



wwPDB EM Validation Summary Report ⓘ

Mar 15, 2026 – 07:30 AM UTC

PDB ID : 8DVD / pdb_00008dvd
EMDB ID : EMD-27735
Title : Cryo-EM structure of SIVmac239 SOS-2P Env trimer in complex with human bNAbs PGT145
Authors : Gorman, J.; Kwong, P.D.
Deposited on : 2022-07-28
Resolution : 4.12 Å (reported)
Based on initial model : 6TYB

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

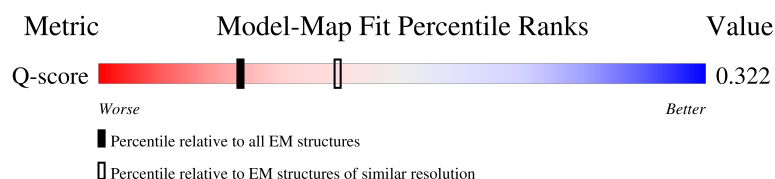
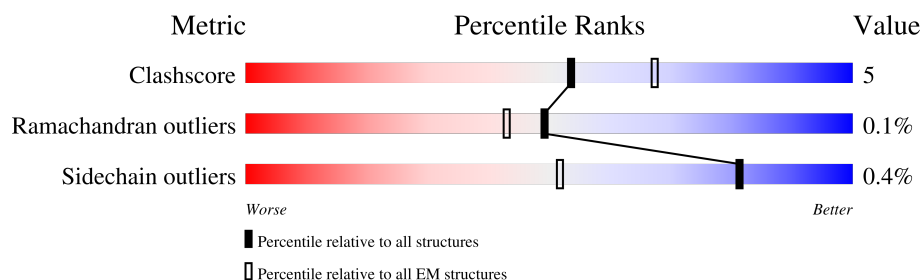
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

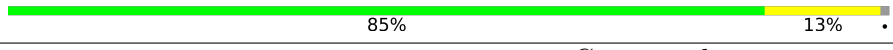
The reported resolution of this entry is 4.12 Å.

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.



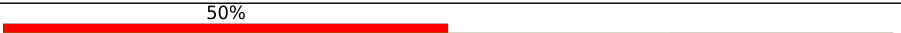
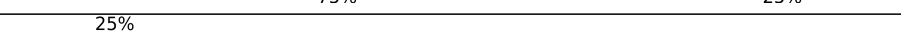
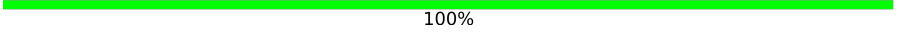
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5662 (3.62 - 4.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	148	
1	B	148	
1	C	148	
2	E	500	

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Mol	Chain	Length	Quality of chain
2	F	500	
2	G	500	
3	H	244	
4	L	219	
5	5	4	
5	7	4	
5	BA	4	
5	CA	4	
5	D	4	
5	I	4	
5	JA	4	
5	K	4	
5	O	4	
5	QA	4	
5	V	4	
5	W	4	
5	d	4	
5	g	4	
5	m	4	
5	q	4	
5	r	4	
5	y	4	
6	1	3	
6	6	3	
6	HA	3	

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Mol	Chain	Length	Quality of chain
6	J	3	
6	MA	3	
6	N	3	
6	Q	3	
6	R	3	
6	RA	3	
6	U	3	
6	Z	3	
6	b	3	
6	k	3	
6	l	3	
6	w	3	
7	0	5	
7	4	5	
7	9	5	
7	DA	5	
7	GA	5	
7	LA	5	
7	M	5	
7	P	5	
7	PA	5	
7	T	5	
7	X	5	
7	a	5	
7	j	5	

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Mol	Chain	Length	Quality of chain
7	o	5	
7	s	5	
7	v	5	
8	2	2	
8	3	2	
8	8	2	
8	AA	2	
8	NA	2	
8	OA	2	
8	S	2	
8	h	2	
8	i	2	
8	n	2	
8	p	2	
9	EA	6	
9	Y	6	
9	t	6	
10	c	8	
11	KA	8	
11	e	8	
11	f	8	
12	FA	4	
12	u	4	
13	IA	7	
13	x	7	

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Mol	Chain	Length	Quality of chain
14	z	7	14% 14% 86%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 20804 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 gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	134	Total	C	N	O	S	0	0
			1059	672	181	201	5		
1	B	135	Total	C	N	O	S	0	0
			1073	683	183	202	5		
1	C	135	Total	C	N	O	S	0	0
			1073	683	183	202	5		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	559	PRO	VAL	conflict	UNP A0A0C5JYT4
A	569	PRO	THR	conflict	UNP A0A0C5JYT4
A	605	CYS	HIS	conflict	UNP A0A0C5JYT4
B	559	PRO	VAL	conflict	UNP A0A0C5JYT4
B	569	PRO	THR	conflict	UNP A0A0C5JYT4
B	605	CYS	HIS	conflict	UNP A0A0C5JYT4
C	559	PRO	VAL	conflict	UNP A0A0C5JYT4
C	569	PRO	THR	conflict	UNP A0A0C5JYT4
C	605	CYS	HIS	conflict	UNP A0A0C5JYT4

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	494	Total	C	N	O	S	0	0
			3962	2483	689	754	36		
2	F	494	Total	C	N	O	S	0	0
			3962	2483	689	754	36		
2	G	494	Total	C	N	O	S	0	0
			3962	2483	689	754	36		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	169	THR	LYS	conflict	UNP A0A4Y5TGK0
E	501	CYS	VAL	conflict	UNP A0A4Y5TGK0
F	169	THR	LYS	conflict	UNP A0A4Y5TGK0
F	501	CYS	VAL	conflict	UNP A0A4Y5TGK0
G	169	THR	LYS	conflict	UNP A0A4Y5TGK0
G	501	CYS	VAL	conflict	UNP A0A4Y5TGK0

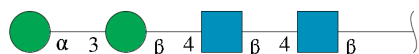
- Molecule 3 is a protein called PGT145 Heavy.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	140	Total	C	N	O	S	0	0
			1102	685	191	219	7		

- Molecule 4 is a protein called PGT145 Light.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	111	Total	C	N	O	S	0	0
			848	536	149	159	4		

- Molecule 5 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.



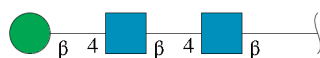
Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	4	Total	C	N	O		0	0
			50	28	2	20			
5	I	4	Total	C	N	O		0	0
			50	28	2	20			
5	K	4	Total	C	N	O		0	0
			50	28	2	20			
5	O	4	Total	C	N	O		0	0
			50	28	2	20			
5	V	4	Total	C	N	O		0	0
			50	28	2	20			
5	W	4	Total	C	N	O		0	0
			50	28	2	20			
5	d	4	Total	C	N	O		0	0
			50	28	2	20			

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	g	4	Total	C	N	O	0	0
			50	28	2	20		
5	m	4	Total	C	N	O	0	0
			50	28	2	20		
5	q	4	Total	C	N	O	0	0
			50	28	2	20		
5	r	4	Total	C	N	O	0	0
			50	28	2	20		
5	y	4	Total	C	N	O	0	0
			50	28	2	20		
5	5	4	Total	C	N	O	0	0
			50	28	2	20		
5	7	4	Total	C	N	O	0	0
			50	28	2	20		
5	BA	4	Total	C	N	O	0	0
			50	28	2	20		
5	CA	4	Total	C	N	O	0	0
			50	28	2	20		
5	JA	4	Total	C	N	O	0	0
			50	28	2	20		
5	QA	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 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.



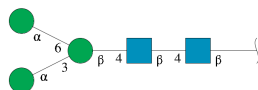
Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	3	Total	C	N	O	0	0
			39	22	2	15		
6	N	3	Total	C	N	O	0	0
			39	22	2	15		
6	Q	3	Total	C	N	O	0	0
			39	22	2	15		
6	R	3	Total	C	N	O	0	0
			39	22	2	15		
6	U	3	Total	C	N	O	0	0
			39	22	2	15		
6	Z	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	b	3	Total	C	N	O	0	0
			39	22	2	15		
6	k	3	Total	C	N	O	0	0
			39	22	2	15		
6	l	3	Total	C	N	O	0	0
			39	22	2	15		
6	w	3	Total	C	N	O	0	0
			39	22	2	15		
6	1	3	Total	C	N	O	0	0
			39	22	2	15		
6	6	3	Total	C	N	O	0	0
			39	22	2	15		
6	HA	3	Total	C	N	O	0	0
			39	22	2	15		
6	MA	3	Total	C	N	O	0	0
			39	22	2	15		
6	RA	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 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
7	M	5	Total	C	N	O	0	0
			61	34	2	25		
7	P	5	Total	C	N	O	0	0
			61	34	2	25		
7	T	5	Total	C	N	O	0	0
			61	34	2	25		
7	X	5	Total	C	N	O	0	0
			61	34	2	25		
7	a	5	Total	C	N	O	0	0
			61	34	2	25		
7	j	5	Total	C	N	O	0	0
			61	34	2	25		
7	o	5	Total	C	N	O	0	0
			61	34	2	25		

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	s	5	Total 61	C 34	N 2	O 25	0	0
7	v	5	Total 61	C 34	N 2	O 25	0	0
7	0	5	Total 61	C 34	N 2	O 25	0	0
7	4	5	Total 61	C 34	N 2	O 25	0	0
7	9	5	Total 61	C 34	N 2	O 25	0	0
7	DA	5	Total 61	C 34	N 2	O 25	0	0
7	GA	5	Total 61	C 34	N 2	O 25	0	0
7	LA	5	Total 61	C 34	N 2	O 25	0	0
7	PA	5	Total 61	C 34	N 2	O 25	0	0

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



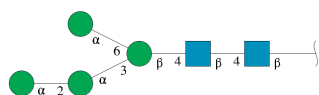
Mol	Chain	Residues	Atoms				AltConf	Trace
8	S	2	Total 28	C 16	N 2	O 10	0	0
8	h	2	Total 28	C 16	N 2	O 10	0	0
8	i	2	Total 28	C 16	N 2	O 10	0	0
8	n	2	Total 28	C 16	N 2	O 10	0	0
8	p	2	Total 28	C 16	N 2	O 10	0	0
8	2	2	Total 28	C 16	N 2	O 10	0	0
8	3	2	Total 28	C 16	N 2	O 10	0	0
8	8	2	Total 28	C 16	N 2	O 10	0	0

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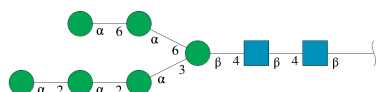
Mol	Chain	Residues	Atoms				AltConf	Trace
8	AA	2	Total	C	N	O	0	0
			28	16	2	10		
8	NA	2	Total	C	N	O	0	0
			28	16	2	10		
8	OA	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 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.



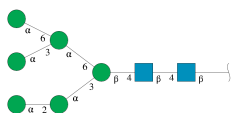
Mol	Chain	Residues	Atoms				AltConf	Trace
9	Y	6	Total	C	N	O	0	0
			72	40	2	30		
9	t	6	Total	C	N	O	0	0
			72	40	2	30		
9	EA	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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
10	c	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 11 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.



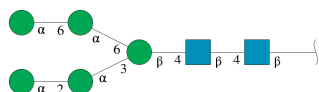
Mol	Chain	Residues	Atoms				AltConf	Trace
11	e	8	Total	C	N	O	0	0
			94	52	2	40		
11	f	8	Total	C	N	O	0	0
			94	52	2	40		
11	KA	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 12 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
12	u	4	Total	C	N	O	0	0
			50	28	2	20		
12	FA	4	Total	C	N	O	0	0
			50	28	2	20		

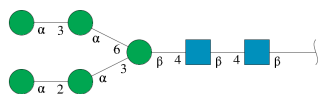
- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
13	x	7	Total	C	N	O	0	0
			83	46	2	35		
13	IA	7	Total	C	N	O	0	0
			83	46	2	35		

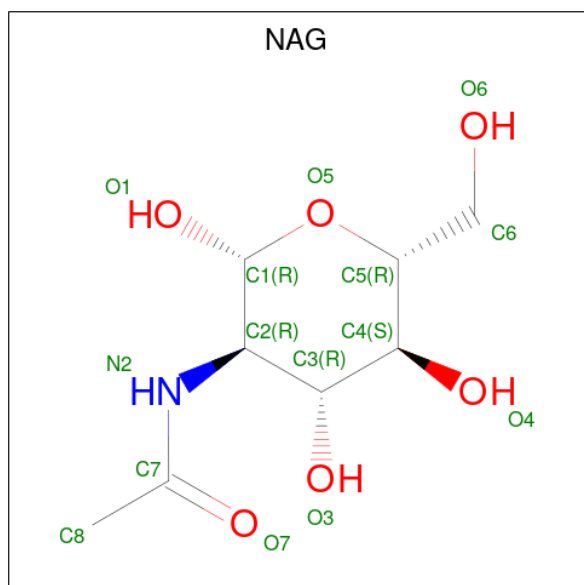
- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyra

nose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



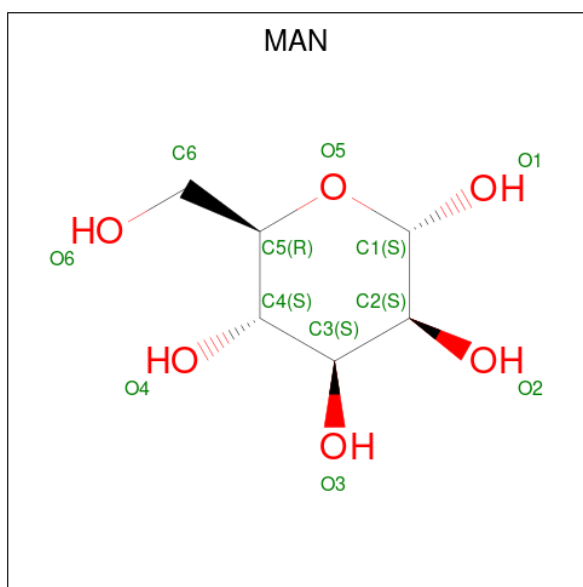
Mol	Chain	Residues	Atoms				AltConf	Trace
14	z	7	Total	C	N	O	0	0
			83	46	2	35		

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



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

- Molecule 16 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
16	F	1	11	6	5	0

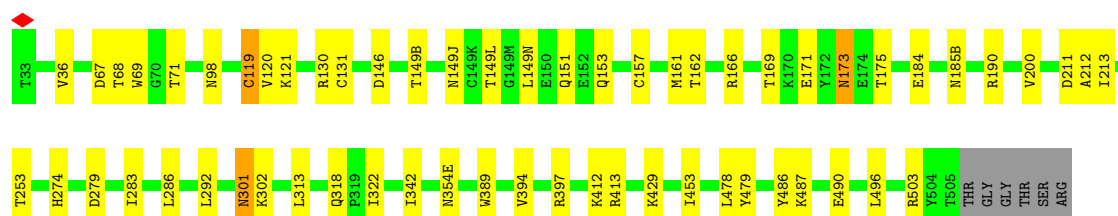
- Molecule 2: Envelope glycoprotein gp160

Chain F:  85% 14%



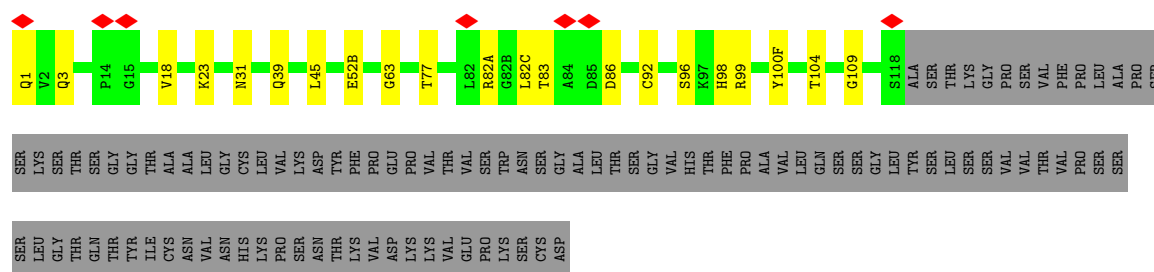
- Molecule 2: Envelope glycoprotein gp160

Chain G:  87% 11%



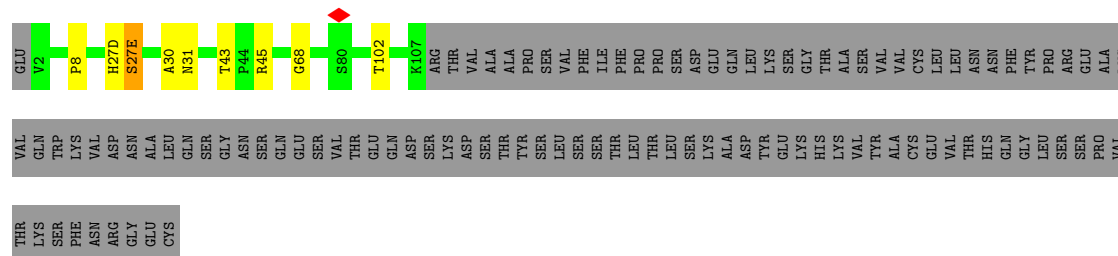
- Molecule 3: PGT145 Heavy

Chain H:  49% 9% 43%



- Molecule 4: PGT145 Light

Chain L:  47% 49%



- Molecule 5: 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 D: 



- Molecule 5: 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 I: 



- Molecule 5: 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 K: 



- Molecule 5: 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 O: 



- Molecule 5: 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 V: 



- Molecule 5: 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 W: 



- Molecule 5: 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 d: 



- Molecule 5: 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 g: 



- Molecule 5: 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 m: 



- Molecule 5: 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 q: 



- Molecule 5: 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 r: 



- Molecule 5: 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 y: 



- Molecule 5: 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 5: 



- Molecule 5: 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 7: 



- Molecule 5: 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 BA: 

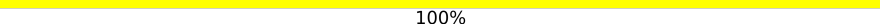


- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain CA: 



- Molecule 5: 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 JA: 



- Molecule 5: 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 QA: 



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 



- Molecule 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 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%

MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  33% 67%

MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:  33% 67%

MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:  100%

MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1:  67% 33%

MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6:  100%

MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain HA:  67% 33%



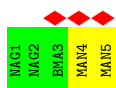
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



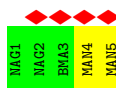
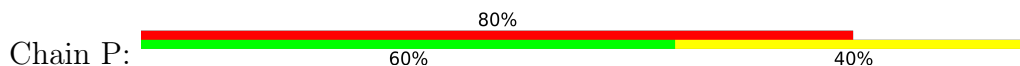
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



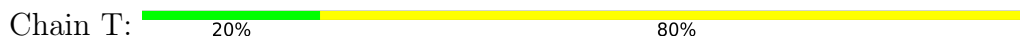
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



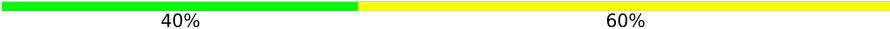
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-3)-[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



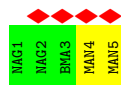
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 



• Molecule 7: 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

Chain a: 

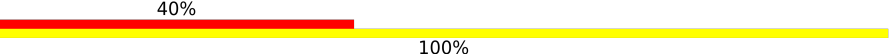


• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j: 

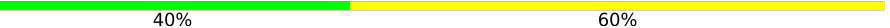


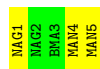
• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o: 



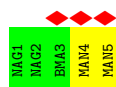
• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s: 

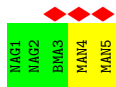


• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v: 



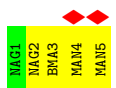
- Molecule 7: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



- Molecule 7: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



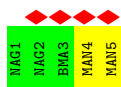
- Molecule 7: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



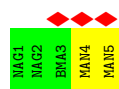
- Molecule 7: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



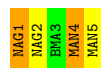
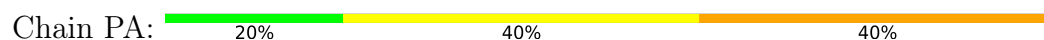
- Molecule 7: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



- Molecule 7: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



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



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



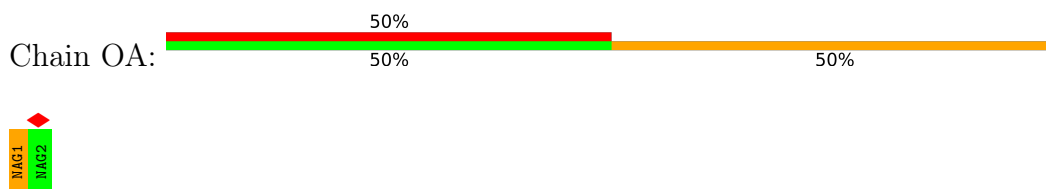
- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



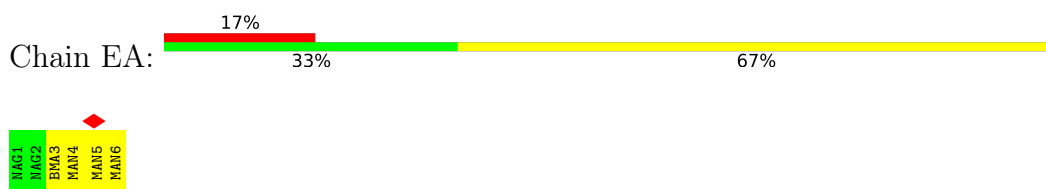
- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 10: alpha-D-mannopyranose-(1-2)-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 11: 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 11: 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 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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

Chain IA: 

MAG1	MAG2	EMA3	MAN4	MAN5	MAN6	MAN7
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- Molecule 14: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain z: 

MAG1	MAG2	EMA3	MAN4	MAN5	MAN6	MAN7
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61881	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 ($e^-/\text{\AA}^2$)	51.15	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.475	Depositor
Minimum map value	-0.550	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	346.56, 346.56, 346.56	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.09	0/1077	0.25	0/1461
1	B	0.14	0/1093	0.26	0/1484
1	C	0.13	0/1093	0.28	0/1484
2	E	0.12	0/4059	0.32	0/5521
2	F	0.12	0/4059	0.31	0/5521
2	G	0.14	0/4059	0.34	0/5521
3	H	0.10	0/1093	0.22	0/1477
4	L	0.10	0/871	0.26	0/1185
All	All	0.12	0/17404	0.31	0/23654

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	119	CYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1059	0	1045	12	0
1	B	1073	0	1055	12	0
1	C	1073	0	1055	10	0
2	E	3962	0	3791	44	0
2	F	3962	0	3791	47	0
2	G	3962	0	3791	46	0
3	H	1102	0	1031	13	0
4	L	848	0	828	5	0
5	5	50	0	43	0	0
5	7	50	0	43	0	0
5	BA	50	0	43	1	0
5	CA	50	0	43	0	0
5	D	50	0	43	0	0
5	I	50	0	43	0	0
5	JA	50	0	43	2	0
5	K	50	0	43	1	0
5	O	50	0	43	0	0
5	QA	50	0	43	0	0
5	V	50	0	43	0	0
5	W	50	0	43	1	0
5	d	50	0	43	0	0
5	g	50	0	43	0	0
5	m	50	0	43	0	0
5	q	50	0	43	0	0
5	r	50	0	43	0	0
5	y	50	0	43	0	0
6	1	39	0	34	1	0
6	6	39	0	34	0	0
6	HA	39	0	34	1	0
6	J	39	0	34	0	0
6	MA	39	0	34	0	0
6	N	39	0	34	0	0
6	Q	39	0	34	0	0
6	R	39	0	34	0	0
6	RA	39	0	34	0	0
6	U	39	0	34	0	0
6	Z	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	b	39	0	34	0	0
6	k	39	0	34	1	0
6	l	39	0	34	1	0
6	w	39	0	34	0	0
7	0	61	0	52	0	0
7	4	61	0	52	0	0
7	9	61	0	52	1	0
7	DA	61	0	52	1	0
7	GA	61	0	52	0	0
7	LA	61	0	52	0	0
7	M	61	0	52	0	0
7	P	61	0	52	0	0
7	PA	61	0	52	4	0
7	T	61	0	52	1	0
7	X	61	0	52	1	0
7	a	61	0	52	0	0
7	j	61	0	52	1	0
7	o	61	0	52	2	0
7	s	61	0	52	1	0
7	v	61	0	52	0	0
8	2	28	0	25	2	0
8	3	28	0	25	2	0
8	8	28	0	25	0	0
8	AA	28	0	25	0	0
8	NA	28	0	25	2	0
8	OA	28	0	25	2	0
8	S	28	0	25	1	0
8	h	28	0	25	0	0
8	i	28	0	25	2	0
8	n	28	0	25	0	0
8	p	28	0	25	0	0
9	EA	72	0	61	0	0
9	Y	72	0	61	0	0
9	t	72	0	61	0	0
10	c	94	0	79	3	0
11	KA	94	0	79	4	0
11	e	94	0	79	1	0
11	f	94	0	79	4	0
12	FA	50	0	43	0	0
12	u	50	0	43	0	0
13	IA	83	0	70	0	0
13	x	83	0	70	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	z	83	0	70	1	0
15	E	14	0	13	0	0
15	F	14	0	13	1	0
15	G	14	0	13	0	0
16	F	11	0	10	0	0
All	All	20804	0	19622	208	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 5.

The worst 5 of 208 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:G:121:LYS:HE3	2:G:200:VAL:HG21	1.34	1.06
11:KA:1:NAG:O3	11:KA:2:NAG:O5	1.93	0.86
2:G:283:ILE:HD13	2:G:453:ILE:HD13	1.67	0.77
2:G:342:ILE:HD12	2:G:394:VAL:HG21	1.68	0.76
1:B:537:LEU:N	1:C:654:GLU:OE2	2.19	0.75

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	A	130/148 (88%)	125 (96%)	5 (4%)	0	100	100
1	B	131/148 (88%)	124 (95%)	7 (5%)	0	100	100
1	C	131/148 (88%)	124 (95%)	7 (5%)	0	100	100
2	E	492/500 (98%)	445 (90%)	47 (10%)	0	100	100
2	F	492/500 (98%)	445 (90%)	47 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	492/500 (98%)	445 (90%)	46 (9%)	1 (0%)	43	76
3	H	136/244 (56%)	132 (97%)	4 (3%)	0	100	100
4	L	109/219 (50%)	103 (94%)	5 (5%)	1 (1%)	14	48
All	All	2113/2407 (88%)	1943 (92%)	168 (8%)	2 (0%)	49	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	429	LYS
4	L	27(E)	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	112/126 (89%)	111 (99%)	1 (1%)	70	76
1	B	113/126 (90%)	112 (99%)	1 (1%)	70	76
1	C	113/126 (90%)	112 (99%)	1 (1%)	70	76
2	E	444/448 (99%)	442 (100%)	2 (0%)	81	82
2	F	444/448 (99%)	443 (100%)	1 (0%)	87	86
2	G	444/448 (99%)	442 (100%)	2 (0%)	81	82
3	H	113/203 (56%)	113 (100%)	0	100	100
4	L	94/191 (49%)	94 (100%)	0	100	100
All	All	1877/2116 (89%)	1869 (100%)	8 (0%)	81	83

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	301	ASN
2	G	173	ASN
2	E	301	ASN
2	E	173	ASN

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Mol	Chain	Res	Type
2	F	173	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	419	HIS
2	G	202	GLN
4	L	27	HIS
2	G	419	HIS
3	H	62	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	TYS	H	100(F)	3	15,16,17	0.70	0	15,22,24	1.03	0
3	TYS	H	100(I)	3	15,16,17	0.66	0	15,22,24	0.93	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	TYS	H	100(F)	3	-	1/10/11/13	0/1/1/1
3	TYS	H	100(I)	3	-	2/10/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	100(F)	TYS	O-C-CA-CB
3	H	100(I)	TYS	CE1-CZ-OH-S
3	H	100(I)	TYS	CE2-CZ-OH-S

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	100(F)	TYS	2	0

5.5 Carbohydrates

298 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	$\# Z > 2$
7	NAG	0	1	2,7	14,14,15	0.22	0	17,19,21	0.39	0
7	NAG	0	2	7	14,14,15	0.23	0	17,19,21	0.50	0
7	BMA	0	3	7	11,11,12	0.54	0	15,15,17	0.70	0
7	MAN	0	4	7	11,11,12	0.65	0	15,15,17	1.10	2 (13%)
7	MAN	0	5	7	11,11,12	0.76	0	15,15,17	1.21	2 (13%)
6	NAG	1	1	6,2	14,14,15	0.67	1 (7%)	17,19,21	0.82	0
6	NAG	1	2	6	14,14,15	0.25	0	17,19,21	0.72	0
6	BMA	1	3	6	11,11,12	0.55	0	15,15,17	0.68	0
8	NAG	2	1	2,8	14,14,15	0.20	0	17,19,21	0.58	0
8	NAG	2	2	8	14,14,15	0.24	0	17,19,21	0.48	0
8	NAG	3	1	2,8	14,14,15	0.34	0	17,19,21	1.02	1 (5%)
8	NAG	3	2	8	14,14,15	0.22	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	4	1	2,7	14,14,15	0.24	0	17,19,21	0.49	0
7	NAG	4	2	7	14,14,15	0.20	0	17,19,21	0.60	0
7	BMA	4	3	7	11,11,12	0.54	0	15,15,17	0.69	0
7	MAN	4	4	7	11,11,12	0.63	0	15,15,17	0.92	2 (13%)
7	MAN	4	5	7	11,11,12	0.64	0	15,15,17	0.93	2 (13%)
5	NAG	5	1	2,5	14,14,15	0.30	0	17,19,21	0.46	0
5	NAG	5	2	5	14,14,15	0.24	0	17,19,21	0.44	0
5	BMA	5	3	5	11,11,12	0.60	0	15,15,17	0.70	0
5	MAN	5	4	5	11,11,12	0.61	0	15,15,17	0.94	2 (13%)
6	NAG	6	1	6,2	14,14,15	0.21	0	17,19,21	0.44	0
6	NAG	6	2	6	14,14,15	0.20	0	17,19,21	0.48	0
6	BMA	6	3	6	11,11,12	0.54	0	15,15,17	0.70	0
5	NAG	7	1	2,5	14,14,15	0.28	0	17,19,21	0.39	0
5	NAG	7	2	5	14,14,15	0.32	0	17,19,21	0.71	0
5	BMA	7	3	5	11,11,12	0.81	0	15,15,17	0.93	1 (6%)
5	MAN	7	4	5	11,11,12	0.72	1 (9%)	15,15,17	0.94	1 (6%)
8	NAG	8	1	2,8	14,14,15	0.20	0	17,19,21	0.42	0
8	NAG	8	2	8	14,14,15	0.22	0	17,19,21	0.44	0
7	NAG	9	1	2,7	14,14,15	0.18	0	17,19,21	0.41	0
7	NAG	9	2	7	14,14,15	0.20	0	17,19,21	0.44	0
7	BMA	9	3	7	11,11,12	0.55	0	15,15,17	0.72	0
7	MAN	9	4	7	11,11,12	0.60	0	15,15,17	0.96	2 (13%)
7	MAN	9	5	7	11,11,12	0.62	0	15,15,17	0.91	2 (13%)
8	NAG	AA	1	2,8	14,14,15	0.22	0	17,19,21	0.43	0
8	NAG	AA	2	8	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	BA	1	2,5	14,14,15	0.14	0	17,19,21	0.63	0
5	NAG	BA	2	5	14,14,15	0.30	0	17,19,21	0.42	0
5	BMA	BA	3	5	11,11,12	0.56	0	15,15,17	0.74	0
5	MAN	BA	4	5	11,11,12	0.60	0	15,15,17	1.01	2 (13%)
5	NAG	CA	1	2,5	14,14,15	0.22	0	17,19,21	0.44	0
5	NAG	CA	2	5	14,14,15	0.24	0	17,19,21	0.40	0
5	BMA	CA	3	5	11,11,12	0.64	0	15,15,17	0.71	0
5	MAN	CA	4	5	11,11,12	0.62	0	15,15,17	0.93	2 (13%)
5	NAG	D	1	1,5	14,14,15	0.28	0	17,19,21	0.54	0
5	NAG	D	2	5	14,14,15	0.24	0	17,19,21	0.45	0
5	BMA	D	3	5	11,11,12	0.58	0	15,15,17	0.68	0
5	MAN	D	4	5	11,11,12	0.67	0	15,15,17	0.92	1 (6%)
7	NAG	DA	1	2,7	14,14,15	0.28	0	17,19,21	0.39	0
7	NAG	DA	2	7	14,14,15	0.18	0	17,19,21	0.45	0
7	BMA	DA	3	7	11,11,12	0.56	0	15,15,17	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	DA	4	7	11,11,12	0.62	0	15,15,17	0.95	2 (13%)
7	MAN	DA	5	7	11,11,12	0.62	0	15,15,17	0.98	2 (13%)
9	NAG	EA	1	2,9	14,14,15	0.30	0	17,19,21	0.42	0
9	NAG	EA	2	9	14,14,15	0.21	0	17,19,21	0.51	0
9	BMA	EA	3	9	11,11,12	0.75	0	15,15,17	0.83	1 (6%)
9	MAN	EA	4	9	11,11,12	0.61	0	15,15,17	0.96	2 (13%)
9	MAN	EA	5	9	11,11,12	0.62	0	15,15,17	0.89	1 (6%)
9	MAN	EA	6	9	11,11,12	0.61	0	15,15,17	0.96	2 (13%)
12	NAG	FA	1	2,12	14,14,15	0.22	0	17,19,21	0.73	0
12	NAG	FA	2	12	14,14,15	0.23	0	17,19,21	0.45	0
12	BMA	FA	3	12	11,11,12	0.54	0	15,15,17	0.65	0
12	MAN	FA	4	12	11,11,12	0.62	0	15,15,17	1.04	2 (13%)
7	NAG	GA	1	2,7	14,14,15	0.20	0	17,19,21	0.42	0
7	NAG	GA	2	7	14,14,15	0.23	0	17,19,21	0.44	0
7	BMA	GA	3	7	11,11,12	0.54	0	15,15,17	0.69	0
7	MAN	GA	4	7	11,11,12	0.63	0	15,15,17	0.96	2 (13%)
7	MAN	GA	5	7	11,11,12	0.61	0	15,15,17	0.97	2 (13%)
6	NAG	HA	1	6,2	14,14,15	0.39	0	17,19,21	0.50	0
6	NAG	HA	2	6	14,14,15	0.24	0	17,19,21	0.58	0
6	BMA	HA	3	6	11,11,12	0.57	0	15,15,17	0.66	0
5	NAG	I	1	1,5	14,14,15	0.24	0	17,19,21	0.37	0
5	NAG	I	2	5	14,14,15	0.20	0	17,19,21	0.44	0
5	BMA	I	3	5	11,11,12	0.53	0	15,15,17	0.70	0
5	MAN	I	4	5	11,11,12	0.60	0	15,15,17	0.97	2 (13%)
13	NAG	IA	1	2,13	14,14,15	0.19	0	17,19,21	0.46	0
13	NAG	IA	2	13	14,14,15	0.21	0	17,19,21	0.43	0
13	BMA	IA	3	13	11,11,12	0.51	0	15,15,17	0.69	0
13	MAN	IA	4	13	11,11,12	0.60	0	15,15,17	0.96	2 (13%)
13	MAN	IA	5	13	11,11,12	0.62	0	15,15,17	1.09	2 (13%)
13	MAN	IA	6	13	11,11,12	0.63	0	15,15,17	1.02	2 (13%)
13	MAN	IA	7	13	11,11,12	0.61	0	15,15,17	0.95	2 (13%)
6	NAG	J	1	6,1	14,14,15	0.21	0	17,19,21	0.39	0
6	NAG	J	2	6	14,14,15	0.23	0	17,19,21	0.45	0
6	BMA	J	3	6	11,11,12	0.57	0	15,15,17	0.71	0
5	NAG	JA	1	2,5	14,14,15	0.56	0	17,19,21	0.59	0
5	NAG	JA	2	5	14,14,15	0.32	0	17,19,21	0.88	0
5	BMA	JA	3	5	11,11,12	0.58	0	15,15,17	0.59	0
5	MAN	JA	4	5	11,11,12	0.53	0	15,15,17	1.02	2 (13%)
5	NAG	K	1	1,5	14,14,15	0.31	0	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	K	2	5	14,14,15	0.39	0	17,19,21	1.10	1 (5%)
5	BMA	K	3	5	11,11,12	0.65	0	15,15,17	0.78	0
5	MAN	K	4	5	11,11,12	0.65	0	15,15,17	1.08	2 (13%)
11	NAG	KA	1	2,11	14,14,15	0.24	0	17,19,21	0.62	0
11	NAG	KA	2	11	14,14,15	0.27	0	17,19,21	0.50	0
11	BMA	KA	3	11	11,11,12	0.65	0	15,15,17	0.96	0
11	MAN	KA	4	11	11,11,12	0.61	0	15,15,17	1.02	2 (13%)
11	MAN	KA	5	11	11,11,12	0.62	0	15,15,17	0.89	2 (13%)
11	MAN	KA	6	11	11,11,12	0.71	0	15,15,17	0.97	2 (13%)
11	MAN	KA	7	11	11,11,12	0.68	0	15,15,17	0.91	1 (6%)
11	MAN	KA	8	11	11,11,12	0.58	0	15,15,17	1.00	2 (13%)
7	NAG	LA	1	2,7	14,14,15	0.16	0	17,19,21	0.46	0
7	NAG	LA	2	7	14,14,15	0.23	0	17,19,21	0.45	0
7	BMA	LA	3	7	11,11,12	0.53	0	15,15,17	0.70	0
7	MAN	LA	4	7	11,11,12	0.60	0	15,15,17	0.98	2 (13%)
7	MAN	LA	5	7	11,11,12	0.61	0	15,15,17	0.97	2 (13%)
7	NAG	M	1	1,7	14,14,15	0.20	0	17,19,21	0.40	0
7	NAG	M	2	7	14,14,15	0.23	0	17,19,21	0.46	0
7	BMA	M	3	7	11,11,12	0.54	0	15,15,17	0.68	0
7	MAN	M	4	7	11,11,12	0.61	0	15,15,17	0.94	2 (13%)
7	MAN	M	5	7	11,11,12	0.63	0	15,15,17	0.97	2 (13%)
6	NAG	MA	1	6,2	14,14,15	0.69	1 (7%)	17,19,21	0.82	0
6	NAG	MA	2	6	14,14,15	0.23	0	17,19,21	0.67	0
6	BMA	MA	3	6	11,11,12	0.55	0	15,15,17	0.70	0
6	NAG	N	1	6,1	14,14,15	0.21	0	17,19,21	0.39	0
6	NAG	N	2	6	14,14,15	0.22	0	17,19,21	0.44	0
6	BMA	N	3	6	11,11,12	0.56	0	15,15,17	0.70	0
8	NAG	NA	1	2,8	14,14,15	0.20	0	17,19,21	0.59	0
8	NAG	NA	2	8	14,14,15	0.24	0	17,19,21	0.48	0
5	NAG	O	1	1,5	14,14,15	0.23	0	17,19,21	0.51	0
5	NAG	O	2	5	14,14,15	0.41	0	17,19,21	0.51	0
5	BMA	O	3	5	11,11,12	0.57	0	15,15,17	0.68	0
5	MAN	O	4	5	11,11,12	0.63	0	15,15,17	1.09	2 (13%)
8	NAG	OA	1	2,8	14,14,15	0.34	0	17,19,21	0.99	1 (5%)
8	NAG	OA	2	8	14,14,15	0.22	0	17,19,21	0.43	0
7	NAG	P	1	1,7	14,14,15	0.26	0	17,19,21	0.44	0
7	NAG	P	2	7	14,14,15	0.25	0	17,19,21	0.45	0
7	BMA	P	3	7	11,11,12	0.54	0	15,15,17	0.69	0
7	MAN	P	4	7	11,11,12	0.61	0	15,15,17	0.94	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	P	5	7	11,11,12	0.63	0	15,15,17	0.96	2 (13%)
7	NAG	PA	1	2,7	14,14,15	0.35	0	17,19,21	0.98	1 (5%)
7	NAG	PA	2	7	14,14,15	0.18	0	17,19,21	0.57	0
7	BMA	PA	3	7	11,11,12	0.56	0	15,15,17	0.74	0
7	MAN	PA	4	7	11,11,12	0.60	0	15,15,17	0.92	2 (13%)
7	MAN	PA	5	7	11,11,12	0.63	0	15,15,17	1.00	2 (13%)
6	NAG	Q	1	6,1	14,14,15	0.22	0	17,19,21	0.39	0
6	NAG	Q	2	6	14,14,15	0.22	0	17,19,21	0.45	0
6	BMA	Q	3	6	11,11,12	0.56	0	15,15,17	0.70	0
5	NAG	QA	1	2,5	14,14,15	0.26	0	17,19,21	0.40	0
5	NAG	QA	2	5	14,14,15	0.24	0	17,19,21	0.45	0
5	BMA	QA	3	5	11,11,12	0.61	0	15,15,17	0.71	0
5	MAN	QA	4	5	11,11,12	0.62	0	15,15,17	0.95	2 (13%)
6	NAG	R	1	6,2	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	R	2	6	14,14,15	0.21	0	17,19,21	0.56	0
6	BMA	R	3	6	11,11,12	0.64	0	15,15,17	0.72	0
6	NAG	RA	1	6,2	14,14,15	0.23	0	17,19,21	0.56	0
6	NAG	RA	2	6	14,14,15	0.26	0	17,19,21	0.47	0
6	BMA	RA	3	6	11,11,12	0.61	0	15,15,17	0.73	0
8	NAG	S	1	2,8	14,14,15	0.21	0	17,19,21	0.43	0
8	NAG	S	2	8	14,14,15	0.22	0	17,19,21	0.43	0
7	NAG	T	1	2,7	14,14,15	0.20	0	17,19,21	0.51	0
7	NAG	T	2	7	14,14,15	0.20	0	17,19,21	0.43	0
7	BMA	T	3	7	11,11,12	0.57	0	15,15,17	0.76	0
7	MAN	T	4	7	11,11,12	0.59	0	15,15,17	0.94	2 (13%)
7	MAN	T	5	7	11,11,12	0.61	0	15,15,17	0.91	2 (13%)
6	NAG	U	1	6,2	14,14,15	0.24	0	17,19,21	0.45	0
6	NAG	U	2	6	14,14,15	0.23	0	17,19,21	0.42	0
6	BMA	U	3	6	11,11,12	0.56	0	15,15,17	0.70	0
5	NAG	V	1	2,5	14,14,15	0.15	0	17,19,21	0.62	0
5	NAG	V	2	5	14,14,15	0.24	0	17,19,21	0.45	0
5	BMA	V	3	5	11,11,12	0.60	0	15,15,17	0.74	0
5	MAN	V	4	5	11,11,12	0.61	0	15,15,17	1.00	2 (13%)
5	NAG	W	1	2,5	14,14,15	0.21	0	17,19,21	0.45	0
5	NAG	W	2	5	14,14,15	0.24	0	17,19,21	0.42	0
5	BMA	W	3	5	11,11,12	0.66	0	15,15,17	0.70	0
5	MAN	W	4	5	11,11,12	0.63	0	15,15,17	0.94	2 (13%)
7	NAG	X	1	2,7	14,14,15	0.20	0	17,19,21	0.44	0
7	NAG	X	2	7	14,14,15	0.19	0	17,19,21	0.40	0
7	BMA	X	3	7	11,11,12	0.59	0	15,15,17	0.69	0
7	MAN	X	4	7	11,11,12	0.61	0	15,15,17	0.95	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	X	5	7	11,11,12	0.64	0	15,15,17	0.97	2 (13%)
9	NAG	Y	1	2,9	14,14,15	0.29	0	17,19,21	0.47	0
9	NAG	Y	2	9	14,14,15	0.23	0	17,19,21	0.53	0
9	BMA	Y	3	9	11,11,12	0.72	0	15,15,17	0.82	0
9	MAN	Y	4	9	11,11,12	0.64	0	15,15,17	0.95	2 (13%)
9	MAN	Y	5	9	11,11,12	0.61	0	15,15,17	0.90	2 (13%)
9	MAN	Y	6	9	11,11,12	0.61	0	15,15,17	0.94	2 (13%)
6	NAG	Z	1	6,2	14,14,15	0.26	0	17,19,21	0.52	0
6	NAG	Z	2	6	14,14,15	0.27	0	17,19,21	1.04	1 (5%)
6	BMA	Z	3	6	11,11,12	0.54	0	15,15,17	0.72	0
7	NAG	a	1	2,7	14,14,15	0.19	0	17,19,21	0.45	0
7	NAG	a	2	7	14,14,15	0.22	0	17,19,21	0.44	0
7	BMA	a	3	7	11,11,12	0.53	0	15,15,17	0.70	0
7	MAN	a	4	7	11,11,12	0.61	0	15,15,17	0.96	2 (13%)
7	MAN	a	5	7	11,11,12	0.61	0	15,15,17	0.98	2 (13%)
6	NAG	b	1	6,2	14,14,15	0.38	0	17,19,21	0.52	0
6	NAG	b	2	6	14,14,15	0.22	0	17,19,21	0.55	0
6	BMA	b	3	6	11,11,12	0.56	0	15,15,17	0.67	0
10	NAG	c	1	2,10	14,14,15	0.29	0	17,19,21	0.48	0
10	NAG	c	2	10	14,14,15	0.23	0	17,19,21	0.40	0
10	BMA	c	3	10	11,11,12	0.50	0	15,15,17	0.74	0
10	MAN	c	4	10	11,11,12	0.49	0	15,15,17	0.92	2 (13%)
10	MAN	c	5	10	11,11,12	1.46	3 (27%)	15,15,17	1.10	1 (6%)
10	MAN	c	6	10	11,11,12	0.62	0	15,15,17	0.87	1 (6%)
10	MAN	c	7	10	11,11,12	0.55	0	15,15,17	0.97	2 (13%)
10	MAN	c	8	10	11,11,12	0.58	0	15,15,17	0.91	2 (13%)
5	NAG	d	1	2,5	14,14,15	1.03	1 (7%)	17,19,21	0.95	1 (5%)
5	NAG	d	2	5	14,14,15	0.31	0	17,19,21	0.44	0
5	BMA	d	3	5	11,11,12	0.53	0	15,15,17	0.80	0
5	MAN	d	4	5	11,11,12	0.55	0	15,15,17	0.96	2 (13%)
11	NAG	e	1	2,11	14,14,15	0.20	0	17,19,21	0.40	0
11	NAG	e	2	11	14,14,15	0.24	0	17,19,21	0.42	0
11	BMA	e	3	11	11,11,12	0.66	0	15,15,17	1.00	0
11	MAN	e	4	11	11,11,12	0.61	0	15,15,17	0.97	2 (13%)
11	MAN	e	5	11	11,11,12	0.62	0	15,15,17	0.90	1 (6%)
11	MAN	e	6	11	11,11,12	0.63	0	15,15,17	0.94	2 (13%)
11	MAN	e	7	11	11,11,12	0.66	0	15,15,17	0.90	1 (6%)
11	MAN	e	8	11	11,11,12	0.61	0	15,15,17	0.93	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	f	1	2,11	14,14,15	0.39	0	17,19,21	0.86	0
11	NAG	f	2	11	14,14,15	0.40	0	17,19,21	0.60	0
11	BMA	f	3	11	11,11,12	0.54	0	15,15,17	0.99	1 (6%)
11	MAN	f	4	11	11,11,12	0.52	0	15,15,17	0.53	0
11	MAN	f	5	11	11,11,12	0.36	0	15,15,17	0.47	0
11	MAN	f	6	11	11,11,12	0.41	0	15,15,17	0.62	0
11	MAN	f	7	11	11,11,12	0.39	0	15,15,17	0.50	0
11	MAN	f	8	11	11,11,12	0.29	0	15,15,17	0.53	0
5	NAG	g	1	2,5	14,14,15	0.27	0	17,19,21	0.43	0
5	NAG	g	2	5	14,14,15	0.20	0	17,19,21	0.45	0
5	BMA	g	3	5	11,11,12	0.61	0	15,15,17	0.89	0
5	MAN	g	4	5	11,11,12	0.63	0	15,15,17	0.92	2 (13%)
8	NAG	h	1	2,8	14,14,15	0.36	0	17,19,21	0.65	0
8	NAG	h	2	8	14,14,15	0.23	0	17,19,21	0.41	0
8	NAG	i	1	2,8	14,14,15	0.35	0	17,19,21	1.02	1 (5%)
8	NAG	i	2	8	14,14,15	0.24	0	17,19,21	0.45	0
7	NAG	j	1	2,7	14,14,15	0.29	0	17,19,21	0.43	0
7	NAG	j	2	7	14,14,15	0.24	0	17,19,21	0.62	0
7	BMA	j	3	7	11,11,12	0.92	0	15,15,17	0.82	0
7	MAN	j	4	7	11,11,12	0.62	0	15,15,17	0.97	2 (13%)
7	MAN	j	5	7	11,11,12	0.67	0	15,15,17	0.94	2 (13%)
6	NAG	k	1	6,2	14,14,15	0.25	0	17,19,21	0.47	0
6	NAG	k	2	6	14,14,15	0.20	0	17,19,21	0.43	0
6	BMA	k	3	6	11,11,12	0.58	0	15,15,17	0.69	0
6	NAG	l	1	6,2	14,14,15	0.21	0	17,19,21	0.63	0
6	NAG	l	2	6	14,14,15	0.26	0	17,19,21	0.47	0
6	BMA	l	3	6	11,11,12	0.58	0	15,15,17	0.78	0
5	NAG	m	1	2,5	14,14,15	0.19	0	17,19,21	0.43	0
5	NAG	m	2	5	14,14,15	0.19	0	17,19,21	0.58	0
5	BMA	m	3	5	11,11,12	0.57	0	15,15,17	0.70	0
5	MAN	m	4	5	11,11,12	0.62	0	15,15,17	1.11	2 (13%)
8	NAG	n	1	2,8	14,14,15	0.21	0	17,19,21	0.44	0
8	NAG	n	2	8	14,14,15	0.24	0	17,19,21	0.44	0
7	NAG	o	1	2,7	14,14,15	0.23	0	17,19,21	0.43	0
7	NAG	o	2	7	14,14,15	0.23	0	17,19,21	0.43	0
7	BMA	o	3	7	11,11,12	0.56	0	15,15,17	0.74	0
7	MAN	o	4	7	11,11,12	0.59	0	15,15,17	0.94	2 (13%)
7	MAN	o	5	7	11,11,12	0.60	0	15,15,17	0.91	2 (13%)
8	NAG	p	1	2,8	14,14,15	0.22	0	17,19,21	0.45	0
8	NAG	p	2	8	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	q	1	2,5	14,14,15	0.17	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	q	2	5	14,14,15	0.19	0	17,19,21	0.47	0
5	BMA	q	3	5	11,11,12	0.60	0	15,15,17	0.77	0
5	MAN	q	4	5	11,11,12	0.61	0	15,15,17	1.02	2 (13%)
5	NAG	r	1	2,5	14,14,15	0.18	0	17,19,21	0.51	0
5	NAG	r	2	5	14,14,15	0.24	0	17,19,21	0.41	0
5	BMA	r	3	5	11,11,12	0.68	0	15,15,17	0.71	0
5	MAN	r	4	5	11,11,12	0.62	0	15,15,17	0.94	2 (13%)
7	NAG	s	1	2,7	14,14,15	0.21	0	17,19,21	0.37	0
7	NAG	s	2	7	14,14,15	0.17	0	17,19,21	0.41	0
7	BMA	s	3	7	11,11,12	0.53	0	15,15,17	0.69	0
7	MAN	s	4	7	11,11,12	0.60	0	15,15,17	0.94	2 (13%)
7	MAN	s	5	7	11,11,12	0.62	0	15,15,17	0.98	2 (13%)
9	NAG	t	1	2,9	14,14,15	0.20	0	17,19,21	0.45	0
9	NAG	t	2	9	14,14,15	0.26	0	17,19,21	0.55	0
9	BMA	t	3	9	11,11,12	0.71	0	15,15,17	0.81	1 (6%)
9	MAN	t	4	9	11,11,12	0.63	0	15,15,17	0.93	1 (6%)
9	MAN	t	5	9	11,11,12	0.60	0	15,15,17	0.89	1 (6%)
9	MAN	t	6	9	11,11,12	0.61	0	15,15,17	0.95	2 (13%)
12	NAG	u	1	2,12	14,14,15	0.33	0	17,19,21	0.74	0
12	NAG	u	2	12	14,14,15	0.24	0	17,19,21	0.45	0
12	BMA	u	3	12	11,11,12	0.54	0	15,15,17	0.70	0
12	MAN	u	4	12	11,11,12	0.62	0	15,15,17	1.03	2 (13%)
7	NAG	v	1	2,7	14,14,15	0.20	0	17,19,21	0.41	0
7	NAG	v	2	7	14,14,15	0.22	0	17,19,21	0.43	0
7	BMA	v	3	7	11,11,12	0.53	0	15,15,17	0.70	0
7	MAN	v	4	7	11,11,12	0.61	0	15,15,17	0.97	2 (13%)
7	MAN	v	5	7	11,11,12	0.62	0	15,15,17	0.97	2 (13%)
6	NAG	w	1	6,2	14,14,15	0.36	0	17,19,21	0.52	0
6	NAG	w	2	6	14,14,15	0.24	0	17,19,21	0.56	0
6	BMA	w	3	6	11,11,12	0.56	0	15,15,17	0.68	0
13	NAG	x	1	2,13	14,14,15	0.21	0	17,19,21	0.48	0
13	NAG	x	2	13	14,14,15	0.26	0	17,19,21	0.39	0
13	BMA	x	3	13	11,11,12	0.55	0	15,15,17	0.72	0
13	MAN	x	4	13	11,11,12	0.63	0	15,15,17	1.00	2 (13%)
13	MAN	x	5	13	11,11,12	0.65	0	15,15,17	1.12	2 (13%)
13	MAN	x	6	13	11,11,12	0.58	0	15,15,17	0.97	2 (13%)
13	MAN	x	7	13	11,11,12	0.58	0	15,15,17	0.96	2 (13%)
5	NAG	y	1	2,5	14,14,15	1.13	1 (7%)	17,19,21	0.96	1 (5%)
5	NAG	y	2	5	14,14,15	0.27	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	y	3	5	11,11,12	0.51	0	15,15,17	0.64	0
5	MAN	y	4	5	11,11,12	0.63	0	15,15,17	0.91	1 (6%)
14	NAG	z	1	2,14	14,14,15	0.16	0	17,19,21	0.48	0
14	NAG	z	2	14	14,14,15	0.22	0	17,19,21	0.46	0
14	BMA	z	3	14	11,11,12	0.63	0	15,15,17	0.78	0
14	MAN	z	4	14	11,11,12	0.61	0	15,15,17	0.98	2 (13%)
14	MAN	z	5	14	11,11,12	0.63	0	15,15,17	0.90	2 (13%)
14	MAN	z	6	14	11,11,12	0.63	0	15,15,17	0.92	1 (6%)
14	MAN	z	7	14	11,11,12	0.68	0	15,15,17	0.93	1 (6%)

