



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 04:06 AM UTC

PDB ID : 8FAE / pdb_00008fae
EMDB ID : EMD-28954
Title : Asymmetric structure of cleaved HIV-1 AE2 envelope glycoprotein trimer in styrene-maleic acid lipid nanoparticles (AE2.1)
Authors : Wang, K.; Zhang, S.; Sodroski, J.; Mao, Y.
Deposited on : 2022-11-26
Resolution : 3.80 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:

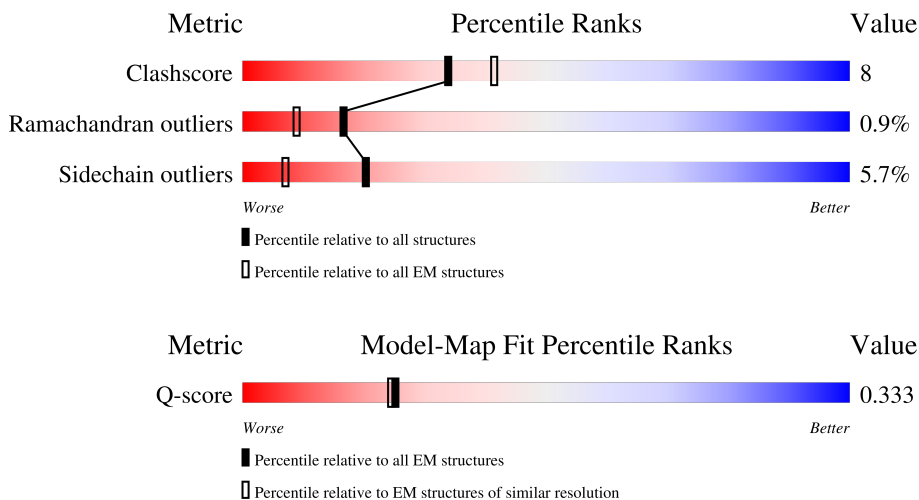
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.80 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.





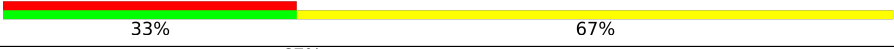



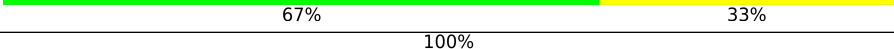


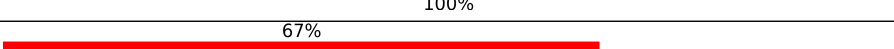
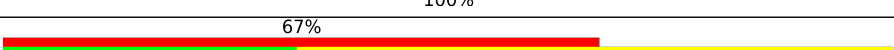



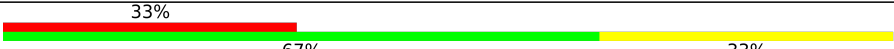
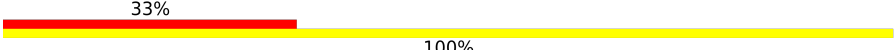





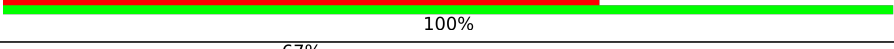



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	B	146	<div> <div>8%</div> <div>76%</div> <div>19%</div> <div>..</div> </div>
1	D	146	<div> <div>7%</div> <div>68%</div> <div>27%</div> <div>..</div> </div>
1	F	146	<div> <div>18%</div> <div>72%</div> <div>24%</div> <div>..</div> </div>
2	A	472	<div> <div>72%</div> <div>25%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	C	472	
2	E	472	
3	0	3	
3	1	3	
3	2	3	
3	4	3	
3	6	3	
3	8	3	
3	CA	3	
3	G	3	
3	IA	3	
3	J	3	
3	JA	3	
3	K	3	
3	L	3	
3	M	3	
3	P	3	
3	Q	3	
3	R	3	
3	V	3	
3	b	3	
3	d	3	
3	h	3	
3	i	3	
3	j	3	

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Mol	Chain	Length	Quality of chain
3	n	3	
3	p	3	
3	r	3	
3	s	3	
3	t	3	
3	x	3	
4	H	3	
4	I	3	
4	LA	3	
4	NA	3	
4	O	3	
4	f	3	
4	g	3	
4	m	3	
5	5	2	
5	7	2	
5	FA	2	
5	MA	2	
5	N	2	
5	U	2	
5	Z	2	
5	c	2	
5	l	2	
6	S	6	
7	T	5	

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Mol	Chain	Length	Quality of chain
8	HA	5	
8	W	5	
8	k	5	
9	EA	7	
9	X	7	
9	v	7	
10	Y	2	
11	a	4	
11	u	4	
11	y	4	
12	KA	4	
12	e	4	
12	z	4	
13	o	4	
14	OA	8	
15	3	4	
15	AA	4	
15	DA	4	
15	GA	4	
15	w	4	
16	9	7	
17	BA	3	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 17693 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 Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	145	Total	C	N	O	S	0	0
			1157	737	196	218	6		
1	D	142	Total	C	N	O	S	0	0
			1132	722	193	211	6		
1	F	143	Total	C	N	O	S	0	0
			1143	731	194	212	6		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	557	LYS	ARG	conflict	UNP O40222
B	567	LYS	GLN	engineered mutation	UNP O40222
B	582	THR	ALA	engineered mutation	UNP O40222
B	633	LYS	ARG	conflict	UNP O40222
B	658	LYS	GLN	conflict	UNP O40222
D	557	LYS	ARG	conflict	UNP O40222
D	567	LYS	GLN	engineered mutation	UNP O40222
D	582	THR	ALA	engineered mutation	UNP O40222
D	633	LYS	ARG	conflict	UNP O40222
D	658	LYS	GLN	conflict	UNP O40222
F	557	LYS	ARG	conflict	UNP O40222
F	567	LYS	GLN	engineered mutation	UNP O40222
F	582	THR	ALA	engineered mutation	UNP O40222
F	633	LYS	ARG	conflict	UNP O40222
F	658	LYS	GLN	conflict	UNP O40222

- Molecule 2 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	467	Total	C	N	O	S	0	0
			3675	2306	641	702	26		
2	E	467	Total	C	N	O	S	0	0
			3675	2306	641	702	26		

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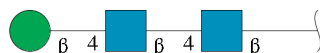
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	468	Total	C	N	O	S	0	0
			3684	2311	642	705	26		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	33	LYS	ASN	conflict	UNP O40222
C	114	GLU	GLN	engineered mutation	UNP O40222
C	166	LYS	ARG	conflict	UNP O40222
C	178	LYS	ARG	conflict	UNP O40222
C	252	LYS	ARG	conflict	UNP O40222
C	315	LYS	ARG	conflict	UNP O40222
C	419	LYS	ARG	conflict	UNP O40222
E	33	LYS	ASN	conflict	UNP O40222
E	114	GLU	GLN	engineered mutation	UNP O40222
E	166	LYS	ARG	conflict	UNP O40222
E	178	LYS	ARG	conflict	UNP O40222
E	252	LYS	ARG	conflict	UNP O40222
E	315	LYS	ARG	conflict	UNP O40222
E	419	LYS	ARG	conflict	UNP O40222
A	33	LYS	ASN	conflict	UNP O40222
A	114	GLU	GLN	engineered mutation	UNP O40222
A	166	LYS	ARG	conflict	UNP O40222
A	178	LYS	ARG	conflict	UNP O40222
A	252	LYS	ARG	conflict	UNP O40222
A	315	LYS	ARG	conflict	UNP O40222
A	419	LYS	ARG	conflict	UNP O40222

- 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	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	J	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		

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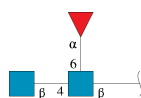
Mol	Chain	Residues	Atoms				AltConf	Trace
3	L	3	Total 39	C 22	N 2	O 15	0	0
3	M	3	Total 39	C 22	N 2	O 15	0	0
3	P	3	Total 39	C 22	N 2	O 15	0	0
3	Q	3	Total 39	C 22	N 2	O 15	0	0
3	R	3	Total 39	C 22	N 2	O 15	0	0
3	V	3	Total 39	C 22	N 2	O 15	0	0
3	b	3	Total 39	C 22	N 2	O 15	0	0
3	d	3	Total 39	C 22	N 2	O 15	0	0
3	h	3	Total 39	C 22	N 2	O 15	0	0
3	i	3	Total 39	C 22	N 2	O 15	0	0
3	j	3	Total 39	C 22	N 2	O 15	0	0
3	n	3	Total 39	C 22	N 2	O 15	0	0
3	p	3	Total 39	C 22	N 2	O 15	0	0
3	r	3	Total 39	C 22	N 2	O 15	0	0
3	s	3	Total 39	C 22	N 2	O 15	0	0
3	t	3	Total 39	C 22	N 2	O 15	0	0
3	x	3	Total 39	C 22	N 2	O 15	0	0
3	0	3	Total 39	C 22	N 2	O 15	0	0
3	1	3	Total 39	C 22	N 2	O 15	0	0
3	2	3	Total 39	C 22	N 2	O 15	0	0
3	4	3	Total 39	C 22	N 2	O 15	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	6	3	Total	C	N	O	0	0
			39	22	2	15		
3	8	3	Total	C	N	O	0	0
			39	22	2	15		
3	CA	3	Total	C	N	O	0	0
			39	22	2	15		
3	IA	3	Total	C	N	O	0	0
			39	22	2	15		
3	JA	3	Total	C	N	O	0	0
			39	22	2	15		

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



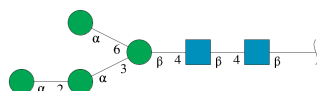
Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	3	Total	C	N	O	0	0
			38	22	2	14		
4	I	3	Total	C	N	O	0	0
			38	22	2	14		
4	O	3	Total	C	N	O	0	0
			38	22	2	14		
4	f	3	Total	C	N	O	0	0
			38	22	2	14		
4	g	3	Total	C	N	O	0	0
			38	22	2	14		
4	m	3	Total	C	N	O	0	0
			38	22	2	14		
4	LA	3	Total	C	N	O	0	0
			38	22	2	14		
4	NA	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



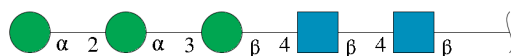
Mol	Chain	Residues	Atoms				AltConf	Trace
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		
5	Z	2	Total	C	N	O	0	0
			28	16	2	10		
5	c	2	Total	C	N	O	0	0
			28	16	2	10		
5	l	2	Total	C	N	O	0	0
			28	16	2	10		
5	5	2	Total	C	N	O	0	0
			28	16	2	10		
5	7	2	Total	C	N	O	0	0
			28	16	2	10		
5	FA	2	Total	C	N	O	0	0
			28	16	2	10		
5	MA	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 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.



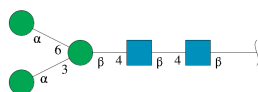
Mol	Chain	Residues	Atoms				AltConf	Trace
6	S	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



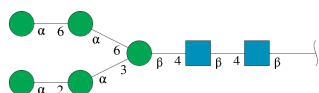
Mol	Chain	Residues	Atoms				AltConf	Trace
7	T	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 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
8	W	5	Total	C	N	O	0	0
			61	34	2	25		
8	k	5	Total	C	N	O	0	0
			61	34	2	25		
8	HA	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



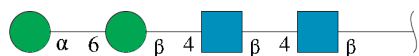
Mol	Chain	Residues	Atoms				AltConf	Trace
9	X	7	Total	C	N	O	0	0
			83	46	2	35		
9	v	7	Total	C	N	O	0	0
			83	46	2	35		
9	EA	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 10 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



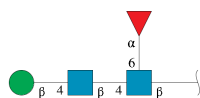
Mol	Chain	Residues	Atoms				AltConf	Trace
10	Y	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 11 is an oligosaccharide called 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.



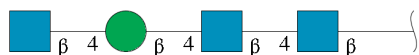
Mol	Chain	Residues	Atoms				AltConf	Trace
11	a	4	Total	C	N	O	0	0
			50	28	2	20		
11	u	4	Total	C	N	O	0	0
			50	28	2	20		
11	y	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 12 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.



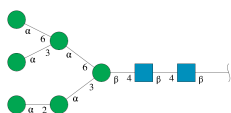
Mol	Chain	Residues	Atoms				AltConf	Trace
12	e	4	Total	C	N	O	0	0
			49	28	2	19		
12	z	4	Total	C	N	O	0	0
			49	28	2	19		
12	KA	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 13 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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	o	4	Total	C	N	O	0	0
			53	30	3	20		

- Molecule 14 is an oligosaccharide called 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.



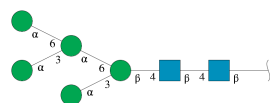
Mol	Chain	Residues	Atoms				AltConf	Trace
14	OA	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 15 is an oligosaccharide called 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.



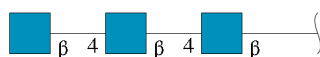
Mol	Chain	Residues	Atoms				AltConf	Trace
15	w	4	Total	C	N	O	0	0
			50	28	2	20		
15	3	4	Total	C	N	O	0	0
			50	28	2	20		
15	AA	4	Total	C	N	O	0	0
			50	28	2	20		
15	DA	4	Total	C	N	O	0	0
			50	28	2	20		
15	GA	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 16 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.



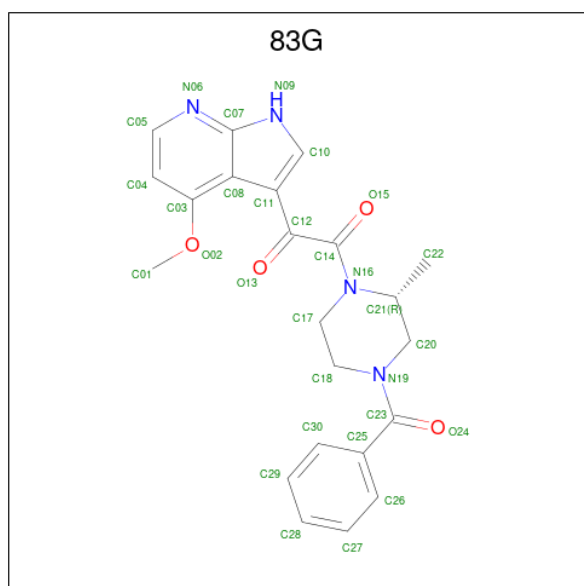
Mol	Chain	Residues	Atoms				AltConf	Trace
16	9	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 17 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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	BA	3	Total	C	N	O	0	0
			42	24	3	15		

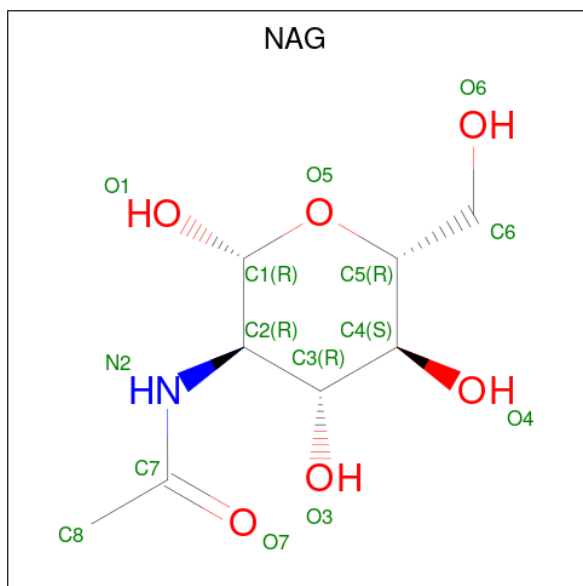
- Molecule 18 is 1-[(2R)-4-(benzenecarbonyl)-2-methylpiperazin-1-yl]-2-(4-methoxy-1H-pyrrolo[2,3-b]pyridin-3-yl)ethane-1,2-dione (CCD ID: 83G) (formula: C₂₂H₂₂N₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
18	C	1	Total	C	N	O	0
			30	22	4	4	
18	E	1	Total	C	N	O	0
			30	22	4	4	
18	A	1	Total	C	N	O	0
			30	22	4	4	

- Molecule 19 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

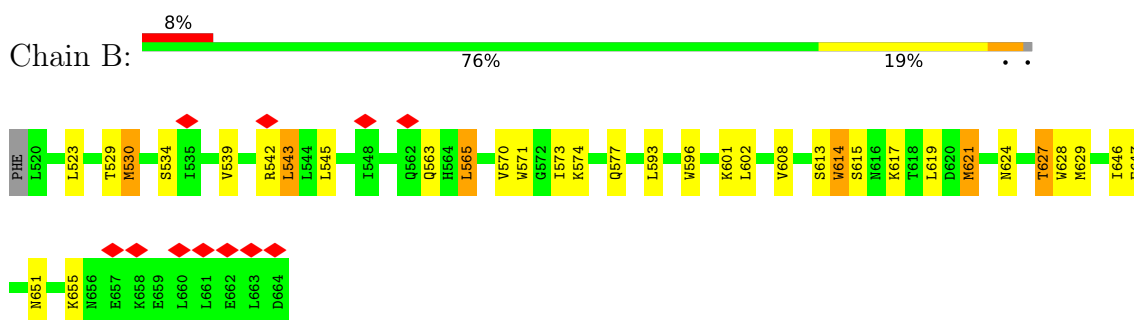


Mol	Chain	Residues	Atoms				AltConf
19	C	1	Total	C	N	O	0
			14	8	1	5	
19	E	1	Total	C	N	O	0
			14	8	1	5	
19	A	1	Total	C	N	O	0
			14	8	1	5	

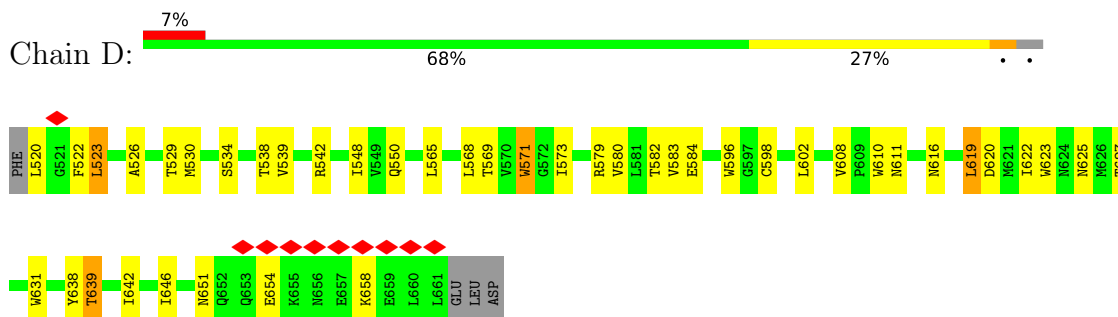
3 Residue-property plots [i](#)

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.

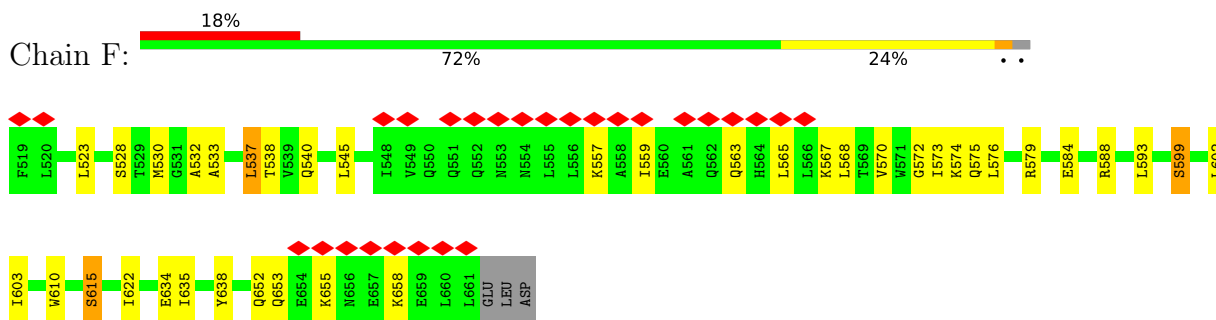
- Molecule 1: Envelope glycoprotein gp41



- Molecule 1: Envelope glycoprotein gp41

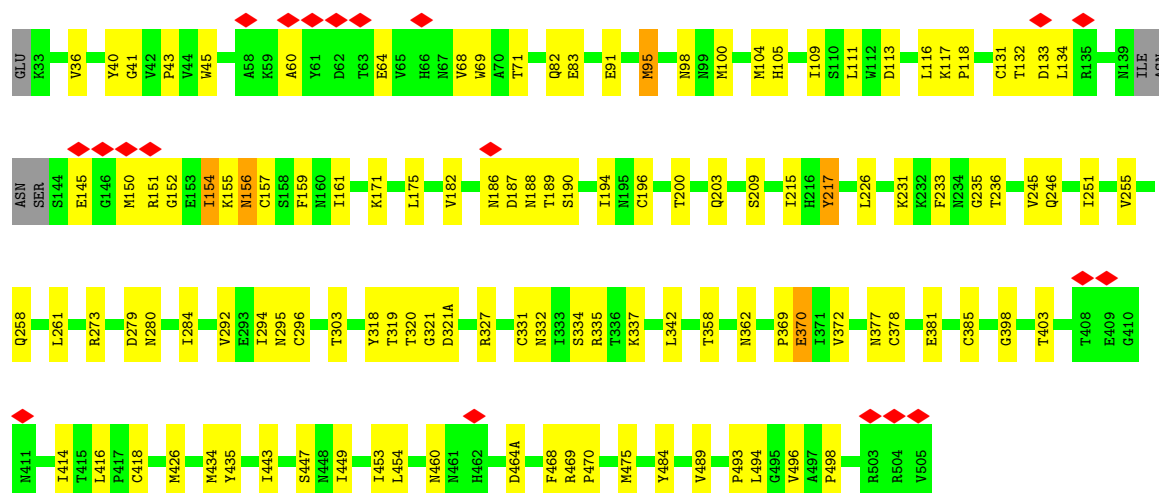


- Molecule 1: Envelope glycoprotein gp41



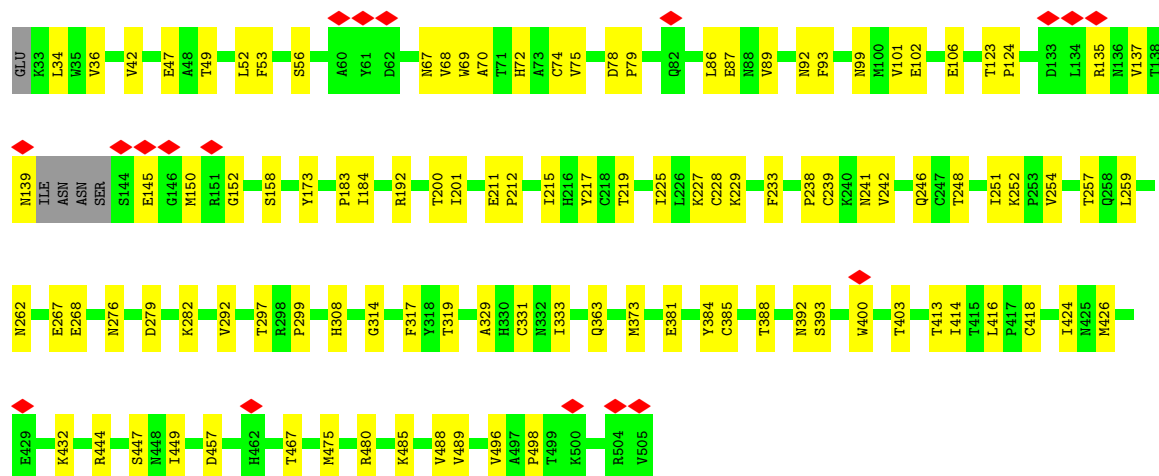
- Molecule 2: Envelope glycoprotein gp120





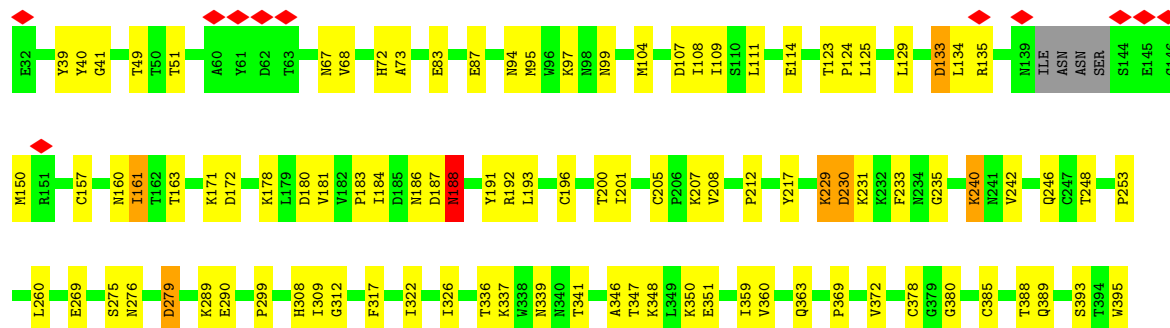
• Molecule 2: Envelope glycoprotein gp120

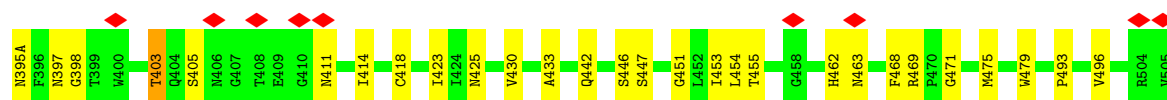
Chain E: 76% 23%



• Molecule 2: Envelope glycoprotein gp120

Chain A: 72% 25%





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



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



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



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



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



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



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



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



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



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



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



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

Chain h: 



- 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 j: 



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

Chain n: 



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

Chain p: 



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

Chain r: 



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



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



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



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



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



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



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



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



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



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



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



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

Chain JA:  67%
100%



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

Chain H:  100%
100%



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

Chain I:  100%
33% 67%



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

Chain O:  100%
100%



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

Chain f:  100%
33% 67%



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

Chain g:  100%
100%



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



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



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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



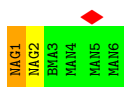
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



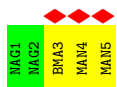
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



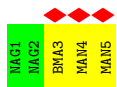
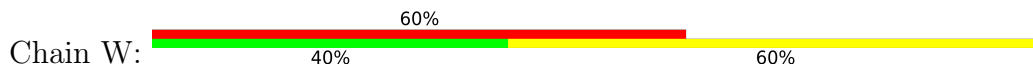
- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



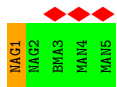
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



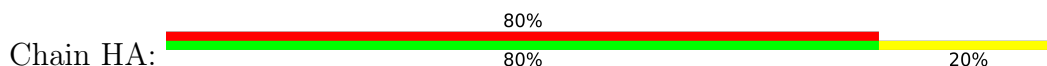
- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

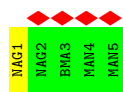


- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 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 9: alpha-D-mannopyranose-(1-2)-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 9: alpha-D-mannopyranose-(1-2)-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



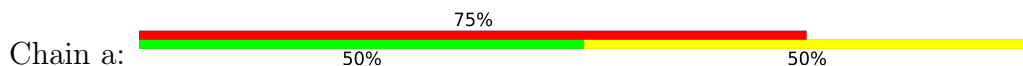
- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: 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 11: 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

Chain u: 




- Molecule 11: 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

Chain y: 



- Molecule 12: 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

Chain e: 




- Molecule 12: 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

Chain z: 




- Molecule 12: 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

Chain KA: 

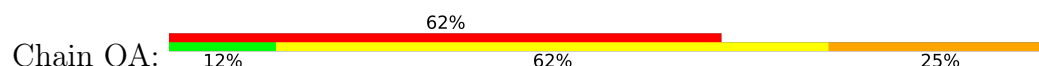


- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

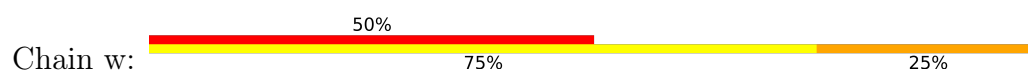
Chain o: 



- Molecule 14: 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



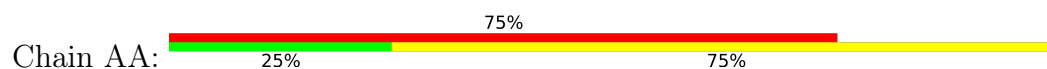
- Molecule 15: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 15: 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 15: 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 15: 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



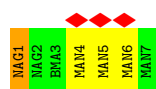
- Molecule 15: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GA: 



- Molecule 16: 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

Chain 9: 



- Molecule 17: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BA: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	140035	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 ($e^-/\text{\AA}^2$)	57	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.145	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	264.0, 264.0, 264.0	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.65, 1.65, 1.65	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, MAN, NAG, 83G, 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	B	0.88	0/1176	1.20	0/1595
1	D	0.87	0/1151	1.19	4/1561 (0.3%)
1	F	0.88	0/1163	1.20	0/1577
2	A	0.83	0/3762	1.06	4/5110 (0.1%)
2	C	0.85	0/3753	1.08	3/5098 (0.1%)
2	E	0.85	0/3753	1.06	1/5098 (0.0%)
All	All	0.85	0/14758	1.10	12/20039 (0.1%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	565	LEU	N-CA-C	-6.67	105.14	113.28
1	D	571	TRP	N-CA-C	-6.24	106.63	114.56
2	C	362	ASN	CA-CB-CG	5.96	118.56	112.60
1	D	611	ASN	CA-CB-CG	5.62	118.22	112.60
2	A	479	TRP	N-CA-C	-5.61	106.48	113.55

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	B	1157	0	1164	20	0
1	D	1132	0	1143	31	0
1	F	1143	0	1152	25	0
2	A	3684	0	3593	80	0
2	C	3675	0	3586	68	0
2	E	3675	0	3587	60	0
3	0	39	0	34	0	0
3	1	39	0	34	4	0
3	2	39	0	34	0	0
3	4	39	0	34	0	0
3	6	39	0	34	0	0
3	8	39	0	34	1	0
3	CA	39	0	34	0	0
3	G	39	0	34	0	0
3	IA	39	0	34	0	0
3	J	39	0	34	0	0
3	JA	39	0	34	0	0
3	K	39	0	34	0	0
3	L	39	0	34	2	0
3	M	39	0	34	0	0
3	P	39	0	34	0	0
3	Q	39	0	34	0	0
3	R	39	0	34	1	0
3	V	39	0	34	0	0
3	b	39	0	34	0	0
3	d	39	0	34	0	0
3	h	39	0	34	0	0
3	i	39	0	34	0	0
3	j	39	0	34	0	0
3	n	39	0	34	6	0
3	p	39	0	34	0	0
3	r	39	0	34	0	0
3	s	39	0	34	0	0
3	t	39	0	34	0	0
3	x	39	0	34	0	0
4	H	38	0	34	0	0
4	I	38	0	34	1	0
4	LA	38	0	34	0	0
4	NA	38	0	34	0	0
4	O	38	0	34	0	0
4	f	38	0	34	0	0
4	g	38	0	34	1	0
4	m	38	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	5	28	0	25	0	0
5	7	28	0	25	0	0
5	FA	28	0	25	0	0
5	MA	28	0	25	0	0
5	N	28	0	25	4	0
5	U	28	0	25	0	0
5	Z	28	0	25	1	0
5	c	28	0	25	1	0
5	l	28	0	25	0	0
6	S	72	0	61	2	0
7	T	61	0	52	0	0
8	HA	61	0	52	0	0
8	W	61	0	52	0	0
8	k	61	0	52	2	0
9	EA	83	0	70	8	0
9	X	83	0	70	7	0
9	v	83	0	70	4	0
10	Y	24	0	22	0	0
11	a	50	0	43	0	0
11	u	50	0	43	0	0
11	y	50	0	43	1	0
12	KA	49	0	43	0	0
12	e	49	0	43	0	0
12	z	49	0	43	1	0
13	o	53	0	46	1	0
14	OA	94	0	80	3	0
15	3	50	0	43	4	0
15	AA	50	0	43	0	0
15	DA	50	0	43	0	0
15	GA	50	0	43	0	0
15	w	50	0	43	2	0
16	9	83	0	70	3	0
17	BA	42	0	37	0	0
18	A	30	0	0	0	0
18	C	30	0	0	1	0
18	E	30	0	0	0	0
19	A	14	0	13	0	0
19	C	14	0	13	0	0
19	E	14	0	13	0	0
All	All	17693	0	16954	282	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 8.

The worst 5 of 282 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)
2:E:467:THR:HG21	15:w:1:NAG:O7	1.66	0.95
2:A:395:TRP:CE3	9:EA:2:NAG:H81	2.19	0.78
2:A:135:ARG:HD3	15:3:1:NAG:H81	1.67	0.77
2:C:335:ARG:HG2	9:X:1:NAG:H81	1.76	0.67
2:A:403:THR:HG21	9:EA:1:NAG:O7	1.94	0.67

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	B	143/146 (98%)	130 (91%)	11 (8%)	2 (1%)	9	37
1	D	140/146 (96%)	128 (91%)	10 (7%)	2 (1%)	9	37
1	F	141/146 (97%)	130 (92%)	10 (7%)	1 (1%)	18	51
2	A	464/472 (98%)	414 (89%)	48 (10%)	2 (0%)	30	62
2	C	463/472 (98%)	423 (91%)	34 (7%)	6 (1%)	9	38
2	E	463/472 (98%)	418 (90%)	41 (9%)	4 (1%)	14	45
All	All	1814/1854 (98%)	1643 (91%)	154 (8%)	17 (1%)	16	45

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	188	ASN
2	C	64	GLU
2	C	156	ASN
1	D	523	LEU
2	E	400	TRP

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	B	125/126 (99%)	112 (90%)	13 (10%)	7	26
1	D	122/126 (97%)	117 (96%)	5 (4%)	27	51
1	F	123/126 (98%)	114 (93%)	9 (7%)	13	39
2	A	420/424 (99%)	390 (93%)	30 (7%)	13	39
2	C	419/424 (99%)	398 (95%)	21 (5%)	22	47
2	E	419/424 (99%)	404 (96%)	15 (4%)	31	54
All	All	1628/1650 (99%)	1535 (94%)	93 (6%)	20	44

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	108	ILE
2	A	337	LYS
2	A	161	ILE
2	A	229	LYS
2	A	350	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	216	HIS
2	A	105	HIS
1	D	590	GLN
2	E	404	GLN
1	D	577	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 ⓘ

