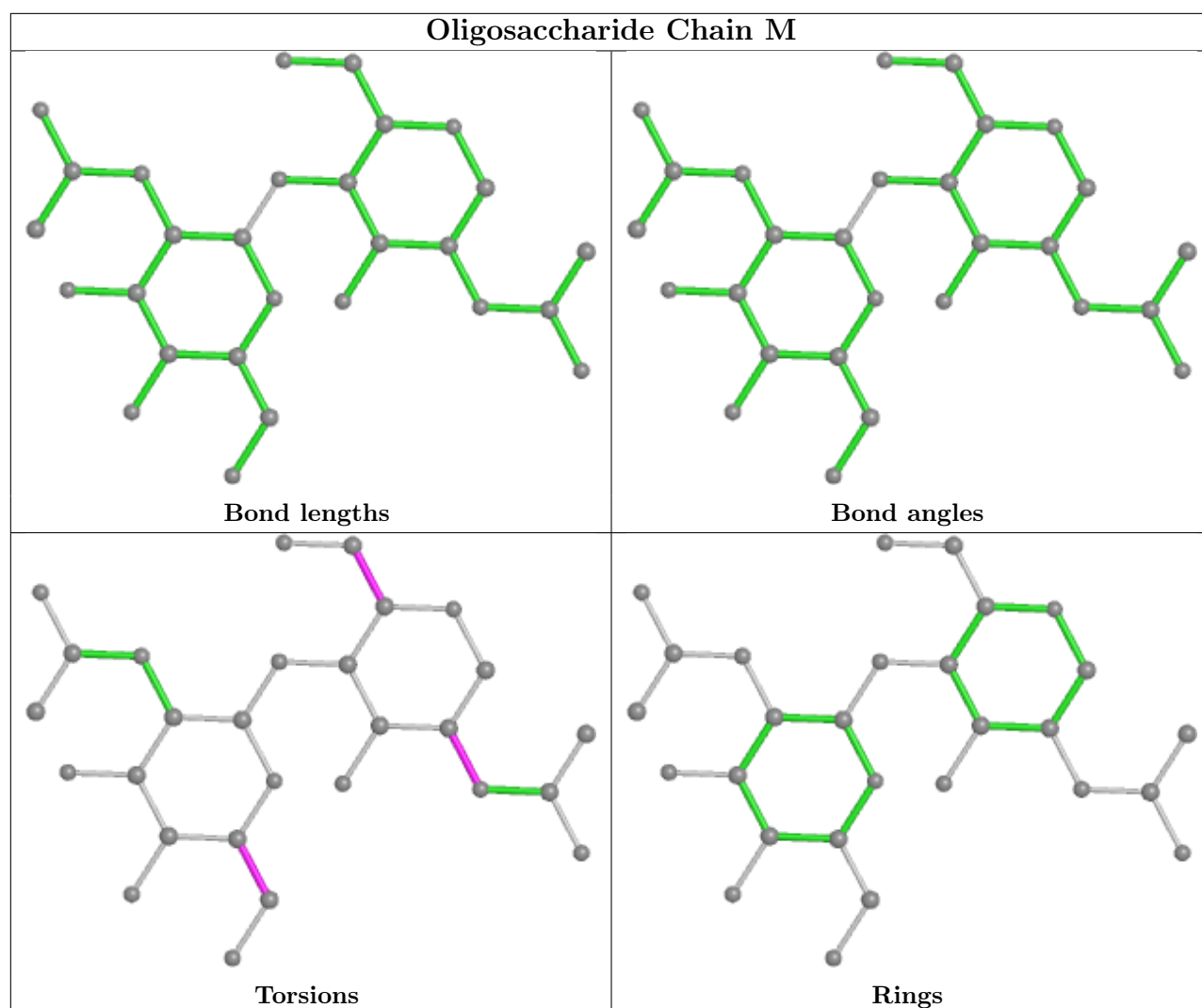


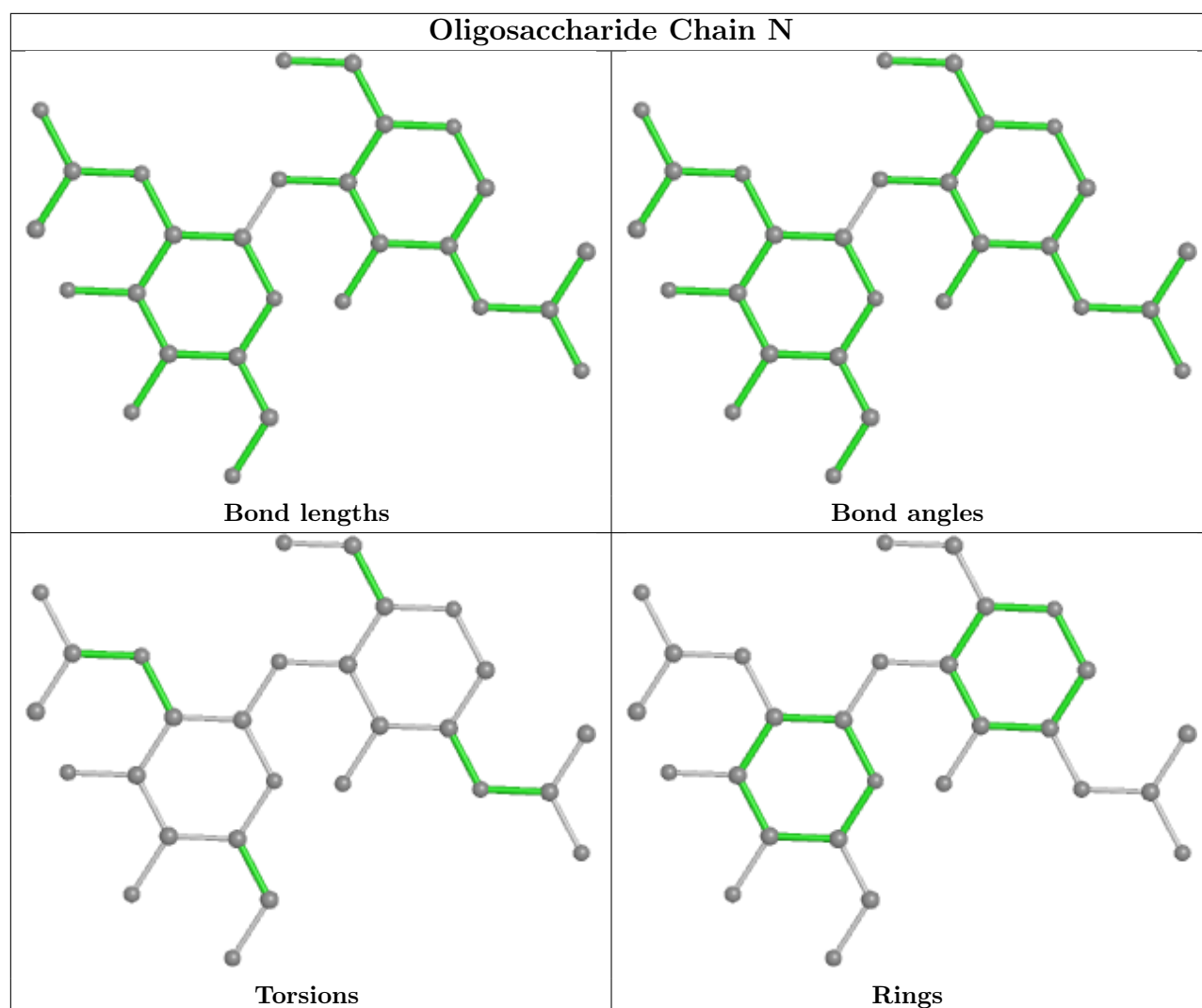


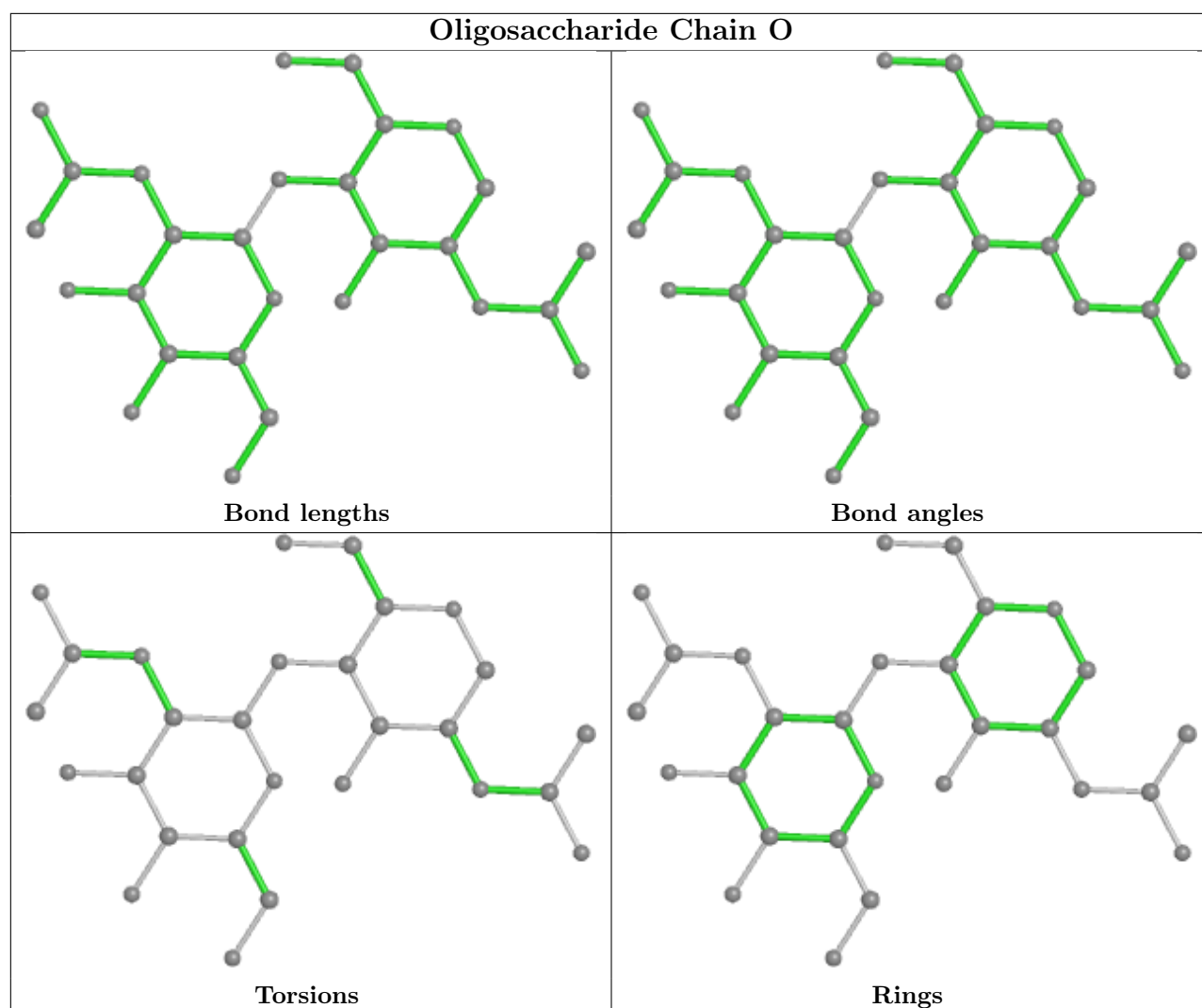


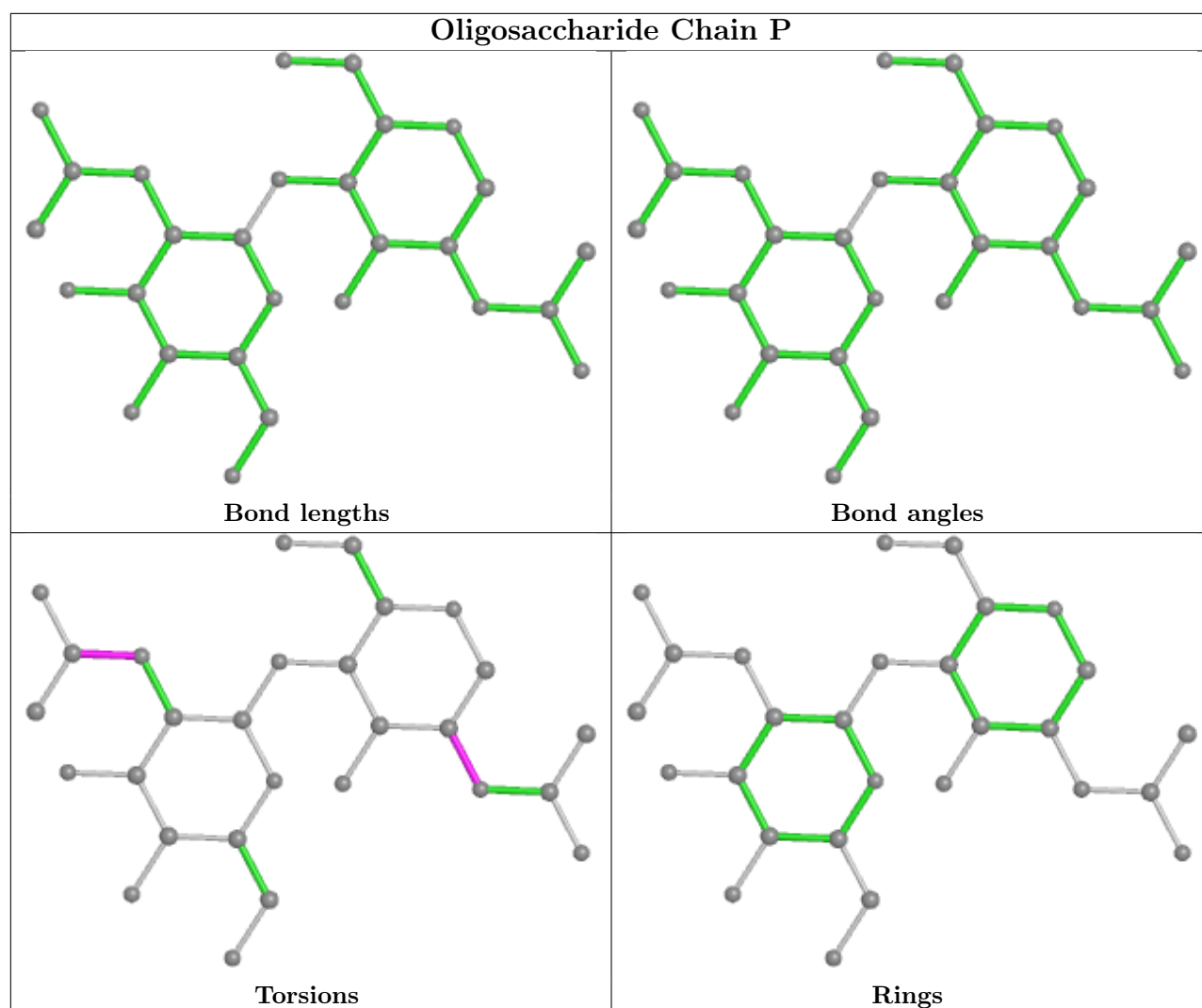


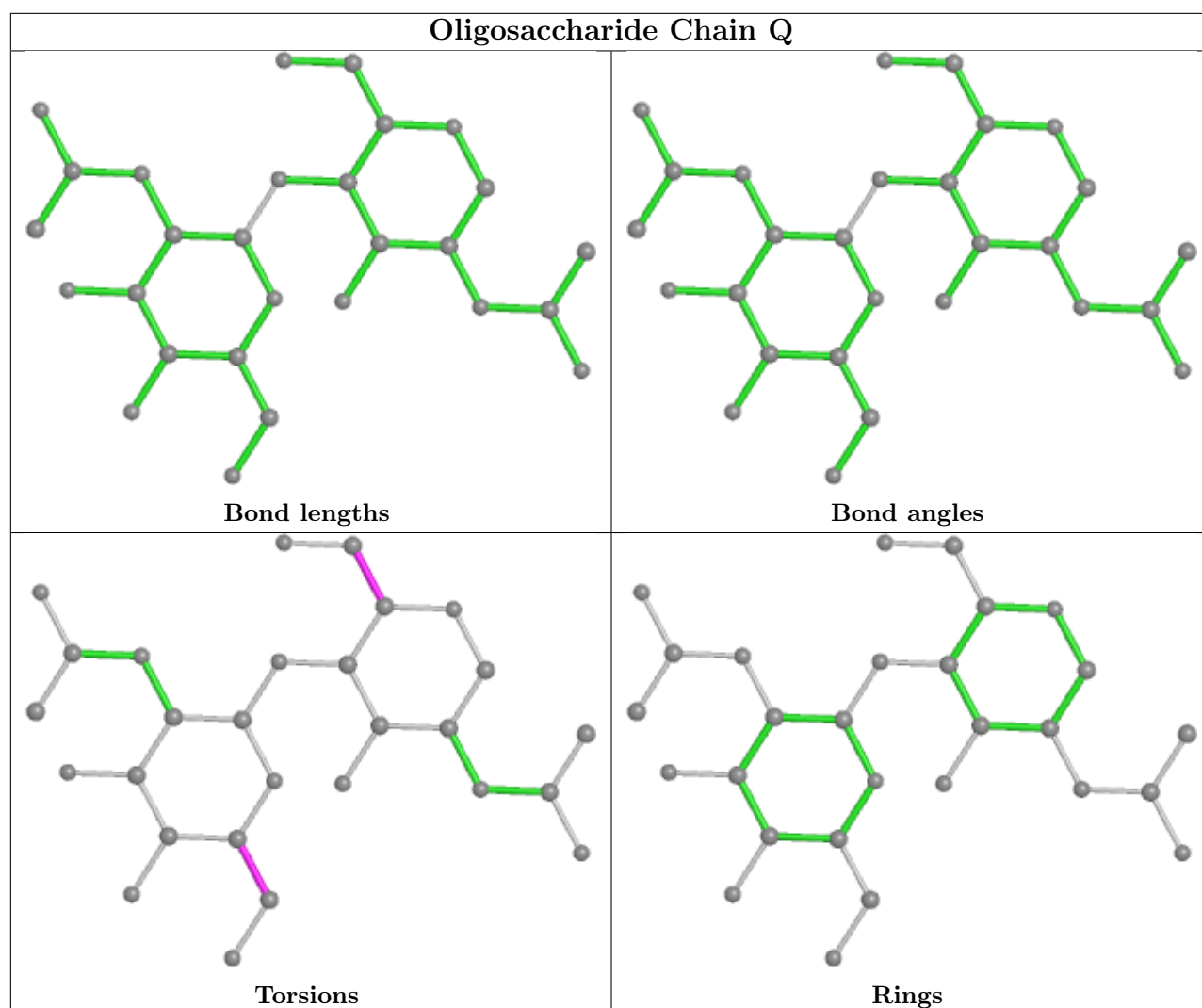


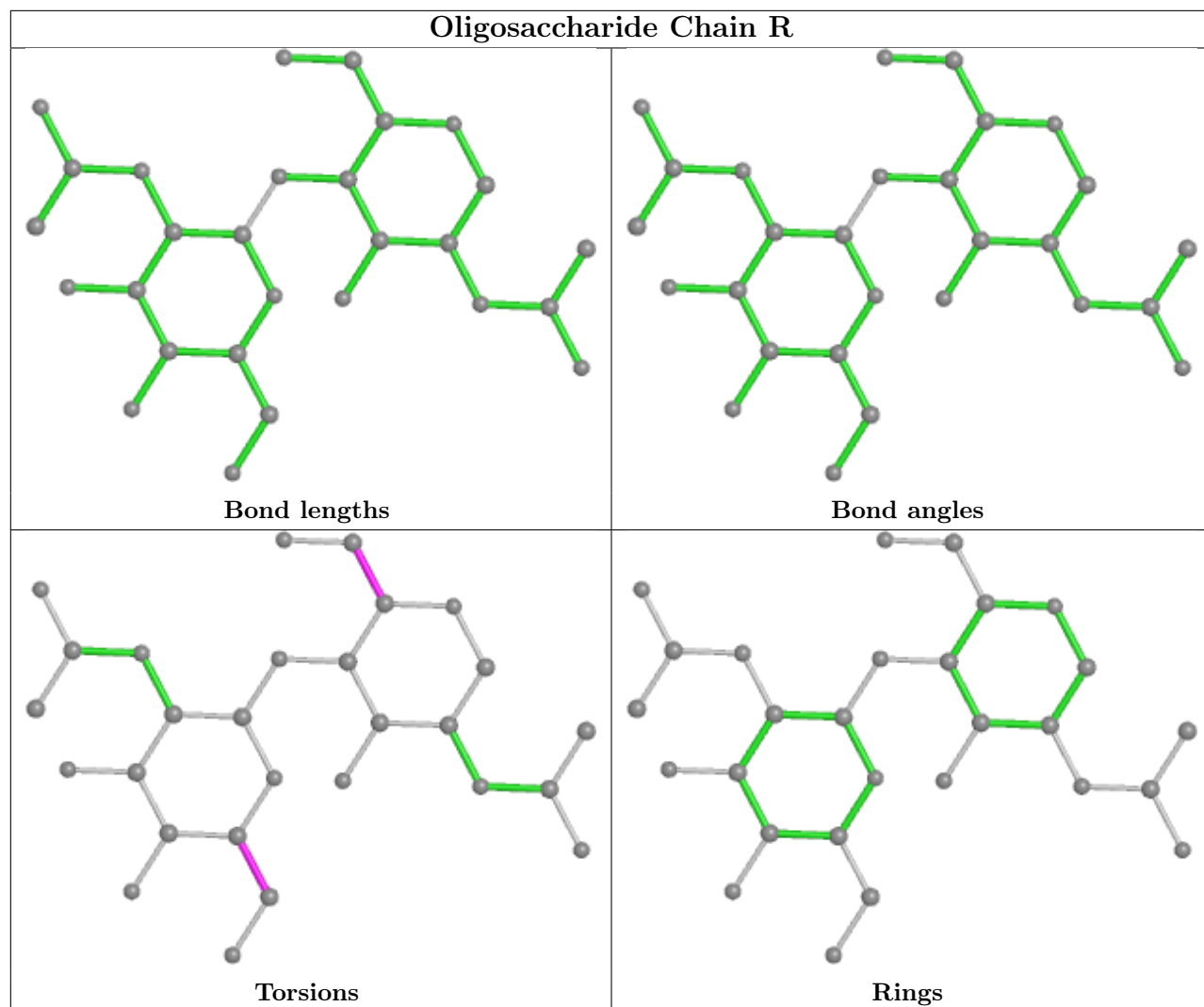


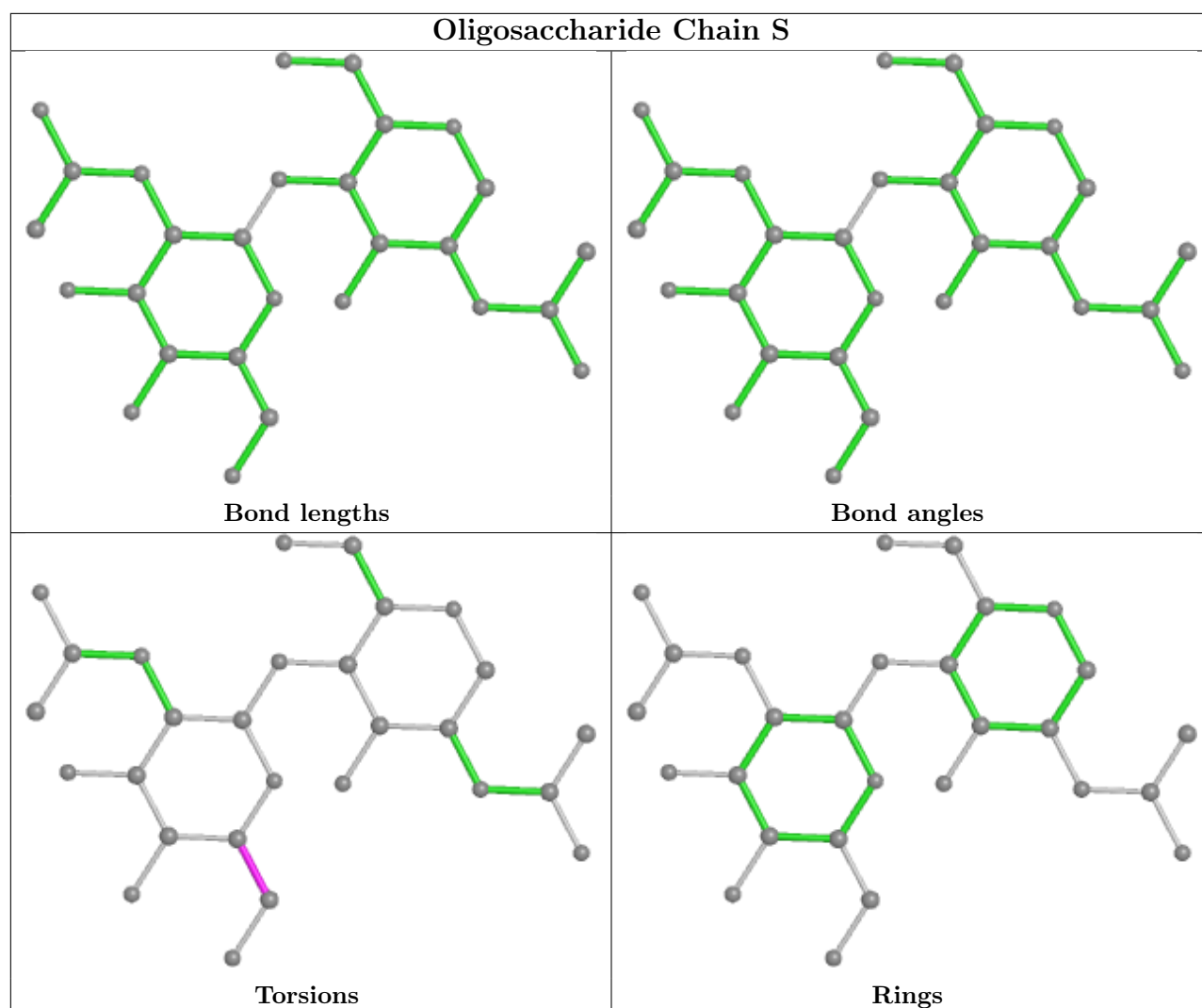


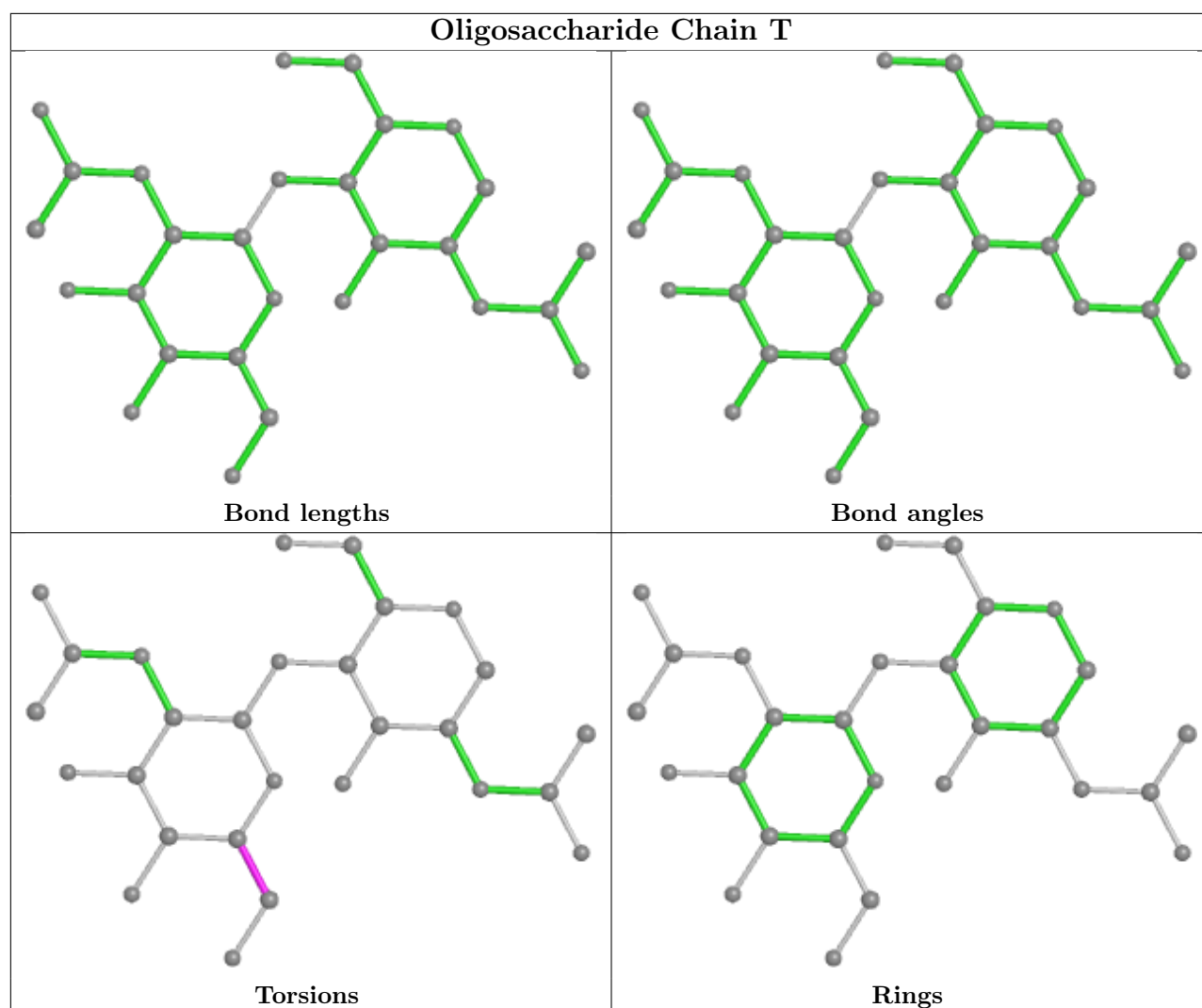


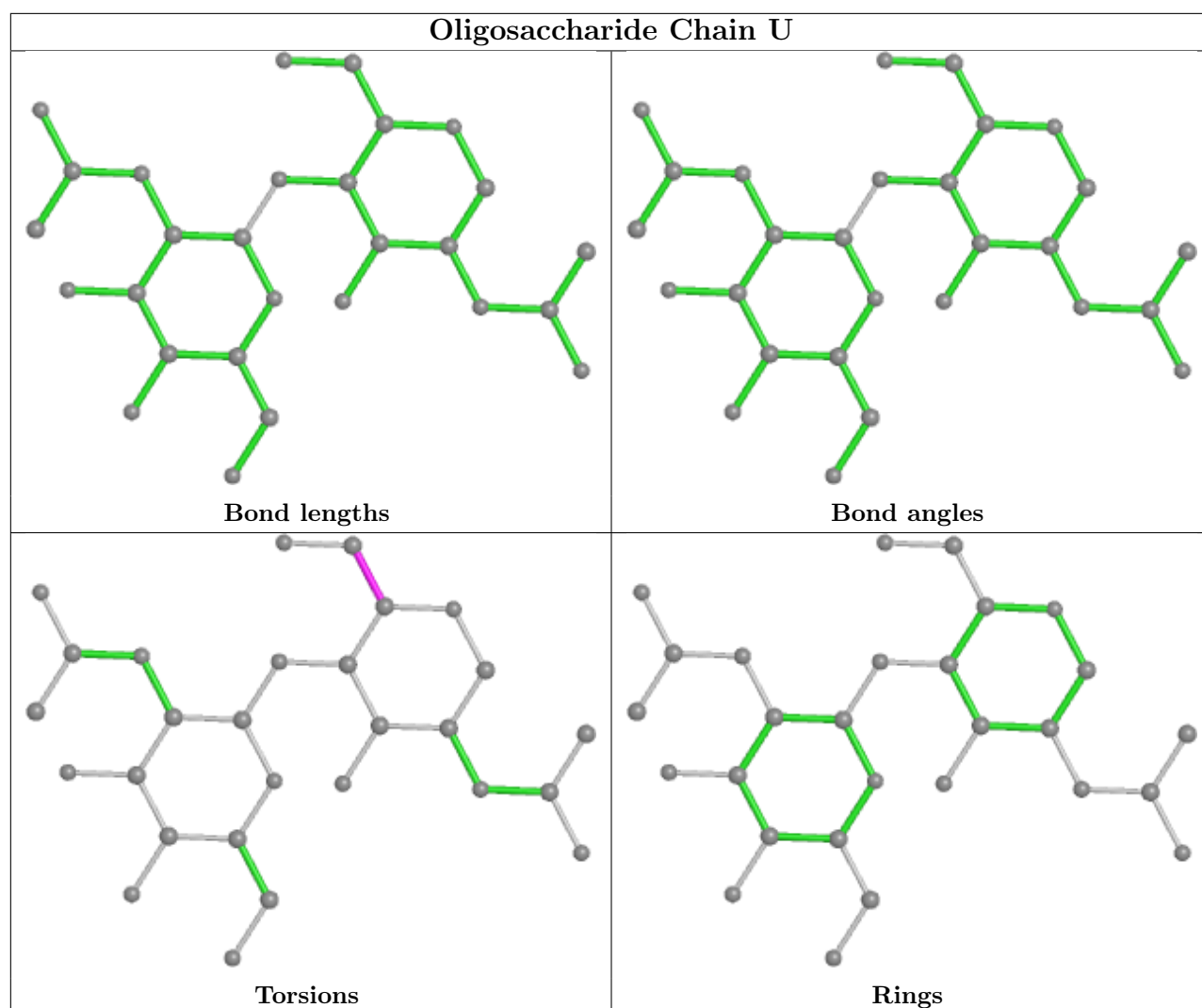


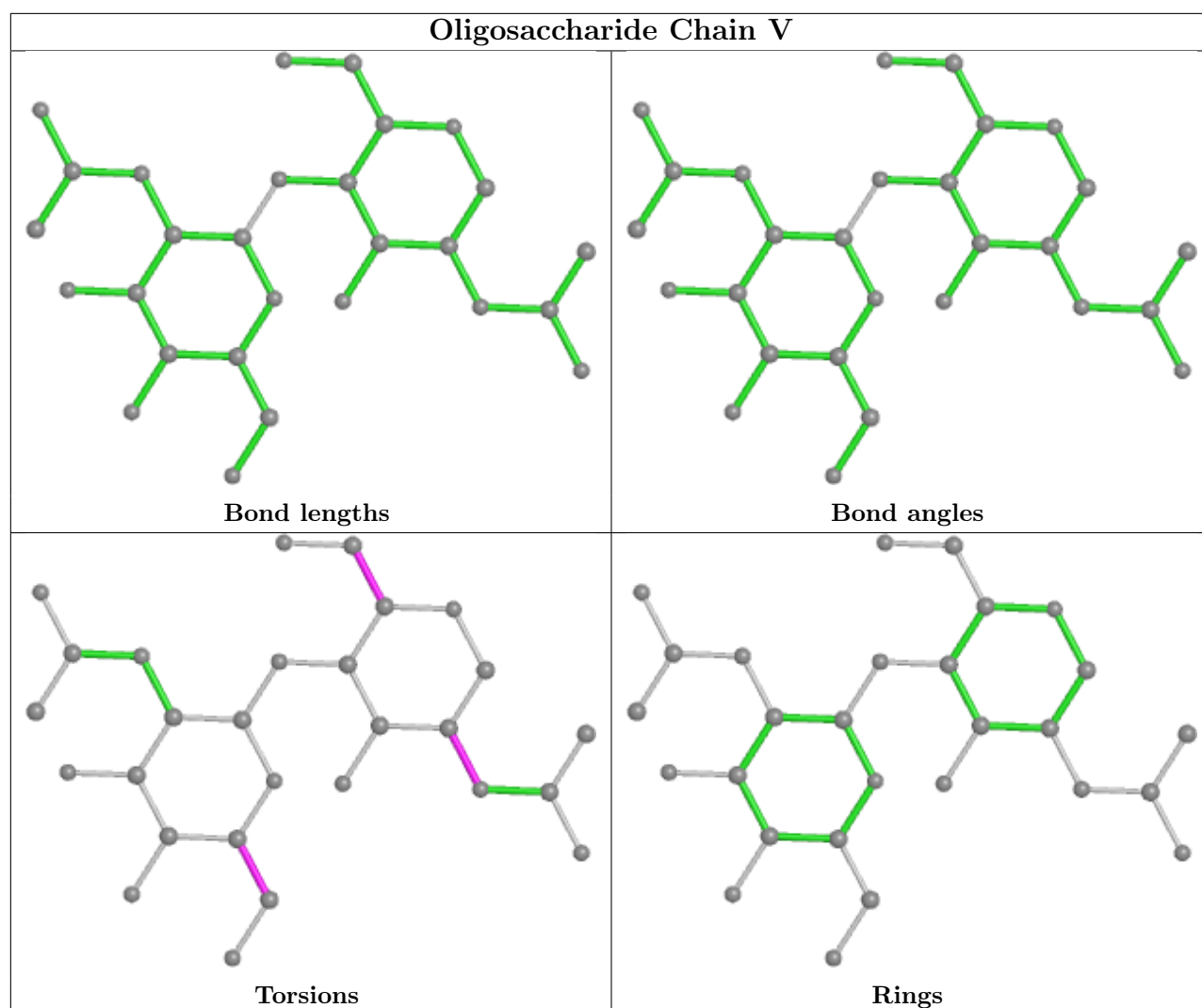


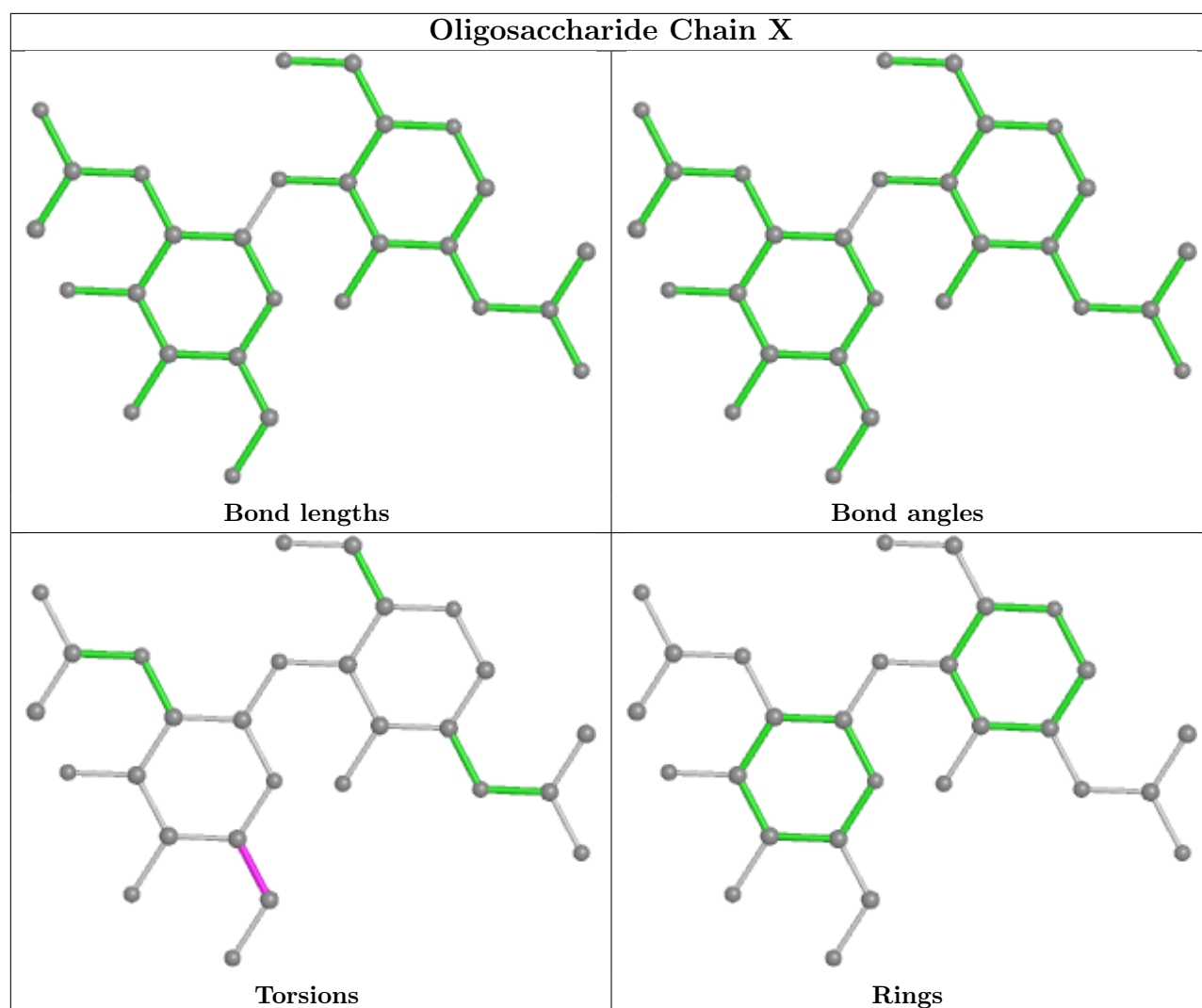


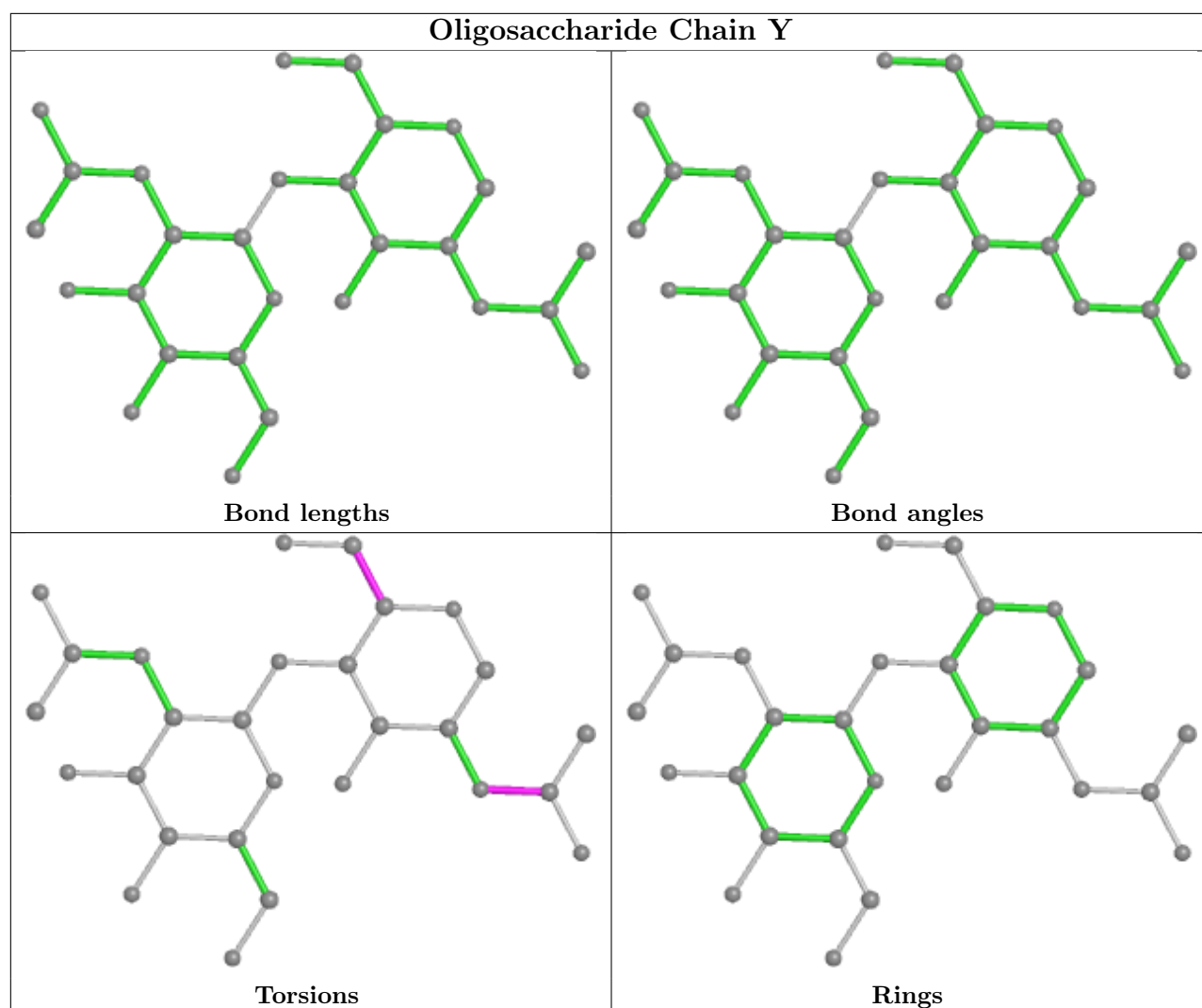


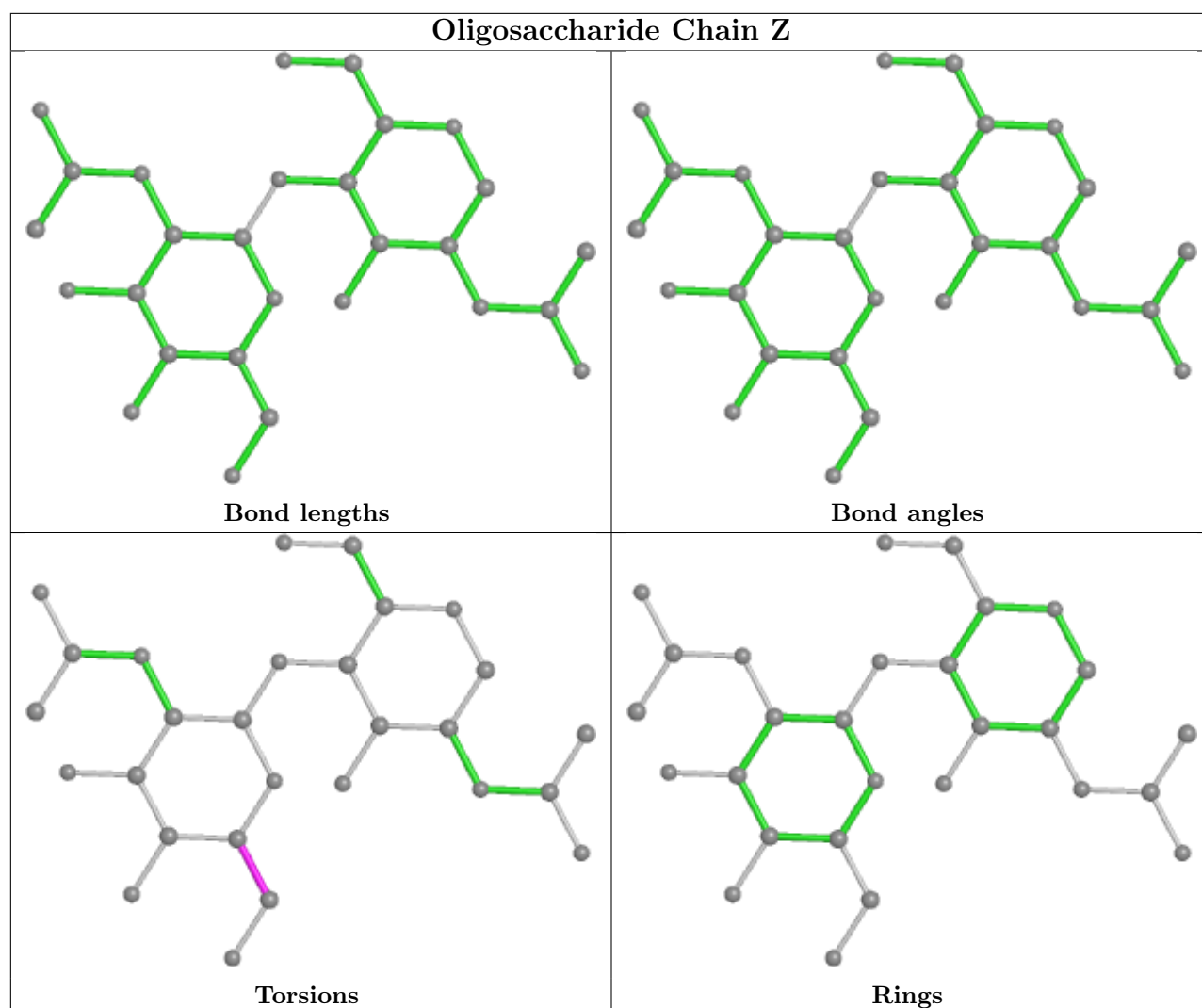


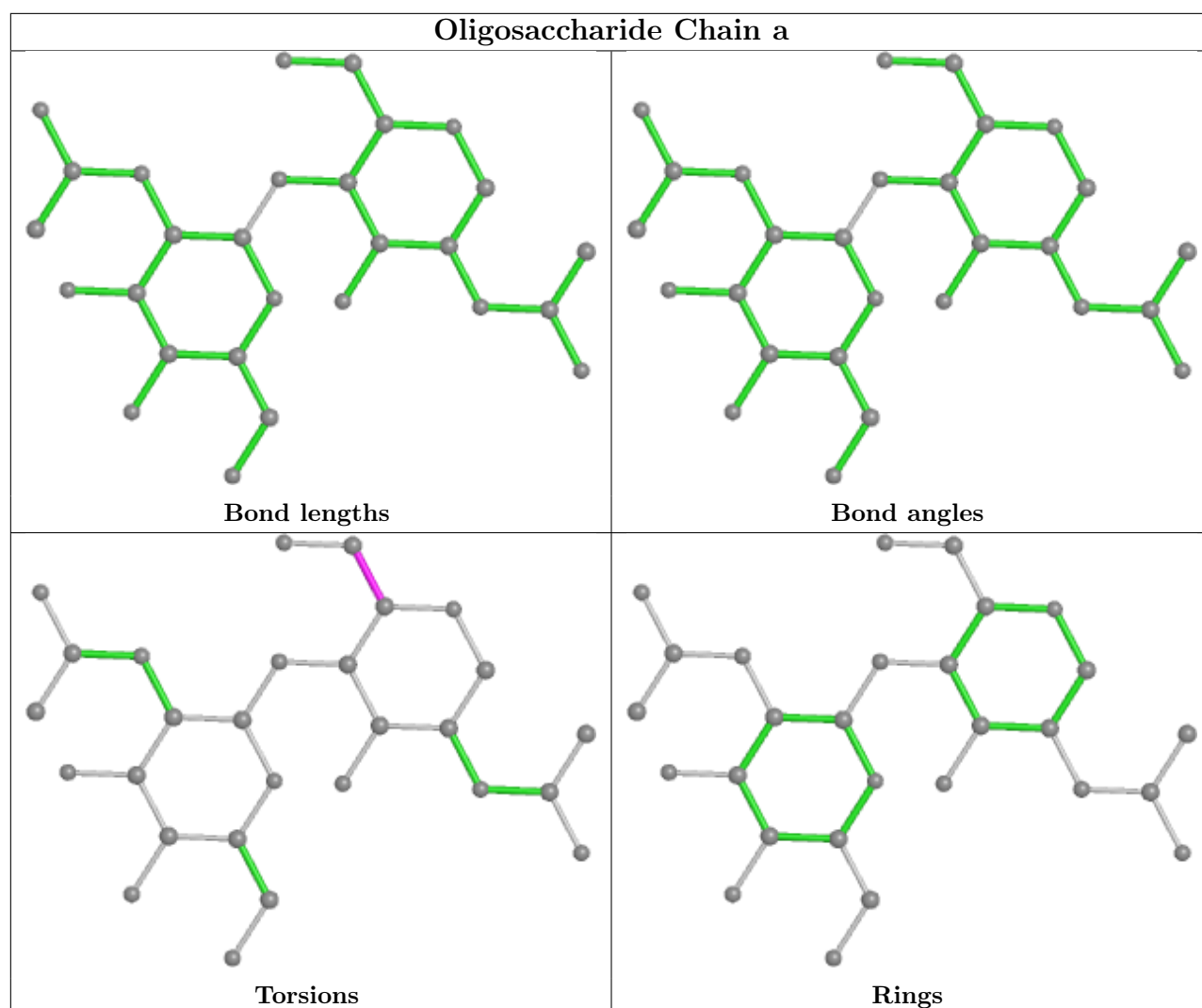


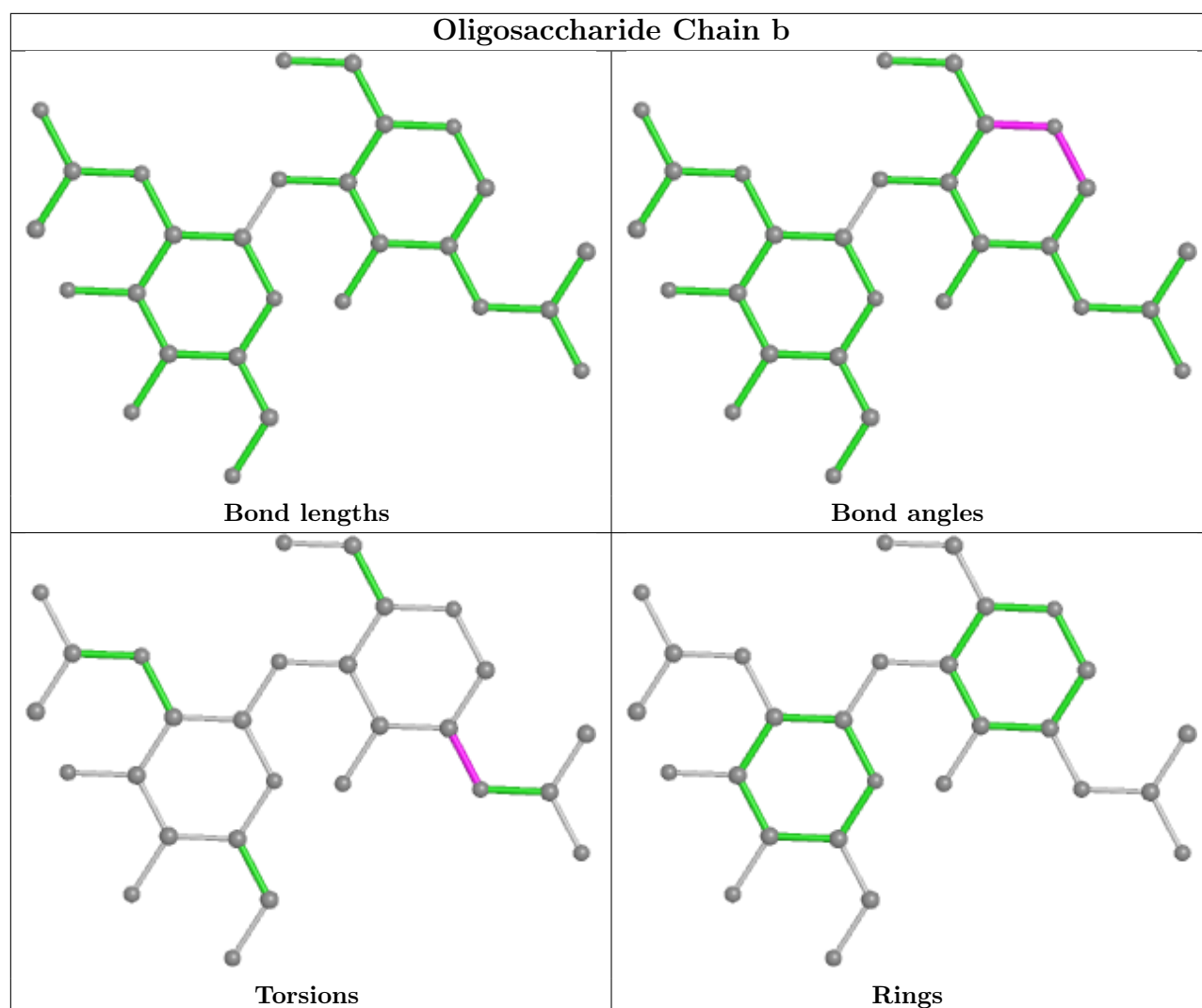


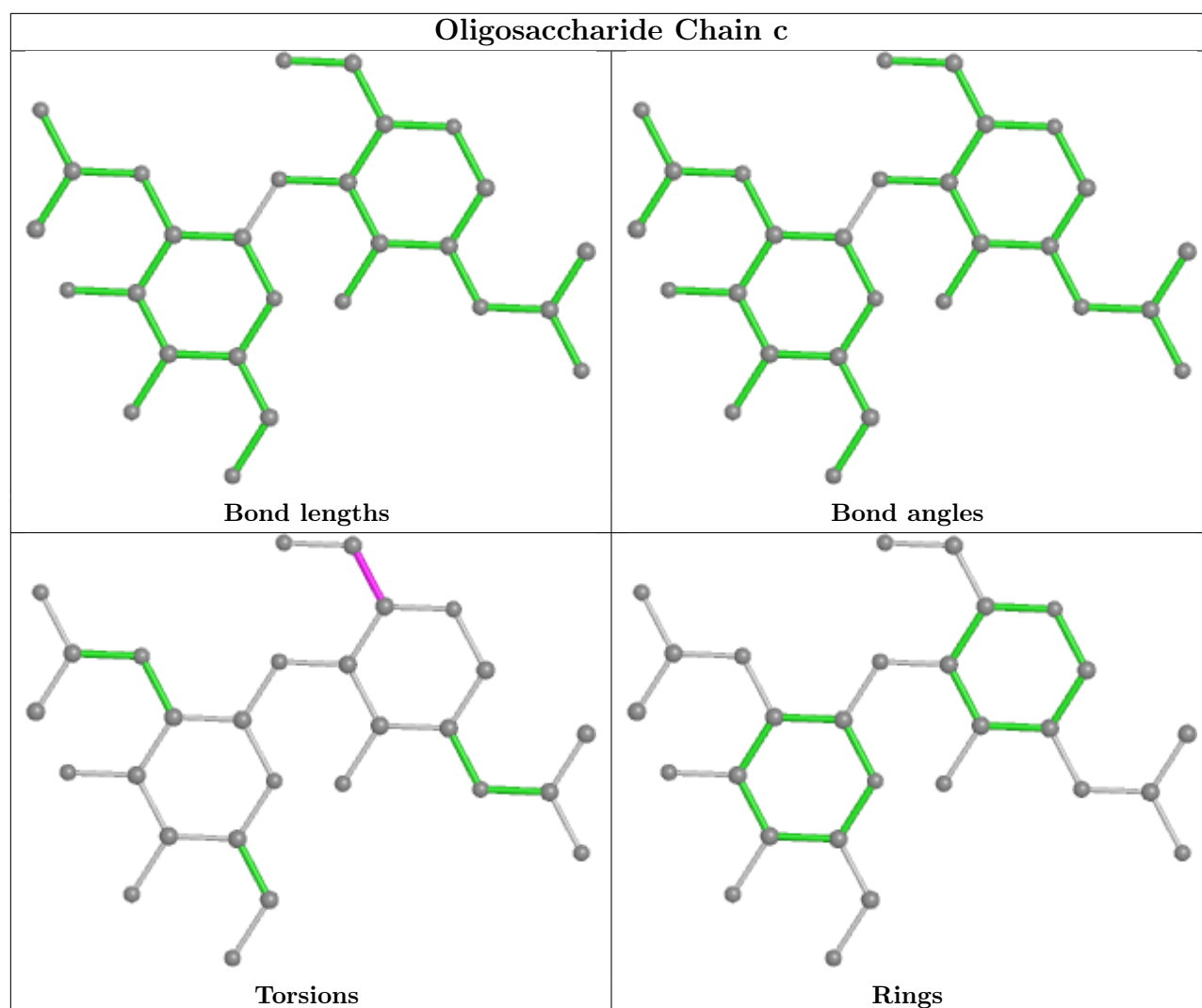


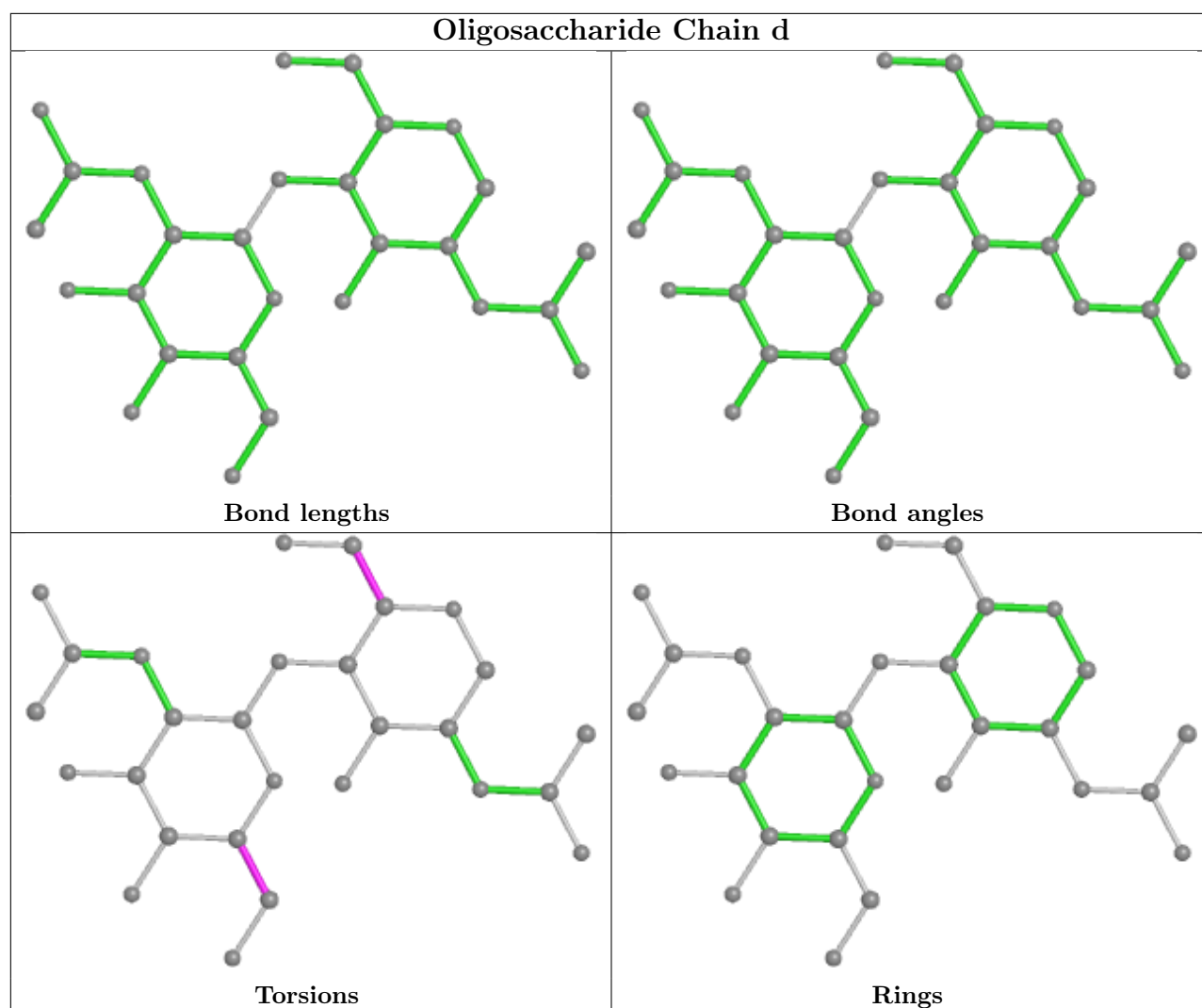


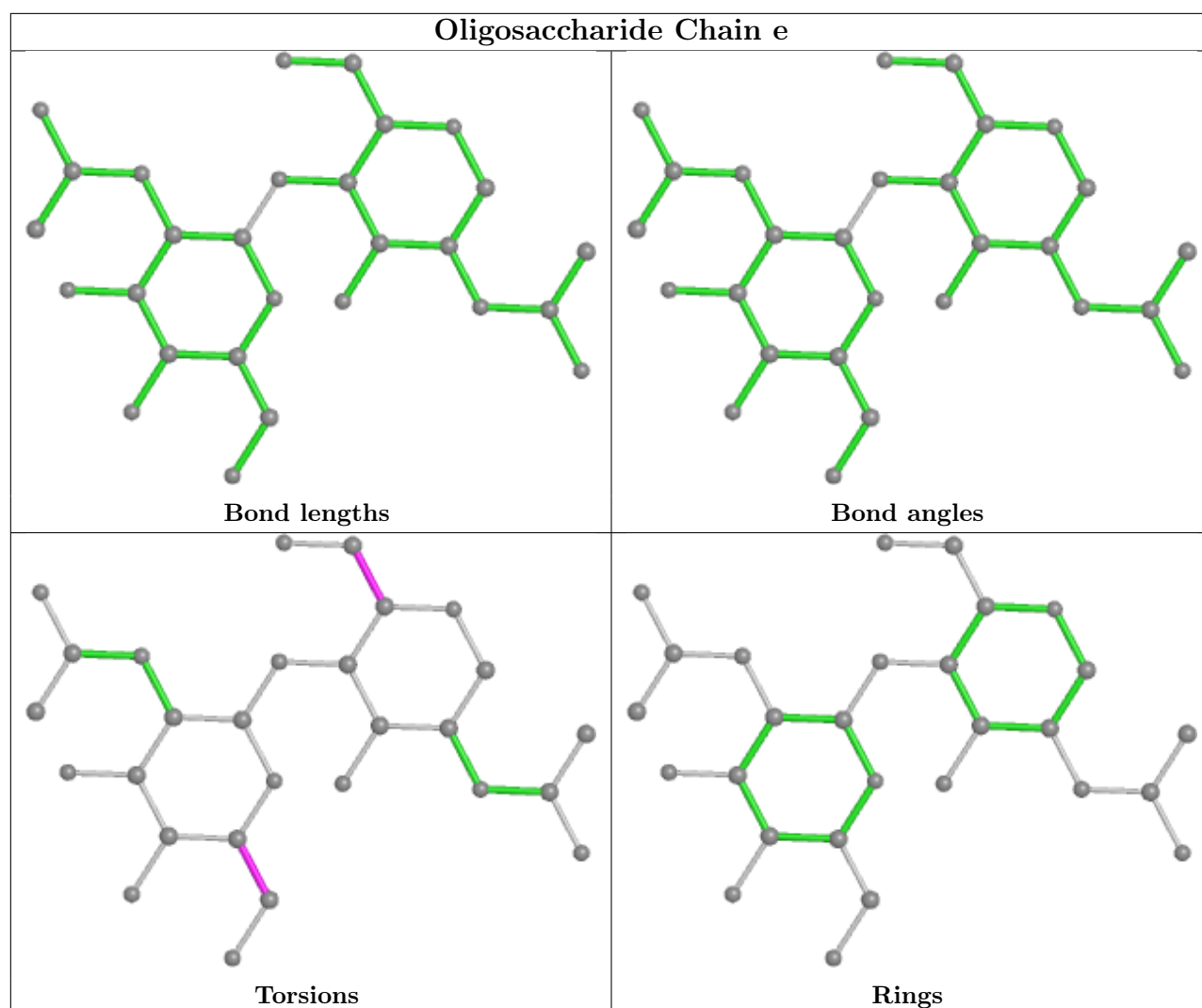


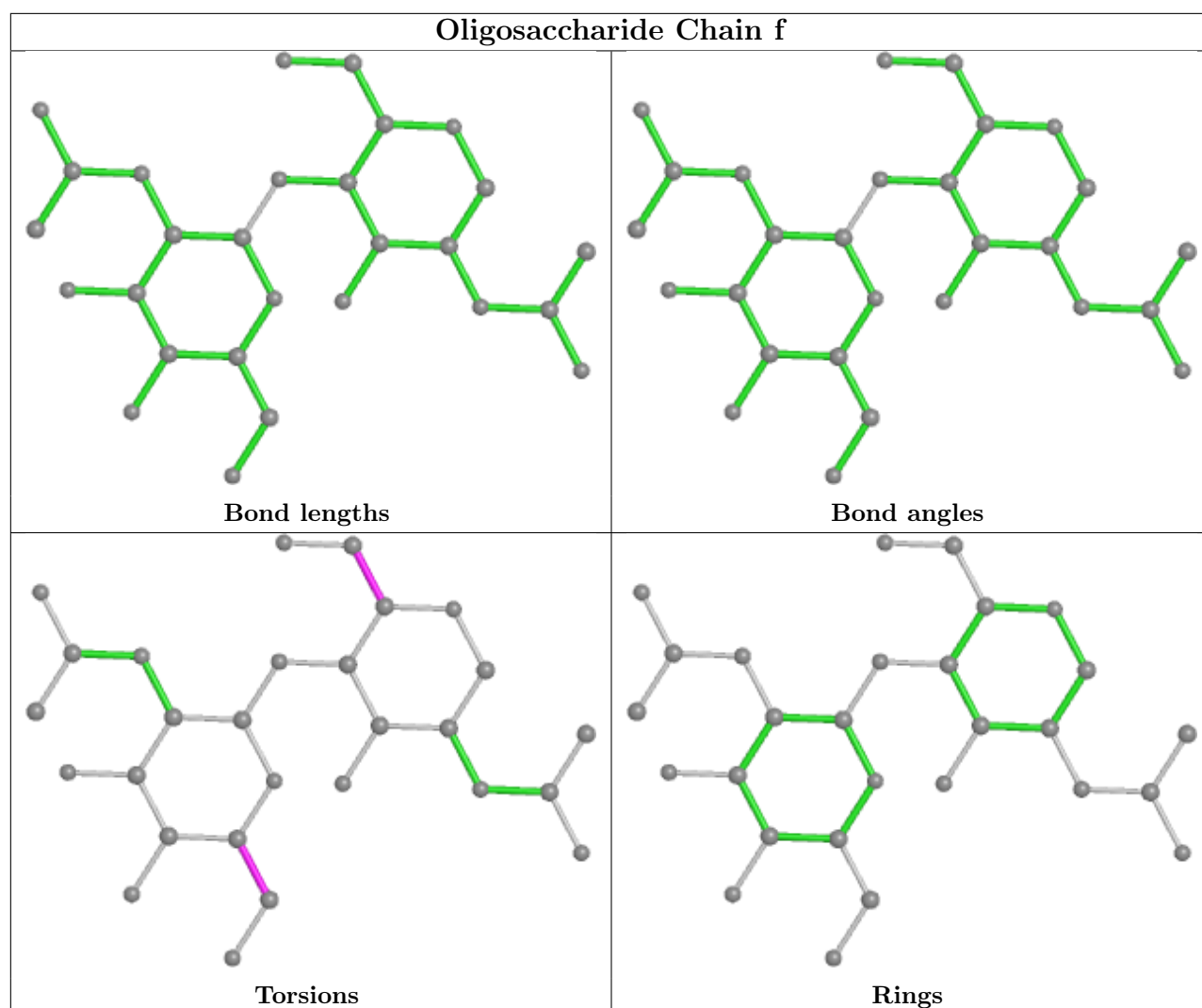


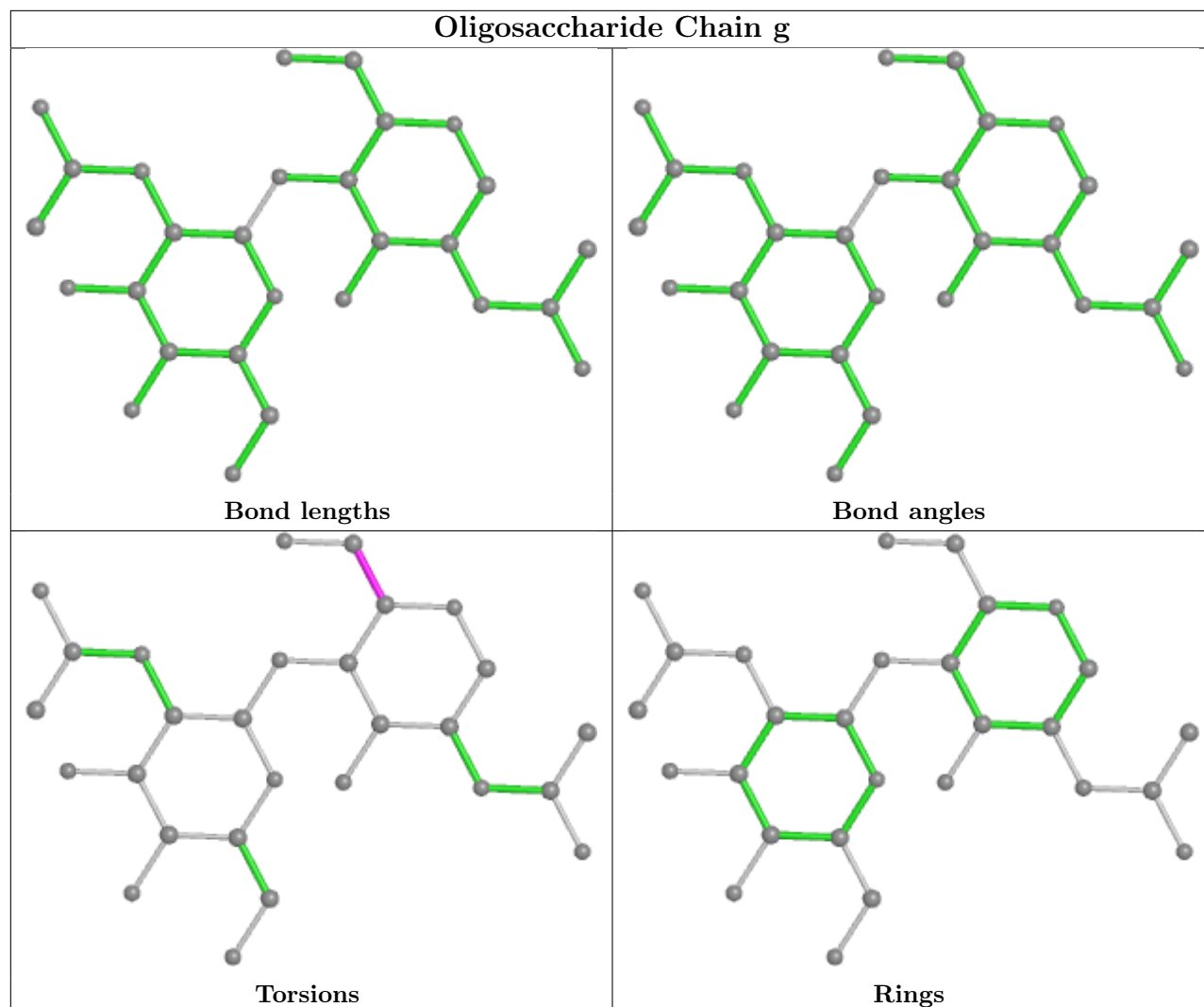


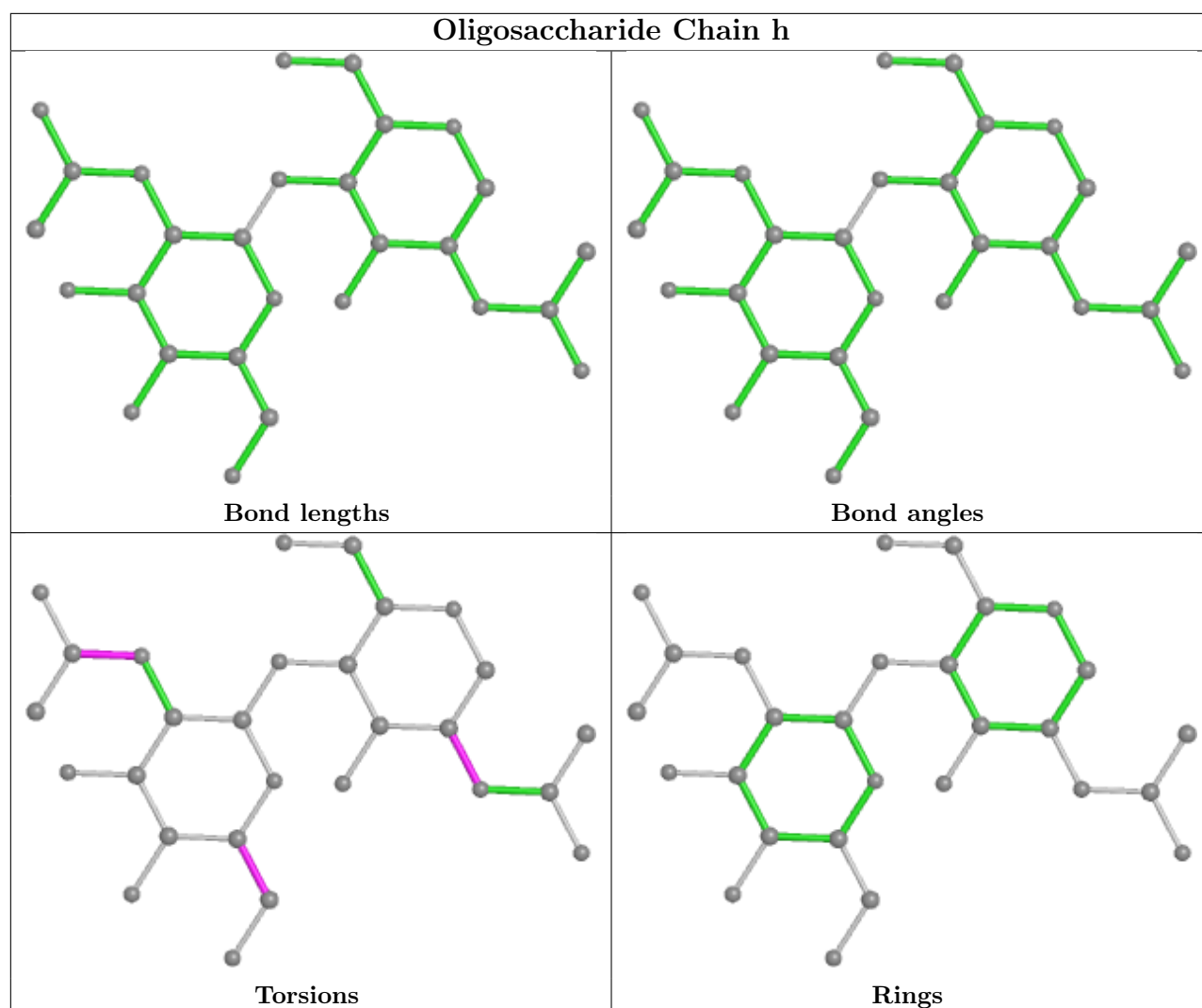


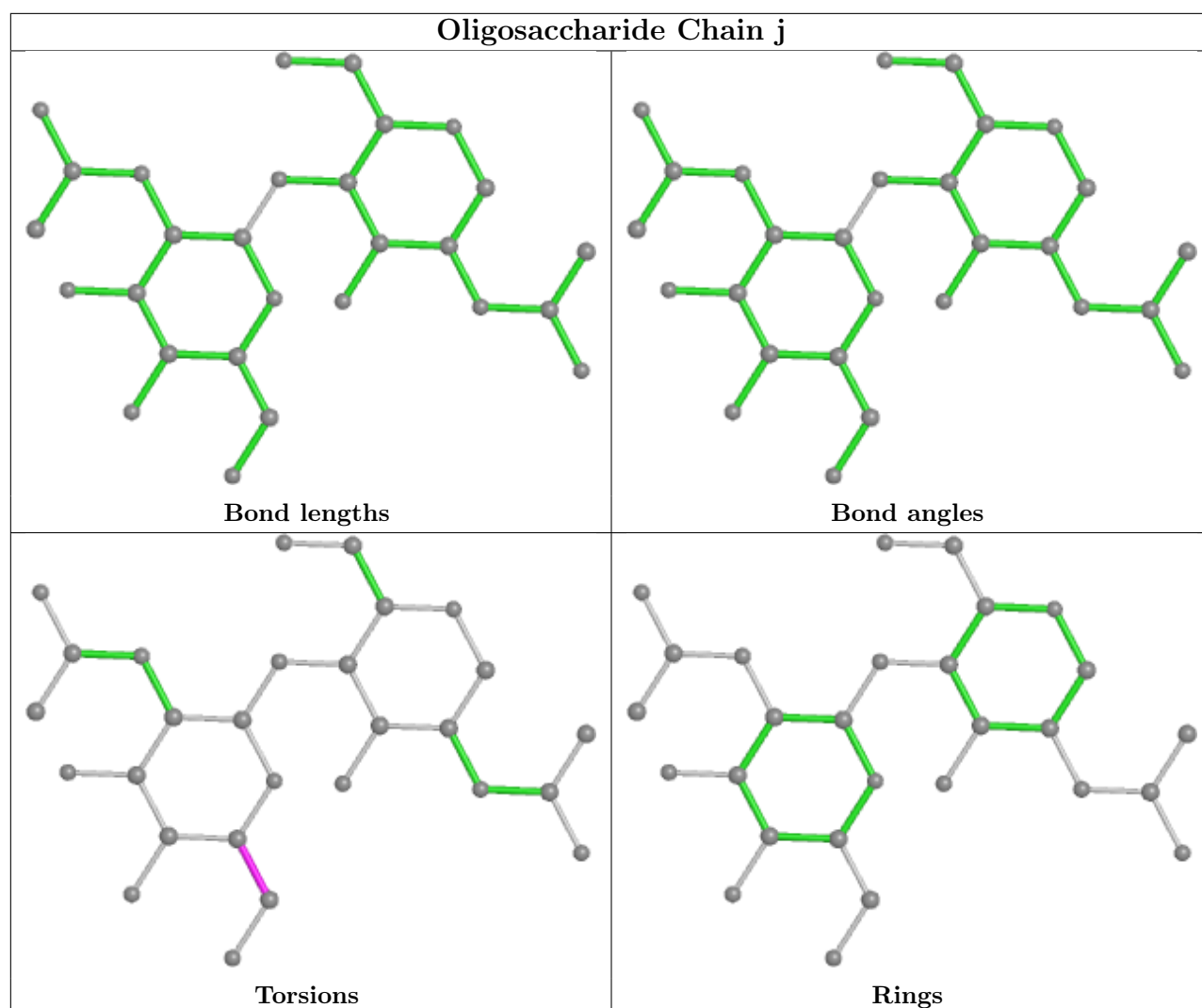


