



wwPDB EM Validation Summary Report ⓘ

May 14, 2026 – 02:07 PM EDT

PDB ID : 9NBY / pdb_00009nby
EMDB ID : EMD-49238
Title : AMC008 v4.2 SOSIP Env trimer in complex with PGT121, VRC01 and 3BC315 Fabs
Authors : Cui, J.; Du, J.; Lin, Z.; Pallesen, J.
Deposited on : 2025-02-14
Resolution : 3.16 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:

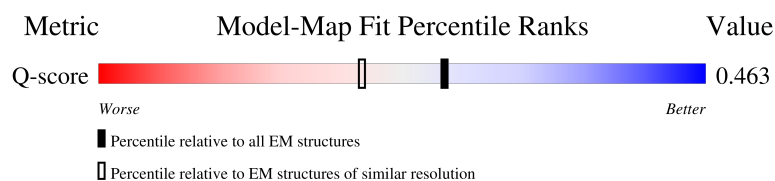
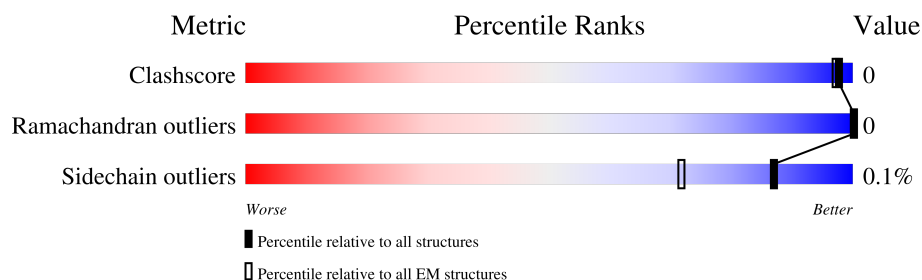
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.16 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14474 (2.66 - 3.66)

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	G	211	
1	K	211	
1	Q	211	
2	H	235	

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Mol	Chain	Length	Quality of chain
2	L	235	
2	R	235	
3	I	224	
3	M	224	
3	P	224	
4	J	210	
4	N	210	
4	O	210	
5	S	232	
6	T	216	
7	A	488	
7	C	488	
7	E	488	
8	B	154	
8	D	154	
8	F	154	
9	0	2	
9	1	2	
9	3	2	
9	4	2	
9	5	2	
9	AA	2	
9	BA	2	
9	CA	2	
9	EA	2	

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Mol	Chain	Length	Quality of chain
9	FA	2	50% 100%
9	GA	2	100%
9	HA	2	100%
9	IA	2	100%
9	JA	2	50% 100% 50%
9	KA	2	100%
9	LA	2	50% 100% 50%
9	MA	2	100%
9	U	2	100%
9	V	2	50% 100% 50%
9	X	2	50% 100%
9	Y	2	50% 50% 50%
9	Z	2	50% 100%
9	a	2	50% 100%
9	d	2	50% 50% 50%
9	g	2	50% 50% 50%
9	h	2	50% 100%
9	i	2	50% 100%
9	j	2	50% 50% 50%
9	k	2	100%
9	l	2	50% 50% 50%
9	m	2	50% 100%
9	p	2	100%
9	q	2	50% 50%
9	s	2	50% 100%

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Mol	Chain	Length	Quality of chain
9	t	2	100%
9	v	2	50% 100%
9	w	2	50% 50% 50%
9	x	2	100% 50% 50%
9	y	2	50% 50% 50%
10	6	3	67% 100%
10	7	3	67% 100%
10	W	3	67% 67% 33%
10	b	3	67% 100%
10	e	3	67% 100%
10	z	3	67% 67% 33%
11	c	6	67% 50% 50%
12	DA	9	44% 78% 22%
12	f	9	44% 89% 11%
12	u	9	44% 78% 22%
13	2	6	67% 50% 50%
13	n	6	33% 83% 17%
14	o	4	75% 75% 25%
15	r	6	67% 50% 33% 17%
16	8	5	80% 80% 20%
17	9	7	71% 100%

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 28589 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 PGT121 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	104	Total	C	N	O	S	0	0
			791	495	137	157	2		
1	K	104	Total	C	N	O	S	0	0
			791	495	137	157	2		
1	Q	104	Total	C	N	O	S	0	0
			791	495	137	157	2		

- Molecule 2 is a protein called PGT121 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	131	Total	C	N	O	S	0	0
			1020	646	174	196	4		
2	L	131	Total	C	N	O	S	0	0
			1020	646	174	196	4		
2	R	131	Total	C	N	O	S	0	0
			1020	646	174	196	4		

- Molecule 3 is a protein called VRC01 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	122	Total	C	N	O	S	0	0
			974	614	176	176	8		
3	M	122	Total	C	N	O	S	0	0
			974	614	176	176	8		
3	P	122	Total	C	N	O	S	0	0
			974	614	176	176	8		

- Molecule 4 is a protein called VRC01 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	99	Total	C	N	O	S	0	0
			766	483	131	150	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	99	Total	C	N	O	S	0	0
			766	483	131	150	2		
4	O	99	Total	C	N	O	S	0	0
			766	483	131	150	2		

- Molecule 5 is a protein called 3BC315 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	128	Total	C	N	O	S	0	0
			1007	643	175	182	7		

- Molecule 6 is a protein called 3BC315 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	109	Total	C	N	O	S	0	0
			808	507	135	163	3		

- Molecule 7 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	454	Total	C	N	O	S	0	0
			3594	2253	627	687	27		
7	A	448	Total	C	N	O	S	0	0
			3540	2220	620	673	27		
7	C	445	Total	C	N	O	S	0	0
			3518	2207	614	670	27		

- Molecule 8 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	143	Total	C	N	O	S	0	0
			1133	714	193	218	8		
8	B	131	Total	C	N	O	S	0	0
			1048	664	176	200	8		
8	D	128	Total	C	N	O	S	0	0
			1026	650	172	196	8		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	514A	THR	ALA	conflict	UNP Q1AII4
F	543	ASN	GLN	conflict	UNP Q1AII4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	559	PRO	ILE	conflict	UNP Q1AII4
F	605	CYS	THR	conflict	UNP Q1AII4
F	607	SER	ALA	conflict	UNP Q1AII4
F	612	THR	ALA	conflict	UNP Q1AII4
F	646	LEU	ILE	conflict	UNP Q1AII4
B	514	THR	ALA	conflict	UNP Q1AII4
B	543	ASN	GLN	conflict	UNP Q1AII4
B	559	PRO	ILE	conflict	UNP Q1AII4
B	605	CYS	THR	conflict	UNP Q1AII4
B	607	SER	ALA	conflict	UNP Q1AII4
B	612	THR	ALA	conflict	UNP Q1AII4
B	646	LEU	ILE	conflict	UNP Q1AII4
D	514	THR	ALA	conflict	UNP Q1AII4
D	543	ASN	GLN	conflict	UNP Q1AII4
D	559	PRO	ILE	conflict	UNP Q1AII4
D	605	CYS	THR	conflict	UNP Q1AII4
D	607	SER	ALA	conflict	UNP Q1AII4
D	612	THR	ALA	conflict	UNP Q1AII4
D	646	LEU	ILE	conflict	UNP Q1AII4

- Molecule 9 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
9	U	2	Total	C	N	O	0	0
			28	16	2	10		
9	V	2	Total	C	N	O	0	0
			28	16	2	10		
9	X	2	Total	C	N	O	0	0
			28	16	2	10		
9	Y	2	Total	C	N	O	0	0
			28	16	2	10		
9	Z	2	Total	C	N	O	0	0
			28	16	2	10		
9	a	2	Total	C	N	O	0	0
			28	16	2	10		
9	d	2	Total	C	N	O	0	0
			28	16	2	10		

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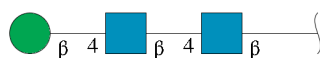
Mol	Chain	Residues	Atoms				AltConf	Trace
9	g	2	Total	C	N	O	0	0
			28	16	2	10		
9	h	2	Total	C	N	O	0	0
			28	16	2	10		
9	i	2	Total	C	N	O	0	0
			28	16	2	10		
9	j	2	Total	C	N	O	0	0
			28	16	2	10		
9	k	2	Total	C	N	O	0	0
			28	16	2	10		
9	l	2	Total	C	N	O	0	0
			28	16	2	10		
9	m	2	Total	C	N	O	0	0
			28	16	2	10		
9	p	2	Total	C	N	O	0	0
			28	16	2	10		
9	q	2	Total	C	N	O	0	0
			28	16	2	10		
9	s	2	Total	C	N	O	0	0
			28	16	2	10		
9	t	2	Total	C	N	O	0	0
			28	16	2	10		
9	v	2	Total	C	N	O	0	0
			28	16	2	10		
9	w	2	Total	C	N	O	0	0
			28	16	2	10		
9	x	2	Total	C	N	O	0	0
			28	16	2	10		
9	y	2	Total	C	N	O	0	0
			28	16	2	10		
9	0	2	Total	C	N	O	0	0
			28	16	2	10		
9	1	2	Total	C	N	O	0	0
			28	16	2	10		
9	3	2	Total	C	N	O	0	0
			28	16	2	10		
9	4	2	Total	C	N	O	0	0
			28	16	2	10		
9	5	2	Total	C	N	O	0	0
			28	16	2	10		
9	AA	2	Total	C	N	O	0	0
			28	16	2	10		

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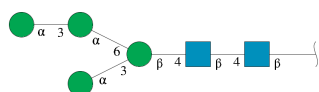
Mol	Chain	Residues	Atoms				AltConf	Trace
9	BA	2	Total	C	N	O	0	0
			28	16	2	10		
9	CA	2	Total	C	N	O	0	0
			28	16	2	10		
9	EA	2	Total	C	N	O	0	0
			28	16	2	10		
9	FA	2	Total	C	N	O	0	0
			28	16	2	10		
9	GA	2	Total	C	N	O	0	0
			28	16	2	10		
9	HA	2	Total	C	N	O	0	0
			28	16	2	10		
9	IA	2	Total	C	N	O	0	0
			28	16	2	10		
9	JA	2	Total	C	N	O	0	0
			28	16	2	10		
9	KA	2	Total	C	N	O	0	0
			28	16	2	10		
9	LA	2	Total	C	N	O	0	0
			28	16	2	10		
9	MA	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 10 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.



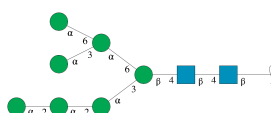
Mol	Chain	Residues	Atoms				AltConf	Trace
10	W	3	Total	C	N	O	0	0
			39	22	2	15		
10	b	3	Total	C	N	O	0	0
			39	22	2	15		
10	e	3	Total	C	N	O	0	0
			39	22	2	15		
10	z	3	Total	C	N	O	0	0
			39	22	2	15		
10	6	3	Total	C	N	O	0	0
			39	22	2	15		
10	7	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



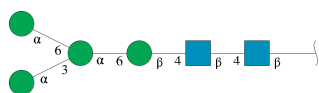
Mol	Chain	Residues	Atoms				AltConf	Trace
11	c	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)]-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



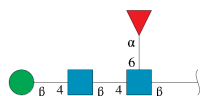
Mol	Chain	Residues	Atoms				AltConf	Trace
12	f	9	Total	C	N	O	0	0
			105	58	2	45		
12	u	9	Total	C	N	O	0	0
			105	58	2	45		
12	DA	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



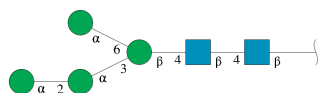
Mol	Chain	Residues	Atoms				AltConf	Trace
13	n	6	Total	C	N	O	0	0
			72	40	2	30		
13	2	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 14 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



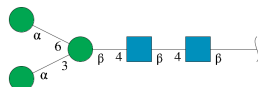
Mol	Chain	Residues	Atoms				AltConf	Trace
14	o	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 15 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



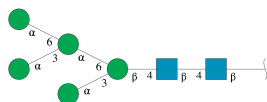
Mol	Chain	Residues	Atoms				AltConf	Trace
15	r	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 16 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



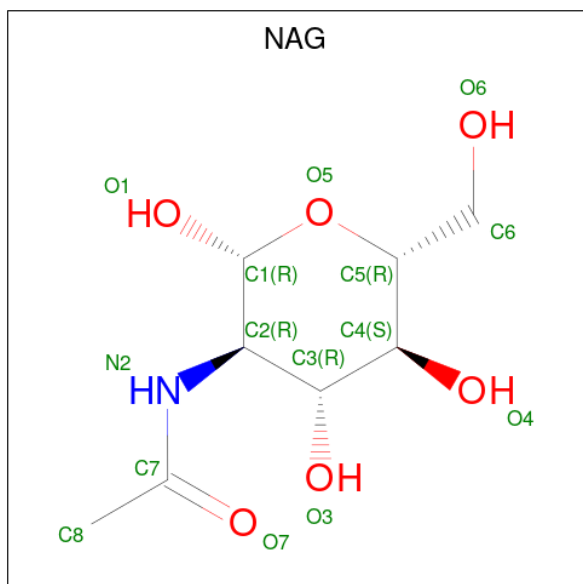
Mol	Chain	Residues	Atoms				AltConf	Trace
16	8	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 17 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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
17	9	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 18 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

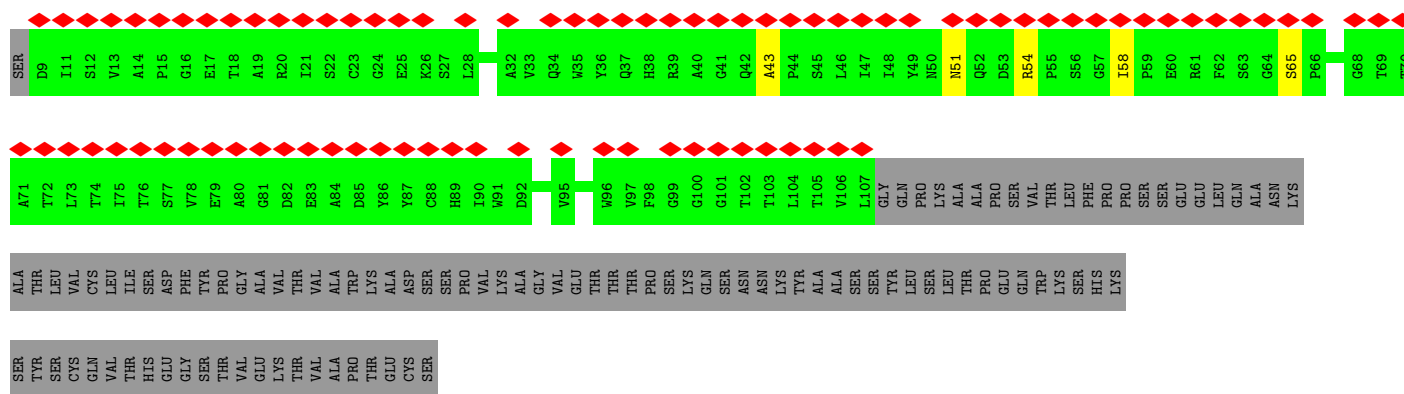


Mol	Chain	Residues	Atoms				AltConf
18	J	1	Total	C	N	O	0
			14	8	1	5	
18	E	1	Total	C	N	O	0
			14	8	1	5	
18	E	1	Total	C	N	O	0
			14	8	1	5	
18	A	1	Total	C	N	O	0
			14	8	1	5	
18	A	1	Total	C	N	O	0
			14	8	1	5	
18	A	1	Total	C	N	O	0
			14	8	1	5	
18	A	1	Total	C	N	O	0
			14	8	1	5	
18	B	1	Total	C	N	O	0
			14	8	1	5	

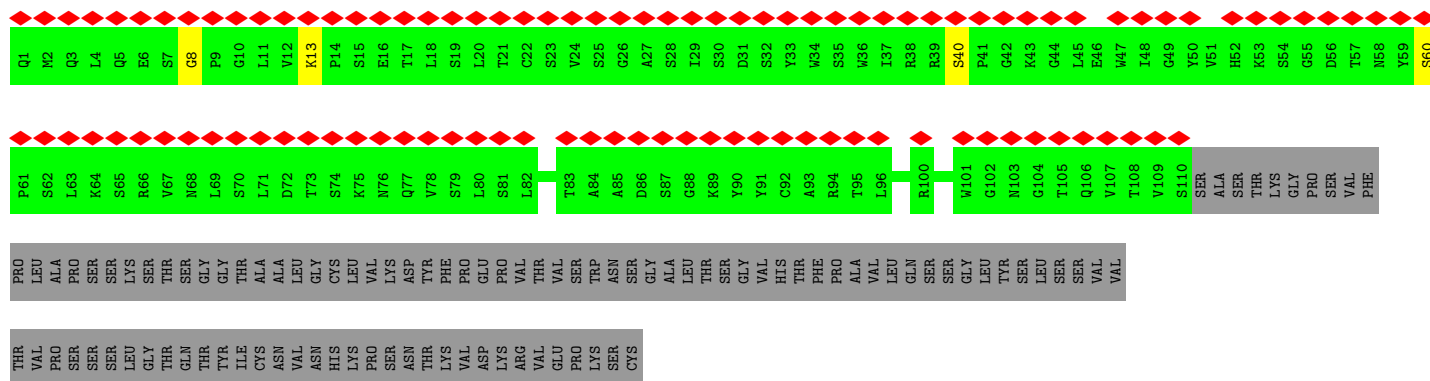
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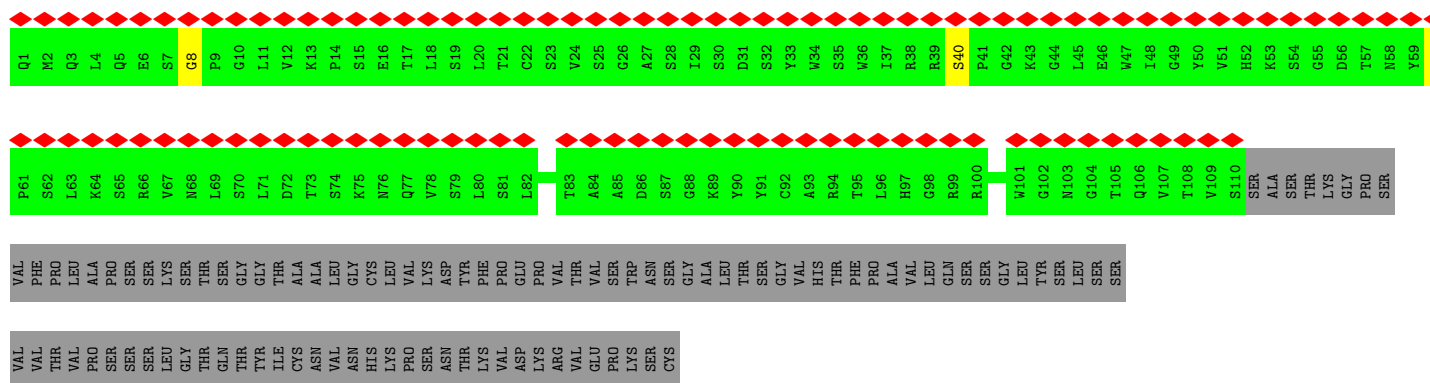
Mol	Chain	Residues	Atoms				AltConf
18	C	1	Total	C	N	O	0
			14	8	1	5	
18	C	1	Total	C	N	O	0
			14	8	1	5	



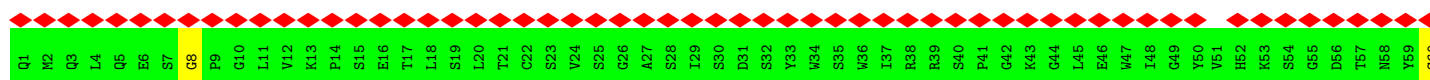
• Molecule 2: PGT121 Fab heavy chain

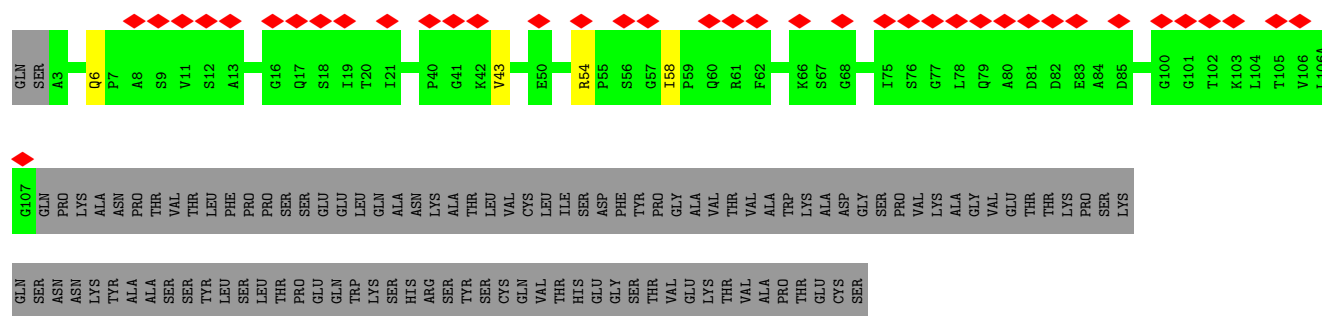


• Molecule 2: PGT121 Fab heavy chain

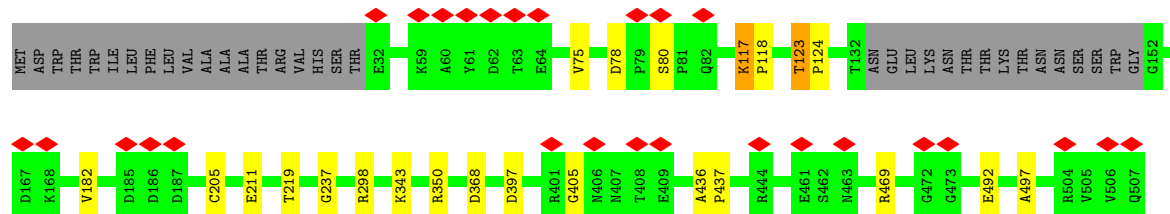
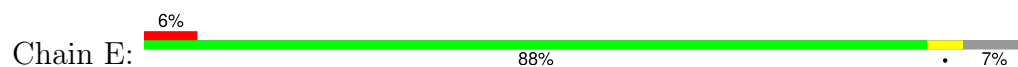


• Molecule 2: PGT121 Fab heavy chain

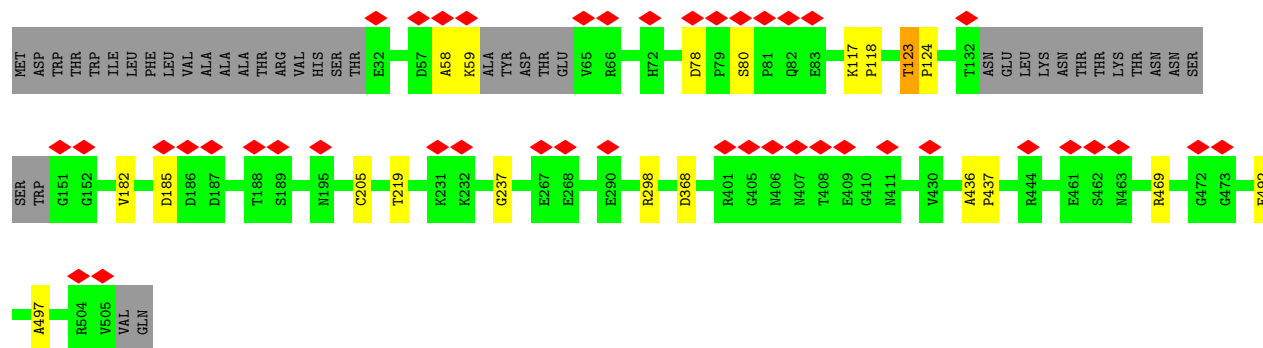
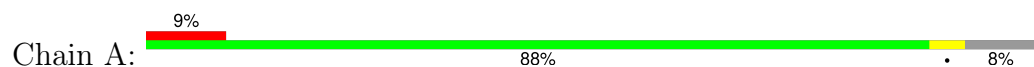




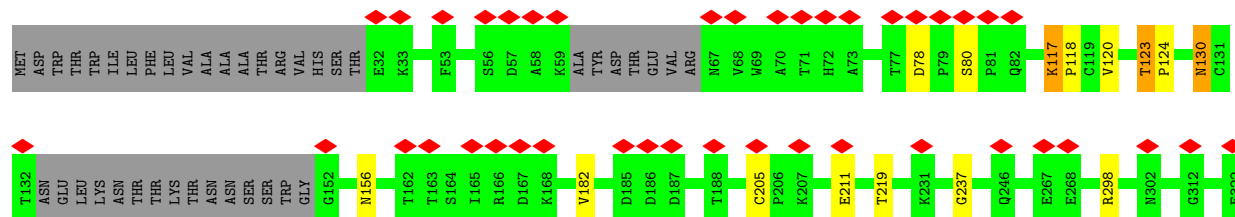
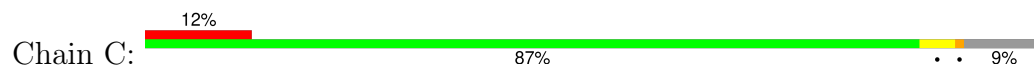
• Molecule 7: Envelope glycoprotein gp120

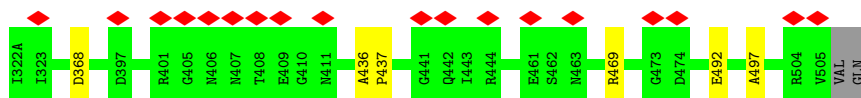


• Molecule 7: Envelope glycoprotein gp120

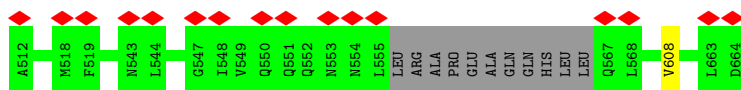


• Molecule 7: Envelope glycoprotein gp120

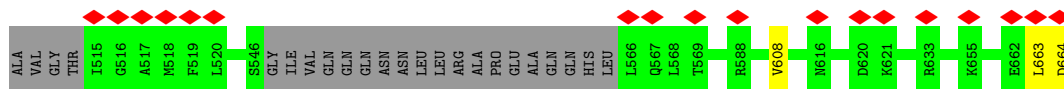
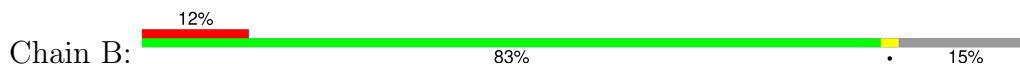




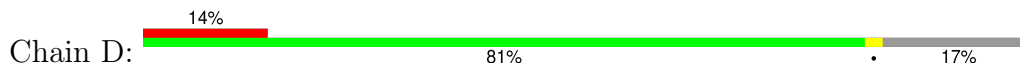
- Molecule 8: Envelope glycoprotein gp41



- Molecule 8: Envelope glycoprotein gp41



- Molecule 8: Envelope glycoprotein gp41



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



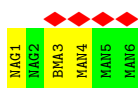
- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



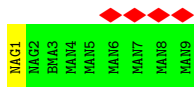
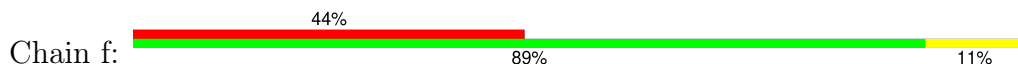
- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



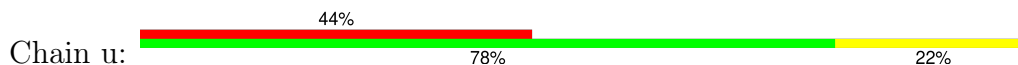
- Molecule 11: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

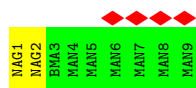


- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

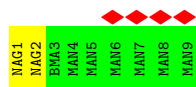
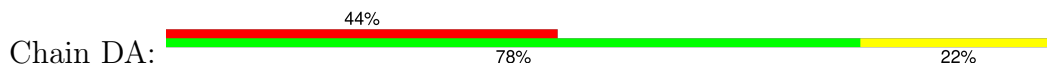


- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

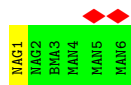
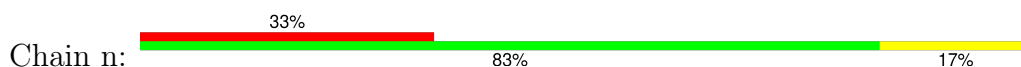




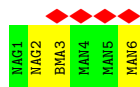
- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

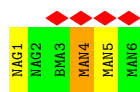


- Molecule 14: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

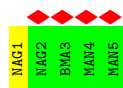
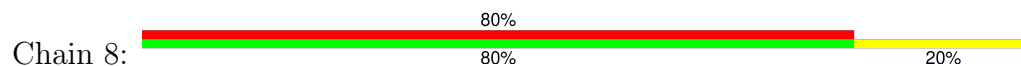


- Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

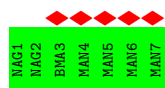




- Molecule 16: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 17: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	117067	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.474	Depositor
Minimum map value	-1.420	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.44	Depositor
Map size (Å)	421.6, 421.6, 421.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.054, 1.054, 1.054	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	G	0.62	0/812	0.95	8/1109 (0.7%)
1	K	0.65	0/812	0.95	8/1109 (0.7%)
1	Q	0.62	0/812	0.97	8/1109 (0.7%)
2	H	0.56	0/1046	0.87	8/1421 (0.6%)
2	L	0.57	0/1046	0.83	6/1421 (0.4%)
2	R	0.58	0/1046	0.84	4/1421 (0.3%)
3	I	0.67	0/1000	0.94	7/1355 (0.5%)
3	M	0.66	0/1000	0.93	4/1355 (0.3%)
3	P	0.68	0/1000	0.92	4/1355 (0.3%)
4	J	0.59	0/786	0.92	6/1069 (0.6%)
4	N	0.61	0/786	0.97	6/1069 (0.6%)
4	O	0.59	0/786	0.94	6/1069 (0.6%)
5	S	0.60	0/1035	0.91	4/1401 (0.3%)
6	T	0.59	0/825	0.99	8/1120 (0.7%)
7	A	0.64	0/3611	0.93	29/4906 (0.6%)
7	C	0.63	0/3589	0.91	33/4877 (0.7%)
7	E	0.65	0/3667	0.93	34/4984 (0.7%)
8	B	0.63	0/1066	0.66	2/1442 (0.1%)
8	D	0.63	0/1044	0.64	2/1412 (0.1%)
8	F	0.65	0/1151	0.65	2/1558 (0.1%)
All	All	0.63	0/26920	0.89	189/36562 (0.5%)

There are no bond length outliers.

The worst 5 of 189 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	436	ALA	CA-C-N	8.22	125.66	119.66
7	E	436	ALA	C-N-CA	8.22	125.66	119.66
4	N	68	GLY	CA-C-N	8.15	127.87	119.56
4	N	68	GLY	C-N-CA	8.15	127.87	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	492	GLU	CA-C-N	8.00	127.64	119.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	791	0	749	0	0
1	K	791	0	749	1	0
1	Q	791	0	749	1	0
2	H	1020	0	989	0	0
2	L	1020	0	989	0	0
2	R	1020	0	989	0	0
3	I	974	0	946	2	0
3	M	974	0	946	2	0
3	P	974	0	946	2	0
4	J	766	0	723	0	0
4	N	766	0	723	0	0
4	O	766	0	723	0	0
5	S	1007	0	970	0	0
6	T	808	0	789	0	0
7	A	3540	0	3465	3	0
7	C	3518	0	3439	4	0
7	E	3594	0	3510	4	0
8	B	1048	0	1032	2	0
8	D	1026	0	1008	1	0
8	F	1133	0	1115	0	0
9	0	28	0	25	0	0
9	1	28	0	25	0	0
9	3	28	0	25	0	0
9	4	28	0	25	0	0
9	5	28	0	25	0	0
9	AA	28	0	25	0	0
9	BA	28	0	25	0	0
9	CA	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	EA	28	0	25	0	0
9	FA	28	0	25	0	0
9	GA	28	0	25	0	0
9	HA	28	0	25	0	0
9	IA	28	0	25	0	0
9	JA	28	0	25	0	0
9	KA	28	0	25	0	0
9	LA	28	0	25	0	0
9	MA	28	0	25	0	0
9	U	28	0	25	0	0
9	V	28	0	25	0	0
9	X	28	0	25	0	0
9	Y	28	0	25	0	0
9	Z	28	0	25	0	0
9	a	28	0	25	0	0
9	d	28	0	25	0	0
9	g	28	0	25	0	0
9	h	28	0	25	0	0
9	i	28	0	25	0	0
9	j	28	0	25	0	0
9	k	28	0	25	0	0
9	l	28	0	25	0	0
9	m	28	0	25	0	0
9	p	28	0	25	0	0
9	q	28	0	25	0	0
9	s	28	0	25	0	0
9	t	28	0	25	0	0
9	v	28	0	25	0	0
9	w	28	0	25	0	0
9	x	28	0	25	0	0
9	y	28	0	25	0	0
10	6	39	0	34	0	0
10	7	39	0	34	0	0
10	W	39	0	34	0	0
10	b	39	0	34	0	0
10	e	39	0	34	0	0
10	z	39	0	34	0	0
11	c	72	0	61	1	0
12	DA	105	0	88	0	0
12	f	105	0	88	0	0
12	u	105	0	88	0	0
13	2	72	0	61	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	n	72	0	61	0	0
14	o	49	0	43	0	0
15	r	72	0	61	1	0
16	8	61	0	52	0	0
17	9	83	0	70	0	0
18	A	56	0	52	0	0
18	B	14	0	13	0	0
18	C	28	0	26	0	0
18	E	28	0	26	0	0
18	J	14	0	13	0	0
All	All	28589	0	27531	25	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

The worst 5 of 25 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:3:BMA:H61	13:2:6:MAN:H61	1.64	0.80
7:A:58:ALA:O	7:A:59:LYS:C	2.52	0.53
7:C:130:ASN:OD1	7:C:130:ASN:C	2.55	0.49
1:K:51:ASN:N	1:K:51:ASN:OD1	2.46	0.48
11:c:3:BMA:H4	11:c:4:MAN:H5	1.96	0.48

There are no symmetry-related clashes.