244 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	$\# Z > 2$
3	NAG	0	1	2,3	14,14,15	0.31	0	17,19,21	0.80	1 (5%)
3	NAG	0	2	3	14,14,15	0.25	0	17,19,21	0.86	1 (5%)
3	BMA	0	3	3	11,11,12	0.22	0	15,15,17	0.58	0
3	NAG	1	1	2,3	14,14,15	0.47	0	17,19,21	0.50	0
3	NAG	1	2	3	14,14,15	0.31	0	17,19,21	0.43	0
3	BMA	1	3	3	11,11,12	0.48	0	15,15,17	0.81	0
3	NAG	2	1	2,3	14,14,15	0.27	0	17,19,21	0.95	1 (5%)
3	NAG	2	2	3	14,14,15	0.21	0	17,19,21	0.88	1 (5%)
3	BMA	2	3	3	11,11,12	0.27	0	15,15,17	0.64	0
15	NAG	3	1	15,2	14,14,15	0.43	0	17,19,21	0.54	0
15	NAG	3	2	15	14,14,15	0.37	0	17,19,21	0.81	0
15	BMA	3	3	15	11,11,12	1.08	0	15,15,17	1.13	2 (13%)
15	MAN	3	4	15	11,11,12	0.62	0	15,15,17	1.03	2 (13%)
3	NAG	4	1	2,3	14,14,15	0.33	0	17,19,21	0.62	0
3	NAG	4	2	3	14,14,15	0.34	0	17,19,21	1.10	2 (11%)
3	BMA	4	3	3	11,11,12	0.23	0	15,15,17	0.49	0
5	NAG	5	1	5,2	14,14,15	0.27	0	17,19,21	0.88	1 (5%)
5	NAG	5	2	5	14,14,15	0.28	0	17,19,21	0.57	0
3	NAG	6	1	2,3	14,14,15	0.27	0	17,19,21	0.57	0
3	NAG	6	2	3	14,14,15	0.33	0	17,19,21	1.59	4 (23%)
3	BMA	6	3	3	11,11,12	0.22	0	15,15,17	0.54	0
5	NAG	7	1	5,2	14,14,15	0.36	0	17,19,21	0.51	0
5	NAG	7	2	5	14,14,15	0.31	0	17,19,21	0.57	0
3	NAG	8	1	2,3	14,14,15	0.37	0	17,19,21	0.41	0
3	NAG	8	2	3	14,14,15	0.19	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	8	3	3	11,11,12	0.59	0	15,15,17	0.69	0
16	NAG	9	1	16,2	14,14,15	1.15	1 (7%)	17,19,21	2.93	4 (23%)
16	NAG	9	2	16	14,14,15	0.27	0	17,19,21	0.88	0
16	BMA	9	3	16	11,11,12	0.24	0	15,15,17	0.60	0
16	MAN	9	4	16	11,11,12	1.01	0	15,15,17	1.41	2 (13%)
16	MAN	9	5	16	11,11,12	0.69	0	15,15,17	1.00	2 (13%)
16	MAN	9	6	16	11,11,12	0.69	0	15,15,17	0.99	2 (13%)
16	MAN	9	7	16	11,11,12	0.19	0	15,15,17	0.62	0
15	NAG	AA	1	15,2	14,14,15	0.60	1 (7%)	17,19,21	0.71	0
15	NAG	AA	2	15	14,14,15	0.20	0	17,19,21	0.85	0
15	BMA	AA	3	15	11,11,12	1.26	1 (9%)	15,15,17	1.77	3 (20%)
15	MAN	AA	4	15	11,11,12	0.67	0	15,15,17	0.92	1 (6%)
17	NAG	BA	1	17,2	14,14,15	0.29	0	17,19,21	0.68	1 (5%)
17	NAG	BA	2	17	14,14,15	0.28	0	17,19,21	0.57	0
17	NAG	BA	3	17	14,14,15	0.27	0	17,19,21	0.57	0
3	NAG	CA	1	2,3	14,14,15	0.29	0	17,19,21	0.51	0
3	NAG	CA	2	3	14,14,15	0.26	0	17,19,21	0.89	1 (5%)
3	BMA	CA	3	3	11,11,12	0.21	0	15,15,17	0.56	0
15	NAG	DA	1	15,2	14,14,15	0.30	0	17,19,21	0.50	0
15	NAG	DA	2	15	14,14,15	0.20	0	17,19,21	0.75	0
15	BMA	DA	3	15	11,11,12	0.90	1 (9%)	15,15,17	0.86	0
15	MAN	DA	4	15	11,11,12	0.71	1 (9%)	15,15,17	1.35	2 (13%)
9	NAG	EA	1	2,9	14,14,15	0.69	1 (7%)	17,19,21	0.79	0
9	NAG	EA	2	9	14,14,15	0.21	0	17,19,21	0.41	0
9	BMA	EA	3	9	11,11,12	0.91	1 (9%)	15,15,17	1.09	2 (13%)
9	MAN	EA	4	9	11,11,12	1.32	2 (18%)	15,15,17	1.85	2 (13%)
9	MAN	EA	5	9	11,11,12	0.83	0	15,15,17	1.05	2 (13%)
9	MAN	EA	6	9	11,11,12	0.58	0	15,15,17	1.23	2 (13%)
9	MAN	EA	7	9	11,11,12	0.70	0	15,15,17	1.08	2 (13%)
5	NAG	FA	1	5,2	14,14,15	0.38	0	17,19,21	0.84	2 (11%)
5	NAG	FA	2	5	14,14,15	0.51	0	17,19,21	0.81	1 (5%)
3	NAG	G	1	3,1	14,14,15	0.32	0	17,19,21	0.55	0
3	NAG	G	2	3	14,14,15	0.30	0	17,19,21	0.61	0
3	BMA	G	3	3	11,11,12	0.24	0	15,15,17	0.56	0
15	NAG	GA	1	15,2	14,14,15	0.25	0	17,19,21	1.06	2 (11%)
15	NAG	GA	2	15	14,14,15	0.33	0	17,19,21	1.58	4 (23%)
15	BMA	GA	3	15	11,11,12	0.20	0	15,15,17	0.59	0
15	MAN	GA	4	15	11,11,12	0.20	0	15,15,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	H	1	4,1	14,14,15	0.33	0	17,19,21	1.09	1 (5%)
4	NAG	H	2	4	14,14,15	0.41	0	17,19,21	0.95	2 (11%)
4	FUC	H	3	4	10,10,11	0.26	0	14,14,16	0.80	1 (7%)
8	NAG	HA	1	2,8	14,14,15	0.31	0	17,19,21	0.66	1 (5%)
8	NAG	HA	2	8	14,14,15	0.31	0	17,19,21	0.79	0
8	BMA	HA	3	8	11,11,12	0.19	0	15,15,17	0.62	0
8	MAN	HA	4	8	11,11,12	0.19	0	15,15,17	0.53	0
8	MAN	HA	5	8	11,11,12	0.20	0	15,15,17	0.54	0
4	NAG	I	1	4,1	14,14,15	0.33	0	17,19,21	1.09	1 (5%)
4	NAG	I	2	4	14,14,15	0.40	0	17,19,21	0.95	2 (11%)
4	FUC	I	3	4	10,10,11	0.25	0	14,14,16	0.81	1 (7%)
3	NAG	IA	1	2,3	14,14,15	0.30	0	17,19,21	0.58	0
3	NAG	IA	2	3	14,14,15	0.32	0	17,19,21	0.77	0
3	BMA	IA	3	3	11,11,12	0.21	0	15,15,17	0.55	0
3	NAG	J	1	3,1	14,14,15	0.30	0	17,19,21	1.30	2 (11%)
3	NAG	J	2	3	14,14,15	0.30	0	17,19,21	0.63	0
3	BMA	J	3	3	11,11,12	0.58	0	15,15,17	2.37	2 (13%)
3	NAG	JA	1	2,3	14,14,15	0.31	0	17,19,21	0.79	0
3	NAG	JA	2	3	14,14,15	0.30	0	17,19,21	0.53	0
3	BMA	JA	3	3	11,11,12	0.21	0	15,15,17	0.54	0
3	NAG	K	1	2,3	14,14,15	0.30	0	17,19,21	0.54	0
3	NAG	K	2	3	14,14,15	0.31	0	17,19,21	0.63	0
3	BMA	K	3	3	11,11,12	0.23	0	15,15,17	0.64	0
12	NAG	KA	1	12,1	14,14,15	1.12	1 (7%)	17,19,21	2.23	5 (29%)
12	NAG	KA	2	12	14,14,15	0.30	0	17,19,21	0.57	0
12	BMA	KA	3	12	11,11,12	0.20	0	15,15,17	0.63	0
12	FUC	KA	4	12	10,10,11	0.25	0	14,14,16	0.52	0
3	NAG	L	1	2,3	14,14,15	0.31	0	17,19,21	0.85	1 (5%)
3	NAG	L	2	3	14,14,15	0.29	0	17,19,21	0.62	0
3	BMA	L	3	3	11,11,12	0.65	0	15,15,17	0.77	0
4	NAG	LA	1	4,1	14,14,15	0.33	0	17,19,21	0.52	0
4	NAG	LA	2	4	14,14,15	0.28	0	17,19,21	0.69	0
4	FUC	LA	3	4	10,10,11	0.25	0	14,14,16	0.52	0
3	NAG	M	1	2,3	14,14,15	0.42	0	17,19,21	0.55	0
3	NAG	M	2	3	14,14,15	0.38	0	17,19,21	0.81	0
3	BMA	M	3	3	11,11,12	1.08	0	15,15,17	1.14	2 (13%)
5	NAG	MA	1	5,1	14,14,15	0.28	0	17,19,21	0.60	0
5	NAG	MA	2	5	14,14,15	0.40	0	17,19,21	2.01	4 (23%)
5	NAG	N	1	5,2	14,14,15	0.35	0	17,19,21	0.92	0
5	NAG	N	2	5	14,14,15	0.34	0	17,19,21	1.19	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	NA	1	4,1	14,14,15	0.31	0	17,19,21	1.19	1 (5%)
4	NAG	NA	2	4	14,14,15	0.29	0	17,19,21	0.57	0
4	FUC	NA	3	4	10,10,11	0.22	0	14,14,16	0.52	0
4	NAG	O	1	2,4	14,14,15	0.30	0	17,19,21	0.71	0
4	NAG	O	2	4	14,14,15	0.30	0	17,19,21	0.53	0
4	FUC	O	3	4	10,10,11	0.23	0	14,14,16	0.51	0
14	NAG	OA	1	2,14	14,14,15	0.22	0	17,19,21	0.61	0
14	NAG	OA	2	14	14,14,15	0.34	0	17,19,21	0.54	0
14	BMA	OA	3	14	11,11,12	0.63	0	15,15,17	0.66	0
14	MAN	OA	4	14	11,11,12	0.64	0	15,15,17	1.18	1 (6%)
14	MAN	OA	5	14	11,11,12	0.79	1 (9%)	15,15,17	1.39	1 (6%)
14	MAN	OA	6	14	11,11,12	1.02	0	15,15,17	1.40	2 (13%)
14	MAN	OA	7	14	11,11,12	0.72	0	15,15,17	1.00	2 (13%)
14	MAN	OA	8	14	11,11,12	0.67	0	15,15,17	0.98	2 (13%)
3	NAG	P	1	2,3	14,14,15	0.46	0	17,19,21	1.47	4 (23%)
3	NAG	P	2	3	14,14,15	0.38	0	17,19,21	1.00	1 (5%)
3	BMA	P	3	3	11,11,12	0.32	0	15,15,17	1.75	3 (20%)
3	NAG	Q	1	2,3	14,14,15	0.55	0	17,19,21	0.71	0
3	NAG	Q	2	3	14,14,15	0.21	0	17,19,21	0.84	0
3	BMA	Q	3	3	11,11,12	1.25	1 (9%)	15,15,17	1.77	3 (20%)
3	NAG	R	1	2,3	14,14,15	0.32	0	17,19,21	0.94	1 (5%)
3	NAG	R	2	3	14,14,15	0.28	0	17,19,21	0.56	0
3	BMA	R	3	3	11,11,12	0.21	0	15,15,17	0.57	0
6	NAG	S	1	2,6	14,14,15	1.28	1 (7%)	17,19,21	3.34	6 (35%)
6	NAG	S	2	6	14,14,15	0.28	0	17,19,21	1.17	2 (11%)
6	BMA	S	3	6	11,11,12	0.23	0	15,15,17	0.71	0
6	MAN	S	4	6	11,11,12	0.17	0	15,15,17	0.63	0
6	MAN	S	5	6	11,11,12	0.22	0	15,15,17	0.55	0
6	MAN	S	6	6	11,11,12	0.21	0	15,15,17	0.57	0
7	NAG	T	1	7,2	14,14,15	0.57	0	17,19,21	0.70	0
7	NAG	T	2	7	14,14,15	0.22	0	17,19,21	0.85	0
7	BMA	T	3	7	11,11,12	1.26	1 (9%)	15,15,17	1.77	3 (20%)
7	MAN	T	4	7	11,11,12	0.69	0	15,15,17	0.93	1 (6%)
7	MAN	T	5	7	11,11,12	0.85	0	15,15,17	1.09	1 (6%)
5	NAG	U	1	5,2	14,14,15	0.31	0	17,19,21	0.55	0
5	NAG	U	2	5	14,14,15	0.26	0	17,19,21	0.55	0
3	NAG	V	1	2,3	14,14,15	0.32	0	17,19,21	0.69	0
3	NAG	V	2	3	14,14,15	0.26	0	17,19,21	0.89	1 (5%)
3	BMA	V	3	3	11,11,12	0.22	0	15,15,17	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	W	1	2,8	14,14,15	0.32	0	17,19,21	0.50	0
8	NAG	W	2	8	14,14,15	0.22	0	17,19,21	0.74	0
8	BMA	W	3	8	11,11,12	0.90	1 (9%)	15,15,17	0.87	0
8	MAN	W	4	8	11,11,12	0.71	1 (9%)	15,15,17	1.36	2 (13%)
8	MAN	W	5	8	11,11,12	0.66	0	15,15,17	1.05	2 (13%)
9	NAG	X	1	2,9	14,14,15	0.71	1 (7%)	17,19,21	0.79	0
9	NAG	X	2	9	14,14,15	0.19	0	17,19,21	0.39	0
9	BMA	X	3	9	11,11,12	0.92	1 (9%)	15,15,17	1.09	2 (13%)
9	MAN	X	4	9	11,11,12	1.34	2 (18%)	15,15,17	1.83	2 (13%)
9	MAN	X	5	9	11,11,12	0.85	1 (9%)	15,15,17	1.05	2 (13%)
9	MAN	X	6	9	11,11,12	0.60	0	15,15,17	1.23	2 (13%)
9	MAN	X	7	9	11,11,12	0.70	0	15,15,17	1.11	2 (13%)
10	NAG	Y	1	2,10	14,14,15	0.23	0	17,19,21	0.95	2 (11%)
10	FUC	Y	2	10	10,10,11	0.37	0	14,14,16	1.16	1 (7%)
5	NAG	Z	1	5,2	14,14,15	0.38	0	17,19,21	0.85	2 (11%)
5	NAG	Z	2	5	14,14,15	0.51	0	17,19,21	0.80	1 (5%)
11	NAG	a	1	2,11	14,14,15	0.34	0	17,19,21	1.11	1 (5%)
11	NAG	a	2	11	14,14,15	0.26	0	17,19,21	0.91	1 (5%)
11	BMA	a	3	11	11,11,12	0.22	0	15,15,17	0.58	0
11	MAN	a	4	11	11,11,12	0.20	0	15,15,17	0.55	0
3	NAG	b	1	2,3	14,14,15	0.35	0	17,19,21	0.66	0
3	NAG	b	2	3	14,14,15	0.25	0	17,19,21	0.84	0
3	BMA	b	3	3	11,11,12	0.21	0	15,15,17	0.54	0
5	NAG	c	1	5,2	14,14,15	0.35	0	17,19,21	1.13	1 (5%)
5	NAG	c	2	5	14,14,15	0.39	0	17,19,21	1.01	1 (5%)
3	NAG	d	1	2,3	14,14,15	0.28	0	17,19,21	0.46	0
3	NAG	d	2	3	14,14,15	0.26	0	17,19,21	0.48	0
3	BMA	d	3	3	11,11,12	0.94	0	15,15,17	1.09	2 (13%)
12	NAG	e	1	12,1	14,14,15	1.13	1 (7%)	17,19,21	2.23	5 (29%)
12	NAG	e	2	12	14,14,15	0.33	0	17,19,21	0.57	0
12	BMA	e	3	12	11,11,12	0.21	0	15,15,17	0.63	0
12	FUC	e	4	12	10,10,11	0.25	0	14,14,16	0.52	0
4	NAG	f	1	4,1	14,14,15	0.33	0	17,19,21	0.93	1 (5%)
4	NAG	f	2	4	14,14,15	0.41	0	17,19,21	2.01	4 (23%)
4	FUC	f	3	4	10,10,11	0.22	0	14,14,16	0.52	0
4	NAG	g	1	4,1	14,14,15	0.34	0	17,19,21	0.94	1 (5%)
4	NAG	g	2	4	14,14,15	0.42	0	17,19,21	2.00	4 (23%)
4	FUC	g	3	4	10,10,11	0.22	0	14,14,16	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	h	1	3,1	14,14,15	0.29	0	17,19,21	0.46	0
3	NAG	h	2	3	14,14,15	0.28	0	17,19,21	0.58	0
3	BMA	h	3	3	11,11,12	0.22	0	15,15,17	0.59	0
3	NAG	i	1	2,3	14,14,15	0.27	0	17,19,21	0.52	0
3	NAG	i	2	3	14,14,15	0.25	0	17,19,21	0.86	1 (5%)
3	BMA	i	3	3	11,11,12	0.21	0	15,15,17	0.56	0
3	NAG	j	1	2,3	14,14,15	0.25	0	17,19,21	0.94	1 (5%)
3	NAG	j	2	3	14,14,15	0.25	0	17,19,21	0.90	1 (5%)
3	BMA	j	3	3	11,11,12	0.21	0	15,15,17	0.57	0
8	NAG	k	1	2,8	14,14,15	0.28	0	17,19,21	0.85	1 (5%)
8	NAG	k	2	8	14,14,15	0.29	0	17,19,21	0.63	0
8	BMA	k	3	8	11,11,12	0.23	0	15,15,17	0.64	0
8	MAN	k	4	8	11,11,12	0.20	0	15,15,17	0.56	0
8	MAN	k	5	8	11,11,12	0.22	0	15,15,17	0.55	0
5	NAG	l	1	5,2	14,14,15	0.36	0	17,19,21	1.03	1 (5%)
5	NAG	l	2	5	14,14,15	0.25	0	17,19,21	0.66	0
4	NAG	m	1	2,4	14,14,15	0.35	0	17,19,21	1.60	2 (11%)
4	NAG	m	2	4	14,14,15	0.31	0	17,19,21	0.64	0
4	FUC	m	3	4	10,10,11	0.42	0	14,14,16	1.51	3 (21%)
3	NAG	n	1	2,3	14,14,15	0.85	1 (7%)	17,19,21	0.72	0
3	NAG	n	2	3	14,14,15	0.39	0	17,19,21	0.96	2 (11%)
3	BMA	n	3	3	11,11,12	0.48	0	15,15,17	0.94	1 (6%)
13	NAG	o	1	2,13	14,14,15	0.49	0	17,19,21	1.69	5 (29%)
13	NAG	o	2	13	14,14,15	0.28	0	17,19,21	0.87	2 (11%)
13	BMA	o	3	13	11,11,12	0.30	0	15,15,17	0.99	0
13	NAG	o	4	13	14,14,15	0.39	0	17,19,21	0.88	1 (5%)
3	NAG	p	1	2,3	14,14,15	0.28	0	17,19,21	0.85	0
3	NAG	p	2	3	14,14,15	0.30	0	17,19,21	0.65	0
3	BMA	p	3	3	11,11,12	0.20	0	15,15,17	0.59	0
3	NAG	r	1	2,3	14,14,15	0.58	0	17,19,21	0.71	0
3	NAG	r	2	3	14,14,15	0.23	0	17,19,21	0.84	0
3	BMA	r	3	3	11,11,12	1.26	1 (9%)	15,15,17	1.76	3 (20%)
3	NAG	s	1	2,3	14,14,15	0.30	0	17,19,21	0.60	0
3	NAG	s	2	3	14,14,15	0.23	0	17,19,21	0.75	0
3	BMA	s	3	3	11,11,12	0.20	0	15,15,17	0.57	0
3	NAG	t	1	2,3	14,14,15	0.28	0	17,19,21	0.61	0
3	NAG	t	2	3	14,14,15	0.29	0	17,19,21	0.55	0
3	BMA	t	3	3	11,11,12	0.22	0	15,15,17	0.55	0
11	NAG	u	1	2,11	14,14,15	0.29	0	17,19,21	0.42	0
11	NAG	u	2	11	14,14,15	0.30	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BMA	u	3	11	11,11,12	0.25	0	15,15,17	0.62	0
11	MAN	u	4	11	11,11,12	0.20	0	15,15,17	0.66	0
9	NAG	v	1	2,9	14,14,15	0.70	1 (7%)	17,19,21	0.78	0
9	NAG	v	2	9	14,14,15	0.18	0	17,19,21	0.40	0
9	BMA	v	3	9	11,11,12	0.92	1 (9%)	15,15,17	1.08	1 (6%)
9	MAN	v	4	9	11,11,12	1.33	2 (18%)	15,15,17	1.84	2 (13%)
9	MAN	v	5	9	11,11,12	0.84	1 (9%)	15,15,17	1.04	2 (13%)
9	MAN	v	6	9	11,11,12	0.61	0	15,15,17	1.23	2 (13%)
9	MAN	v	7	9	11,11,12	0.70	0	15,15,17	1.08	2 (13%)
15	NAG	w	1	15,2	14,14,15	0.35	0	17,19,21	0.85	2 (11%)
15	NAG	w	2	15	14,14,15	0.50	0	17,19,21	0.80	1 (5%)
15	BMA	w	3	15	11,11,12	1.02	1 (9%)	15,15,17	0.94	1 (6%)
15	MAN	w	4	15	11,11,12	0.74	0	15,15,17	1.27	2 (13%)
3	NAG	x	1	2,3	14,14,15	0.26	0	17,19,21	0.97	1 (5%)
3	NAG	x	2	3	14,14,15	0.30	0	17,19,21	0.61	0
3	BMA	x	3	3	11,11,12	0.21	0	15,15,17	0.57	0
11	NAG	y	1	2,11	14,14,15	0.28	0	17,19,21	0.60	0
11	NAG	y	2	11	14,14,15	0.26	0	17,19,21	1.00	1 (5%)
11	BMA	y	3	11	11,11,12	0.24	0	15,15,17	0.57	0
11	MAN	y	4	11	11,11,12	0.21	0	15,15,17	0.55	0
12	NAG	z	1	2,12	14,14,15	0.37	0	17,19,21	1.29	3 (17%)
12	NAG	z	2	12	14,14,15	0.42	0	17,19,21	1.08	1 (5%)
12	BMA	z	3	12	11,11,12	0.20	0	15,15,17	0.56	0
12	FUC	z	4	12	10,10,11	0.23	0	14,14,16	0.60	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
3	NAG	0	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	0	2	3	-	4/6/23/26	0/1/1/1
3	BMA	0	3	3	-	0/2/19/22	0/1/1/1
3	NAG	1	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	1	2	3	-	0/6/23/26	0/1/1/1
3	BMA	1	3	3	-	2/2/19/22	0/1/1/1
3	NAG	2	1	2,3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	2	2	3	-	3/6/23/26	0/1/1/1
3	BMA	2	3	3	-	0/2/19/22	0/1/1/1
15	NAG	3	1	15,2	-	2/6/23/26	0/1/1/1
15	NAG	3	2	15	-	2/6/23/26	0/1/1/1
15	BMA	3	3	15	-	1/2/19/22	0/1/1/1
15	MAN	3	4	15	-	0/2/19/22	0/1/1/1
3	NAG	4	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	4	2	3	-	3/6/23/26	0/1/1/1
3	BMA	4	3	3	-	1/2/19/22	0/1/1/1
5	NAG	5	1	5,2	-	3/6/23/26	0/1/1/1
5	NAG	5	2	5	-	0/6/23/26	0/1/1/1
3	NAG	6	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	6	2	3	-	3/6/23/26	0/1/1/1
3	BMA	6	3	3	-	0/2/19/22	0/1/1/1
5	NAG	7	1	5,2	-	1/6/23/26	0/1/1/1
5	NAG	7	2	5	-	2/6/23/26	0/1/1/1
3	NAG	8	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	8	2	3	-	1/6/23/26	0/1/1/1
3	BMA	8	3	3	-	0/2/19/22	0/1/1/1
16	NAG	9	1	16,2	-	2/6/23/26	0/1/1/1
16	NAG	9	2	16	-	5/6/23/26	0/1/1/1
16	BMA	9	3	16	-	2/2/19/22	0/1/1/1
16	MAN	9	4	16	-	1/2/19/22	0/1/1/1
16	MAN	9	5	16	-	0/2/19/22	0/1/1/1
16	MAN	9	6	16	-	0/2/19/22	0/1/1/1
16	MAN	9	7	16	-	0/2/19/22	0/1/1/1
15	NAG	AA	1	15,2	-	2/6/23/26	0/1/1/1
15	NAG	AA	2	15	-	4/6/23/26	0/1/1/1
15	BMA	AA	3	15	-	1/2/19/22	0/1/1/1
15	MAN	AA	4	15	-	0/2/19/22	0/1/1/1
17	NAG	BA	1	17,2	-	0/6/23/26	0/1/1/1
17	NAG	BA	2	17	-	1/6/23/26	0/1/1/1
17	NAG	BA	3	17	-	1/6/23/26	0/1/1/1
3	NAG	CA	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	CA	2	3	-	5/6/23/26	0/1/1/1
3	BMA	CA	3	3	-	0/2/19/22	0/1/1/1
15	NAG	DA	1	15,2	-	2/6/23/26	0/1/1/1
15	NAG	DA	2	15	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BMA	DA	3	15	-	0/2/19/22	0/1/1/1
15	MAN	DA	4	15	-	2/2/19/22	0/1/1/1
9	NAG	EA	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	EA	2	9	-	0/6/23/26	0/1/1/1
9	BMA	EA	3	9	-	2/2/19/22	0/1/1/1
9	MAN	EA	4	9	-	0/2/19/22	0/1/1/1
9	MAN	EA	5	9	-	0/2/19/22	0/1/1/1
9	MAN	EA	6	9	-	0/2/19/22	0/1/1/1
9	MAN	EA	7	9	-	0/2/19/22	0/1/1/1
5	NAG	FA	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	FA	2	5	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
15	NAG	GA	1	15,2	-	3/6/23/26	0/1/1/1
15	NAG	GA	2	15	-	3/6/23/26	0/1/1/1
15	BMA	GA	3	15	-	0/2/19/22	0/1/1/1
15	MAN	GA	4	15	-	1/2/19/22	0/1/1/1
4	NAG	H	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1
4	FUC	H	3	4	-	-	0/1/1/1
8	NAG	HA	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	HA	2	8	-	0/6/23/26	0/1/1/1
8	BMA	HA	3	8	-	0/2/19/22	0/1/1/1
8	MAN	HA	4	8	-	0/2/19/22	0/1/1/1
8	MAN	HA	5	8	-	0/2/19/22	0/1/1/1
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	1/6/23/26	0/1/1/1
4	FUC	I	3	4	-	-	0/1/1/1
3	NAG	IA	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	IA	2	3	-	3/6/23/26	0/1/1/1
3	BMA	IA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
3	NAG	JA	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	JA	2	3	-	0/6/23/26	0/1/1/1
3	BMA	JA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	K	1	2,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	K	2	3	-	3/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
12	NAG	KA	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	KA	2	12	-	0/6/23/26	0/1/1/1
12	BMA	KA	3	12	-	0/2/19/22	0/1/1/1
12	FUC	KA	4	12	-	-	0/1/1/1
3	NAG	L	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1
3	BMA	L	3	3	-	2/2/19/22	0/1/1/1
4	NAG	LA	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	LA	2	4	-	0/6/23/26	0/1/1/1
4	FUC	LA	3	4	-	-	0/1/1/1
3	NAG	M	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	BMA	M	3	3	-	1/2/19/22	0/1/1/1
5	NAG	MA	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	MA	2	5	-	1/6/23/26	0/1/1/1
5	NAG	N	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	3/6/23/26	0/1/1/1
4	NAG	NA	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	NA	2	4	-	2/6/23/26	0/1/1/1
4	FUC	NA	3	4	-	-	0/1/1/1
4	NAG	O	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	FUC	O	3	4	-	-	0/1/1/1
14	NAG	OA	1	2,14	-	0/6/23/26	0/1/1/1
14	NAG	OA	2	14	-	2/6/23/26	0/1/1/1
14	BMA	OA	3	14	-	0/2/19/22	0/1/1/1
14	MAN	OA	4	14	-	0/2/19/22	0/1/1/1
14	MAN	OA	5	14	-	0/2/19/22	0/1/1/1
14	MAN	OA	6	14	-	1/2/19/22	0/1/1/1
14	MAN	OA	7	14	-	0/2/19/22	0/1/1/1
14	MAN	OA	8	14	-	0/2/19/22	0/1/1/1
3	NAG	P	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
3	BMA	P	3	3	-	1/2/19/22	0/1/1/1
3	NAG	Q	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	Q	3	3	-	1/2/19/22	0/1/1/1
3	NAG	R	1	2,3	-	4/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	BMA	R	3	3	-	0/2/19/22	0/1/1/1
6	NAG	S	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	3/6/23/26	0/1/1/1
6	BMA	S	3	6	-	0/2/19/22	0/1/1/1
6	MAN	S	4	6	-	0/2/19/22	0/1/1/1
6	MAN	S	5	6	-	1/2/19/22	0/1/1/1
6	MAN	S	6	6	-	0/2/19/22	0/1/1/1
7	NAG	T	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	T	2	7	-	4/6/23/26	0/1/1/1
7	BMA	T	3	7	-	1/2/19/22	0/1/1/1
7	MAN	T	4	7	-	0/2/19/22	0/1/1/1
7	MAN	T	5	7	-	0/2/19/22	0/1/1/1
5	NAG	U	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	U	2	5	-	2/6/23/26	0/1/1/1
3	NAG	V	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	V	2	3	-	4/6/23/26	0/1/1/1
3	BMA	V	3	3	-	0/2/19/22	0/1/1/1
8	NAG	W	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	W	2	8	-	4/6/23/26	0/1/1/1
8	BMA	W	3	8	-	0/2/19/22	0/1/1/1
8	MAN	W	4	8	-	2/2/19/22	0/1/1/1
8	MAN	W	5	8	-	0/2/19/22	0/1/1/1
9	NAG	X	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	X	2	9	-	0/6/23/26	0/1/1/1
9	BMA	X	3	9	-	2/2/19/22	0/1/1/1
9	MAN	X	4	9	-	0/2/19/22	0/1/1/1
9	MAN	X	5	9	-	0/2/19/22	0/1/1/1
9	MAN	X	6	9	-	0/2/19/22	0/1/1/1
9	MAN	X	7	9	-	0/2/19/22	0/1/1/1
10	NAG	Y	1	2,10	-	5/6/23/26	0/1/1/1
10	FUC	Y	2	10	-	-	0/1/1/1
5	NAG	Z	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	2/6/23/26	0/1/1/1
11	NAG	a	1	2,11	-	2/6/23/26	0/1/1/1
11	NAG	a	2	11	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BMA	a	3	11	-	0/2/19/22	0/1/1/1
11	MAN	a	4	11	-	0/2/19/22	0/1/1/1
3	NAG	b	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	b	2	3	-	3/6/23/26	0/1/1/1
3	BMA	b	3	3	-	0/2/19/22	0/1/1/1
5	NAG	c	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	1/6/23/26	0/1/1/1
3	NAG	d	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	d	2	3	-	2/6/23/26	0/1/1/1
3	BMA	d	3	3	-	2/2/19/22	0/1/1/1
12	NAG	e	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	e	2	12	-	0/6/23/26	0/1/1/1
12	BMA	e	3	12	-	0/2/19/22	0/1/1/1
12	FUC	e	4	12	-	-	0/1/1/1
4	NAG	f	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	f	2	4	-	1/6/23/26	0/1/1/1
4	FUC	f	3	4	-	-	0/1/1/1
4	NAG	g	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	g	2	4	-	1/6/23/26	0/1/1/1
4	FUC	g	3	4	-	-	0/1/1/1
3	NAG	h	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	h	2	3	-	1/6/23/26	0/1/1/1
3	BMA	h	3	3	-	1/2/19/22	0/1/1/1
3	NAG	i	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	i	2	3	-	3/6/23/26	0/1/1/1
3	BMA	i	3	3	-	0/2/19/22	0/1/1/1
3	NAG	j	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	j	2	3	-	4/6/23/26	0/1/1/1
3	BMA	j	3	3	-	0/2/19/22	0/1/1/1
8	NAG	k	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	k	2	8	-	2/6/23/26	0/1/1/1
8	BMA	k	3	8	-	0/2/19/22	0/1/1/1
8	MAN	k	4	8	-	1/2/19/22	0/1/1/1
8	MAN	k	5	8	-	0/2/19/22	0/1/1/1
5	NAG	l	1	5,2	-	4/6/23/26	0/1/1/1
5	NAG	l	2	5	-	0/6/23/26	0/1/1/1
4	NAG	m	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	m	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUC	m	3	4	-	-	0/1/1/1
3	NAG	n	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	n	2	3	-	1/6/23/26	0/1/1/1
3	BMA	n	3	3	-	0/2/19/22	0/1/1/1
13	NAG	o	1	2,13	-	2/6/23/26	0/1/1/1
13	NAG	o	2	13	-	3/6/23/26	0/1/1/1
13	BMA	o	3	13	-	0/2/19/22	0/1/1/1
13	NAG	o	4	13	-	0/6/23/26	0/1/1/1
3	NAG	p	1	2,3	-	5/6/23/26	0/1/1/1
3	NAG	p	2	3	-	2/6/23/26	0/1/1/1
3	BMA	p	3	3	-	0/2/19/22	0/1/1/1
3	NAG	r	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	r	2	3	-	4/6/23/26	0/1/1/1
3	BMA	r	3	3	-	1/2/19/22	0/1/1/1
3	NAG	s	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	s	2	3	-	3/6/23/26	0/1/1/1
3	BMA	s	3	3	-	0/2/19/22	0/1/1/1
3	NAG	t	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	t	2	3	-	0/6/23/26	0/1/1/1
3	BMA	t	3	3	-	0/2/19/22	0/1/1/1
11	NAG	u	1	2,11	-	1/6/23/26	0/1/1/1
11	NAG	u	2	11	-	2/6/23/26	0/1/1/1
11	BMA	u	3	11	-	2/2/19/22	0/1/1/1
11	MAN	u	4	11	-	0/2/19/22	0/1/1/1
9	NAG	v	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	v	2	9	-	0/6/23/26	0/1/1/1
9	BMA	v	3	9	-	2/2/19/22	0/1/1/1
9	MAN	v	4	9	-	0/2/19/22	0/1/1/1
9	MAN	v	5	9	-	0/2/19/22	0/1/1/1
9	MAN	v	6	9	-	0/2/19/22	0/1/1/1
9	MAN	v	7	9	-	0/2/19/22	0/1/1/1
15	NAG	w	1	15,2	-	0/6/23/26	0/1/1/1
15	NAG	w	2	15	-	2/6/23/26	0/1/1/1
15	BMA	w	3	15	-	0/2/19/22	0/1/1/1
15	MAN	w	4	15	-	0/2/19/22	0/1/1/1
3	NAG	x	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	x	2	3	-	0/6/23/26	0/1/1/1
3	BMA	x	3	3	-	0/2/19/22	0/1/1/1
11	NAG	y	1	2,11	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	y	2	11	-	3/6/23/26	0/1/1/1
11	BMA	y	3	11	-	2/2/19/22	0/1/1/1
11	MAN	y	4	11	-	1/2/19/22	0/1/1/1
12	NAG	z	1	2,12	-	3/6/23/26	0/1/1/1
12	NAG	z	2	12	-	1/6/23/26	0/1/1/1
12	BMA	z	3	12	-	0/2/19/22	0/1/1/1
12	FUC	z	4	12	-	-	0/1/1/1

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	1	NAG	C1-C2	4.22	1.58	1.52
12	e	1	NAG	C1-C2	4.01	1.57	1.52
12	KA	1	NAG	C1-C2	4.00	1.57	1.52
16	9	1	NAG	C1-C2	3.85	1.57	1.52
7	T	3	BMA	O5-C5	3.38	1.50	1.43

The worst 5 of 199 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	1	NAG	C1-O5-C5	10.01	125.59	112.19
16	9	1	NAG	O5-C1-C2	-8.95	97.44	111.29
3	J	3	BMA	O2-C2-C3	8.25	127.23	110.15
12	e	1	NAG	O5-C1-C2	-7.46	99.75	111.29
12	KA	1	NAG	O5-C1-C2	-7.46	99.75	111.29

There are no chirality outliers.

5 of 296 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	1	NAG	C1-C2-N2-C7
3	J	1	NAG	C8-C7-N2-C2
3	J	1	NAG	O7-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	K	2	NAG	C8-C7-N2-C2

There are no ring outliers.

47 monomers are involved in 58 short contacts:

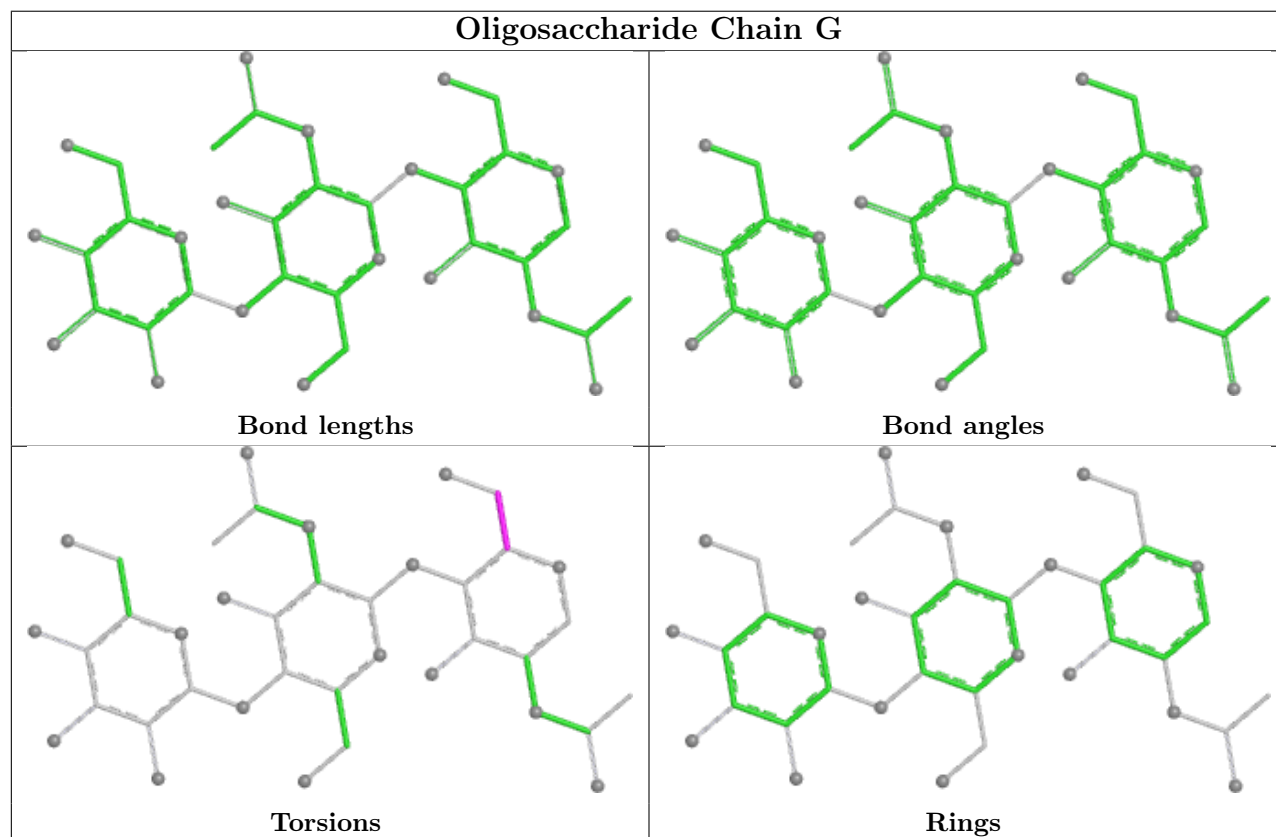
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	z	1	NAG	1	0
8	k	1	NAG	2	0
9	X	5	MAN	1	0
5	N	2	NAG	1	0
9	EA	3	BMA	2	0
5	N	1	NAG	4	0
9	EA	2	NAG	2	0
9	v	1	NAG	1	0
9	EA	6	MAN	1	0
9	v	3	BMA	2	0
4	I	1	NAG	1	0
5	c	2	NAG	1	0
16	9	1	NAG	3	0
9	X	1	NAG	2	0
3	n	2	NAG	5	0
3	8	1	NAG	1	0
9	EA	5	MAN	1	0
9	X	3	BMA	2	0
5	c	1	NAG	1	0
5	Z	1	NAG	1	0
3	L	1	NAG	2	0
6	S	1	NAG	2	0
9	v	4	MAN	3	0
14	OA	6	MAN	2	0
11	y	4	MAN	1	0
3	R	1	NAG	1	0
9	X	2	NAG	1	0
14	OA	8	MAN	1	0
14	OA	3	BMA	1	0
15	w	1	NAG	2	0
9	EA	1	NAG	2	0
9	EA	4	MAN	3	0
9	v	5	MAN	1	0
12	z	2	NAG	1	0
3	n	1	NAG	1	0
13	o	3	BMA	1	0
14	OA	1	NAG	1	0
11	y	2	NAG	1	0
13	o	4	NAG	1	0
4	g	3	FUC	1	0
9	X	4	MAN	3	0
3	8	2	NAG	1	0
4	I	2	NAG	1	0

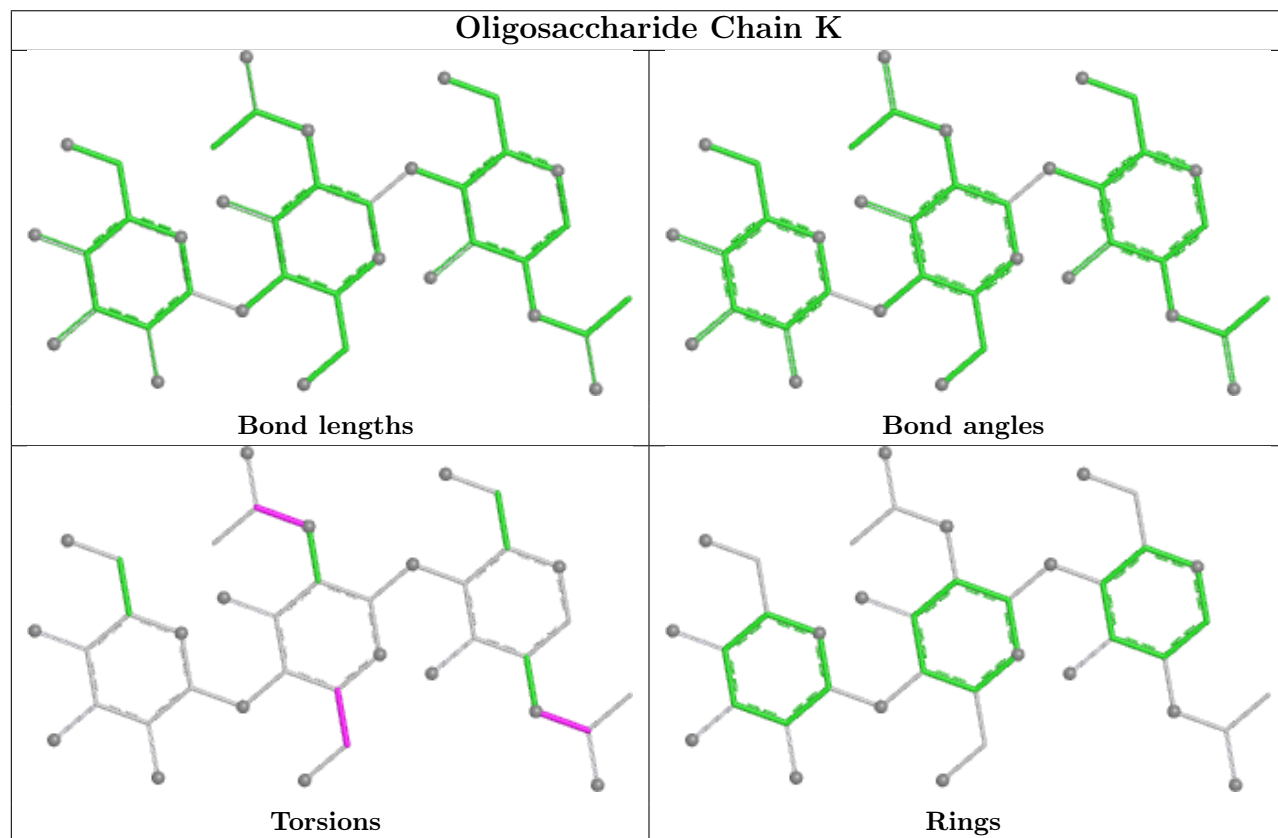
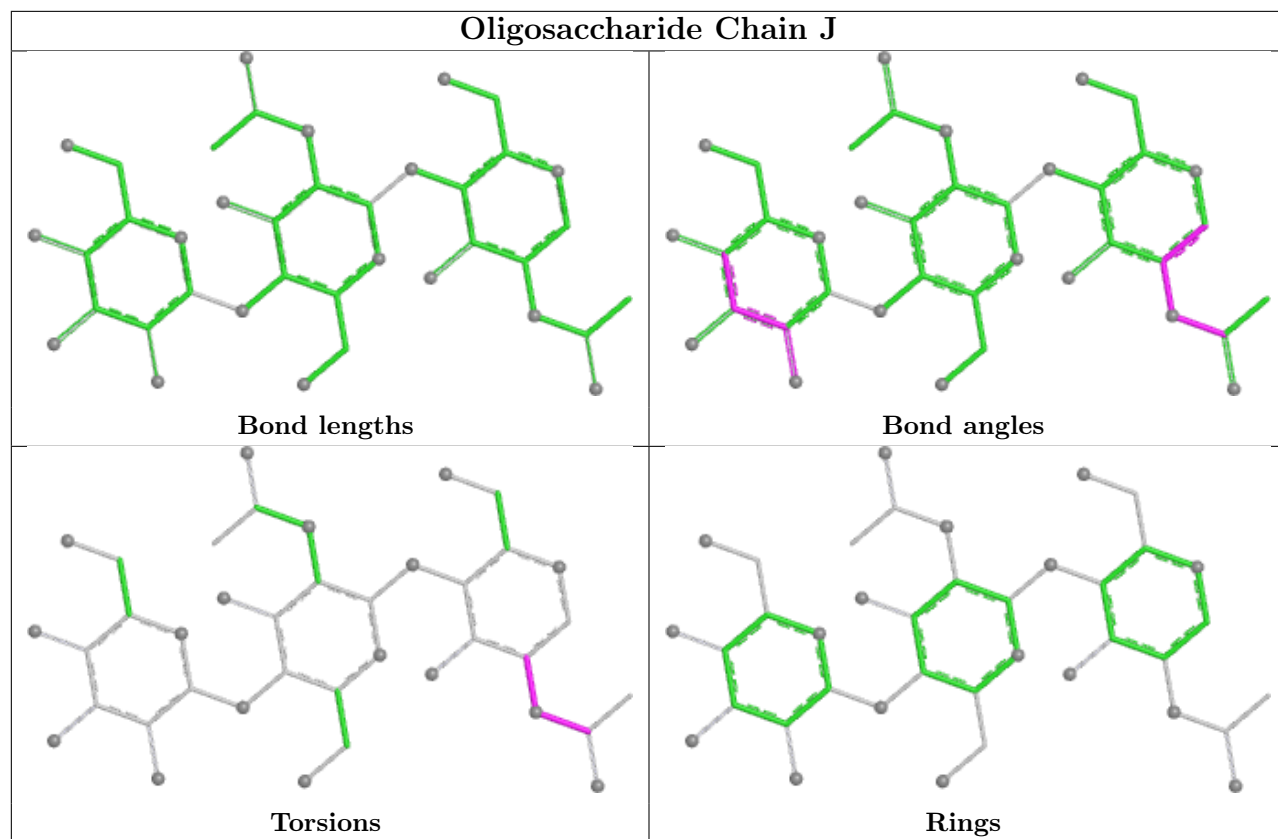
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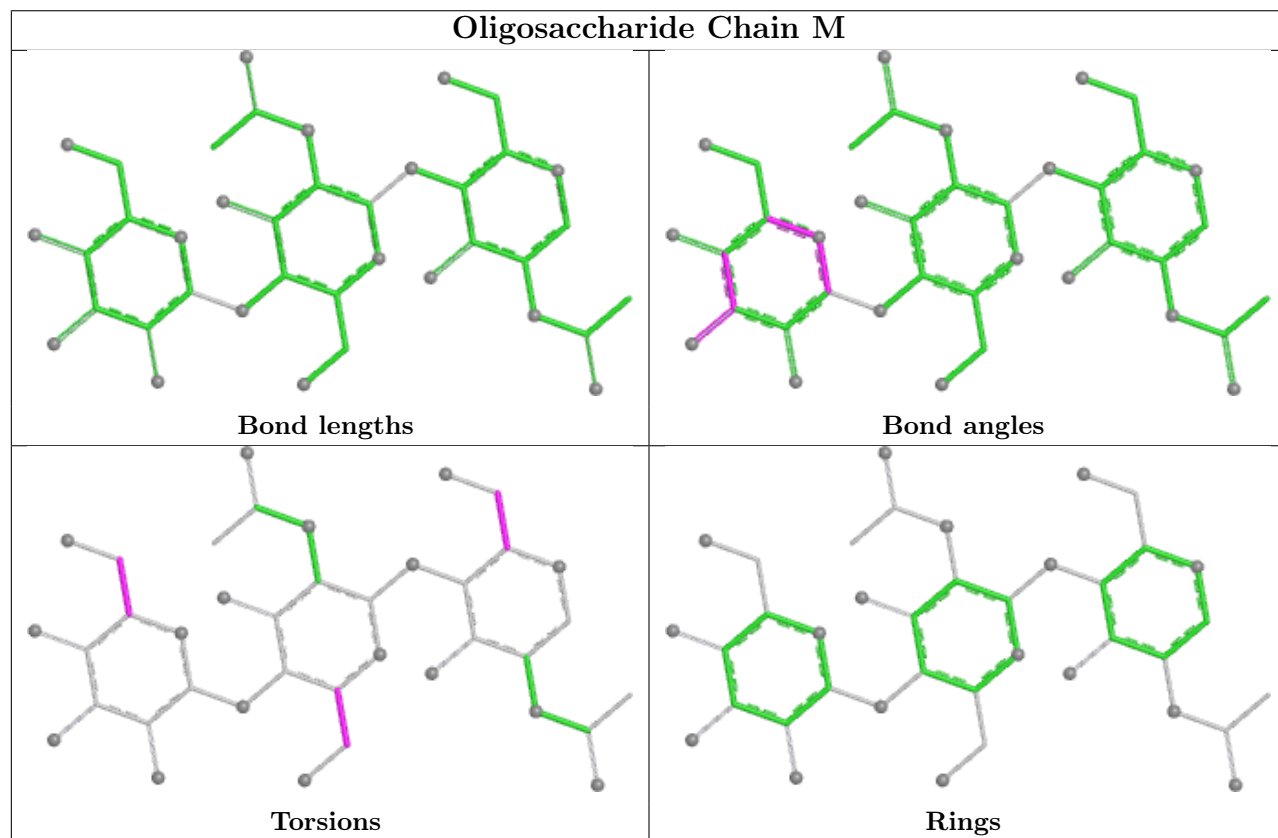
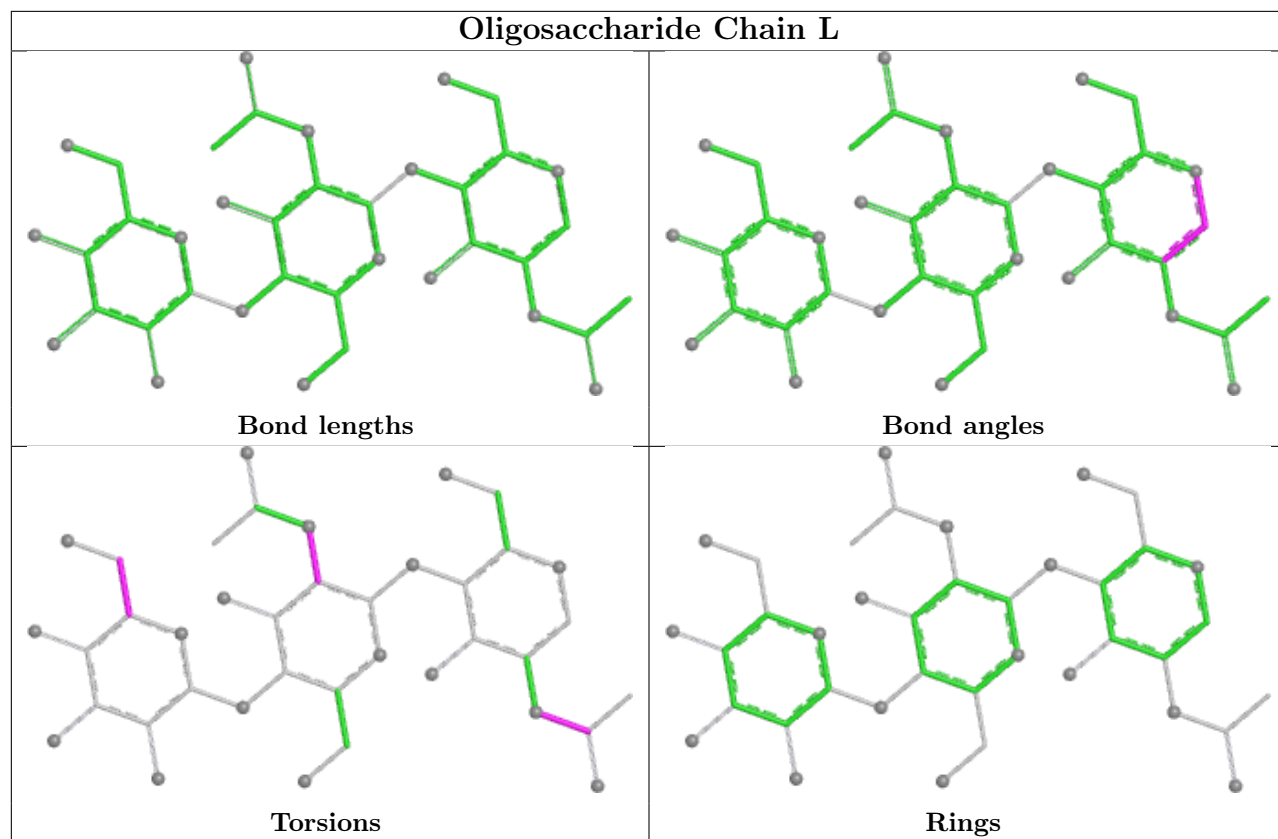
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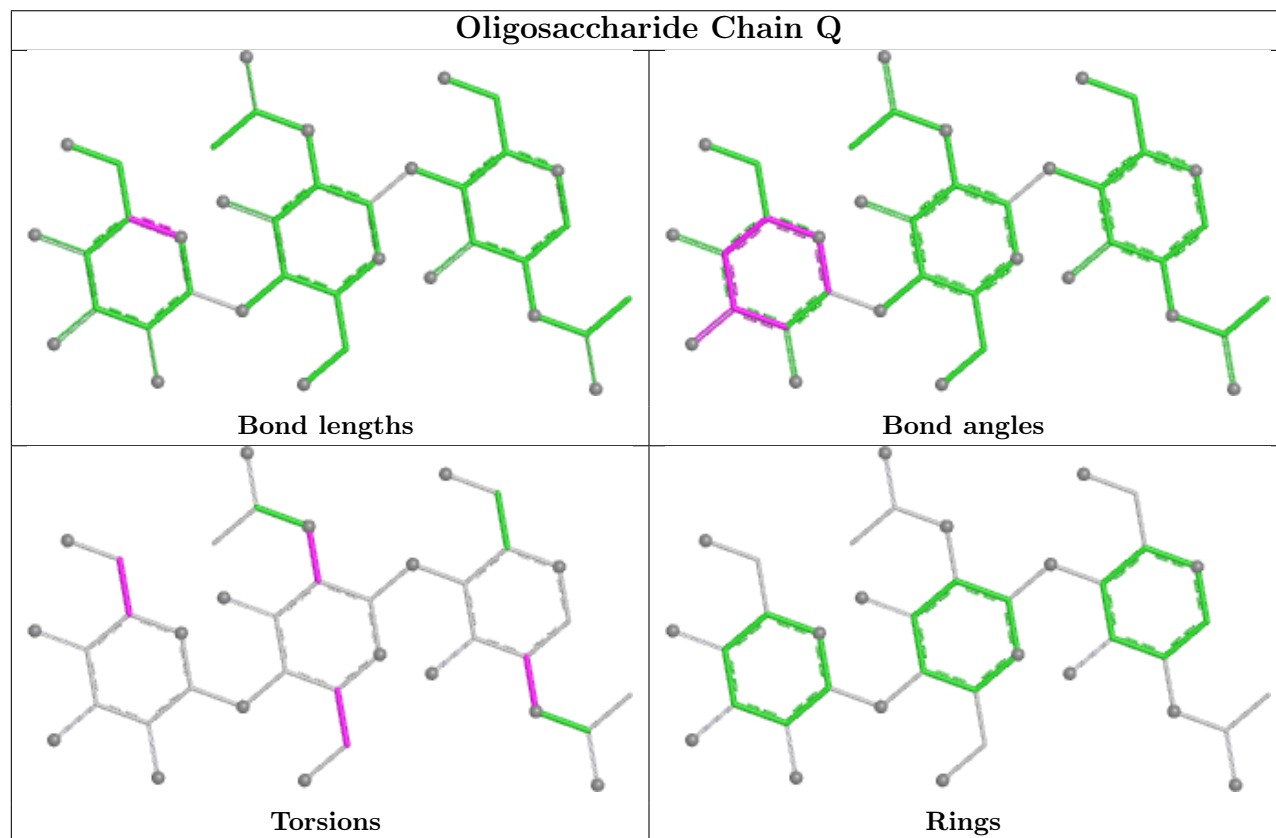
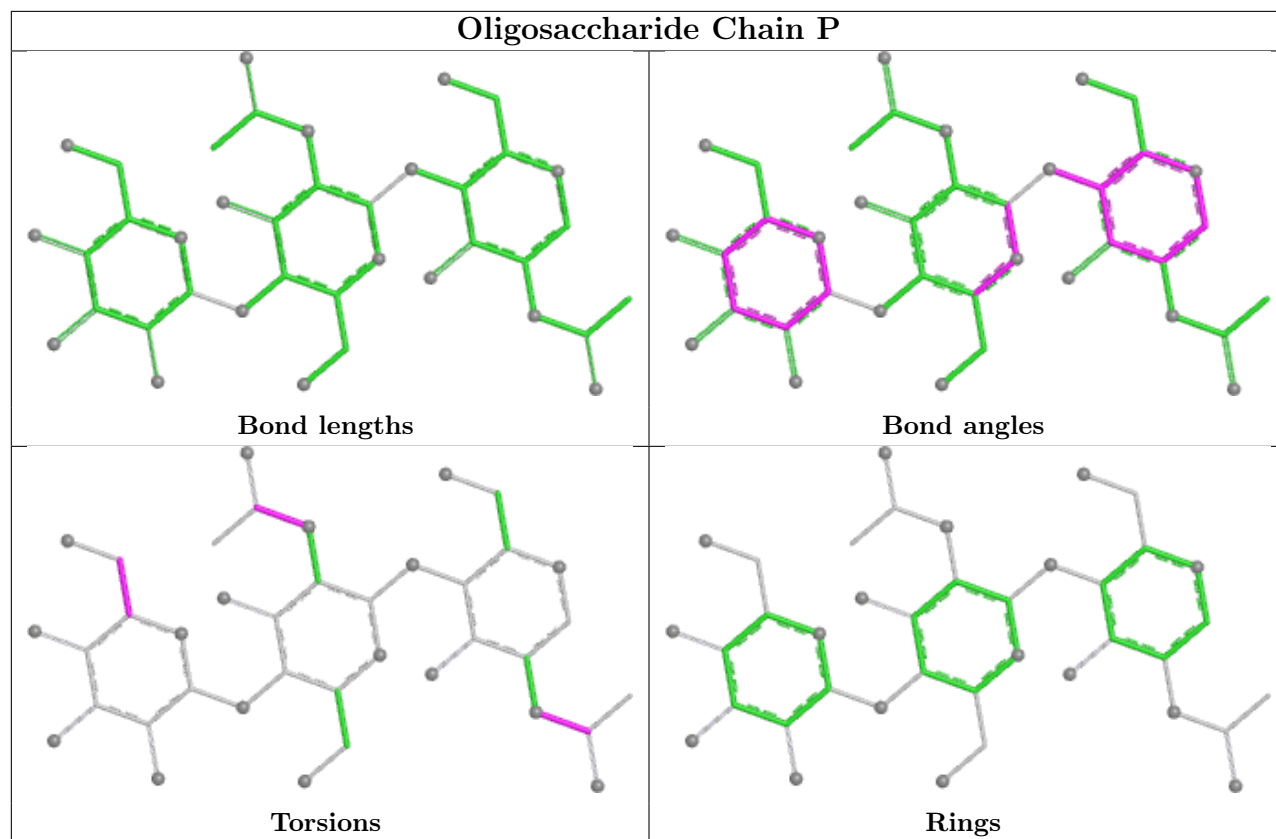
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1	1	NAG	4	0
9	X	6	MAN	2	0
9	v	2	NAG	1	0
15	3	1	NAG	4	0