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
7	NAG	0	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	0	2	7	-	2/6/23/26	0/1/1/1
7	BMA	0	3	7	-	2/2/19/22	0/1/1/1
7	MAN	0	4	7	-	0/2/19/22	1/1/1/1
7	MAN	0	5	7	-	1/2/19/22	1/1/1/1
6	NAG	1	1	6,2	-	4/6/23/26	0/1/1/1
6	NAG	1	2	6	-	4/6/23/26	0/1/1/1
6	BMA	1	3	6	-	1/2/19/22	0/1/1/1
8	NAG	2	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	2	2	8	-	2/6/23/26	0/1/1/1
8	NAG	3	1	2,8	-	3/6/23/26	0/1/1/1
8	NAG	3	2	8	-	1/6/23/26	0/1/1/1
7	NAG	4	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	4	2	7	-	4/6/23/26	0/1/1/1
7	BMA	4	3	7	-	2/2/19/22	0/1/1/1
7	MAN	4	4	7	-	0/2/19/22	0/1/1/1
7	MAN	4	5	7	-	0/2/19/22	0/1/1/1
5	NAG	5	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	5	2	5	-	0/6/23/26	0/1/1/1
5	BMA	5	3	5	-	0/2/19/22	0/1/1/1
5	MAN	5	4	5	-	0/2/19/22	0/1/1/1
6	NAG	6	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	6	2	6	-	0/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BMA	FA	3	12	-	1/2/19/22	0/1/1/1
12	MAN	FA	4	12	-	1/2/19/22	1/1/1/1
7	NAG	GA	1	2,7	-	4/6/23/26	0/1/1/1
7	NAG	GA	2	7	-	0/6/23/26	0/1/1/1
7	BMA	GA	3	7	-	0/2/19/22	0/1/1/1
7	MAN	GA	4	7	-	0/2/19/22	0/1/1/1
7	MAN	GA	5	7	-	1/2/19/22	0/1/1/1
6	NAG	HA	1	6,2	-	1/6/23/26	0/1/1/1
6	NAG	HA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	HA	3	6	-	0/2/19/22	0/1/1/1
5	NAG	I	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
5	MAN	I	4	5	-	0/2/19/22	0/1/1/1
13	NAG	IA	1	2,13	-	1/6/23/26	0/1/1/1
13	NAG	IA	2	13	-	1/6/23/26	0/1/1/1
13	BMA	IA	3	13	-	0/2/19/22	0/1/1/1
13	MAN	IA	4	13	-	0/2/19/22	0/1/1/1
13	MAN	IA	5	13	-	0/2/19/22	1/1/1/1
13	MAN	IA	6	13	-	0/2/19/22	0/1/1/1
13	MAN	IA	7	13	-	0/2/19/22	0/1/1/1
6	NAG	J	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	1/6/23/26	0/1/1/1
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1
5	NAG	JA	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	JA	2	5	-	2/6/23/26	0/1/1/1
5	BMA	JA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	JA	4	5	-	1/2/19/22	0/1/1/1
5	NAG	K	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	K	2	5	-	6/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	MAN	K	4	5	-	2/2/19/22	0/1/1/1
11	NAG	KA	1	2,11	-	3/6/23/26	0/1/1/1
11	NAG	KA	2	11	-	2/6/23/26	0/1/1/1
11	BMA	KA	3	11	-	0/2/19/22	0/1/1/1
11	MAN	KA	4	11	-	0/2/19/22	0/1/1/1
11	MAN	KA	5	11	-	0/2/19/22	0/1/1/1
11	MAN	KA	6	11	-	1/2/19/22	0/1/1/1
11	MAN	KA	7	11	-	0/2/19/22	0/1/1/1
11	MAN	KA	8	11	-	0/2/19/22	0/1/1/1

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	Z	2	6	-	4/6/23/26	0/1/1/1
6	BMA	Z	3	6	-	0/2/19/22	0/1/1/1
7	NAG	a	1	2,7	-	4/6/23/26	0/1/1/1
7	NAG	a	2	7	-	0/6/23/26	0/1/1/1
7	BMA	a	3	7	-	0/2/19/22	0/1/1/1
7	MAN	a	4	7	-	0/2/19/22	0/1/1/1
7	MAN	a	5	7	-	1/2/19/22	0/1/1/1
6	NAG	b	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	b	2	6	-	0/6/23/26	0/1/1/1
6	BMA	b	3	6	-	0/2/19/22	0/1/1/1
10	NAG	c	1	2,10	-	2/6/23/26	0/1/1/1
10	NAG	c	2	10	-	0/6/23/26	0/1/1/1
10	BMA	c	3	10	-	0/2/19/22	0/1/1/1
10	MAN	c	4	10	-	0/2/19/22	0/1/1/1
10	MAN	c	5	10	-	2/2/19/22	0/1/1/1
10	MAN	c	6	10	-	1/2/19/22	0/1/1/1
10	MAN	c	7	10	-	2/2/19/22	0/1/1/1
10	MAN	c	8	10	-	0/2/19/22	0/1/1/1
5	NAG	d	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	d	2	5	-	1/6/23/26	0/1/1/1
5	BMA	d	3	5	-	0/2/19/22	0/1/1/1
5	MAN	d	4	5	-	1/2/19/22	0/1/1/1
11	NAG	e	1	2,11	-	2/6/23/26	0/1/1/1
11	NAG	e	2	11	-	4/6/23/26	0/1/1/1
11	BMA	e	3	11	-	0/2/19/22	0/1/1/1
11	MAN	e	4	11	-	0/2/19/22	0/1/1/1
11	MAN	e	5	11	-	0/2/19/22	0/1/1/1
11	MAN	e	6	11	-	1/2/19/22	0/1/1/1
11	MAN	e	7	11	-	0/2/19/22	0/1/1/1
11	MAN	e	8	11	-	0/2/19/22	0/1/1/1
11	NAG	f	1	2,11	-	1/6/23/26	0/1/1/1
11	NAG	f	2	11	-	1/6/23/26	0/1/1/1
11	BMA	f	3	11	-	0/2/19/22	0/1/1/1
11	MAN	f	4	11	-	0/2/19/22	0/1/1/1
11	MAN	f	5	11	-	0/2/19/22	0/1/1/1
11	MAN	f	6	11	-	0/2/19/22	0/1/1/1
11	MAN	f	7	11	-	0/2/19/22	0/1/1/1
11	MAN	f	8	11	-	0/2/19/22	0/1/1/1
5	NAG	g	1	2,5	-	4/6/23/26	0/1/1/1
5	NAG	g	2	5	-	2/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	s	2	7	-	1/6/23/26	0/1/1/1
7	BMA	s	3	7	-	0/2/19/22	0/1/1/1
7	MAN	s	4	7	-	0/2/19/22	0/1/1/1
7	MAN	s	5	7	-	0/2/19/22	0/1/1/1
9	NAG	t	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	t	2	9	-	0/6/23/26	0/1/1/1
9	BMA	t	3	9	-	0/2/19/22	0/1/1/1
9	MAN	t	4	9	-	0/2/19/22	0/1/1/1
9	MAN	t	5	9	-	1/2/19/22	0/1/1/1
9	MAN	t	6	9	-	0/2/19/22	0/1/1/1
12	NAG	u	1	2,12	-	2/6/23/26	0/1/1/1
12	NAG	u	2	12	-	0/6/23/26	0/1/1/1
12	BMA	u	3	12	-	1/2/19/22	0/1/1/1
12	MAN	u	4	12	-	1/2/19/22	1/1/1/1
7	NAG	v	1	2,7	-	4/6/23/26	0/1/1/1
7	NAG	v	2	7	-	0/6/23/26	0/1/1/1
7	BMA	v	3	7	-	0/2/19/22	0/1/1/1
7	MAN	v	4	7	-	0/2/19/22	0/1/1/1
7	MAN	v	5	7	-	1/2/19/22	0/1/1/1
6	NAG	w	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	w	2	6	-	0/6/23/26	0/1/1/1
6	BMA	w	3	6	-	0/2/19/22	0/1/1/1
13	NAG	x	1	2,13	-	1/6/23/26	0/1/1/1
13	NAG	x	2	13	-	2/6/23/26	0/1/1/1
13	BMA	x	3	13	-	0/2/19/22	0/1/1/1
13	MAN	x	4	13	-	0/2/19/22	0/1/1/1
13	MAN	x	5	13	-	0/2/19/22	1/1/1/1
13	MAN	x	6	13	-	2/2/19/22	0/1/1/1
13	MAN	x	7	13	-	0/2/19/22	0/1/1/1
5	NAG	y	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	y	2	5	-	2/6/23/26	0/1/1/1
5	BMA	y	3	5	-	0/2/19/22	0/1/1/1
5	MAN	y	4	5	-	1/2/19/22	0/1/1/1
14	NAG	z	1	2,14	-	4/6/23/26	0/1/1/1
14	NAG	z	2	14	-	2/6/23/26	0/1/1/1
14	BMA	z	3	14	-	0/2/19/22	0/1/1/1
14	MAN	z	4	14	-	0/2/19/22	0/1/1/1
14	MAN	z	5	14	-	0/2/19/22	0/1/1/1
14	MAN	z	6	14	-	1/2/19/22	0/1/1/1
14	MAN	z	7	14	-	0/2/19/22	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	y	1	NAG	O5-C1	-3.88	1.37	1.43
10	c	5	MAN	C2-C3	3.45	1.57	1.52
5	d	1	NAG	O5-C1	-3.38	1.38	1.43
6	MA	1	NAG	O5-C1	-2.44	1.39	1.43
6	1	1	NAG	O5-C1	-2.39	1.39	1.43

The worst 5 of 175 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	0	5	MAN	C1-O5-C5	3.69	117.13	112.19
5	K	2	NAG	C2-N2-C7	3.40	127.46	122.90
6	Z	2	NAG	C2-N2-C7	3.40	127.46	122.90
13	x	5	MAN	C1-O5-C5	3.31	116.62	112.19
5	m	4	MAN	C1-O5-C5	3.28	116.59	112.19

There are no chirality outliers.

5 of 298 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	g	1	NAG	C1-C2-N2-C7
5	g	2	NAG	C1-C2-N2-C7
7	PA	1	NAG	C1-C2-N2-C7
8	i	1	NAG	C1-C2-N2-C7
8	3	1	NAG	C1-C2-N2-C7

5 of 8 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	j	5	MAN	C1-C2-C3-C4-C5-O5
12	u	4	MAN	C1-C2-C3-C4-C5-O5
12	FA	4	MAN	C1-C2-C3-C4-C5-O5
7	0	4	MAN	C1-C2-C3-C4-C5-O5
7	0	5	MAN	C1-C2-C3-C4-C5-O5

49 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	f	5	MAN	1	0
11	f	7	MAN	1	0
8	S	2	NAG	1	0
8	2	1	NAG	2	0

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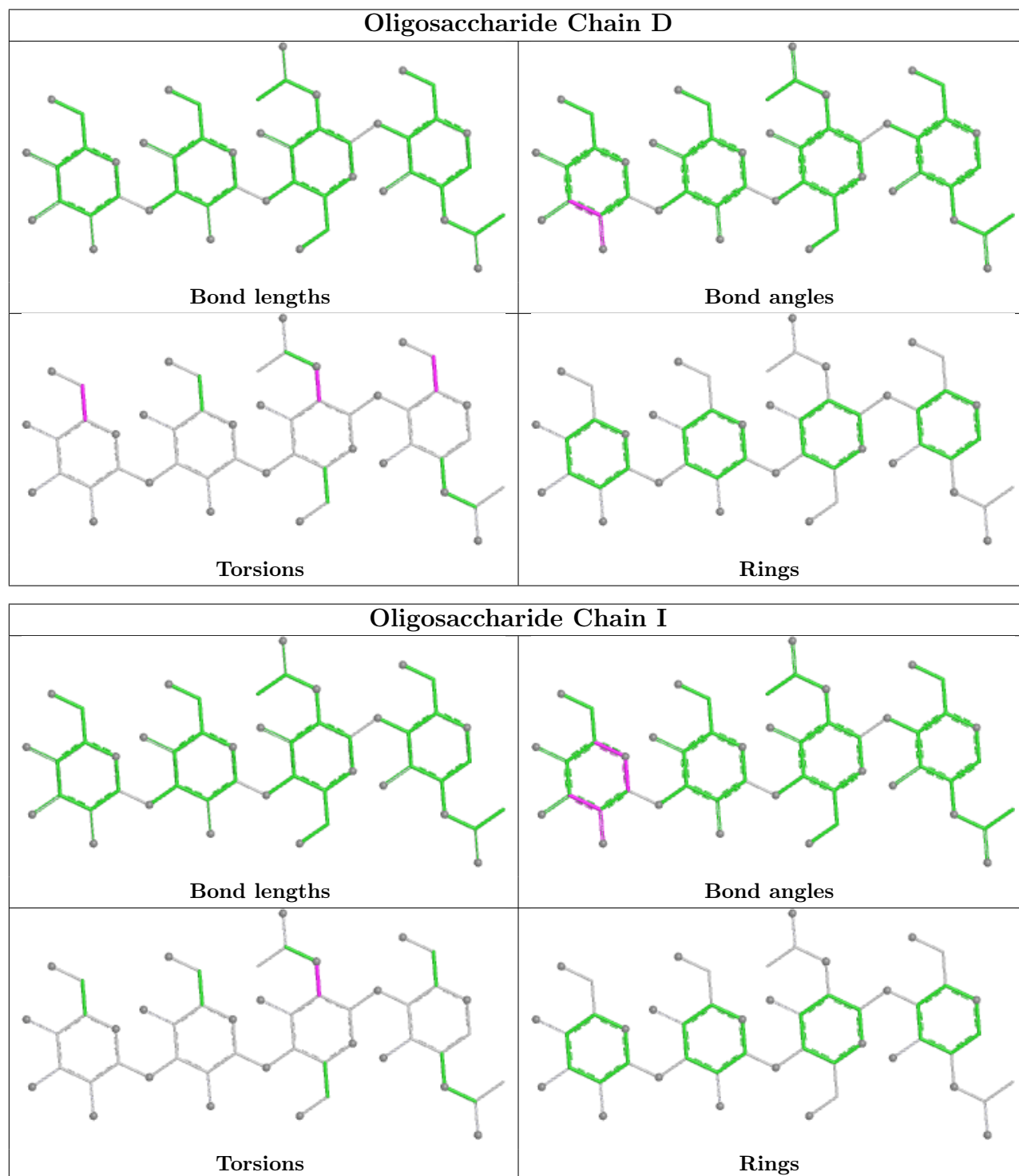
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	BA	2	NAG	1	0
8	NA	2	NAG	1	0
7	o	3	BMA	1	0
8	2	2	NAG	1	0
11	KA	3	BMA	1	0
11	e	1	NAG	1	0
11	f	6	MAN	1	0
7	s	1	NAG	1	0
8	NA	1	NAG	2	0
7	T	2	NAG	1	0
11	f	3	BMA	1	0
7	PA	4	MAN	1	0
7	X	1	NAG	1	0
6	k	2	NAG	1	0
5	K	2	NAG	1	0
7	o	2	NAG	1	0
7	DA	1	NAG	1	0
14	z	1	NAG	1	0
11	f	8	MAN	1	0
11	e	2	NAG	1	0
10	c	1	NAG	3	0
7	T	3	BMA	1	0
6	l	1	NAG	1	0
8	OA	1	NAG	2	0
5	W	1	NAG	1	0
5	JA	1	NAG	1	0
8	i	1	NAG	2	0
8	S	1	NAG	1	0
14	z	2	NAG	1	0
11	KA	2	NAG	3	0
7	j	1	NAG	1	0
7	o	1	NAG	1	0
5	JA	3	BMA	1	0
5	JA	2	NAG	1	0
8	3	1	NAG	2	0
6	HA	1	NAG	1	0
7	PA	1	NAG	3	0
11	KA	1	NAG	3	0
6	Z	2	NAG	1	0
7	9	2	NAG	1	0
7	9	3	BMA	1	0
6	k	3	BMA	1	0

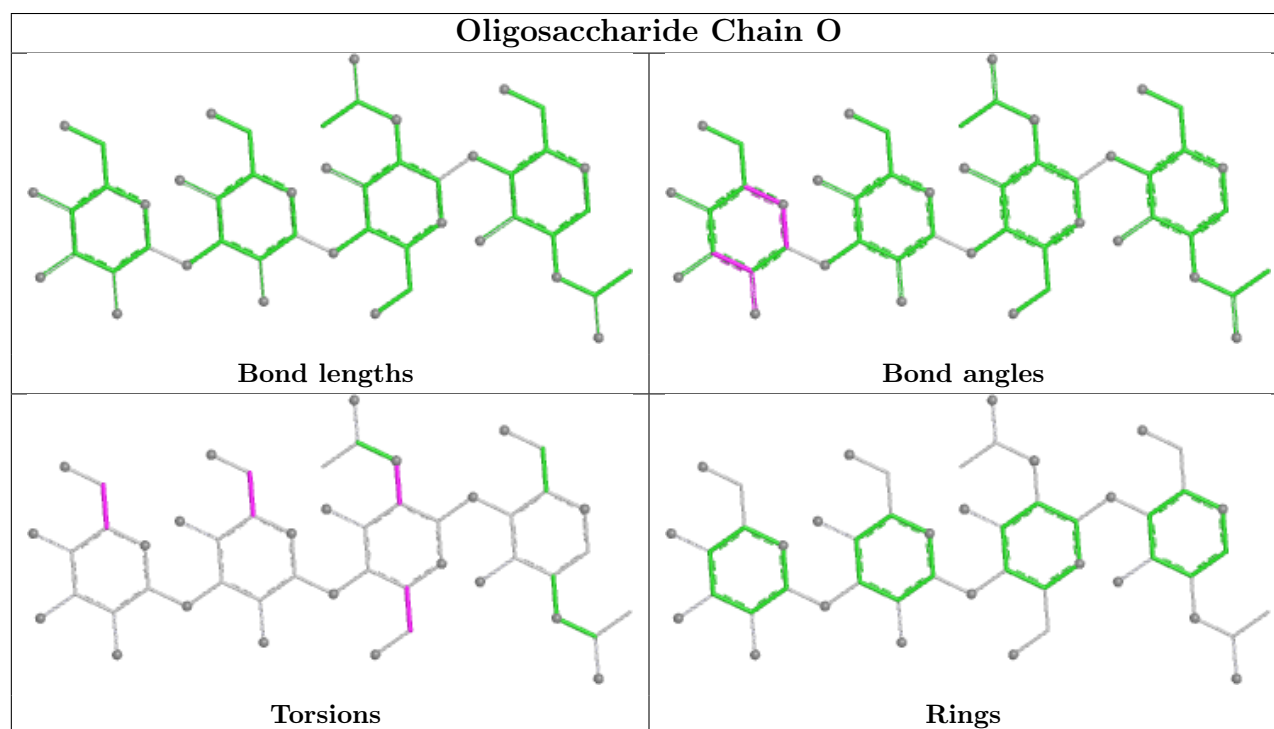
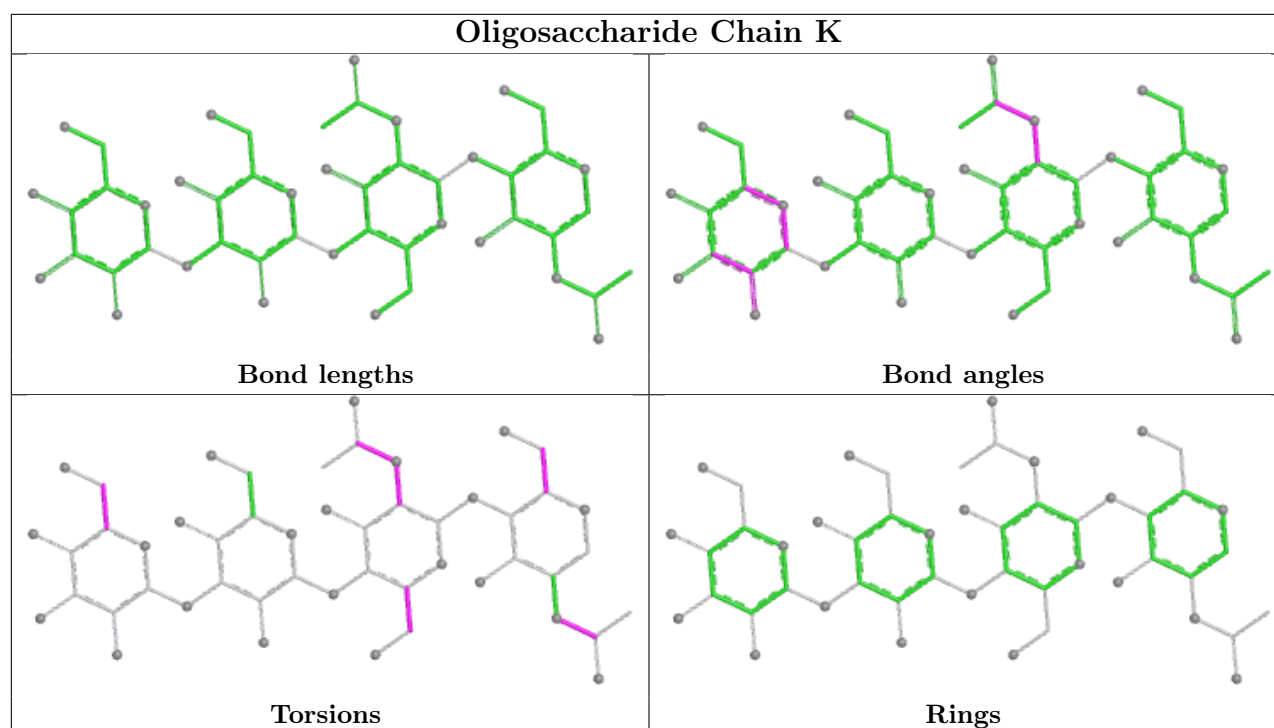
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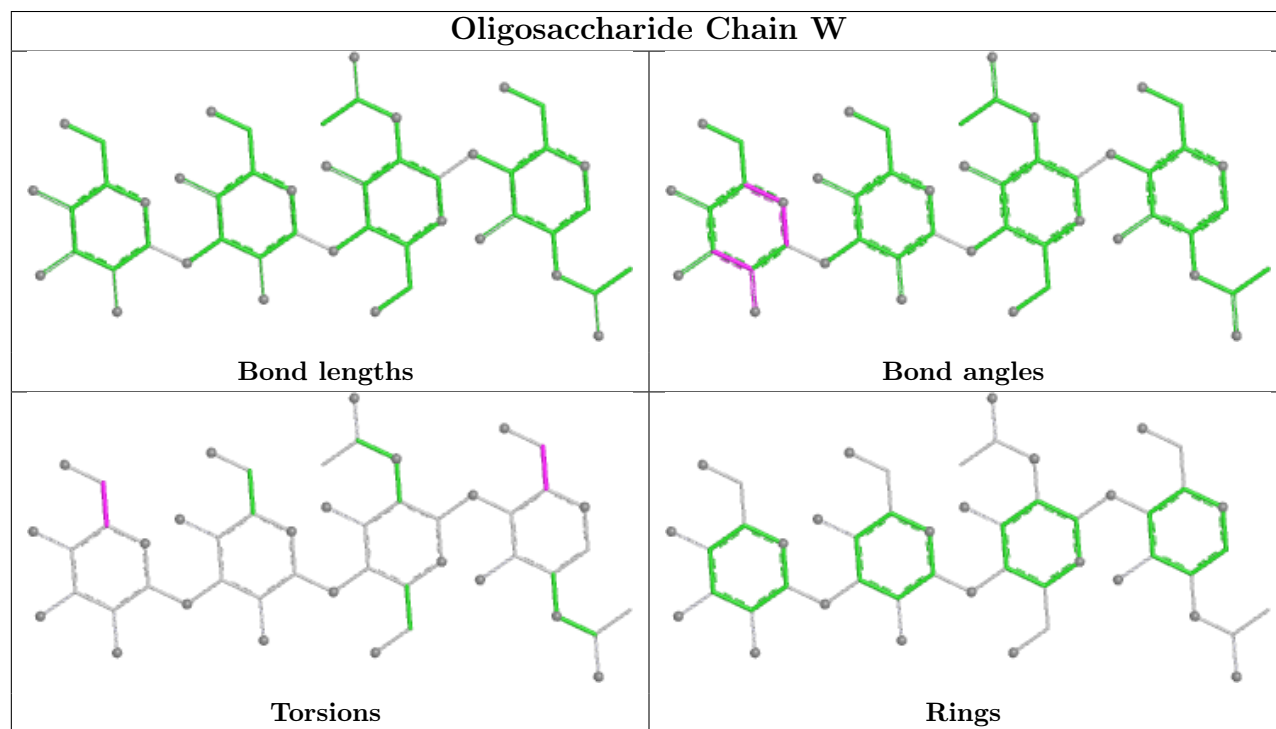
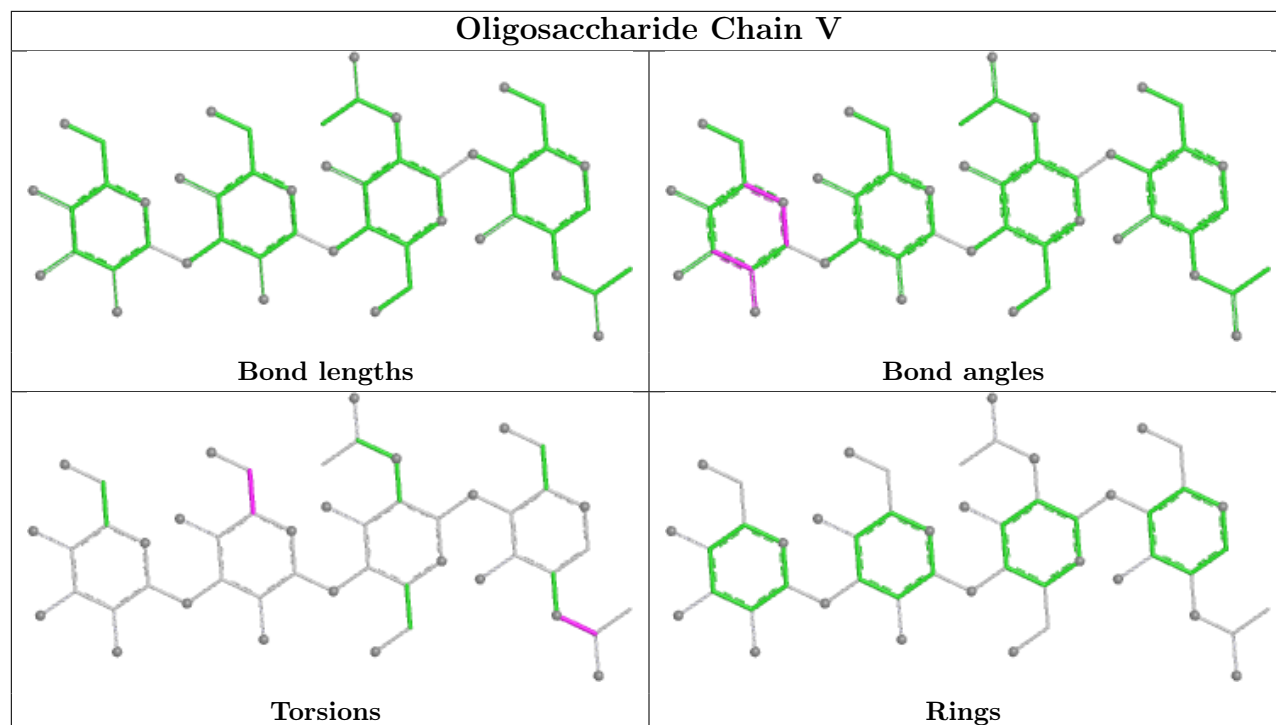
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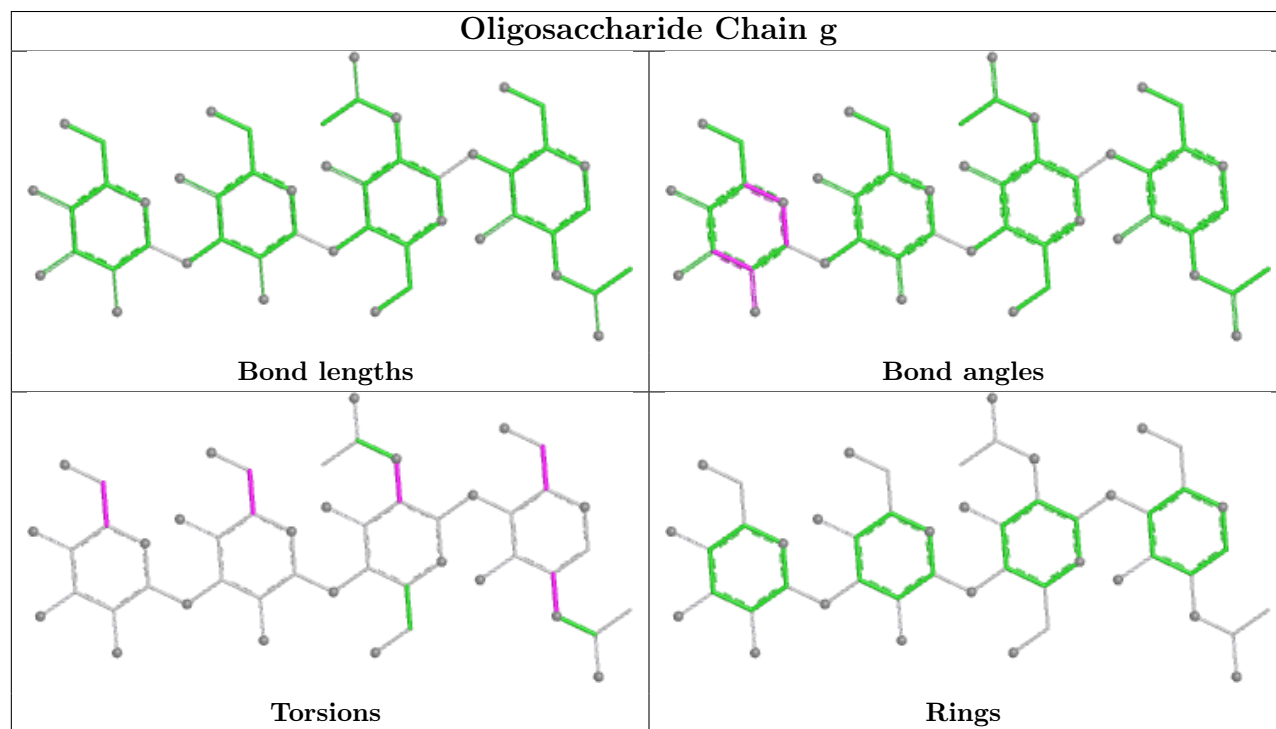
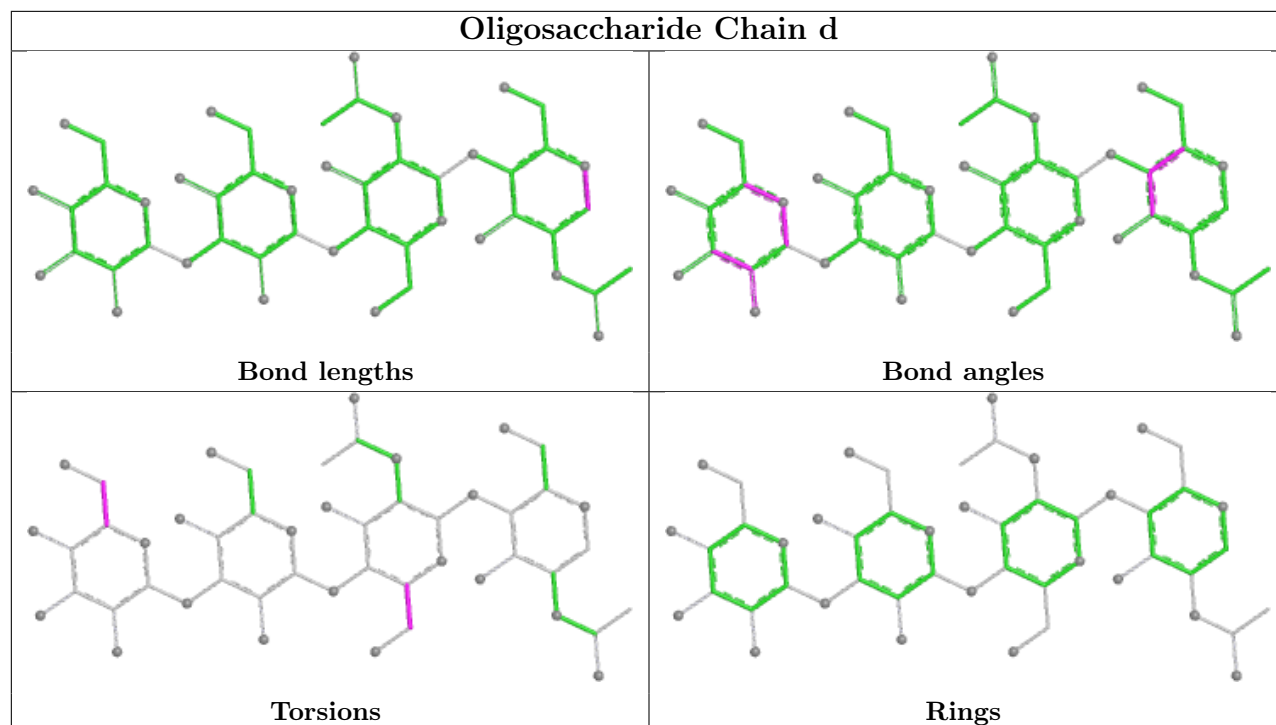
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	1	NAG	1	0
7	PA	2	NAG	1	0
6	1	2	NAG	1	0