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	G	102/211 (48%)	100 (98%)	2 (2%)	0	100	100
1	K	102/211 (48%)	100 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	102/211 (48%)	101 (99%)	1 (1%)	0	100	100
2	H	129/235 (55%)	128 (99%)	1 (1%)	0	100	100
2	L	129/235 (55%)	127 (98%)	2 (2%)	0	100	100
2	R	129/235 (55%)	128 (99%)	1 (1%)	0	100	100
3	I	120/224 (54%)	120 (100%)	0	0	100	100
3	M	120/224 (54%)	120 (100%)	0	0	100	100
3	P	120/224 (54%)	120 (100%)	0	0	100	100
4	J	97/210 (46%)	95 (98%)	2 (2%)	0	100	100
4	N	97/210 (46%)	95 (98%)	2 (2%)	0	100	100
4	O	97/210 (46%)	95 (98%)	2 (2%)	0	100	100
5	S	126/232 (54%)	126 (100%)	0	0	100	100
6	T	107/216 (50%)	105 (98%)	2 (2%)	0	100	100
7	A	442/488 (91%)	436 (99%)	6 (1%)	0	100	100
7	C	439/488 (90%)	433 (99%)	6 (1%)	0	100	100
7	E	450/488 (92%)	446 (99%)	4 (1%)	0	100	100
8	B	127/154 (82%)	125 (98%)	2 (2%)	0	100	100
8	D	124/154 (80%)	122 (98%)	2 (2%)	0	100	100
8	F	139/154 (90%)	139 (100%)	0	0	100	100
All	All	3298/5014 (66%)	3261 (99%)	37 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	85/177 (48%)	85 (100%)	0	100	100
1	K	85/177 (48%)	84 (99%)	1 (1%)	63	74
1	Q	85/177 (48%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	112/202 (55%)	112 (100%)	0	100	100
2	L	112/202 (55%)	112 (100%)	0	100	100
2	R	112/202 (55%)	112 (100%)	0	100	100
3	I	104/193 (54%)	104 (100%)	0	100	100
3	M	104/193 (54%)	104 (100%)	0	100	100
3	P	104/193 (54%)	104 (100%)	0	100	100
4	J	82/182 (45%)	82 (100%)	0	100	100
4	N	82/182 (45%)	82 (100%)	0	100	100
4	O	82/182 (45%)	82 (100%)	0	100	100
5	S	106/196 (54%)	106 (100%)	0	100	100
6	T	89/182 (49%)	89 (100%)	0	100	100
7	A	405/441 (92%)	405 (100%)	0	100	100
7	C	403/441 (91%)	402 (100%)	1 (0%)	87	87
7	E	411/441 (93%)	411 (100%)	0	100	100
8	B	114/132 (86%)	114 (100%)	0	100	100
8	D	112/132 (85%)	112 (100%)	0	100	100
8	F	123/132 (93%)	123 (100%)	0	100	100
All	All	2912/4359 (67%)	2910 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	51	ASN
7	C	130	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
7	E	190	ASN
7	C	337	GLN
8	F	540	GLN
8	B	591	GLN
7	E	422	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

163 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	$\# Z > 2$
9	NAG	0	1	9,7	14,14,15	0.38	0	17,19,21	0.65	0
9	NAG	0	2	9	14,14,15	0.41	0	17,19,21	0.42	0
9	NAG	1	1	9,7	14,14,15	0.39	0	17,19,21	0.80	0
9	NAG	1	2	9	14,14,15	0.39	0	17,19,21	0.56	0
13	NAG	2	1	7,13	14,14,15	0.41	0	17,19,21	0.84	0
13	NAG	2	2	13	14,14,15	0.38	0	17,19,21	0.81	1 (5%)
13	BMA	2	3	13	11,11,12	0.40	0	15,15,17	0.53	0
13	MAN	2	4	13	11,11,12	0.40	0	15,15,17	0.62	0
13	MAN	2	5	13	11,11,12	0.30	0	15,15,17	0.51	0
13	MAN	2	6	13	11,11,12	0.36	0	15,15,17	0.59	0
9	NAG	3	1	9,7	14,14,15	0.38	0	17,19,21	1.83	2 (11%)
9	NAG	3	2	9	14,14,15	0.37	0	17,19,21	0.76	1 (5%)
9	NAG	4	1	9,7	14,14,15	0.38	0	17,19,21	0.86	0
9	NAG	4	2	9	14,14,15	0.39	0	17,19,21	0.63	0
9	NAG	5	1	9,7	14,14,15	0.37	0	17,19,21	0.85	1 (5%)
9	NAG	5	2	9	14,14,15	0.35	0	17,19,21	0.59	0
10	NAG	6	1	7,10	14,14,15	0.37	0	17,19,21	0.87	0
10	NAG	6	2	10	14,14,15	0.39	0	17,19,21	0.56	0
10	BMA	6	3	10	11,11,12	0.22	0	15,15,17	0.56	0
10	NAG	7	1	7,10	14,14,15	0.41	0	17,19,21	0.65	0
10	NAG	7	2	10	14,14,15	0.36	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BMA	7	3	10	11,11,12	0.25	0	15,15,17	0.55	0
16	NAG	8	1	7,16	14,14,15	0.40	0	17,19,21	0.64	1 (5%)
16	NAG	8	2	16	14,14,15	0.40	0	17,19,21	0.58	0
16	BMA	8	3	16	11,11,12	0.47	0	15,15,17	0.88	0
16	MAN	8	4	16	11,11,12	0.31	0	15,15,17	0.53	0
16	MAN	8	5	16	11,11,12	0.29	0	15,15,17	0.51	0
17	NAG	9	1	7,17	14,14,15	0.37	0	17,19,21	0.77	0
17	NAG	9	2	17	14,14,15	0.37	0	17,19,21	0.54	0
17	BMA	9	3	17	11,11,12	0.27	0	15,15,17	0.58	0
17	MAN	9	4	17	11,11,12	0.42	0	15,15,17	0.64	0
17	MAN	9	5	17	11,11,12	0.34	0	15,15,17	0.60	0
17	MAN	9	6	17	11,11,12	0.32	0	15,15,17	0.50	0
17	MAN	9	7	17	11,11,12	0.30	0	15,15,17	0.60	0
9	NAG	AA	1	9,7	14,14,15	0.35	0	17,19,21	0.84	1 (5%)
9	NAG	AA	2	9	14,14,15	0.39	0	17,19,21	0.50	0
9	NAG	BA	1	9,7	14,14,15	0.39	0	17,19,21	0.78	1 (5%)
9	NAG	BA	2	9	14,14,15	0.38	0	17,19,21	0.68	0
9	NAG	CA	1	9,7	14,14,15	0.38	0	17,19,21	0.57	0
9	NAG	CA	2	9	14,14,15	0.38	0	17,19,21	0.47	0
12	NAG	DA	1	12,7	14,14,15	0.41	0	17,19,21	0.81	1 (5%)
12	NAG	DA	2	12	14,14,15	0.40	0	17,19,21	0.89	2 (11%)
12	BMA	DA	3	12	11,11,12	0.65	0	15,15,17	0.62	0
12	MAN	DA	4	12	11,11,12	0.53	0	15,15,17	0.57	0
12	MAN	DA	5	12	11,11,12	0.42	0	15,15,17	0.59	0
12	MAN	DA	6	12	11,11,12	0.35	0	15,15,17	0.55	0
12	MAN	DA	7	12	11,11,12	0.28	0	15,15,17	0.56	0
12	MAN	DA	8	12	11,11,12	0.27	0	15,15,17	0.51	0
12	MAN	DA	9	12	11,11,12	0.33	0	15,15,17	0.58	0
9	NAG	EA	1	9,7	14,14,15	0.39	0	17,19,21	0.71	0
9	NAG	EA	2	9	14,14,15	0.37	0	17,19,21	0.53	0
9	NAG	FA	1	9,7	14,14,15	0.38	0	17,19,21	0.63	0
9	NAG	FA	2	9	14,14,15	0.39	0	17,19,21	0.74	0
9	NAG	GA	1	9,7	14,14,15	0.40	0	17,19,21	0.72	0
9	NAG	GA	2	9	14,14,15	0.38	0	17,19,21	0.47	0
9	NAG	HA	1	9,7	14,14,15	0.40	0	17,19,21	0.48	0
9	NAG	HA	2	9	14,14,15	0.39	0	17,19,21	0.50	0
9	NAG	IA	1	9,7	14,14,15	0.37	0	17,19,21	1.15	2 (11%)
9	NAG	IA	2	9	14,14,15	0.39	0	17,19,21	0.63	0
9	NAG	JA	1	9,7	14,14,15	0.39	0	17,19,21	1.09	1 (5%)
9	NAG	JA	2	9	14,14,15	0.38	0	17,19,21	0.87	1 (5%)
9	NAG	KA	1	9,7	14,14,15	0.41	0	17,19,21	1.16	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	KA	2	9	14,14,15	0.39	0	17,19,21	0.44	0
9	NAG	LA	1	9,7	14,14,15	0.39	0	17,19,21	0.50	0
9	NAG	LA	2	9	14,14,15	0.41	0	17,19,21	0.90	1 (5%)
9	NAG	MA	1	9,8	14,14,15	0.38	0	17,19,21	0.69	0
9	NAG	MA	2	9	14,14,15	0.37	0	17,19,21	0.48	0
9	NAG	U	1	4,9	14,14,15	0.41	0	17,19,21	0.96	2 (11%)
9	NAG	U	2	9	14,14,15	0.39	0	17,19,21	0.56	0
9	NAG	V	1	4,9	14,14,15	0.39	0	17,19,21	0.73	1 (5%)
9	NAG	V	2	9	14,14,15	0.38	0	17,19,21	0.41	0
10	NAG	W	1	7,10	14,14,15	0.40	0	17,19,21	0.68	1 (5%)
10	NAG	W	2	10	14,14,15	0.40	0	17,19,21	0.60	0
10	BMA	W	3	10	11,11,12	0.31	0	15,15,17	0.47	0
9	NAG	X	1	9,7	14,14,15	0.42	0	17,19,21	0.60	0
9	NAG	X	2	9	14,14,15	0.37	0	17,19,21	0.48	0
9	NAG	Y	1	9,7	14,14,15	0.41	0	17,19,21	0.82	1 (5%)
9	NAG	Y	2	9	14,14,15	0.39	0	17,19,21	0.55	0
9	NAG	Z	1	9,7	14,14,15	0.36	0	17,19,21	1.19	2 (11%)
9	NAG	Z	2	9	14,14,15	0.38	0	17,19,21	0.87	1 (5%)
9	NAG	a	1	9,7	14,14,15	0.42	0	17,19,21	0.89	0
9	NAG	a	2	9	14,14,15	0.38	0	17,19,21	0.61	0
10	NAG	b	1	7,10	14,14,15	0.40	0	17,19,21	0.88	0
10	NAG	b	2	10	14,14,15	0.40	0	17,19,21	0.59	0
10	BMA	b	3	10	11,11,12	0.42	0	15,15,17	0.51	0
11	NAG	c	1	7,11	14,14,15	0.43	0	17,19,21	0.74	1 (5%)
11	NAG	c	2	11	14,14,15	0.38	0	17,19,21	0.65	0
11	BMA	c	3	11	11,11,12	0.39	0	15,15,17	0.82	0
11	MAN	c	4	11	11,11,12	0.37	0	15,15,17	0.64	0
11	MAN	c	5	11	11,11,12	0.41	0	15,15,17	0.47	0
11	MAN	c	6	11	11,11,12	0.48	0	15,15,17	0.61	0
9	NAG	d	1	9,7	14,14,15	0.38	0	17,19,21	0.92	1 (5%)
9	NAG	d	2	9	14,14,15	0.38	0	17,19,21	0.52	0
10	NAG	e	1	7,10	14,14,15	0.42	0	17,19,21	0.72	0
10	NAG	e	2	10	14,14,15	0.39	0	17,19,21	0.62	0
10	BMA	e	3	10	11,11,12	0.31	0	15,15,17	0.56	0
12	NAG	f	1	12,7	14,14,15	0.43	0	17,19,21	0.99	1 (5%)
12	NAG	f	2	12	14,14,15	0.43	0	17,19,21	0.67	0
12	BMA	f	3	12	11,11,12	0.62	0	15,15,17	0.60	0
12	MAN	f	4	12	11,11,12	0.49	0	15,15,17	0.58	0
12	MAN	f	5	12	11,11,12	0.66	0	15,15,17	0.67	0
12	MAN	f	6	12	11,11,12	0.38	0	15,15,17	0.55	0
12	MAN	f	7	12	11,11,12	0.45	0	15,15,17	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MAN	f	8	12	11,11,12	0.37	0	15,15,17	0.48	0
12	MAN	f	9	12	11,11,12	0.33	0	15,15,17	0.51	0
9	NAG	g	1	9,7	14,14,15	0.37	0	17,19,21	0.79	1 (5%)
9	NAG	g	2	9	14,14,15	0.38	0	17,19,21	0.60	0
9	NAG	h	1	9,7	14,14,15	0.39	0	17,19,21	0.87	0
9	NAG	h	2	9	14,14,15	0.37	0	17,19,21	0.43	0
9	NAG	i	1	9,7	14,14,15	0.41	0	17,19,21	0.61	0
9	NAG	i	2	9	14,14,15	0.37	0	17,19,21	0.59	0
9	NAG	j	1	9,7	14,14,15	0.39	0	17,19,21	0.94	1 (5%)
9	NAG	j	2	9	14,14,15	0.39	0	17,19,21	0.47	0
9	NAG	k	1	9,7	14,14,15	0.41	0	17,19,21	0.67	0
9	NAG	k	2	9	14,14,15	0.39	0	17,19,21	0.48	0
9	NAG	l	1	9,7	14,14,15	0.40	0	17,19,21	2.10	2 (11%)
9	NAG	l	2	9	14,14,15	0.41	0	17,19,21	0.67	0
9	NAG	m	1	9,7	14,14,15	0.40	0	17,19,21	0.67	0
9	NAG	m	2	9	14,14,15	0.38	0	17,19,21	0.60	0
13	NAG	n	1	7,13	14,14,15	0.41	0	17,19,21	0.87	1 (5%)
13	NAG	n	2	13	14,14,15	0.40	0	17,19,21	0.70	0
13	BMA	n	3	13	11,11,12	0.37	0	15,15,17	0.55	0
13	MAN	n	4	13	11,11,12	0.47	0	15,15,17	0.60	0
13	MAN	n	5	13	11,11,12	0.37	0	15,15,17	0.52	0
13	MAN	n	6	13	11,11,12	0.37	0	15,15,17	0.51	0
14	NAG	o	1	14,8	14,14,15	0.40	0	17,19,21	0.68	1 (5%)
14	NAG	o	2	14	14,14,15	0.37	0	17,19,21	0.67	0
14	BMA	o	3	14	11,11,12	0.31	0	15,15,17	0.51	0
14	FUC	o	4	14	10,10,11	0.49	0	14,14,16	0.37	0
9	NAG	p	1	9,7	14,14,15	0.37	0	17,19,21	0.94	1 (5%)
9	NAG	p	2	9	14,14,15	0.38	0	17,19,21	0.40	0
9	NAG	q	1	9,7	14,14,15	0.40	0	17,19,21	0.59	0
9	NAG	q	2	9	14,14,15	0.40	0	17,19,21	0.58	0
15	NAG	r	1	7,15	14,14,15	0.42	0	17,19,21	0.76	1 (5%)
15	NAG	r	2	15	14,14,15	0.42	0	17,19,21	0.66	0
15	BMA	r	3	15	11,11,12	0.52	0	15,15,17	0.57	0
15	MAN	r	4	15	11,11,12	0.27	0	15,15,17	0.77	1 (6%)
15	MAN	r	5	15	11,11,12	0.19	0	15,15,17	0.68	0
15	MAN	r	6	15	11,11,12	0.33	0	15,15,17	0.54	0
9	NAG	s	1	9,7	14,14,15	0.39	0	17,19,21	0.87	0
9	NAG	s	2	9	14,14,15	0.38	0	17,19,21	0.50	0
9	NAG	t	1	9,7	14,14,15	0.39	0	17,19,21	0.69	0
9	NAG	t	2	9	14,14,15	0.39	0	17,19,21	0.53	0
12	NAG	u	1	12,7	14,14,15	0.41	0	17,19,21	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	u	2	12	14,14,15	0.39	0	17,19,21	0.82	1 (5%)
12	BMA	u	3	12	11,11,12	0.60	0	15,15,17	0.61	0
12	MAN	u	4	12	11,11,12	0.63	0	15,15,17	0.70	0
12	MAN	u	5	12	11,11,12	0.35	0	15,15,17	0.48	0
12	MAN	u	6	12	11,11,12	0.39	0	15,15,17	0.57	0
12	MAN	u	7	12	11,11,12	0.35	0	15,15,17	0.62	0
12	MAN	u	8	12	11,11,12	0.35	0	15,15,17	0.45	0
12	MAN	u	9	12	11,11,12	0.32	0	15,15,17	0.52	0
9	NAG	v	1	9,7	14,14,15	0.37	0	17,19,21	0.73	0
9	NAG	v	2	9	14,14,15	0.35	0	17,19,21	0.54	0
9	NAG	w	1	9,7	14,14,15	0.40	0	17,19,21	0.69	0
9	NAG	w	2	9	14,14,15	0.38	0	17,19,21	0.73	1 (5%)
9	NAG	x	1	9,7	14,14,15	0.39	0	17,19,21	0.87	1 (5%)
9	NAG	x	2	9	14,14,15	0.38	0	17,19,21	0.45	0
9	NAG	y	1	9,7	14,14,15	0.39	0	17,19,21	1.22	2 (11%)
9	NAG	y	2	9	14,14,15	0.38	0	17,19,21	0.65	0
10	NAG	z	1	7,10	14,14,15	0.38	0	17,19,21	0.80	1 (5%)
10	NAG	z	2	10	14,14,15	0.39	0	17,19,21	0.50	0
10	BMA	z	3	10	11,11,12	0.37	0	15,15,17	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
9	NAG	0	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	0	2	9	-	0/6/23/26	0/1/1/1
9	NAG	1	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	1	2	9	-	1/6/23/26	0/1/1/1
13	NAG	2	1	7,13	-	0/6/23/26	0/1/1/1
13	NAG	2	2	13	-	0/6/23/26	0/1/1/1
13	BMA	2	3	13	-	0/2/19/22	0/1/1/1
13	MAN	2	4	13	-	0/2/19/22	0/1/1/1
13	MAN	2	5	13	-	1/2/19/22	0/1/1/1
13	MAN	2	6	13	-	1/2/19/22	0/1/1/1
9	NAG	3	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	3	2	9	-	1/6/23/26	0/1/1/1
9	NAG	4	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	4	2	9	-	1/6/23/26	0/1/1/1
9	NAG	5	1	9,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	5	2	9	-	1/6/23/26	0/1/1/1
10	NAG	6	1	7,10	-	0/6/23/26	0/1/1/1
10	NAG	6	2	10	-	0/6/23/26	0/1/1/1
10	BMA	6	3	10	-	0/2/19/22	0/1/1/1
10	NAG	7	1	7,10	-	0/6/23/26	0/1/1/1
10	NAG	7	2	10	-	0/6/23/26	0/1/1/1
10	BMA	7	3	10	-	0/2/19/22	0/1/1/1
16	NAG	8	1	7,16	-	0/6/23/26	0/1/1/1
16	NAG	8	2	16	-	0/6/23/26	0/1/1/1
16	BMA	8	3	16	-	0/2/19/22	0/1/1/1
16	MAN	8	4	16	-	1/2/19/22	0/1/1/1
16	MAN	8	5	16	-	0/2/19/22	0/1/1/1
17	NAG	9	1	7,17	-	0/6/23/26	0/1/1/1
17	NAG	9	2	17	-	0/6/23/26	0/1/1/1
17	BMA	9	3	17	-	0/2/19/22	0/1/1/1
17	MAN	9	4	17	-	0/2/19/22	0/1/1/1
17	MAN	9	5	17	-	0/2/19/22	0/1/1/1
17	MAN	9	6	17	-	0/2/19/22	0/1/1/1
17	MAN	9	7	17	-	1/2/19/22	0/1/1/1
9	NAG	AA	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	AA	2	9	-	0/6/23/26	0/1/1/1
9	NAG	BA	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	BA	2	9	-	1/6/23/26	0/1/1/1
9	NAG	CA	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	CA	2	9	-	1/6/23/26	0/1/1/1
12	NAG	DA	1	12,7	-	0/6/23/26	0/1/1/1
12	NAG	DA	2	12	-	0/6/23/26	0/1/1/1
12	BMA	DA	3	12	-	0/2/19/22	0/1/1/1
12	MAN	DA	4	12	-	0/2/19/22	0/1/1/1
12	MAN	DA	5	12	-	1/2/19/22	0/1/1/1
12	MAN	DA	6	12	-	1/2/19/22	0/1/1/1
12	MAN	DA	7	12	-	0/2/19/22	0/1/1/1
12	MAN	DA	8	12	-	1/2/19/22	0/1/1/1
12	MAN	DA	9	12	-	1/2/19/22	0/1/1/1
9	NAG	EA	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	EA	2	9	-	0/6/23/26	0/1/1/1
9	NAG	FA	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	FA	2	9	-	1/6/23/26	0/1/1/1
9	NAG	GA	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	GA	2	9	-	1/6/23/26	0/1/1/1
9	NAG	HA	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	HA	2	9	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	IA	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	IA	2	9	-	0/6/23/26	0/1/1/1
9	NAG	JA	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	JA	2	9	-	0/6/23/26	0/1/1/1
9	NAG	KA	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	KA	2	9	-	1/6/23/26	0/1/1/1
9	NAG	LA	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	LA	2	9	-	0/6/23/26	0/1/1/1
9	NAG	MA	1	9,8	-	0/6/23/26	0/1/1/1
9	NAG	MA	2	9	-	0/6/23/26	0/1/1/1
9	NAG	U	1	4,9	-	0/6/23/26	0/1/1/1
9	NAG	U	2	9	-	1/6/23/26	0/1/1/1
9	NAG	V	1	4,9	-	0/6/23/26	0/1/1/1
9	NAG	V	2	9	-	0/6/23/26	0/1/1/1
10	NAG	W	1	7,10	-	0/6/23/26	0/1/1/1
10	NAG	W	2	10	-	0/6/23/26	0/1/1/1
10	BMA	W	3	10	-	0/2/19/22	0/1/1/1
9	NAG	X	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	X	2	9	-	1/6/23/26	0/1/1/1
9	NAG	Y	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	0/6/23/26	0/1/1/1
9	NAG	Z	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	0/6/23/26	0/1/1/1
9	NAG	a	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	a	2	9	-	0/6/23/26	0/1/1/1
10	NAG	b	1	7,10	-	1/6/23/26	0/1/1/1
10	NAG	b	2	10	-	0/6/23/26	0/1/1/1
10	BMA	b	3	10	-	1/2/19/22	0/1/1/1
11	NAG	c	1	7,11	-	0/6/23/26	0/1/1/1
11	NAG	c	2	11	-	0/6/23/26	0/1/1/1
11	BMA	c	3	11	-	0/2/19/22	0/1/1/1
11	MAN	c	4	11	-	0/2/19/22	0/1/1/1
11	MAN	c	5	11	-	0/2/19/22	0/1/1/1
11	MAN	c	6	11	-	1/2/19/22	0/1/1/1
9	NAG	d	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	d	2	9	-	0/6/23/26	0/1/1/1
10	NAG	e	1	7,10	-	0/6/23/26	0/1/1/1
10	NAG	e	2	10	-	0/6/23/26	0/1/1/1
10	BMA	e	3	10	-	1/2/19/22	0/1/1/1
12	NAG	f	1	12,7	-	0/6/23/26	0/1/1/1
12	NAG	f	2	12	-	1/6/23/26	0/1/1/1
12	BMA	f	3	12	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	f	4	12	-	1/2/19/22	0/1/1/1
12	MAN	f	5	12	-	0/2/19/22	0/1/1/1
12	MAN	f	6	12	-	0/2/19/22	0/1/1/1
12	MAN	f	7	12	-	0/2/19/22	0/1/1/1
12	MAN	f	8	12	-	0/2/19/22	0/1/1/1
12	MAN	f	9	12	-	0/2/19/22	0/1/1/1
9	NAG	g	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	g	2	9	-	0/6/23/26	0/1/1/1
9	NAG	h	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	h	2	9	-	0/6/23/26	0/1/1/1
9	NAG	i	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	i	2	9	-	0/6/23/26	0/1/1/1
9	NAG	j	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	j	2	9	-	0/6/23/26	0/1/1/1
9	NAG	k	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	k	2	9	-	1/6/23/26	0/1/1/1
9	NAG	l	1	9,7	-	1/6/23/26	0/1/1/1
9	NAG	l	2	9	-	1/6/23/26	0/1/1/1
9	NAG	m	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	m	2	9	-	1/6/23/26	0/1/1/1
13	NAG	n	1	7,13	-	0/6/23/26	0/1/1/1
13	NAG	n	2	13	-	0/6/23/26	0/1/1/1
13	BMA	n	3	13	-	0/2/19/22	0/1/1/1
13	MAN	n	4	13	-	0/2/19/22	0/1/1/1
13	MAN	n	5	13	-	1/2/19/22	0/1/1/1
13	MAN	n	6	13	-	0/2/19/22	0/1/1/1
14	NAG	o	1	14,8	-	0/6/23/26	0/1/1/1
14	NAG	o	2	14	-	0/6/23/26	0/1/1/1
14	BMA	o	3	14	-	0/2/19/22	0/1/1/1
14	FUC	o	4	14	-	-	0/1/1/1
9	NAG	p	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	p	2	9	-	0/6/23/26	0/1/1/1
9	NAG	q	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	q	2	9	-	1/6/23/26	0/1/1/1
15	NAG	r	1	7,15	-	0/6/23/26	0/1/1/1
15	NAG	r	2	15	-	0/6/23/26	0/1/1/1
15	BMA	r	3	15	-	0/2/19/22	0/1/1/1
15	MAN	r	4	15	-	1/2/19/22	0/1/1/1
15	MAN	r	5	15	-	0/2/19/22	0/1/1/1
15	MAN	r	6	15	-	0/2/19/22	0/1/1/1
9	NAG	s	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	s	2	9	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	t	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	t	2	9	-	0/6/23/26	0/1/1/1
12	NAG	u	1	12,7	-	0/6/23/26	0/1/1/1
12	NAG	u	2	12	-	0/6/23/26	0/1/1/1
12	BMA	u	3	12	-	0/2/19/22	0/1/1/1
12	MAN	u	4	12	-	1/2/19/22	0/1/1/1
12	MAN	u	5	12	-	1/2/19/22	0/1/1/1
12	MAN	u	6	12	-	1/2/19/22	0/1/1/1
12	MAN	u	7	12	-	0/2/19/22	0/1/1/1
12	MAN	u	8	12	-	1/2/19/22	0/1/1/1
12	MAN	u	9	12	-	0/2/19/22	0/1/1/1
9	NAG	v	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	v	2	9	-	0/6/23/26	0/1/1/1
9	NAG	w	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	w	2	9	-	0/6/23/26	0/1/1/1
9	NAG	x	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	x	2	9	-	0/6/23/26	0/1/1/1
9	NAG	y	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	y	2	9	-	0/6/23/26	0/1/1/1
10	NAG	z	1	7,10	-	0/6/23/26	0/1/1/1
10	NAG	z	2	10	-	0/6/23/26	0/1/1/1
10	BMA	z	3	10	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	3	1	NAG	C2-N2-C7	6.51	131.63	122.90
9	l	1	NAG	C2-N2-C7	6.43	131.52	122.90
9	l	1	NAG	C1-C2-N2	-4.95	102.63	110.43
9	Z	1	NAG	C2-N2-C7	3.61	127.73	122.90
9	LA	2	NAG	C1-C2-N2	3.30	115.63	110.43

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	l	1	NAG	C3-C2-N2-C7
9	q	2	NAG	O5-C5-C6-O6
12	DA	9	MAN	O5-C5-C6-O6
16	8	4	MAN	O5-C5-C6-O6

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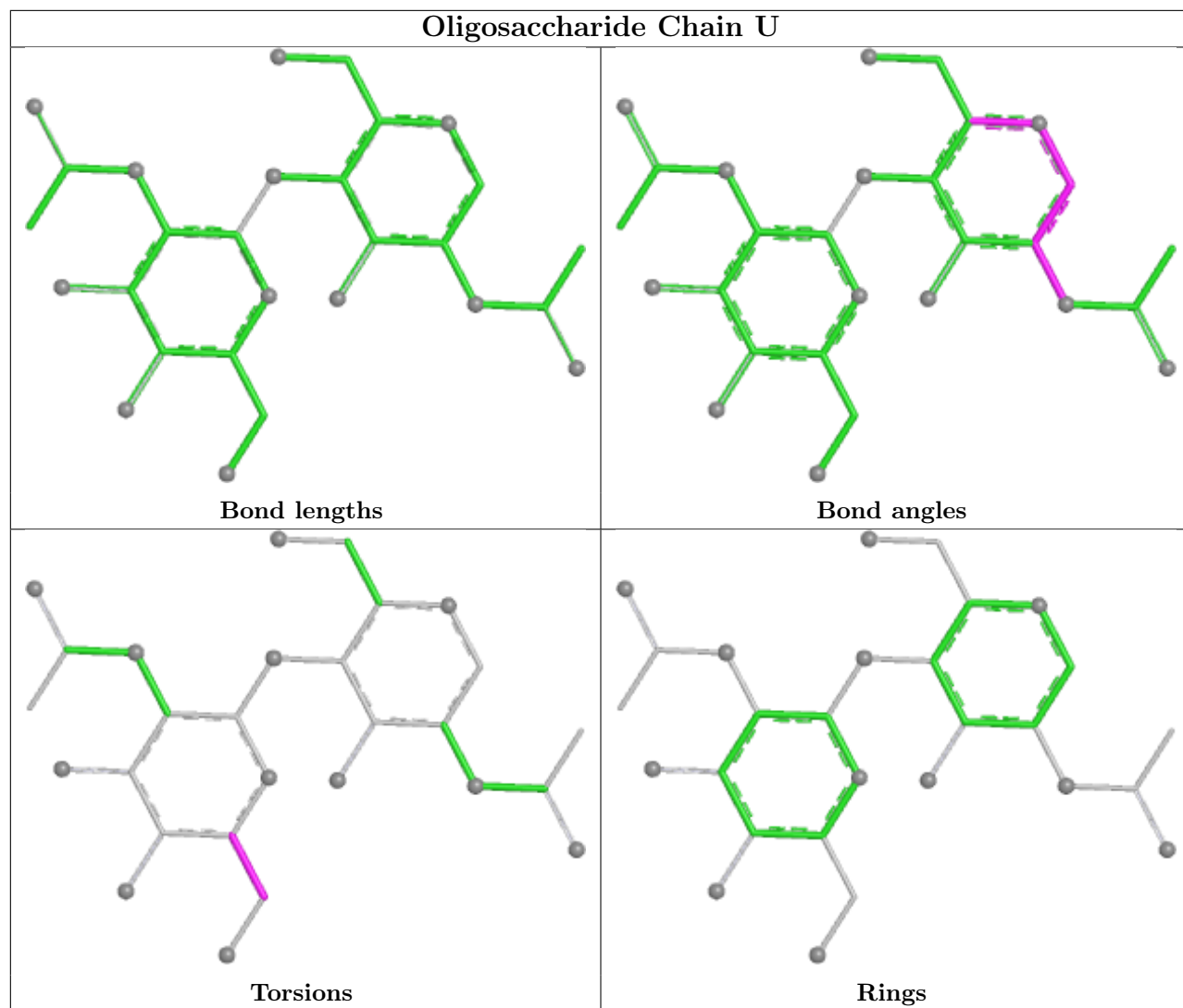
Mol	Chain	Res	Type	Atoms
9	U	2	NAG	O5-C5-C6-O6

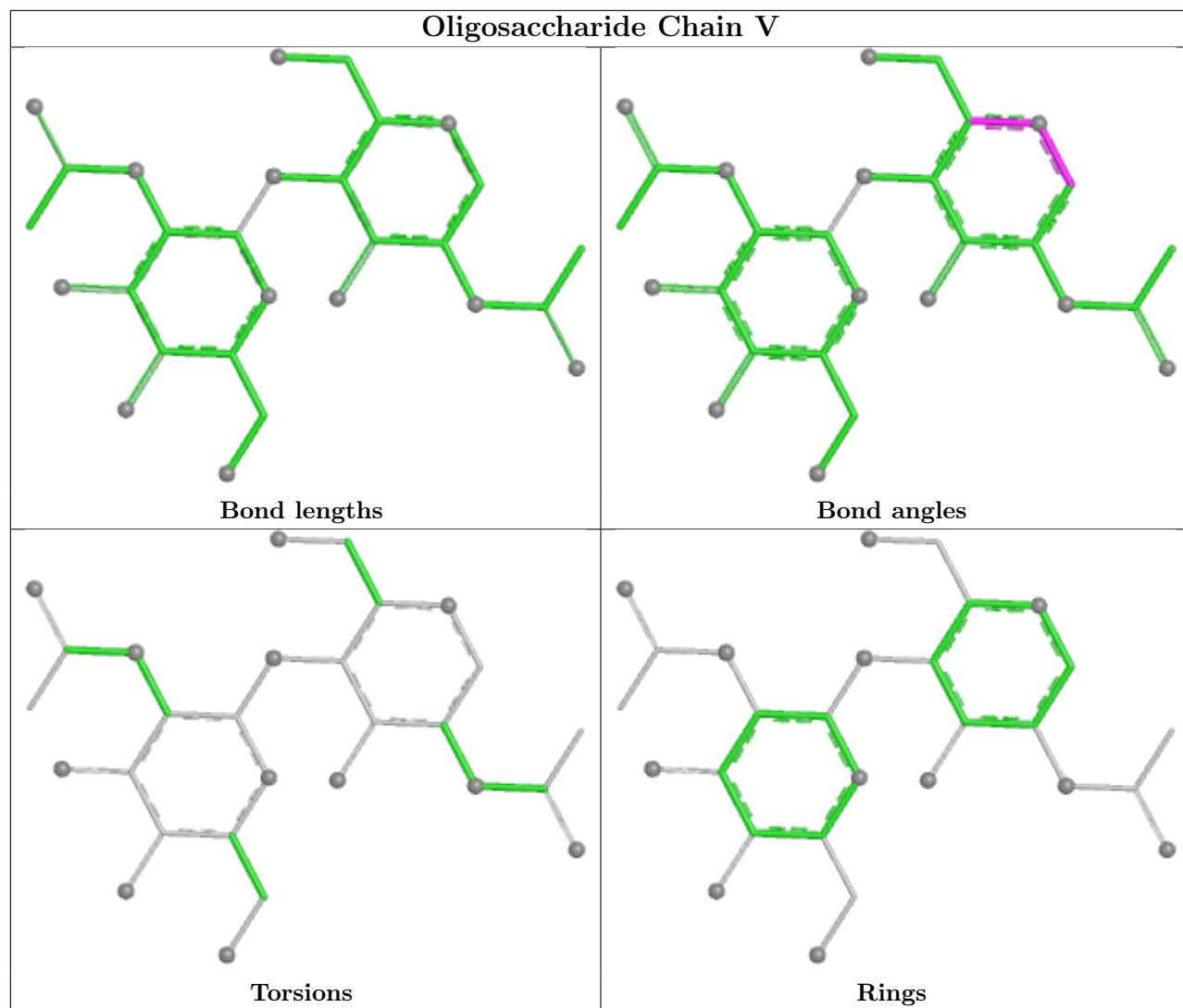
There are no ring outliers.

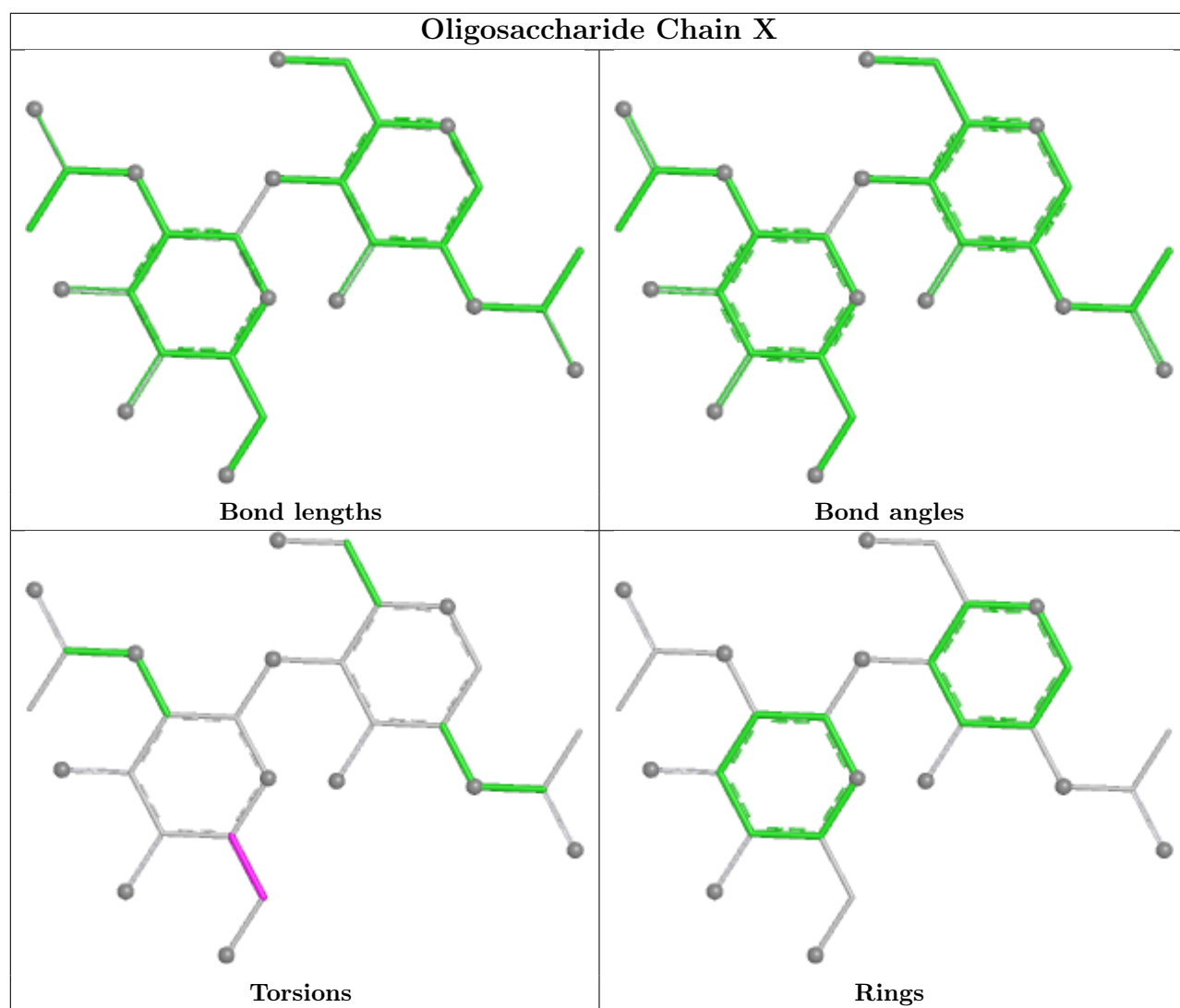
6 monomers are involved in 3 short contacts:

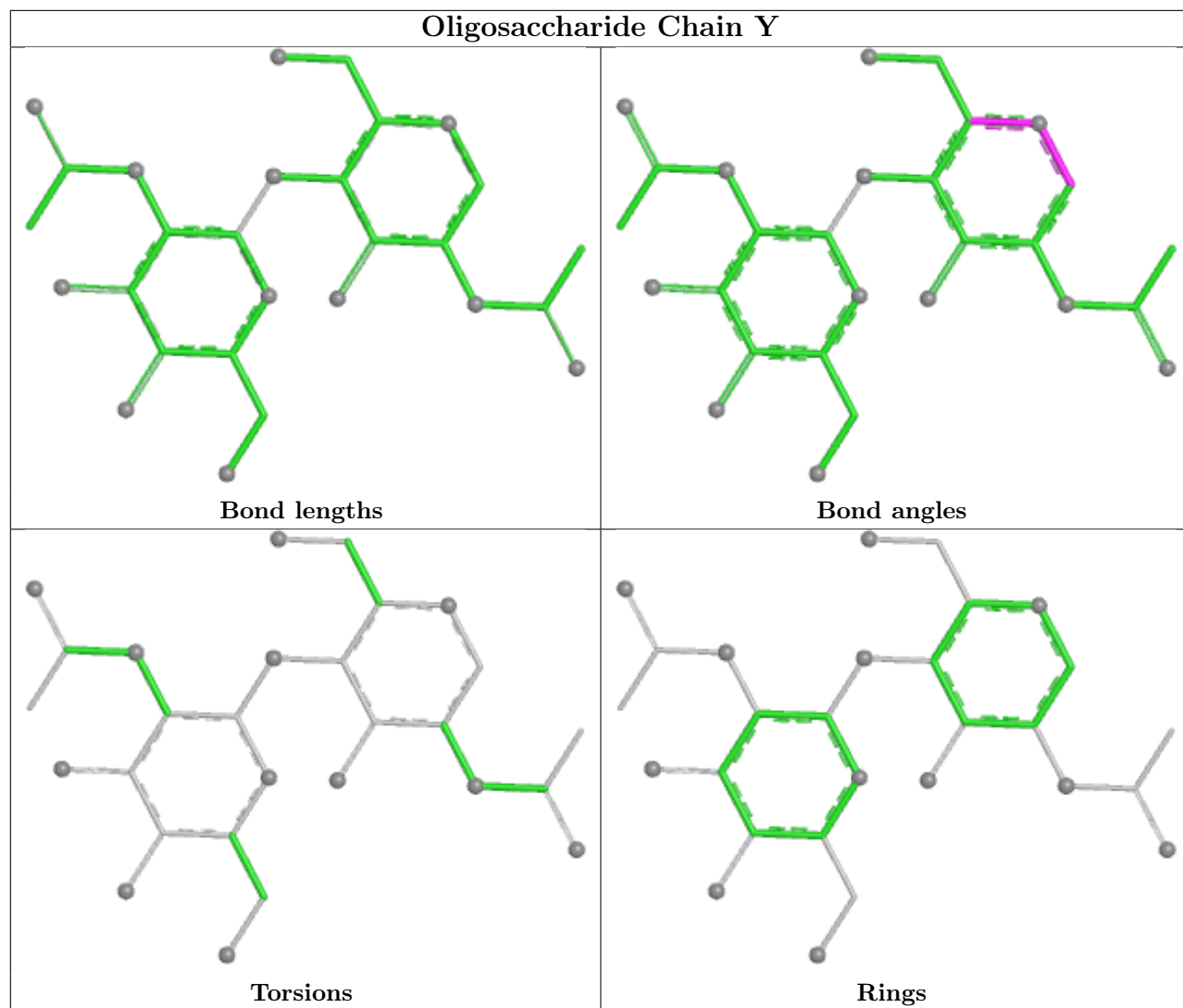
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	r	5	MAN	1	0
13	2	6	MAN	1	0
13	2	3	BMA	1	0
11	c	4	MAN	1	0
11	c	3	BMA	1	0
15	r	4	MAN	1	0