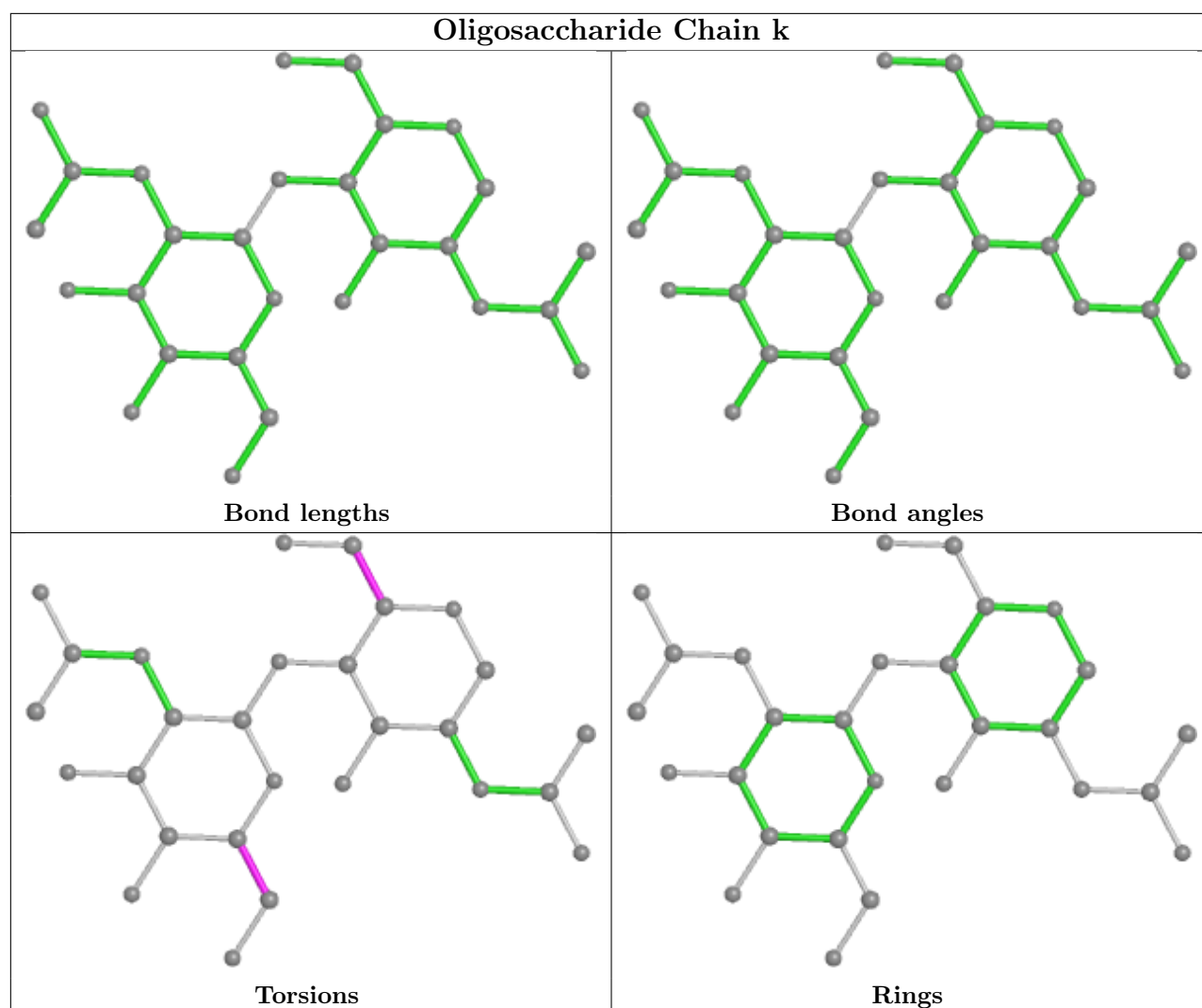


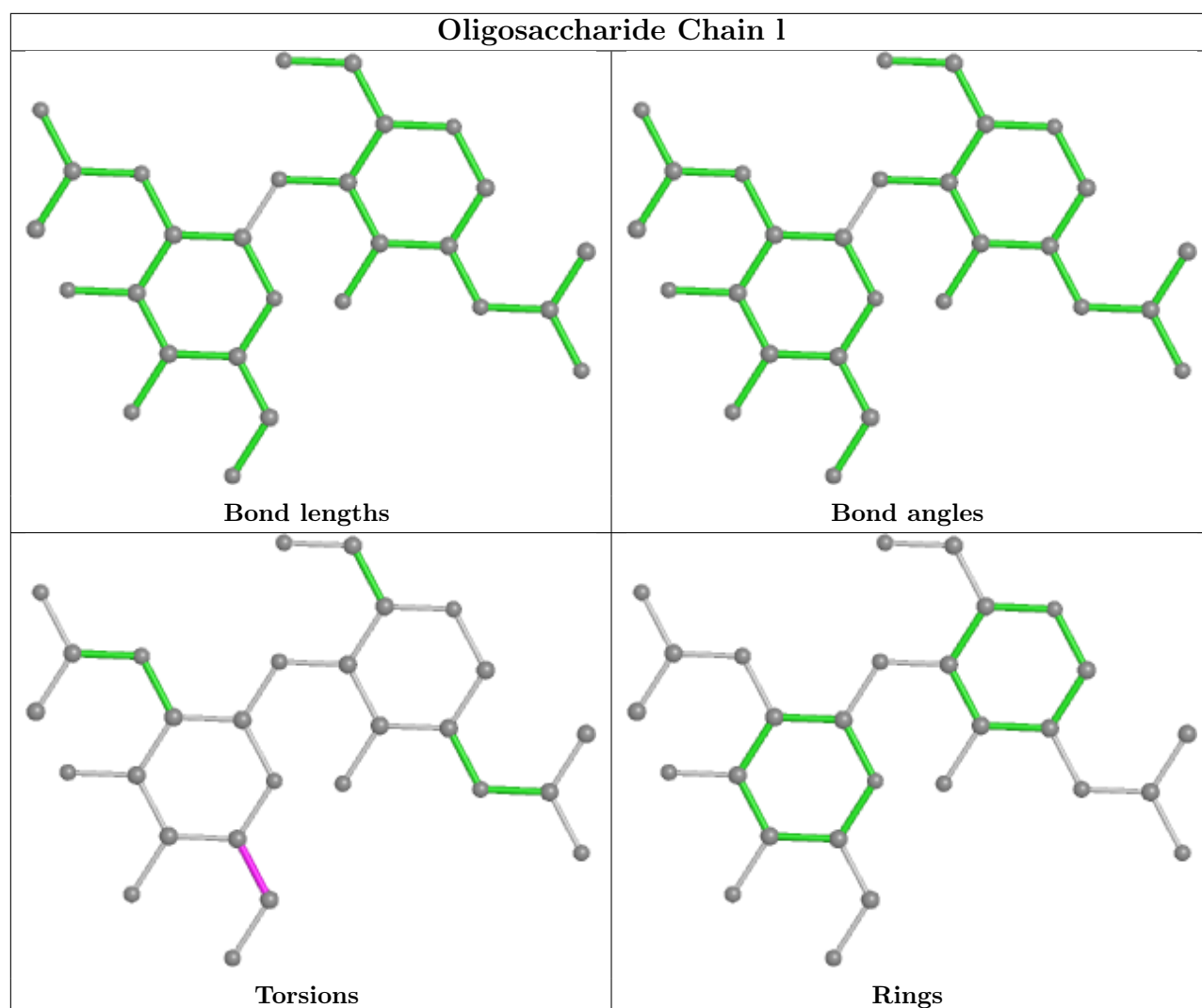


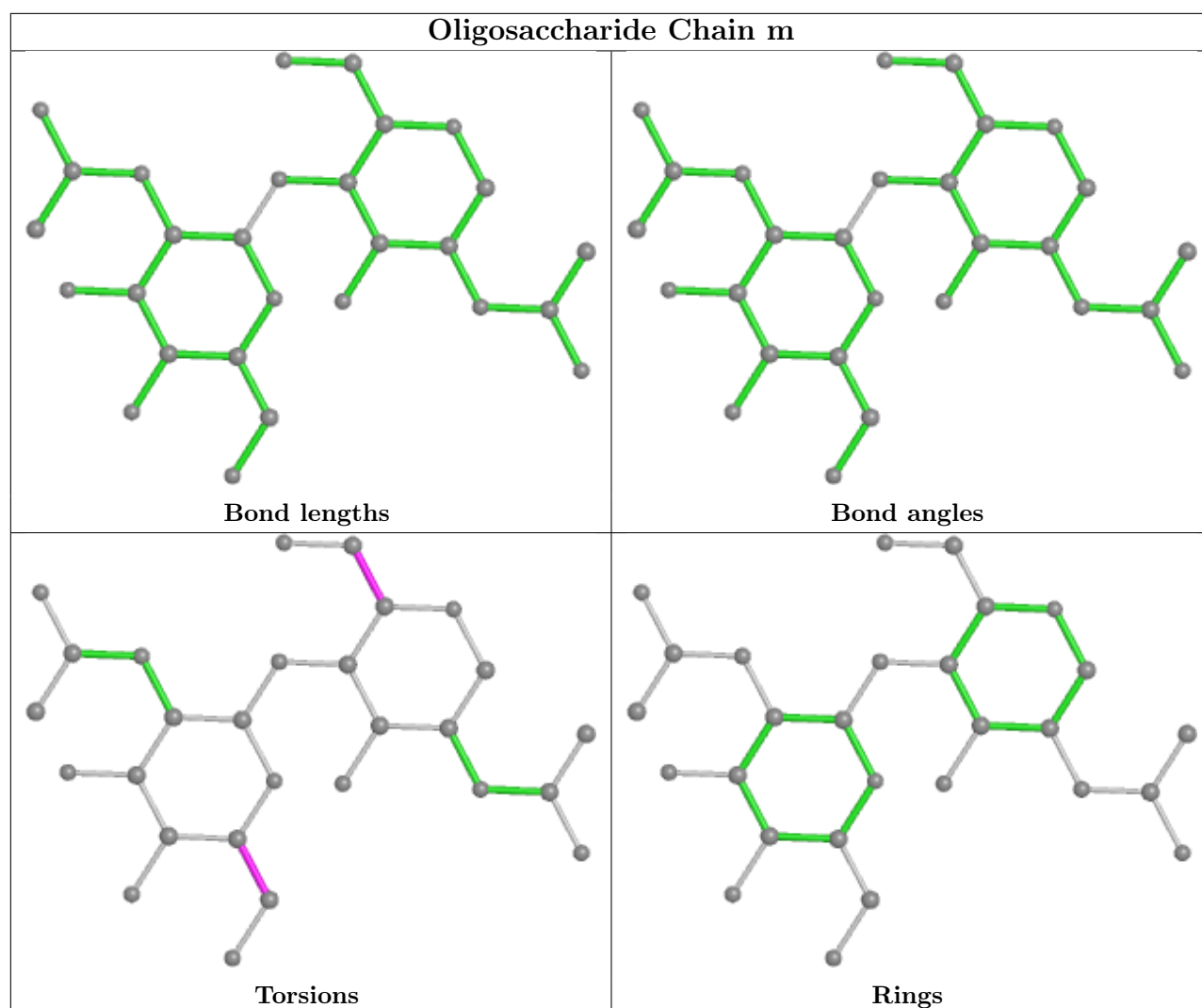


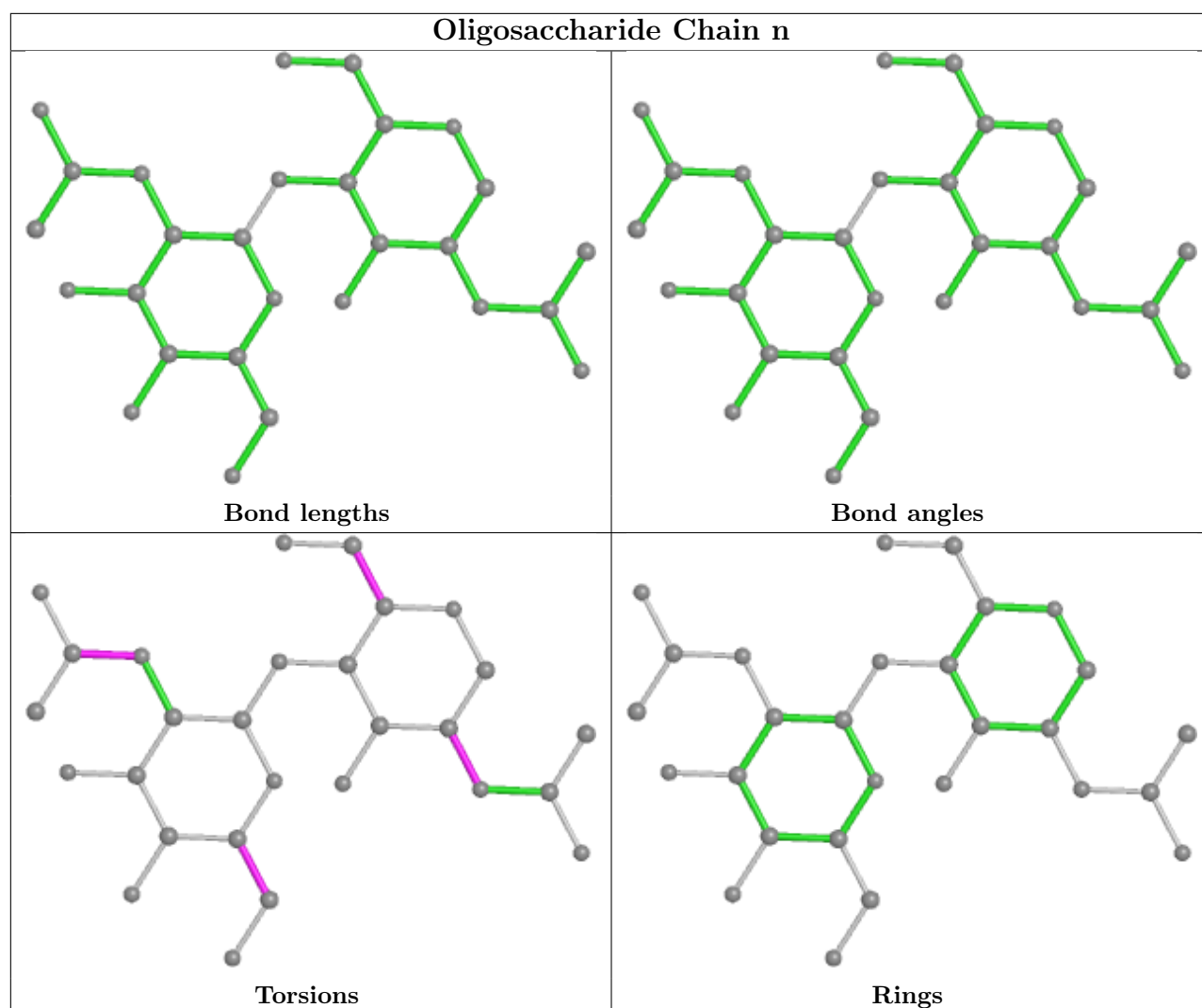


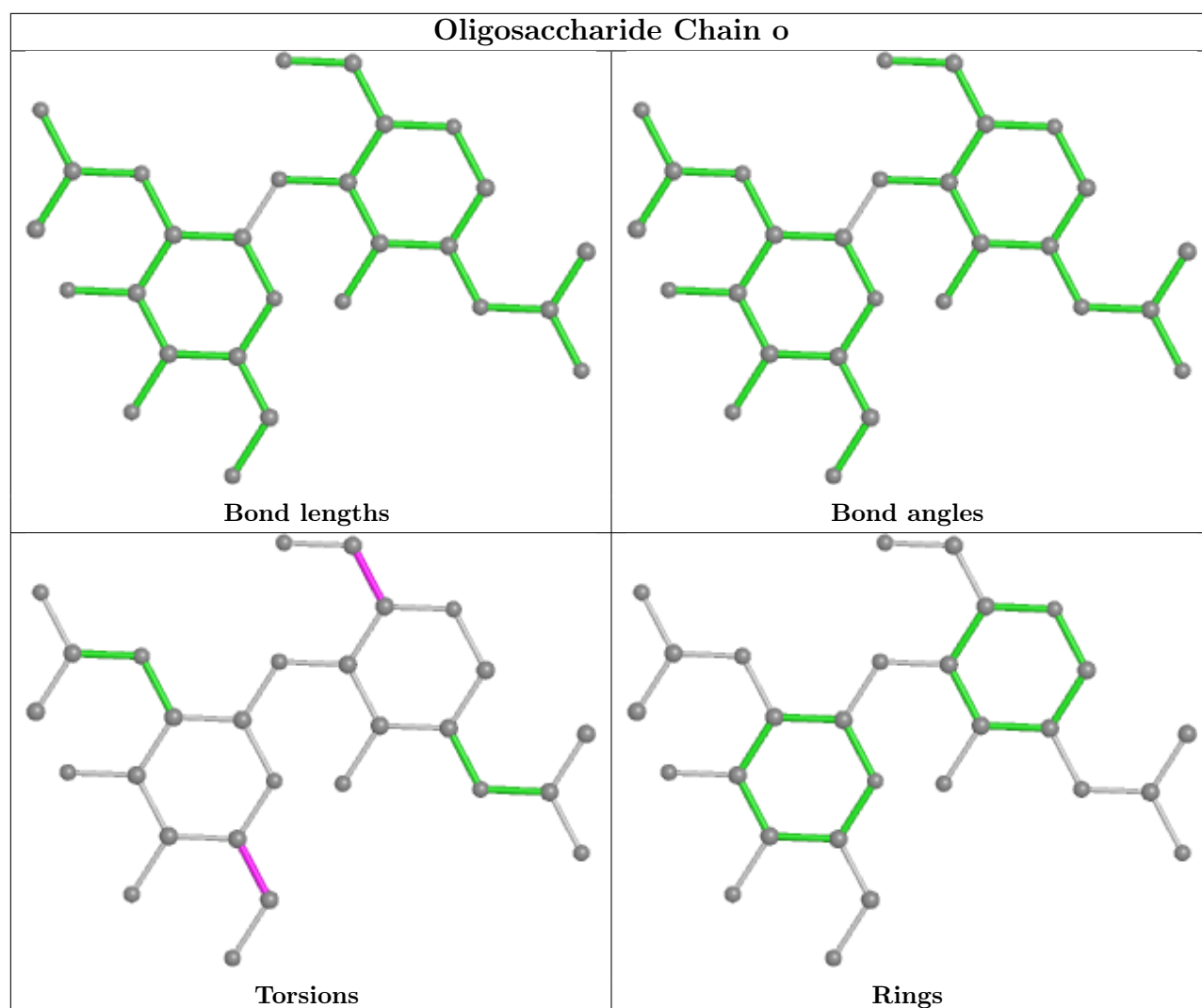


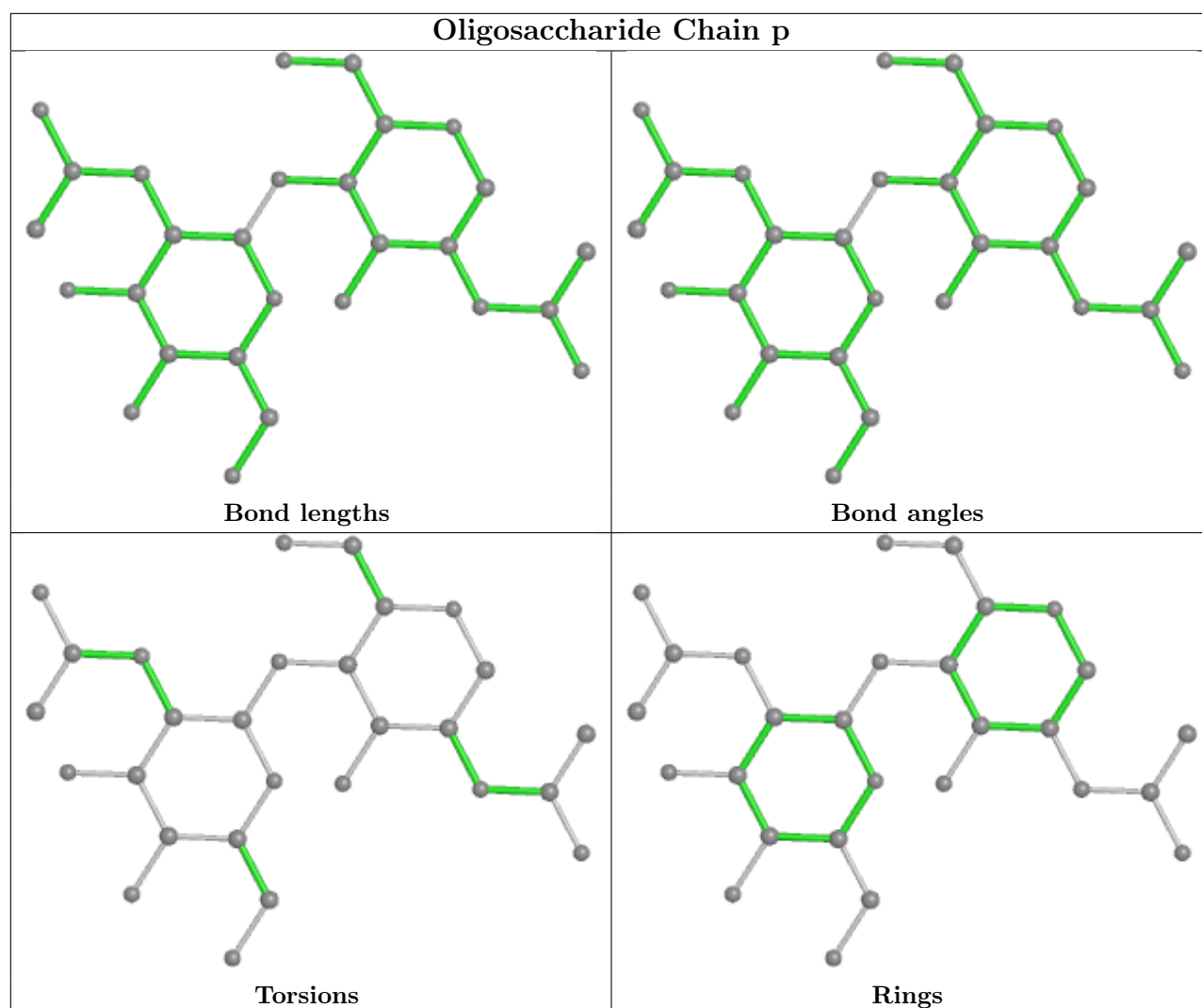


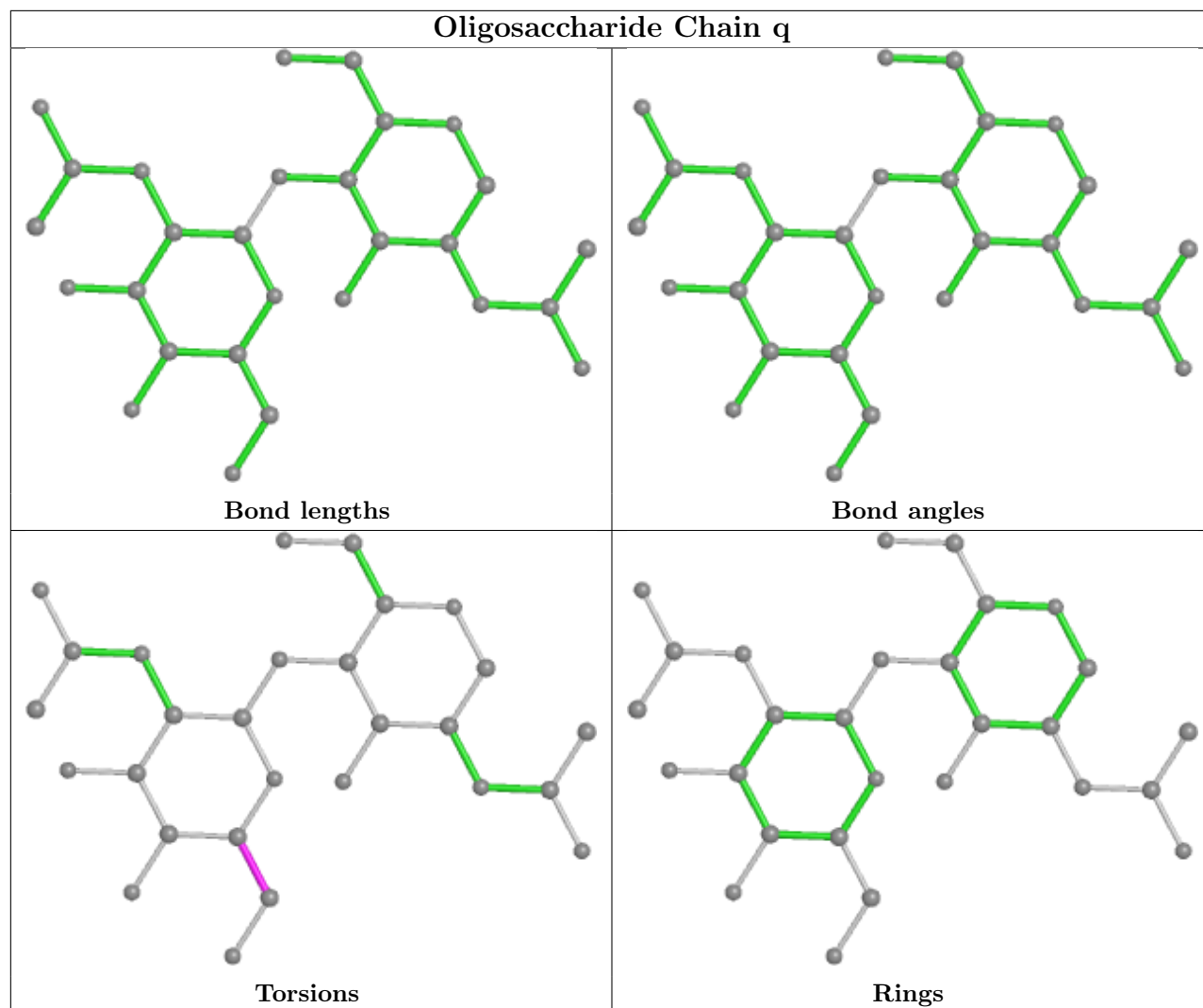


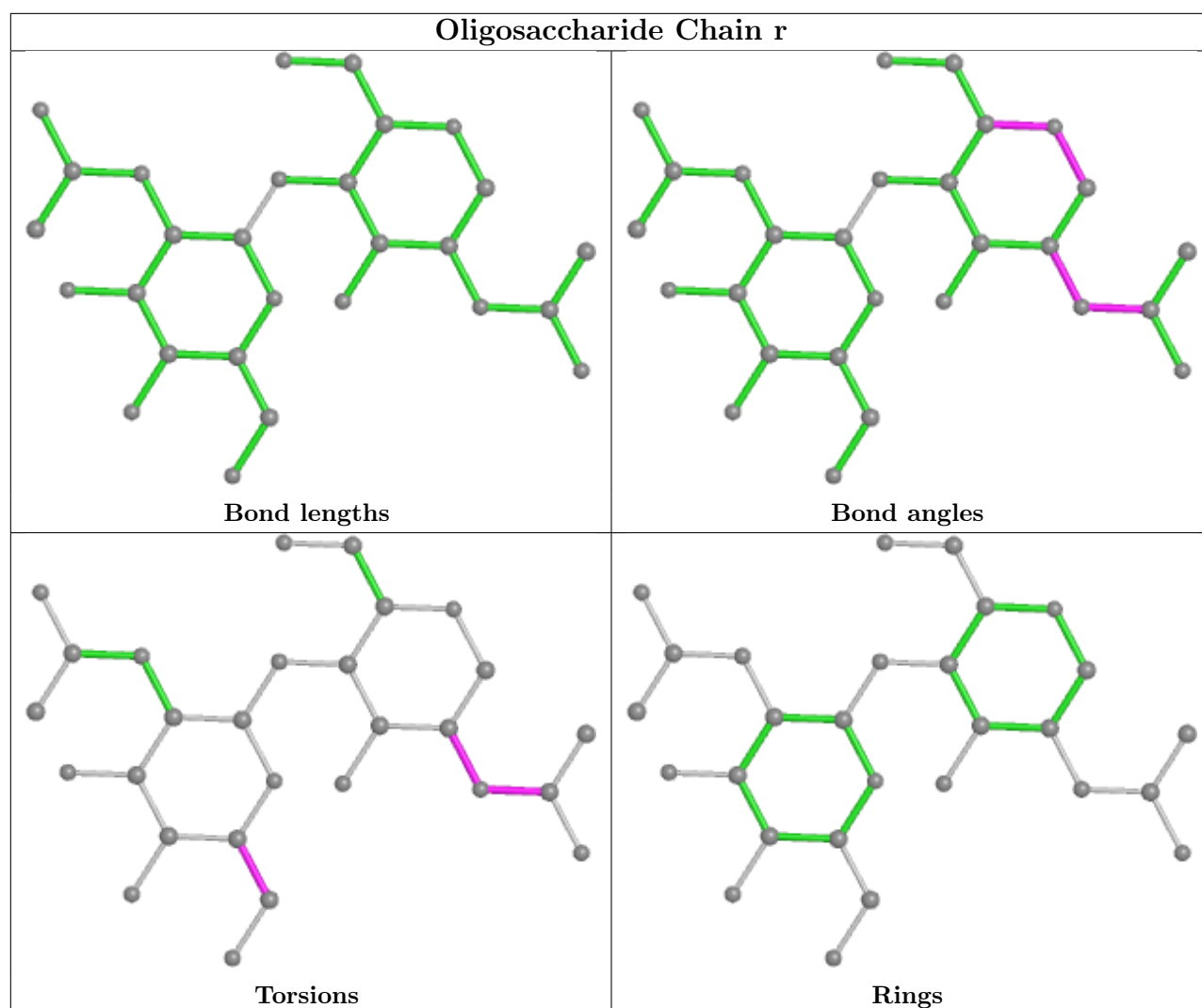


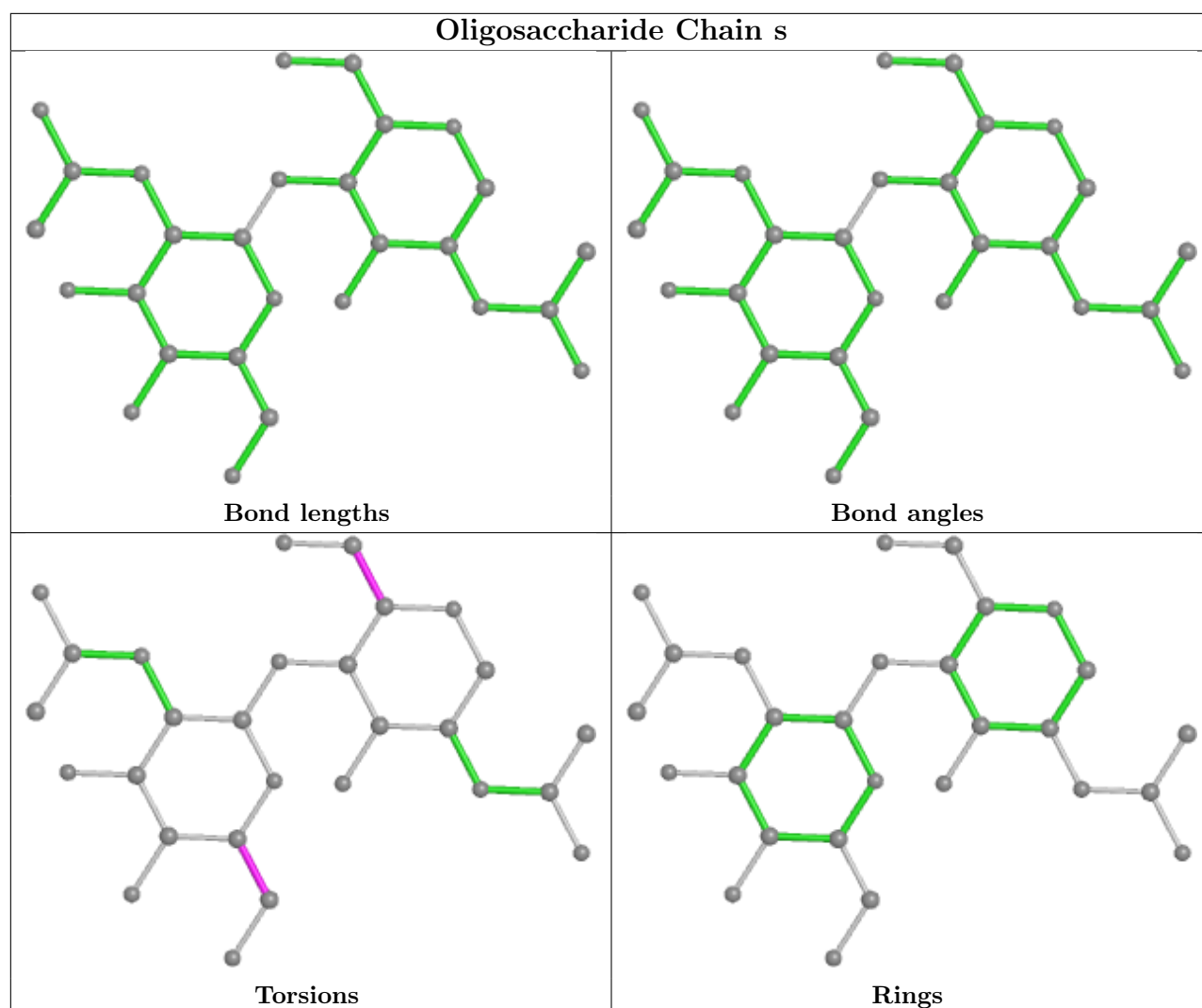


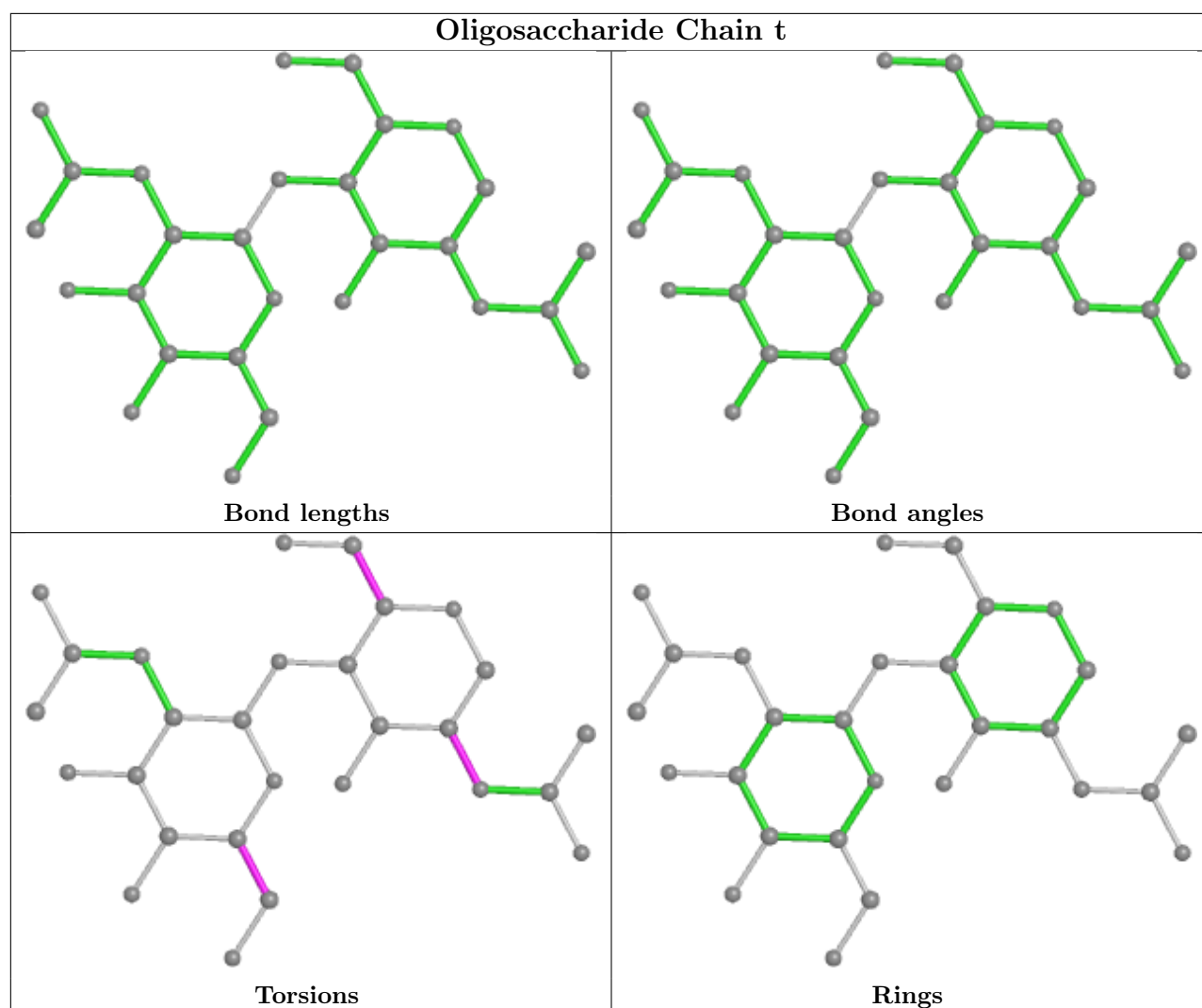


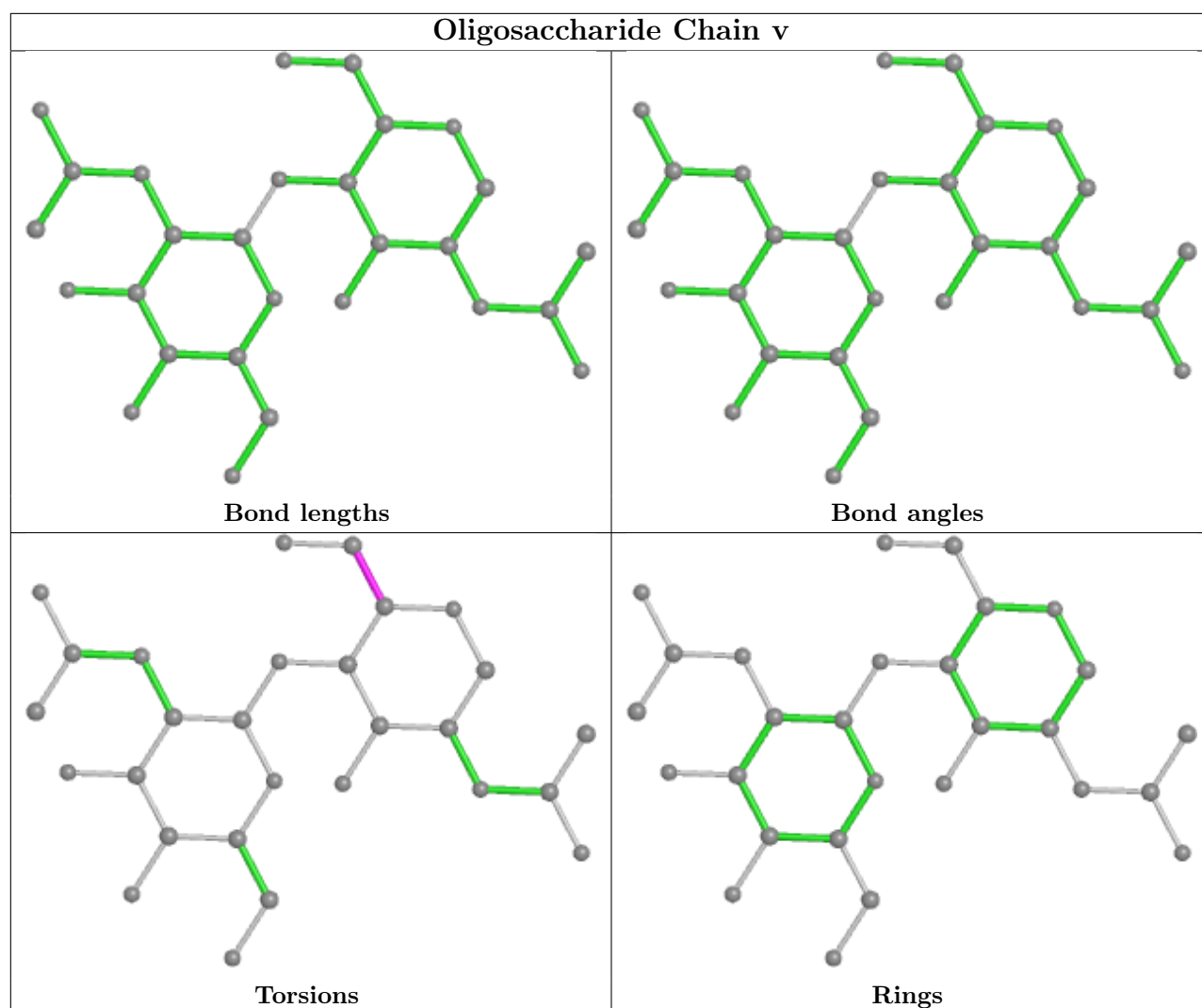


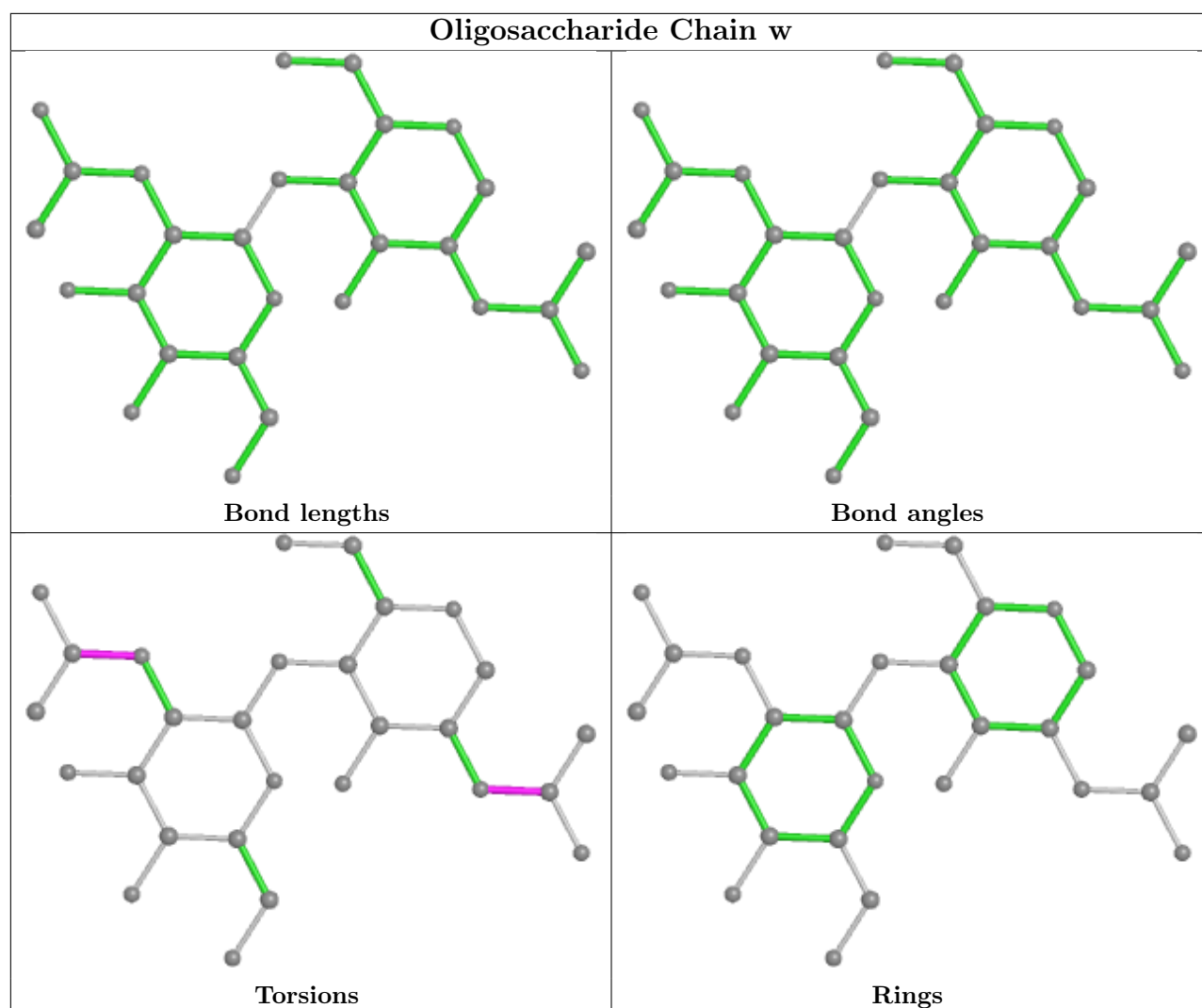


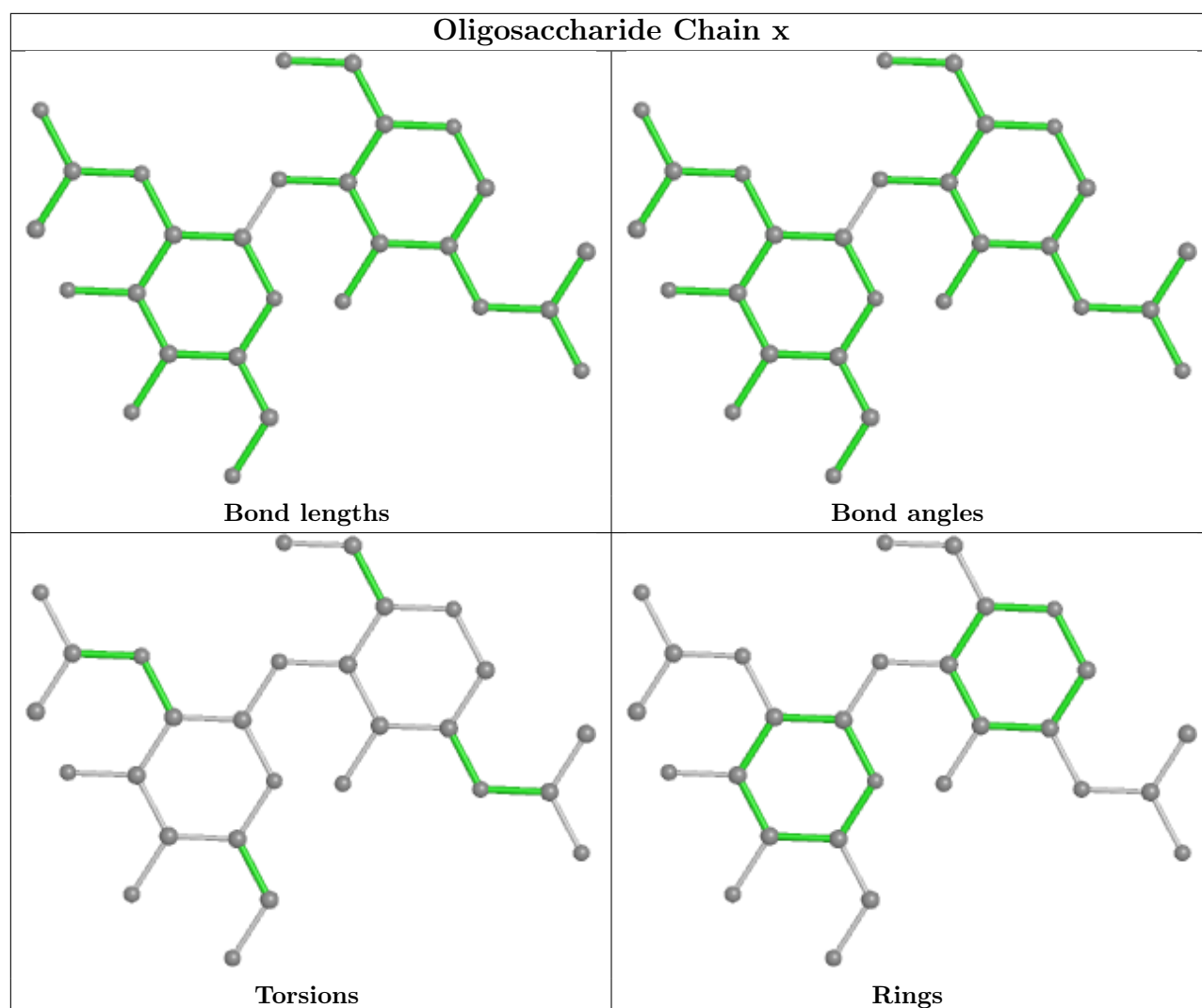


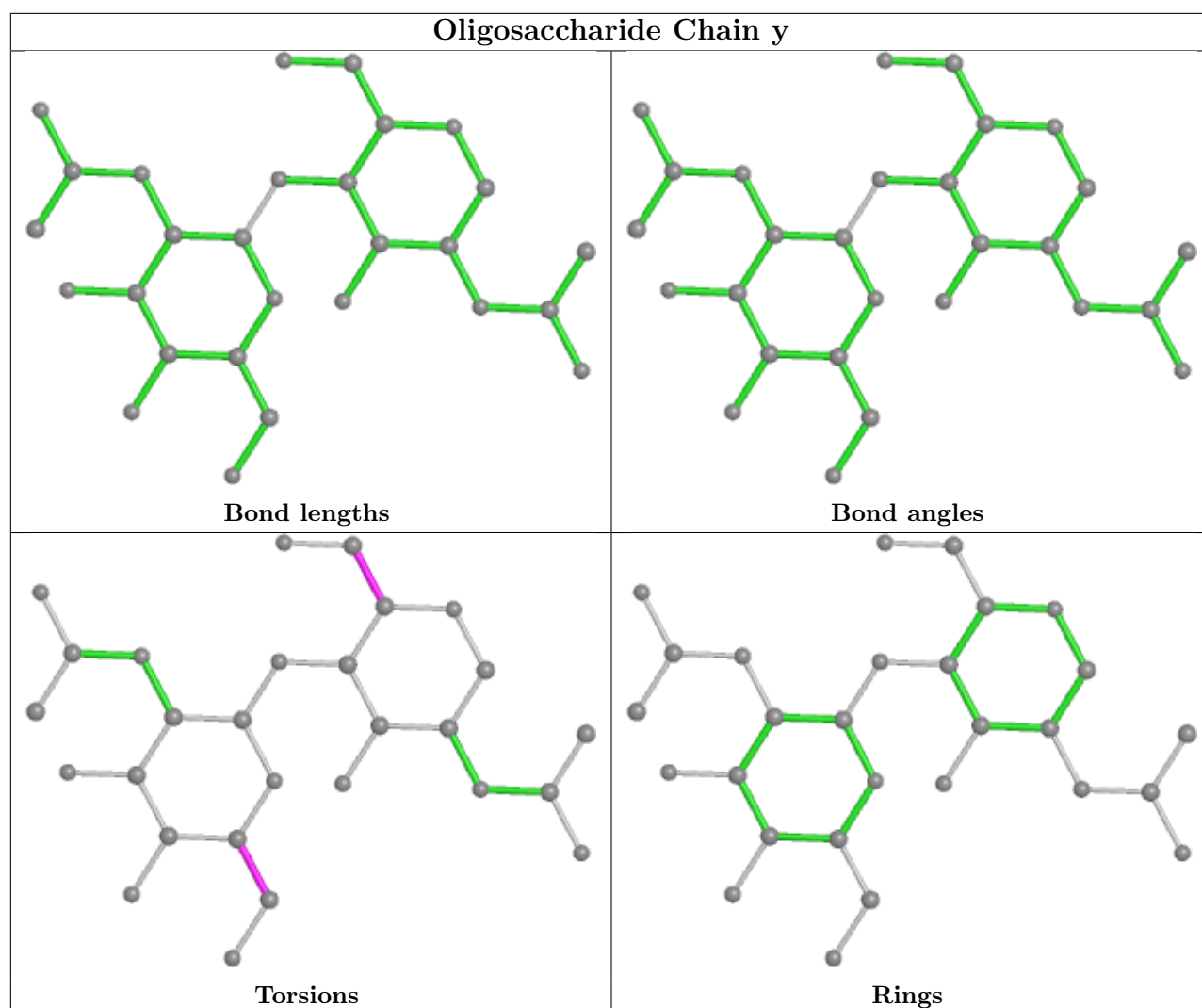


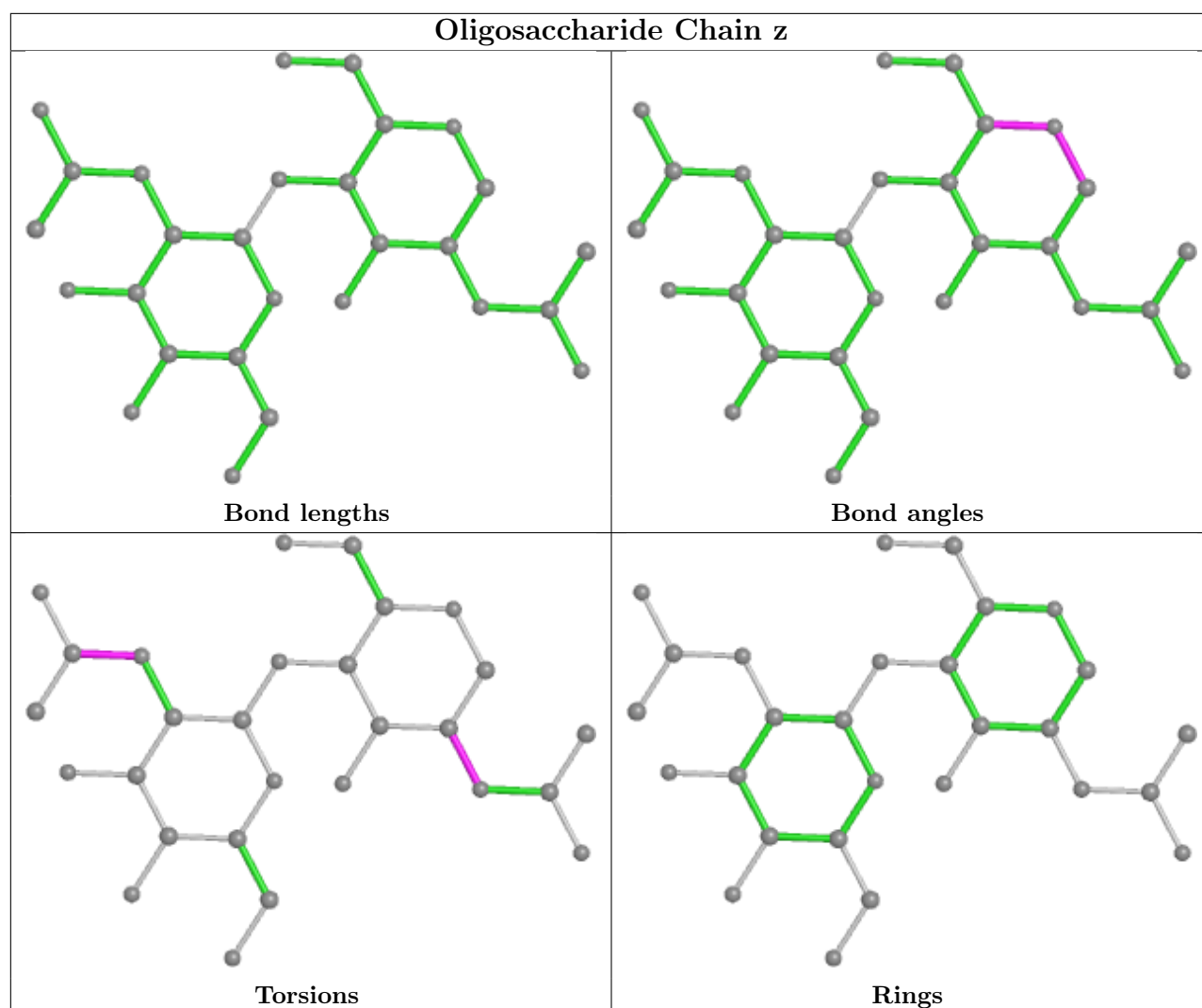


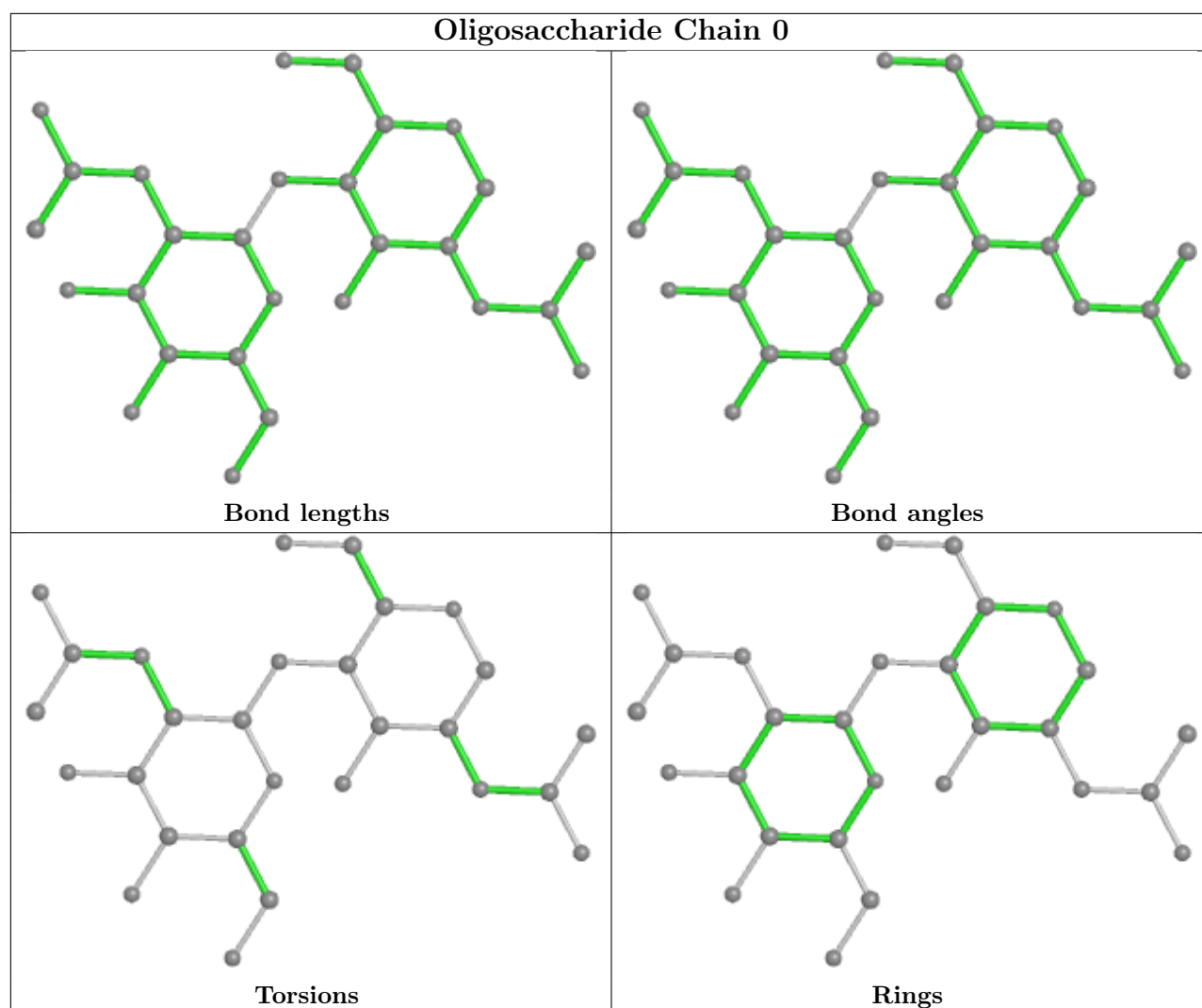


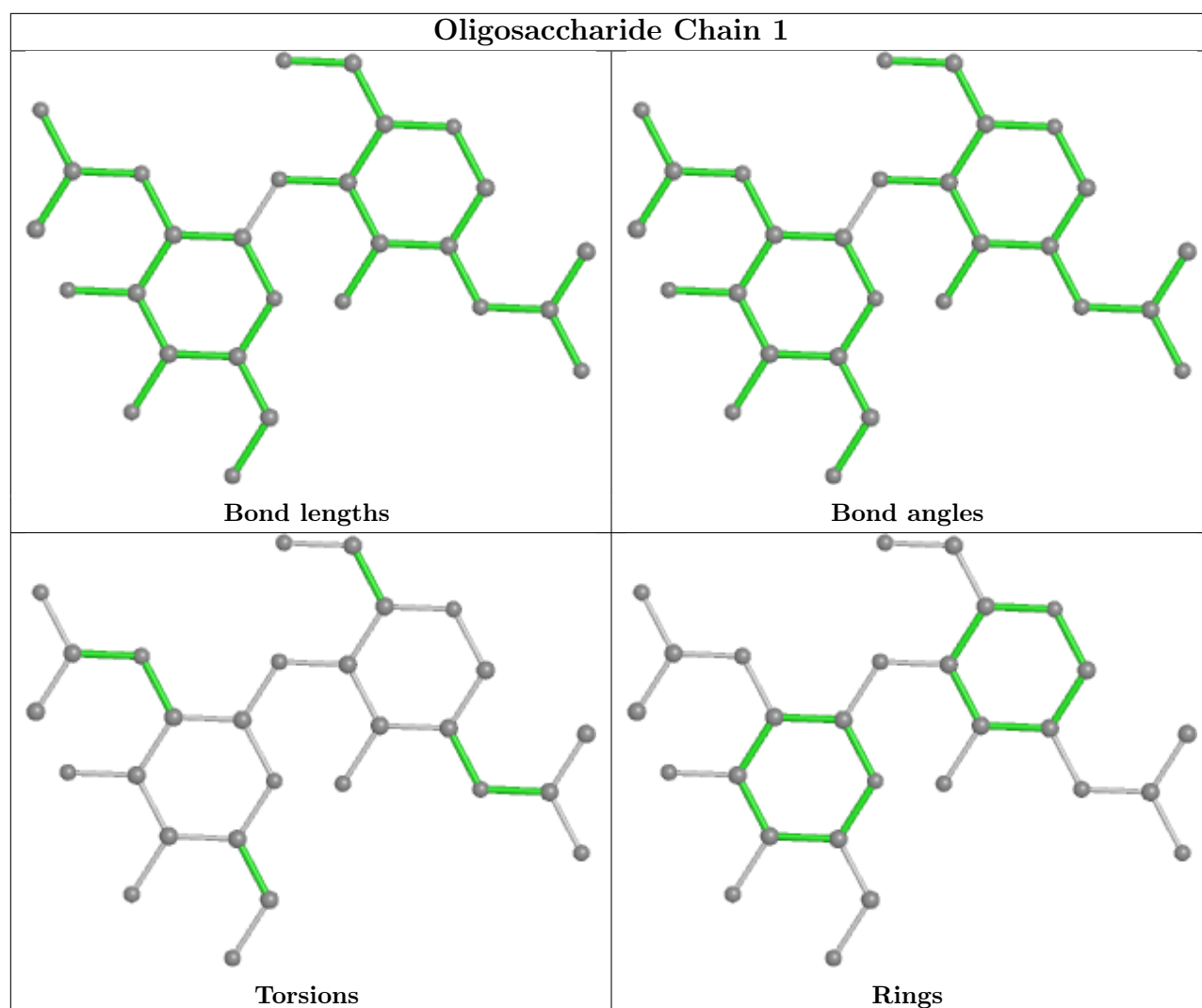


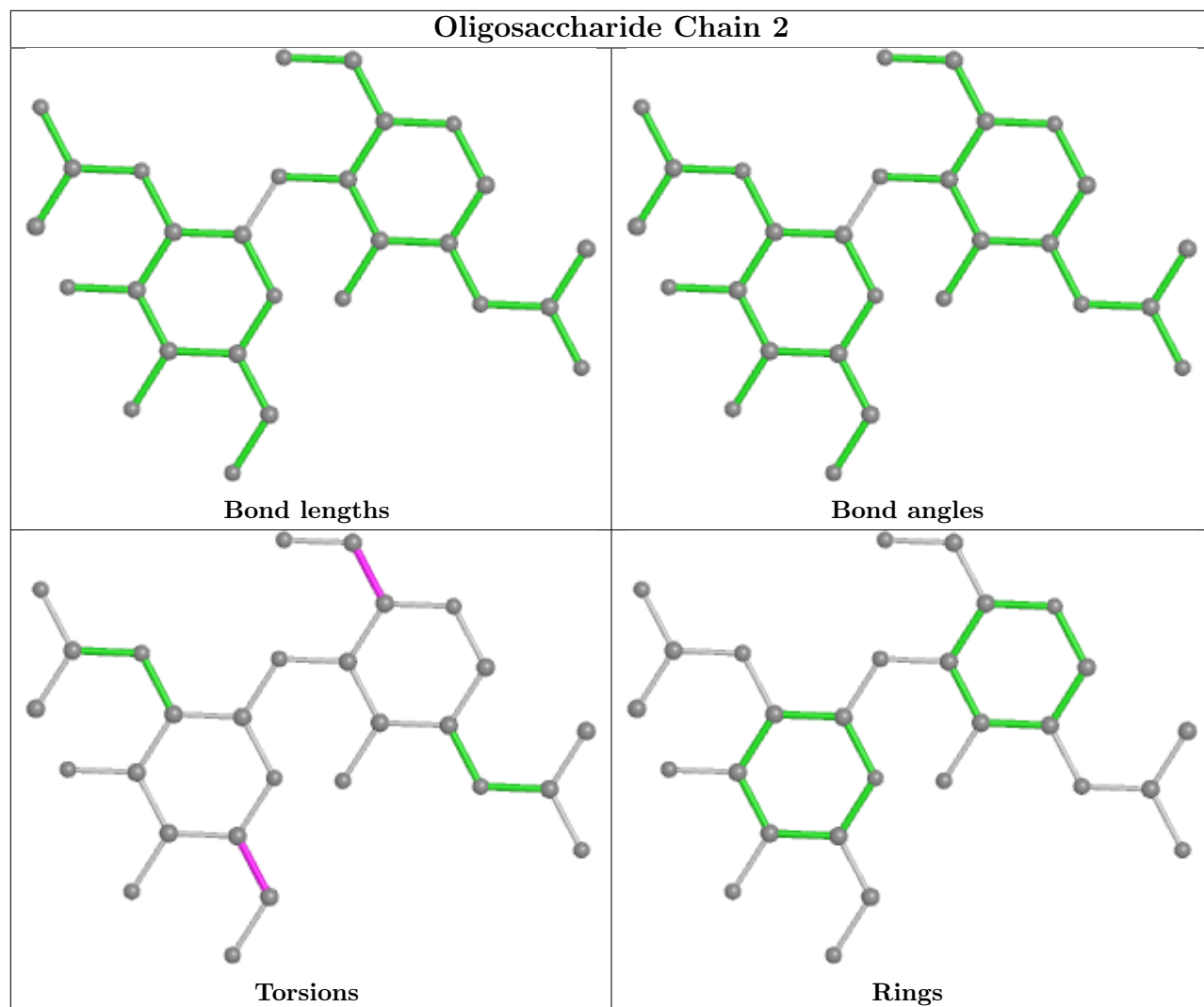


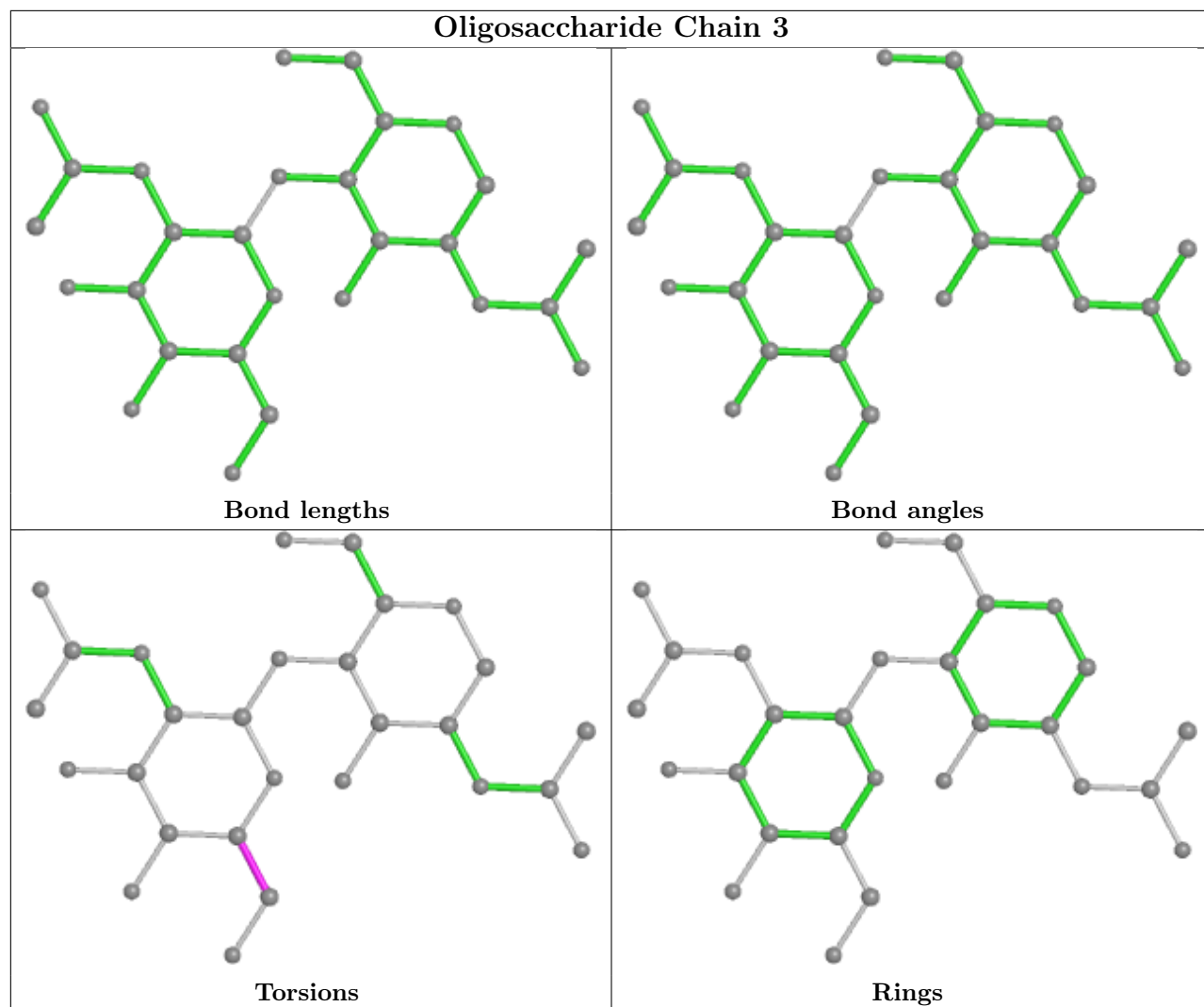


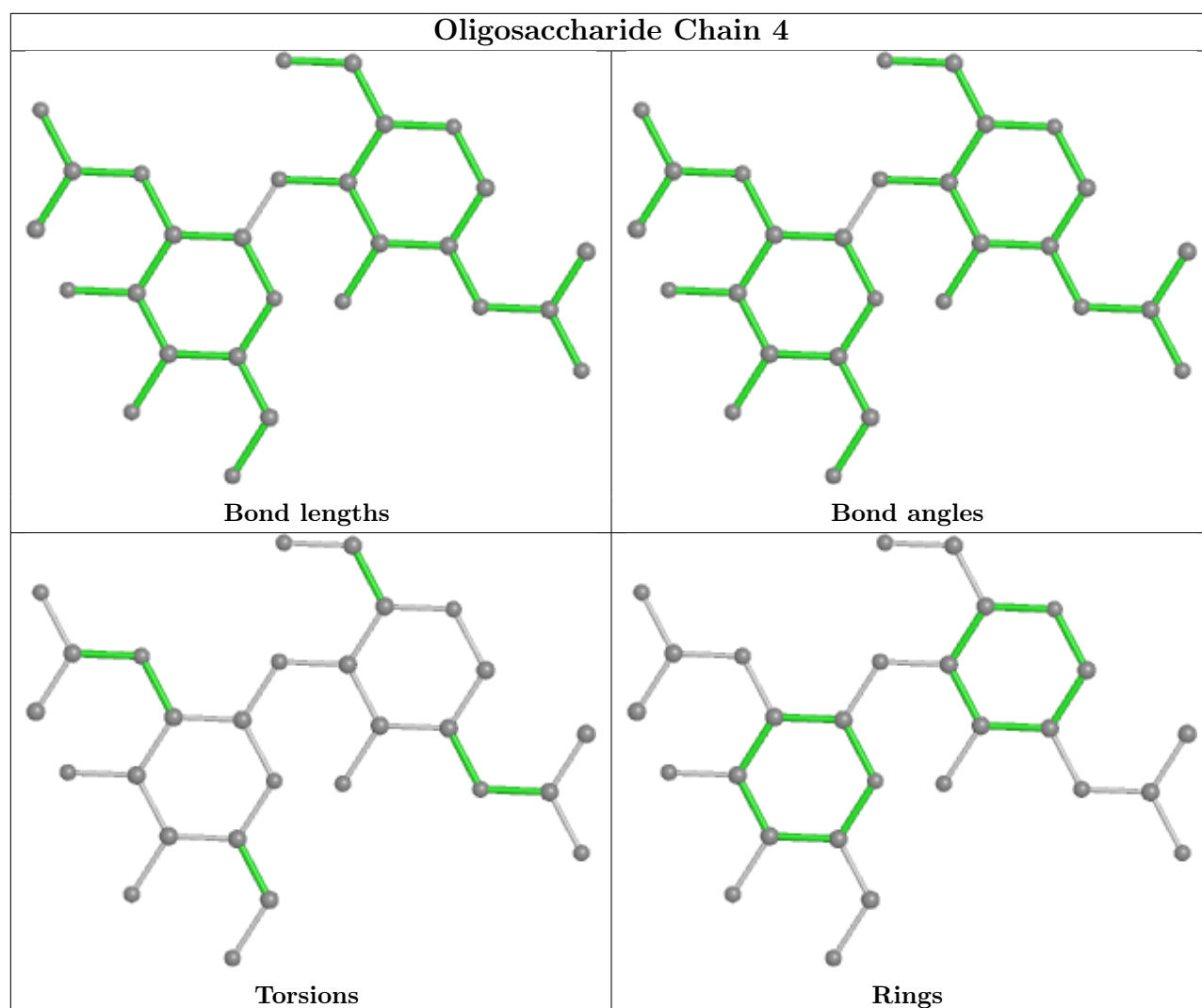


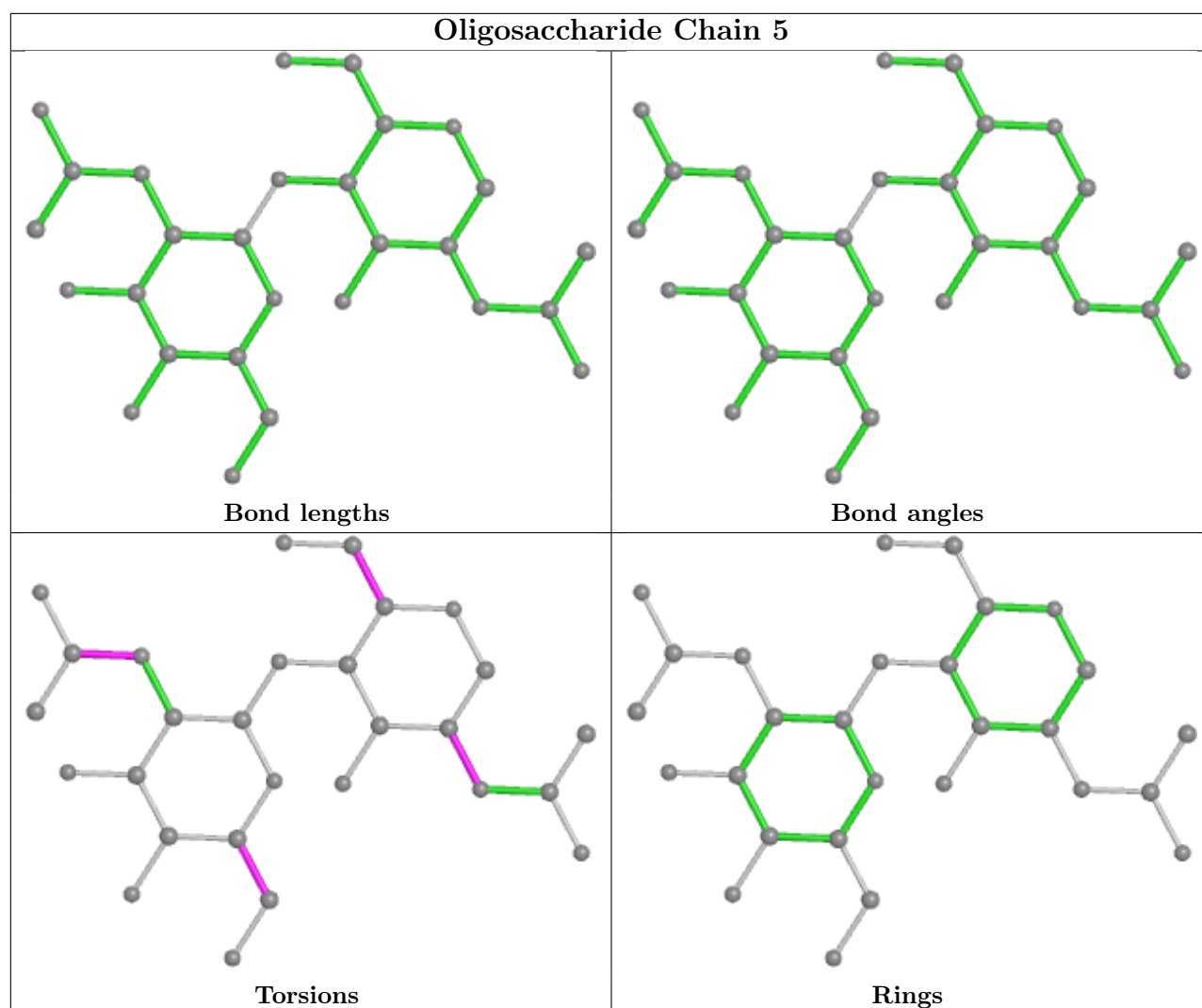


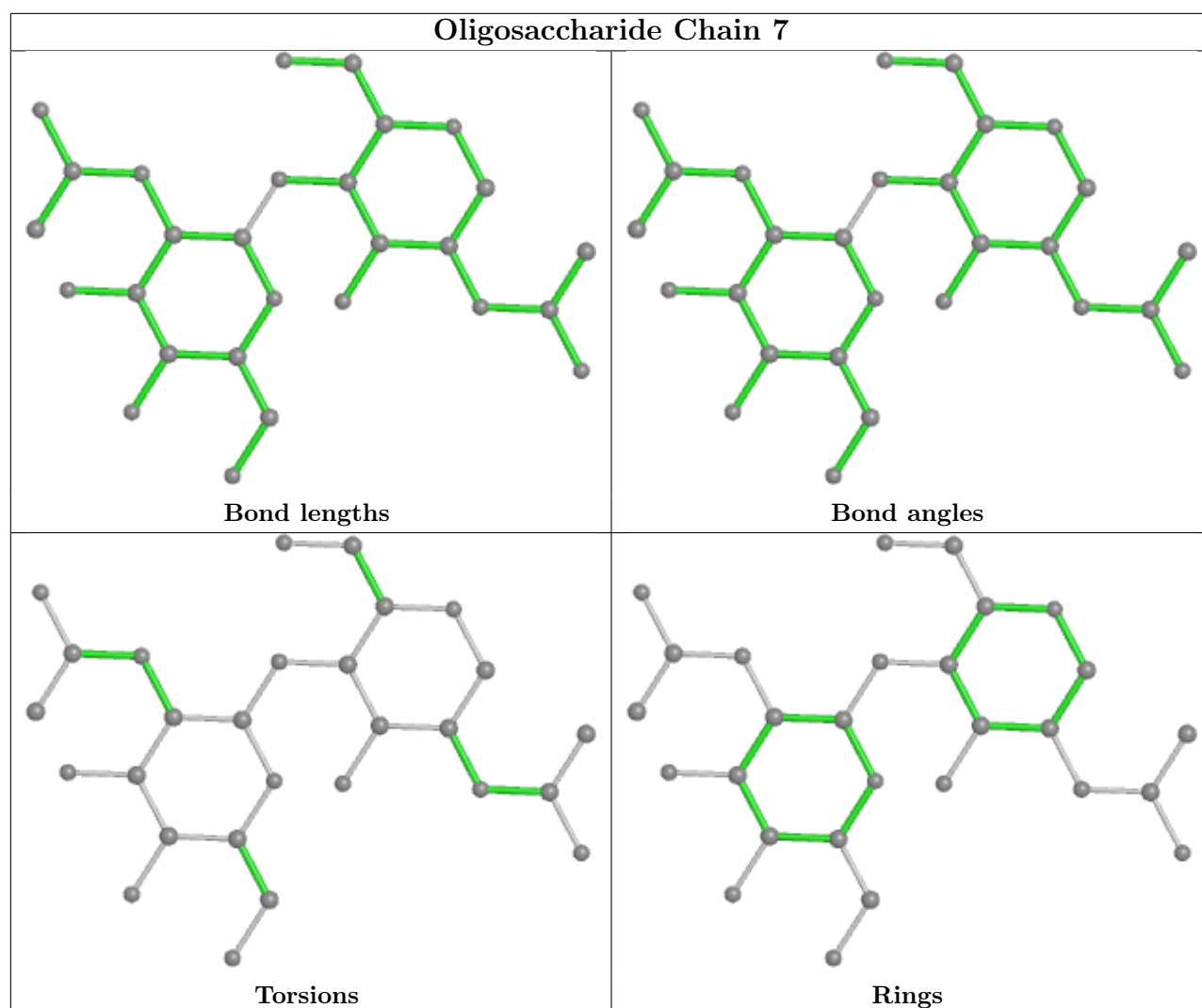