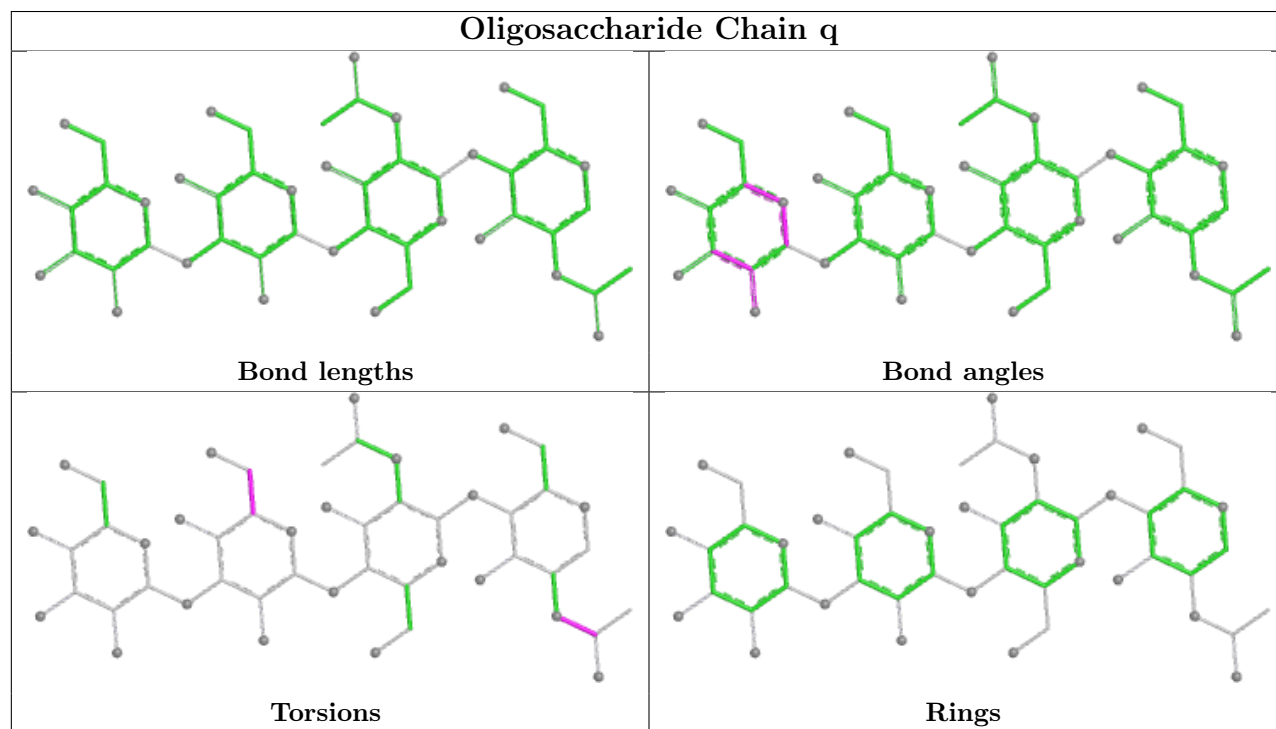
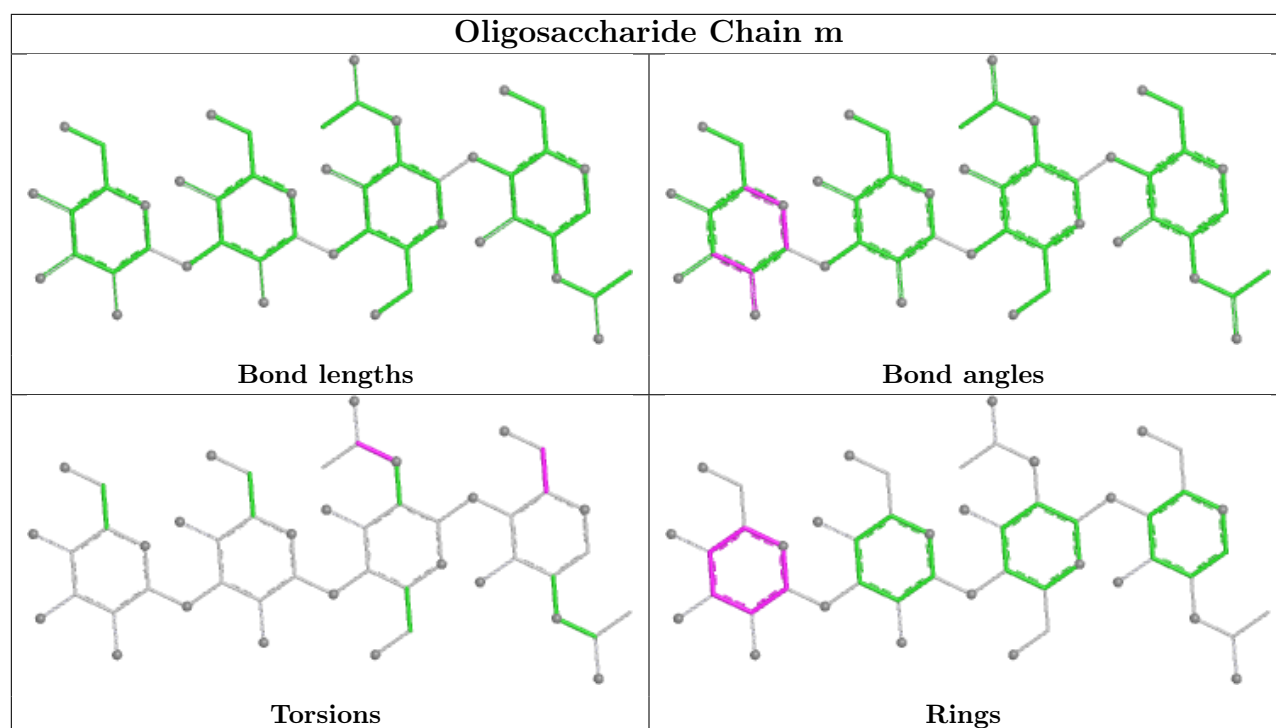
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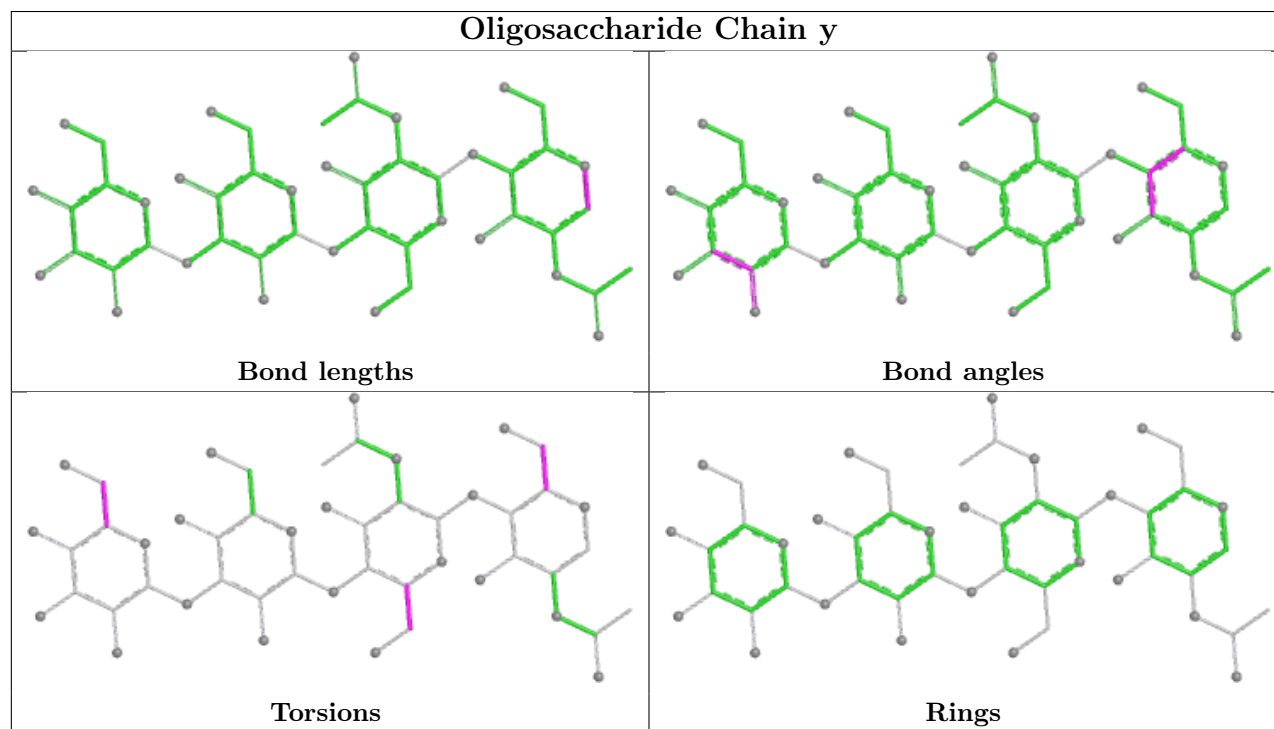
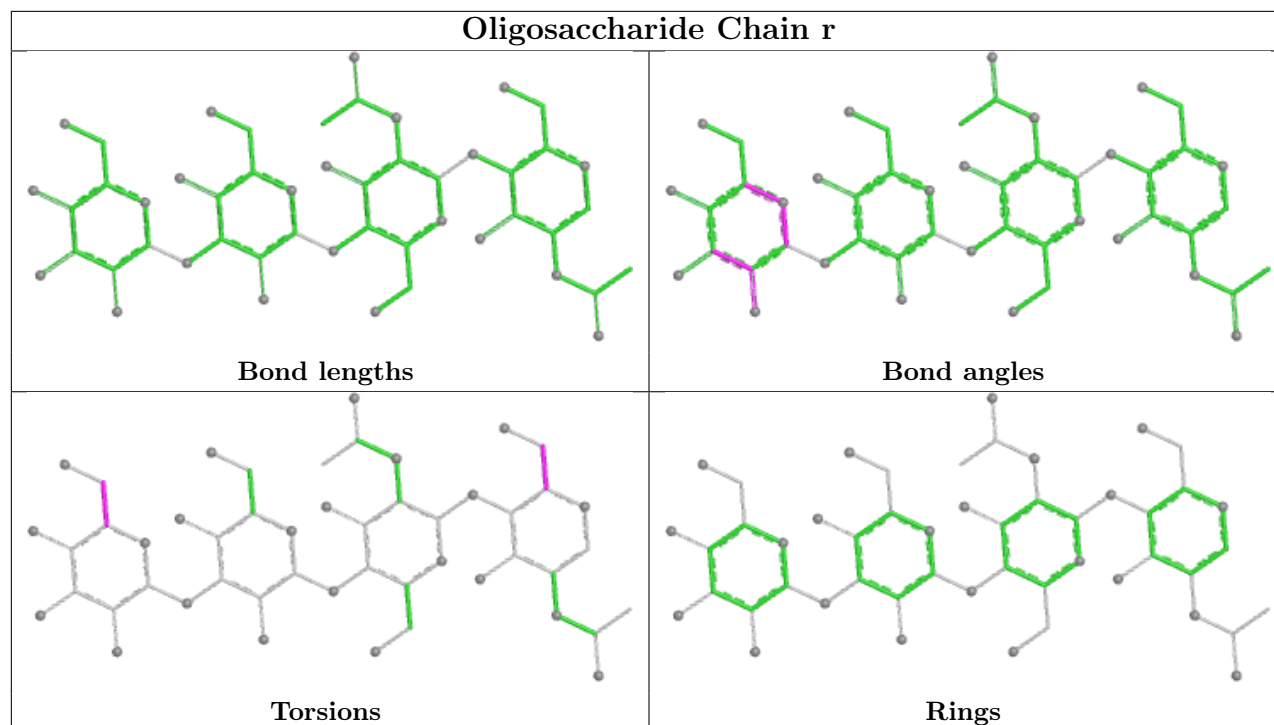


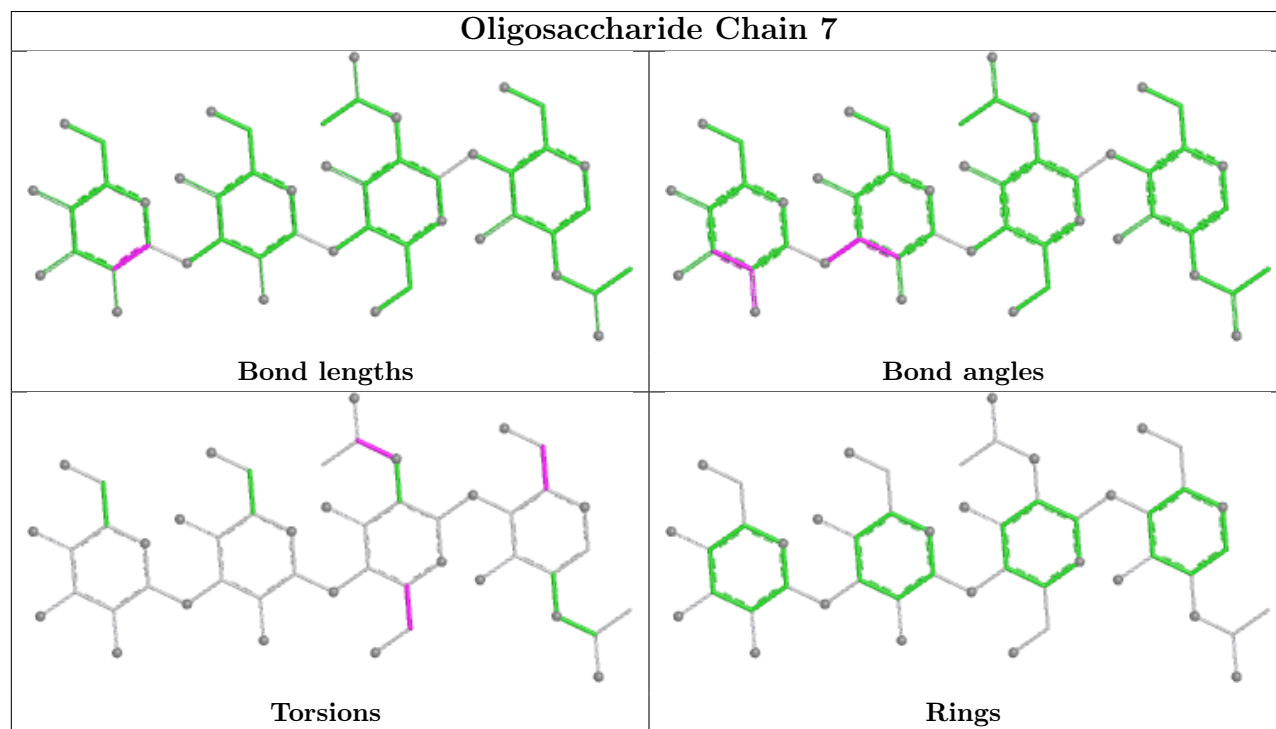
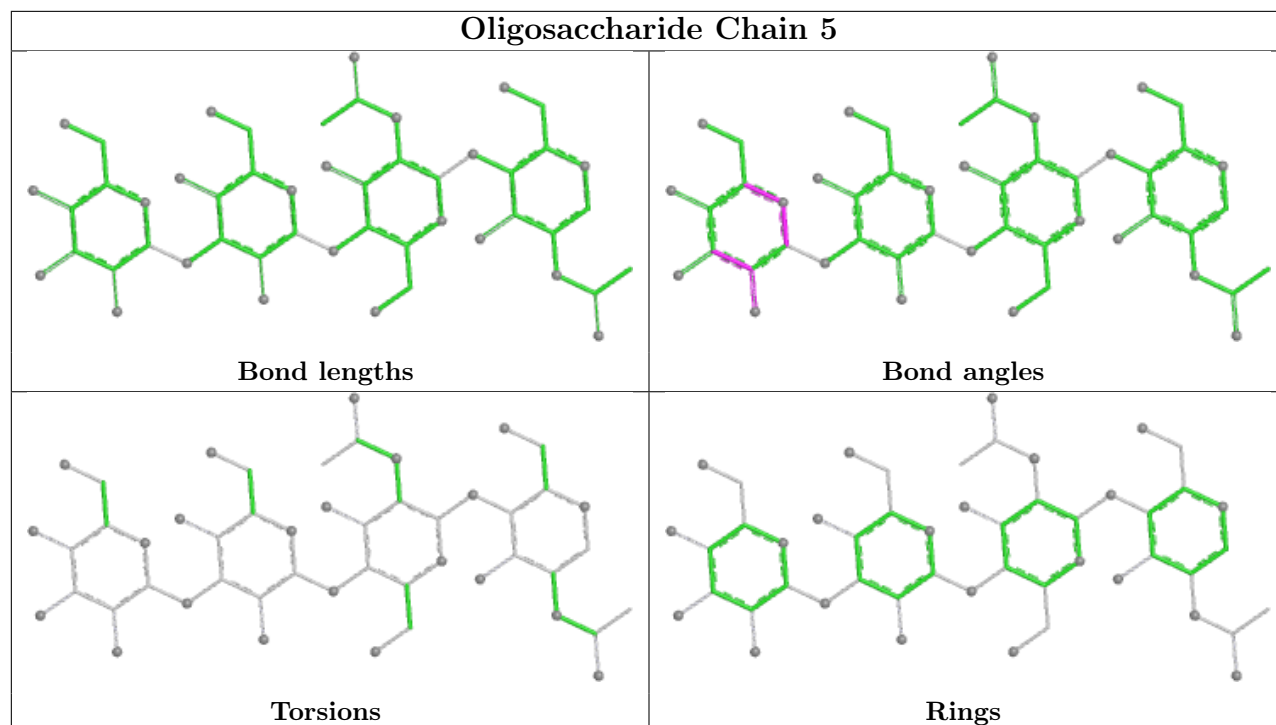


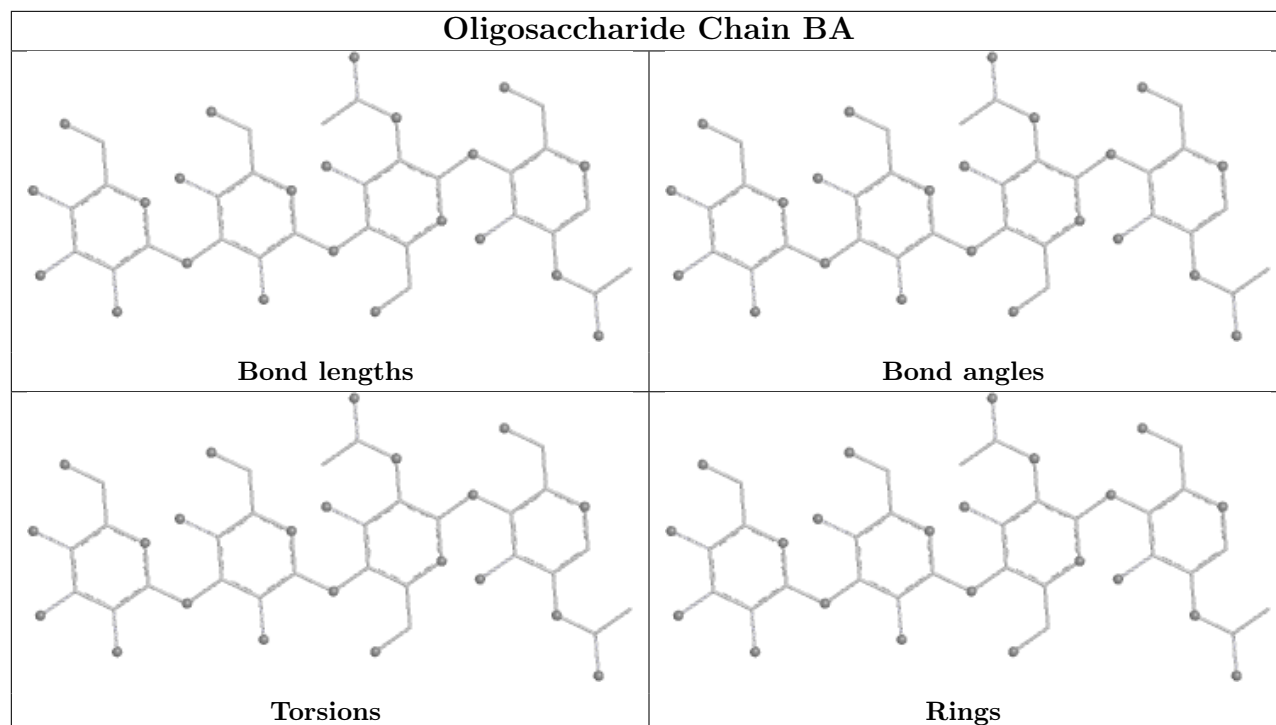
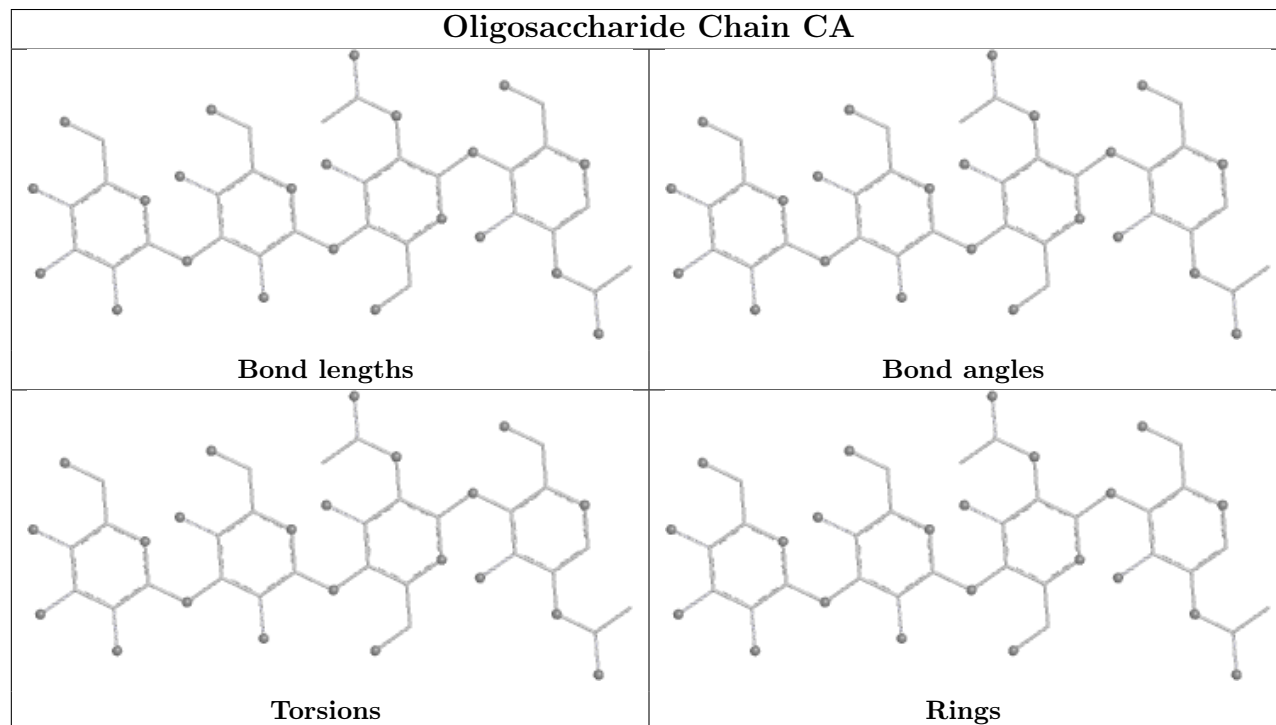


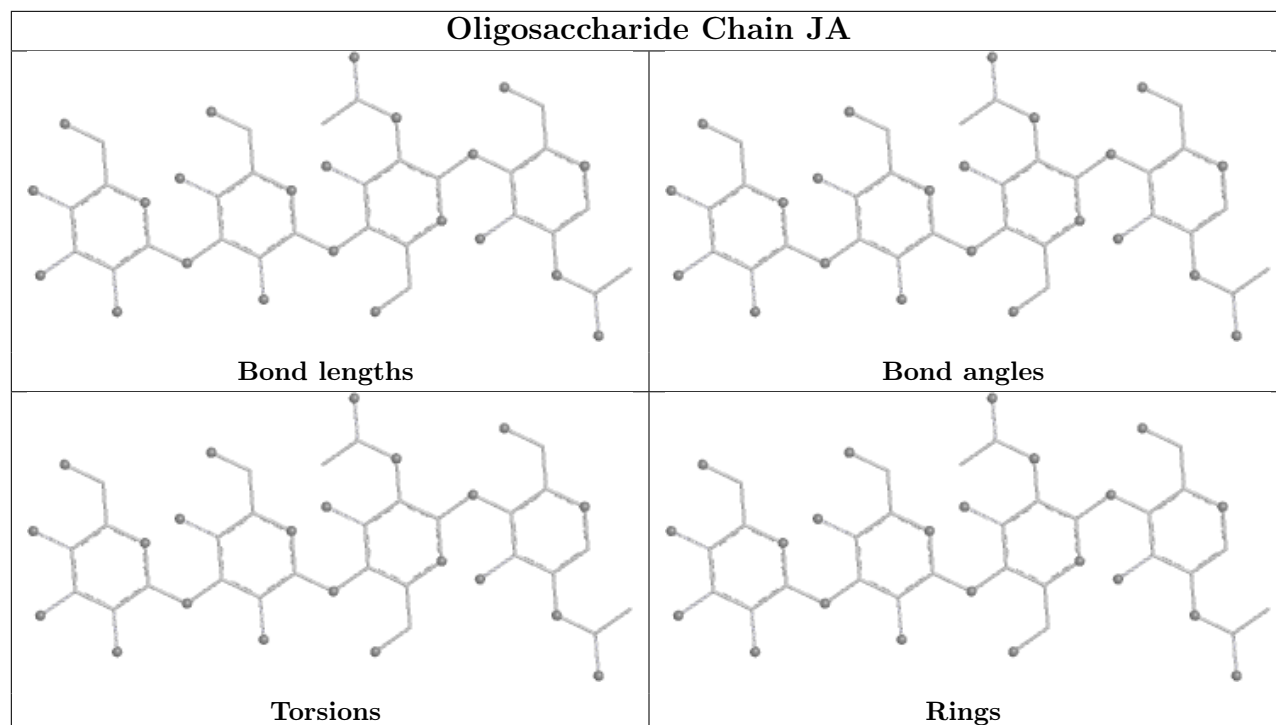
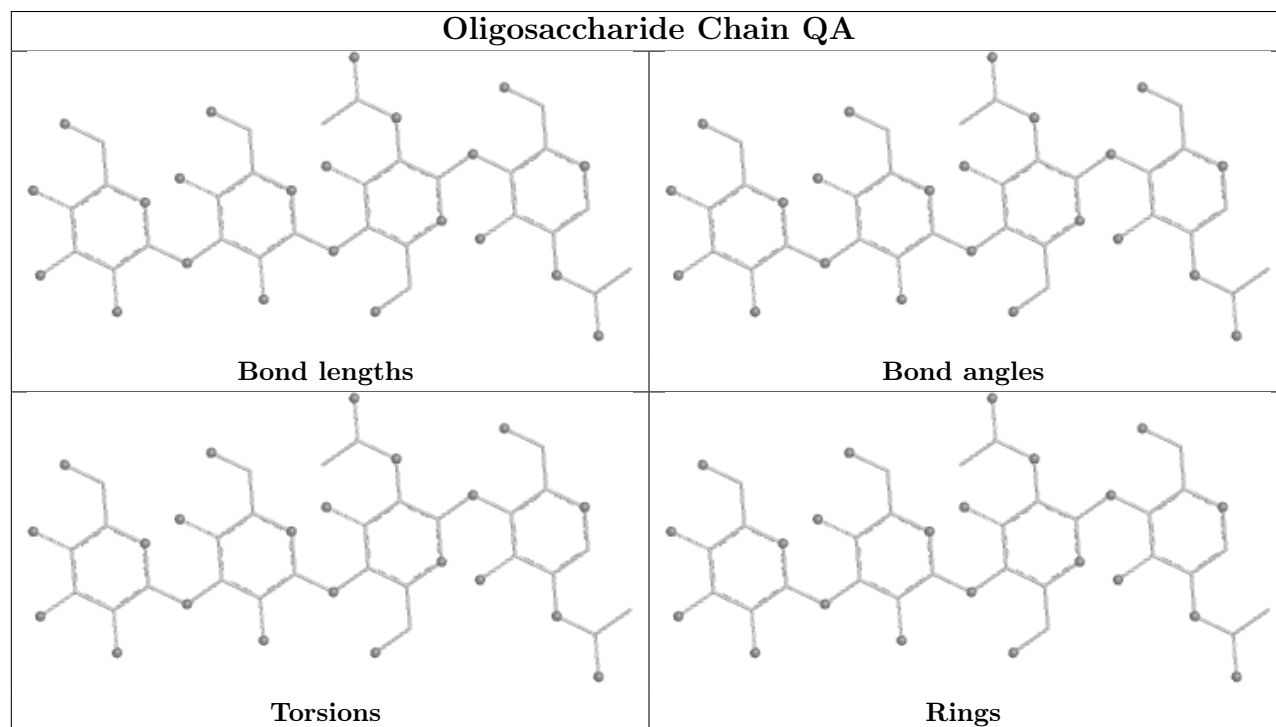


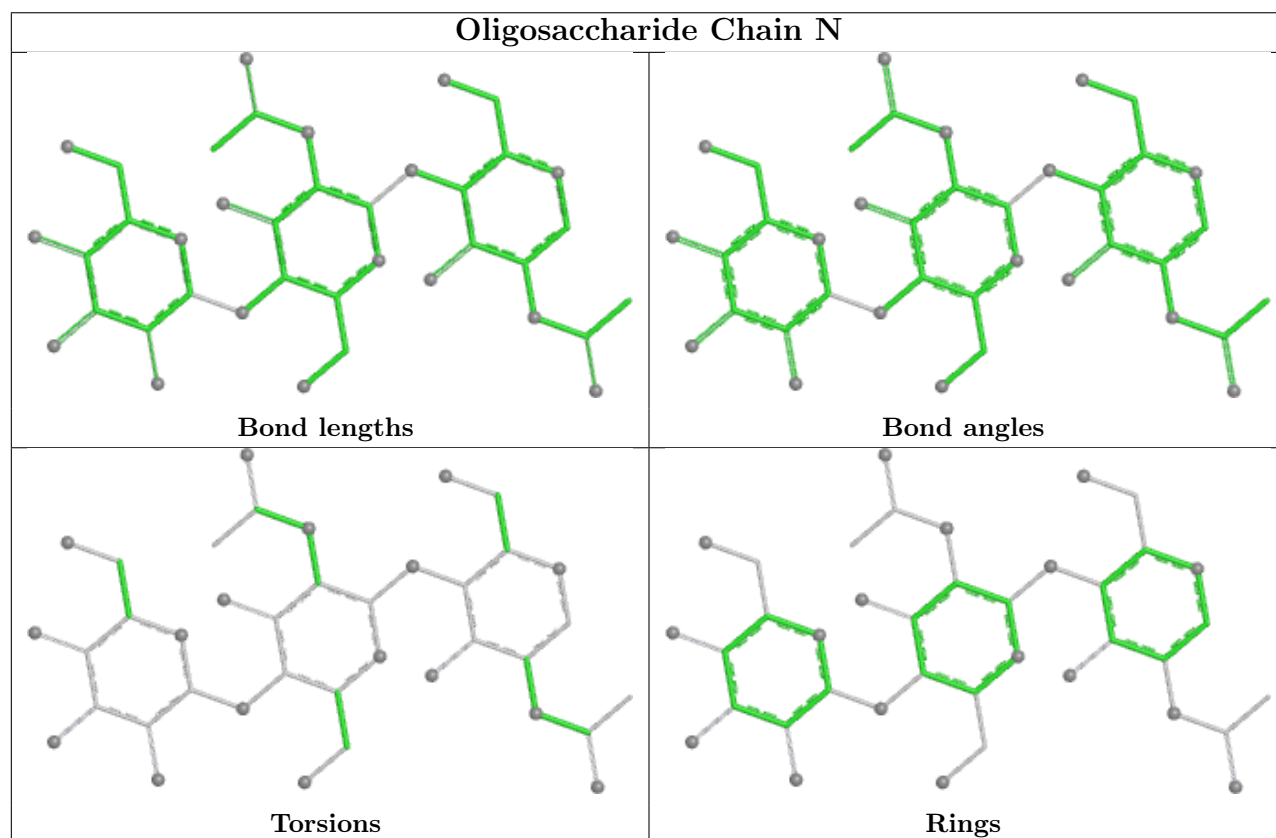
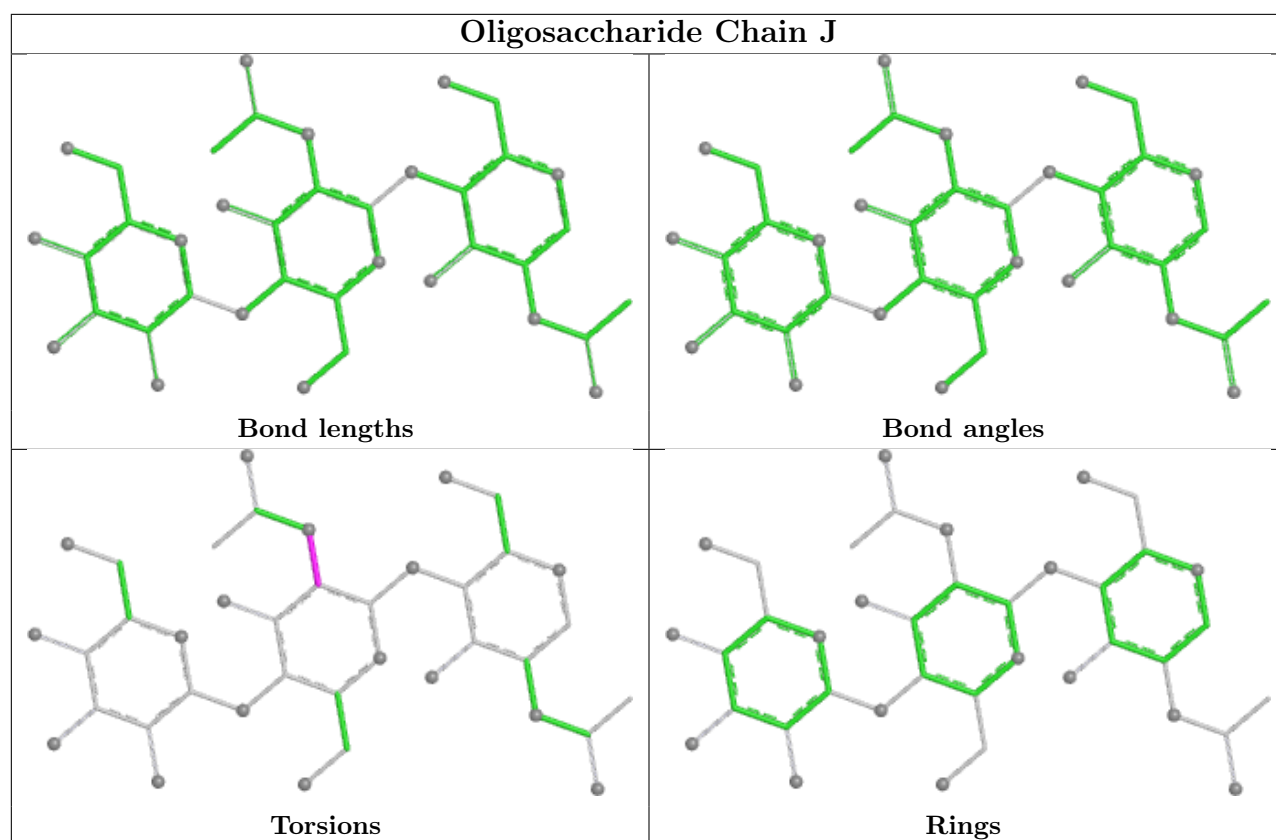


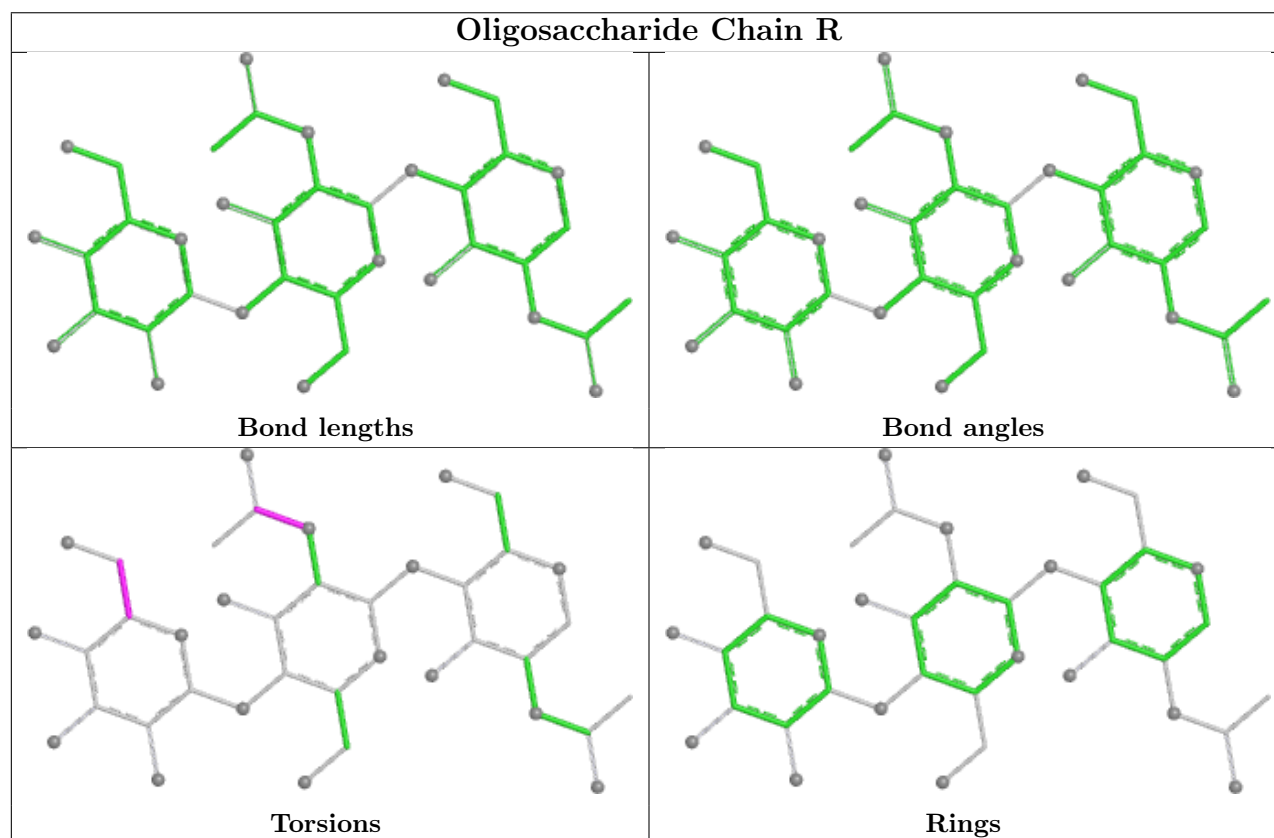
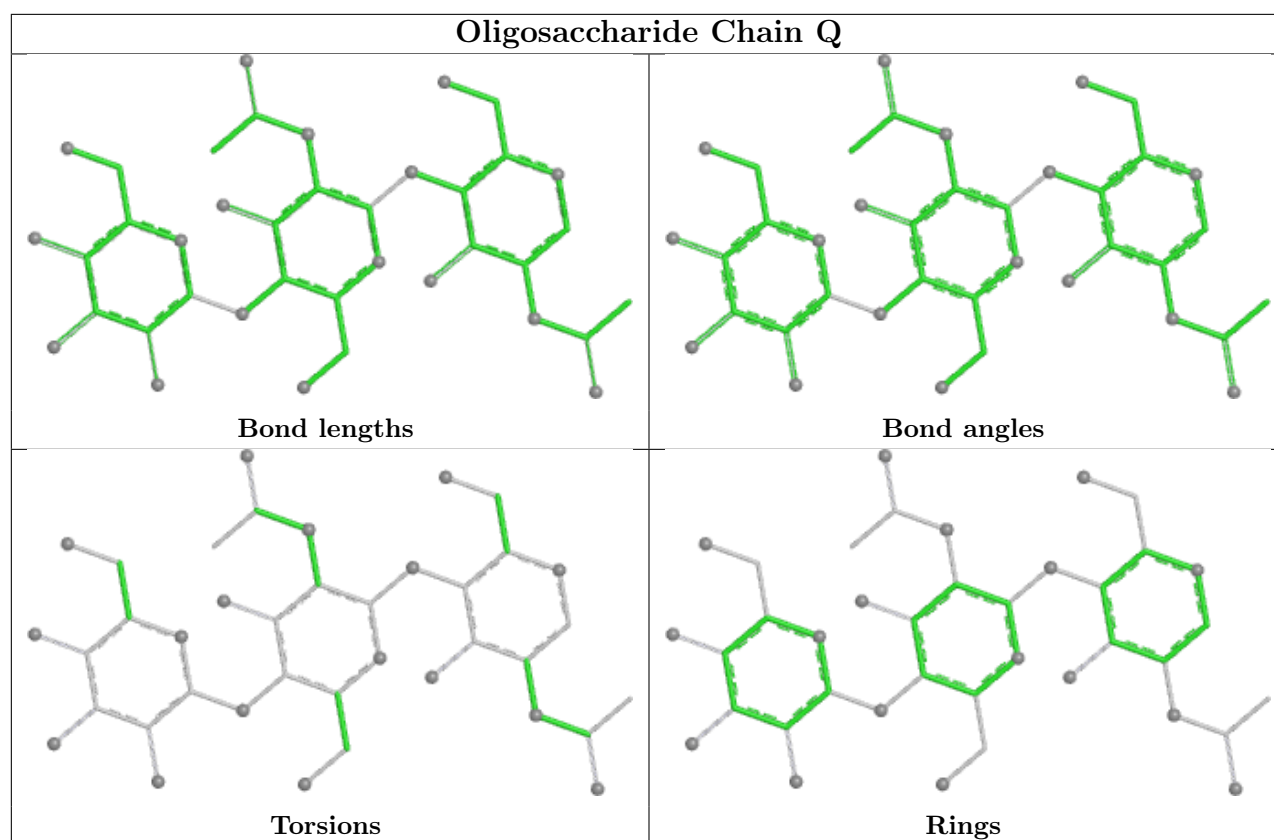


