



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 02:30 AM UTC

PDB ID : 8FR7 / pdb_00008fr7
EMDB ID : EMD-22889
Title : A hinge glycan regulates spike bending and impacts coronavirus infectivity
Authors : Pintilie, G.; Wilson, E.; Chmielewski, D.; Schmid, M.F.; Jin, J.; Chen, M.; Singharoy, A.; Chiu, W.
Deposited on : 2023-01-06
Resolution : 3.39 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

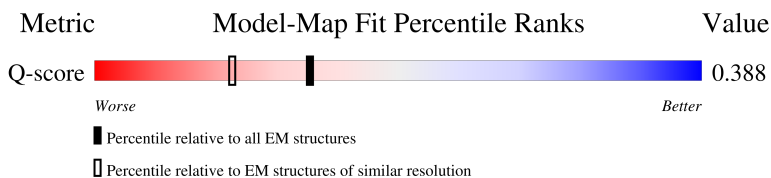
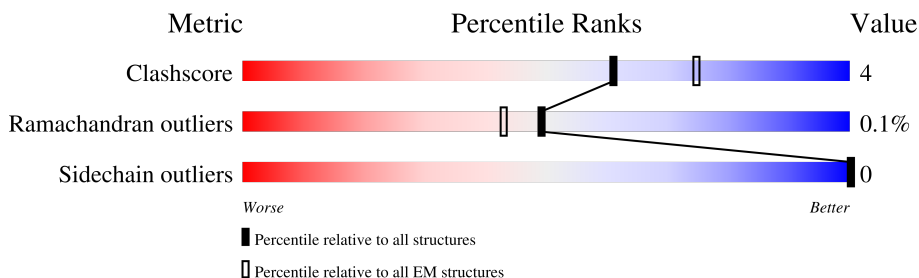
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.39 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	14220 (2.89 - 3.89)

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	1356	
1	B	1356	
1	C	1356	
2	2	7	

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Mol	Chain	Length	Quality of chain
2	3	7	
2	4	7	
2	7	7	
2	AA	7	
2	CA	7	
2	D	7	
2	FA	7	
2	JA	7	
2	L	7	
2	LA	7	
2	NA	7	
2	PA	7	
2	R	7	
2	S	7	
2	T	7	
2	W	7	
2	XA	7	
2	Z	7	
2	b	7	
2	dA	7	
2	e	7	
2	eA	7	
2	fA	7	
2	i	7	
2	iA	7	

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Mol	Chain	Length	Quality of chain
2	k	7	
2	lA	7	
2	m	7	
2	nA	7	
2	o	7	
2	qA	7	
2	uA	7	
2	w	7	
2	wA	7	
2	yA	7	
3	0	7	
3	1	7	
3	5	7	
3	6	7	
3	8	7	
3	9	7	
3	BA	7	
3	DA	7	
3	E	7	
3	GA	7	
3	H	7	
3	HA	7	
3	I	7	
3	IA	7	
3	J	7	

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Mol	Chain	Length	Quality of chain
3	K	7	
3	MA	7	
3	N	7	
3	O	7	
3	P	7	
3	Q	7	
3	QA	7	
3	TA	7	
3	U	7	
3	UA	7	
3	V	7	
3	VA	7	
3	WA	7	
3	X	7	
3	Y	7	
3	ZA	7	
3	a	7	
3	aA	7	
3	bA	7	
3	c	7	
3	cA	7	
3	f	7	
3	g	7	
3	gA	7	
3	h	7	

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Mol	Chain	Length	Quality of chain
3	hA	7	
3	jA	7	
3	kA	7	
3	l	7	
3	mA	7	
3	oA	7	
3	p	7	
3	rA	7	
3	s	7	
3	sA	7	
3	t	7	
3	tA	7	
3	u	7	
3	v	7	
3	xA	7	
3	y	7	
3	z	7	
4	F	9	
4	RA	9	
4	q	9	
5	G	9	
5	SA	9	
5	r	9	
6	M	8	
6	YA	8	

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Mol	Chain	Length	Quality of chain
6	x	8	
7	EA	12	
7	d	12	
7	pA	12	
8	KA	5	
8	j	5	
8	vA	5	
9	OA	2	
9	n	2	
9	zA	2	
10	0A	7	
10	1A	7	
10	2A	7	
10	3A	7	
10	4A	7	
10	5A	7	
10	6A	7	
10	7A	7	

2 Entry composition [i](#)

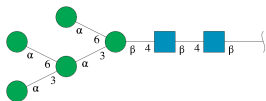
There are 10 unique types of molecules in this entry. The entry contains 39808 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1275	Total	C	N	O	S	0	0
			9930	6331	1657	1899	43		
1	C	1275	Total	C	N	O	S	0	0
			9930	6331	1657	1899	43		
1	B	1275	Total	C	N	O	S	0	0
			9930	6331	1657	1899	43		

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
2	D	7	Total	C	N	O	0	0
			83	46	2	35		
2	L	7	Total	C	N	O	0	0
			83	46	2	35		
2	R	7	Total	C	N	O	0	0
			83	46	2	35		
2	S	7	Total	C	N	O	0	0
			83	46	2	35		
2	T	7	Total	C	N	O	0	0
			83	46	2	35		
2	W	7	Total	C	N	O	0	0
			83	46	2	35		
2	Z	7	Total	C	N	O	0	0
			83	46	2	35		
2	b	7	Total	C	N	O	0	0
			83	46	2	35		

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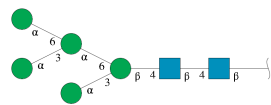
Mol	Chain	Residues	Atoms				AltConf	Trace
2	e	7	Total 83	C 46	N 2	O 35	0	0
2	i	7	Total 83	C 46	N 2	O 35	0	0
2	k	7	Total 83	C 46	N 2	O 35	0	0
2	m	7	Total 83	C 46	N 2	O 35	0	0
2	o	7	Total 83	C 46	N 2	O 35	0	0
2	w	7	Total 83	C 46	N 2	O 35	0	0
2	2	7	Total 83	C 46	N 2	O 35	0	0
2	3	7	Total 83	C 46	N 2	O 35	0	0
2	4	7	Total 83	C 46	N 2	O 35	0	0
2	7	7	Total 83	C 46	N 2	O 35	0	0
2	AA	7	Total 83	C 46	N 2	O 35	0	0
2	CA	7	Total 83	C 46	N 2	O 35	0	0
2	FA	7	Total 83	C 46	N 2	O 35	0	0
2	JA	7	Total 83	C 46	N 2	O 35	0	0
2	LA	7	Total 83	C 46	N 2	O 35	0	0
2	NA	7	Total 83	C 46	N 2	O 35	0	0
2	PA	7	Total 83	C 46	N 2	O 35	0	0
2	XA	7	Total 83	C 46	N 2	O 35	0	0
2	dA	7	Total 83	C 46	N 2	O 35	0	0
2	eA	7	Total 83	C 46	N 2	O 35	0	0
2	fA	7	Total 83	C 46	N 2	O 35	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	iA	7	Total	C	N	O	0	0
			83	46	2	35		
2	lA	7	Total	C	N	O	0	0
			83	46	2	35		
2	nA	7	Total	C	N	O	0	0
			83	46	2	35		
2	qA	7	Total	C	N	O	0	0
			83	46	2	35		
2	uA	7	Total	C	N	O	0	0
			83	46	2	35		
2	wA	7	Total	C	N	O	0	0
			83	46	2	35		
2	yA	7	Total	C	N	O	0	0
			83	46	2	35		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	7	Total	C	N	O	0	0
			83	46	2	35		
3	H	7	Total	C	N	O	0	0
			83	46	2	35		
3	I	7	Total	C	N	O	0	0
			83	46	2	35		
3	J	7	Total	C	N	O	0	0
			83	46	2	35		
3	K	7	Total	C	N	O	0	0
			83	46	2	35		
3	N	7	Total	C	N	O	0	0
			83	46	2	35		
3	O	7	Total	C	N	O	0	0
			83	46	2	35		
3	P	7	Total	C	N	O	0	0
			83	46	2	35		
3	Q	7	Total	C	N	O	0	0
			83	46	2	35		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	U	7	Total	C	N	O	0	0
			83	46	2	35		
3	V	7	Total	C	N	O	0	0
			83	46	2	35		
3	X	7	Total	C	N	O	0	0
			83	46	2	35		
3	Y	7	Total	C	N	O	0	0
			83	46	2	35		
3	a	7	Total	C	N	O	0	0
			83	46	2	35		
3	c	7	Total	C	N	O	0	0
			83	46	2	35		
3	f	7	Total	C	N	O	0	0
			83	46	2	35		
3	g	7	Total	C	N	O	0	0
			83	46	2	35		
3	h	7	Total	C	N	O	0	0
			83	46	2	35		
3	l	7	Total	C	N	O	0	0
			83	46	2	35		
3	p	7	Total	C	N	O	0	0
			83	46	2	35		
3	s	7	Total	C	N	O	0	0
			83	46	2	35		
3	t	7	Total	C	N	O	0	0
			83	46	2	35		
3	u	7	Total	C	N	O	0	0
			83	46	2	35		
3	v	7	Total	C	N	O	0	0
			83	46	2	35		
3	y	7	Total	C	N	O	0	0
			83	46	2	35		
3	z	7	Total	C	N	O	0	0
			83	46	2	35		
3	0	7	Total	C	N	O	0	0
			83	46	2	35		
3	1	7	Total	C	N	O	0	0
			83	46	2	35		
3	5	7	Total	C	N	O	0	0
			83	46	2	35		
3	6	7	Total	C	N	O	0	0
			83	46	2	35		

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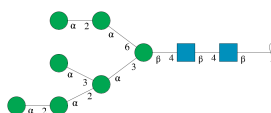
Mol	Chain	Residues	Atoms				AltConf	Trace
3	8	7	Total	C	N	O	0	0
			83	46	2	35		
3	9	7	Total	C	N	O	0	0
			83	46	2	35		
3	BA	7	Total	C	N	O	0	0
			83	46	2	35		
3	DA	7	Total	C	N	O	0	0
			83	46	2	35		
3	GA	7	Total	C	N	O	0	0
			83	46	2	35		
3	HA	7	Total	C	N	O	0	0
			83	46	2	35		
3	IA	7	Total	C	N	O	0	0
			83	46	2	35		
3	MA	7	Total	C	N	O	0	0
			83	46	2	35		
3	QA	7	Total	C	N	O	0	0
			83	46	2	35		
3	TA	7	Total	C	N	O	0	0
			83	46	2	35		
3	UA	7	Total	C	N	O	0	0
			83	46	2	35		
3	VA	7	Total	C	N	O	0	0
			83	46	2	35		
3	WA	7	Total	C	N	O	0	0
			83	46	2	35		
3	ZA	7	Total	C	N	O	0	0
			83	46	2	35		
3	aA	7	Total	C	N	O	0	0
			83	46	2	35		
3	bA	7	Total	C	N	O	0	0
			83	46	2	35		
3	cA	7	Total	C	N	O	0	0
			83	46	2	35		
3	gA	7	Total	C	N	O	0	0
			83	46	2	35		
3	hA	7	Total	C	N	O	0	0
			83	46	2	35		
3	jA	7	Total	C	N	O	0	0
			83	46	2	35		
3	kA	7	Total	C	N	O	0	0
			83	46	2	35		

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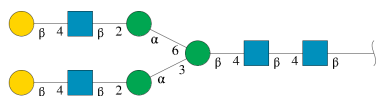
Mol	Chain	Residues	Atoms				AltConf	Trace
3	mA	7	Total	C	N	O	0	0
			83	46	2	35		
3	oA	7	Total	C	N	O	0	0
			83	46	2	35		
3	rA	7	Total	C	N	O	0	0
			83	46	2	35		
3	sA	7	Total	C	N	O	0	0
			83	46	2	35		
3	tA	7	Total	C	N	O	0	0
			83	46	2	35		
3	xA	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-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.



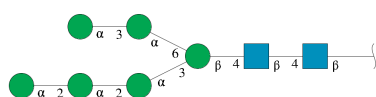
Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	9	Total	C	N	O	0	0
			105	58	2	45		
4	q	9	Total	C	N	O	0	0
			105	58	2	45		
4	RA	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 5 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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.



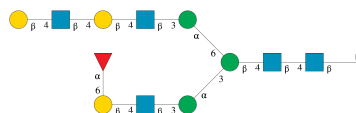
Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	9	Total	C	N	O	0	0
			111	62	4	45		
5	r	9	Total	C	N	O	0	0
			111	62	4	45		
5	SA	9	Total	C	N	O	0	0
			111	62	4	45		

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



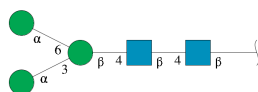
Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	8	Total	C	N	O	0	0
			94	52	2	40		
6	x	8	Total	C	N	O	0	0
			94	52	2	40		
6	YA	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 7 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-L-fucopyranose-(1-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	d	12	Total	C	N	O	0	0
			146	82	5	59		
7	EA	12	Total	C	N	O	0	0
			146	82	5	59		
7	pA	12	Total	C	N	O	0	0
			146	82	5	59		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



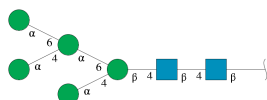
Mol	Chain	Residues	Atoms				AltConf	Trace
8	j	5	Total	C	N	O	0	0
			61	34	2	25		
8	KA	5	Total	C	N	O	0	0
			61	34	2	25		
8	vA	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
9	n	2	Total	C	N	O	0	0
			28	16	2	10		
9	OA	2	Total	C	N	O	0	0
			28	16	2	10		
9	zA	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-4)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
10	0A	7	Total	C	N	O	0	0
			83	46	2	35		

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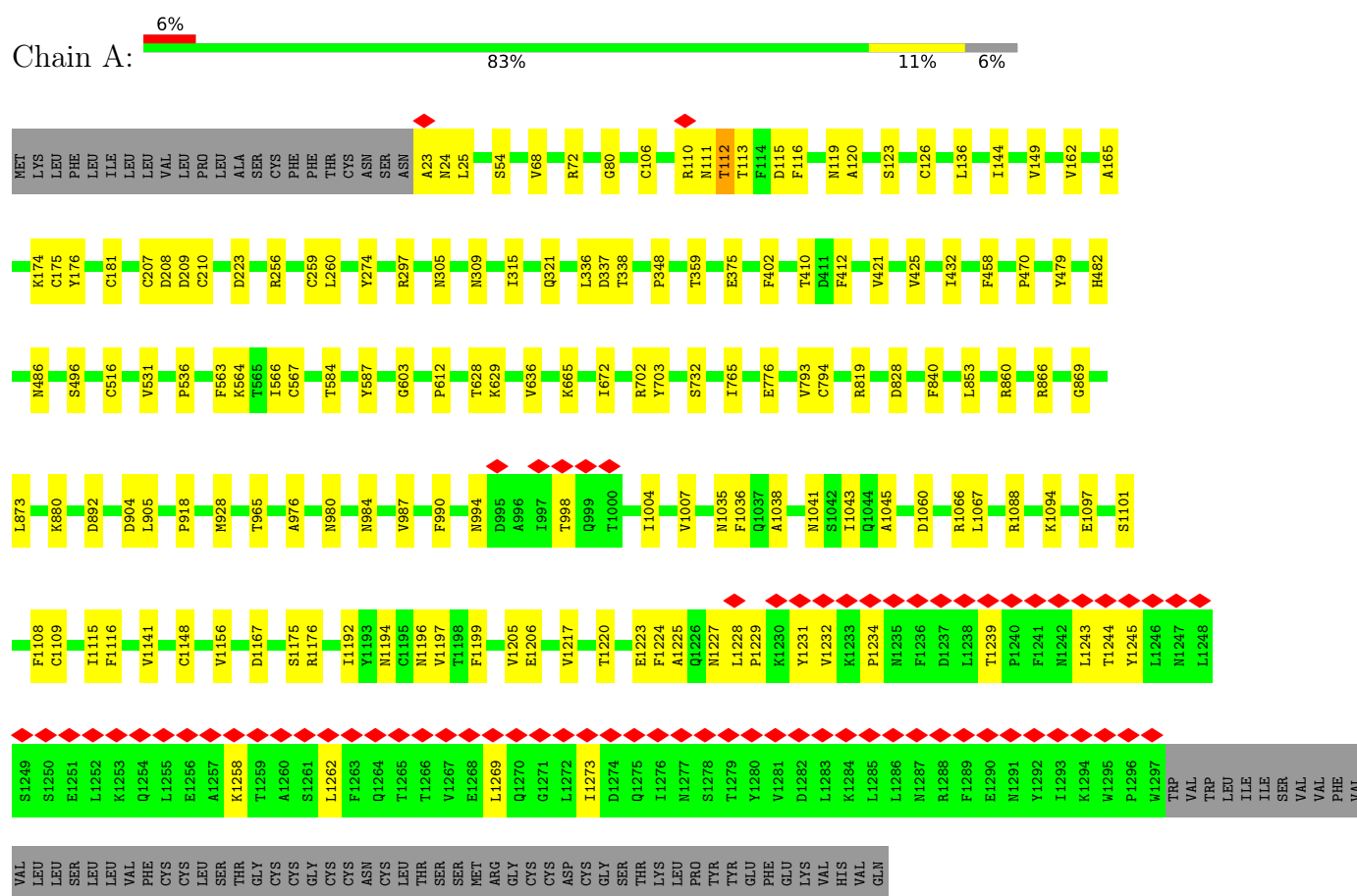
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Mol	Chain	Residues	Atoms				AltConf	Trace
10	1A	7	Total 83	C 46	N 2	O 35	0	0
10	2A	7	Total 83	C 46	N 2	O 35	0	0
10	3A	7	Total 83	C 46	N 2	O 35	0	0
10	4A	7	Total 83	C 46	N 2	O 35	0	0
10	5A	7	Total 83	C 46	N 2	O 35	0	0
10	6A	7	Total 83	C 46	N 2	O 35	0	0
10	7A	7	Total 83	C 46	N 2	O 35	0	0