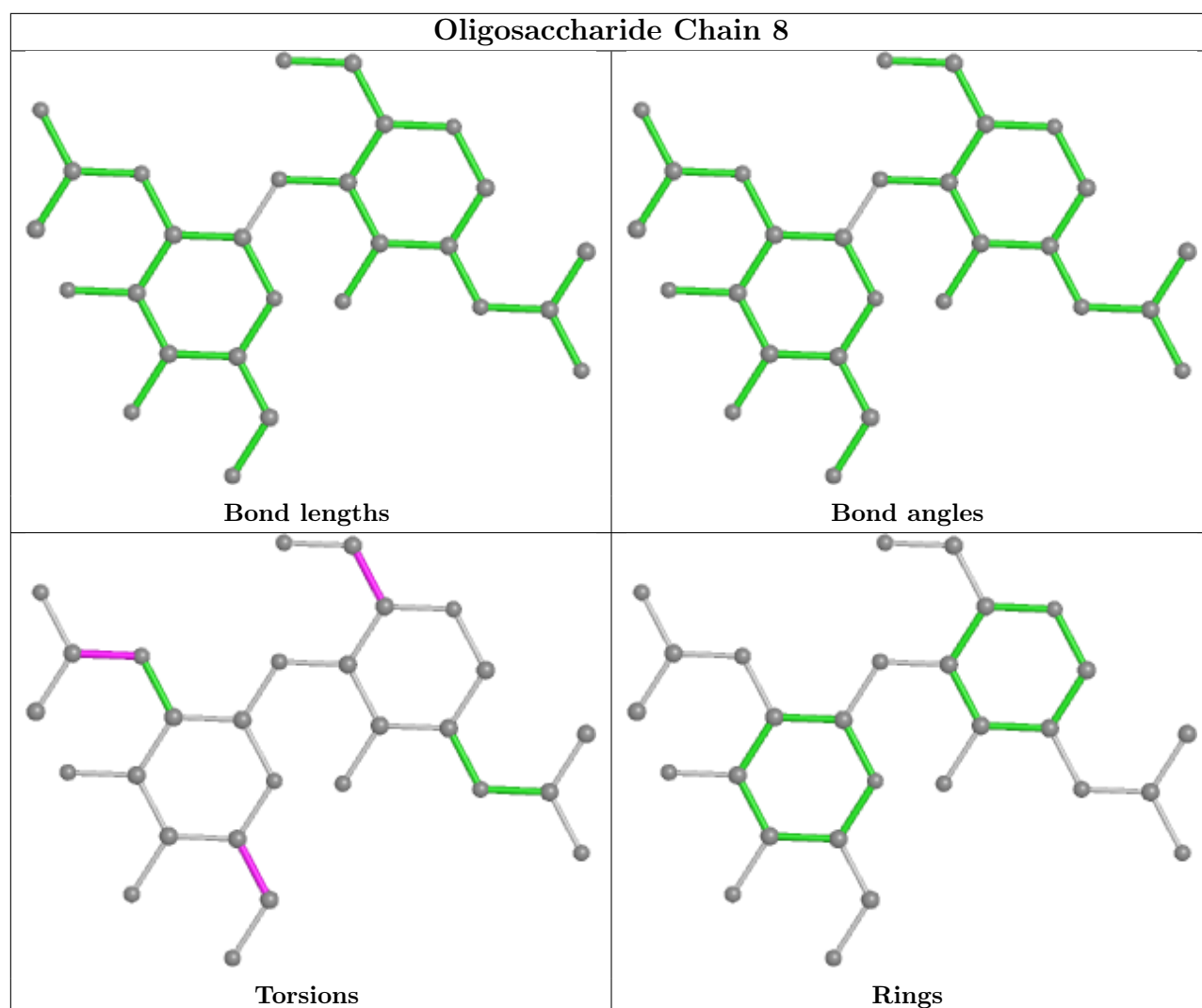


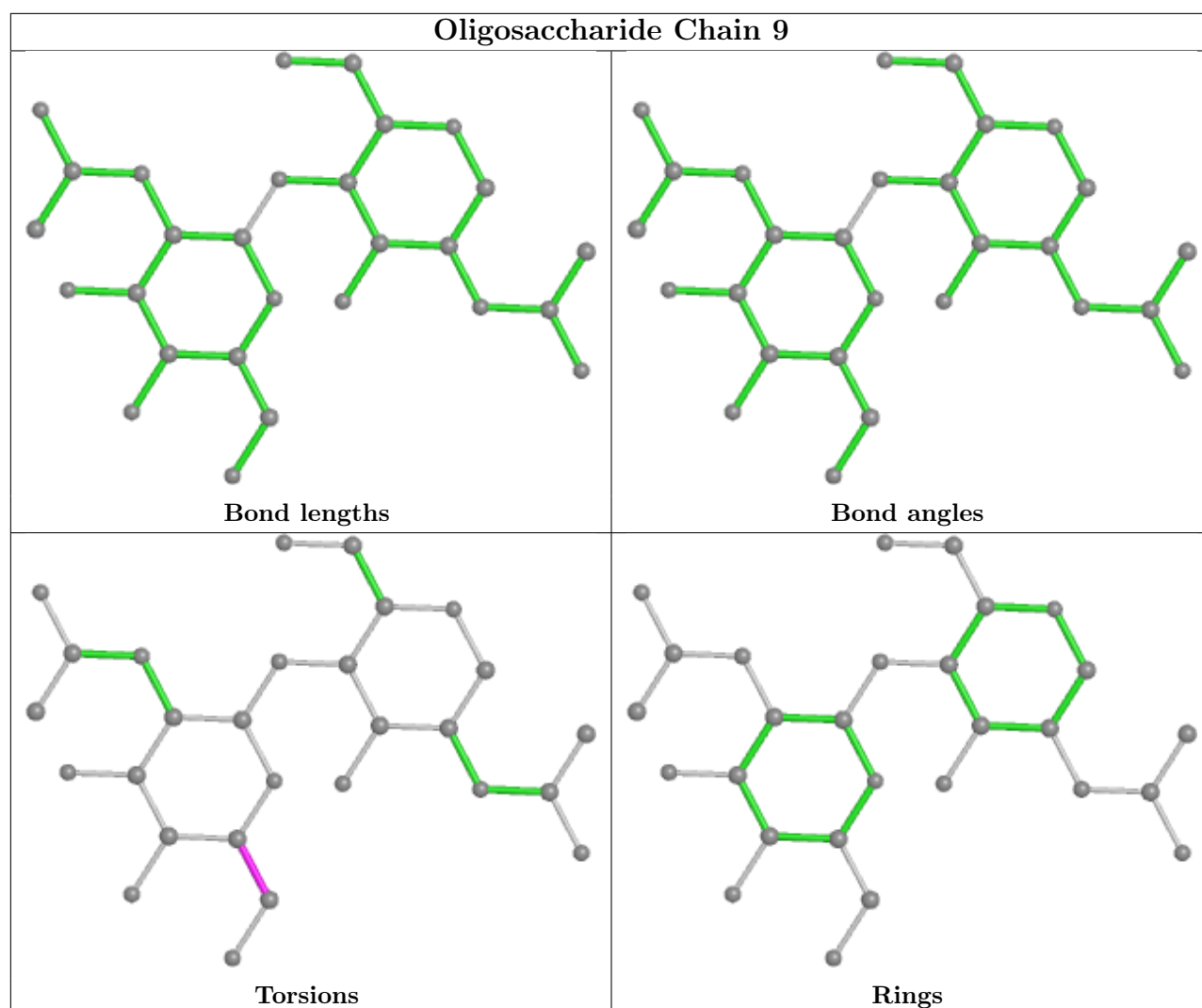


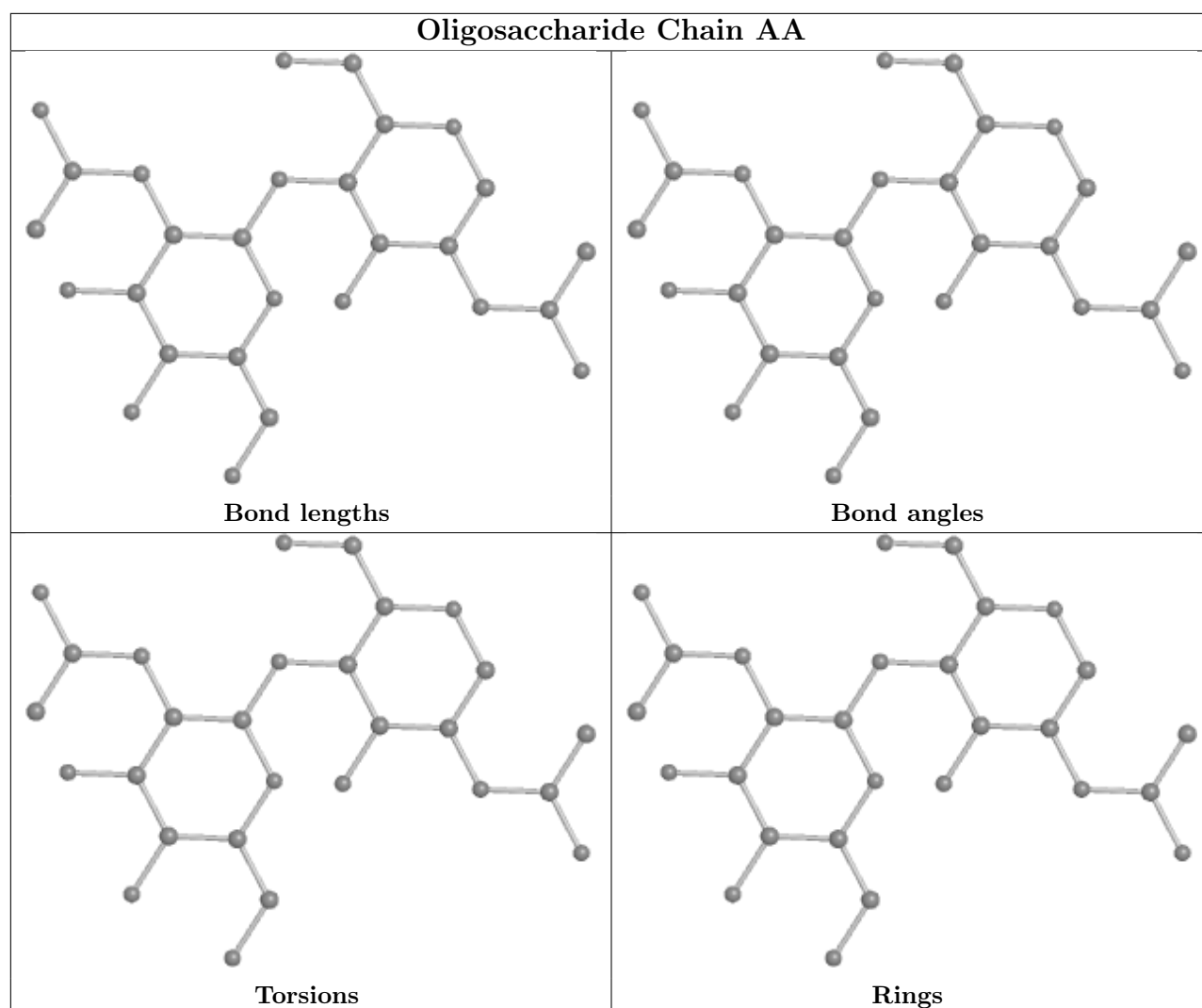


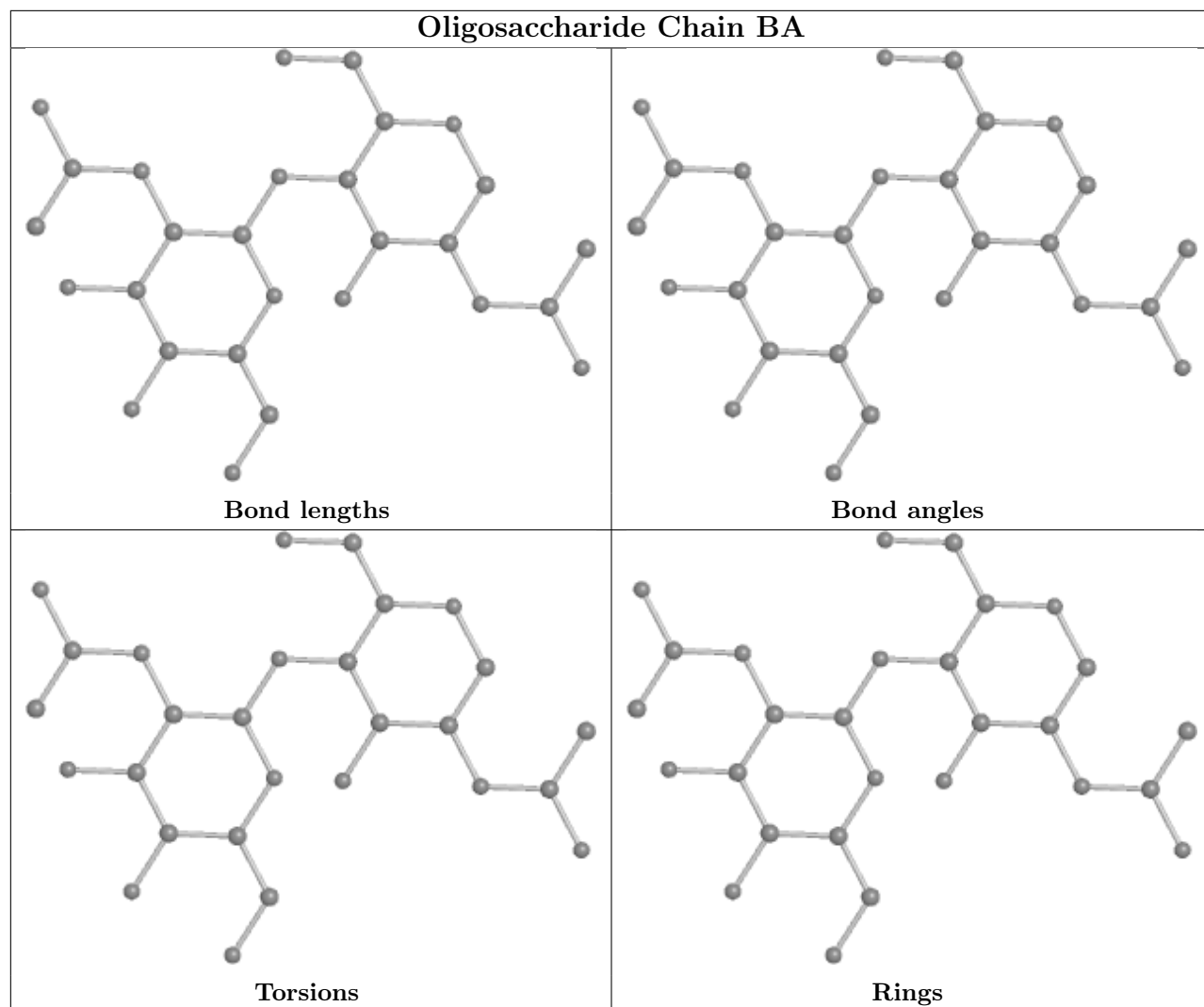


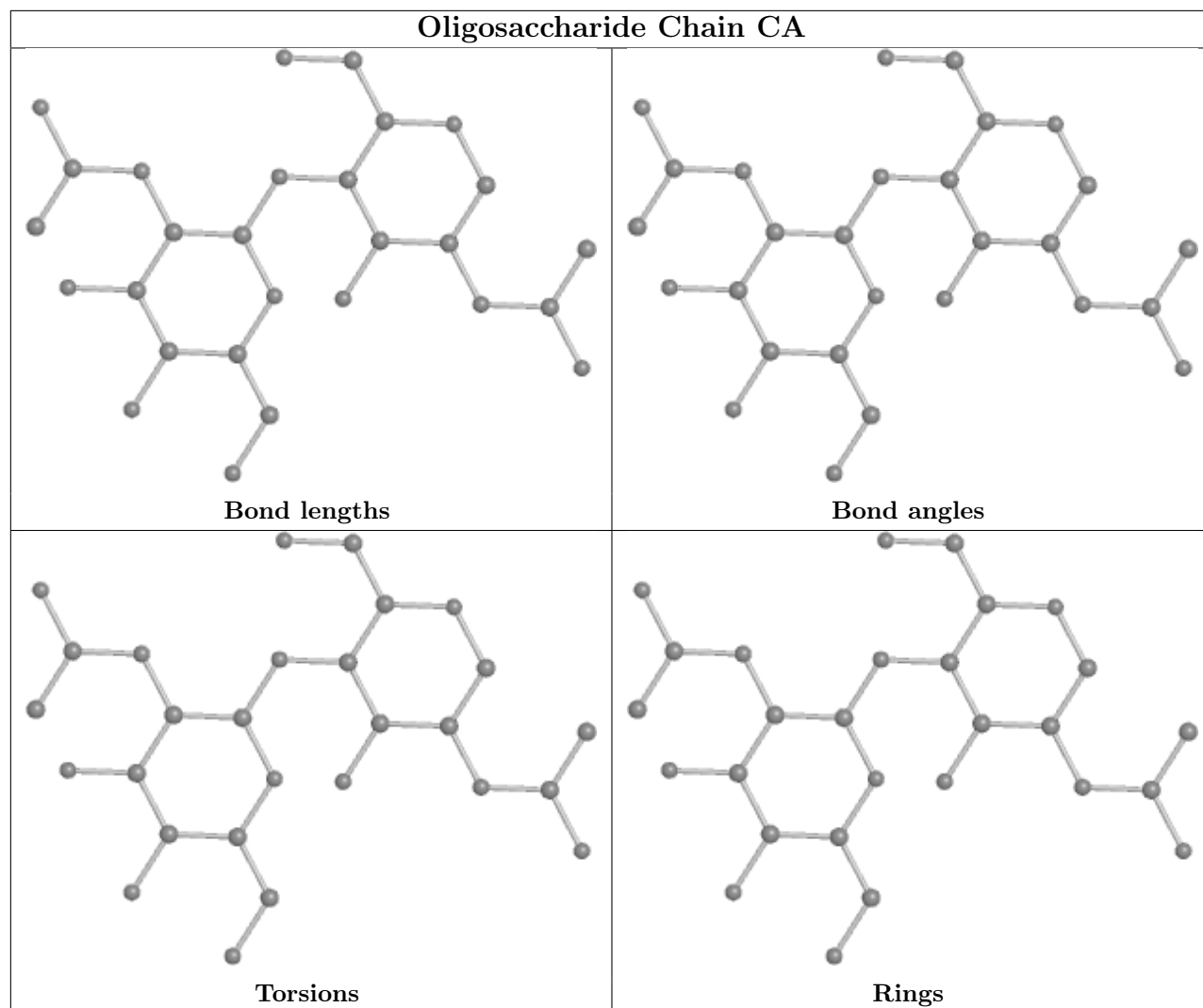


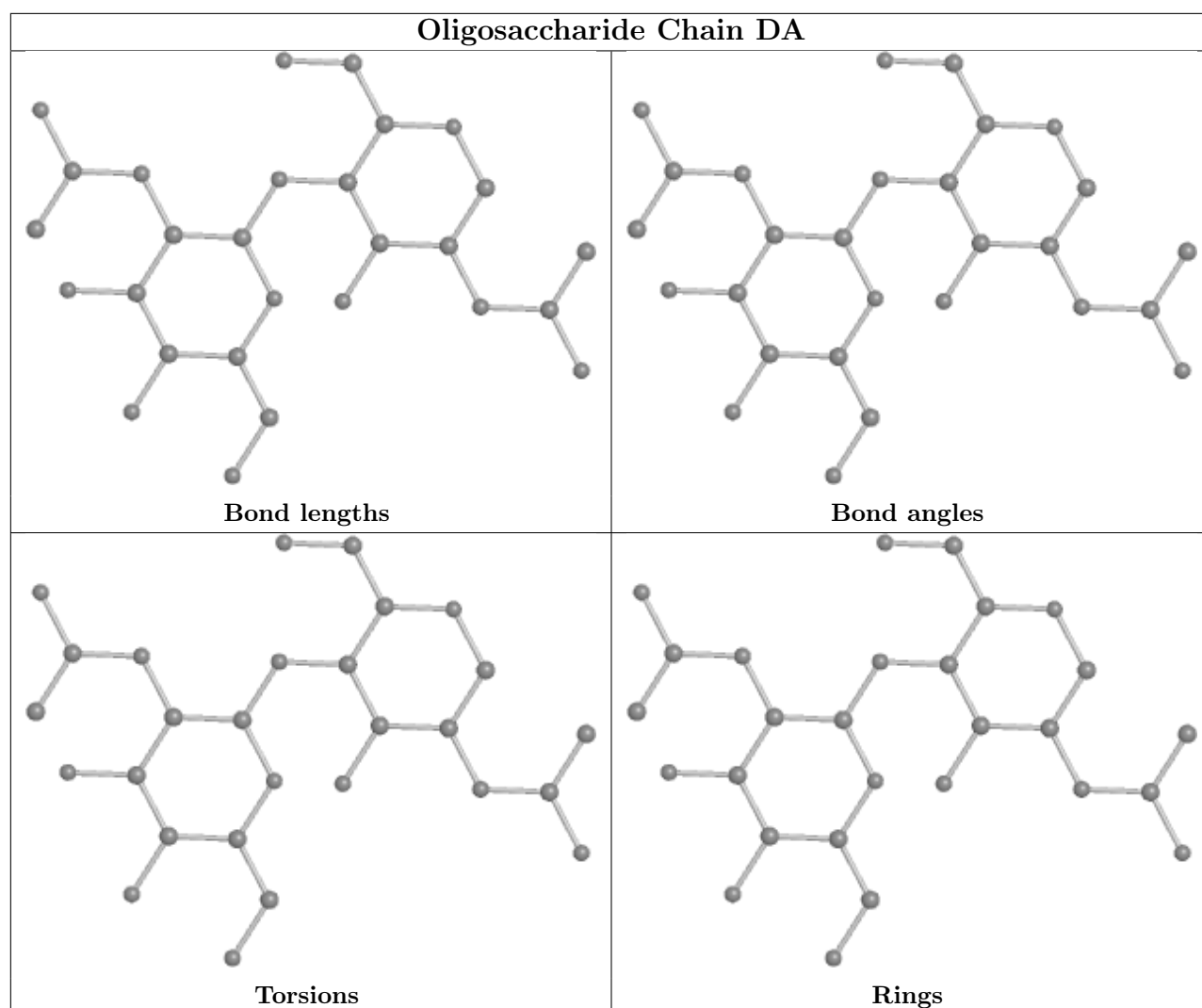


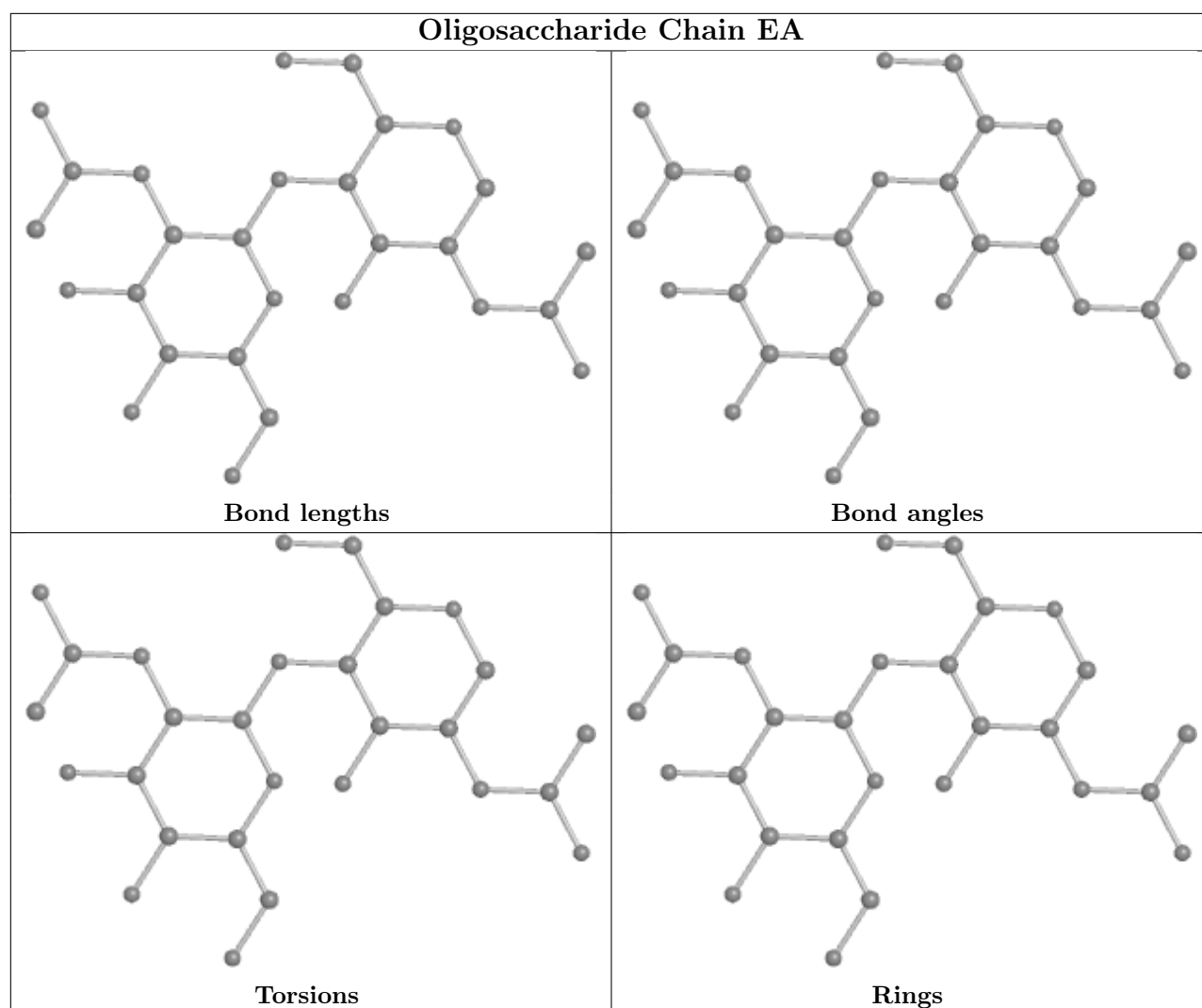


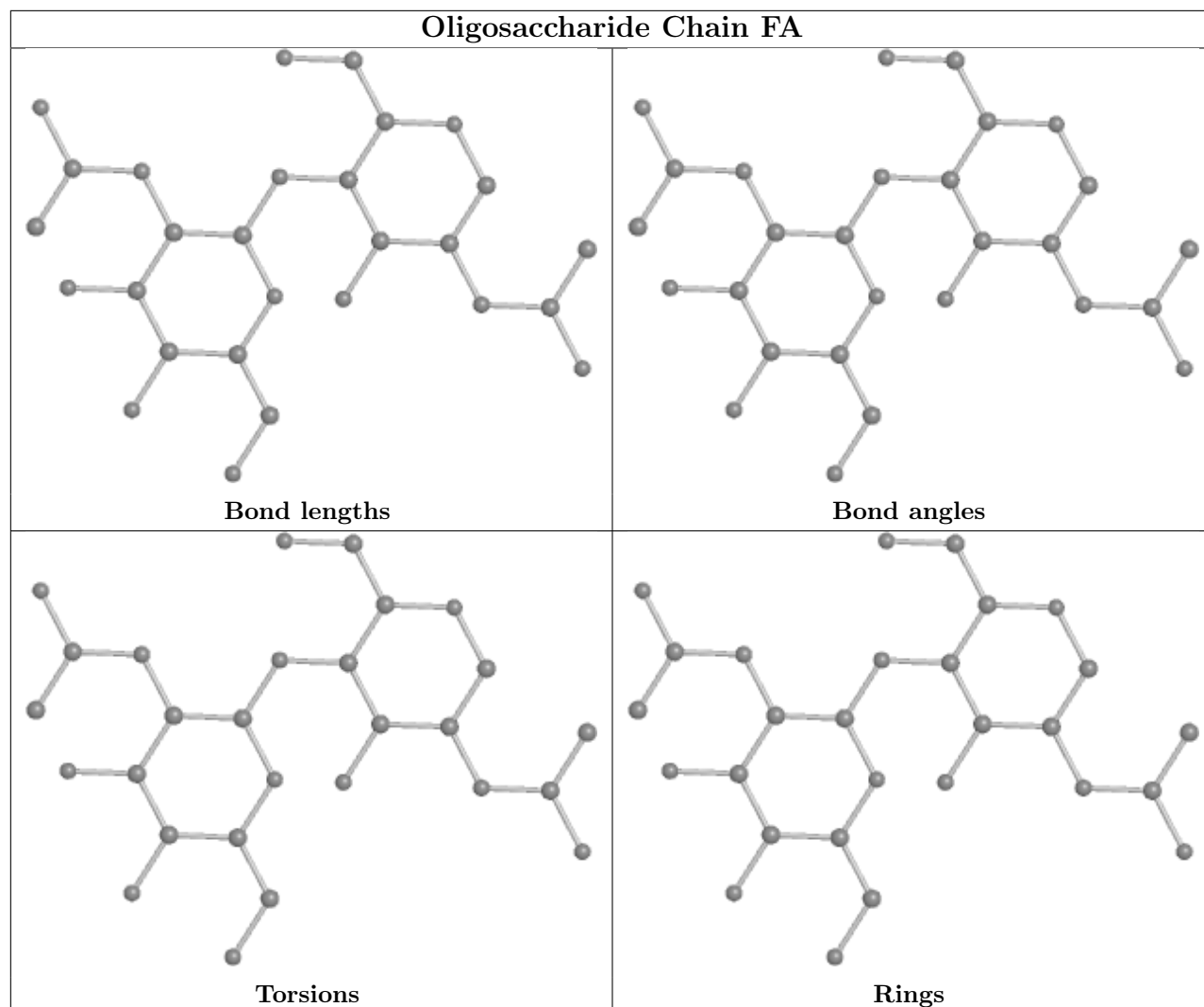


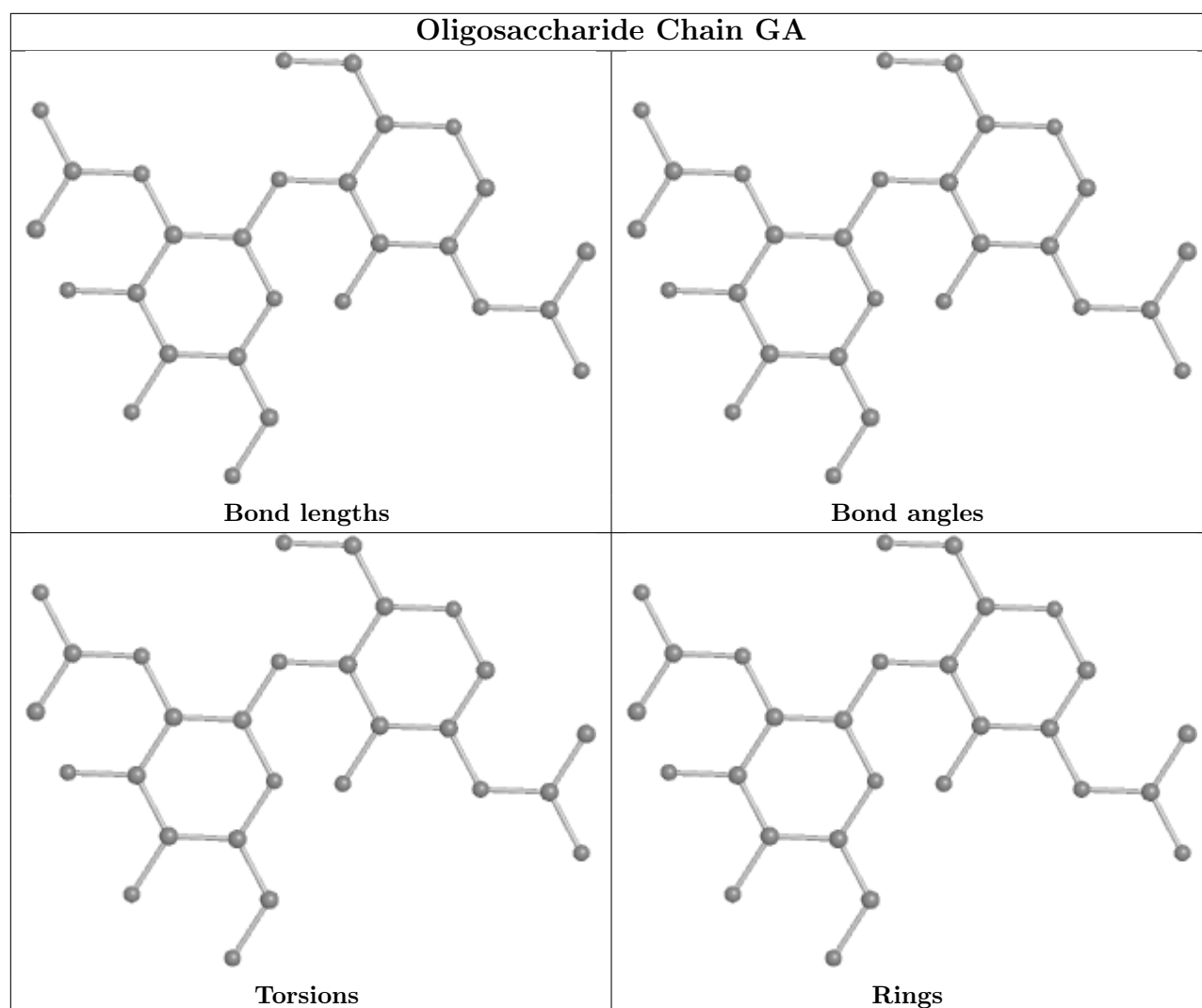


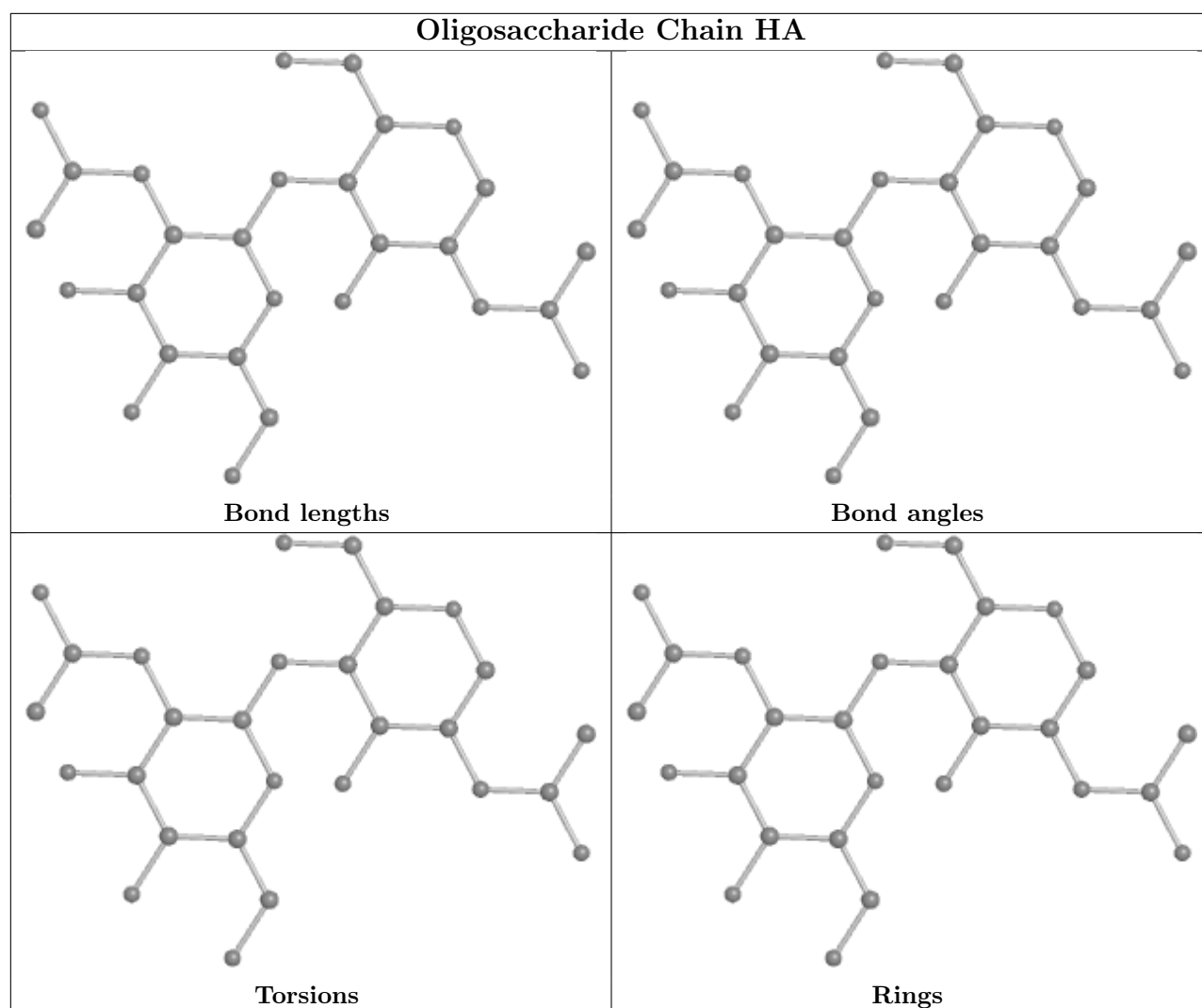


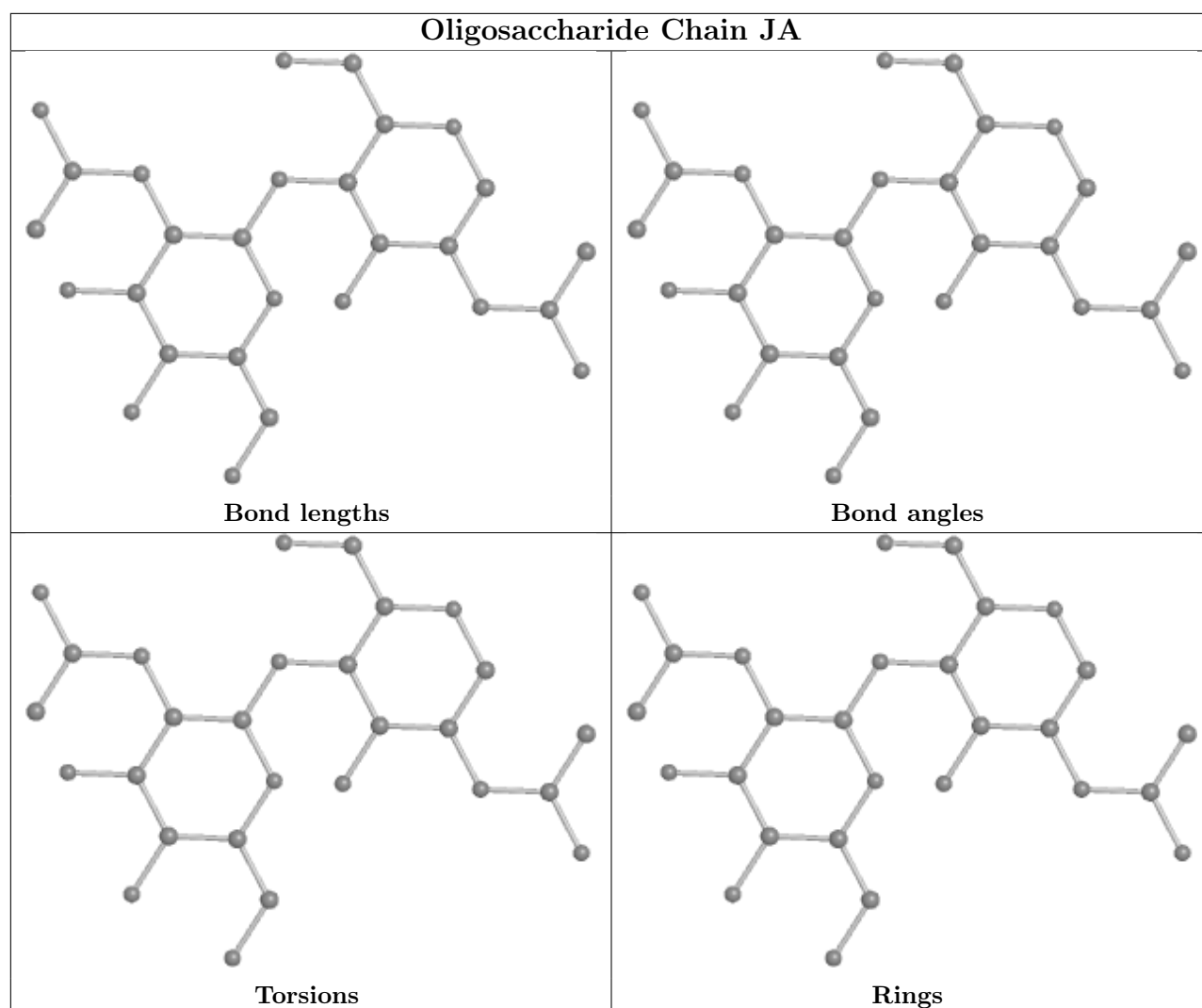


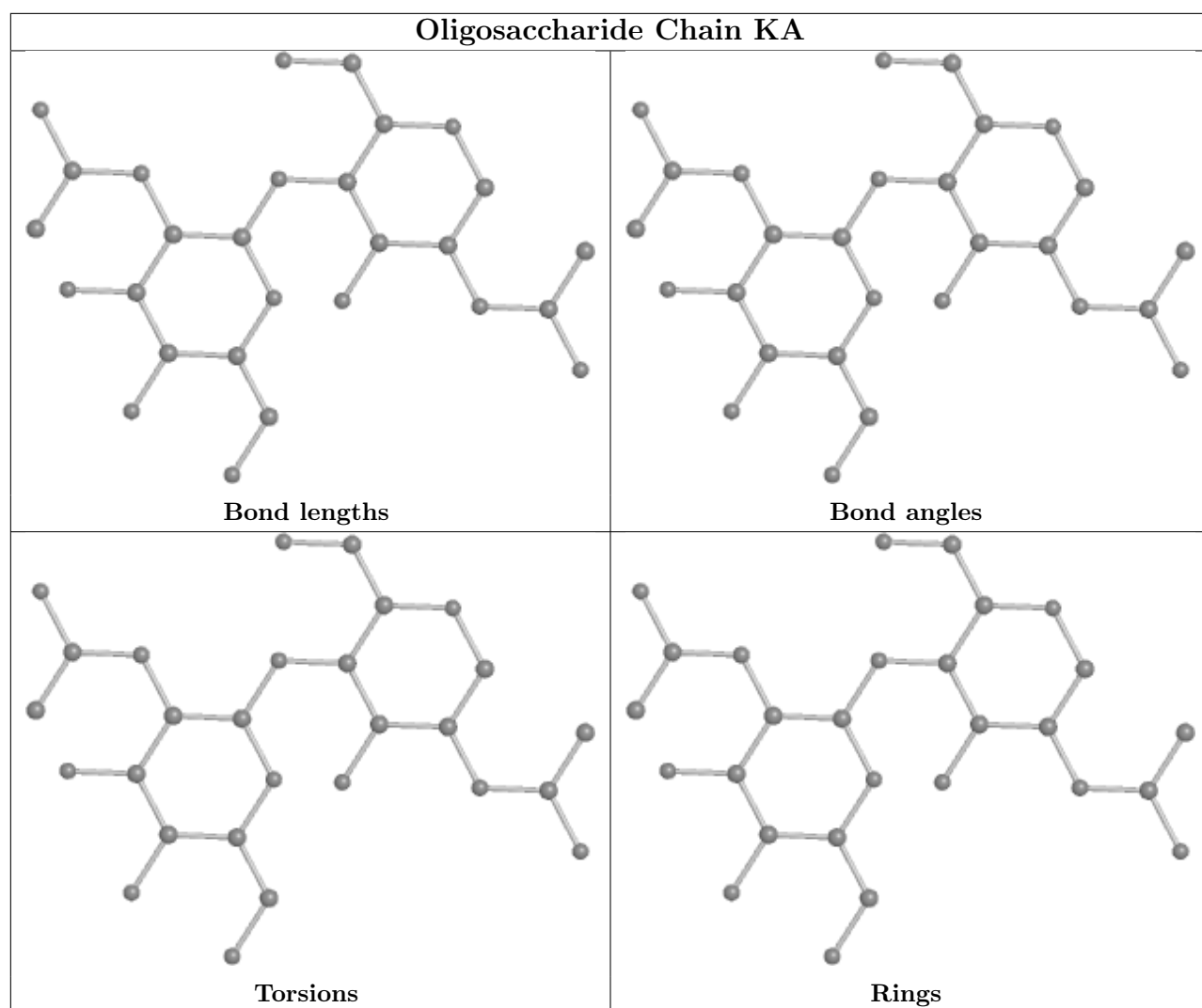


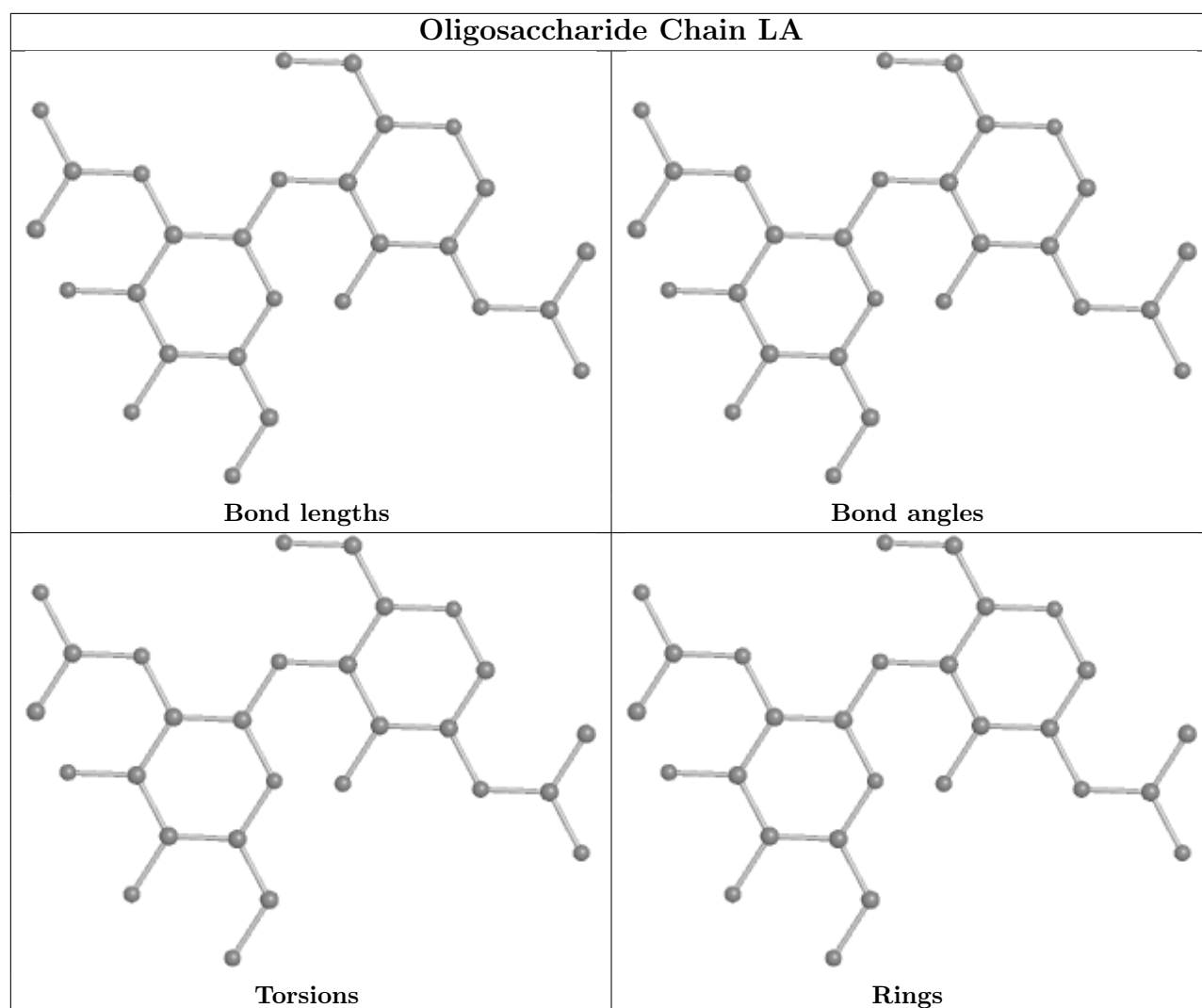


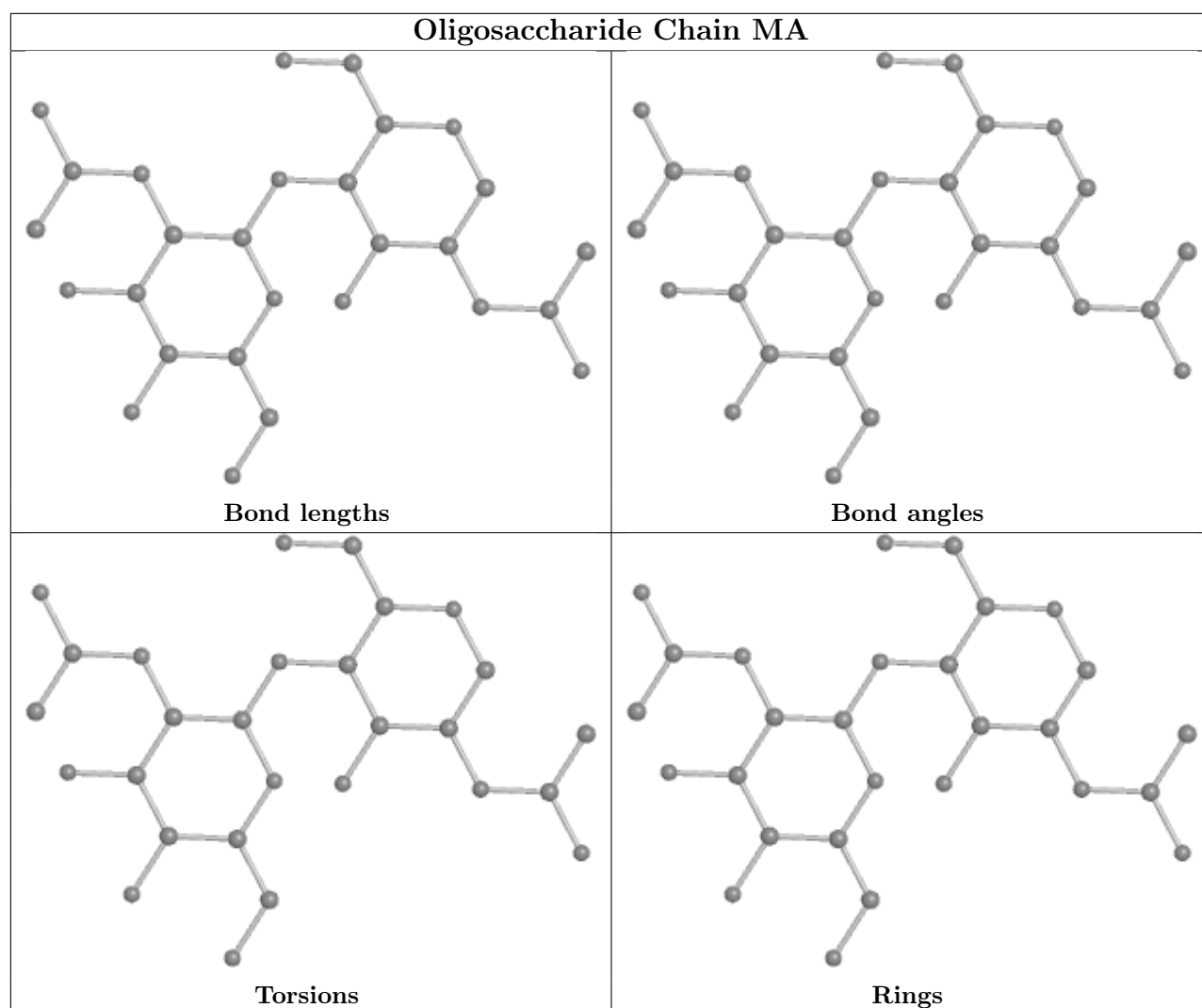


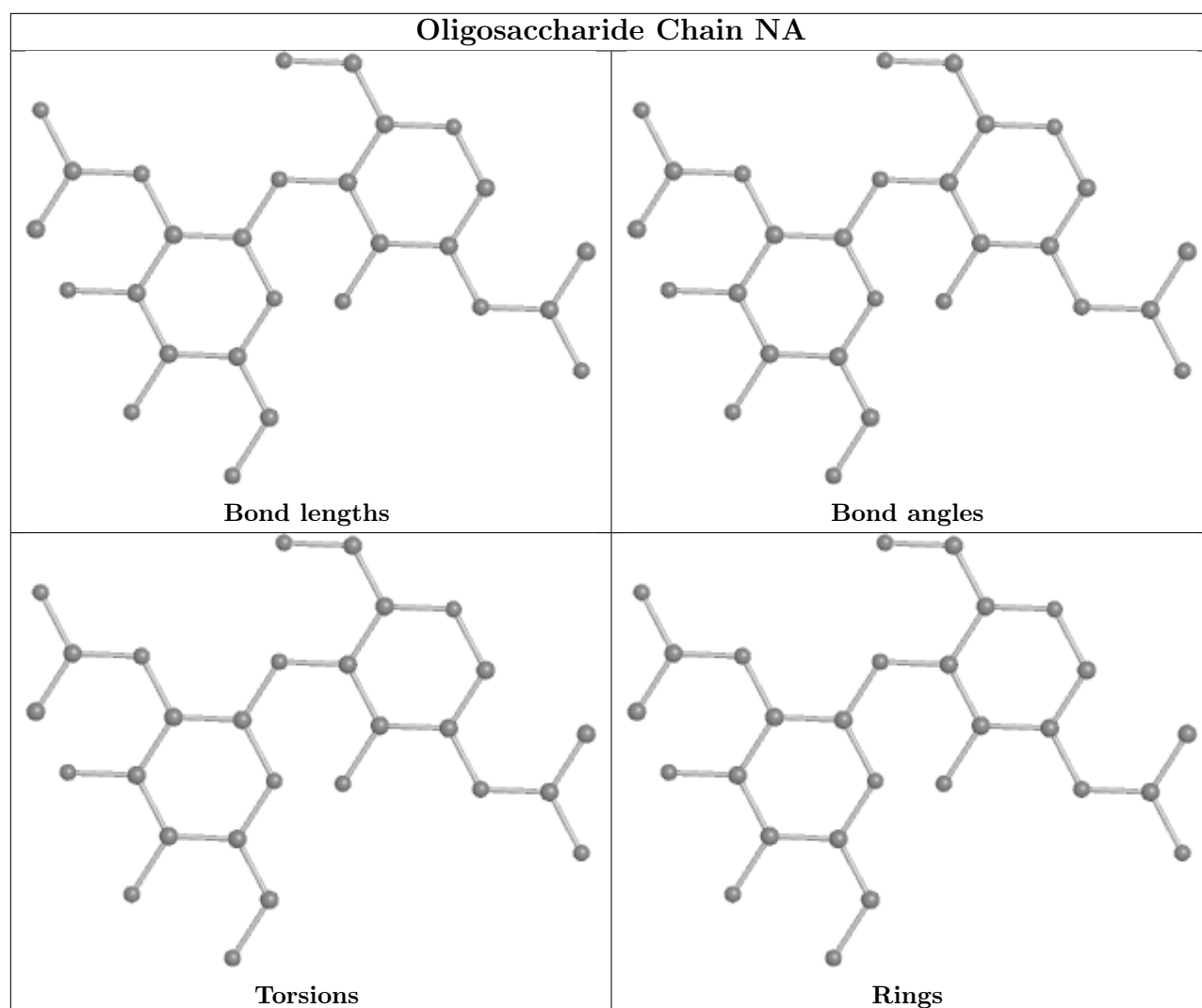


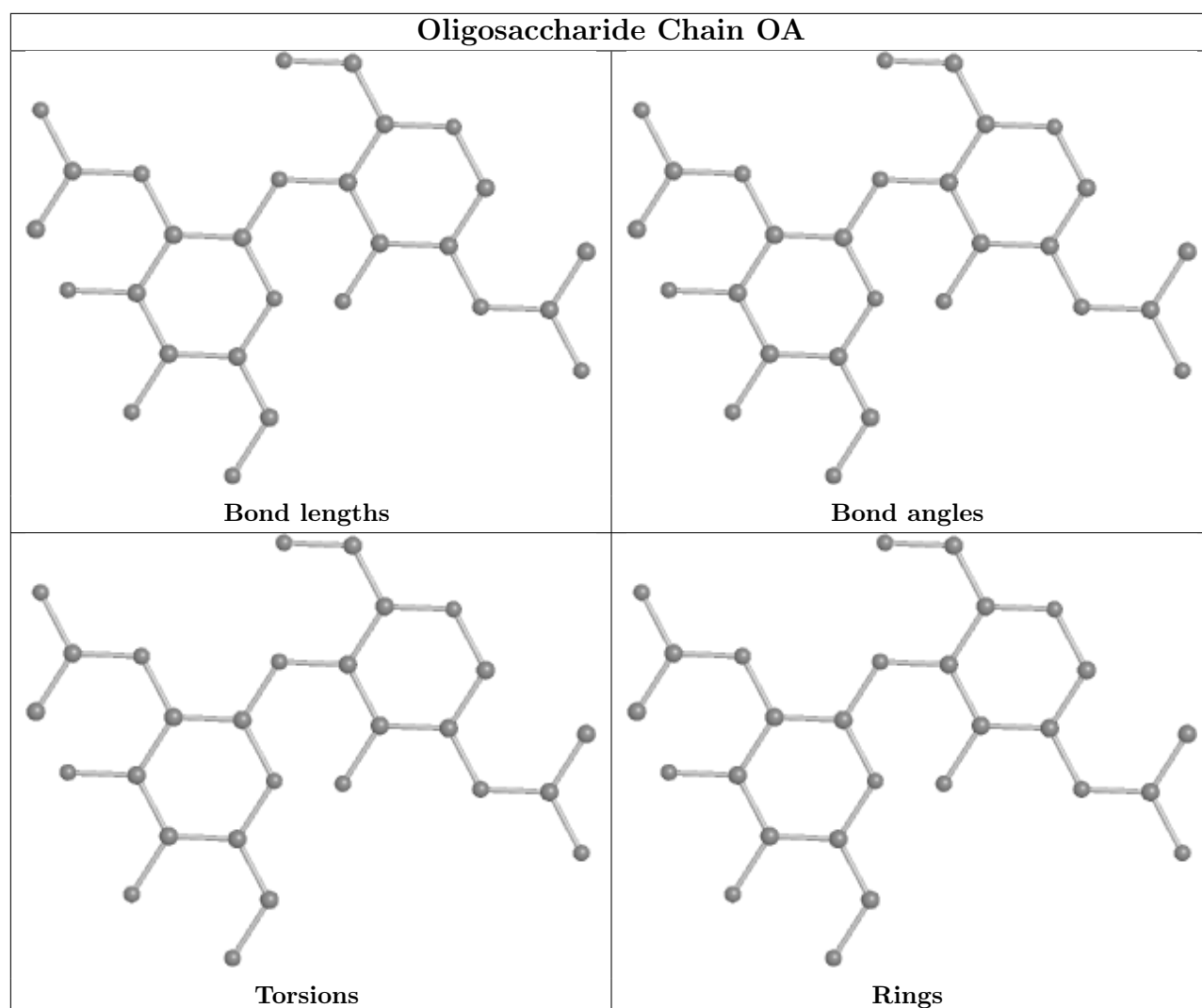


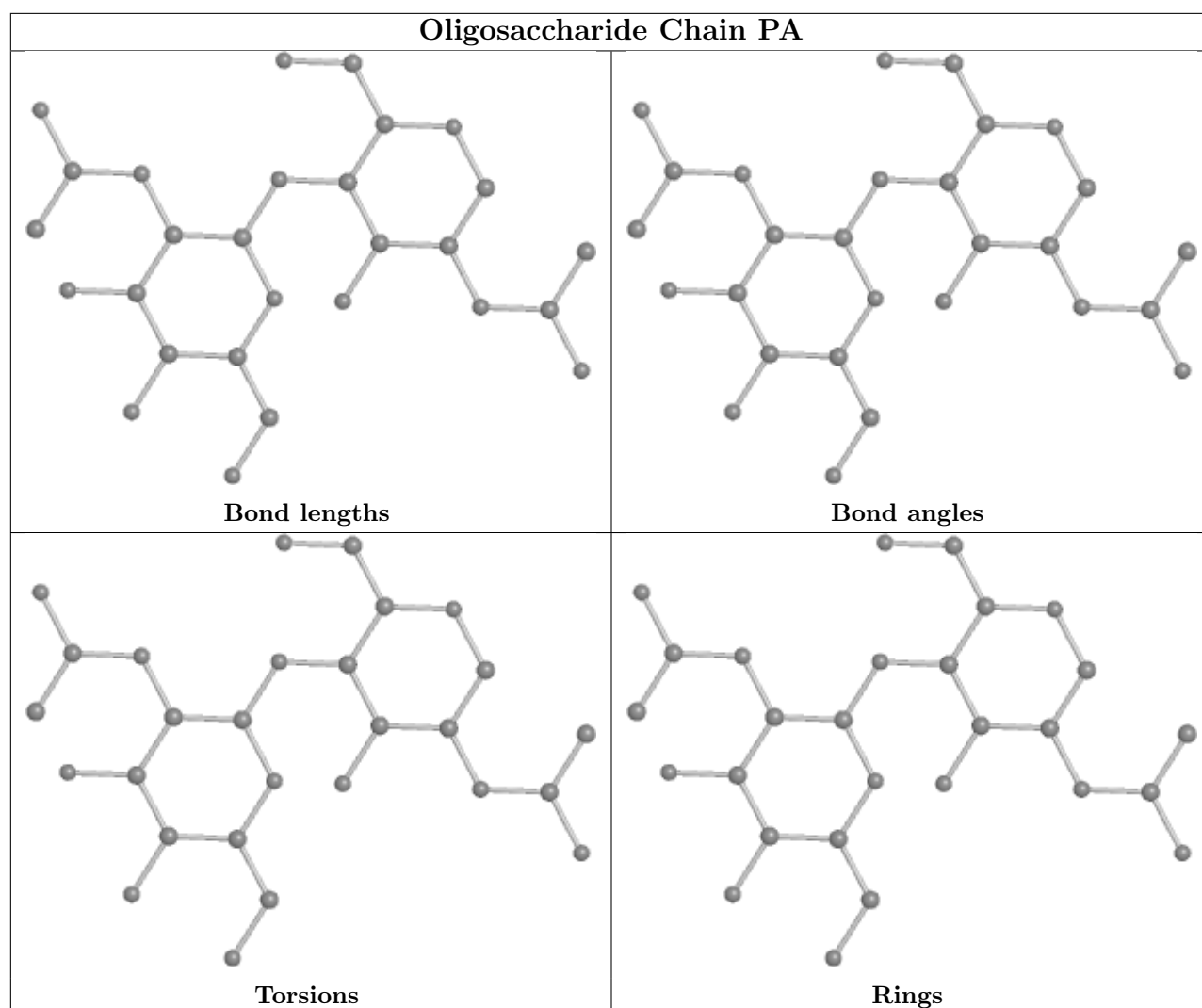


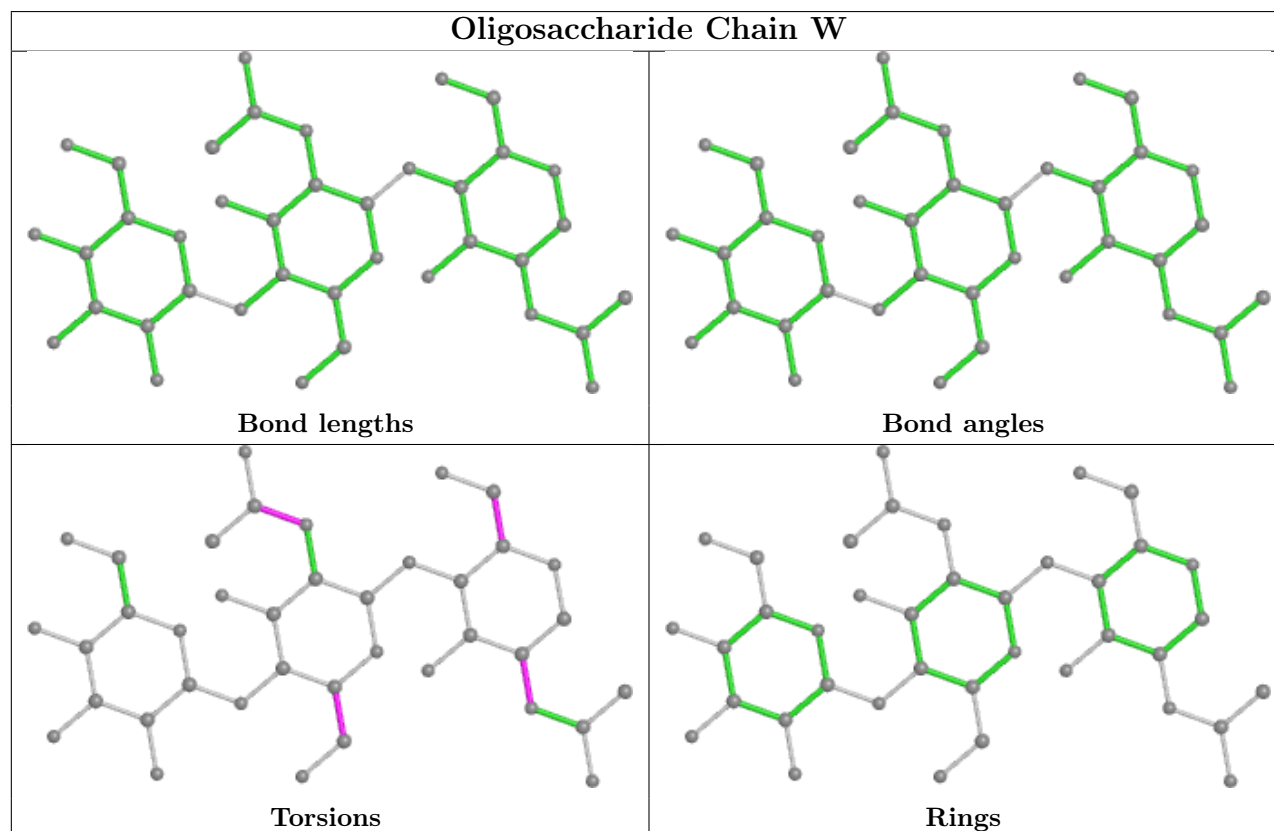
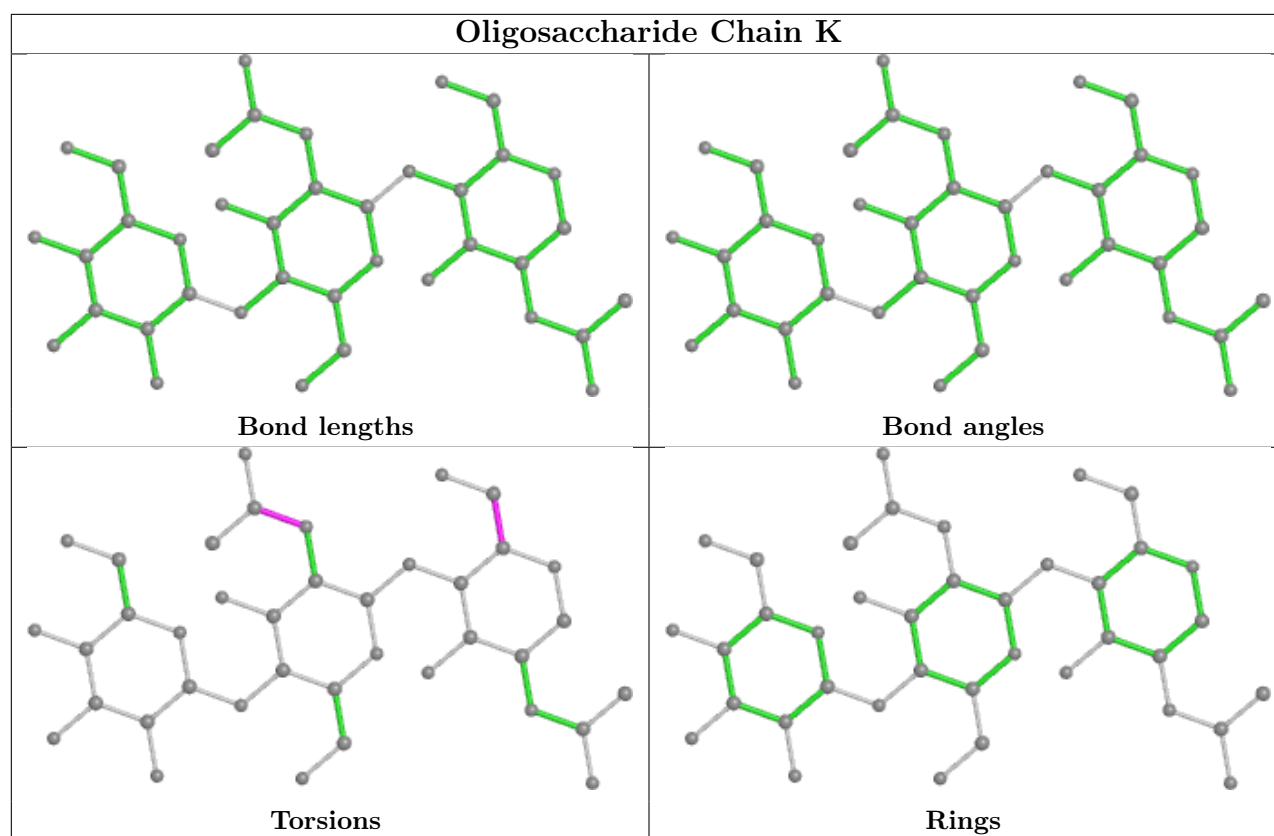


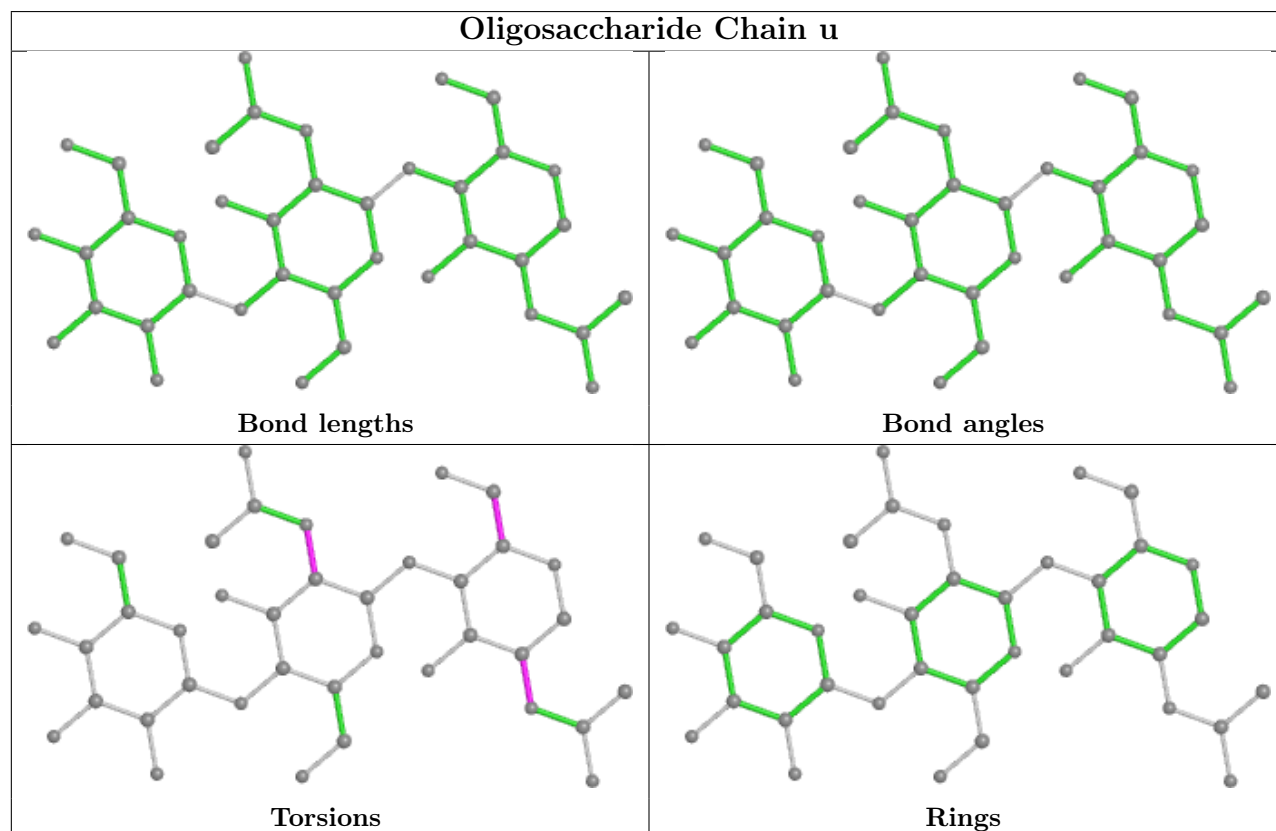
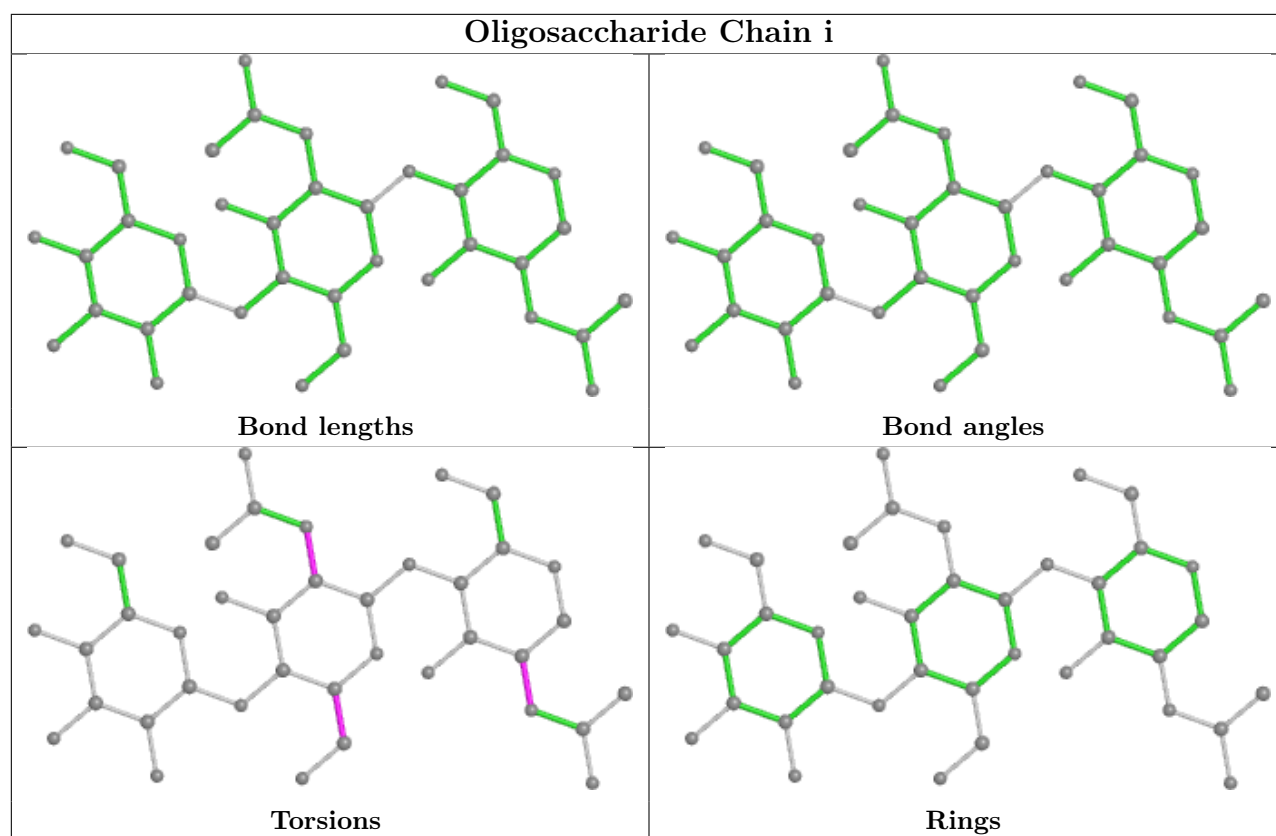


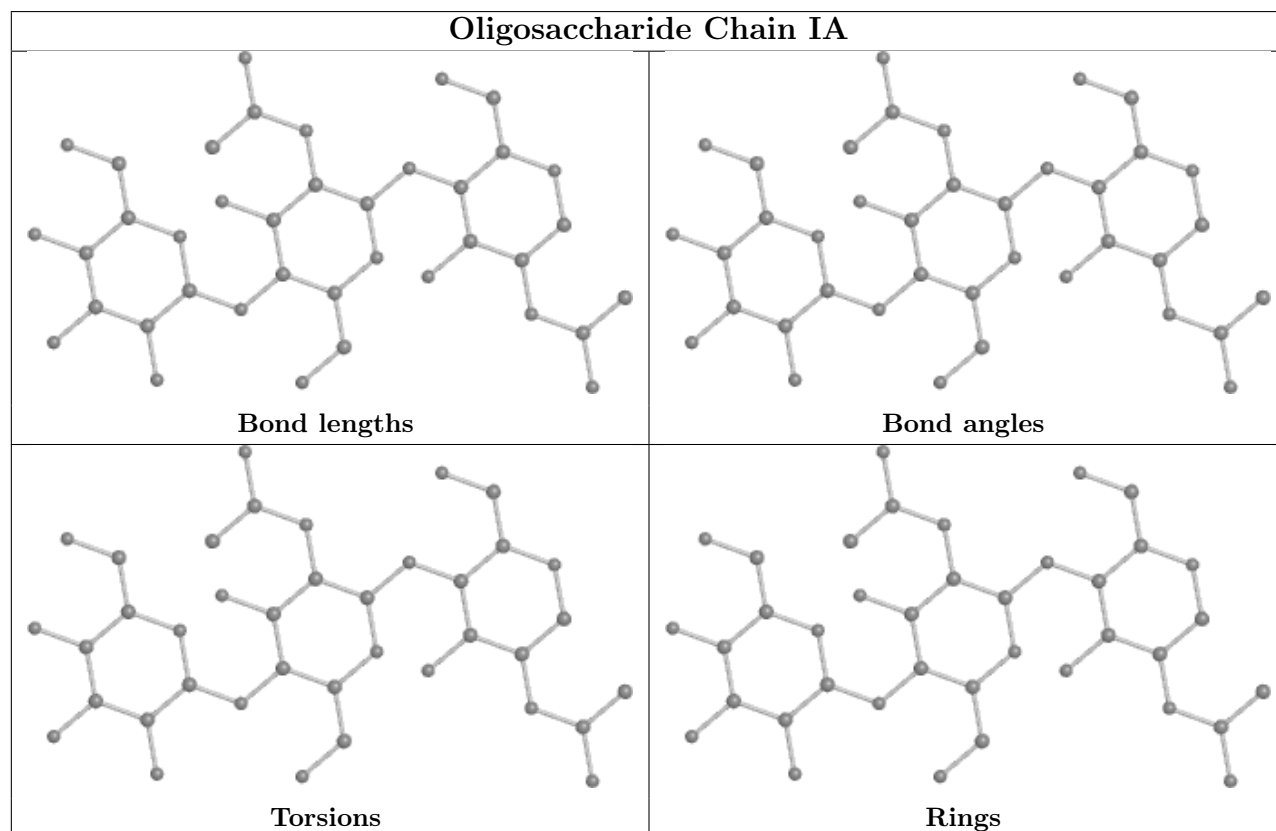