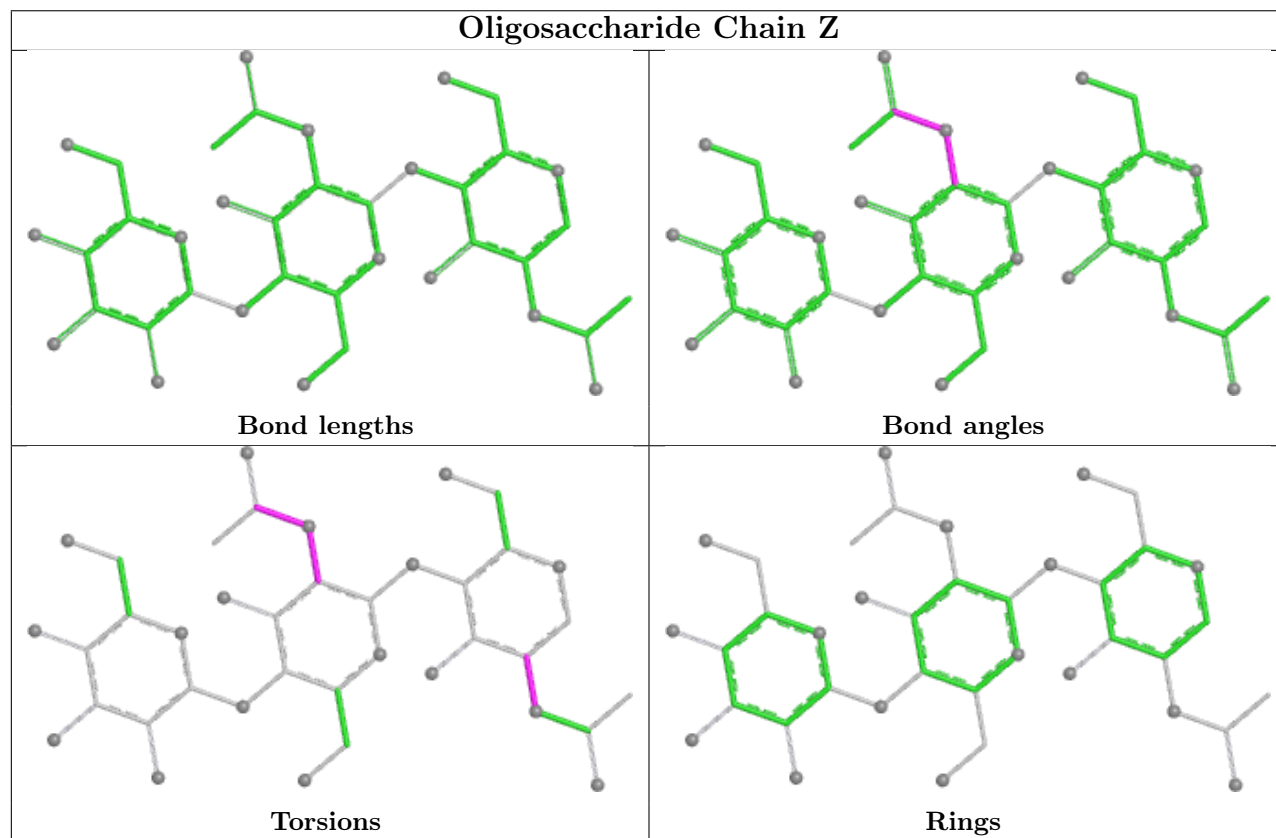
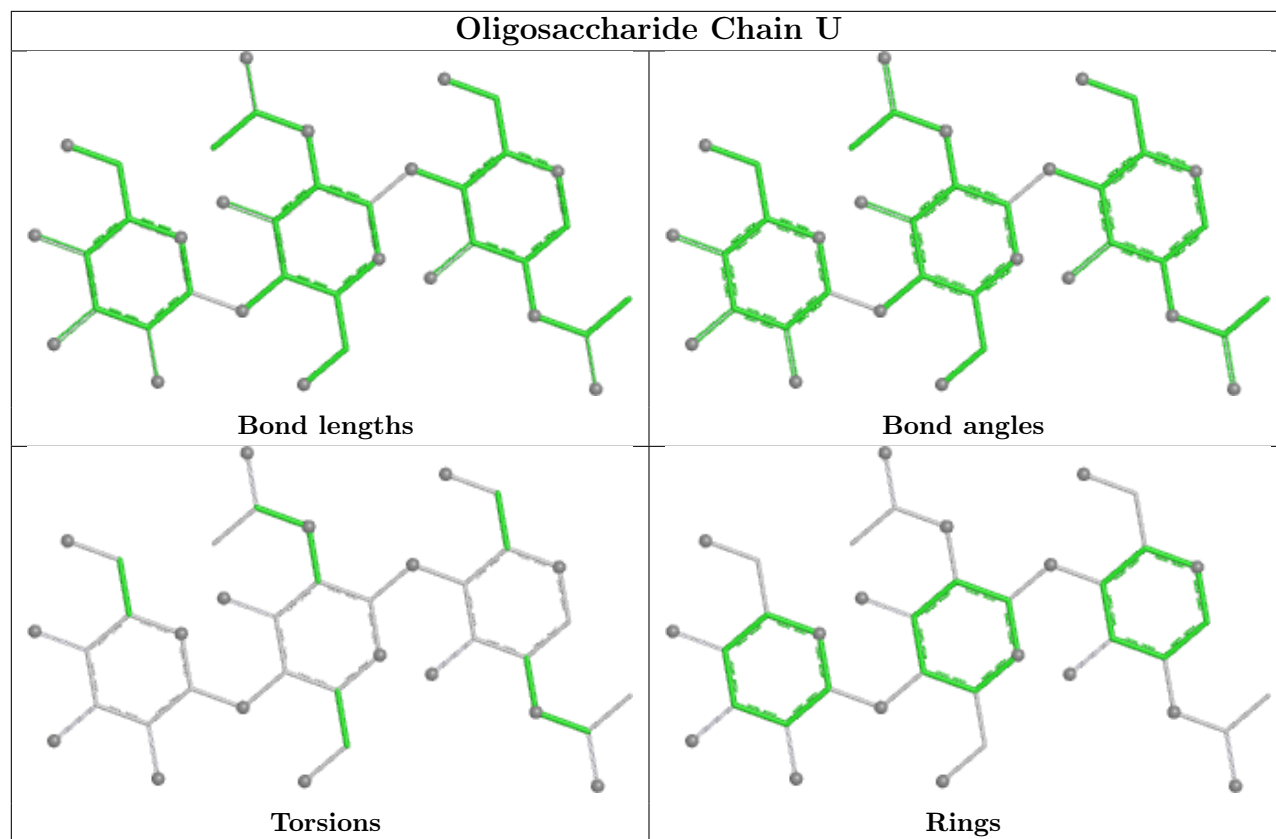


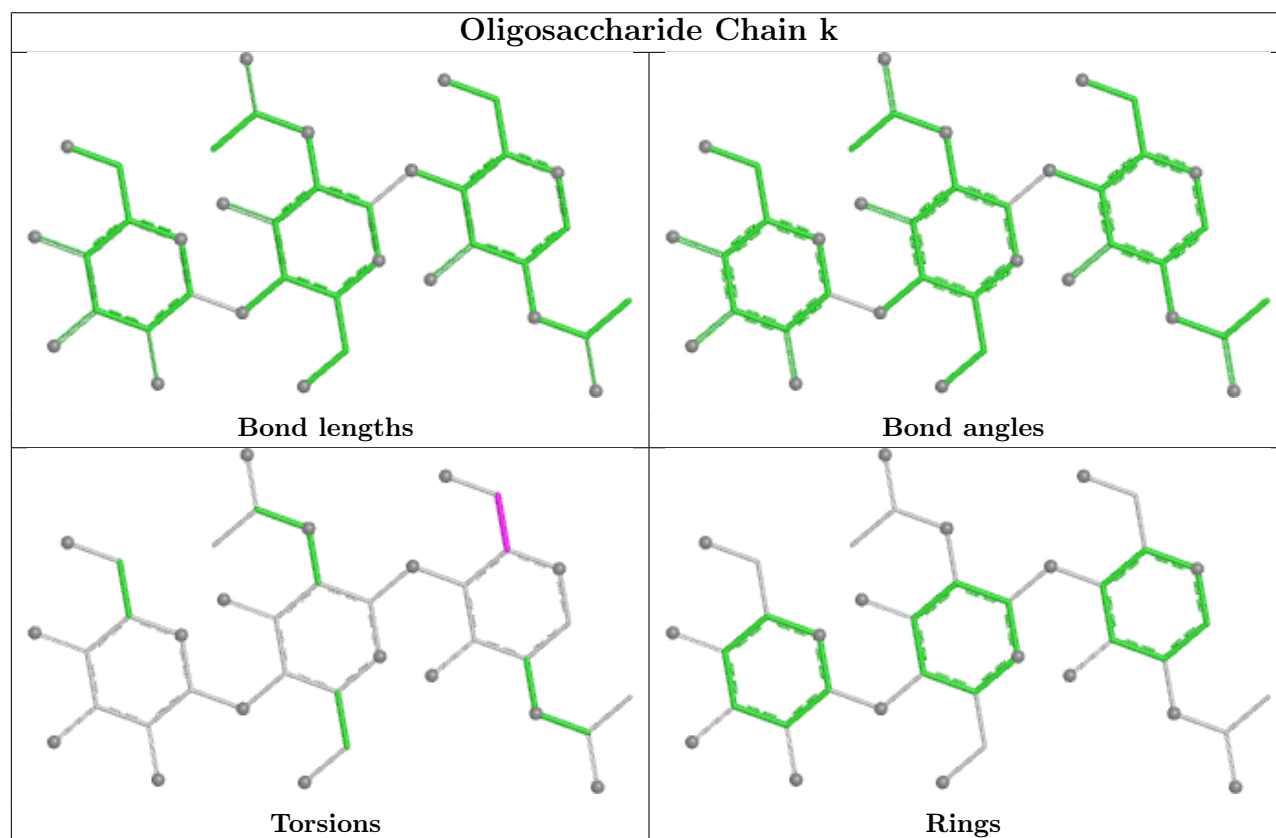
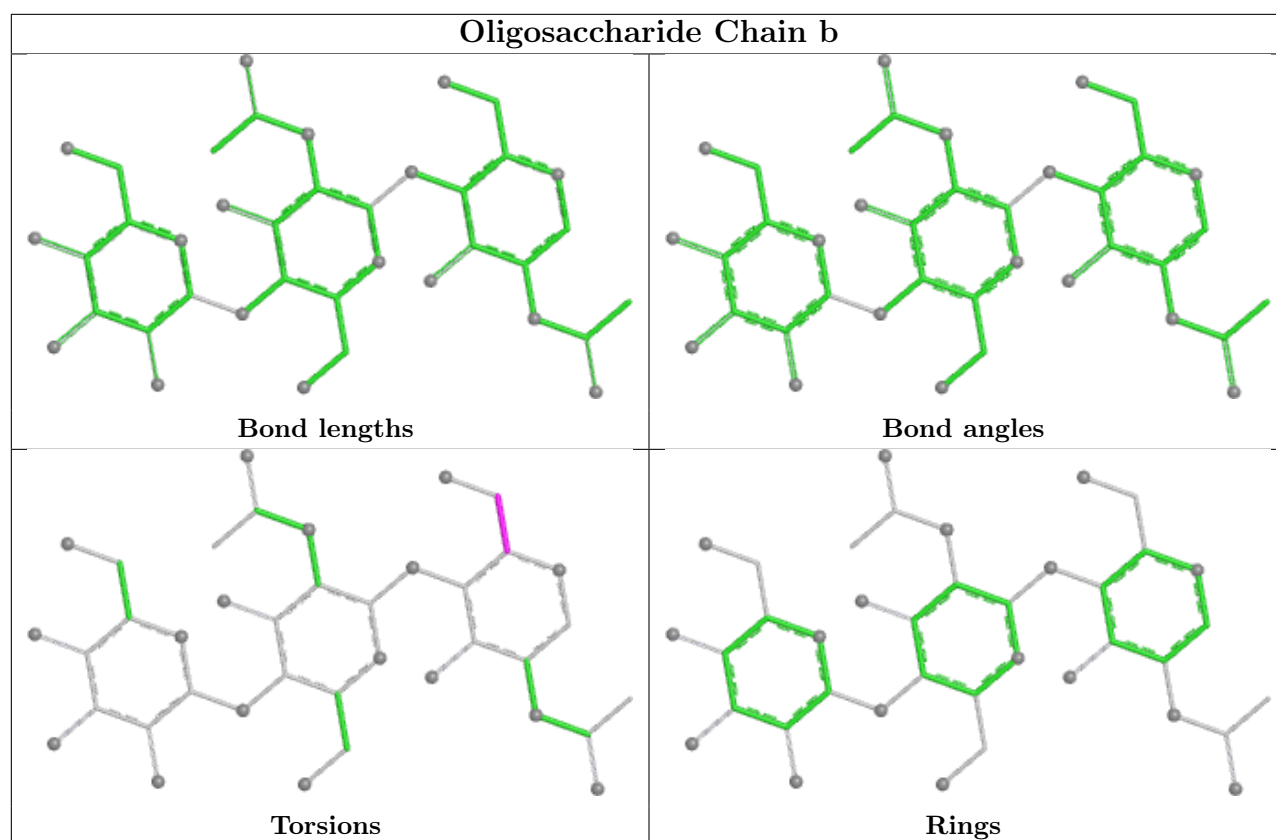
Oligosaccharide Chain BA**Oligosaccharide Chain CA**

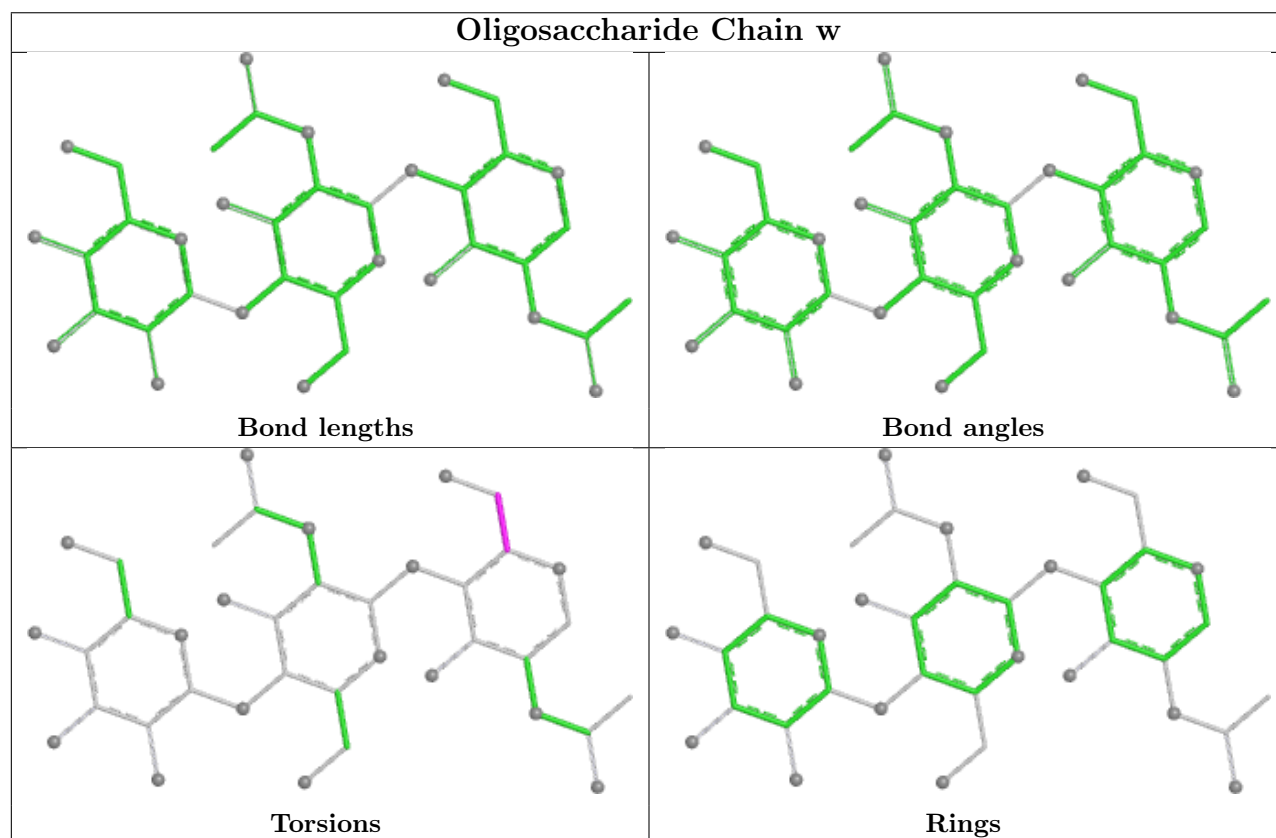
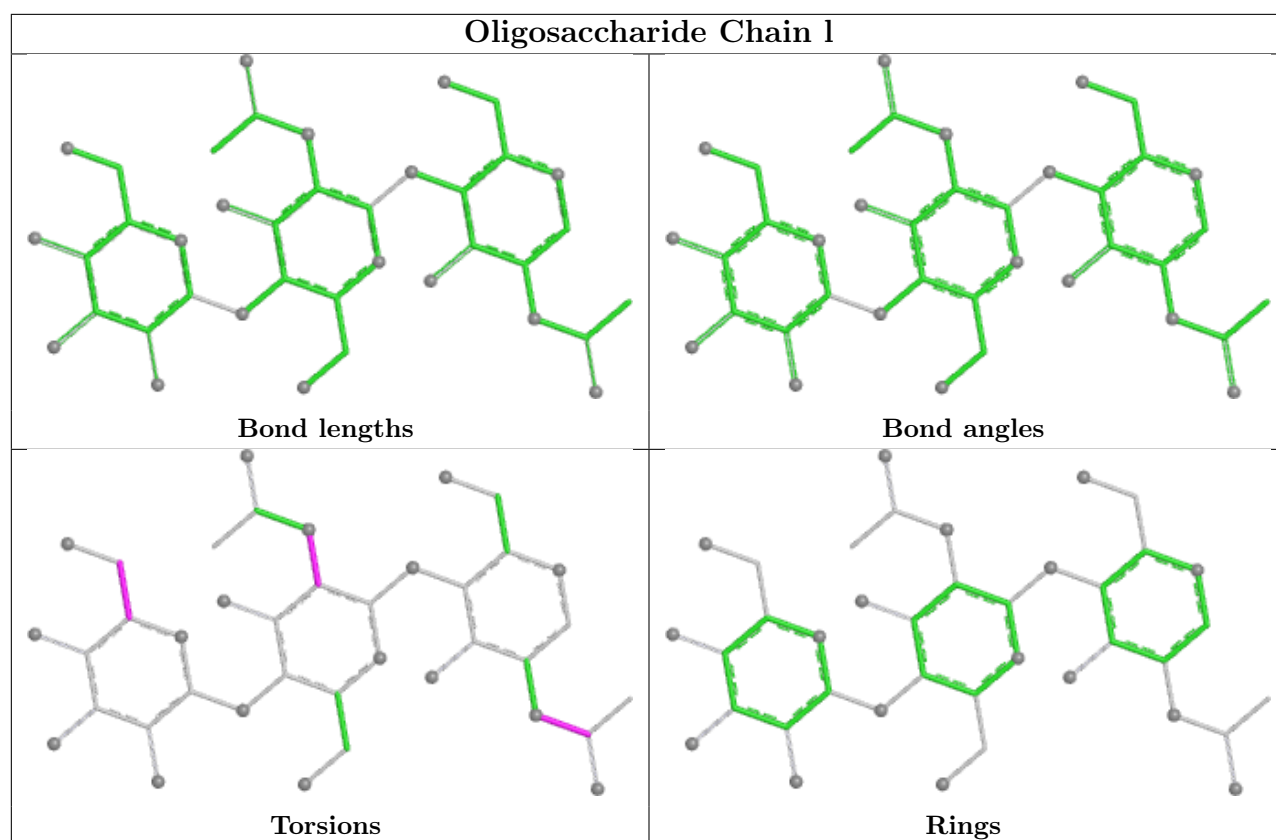
Oligosaccharide Chain JA**Oligosaccharide Chain QA**

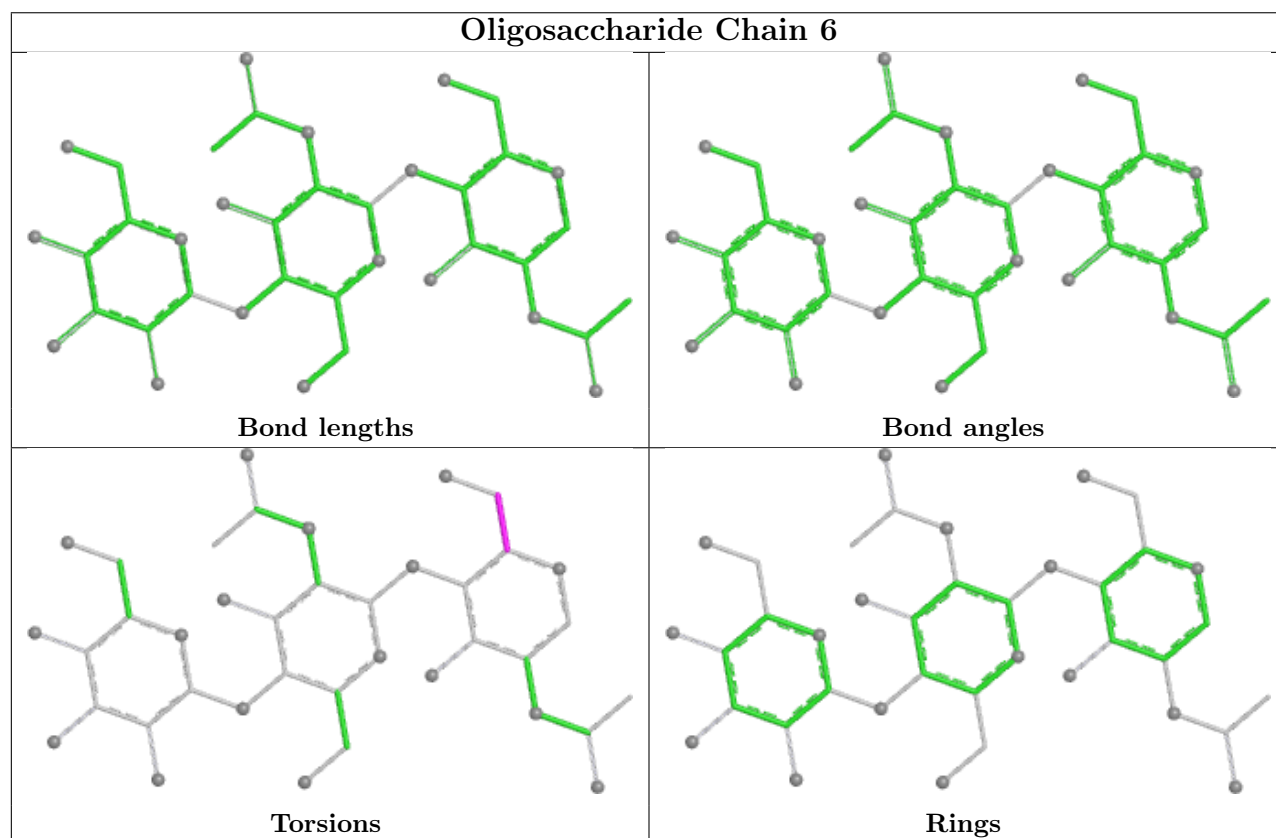
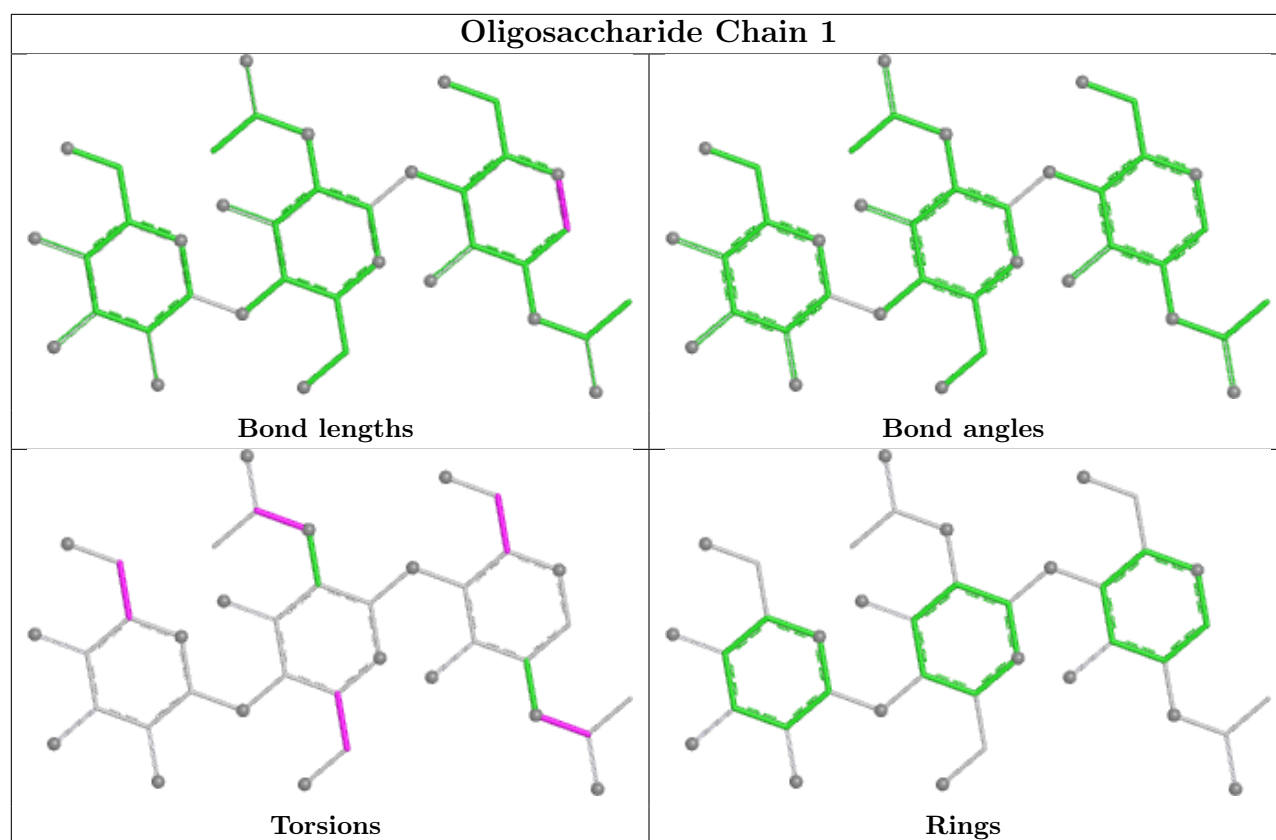


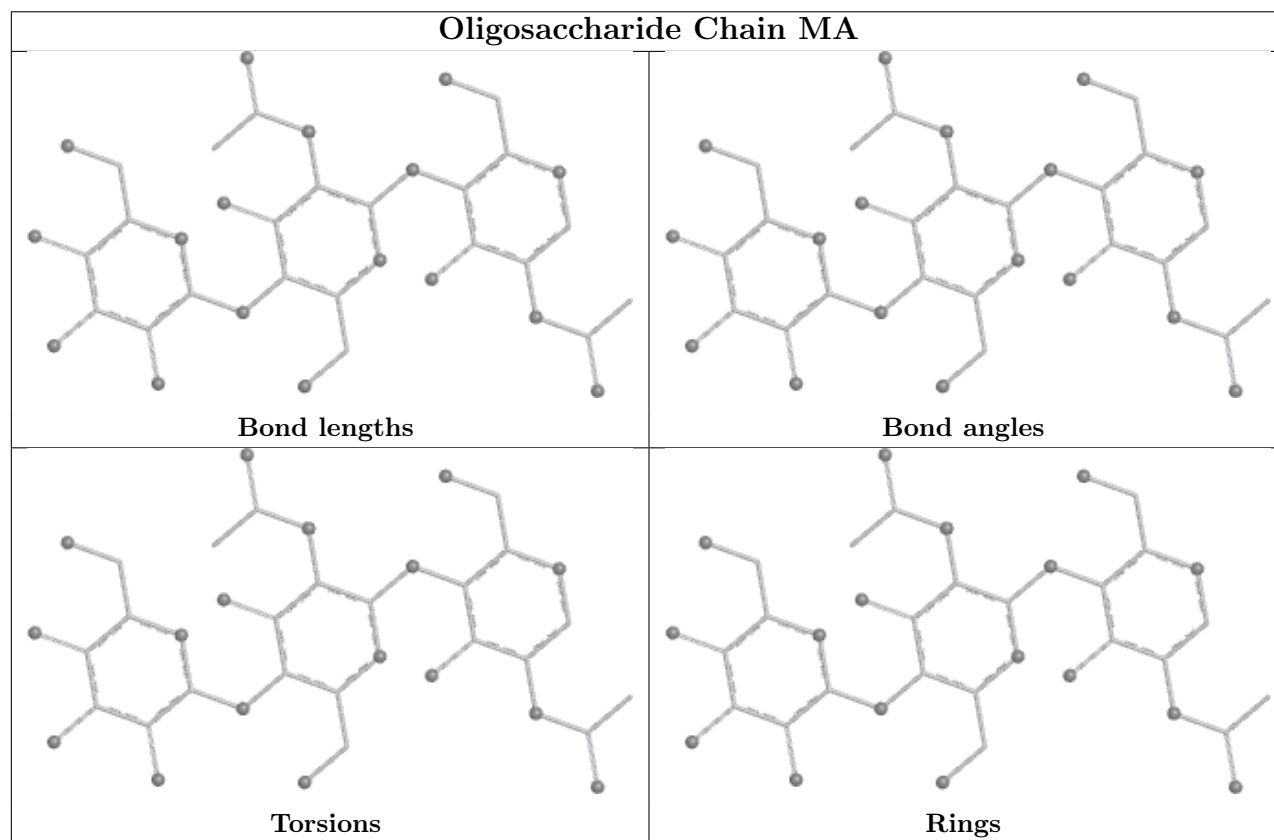
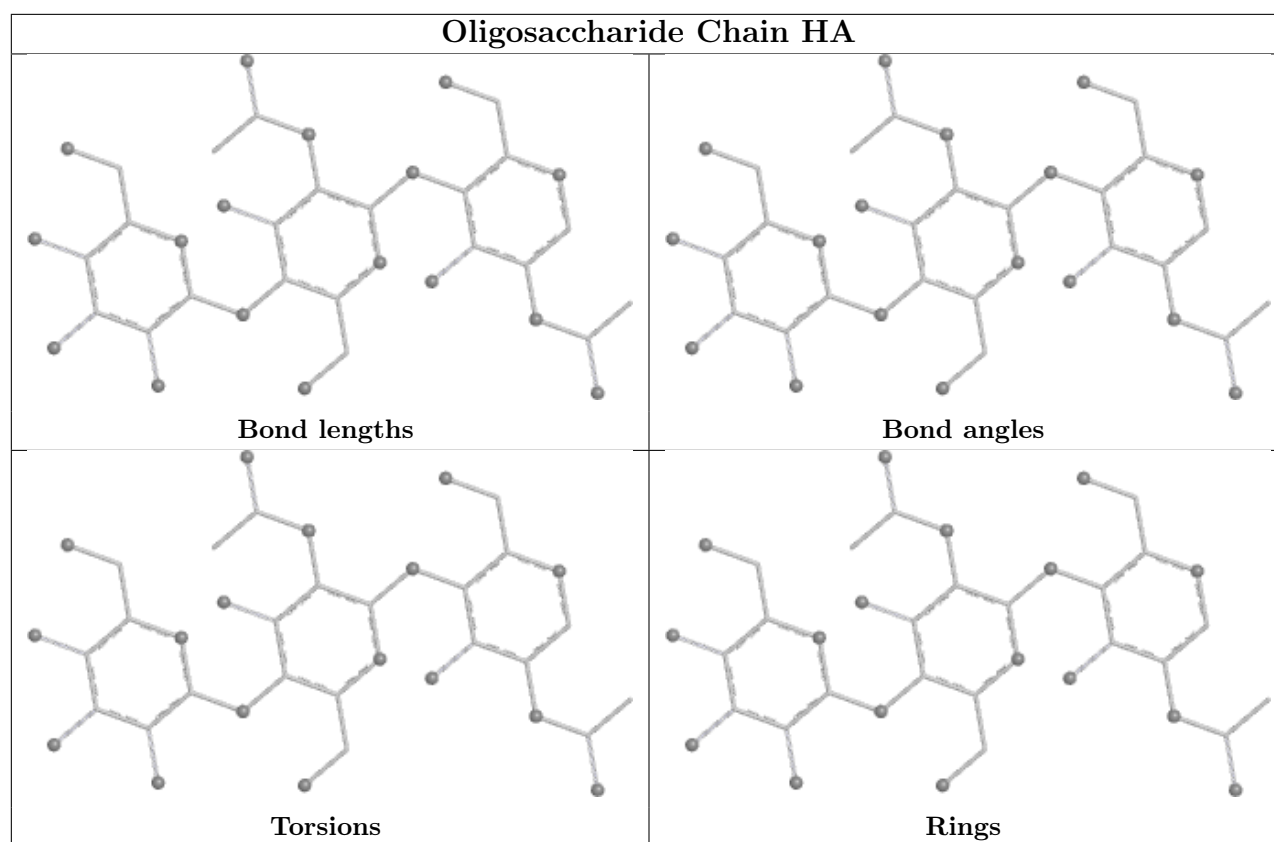


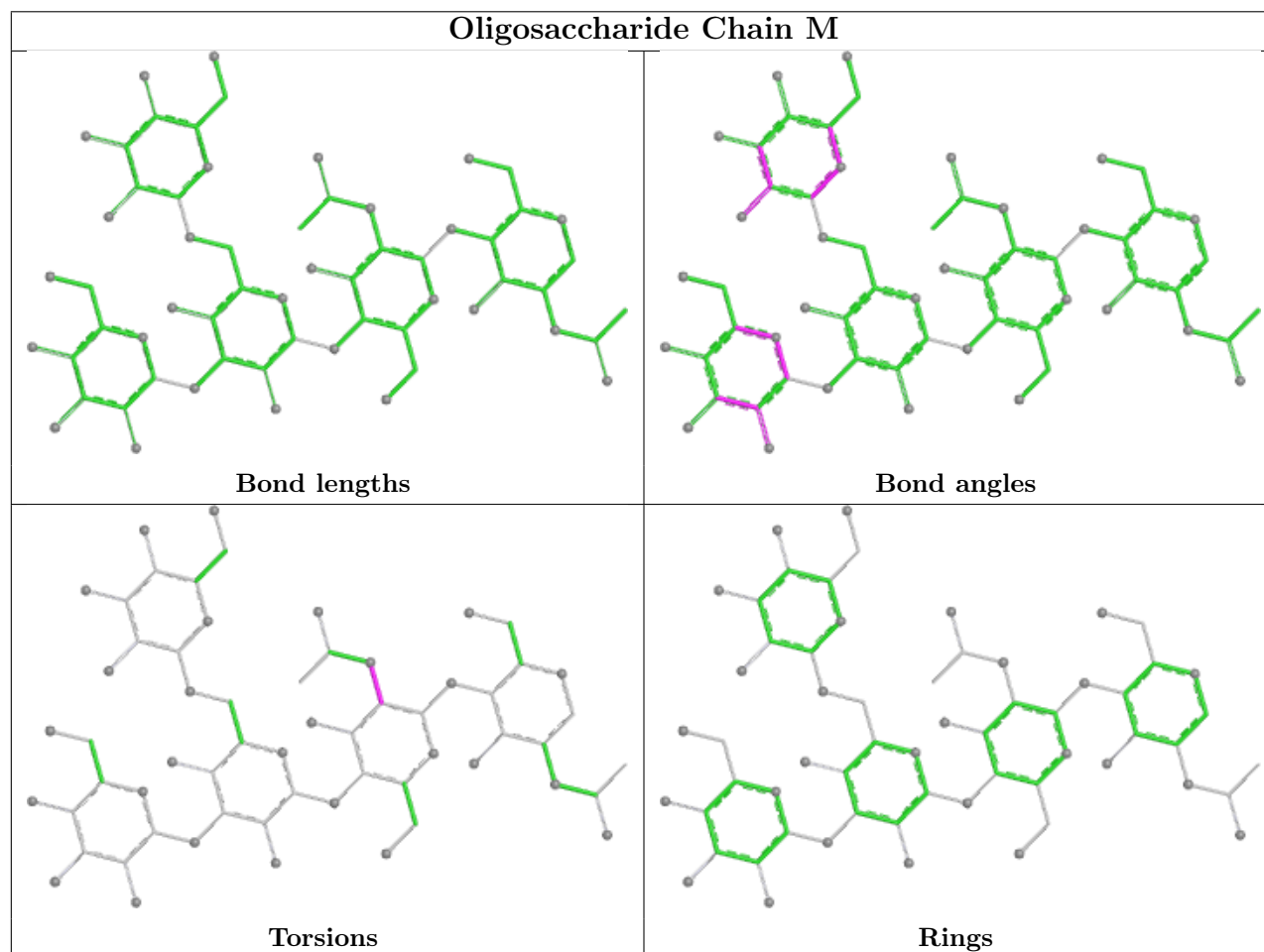
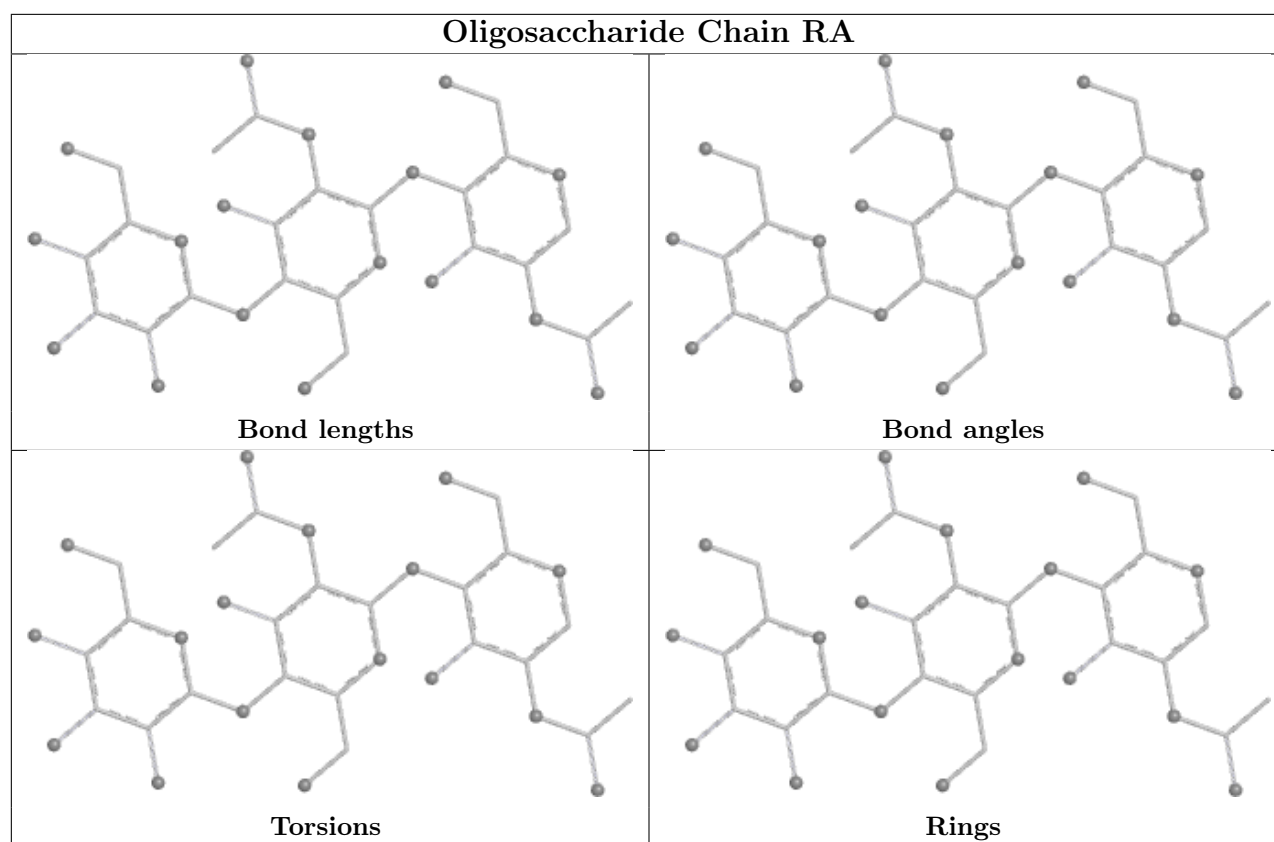