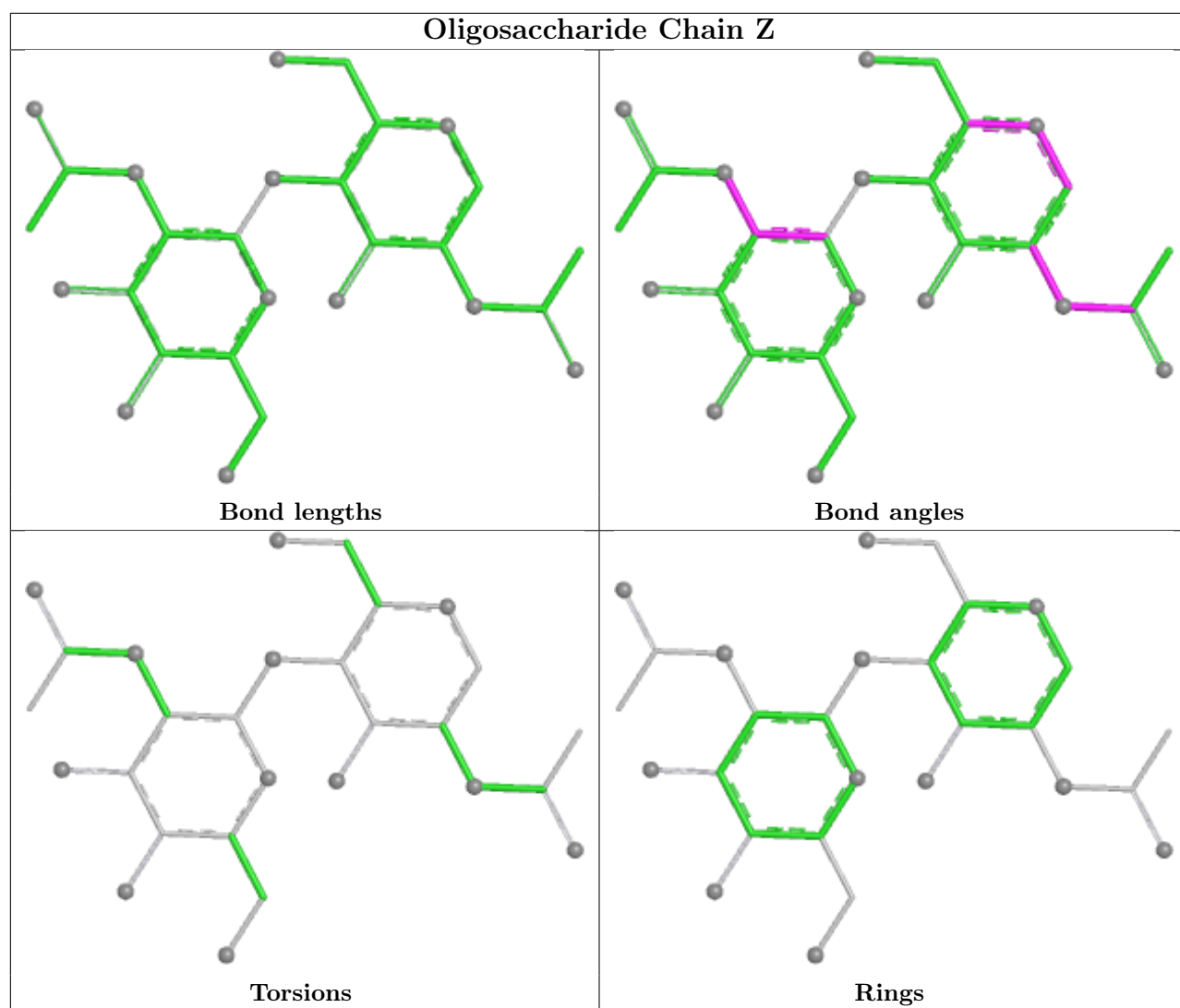
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