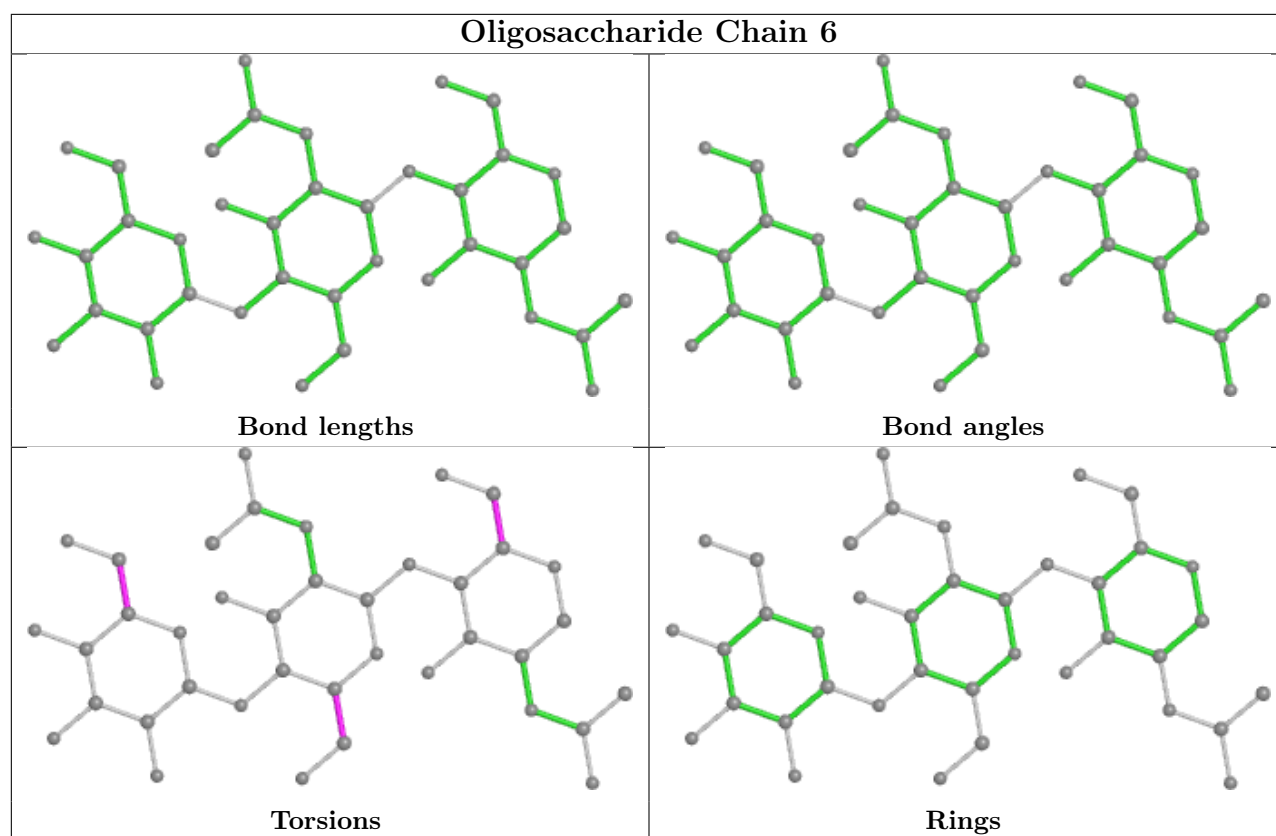












5.6 Ligand geometry

24 ligands 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	E	2003	1	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	D	2004	1	14,14,15	0.26	0	17,19,21	0.40	0
4	NAG	C	2002	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	E	2002	1	14,14,15	0.18	0	17,19,21	0.46	0
4	NAG	D	2001	1	14,14,15	0.26	0	17,19,21	0.32	0
4	NAG	F	2001	1	14,14,15	0.30	0	17,19,21	0.33	0
4	NAG	B	2004	1	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	E	2001	1	14,14,15	0.28	0	17,19,21	0.33	0
4	NAG	C	2004	1	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	D	2003	1	14,14,15	0.24	0	17,19,21	0.38	0
4	NAG	F	2003	1	14,14,15	0.19	0	17,19,21	0.49	0
4	NAG	D	2002	1	14,14,15	0.39	0	17,19,21	0.43	0
4	NAG	B	2001	1	14,14,15	0.29	0	17,19,21	0.47	0
4	NAG	A	2003	1	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	A	2004	-	14,14,15	0.22	0	17,19,21	0.40	0
4	NAG	F	2002	1	14,14,15	0.24	0	17,19,21	0.48	0