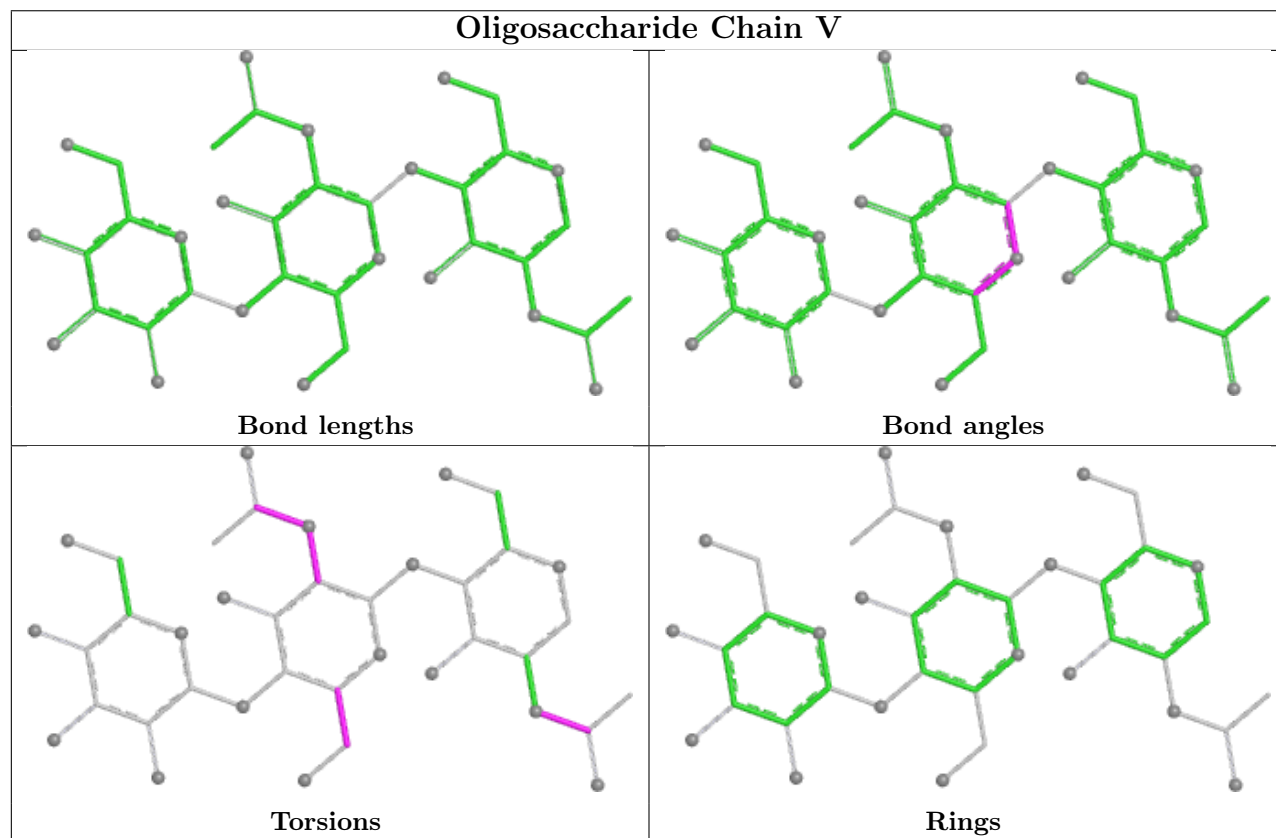
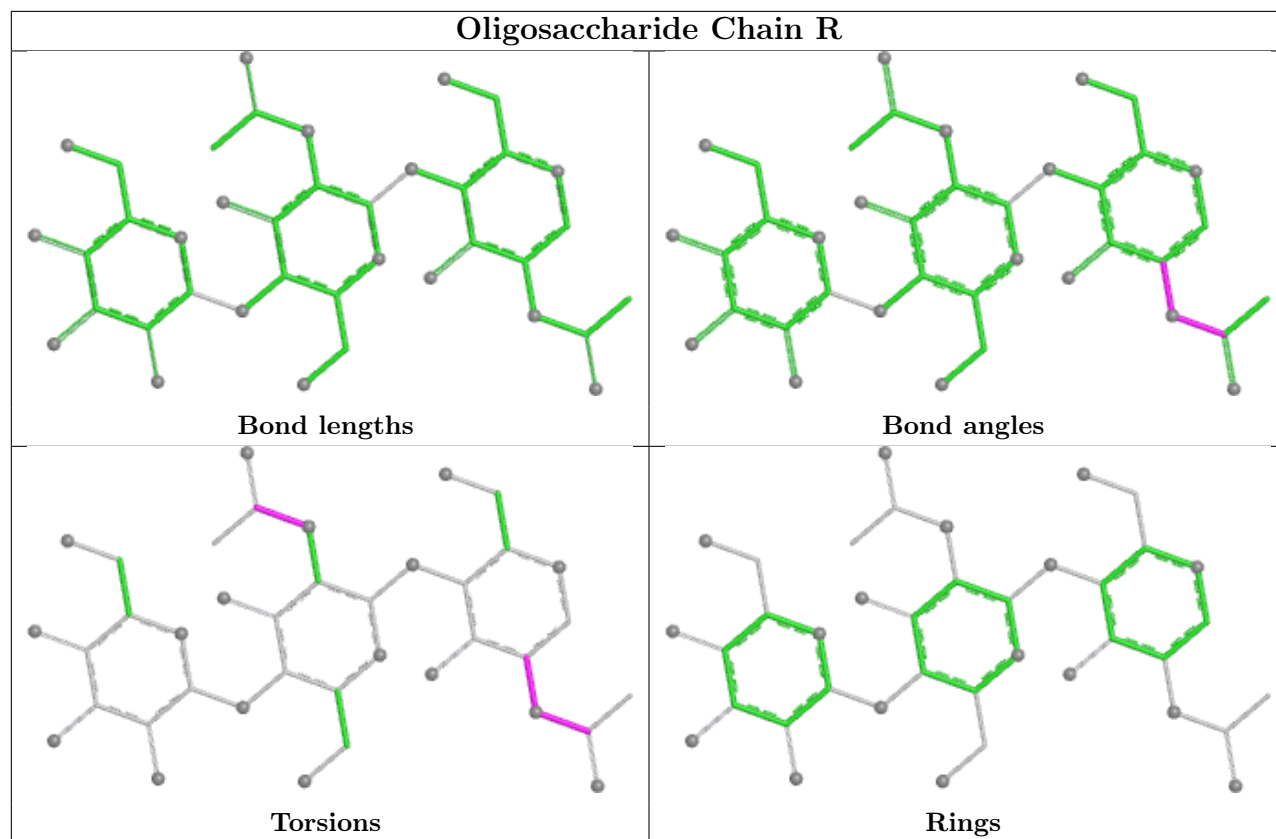
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

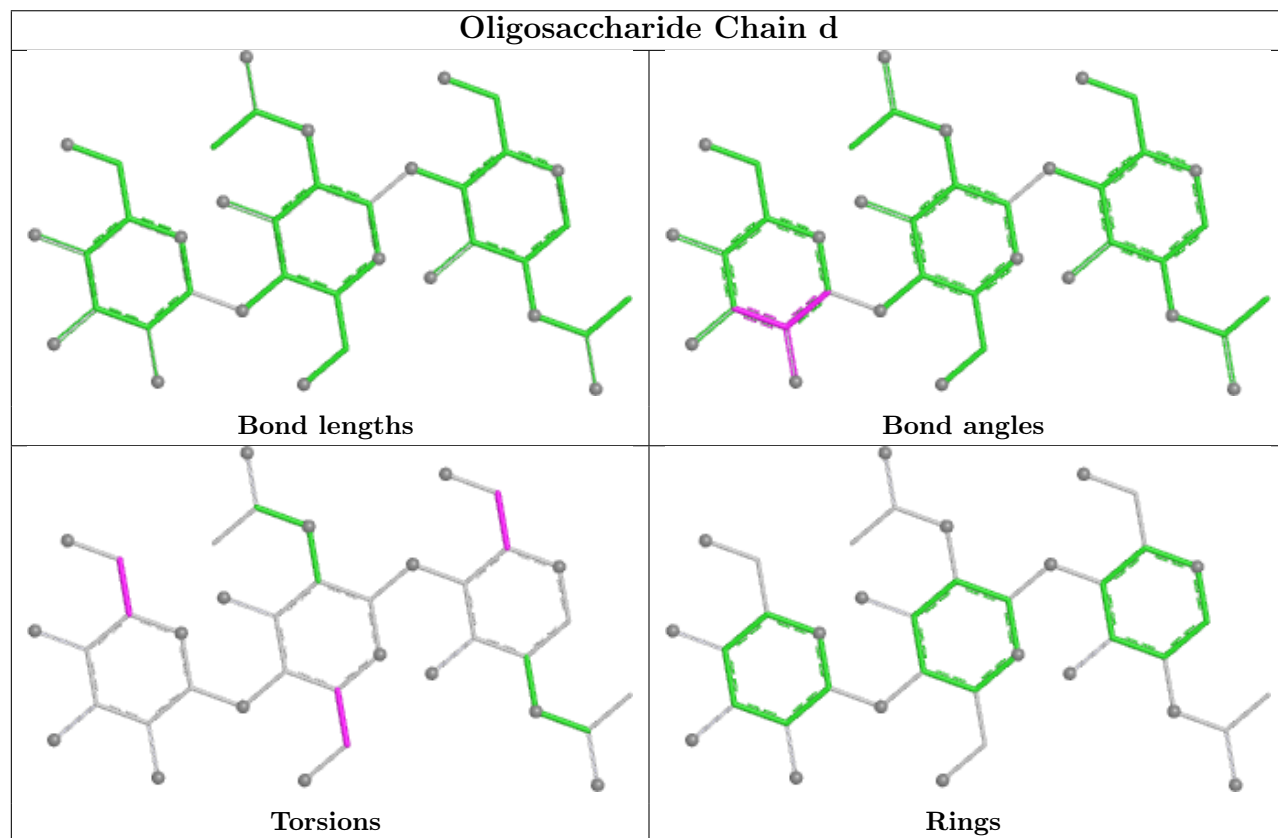
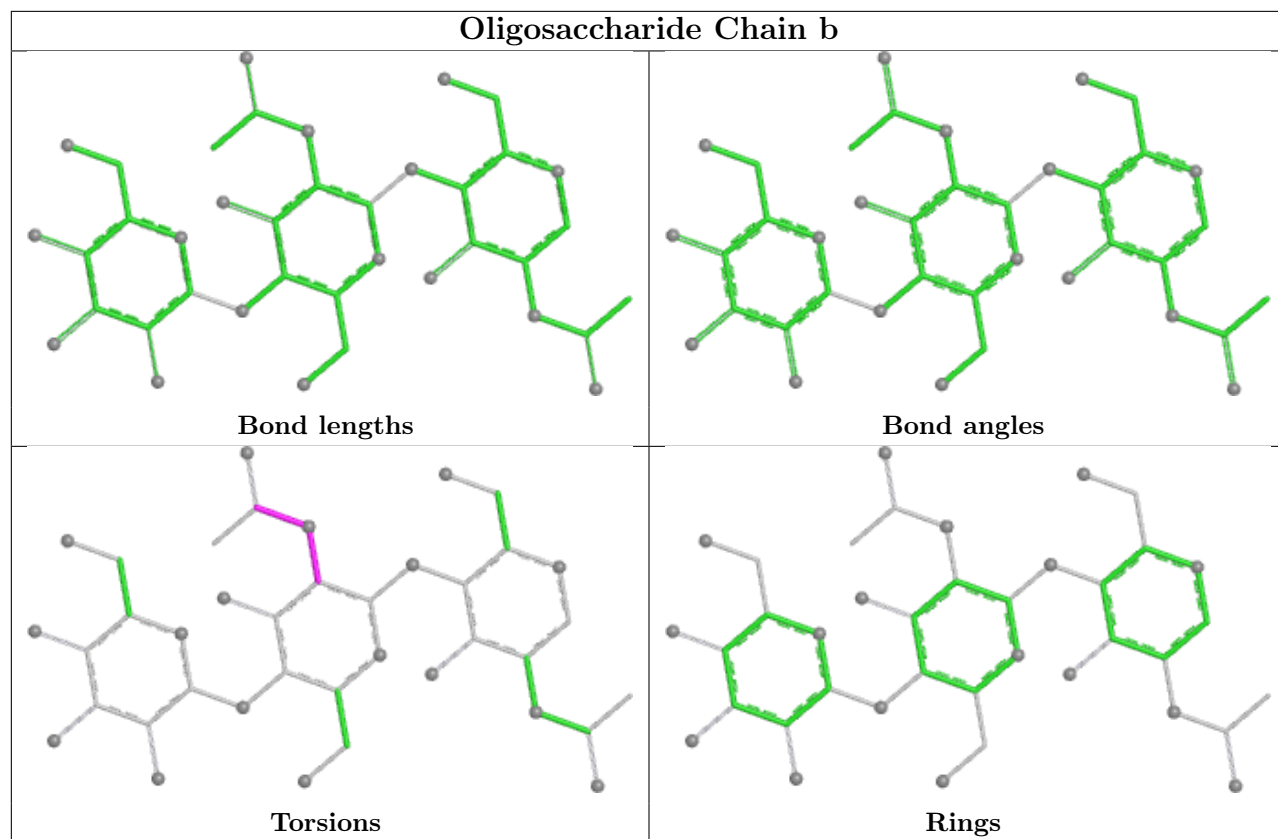


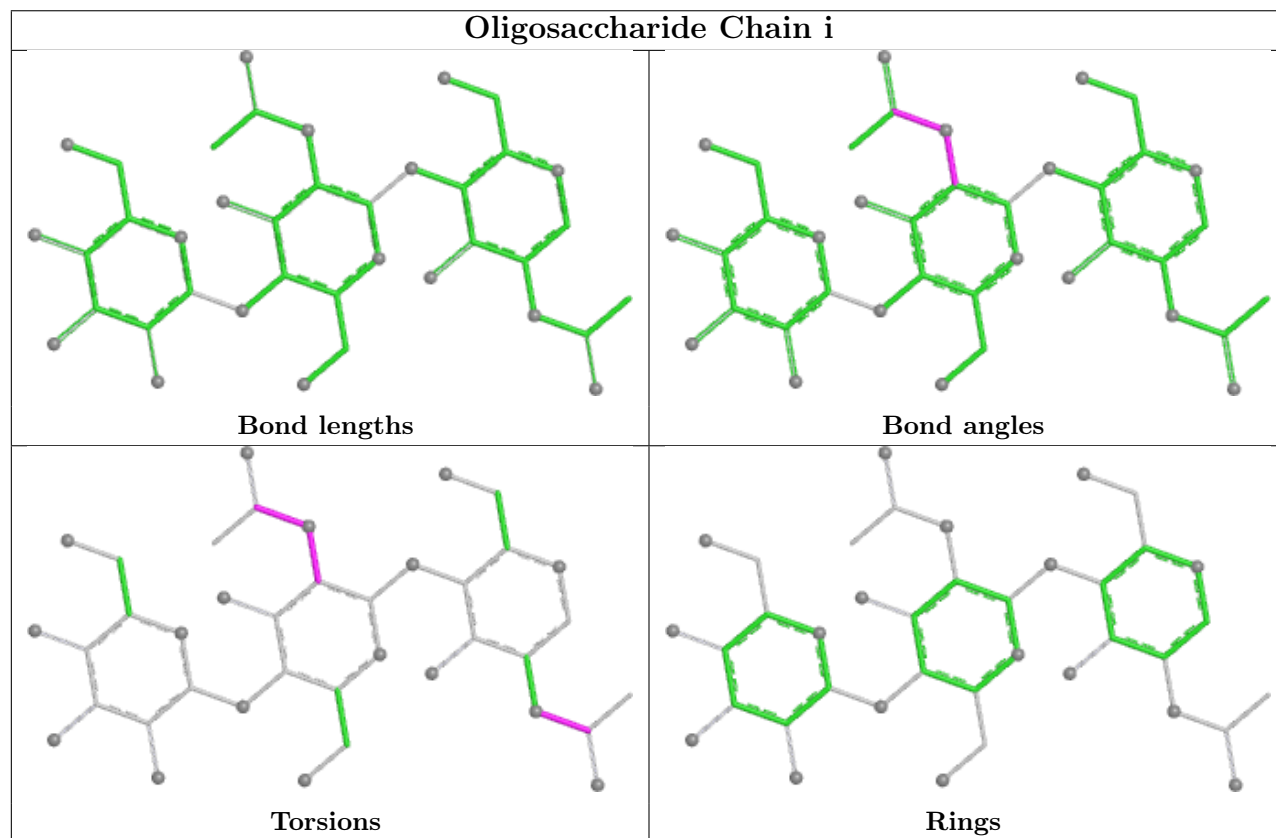
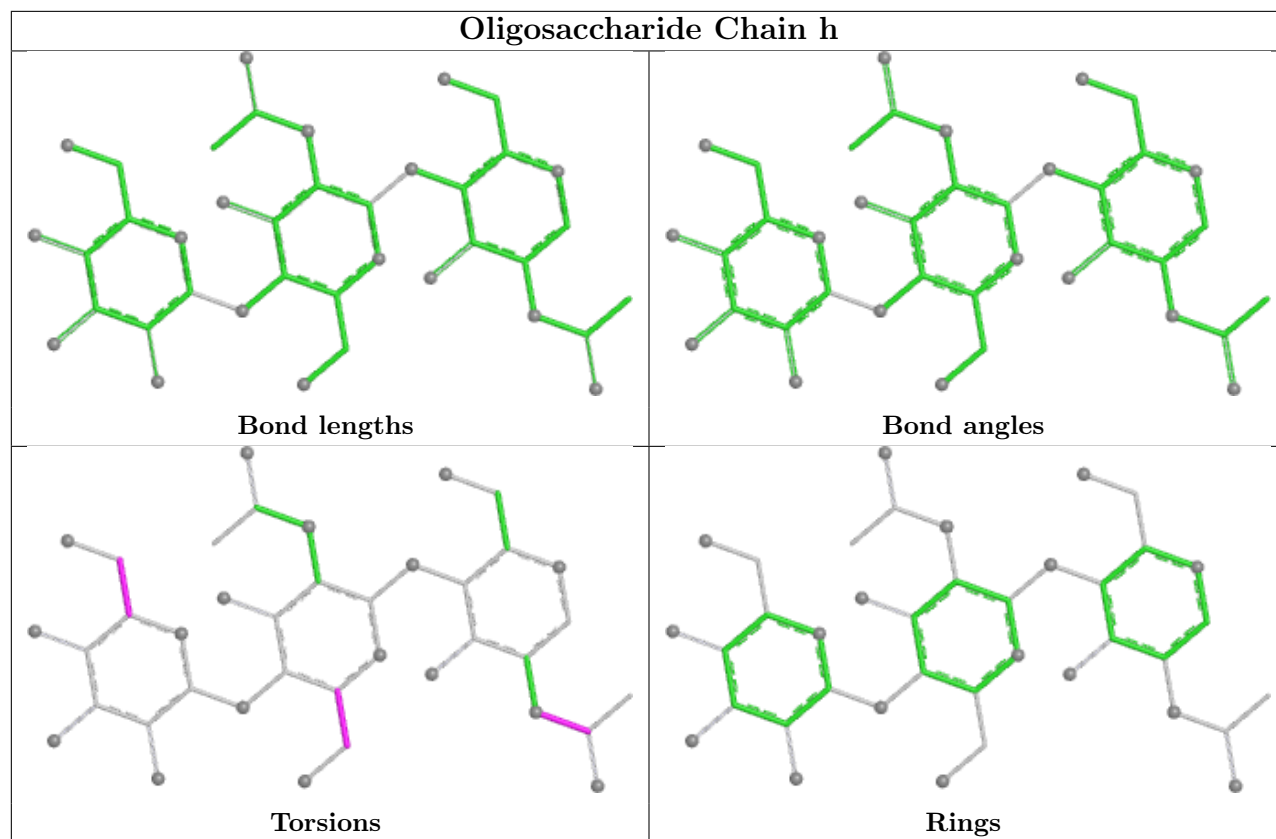


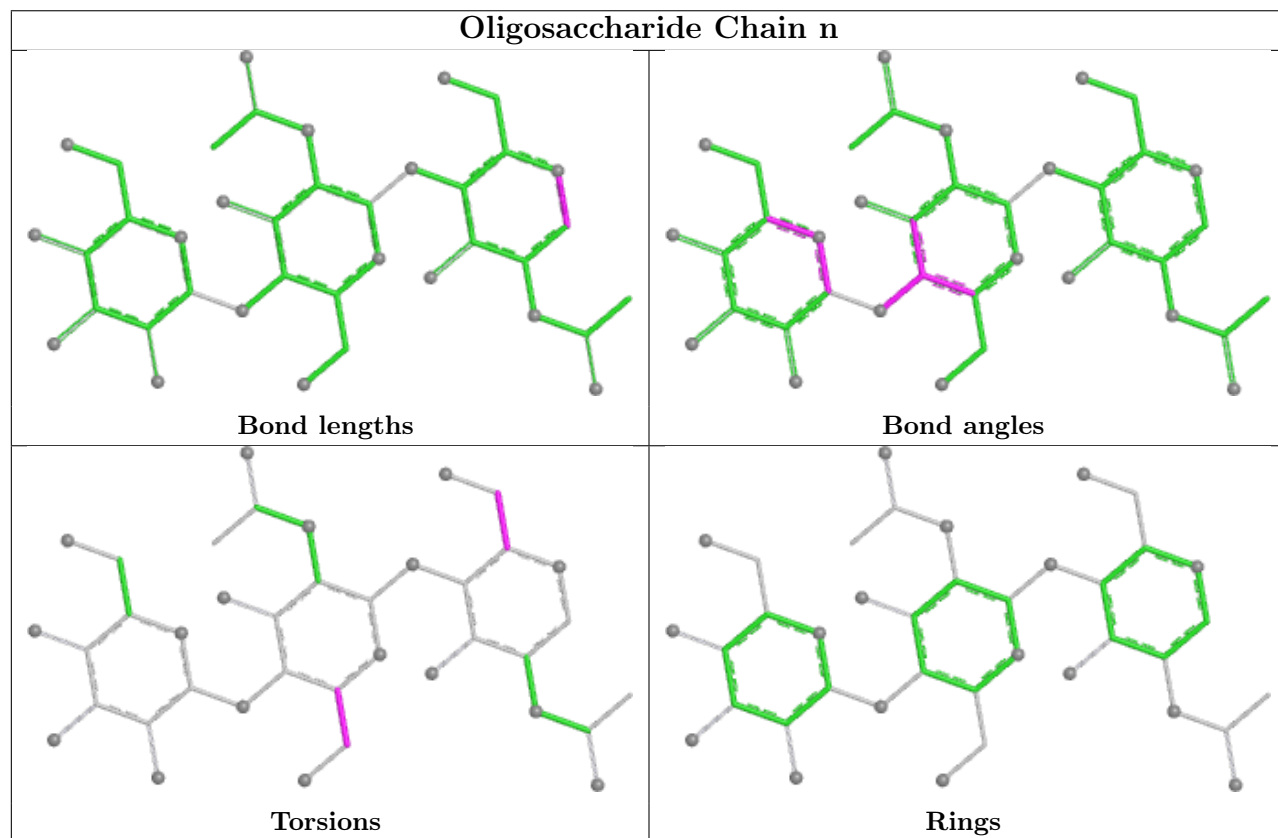
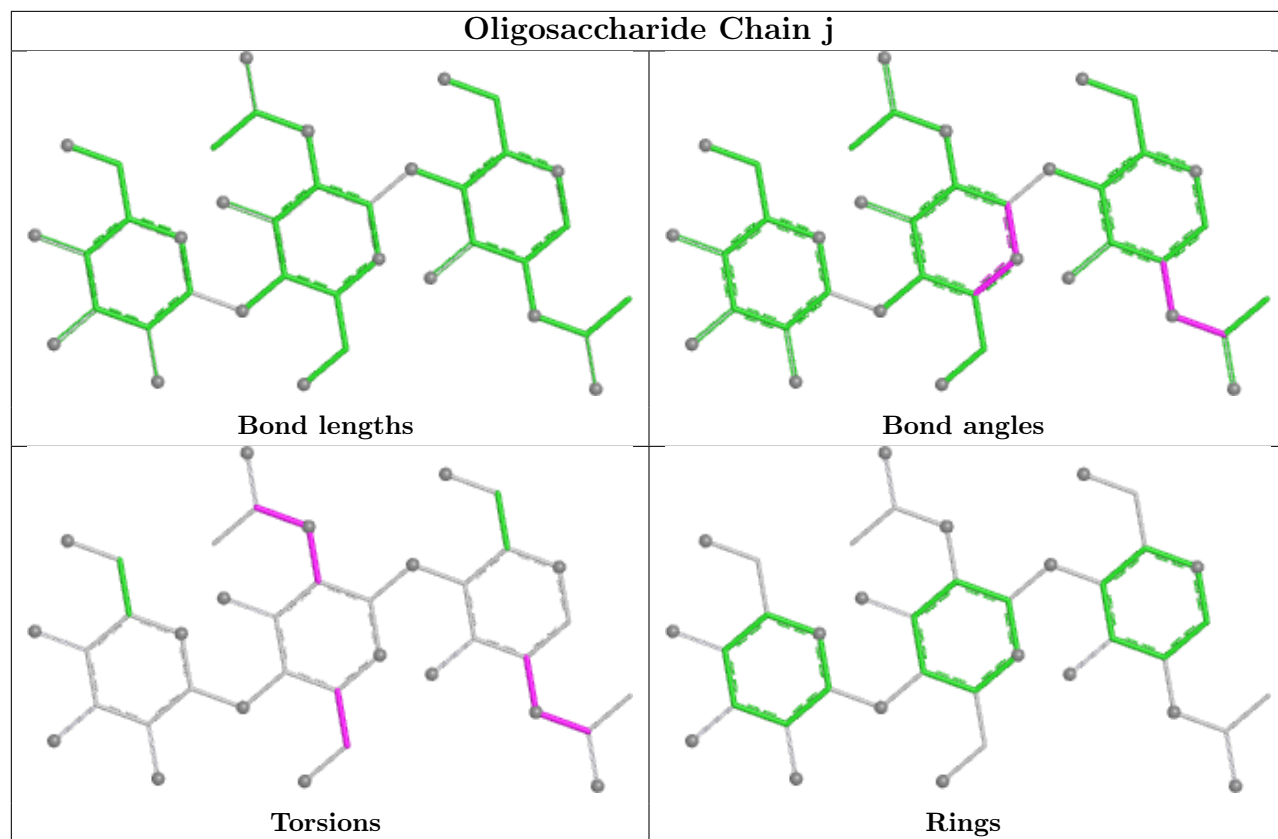


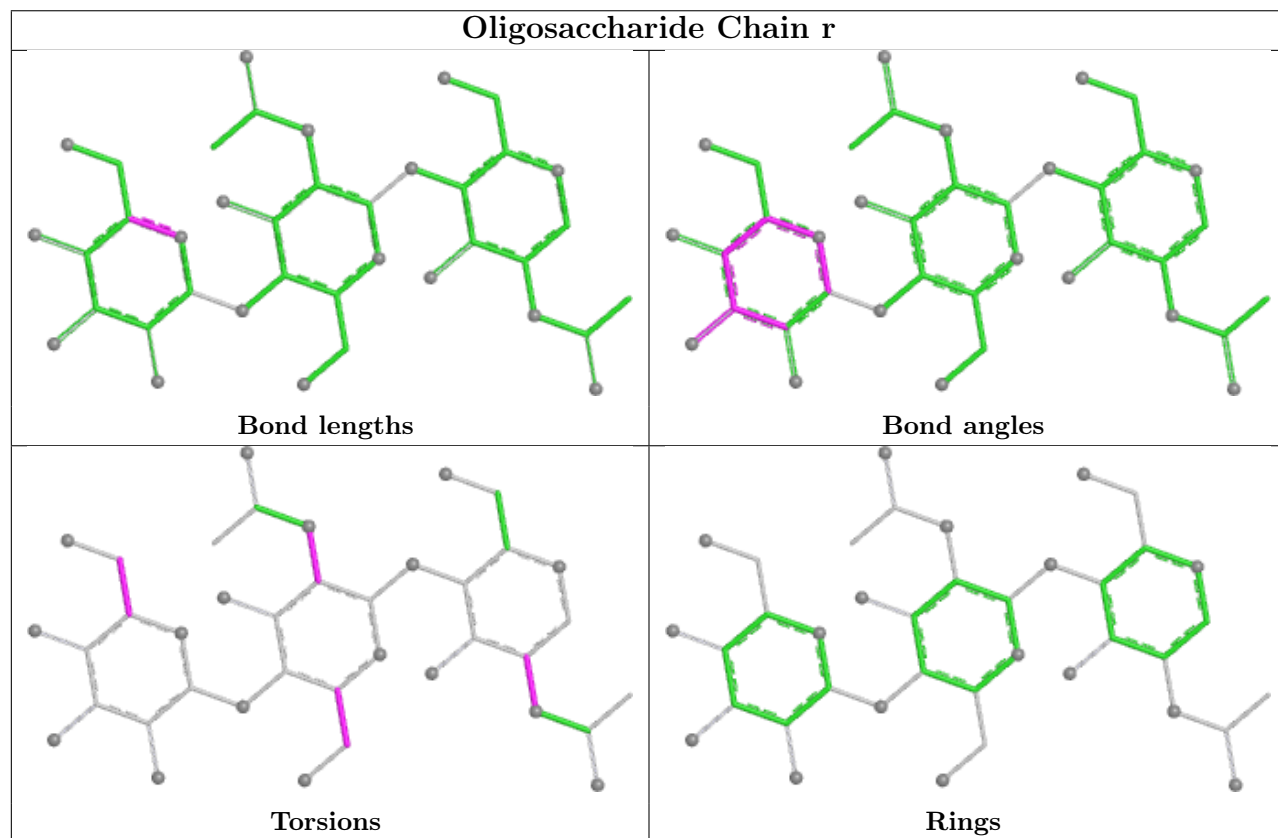
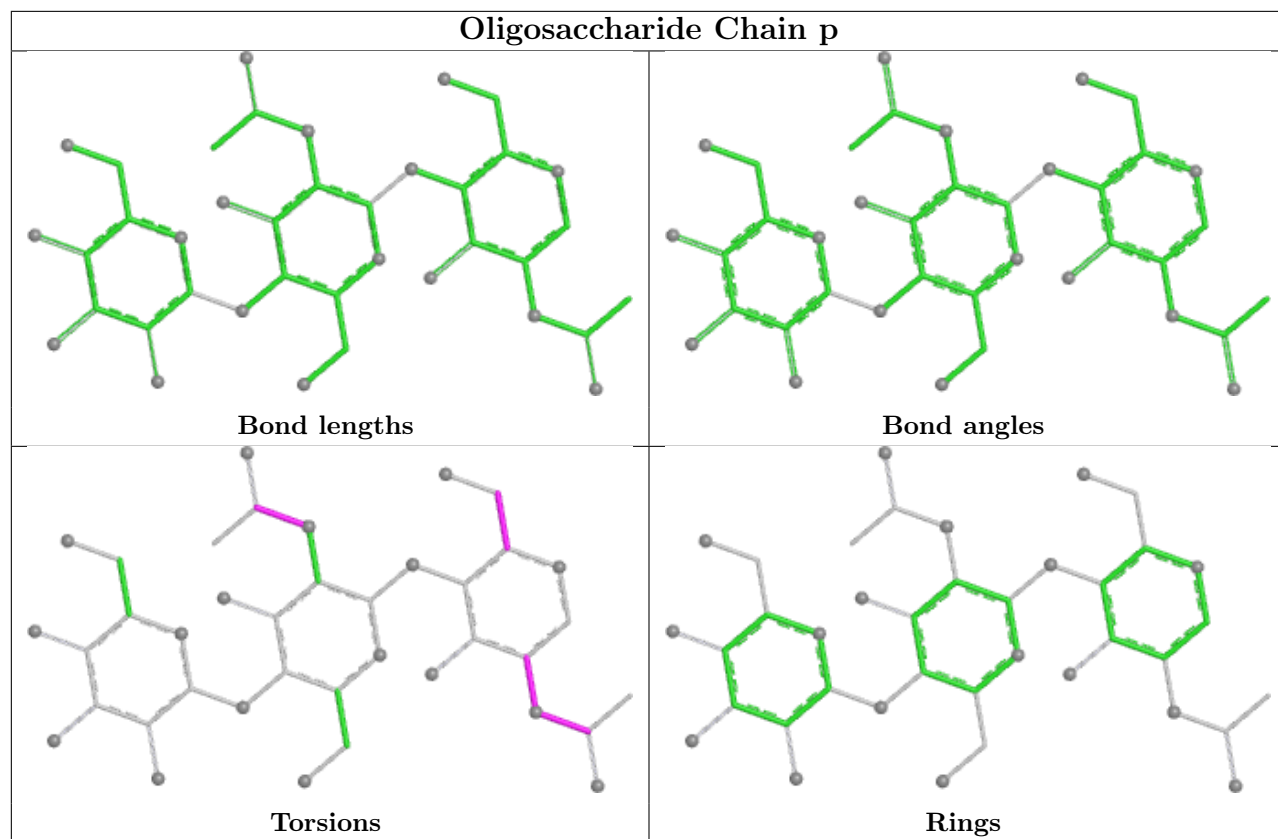


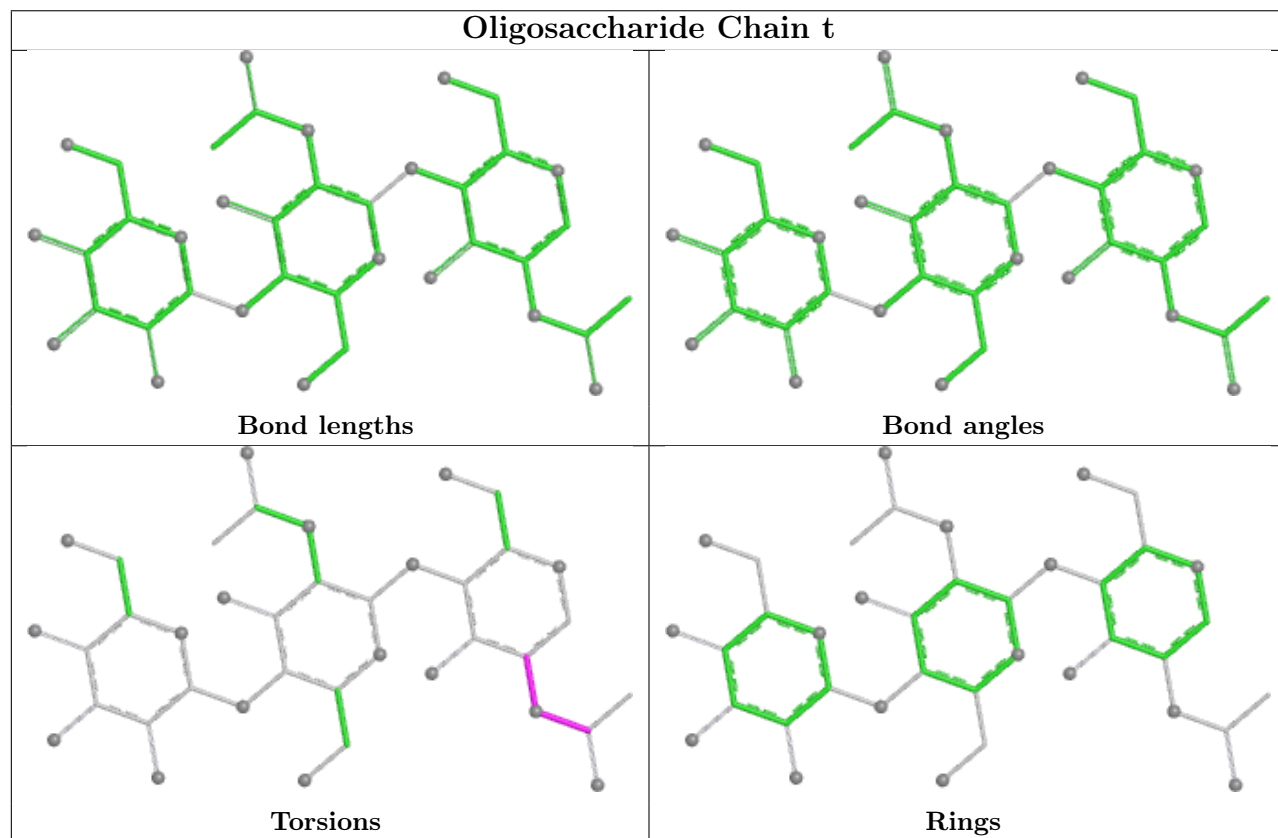
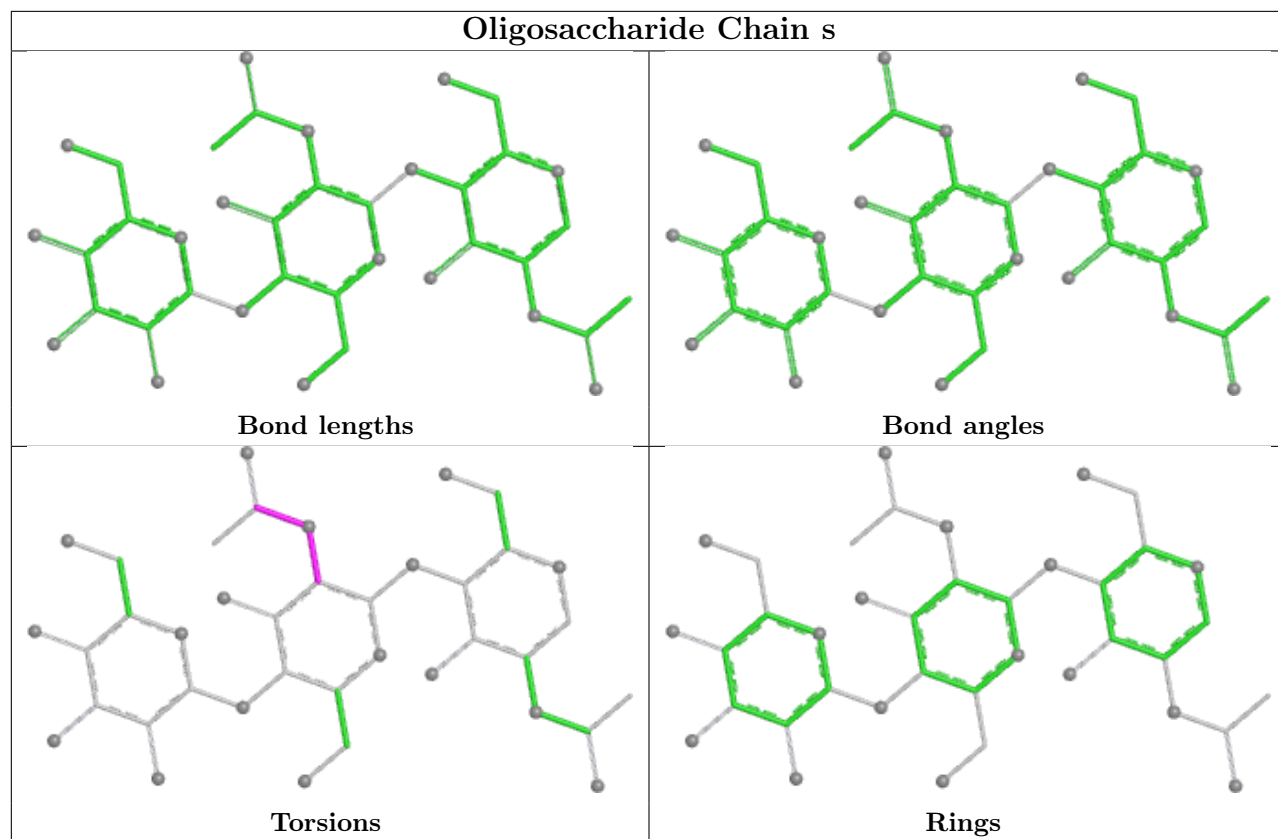


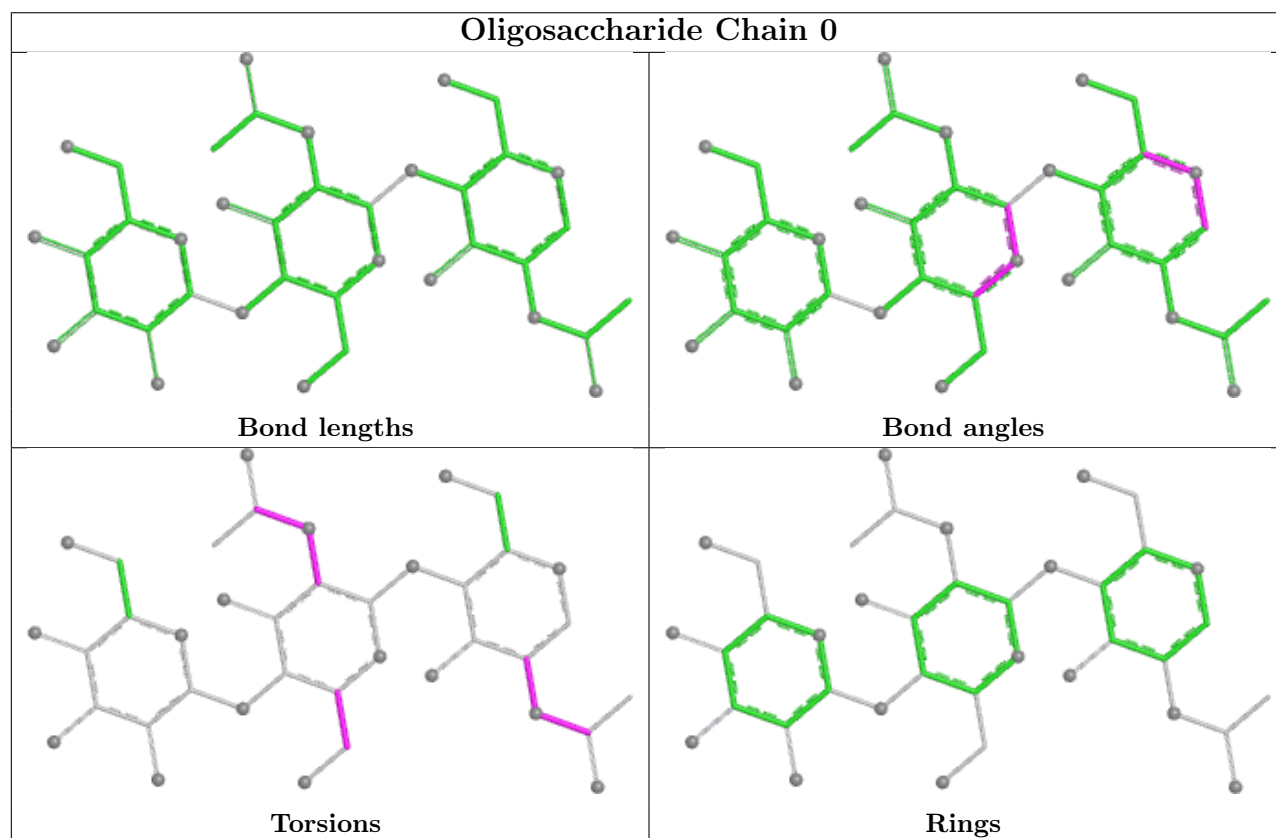
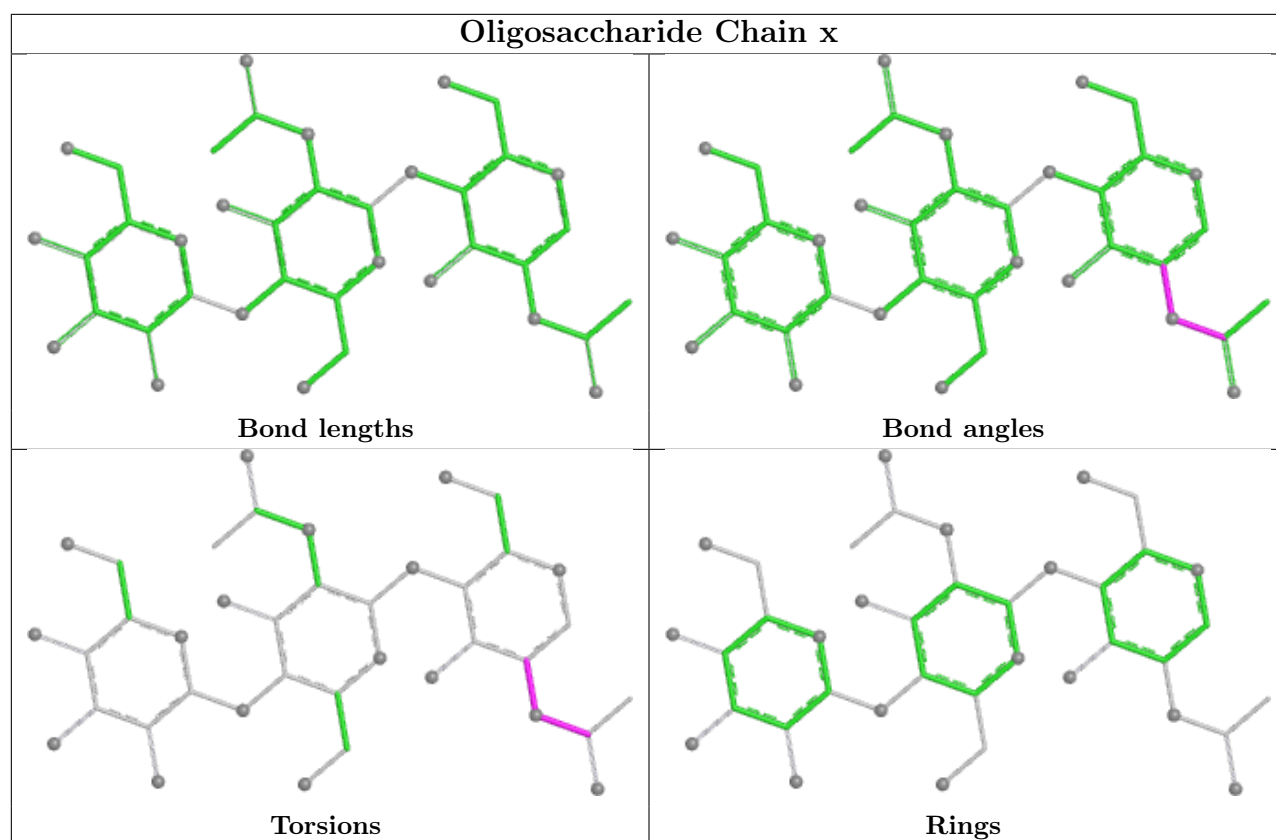