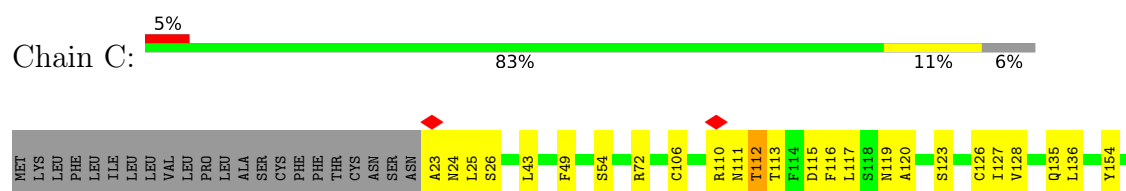
3 Residue-property plots [i](#)

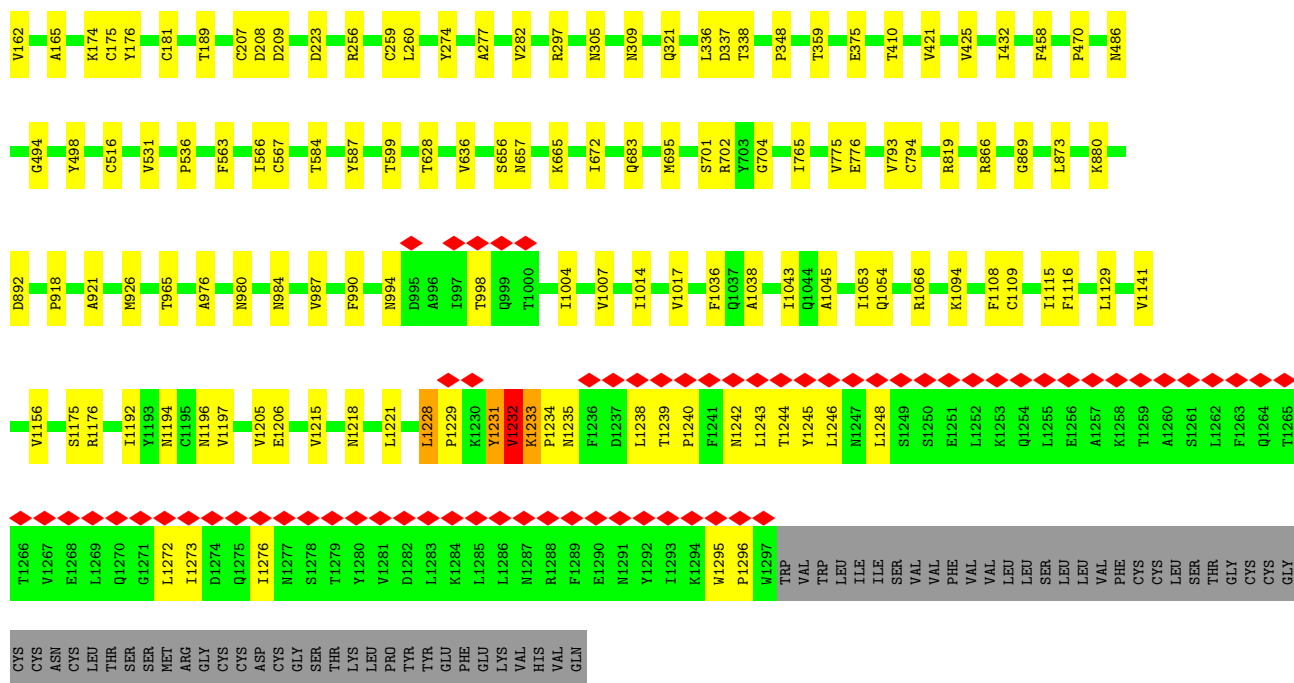
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein

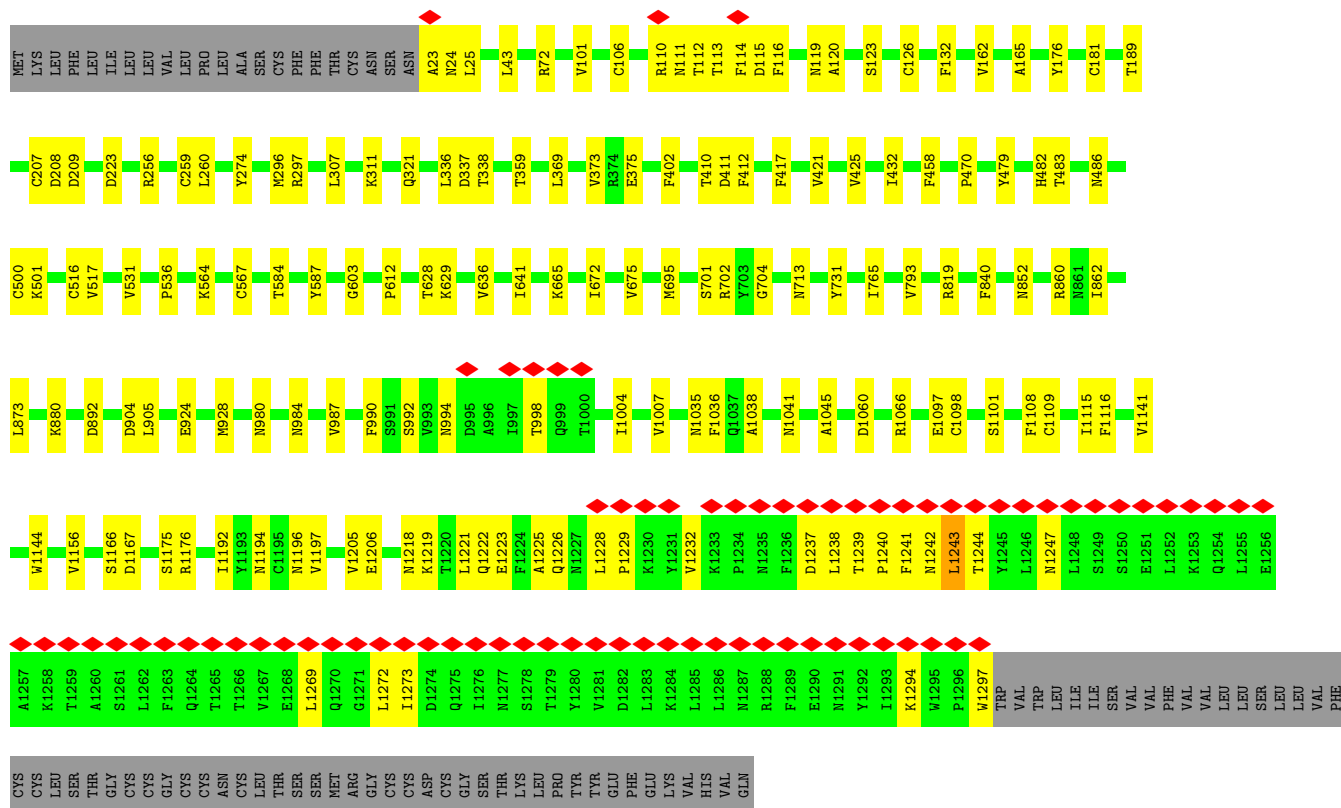
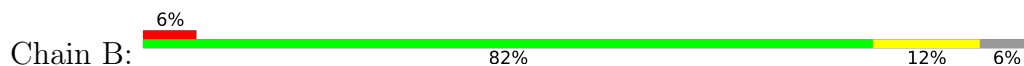


• Molecule 1: Spike glycoprotein



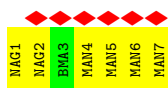
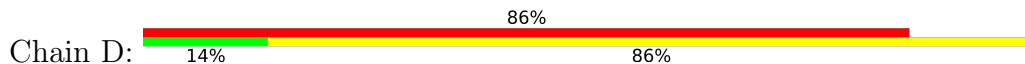


• Molecule 1: Spike glycoprotein

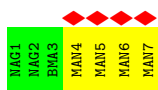
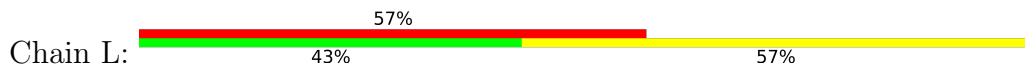


• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-

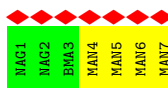
D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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



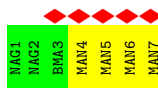
- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



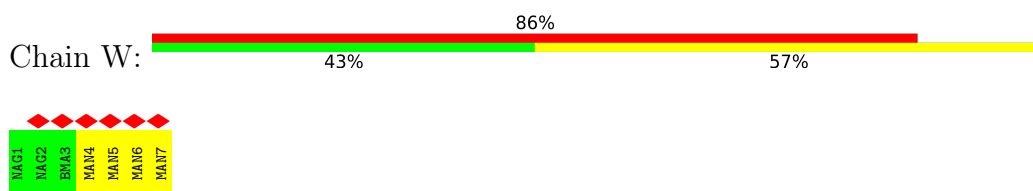
- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



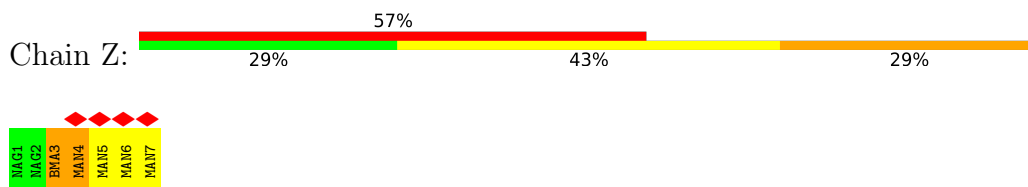
- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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



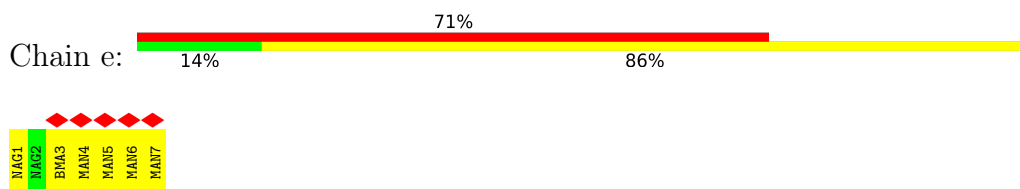
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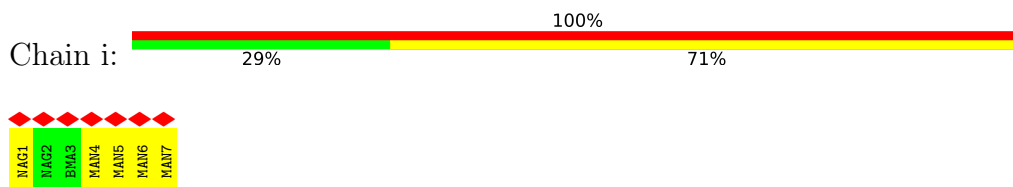
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• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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

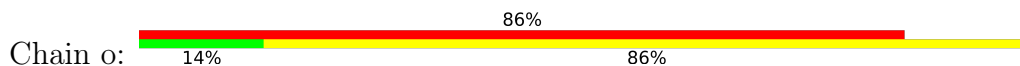




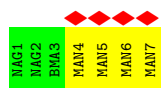
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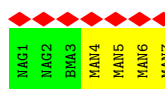
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- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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

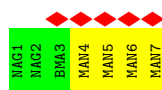


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

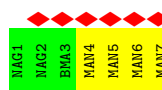
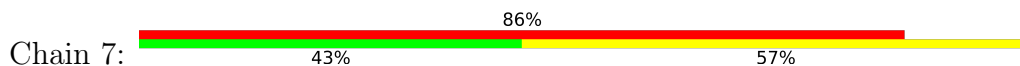




- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



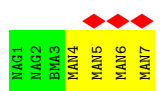
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- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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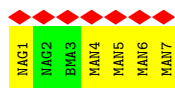


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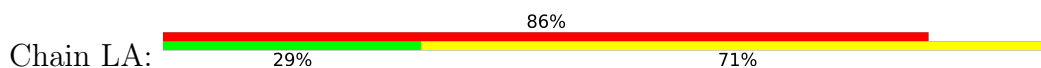




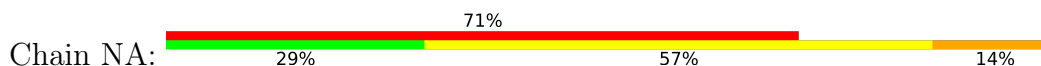
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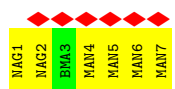
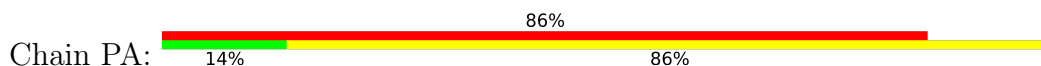
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- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

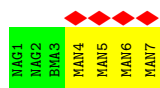


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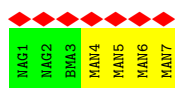


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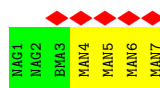
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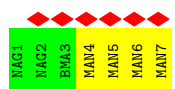
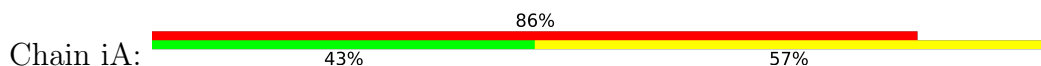
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- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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

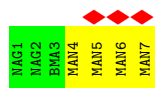


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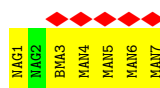
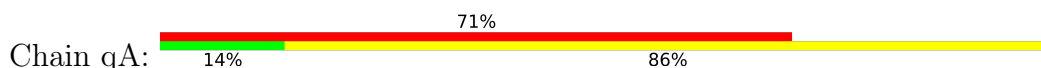




- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



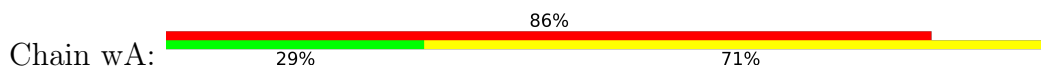
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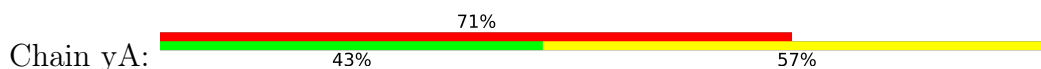
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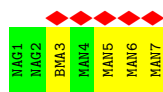


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

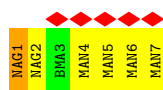


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





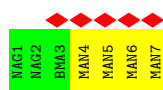
- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



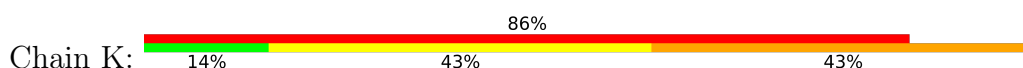
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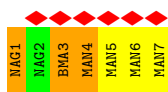


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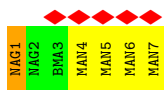


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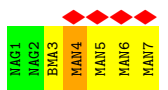




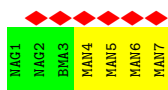
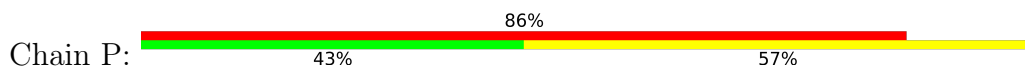
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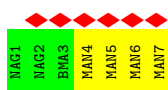
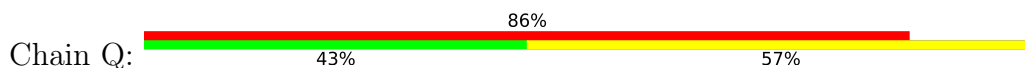
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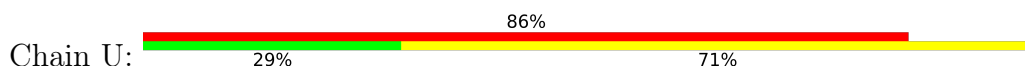
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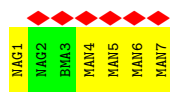


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- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

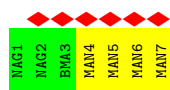
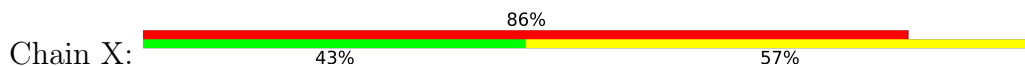




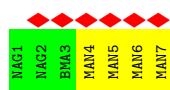
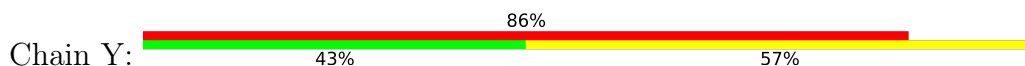
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- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

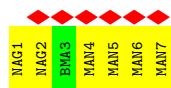
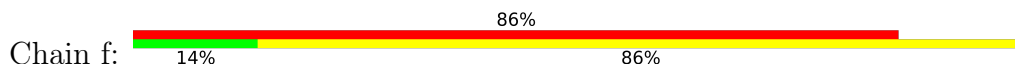


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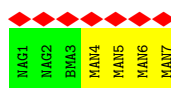




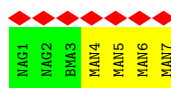
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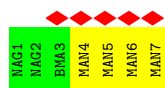
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- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

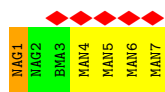


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- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

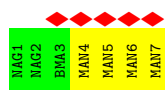




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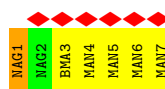
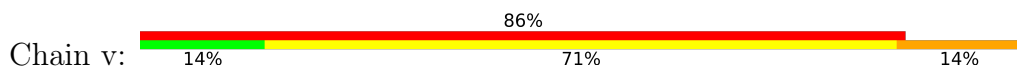
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- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

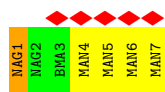


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- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

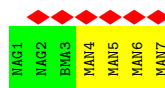
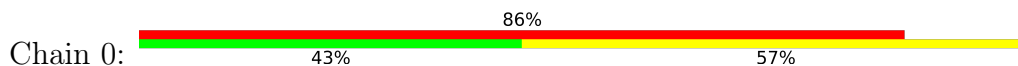