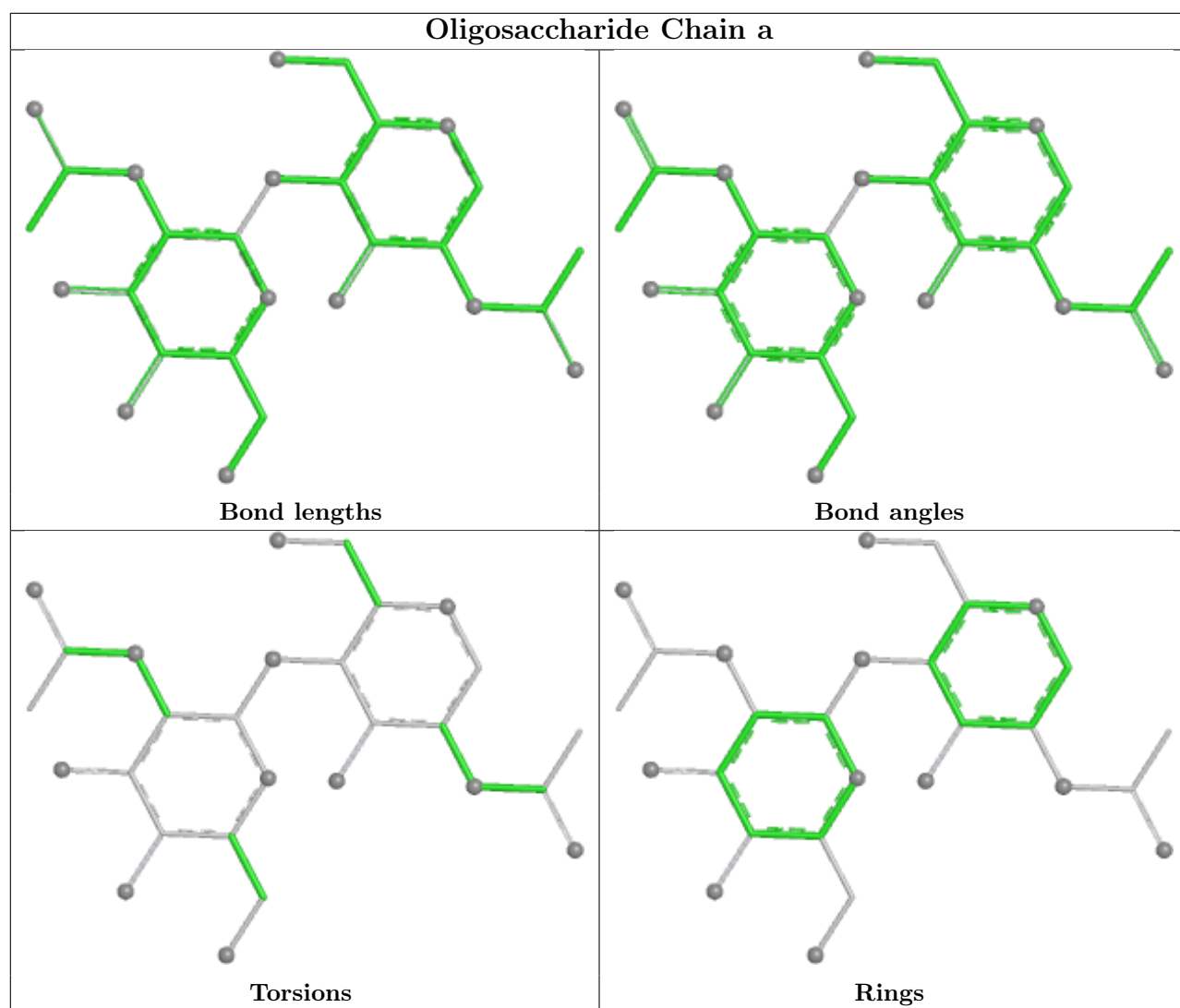


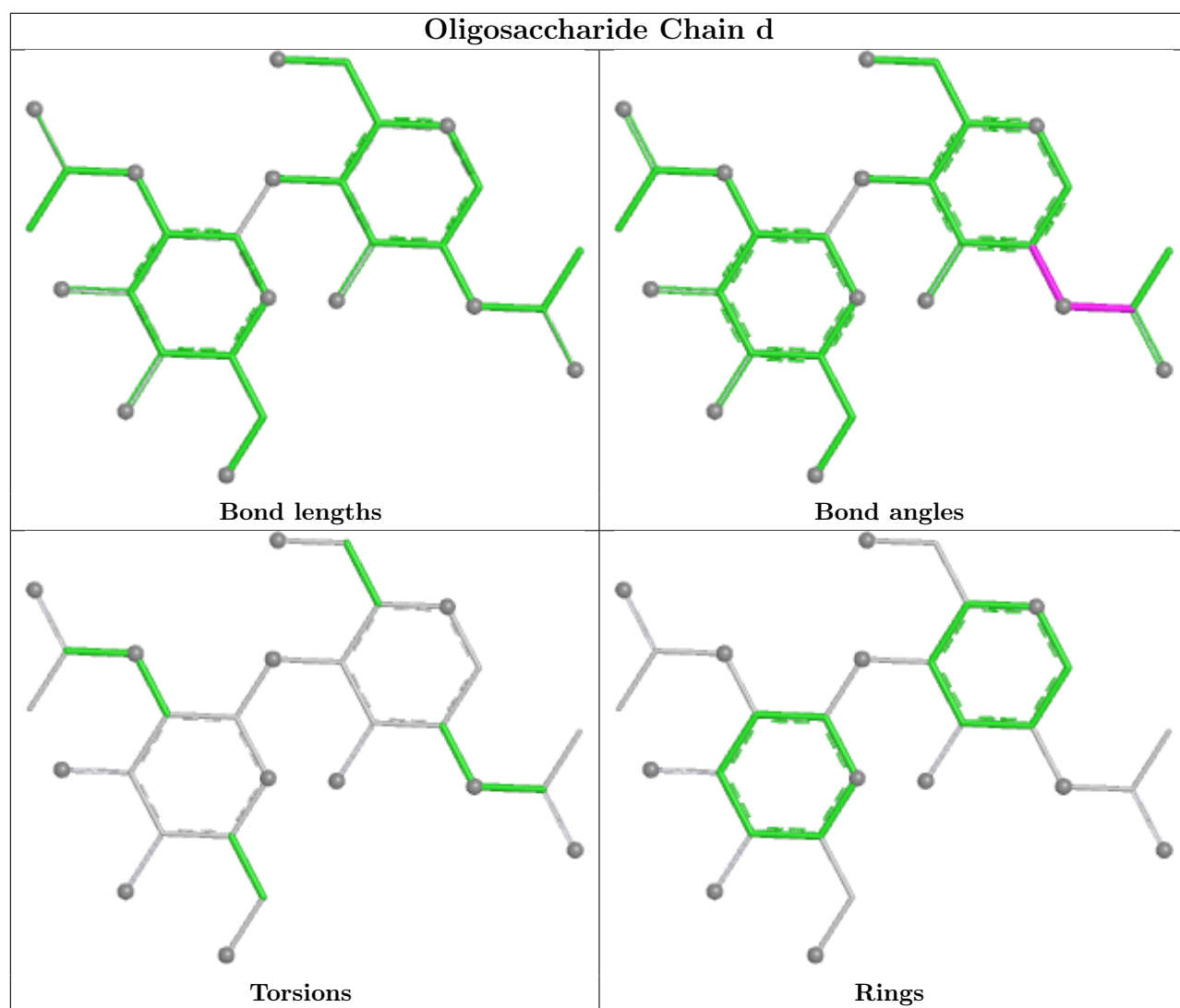


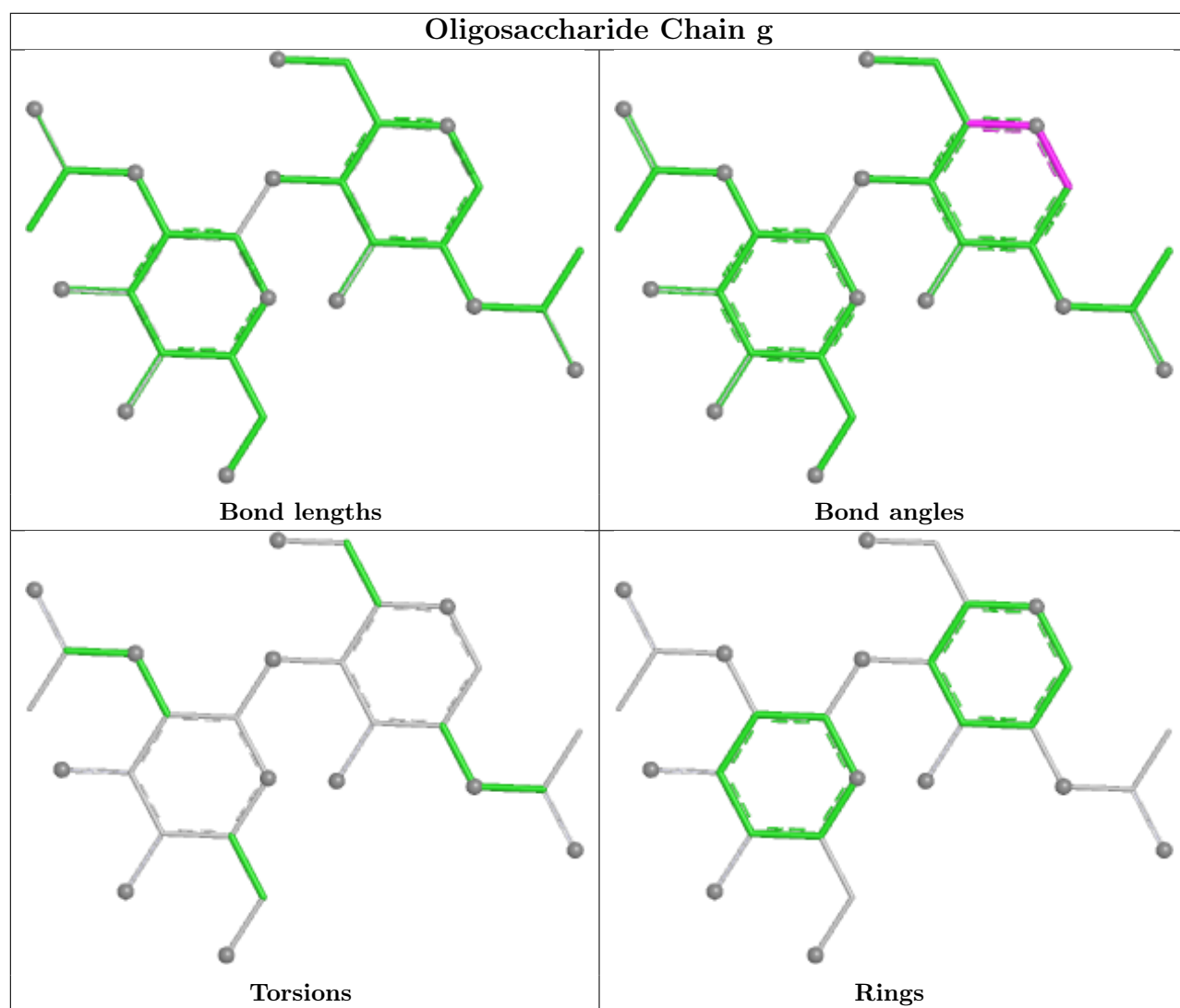


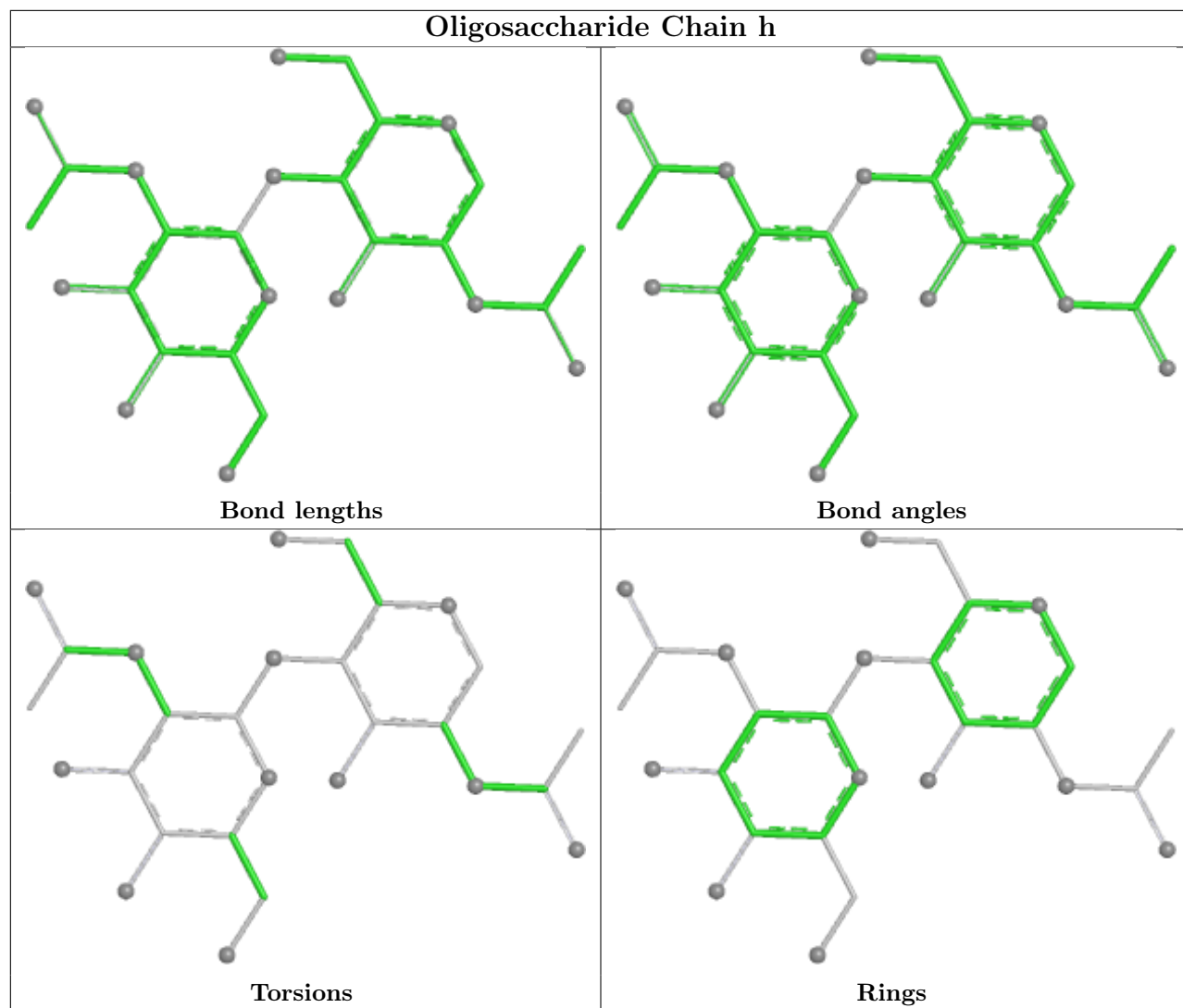


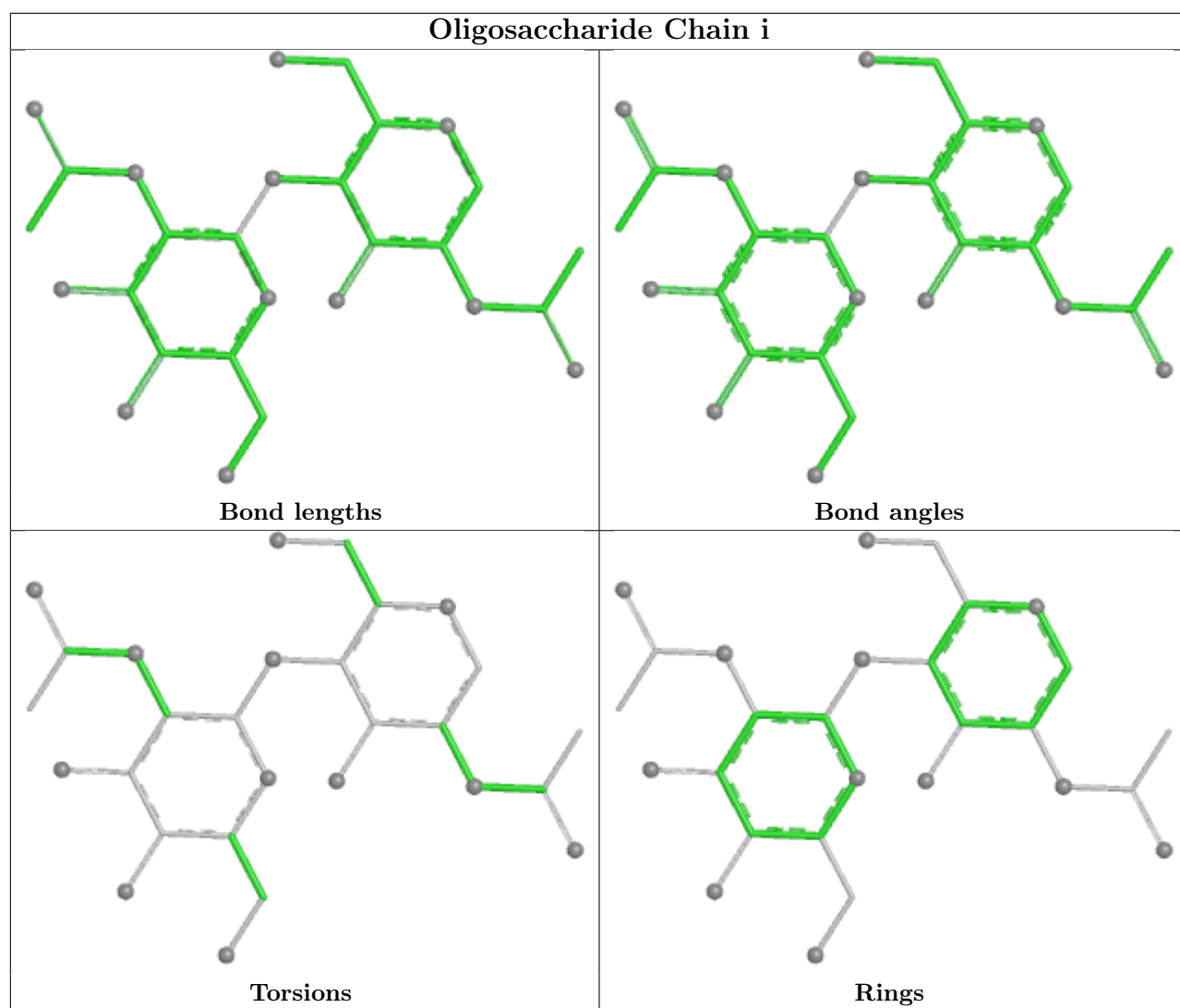


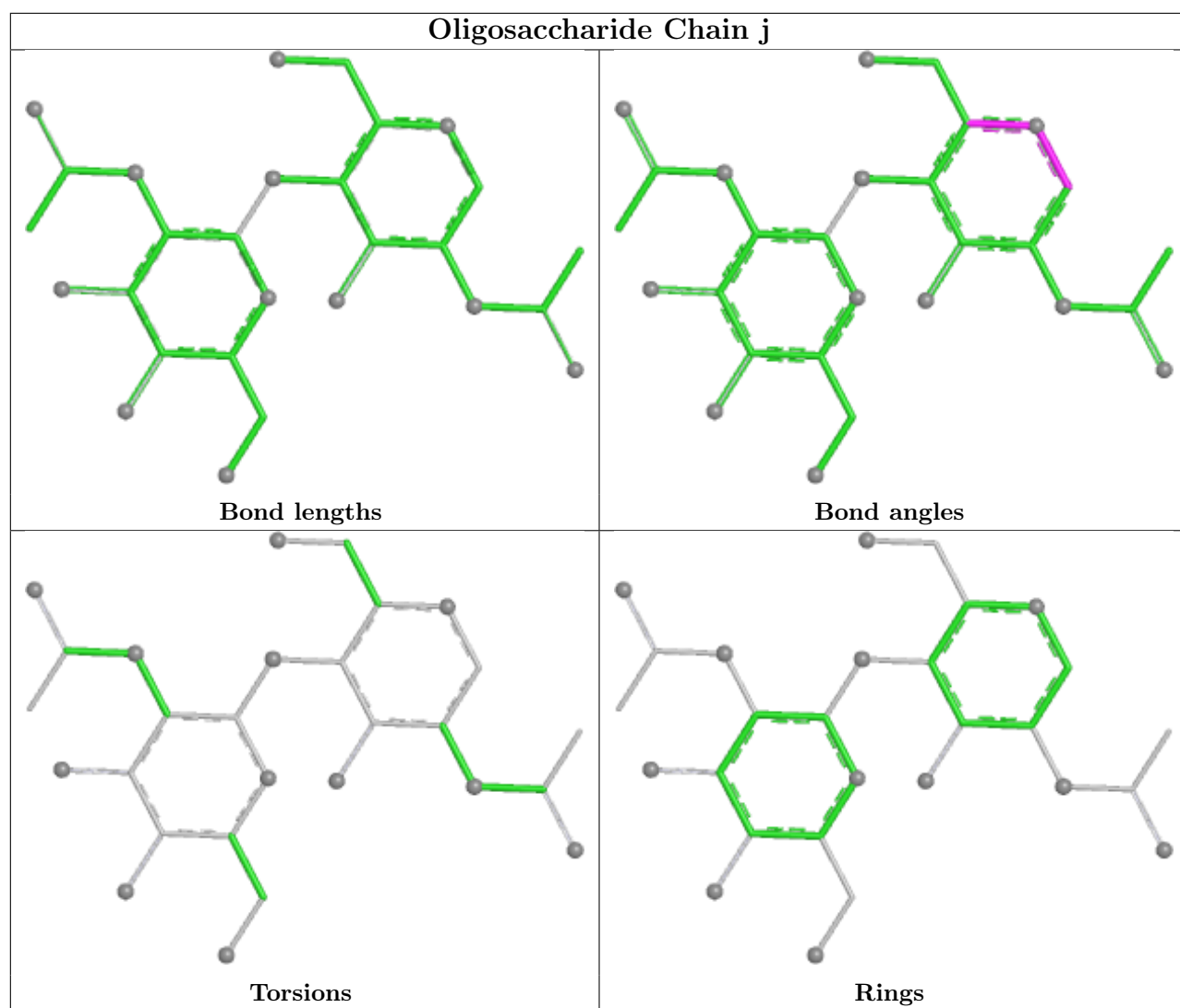


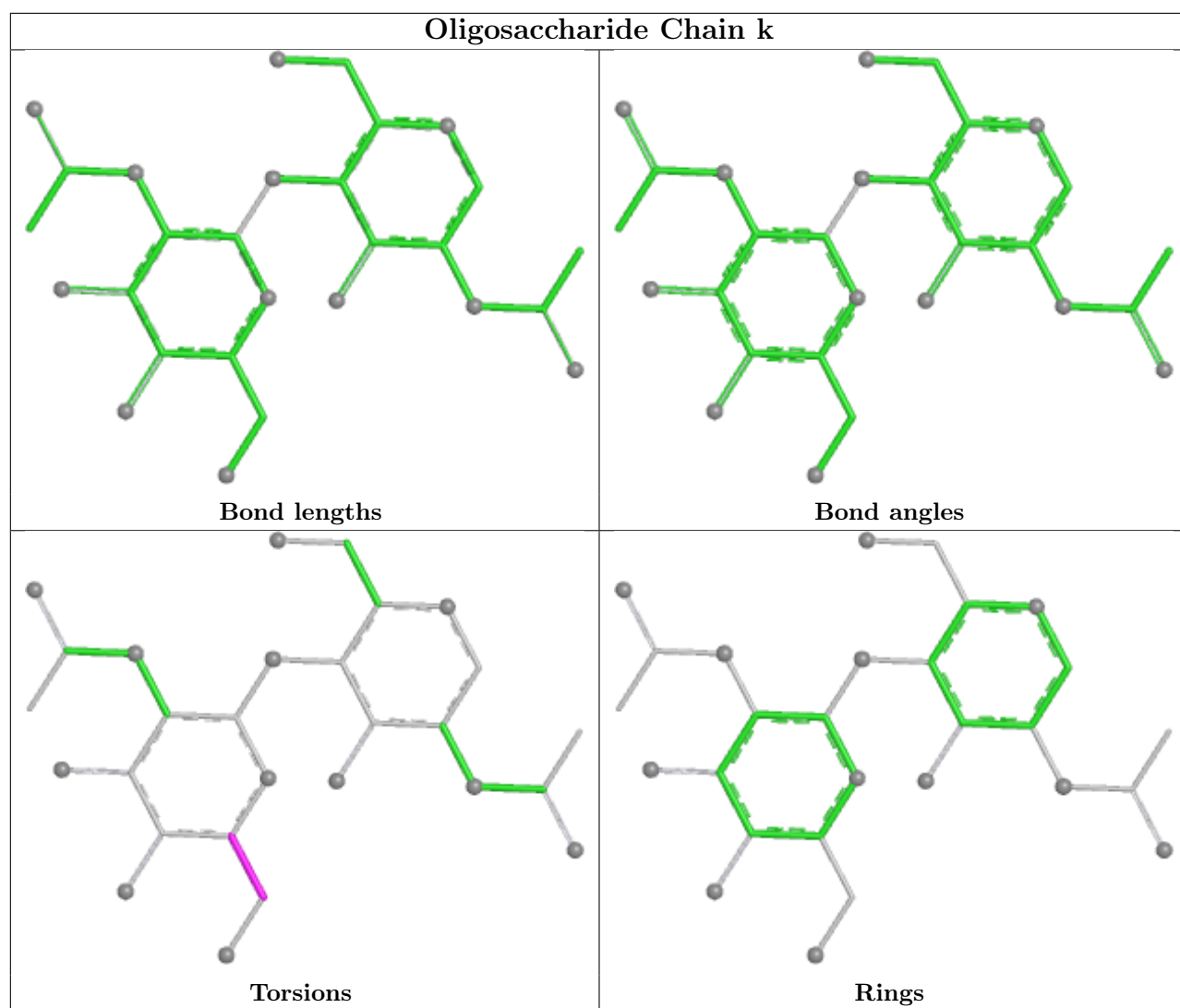


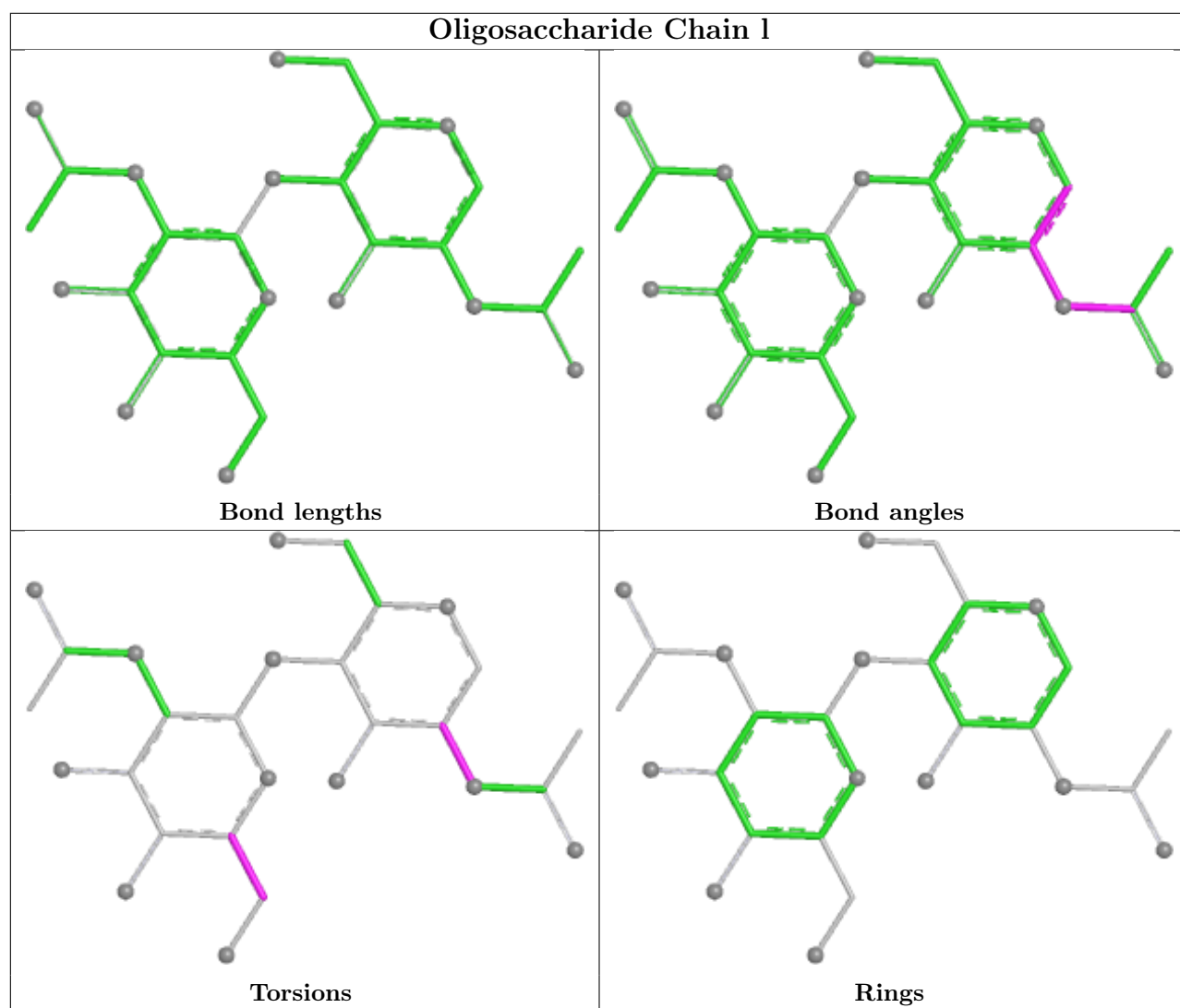


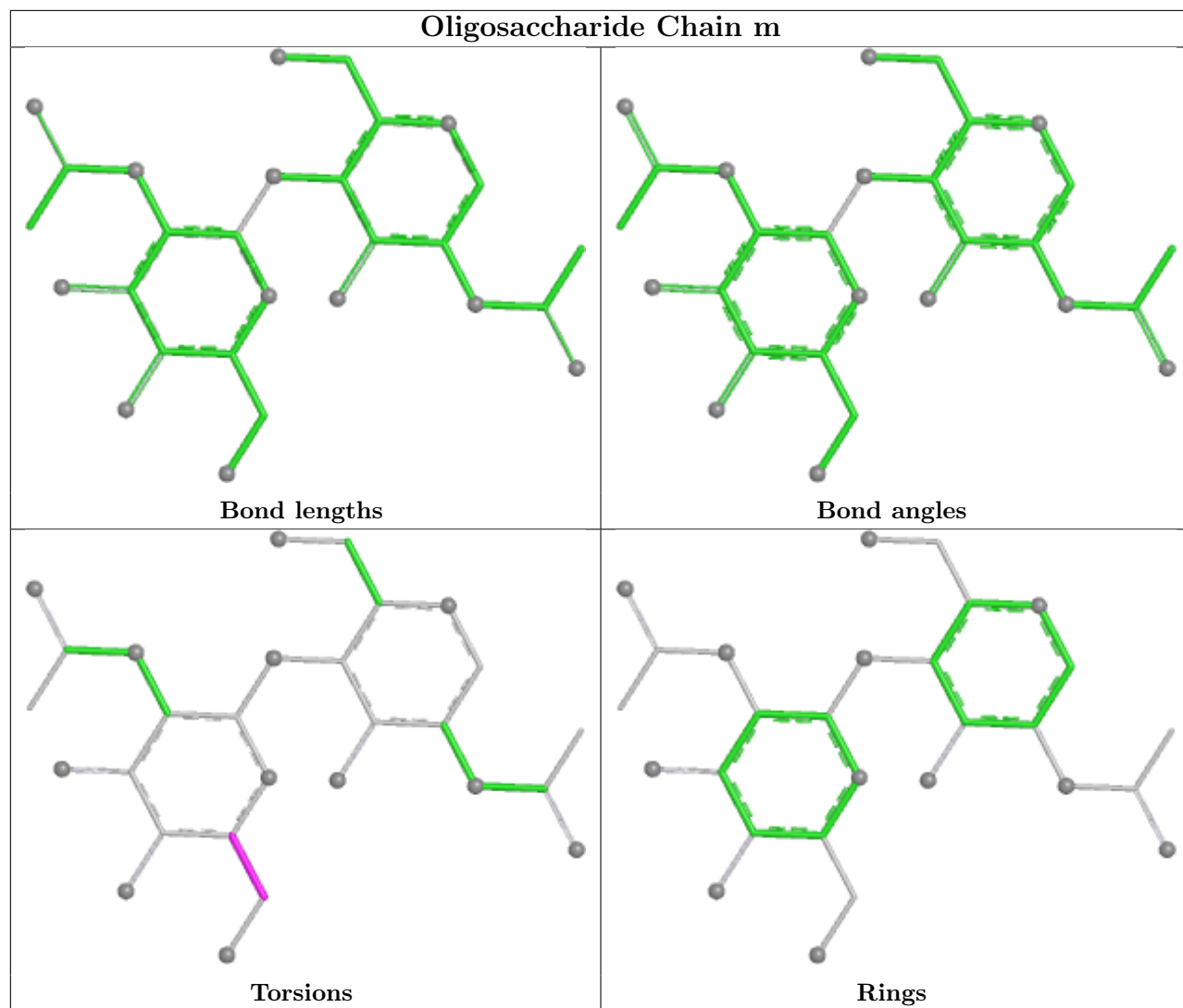


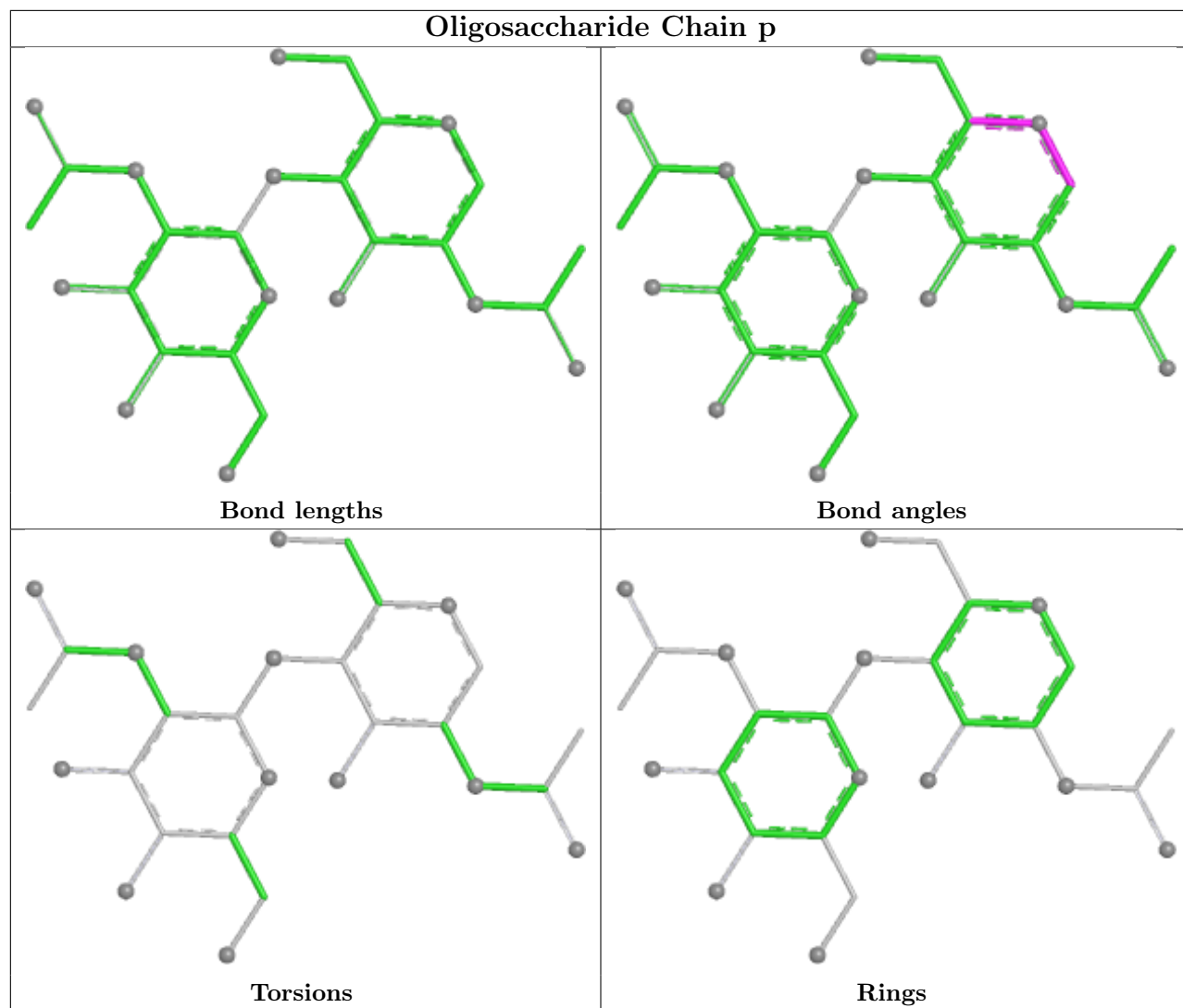


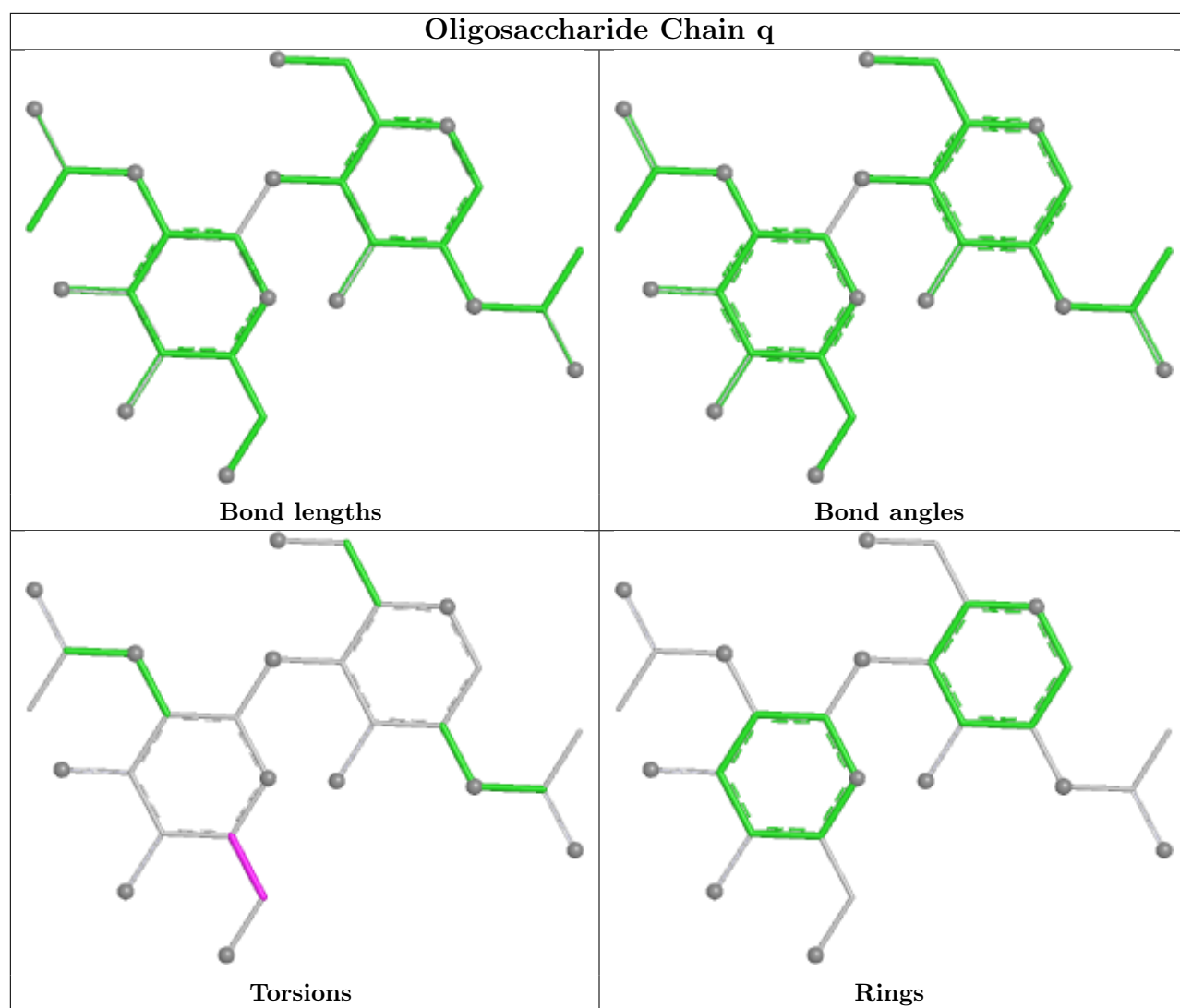


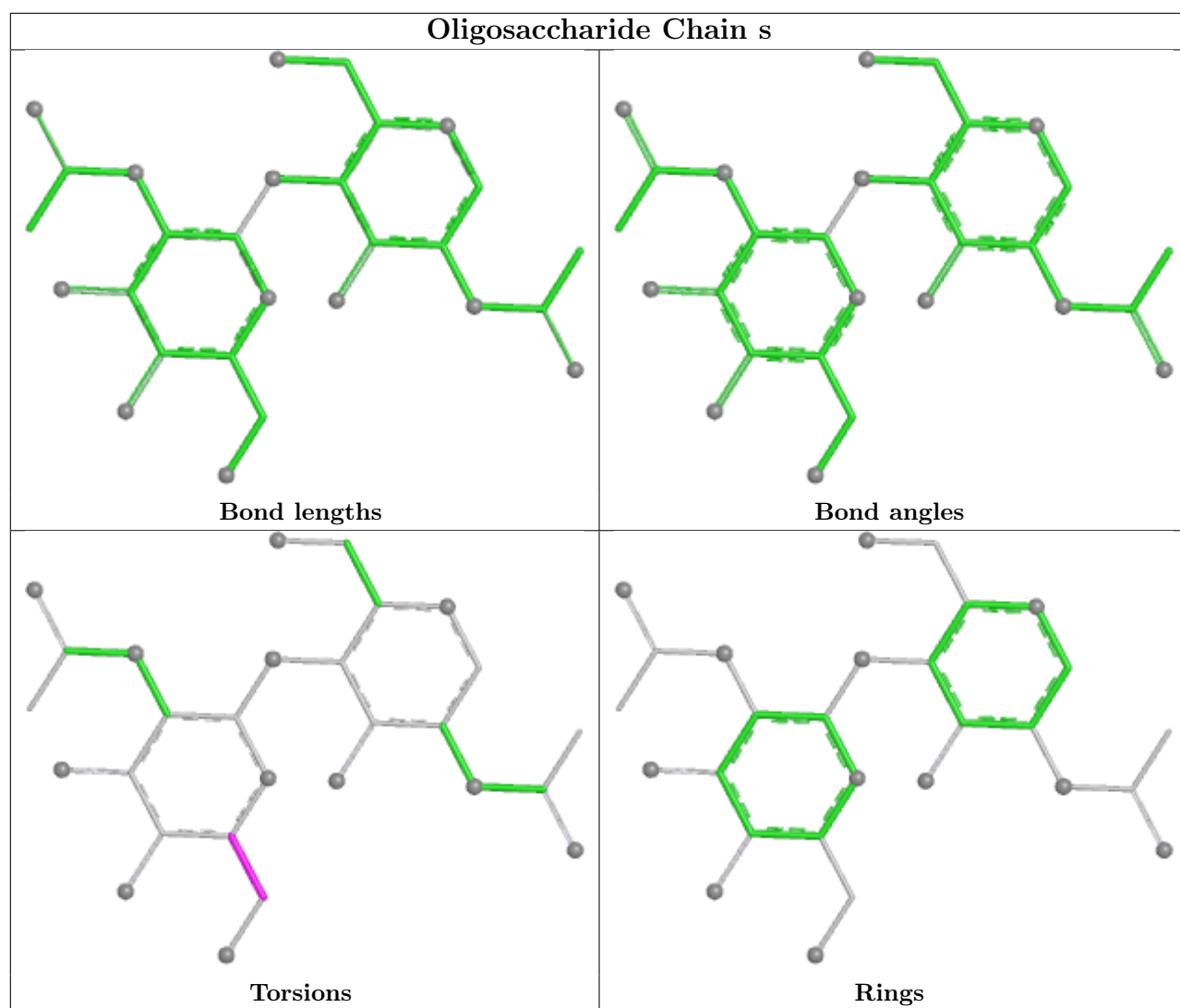


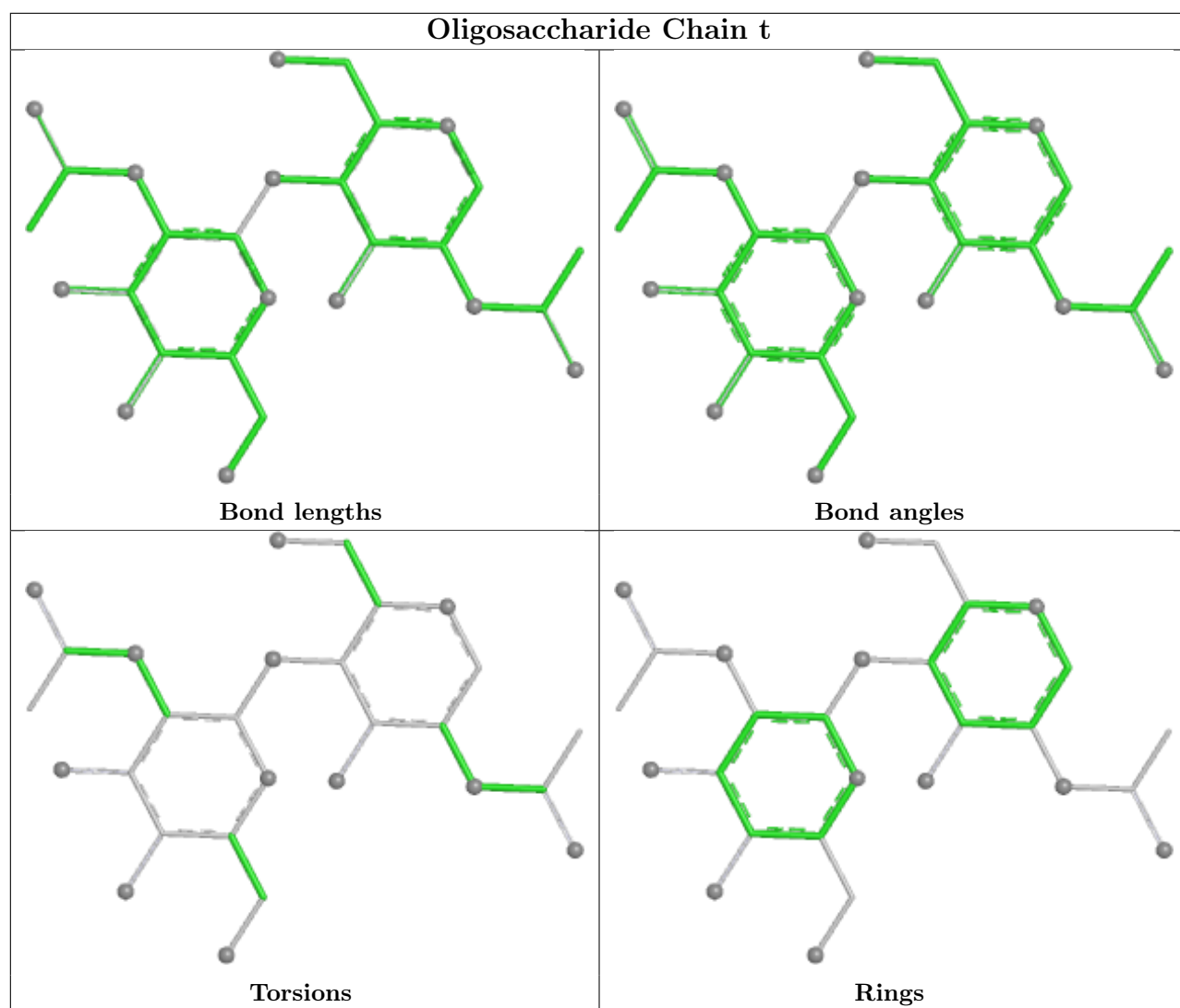