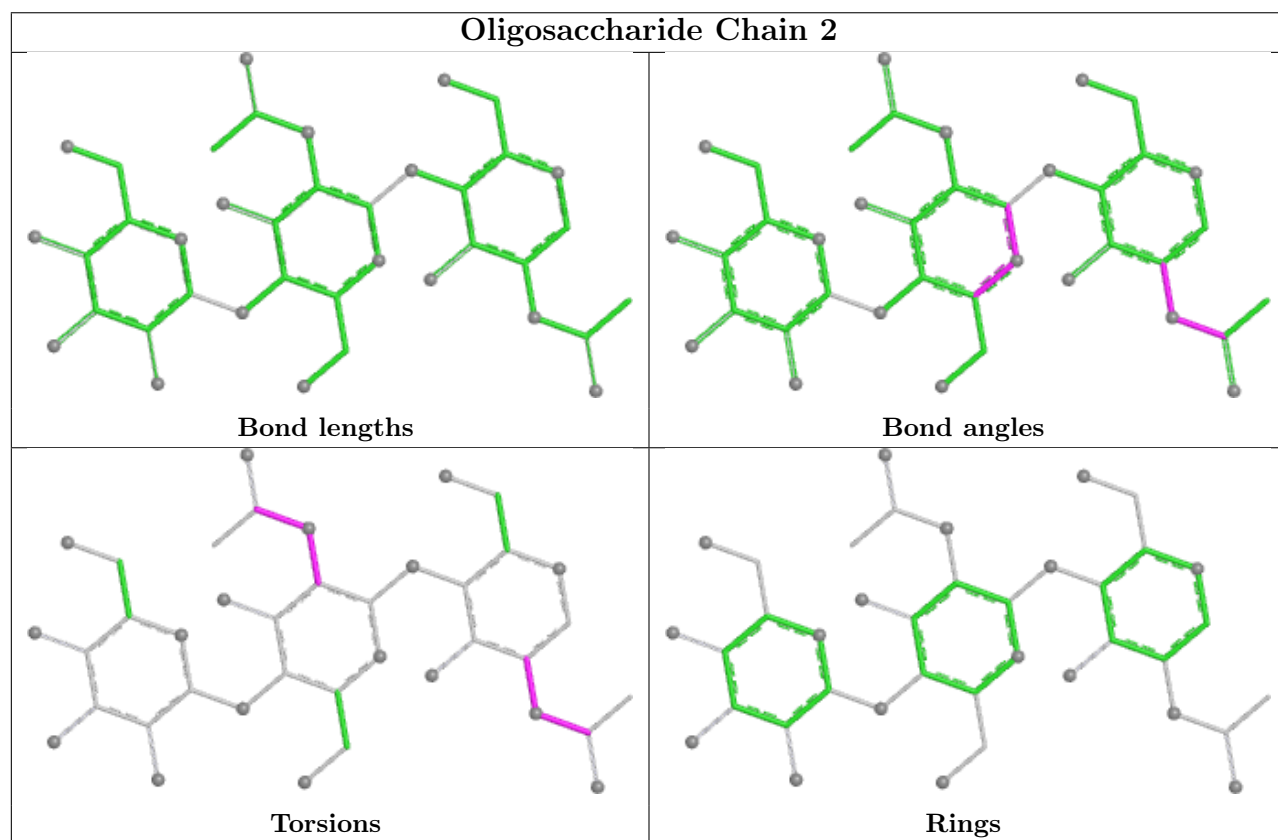
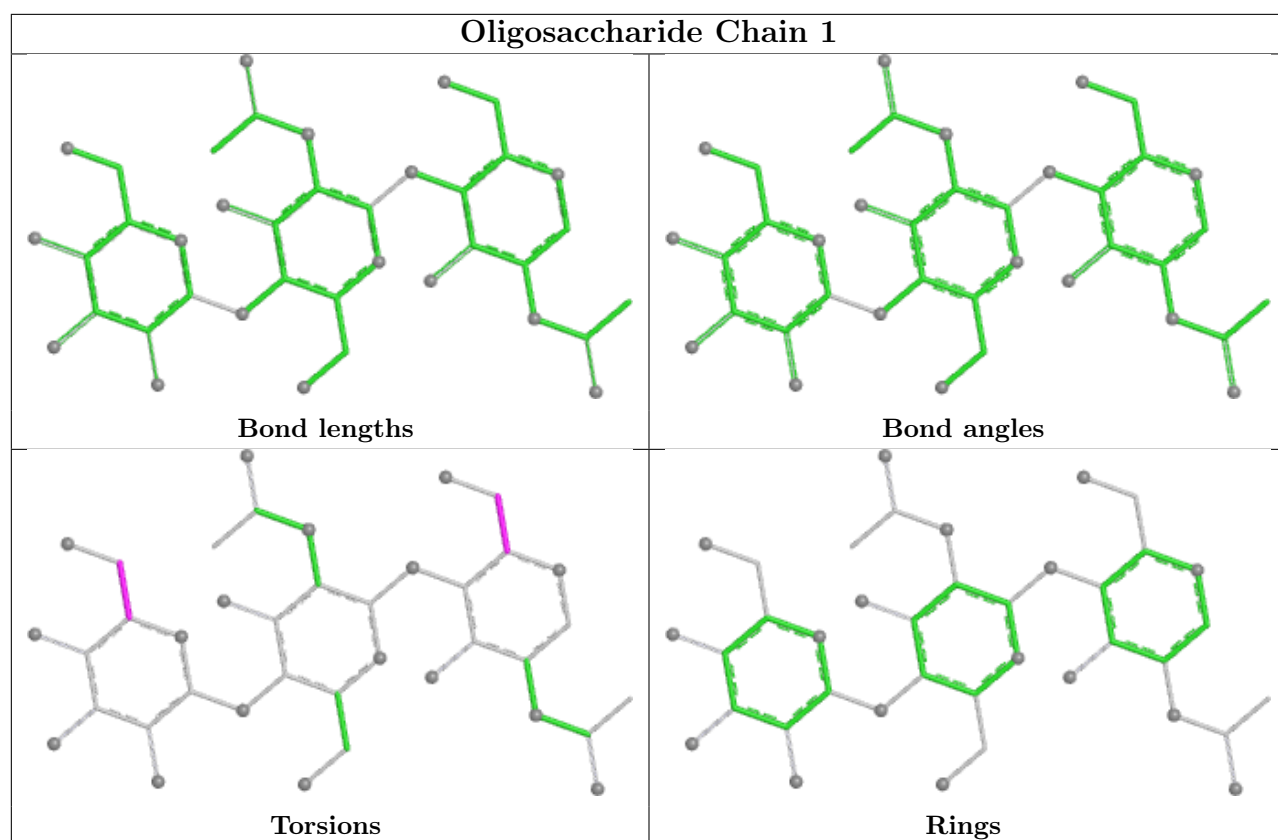


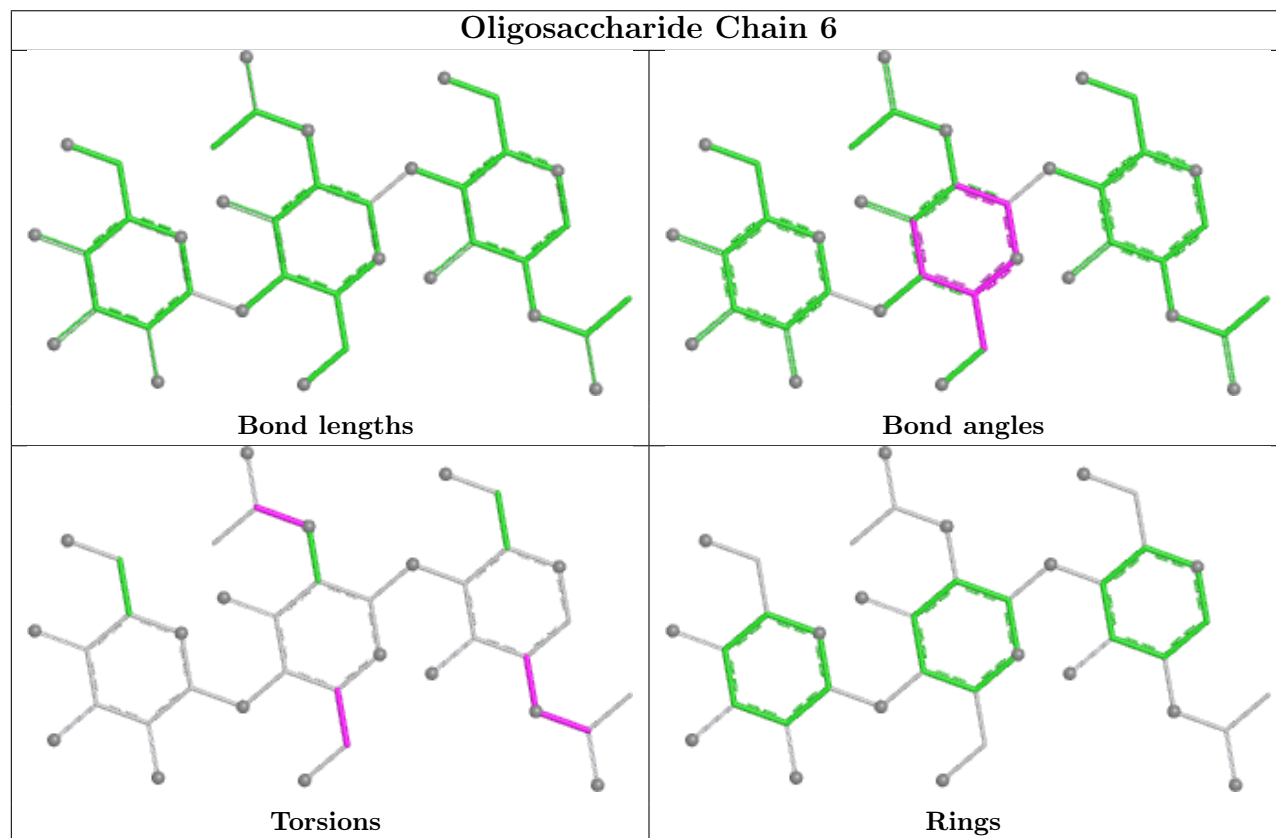
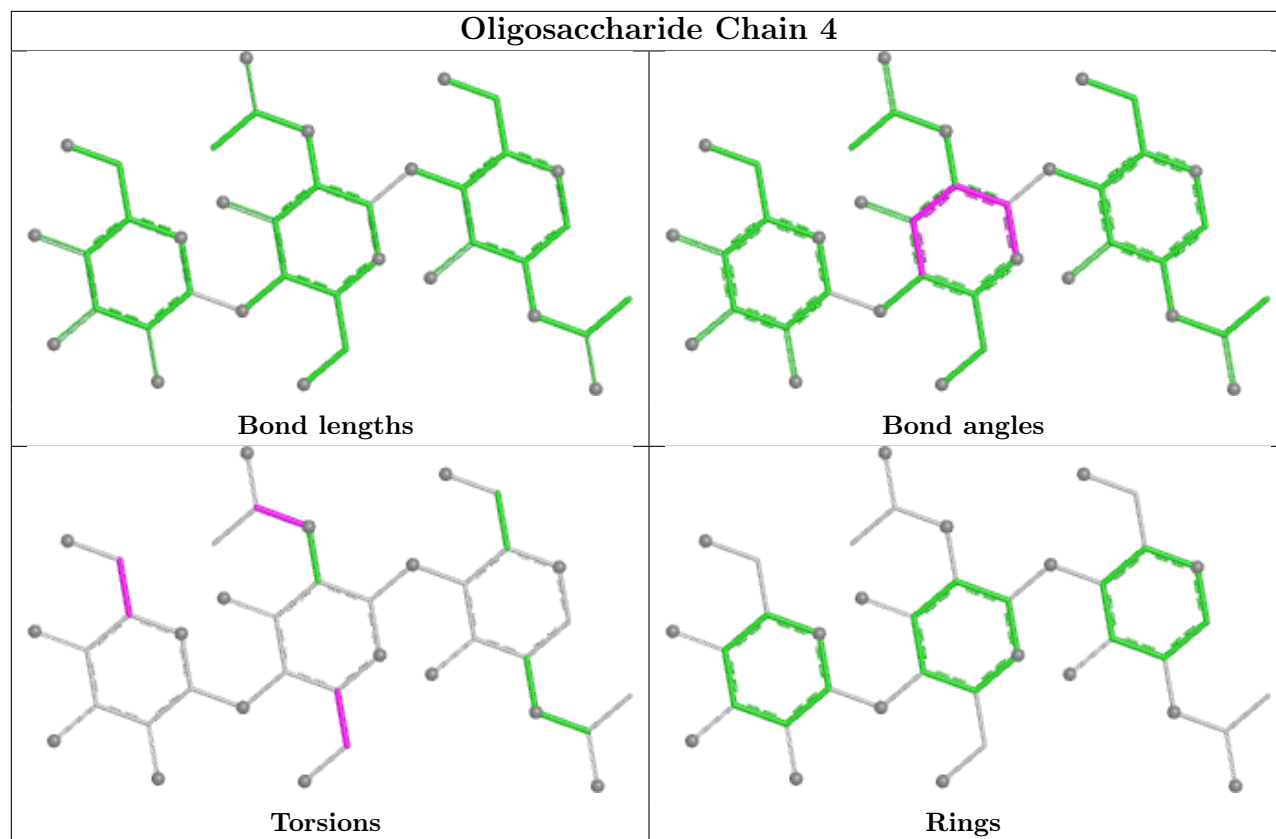


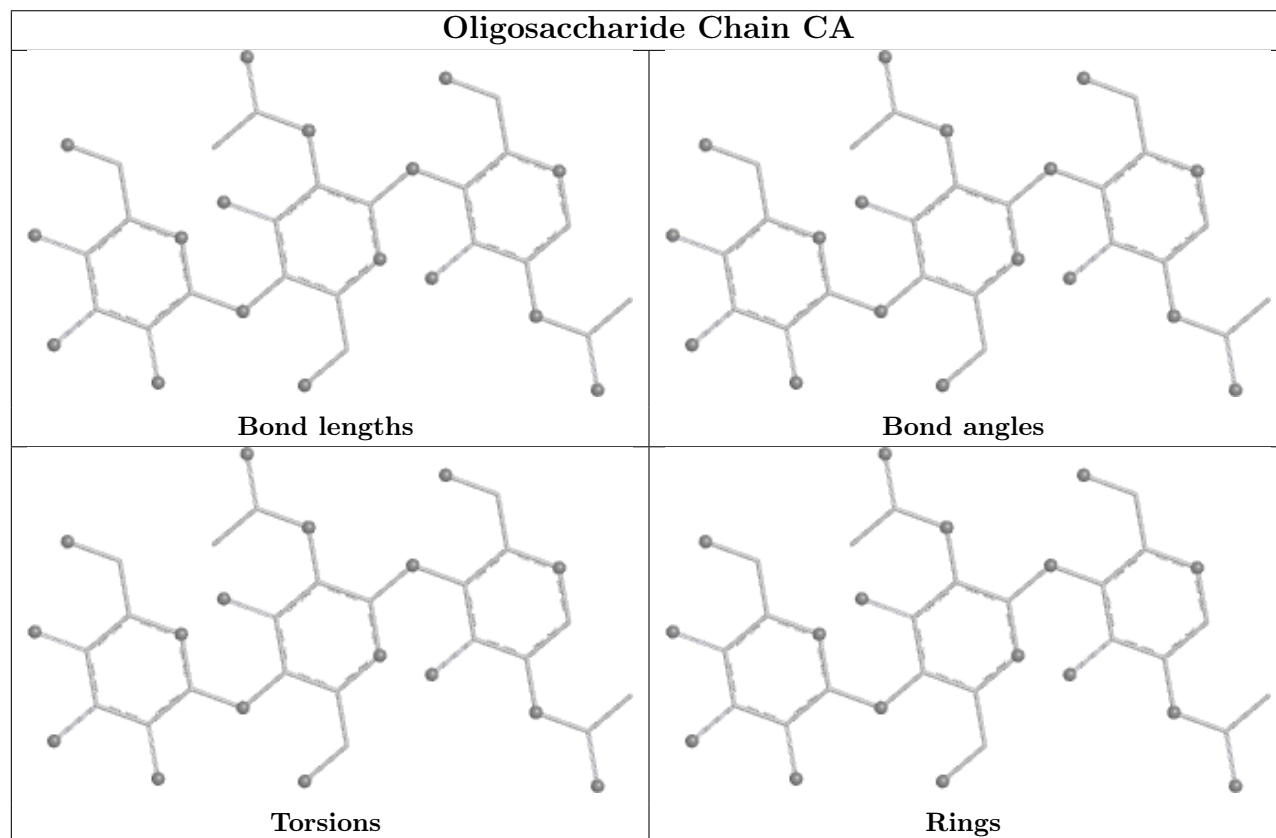
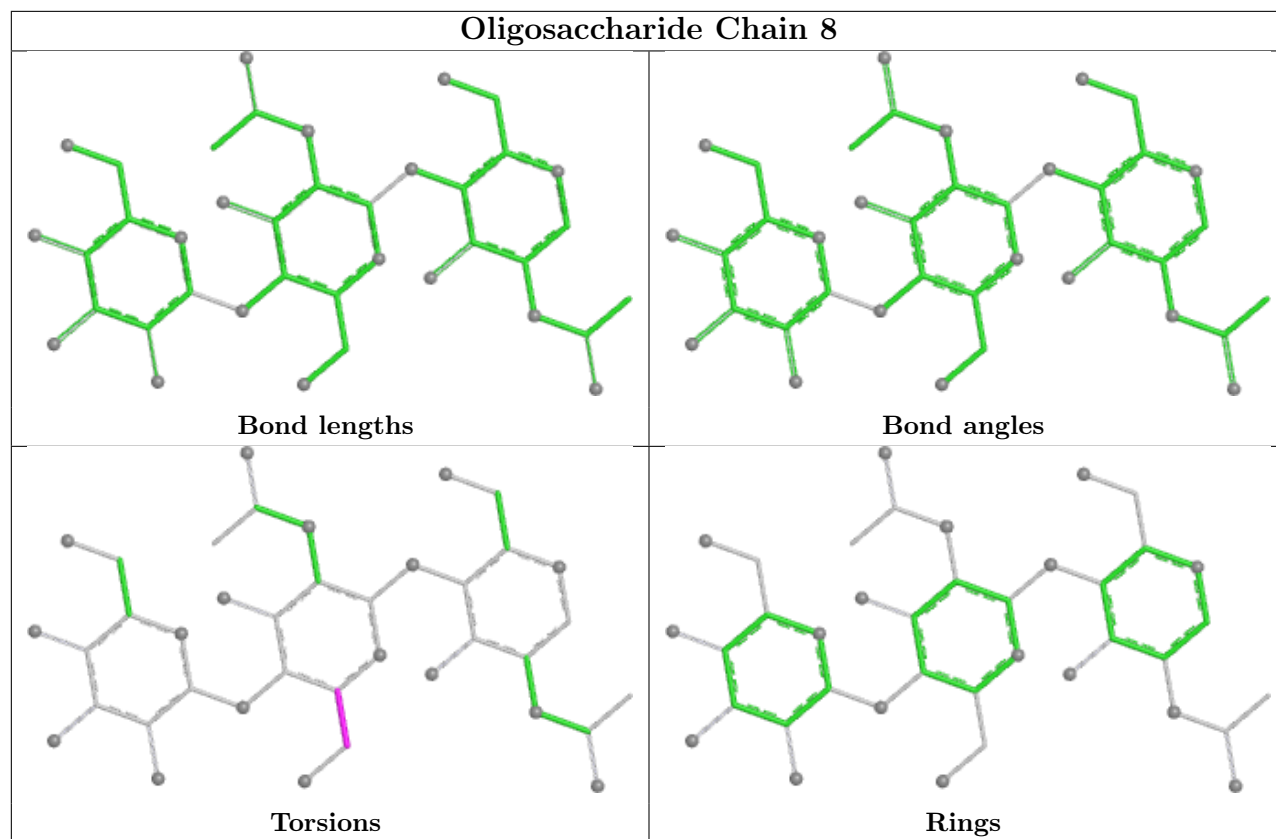


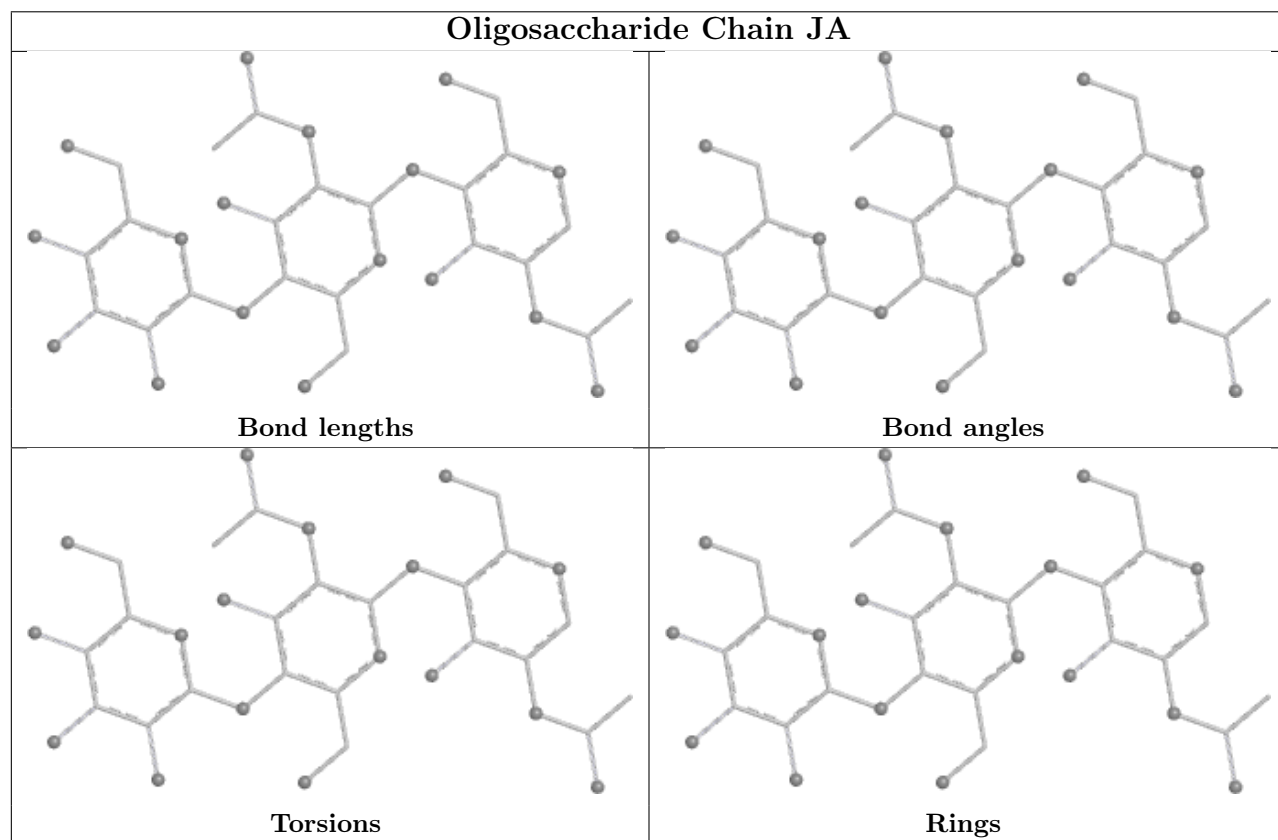
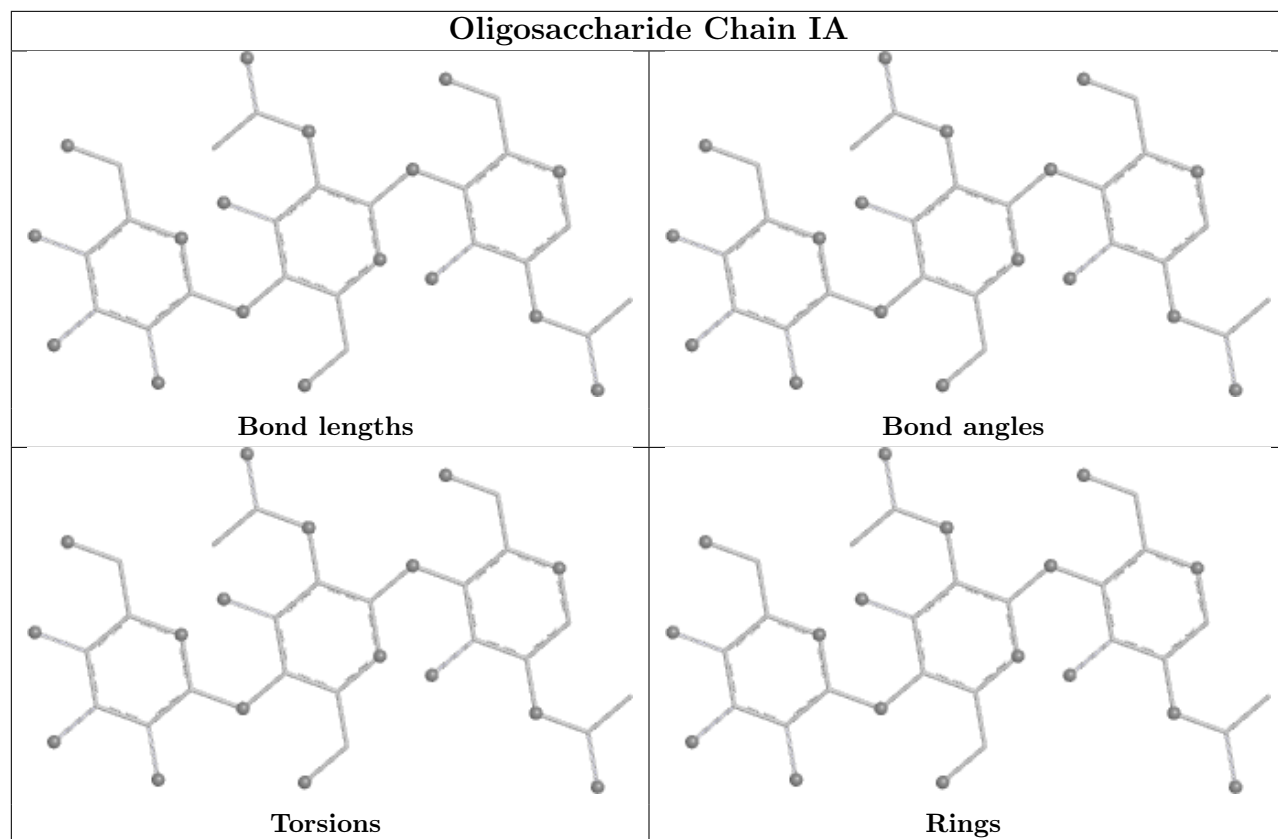