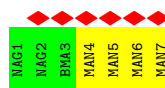
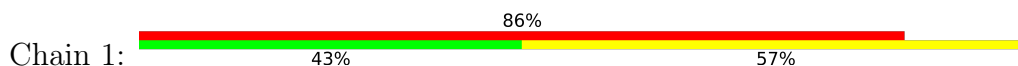
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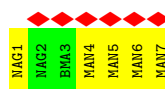
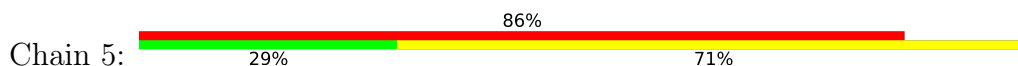
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- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

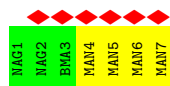
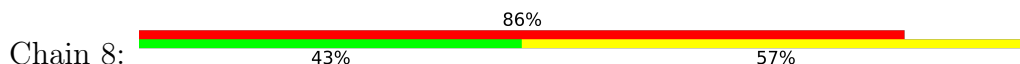


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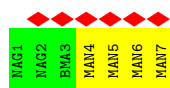
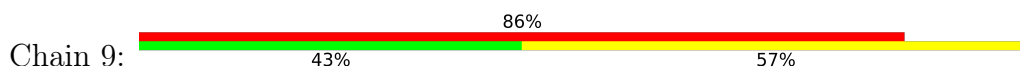




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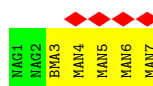
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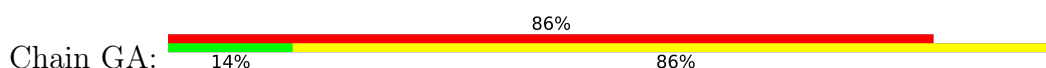
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- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

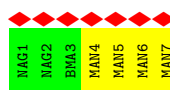


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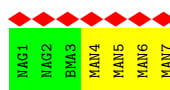




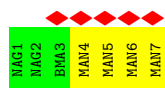
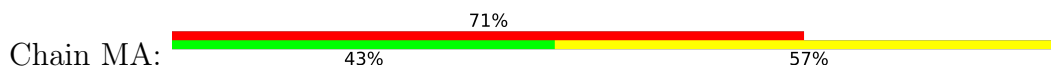
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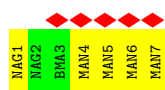
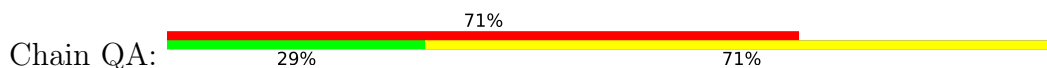
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- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

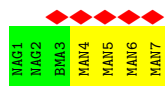
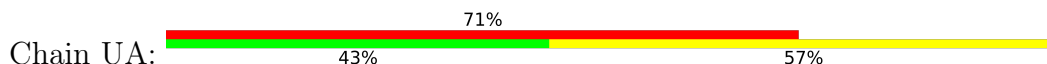


- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





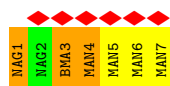
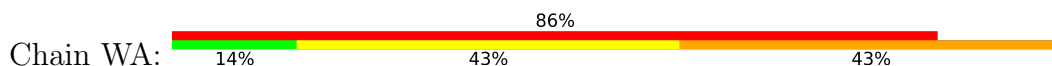
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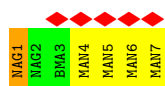
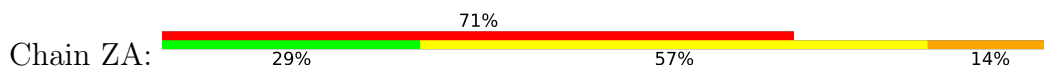
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- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

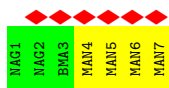
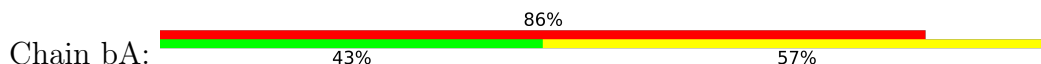


- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

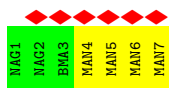
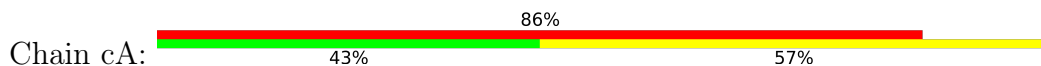




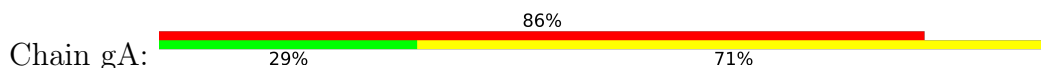
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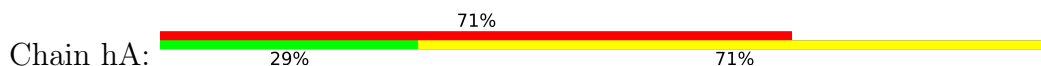
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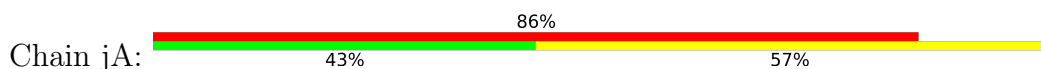
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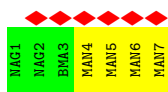


- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

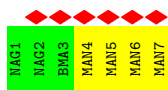
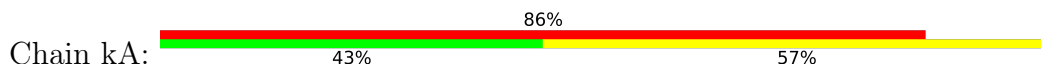


- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





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



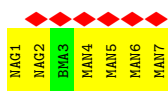
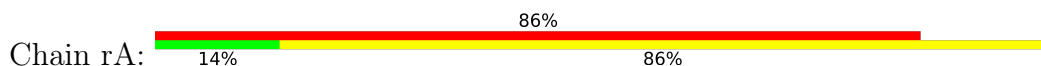
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- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

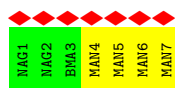


- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

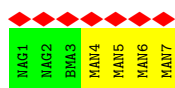


- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

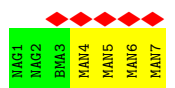
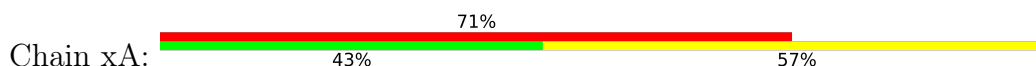




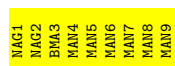
- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



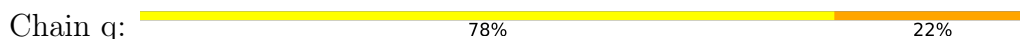
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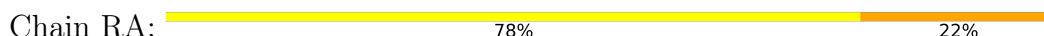
- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-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

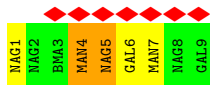
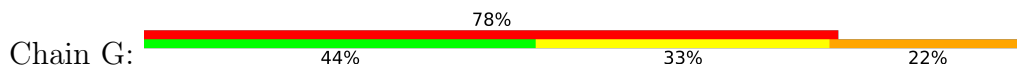


- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

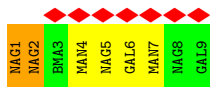
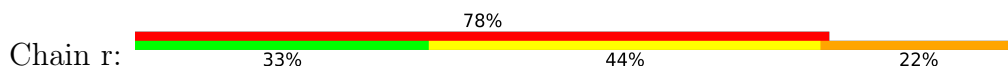




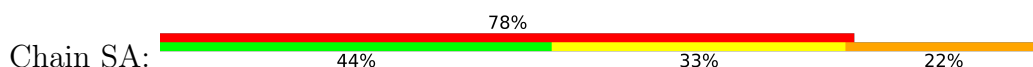
- Molecule 5: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



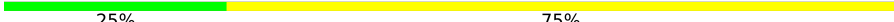
- Molecule 5: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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:  25% 75%

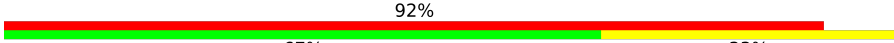


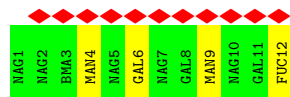
- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain YA:  25% 75%

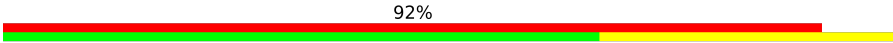


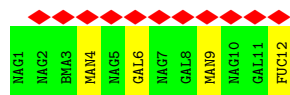
- Molecule 7: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-L-fucopyranose-(1-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido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

Chain d:  92% 67% 33%



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

Chain EA:  92% 67% 33%

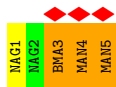


- Molecule 7: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-L-fucopyranose-(1-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido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

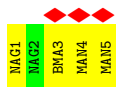
Chain pA:  92% 42% 50% 8%



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



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



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



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



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

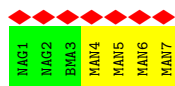


- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

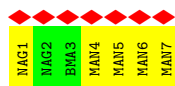




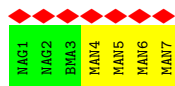
- Molecule 10: alpha-D-mannopyranose-(1-4)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-4)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



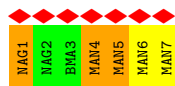
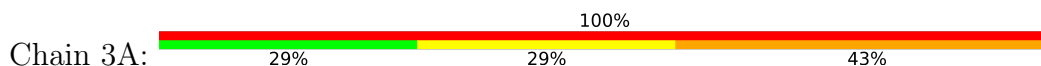
- Molecule 10: alpha-D-mannopyranose-(1-4)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-4)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

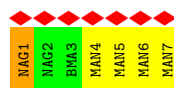


- Molecule 10: alpha-D-mannopyranose-(1-4)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-4)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

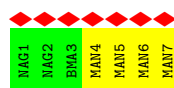


- Molecule 10: alpha-D-mannopyranose-(1-4)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-4)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

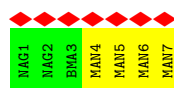




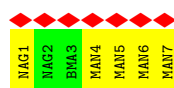
- Molecule 10: alpha-D-mannopyranose-(1-4)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-4)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82030	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	30000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.420	Depositor
Minimum map value	-1.848	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.142	Depositor
Recommended contour level	0.528	Depositor
Map size ($\text{\AA}$)	358.4, 358.4, 358.4	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.15	0/10155	0.38	0/13860
1	B	0.16	0/10155	0.39	1/13860 (0.0%)
1	C	0.16	0/10155	0.39	0/13860
All	All	0.16	0/30465	0.39	1/41580 (0.0%)

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
1	A	0	3
1	B	0	2
1	C	0	6
All	All	0	11

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1243	LEU	CB-CA-C	5.68	121.72	110.42

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ARG	Peptide
1	A	112	THR	Peptide
1	A	1194	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	B	110	ARG	Peptide
1	B	1194	ASN	Peptide
1	C	110	ARG	Peptide
1	C	112	THR	Peptide
1	C	1194	ASN	Peptide
1	C	1228	LEU	Peptide
1	C	1231	TYR	Peptide
1	C	1232	VAL	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	9930	0	9652	108	0
1	B	9930	0	9653	106	0
1	C	9930	0	9654	110	0
2	2	83	0	70	0	0
2	3	83	0	70	0	0
2	4	83	0	70	0	0
2	7	83	0	70	0	0
2	AA	83	0	70	0	0
2	CA	83	0	70	0	0
2	D	83	0	70	1	0
2	FA	83	0	70	1	0
2	JA	83	0	70	0	0
2	L	83	0	70	0	0
2	LA	83	0	70	0	0
2	NA	83	0	70	1	0
2	PA	83	0	70	1	0
2	R	83	0	70	0	0
2	S	83	0	70	0	0
2	T	83	0	70	0	0
2	W	83	0	70	0	0
2	XA	83	0	70	0	0
2	Z	83	0	70	1	0
2	b	83	0	70	0	0
2	dA	83	0	70	0	0
2	e	83	0	70	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	eA	83	0	70	0	0
2	fA	83	0	70	0	0
2	i	83	0	70	0	0
2	iA	83	0	70	0	0
2	k	83	0	70	0	0
2	lA	83	0	70	1	0
2	m	83	0	70	1	0
2	nA	83	0	70	0	0
2	o	83	0	70	1	0
2	qA	83	0	70	1	0
2	uA	83	0	70	0	0
2	w	83	0	70	0	0
2	wA	83	0	70	0	0
2	yA	83	0	70	0	0
3	0	83	0	70	0	0
3	1	83	0	70	0	0
3	5	83	0	70	0	0
3	6	83	0	70	0	0
3	8	83	0	70	0	0
3	9	83	0	70	0	0
3	BA	83	0	70	1	0
3	DA	83	0	70	0	0
3	E	83	0	70	1	0
3	GA	83	0	70	1	0
3	H	83	0	70	1	0
3	HA	83	0	70	0	0
3	I	83	0	70	0	0
3	IA	83	0	70	0	0
3	J	83	0	70	1	0
3	K	83	0	70	2	0
3	MA	83	0	70	0	0
3	N	83	0	70	1	0
3	O	83	0	70	1	0
3	P	83	0	70	0	0
3	Q	83	0	70	0	0
3	QA	83	0	70	0	0
3	TA	83	0	70	1	0
3	U	83	0	70	0	0
3	UA	83	0	70	0	0
3	V	83	0	70	0	0
3	VA	83	0	70	1	0
3	WA	83	0	70	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	X	83	0	70	0	0
3	Y	83	0	70	0	0
3	ZA	83	0	70	1	0
3	a	83	0	70	1	0
3	aA	83	0	70	1	0
3	bA	83	0	70	0	0
3	c	83	0	70	0	0
3	cA	83	0	70	0	0
3	f	83	0	70	1	0
3	g	83	0	70	0	0
3	gA	83	0	70	0	0
3	h	83	0	70	0	0
3	hA	83	0	70	0	0
3	jA	83	0	70	0	0
3	kA	83	0	70	0	0
3	l	83	0	70	0	0
3	mA	83	0	70	1	0
3	oA	83	0	70	0	0
3	p	83	0	70	3	0
3	rA	83	0	70	1	0
3	s	83	0	70	1	0
3	sA	83	0	70	0	0
3	t	83	0	70	0	0
3	tA	83	0	70	0	0
3	u	83	0	70	1	0
3	v	83	0	70	1	0
3	xA	83	0	70	0	0
3	y	83	0	70	1	0
3	z	83	0	70	1	0
4	F	105	0	88	1	0
4	RA	105	0	88	2	0
4	q	105	0	88	2	0
5	G	111	0	94	2	0
5	SA	111	0	94	2	0
5	r	111	0	94	2	0
6	M	94	0	79	0	0
6	YA	94	0	79	0	0
6	x	94	0	79	0	0
7	EA	146	0	124	0	0
7	d	146	0	124	0	0
7	pA	146	0	121	1	0
8	KA	61	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	j	61	0	52	2	0
8	vA	61	0	52	1	0
9	OA	28	0	25	2	0
9	n	28	0	25	2	0
9	zA	28	0	25	1	0
10	0A	83	0	70	0	0
10	1A	83	0	70	0	0
10	2A	83	0	70	0	0
10	3A	83	0	70	3	0
10	4A	83	0	70	1	0
10	5A	83	0	70	0	0
10	6A	83	0	70	0	0
10	7A	83	0	70	0	0
All	All	39808	0	37412	343	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 4.