4	NAG	E	2004	1	14,14,15	0.16	0	17,19,21	0.42	0
4	NAG	C	2003	1	14,14,15	0.28	0	17,19,21	0.50	0
4	NAG	A	2001	1	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	B	2002	1	14,14,15	0.18	0	17,19,21	0.43	0
4	NAG	B	2003	1	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	C	2001	1	14,14,15	0.30	0	17,19,21	0.32	0
4	NAG	A	2002	1	14,14,15	0.25	0	17,19,21	0.37	0
4	NAG	F	2004	1	14,14,15	0.24	0	17,19,21	0.49	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	E	2003	1	-	4/6/23/26	0/1/1/1
4	NAG	D	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	E	2002	1	-	0/6/23/26	0/1/1/1
4	NAG	D	2001	1	-	4/6/23/26	0/1/1/1
4	NAG	F	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	E	2001	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	D	2003	1	-	0/6/23/26	0/1/1/1
4	NAG	F	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	D	2002	1	-	4/6/23/26	0/1/1/1
4	NAG	B	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2003	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2004	-	-	2/6/23/26	0/1/1/1
4	NAG	F	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	E	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2003	1	-	4/6/23/26	0/1/1/1
4	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2001	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2002	1	-	0/6/23/26	0/1/1/1
4	NAG	F	2004	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

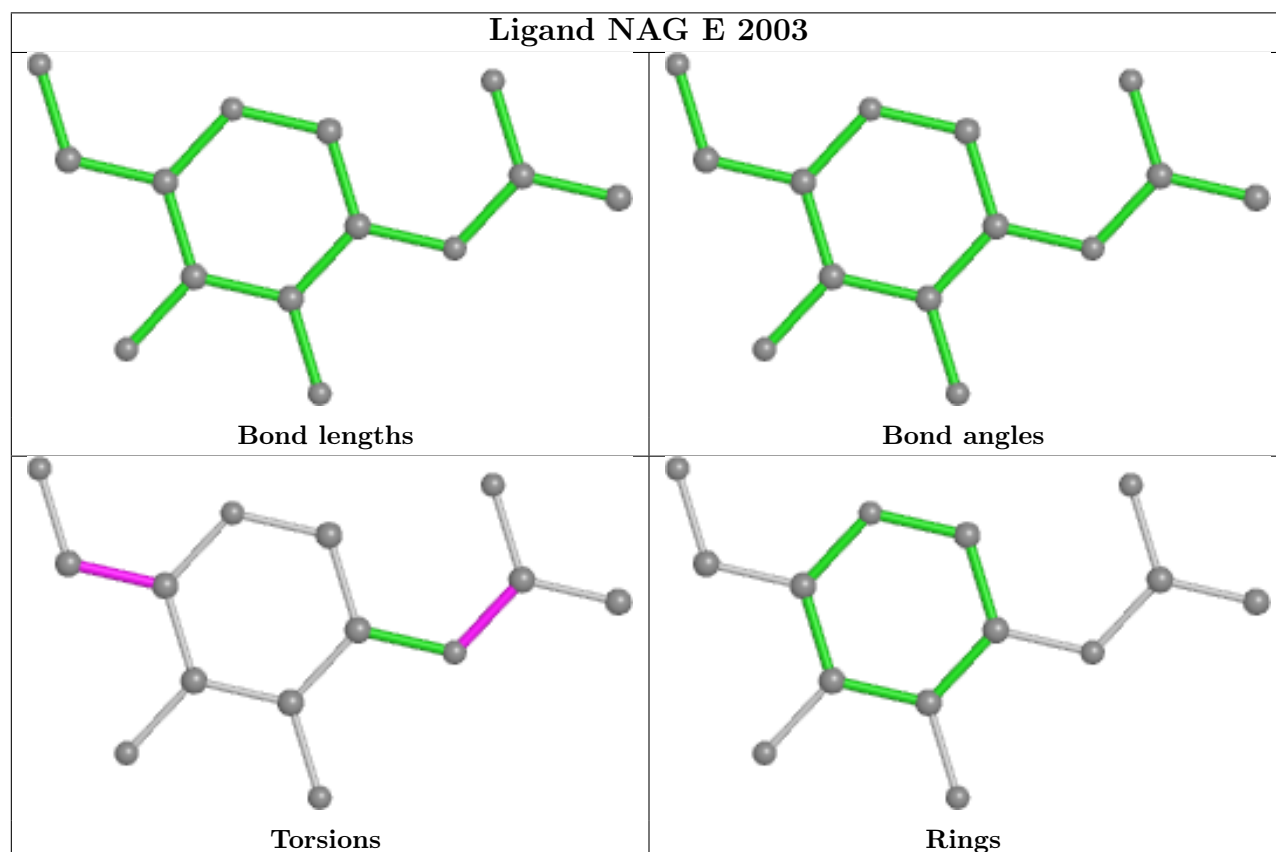
5 of 44 torsion outliers are listed below:

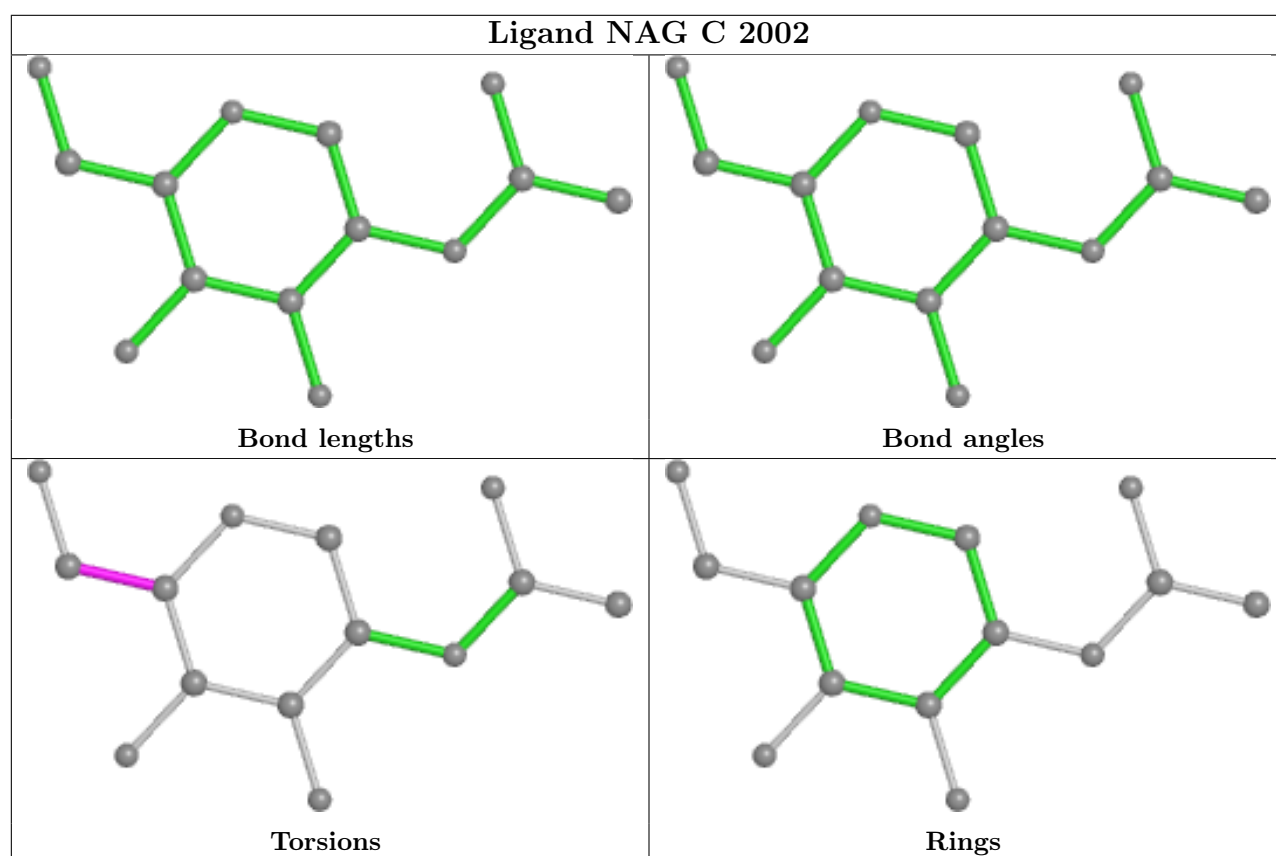
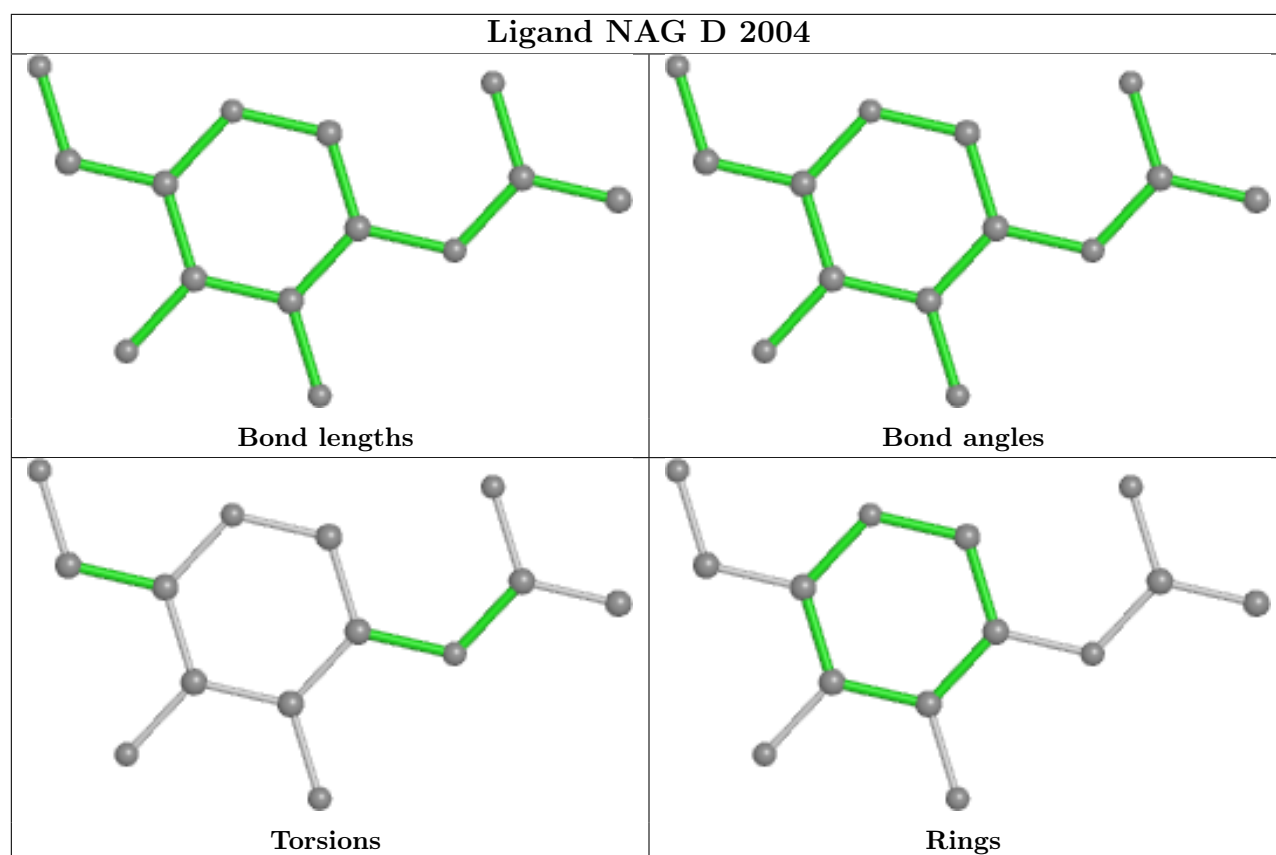
Mol	Chain	Res	Type	Atoms
4	A	2004	NAG	O5-C5-C6-O6
4	B	2004	NAG	O5-C5-C6-O6
4	E	2004	NAG	C4-C5-C6-O6
4	F	2004	NAG	O5-C5-C6-O6
4	A	2004	NAG	C4-C5-C6-O6

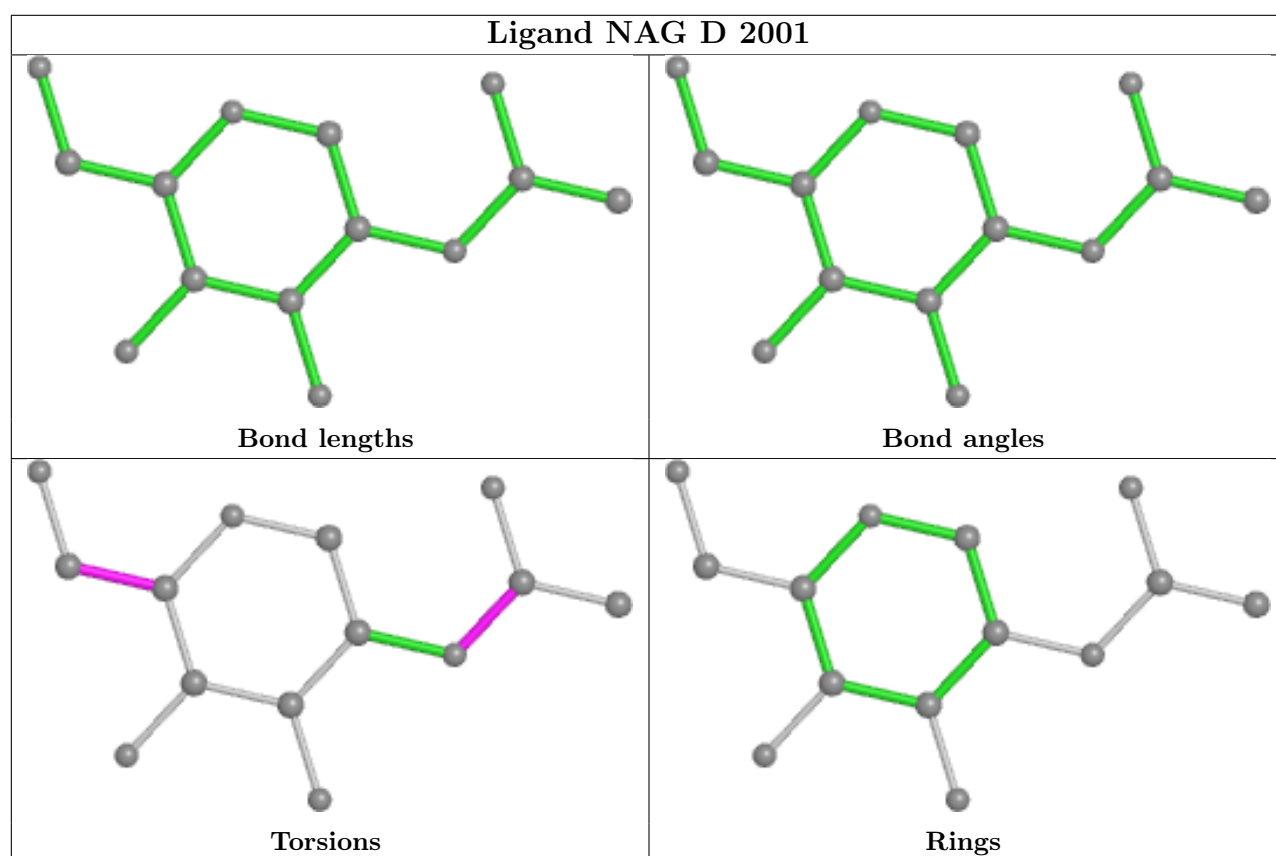
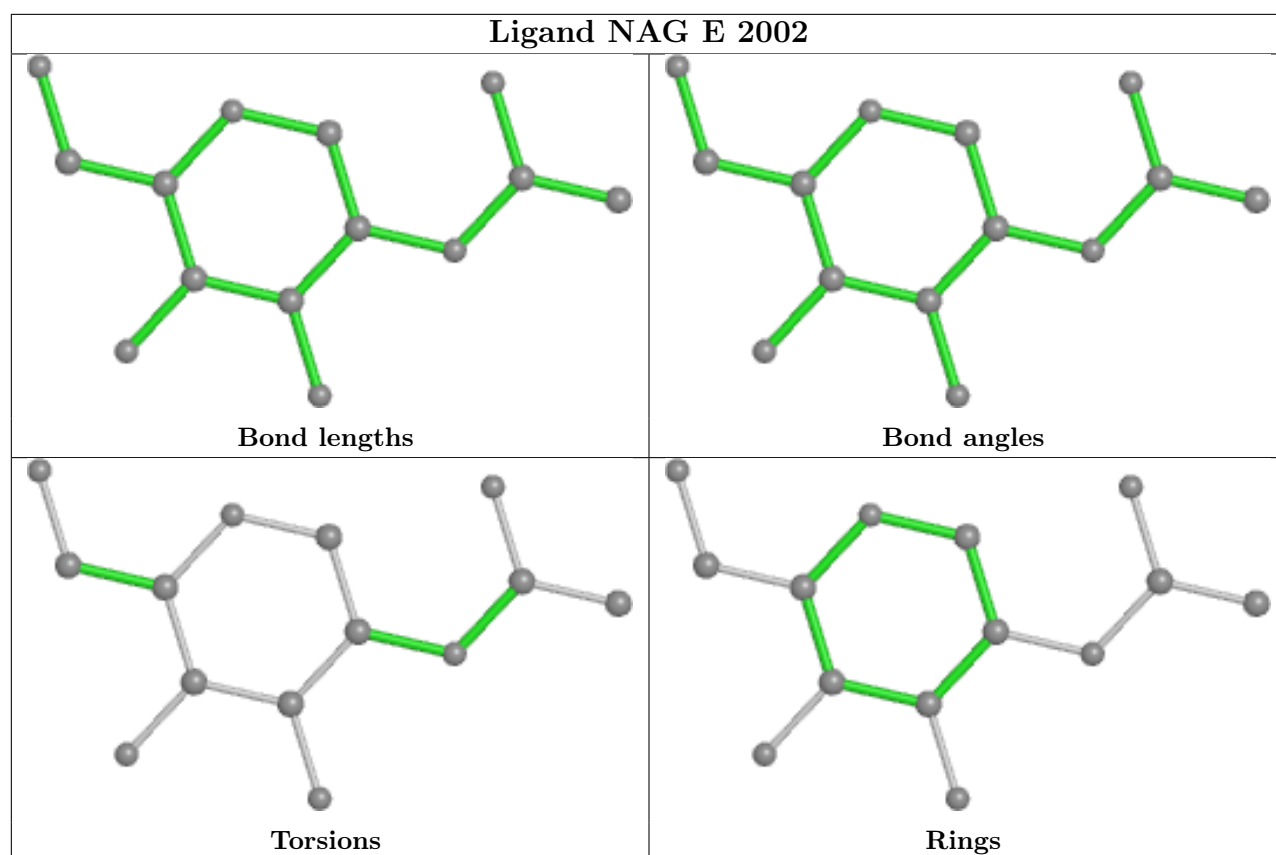
There are no ring outliers.

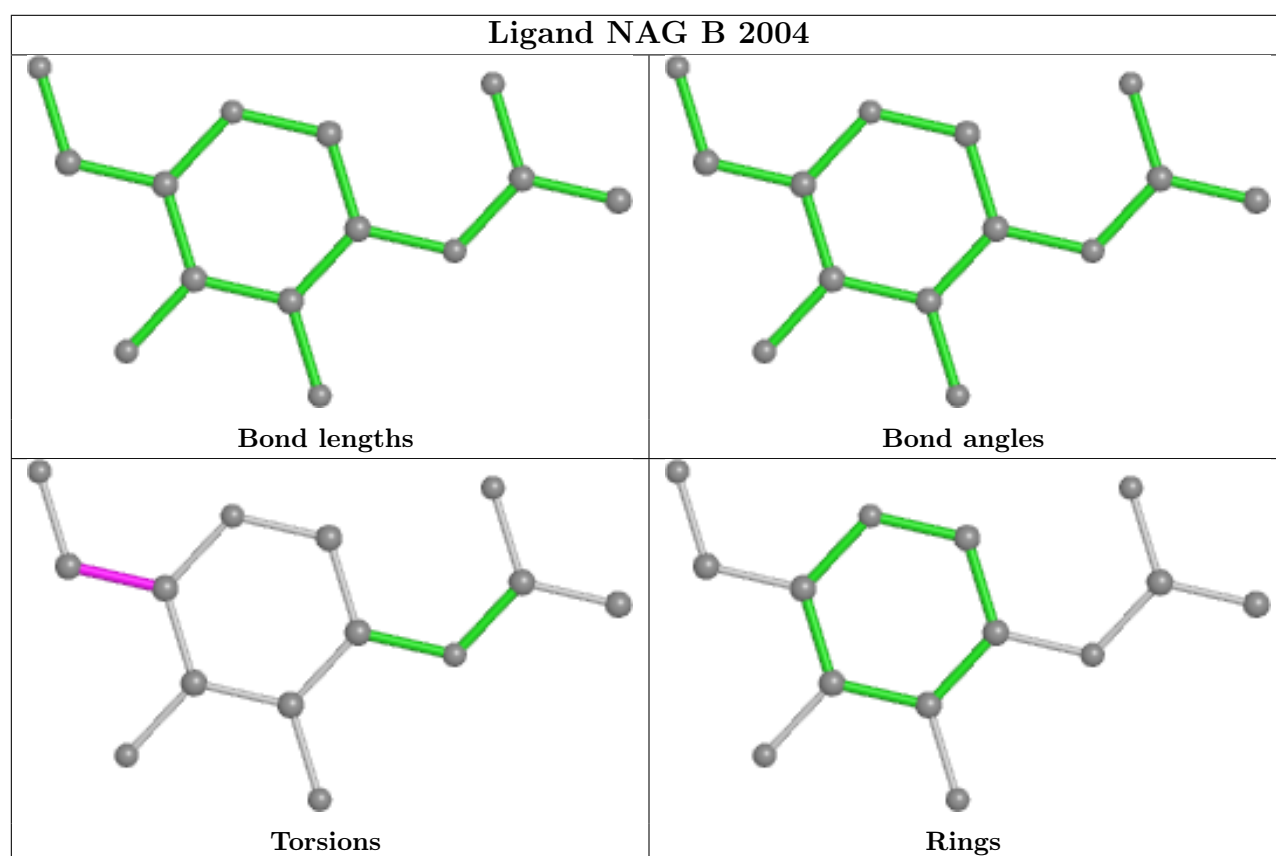
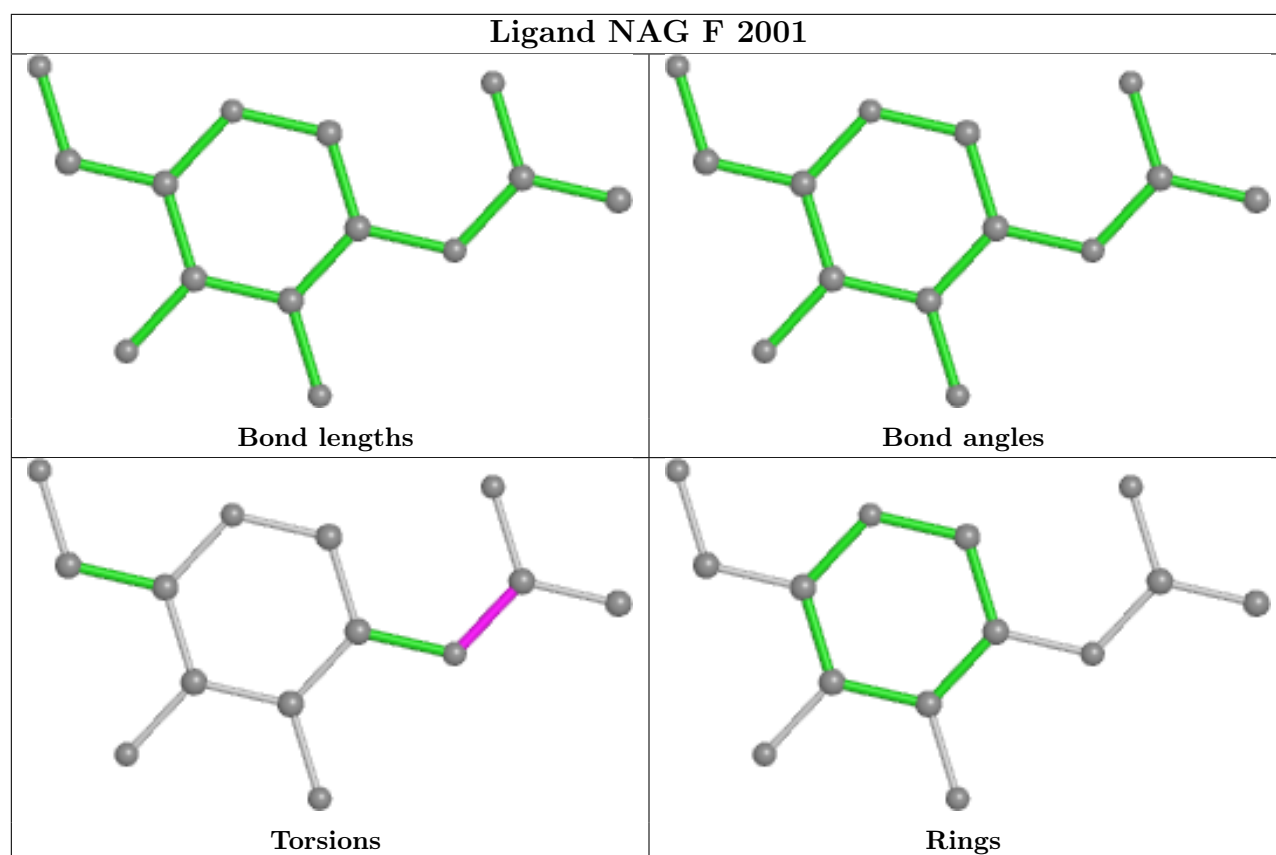
No monomer is involved in short contacts.