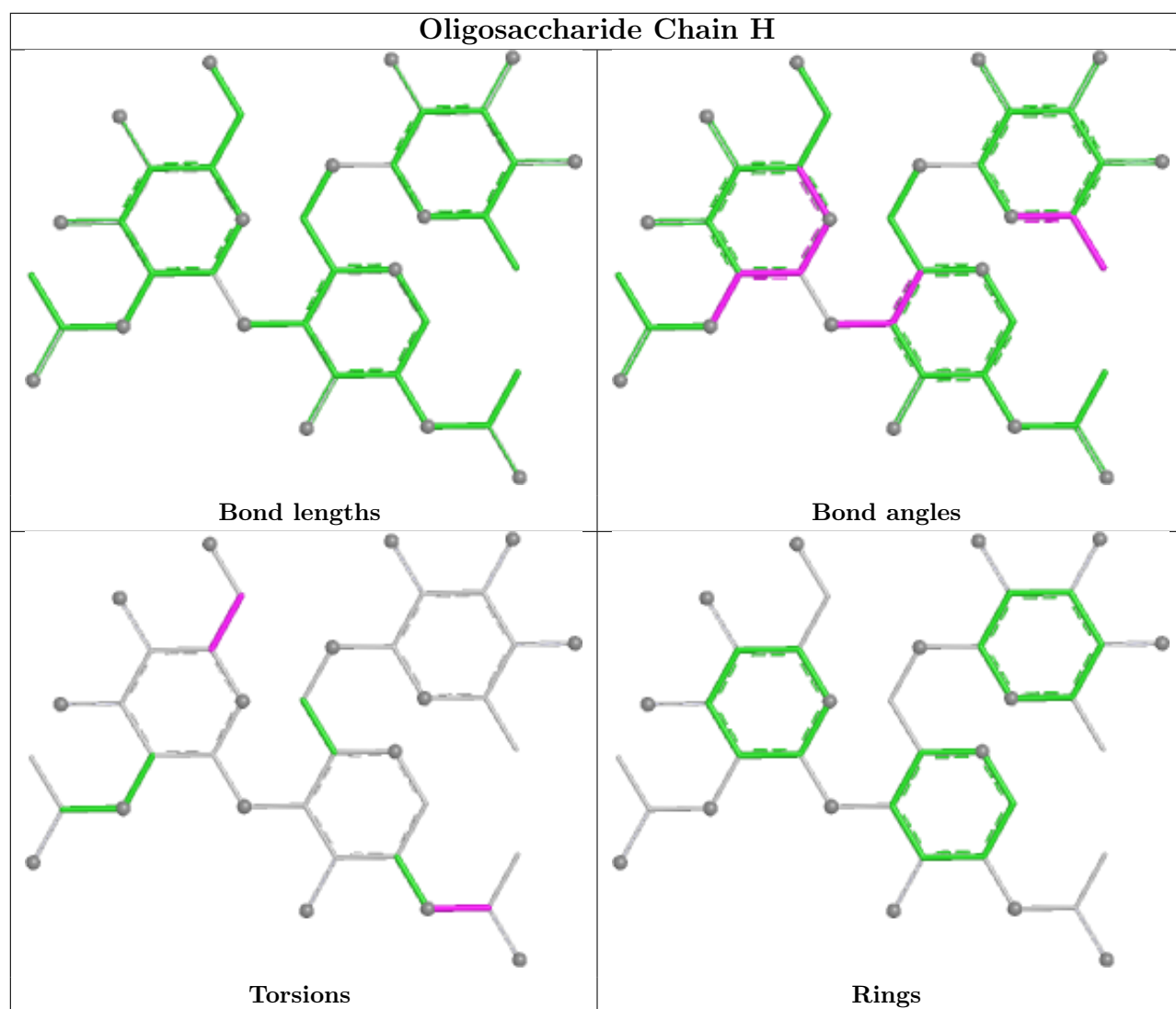


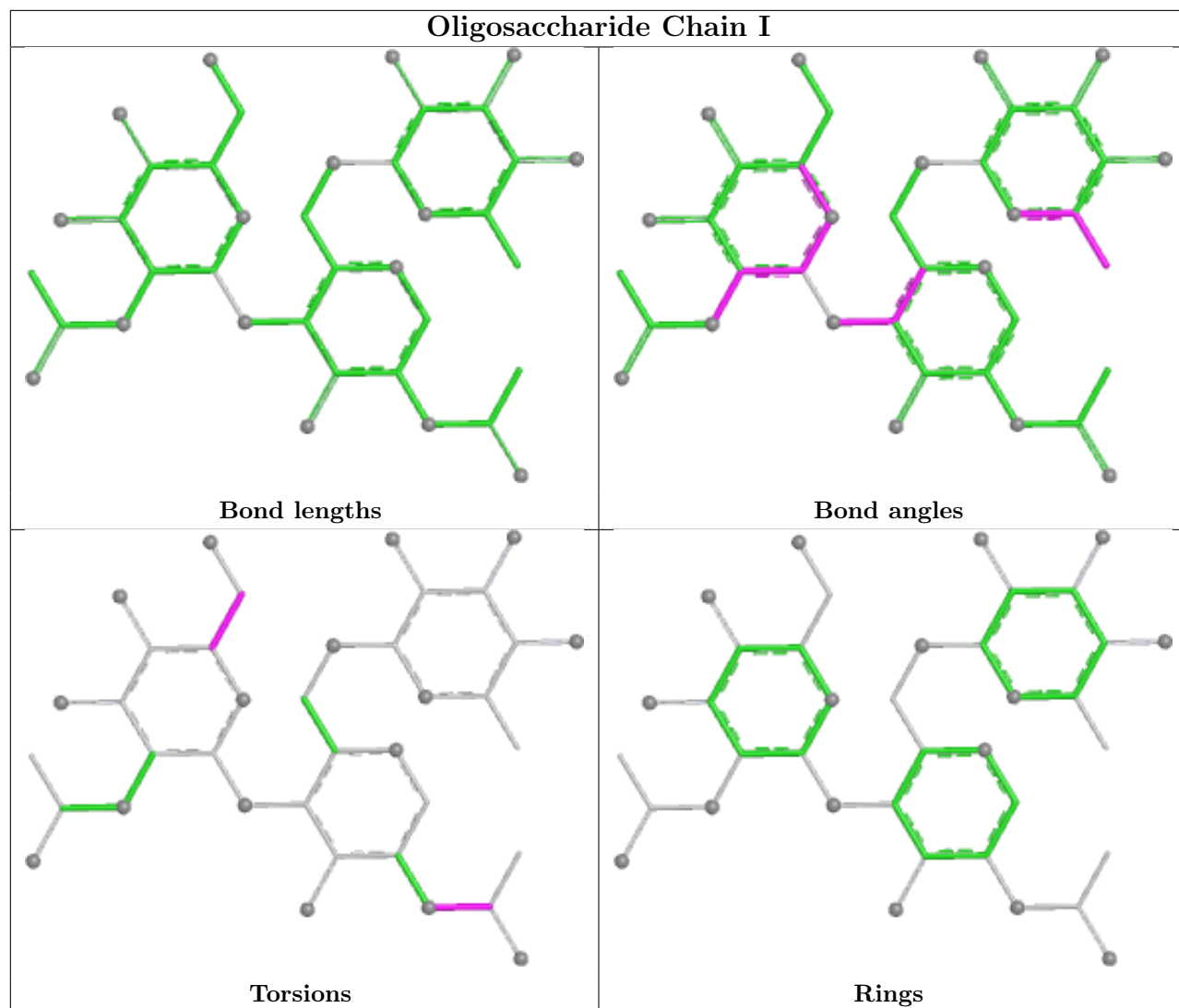


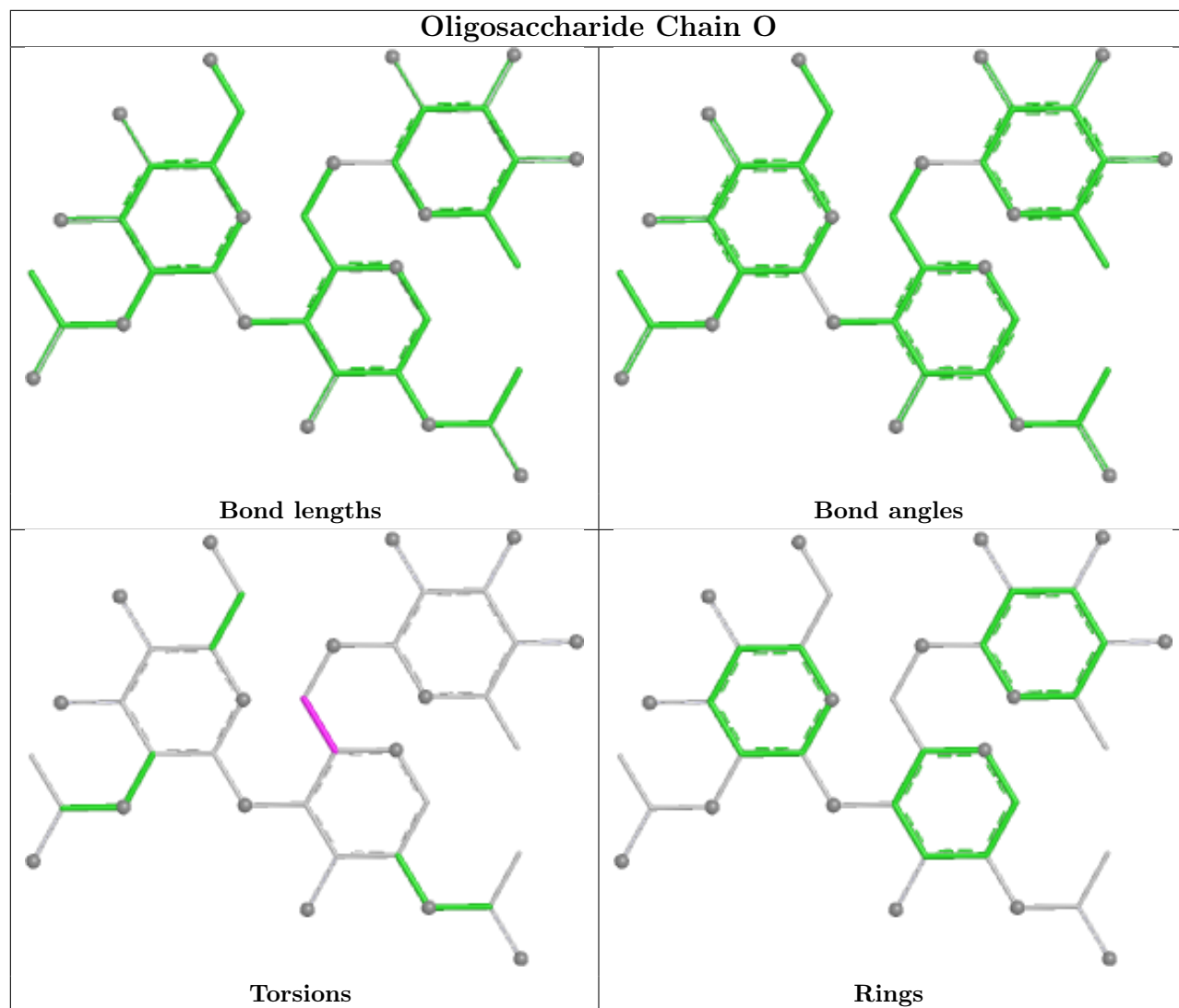


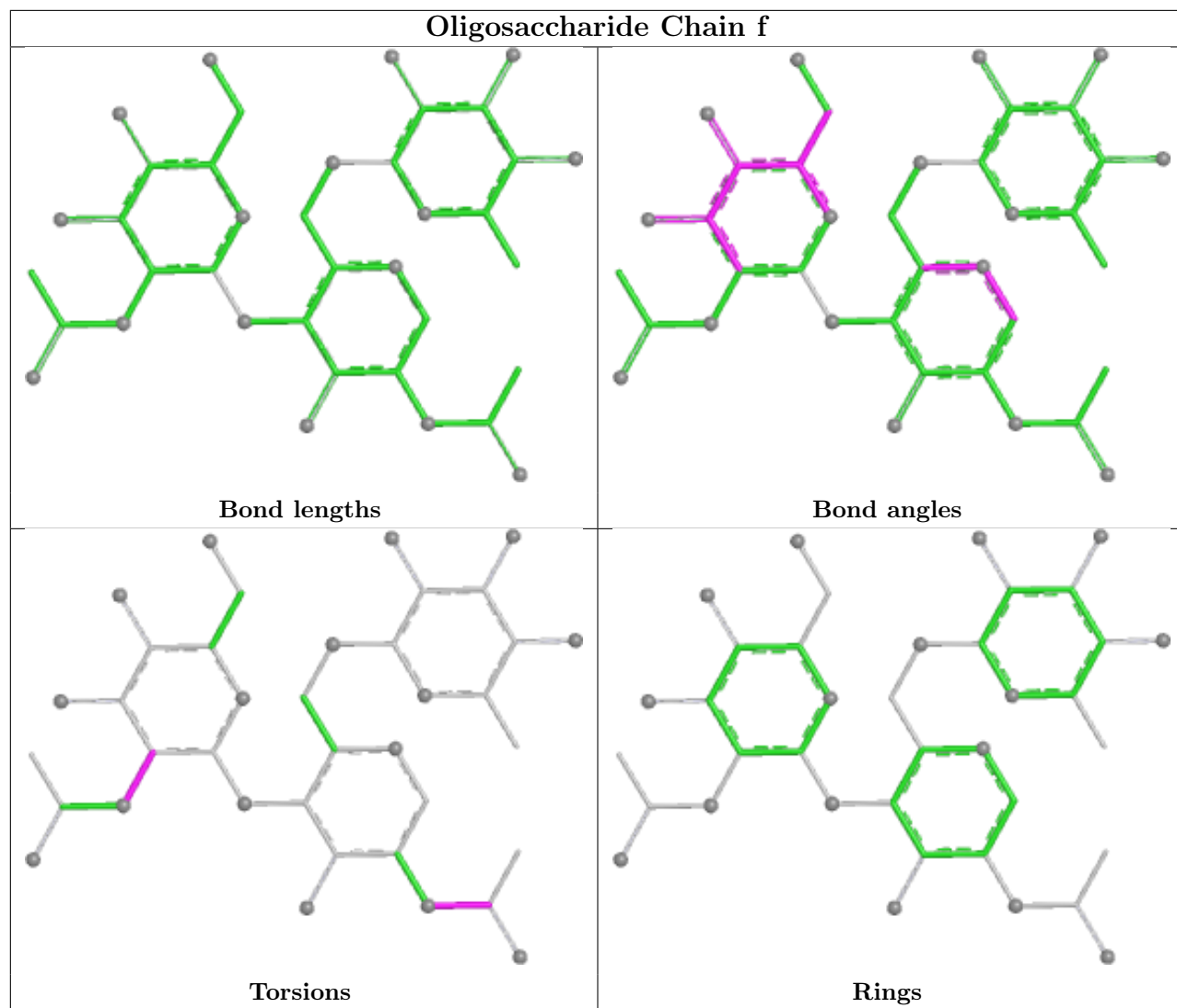


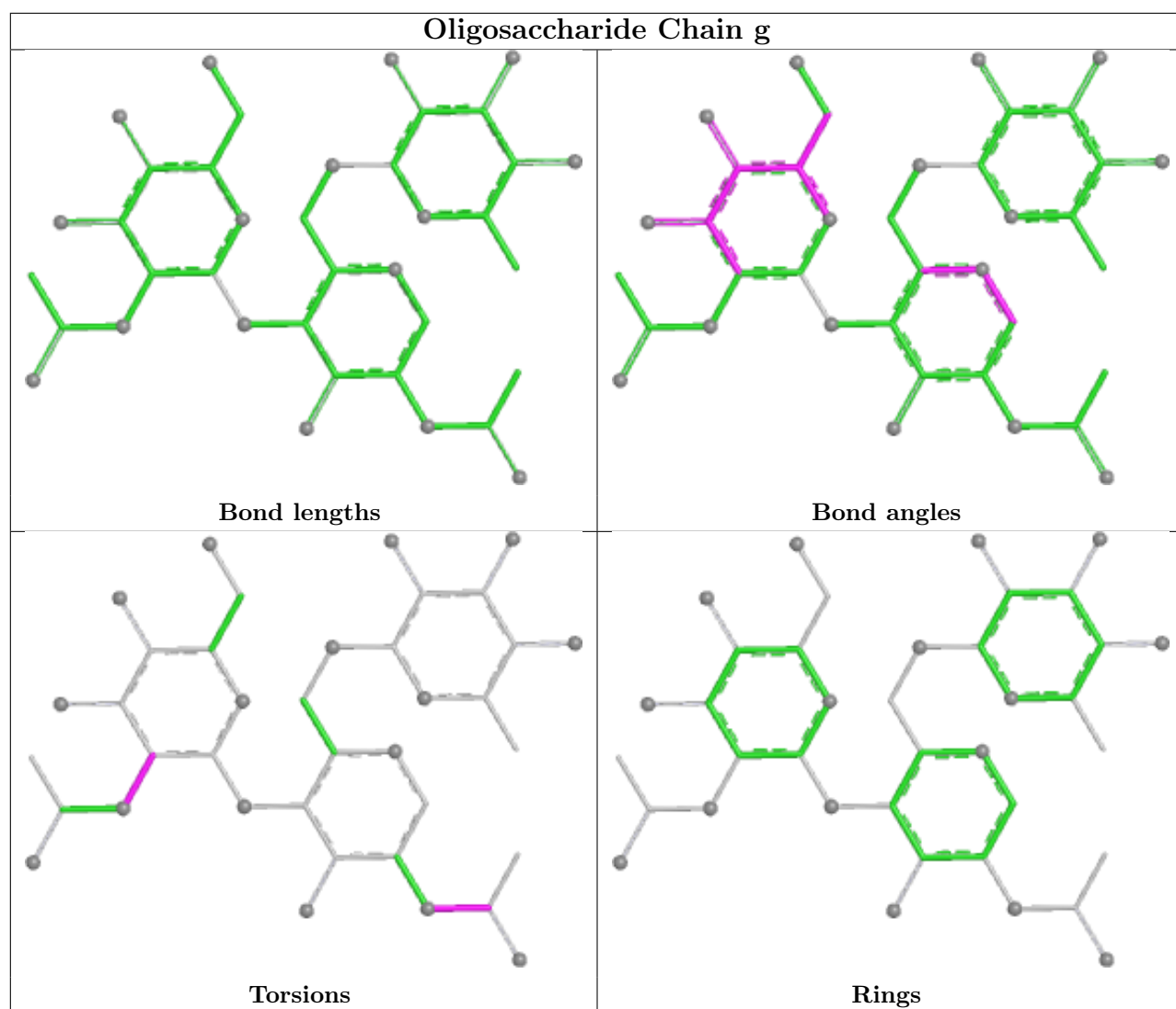


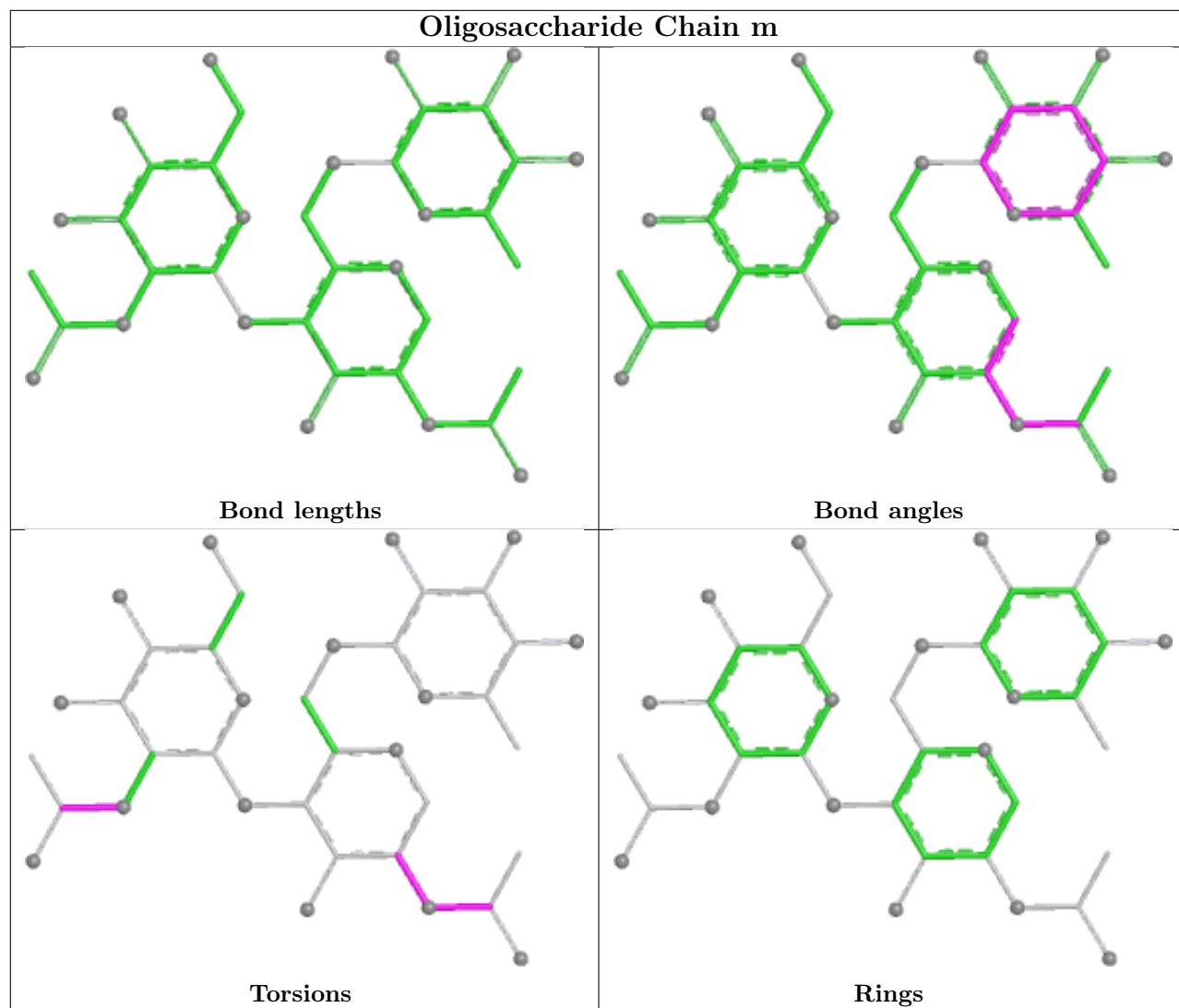


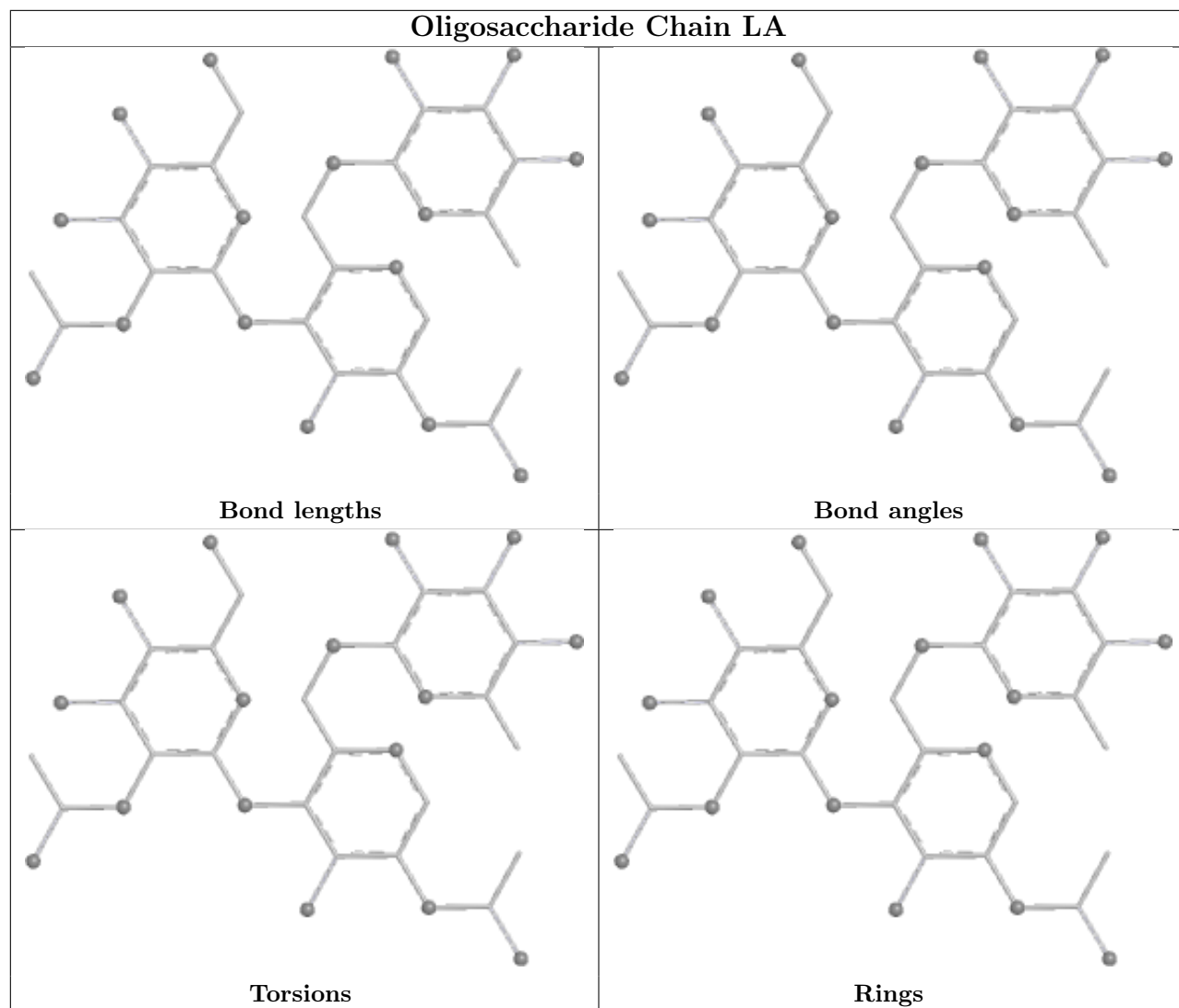


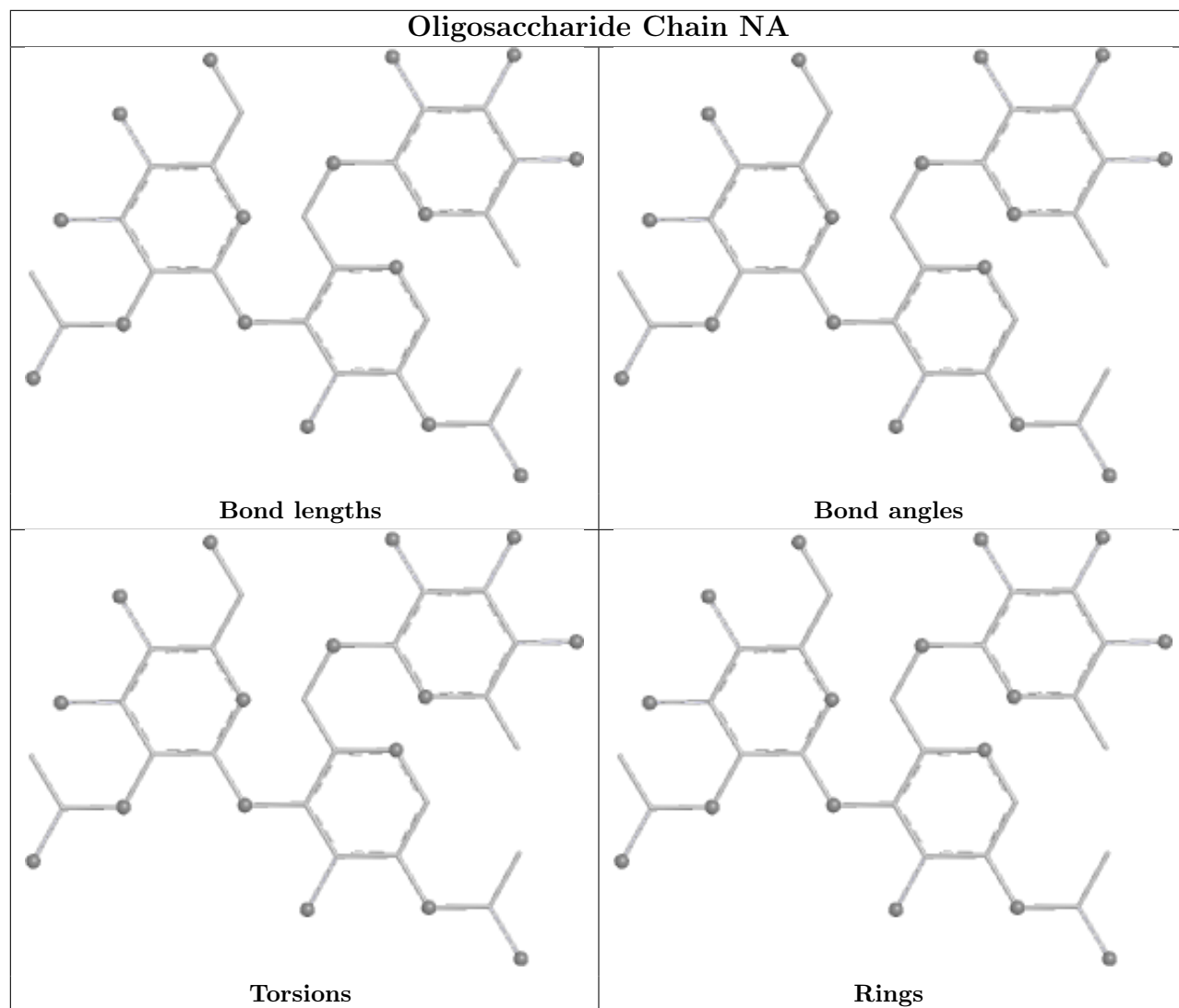


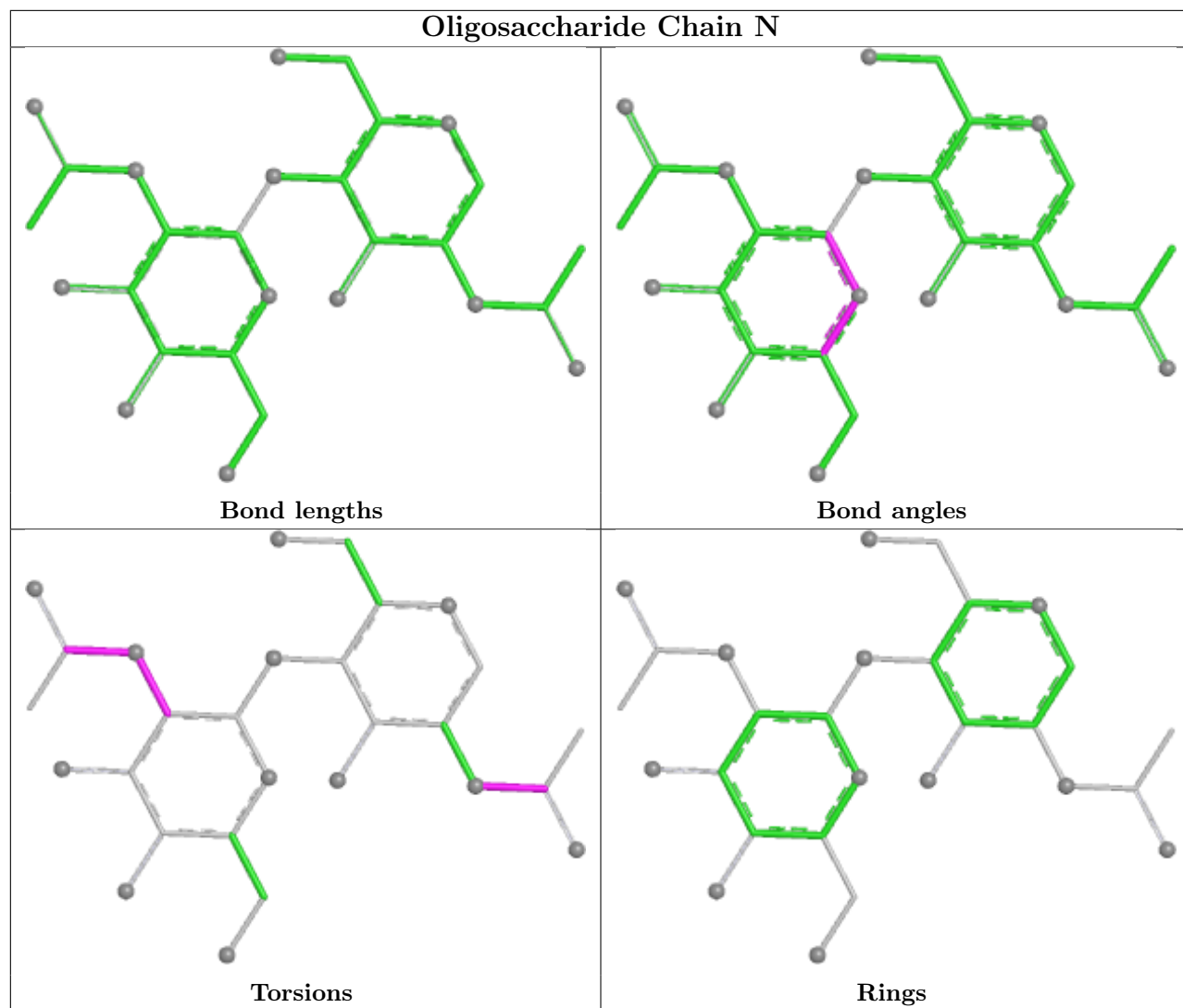


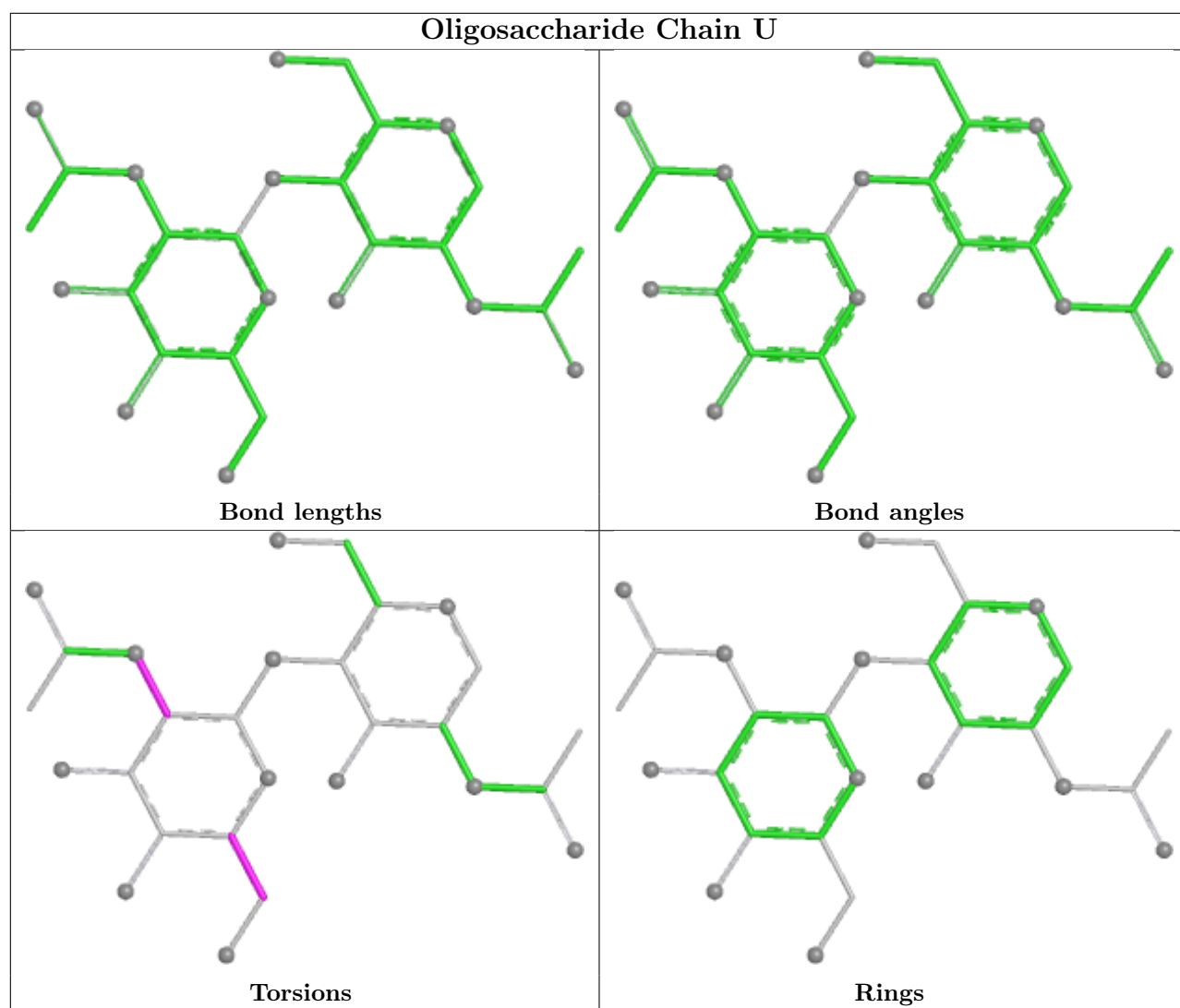


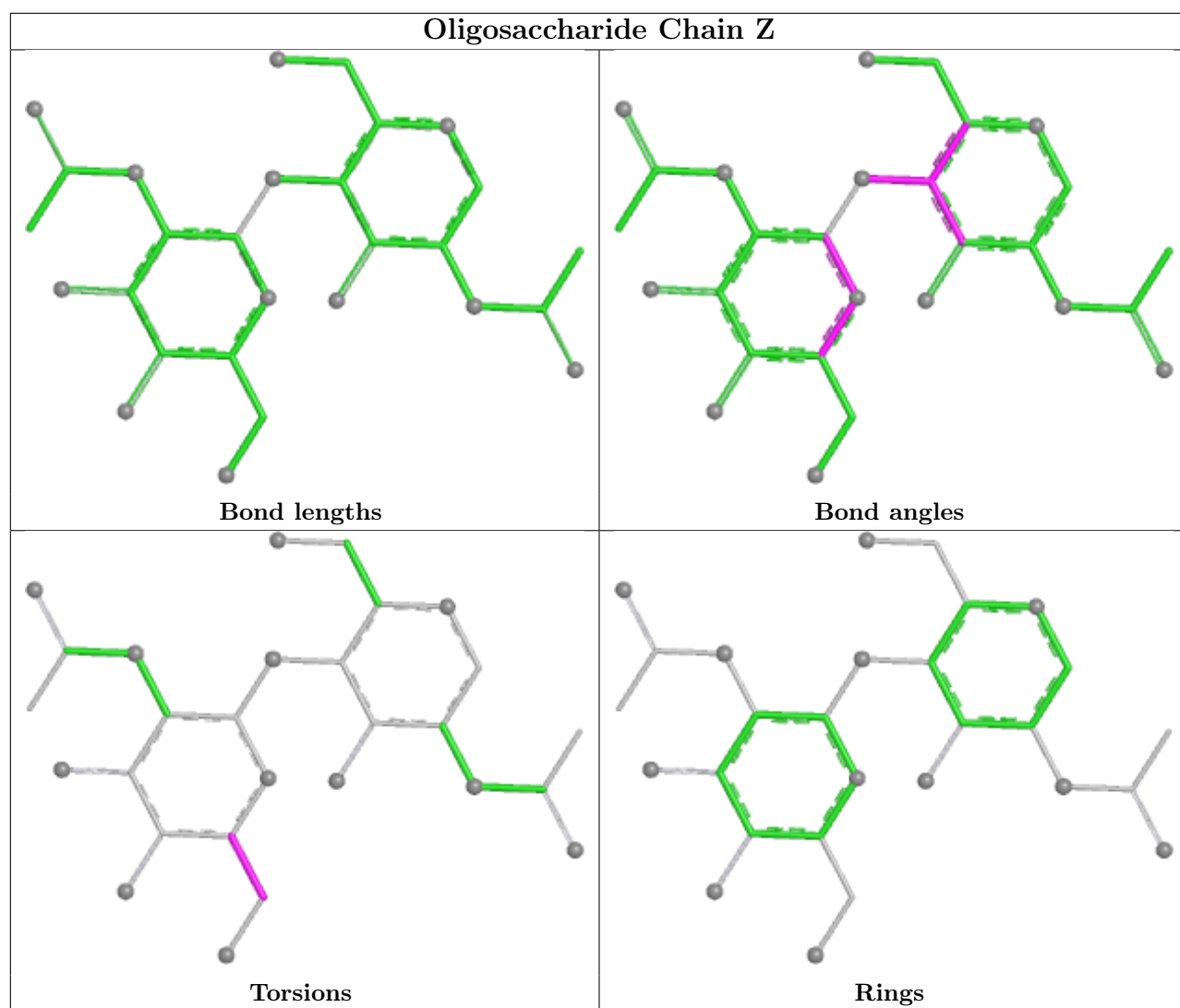


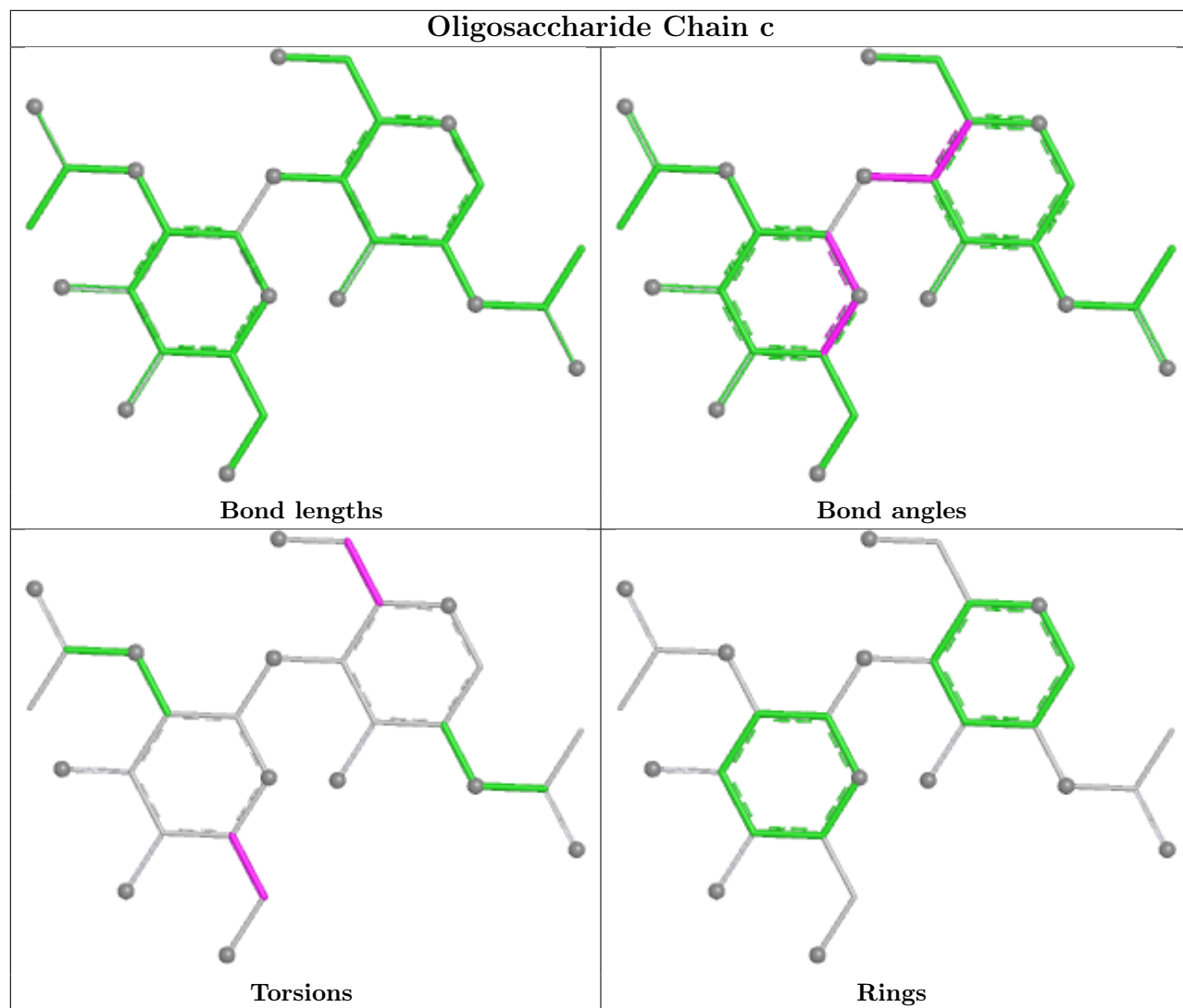


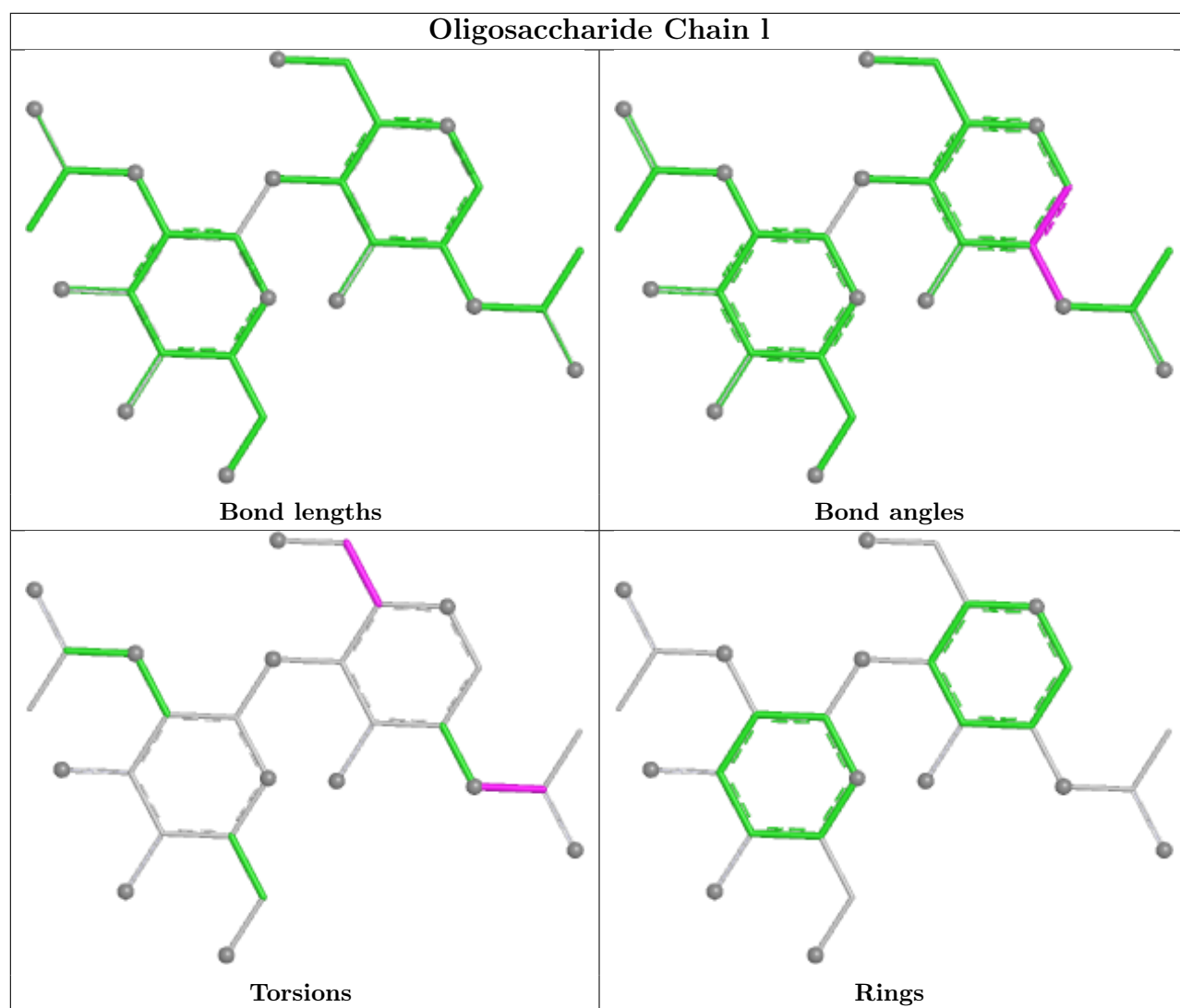


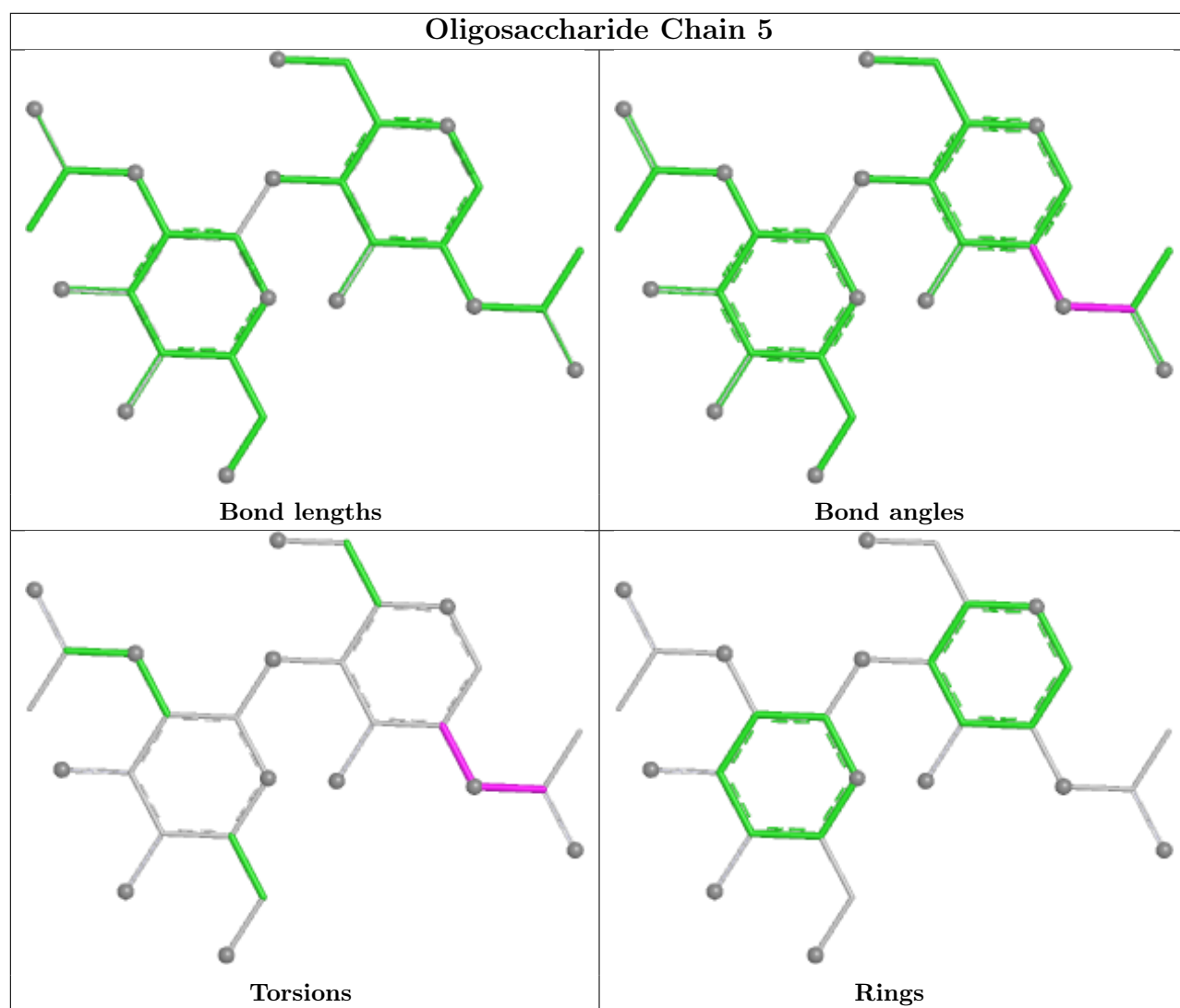


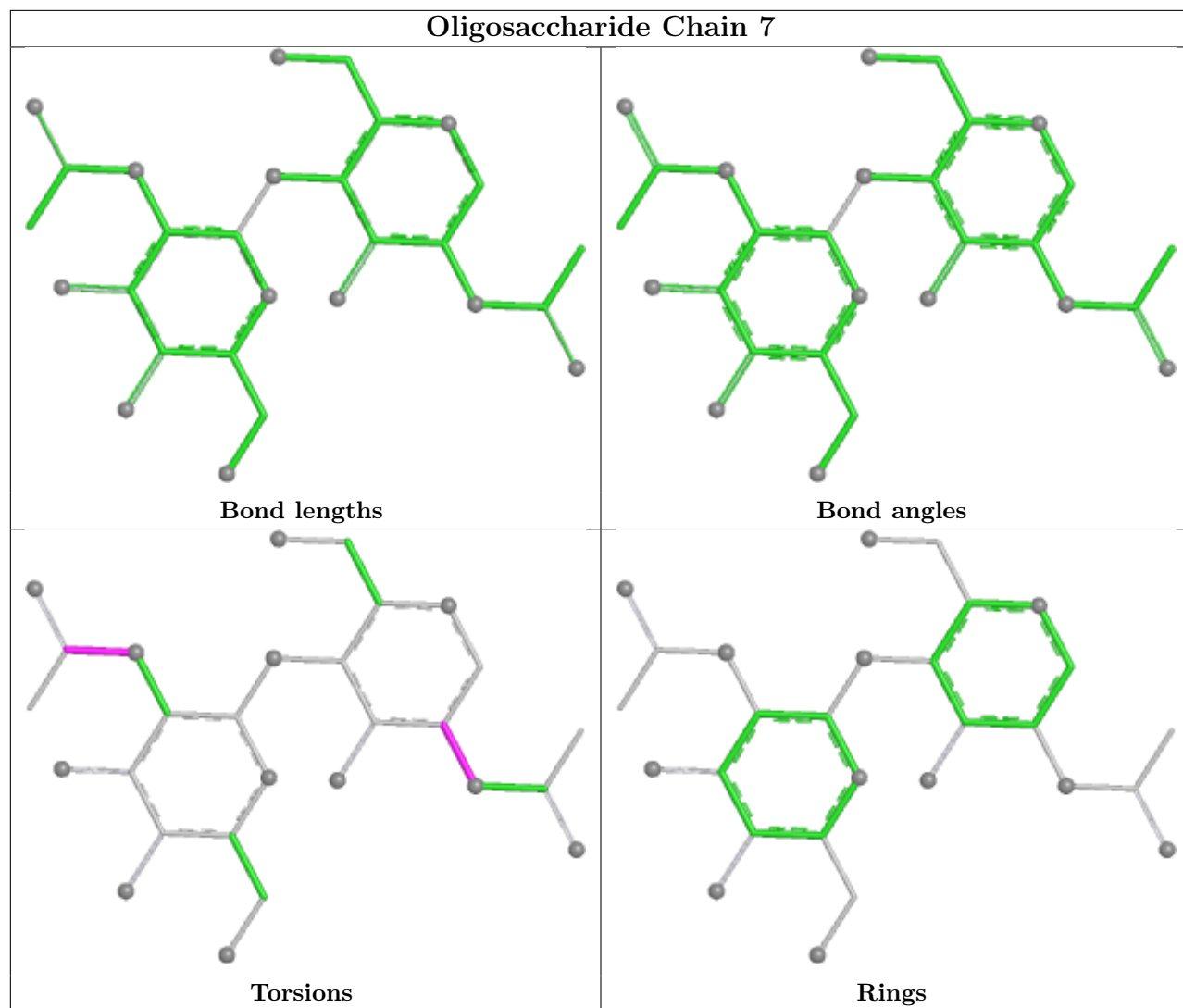


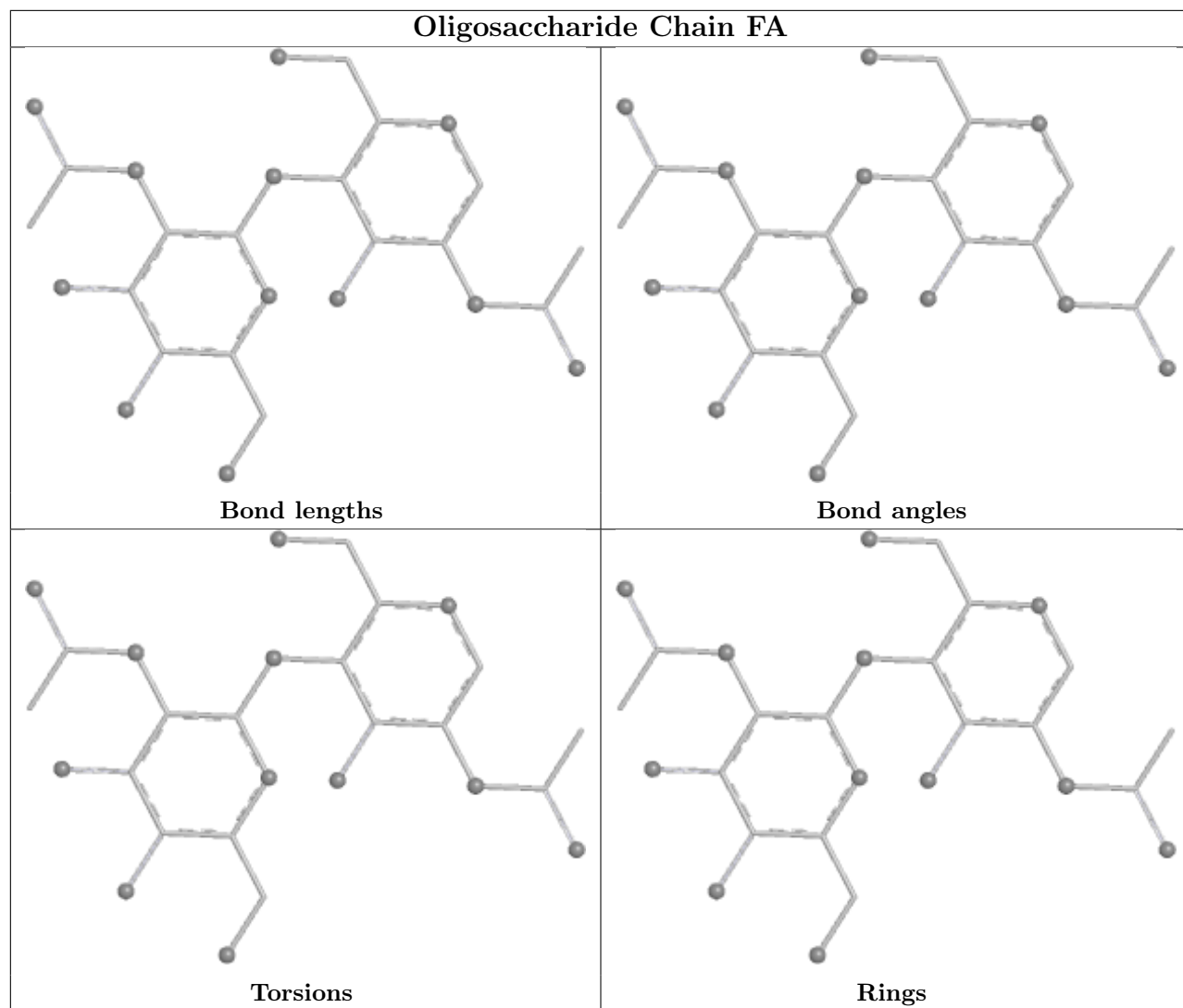


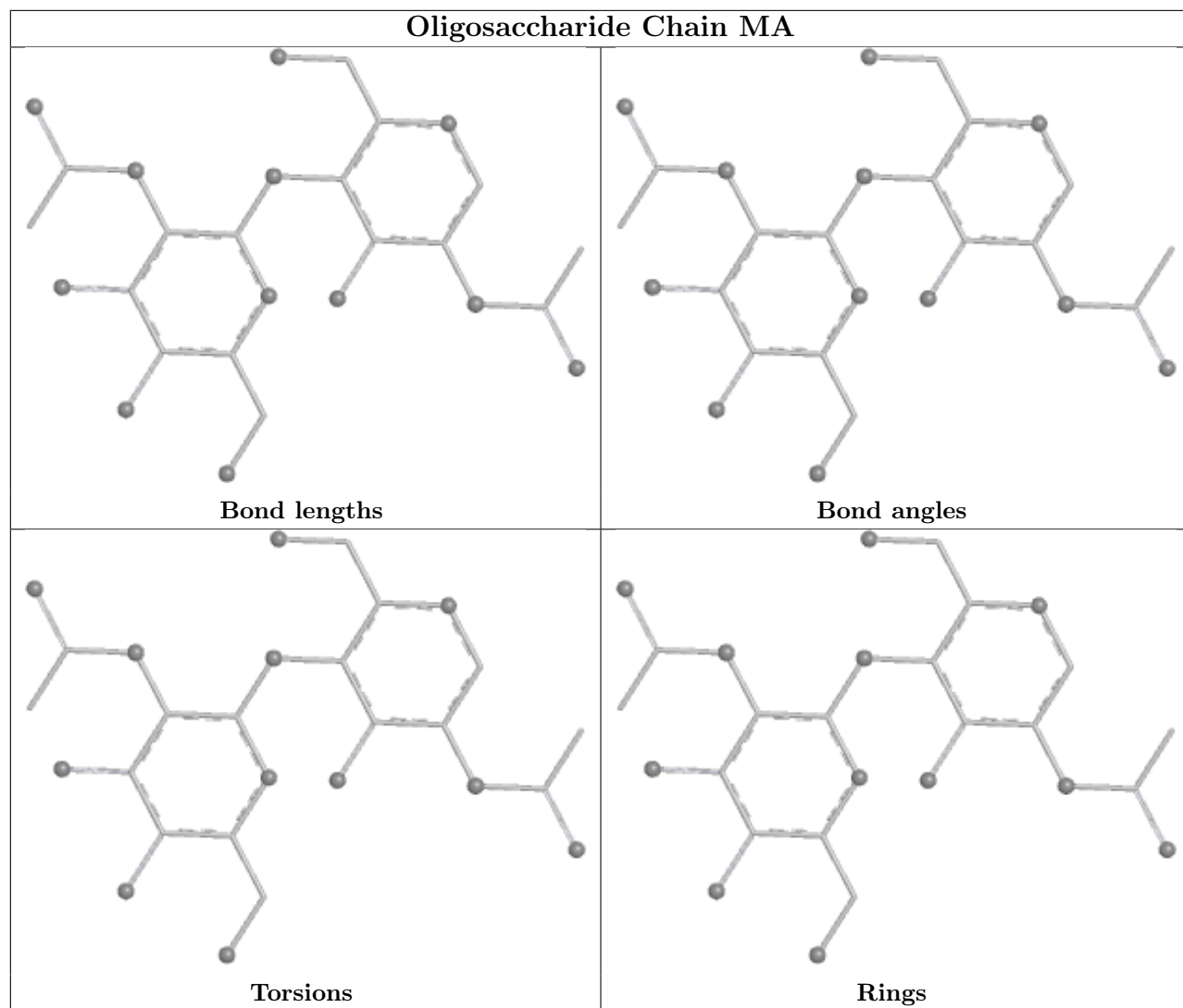


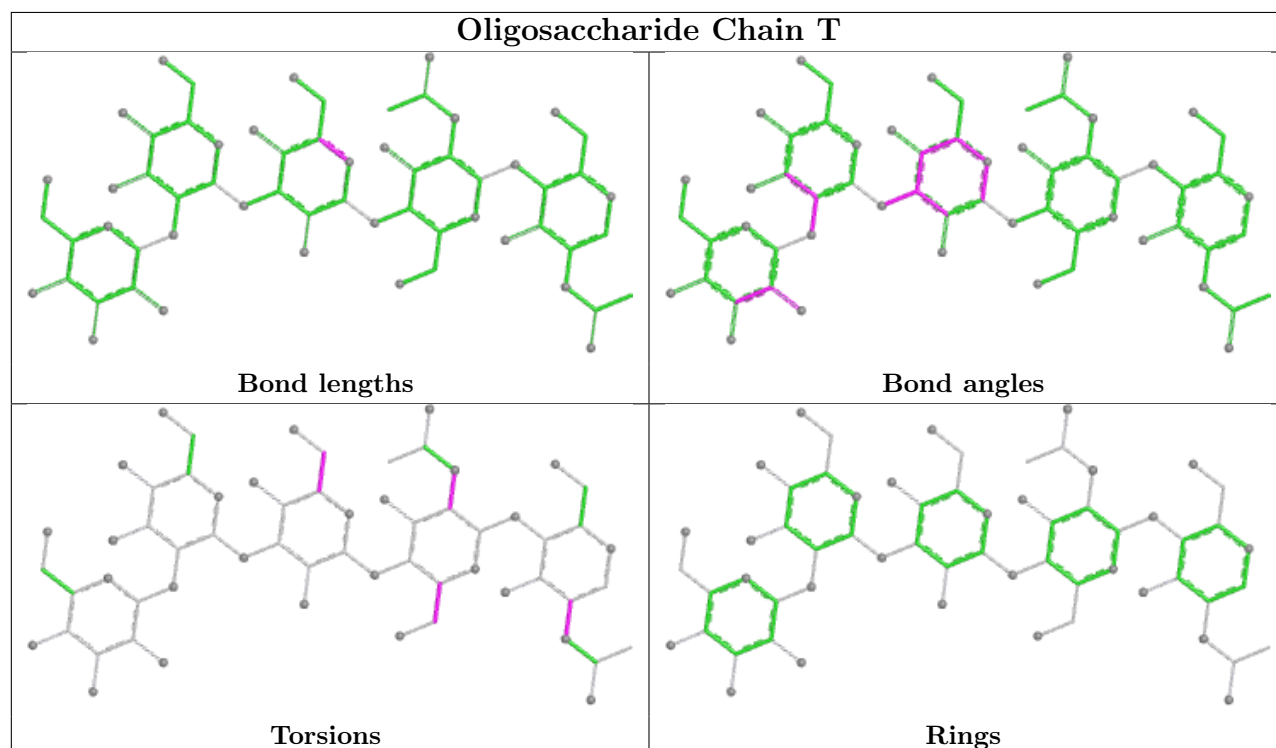
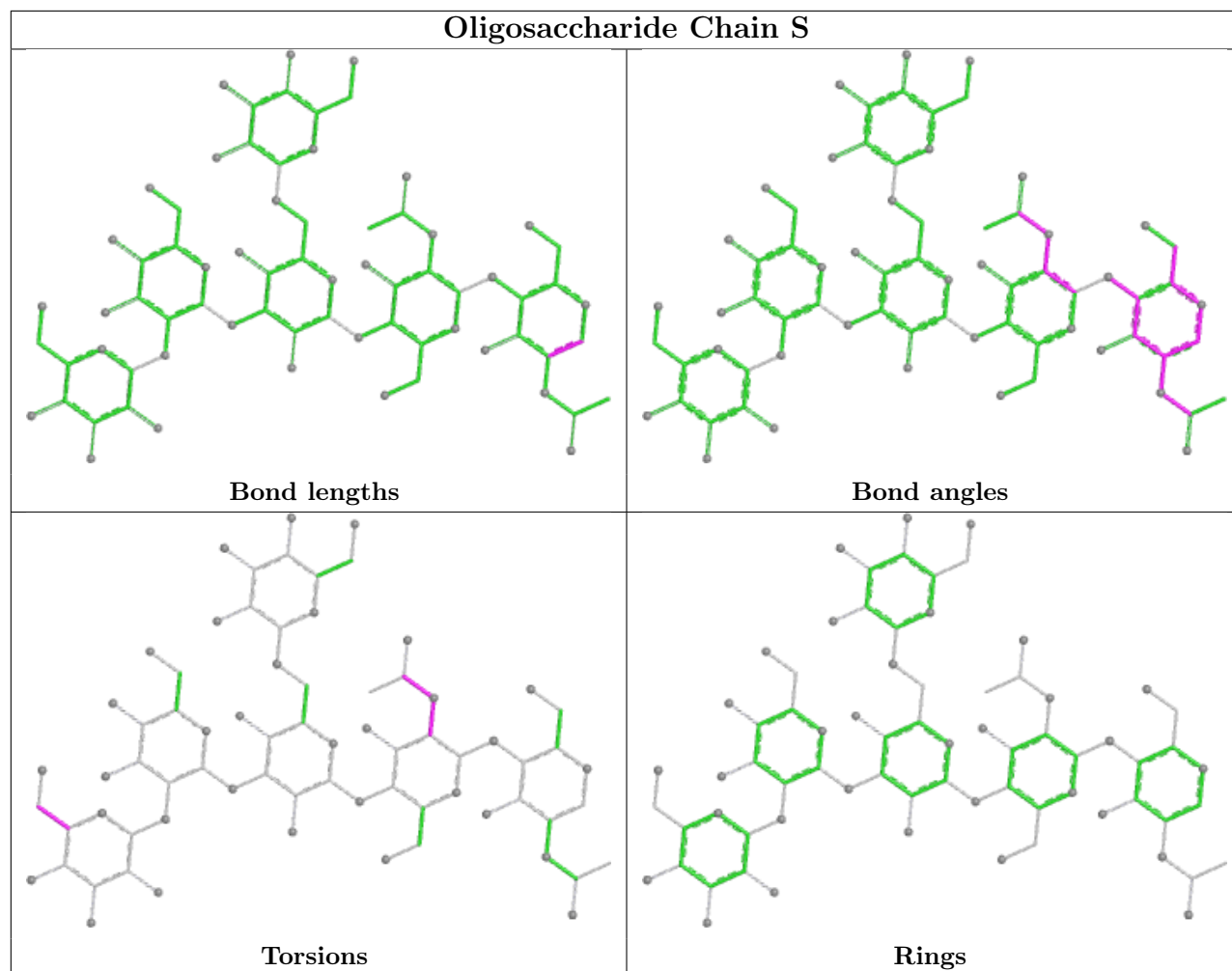