All (343) 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)
1:C:516:CYS:HB3	1:C:567:CYS:HA	1.48	0.96
1:B:516:CYS:HB3	1:B:567:CYS:HA	1.45	0.95
1:A:516:CYS:HB3	1:A:567:CYS:HA	1.50	0.92
1:A:702:ARG:HG3	1:A:703:TYR:H	1.40	0.84
1:C:106:CYS:HB3	1:C:126:CYS:HA	1.60	0.81
1:C:1228:LEU:HG	1:C:1229:PRO:HD2	1.63	0.81
1:C:1235:ASN:H	1:C:1238:LEU:HD22	1.47	0.80
1:B:1243:LEU:HB2	1:B:1244:THR:HA	1.65	0.76
1:A:106:CYS:HB3	1:A:126:CYS:HA	1.65	0.76
1:B:106:CYS:HB3	1:B:126:CYS:HA	1.67	0.76
1:A:68:VAL:HG23	1:A:136:LEU:HD21	1.71	0.73
1:B:119:ASN:OD1	1:B:120:ALA:N	2.22	0.72
1:C:1156:VAL:HG13	1:C:1192:ILE:HG21	1.71	0.71
1:B:1156:VAL:HG13	1:B:1192:ILE:HG21	1.74	0.70
1:A:840:PHE:HE2	1:A:860:ARG:HH12	1.43	0.67
1:C:127:ILE:HG22	1:C:128:VAL:HG23	1.77	0.67
1:A:516:CYS:CB	1:A:567:CYS:HA	2.24	0.66
1:B:1223:GLU:HA	1:B:1226:GLN:HB2	1.78	0.66
1:A:1156:VAL:HG13	1:A:1192:ILE:HG21	1.77	0.65
1:B:516:CYS:CB	1:B:567:CYS:HA	2.24	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:866:ARG:HH12	1:A:869:GLY:HA2	1.60	0.65
1:C:516:CYS:CB	1:C:567:CYS:HA	2.23	0.64
1:C:866:ARG:HH22	1:C:869:GLY:HA2	1.61	0.64
1:A:486:ASN:OD1	3:N:1:NAG:N2	2.31	0.63
1:C:486:ASN:OD1	3:y:1:NAG:N2	2.31	0.63
1:C:259:CYS:SG	1:C:260:LEU:N	2.72	0.63
1:A:111:ASN:O	1:A:112:THR:OG1	2.16	0.63
1:B:486:ASN:OD1	3:ZA:1:NAG:N2	2.32	0.63
1:C:111:ASN:O	1:C:112:THR:OG1	2.17	0.63
1:B:111:ASN:O	1:B:112:THR:OG1	2.18	0.62
1:A:1045:ALA:HB2	1:B:636:VAL:HG21	1.82	0.62
1:B:1222:GLN:O	1:B:1226:GLN:N	2.33	0.62
1:B:1243:LEU:CB	1:B:1244:THR:HA	2.30	0.61
1:A:259:CYS:SG	1:A:260:LEU:N	2.73	0.61
1:C:54:SER:O	1:C:174:LYS:NZ	2.28	0.61
1:B:840:PHE:HE2	1:B:860:ARG:HH12	1.49	0.61
1:C:24:ASN:HB2	2:FA:1:NAG:O5	2.01	0.61
1:B:256:ARG:HE	1:B:421:VAL:HG21	1.66	0.60
1:A:1243:LEU:HB2	10:3A:1:NAG:H5	1.84	0.60
1:C:1228:LEU:HG	1:C:1229:PRO:CD	2.31	0.60
1:A:305:ASN:O	1:A:309:ASN:ND2	2.35	0.59
1:A:1004:ILE:HA	1:A:1007:VAL:HG12	1.84	0.59
1:B:500:CYS:SG	1:B:501:LYS:N	2.75	0.59
5:r:2:NAG:H3	5:r:2:NAG:H83	1.84	0.59
1:B:259:CYS:SG	1:B:260:LEU:N	2.76	0.59
1:C:880:LYS:NZ	1:C:990:PHE:O	2.35	0.58
1:C:458:PHE:O	1:B:819:ARG:NH1	2.36	0.58
1:B:470:PRO:HG2	1:B:628:THR:HG22	1.85	0.58
1:B:1004:ILE:HA	1:B:1007:VAL:HG12	1.86	0.58
1:B:880:LYS:NZ	1:B:990:PHE:O	2.35	0.58
1:C:470:PRO:HG2	1:C:628:THR:HG22	1.86	0.58
1:B:24:ASN:HB2	2:qA:1:NAG:O5	2.02	0.58
9:OA:1:NAG:H83	9:OA:1:NAG:H3	1.85	0.57
9:n:1:NAG:H3	9:n:1:NAG:H83	1.86	0.57
1:A:24:ASN:HB2	2:e:1:NAG:O5	2.03	0.57
1:A:297:ARG:NH1	1:A:375:GLU:OE2	2.38	0.57
1:C:1231:TYR:O	1:C:1232:VAL:HG22	2.05	0.57
10:3A:4:MAN:H62	10:3A:5:MAN:H5	1.85	0.57
1:A:119:ASN:OD1	1:A:120:ALA:N	2.37	0.56
1:A:458:PHE:O	1:C:819:ARG:NH1	2.38	0.56
3:WA:1:NAG:H83	3:WA:1:NAG:H3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:zA:1:NAG:H3	9:zA:1:NAG:H83	1.86	0.56
1:C:23:ALA:HB3	1:C:25:LEU:HD22	1.87	0.56
3:K:1:NAG:H83	3:K:1:NAG:H3	1.88	0.56
3:v:1:NAG:H3	3:v:1:NAG:H83	1.88	0.56
1:C:119:ASN:OD1	1:C:120:ALA:N	2.38	0.56
1:A:880:LYS:NZ	1:A:990:PHE:O	2.36	0.56
1:A:54:SER:O	1:A:174:LYS:NZ	2.30	0.55
1:A:819:ARG:NH1	1:B:458:PHE:O	2.39	0.55
1:C:1004:ILE:HA	1:C:1007:VAL:HG12	1.87	0.55
1:C:775:VAL:HG12	1:C:1129:LEU:HD23	1.88	0.55
3:mA:2:NAG:H3	3:mA:2:NAG:H83	1.89	0.55
1:B:114:PHE:HB3	8:vA:2:NAG:H81	1.89	0.55
1:C:793:VAL:O	1:C:1066:ARG:NH1	2.37	0.55
1:B:1144:TRP:NE1	1:B:1166:SER:OG	2.30	0.55
1:C:123:SER:HB3	1:C:126:CYS:SG	2.48	0.54
1:C:1272:LEU:O	1:C:1276:ILE:HG12	2.08	0.54
3:a:2:NAG:H3	3:a:2:NAG:H83	1.89	0.54
1:C:297:ARG:NH1	1:C:375:GLU:OE2	2.40	0.54
1:A:123:SER:HB3	1:A:126:CYS:SG	2.48	0.54
1:A:990:PHE:HE1	1:A:1007:VAL:HG23	1.73	0.54
1:B:665:LYS:HD3	1:B:672:ILE:HG22	1.90	0.53
1:B:1218:ASN:HA	1:B:1221:LEU:HG	1.90	0.53
1:C:223:ASP:O	1:C:256:ARG:NH1	2.42	0.53
1:C:1231:TYR:HB3	1:C:1235:ASN:HD22	1.74	0.53
1:B:840:PHE:HE1	1:B:928:MET:HA	1.72	0.53
3:BA:2:NAG:H83	3:BA:2:NAG:H3	1.89	0.53
1:A:1035:ASN:HB3	1:A:1041:ASN:HB3	1.91	0.53
1:B:297:ARG:NH1	1:B:375:GLU:OE2	2.42	0.53
1:C:873:LEU:HD11	1:C:990:PHE:HD2	1.74	0.53
1:B:72:ARG:HD2	1:B:116:PHE:HB3	1.91	0.53
1:A:470:PRO:HG2	1:A:628:THR:HG22	1.89	0.53
1:B:123:SER:HB3	1:B:126:CYS:SG	2.48	0.53
1:B:793:VAL:O	1:B:1066:ARG:NH1	2.39	0.53
1:B:223:ASP:O	1:B:256:ARG:NH1	2.42	0.52
1:B:1035:ASN:HB3	1:B:1041:ASN:HB3	1.91	0.52
1:A:162:VAL:HG13	1:A:165:ALA:HB2	1.90	0.52
1:A:223:ASP:O	1:A:256:ARG:NH1	2.43	0.52
1:B:162:VAL:HG13	1:B:165:ALA:HB2	1.90	0.52
1:A:315:ILE:HG12	1:A:402:PHE:CD1	2.43	0.52
1:A:873:LEU:HD11	1:A:990:PHE:HD2	1.75	0.52
1:A:1036:PHE:O	1:A:1038:ALA:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:VAL:HG13	1:B:432:ILE:HG23	1.92	0.52
1:C:162:VAL:HG13	1:C:165:ALA:HB2	1.92	0.52
1:C:336:LEU:HD23	1:C:336:LEU:H	1.75	0.52
1:C:494:GLY:HA2	1:C:498:TYR:CE1	2.44	0.52
1:B:336:LEU:H	1:B:336:LEU:HD23	1.74	0.52
1:C:49:PHE:HZ	3:p:1:NAG:H81	1.74	0.52
1:B:23:ALA:HB3	1:B:25:LEU:HD22	1.91	0.51
1:C:1295:TRP:CG	1:C:1296:PRO:HD3	2.45	0.51
1:A:1245:TYR:HB2	1:C:1242:ASN:HB2	1.92	0.51
1:B:924:GLU:HG2	1:B:928:MET:HE2	1.91	0.51
1:A:336:LEU:HD23	1:A:336:LEU:H	1.75	0.51
1:C:665:LYS:HD3	1:C:672:ILE:HG22	1.91	0.51
1:B:207:CYS:HB3	1:B:209:ASP:O	2.11	0.51
1:A:256:ARG:HE	1:A:421:VAL:HG21	1.75	0.51
1:C:207:CYS:HB3	1:C:209:ASP:O	2.11	0.51
1:C:1036:PHE:O	1:C:1038:ALA:N	2.43	0.51
1:C:656:SER:OG	1:C:657:ASN:N	2.44	0.51
1:B:482:HIS:CE1	1:B:612:PRO:HB3	2.45	0.51
1:C:1248:LEU:HD13	10:4A:1:NAG:H82	1.93	0.51
1:C:1243:LEU:HD13	1:C:1246:LEU:HG	1.92	0.50
4:RA:1:NAG:O6	4:RA:2:NAG:N2	2.42	0.50
1:B:410:THR:OG1	3:TA:1:NAG:H2	2.12	0.50
1:A:23:ALA:HB3	1:A:25:LEU:HD22	1.93	0.50
1:C:990:PHE:HE1	1:C:1007:VAL:HG23	1.75	0.50
4:q:1:NAG:O6	4:q:2:NAG:N2	2.45	0.50
1:C:1229:PRO:HA	1:B:1225:ALA:HB2	1.93	0.50
1:A:665:LYS:HD3	1:A:672:ILE:HG22	1.93	0.50
1:C:410:THR:OG1	3:s:1:NAG:H2	2.11	0.50
1:C:1205:VAL:HG13	1:C:1206:GLU:HG2	1.94	0.50
3:VA:2:NAG:H4	3:VA:3:BMA:O2	2.12	0.50
1:B:402:PHE:CE2	1:B:412:PHE:HZ	2.30	0.50
4:F:1:NAG:O6	4:F:2:NAG:N2	2.44	0.50
1:A:112:THR:HG22	1:A:113:THR:N	2.27	0.49
1:C:1231:TYR:HB3	1:C:1235:ASN:ND2	2.27	0.49
1:B:483:THR:HG21	1:B:517:VAL:HG12	1.94	0.49
1:A:1239:THR:HG22	1:A:1243:LEU:HD11	1.93	0.49
1:B:112:THR:HG22	1:B:113:THR:N	2.27	0.49
1:C:72:ARG:HG3	1:C:116:PHE:HD2	1.76	0.49
3:J:2:NAG:H4	3:J:3:BMA:O2	2.12	0.49
3:u:2:NAG:H4	3:u:3:BMA:O2	2.12	0.49
1:A:853:LEU:O	1:A:853:LEU:HD23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1175:SER:OG	1:B:1176:ARG:N	2.46	0.49
1:B:176:TYR:O	1:B:181:CYS:HB3	2.12	0.49
1:B:1097:GLU:O	1:B:1101:SER:OG	2.30	0.49
1:C:112:THR:HG22	1:C:113:THR:N	2.27	0.49
1:B:1036:PHE:O	1:B:1038:ALA:N	2.42	0.49
1:B:1294:LYS:HB2	1:B:1297:TRP:NE1	2.27	0.48
1:A:207:CYS:HB3	1:A:209:ASP:O	2.12	0.48
1:A:702:ARG:HG3	1:A:703:TYR:N	2.19	0.48
1:A:482:HIS:CE1	1:A:612:PRO:HB3	2.48	0.48
1:C:921:ALA:HB1	1:C:926:MET:HE3	1.94	0.48
1:A:410:THR:OG1	3:H:1:NAG:H2	2.13	0.48
1:A:793:VAL:O	1:A:1066:ARG:NH1	2.41	0.48
1:A:892:ASP:OD1	1:A:892:ASP:N	2.47	0.48
1:C:72:ARG:HH12	1:C:117:LEU:HD12	1.78	0.48
1:C:1115:ILE:HG22	1:C:1116:PHE:HD2	1.79	0.48
1:C:976:ALA:O	1:C:980:ASN:ND2	2.46	0.48
1:B:1269:LEU:O	1:B:1273:ILE:HG13	2.14	0.48
1:A:115:ASP:N	1:A:115:ASP:OD1	2.45	0.48
1:A:1231:TYR:HA	1:A:1232:VAL:HA	1.68	0.48
1:A:1244:THR:OG1	1:C:1244:THR:OG1	2.32	0.48
1:A:976:ALA:O	1:A:980:ASN:ND2	2.46	0.48
1:B:101:VAL:HB	1:B:132:PHE:HB2	1.96	0.47
1:A:176:TYR:O	1:A:181:CYS:HB3	2.14	0.47
1:A:425:VAL:HG13	1:A:432:ILE:HG23	1.96	0.47
1:A:776:GLU:OE1	1:A:1094:LYS:NZ	2.46	0.47
1:B:765:ILE:HD12	1:B:1141:VAL:HG21	1.96	0.47
1:A:873:LEU:HD11	1:A:990:PHE:CD2	2.50	0.47
1:A:828:ASP:OD2	1:A:1088:ARG:NH2	2.47	0.47
1:A:1175:SER:OG	1:A:1176:ARG:N	2.47	0.47
1:A:1205:VAL:HG13	1:A:1206:GLU:HG2	1.97	0.47
1:C:1245:TYR:HD1	1:C:1248:LEU:HD12	1.80	0.47