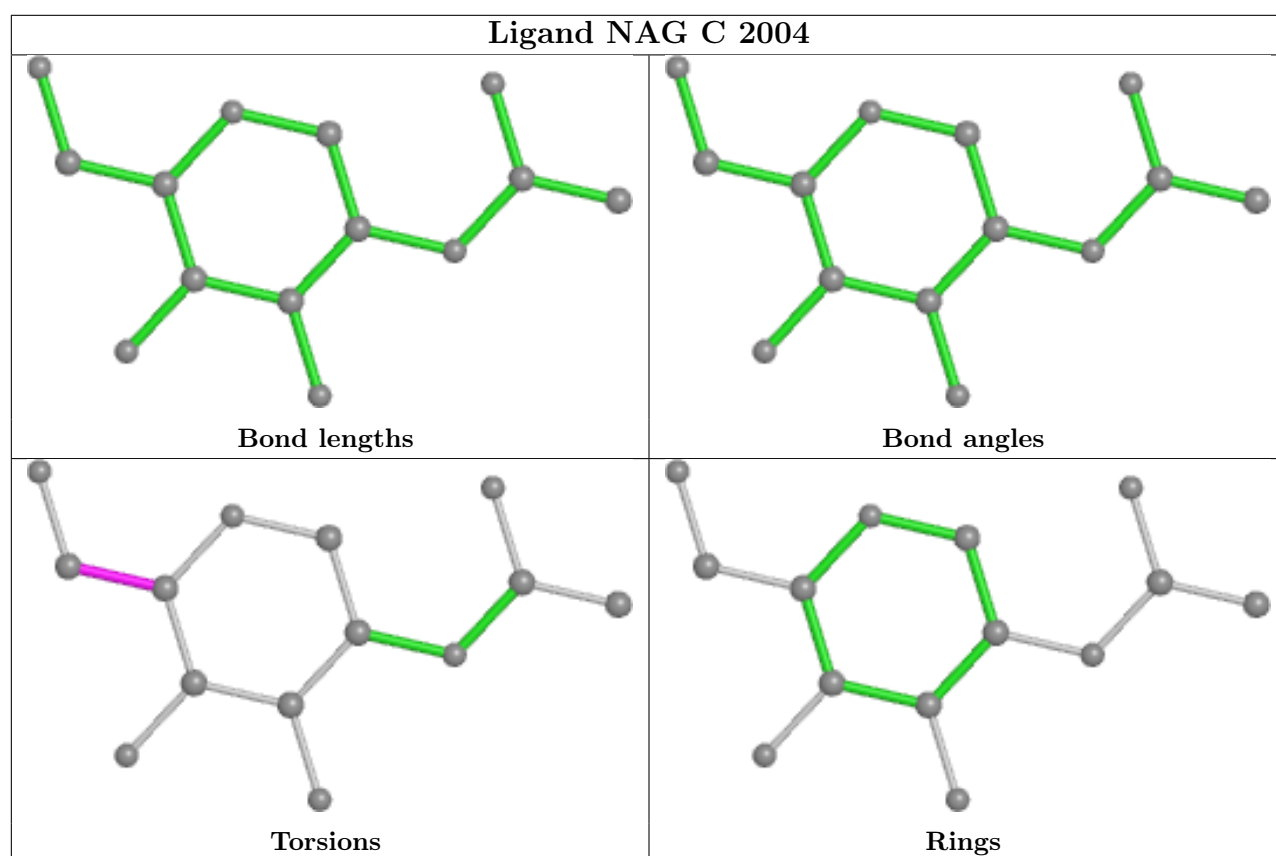
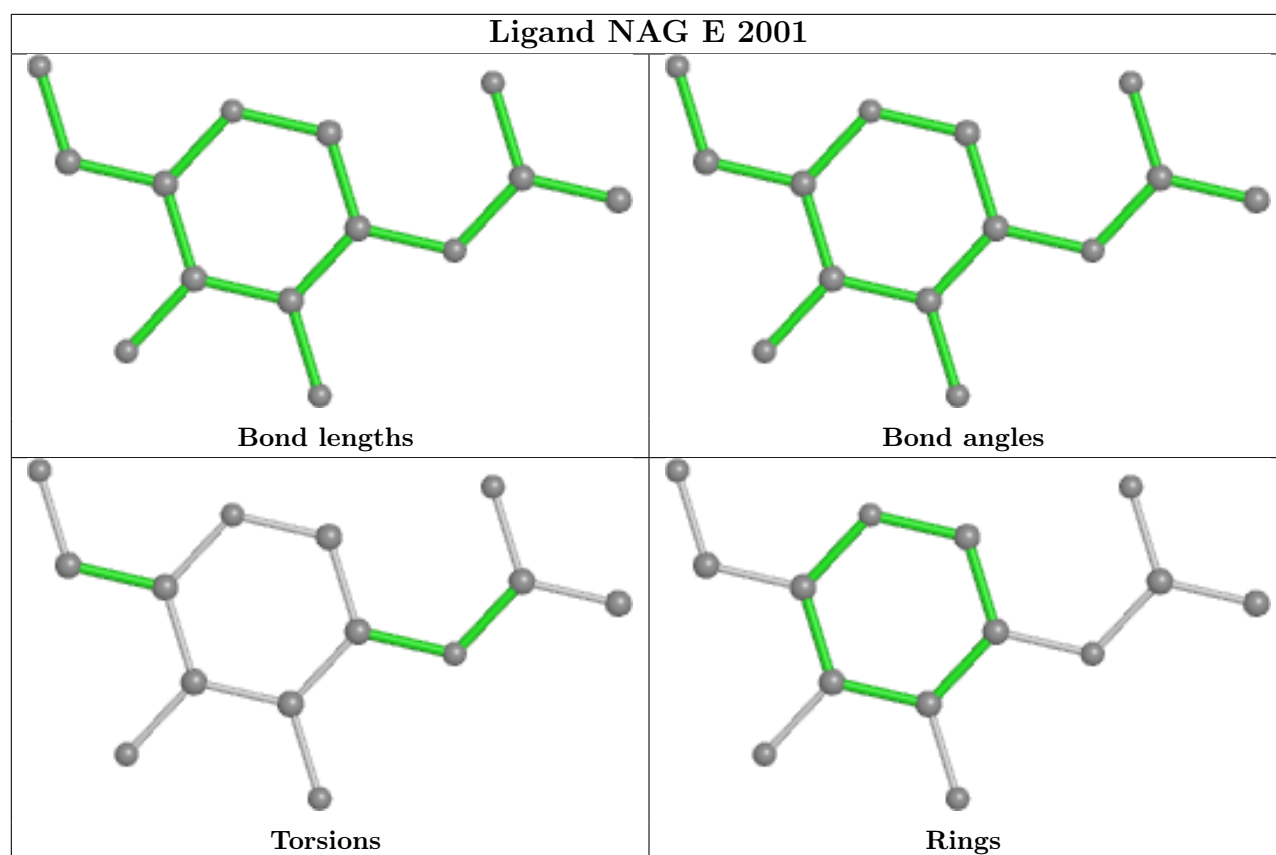
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

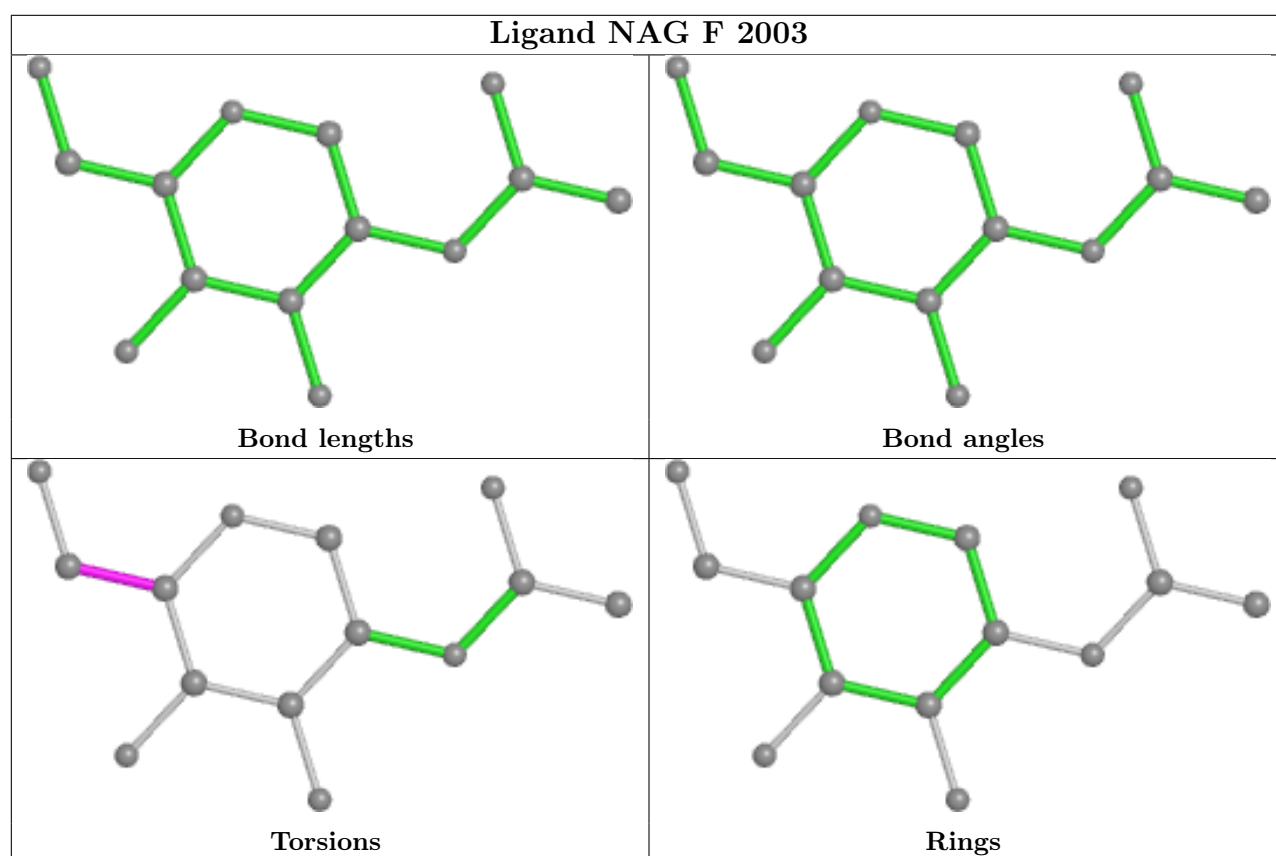
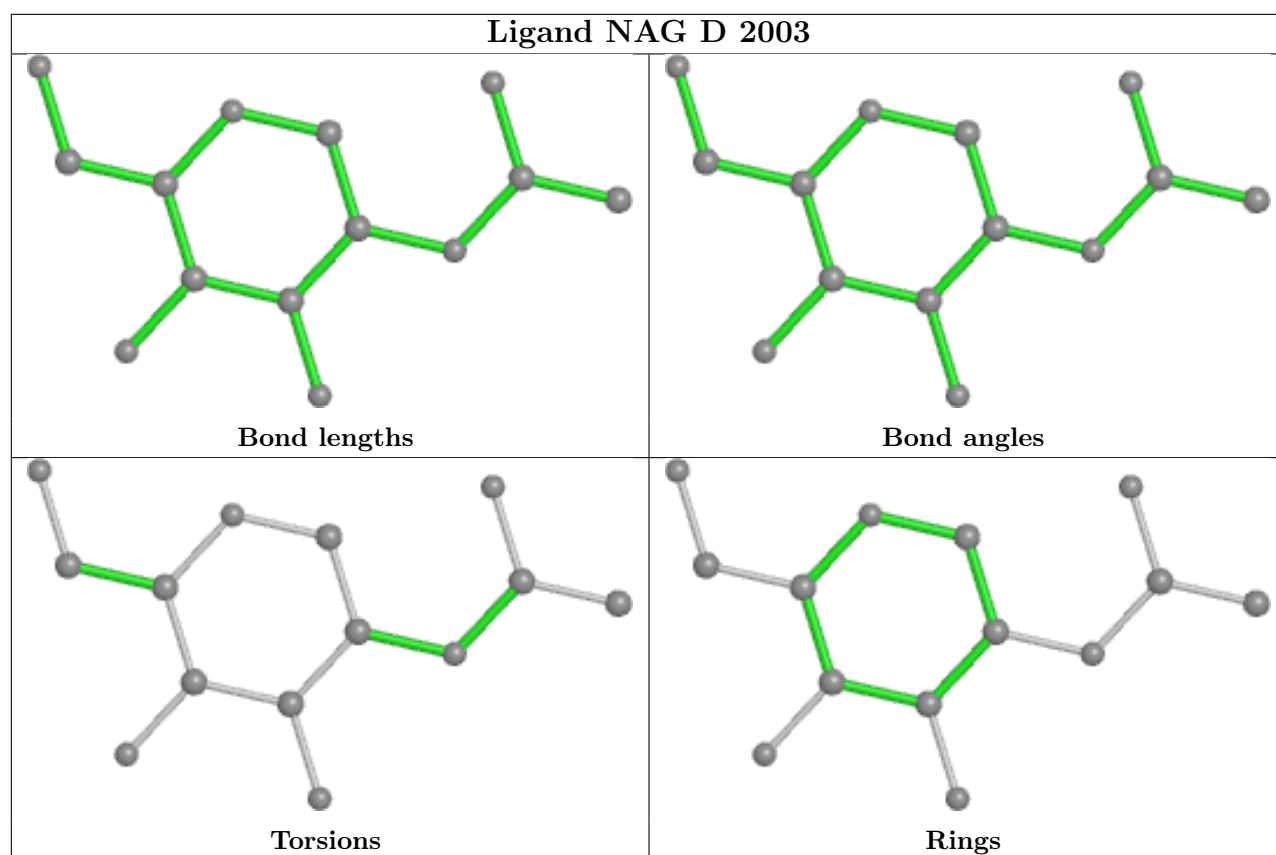


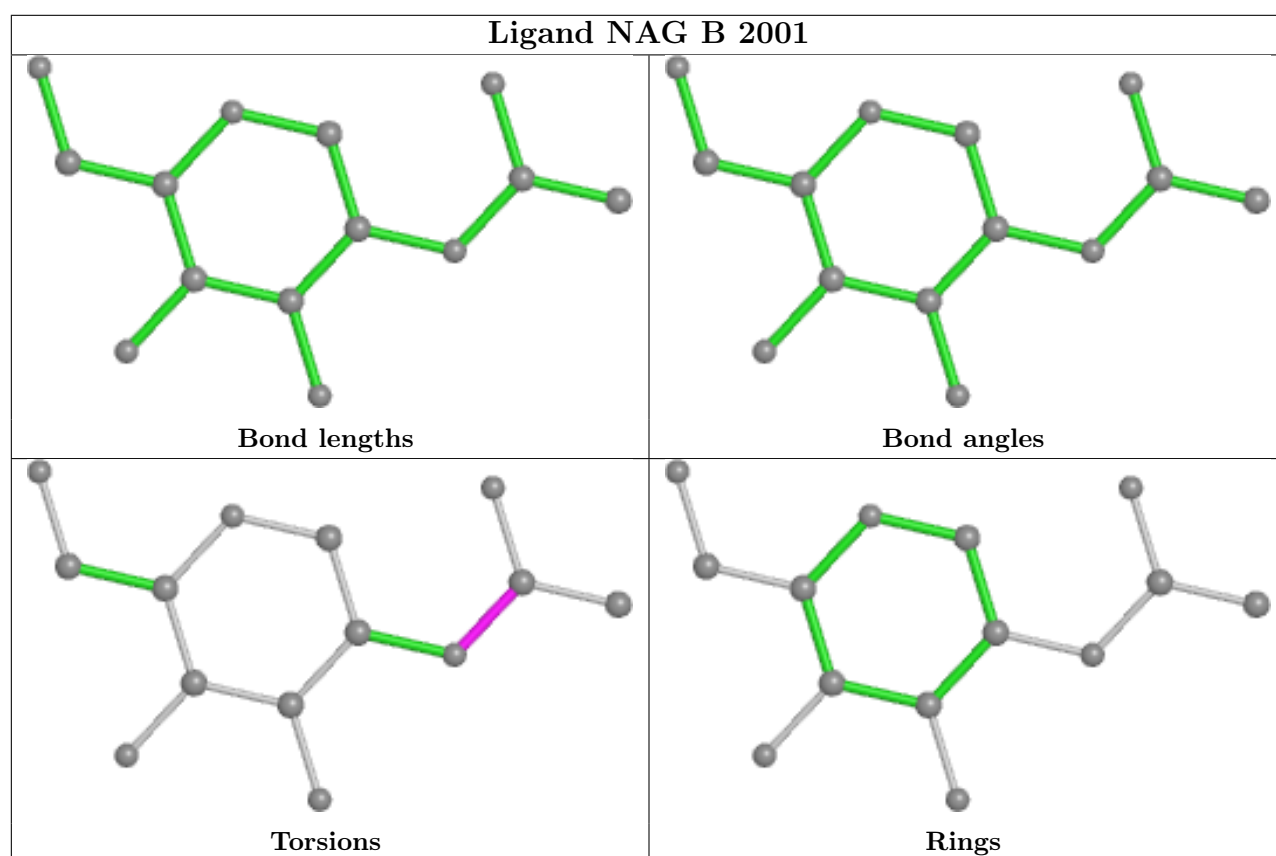
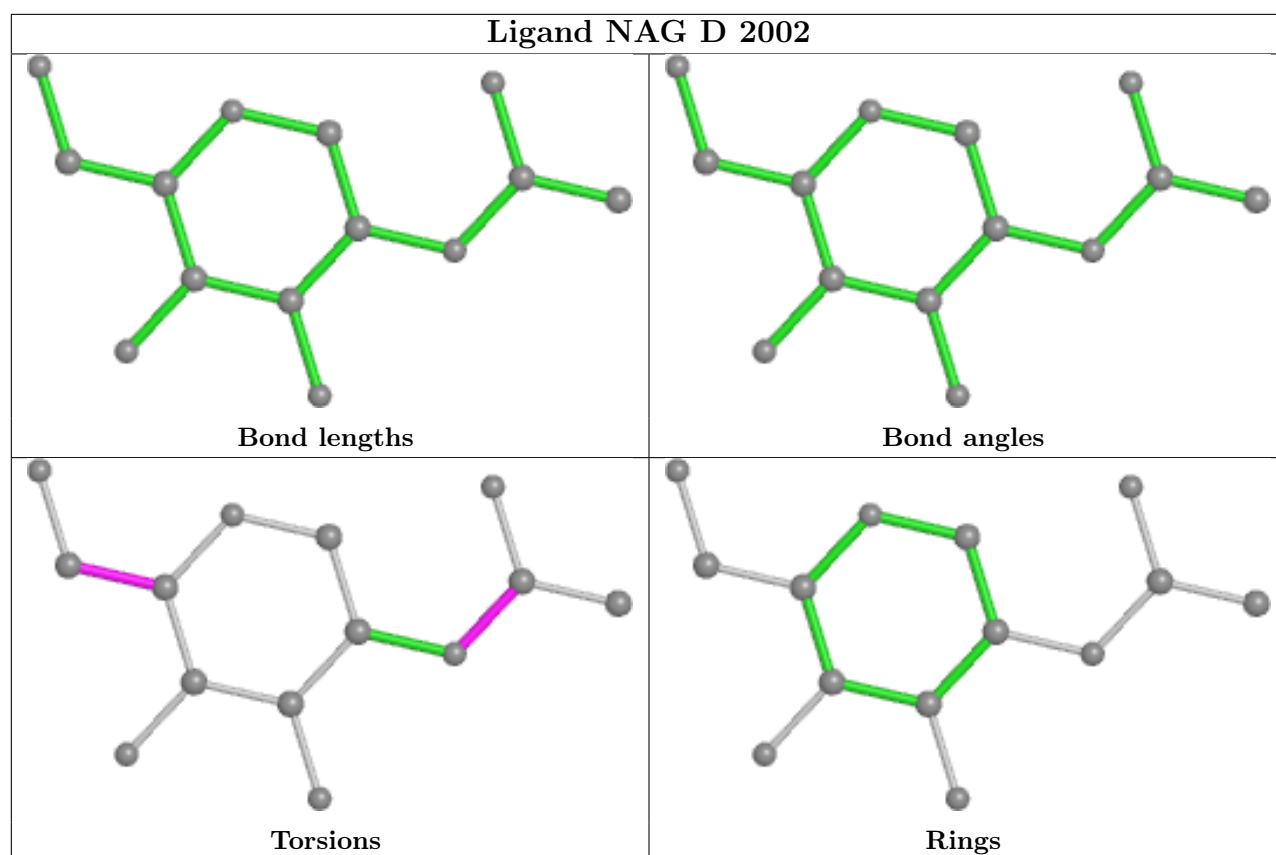


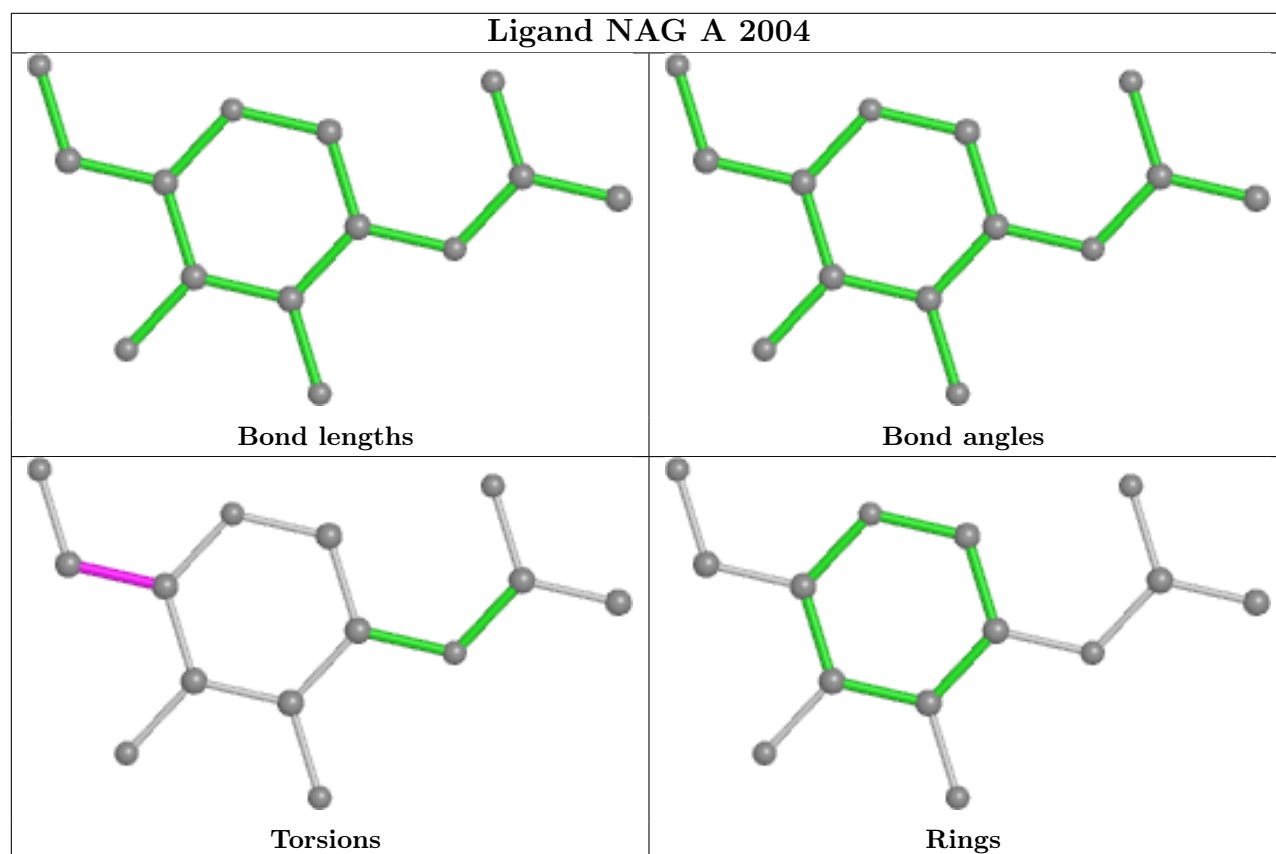
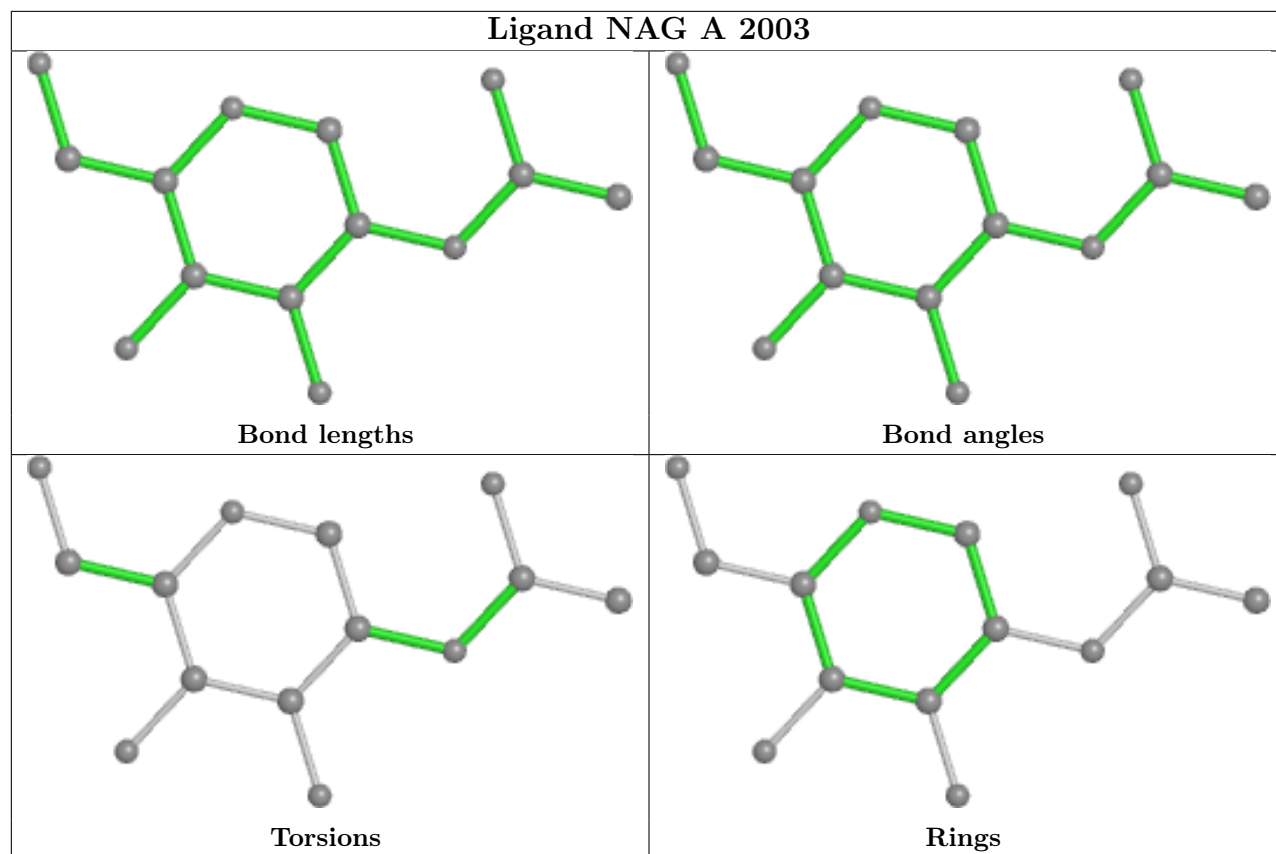


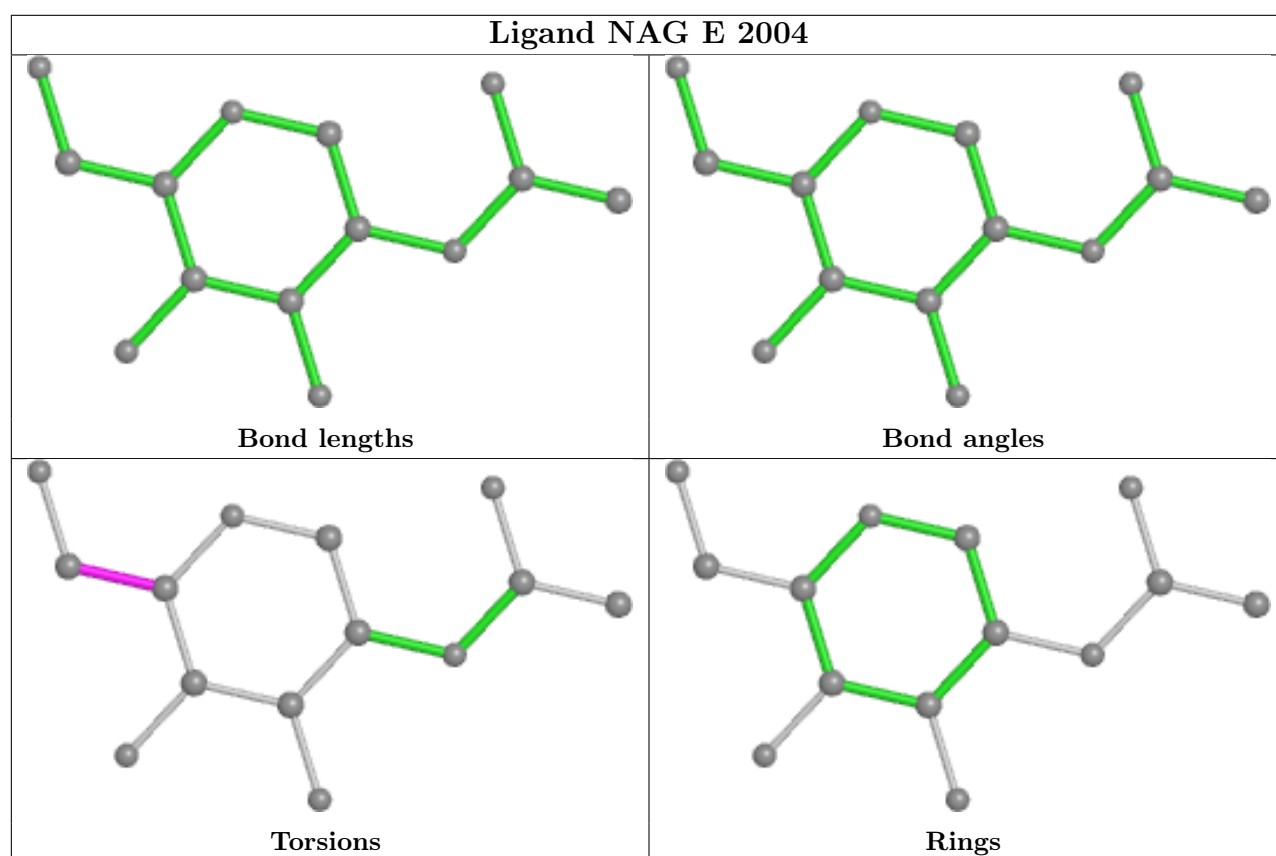
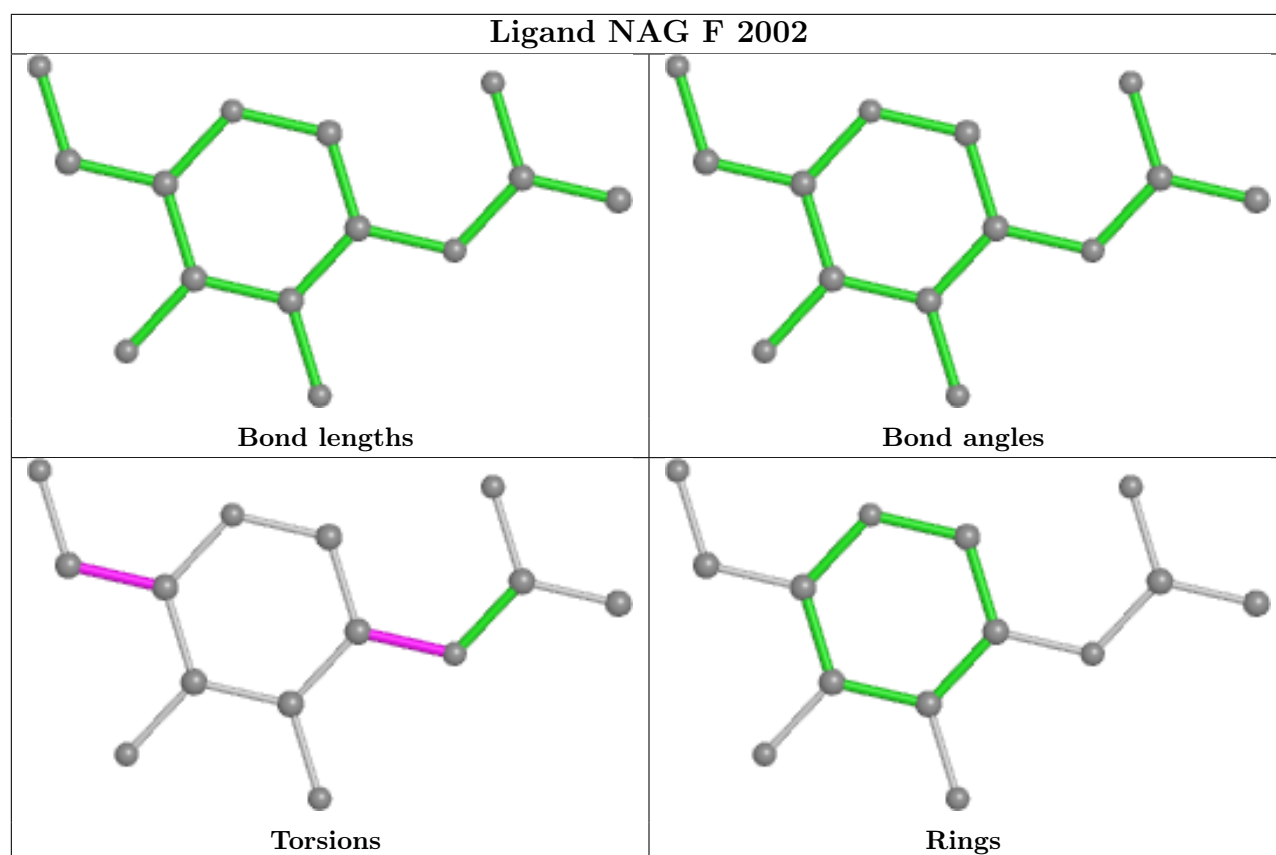


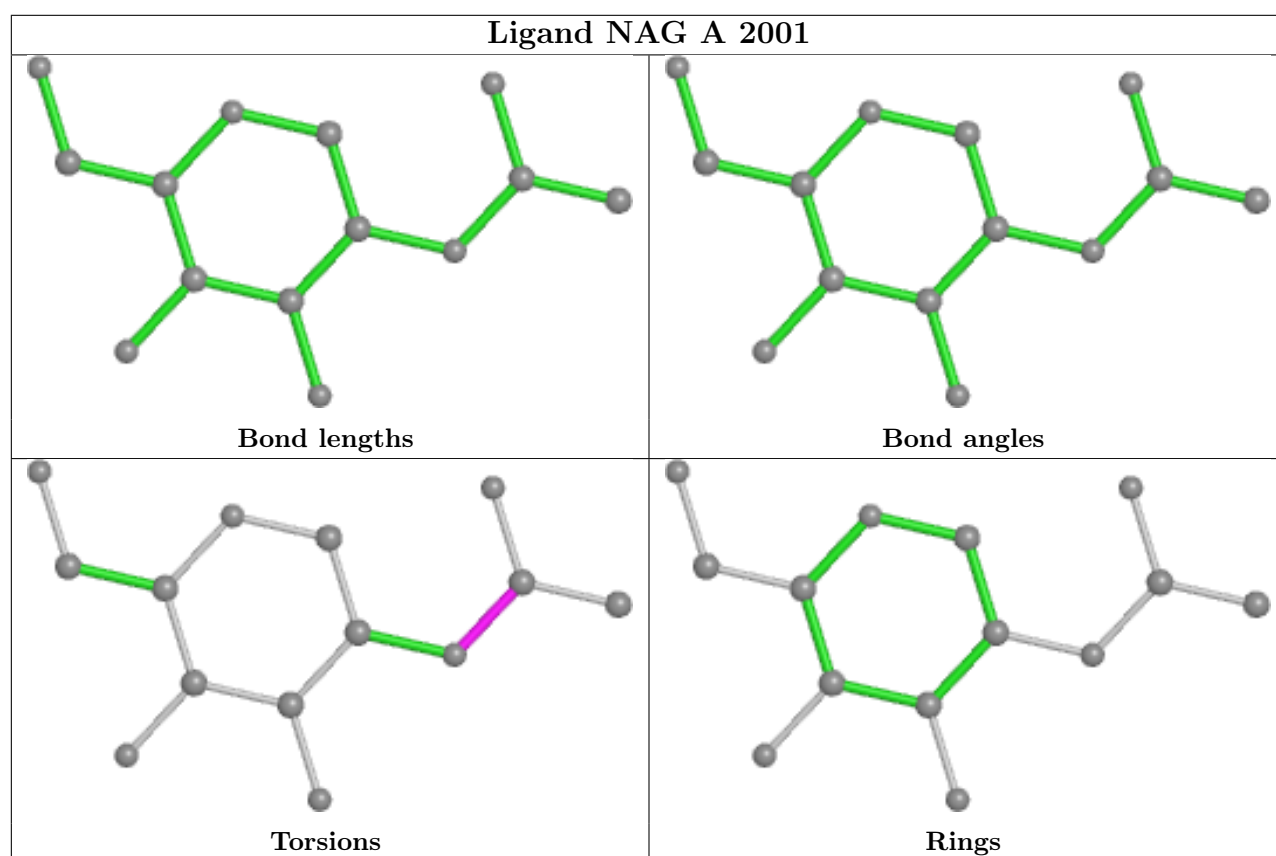
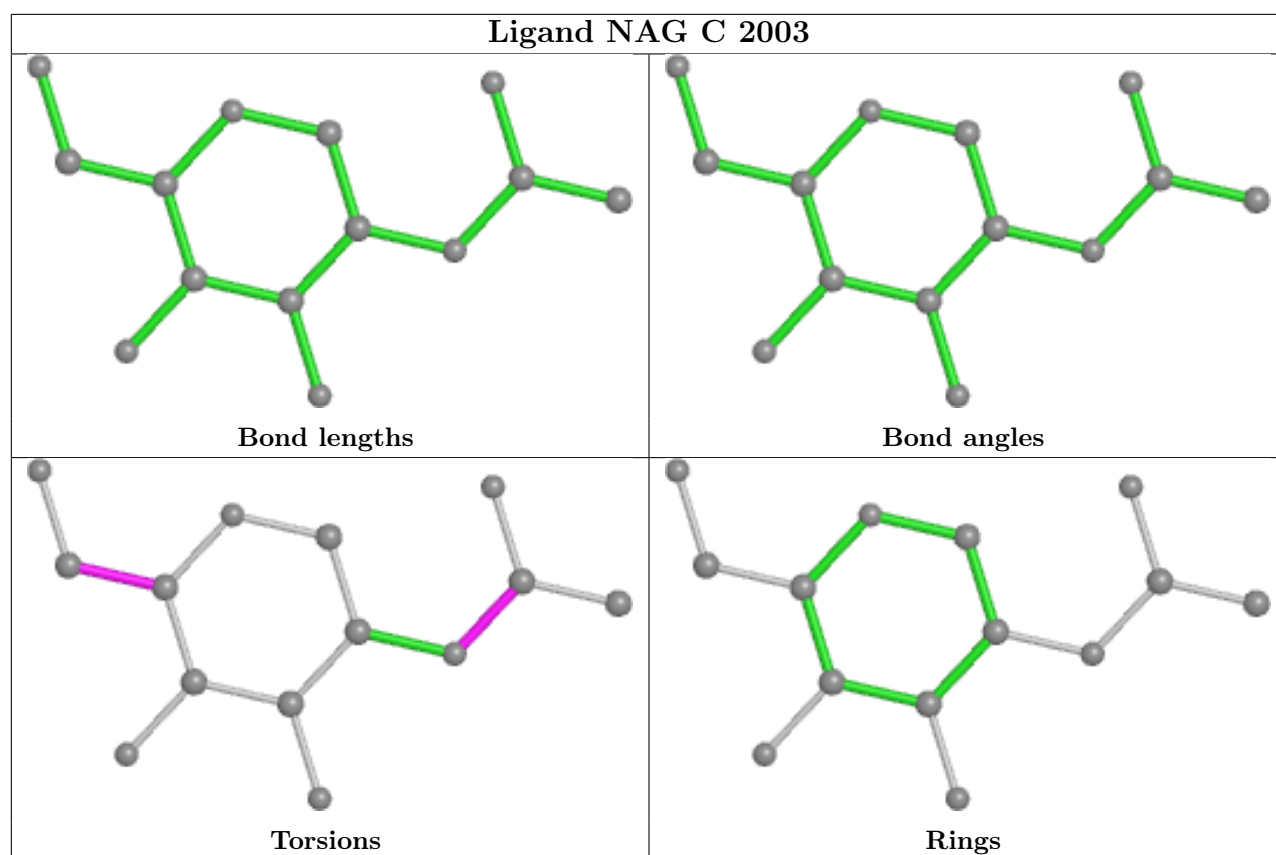