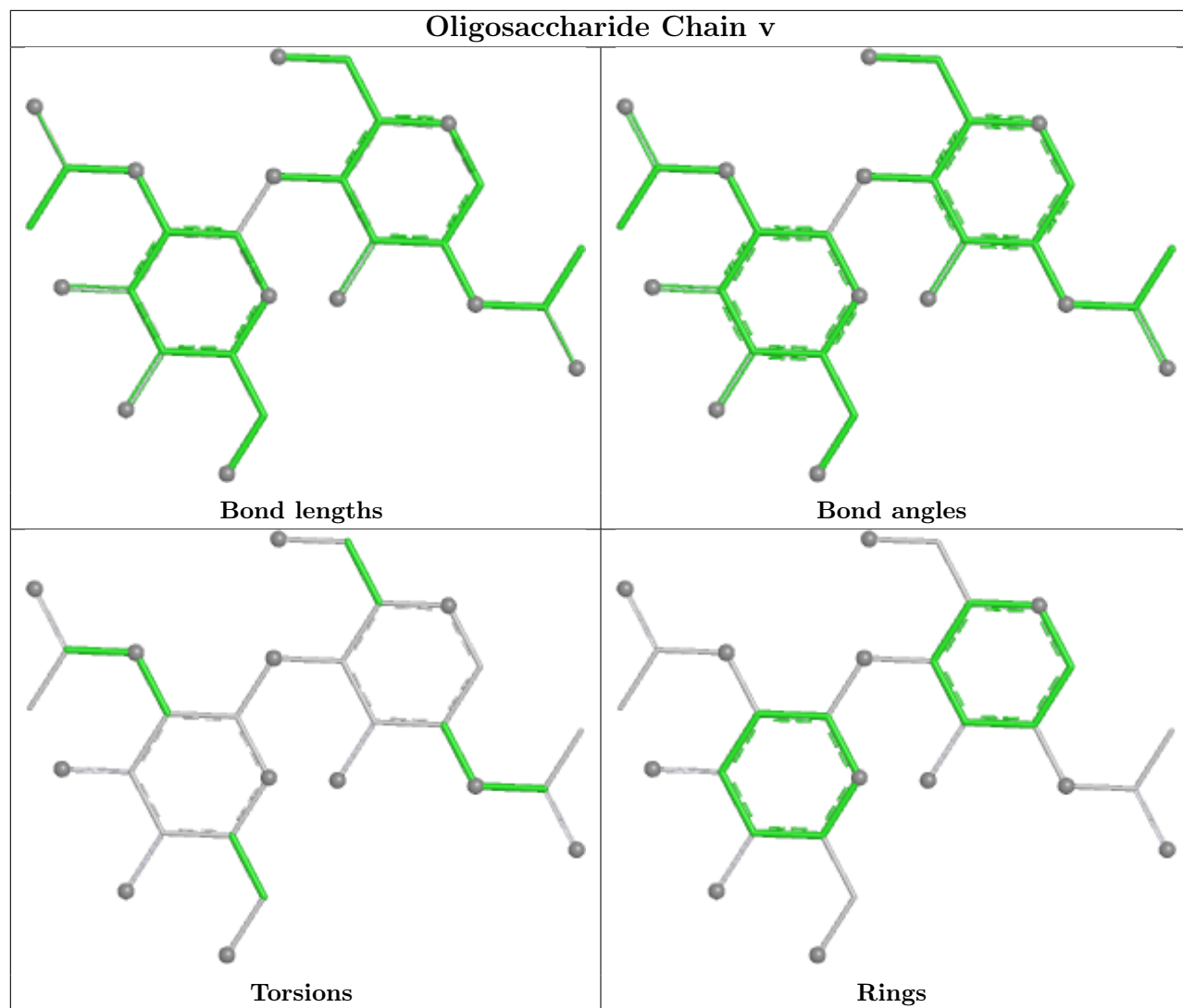


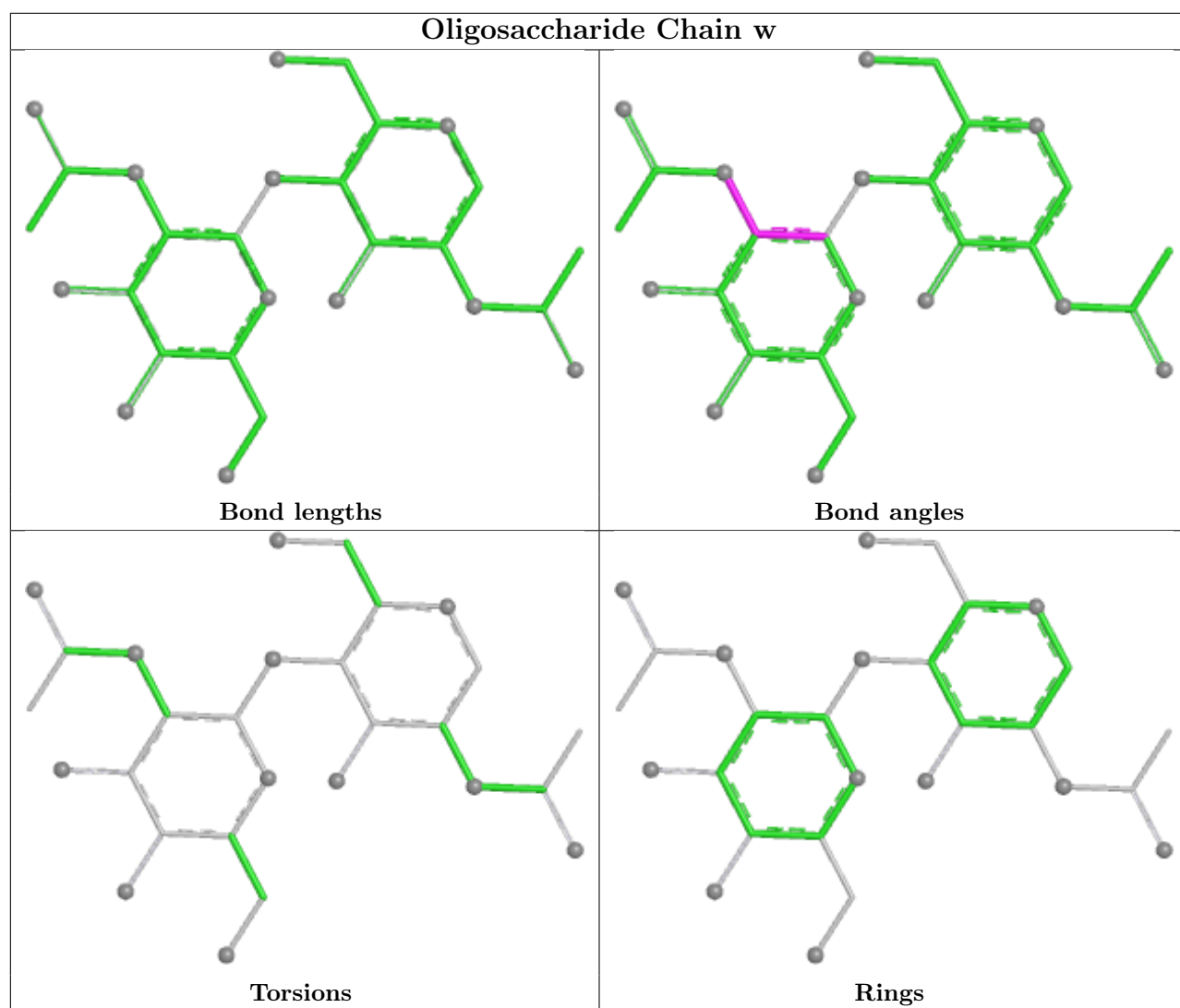


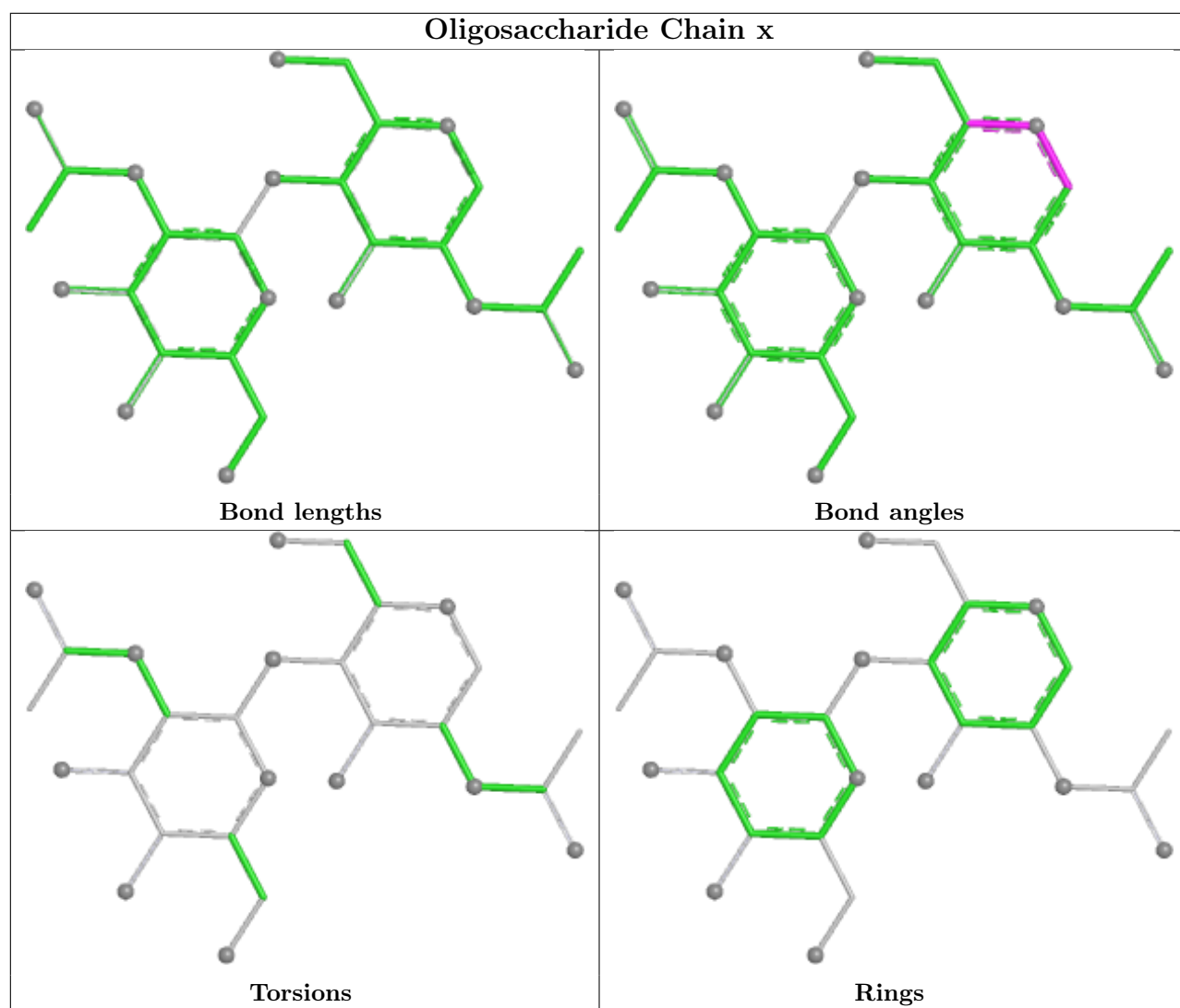


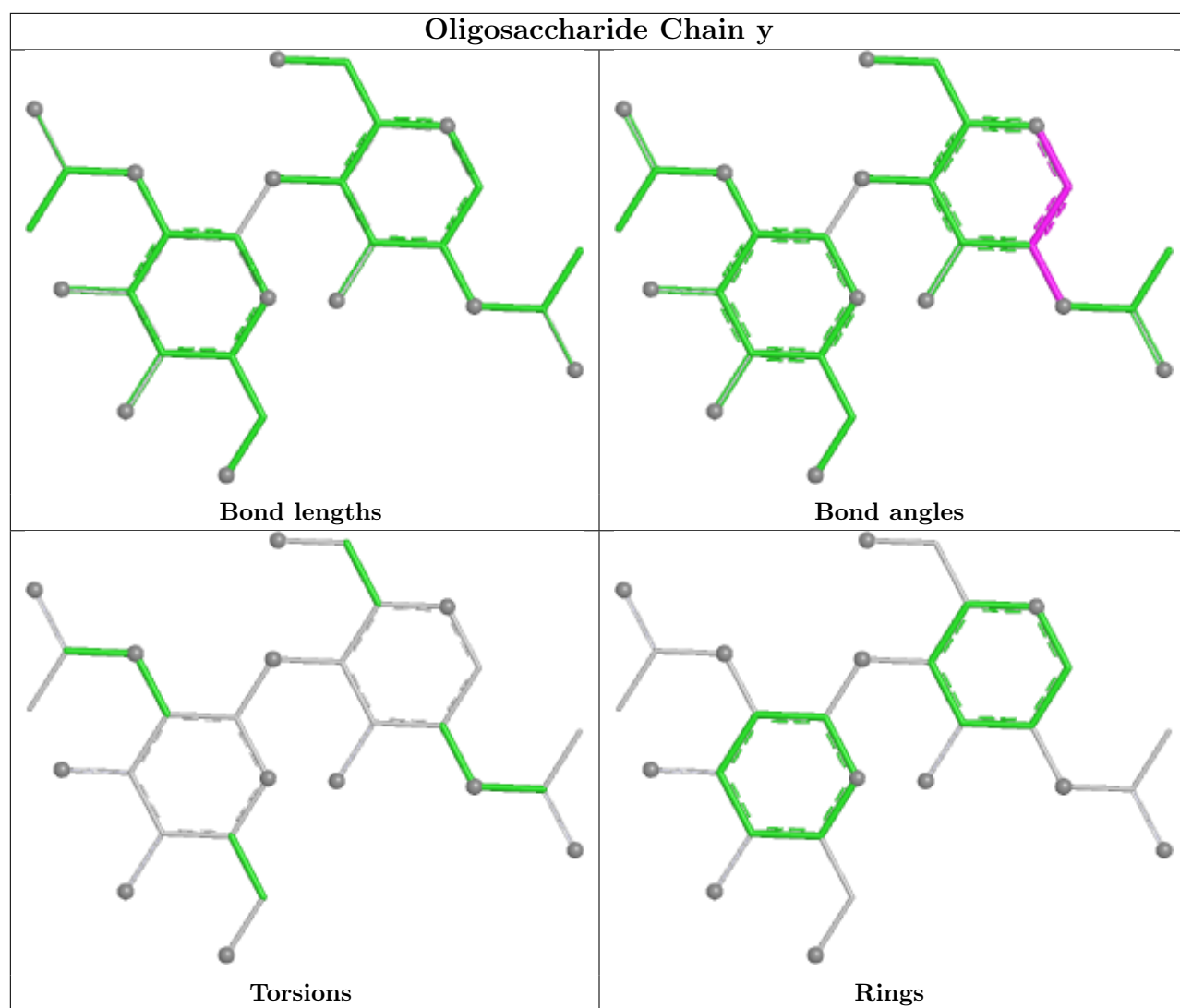


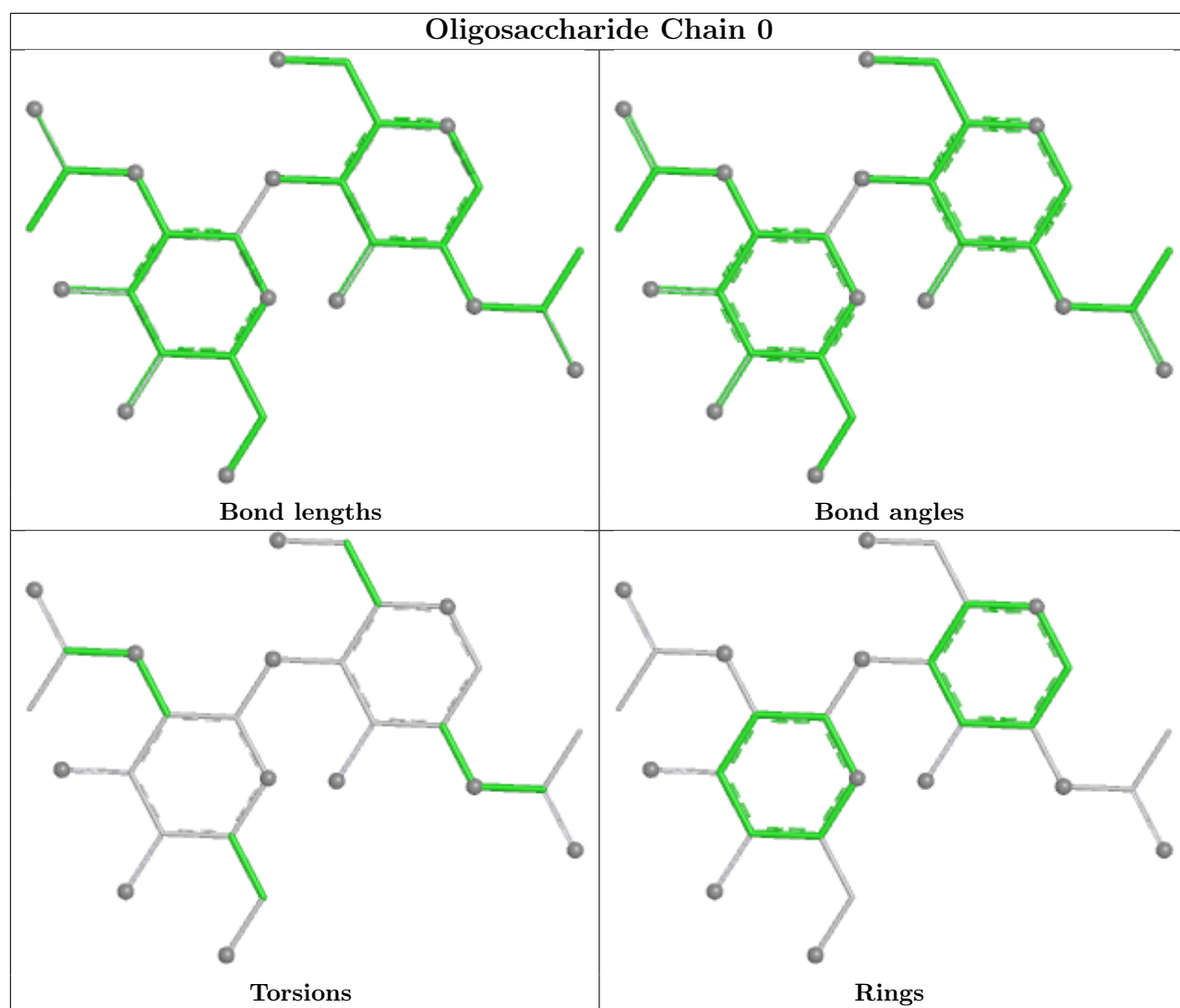


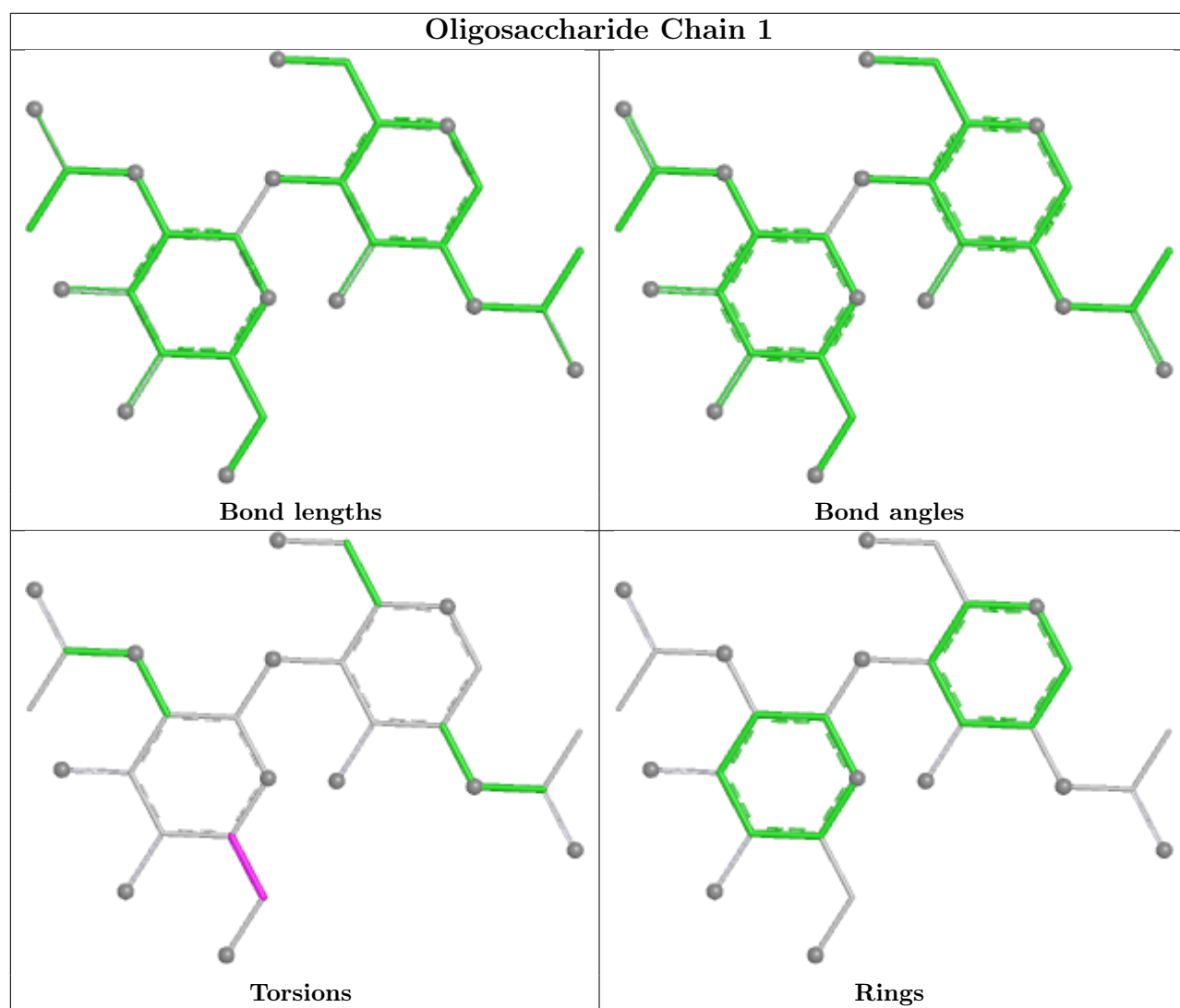


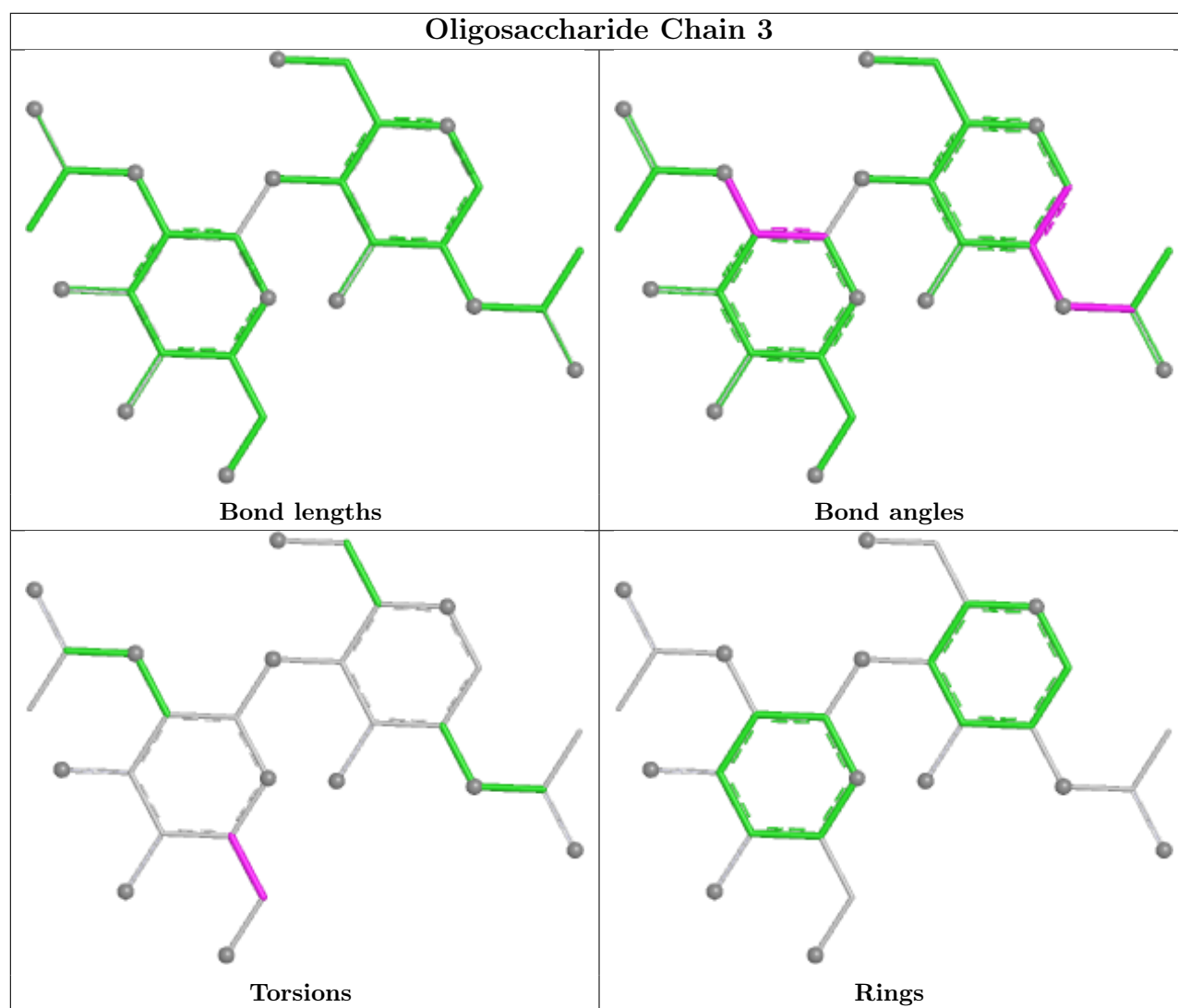


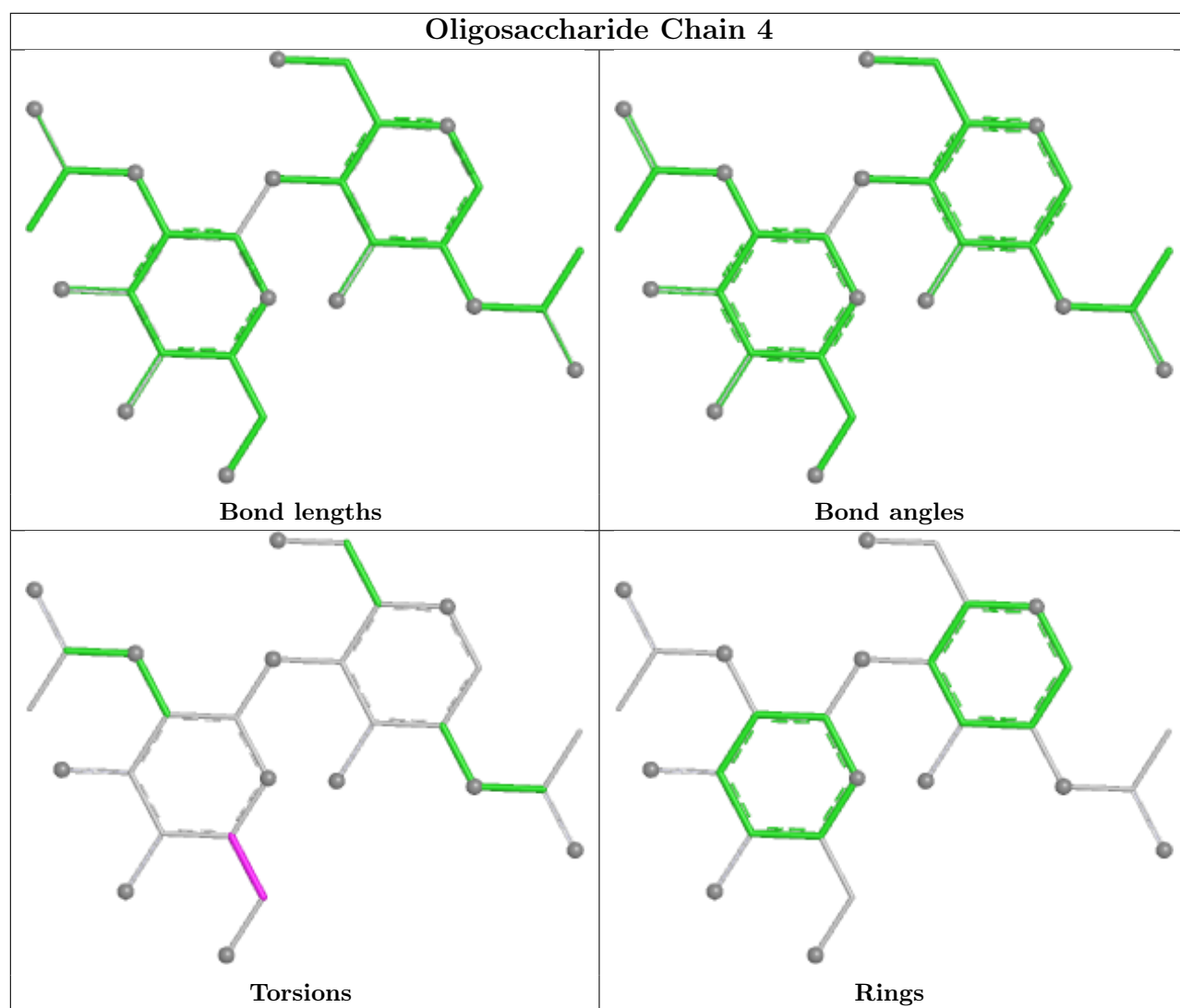


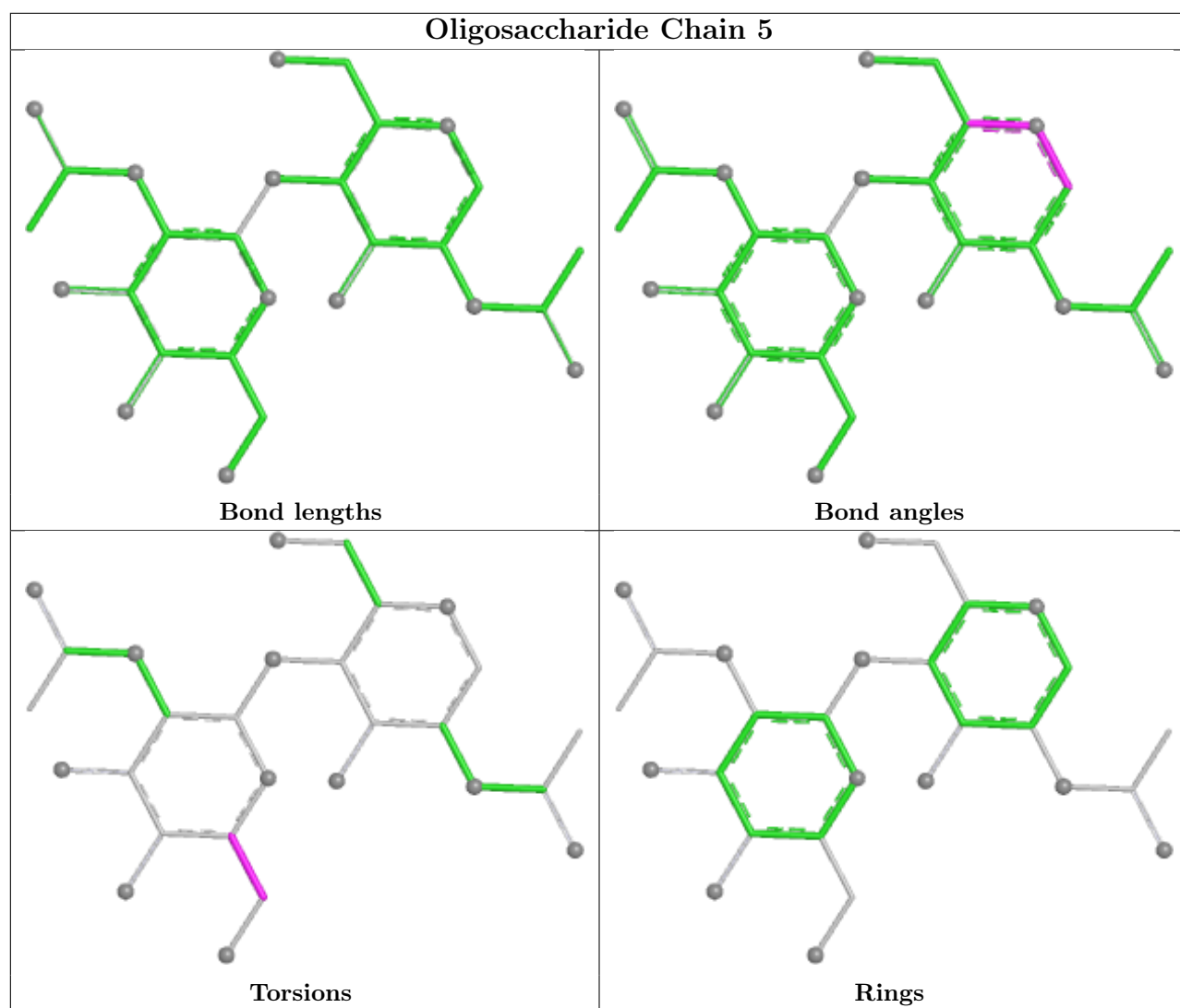


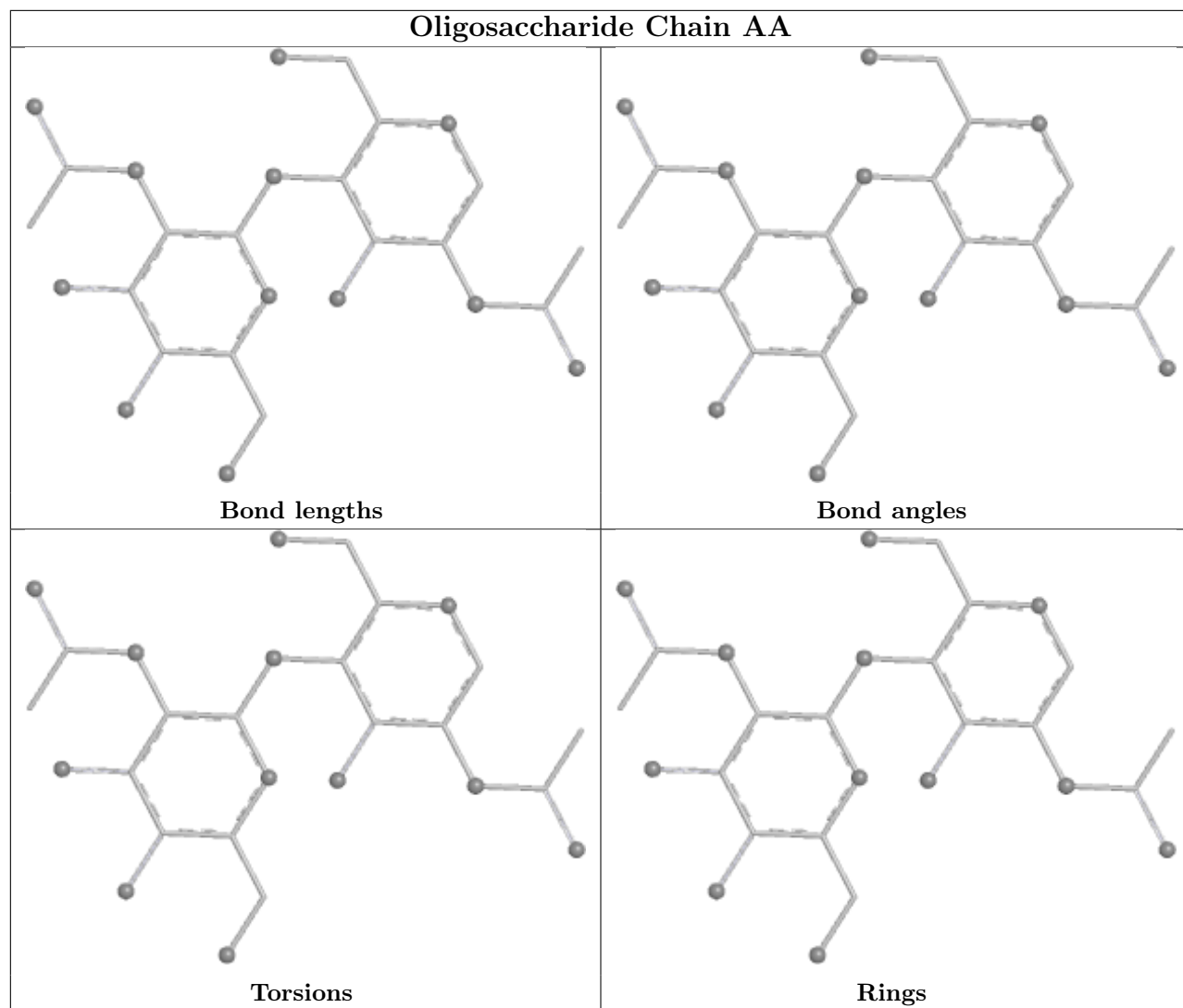


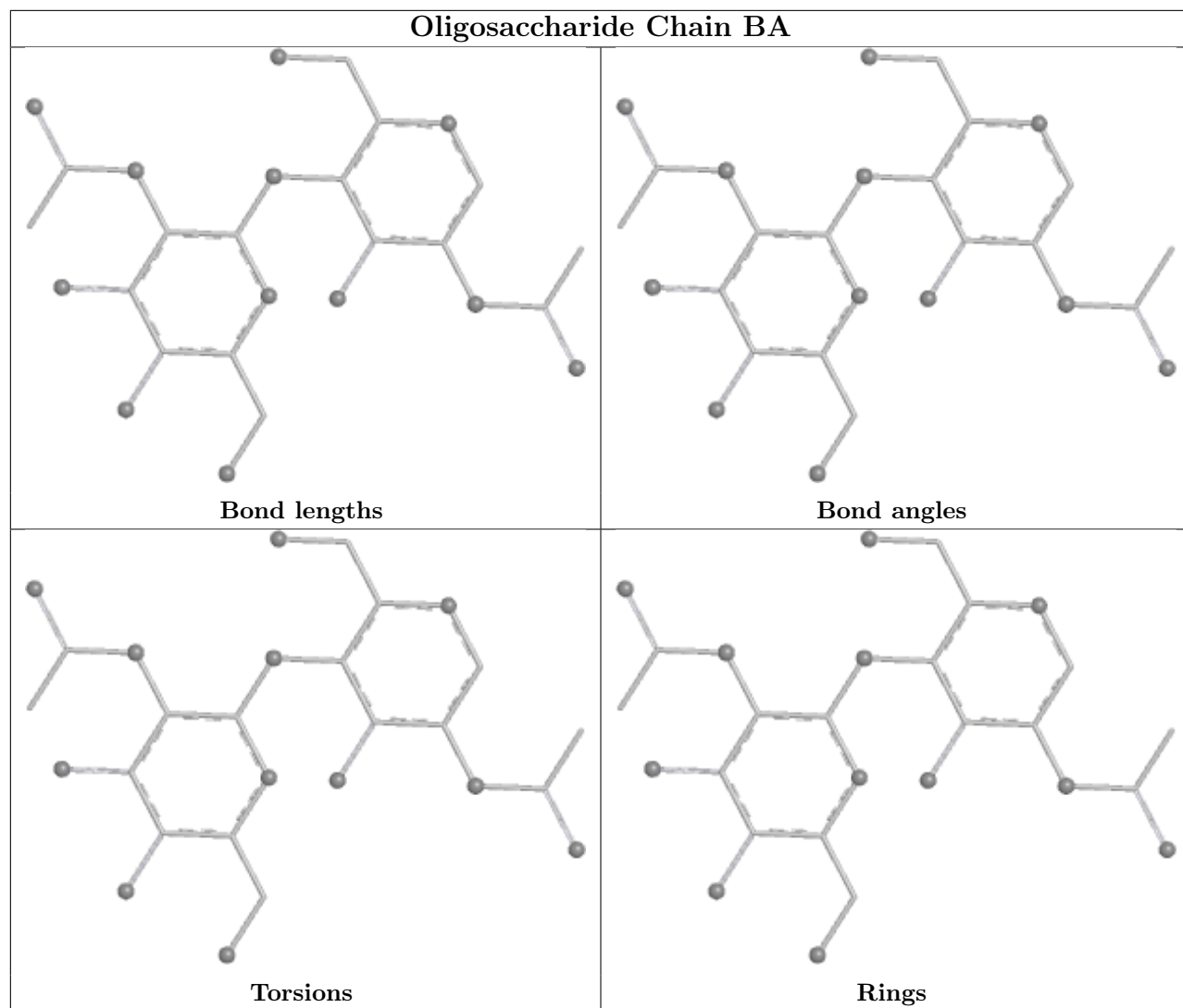


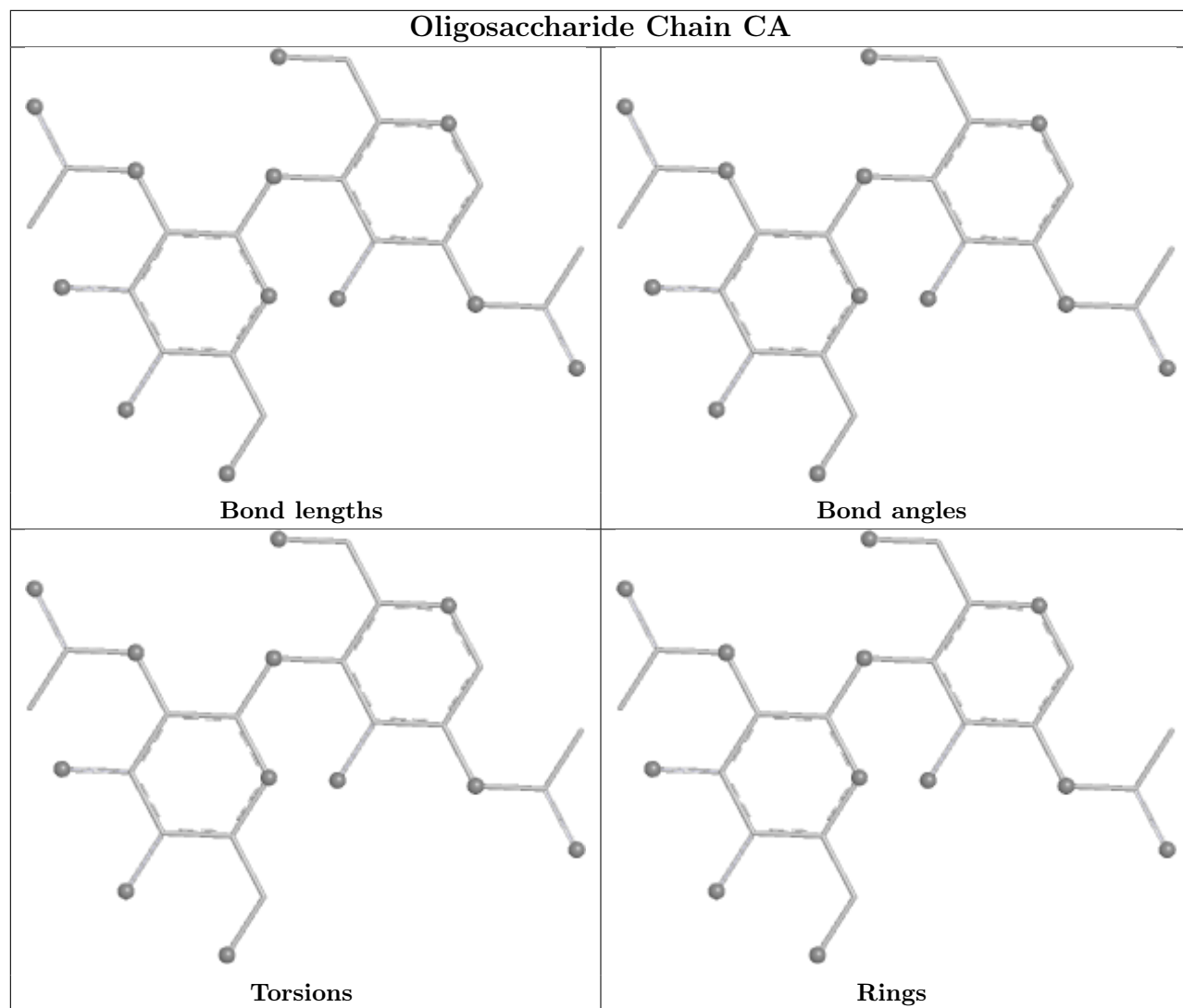


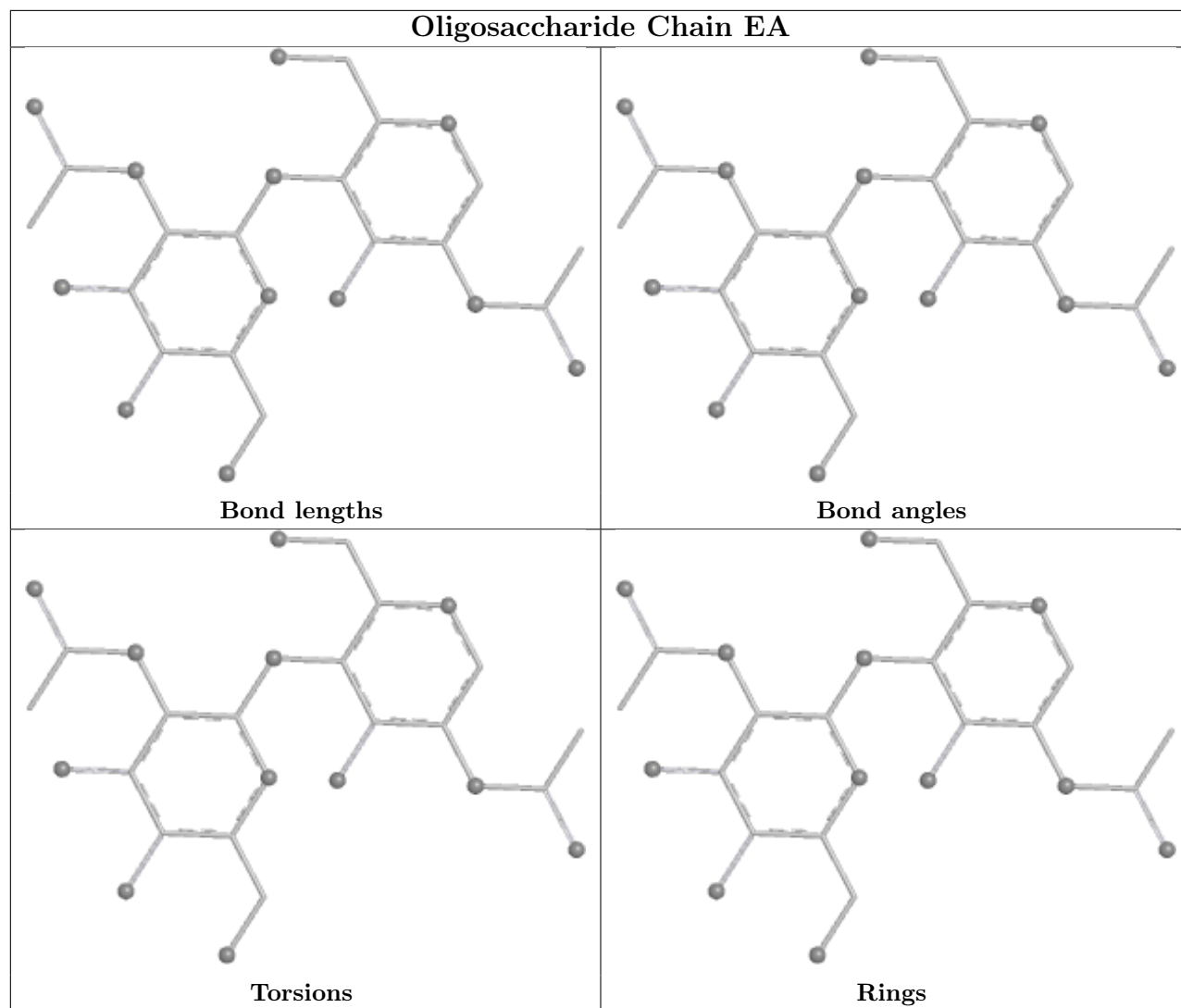


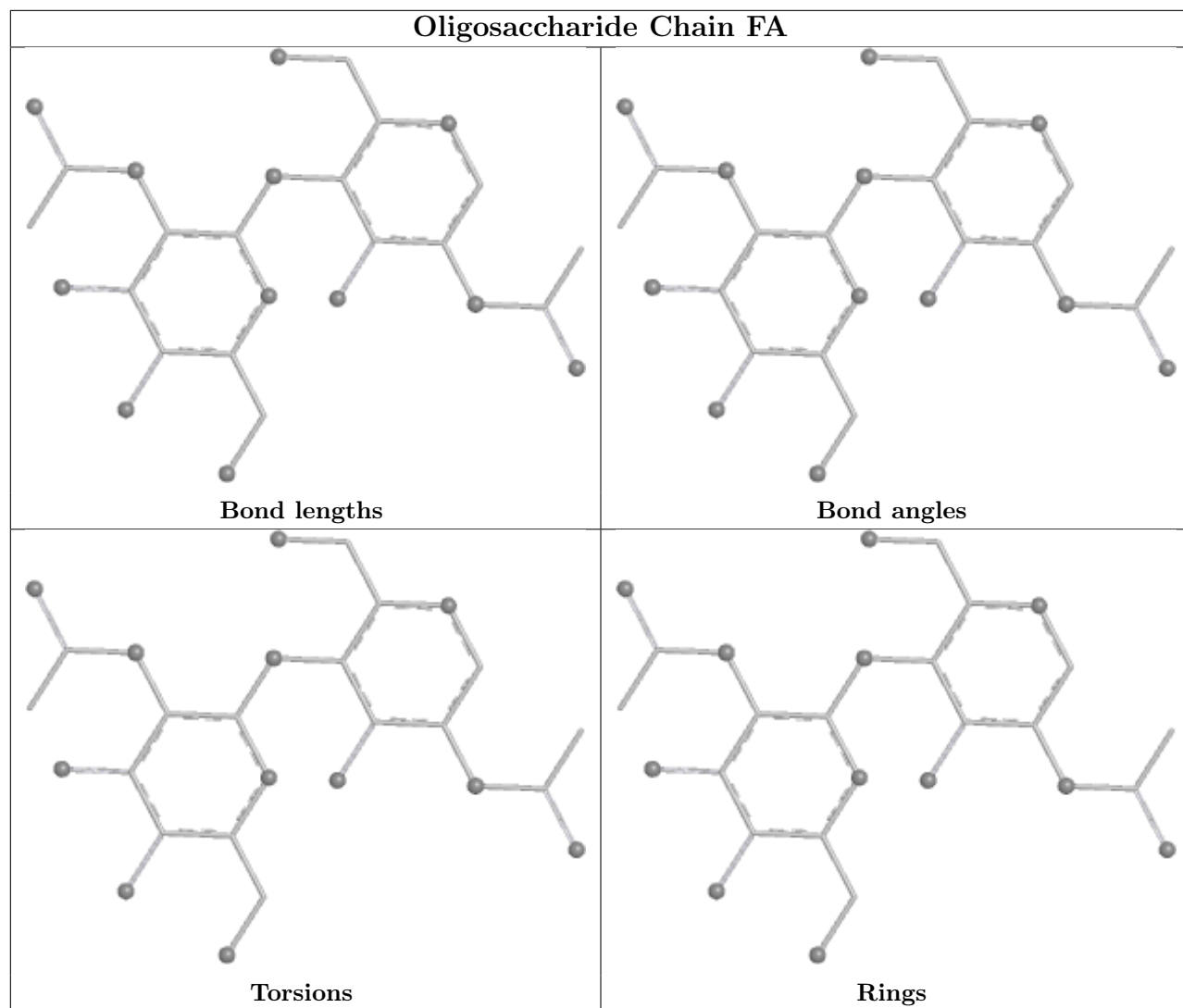