1:B:695:MET:HE1	1:B:731:TYR:CZ	2.50	0.47
1:A:531:VAL:HG12	1:A:531:VAL:O	2.15	0.47
1:A:1258:LYS:HE2	1:A:1262:LEU:HD12	1.97	0.47
1:B:873:LEU:HD11	1:B:990:PHE:HD2	1.79	0.47
1:A:72:ARG:HD2	1:A:116:PHE:HB3	1.97	0.47
1:C:26:SER:HB3	1:C:154:TYR:CE1	2.49	0.47
1:C:115:ASP:N	1:C:115:ASP:OD1	2.48	0.47
1:C:984:ASN:HA	1:C:987:VAL:HG22	1.97	0.47
1:C:176:TYR:O	1:C:181:CYS:HB3	2.15	0.47
1:B:1205:VAL:HG13	1:B:1206:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1220:THR:O	1:A:1224:PHE:N	2.47	0.46
1:C:425:VAL:HG13	1:C:432:ILE:HG23	1.96	0.46
1:C:566:ILE:O	1:C:599:THR:OG1	2.29	0.46
1:B:115:ASP:OD1	1:B:115:ASP:N	2.47	0.46
1:B:1238:LEU:HB3	1:B:1240:PRO:HD2	1.96	0.46
1:A:1229:PRO:HA	1:A:1234:PRO:HD3	1.98	0.46
1:B:208:ASP:OD1	1:B:208:ASP:N	2.49	0.46
1:B:531:VAL:O	1:B:531:VAL:HG12	2.15	0.46
1:C:321:GLN:HE22	1:C:536:PRO:HG2	1.81	0.46
1:B:321:GLN:HE22	1:B:536:PRO:HG2	1.80	0.46
1:C:765:ILE:HD12	1:C:1141:VAL:HG21	1.97	0.46
1:C:1228:LEU:HD12	1:B:1228:LEU:O	2.16	0.46
1:A:1228:LEU:N	1:A:1229:PRO:HD2	2.30	0.46
1:C:337:ASP:OD1	1:C:338:THR:N	2.49	0.46
1:A:144:ILE:HG12	1:A:149:VAL:HG22	1.97	0.45
1:C:531:VAL:HG12	1:C:531:VAL:O	2.15	0.45
1:C:1245:TYR:CD1	1:C:1248:LEU:HD12	2.52	0.45
1:B:337:ASP:OD1	1:B:338:THR:N	2.50	0.45
4:RA:8:MAN:H2	4:RA:9:MAN:H2	1.72	0.45
1:A:274:TYR:HB3	5:G:1:NAG:H62	1.98	0.45
1:A:965:THR:HA	1:B:1192:ILE:HD11	1.98	0.45
1:C:256:ARG:HE	1:C:421:VAL:HG21	1.81	0.45
1:C:873:LEU:HD11	1:C:990:PHE:CD2	2.51	0.45
1:C:1108:PHE:O	1:C:1109:CYS:C	2.60	0.45
1:C:1218:ASN:O	1:C:1221:LEU:HG	2.17	0.45
1:A:984:ASN:HA	1:A:987:VAL:HG22	1.99	0.45
1:C:683:GLN:HB2	1:C:695:MET:HB3	1.97	0.45
1:B:274:TYR:HB3	5:SA:1:NAG:H62	1.99	0.45
1:B:369:LEU:HD13	1:B:373:VAL:HG21	1.98	0.45
1:A:174:LYS:HE3	1:A:174:LYS:HB3	1.83	0.45
1:A:1097:GLU:O	1:A:1101:SER:OG	2.35	0.45
1:A:1108:PHE:O	1:A:1109:CYS:C	2.60	0.45
1:C:1243:LEU:HB3	1:C:1246:LEU:HD23	1.98	0.45
1:B:584:THR:HG21	1:B:587:TYR:HA	1.99	0.45
1:A:496:SER:HB2	9:n:1:NAG:H82	1.99	0.44
1:A:794:CYS:HB2	1:A:1043:ILE:HD12	1.99	0.44
1:C:1053:ILE:HG23	1:C:1054:GLN:NE2	2.32	0.44
1:C:1233:LYS:NZ	1:B:1237:ASP:OD1	2.46	0.44
1:C:1239:THR:N	1:C:1240:PRO:HD2	2.32	0.44
1:B:984:ASN:HA	1:B:987:VAL:HG22	1.98	0.44
5:SA:4:MAN:H2	5:SA:5:NAG:H2	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1196:ASN:OD1	1:B:1197:VAL:N	2.50	0.44
3:WA:3:BMA:H62	3:WA:4:MAN:H2	1.69	0.44
1:A:584:THR:HG21	1:A:587:TYR:HA	1.99	0.44
1:B:564:LYS:HB2	1:B:603:GLY:HA3	1.98	0.44
1:B:873:LEU:HD11	1:B:990:PHE:CD2	2.52	0.44
1:A:564:LYS:HB2	1:A:603:GLY:HA3	1.98	0.44
1:C:1234:PRO:HB2	1:B:1241:PHE:CE1	2.51	0.44
2:NA:4:MAN:H62	2:NA:6:MAN:H2	1.72	0.44
1:B:1247:ASN:HB2	10:3A:1:NAG:H81	1.99	0.44
2:m:4:MAN:H62	2:m:6:MAN:H2	1.73	0.44
3:rA:1:NAG:H4	3:rA:2:NAG:H2	1.70	0.44
1:A:321:GLN:HE22	1:A:536:PRO:HG2	1.82	0.44
1:A:337:ASP:OD1	1:A:338:THR:N	2.50	0.44
1:C:1196:ASN:OD1	1:C:1197:VAL:N	2.51	0.44
3:z:3:BMA:H62	3:z:4:MAN:H2	1.72	0.44
1:A:765:ILE:HD12	1:A:1141:VAL:HG21	1.99	0.44
1:C:208:ASP:OD1	1:C:208:ASP:N	2.48	0.44
1:C:636:VAL:HG21	1:B:1045:ALA:HB2	1.99	0.44
1:A:209:ASP:CG	1:A:210:CYS:H	2.24	0.44
3:f:1:NAG:H4	3:f:2:NAG:H2	1.70	0.44
1:A:1217:VAL:HG11	1:C:1215:VAL:HG11	2.00	0.43
1:B:1108:PHE:O	1:B:1109:CYS:C	2.60	0.43
1:A:1196:ASN:OD1	1:A:1197:VAL:N	2.50	0.43
1:B:892:ASP:OD1	1:B:892:ASP:N	2.47	0.43
1:A:1148:CYS:HB2	1:A:1199:PHE:HD2	1.83	0.43
1:B:641:ILE:HG12	1:B:675:VAL:HG22	1.99	0.43
1:A:994:ASN:O	1:A:998:THR:HG23	2.19	0.43
1:A:1115:ILE:HG22	1:A:1116:PHE:HD2	1.84	0.43
1:B:1060:ASP:OD1	1:B:1060:ASP:N	2.51	0.43
1:B:1242:ASN:C	1:B:1243:LEU:HD23	2.42	0.43
2:o:1:NAG:H61	2:o:2:NAG:H82	2.00	0.43
1:B:25:LEU:HD23	1:B:25:LEU:H	1.83	0.43
1:B:311:LYS:NZ	1:B:411:ASP:OD1	2.48	0.43
4:q:8:MAN:H2	4:q:9:MAN:H2	1.70	0.43
1:A:702:ARG:CG	1:A:703:TYR:H	2.21	0.43
1:A:1223:GLU:O	1:A:1227:ASN:ND2	2.38	0.43
1:A:1269:LEU:O	1:A:1273:ILE:HG13	2.17	0.43
1:C:25:LEU:H	1:C:25:LEU:HD23	1.83	0.43
1:C:1273:ILE:HG12	1:B:1272:LEU:HD22	2.01	0.43
1:B:990:PHE:HE1	1:B:1007:VAL:HG23	1.82	0.43
1:C:584:THR:HG21	1:C:587:TYR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:904:ASP:OD1	1:B:905:LEU:N	2.47	0.43
2:D:1:NAG:H61	2:D:2:NAG:H82	2.00	0.43
2:1A:3:BMA:H3	2:1A:4:MAN:H2	1.84	0.43
2:PA:1:NAG:H61	2:PA:2:NAG:H82	2.01	0.43
1:C:135:GLN:NE2	1:C:136:LEU:O	2.41	0.42
1:A:175:CYS:SG	1:A:176:TYR:N	2.92	0.42
1:A:1060:ASP:N	1:A:1060:ASP:OD1	2.51	0.42
1:C:1228:LEU:HA	1:B:1232:VAL:H	1.84	0.42
5:G:4:MAN:H2	5:G:5:NAG:H2	1.77	0.42
1:C:72:ARG:HH12	1:C:117:LEU:CD1	2.32	0.42
1:B:307:LEU:HD23	1:B:307:LEU:H	1.85	0.42
1:A:904:ASP:OD1	1:A:905:LEU:N	2.48	0.42
1:C:1295:TRP:CD1	1:C:1296:PRO:HD3	2.55	0.42
1:A:1167:ASP:OD1	1:A:1167:ASP:N	2.53	0.42
1:C:794:CYS:HB2	1:C:1043:ILE:HD12	2.02	0.42
1:B:1239:THR:N	1:B:1240:PRO:HD2	2.34	0.42
3:K:3:BMA:H62	3:K:4:MAN:H2	1.68	0.42
1:A:25:LEU:H	1:A:25:LEU:HD23	1.84	0.42
1:A:208:ASP:OD1	1:A:208:ASP:N	2.49	0.42
1:A:563:PHE:CD2	1:A:566:ILE:HD11	2.55	0.42
1:A:1192:ILE:HD11	1:C:965:THR:HA	2.01	0.42
1:A:1231:TYR:CE1	7:pA:2:NAG:H5	2.55	0.42
1:C:1175:SER:OG	1:C:1176:ARG:N	2.53	0.42
1:B:1115:ILE:HG22	1:B:1116:PHE:HD2	1.84	0.42
1:A:1067:LEU:HD23	1:A:1067:LEU:HA	1.89	0.42
1:C:72:ARG:HG3	1:C:116:PHE:CD2	2.55	0.42
1:C:410:THR:HG23	1:C:410:THR:O	2.20	0.42
1:C:274:TYR:HB3	5:r:1:NAG:H62	2.01	0.41
1:B:1098:CYS:SG	1:B:1108:PHE:CE2	3.13	0.41
1:C:1014:ILE:O	1:C:1017:VAL:HG12	2.20	0.41
1:A:359:THR:HG22	1:A:359:THR:O	2.20	0.41
1:A:410:THR:HG23	1:A:410:THR:O	2.20	0.41
1:A:840:PHE:HE1	1:A:928:MET:HA	1.85	0.41
1:C:305:ASN:O	1:C:309:ASN:ND2	2.53	0.41
1:A:918:PRO:HG3	1:B:713:ASN:HD21	1.86	0.41
1:C:702:ARG:O	1:C:704:GLY:N	2.53	0.41
1:C:994:ASN:O	1:C:998:THR:HG23	2.20	0.41
1:B:862:ILE:HG22	1:B:862:ILE:O	2.20	0.41
1:B:701:SER:O	1:B:702:ARG:HD2	2.20	0.41
3:p:1:NAG:O7	3:p:1:NAG:O3	2.35	0.41
1:B:880:LYS:HE2	1:B:992:SER:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:3:BMA:H3	2:Z:4:MAN:H2	1.84	0.41
1:A:402:PHE:CE2	1:A:412:PHE:HZ	2.39	0.41
1:C:701:SER:O	1:C:702:ARG:HD2	2.21	0.41
1:B:296:MET:HE2	1:B:417:PHE:HE1	1.86	0.41
1:B:359:THR:HG22	1:B:359:THR:O	2.21	0.41
1:B:1242:ASN:O	1:B:1243:LEU:HD23	2.20	0.41
1:A:629:LYS:HB3	1:A:629:LYS:HE2	1.89	0.41
1:A:636:VAL:HG21	1:C:1045:ALA:HB2	2.02	0.41
1:A:732:SER:HB2	1:C:918:PRO:O	2.21	0.41
1:A:998:THR:HG22	1:A:1004:ILE:HD13	2.02	0.41
1:C:175:CYS:SG	1:C:176:TYR:N	2.93	0.41
1:C:563:PHE:CD2	1:C:566:ILE:HD11	2.56	0.41
1:B:702:ARG:O	1:B:704:GLY:N	2.54	0.41
1:B:1167:ASP:OD1	1:B:1167:ASP:N	2.53	0.41
1:B:1218:ASN:OD1	1:B:1219:LYS:N	2.54	0.41
3:E:1:NAG:H61	3:E:2:NAG:C7	2.51	0.41
3:GA:1:NAG:H4	3:GA:2:NAG:H2	1.70	0.41
1:B:994:ASN:O	1:B:998:THR:HG23	2.20	0.41
1:A:111:ASN:OD1	1:A:112:THR:N	2.51	0.40
1:A:479:TYR:HD2	1:C:348:PRO:HG3	1.85	0.40
8:j:3:BMA:H62	8:j:5:MAN:H2	1.82	0.40
3:aA:3:BMA:H62	3:aA:4:MAN:H2	1.73	0.40
1:A:80:GLY:O	8:j:4:MAN:O6	2.36	0.40
1:B:43:LEU:HD23	1:B:189:THR:H	1.86	0.40
1:B:629:LYS:HB3	1:B:629:LYS:HE2	1.90	0.40
1:B:1228:LEU:HB2	1:B:1229:PRO:HD3	2.03	0.40
1:A:348:PRO:HG3	1:B:479:TYR:HD2	1.86	0.40
1:C:49:PHE:CZ	3:p:1:NAG:H81	2.56	0.40
1:C:776:GLU:OE1	1:C:1094:LYS:NZ	2.53	0.40
1:C:43:LEU:HD23	1:C:189:THR:H	1.86	0.40
1:C:359:THR:HG22	1:C:359:THR:O	2.22	0.40
1:C:892:ASP:OD1	1:C:892:ASP:N	2.47	0.40
3:O:3:BMA:H62	3:O:4:MAN:H2	1.72	0.40
9:OA:1:NAG:H61	9:OA:2:NAG:O5	2.22	0.40
1:C:277:ALA:HB1	1:C:282:VAL:HG11	2.02	0.40
1:B:852:ASN:H	1:B:980:ASN:HD21	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1273/1356 (94%)	1176 (92%)	96 (8%)	1 (0%)	48	78
1	B	1273/1356 (94%)	1182 (93%)	91 (7%)	0	100	100
1	C	1273/1356 (94%)	1170 (92%)	101 (8%)	2 (0%)	43	71
All	All	3819/4068 (94%)	3528 (92%)	288 (8%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1233	LYS
1	A	1225	ALA
1	C	1232	VAL