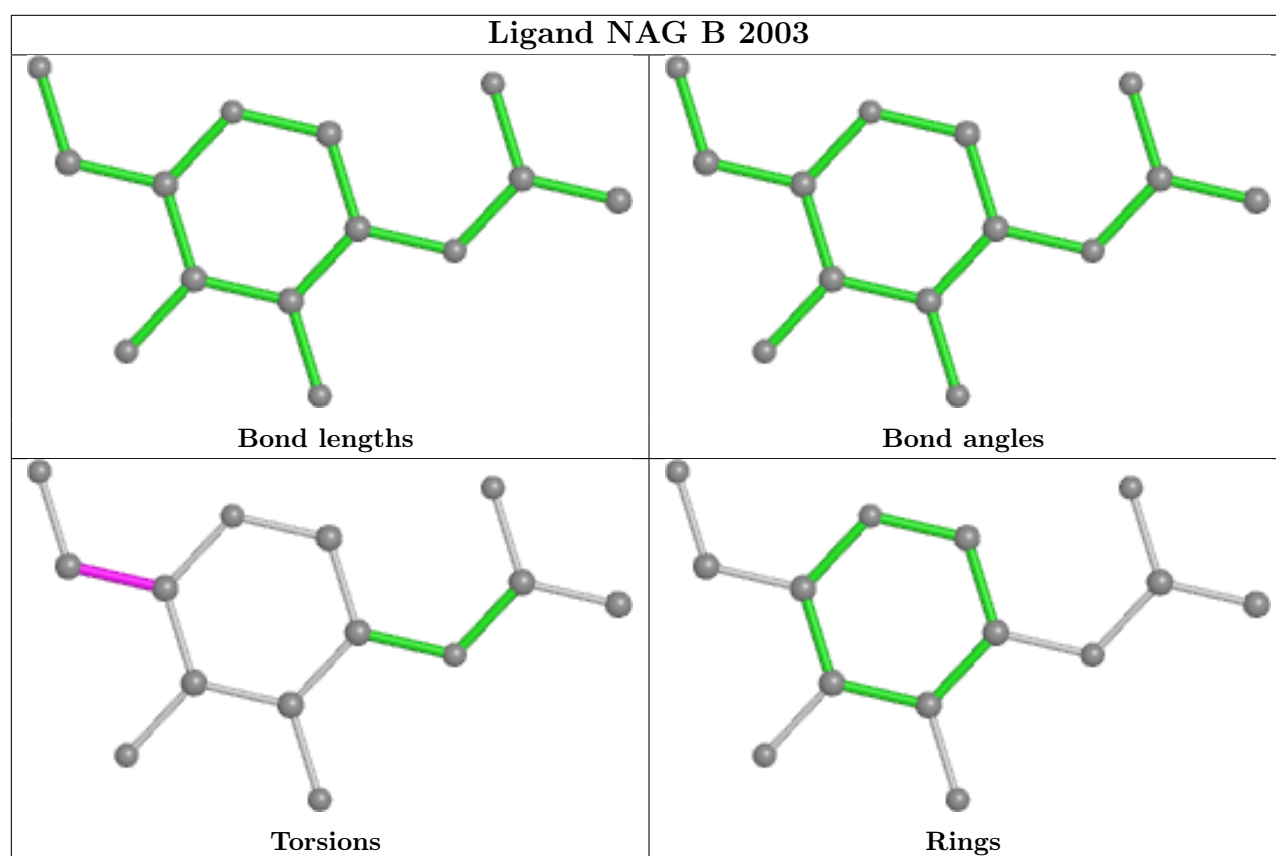
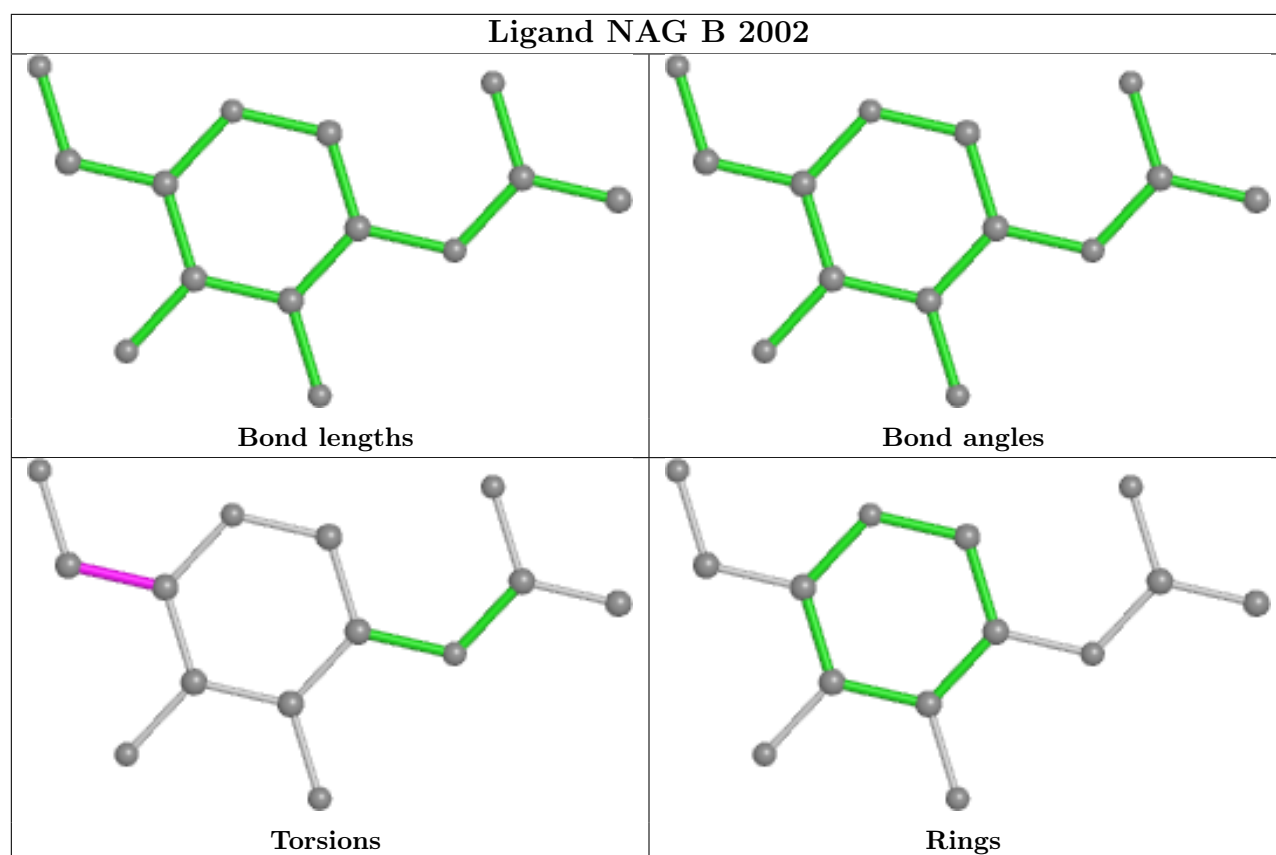


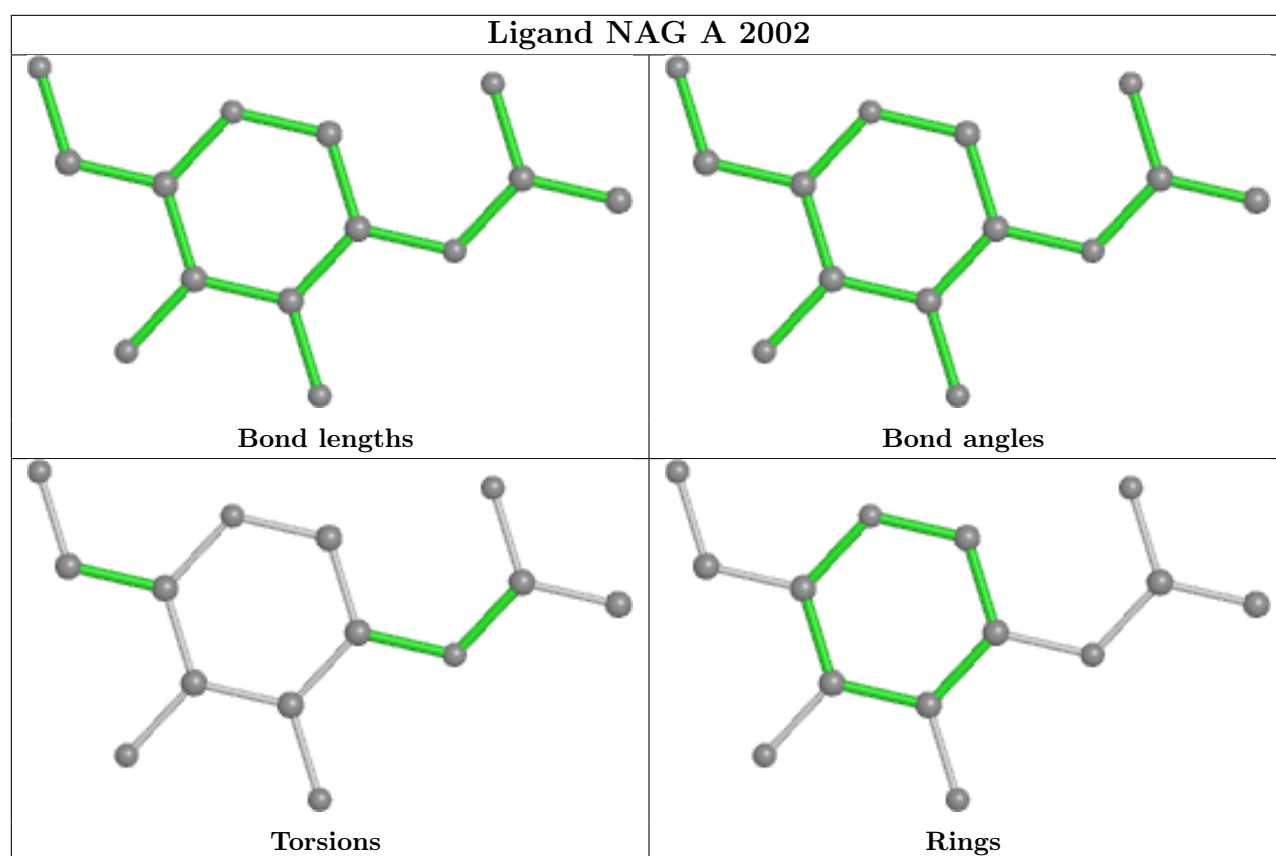
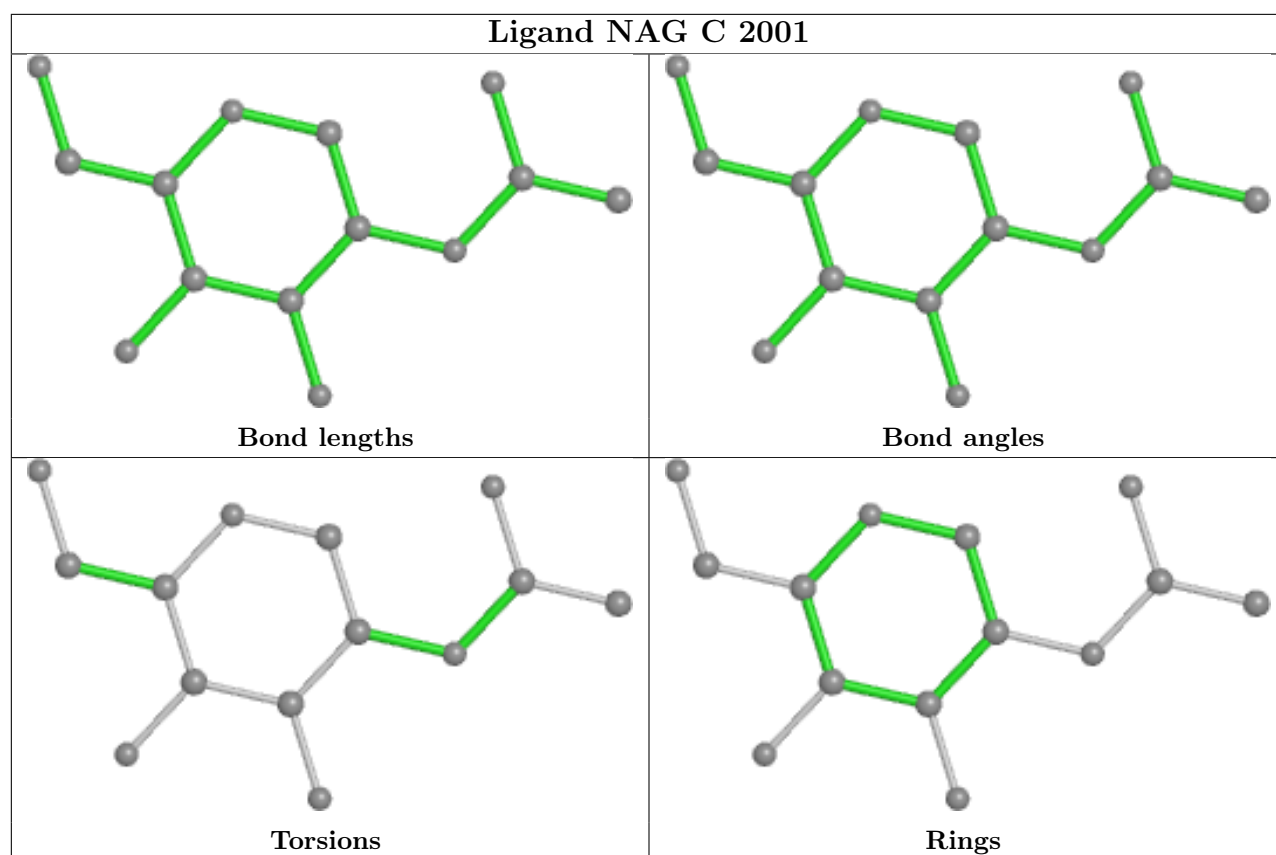


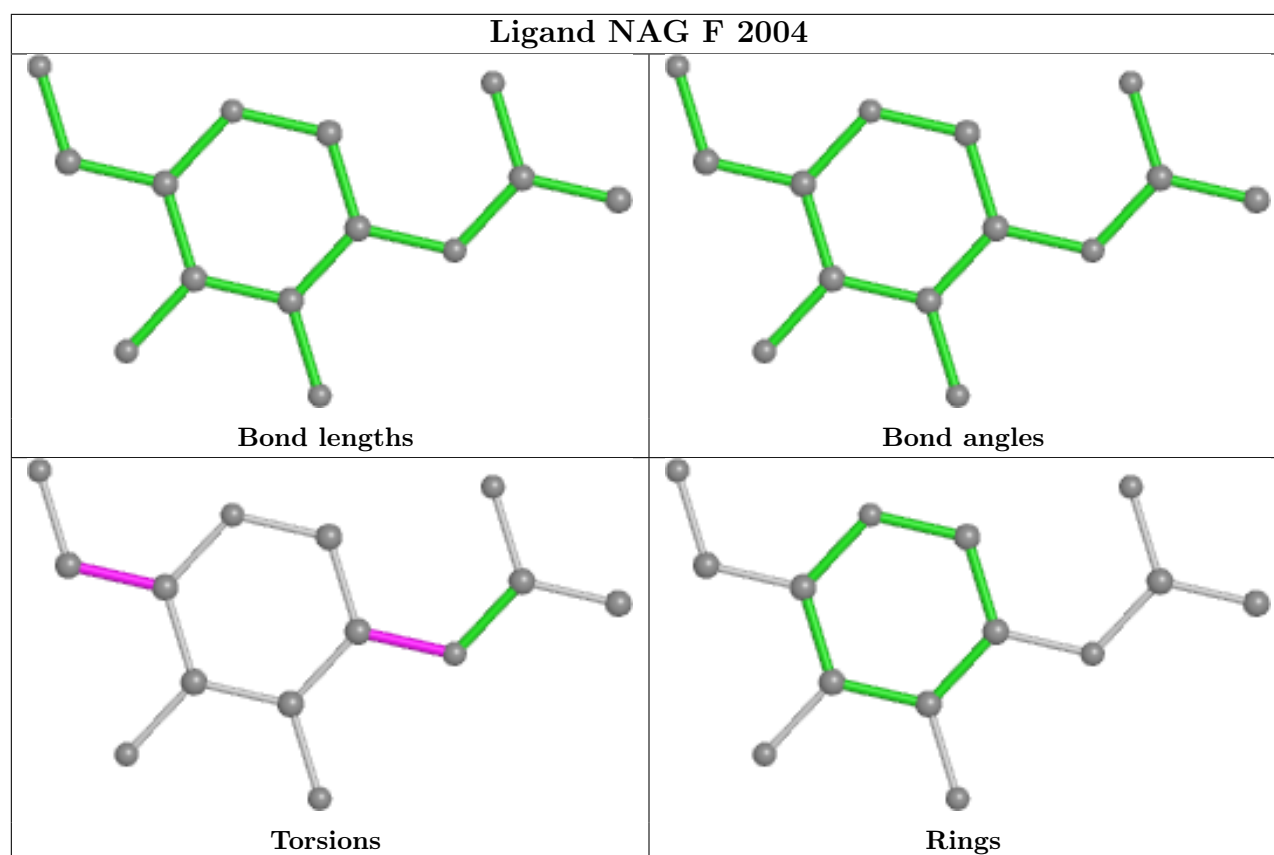












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

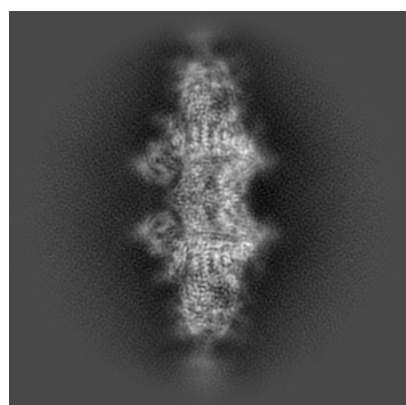
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31772. These allow visual inspection of the internal detail of the map and identification of artifacts.

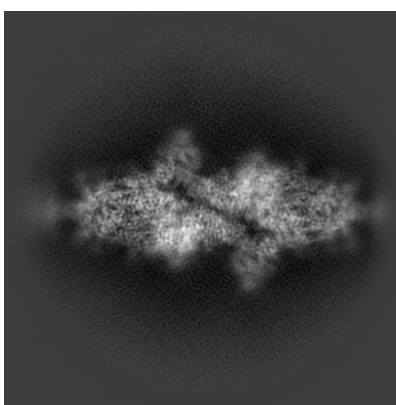
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

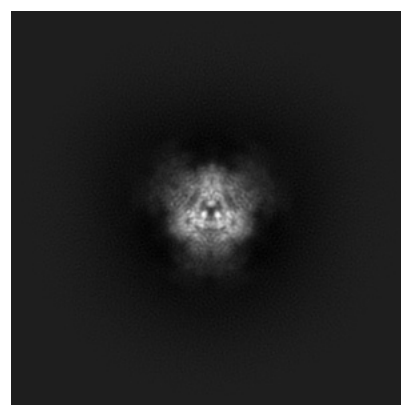
6.1.1 Primary map



X



Y

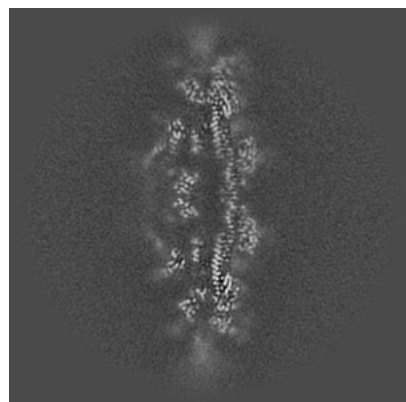


Z

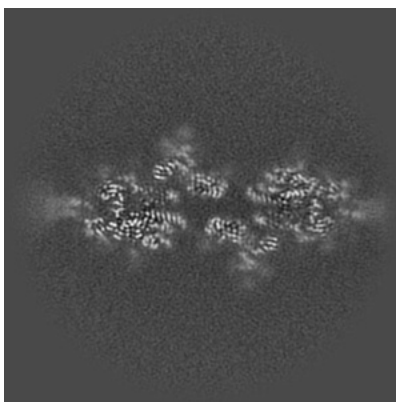
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

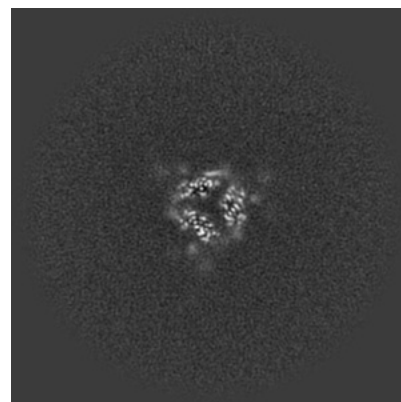
6.2.1 Primary map



X Index: 192



Y Index: 192

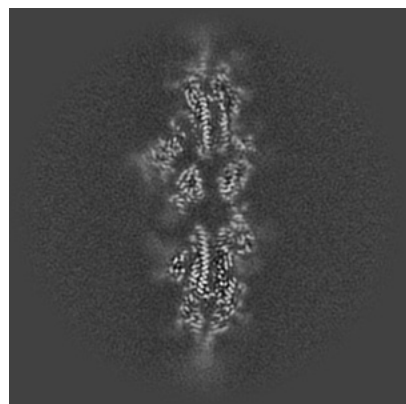


Z Index: 192

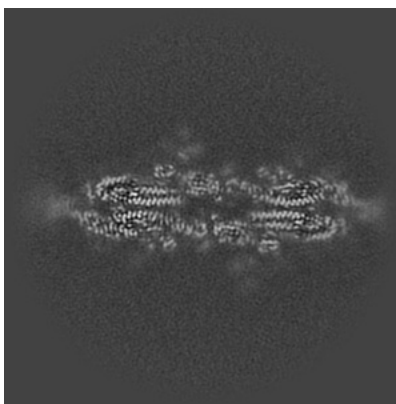
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

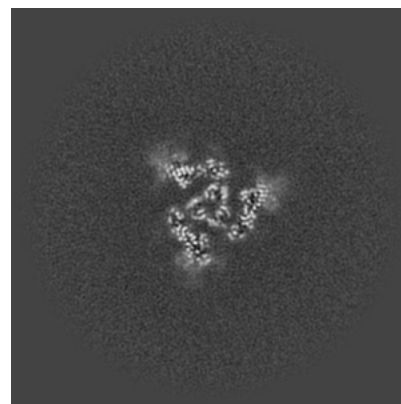
6.3.1 Primary map



X Index: 198



Y Index: 187

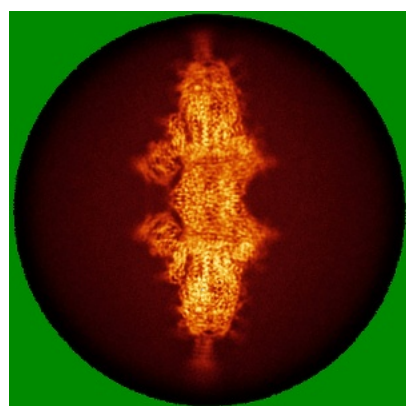


Z Index: 160

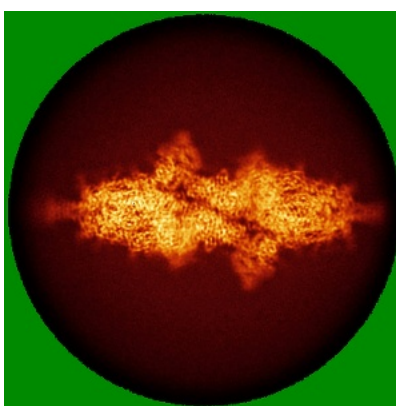
The images above show the largest variance slices of the map in three orthogonal directions.

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

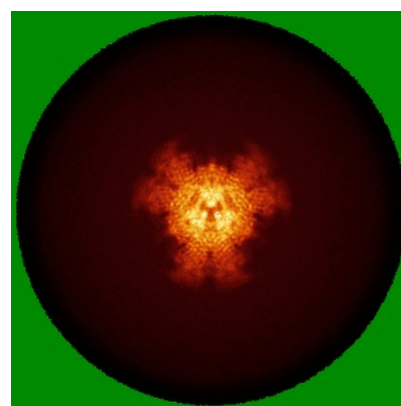
6.4.1 Primary map



X



Y



Z

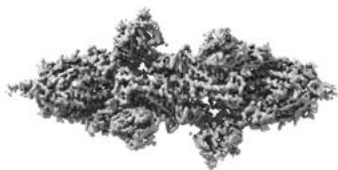
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

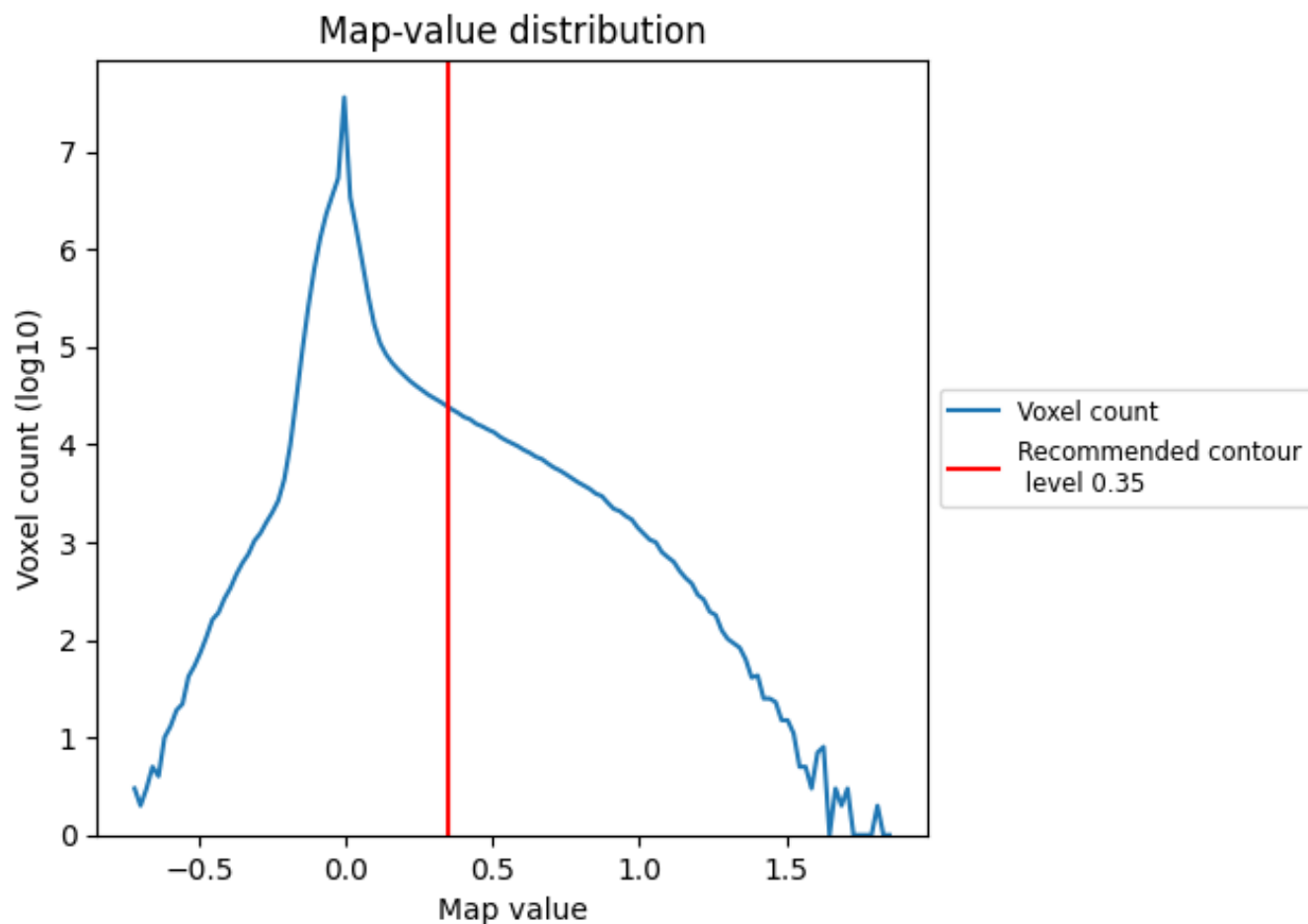
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

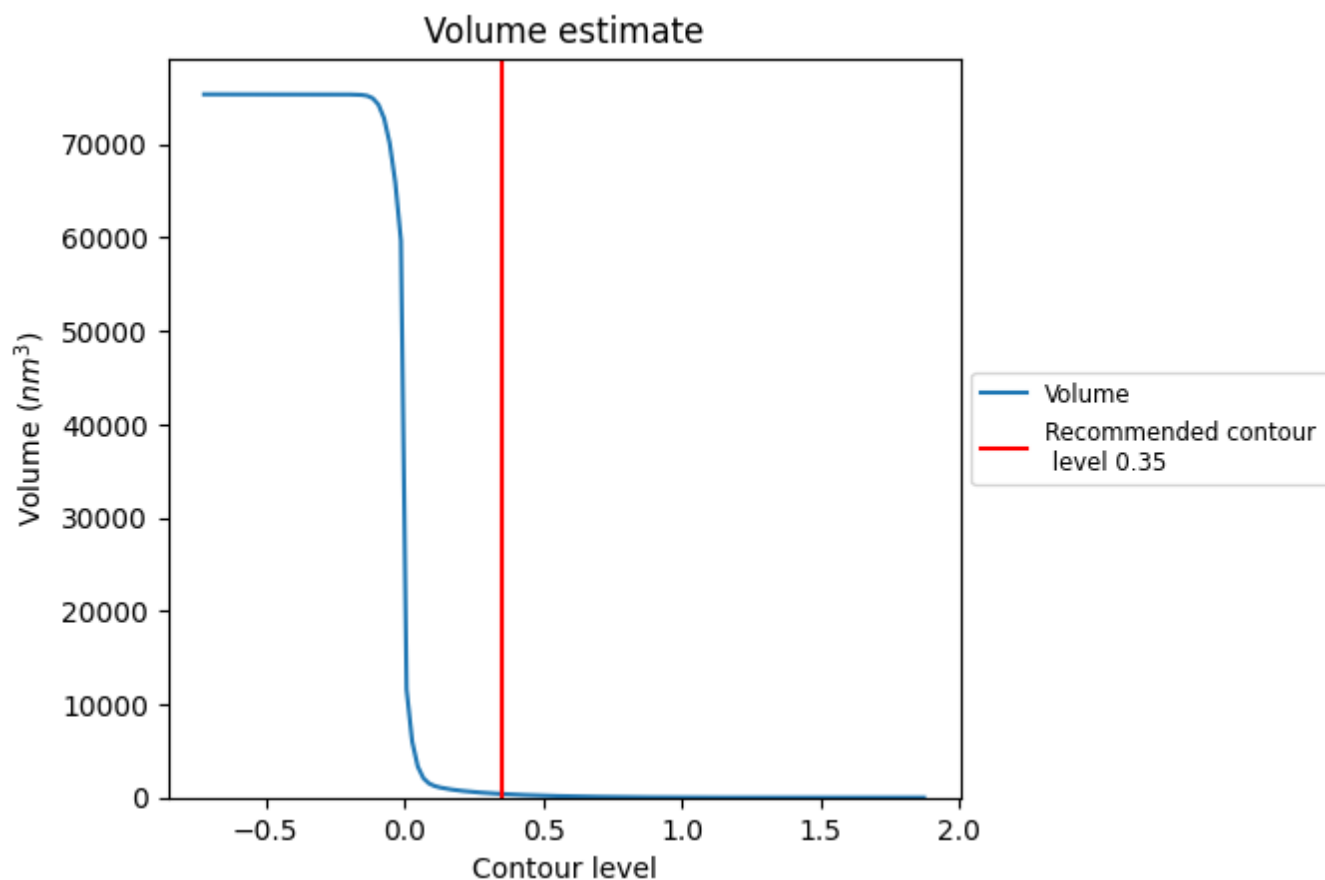
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

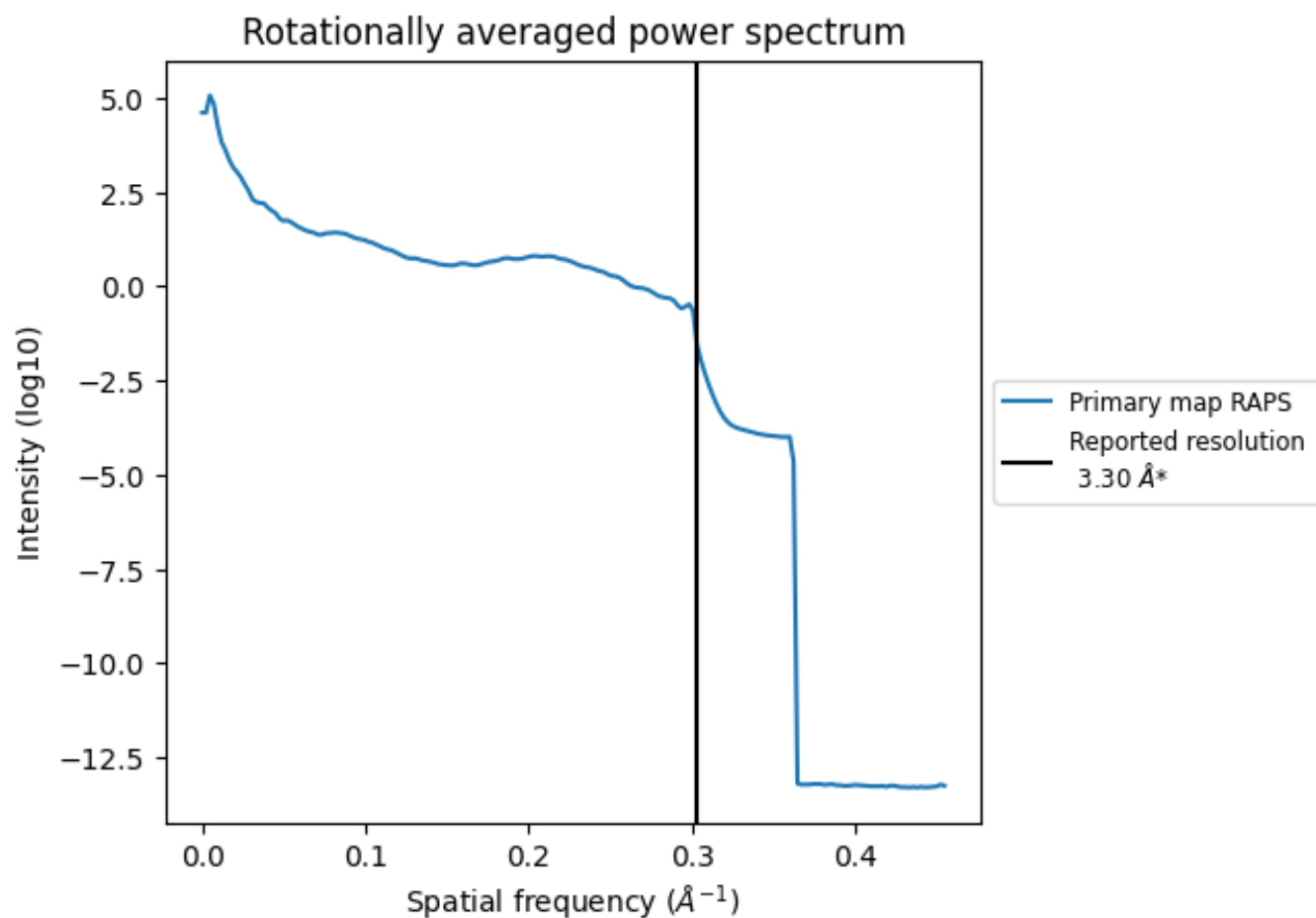
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 389 nm³; this corresponds to an approximate mass of 352 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 0.303 Å⁻¹

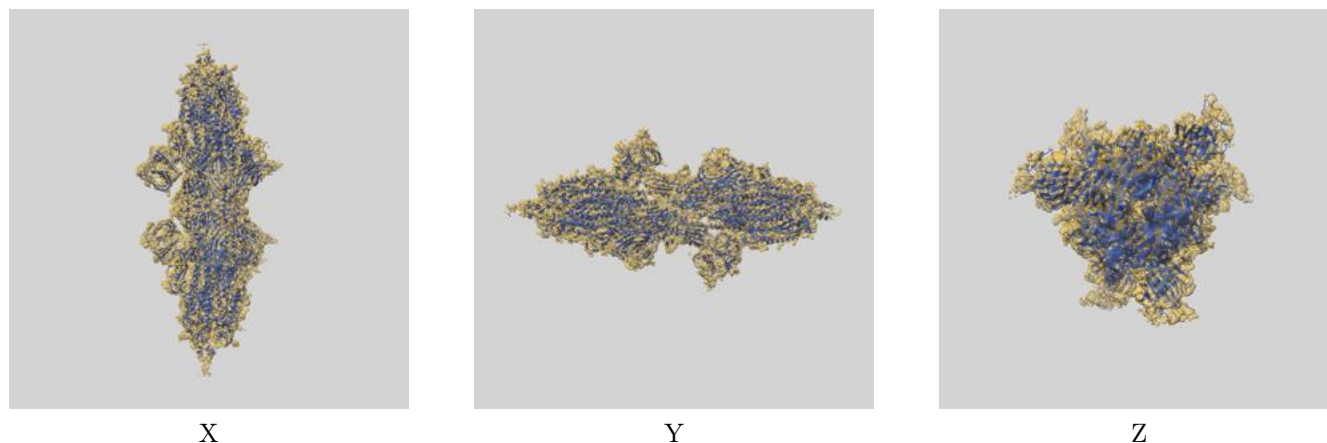
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

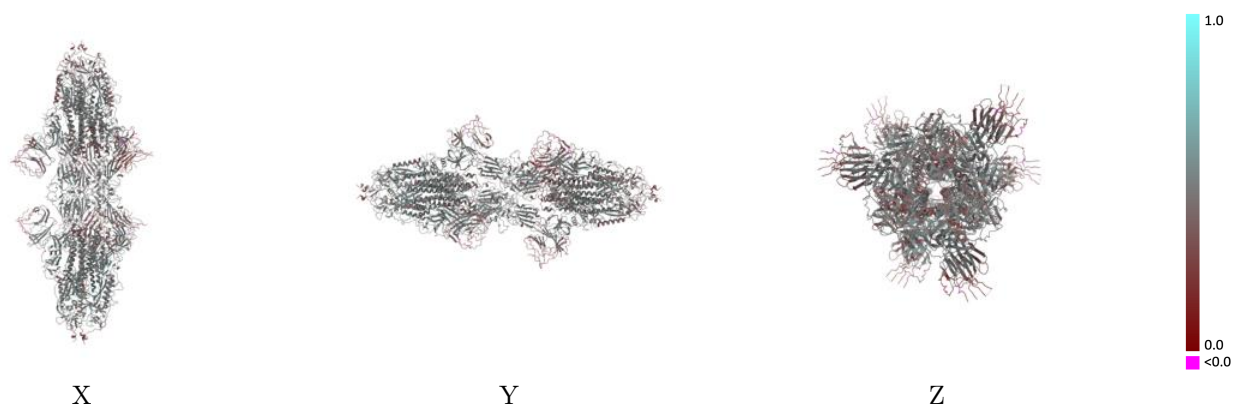
This section contains information regarding the fit between EMDB map EMD-31772 and PDB model 7V7I. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay [i](#)



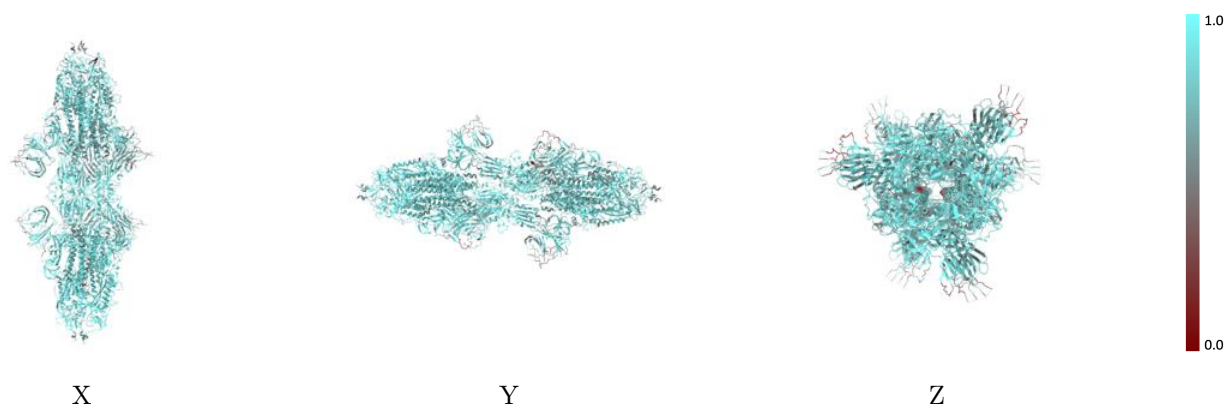
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



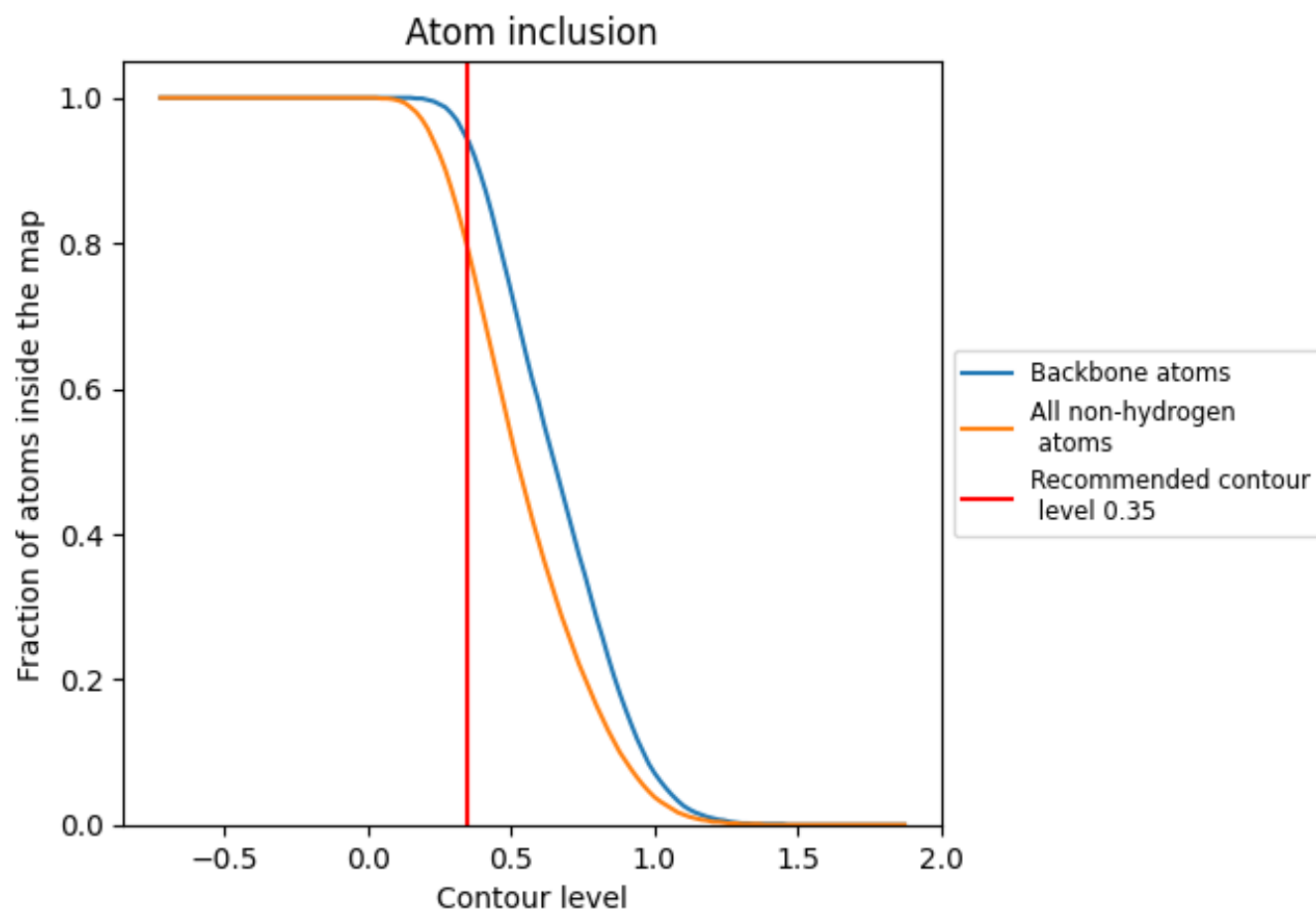
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 79% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7920	 0.4470
0	 0.3930	 0.2990
1	 0.4290	 0.3630
2	 0.2860	 0.3240
3	 0.0360	 0.2560
4	 0.0710	 0.3650
5	 0.3210	 0.3200
6	 0.4620	 0.4190
7	 0.3210	 0.4120
8	 0.1790	 0.1540
9	 0.4640	 0.3840
A	 0.8370	 0.4620
AA	 0.5000	 0.3570
B	 0.8350	 0.4590
BA	 0.1790	 0.3630
C	 0.8430	 0.4650
CA	 0.3570	 0.3320
D	 0.7760	 0.4360
DA	 0.3570	 0.3870
E	 0.7810	 0.4420
EA	 0.2140	 0.2160
F	 0.7920	 0.4430
FA	 0.1430	 0.2540
G	 0.3930	 0.2480
GA	 0.2140	 0.3550
H	 0.1070	 0.2420
HA	 0.3210	 0.3370
I	 0.3570	 0.3830
IA	 0.5380	 0.3600
J	 0.3570	 0.3950
JA	 0.2140	 0.2920
K	 0.6150	 0.4390
KA	 0.2500	 0.3770
L	 0.3570	 0.3360
LA	 0.4640	 0.3880







Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
M	 0.3570	 0.4090
MA	 0.4640	 0.4430
N	 0.6070	 0.4180
NA	 0.0360	 0.2780
O	 0.5710	 0.3940
OA	 0.3570	 0.2800
P	 0.2500	 0.2690
PA	 0.3210	 0.3920
Q	 0.6070	 0.3970
R	 0.5360	 0.4060
S	 0.3930	 0.3960
T	 0.0710	 0.1810
U	 0.3210	 0.3130
V	 0.3210	 0.4130
W	 0.4870	 0.4100
X	 0.2860	 0.2910
Y	 0.3210	 0.3560
Z	 0.4640	 0.3660
a	 0.6430	 0.4010
b	 0.1430	 0.3530
c	 0.4290	 0.3630
d	 0.5710	 0.3960
e	 0.4290	 0.3130
f	 0.0710	 0.3230
g	 0.2860	 0.3340
h	 0.4290	 0.3050
i	 0.5640	 0.3690
j	 0.2500	 0.4110
k	 0.2860	 0.3780
l	 0.6790	 0.4690
m	 0.5000	 0.3750
n	 0.3210	 0.4690
o	 0.6070	 0.3920
p	 0.6070	 0.4630
q	 0.3210	 0.3340
r	 0.1070	 0.2560
s	 0.1430	 0.3310
t	 0.3570	 0.4800
u	 0.5130	 0.4000
v	 0.2500	 0.3640
w	 0.0710	 0.3750
x	 0.5000	 0.3570

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
y	 0.4290	 0.4210
z	 0.0710	 0.2970