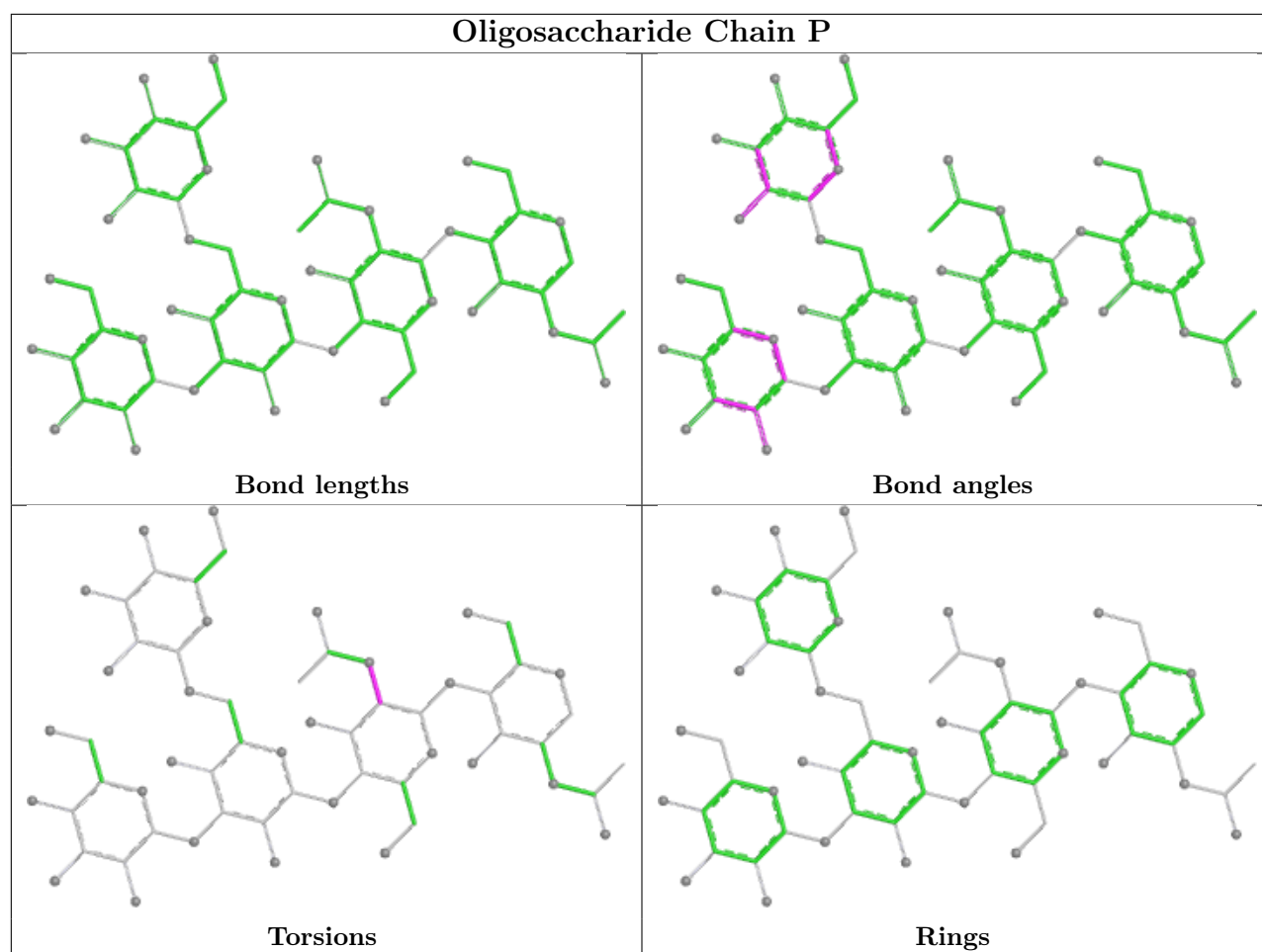


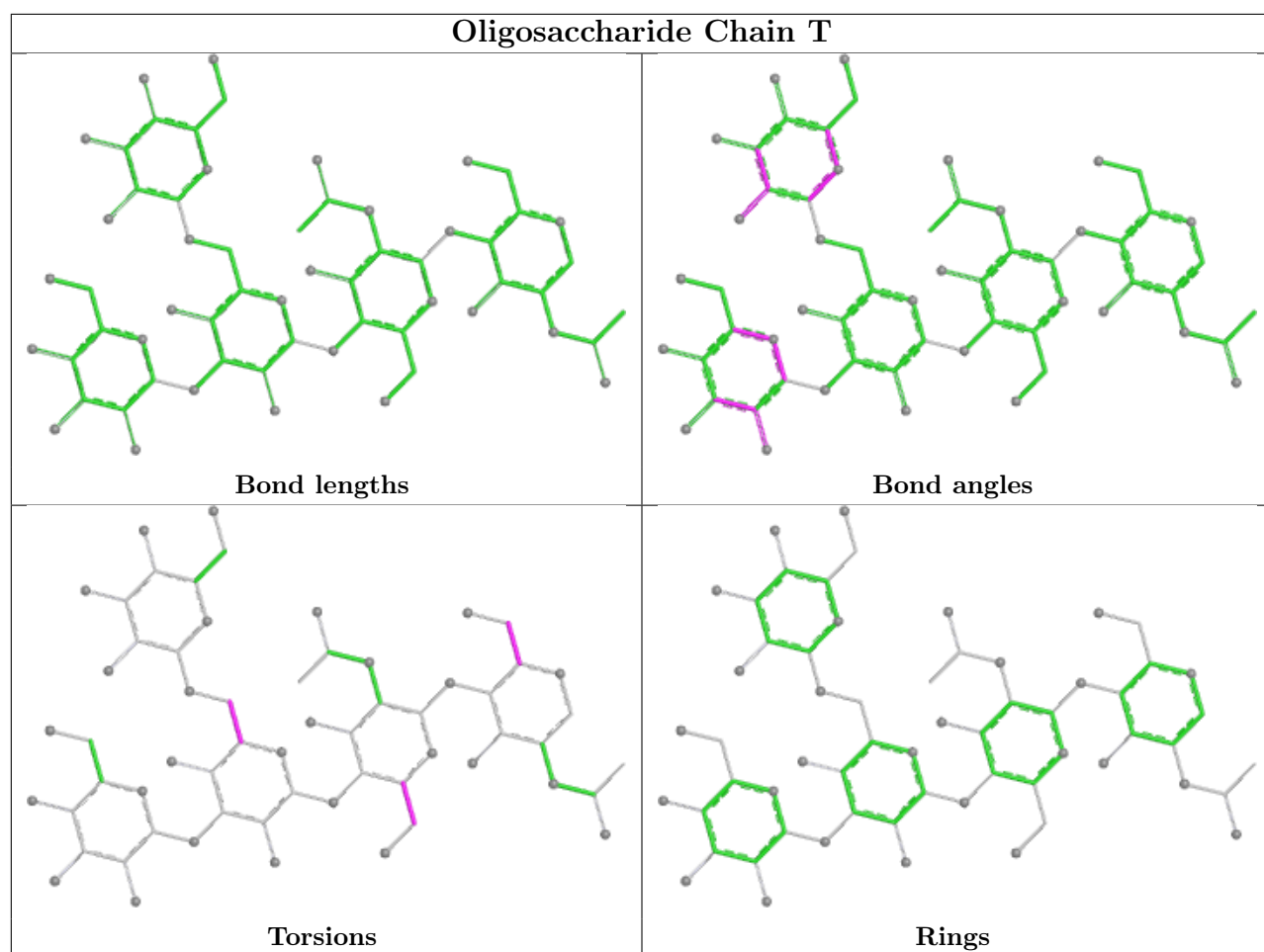


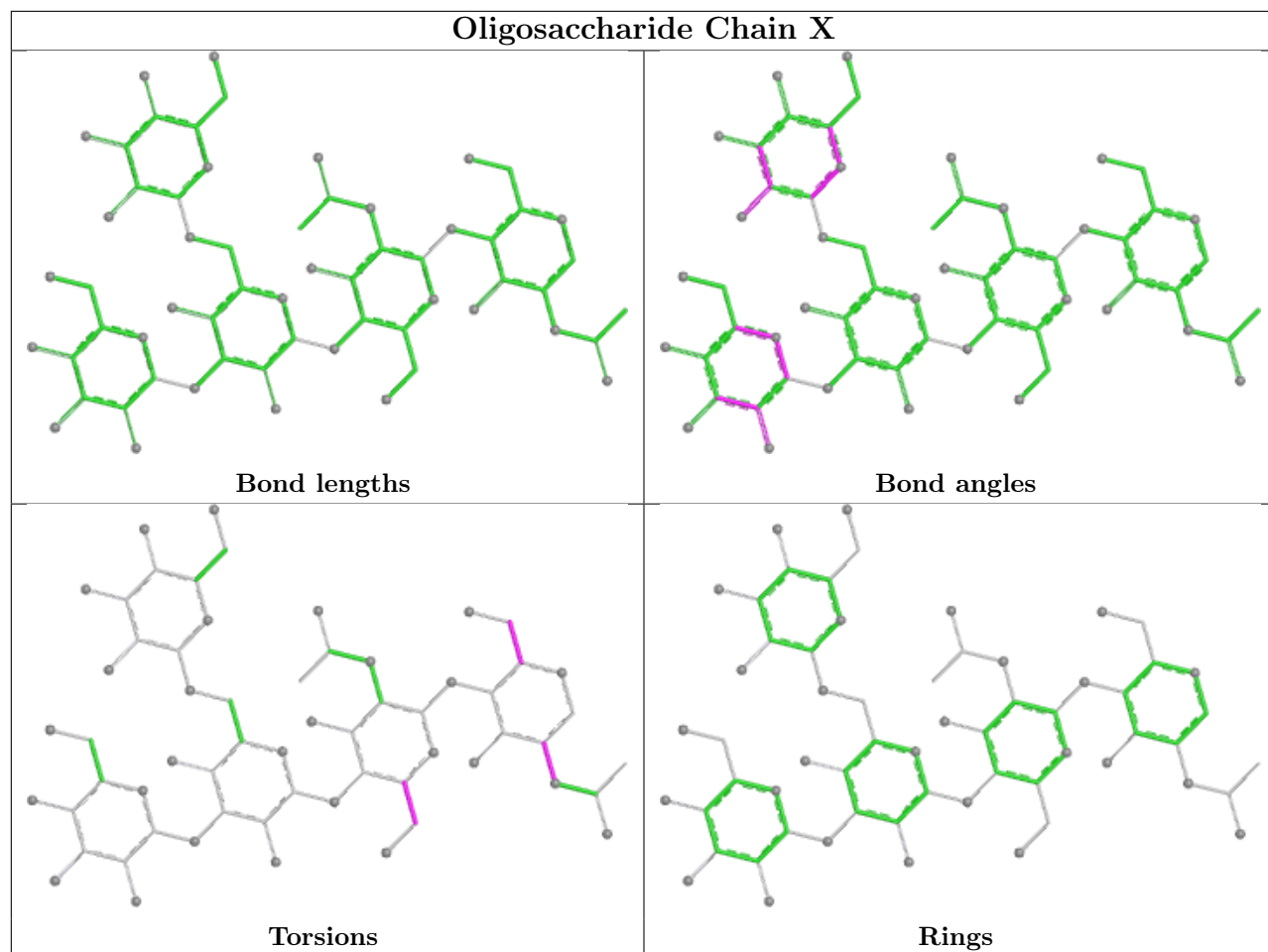


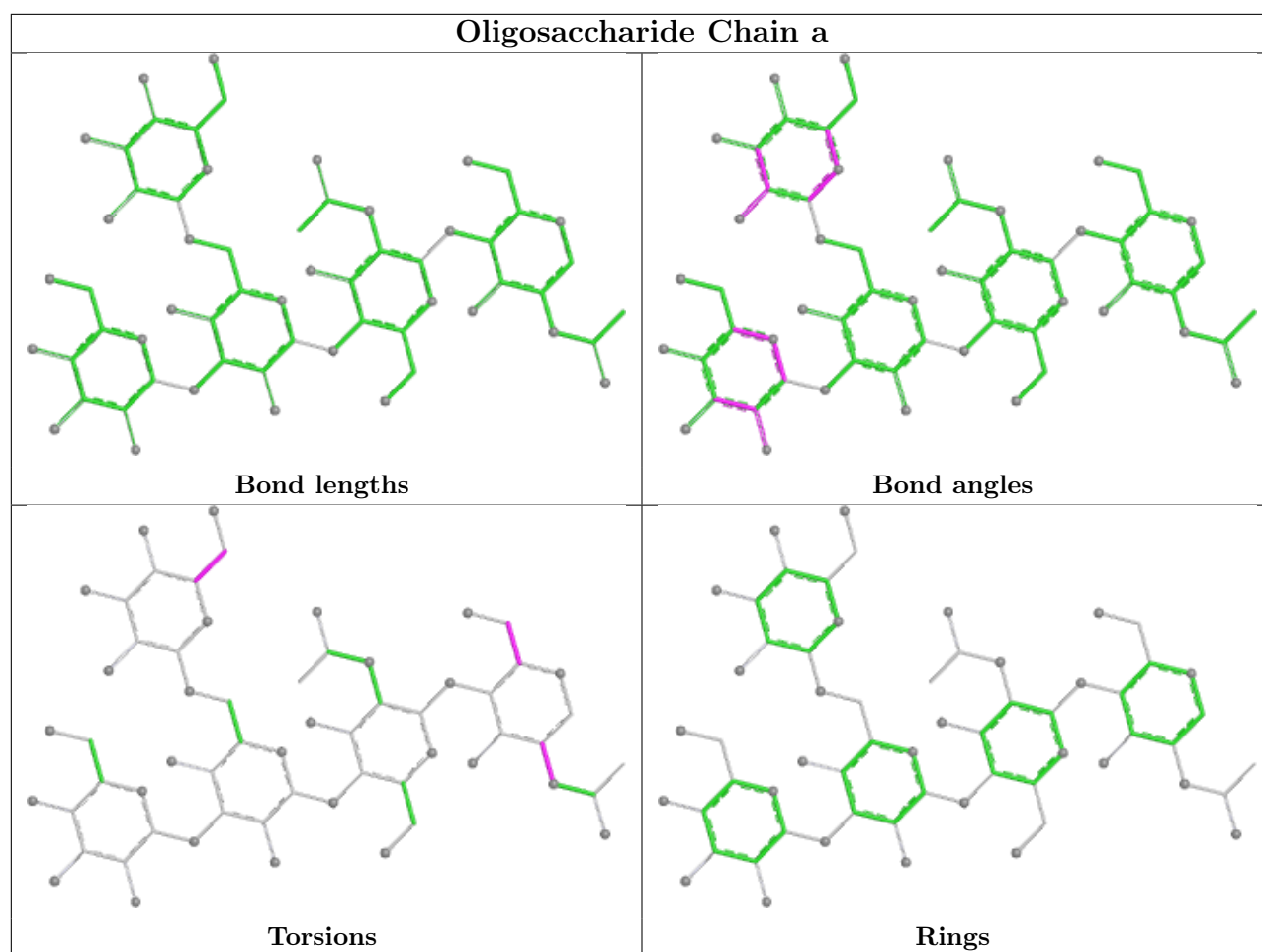


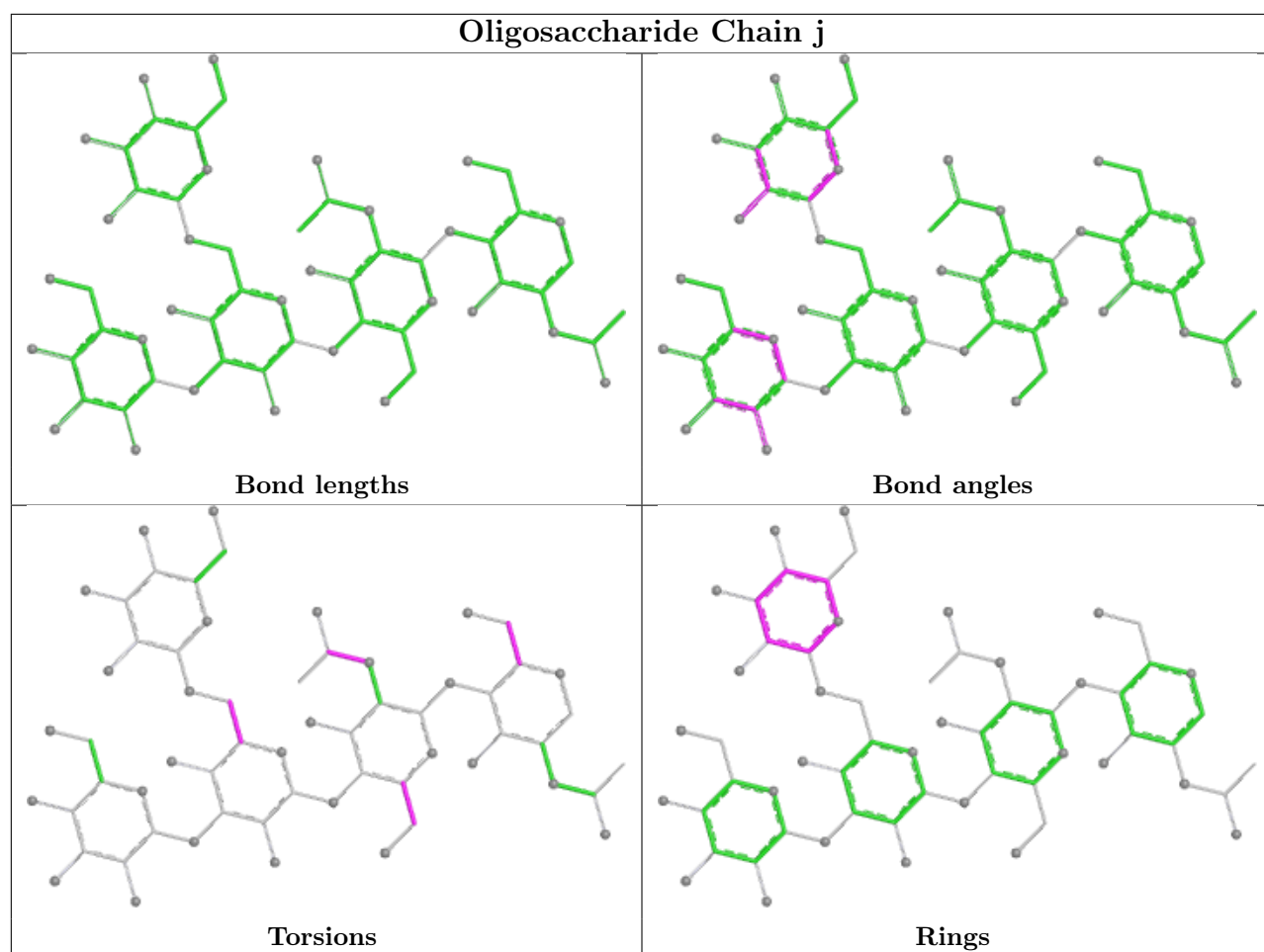


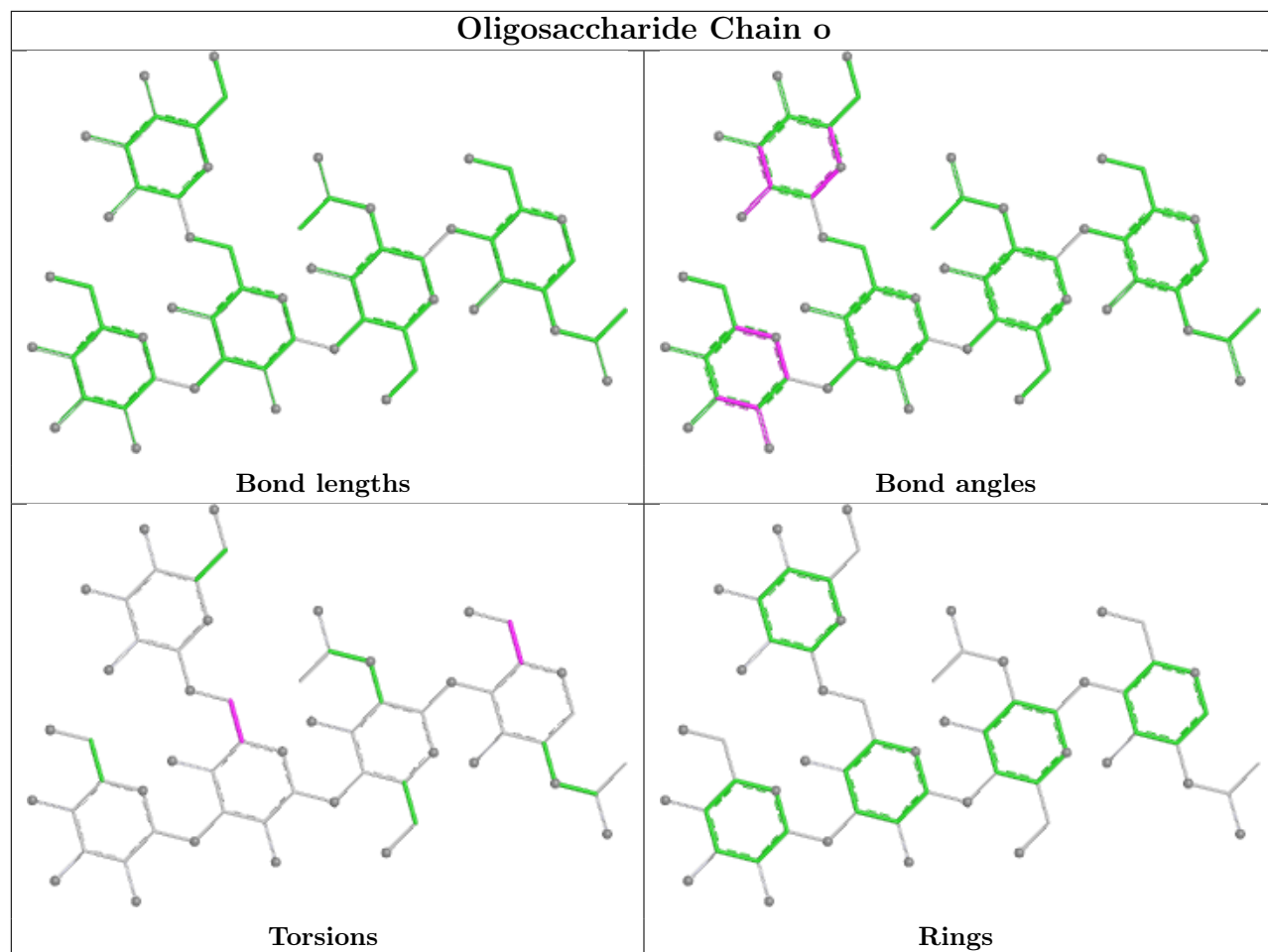


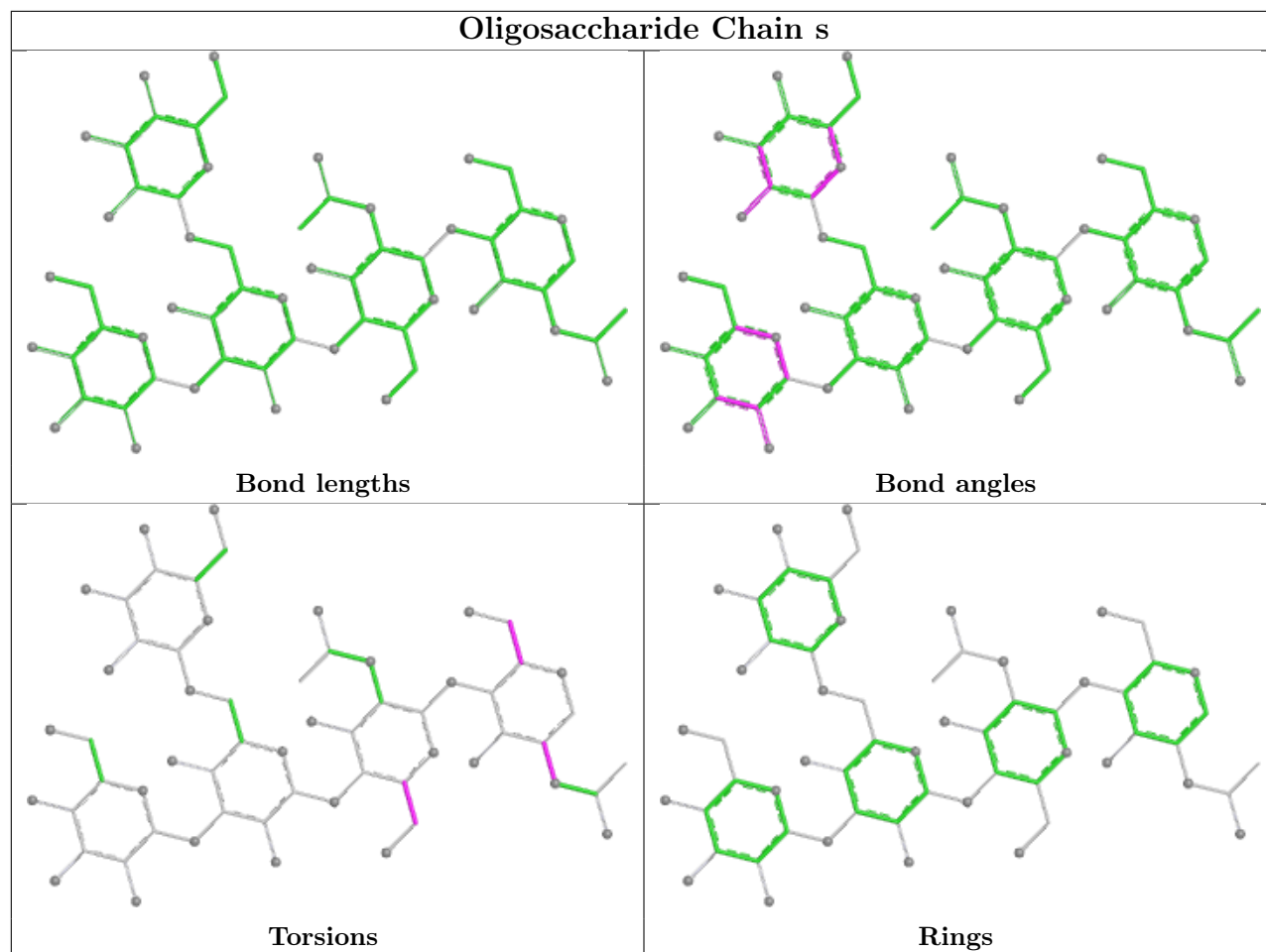


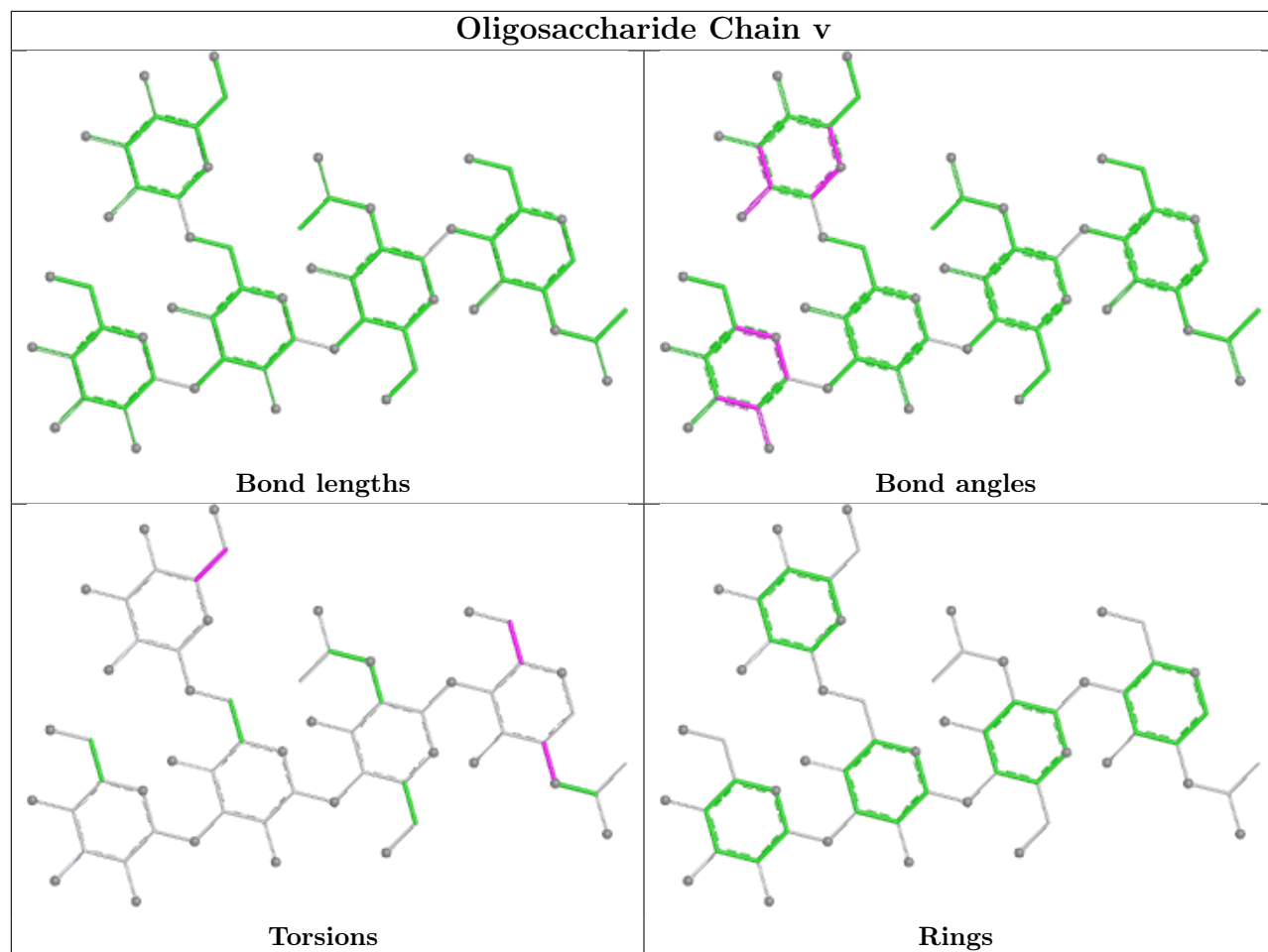


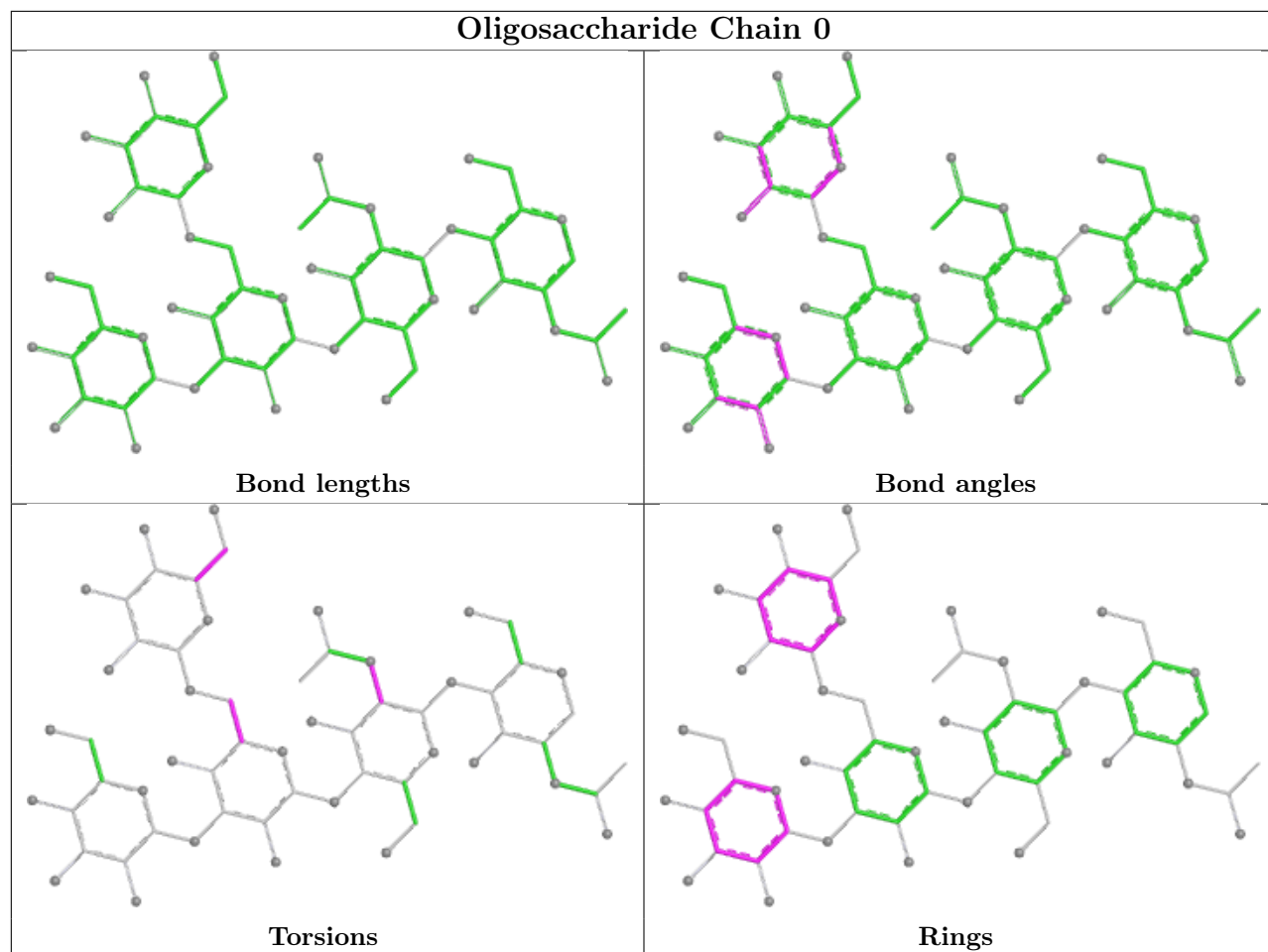


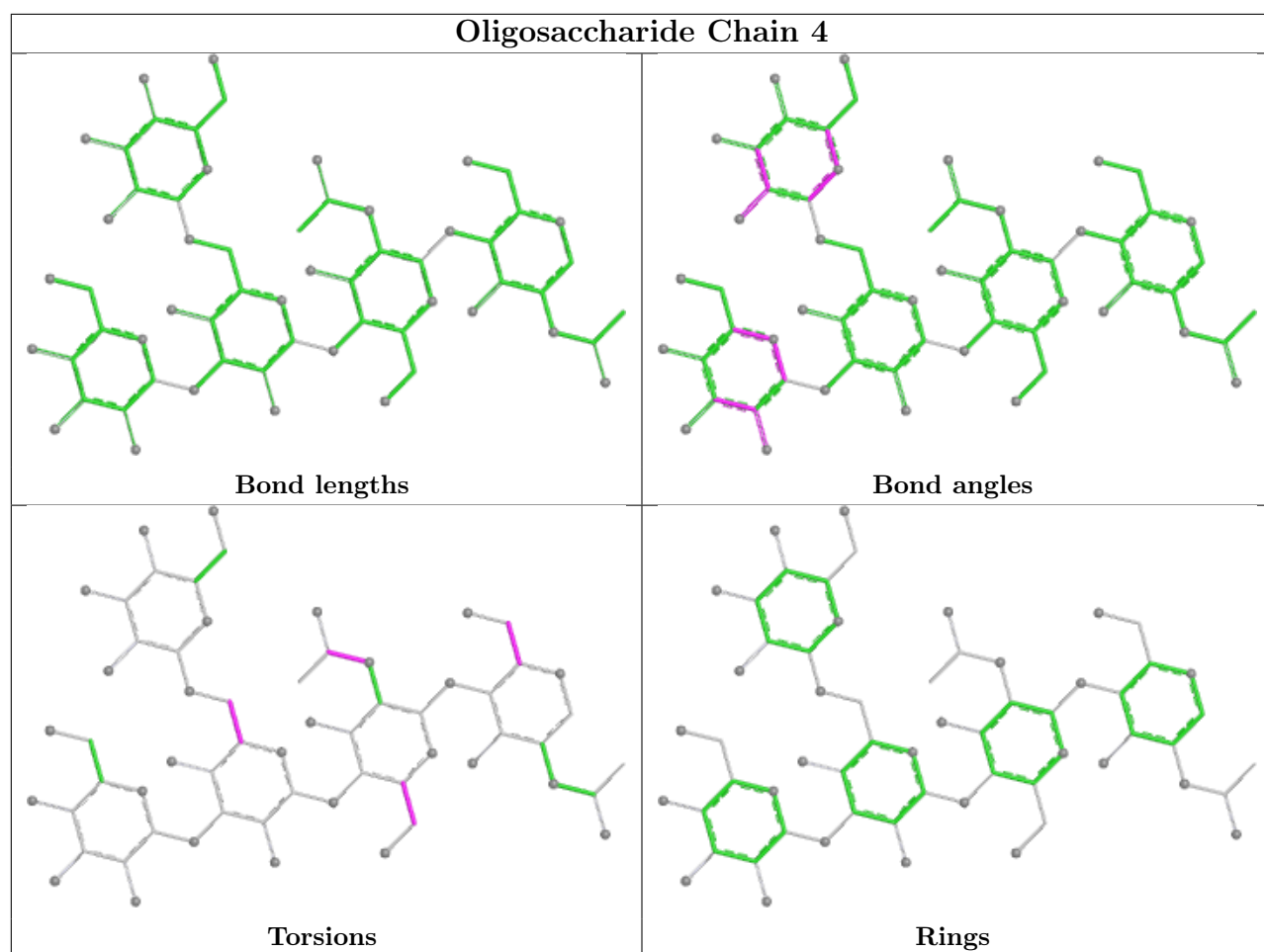


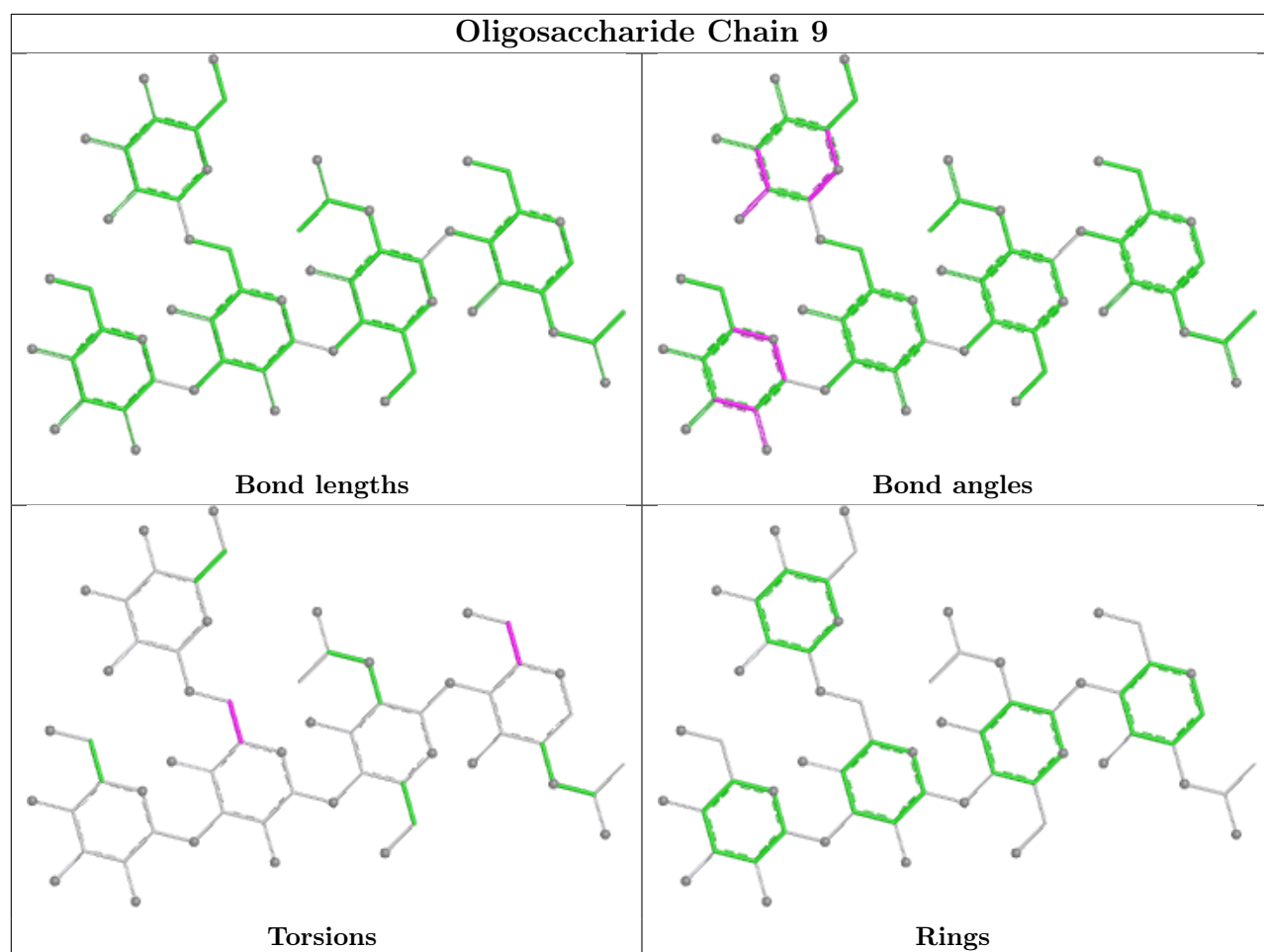


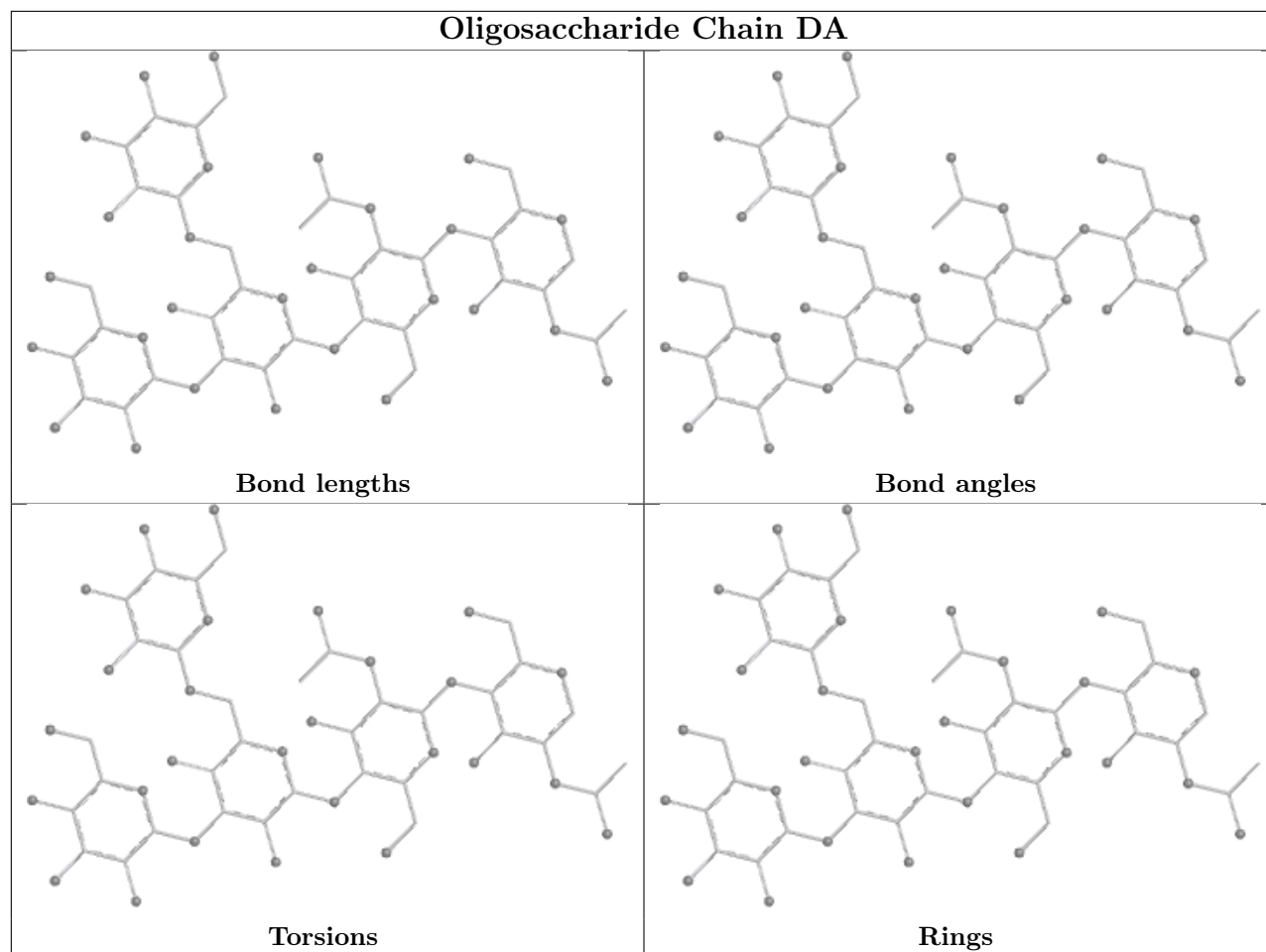


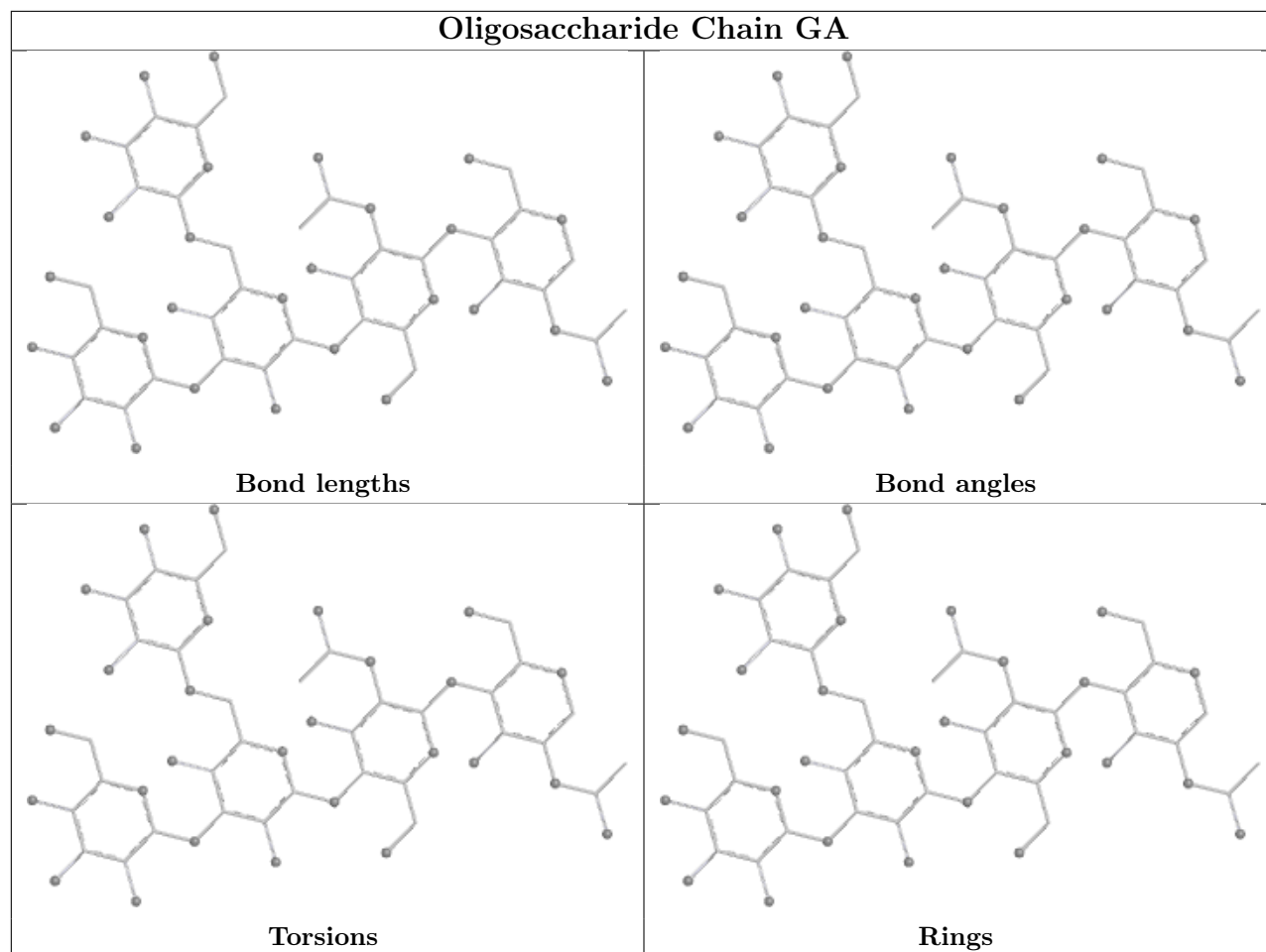


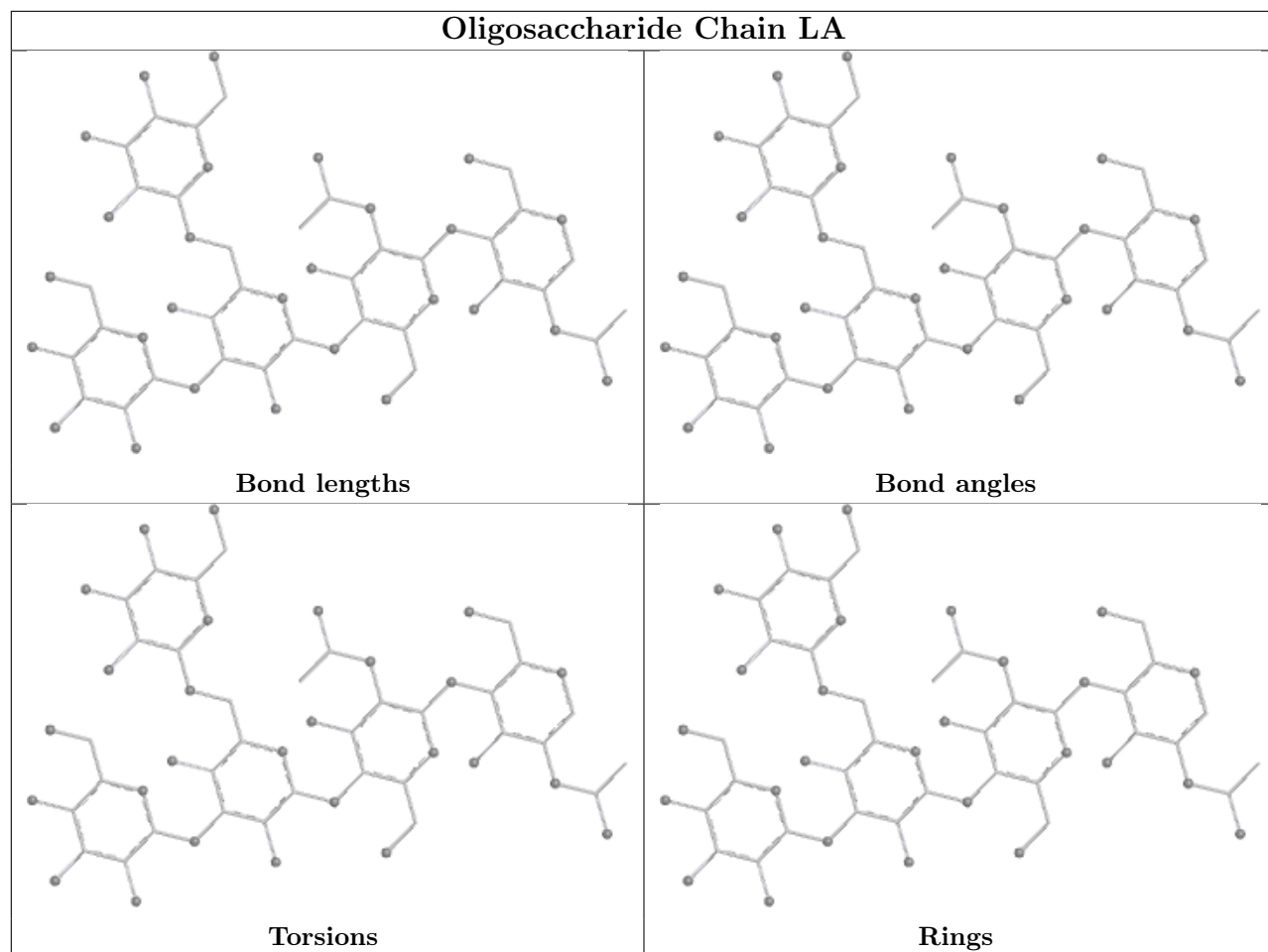


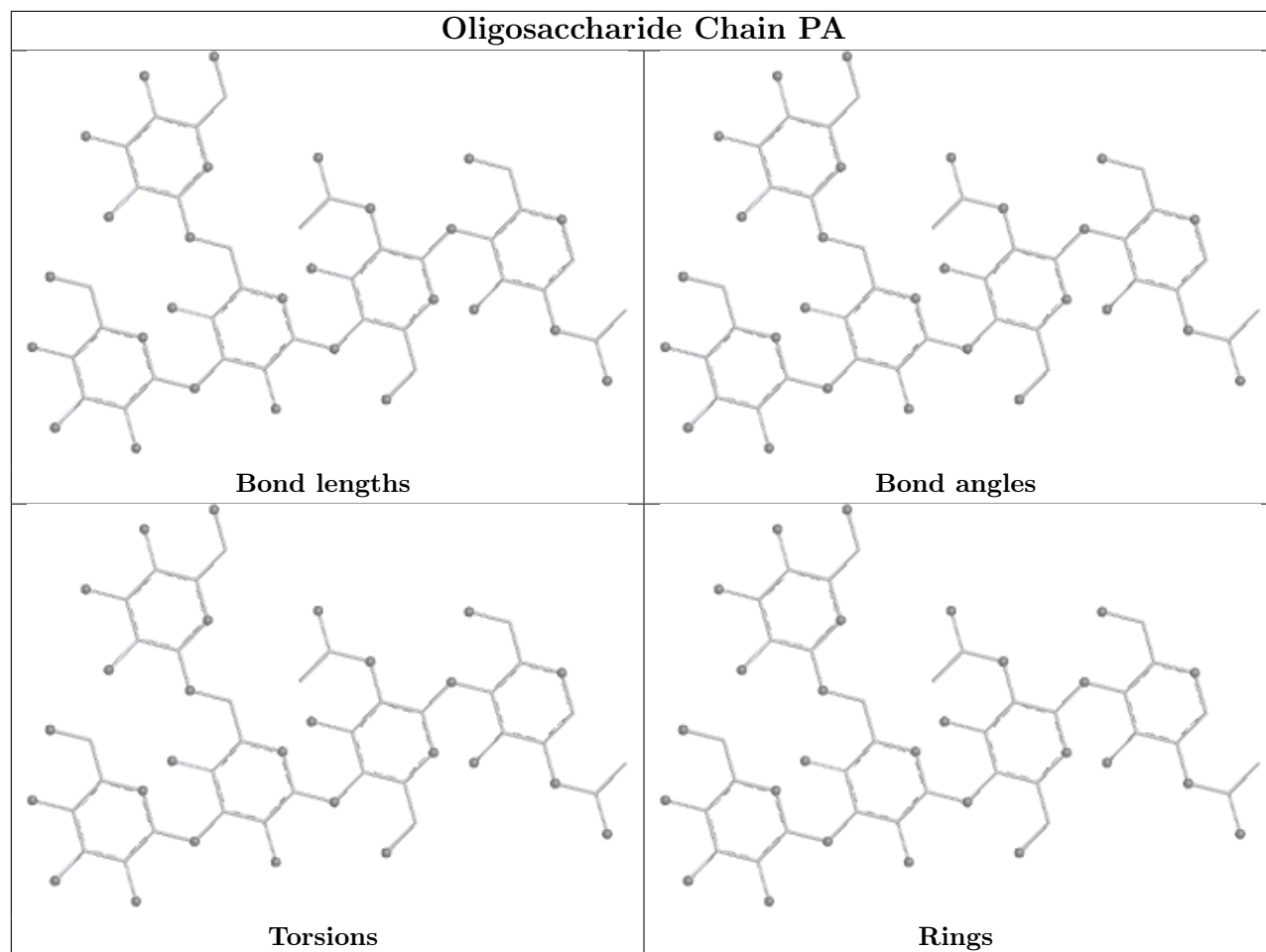


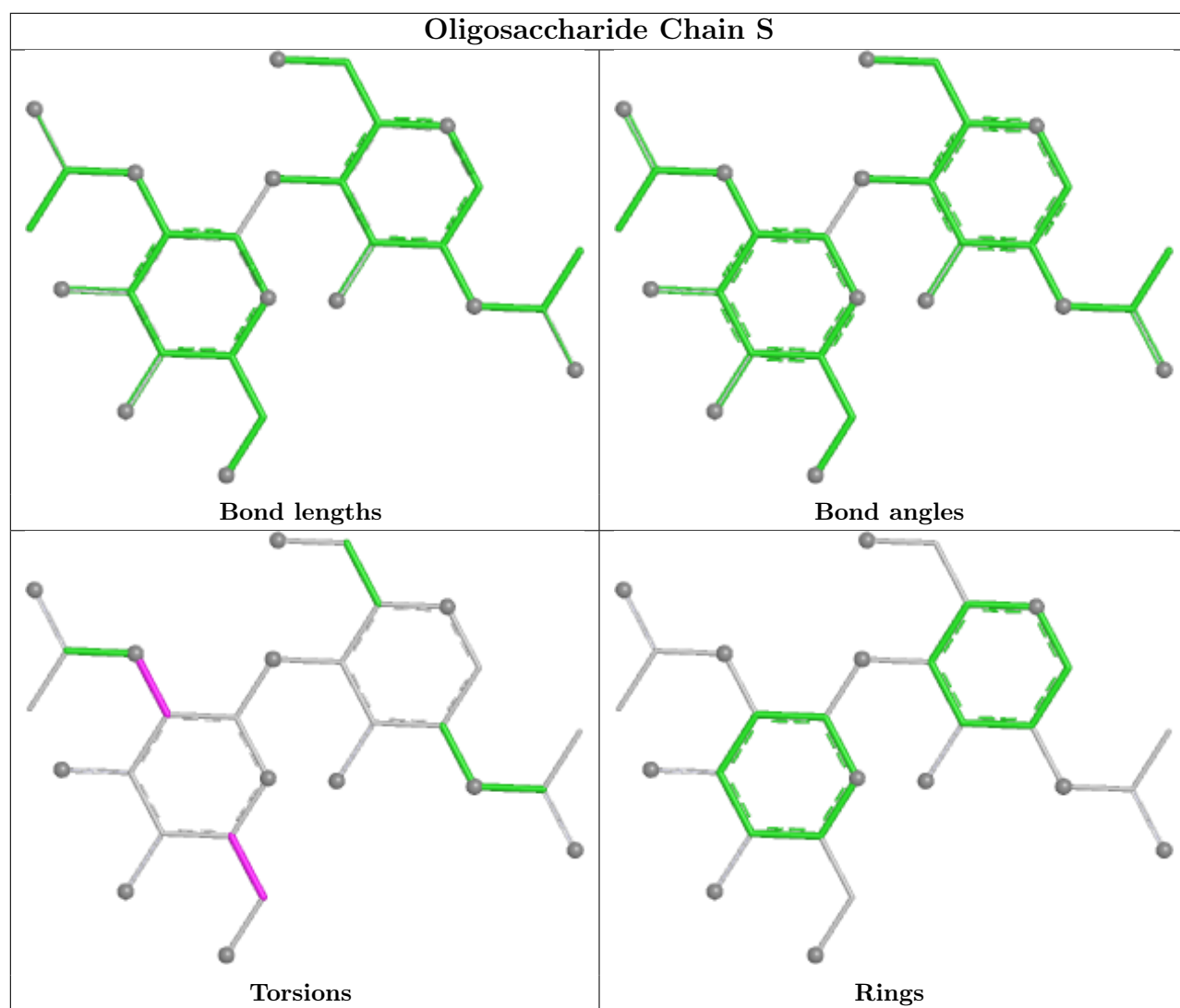


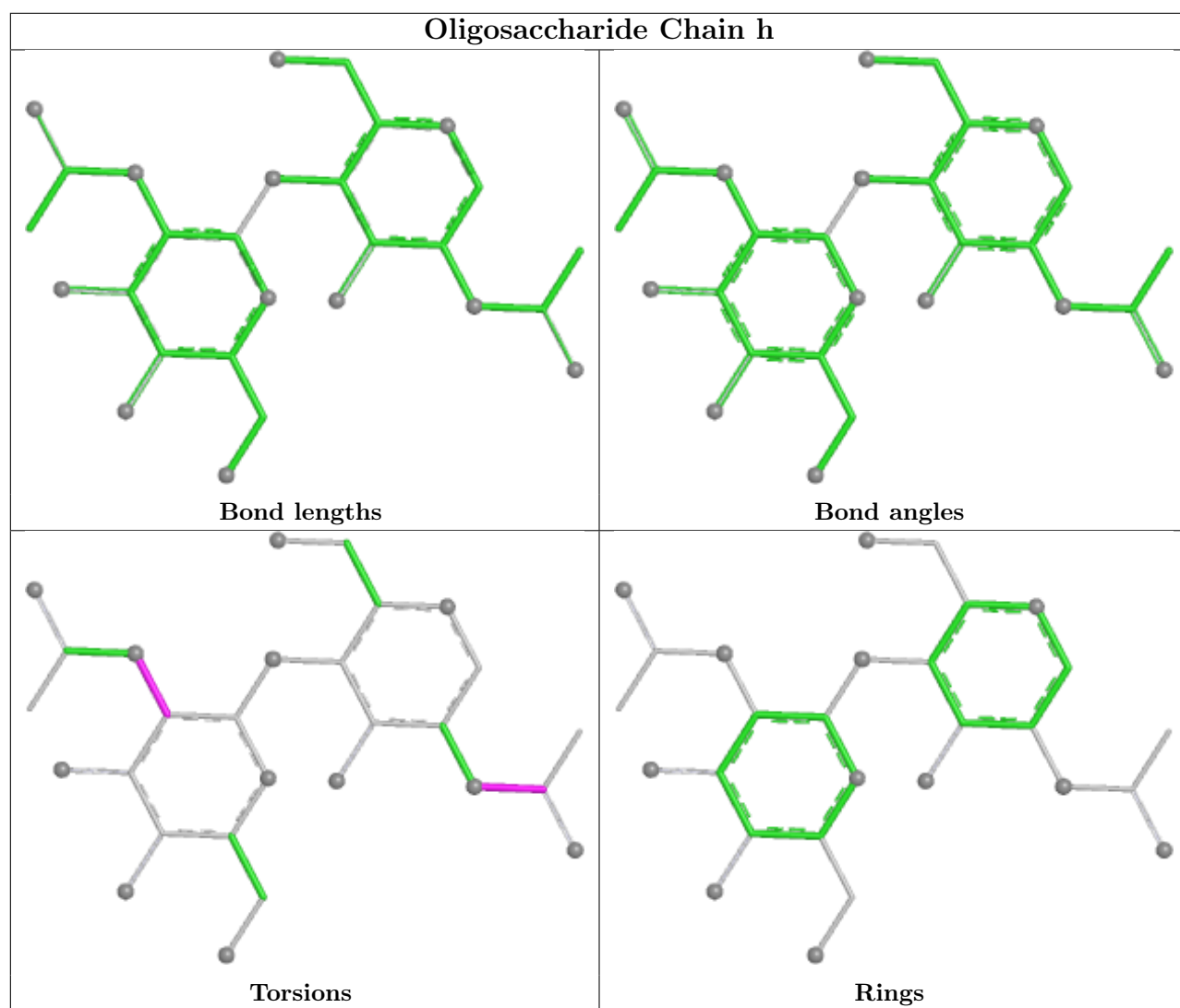


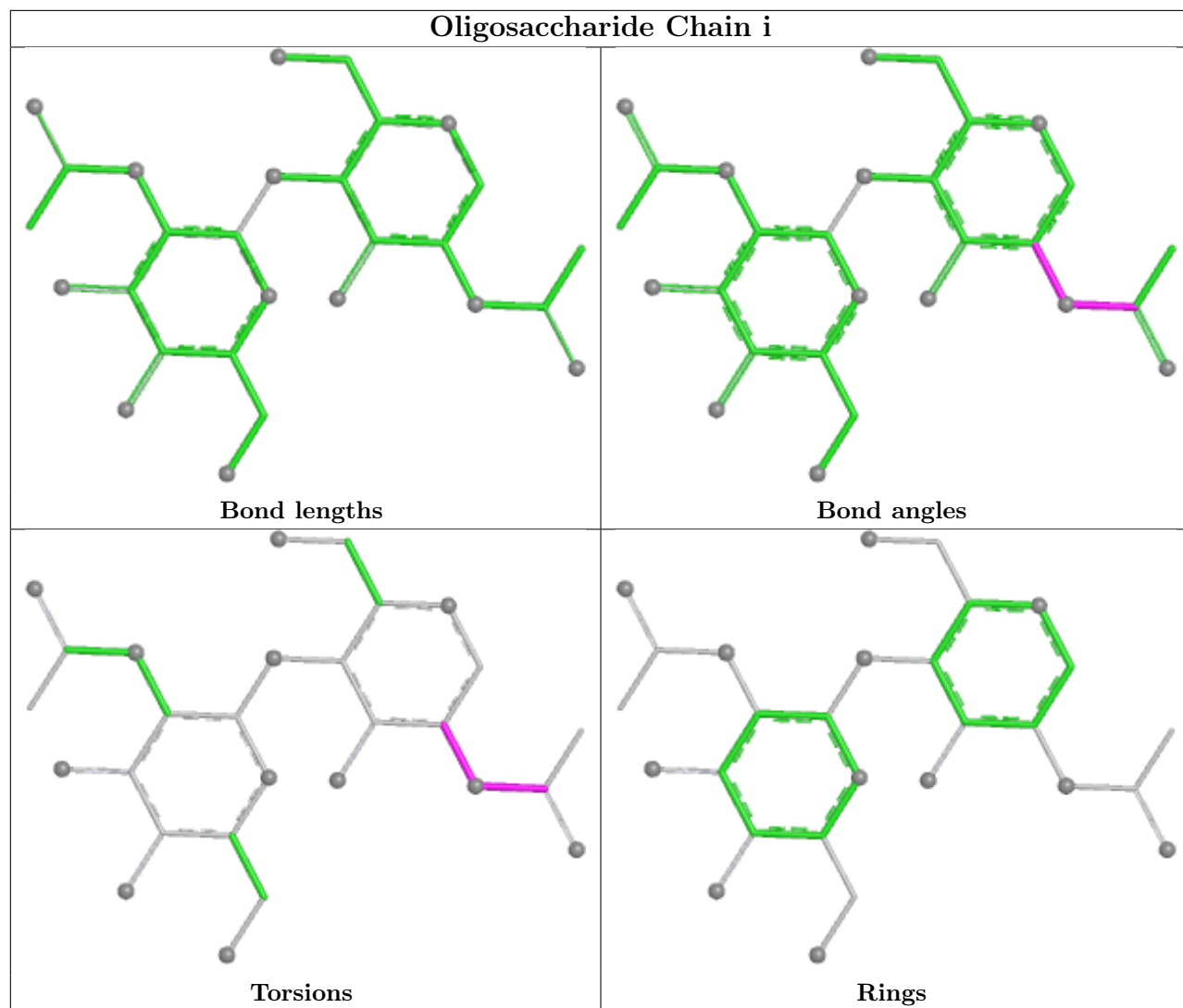


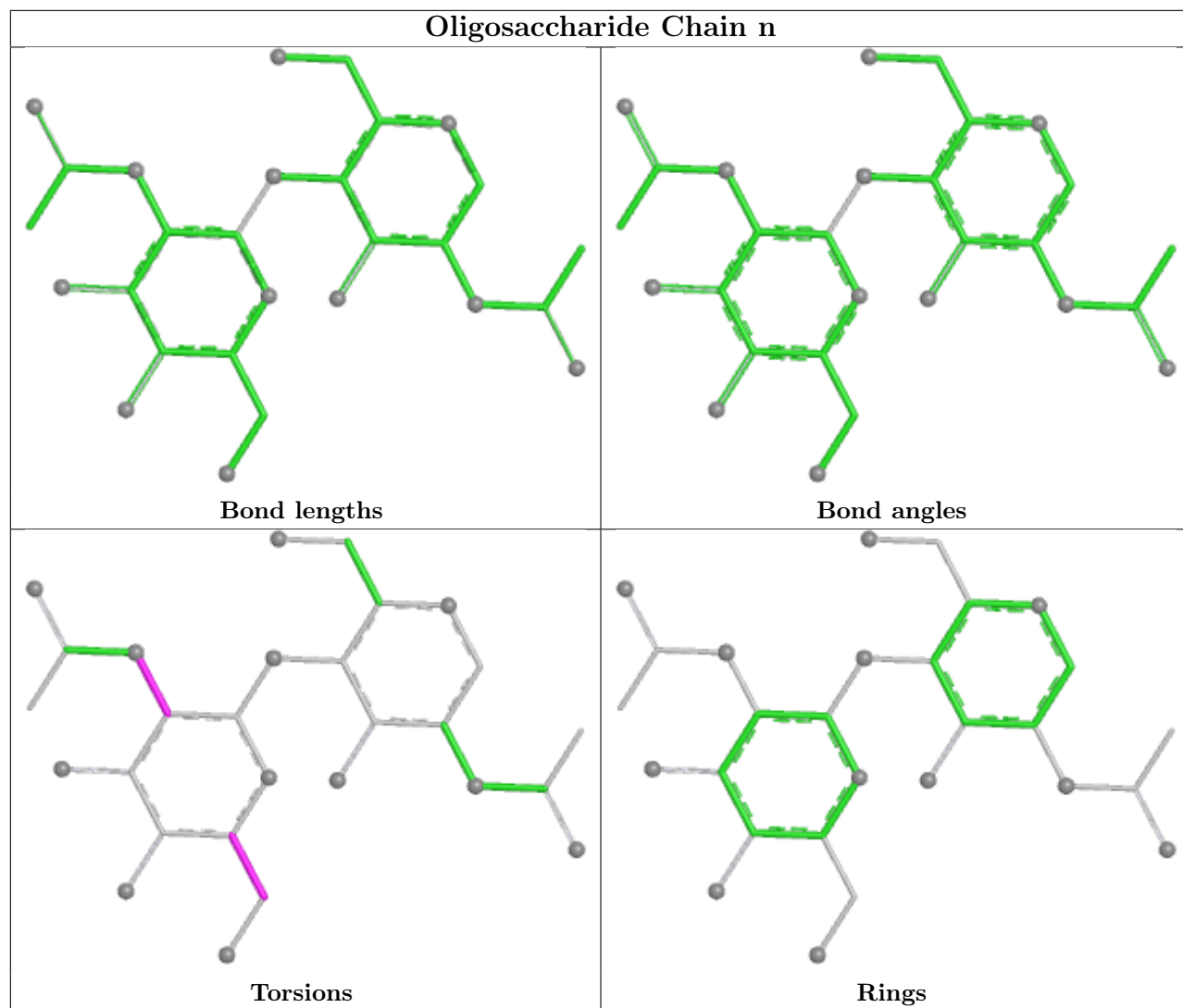


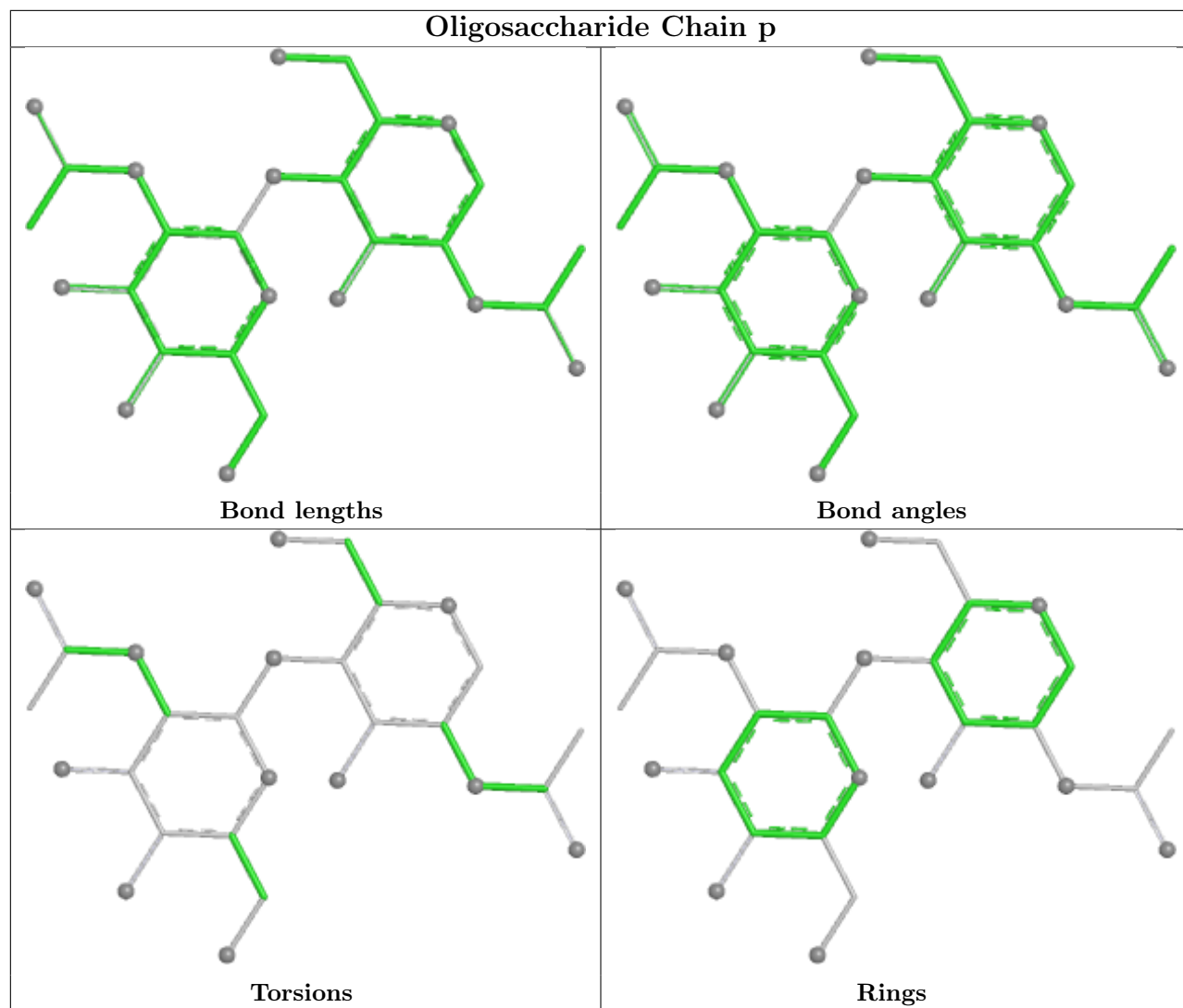