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	1121/1197 (94%)	1121 (100%)	0	100	100
1	B	1121/1197 (94%)	1121 (100%)	0	100	100
1	C	1121/1197 (94%)	1121 (100%)	0	100	100
All	All	3363/3591 (94%)	3363 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	321	GLN
1	A	434	ASN
1	A	503	HIS
1	A	969	GLN
1	A	972	GLN
1	A	1026	ASN
1	A	1291	ASN
1	C	969	GLN
1	C	980	ASN
1	C	1026	ASN
1	C	1287	ASN
1	B	401	ASN
1	B	434	ASN
1	B	969	GLN
1	B	980	ASN
1	B	1026	ASN
1	B	1227	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

842 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	0	1	3,1	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	0	2	3	14,14,15	0.26	0	17,19,21	0.46	0
3	BMA	0	3	3	11,11,12	0.70	0	15,15,17	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	0	4	3	11,11,12	1.40	2 (18%)	15,15,17	1.28	2 (13%)
3	MAN	0	5	3	11,11,12	0.72	1 (9%)	15,15,17	1.12	2 (13%)
3	MAN	0	6	3	11,11,12	0.65	0	15,15,17	1.09	2 (13%)
3	MAN	0	7	3	11,11,12	0.59	0	15,15,17	1.03	2 (13%)
10	NAG	0A	1	10,1	14,14,15	0.37	0	17,19,21	0.50	0
10	NAG	0A	2	10	14,14,15	0.23	0	17,19,21	0.44	0
10	BMA	0A	3	10	11,11,12	0.73	0	15,15,17	0.77	0
10	MAN	0A	4	10	11,11,12	0.70	0	15,15,17	0.87	1 (6%)
10	MAN	0A	5	10	11,11,12	0.62	0	15,15,17	0.98	2 (13%)
10	MAN	0A	6	10	11,11,12	0.63	0	15,15,17	0.99	2 (13%)
10	MAN	0A	7	10	11,11,12	0.67	0	15,15,17	0.99	2 (13%)
3	NAG	1	1	3,1	14,14,15	0.21	0	17,19,21	0.50	0
3	NAG	1	2	3	14,14,15	0.28	0	17,19,21	0.55	0
3	BMA	1	3	3	11,11,12	0.55	0	15,15,17	0.78	0
3	MAN	1	4	3	11,11,12	0.67	0	15,15,17	1.05	2 (13%)
3	MAN	1	5	3	11,11,12	0.65	0	15,15,17	0.99	2 (13%)
3	MAN	1	6	3	11,11,12	0.68	0	15,15,17	1.05	2 (13%)
3	MAN	1	7	3	11,11,12	0.68	0	15,15,17	1.00	2 (13%)
10	NAG	1A	1	10,1	14,14,15	0.41	0	17,19,21	0.74	1 (5%)
10	NAG	1A	2	10	14,14,15	0.24	0	17,19,21	0.39	0
10	BMA	1A	3	10	11,11,12	0.58	0	15,15,17	0.64	0
10	MAN	1A	4	10	11,11,12	0.69	0	15,15,17	0.98	2 (13%)
10	MAN	1A	5	10	11,11,12	0.65	0	15,15,17	0.91	1 (6%)
10	MAN	1A	6	10	11,11,12	0.67	0	15,15,17	0.99	2 (13%)
10	MAN	1A	7	10	11,11,12	0.65	0	15,15,17	0.93	2 (13%)
2	NAG	2	1	2,1	14,14,15	0.25	0	17,19,21	0.56	0
2	NAG	2	2	2	14,14,15	0.23	0	17,19,21	0.45	0
2	BMA	2	3	2	11,11,12	0.72	0	15,15,17	0.71	0
2	MAN	2	4	2	11,11,12	1.02	0	15,15,17	0.95	1 (6%)
2	MAN	2	5	2	11,11,12	0.65	0	15,15,17	0.94	2 (13%)
2	MAN	2	6	2	11,11,12	0.63	0	15,15,17	1.00	2 (13%)
2	MAN	2	7	2	11,11,12	0.61	0	15,15,17	0.93	2 (13%)
10	NAG	2A	1	10,1	14,14,15	0.21	0	17,19,21	0.40	0
10	NAG	2A	2	10	14,14,15	0.24	0	17,19,21	0.43	0
10	BMA	2A	3	10	11,11,12	0.58	0	15,15,17	0.81	0
10	MAN	2A	4	10	11,11,12	0.69	0	15,15,17	0.88	1 (6%)
10	MAN	2A	5	10	11,11,12	0.61	0	15,15,17	1.00	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	2A	6	10	11,11,12	0.64	0	15,15,17	0.97	2 (13%)
10	MAN	2A	7	10	11,11,12	0.62	0	15,15,17	1.01	2 (13%)
2	NAG	3	1	2,1	14,14,15	0.26	0	17,19,21	0.48	0
2	NAG	3	2	2	14,14,15	0.24	0	17,19,21	0.44	0
2	BMA	3	3	2	11,11,12	0.91	1 (9%)	15,15,17	0.91	1 (6%)
2	MAN	3	4	2	11,11,12	0.69	0	15,15,17	0.94	2 (13%)
2	MAN	3	5	2	11,11,12	0.67	0	15,15,17	0.98	2 (13%)
2	MAN	3	6	2	11,11,12	0.65	0	15,15,17	0.94	2 (13%)
2	MAN	3	7	2	11,11,12	0.67	0	15,15,17	1.08	2 (13%)
10	NAG	3A	1	10,1	14,14,15	0.33	0	17,19,21	0.69	1 (5%)
10	NAG	3A	2	10	14,14,15	0.20	0	17,19,21	0.50	0
10	BMA	3A	3	10	11,11,12	0.60	0	15,15,17	0.78	0
10	MAN	3A	4	10	11,11,12	0.72	0	15,15,17	0.94	2 (13%)
10	MAN	3A	5	10	11,11,12	0.63	0	15,15,17	1.12	2 (13%)
10	MAN	3A	6	10	11,11,12	0.67	0	15,15,17	0.98	2 (13%)
10	MAN	3A	7	10	11,11,12	0.61	0	15,15,17	1.01	2 (13%)
2	NAG	4	1	2,1	14,14,15	0.24	0	17,19,21	0.42	0
2	NAG	4	2	2	14,14,15	0.23	0	17,19,21	0.49	0
2	BMA	4	3	2	11,11,12	0.57	0	15,15,17	0.68	0
2	MAN	4	4	2	11,11,12	0.93	0	15,15,17	1.18	2 (13%)
2	MAN	4	5	2	11,11,12	0.60	0	15,15,17	1.05	2 (13%)
2	MAN	4	6	2	11,11,12	0.66	0	15,15,17	1.02	2 (13%)
2	MAN	4	7	2	11,11,12	0.65	0	15,15,17	1.01	2 (13%)
10	NAG	4A	1	10,1	14,14,15	0.47	0	17,19,21	0.71	1 (5%)
10	NAG	4A	2	10	14,14,15	0.22	0	17,19,21	0.40	0
10	BMA	4A	3	10	11,11,12	0.58	0	15,15,17	0.66	0
10	MAN	4A	4	10	11,11,12	0.65	0	15,15,17	0.90	1 (6%)
10	MAN	4A	5	10	11,11,12	0.61	0	15,15,17	0.93	2 (13%)
10	MAN	4A	6	10	11,11,12	0.65	0	15,15,17	1.00	2 (13%)
10	MAN	4A	7	10	11,11,12	0.61	0	15,15,17	0.95	2 (13%)
3	NAG	5	1	3,1	14,14,15	0.44	0	17,19,21	0.82	1 (5%)
3	NAG	5	2	3	14,14,15	0.26	0	17,19,21	0.41	0
3	BMA	5	3	3	11,11,12	0.60	0	15,15,17	0.61	0
3	MAN	5	4	3	11,11,12	0.88	1 (9%)	15,15,17	1.20	3 (20%)
3	MAN	5	5	3	11,11,12	0.64	0	15,15,17	0.92	2 (13%)
3	MAN	5	6	3	11,11,12	0.64	0	15,15,17	0.95	2 (13%)
3	MAN	5	7	3	11,11,12	0.64	0	15,15,17	0.99	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	5A	1	10,1	14,14,15	0.31	0	17,19,21	0.44	0
10	NAG	5A	2	10	14,14,15	0.25	0	17,19,21	0.41	0
10	BMA	5A	3	10	11,11,12	0.55	0	15,15,17	0.79	0
10	MAN	5A	4	10	11,11,12	0.66	0	15,15,17	0.98	2 (13%)
10	MAN	5A	5	10	11,11,12	0.62	0	15,15,17	0.96	2 (13%)
10	MAN	5A	6	10	11,11,12	0.66	0	15,15,17	0.96	2 (13%)
10	MAN	5A	7	10	11,11,12	0.65	0	15,15,17	1.02	2 (13%)
3	NAG	6	1	3,1	14,14,15	0.47	0	17,19,21	0.65	0
3	NAG	6	2	3	14,14,15	0.21	0	17,19,21	0.44	0
3	BMA	6	3	3	11,11,12	1.04	1 (9%)	15,15,17	0.96	0
3	MAN	6	4	3	11,11,12	0.79	1 (9%)	15,15,17	1.25	2 (13%)
3	MAN	6	5	3	11,11,12	0.70	0	15,15,17	0.89	1 (6%)
3	MAN	6	6	3	11,11,12	0.63	0	15,15,17	1.02	2 (13%)
3	MAN	6	7	3	11,11,12	0.61	0	15,15,17	1.02	2 (13%)
10	NAG	6A	1	10,1	14,14,15	0.35	0	17,19,21	0.52	0
10	NAG	6A	2	10	14,14,15	0.27	0	17,19,21	0.45	0
10	BMA	6A	3	10	11,11,12	0.58	0	15,15,17	0.66	0
10	MAN	6A	4	10	11,11,12	0.69	0	15,15,17	0.94	2 (13%)
10	MAN	6A	5	10	11,11,12	0.63	0	15,15,17	0.98	2 (13%)
10	MAN	6A	6	10	11,11,12	0.63	0	15,15,17	0.97	2 (13%)
10	MAN	6A	7	10	11,11,12	0.63	0	15,15,17	0.99	2 (13%)
2	NAG	7	1	2,1	14,14,15	0.30	0	17,19,21	0.61	0
2	NAG	7	2	2	14,14,15	0.29	0	17,19,21	0.44	0
2	BMA	7	3	2	11,11,12	0.60	0	15,15,17	0.72	0
2	MAN	7	4	2	11,11,12	0.60	0	15,15,17	0.96	2 (13%)
2	MAN	7	5	2	11,11,12	0.66	0	15,15,17	0.95	2 (13%)
2	MAN	7	6	2	11,11,12	1.50	2 (18%)	15,15,17	2.10	4 (26%)
2	MAN	7	7	2	11,11,12	0.63	0	15,15,17	1.00	2 (13%)
10	NAG	7A	1	10,1	14,14,15	0.64	1 (7%)	17,19,21	0.71	1 (5%)
10	NAG	7A	2	10	14,14,15	0.24	0	17,19,21	0.41	0
10	BMA	7A	3	10	11,11,12	0.71	0	15,15,17	0.70	0
10	MAN	7A	4	10	11,11,12	0.69	0	15,15,17	0.87	1 (6%)
10	MAN	7A	5	10	11,11,12	0.63	0	15,15,17	0.97	2 (13%)
10	MAN	7A	6	10	11,11,12	0.67	0	15,15,17	1.02	2 (13%)
10	MAN	7A	7	10	11,11,12	0.63	0	15,15,17	0.99	2 (13%)
3	NAG	8	1	3,1	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	8	2	3	14,14,15	0.26	0	17,19,21	0.57	0
3	BMA	8	3	3	11,11,12	0.57	0	15,15,17	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	8	4	3	11,11,12	0.78	1 (9%)	15,15,17	1.16	2 (13%)
3	MAN	8	5	3	11,11,12	0.65	0	15,15,17	0.93	2 (13%)
3	MAN	8	6	3	11,11,12	0.76	1 (9%)	15,15,17	1.19	2 (13%)
3	MAN	8	7	3	11,11,12	0.61	0	15,15,17	0.99	2 (13%)
3	NAG	9	1	3,1	14,14,15	0.24	0	17,19,21	0.60	0
3	NAG	9	2	3	14,14,15	0.18	0	17,19,21	0.37	0
3	BMA	9	3	3	11,11,12	0.92	0	15,15,17	0.83	0
3	MAN	9	4	3	11,11,12	0.63	0	15,15,17	1.09	2 (13%)
3	MAN	9	5	3	11,11,12	0.65	0	15,15,17	0.91	2 (13%)
3	MAN	9	6	3	11,11,12	0.66	0	15,15,17	0.97	2 (13%)
3	MAN	9	7	3	11,11,12	0.66	0	15,15,17	1.01	2 (13%)
2	NAG	AA	1	2,1	14,14,15	0.22	0	17,19,21	0.41	0
2	NAG	AA	2	2	14,14,15	0.21	0	17,19,21	0.58	0
2	BMA	AA	3	2	11,11,12	0.59	0	15,15,17	1.01	1 (6%)
2	MAN	AA	4	2	11,11,12	0.59	0	15,15,17	0.89	2 (13%)
2	MAN	AA	5	2	11,11,12	0.64	0	15,15,17	0.92	2 (13%)
2	MAN	AA	6	2	11,11,12	0.68	0	15,15,17	1.05	2 (13%)
2	MAN	AA	7	2	11,11,12	0.64	0	15,15,17	1.00	2 (13%)
3	NAG	BA	1	3,1	14,14,15	0.33	0	17,19,21	0.60	0
3	NAG	BA	2	3	14,14,15	0.44	0	17,19,21	1.41	2 (11%)
3	BMA	BA	3	3	11,11,12	0.83	1 (9%)	15,15,17	0.92	0
3	MAN	BA	4	3	11,11,12	0.70	0	15,15,17	1.05	2 (13%)
3	MAN	BA	5	3	11,11,12	0.69	0	15,15,17	1.21	2 (13%)
3	MAN	BA	6	3	11,11,12	0.60	0	15,15,17	0.94	2 (13%)
3	MAN	BA	7	3	11,11,12	0.67	0	15,15,17	1.12	2 (13%)
2	NAG	CA	1	2,1	14,14,15	0.24	0	17,19,21	0.56	0
2	NAG	CA	2	2	14,14,15	0.20	0	17,19,21	0.47	0
2	BMA	CA	3	2	11,11,12	0.62	0	15,15,17	0.79	0
2	MAN	CA	4	2	11,11,12	0.61	0	15,15,17	0.92	2 (13%)
2	MAN	CA	5	2	11,11,12	0.63	0	15,15,17	0.96	2 (13%)
2	MAN	CA	6	2	11,11,12	0.67	0	15,15,17	1.07	2 (13%)
2	MAN	CA	7	2	11,11,12	0.62	0	15,15,17	0.95	2 (13%)
2	NAG	D	1	2,1	14,14,15	0.22	0	17,19,21	0.45	0
2	NAG	D	2	2	14,14,15	0.22	0	17,19,21	0.43	0
2	BMA	D	3	2	11,11,12	0.57	0	15,15,17	0.83	0
2	MAN	D	4	2	11,11,12	0.62	0	15,15,17	0.90	2 (13%)
2	MAN	D	5	2	11,11,12	0.60	0	15,15,17	0.96	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	D	6	2	11,11,12	0.65	0	15,15,17	0.99	2 (13%)
2	MAN	D	7	2	11,11,12	1.56	2 (18%)	15,15,17	2.15	4 (26%)
3	NAG	DA	1	3,1	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	DA	2	3	14,14,15	0.30	0	17,19,21	0.67	0
3	BMA	DA	3	3	11,11,12	0.58	0	15,15,17	1.02	1 (6%)
3	MAN	DA	4	3	11,11,12	0.72	0	15,15,17	1.21	2 (13%)
3	MAN	DA	5	3	11,11,12	0.64	0	15,15,17	0.97	2 (13%)
3	MAN	DA	6	3	11,11,12	0.61	0	15,15,17	0.99	2 (13%)
3	MAN	DA	7	3	11,11,12	0.64	0	15,15,17	0.99	2 (13%)
3	NAG	E	1	3,1	14,14,15	0.69	1 (7%)	17,19,21	0.81	1 (5%)
3	NAG	E	2	3	14,14,15	0.29	0	17,19,21	0.60	0
3	BMA	E	3	3	11,11,12	0.53	0	15,15,17	0.78	0
3	MAN	E	4	3	11,11,12	0.99	0	15,15,17	1.03	1 (6%)
3	MAN	E	5	3	11,11,12	0.68	0	15,15,17	0.98	2 (13%)
3	MAN	E	6	3	11,11,12	0.61	0	15,15,17	1.02	2 (13%)
3	MAN	E	7	3	11,11,12	0.64	0	15,15,17	0.91	2 (13%)
7	NAG	EA	1	7,1	14,14,15	0.27	0	17,19,21	0.46	0
7	NAG	EA	10	7	14,14,15	0.23	0	17,19,21	0.42	0
7	GAL	EA	11	7	11,11,12	0.50	0	15,15,17	0.90	0
7	FUC	EA	12	7	10,10,11	1.55	2 (20%)	14,14,16	1.62	3 (21%)
7	NAG	EA	2	7	14,14,15	0.28	0	17,19,21	0.46	0
7	BMA	EA	3	7	11,11,12	0.78	0	15,15,17	0.81	0
7	MAN	EA	4	7	11,11,12	1.18	2 (18%)	15,15,17	1.00	1 (6%)
7	NAG	EA	5	7	14,14,15	0.20	0	17,19,21	0.45	0
7	GAL	EA	6	7	11,11,12	0.71	0	15,15,17	1.39	2 (13%)
7	NAG	EA	7	7	14,14,15	0.32	0	17,19,21	0.56	0
7	GAL	EA	8	7	11,11,12	0.50	0	15,15,17	0.87	0
7	MAN	EA	9	7	11,11,12	0.69	0	15,15,17	1.17	2 (13%)
4	NAG	F	1	4,1	14,14,15	0.20	0	17,19,21	0.50	0
4	NAG	F	2	4	14,14,15	0.19	0	17,19,21	0.51	0
4	BMA	F	3	4	11,11,12	1.04	1 (9%)	15,15,17	1.25	2 (13%)
4	MAN	F	4	4	11,11,12	0.65	0	15,15,17	1.19	2 (13%)
4	MAN	F	5	4	11,11,12	0.96	1 (9%)	15,15,17	1.24	2 (13%)
4	MAN	F	6	4	11,11,12	0.63	0	15,15,17	0.92	2 (13%)
4	MAN	F	7	4	11,11,12	0.67	0	15,15,17	1.11	2 (13%)
4	MAN	F	8	4	11,11,12	0.57	0	15,15,17	1.14	2 (13%)
4	MAN	F	9	4	11,11,12	0.69	0	15,15,17	0.92	2 (13%)
2	NAG	FA	1	2,1	14,14,15	0.26	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	FA	2	2	14,14,15	0.21	0	17,19,21	0.41	0
2	BMA	FA	3	2	11,11,12	1.20	3 (27%)	15,15,17	1.20	2 (13%)
2	MAN	FA	4	2	11,11,12	0.65	0	15,15,17	1.10	2 (13%)
2	MAN	FA	5	2	11,11,12	0.67	0	15,15,17	1.03	2 (13%)
2	MAN	FA	6	2	11,11,12	0.68	0	15,15,17	0.99	2 (13%)
2	MAN	FA	7	2	11,11,12	0.65	0	15,15,17	0.95	2 (13%)
5	NAG	G	1	1,5	14,14,15	0.52	0	17,19,21	0.55	0
5	NAG	G	2	5	14,14,15	0.20	0	17,19,21	0.42	0
5	BMA	G	3	5	11,11,12	0.45	0	15,15,17	0.75	0
5	MAN	G	4	5	11,11,12	0.76	1 (9%)	15,15,17	1.20	1 (6%)
5	NAG	G	5	5	14,14,15	0.22	0	17,19,21	0.79	1 (5%)
5	GAL	G	6	5	11,11,12	0.49	0	15,15,17	1.05	1 (6%)
5	MAN	G	7	5	11,11,12	0.60	0	15,15,17	0.94	2 (13%)
5	NAG	G	8	5	14,14,15	0.27	0	17,19,21	0.51	0
5	GAL	G	9	5	11,11,12	0.50	0	15,15,17	0.85	0
3	NAG	GA	1	3,1	14,14,15	0.32	0	17,19,21	0.48	0
3	NAG	GA	2	3	14,14,15	0.45	0	17,19,21	0.55	0
3	BMA	GA	3	3	11,11,12	0.86	0	15,15,17	0.83	0
3	MAN	GA	4	3	11,11,12	1.25	3 (27%)	15,15,17	0.96	0
3	MAN	GA	5	3	11,11,12	0.69	0	15,15,17	0.99	2 (13%)