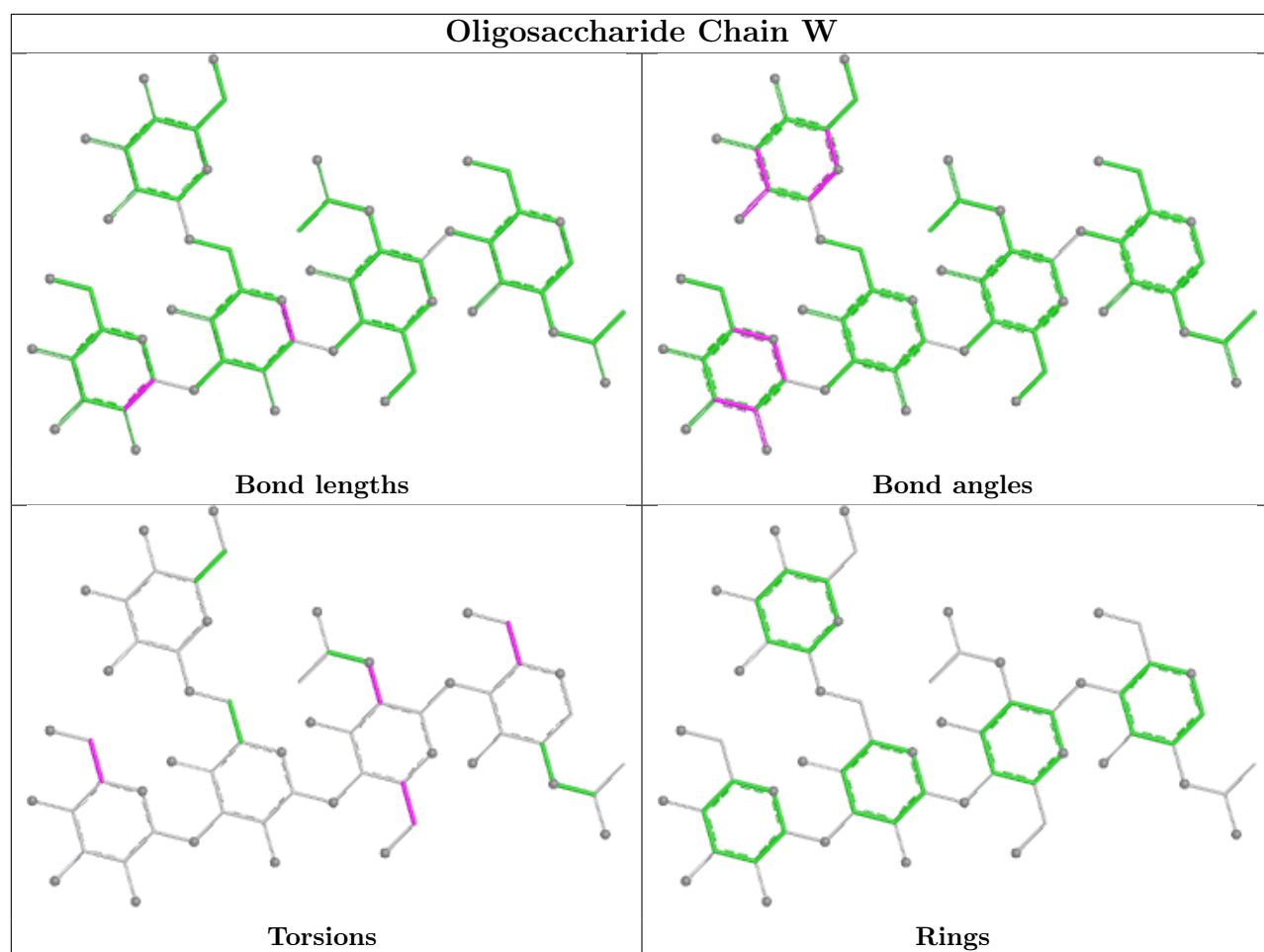


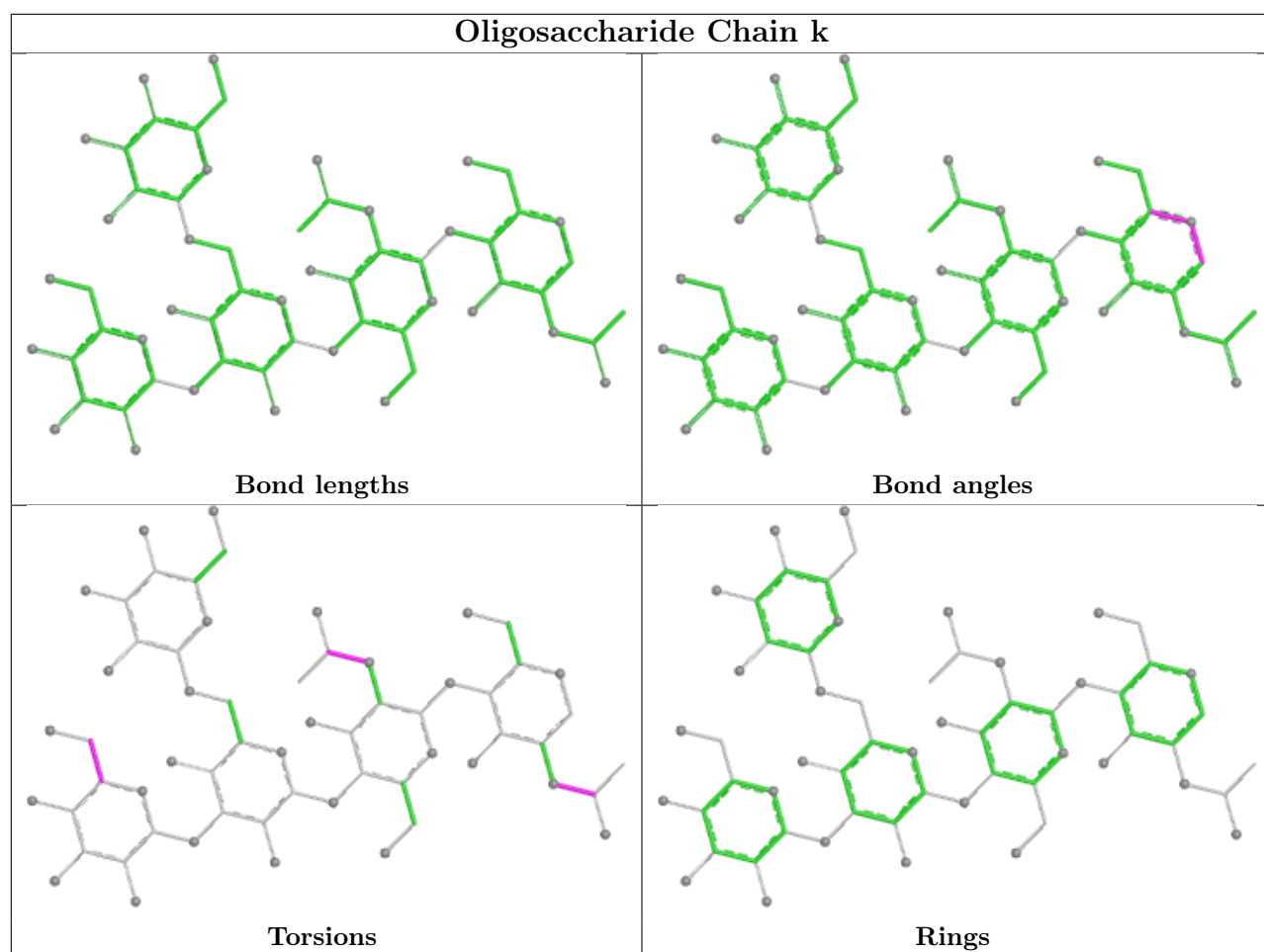


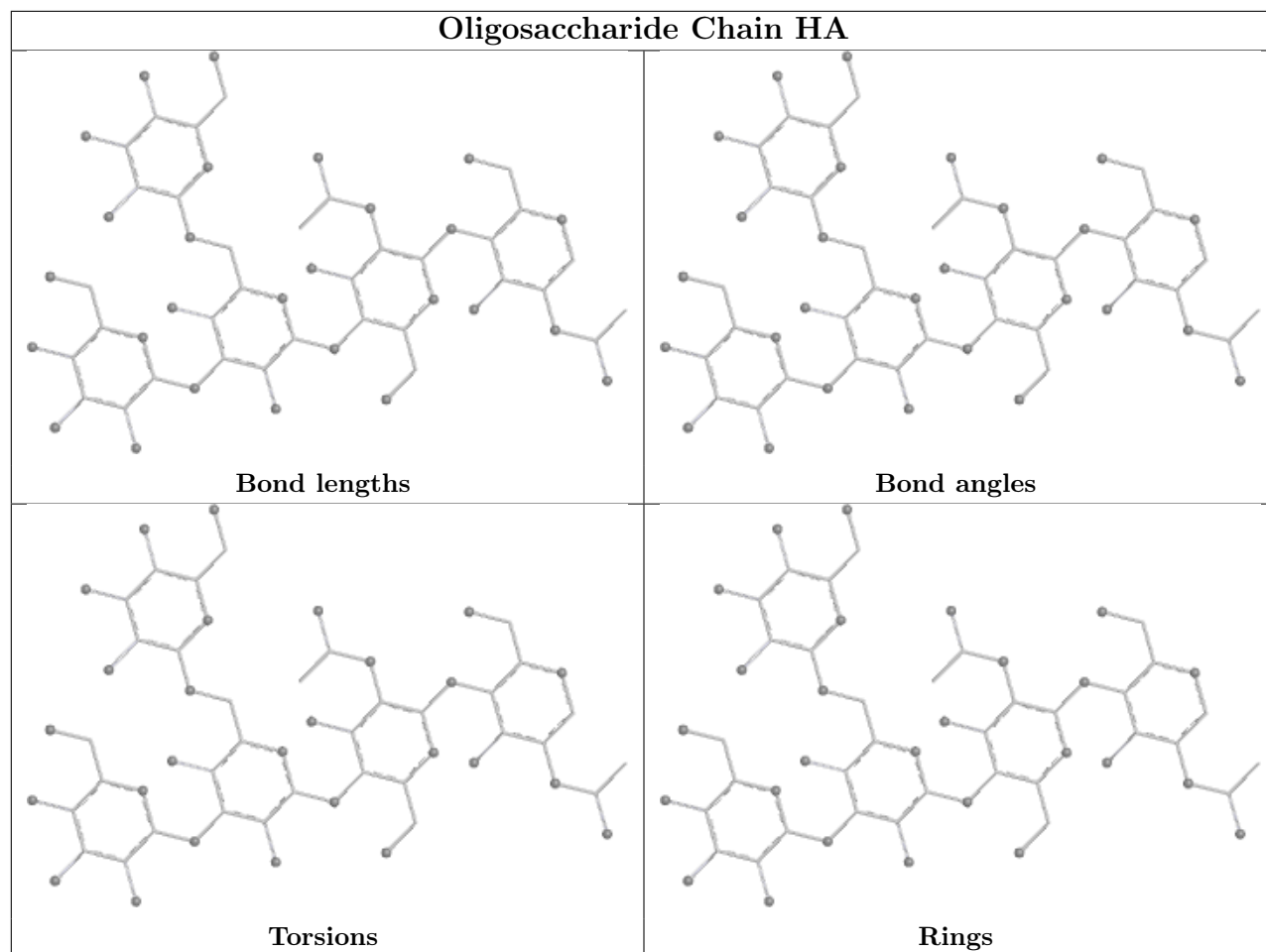


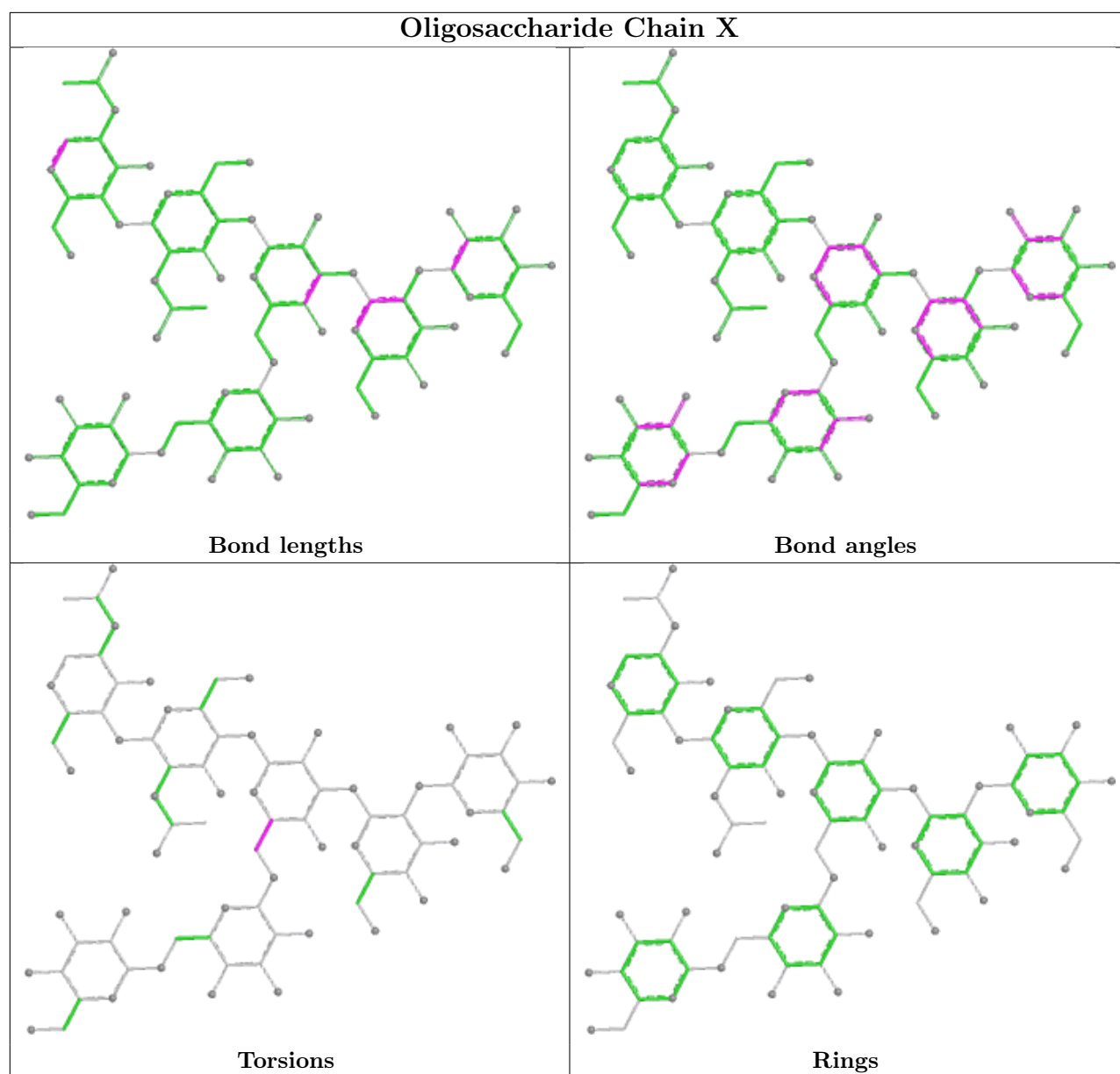


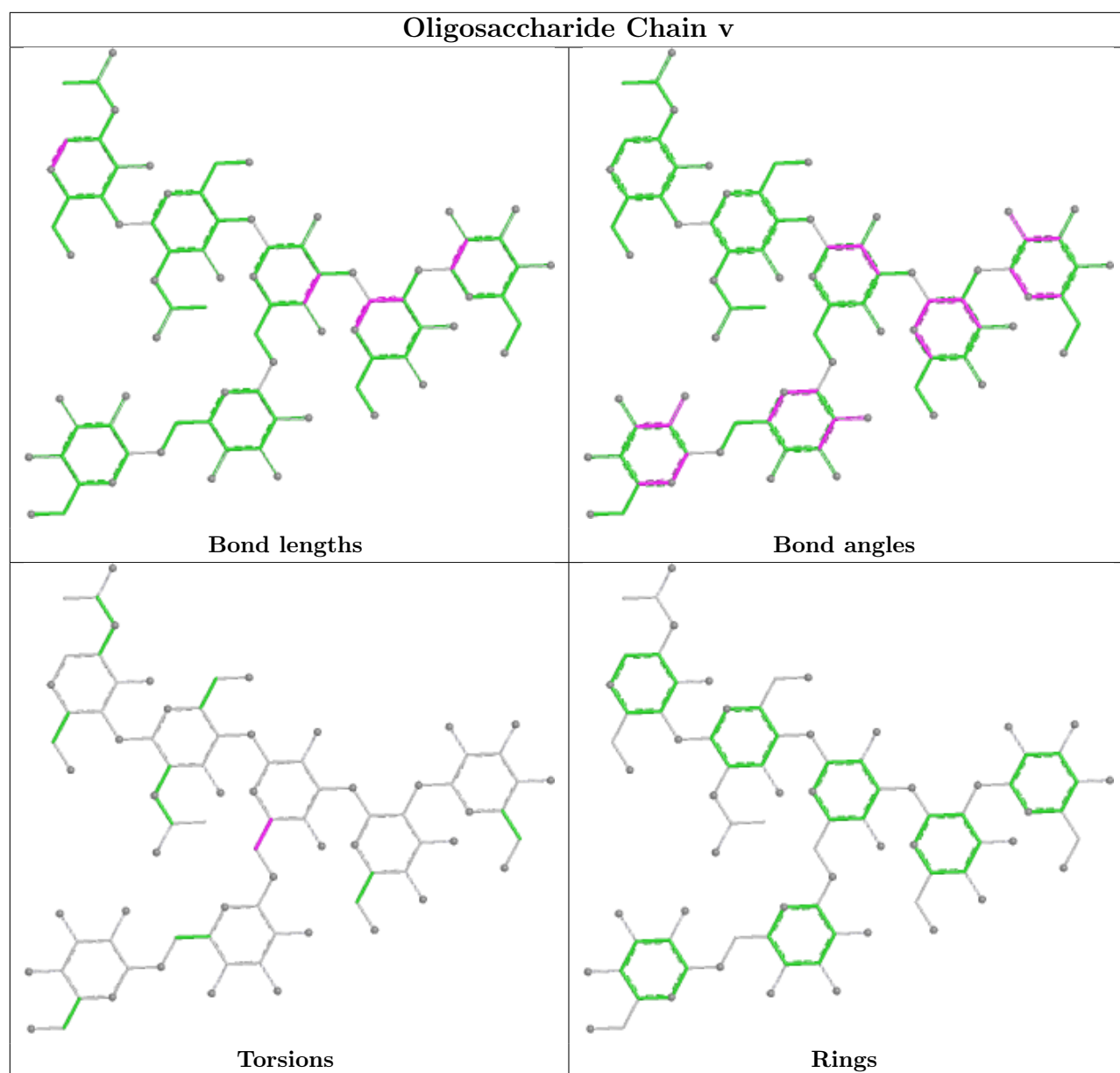


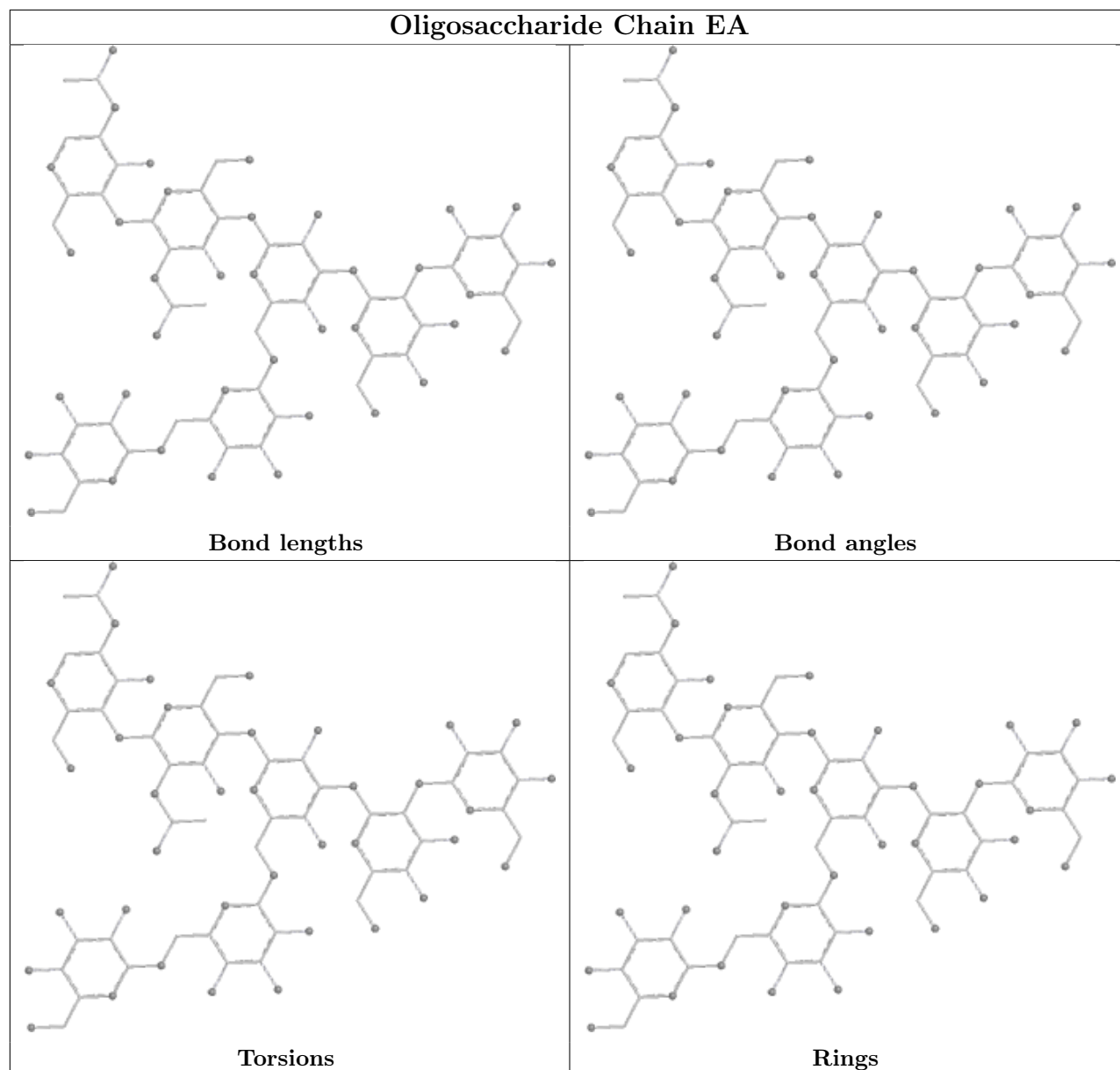


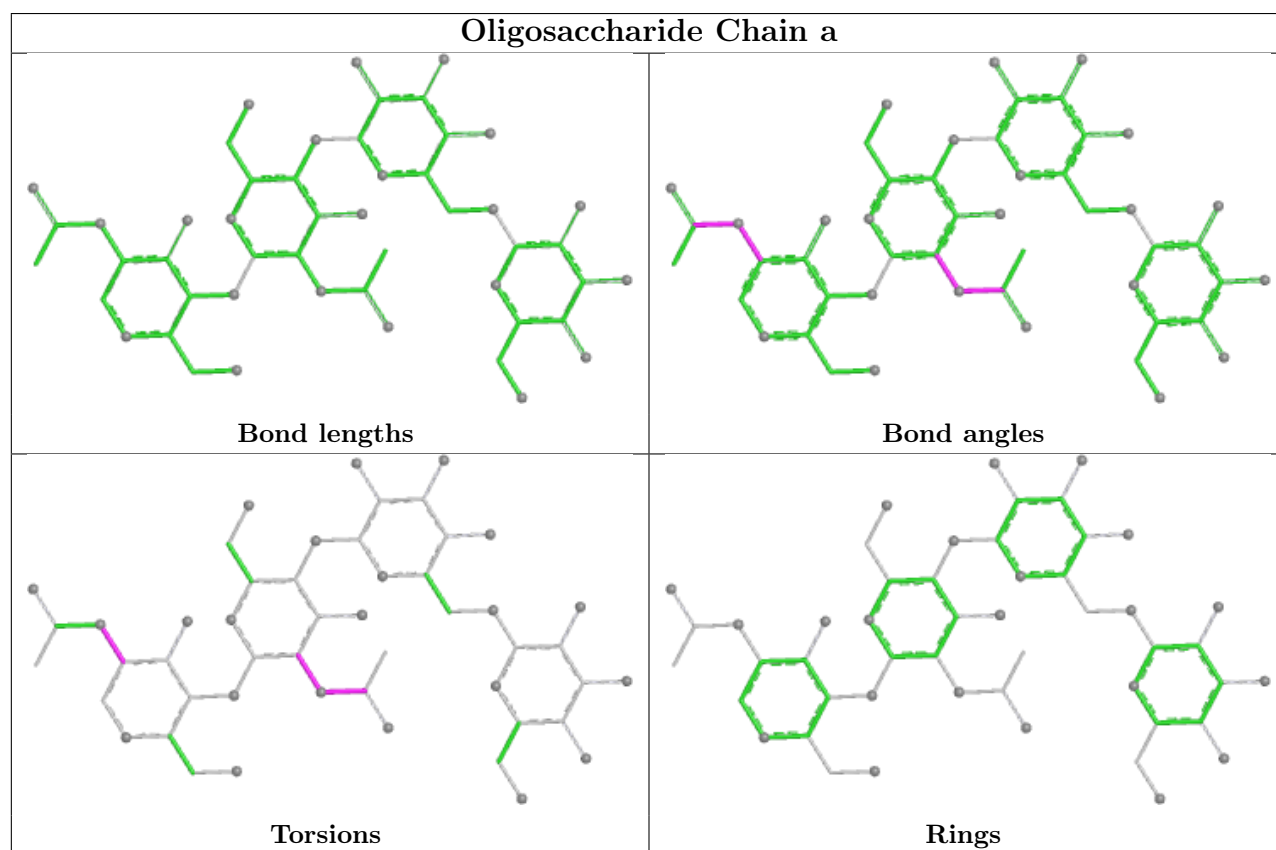
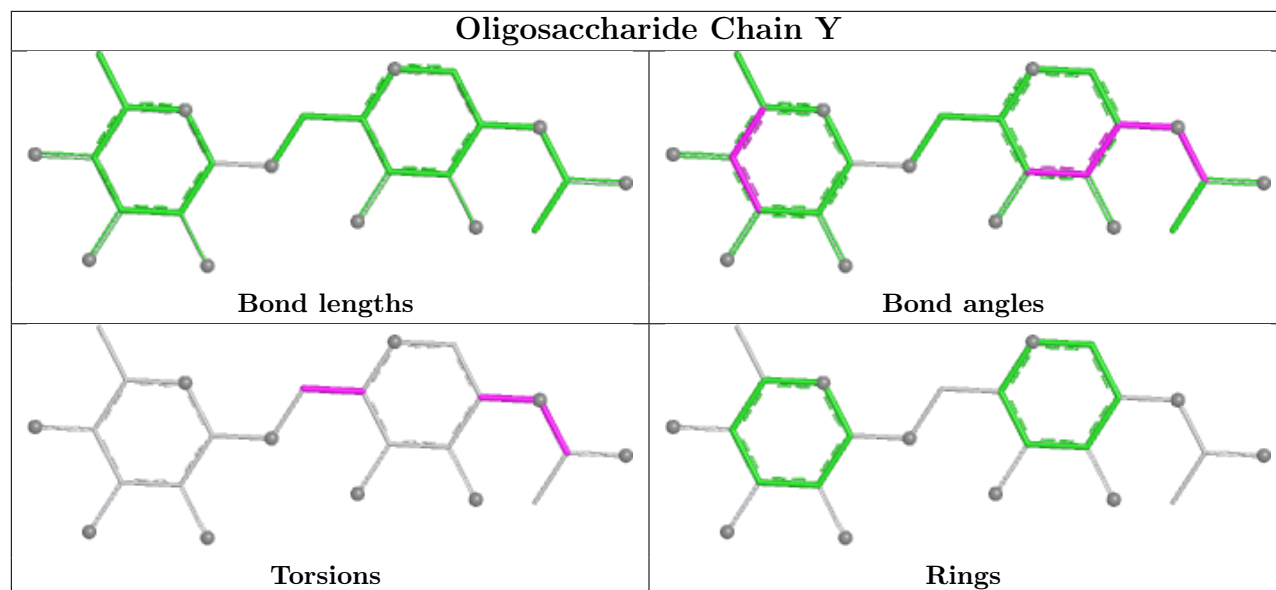


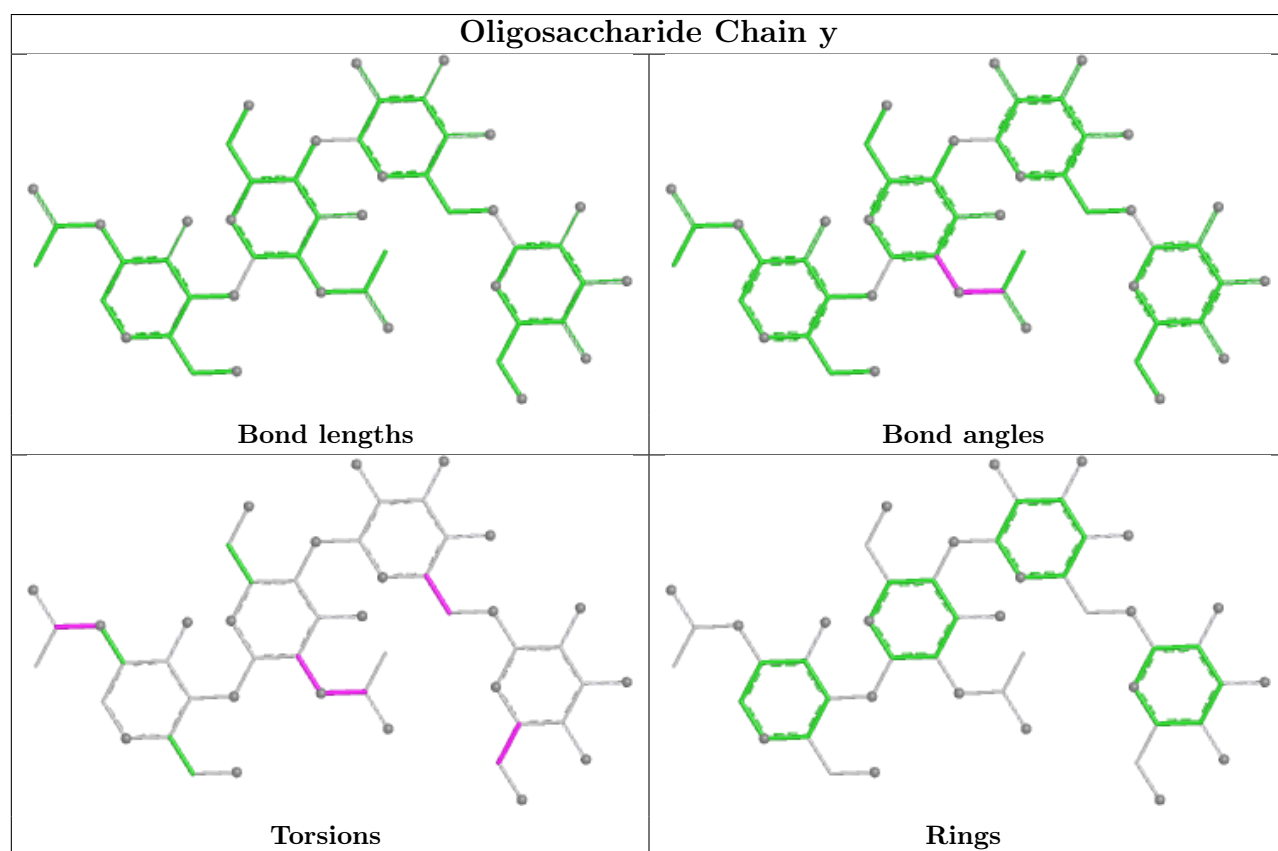
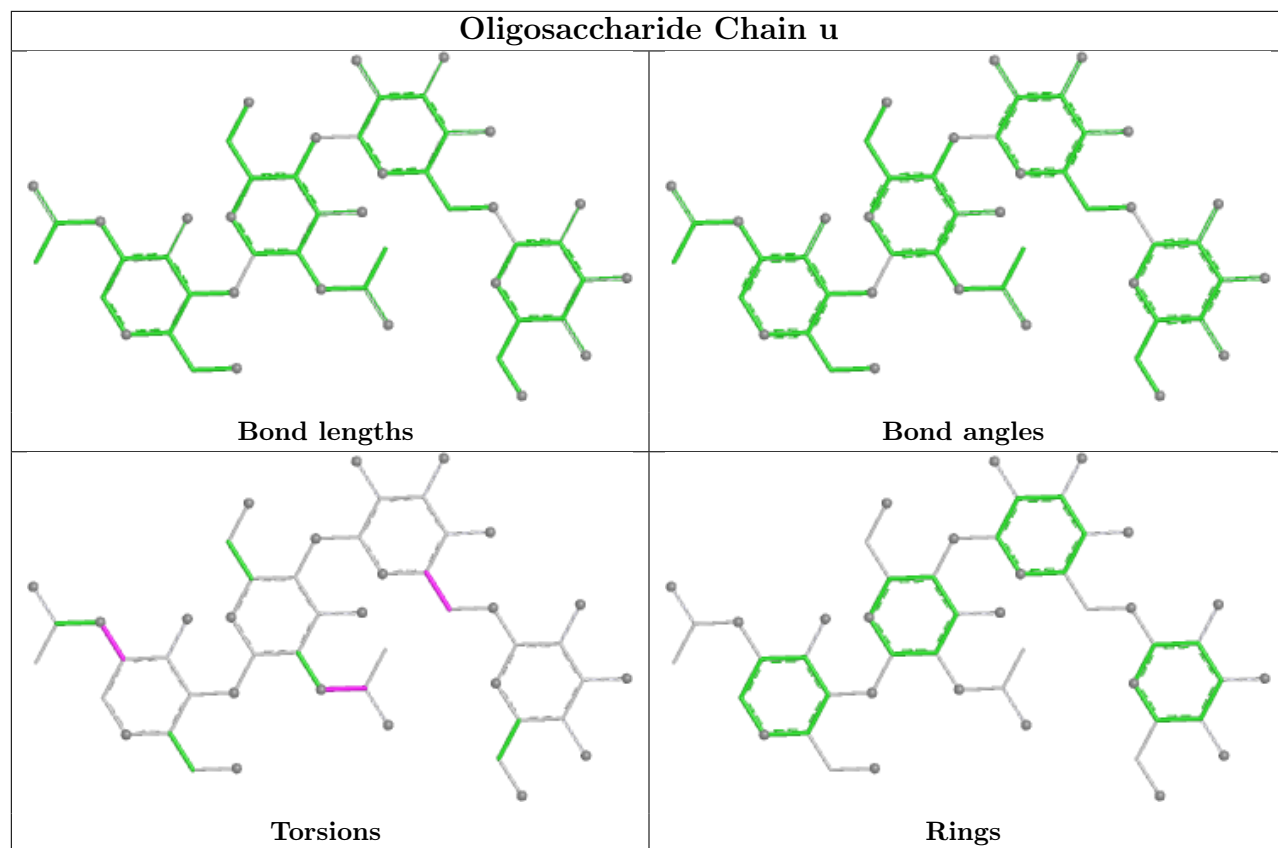


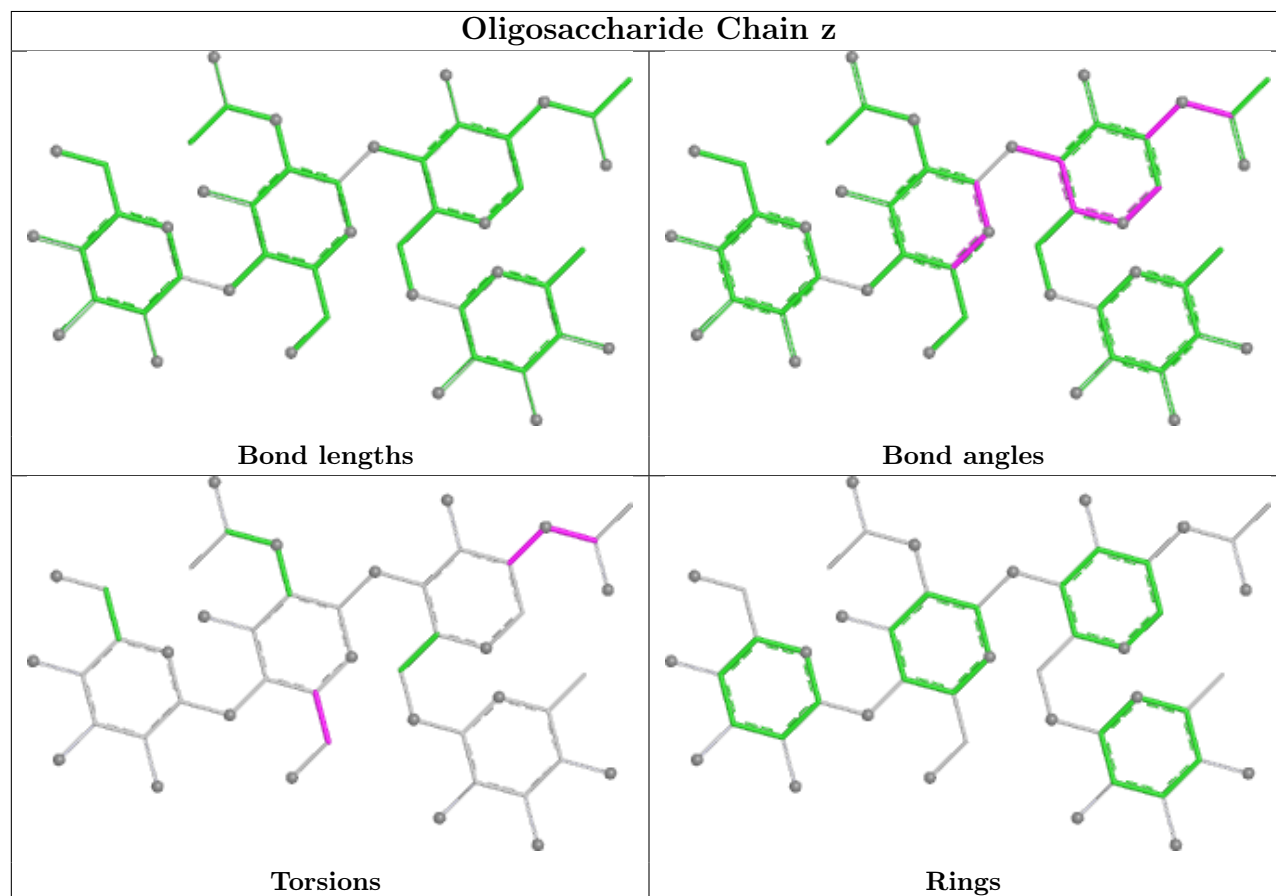
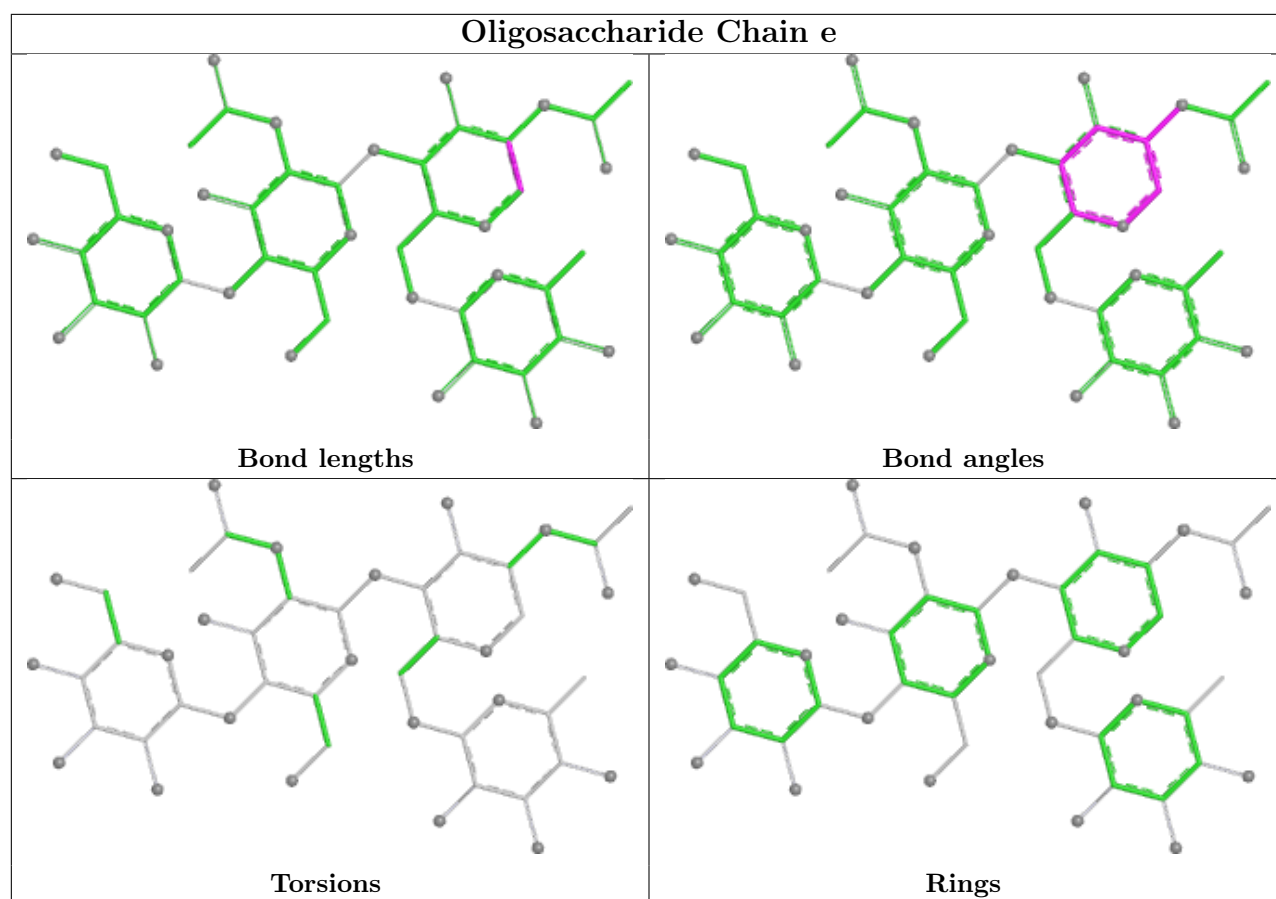