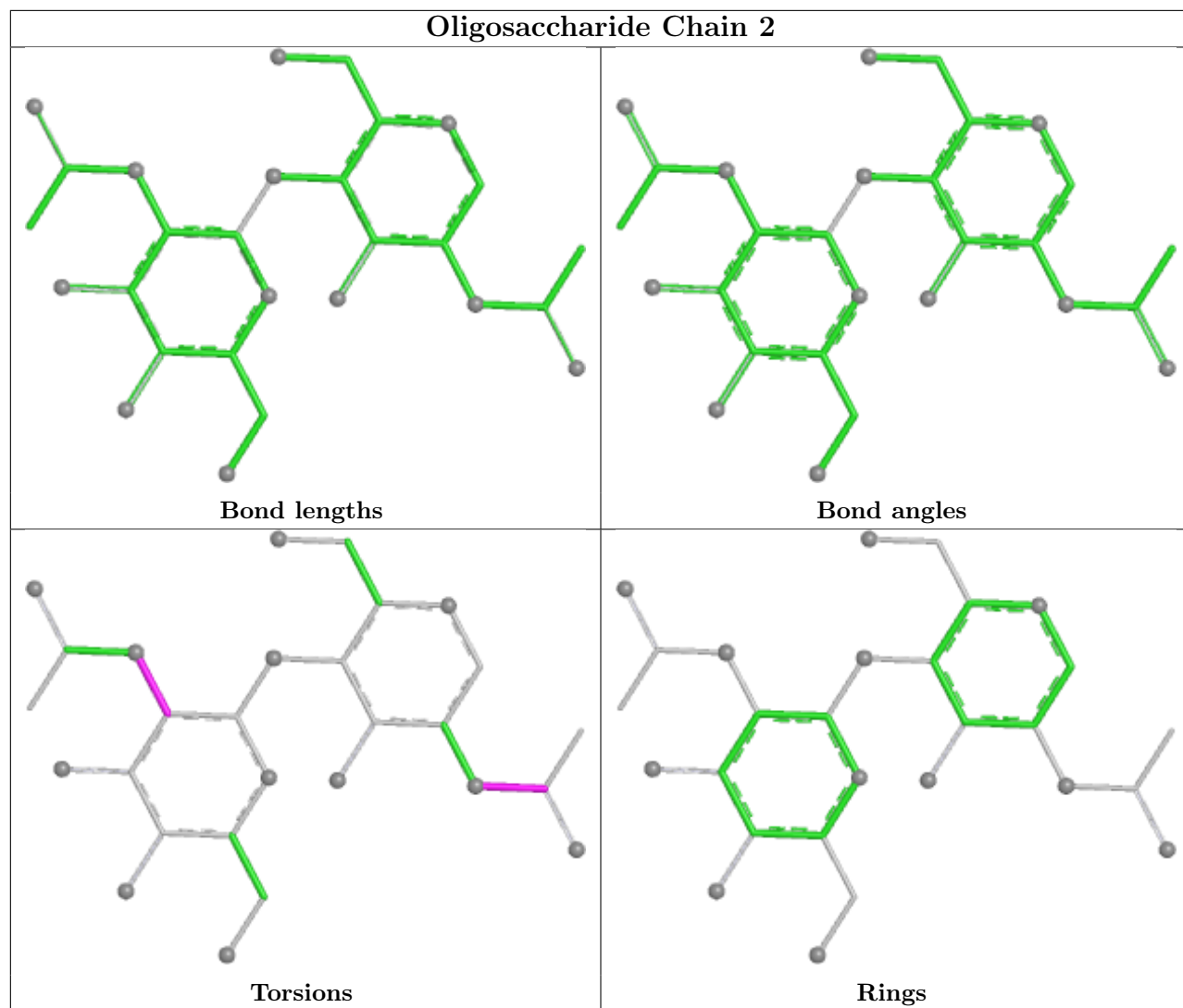


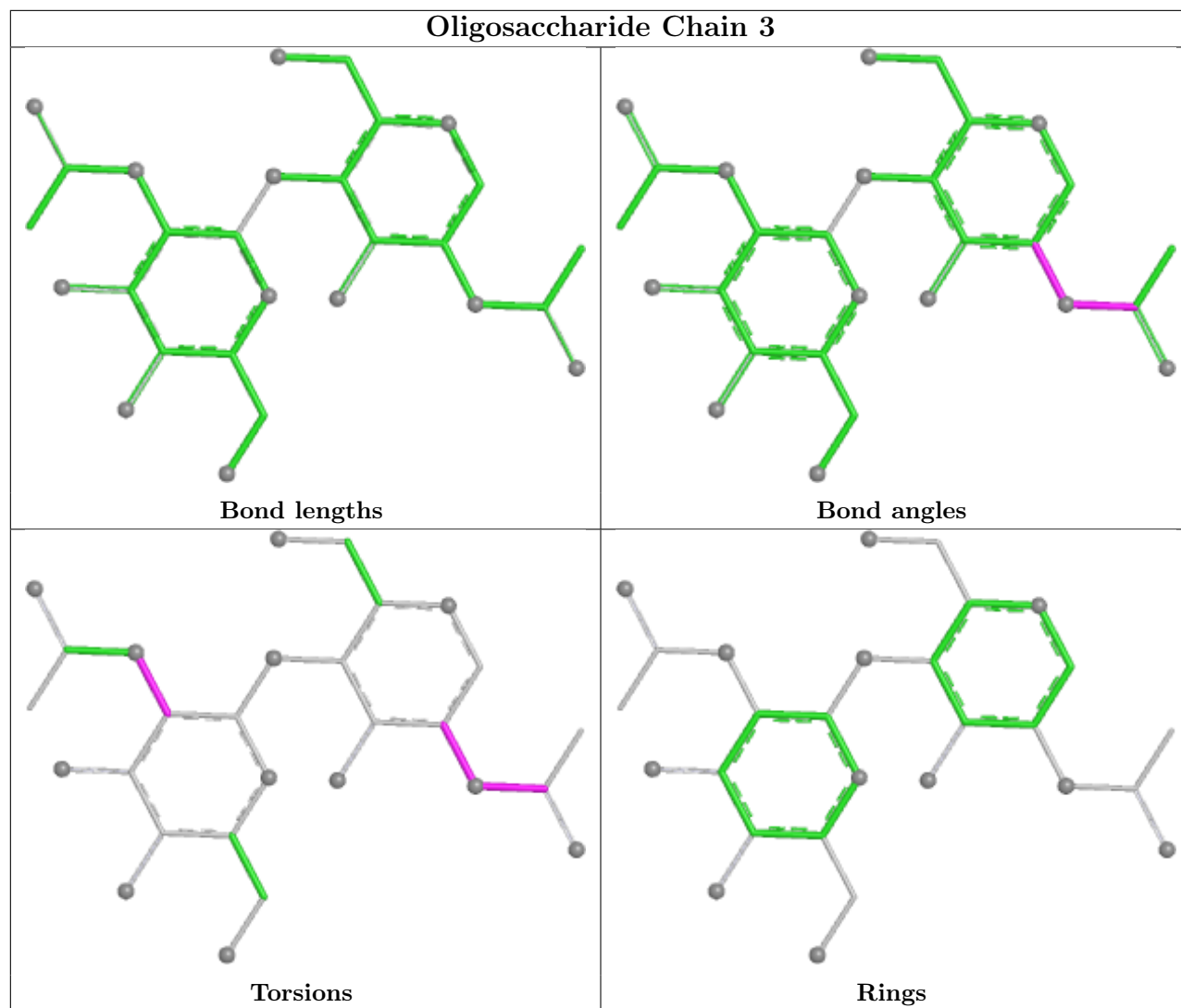


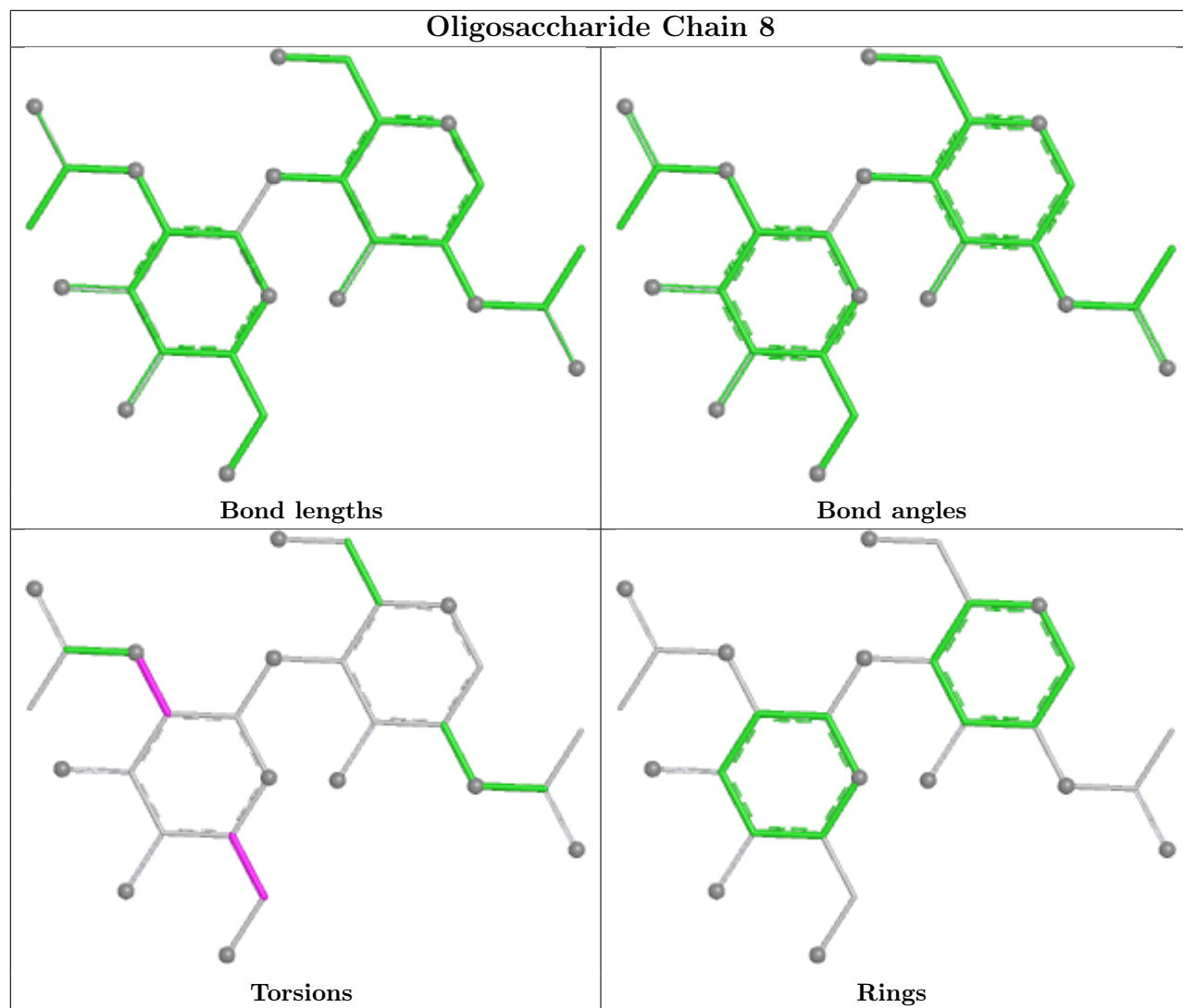


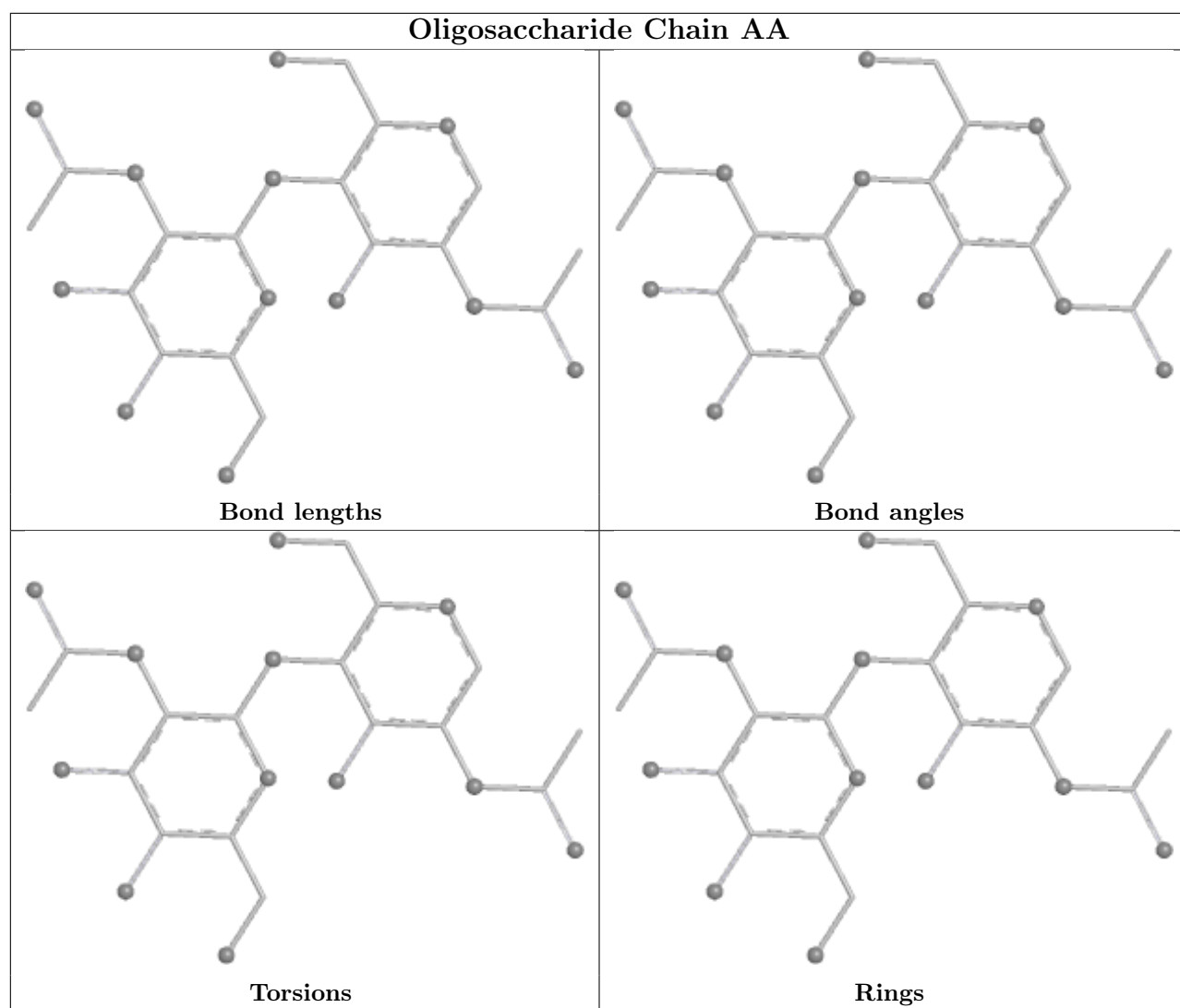


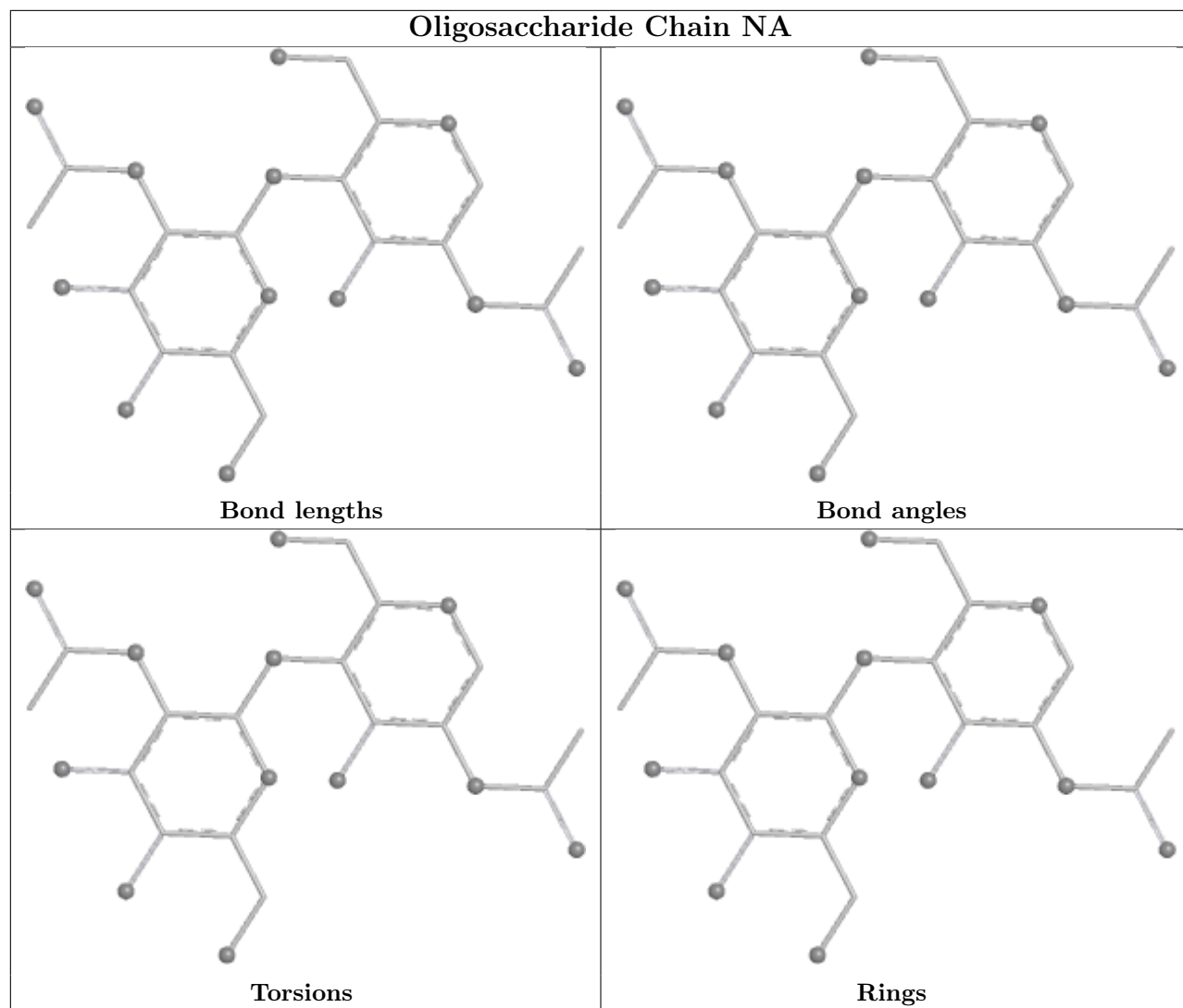


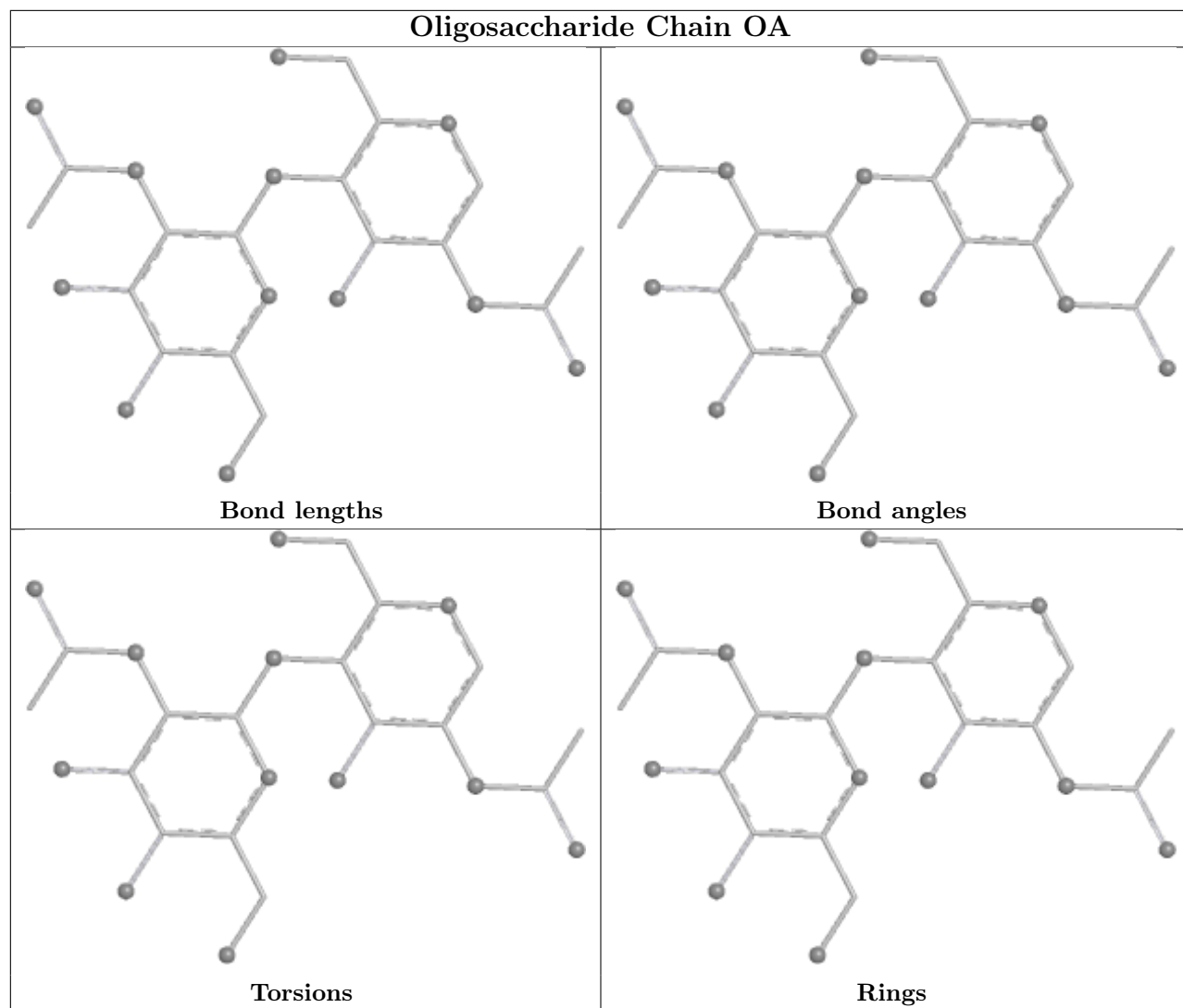


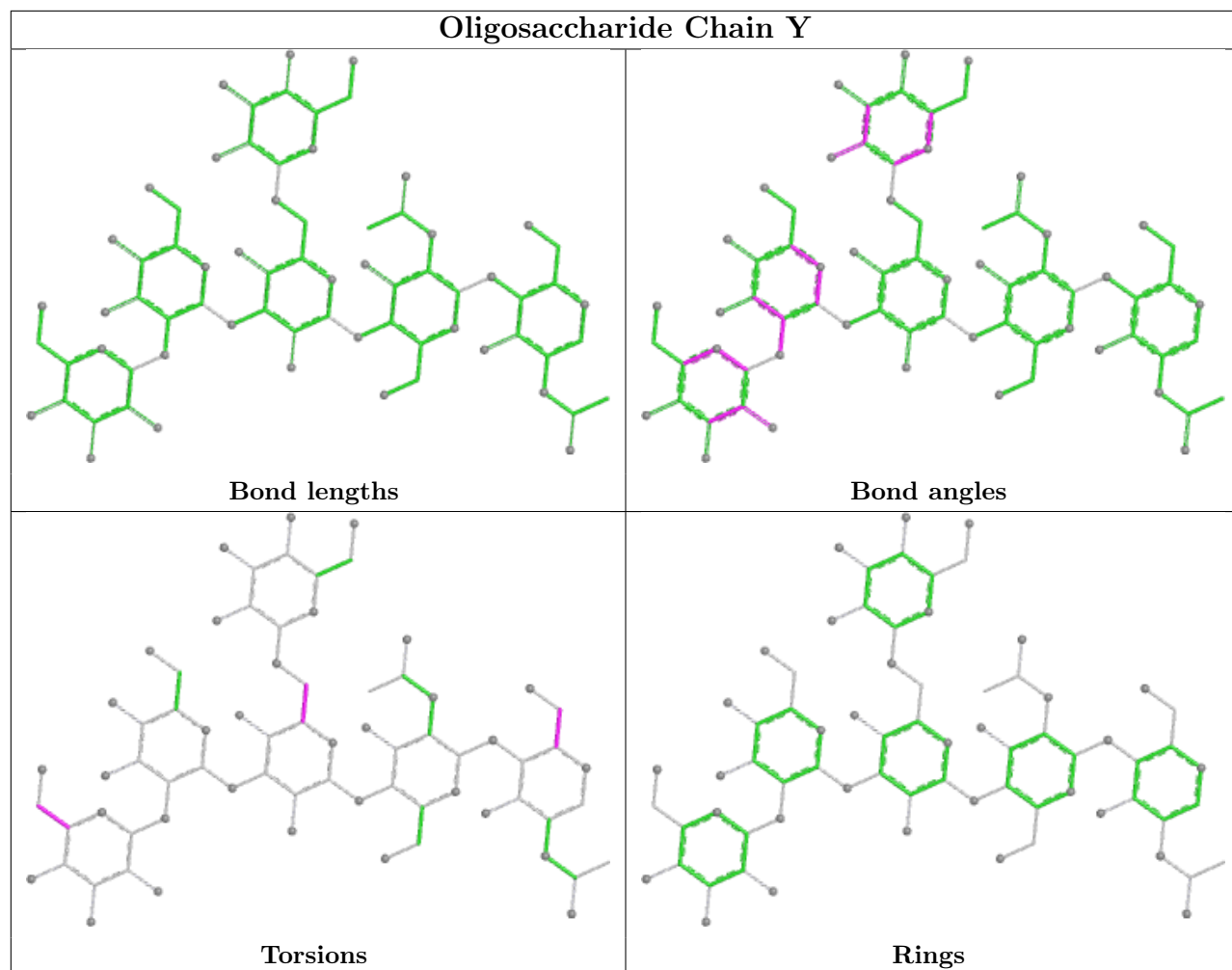


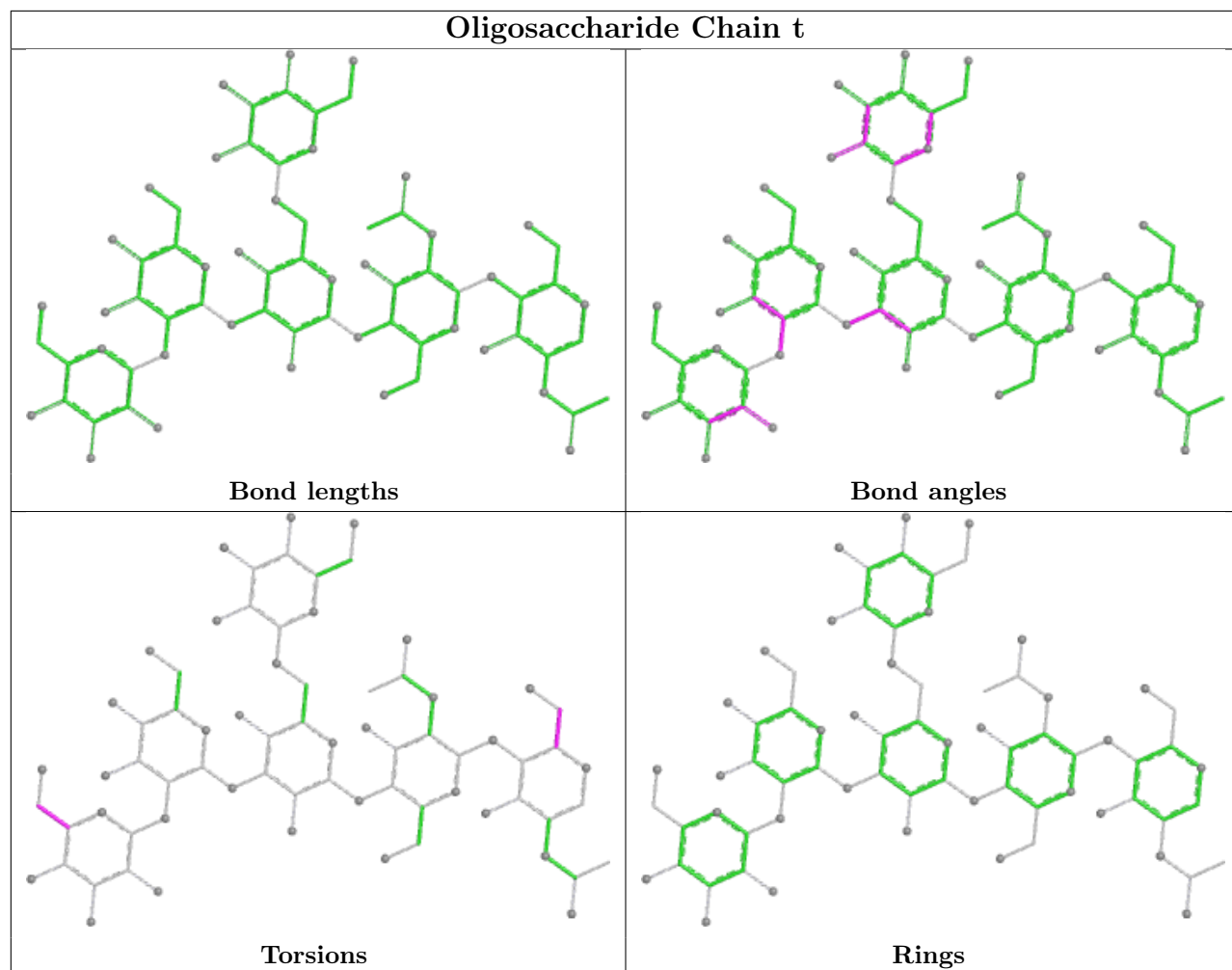


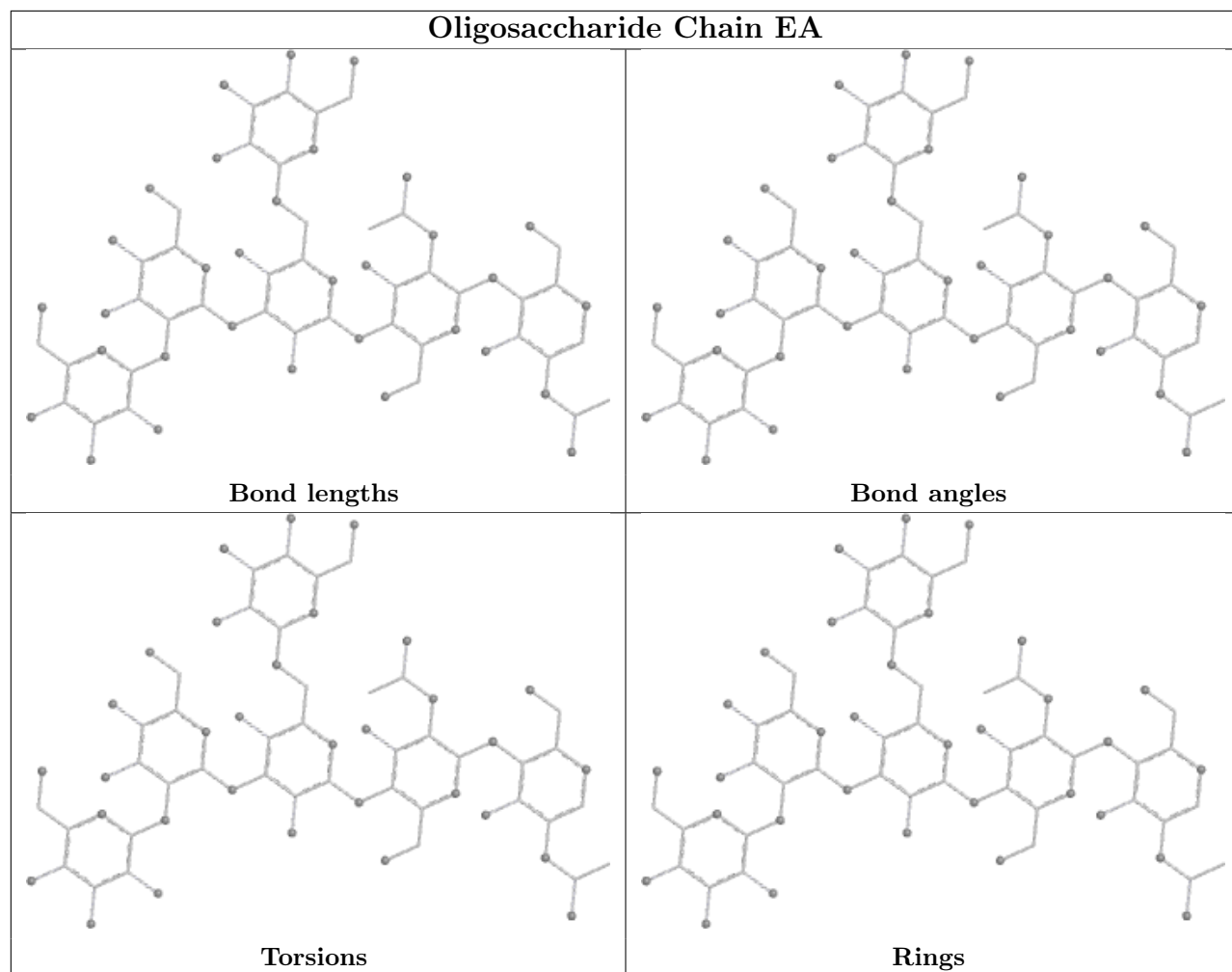


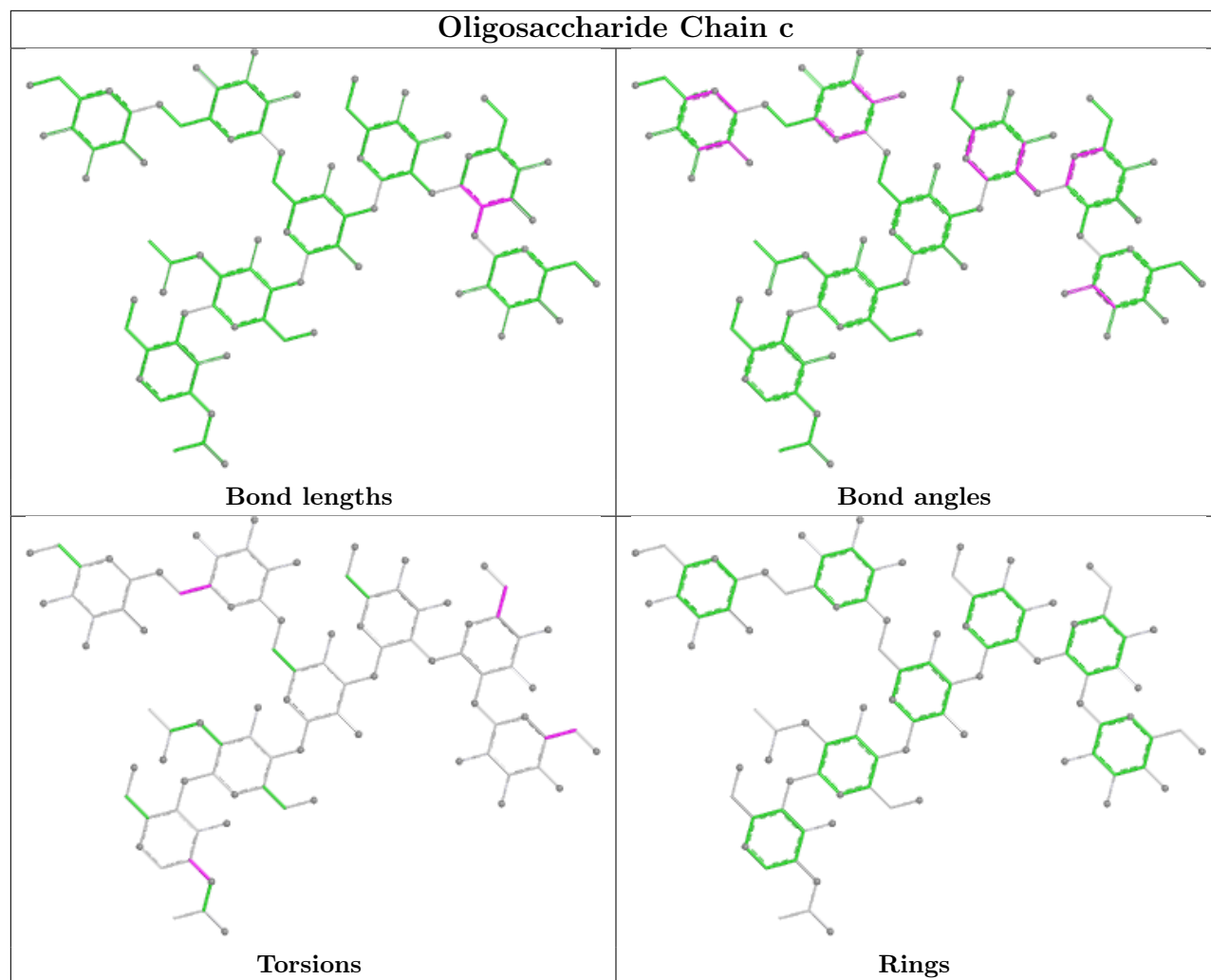


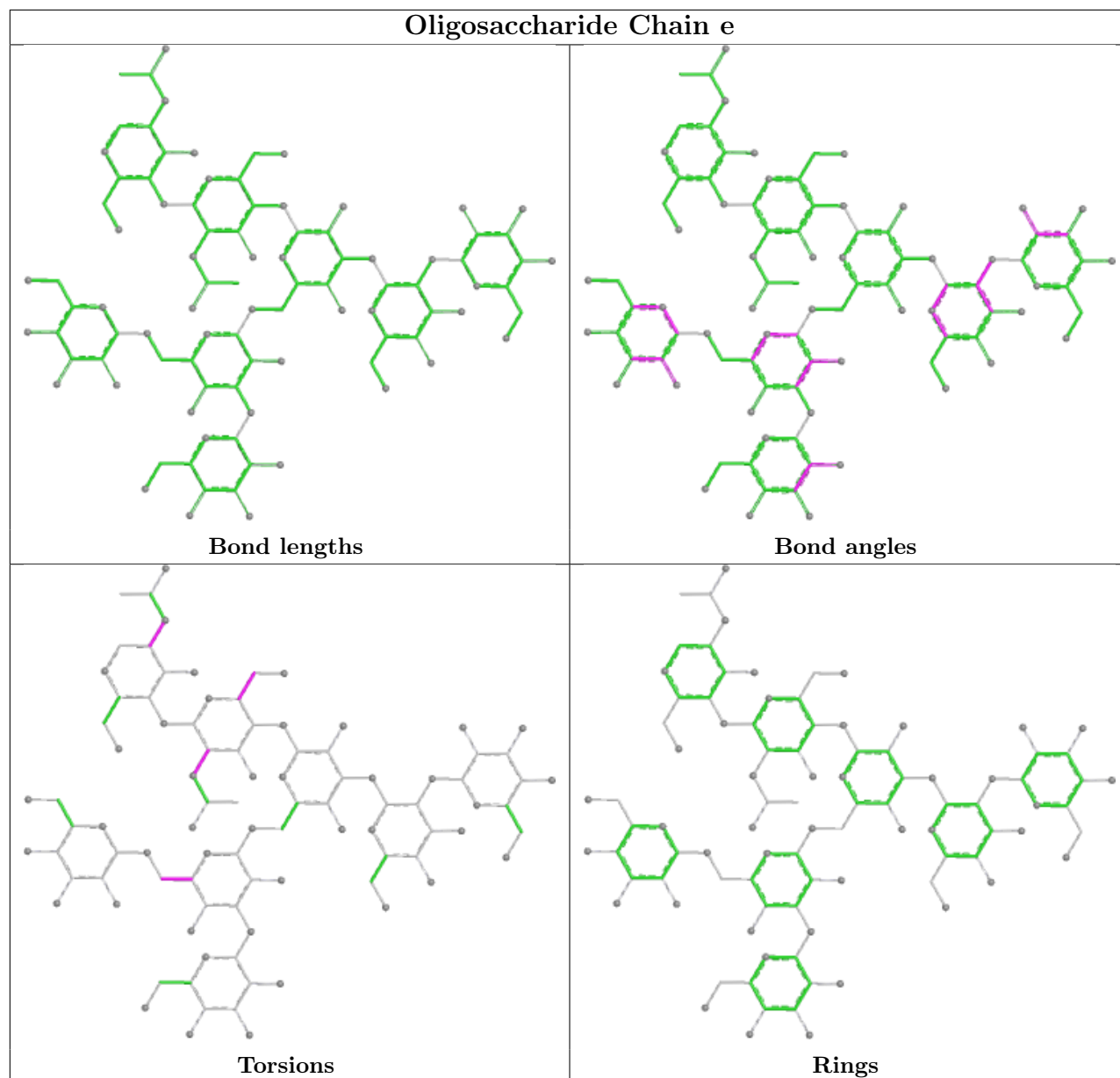


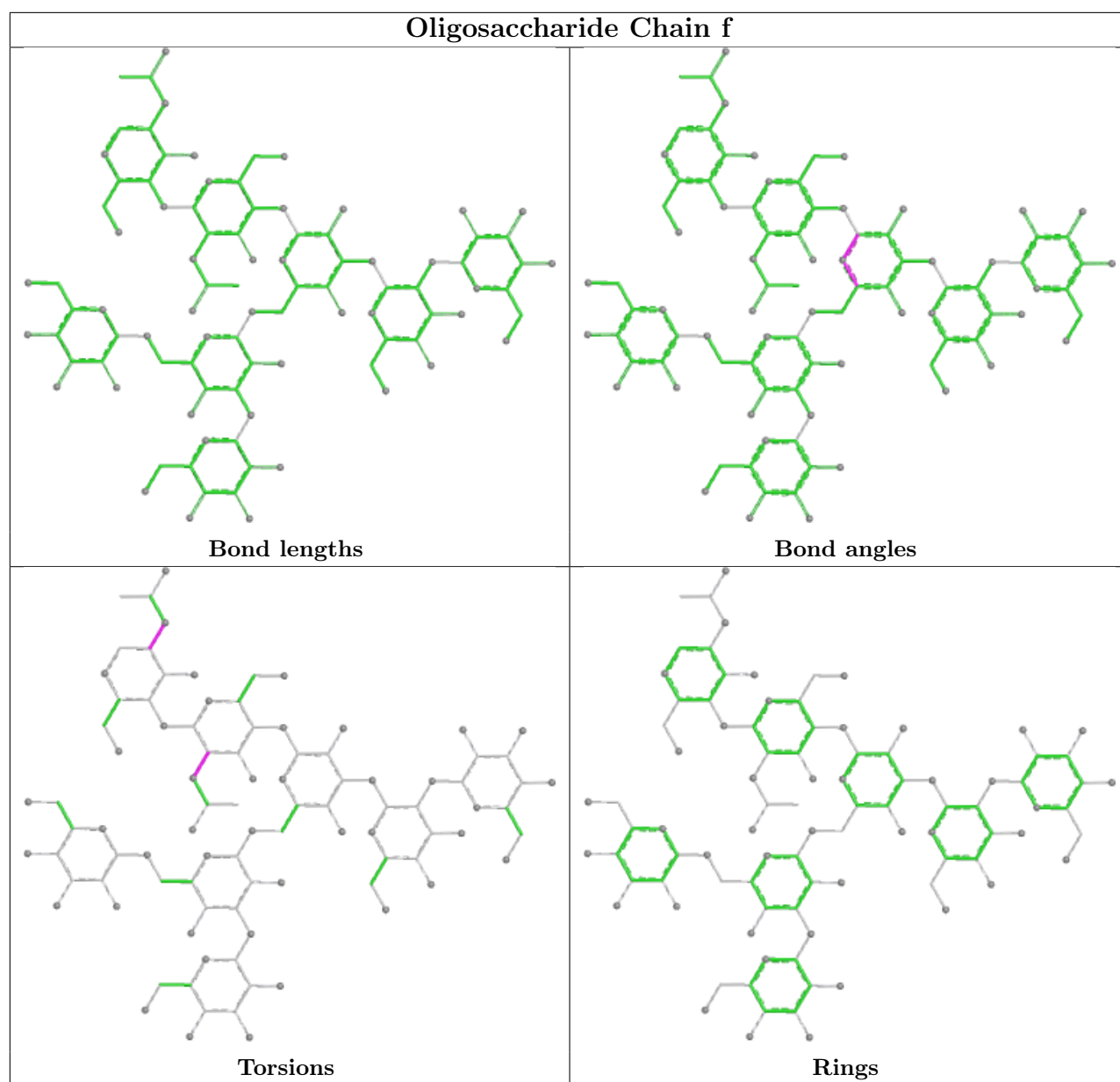


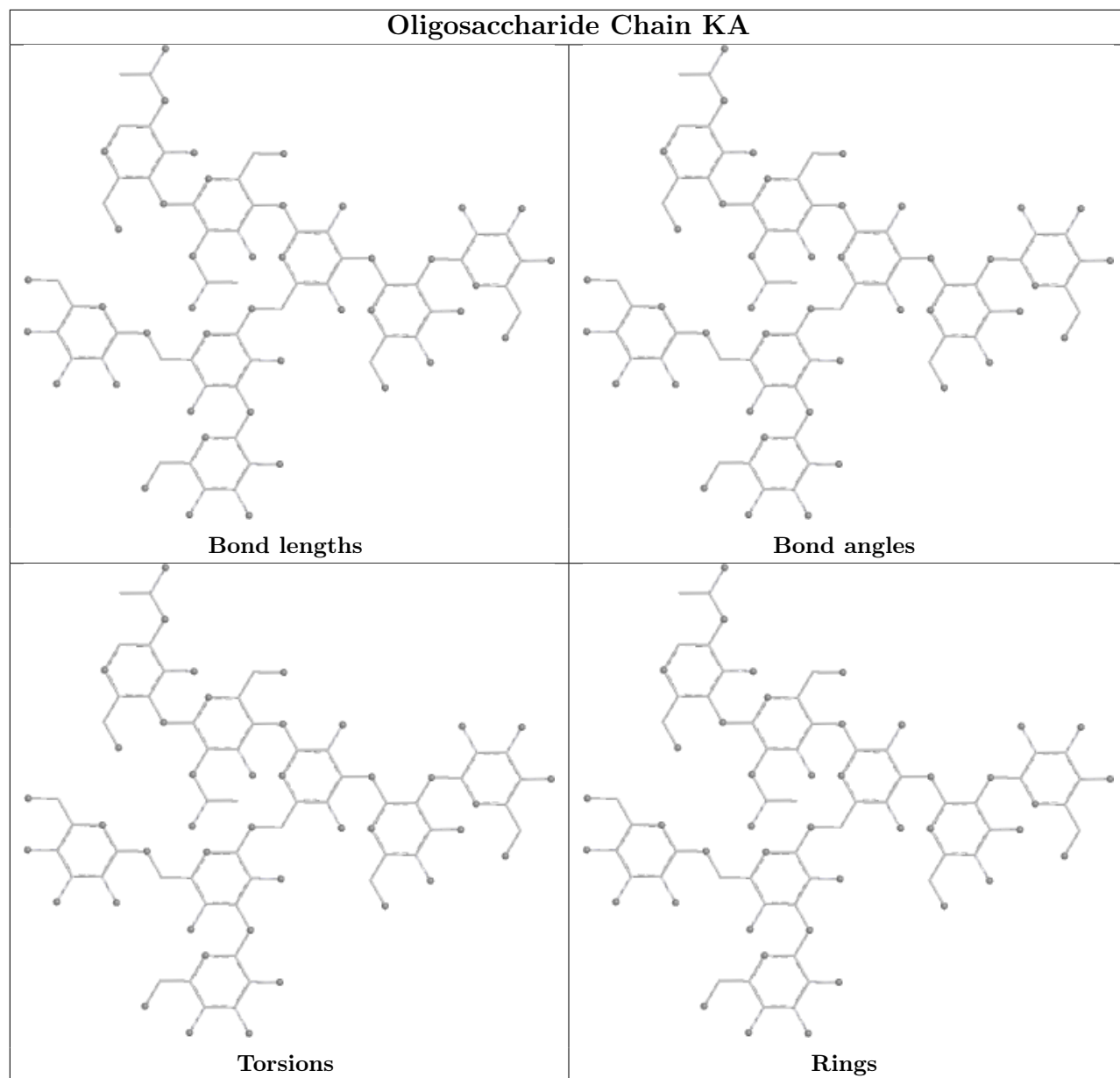


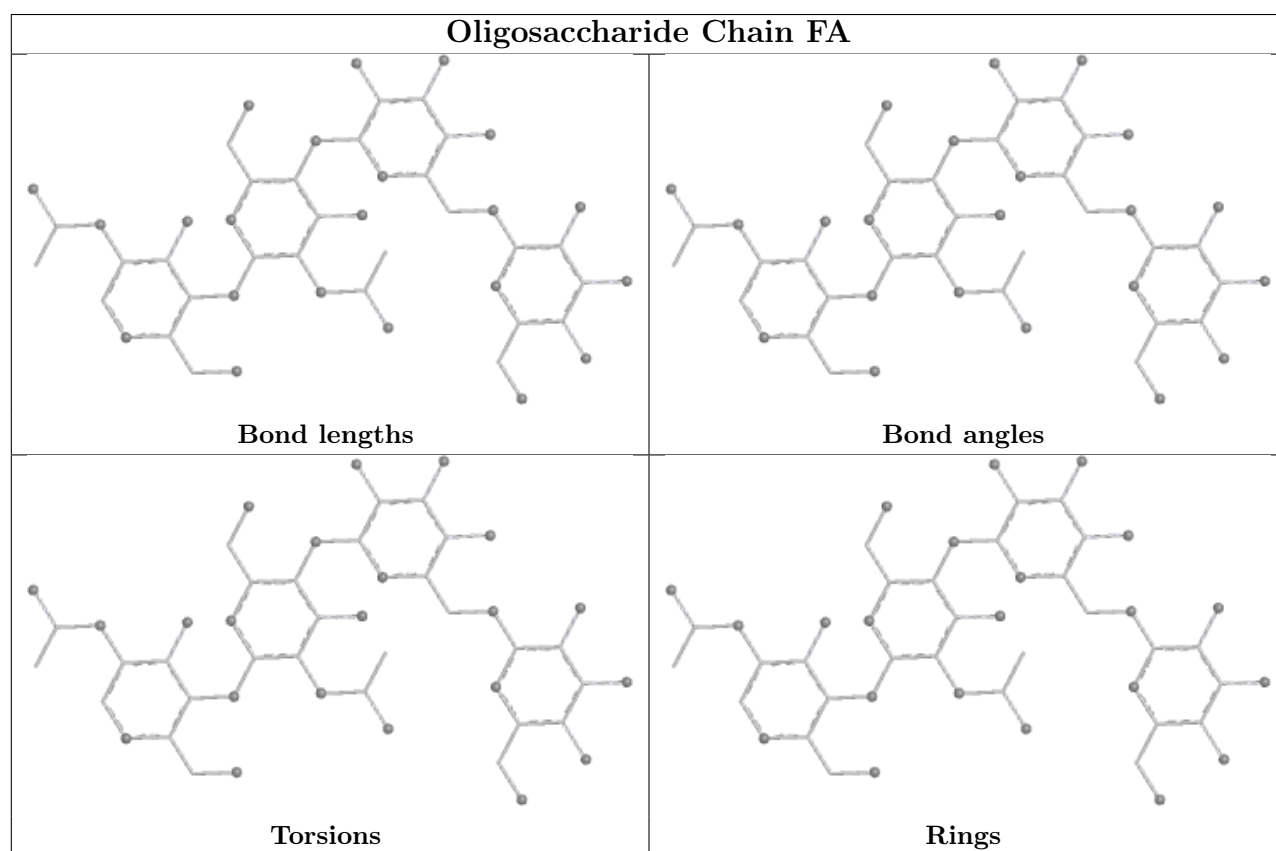
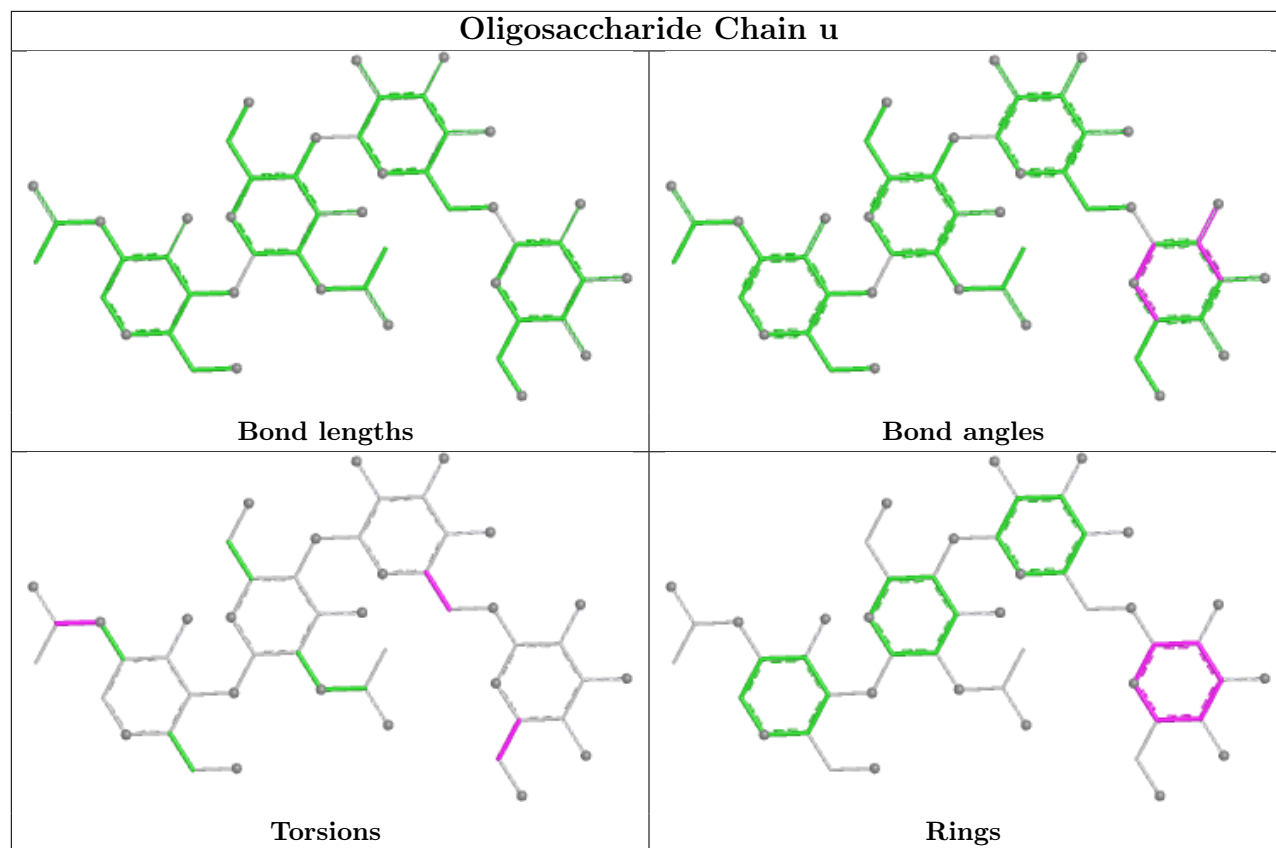
Oligosaccharide Chain EA

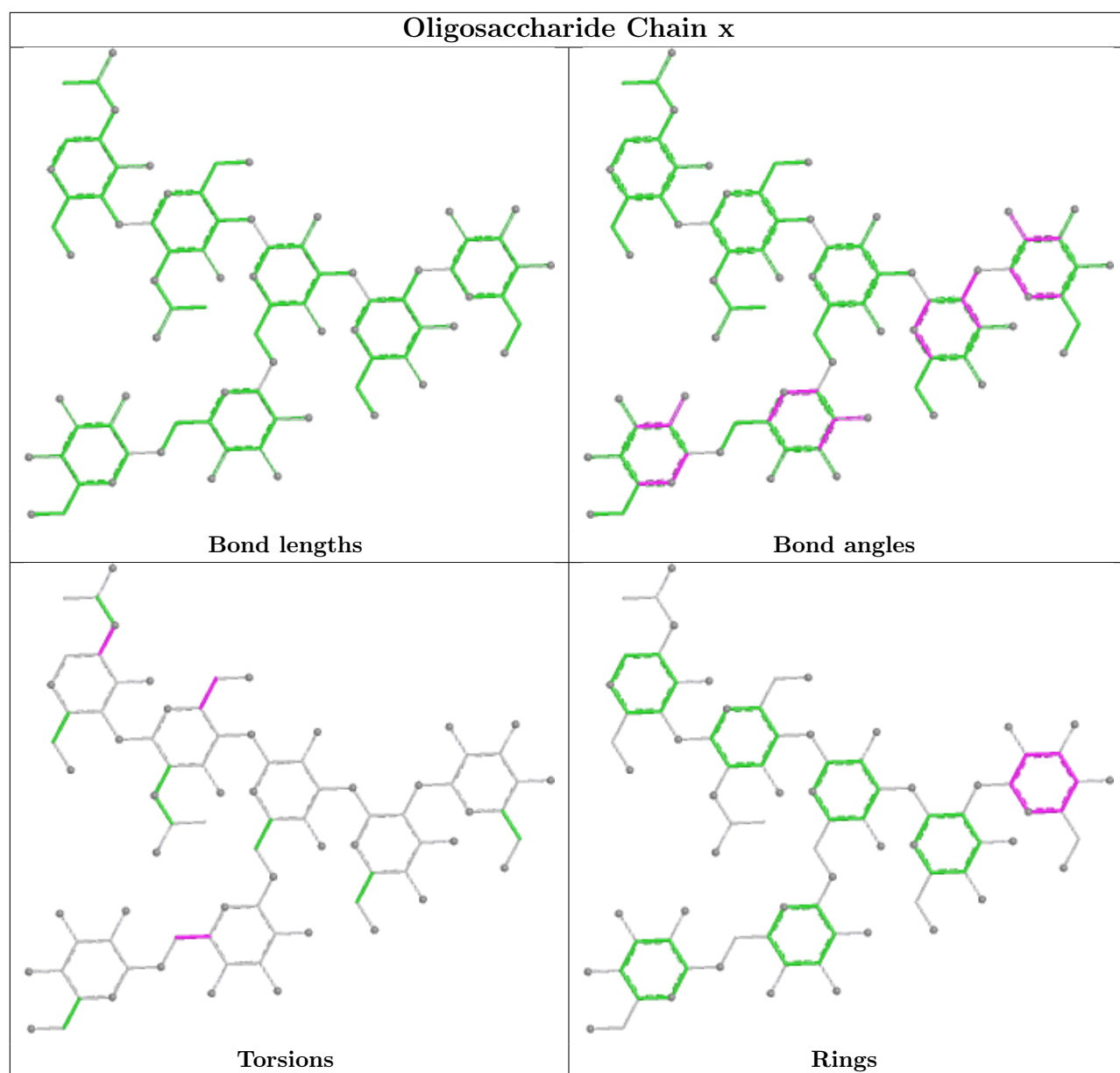


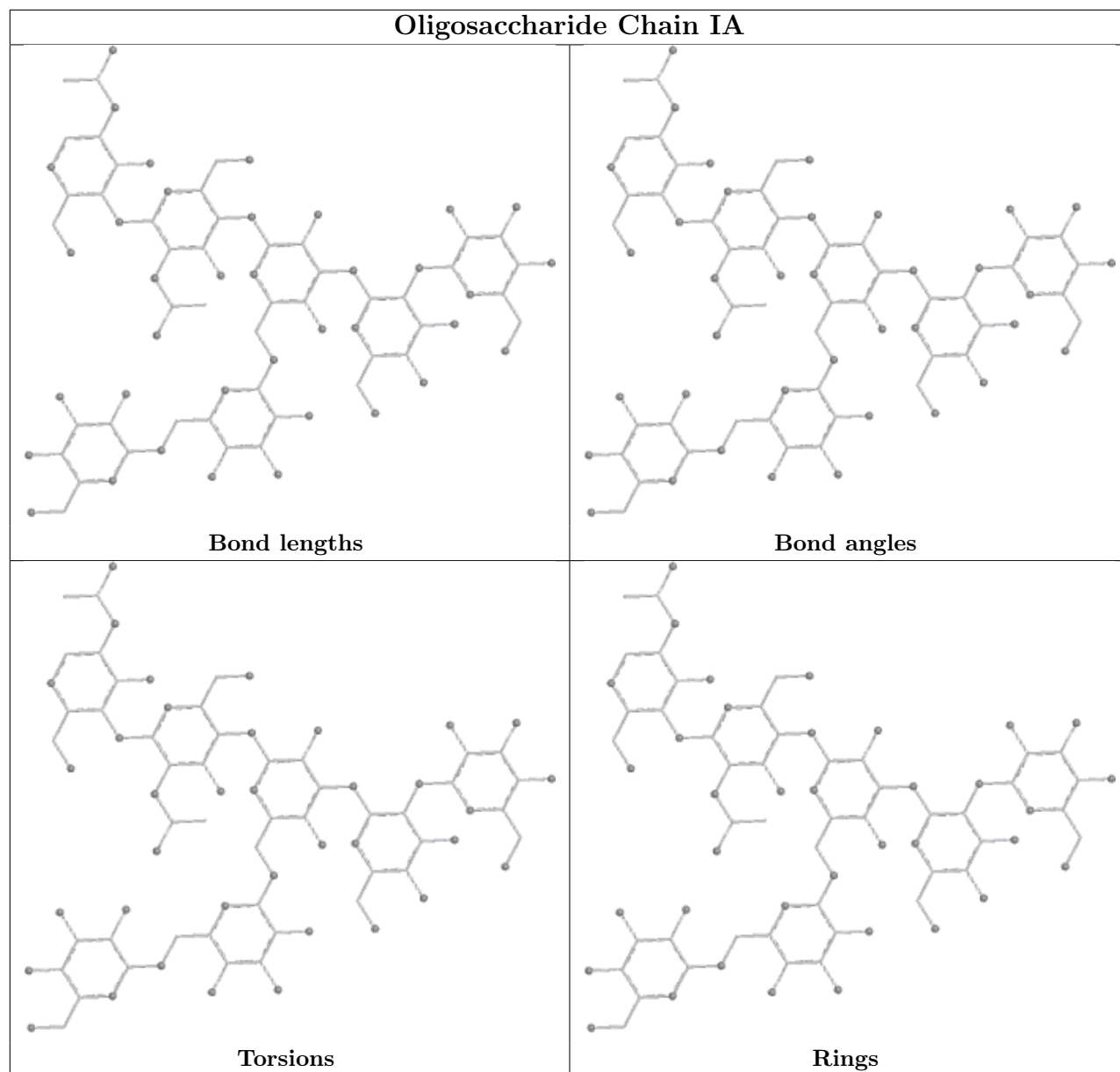


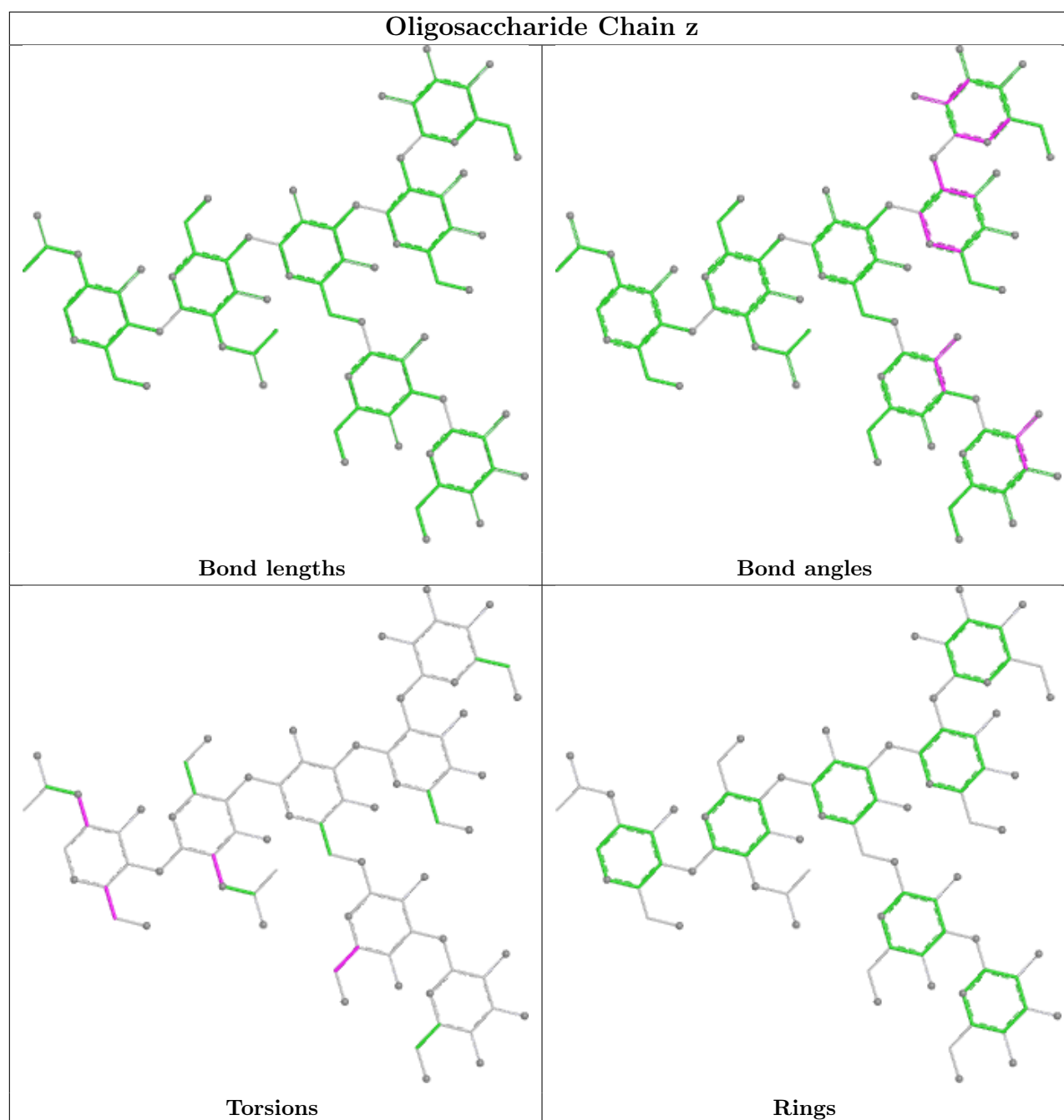












5.6 Ligand geometry [i](#)