3	MAN	GA	6	3	11,11,12	0.67	0	15,15,17	1.03	2 (13%)
3	MAN	GA	7	3	11,11,12	0.68	1 (9%)	15,15,17	1.16	2 (13%)
3	NAG	H	1	3,1	14,14,15	0.25	0	17,19,21	0.47	0
3	NAG	H	2	3	14,14,15	0.29	0	17,19,21	0.78	1 (5%)
3	BMA	H	3	3	11,11,12	0.56	0	15,15,17	1.04	1 (6%)
3	MAN	H	4	3	11,11,12	1.18	1 (9%)	15,15,17	1.04	0
3	MAN	H	5	3	11,11,12	0.71	1 (9%)	15,15,17	1.08	2 (13%)
3	MAN	H	6	3	11,11,12	0.65	0	15,15,17	1.05	2 (13%)
3	MAN	H	7	3	11,11,12	0.62	0	15,15,17	0.98	2 (13%)
3	NAG	HA	1	3,1	14,14,15	0.24	0	17,19,21	0.39	0
3	NAG	HA	2	3	14,14,15	0.23	0	17,19,21	0.40	0
3	BMA	HA	3	3	11,11,12	0.57	0	15,15,17	0.74	0
3	MAN	HA	4	3	11,11,12	1.13	1 (9%)	15,15,17	0.96	0
3	MAN	HA	5	3	11,11,12	0.65	0	15,15,17	0.96	2 (13%)
3	MAN	HA	6	3	11,11,12	0.67	0	15,15,17	1.03	2 (13%)
3	MAN	HA	7	3	11,11,12	0.67	0	15,15,17	1.10	2 (13%)
3	NAG	I	1	3,1	14,14,15	0.28	0	17,19,21	0.54	0
3	NAG	I	2	3	14,14,15	0.22	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	I	3	3	11,11,12	0.52	0	15,15,17	0.73	0
3	MAN	I	4	3	11,11,12	0.92	1 (9%)	15,15,17	1.49	1 (6%)
3	MAN	I	5	3	11,11,12	0.73	0	15,15,17	0.87	1 (6%)
3	MAN	I	6	3	11,11,12	0.68	0	15,15,17	0.89	1 (6%)
3	MAN	I	7	3	11,11,12	0.64	0	15,15,17	0.91	2 (13%)
3	NAG	IA	1	3,1	14,14,15	0.41	0	17,19,21	0.65	0
3	NAG	IA	2	3	14,14,15	0.23	0	17,19,21	0.41	0
3	BMA	IA	3	3	11,11,12	0.50	0	15,15,17	0.79	0
3	MAN	IA	4	3	11,11,12	1.04	0	15,15,17	1.25	1 (6%)
3	MAN	IA	5	3	11,11,12	0.61	0	15,15,17	0.96	2 (13%)
3	MAN	IA	6	3	11,11,12	0.62	0	15,15,17	1.02	2 (13%)
3	MAN	IA	7	3	11,11,12	0.65	0	15,15,17	0.89	1 (6%)
3	NAG	J	1	3,1	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	J	2	3	14,14,15	0.24	0	17,19,21	0.52	0
3	BMA	J	3	3	11,11,12	1.04	1 (9%)	15,15,17	1.10	1 (6%)
3	MAN	J	4	3	11,11,12	0.79	0	15,15,17	1.02	2 (13%)
3	MAN	J	5	3	11,11,12	0.74	1 (9%)	15,15,17	1.18	2 (13%)
3	MAN	J	6	3	11,11,12	0.68	0	15,15,17	0.91	1 (6%)
3	MAN	J	7	3	11,11,12	0.63	0	15,15,17	1.01	2 (13%)
2	NAG	JA	1	2,1	14,14,15	1.12	1 (7%)	17,19,21	1.24	1 (5%)
2	NAG	JA	2	2	14,14,15	0.24	0	17,19,21	0.47	0
2	BMA	JA	3	2	11,11,12	0.70	0	15,15,17	0.72	0
2	MAN	JA	4	2	11,11,12	0.87	1 (9%)	15,15,17	1.13	3 (20%)
2	MAN	JA	5	2	11,11,12	0.63	0	15,15,17	1.01	2 (13%)
2	MAN	JA	6	2	11,11,12	0.62	0	15,15,17	1.04	2 (13%)
2	MAN	JA	7	2	11,11,12	0.64	0	15,15,17	0.98	2 (13%)
3	NAG	K	1	3,1	14,14,15	0.93	1 (7%)	17,19,21	1.61	3 (17%)
3	NAG	K	2	3	14,14,15	0.30	0	17,19,21	0.44	0
3	BMA	K	3	3	11,11,12	1.00	1 (9%)	15,15,17	0.78	0
3	MAN	K	4	3	11,11,12	0.71	0	15,15,17	0.93	1 (6%)
3	MAN	K	5	3	11,11,12	0.63	0	15,15,17	0.98	2 (13%)
3	MAN	K	6	3	11,11,12	1.51	2 (18%)	15,15,17	2.10	4 (26%)
3	MAN	K	7	3	11,11,12	0.61	0	15,15,17	0.99	2 (13%)
8	NAG	KA	1	8,1	14,14,15	0.44	0	17,19,21	1.58	2 (11%)
8	NAG	KA	2	8	14,14,15	0.49	0	17,19,21	0.65	0
8	BMA	KA	3	8	11,11,12	1.58	3 (27%)	15,15,17	1.14	2 (13%)
8	MAN	KA	4	8	11,11,12	0.71	0	15,15,17	1.06	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	KA	5	8	11,11,12	0.70	0	15,15,17	0.87	1 (6%)
2	NAG	L	1	2,1	14,14,15	0.19	0	17,19,21	0.53	0
2	NAG	L	2	2	14,14,15	0.30	0	17,19,21	0.45	0
2	BMA	L	3	2	11,11,12	0.53	0	15,15,17	0.75	0
2	MAN	L	4	2	11,11,12	0.59	0	15,15,17	0.98	2 (13%)
2	MAN	L	5	2	11,11,12	0.61	0	15,15,17	1.00	2 (13%)
2	MAN	L	6	2	11,11,12	0.68	0	15,15,17	1.09	2 (13%)
2	MAN	L	7	2	11,11,12	0.64	0	15,15,17	0.96	2 (13%)
2	NAG	LA	1	2,1	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	LA	2	2	14,14,15	0.25	0	17,19,21	0.40	0
2	BMA	LA	3	2	11,11,12	0.97	1 (9%)	15,15,17	0.86	0
2	MAN	LA	4	2	11,11,12	0.77	0	15,15,17	0.95	1 (6%)
2	MAN	LA	5	2	11,11,12	0.60	0	15,15,17	0.97	2 (13%)
2	MAN	LA	6	2	11,11,12	0.71	0	15,15,17	1.04	2 (13%)
2	MAN	LA	7	2	11,11,12	0.63	0	15,15,17	0.97	2 (13%)
6	NAG	M	1	1,6	14,14,15	0.28	0	17,19,21	0.44	0
6	NAG	M	2	6	14,14,15	0.20	0	17,19,21	0.53	0
6	BMA	M	3	6	11,11,12	0.87	0	15,15,17	1.03	1 (6%)
6	MAN	M	4	6	11,11,12	0.88	0	15,15,17	1.21	2 (13%)
6	MAN	M	5	6	11,11,12	0.72	0	15,15,17	0.98	1 (6%)
6	MAN	M	6	6	11,11,12	0.68	0	15,15,17	0.90	1 (6%)
6	MAN	M	7	6	11,11,12	1.00	1 (9%)	15,15,17	1.66	2 (13%)
6	MAN	M	8	6	11,11,12	0.64	0	15,15,17	1.08	2 (13%)
3	NAG	MA	1	3,1	14,14,15	0.35	0	17,19,21	0.66	0
3	NAG	MA	2	3	14,14,15	0.24	0	17,19,21	0.57	0
3	BMA	MA	3	3	11,11,12	0.72	0	15,15,17	0.84	0
3	MAN	MA	4	3	11,11,12	0.75	1 (9%)	15,15,17	1.03	2 (13%)
3	MAN	MA	5	3	11,11,12	0.62	0	15,15,17	0.93	2 (13%)
3	MAN	MA	6	3	11,11,12	0.62	0	15,15,17	1.03	2 (13%)
3	MAN	MA	7	3	11,11,12	0.66	0	15,15,17	1.07	2 (13%)
3	NAG	N	1	3,1	14,14,15	0.46	0	17,19,21	0.68	1 (5%)
3	NAG	N	2	3	14,14,15	0.26	0	17,19,21	0.44	0
3	BMA	N	3	3	11,11,12	0.62	0	15,15,17	0.91	0
3	MAN	N	4	3	11,11,12	0.61	0	15,15,17	0.96	2 (13%)
3	MAN	N	5	3	11,11,12	0.62	0	15,15,17	0.94	2 (13%)
3	MAN	N	6	3	11,11,12	0.61	0	15,15,17	0.97	2 (13%)
3	MAN	N	7	3	11,11,12	0.64	0	15,15,17	1.00	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	NA	1	2,1	14,14,15	0.35	0	17,19,21	0.64	0
2	NAG	NA	2	2	14,14,15	0.22	0	17,19,21	0.47	0
2	BMA	NA	3	2	11,11,12	1.03	1 (9%)	15,15,17	0.90	0
2	MAN	NA	4	2	11,11,12	1.07	0	15,15,17	0.93	0
2	MAN	NA	5	2	11,11,12	0.71	0	15,15,17	0.99	2 (13%)
2	MAN	NA	6	2	11,11,12	0.67	0	15,15,17	0.97	2 (13%)
2	MAN	NA	7	2	11,11,12	0.67	0	15,15,17	1.03	2 (13%)
3	NAG	O	1	3,1	14,14,15	0.23	0	17,19,21	0.47	0
3	NAG	O	2	3	14,14,15	0.18	0	17,19,21	0.45	0
3	BMA	O	3	3	11,11,12	0.56	0	15,15,17	0.80	0
3	MAN	O	4	3	11,11,12	0.60	0	15,15,17	0.95	2 (13%)
3	MAN	O	5	3	11,11,12	0.61	0	15,15,17	0.98	2 (13%)
3	MAN	O	6	3	11,11,12	0.71	0	15,15,17	1.09	2 (13%)
3	MAN	O	7	3	11,11,12	0.71	0	15,15,17	0.99	2 (13%)
9	NAG	OA	1	9,1	14,14,15	0.86	1 (7%)	17,19,21	1.58	4 (23%)
9	NAG	OA	2	9	14,14,15	0.36	0	17,19,21	0.36	0
3	NAG	P	1	3,1	14,14,15	0.23	0	17,19,21	0.40	0
3	NAG	P	2	3	14,14,15	0.27	0	17,19,21	0.46	0
3	BMA	P	3	3	11,11,12	0.70	0	15,15,17	0.87	0
3	MAN	P	4	3	11,11,12	1.40	2 (18%)	15,15,17	1.29	2 (13%)
3	MAN	P	5	3	11,11,12	0.73	1 (9%)	15,15,17	1.13	2 (13%)
3	MAN	P	6	3	11,11,12	0.66	0	15,15,17	1.08	2 (13%)
3	MAN	P	7	3	11,11,12	0.60	0	15,15,17	1.04	2 (13%)
2	NAG	PA	1	2,1	14,14,15	0.23	0	17,19,21	0.46	0
2	NAG	PA	2	2	14,14,15	0.23	0	17,19,21	0.43	0
2	BMA	PA	3	2	11,11,12	0.57	0	15,15,17	0.84	0
2	MAN	PA	4	2	11,11,12	0.61	0	15,15,17	0.90	2 (13%)
2	MAN	PA	5	2	11,11,12	0.60	0	15,15,17	0.96	2 (13%)
2	MAN	PA	6	2	11,11,12	0.65	0	15,15,17	0.99	2 (13%)
2	MAN	PA	7	2	11,11,12	1.56	2 (18%)	15,15,17	2.14	4 (26%)
3	NAG	Q	1	3,1	14,14,15	0.21	0	17,19,21	0.50	0
3	NAG	Q	2	3	14,14,15	0.28	0	17,19,21	0.54	0
3	BMA	Q	3	3	11,11,12	0.56	0	15,15,17	0.77	0
3	MAN	Q	4	3	11,11,12	0.67	0	15,15,17	1.05	2 (13%)
3	MAN	Q	5	3	11,11,12	0.64	0	15,15,17	0.99	2 (13%)
3	MAN	Q	6	3	11,11,12	0.68	0	15,15,17	1.06	2 (13%)
3	MAN	Q	7	3	11,11,12	0.68	0	15,15,17	1.00	2 (13%)
3	NAG	QA	1	3,1	14,14,15	0.68	1 (7%)	17,19,21	0.79	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	QA	2	3	14,14,15	0.28	0	17,19,21	0.60	0
3	BMA	QA	3	3	11,11,12	0.53	0	15,15,17	0.77	0
3	MAN	QA	4	3	11,11,12	0.98	0	15,15,17	1.03	1 (6%)
3	MAN	QA	5	3	11,11,12	0.68	0	15,15,17	0.98	2 (13%)
3	MAN	QA	6	3	11,11,12	0.61	0	15,15,17	1.01	2 (13%)
3	MAN	QA	7	3	11,11,12	0.64	0	15,15,17	0.91	2 (13%)
2	NAG	R	1	2,1	14,14,15	0.24	0	17,19,21	0.56	0
2	NAG	R	2	2	14,14,15	0.23	0	17,19,21	0.44	0
2	BMA	R	3	2	11,11,12	0.71	0	15,15,17	0.72	0
2	MAN	R	4	2	11,11,12	1.03	0	15,15,17	0.94	1 (6%)
2	MAN	R	5	2	11,11,12	0.63	0	15,15,17	0.95	2 (13%)
2	MAN	R	6	2	11,11,12	0.63	0	15,15,17	1.01	2 (13%)
2	MAN	R	7	2	11,11,12	0.60	0	15,15,17	0.93	2 (13%)
4	NAG	RA	1	4,1	14,14,15	0.21	0	17,19,21	0.50	0
4	NAG	RA	2	4	14,14,15	0.22	0	17,19,21	0.51	0
4	BMA	RA	3	4	11,11,12	1.09	1 (9%)	15,15,17	1.23	2 (13%)
4	MAN	RA	4	4	11,11,12	0.67	0	15,15,17	1.21	2 (13%)
4	MAN	RA	5	4	11,11,12	0.98	1 (9%)	15,15,17	1.23	2 (13%)
4	MAN	RA	6	4	11,11,12	0.62	0	15,15,17	0.92	2 (13%)
4	MAN	RA	7	4	11,11,12	0.66	0	15,15,17	1.12	2 (13%)
4	MAN	RA	8	4	11,11,12	0.58	0	15,15,17	1.15	2 (13%)
4	MAN	RA	9	4	11,11,12	0.70	0	15,15,17	0.92	2 (13%)
2	NAG	S	1	2,1	14,14,15	0.26	0	17,19,21	0.49	0
2	NAG	S	2	2	14,14,15	0.25	0	17,19,21	0.44	0
2	BMA	S	3	2	11,11,12	0.92	1 (9%)	15,15,17	0.91	1 (6%)
2	MAN	S	4	2	11,11,12	0.69	0	15,15,17	0.94	2 (13%)
2	MAN	S	5	2	11,11,12	0.68	0	15,15,17	0.99	2 (13%)
2	MAN	S	6	2	11,11,12	0.65	0	15,15,17	0.93	2 (13%)
2	MAN	S	7	2	11,11,12	0.68	0	15,15,17	1.08	2 (13%)
5	NAG	SA	1	1,5	14,14,15	0.54	0	17,19,21	0.53	0
5	NAG	SA	2	5	14,14,15	0.19	0	17,19,21	0.44	0
5	BMA	SA	3	5	11,11,12	0.45	0	15,15,17	0.78	0
5	MAN	SA	4	5	11,11,12	0.76	1 (9%)	15,15,17	1.19	1 (6%)
5	NAG	SA	5	5	14,14,15	0.22	0	17,19,21	0.80	1 (5%)
5	GAL	SA	6	5	11,11,12	0.49	0	15,15,17	1.04	1 (6%)
5	MAN	SA	7	5	11,11,12	0.60	0	15,15,17	0.95	2 (13%)
5	NAG	SA	8	5	14,14,15	0.27	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GAL	SA	9	5	11,11,12	0.49	0	15,15,17	0.85	0
2	NAG	T	1	2,1	14,14,15	0.27	0	17,19,21	0.42	0
2	NAG	T	2	2	14,14,15	0.23	0	17,19,21	0.47	0
2	BMA	T	3	2	11,11,12	0.57	0	15,15,17	0.68	0
2	MAN	T	4	2	11,11,12	0.93	0	15,15,17	1.18	2 (13%)
2	MAN	T	5	2	11,11,12	0.61	0	15,15,17	1.05	2 (13%)
2	MAN	T	6	2	11,11,12	0.65	0	15,15,17	1.01	2 (13%)
2	MAN	T	7	2	11,11,12	0.66	0	15,15,17	1.03	2 (13%)
3	NAG	TA	1	3,1	14,14,15	0.26	0	17,19,21	0.48	0
3	NAG	TA	2	3	14,14,15	0.29	0	17,19,21	0.78	1 (5%)
3	BMA	TA	3	3	11,11,12	0.56	0	15,15,17	1.06	1 (6%)
3	MAN	TA	4	3	11,11,12	1.17	1 (9%)	15,15,17	1.04	0
3	MAN	TA	5	3	11,11,12	0.71	1 (9%)	15,15,17	1.07	2 (13%)
3	MAN	TA	6	3	11,11,12	0.66	0	15,15,17	1.04	2 (13%)
3	MAN	TA	7	3	11,11,12	0.62	0	15,15,17	0.97	2 (13%)
3	NAG	U	1	3,1	14,14,15	0.47	0	17,19,21	0.84	1 (5%)
3	NAG	U	2	3	14,14,15	0.26	0	17,19,21	0.42	0
3	BMA	U	3	3	11,11,12	0.61	0	15,15,17	0.63	0
3	MAN	U	4	3	11,11,12	0.90	1 (9%)	15,15,17	1.22	3 (20%)
3	MAN	U	5	3	11,11,12	0.65	0	15,15,17	0.91	2 (13%)
3	MAN	U	6	3	11,11,12	0.64	0	15,15,17	0.96	2 (13%)
3	MAN	U	7	3	11,11,12	0.64	0	15,15,17	0.99	2 (13%)
3	NAG	UA	1	3,1	14,14,15	0.28	0	17,19,21	0.54	0
3	NAG	UA	2	3	14,14,15	0.22	0	17,19,21	0.45	0
3	BMA	UA	3	3	11,11,12	0.51	0	15,15,17	0.73	0
3	MAN	UA	4	3	11,11,12	0.93	1 (9%)	15,15,17	1.49	2 (13%)
3	MAN	UA	5	3	11,11,12	0.74	0	15,15,17	0.87	1 (6%)
3	MAN	UA	6	3	11,11,12	0.68	0	15,15,17	0.89	1 (6%)
3	MAN	UA	7	3	11,11,12	0.63	0	15,15,17	0.90	2 (13%)
3	NAG	V	1	3,1	14,14,15	0.47	0	17,19,21	0.66	0
3	NAG	V	2	3	14,14,15	0.22	0	17,19,21	0.44	0
3	BMA	V	3	3	11,11,12	1.03	1 (9%)	15,15,17	0.94	0
3	MAN	V	4	3	11,11,12	0.78	1 (9%)	15,15,17	1.24	2 (13%)
3	MAN	V	5	3	11,11,12	0.69	0	15,15,17	0.88	1 (6%)
3	MAN	V	6	3	11,11,12	0.63	0	15,15,17	1.03	2 (13%)
3	MAN	V	7	3	11,11,12	0.61	0	15,15,17	1.02	2 (13%)
3	NAG	VA	1	3,1	14,14,15	0.22	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	VA	2	3	14,14,15	0.22	0	17,19,21	0.52	0
3	BMA	VA	3	3	11,11,12	1.05	1 (9%)	15,15,17	1.10	1 (6%)
3	MAN	VA	4	3	11,11,12	0.78	0	15,15,17	1.01	2 (13%)
3	MAN	VA	5	3	11,11,12	0.73	1 (9%)	15,15,17	1.17	2 (13%)
3	MAN	VA	6	3	11,11,12	0.68	0	15,15,17	0.91	1 (6%)
3	MAN	VA	7	3	11,11,12	0.63	0	15,15,17	1.01	2 (13%)
2	NAG	W	1	2,1	14,14,15	0.31	0	17,19,21	0.61	0
2	NAG	W	2	2	14,14,15	0.28	0	17,19,21	0.43	0
2	BMA	W	3	2	11,11,12	0.60	0	15,15,17	0.74	0
2	MAN	W	4	2	11,11,12	0.60	0	15,15,17	0.96	2 (13%)
2	MAN	W	5	2	11,11,12	0.67	0	15,15,17	0.95	2 (13%)
2	MAN	W	6	2	11,11,12	1.51	2 (18%)	15,15,17	2.09	4 (26%)
2	MAN	W	7	2	11,11,12	0.62	0	15,15,17	1.01	2 (13%)
3	NAG	WA	1	3,1	14,14,15	0.94	1 (7%)	17,19,21	1.60	3 (17%)
3	NAG	WA	2	3	14,14,15	0.30	0	17,19,21	0.44	0
3	BMA	WA	3	3	11,11,12	0.98	1 (9%)	15,15,17	0.78	0
3	MAN	WA	4	3	11,11,12	0.71	0	15,15,17	0.93	1 (6%)
3	MAN	WA	5	3	11,11,12	0.65	0	15,15,17	0.96	2 (13%)