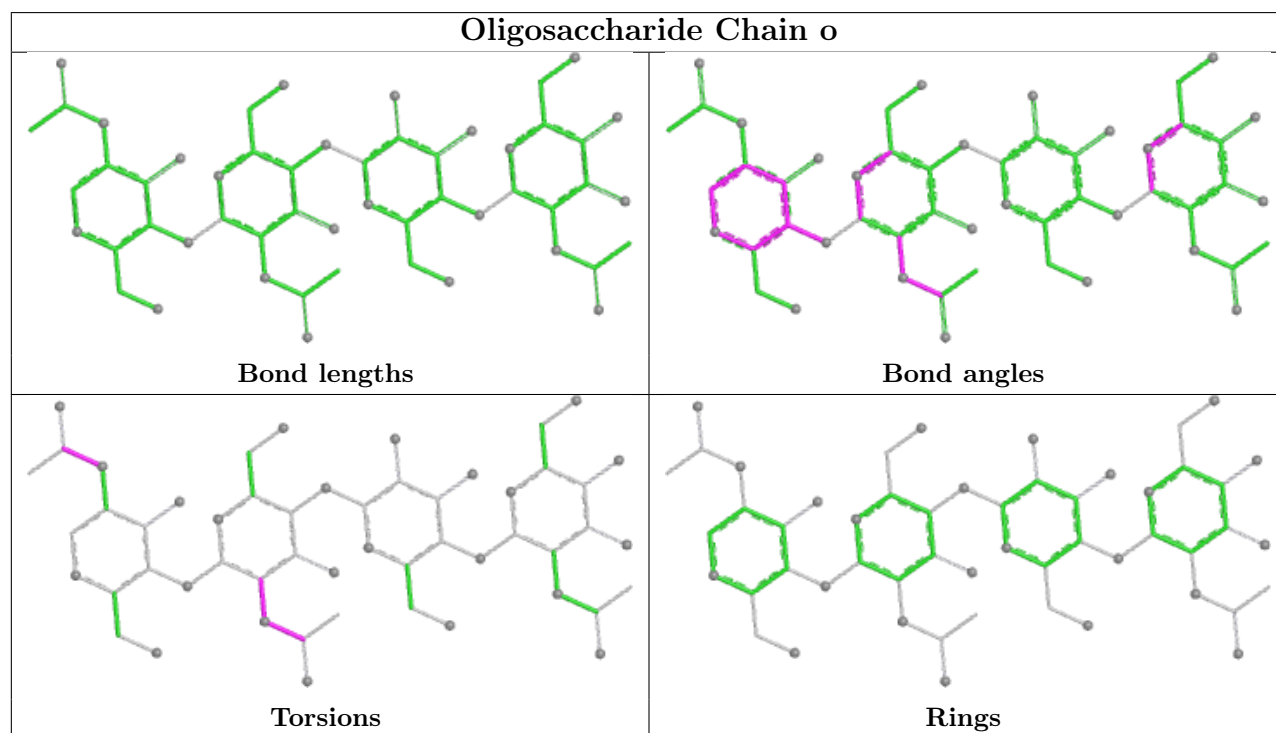
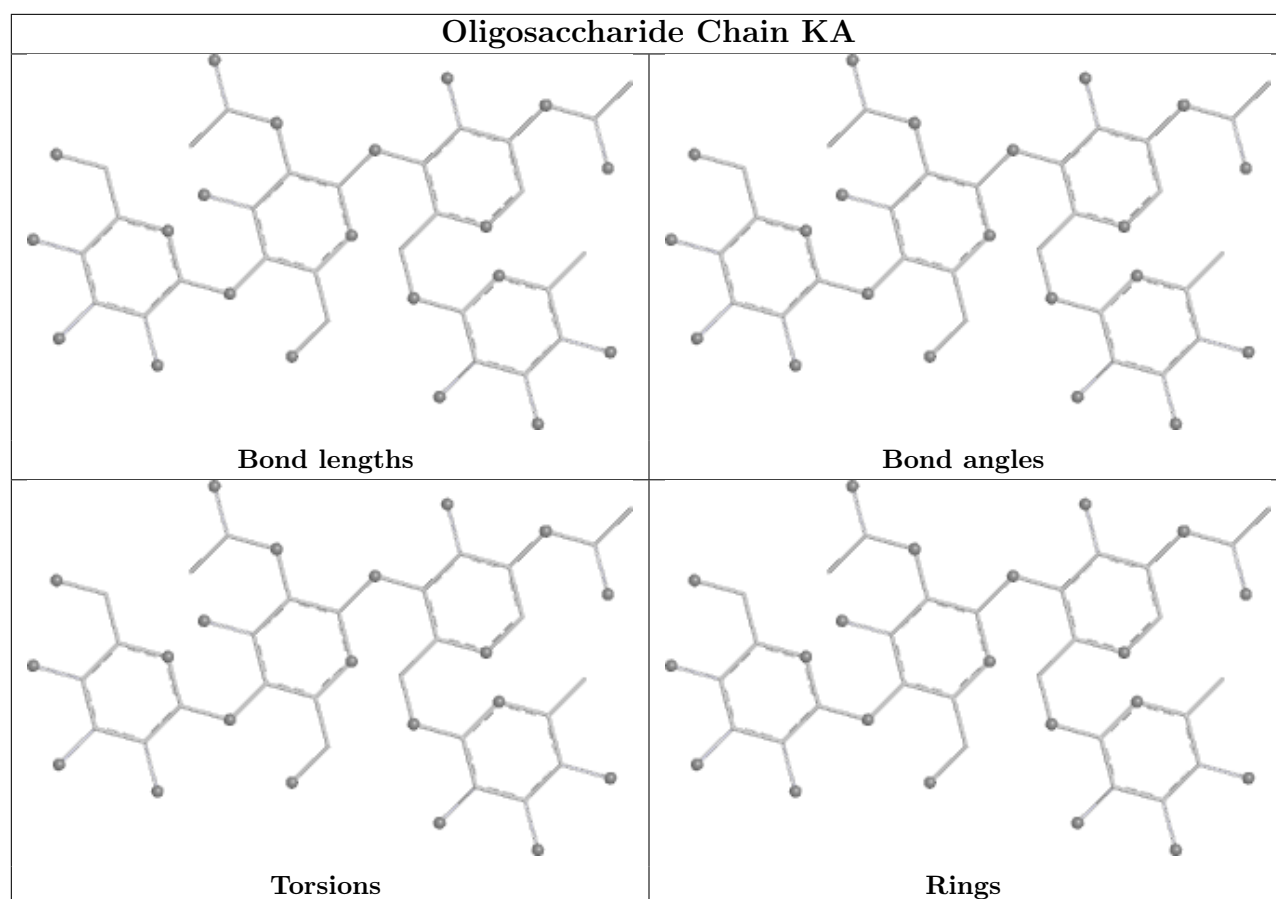


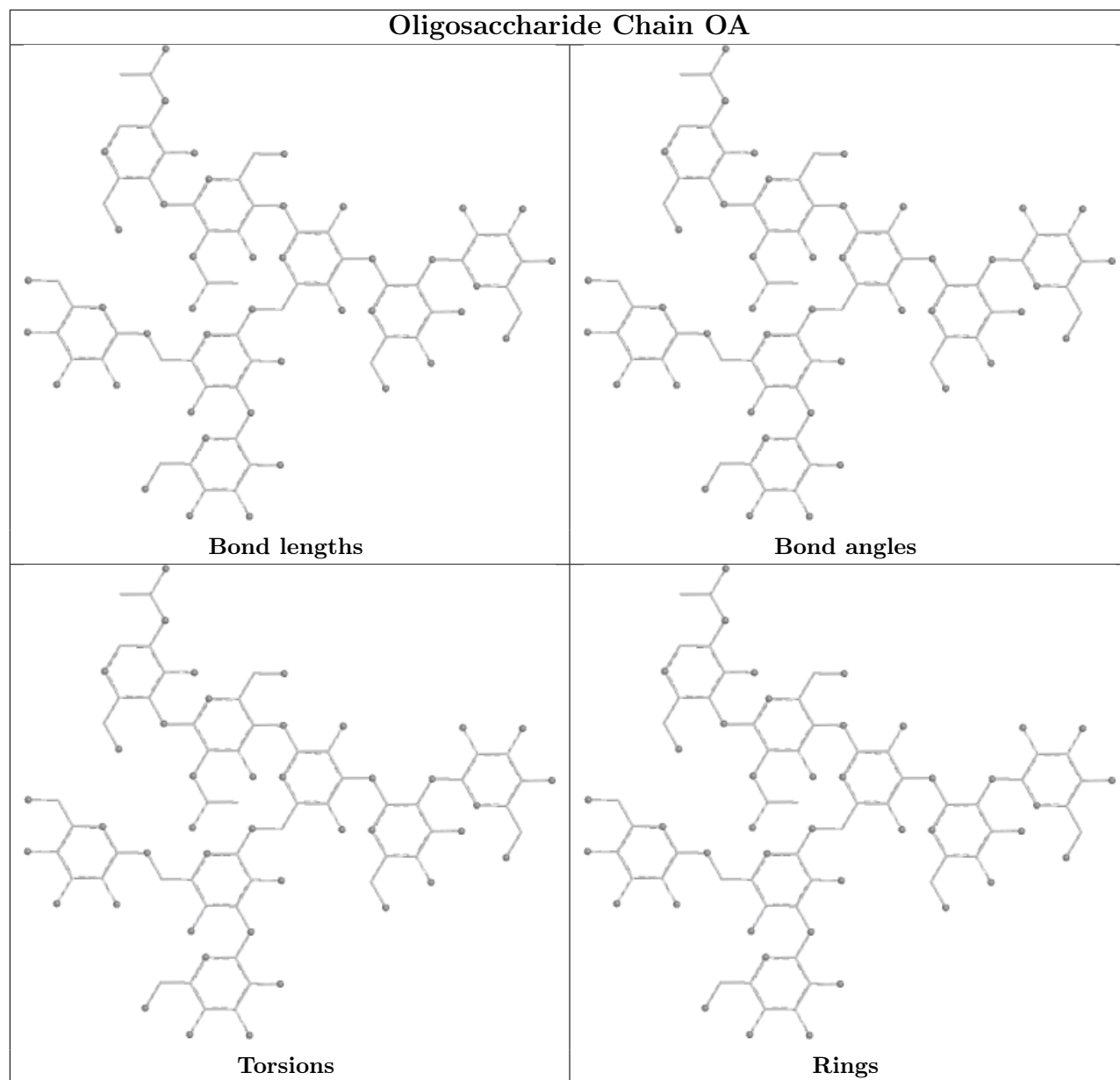
Oligosaccharide Chain EA

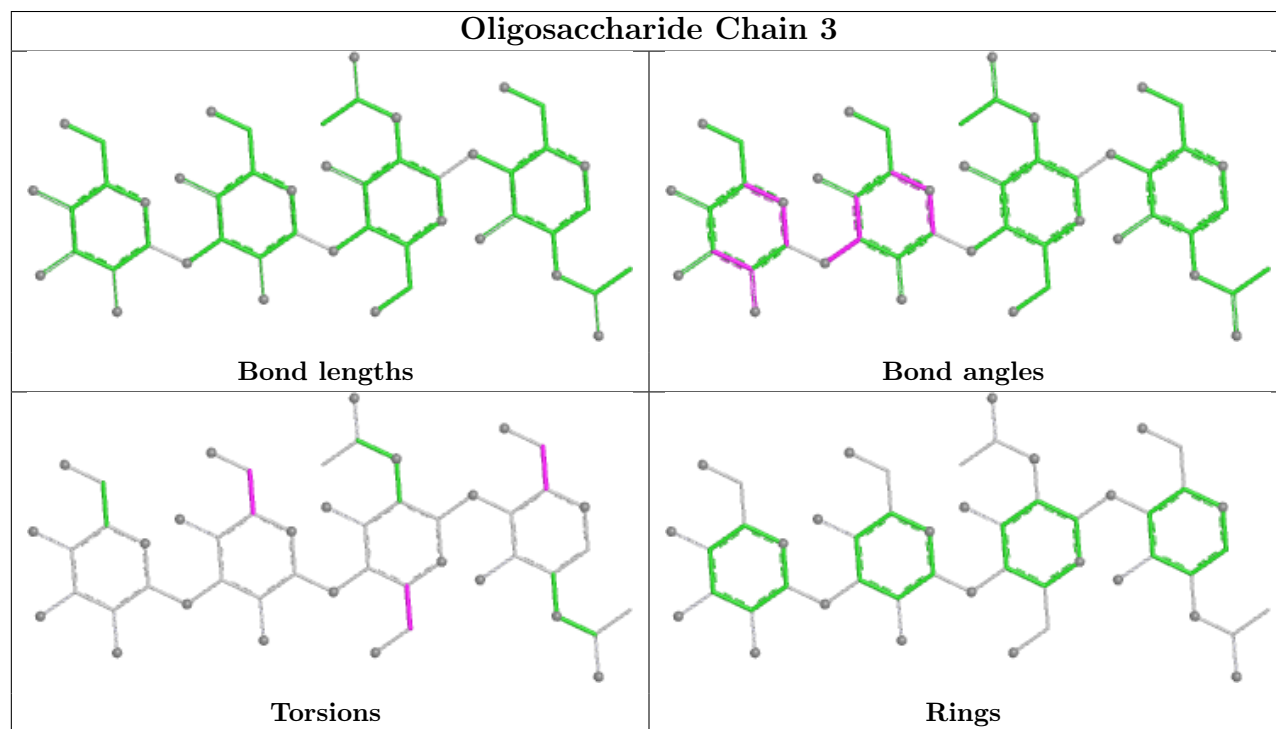
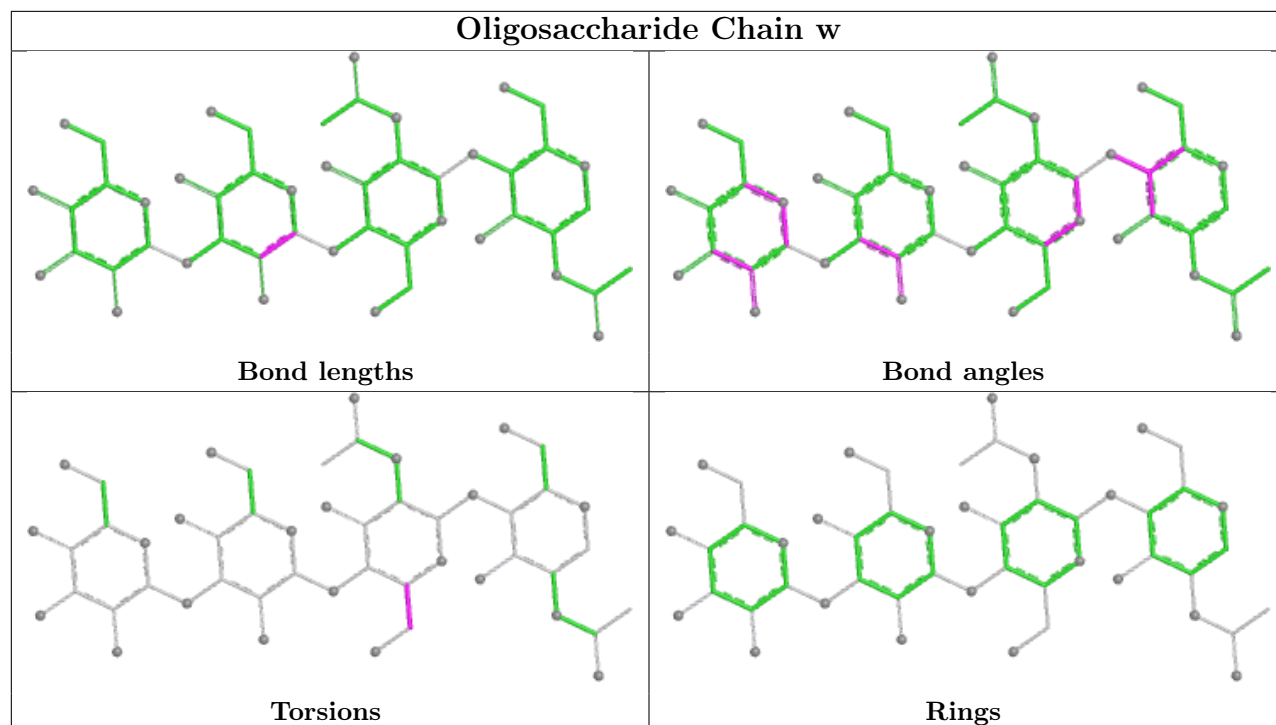


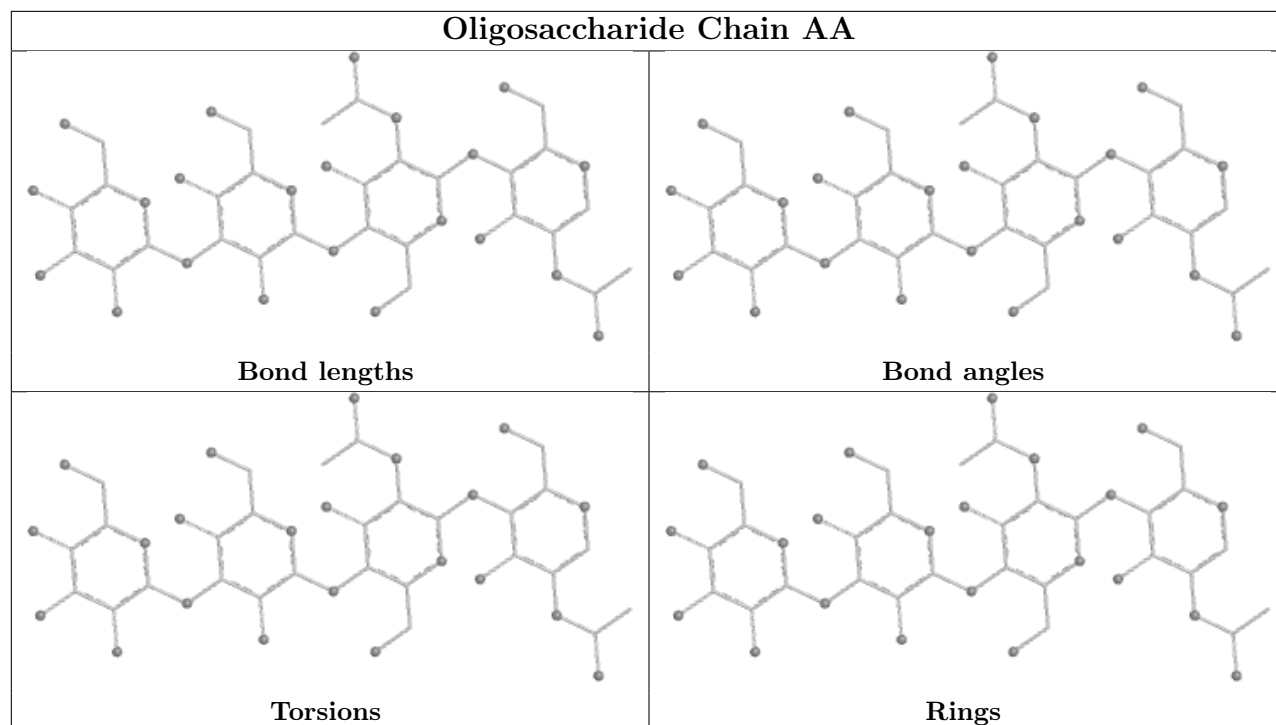
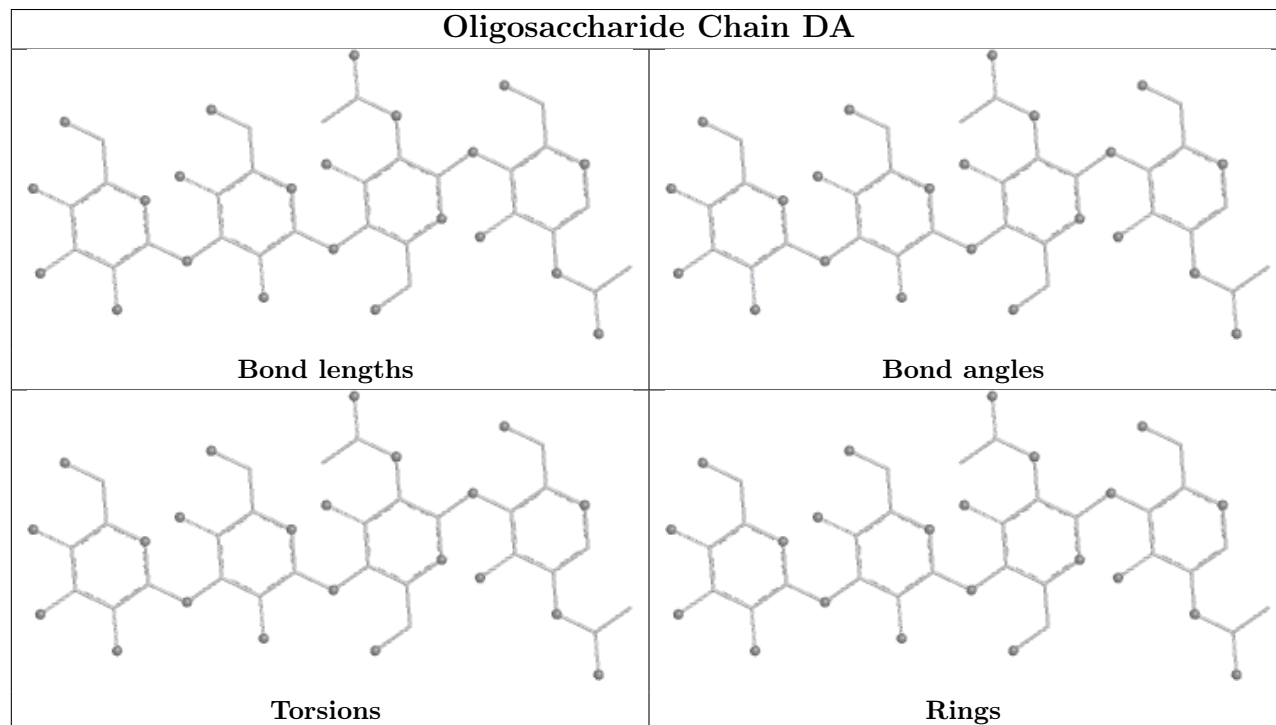


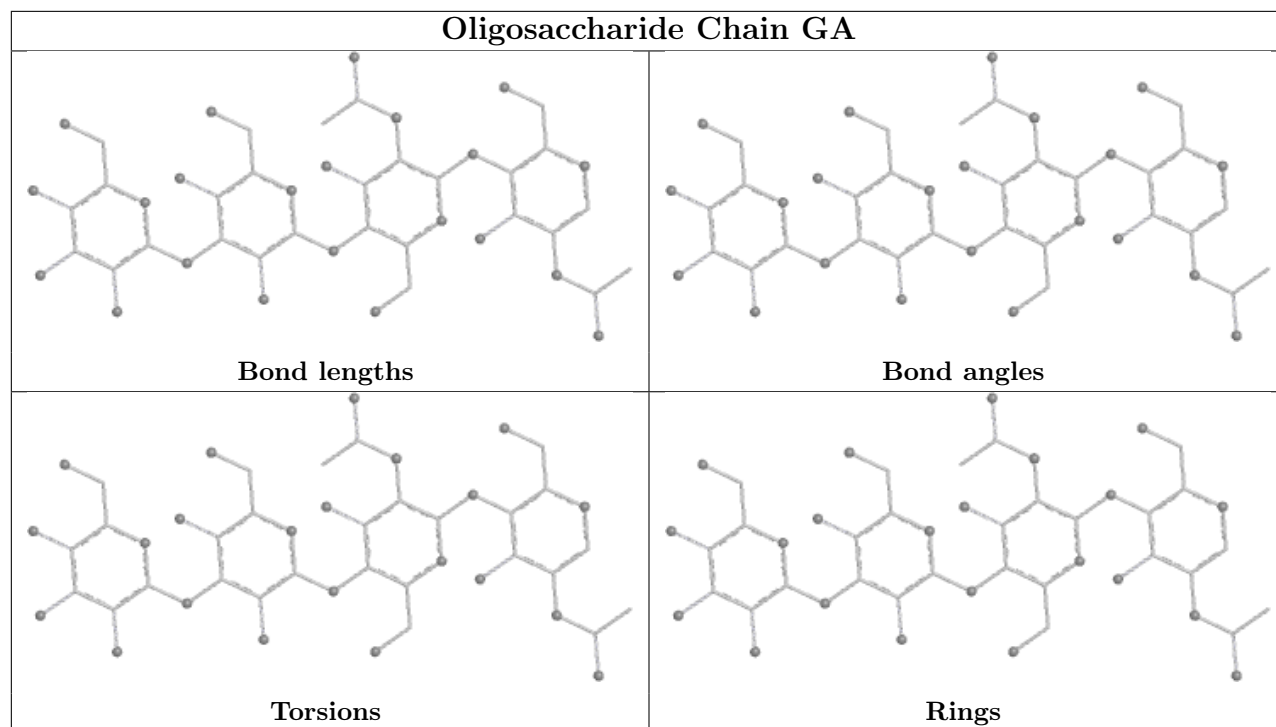


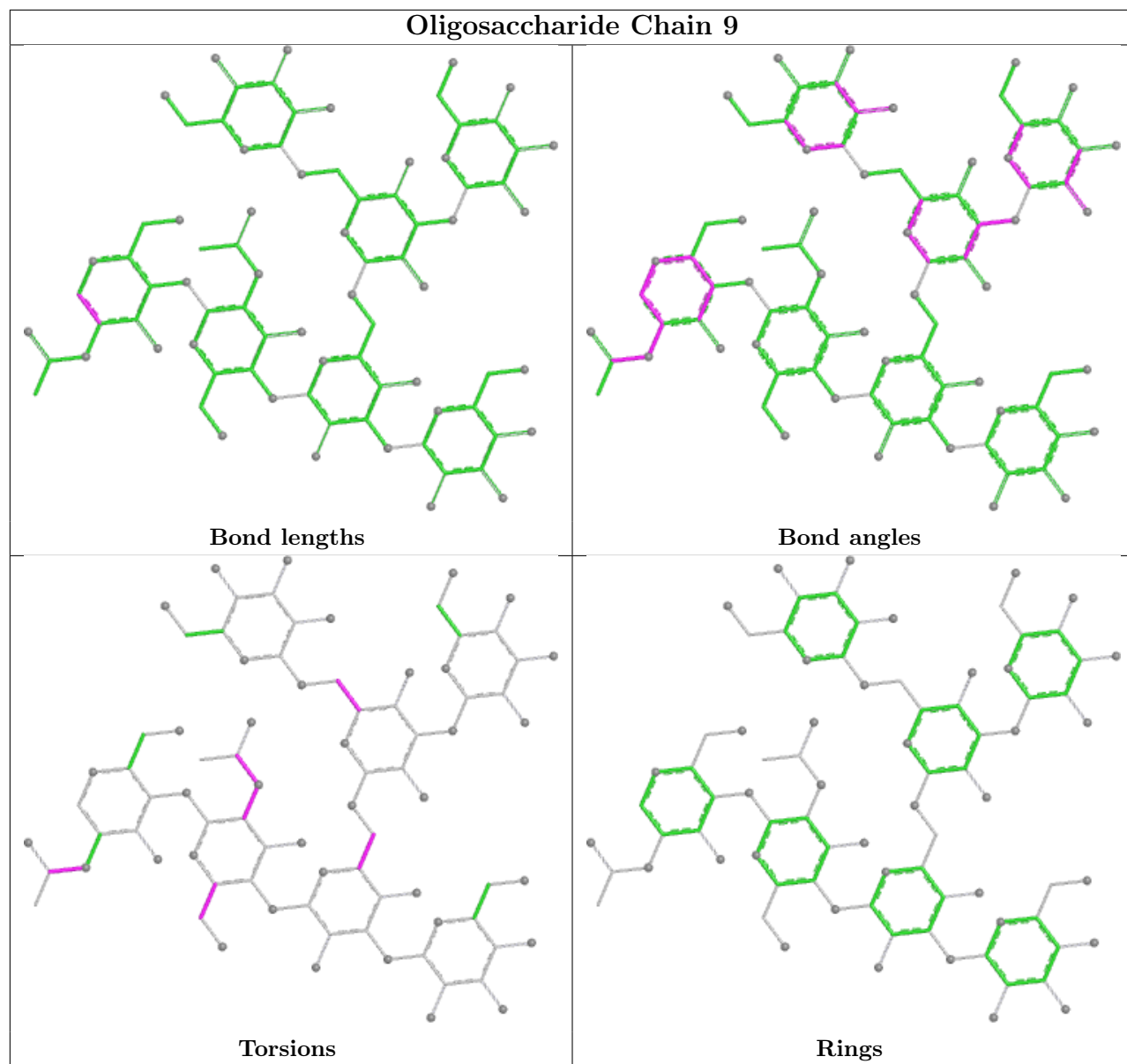


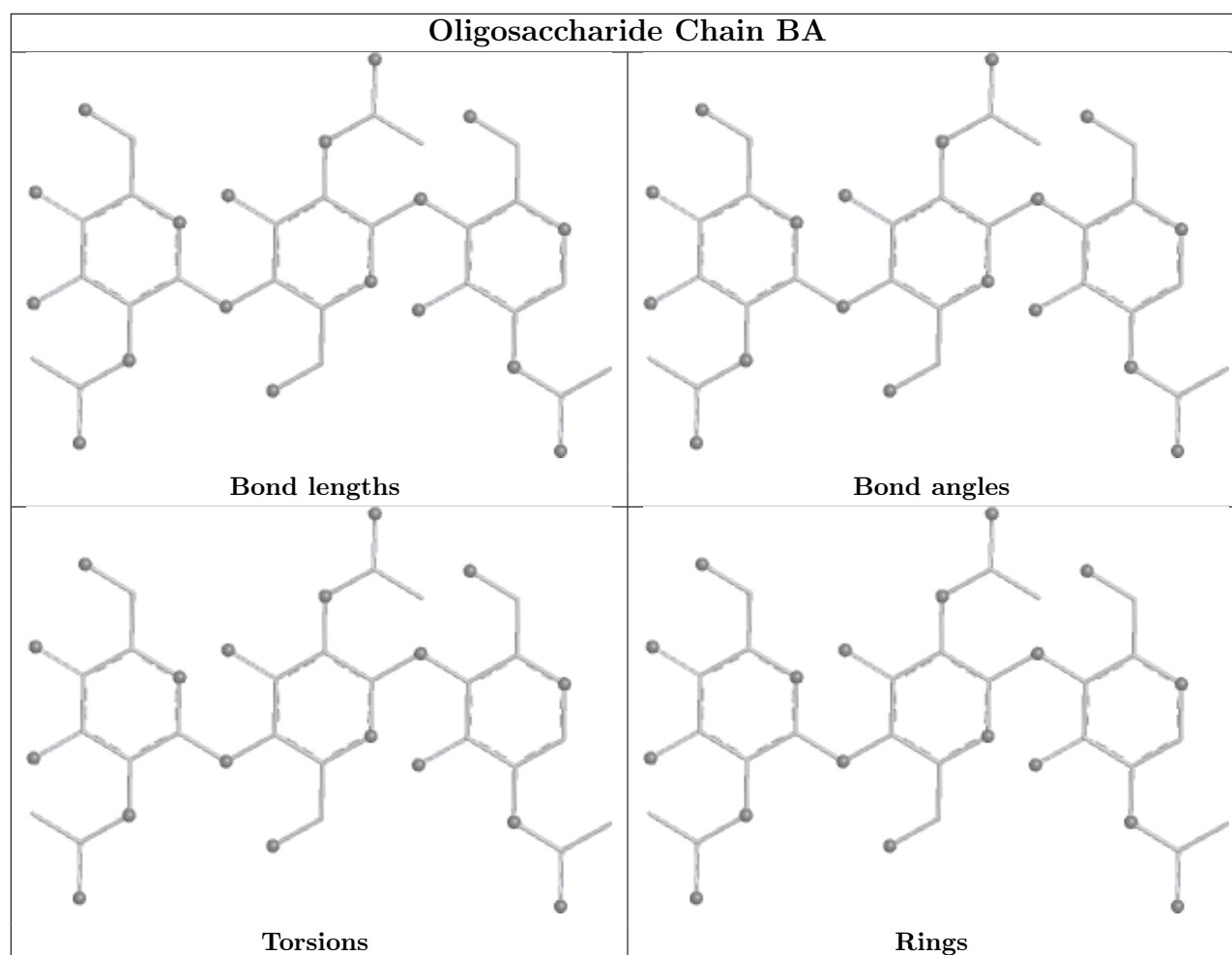




Oligosaccharide Chain AA**Oligosaccharide Chain DA**







5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
19	NAG	A	602	2	14,14,15	0.35	0	17,19,21	0.51	0
18	83G	E	601	-	33,33,33	0.44	0	44,47,47	1.02	3 (6%)
19	NAG	C	602	2	14,14,15	0.30	0	17,19,21	0.64	0
18	83G	C	601	-	33,33,33	0.40	0	44,47,47	0.85	2 (4%)
18	83G	A	601	-	33,33,33	0.41	0	44,47,47	0.82	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	NAG	E	602	2	14,14,15	0.42	0	17,19,21	0.75	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
19	NAG	A	602	2	-	1/6/23/26	0/1/1/1
18	83G	E	601	-	-	6/22/35/35	0/4/4/4
19	NAG	C	602	2	-	2/6/23/26	0/1/1/1
18	83G	C	601	-	-	8/22/35/35	0/4/4/4
18	83G	A	601	-	-	13/22/35/35	0/4/4/4
19	NAG	E	602	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	E	601	83G	C11-C12-C14	2.74	124.19	118.82
18	C	601	83G	O02-C03-C08	2.55	119.46	115.84
18	E	601	83G	O02-C03-C08	2.45	119.32	115.84
18	A	601	83G	C12-C14-N16	2.17	121.03	118.81
18	C	601	83G	C11-C12-C14	2.09	122.93	118.82

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

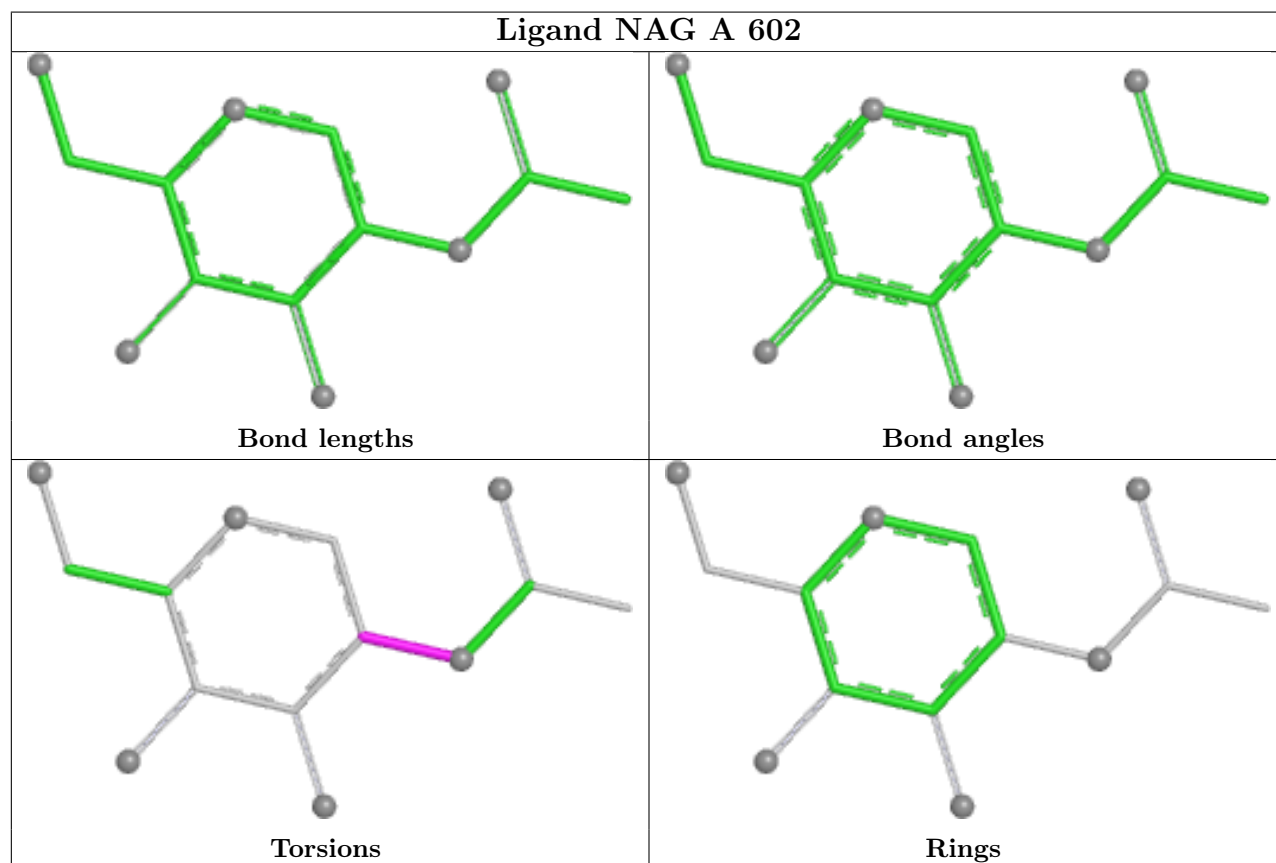
Mol	Chain	Res	Type	Atoms
18	C	601	83G	O15-C14-N16-C17
18	C	601	83G	C08-C11-C12-O13
18	A	601	83G	O15-C14-N16-C17
18	A	601	83G	C10-C11-C12-O13
18	A	601	83G	C08-C11-C12-C14

There are no ring outliers.

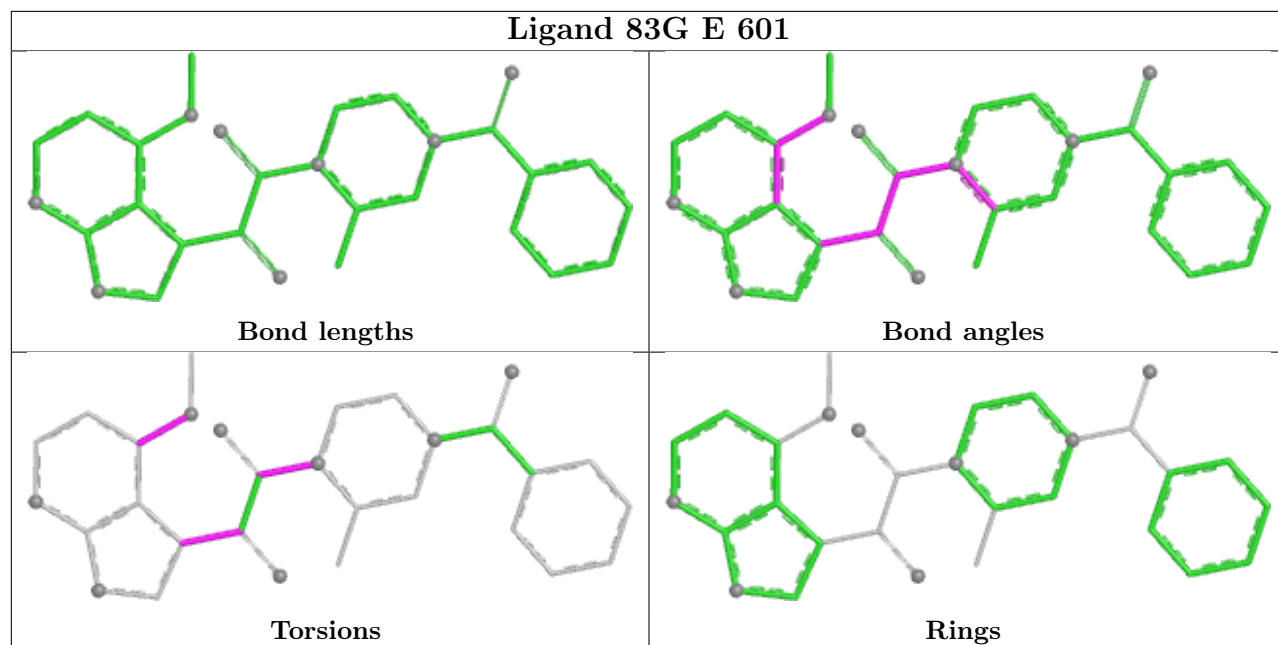
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	601	83G	1	0

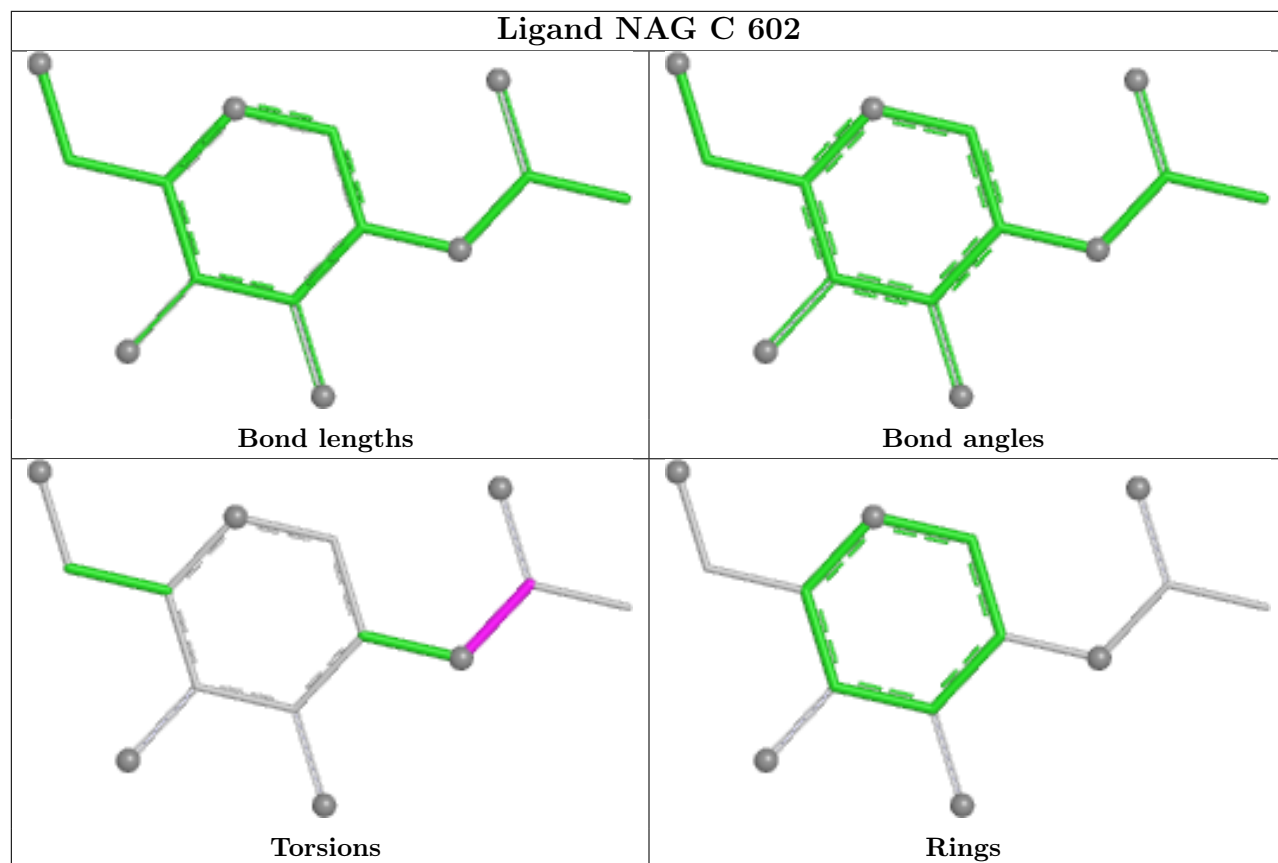
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

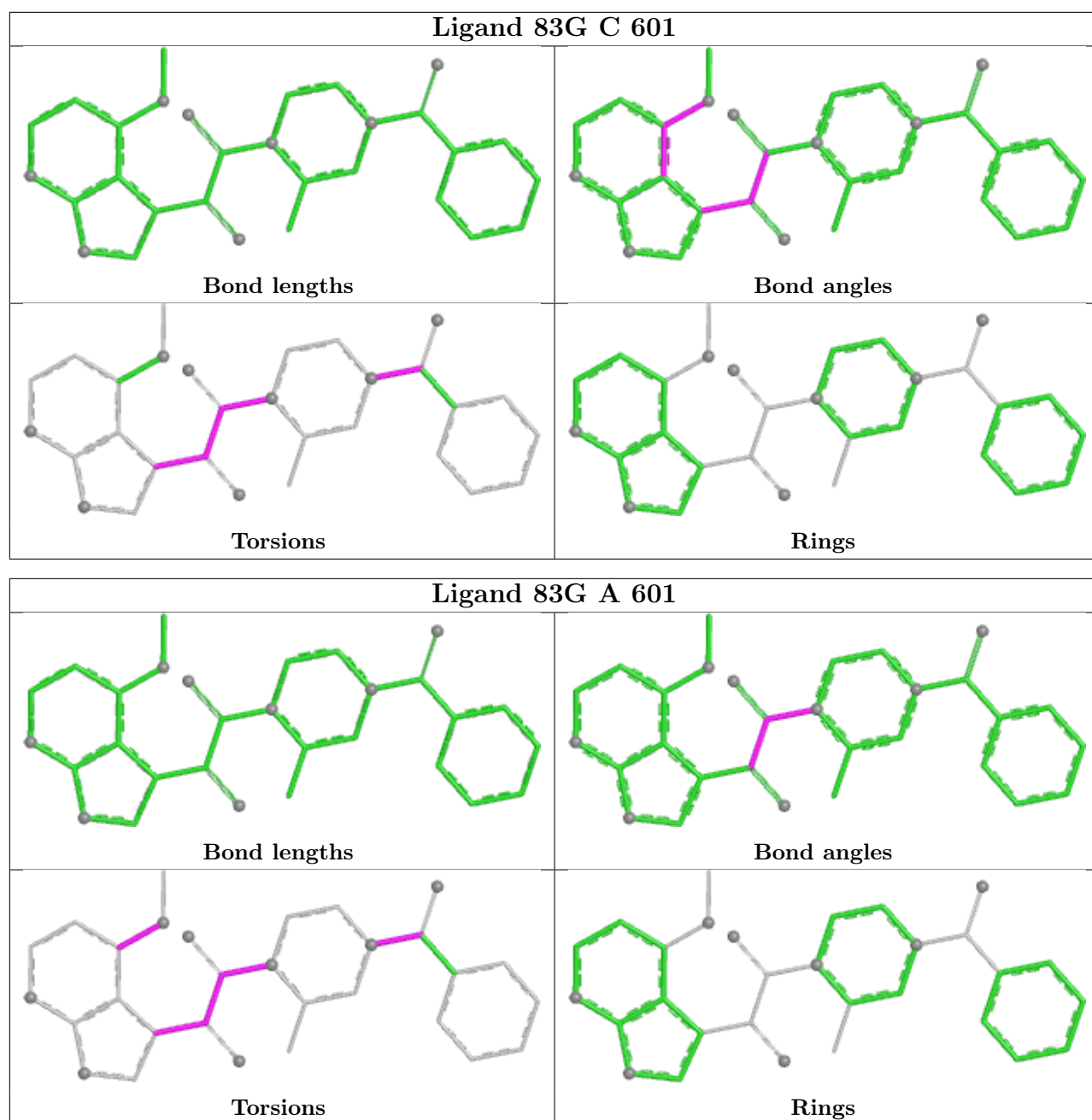


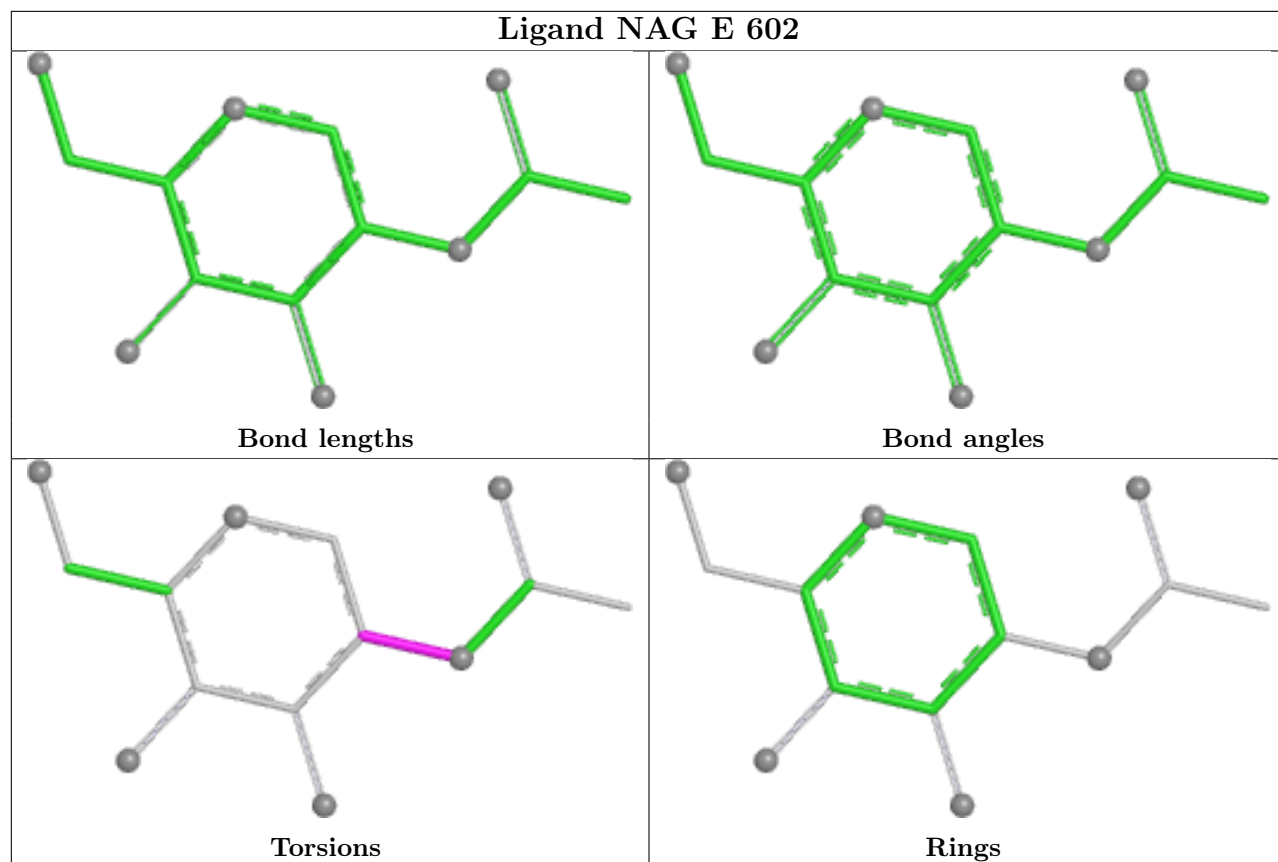
Ligand 83G E 601



Ligand NAG C 602







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.