4 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
15	NAG	F	602	2	14,14,15	0.24	0	17,19,21	0.46	0
16	MAN	F	601	-	11,11,12	0.66	0	15,15,17	0.99	2 (13%)
15	NAG	E	601	2	14,14,15	0.28	0	17,19,21	0.48	0
15	NAG	G	601	2	14,14,15	0.23	0	17,19,21	0.44	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
15	NAG	F	602	2	-	0/6/23/26	0/1/1/1
16	MAN	F	601	-	-	0/2/19/22	0/1/1/1
15	NAG	E	601	2	-	0/6/23/26	0/1/1/1
15	NAG	G	601	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	F	601	MAN	C1-O5-C5	2.27	115.23	112.19
16	F	601	MAN	O2-C2-C3	-2.20	105.60	110.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	F	602	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

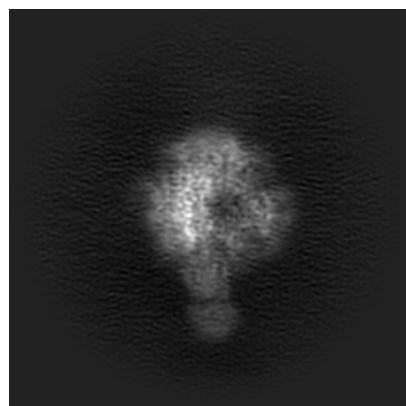
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27735. These allow visual inspection of the internal detail of the map and identification of artifacts.