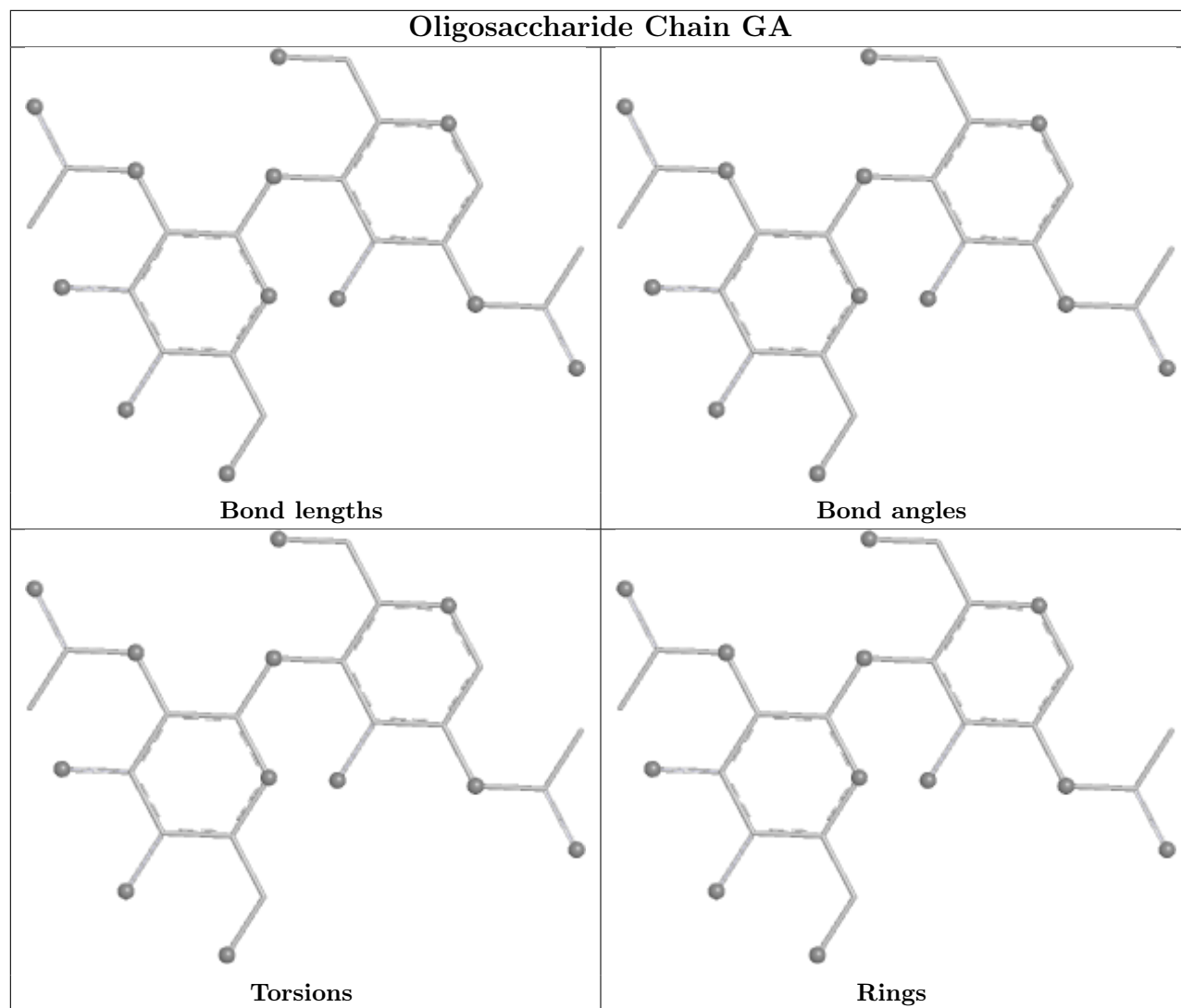


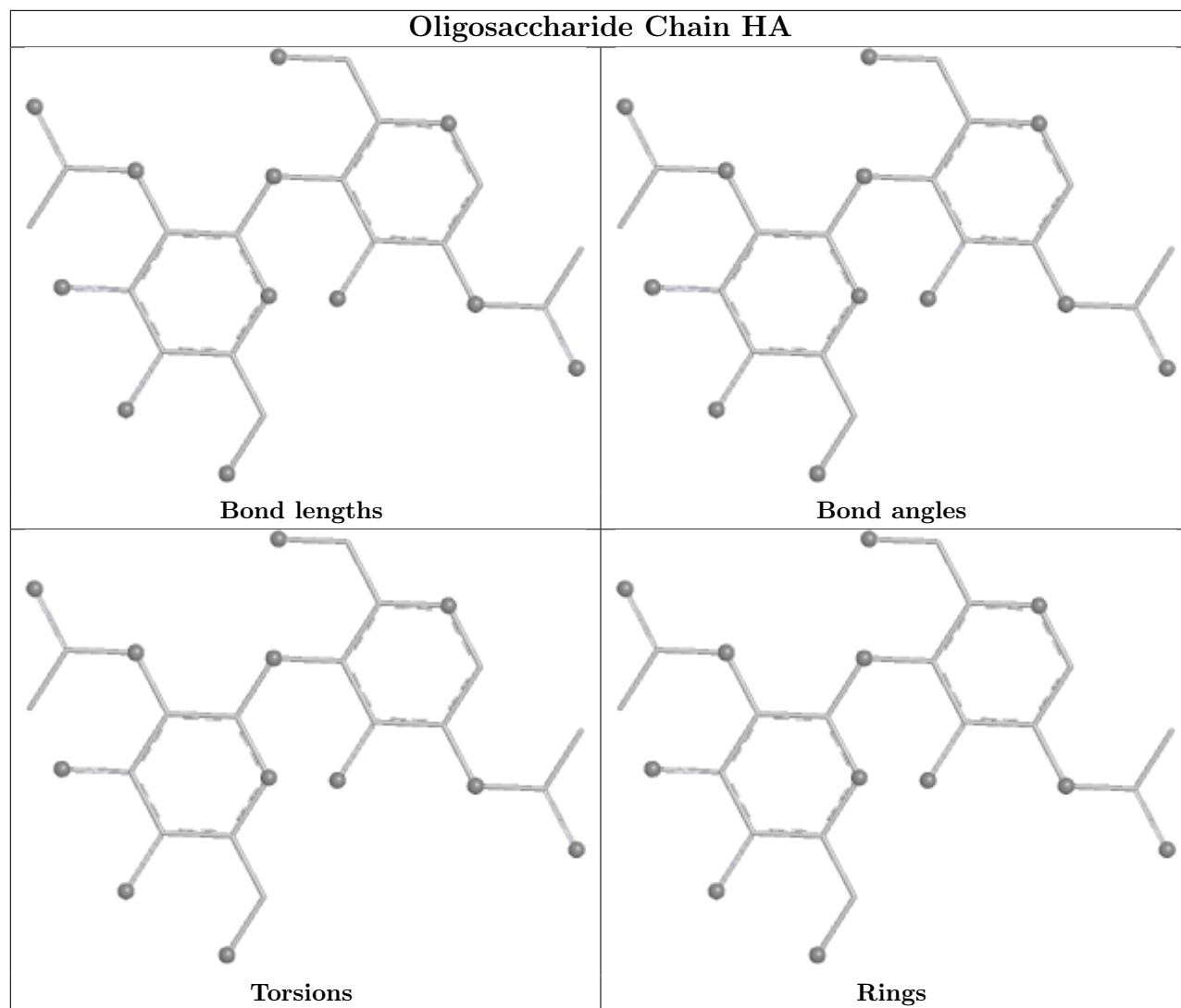


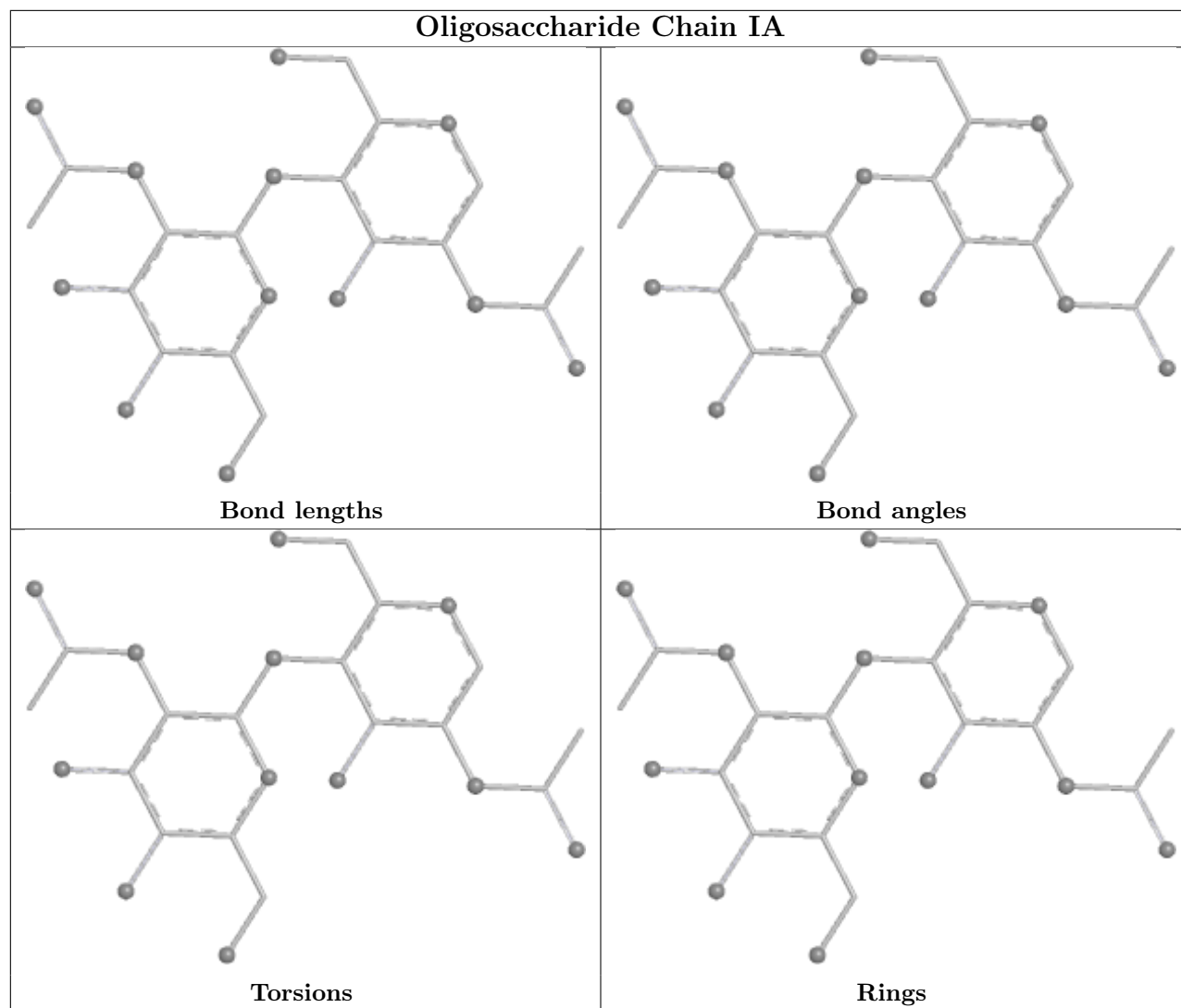


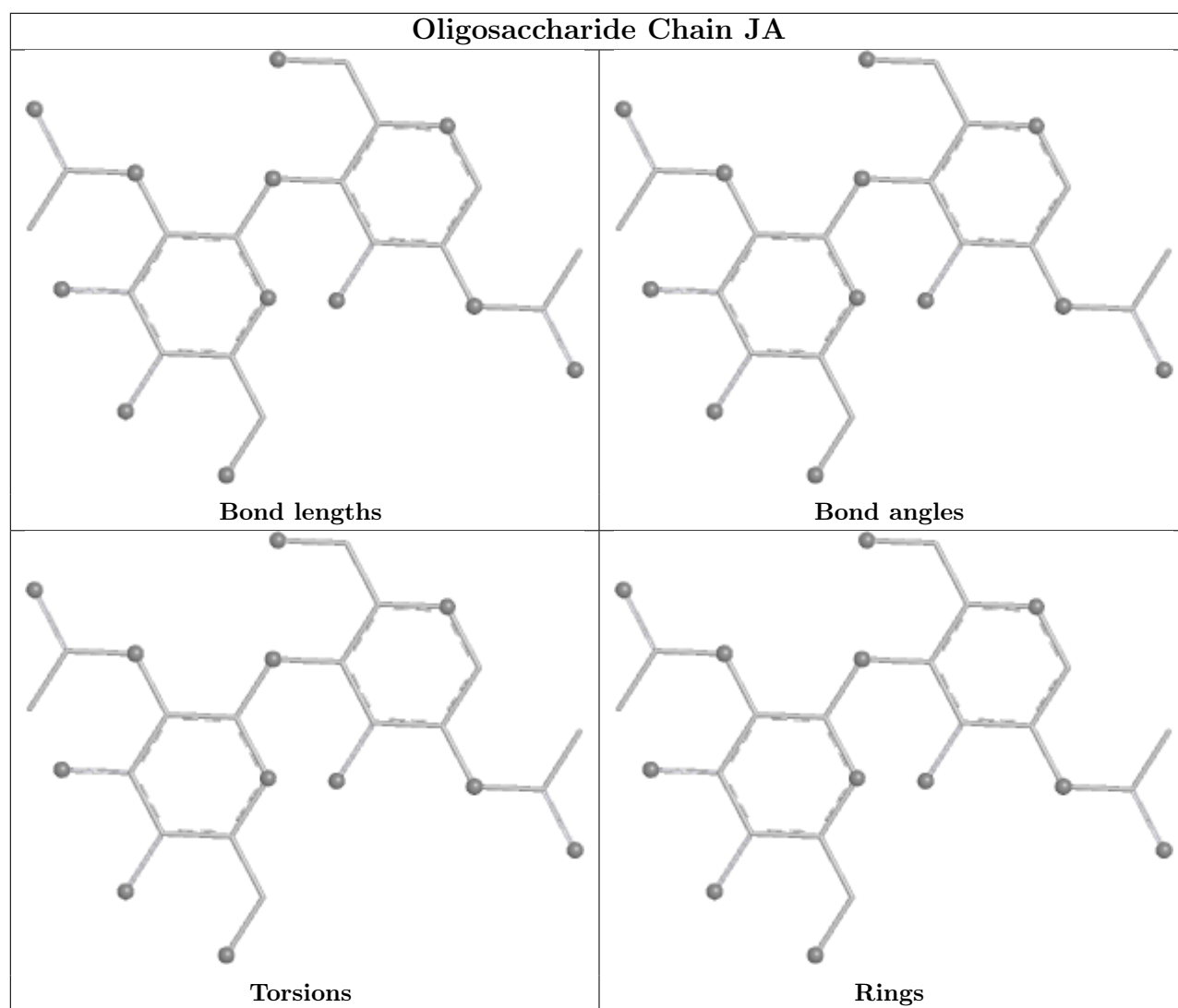


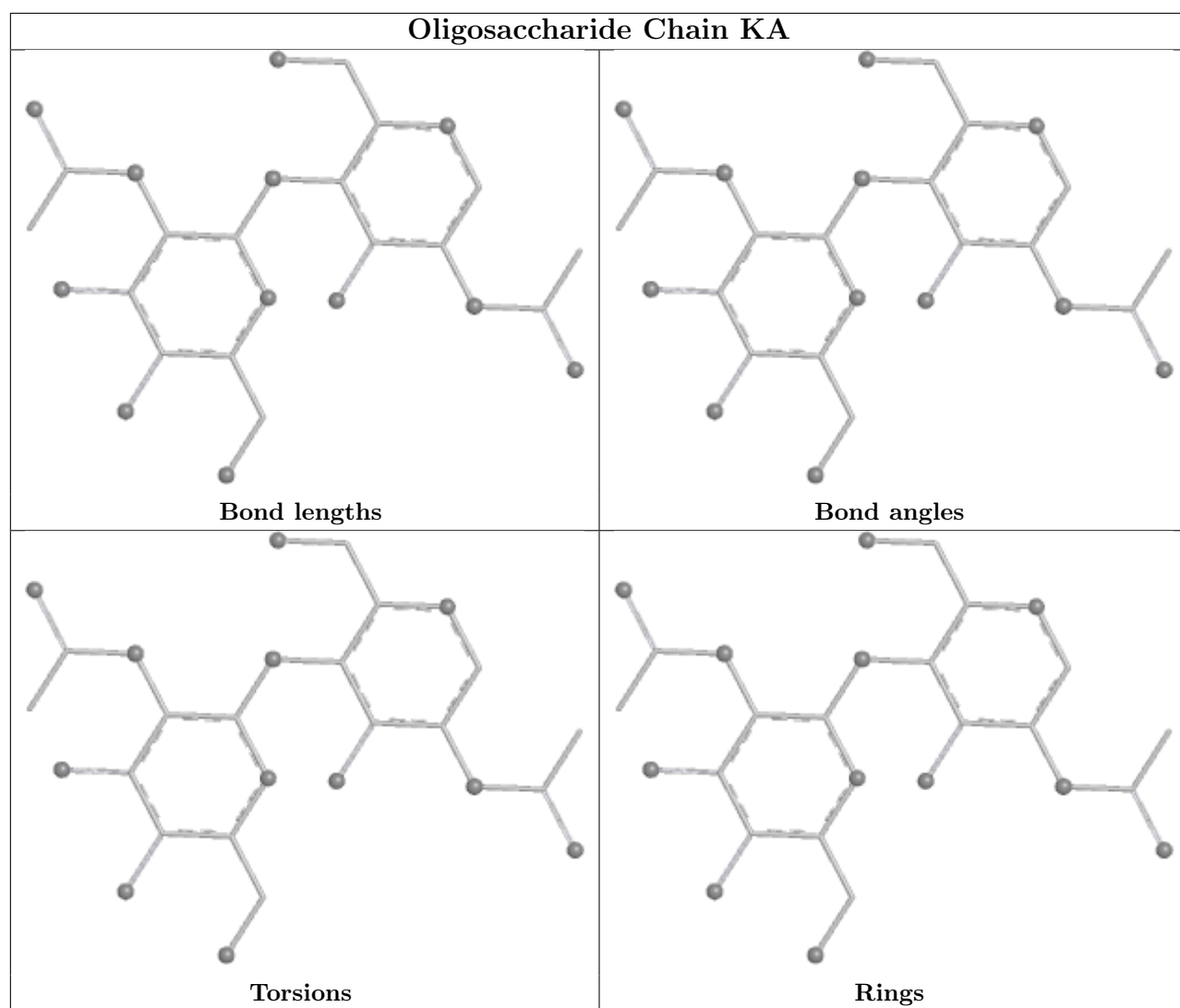


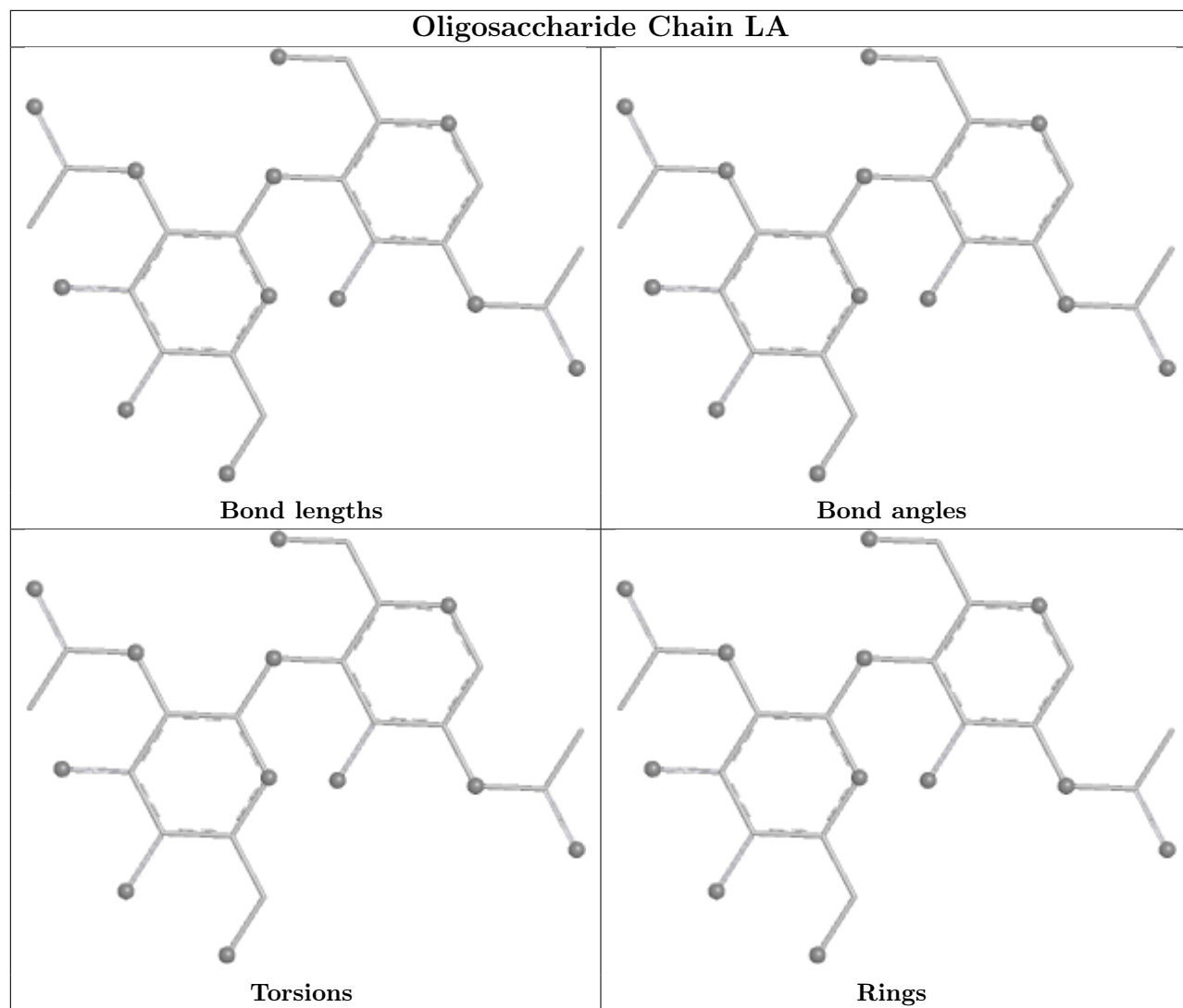


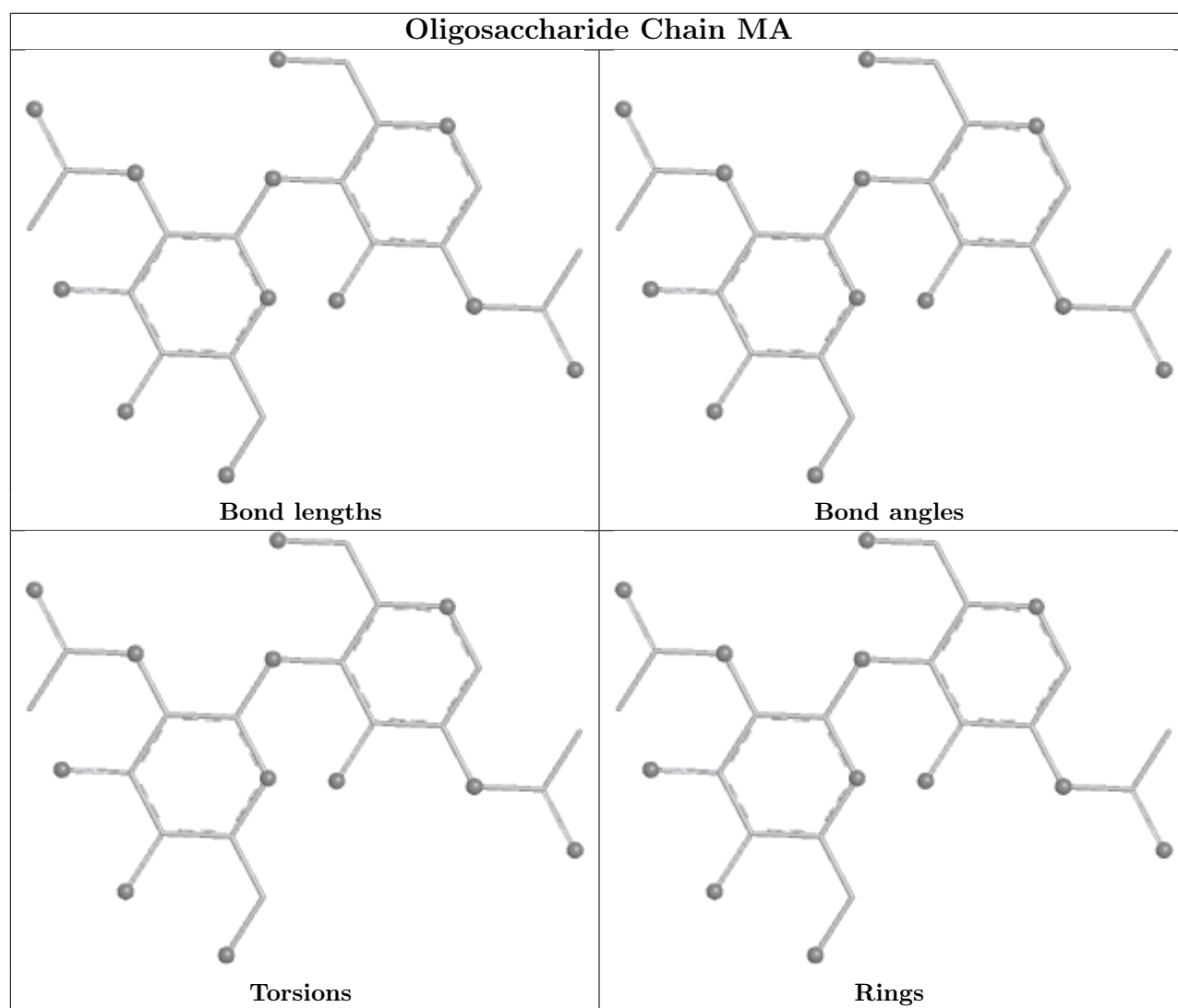


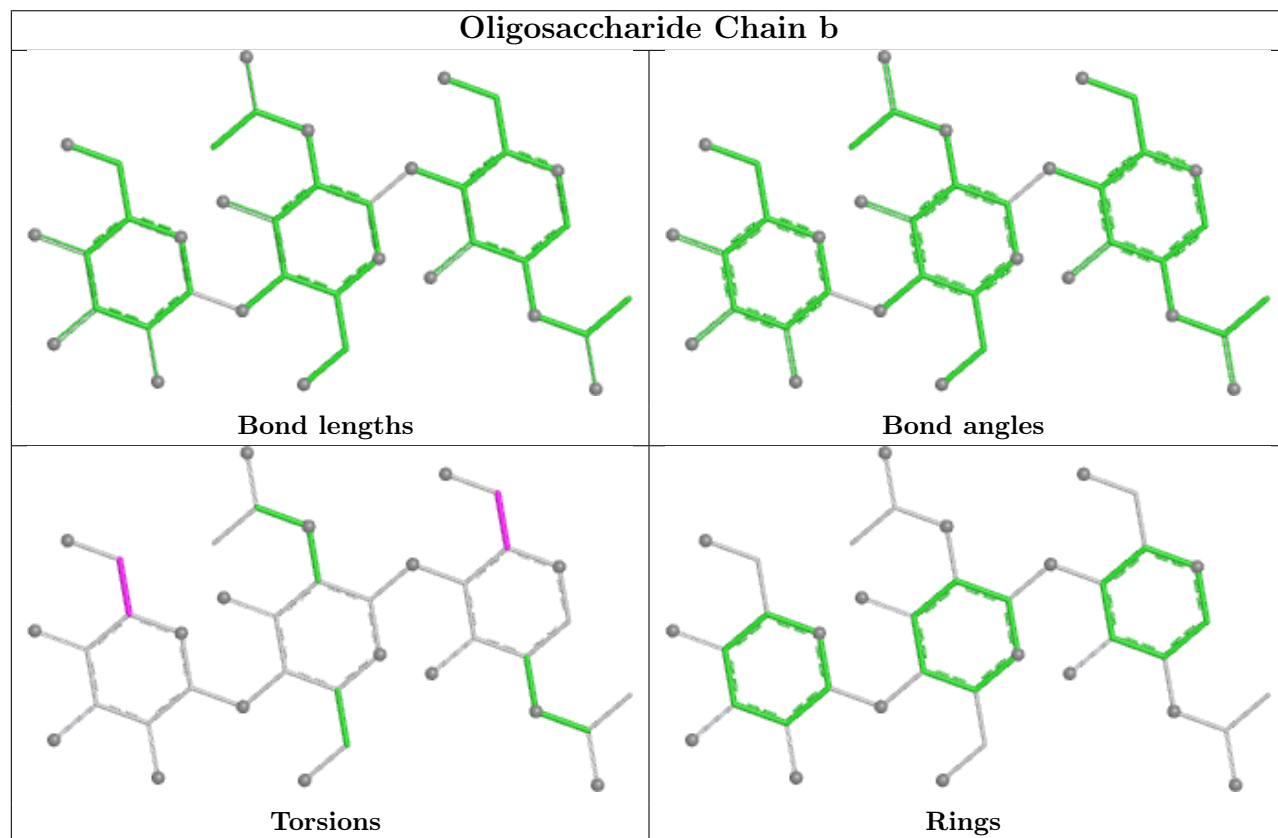
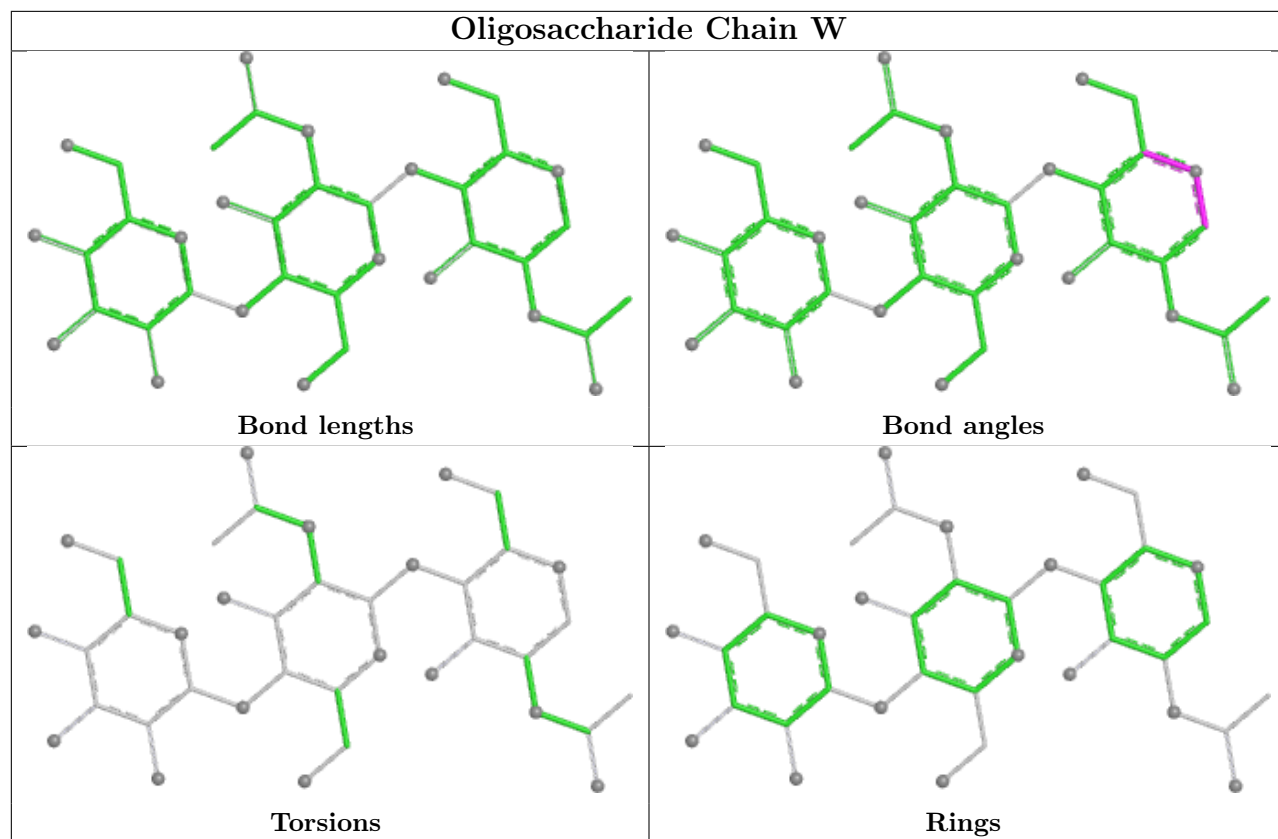


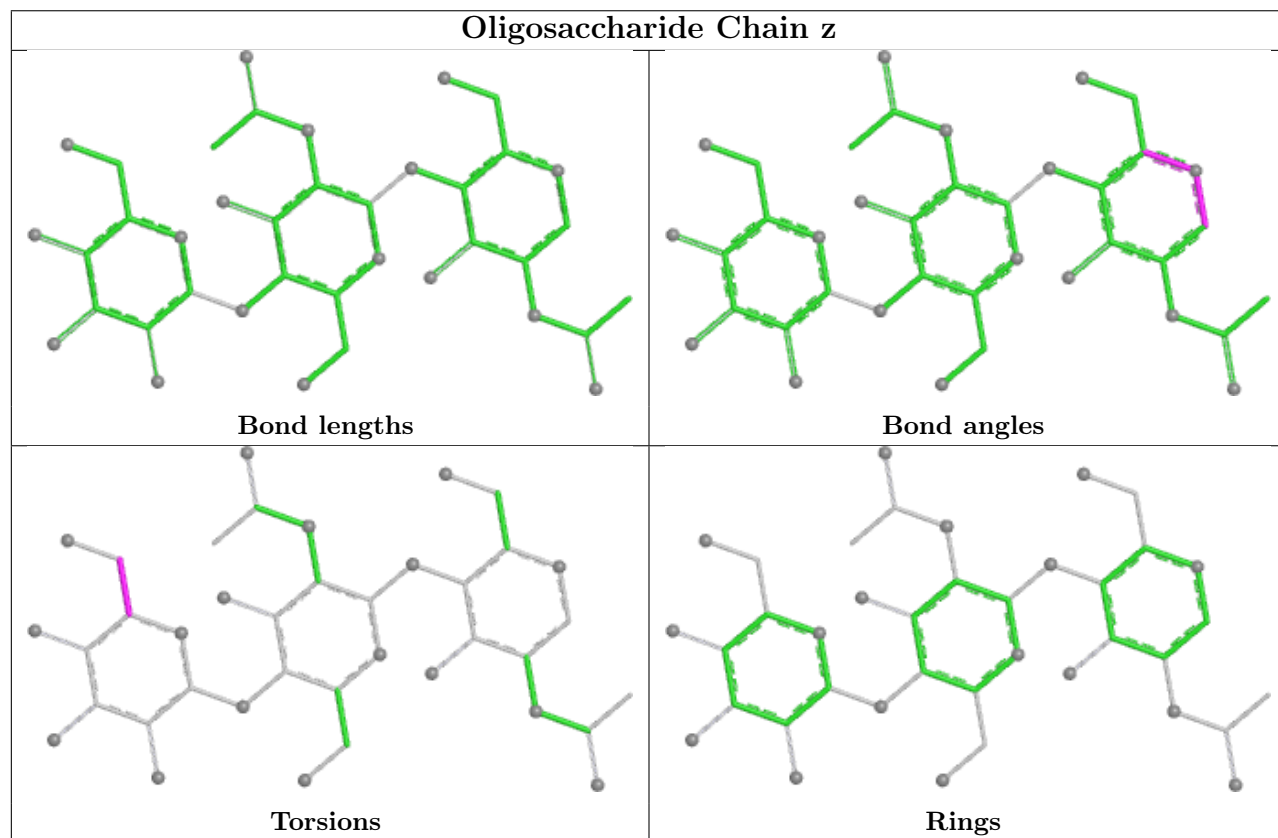
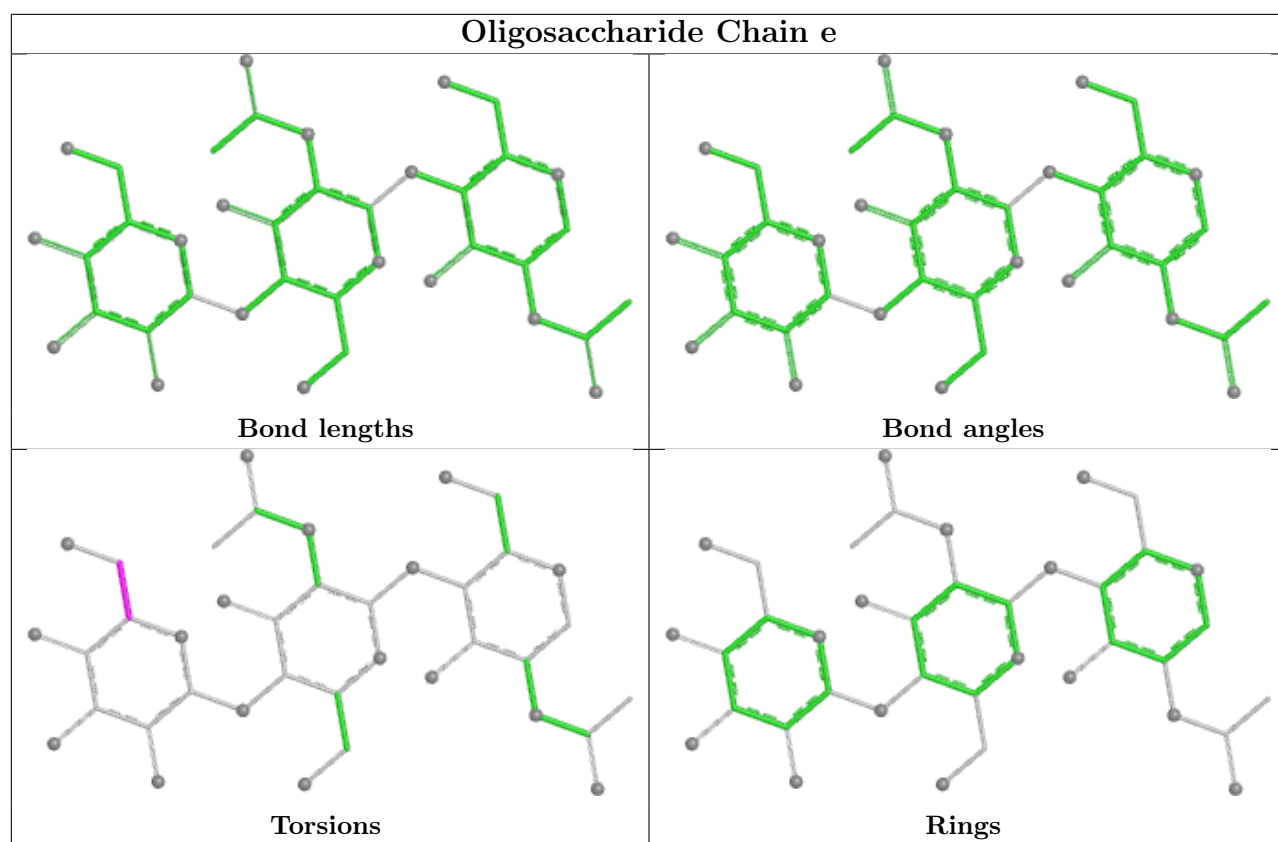


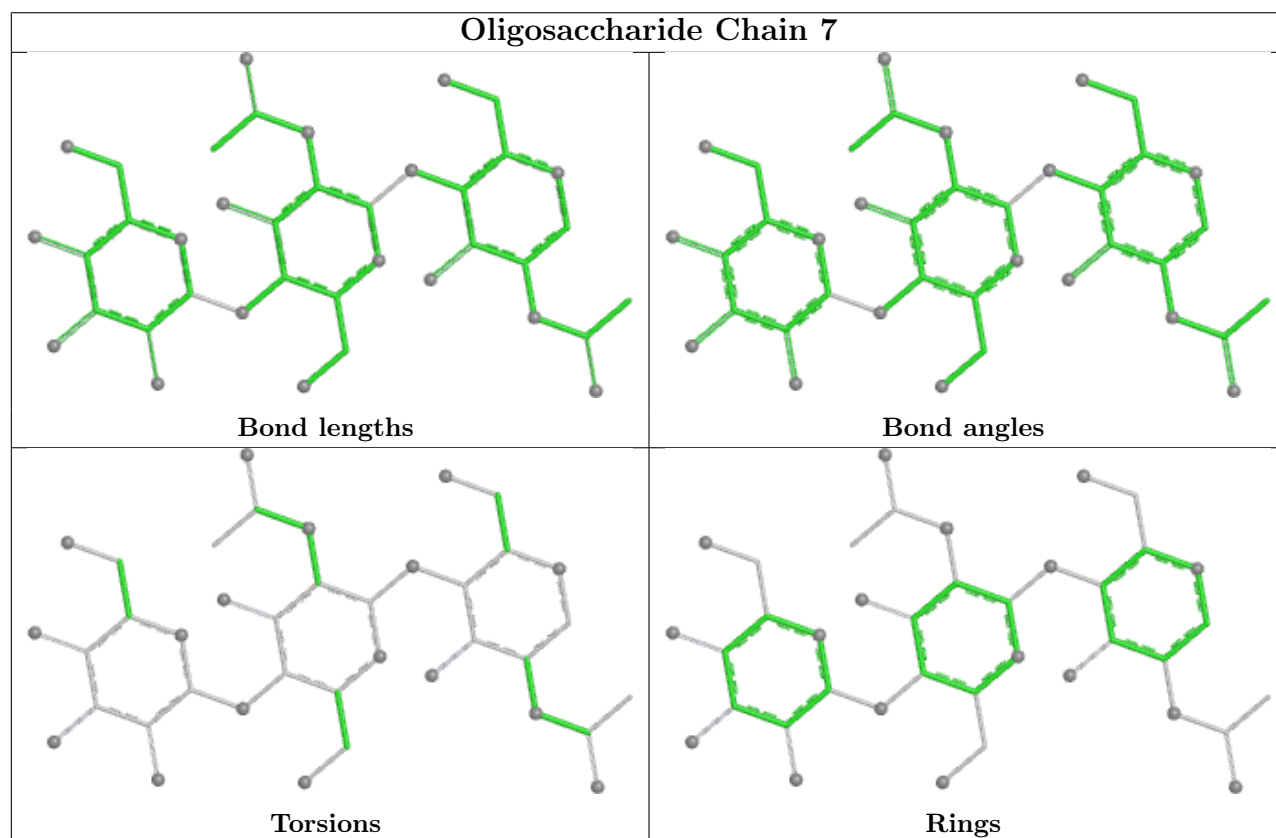
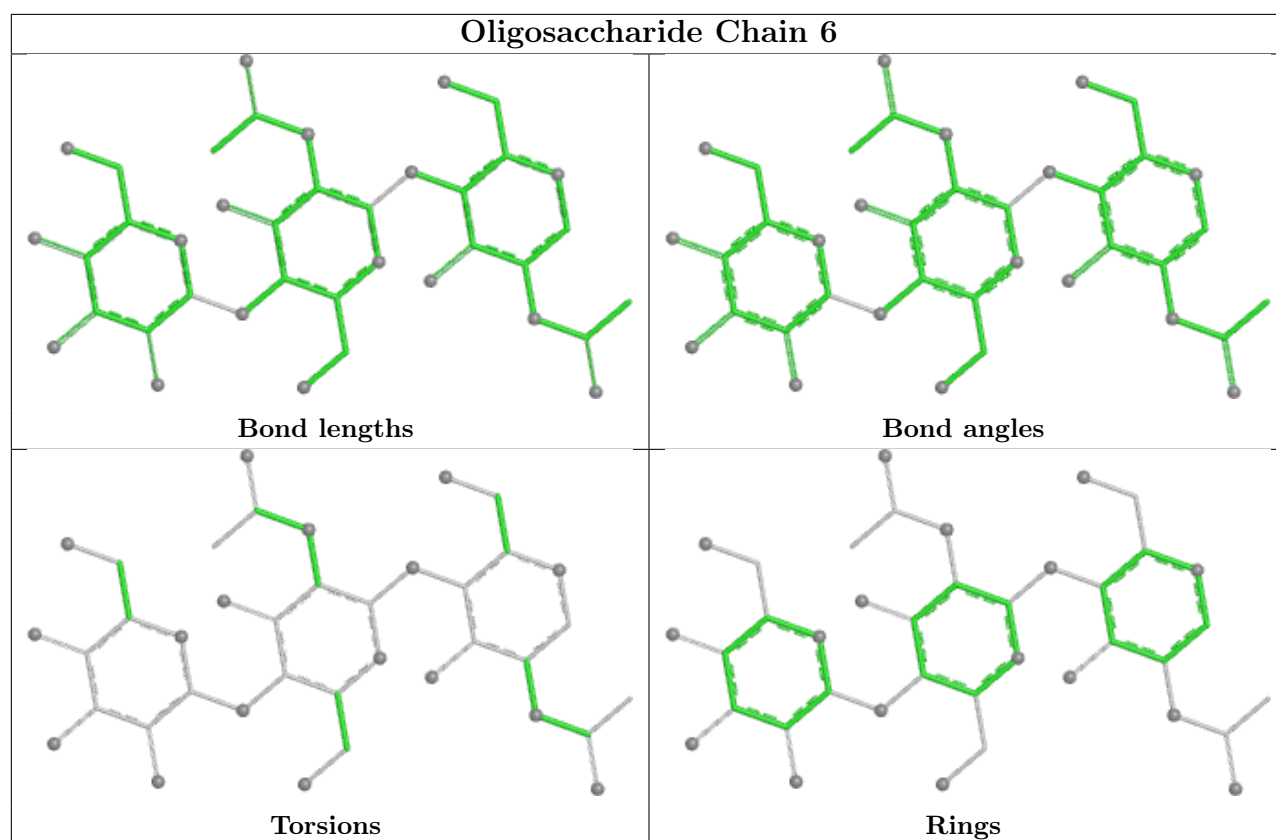