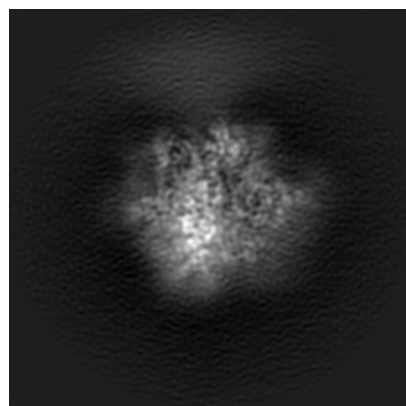
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28954. These allow visual inspection of the internal detail of the map and identification of artifacts.

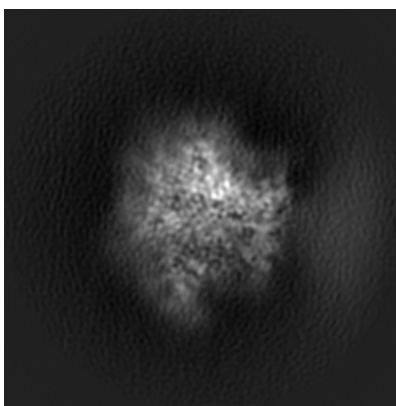
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

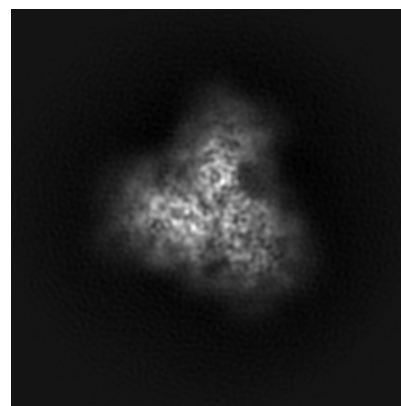
6.1.1 Primary map



X

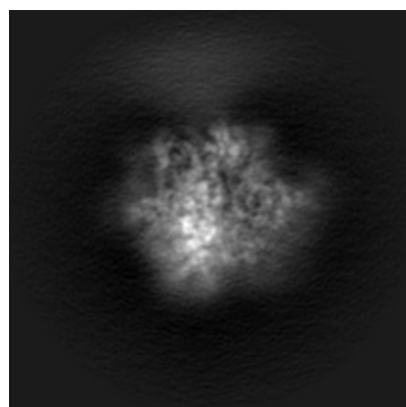


Y

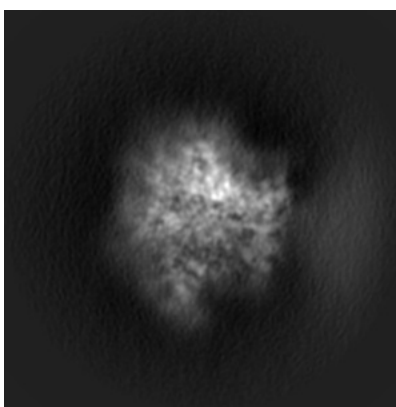


Z

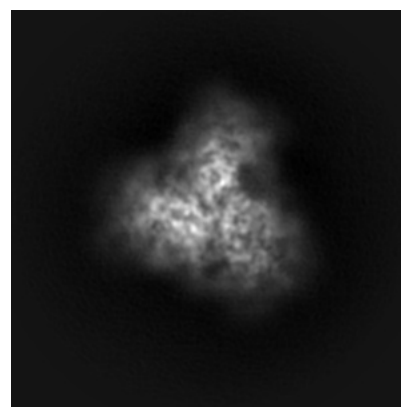
6.1.2 Raw map



X



Y

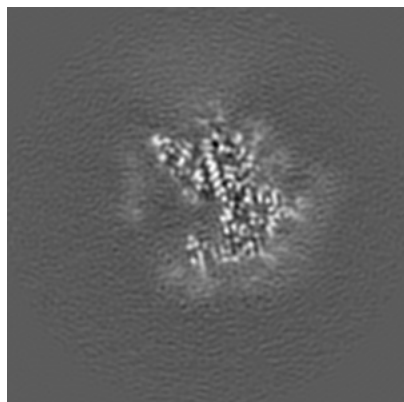


Z

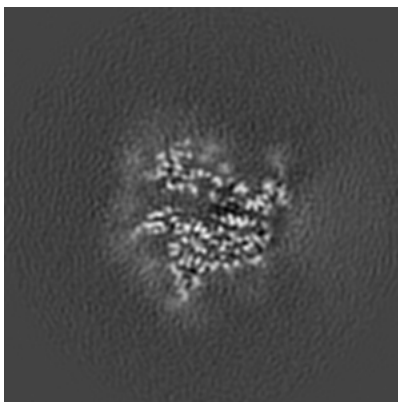
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

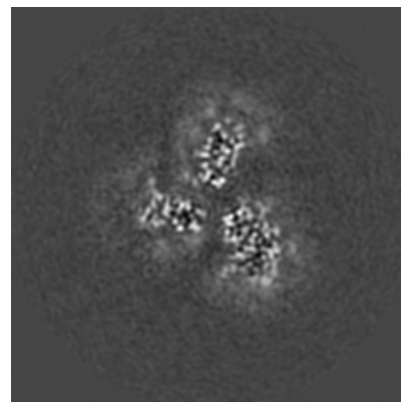
6.2.1 Primary map



X Index: 80

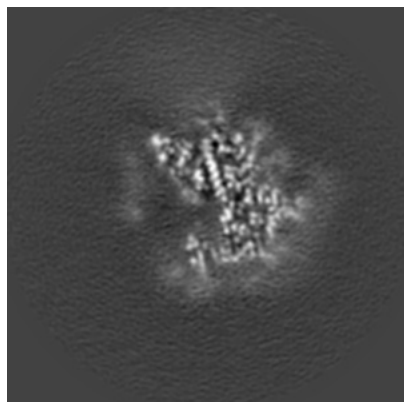


Y Index: 80

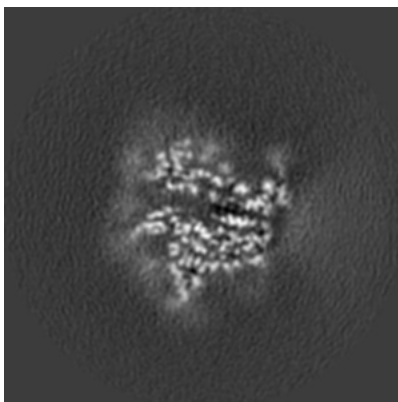


Z Index: 80

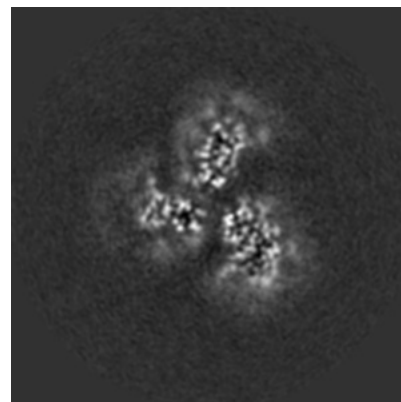
6.2.2 Raw map



X Index: 80



Y Index: 80

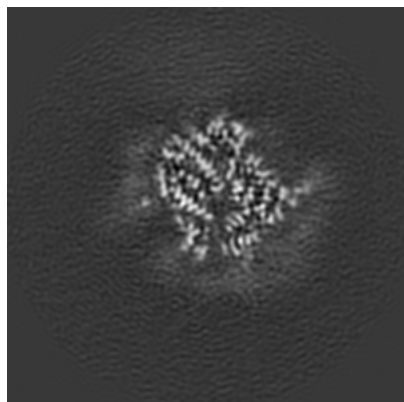


Z Index: 80

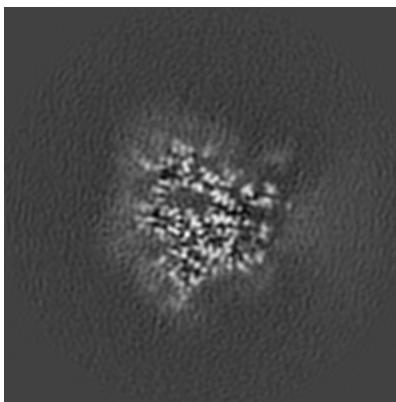
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

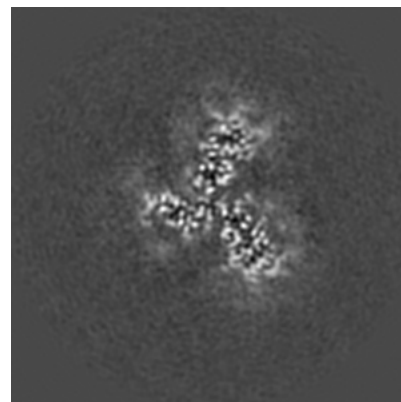
6.3.1 Primary map



X Index: 86

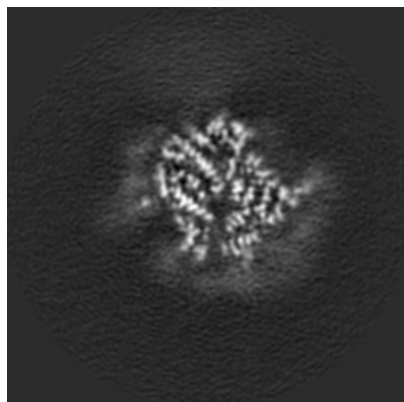


Y Index: 78

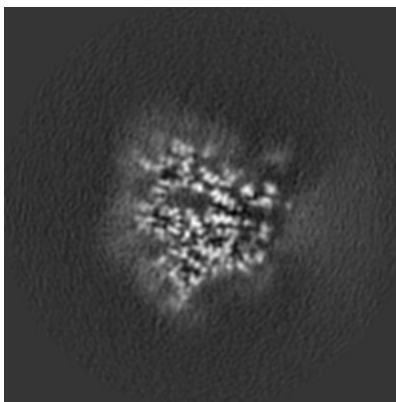


Z Index: 83

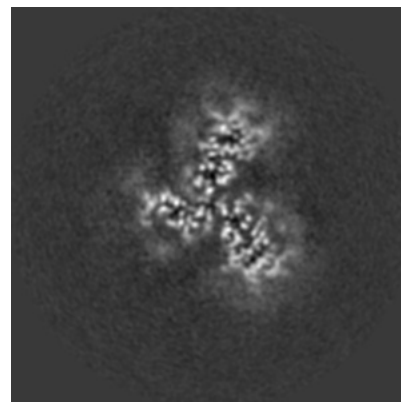
6.3.2 Raw map



X Index: 86



Y Index: 78

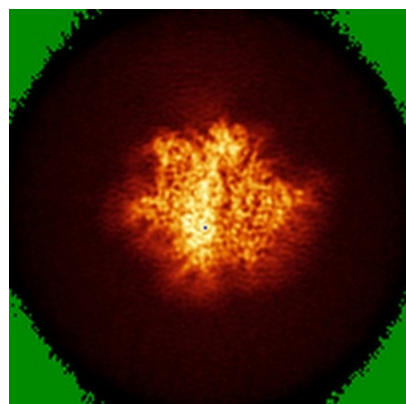


Z Index: 83

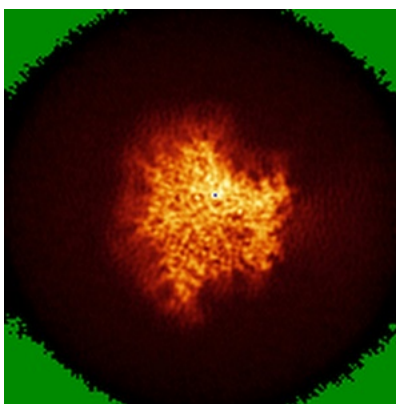
The images above show the largest variance slices of the map in three orthogonal directions.

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

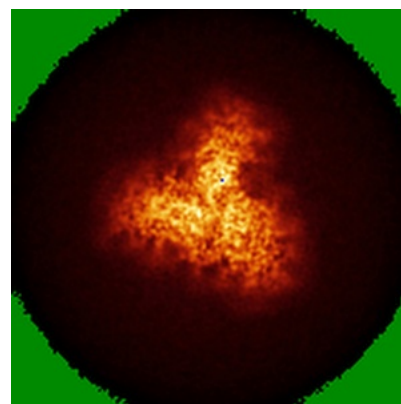
6.4.1 Primary map



X

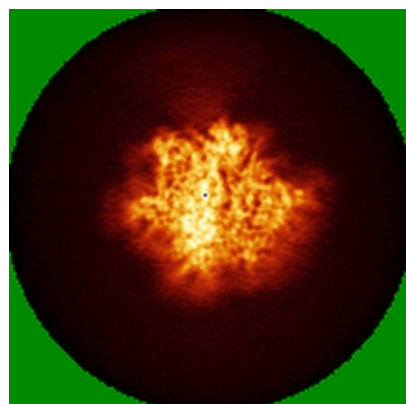


Y

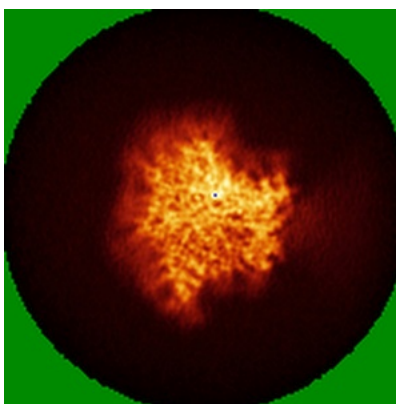


Z

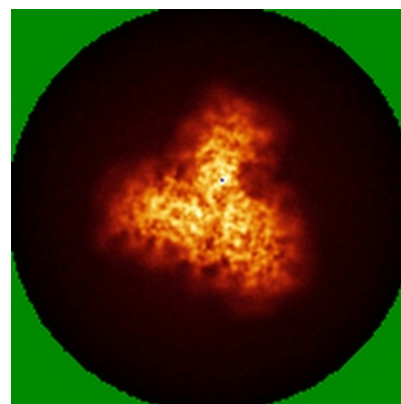
6.4.2 Raw map



X



Y

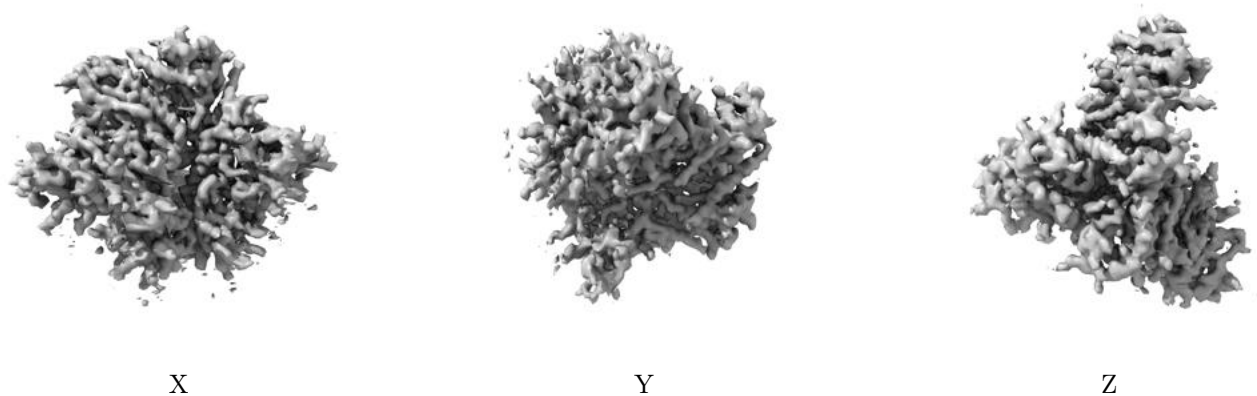


Z

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.

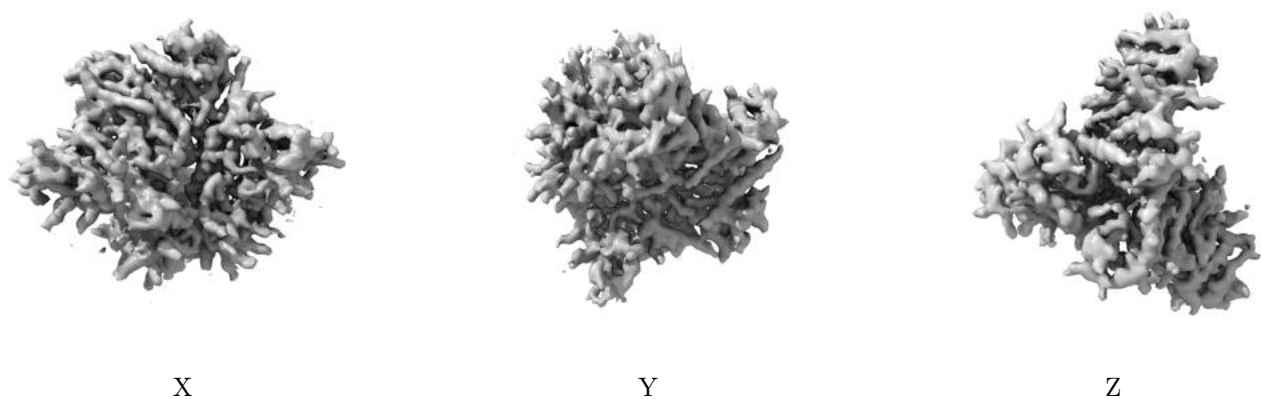
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. 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.

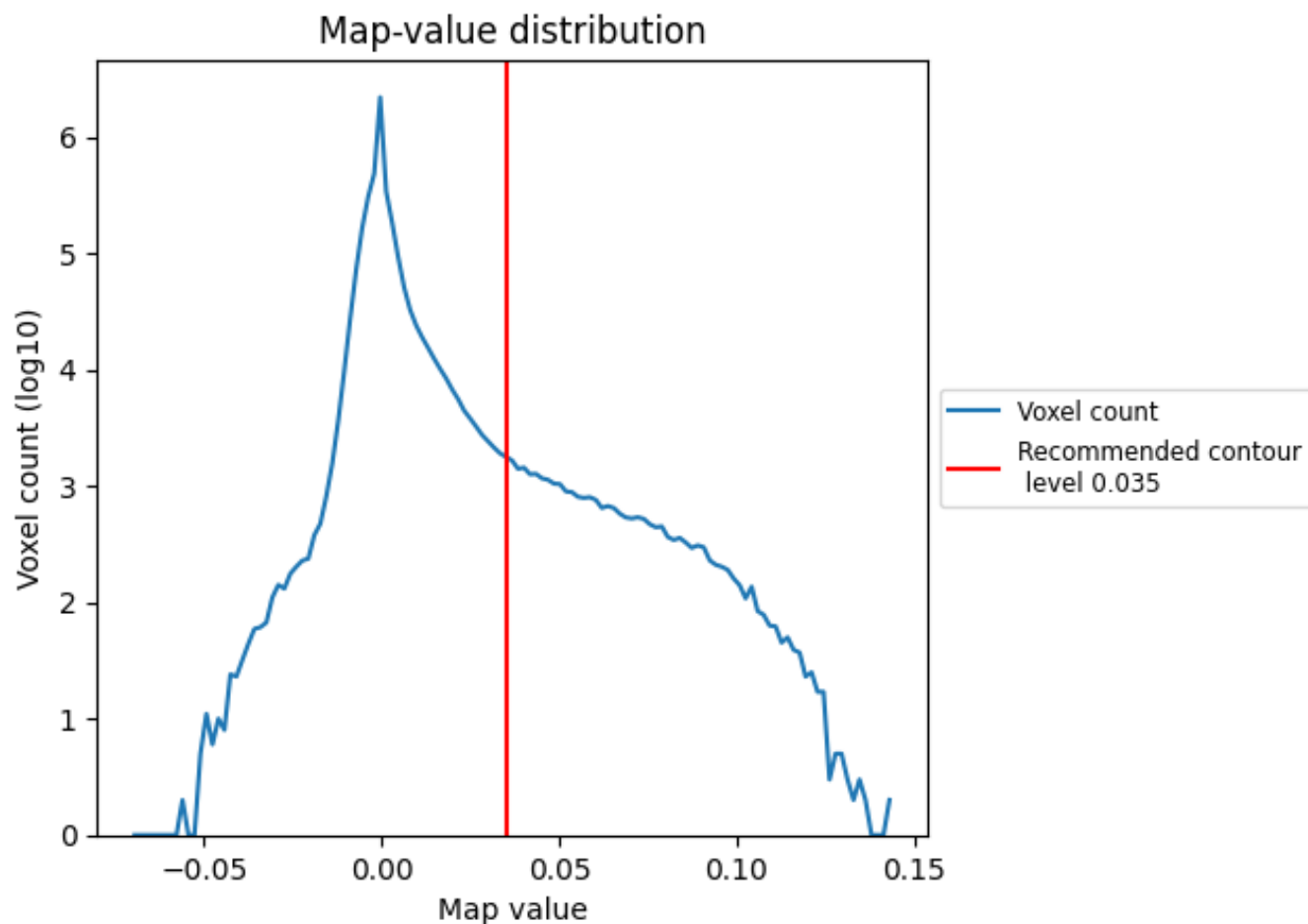
6.6 Mask visualisation [i](#)

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

7 Map analysis ⓘ

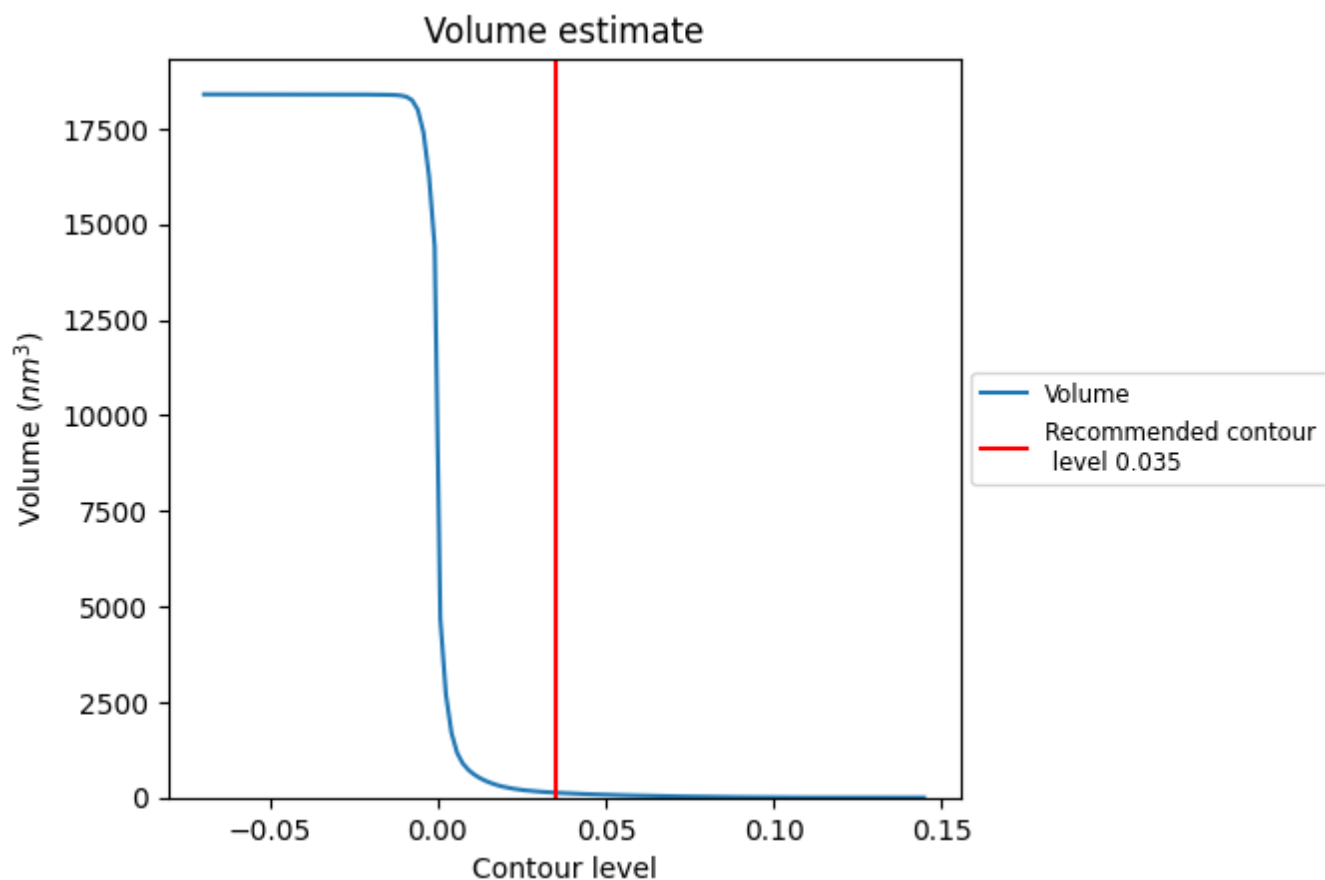
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

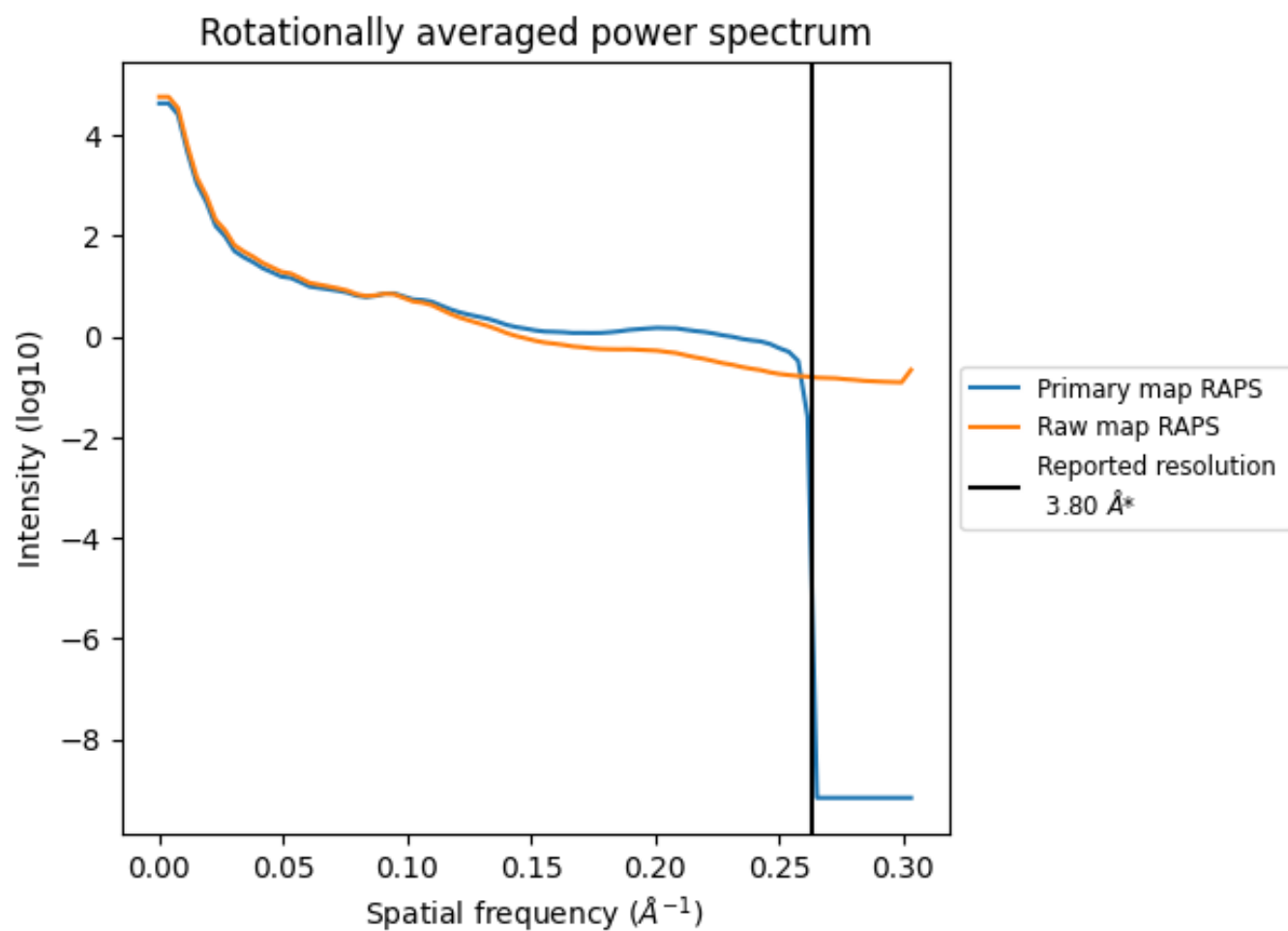
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 128 nm³; this corresponds to an approximate mass of 115 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 ⓘ

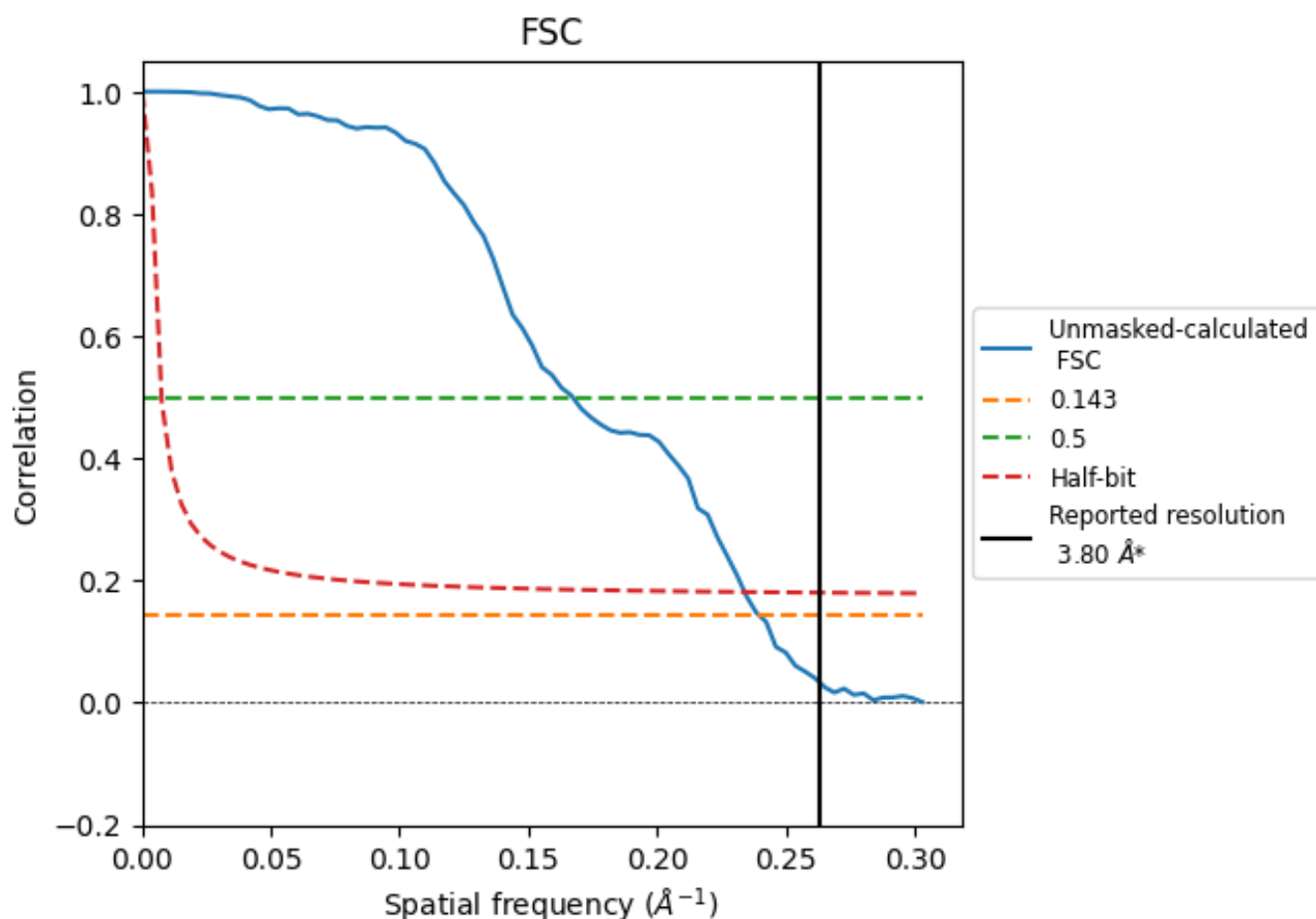


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

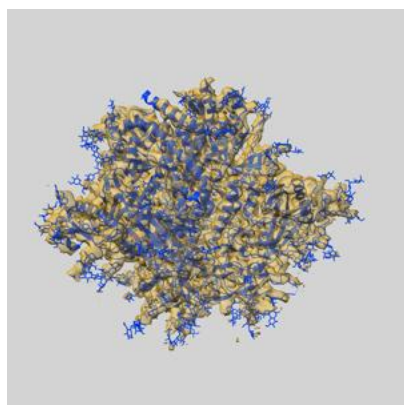
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.17	5.98	4.27

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

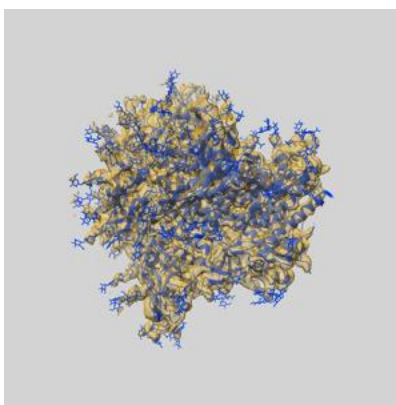
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28954 and PDB model 8FAE. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

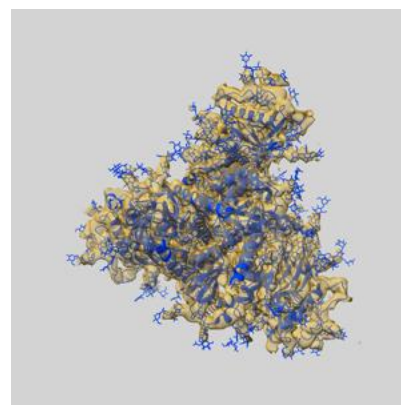
9.1 Map-model overlay [i](#)



X



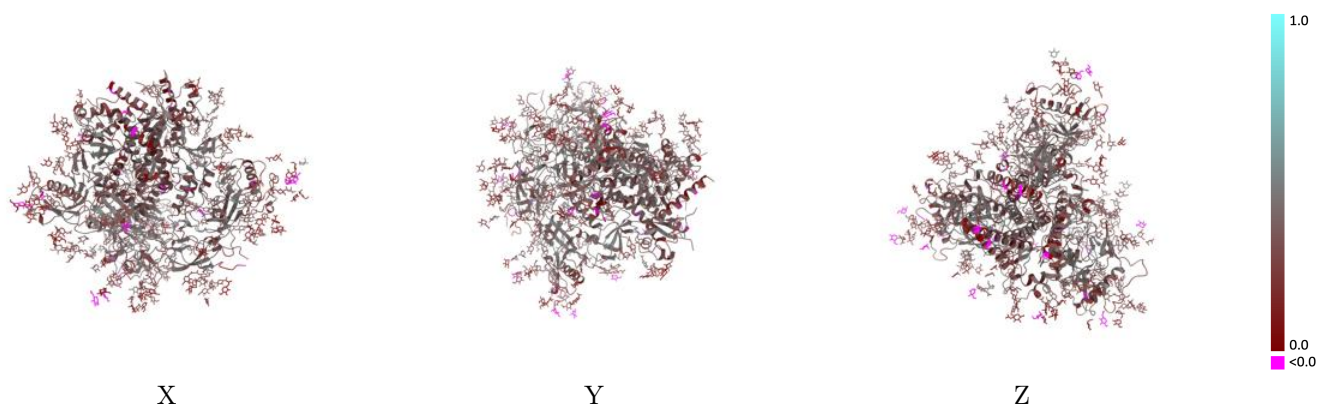
Y



Z

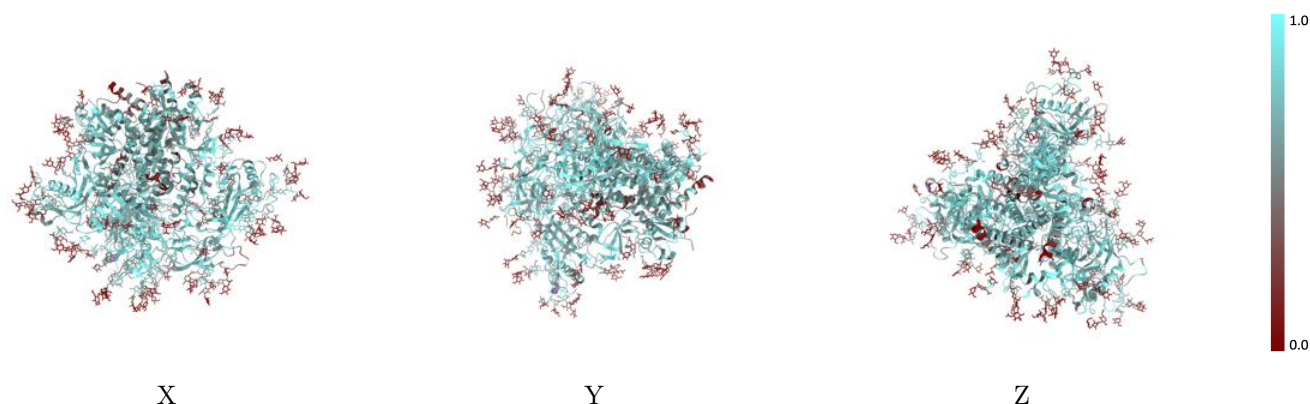
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



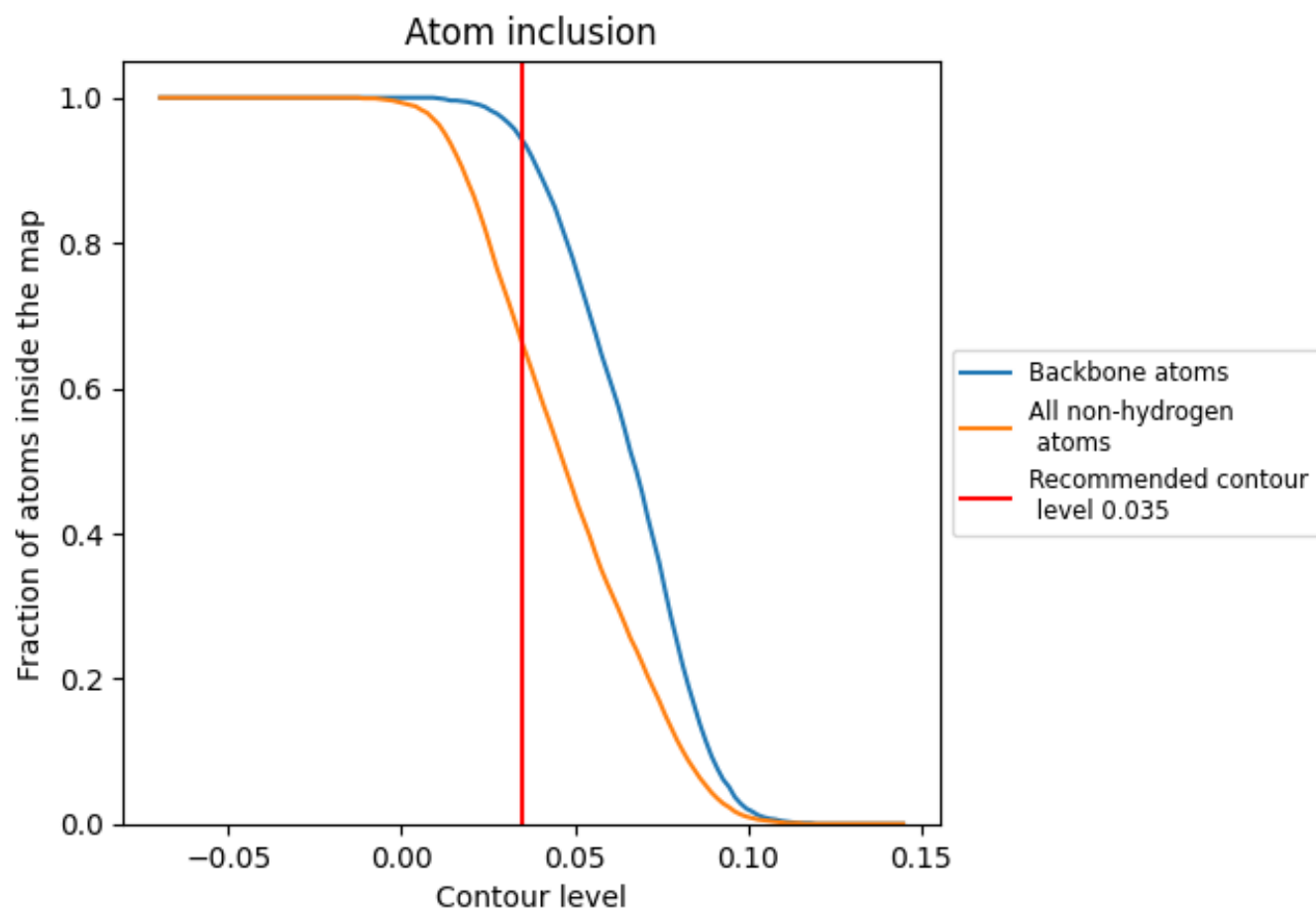
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 66% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6600	 0.3330
0	 0.3850	 0.3230
1	 0.2560	 0.2240
2	 0.4360	 0.2580
3	 0.4000	 0.1390
4	 0.2560	 0.2200
5	 0.1790	 0.2130
6	 0.2820	 0.2460
7	 0.4640	 0.3100
8	 0.1280	 0.1240
9	 0.4820	 0.2690
A	 0.7570	 0.3740
AA	 0.3200	 0.2340
B	 0.6790	 0.2900
BA	 0.3090	 0.2960
C	 0.7530	 0.3770
CA	 0.3330	 0.3390
D	 0.6790	 0.2970
DA	 0.4600	 0.2360
E	 0.7550	 0.3760
EA	 0.4580	 0.1680
F	 0.6210	 0.2970
FA	 0.6070	 0.2260
G	 0.3590	 0.3060
GA	 0.3800	 0.2690
H	 0.0790	 0.1720
HA	 0.1800	 0.1600
I	 0.1320	 0.0780
IA	 0.2050	 0.1160
J	 0.2310	 0.2540
JA	 0.3330	 0.2370
K	 0.3330	 0.2660
KA	 0.3670	 0.2700
L	 0.3080	 0.2150
LA	 0.0790	 0.1210



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Chain	Atom inclusion	Q-score
M	 0.5130	 0.3370
MA	 0.1070	 0.3350
N	 0.2140	 0.1740
NA	 0.1320	 0.1800
O	 0.0260	 -0.0160
OA	 0.3620	 0.2160
P	 0.4360	 0.2290
Q	 0.2820	 0.1650
R	 0.1030	 0.1470
S	 0.5560	 0.2920
T	 0.2620	 0.1250
U	 0.4640	 0.2930
V	 0.2560	 0.3200
W	 0.3280	 0.2550
X	 0.4220	 0.1960
Y	 0.0000	 0.0930
Z	 0.5710	 0.2190
a	 0.3200	 0.3080
b	 0.3080	 0.2070
c	 0.3930	 0.2910
d	 0.3850	 0.2590
e	 0.3270	 0.2380
f	 0.1320	 0.1820
g	 0.1840	 0.1610
h	 0.1790	 0.2350
i	 0.3590	 0.3430
j	 0.3850	 0.2950
k	 0.3280	 0.2250
l	 0.1430	 0.1170
m	 0.1840	 0.1390
n	 0.3850	 0.2200
o	 0.2070	 0.2930
p	 0.2820	 0.1610
r	 0.4360	 0.2150
s	 0.3080	 0.3260
t	 0.3850	 0.2960
u	 0.4400	 0.2960
v	 0.4580	 0.1600
w	 0.3600	 0.2060
x	 0.4360	 0.2830
y	 0.2400	 0.1530
z	 0.1430	 0.2010