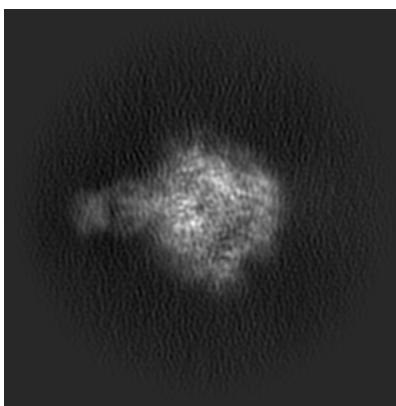
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

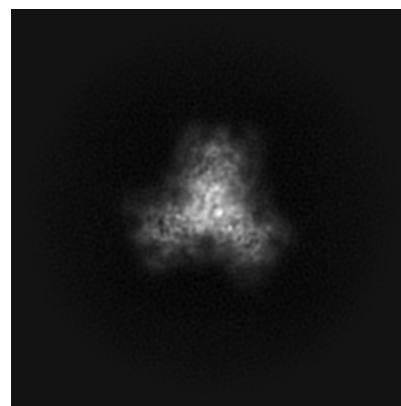
6.1.1 Primary map



X

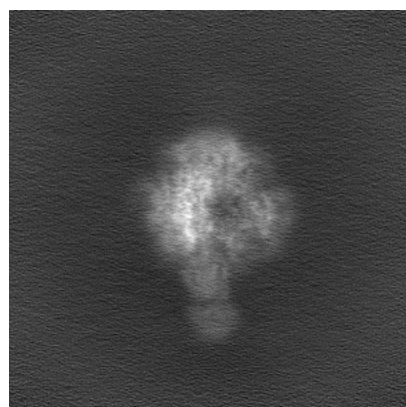


Y

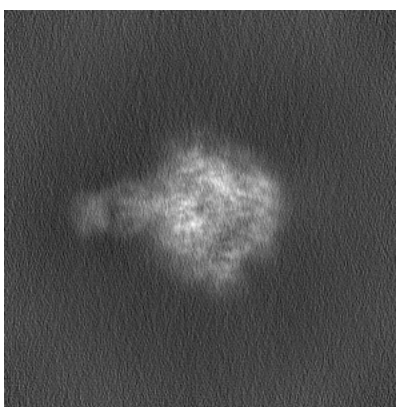


Z

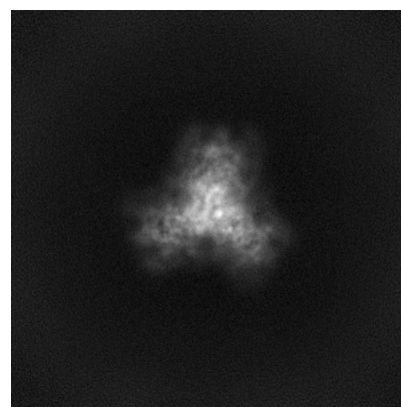
6.1.2 Raw map



X



Y

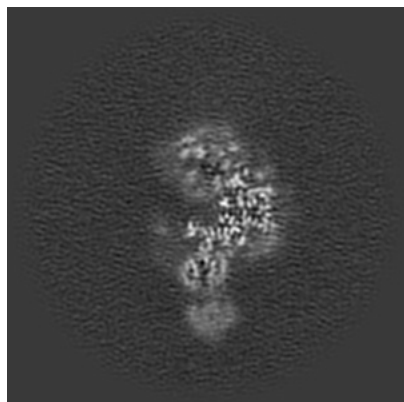


Z

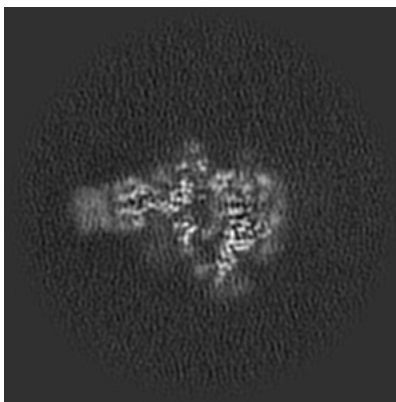
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

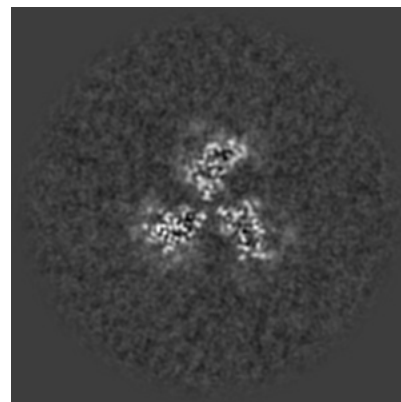
6.2.1 Primary map



X Index: 160

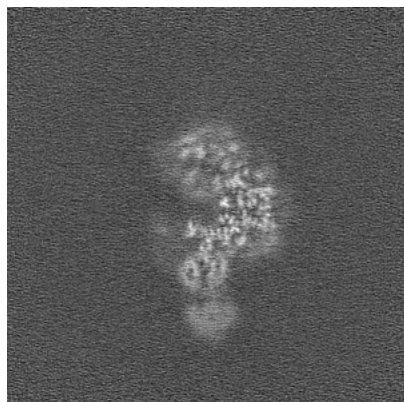


Y Index: 160

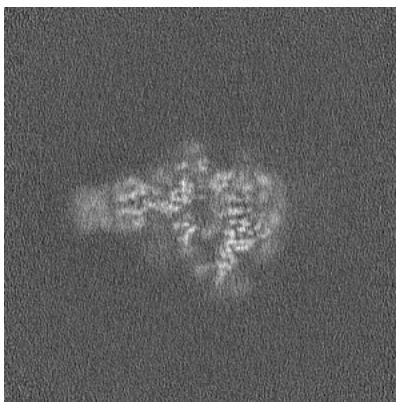


Z Index: 160

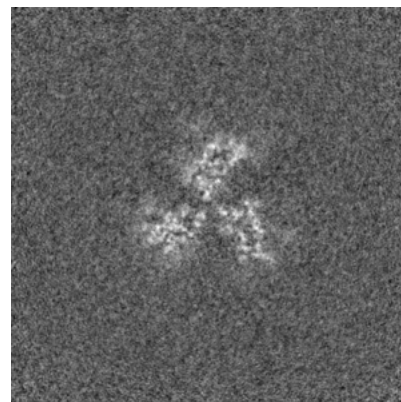
6.2.2 Raw map



X Index: 160



Y Index: 160

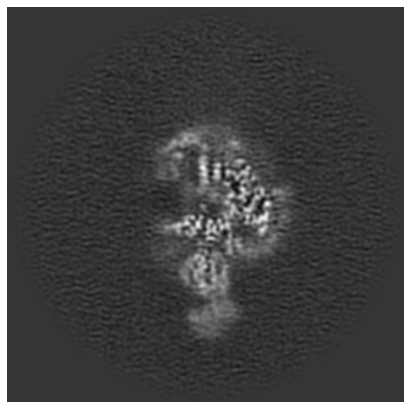


Z Index: 160

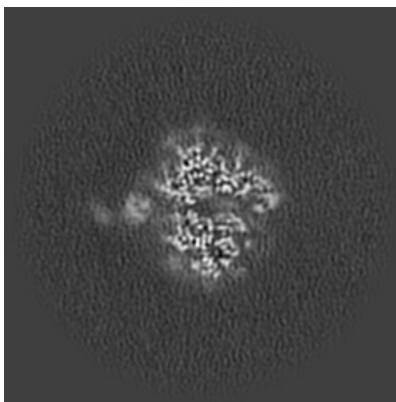
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

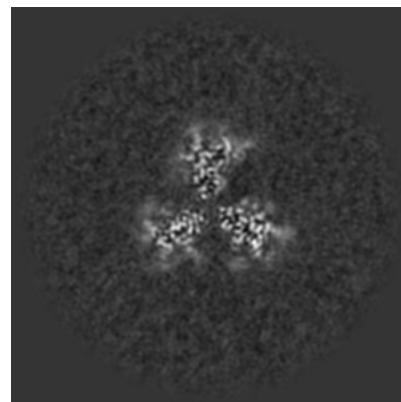
6.3.1 Primary map



X Index: 165

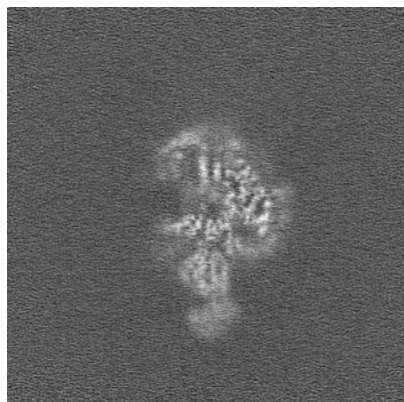


Y Index: 143

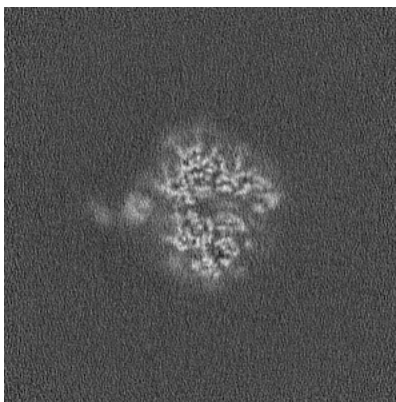


Z Index: 155

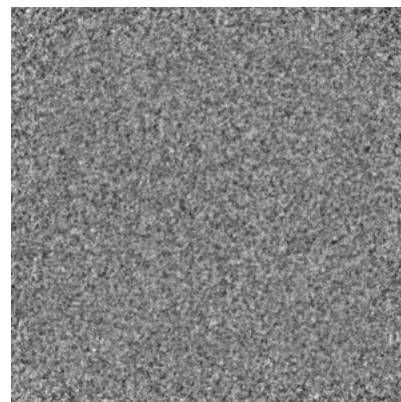
6.3.2 Raw map



X Index: 165



Y Index: 143

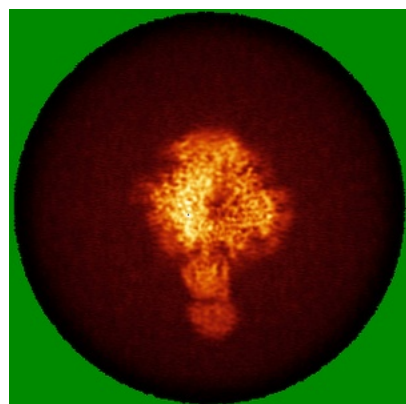


Z Index: 0

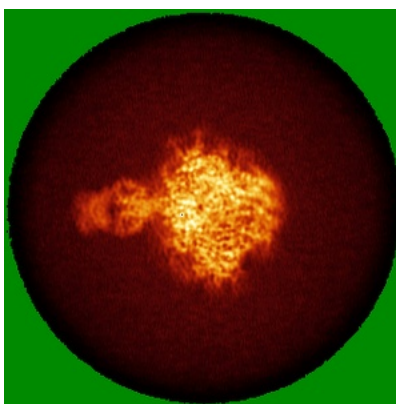
The images above show the largest variance slices of the map in three orthogonal directions.

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

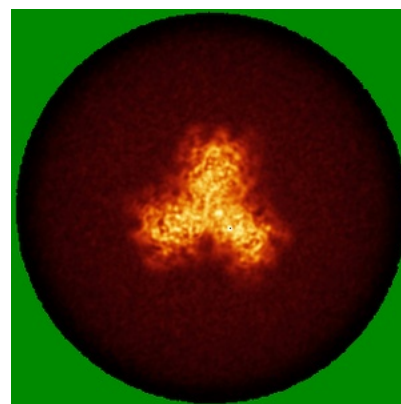
6.4.1 Primary map



X

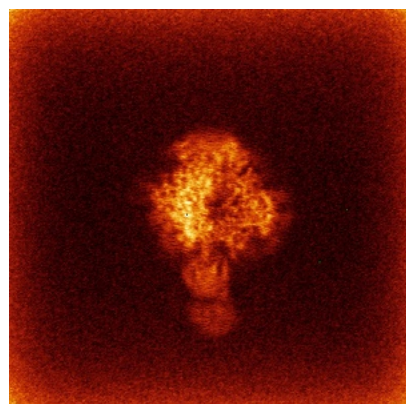


Y

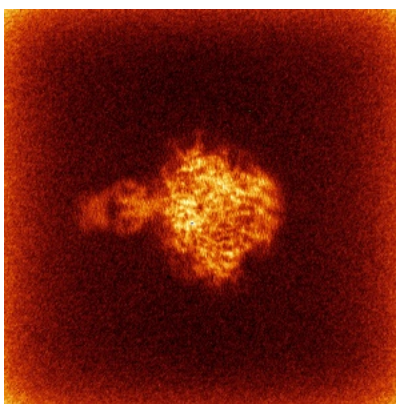


Z

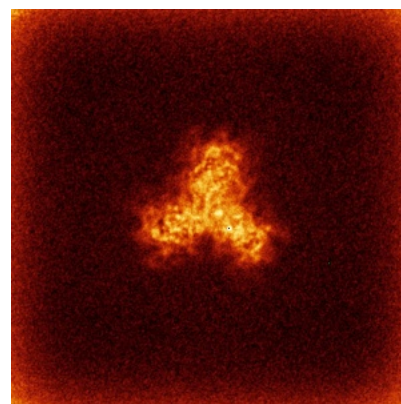
6.4.2 Raw map



X



Y



Z

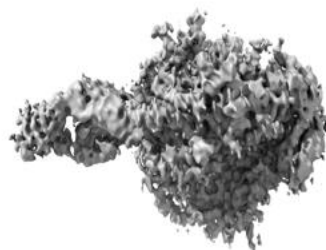
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



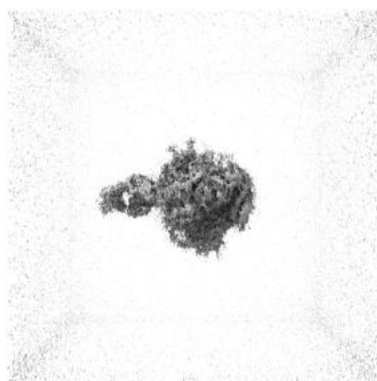
Z

The images above show the 3D surface view of the map at the recommended contour level 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

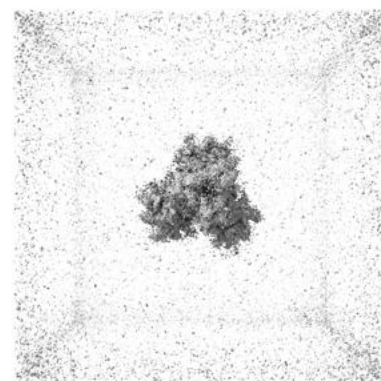
6.5.2 Raw map



X



Y



Z

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.

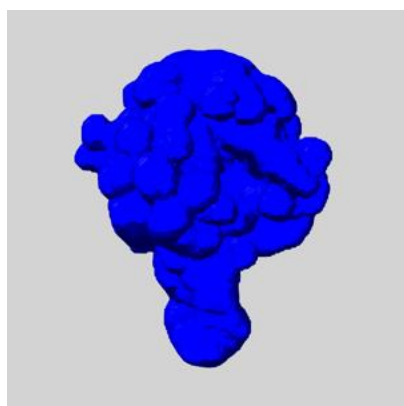
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

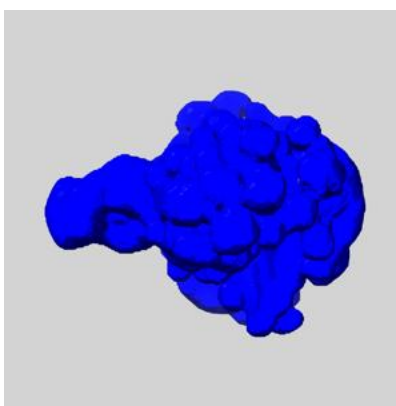
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

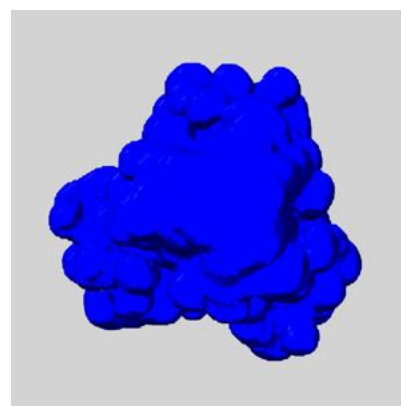
6.6.1 emd_27735_msk_1.map [i](#)



X



Y

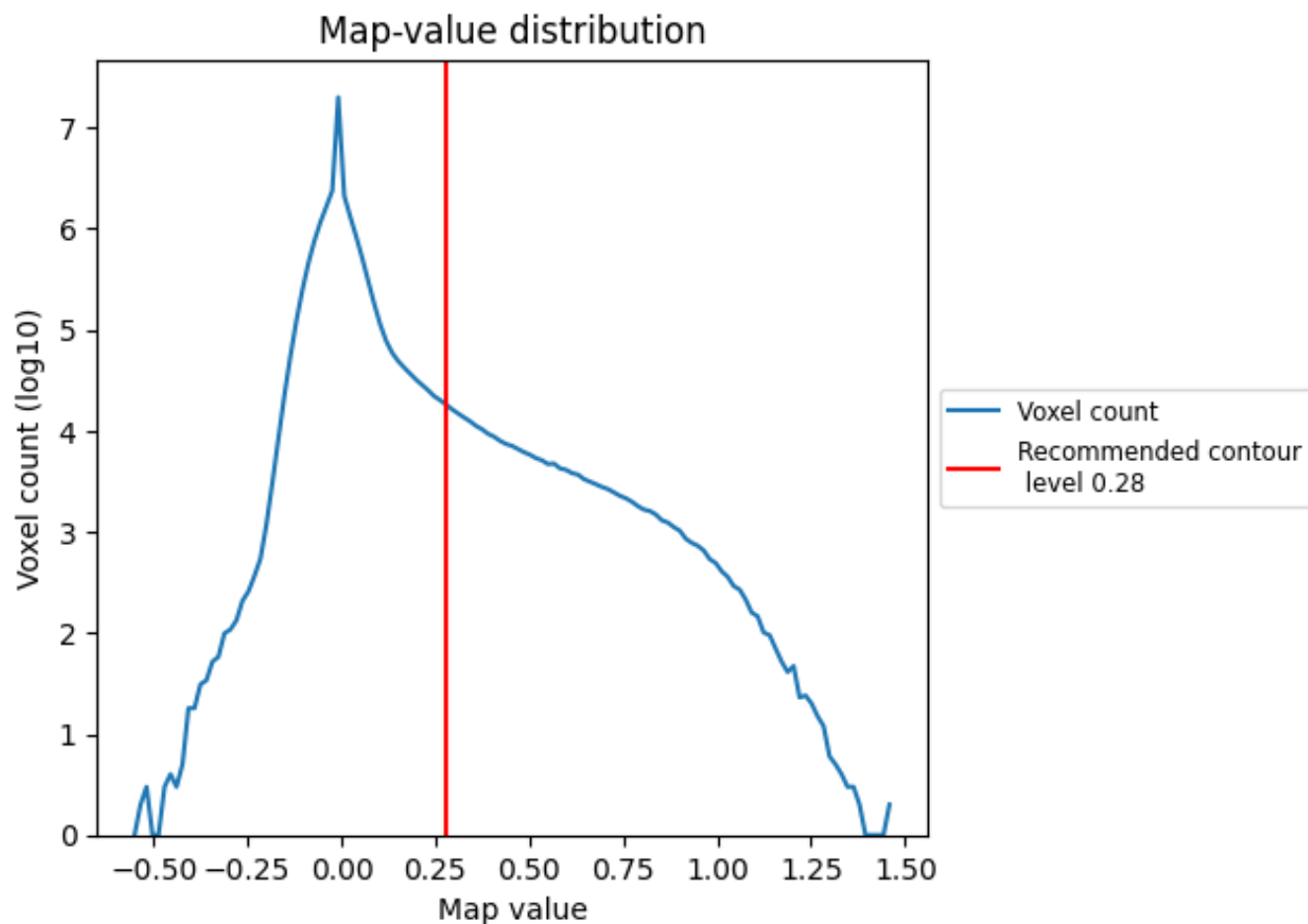


Z

7 Map analysis [i](#)

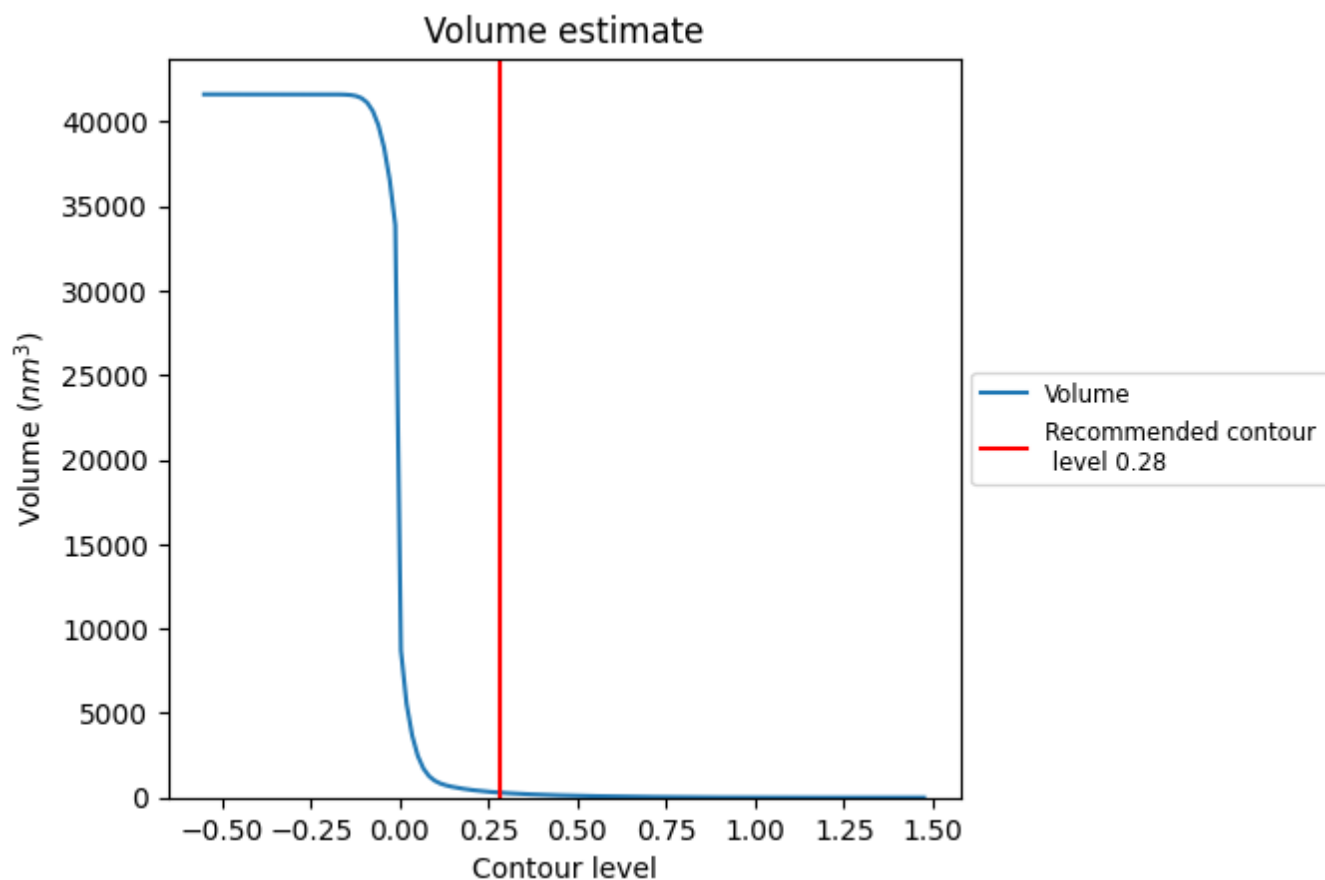
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

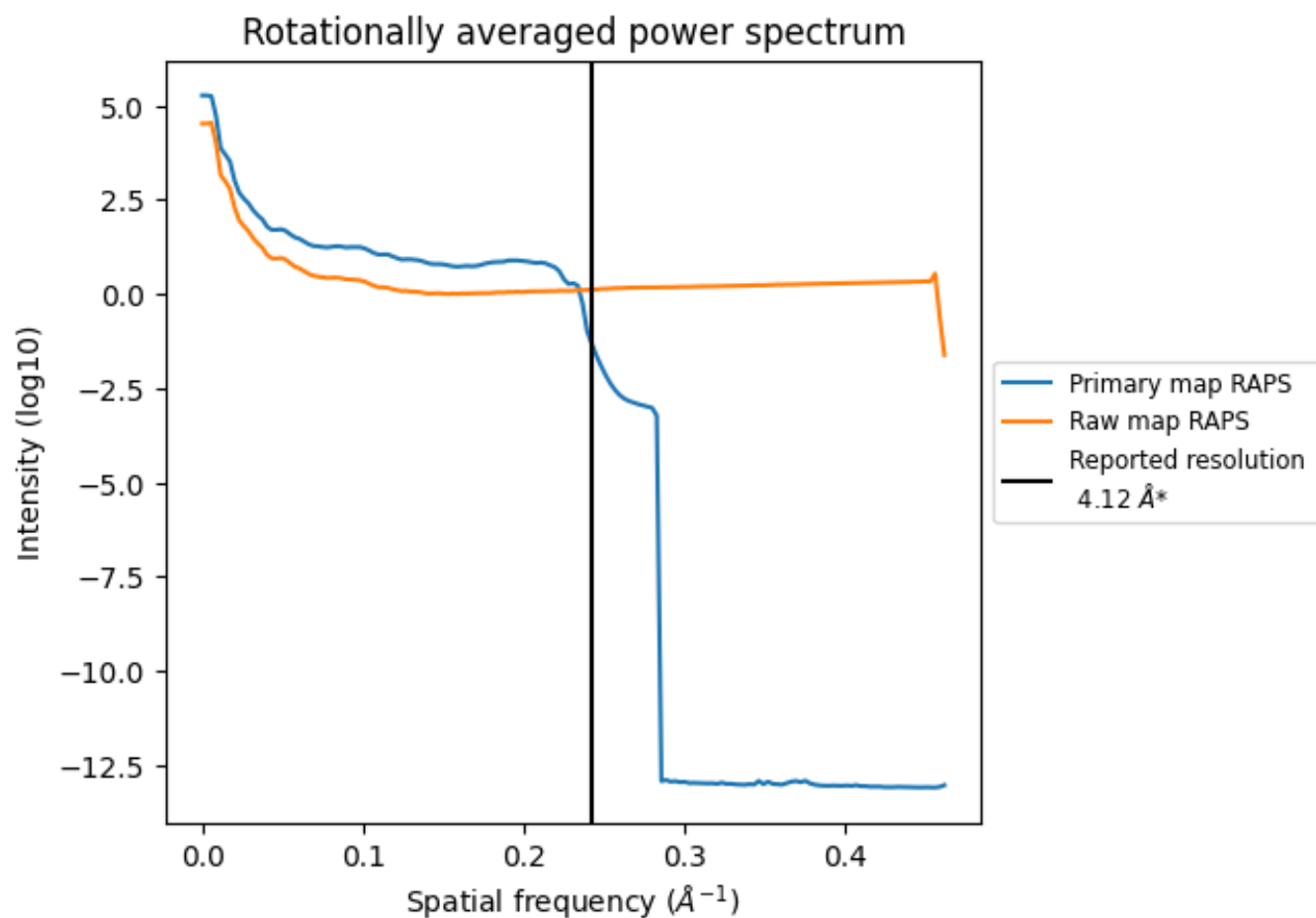
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 294 nm^3 ; this corresponds to an approximate mass of 266 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 ⓘ

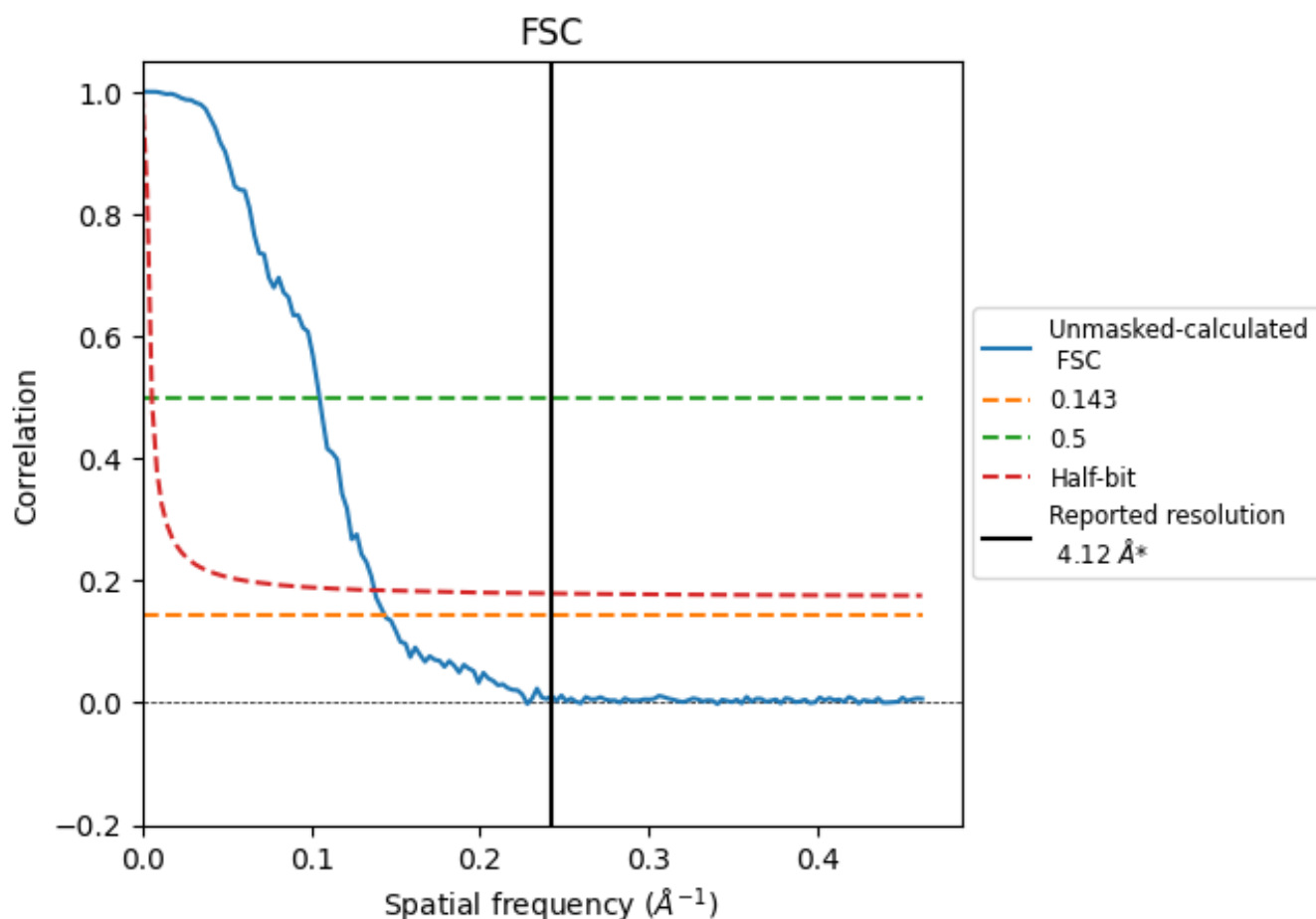


*Reported resolution corresponds to spatial frequency of 0.243 Å⁻¹

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 0.243 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

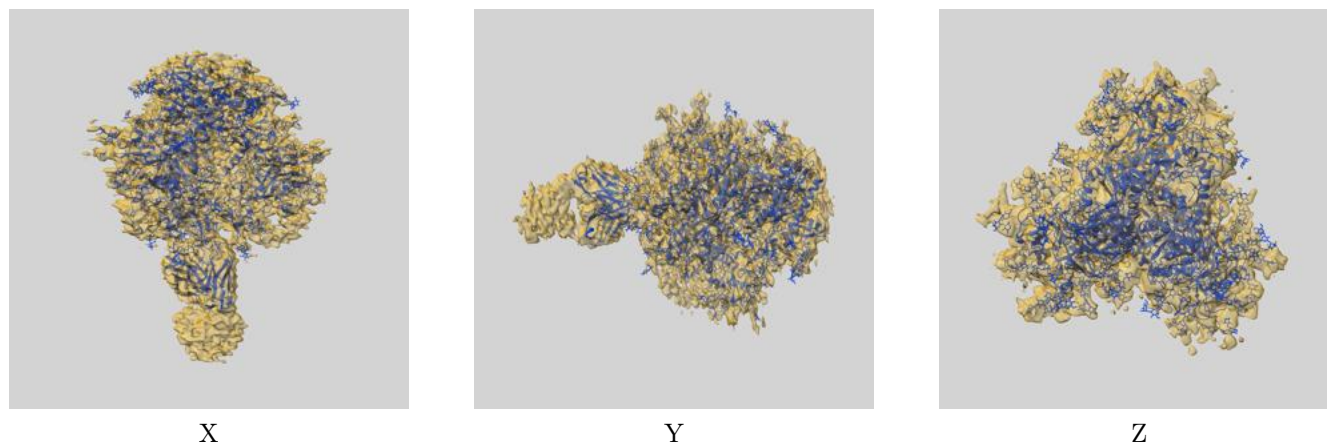
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.12	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.96	9.53	7.27

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.96 differs from the reported value 4.12 by more than 10 %

9 Map-model fit [i](#)

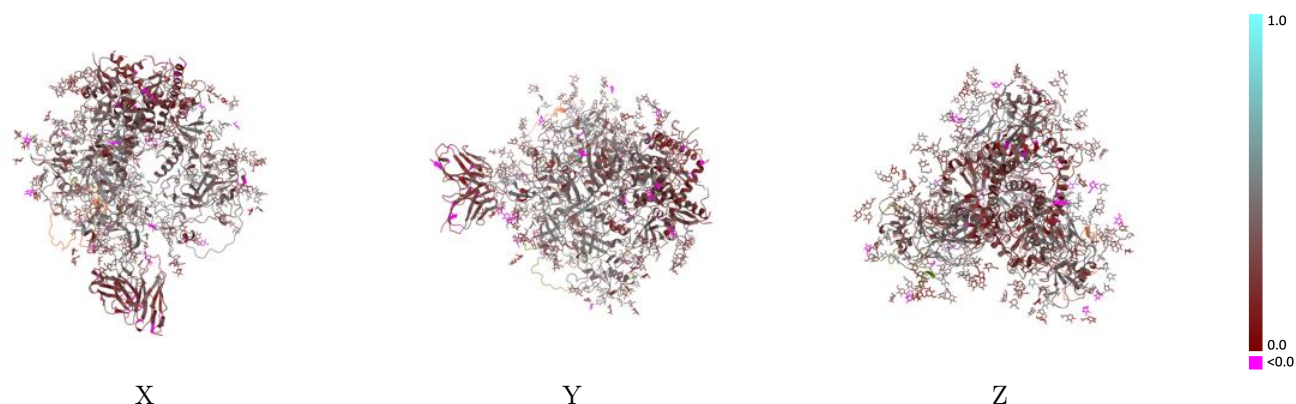
This section contains information regarding the fit between EMDB map EMD-27735 and PDB model 8DVD. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.28 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](#)

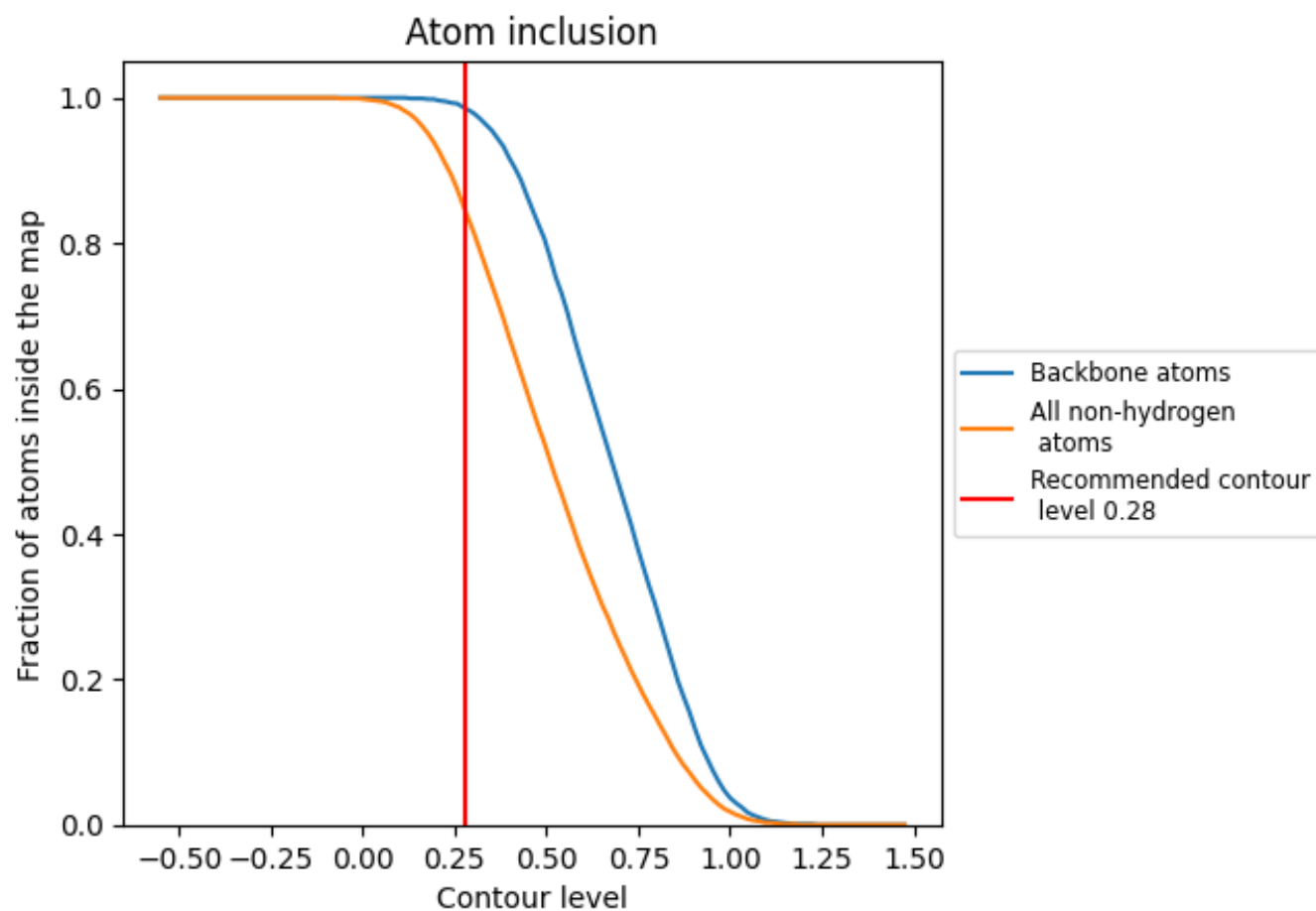


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 84% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8430	 0.3220
0	 0.3440	 0.1610
1	 0.7690	 0.3330
2	 0.3570	 0.2290
3	 0.7860	 0.2500
4	 0.9020	 0.3920
5	 0.7200	 0.3420
6	 0.8210	 0.3630
7	 0.5000	 0.2350
8	 0.4290	 0.1810
9	 0.5410	 0.2040
A	 0.7970	 0.2300
AA	 0.4290	 0.1590
B	 0.8080	 0.2460
BA	 0.8600	 0.3360
C	 0.7930	 0.2460
CA	 0.6800	 0.3740
D	 0.3800	 0.3110
DA	 0.9020	 0.3950
E	 0.9040	 0.3680
EA	 0.8190	 0.2520
F	 0.9020	 0.3640
FA	 0.9600	 0.4070
G	 0.9070	 0.3680
GA	 0.2300	 0.0730
H	 0.8110	 0.2420
HA	 0.8460	 0.3080
I	 0.2600	 0.2330
IA	 0.9040	 0.4230
J	 0.3080	 0.1300
JA	 0.8800	 0.2670
K	 0.4600	 0.3280
KA	 0.7550	 0.2890
L	 0.8730	 0.2310
LA	 0.4100	 0.2680



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Chain	Atom inclusion	Q-score
M	 0.3110	 0.2910
MA	 0.7690	 0.2860
N	 0.4620	 0.1750
NA	 0.1430	 0.0310
O	 0.4800	 0.2560
OA	 0.5710	 0.2040
P	 0.2460	 0.2700
PA	 0.8690	 0.3110
Q	 0.4100	 0.1310
QA	 0.7800	 0.3320
R	 0.8460	 0.3500
RA	 0.7440	 0.2710
S	 0.3930	 0.2260
T	 0.8530	 0.3210
U	 0.4360	 0.2360
V	 0.9200	 0.3550
W	 0.7600	 0.3520
X	 0.9340	 0.3720
Y	 0.8190	 0.2410
Z	 1.0000	 0.4410
a	 0.2790	 0.2300
b	 0.8970	 0.2830
c	 0.9150	 0.4470
d	 0.9200	 0.3510
e	 0.7550	 0.3240
f	 0.9250	 0.4020
g	 0.5800	 0.2550
h	 0.2500	 0.1690
i	 0.5710	 0.0700
j	 0.8850	 0.3410
k	 0.9230	 0.3940
l	 0.7440	 0.2540
m	 0.7600	 0.2500
n	 0.4290	 0.2630
o	 0.5900	 0.1850
p	 0.5360	 0.1870
q	 0.9000	 0.3040
r	 0.7800	 0.3000
s	 0.8850	 0.3350
t	 0.9030	 0.3200
u	 0.9200	 0.3120
v	 0.2950	 0.2150

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Chain	Atom inclusion	Q-score
w	 0.8970	 0.2880
x	 0.9160	 0.3890
y	 0.8000	 0.2570
z	 0.7830	 0.3410