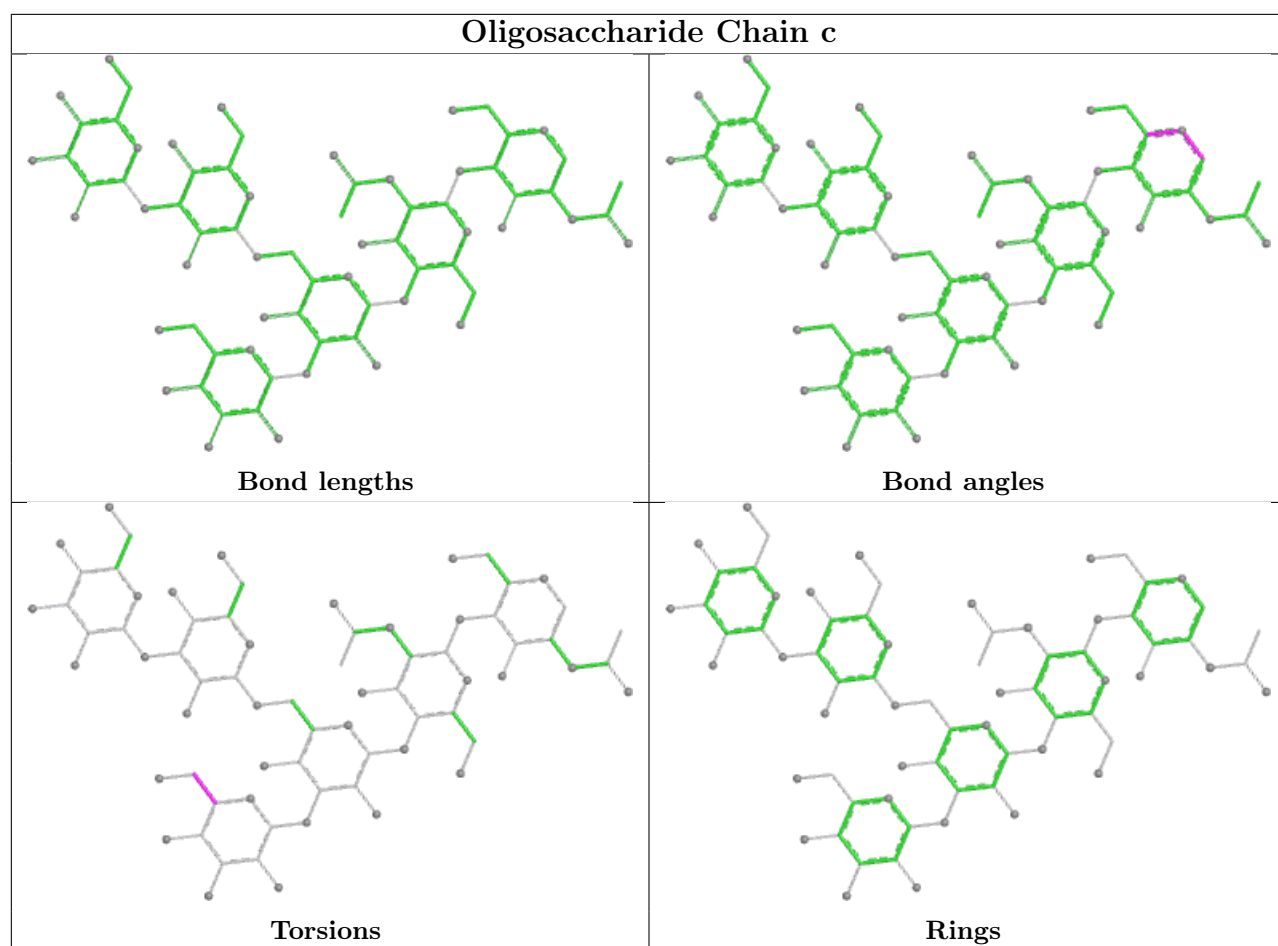


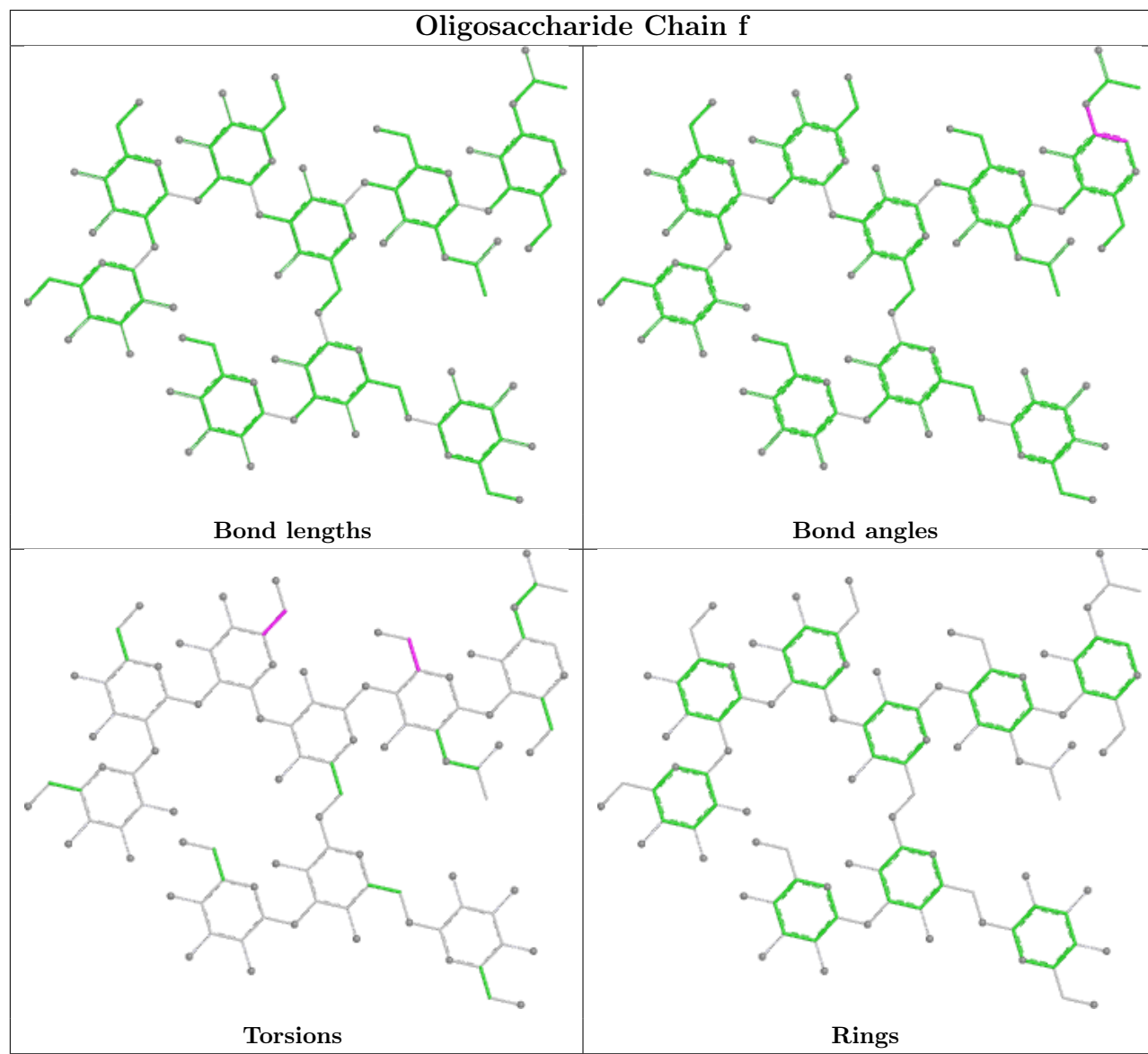


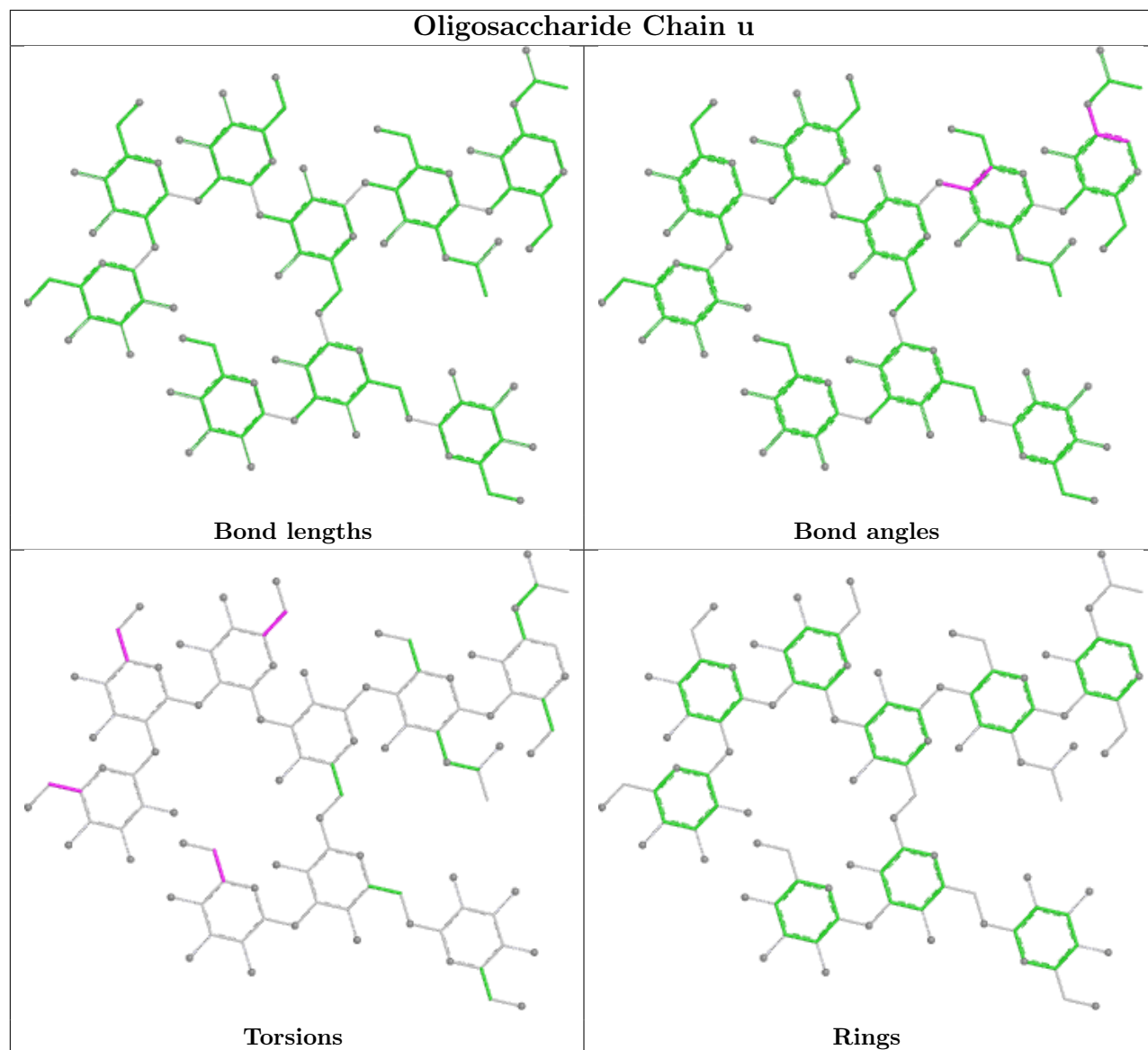


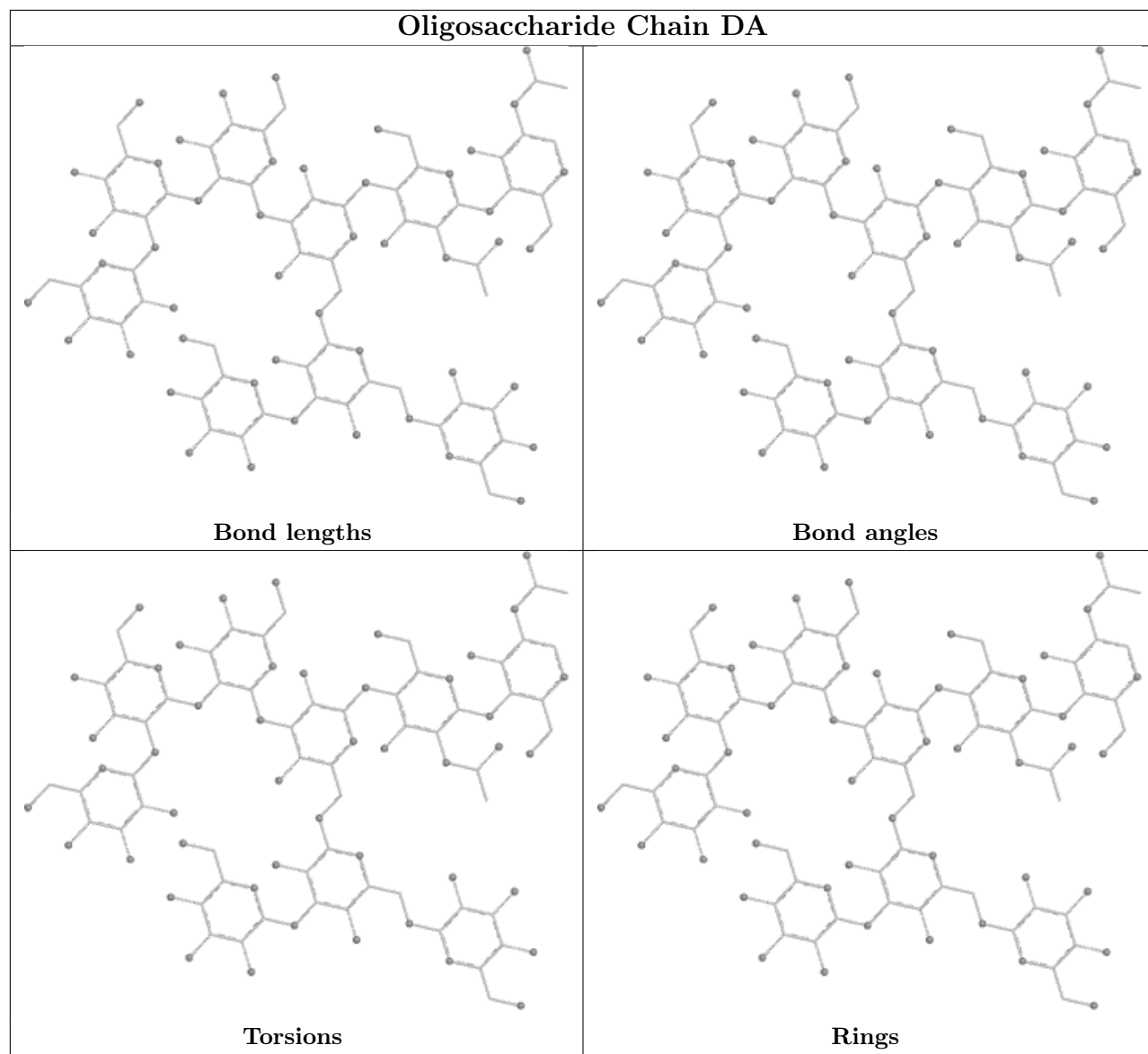


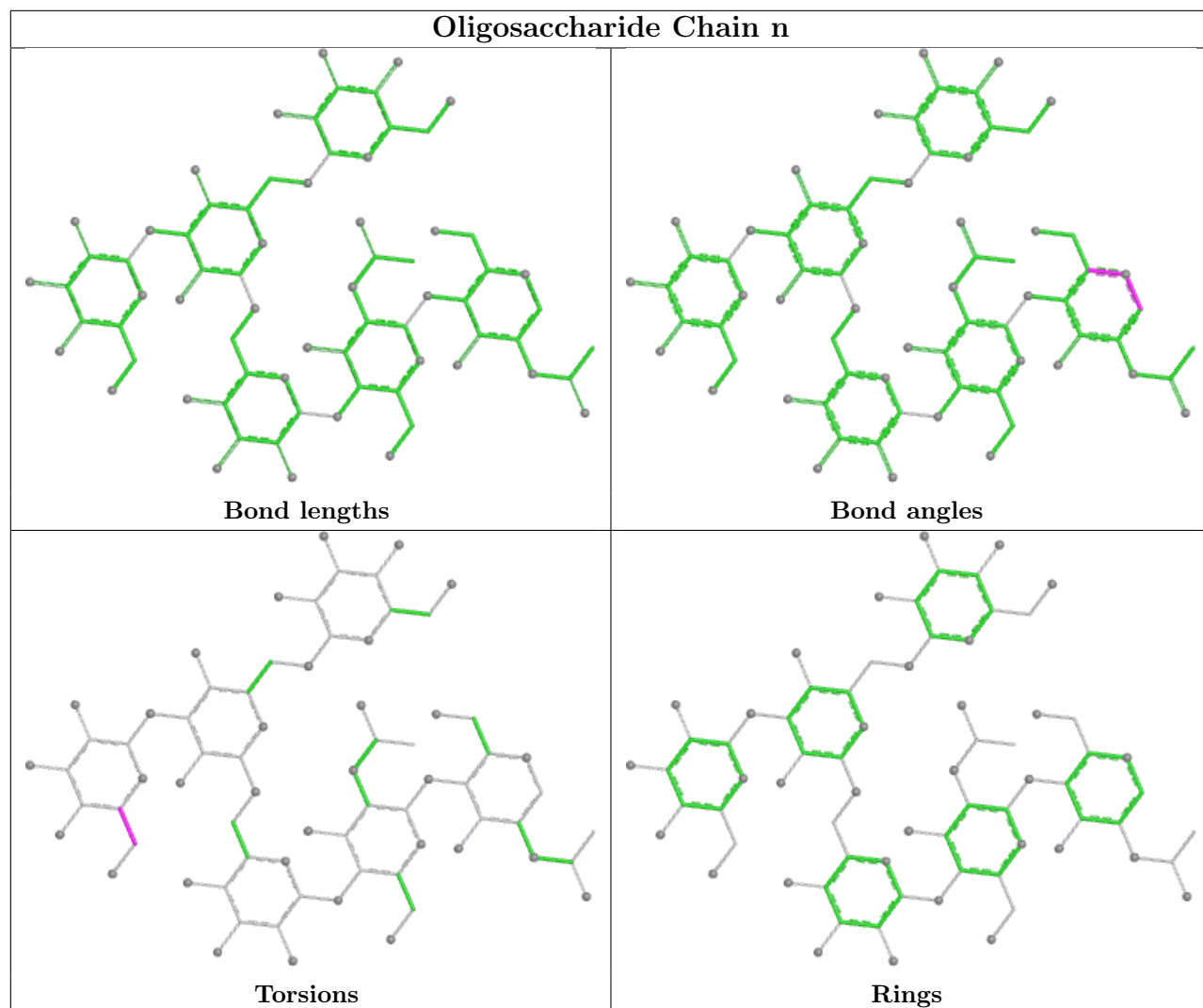


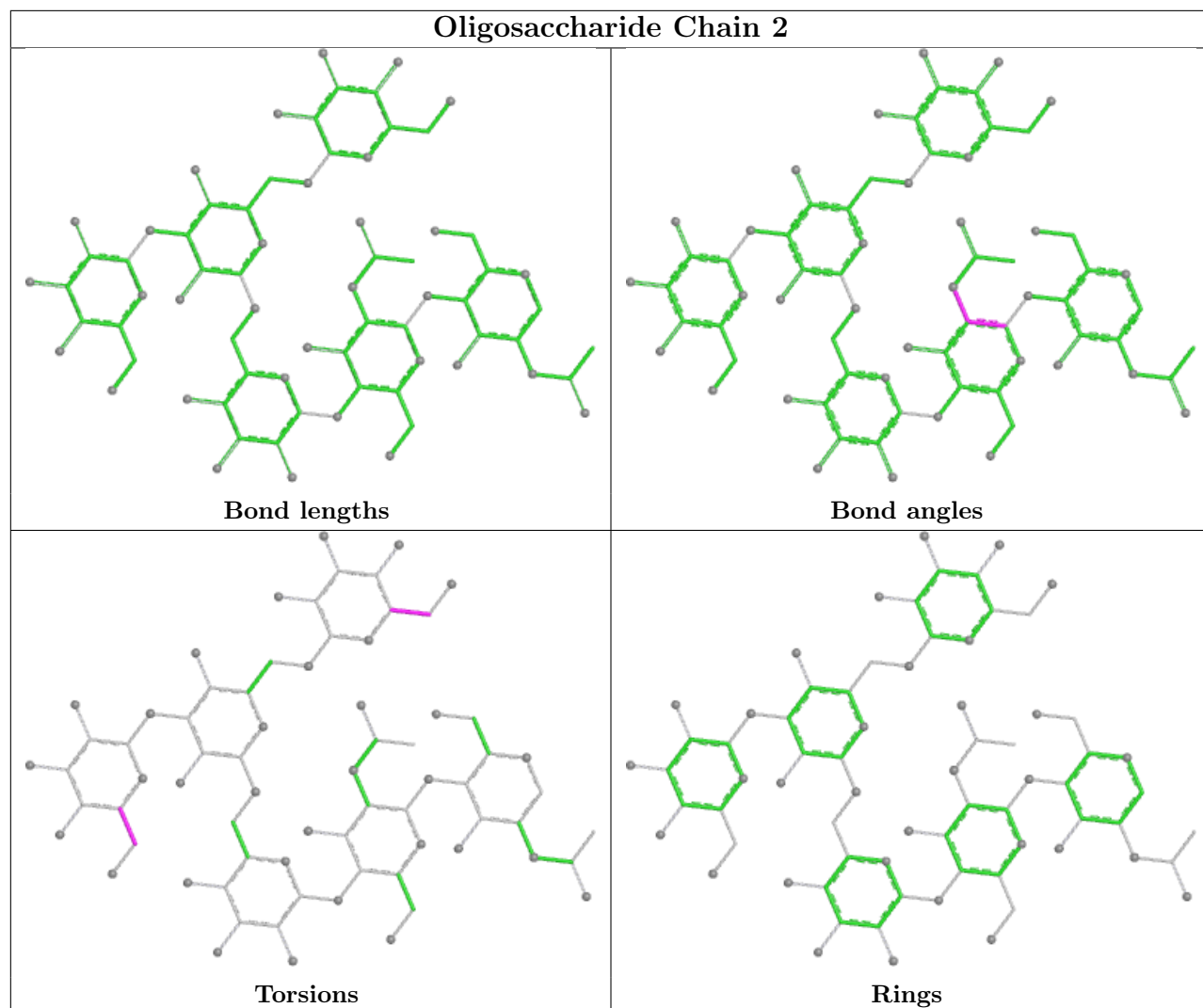


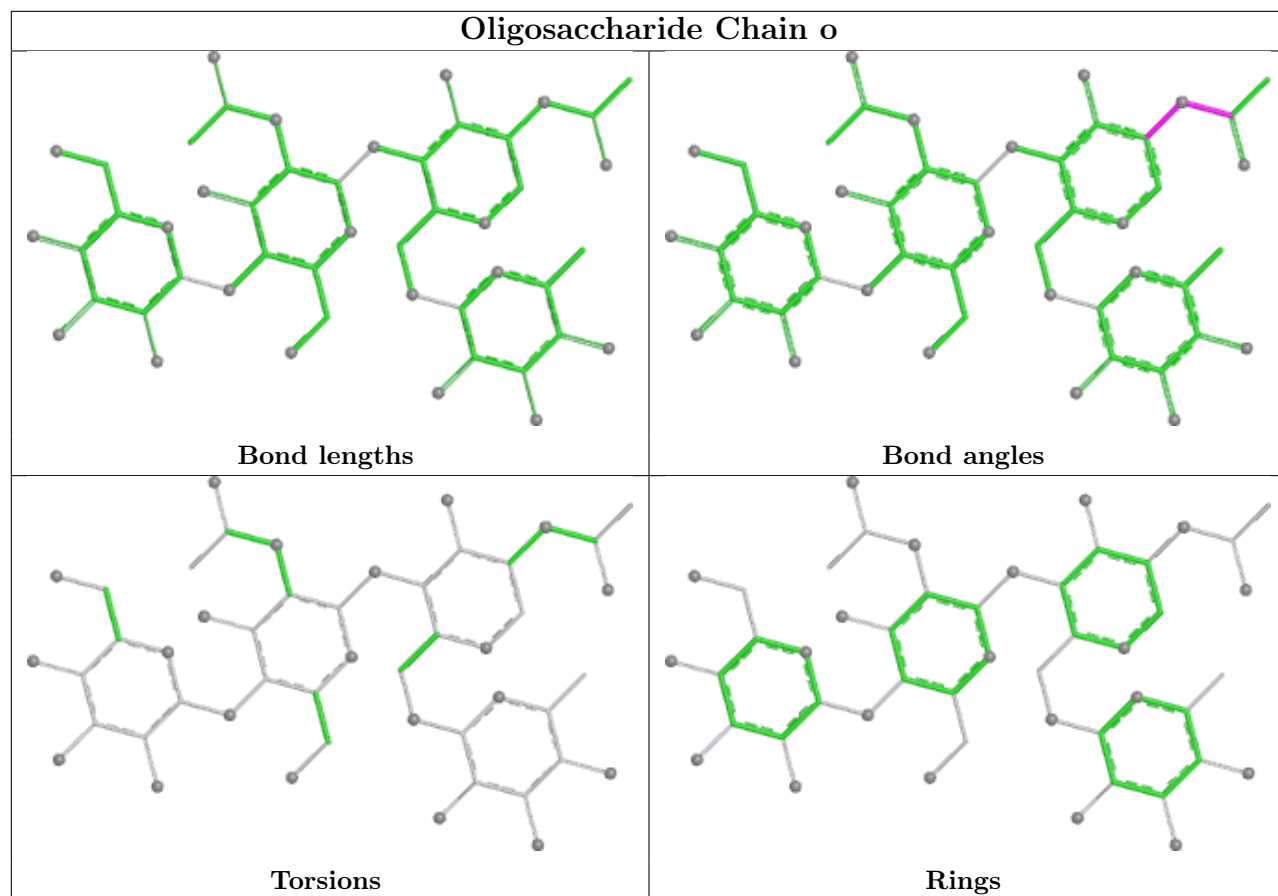


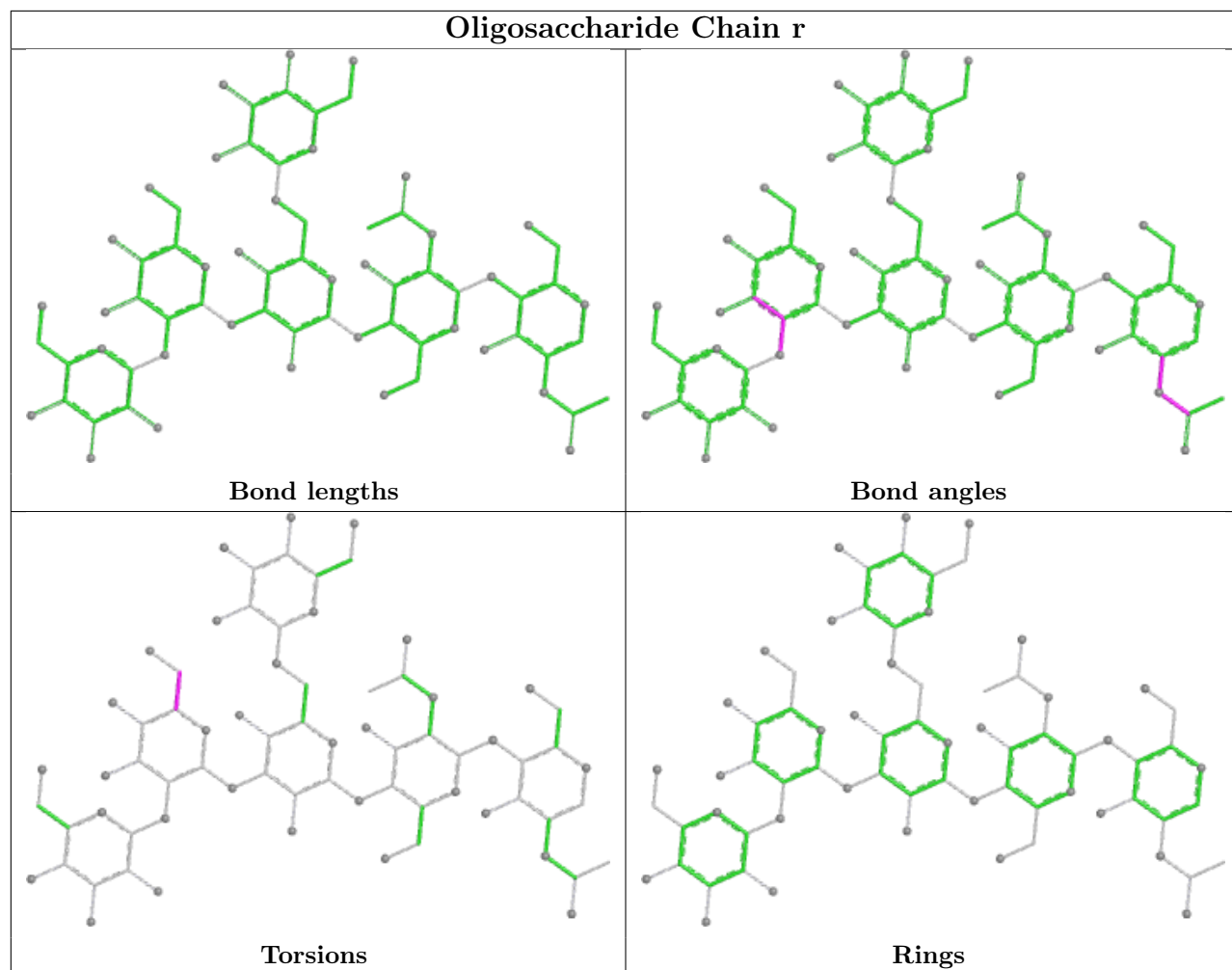


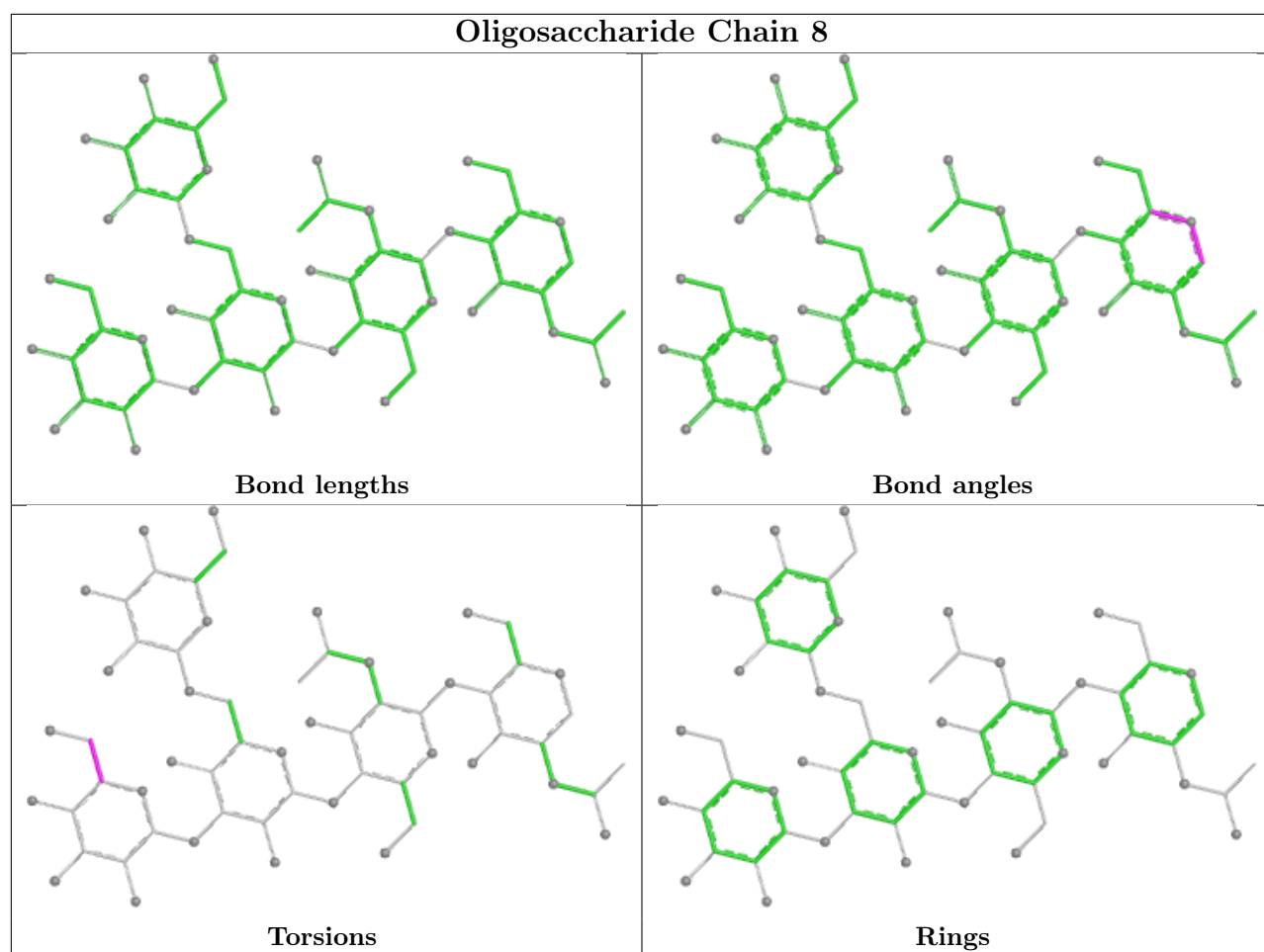


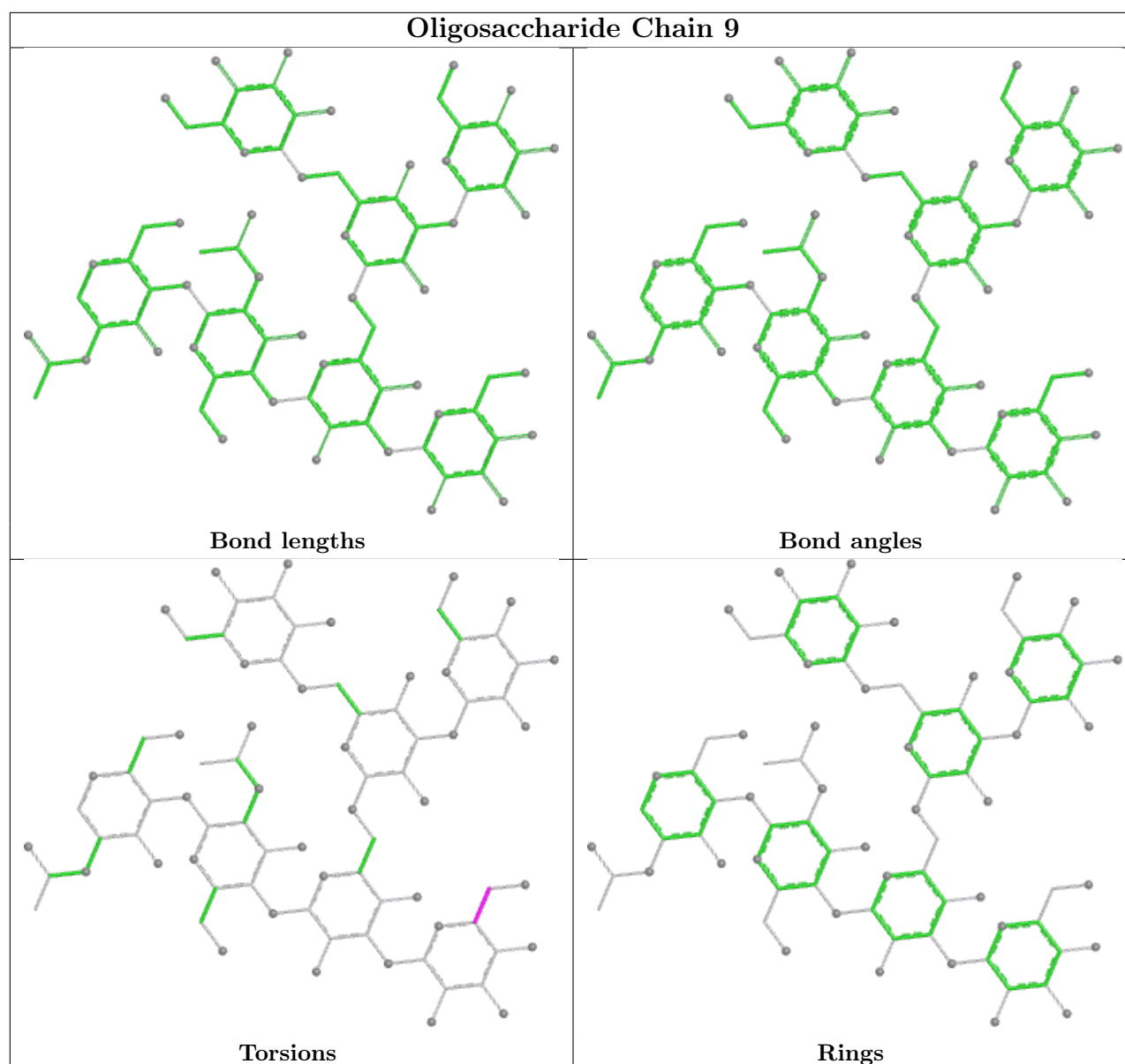












5.6 Ligand geometry [i](#)

10 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
18	NAG	A	603	7	14,14,15	0.40	0	17,19,21	0.73	0
18	NAG	C	602	7	14,14,15	0.38	0	17,19,21	0.74	0
18	NAG	A	602	7	14,14,15	0.38	0	17,19,21	1.10	2 (11%)
18	NAG	B	701	8	14,14,15	0.39	0	17,19,21	0.80	1 (5%)
18	NAG	A	604	7	14,14,15	0.37	0	17,19,21	0.56	0
18	NAG	C	601	7	14,14,15	0.38	0	17,19,21	0.53	0
18	NAG	J	301	4	14,14,15	0.38	0	17,19,21	0.55	0
18	NAG	E	601	7	14,14,15	0.39	0	17,19,21	1.04	1 (5%)
18	NAG	E	602	7	14,14,15	0.38	0	17,19,21	0.67	0
18	NAG	A	601	7	14,14,15	0.39	0	17,19,21	0.61	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
18	NAG	A	603	7	-	1/6/23/26	0/1/1/1
18	NAG	C	602	7	-	0/6/23/26	0/1/1/1
18	NAG	A	602	7	-	1/6/23/26	0/1/1/1
18	NAG	B	701	8	-	1/6/23/26	0/1/1/1
18	NAG	A	604	7	-	0/6/23/26	0/1/1/1
18	NAG	C	601	7	-	0/6/23/26	0/1/1/1
18	NAG	J	301	4	-	0/6/23/26	0/1/1/1
18	NAG	E	601	7	-	0/6/23/26	0/1/1/1
18	NAG	E	602	7	-	1/6/23/26	0/1/1/1
18	NAG	A	601	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	E	601	NAG	C2-N2-C7	-3.19	118.62	122.90
18	A	602	NAG	C1-C2-N2	2.62	114.56	110.43
18	B	701	NAG	C1-O5-C5	2.25	115.20	112.19
18	A	602	NAG	C2-N2-C7	-2.14	120.04	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	E	602	NAG	O5-C5-C6-O6
18	A	602	NAG	O5-C5-C6-O6
18	A	603	NAG	O5-C5-C6-O6
18	B	701	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

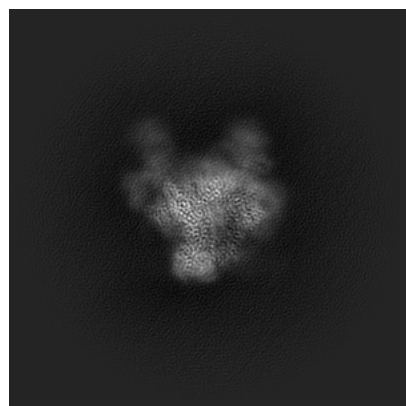
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49238. These allow visual inspection of the internal detail of the map and identification of artifacts.

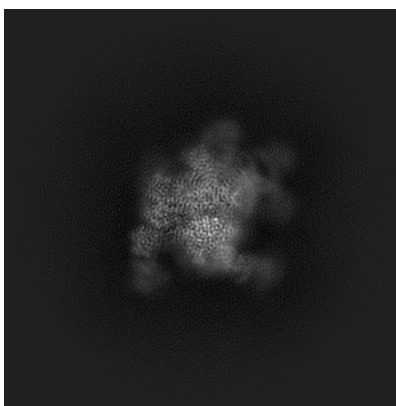
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

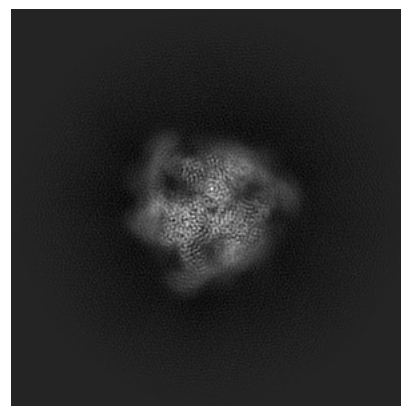
6.1.1 Primary map



X

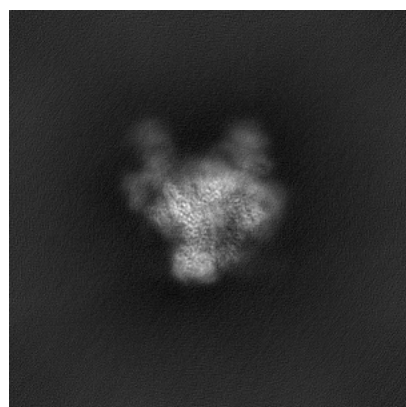


Y

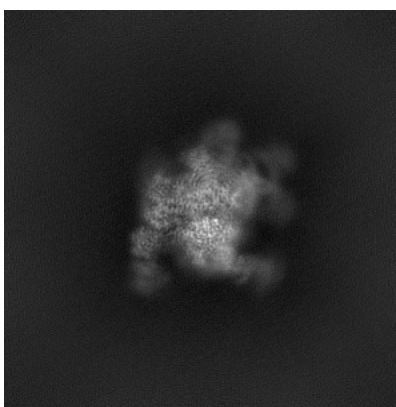


Z

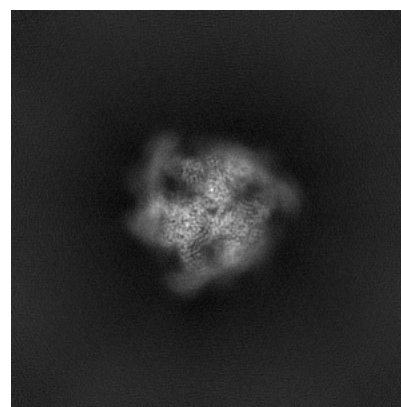
6.1.2 Raw map



X



Y

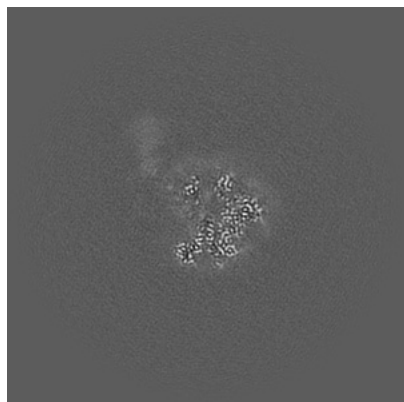


Z

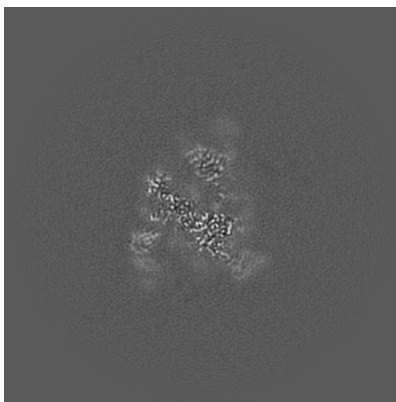
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

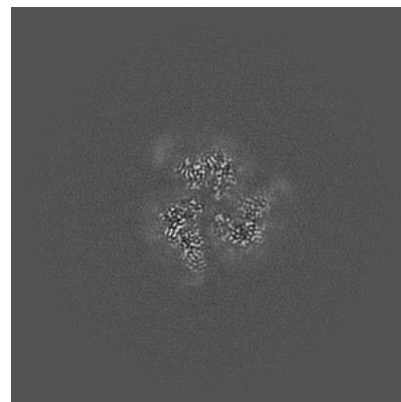
6.2.1 Primary map



X Index: 200

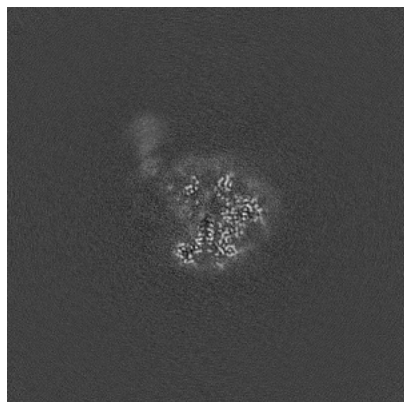


Y Index: 200

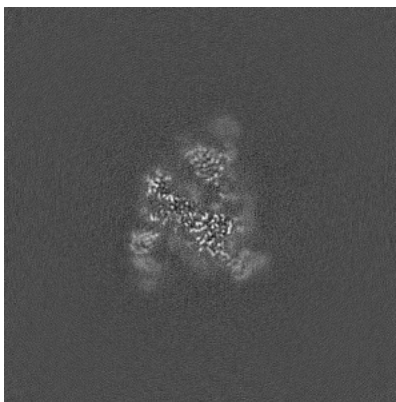


Z Index: 200

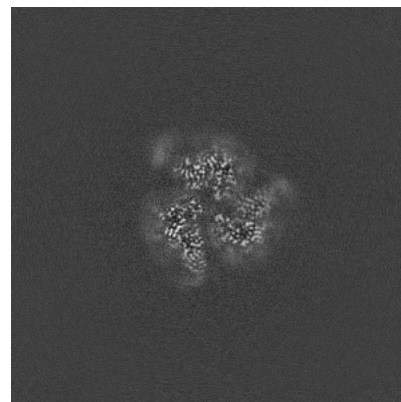
6.2.2 Raw map



X Index: 200



Y Index: 200

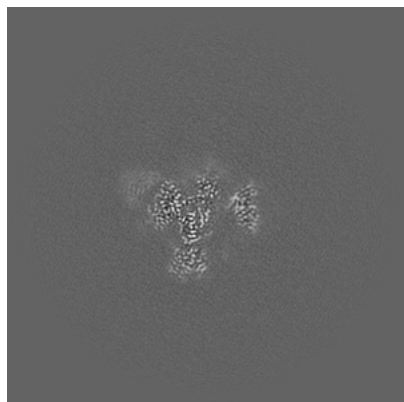


Z Index: 200

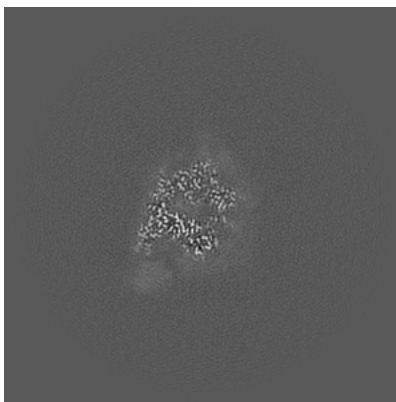
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

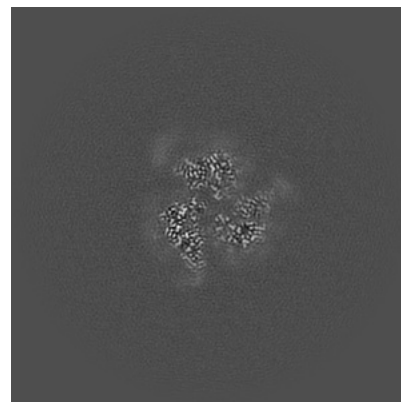
6.3.1 Primary map



X Index: 176

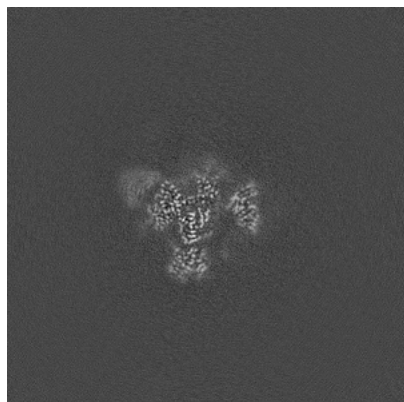


Y Index: 184

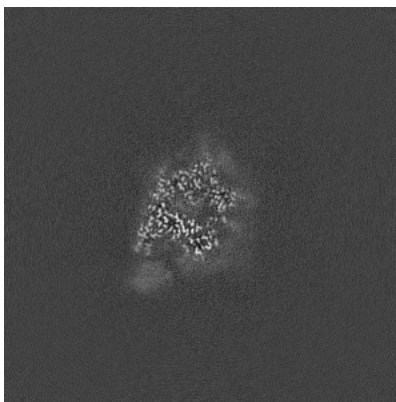


Z Index: 201

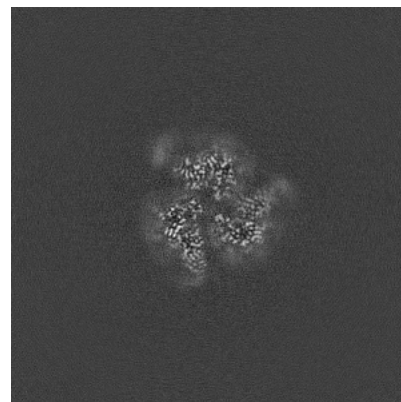
6.3.2 Raw map



X Index: 176



Y Index: 184

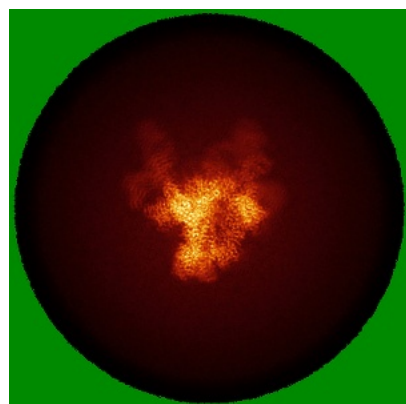


Z Index: 200

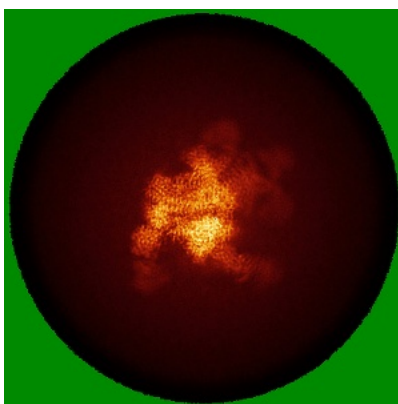
The images above show the largest variance slices of the map in three orthogonal directions.

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

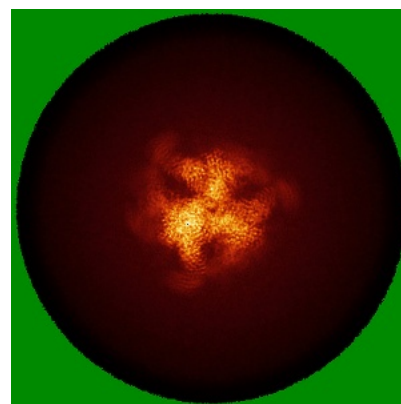
6.4.1 Primary map



X



Y

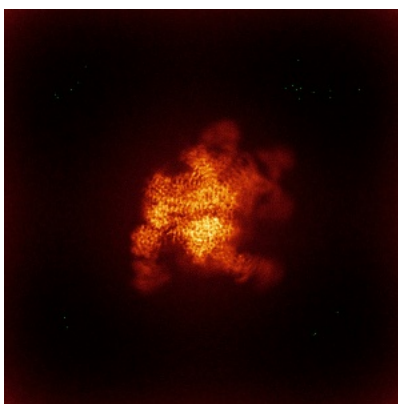


Z

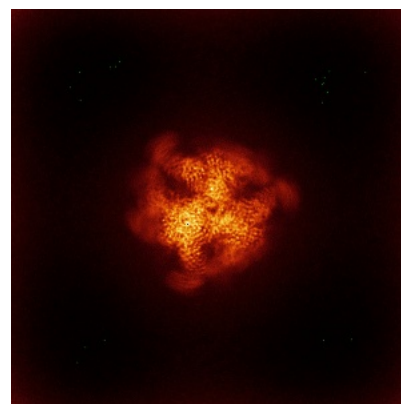
6.4.2 Raw map



X



Y

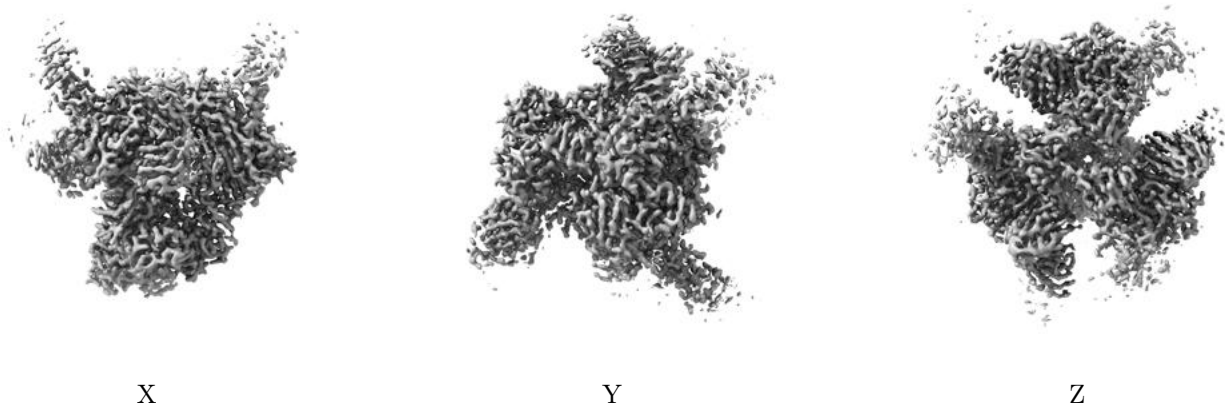


Z

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

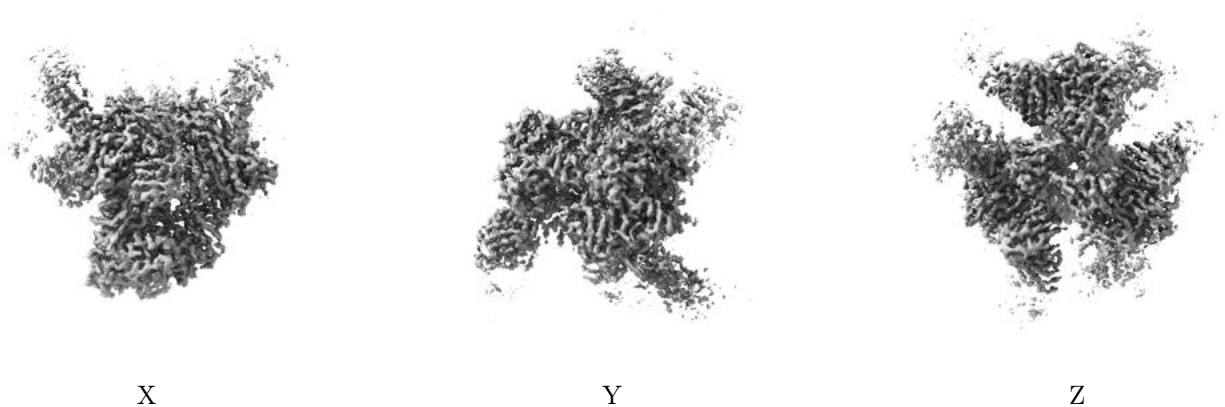
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.44. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

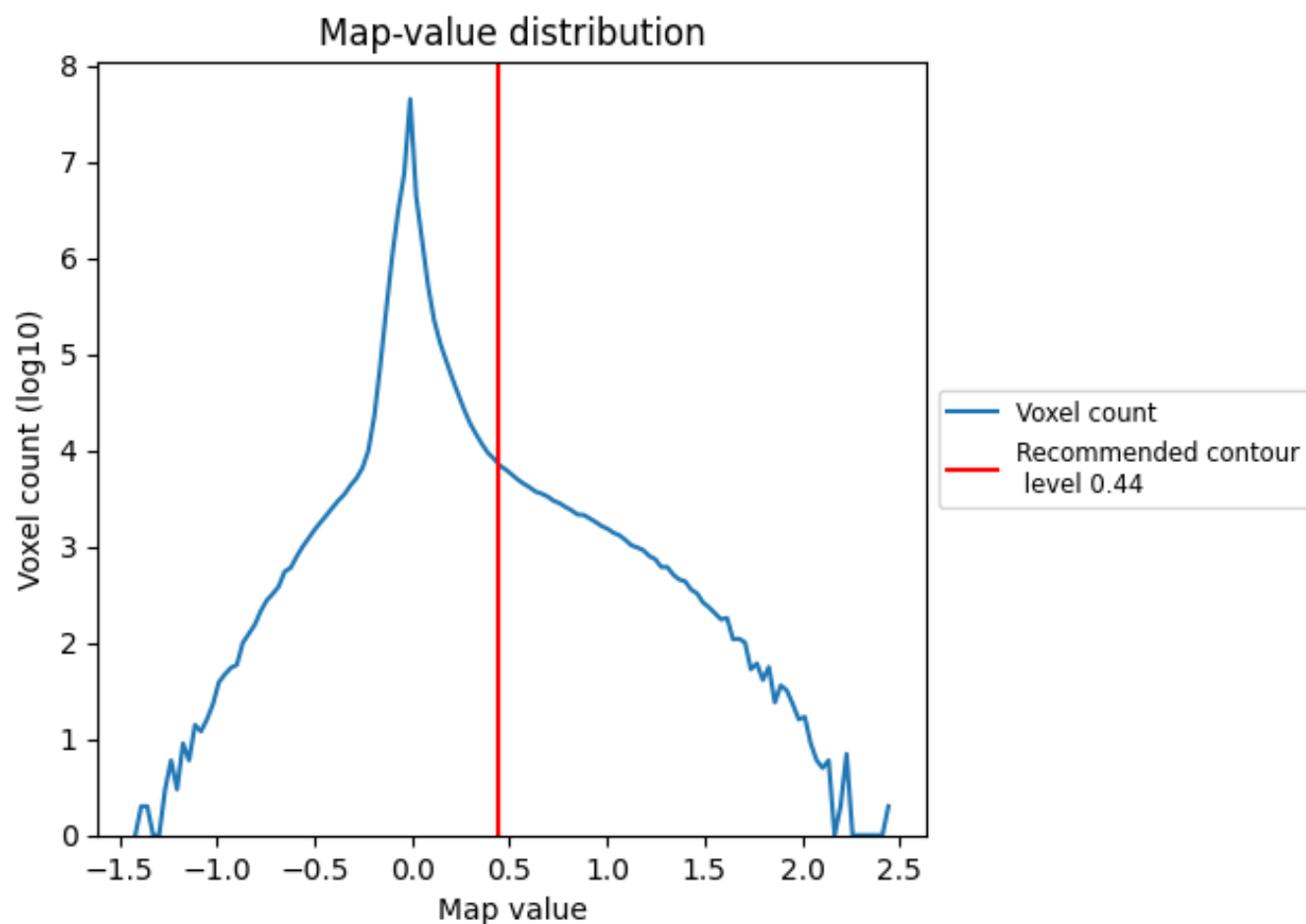
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

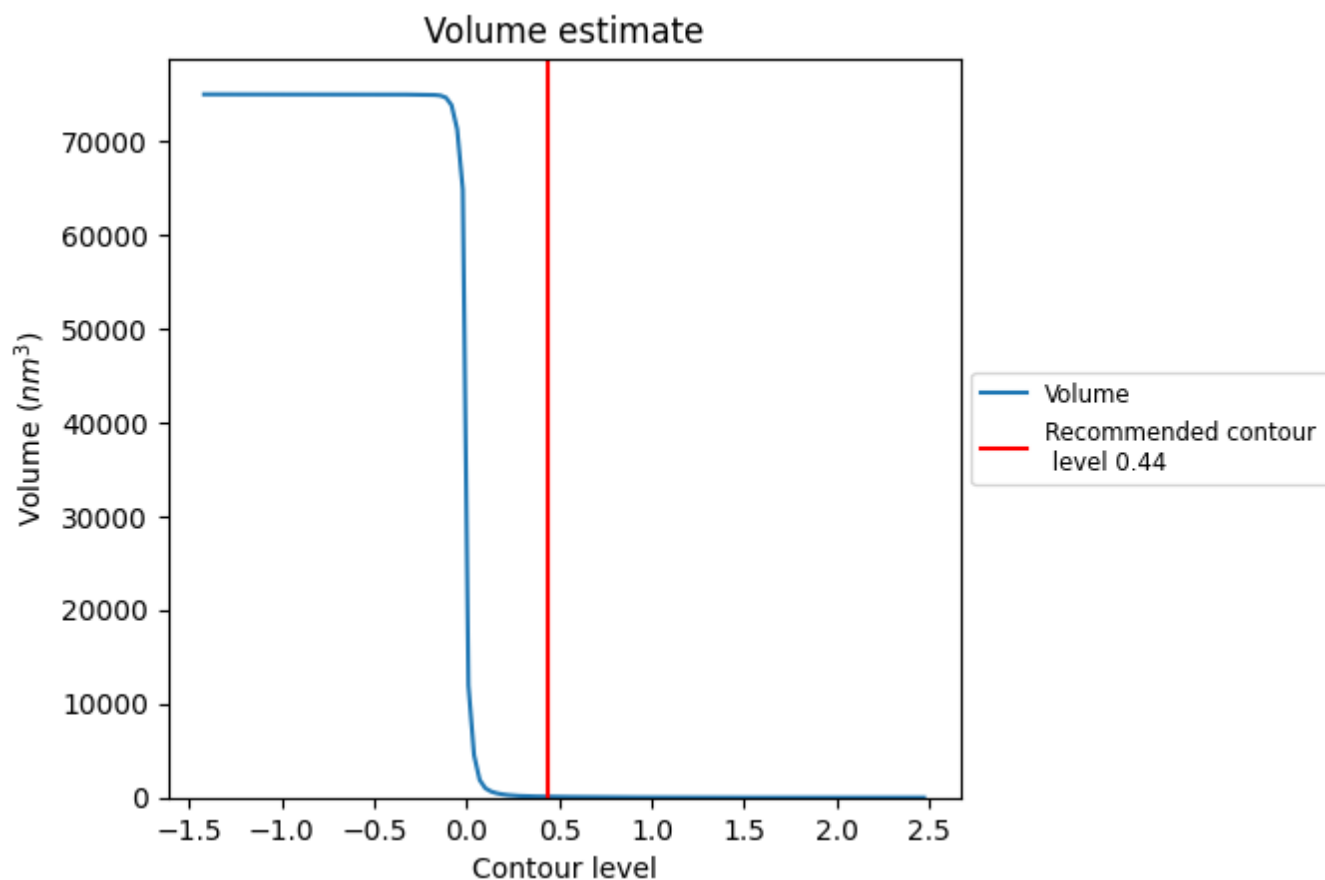
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

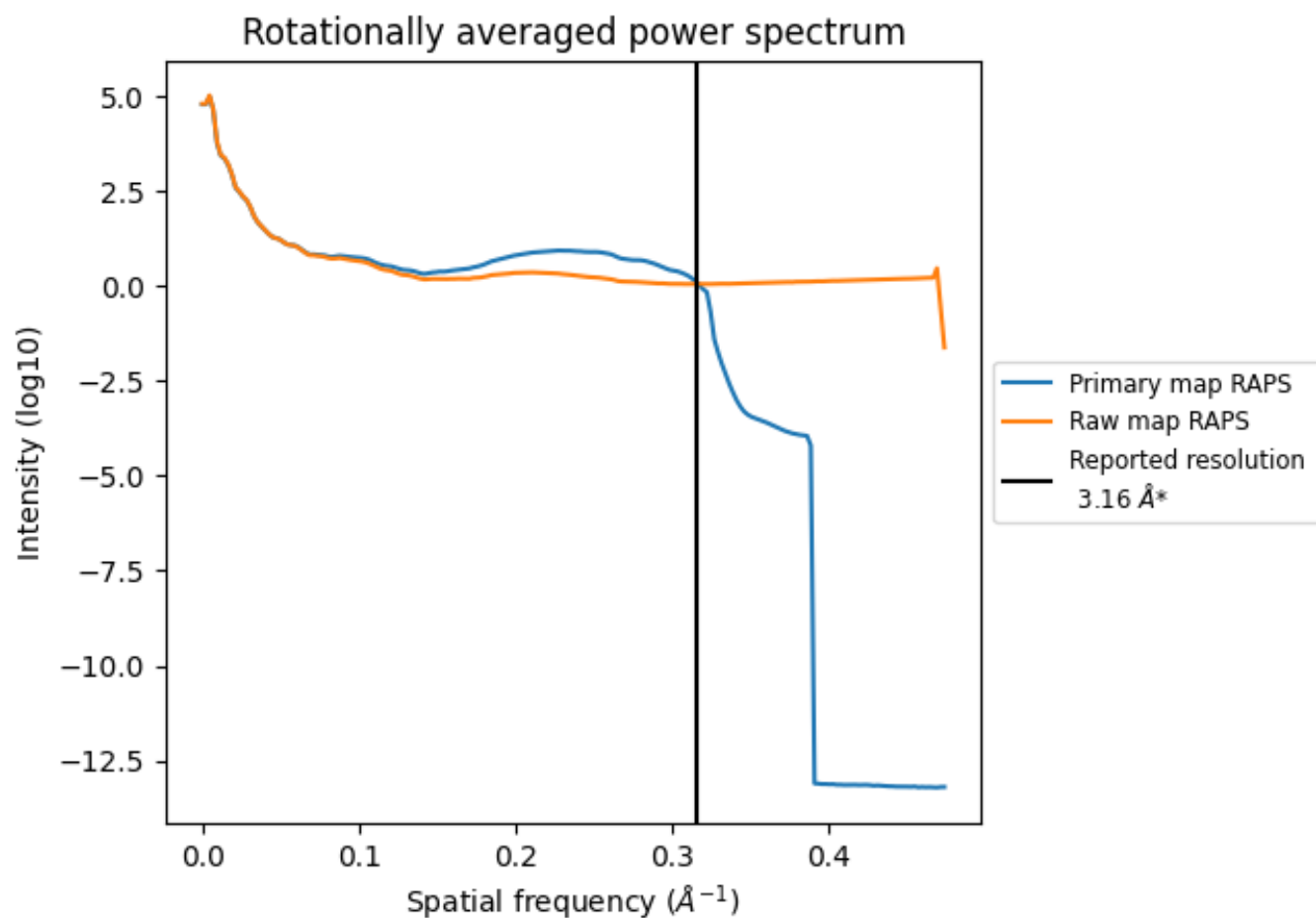
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 95 nm³; this corresponds to an approximate mass of 86 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 ⓘ

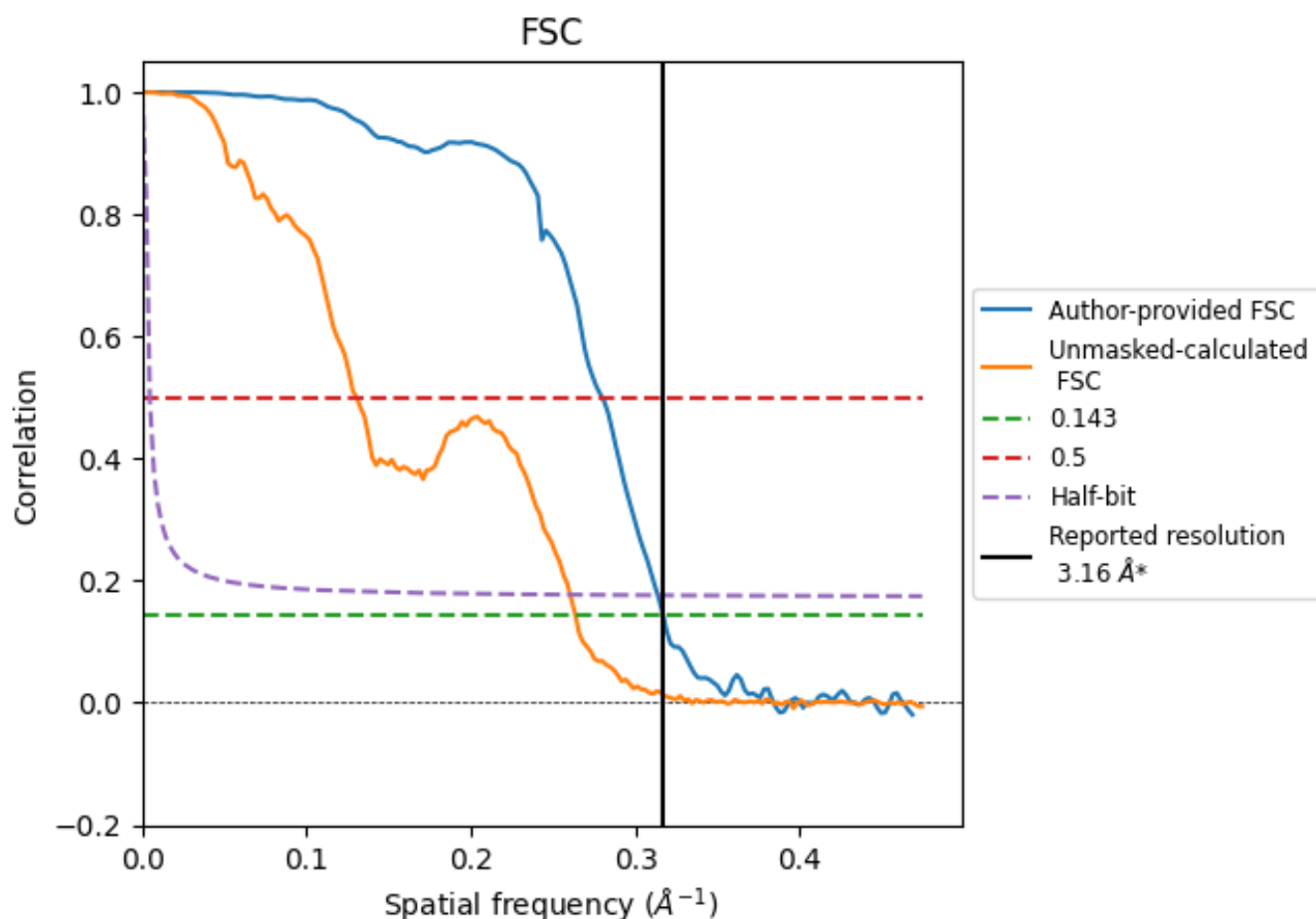


*Reported resolution corresponds to spatial frequency of 0.316 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.316 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

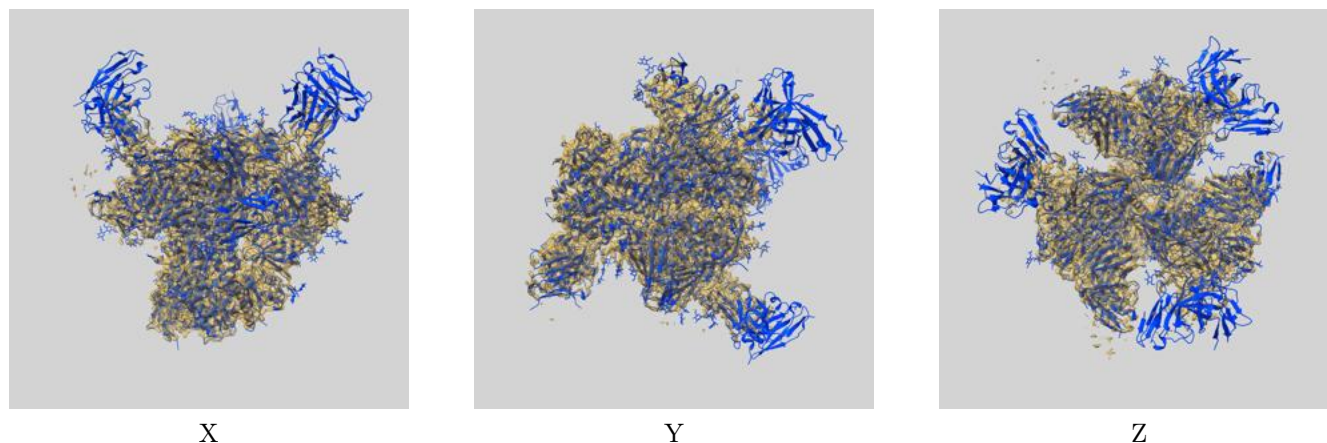
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.16	3.58	3.19
Unmasked-calculated*	3.80	7.67	3.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 3.16 by more than 10 %

9 Map-model fit [i](#)

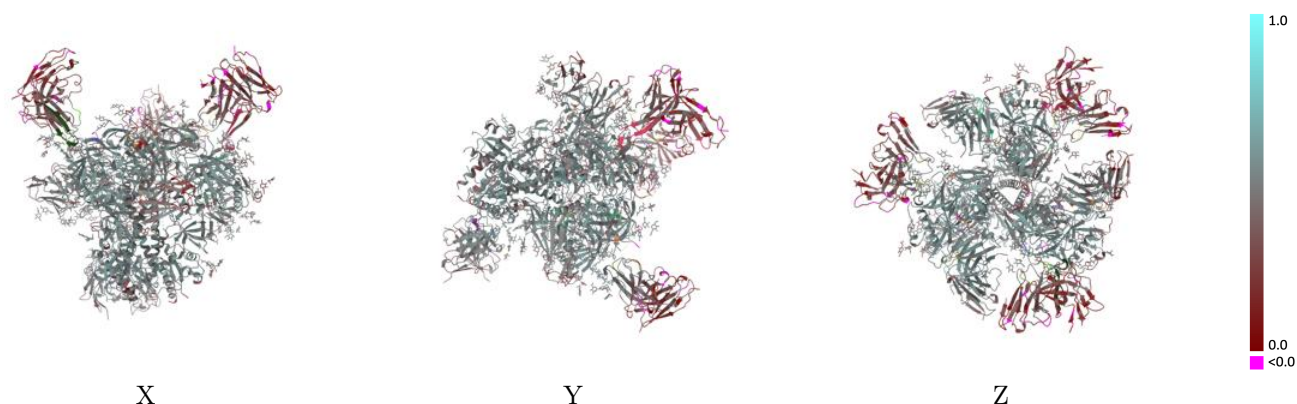
This section contains information regarding the fit between EMDB map EMD-49238 and PDB model 9NBY. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



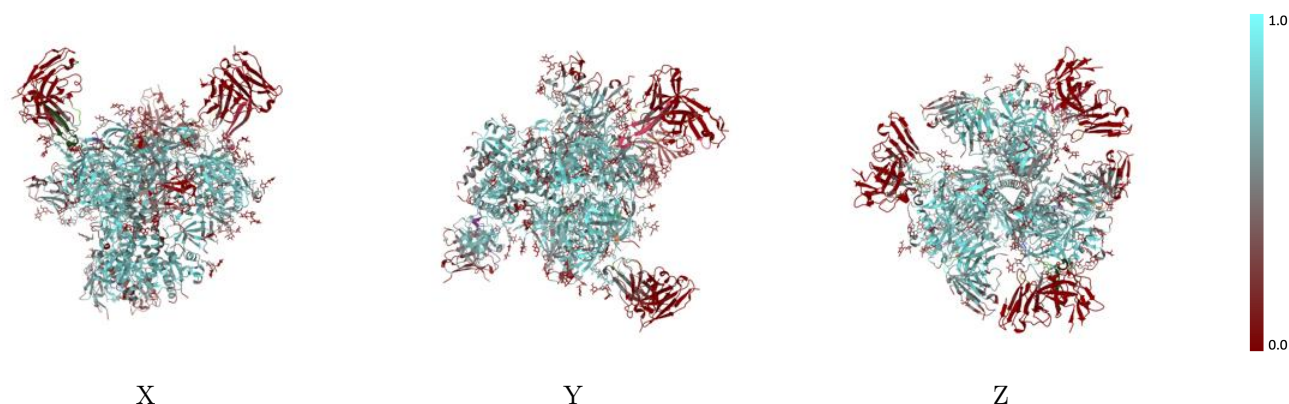
The images above show the 3D surface view of the map at the recommended contour level 0.44 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



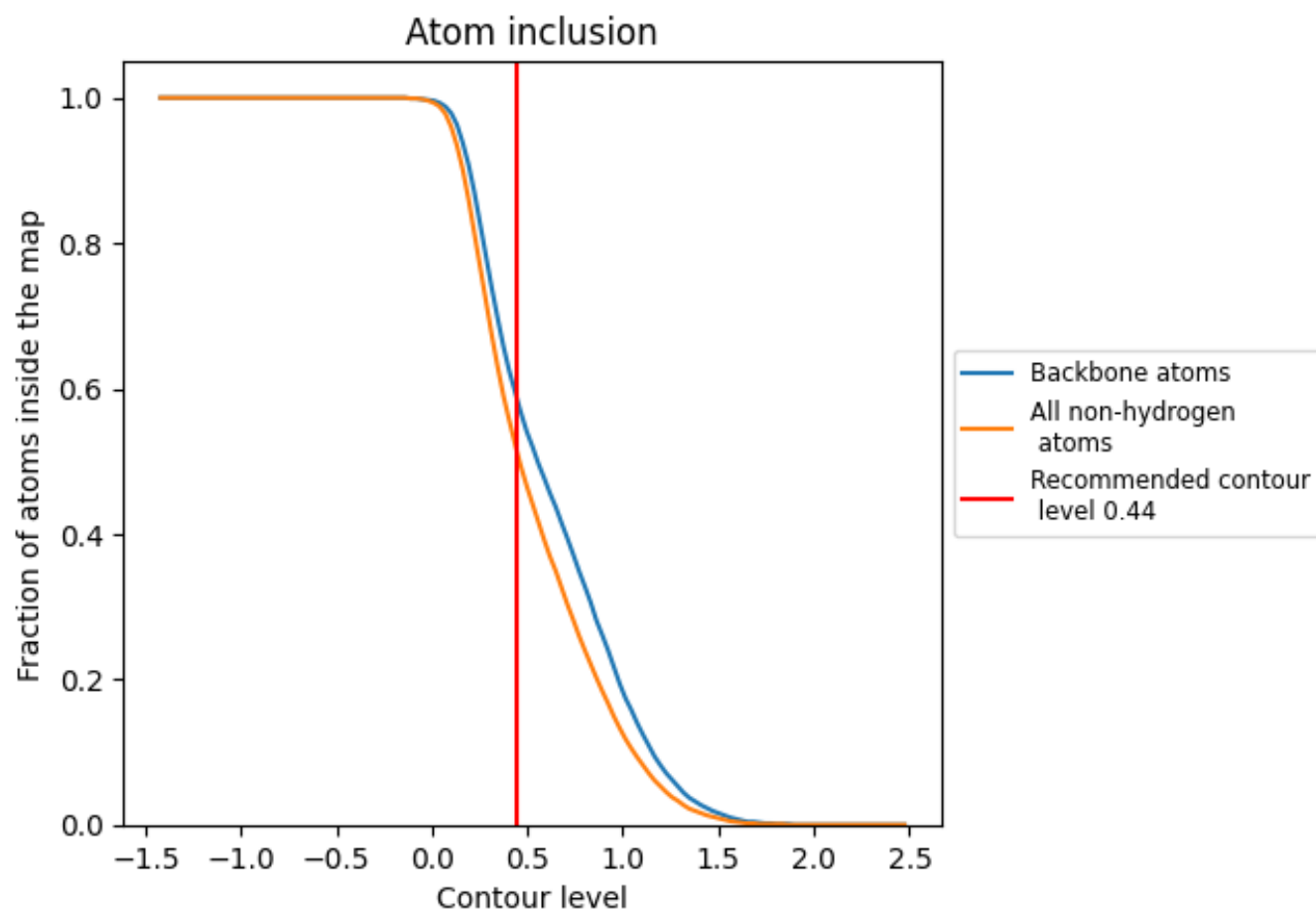
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.44).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 52% 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 (0.44) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5190	 0.4630
0	 0.3930	 0.5020
1	 0.2860	 0.4620
2	 0.2640	 0.4500
3	 0.1070	 0.2540
4	 0.2140	 0.3950
5	 0.1430	 0.4580
6	 0.2560	 0.4750
7	 0.1540	 0.4470
8	 0.3110	 0.5100
9	 0.2890	 0.4770
A	 0.6740	 0.5160
AA	 0.2860	 0.4530
B	 0.6330	 0.5010
BA	 0.2860	 0.4630
C	 0.6510	 0.5050
CA	 0.0000	 0.3890
D	 0.6130	 0.4990
DA	 0.3430	 0.5040
E	 0.7440	 0.5410
EA	 0.3570	 0.4380
F	 0.6660	 0.5200
FA	 0.3930	 0.4150
G	 0.2270	 0.3580
GA	 0.1790	 0.4070
H	 0.1450	 0.3030
HA	 0.0360	 0.2970
I	 0.6980	 0.5250
IA	 0.1790	 0.4820
J	 0.5320	 0.4790
JA	 0.2140	 0.4070
K	 0.1010	 0.3100
KA	 0.1430	 0.3680
L	 0.1050	 0.2650
LA	 0.0000	 0.4420



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Chain	Atom inclusion	Q-score
M	 0.5280	 0.4590
MA	 0.1070	 0.4100
N	 0.3330	 0.4090
O	 0.6280	 0.5020
P	 0.7360	 0.5340
Q	 0.1130	 0.3010
R	 0.1120	 0.2690
S	 0.5590	 0.4720
T	 0.5200	 0.4760
U	 0.0000	 0.4540
V	 0.0360	 0.4220
W	 0.2050	 0.4690
X	 0.2500	 0.4680
Y	 0.4290	 0.4840
Z	 0.2500	 0.4130
a	 0.4290	 0.4830
b	 0.2820	 0.4490
c	 0.3470	 0.4630
d	 0.3570	 0.4230
e	 0.3080	 0.4280
f	 0.4760	 0.5290
g	 0.2500	 0.4100
h	 0.4640	 0.4460
i	 0.3930	 0.5320
j	 0.2500	 0.5090
k	 0.0710	 0.3440
l	 0.2500	 0.4570
m	 0.2500	 0.4910
n	 0.4860	 0.4870
o	 0.2860	 0.4510
p	 0.1070	 0.4910
q	 0.3210	 0.4670
r	 0.3470	 0.5140
s	 0.3210	 0.4470
t	 0.1790	 0.4910
u	 0.4000	 0.4840
v	 0.2860	 0.4280
w	 0.3930	 0.4680
x	 0.0710	 0.4210
y	 0.2500	 0.3660
z	 0.1540	 0.4650