3	MAN	WA	6	3	11,11,12	1.51	2 (18%)	15,15,17	2.09	4 (26%)
3	MAN	WA	7	3	11,11,12	0.60	0	15,15,17	0.99	2 (13%)
3	NAG	X	1	3,1	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	X	2	3	14,14,15	0.26	0	17,19,21	0.59	0
3	BMA	X	3	3	11,11,12	0.57	0	15,15,17	0.75	0
3	MAN	X	4	3	11,11,12	0.77	1 (9%)	15,15,17	1.15	2 (13%)
3	MAN	X	5	3	11,11,12	0.65	0	15,15,17	0.94	2 (13%)
3	MAN	X	6	3	11,11,12	0.77	1 (9%)	15,15,17	1.19	2 (13%)
3	MAN	X	7	3	11,11,12	0.61	0	15,15,17	0.97	2 (13%)
2	NAG	XA	1	2,1	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	XA	2	2	14,14,15	0.31	0	17,19,21	0.43	0
2	BMA	XA	3	2	11,11,12	0.55	0	15,15,17	0.75	0
2	MAN	XA	4	2	11,11,12	0.60	0	15,15,17	0.98	2 (13%)
2	MAN	XA	5	2	11,11,12	0.62	0	15,15,17	0.99	2 (13%)
2	MAN	XA	6	2	11,11,12	0.68	0	15,15,17	1.11	2 (13%)
2	MAN	XA	7	2	11,11,12	0.63	0	15,15,17	0.96	2 (13%)
3	NAG	Y	1	3,1	14,14,15	0.27	0	17,19,21	0.46	0
3	NAG	Y	2	3	14,14,15	0.20	0	17,19,21	0.41	0
3	BMA	Y	3	3	11,11,12	0.94	0	15,15,17	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	Y	4	3	11,11,12	0.64	0	15,15,17	1.08	2 (13%)
3	MAN	Y	5	3	11,11,12	0.64	0	15,15,17	0.92	2 (13%)
3	MAN	Y	6	3	11,11,12	0.67	0	15,15,17	0.98	2 (13%)
3	MAN	Y	7	3	11,11,12	0.65	0	15,15,17	0.98	2 (13%)
6	NAG	YA	1	1,6	14,14,15	0.30	0	17,19,21	0.43	0
6	NAG	YA	2	6	14,14,15	0.20	0	17,19,21	0.53	0
6	BMA	YA	3	6	11,11,12	0.87	0	15,15,17	0.99	1 (6%)
6	MAN	YA	4	6	11,11,12	0.89	0	15,15,17	1.23	2 (13%)
6	MAN	YA	5	6	11,11,12	0.71	0	15,15,17	0.99	1 (6%)
6	MAN	YA	6	6	11,11,12	0.66	0	15,15,17	0.89	1 (6%)
6	MAN	YA	7	6	11,11,12	0.98	1 (9%)	15,15,17	1.65	2 (13%)
6	MAN	YA	8	6	11,11,12	0.63	0	15,15,17	1.08	2 (13%)
2	NAG	Z	1	2,1	14,14,15	0.19	0	17,19,21	0.40	0
2	NAG	Z	2	2	14,14,15	0.21	0	17,19,21	0.58	0
2	BMA	Z	3	2	11,11,12	0.59	0	15,15,17	1.00	1 (6%)
2	MAN	Z	4	2	11,11,12	0.60	0	15,15,17	0.90	2 (13%)
2	MAN	Z	5	2	11,11,12	0.63	0	15,15,17	0.93	2 (13%)
2	MAN	Z	6	2	11,11,12	0.67	0	15,15,17	1.06	2 (13%)
2	MAN	Z	7	2	11,11,12	0.64	0	15,15,17	1.00	2 (13%)
3	NAG	ZA	1	3,1	14,14,15	0.48	0	17,19,21	0.68	1 (5%)
3	NAG	ZA	2	3	14,14,15	0.26	0	17,19,21	0.44	0
3	BMA	ZA	3	3	11,11,12	0.61	0	15,15,17	0.90	0
3	MAN	ZA	4	3	11,11,12	0.62	0	15,15,17	0.96	2 (13%)
3	MAN	ZA	5	3	11,11,12	0.61	0	15,15,17	0.94	2 (13%)
3	MAN	ZA	6	3	11,11,12	0.61	0	15,15,17	0.97	2 (13%)
3	MAN	ZA	7	3	11,11,12	0.63	0	15,15,17	1.01	2 (13%)
3	NAG	a	1	3,1	14,14,15	0.35	0	17,19,21	0.61	0
3	NAG	a	2	3	14,14,15	0.44	0	17,19,21	1.40	2 (11%)
3	BMA	a	3	3	11,11,12	0.84	1 (9%)	15,15,17	0.93	0
3	MAN	a	4	3	11,11,12	0.69	0	15,15,17	1.04	2 (13%)
3	MAN	a	5	3	11,11,12	0.69	0	15,15,17	1.21	2 (13%)
3	MAN	a	6	3	11,11,12	0.60	0	15,15,17	0.93	2 (13%)
3	MAN	a	7	3	11,11,12	0.69	1 (9%)	15,15,17	1.13	2 (13%)
3	NAG	aA	1	3,1	14,14,15	0.22	0	17,19,21	0.48	0
3	NAG	aA	2	3	14,14,15	0.19	0	17,19,21	0.45	0
3	BMA	aA	3	3	11,11,12	0.57	0	15,15,17	0.79	0
3	MAN	aA	4	3	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
3	MAN	aA	5	3	11,11,12	0.61	0	15,15,17	0.98	2 (13%)
3	MAN	aA	6	3	11,11,12	0.68	0	15,15,17	1.10	2 (13%)
3	MAN	aA	7	3	11,11,12	0.71	0	15,15,17	0.99	2 (13%)
2	NAG	b	1	2,1	14,14,15	0.22	0	17,19,21	0.55	0
2	NAG	b	2	2	14,14,15	0.21	0	17,19,21	0.47	0
2	BMA	b	3	2	11,11,12	0.62	0	15,15,17	0.77	0
2	MAN	b	4	2	11,11,12	0.60	0	15,15,17	0.92	2 (13%)
2	MAN	b	5	2	11,11,12	0.62	0	15,15,17	0.96	2 (13%)
2	MAN	b	6	2	11,11,12	0.68	0	15,15,17	1.07	2 (13%)
2	MAN	b	7	2	11,11,12	0.62	0	15,15,17	0.95	2 (13%)
3	NAG	bA	1	3,1	14,14,15	0.22	0	17,19,21	0.40	0
3	NAG	bA	2	3	14,14,15	0.27	0	17,19,21	0.46	0
3	BMA	bA	3	3	11,11,12	0.70	0	15,15,17	0.89	0
3	MAN	bA	4	3	11,11,12	1.41	2 (18%)	15,15,17	1.30	2 (13%)
3	MAN	bA	5	3	11,11,12	0.72	1 (9%)	15,15,17	1.14	2 (13%)
3	MAN	bA	6	3	11,11,12	0.66	0	15,15,17	1.09	2 (13%)
3	MAN	bA	7	3	11,11,12	0.60	0	15,15,17	1.04	2 (13%)
3	NAG	c	1	3,1	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	c	2	3	14,14,15	0.31	0	17,19,21	0.67	0
3	BMA	c	3	3	11,11,12	0.58	0	15,15,17	1.02	1 (6%)
3	MAN	c	4	3	11,11,12	0.72	0	15,15,17	1.21	2 (13%)
3	MAN	c	5	3	11,11,12	0.65	0	15,15,17	0.96	2 (13%)
3	MAN	c	6	3	11,11,12	0.61	0	15,15,17	0.99	2 (13%)
3	MAN	c	7	3	11,11,12	0.64	0	15,15,17	0.99	2 (13%)
3	NAG	cA	1	3,1	14,14,15	0.21	0	17,19,21	0.49	0
3	NAG	cA	2	3	14,14,15	0.28	0	17,19,21	0.55	0
3	BMA	cA	3	3	11,11,12	0.56	0	15,15,17	0.78	0
3	MAN	cA	4	3	11,11,12	0.67	0	15,15,17	1.07	2 (13%)
3	MAN	cA	5	3	11,11,12	0.64	0	15,15,17	1.00	2 (13%)
3	MAN	cA	6	3	11,11,12	0.68	0	15,15,17	1.05	2 (13%)
3	MAN	cA	7	3	11,11,12	0.68	0	15,15,17	0.99	2 (13%)
7	NAG	d	1	7,1	14,14,15	0.27	0	17,19,21	0.45	0
7	NAG	d	10	7	14,14,15	0.23	0	17,19,21	0.41	0
7	GAL	d	11	7	11,11,12	0.50	0	15,15,17	0.91	0
7	FUC	d	12	7	10,10,11	1.57	2 (20%)	14,14,16	1.61	3 (21%)
7	NAG	d	2	7	14,14,15	0.26	0	17,19,21	0.46	0
7	BMA	d	3	7	11,11,12	0.75	0	15,15,17	0.81	0
7	MAN	d	4	7	11,11,12	1.15	2 (18%)	15,15,17	0.98	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	d	5	7	14,14,15	0.20	0	17,19,21	0.45	0
7	GAL	d	6	7	11,11,12	0.70	0	15,15,17	1.39	2 (13%)
7	NAG	d	7	7	14,14,15	0.33	0	17,19,21	0.55	0
7	GAL	d	8	7	11,11,12	0.50	0	15,15,17	0.86	0
7	MAN	d	9	7	11,11,12	0.68	0	15,15,17	1.19	2 (13%)
2	NAG	dA	1	2,1	14,14,15	0.24	0	17,19,21	0.56	0
2	NAG	dA	2	2	14,14,15	0.24	0	17,19,21	0.45	0
2	BMA	dA	3	2	11,11,12	0.71	0	15,15,17	0.71	0
2	MAN	dA	4	2	11,11,12	1.03	0	15,15,17	0.94	1 (6%)
2	MAN	dA	5	2	11,11,12	0.63	0	15,15,17	0.95	2 (13%)
2	MAN	dA	6	2	11,11,12	0.65	0	15,15,17	1.00	2 (13%)
2	MAN	dA	7	2	11,11,12	0.61	0	15,15,17	0.93	2 (13%)
2	NAG	e	1	2,1	14,14,15	0.25	0	17,19,21	0.42	0
2	NAG	e	2	2	14,14,15	0.20	0	17,19,21	0.42	0
2	BMA	e	3	2	11,11,12	1.21	2 (18%)	15,15,17	1.20	2 (13%)
2	MAN	e	4	2	11,11,12	0.64	0	15,15,17	1.08	2 (13%)
2	MAN	e	5	2	11,11,12	0.66	0	15,15,17	1.02	2 (13%)
2	MAN	e	6	2	11,11,12	0.68	0	15,15,17	0.99	2 (13%)
2	MAN	e	7	2	11,11,12	0.64	0	15,15,17	0.95	2 (13%)
2	NAG	eA	1	2,1	14,14,15	0.26	0	17,19,21	0.49	0
2	NAG	eA	2	2	14,14,15	0.22	0	17,19,21	0.44	0
2	BMA	eA	3	2	11,11,12	0.93	1 (9%)	15,15,17	0.92	1 (6%)
2	MAN	eA	4	2	11,11,12	0.68	0	15,15,17	0.95	2 (13%)
2	MAN	eA	5	2	11,11,12	0.69	0	15,15,17	0.98	2 (13%)
2	MAN	eA	6	2	11,11,12	0.64	0	15,15,17	0.94	2 (13%)
2	MAN	eA	7	2	11,11,12	0.69	0	15,15,17	1.10	2 (13%)
3	NAG	f	1	3,1	14,14,15	0.34	0	17,19,21	0.48	0
3	NAG	f	2	3	14,14,15	0.45	0	17,19,21	0.55	0
3	BMA	f	3	3	11,11,12	0.85	0	15,15,17	0.82	0
3	MAN	f	4	3	11,11,12	1.25	2 (18%)	15,15,17	0.97	0
3	MAN	f	5	3	11,11,12	0.69	0	15,15,17	1.00	2 (13%)
3	MAN	f	6	3	11,11,12	0.66	0	15,15,17	1.03	2 (13%)
3	MAN	f	7	3	11,11,12	0.68	0	15,15,17	1.16	2 (13%)
2	NAG	fA	1	2,1	14,14,15	0.26	0	17,19,21	0.42	0
2	NAG	fA	2	2	14,14,15	0.24	0	17,19,21	0.48	0
2	BMA	fA	3	2	11,11,12	0.56	0	15,15,17	0.67	0
2	MAN	fA	4	2	11,11,12	0.93	0	15,15,17	1.16	2 (13%)
2	MAN	fA	5	2	11,11,12	0.61	0	15,15,17	1.05	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	fA	6	2	11,11,12	0.65	0	15,15,17	1.01	2 (13%)
2	MAN	fA	7	2	11,11,12	0.65	0	15,15,17	1.02	2 (13%)
3	NAG	g	1	3,1	14,14,15	0.26	0	17,19,21	0.39	0
3	NAG	g	2	3	14,14,15	0.23	0	17,19,21	0.40	0
3	BMA	g	3	3	11,11,12	0.56	0	15,15,17	0.73	0
3	MAN	g	4	3	11,11,12	1.12	1 (9%)	15,15,17	0.96	0
3	MAN	g	5	3	11,11,12	0.65	0	15,15,17	0.96	2 (13%)
3	MAN	g	6	3	11,11,12	0.65	0	15,15,17	1.03	2 (13%)
3	MAN	g	7	3	11,11,12	0.67	0	15,15,17	1.09	2 (13%)
3	NAG	gA	1	3,1	14,14,15	0.44	0	17,19,21	0.83	1 (5%)
3	NAG	gA	2	3	14,14,15	0.27	0	17,19,21	0.41	0
3	BMA	gA	3	3	11,11,12	0.59	0	15,15,17	0.63	0
3	MAN	gA	4	3	11,11,12	0.88	1 (9%)	15,15,17	1.21	2 (13%)
3	MAN	gA	5	3	11,11,12	0.64	0	15,15,17	0.91	2 (13%)
3	MAN	gA	6	3	11,11,12	0.64	0	15,15,17	0.96	2 (13%)
3	MAN	gA	7	3	11,11,12	0.65	0	15,15,17	0.99	2 (13%)
3	NAG	h	1	3,1	14,14,15	0.41	0	17,19,21	0.65	0
3	NAG	h	2	3	14,14,15	0.23	0	17,19,21	0.40	0
3	BMA	h	3	3	11,11,12	0.51	0	15,15,17	0.78	0
3	MAN	h	4	3	11,11,12	1.05	0	15,15,17	1.27	1 (6%)
3	MAN	h	5	3	11,11,12	0.62	0	15,15,17	0.95	2 (13%)
3	MAN	h	6	3	11,11,12	0.62	0	15,15,17	1.01	2 (13%)
3	MAN	h	7	3	11,11,12	0.65	0	15,15,17	0.89	1 (6%)
3	NAG	hA	1	3,1	14,14,15	0.47	0	17,19,21	0.67	0
3	NAG	hA	2	3	14,14,15	0.22	0	17,19,21	0.45	0
3	BMA	hA	3	3	11,11,12	1.04	1 (9%)	15,15,17	0.94	0
3	MAN	hA	4	3	11,11,12	0.80	1 (9%)	15,15,17	1.25	2 (13%)
3	MAN	hA	5	3	11,11,12	0.69	0	15,15,17	0.88	1 (6%)
3	MAN	hA	6	3	11,11,12	0.63	0	15,15,17	1.02	2 (13%)
3	MAN	hA	7	3	11,11,12	0.62	0	15,15,17	1.04	2 (13%)
2	NAG	i	1	2,1	14,14,15	1.13	1 (7%)	17,19,21	1.22	1 (5%)
2	NAG	i	2	2	14,14,15	0.24	0	17,19,21	0.47	0
2	BMA	i	3	2	11,11,12	0.70	0	15,15,17	0.72	0
2	MAN	i	4	2	11,11,12	0.88	1 (9%)	15,15,17	1.14	3 (20%)
2	MAN	i	5	2	11,11,12	0.64	0	15,15,17	1.01	2 (13%)
2	MAN	i	6	2	11,11,12	0.61	0	15,15,17	1.06	2 (13%)
2	MAN	i	7	2	11,11,12	0.64	0	15,15,17	0.99	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	iA	1	2,1	14,14,15	0.30	0	17,19,21	0.59	0
2	NAG	iA	2	2	14,14,15	0.29	0	17,19,21	0.44	0
2	BMA	iA	3	2	11,11,12	0.61	0	15,15,17	0.73	0
2	MAN	iA	4	2	11,11,12	0.59	0	15,15,17	0.97	2 (13%)
2	MAN	iA	5	2	11,11,12	0.67	0	15,15,17	0.95	2 (13%)
2	MAN	iA	6	2	11,11,12	1.50	2 (18%)	15,15,17	2.07	4 (26%)
2	MAN	iA	7	2	11,11,12	0.61	0	15,15,17	1.00	2 (13%)
8	NAG	j	1	8,1	14,14,15	0.45	0	17,19,21	1.57	2 (11%)
8	NAG	j	2	8	14,14,15	0.48	0	17,19,21	0.65	0
8	BMA	j	3	8	11,11,12	1.56	3 (27%)	15,15,17	1.14	2 (13%)
8	MAN	j	4	8	11,11,12	0.71	0	15,15,17	1.03	2 (13%)
8	MAN	j	5	8	11,11,12	0.71	0	15,15,17	0.86	1 (6%)
3	NAG	jA	1	3,1	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	jA	2	3	14,14,15	0.26	0	17,19,21	0.58	0
3	BMA	jA	3	3	11,11,12	0.57	0	15,15,17	0.74	0
3	MAN	jA	4	3	11,11,12	0.76	1 (9%)	15,15,17	1.15	2 (13%)
3	MAN	jA	5	3	11,11,12	0.63	0	15,15,17	0.94	2 (13%)
3	MAN	jA	6	3	11,11,12	0.76	1 (9%)	15,15,17	1.19	2 (13%)
3	MAN	jA	7	3	11,11,12	0.62	0	15,15,17	0.97	2 (13%)
2	NAG	k	1	2,1	14,14,15	0.21	0	17,19,21	0.44	0
2	NAG	k	2	2	14,14,15	0.24	0	17,19,21	0.40	0
2	BMA	k	3	2	11,11,12	0.97	1 (9%)	15,15,17	0.86	0
2	MAN	k	4	2	11,11,12	0.75	0	15,15,17	0.93	1 (6%)
2	MAN	k	5	2	11,11,12	0.60	0	15,15,17	0.97	2 (13%)
2	MAN	k	6	2	11,11,12	0.72	0	15,15,17	1.04	2 (13%)
2	MAN	k	7	2	11,11,12	0.62	0	15,15,17	0.96	2 (13%)
3	NAG	kA	1	3,1	14,14,15	0.27	0	17,19,21	0.46	0
3	NAG	kA	2	3	14,14,15	0.20	0	17,19,21	0.42	0
3	BMA	kA	3	3	11,11,12	0.92	0	15,15,17	0.78	0
3	MAN	kA	4	3	11,11,12	0.63	0	15,15,17	1.08	2 (13%)
3	MAN	kA	5	3	11,11,12	0.63	0	15,15,17	0.92	2 (13%)
3	MAN	kA	6	3	11,11,12	0.66	0	15,15,17	0.97	2 (13%)
3	MAN	kA	7	3	11,11,12	0.63	0	15,15,17	0.99	2 (13%)
3	NAG	l	1	3,1	14,14,15	0.36	0	17,19,21	0.66	0
3	NAG	l	2	3	14,14,15	0.23	0	17,19,21	0.56	0
3	BMA	l	3	3	11,11,12	0.71	0	15,15,17	0.82	0
3	MAN	l	4	3	11,11,12	0.75	1 (9%)	15,15,17	1.05	2 (13%)
3	MAN	l	5	3	11,11,12	0.63	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
3	MAN	l	6	3	11,11,12	0.61	0	15,15,17	1.03	2 (13%)
3	MAN	l	7	3	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
2	NAG	lA	1	2,1	14,14,15	0.21	0	17,19,21	0.40	0
2	NAG	lA	2	2	14,14,15	0.20	0	17,19,21	0.57	0
2	BMA	lA	3	2	11,11,12	0.61	0	15,15,17	1.02	1 (6%)
2	MAN	lA	4	2	11,11,12	0.60	0	15,15,17	0.90	2 (13%)
2	MAN	lA	5	2	11,11,12	0.65	0	15,15,17	0.91	2 (13%)
2	MAN	lA	6	2	11,11,12	0.68	0	15,15,17	1.07	2 (13%)
2	MAN	lA	7	2	11,11,12	0.63	0	15,15,17	0.98	2 (13%)
2	NAG	m	1	2,1	14,14,15	0.34	0	17,19,21	0.64	0
2	NAG	m	2	2	14,14,15	0.22	0	17,19,21	0.47	0
2	BMA	m	3	2	11,11,12	1.01	1 (9%)	15,15,17	0.89	0
2	MAN	m	4	2	11,11,12	1.07	0	15,15,17	0.93	0
2	MAN	m	5	2	11,11,12	0.72	0	15,15,17	0.98	2 (13%)
2	MAN	m	6	2	11,11,12	0.67	0	15,15,17	0.97	2 (13%)
2	MAN	m	7	2	11,11,12	0.67	0	15,15,17	1.03	2 (13%)
3	NAG	mA	1	3,1	14,14,15	0.39	0	17,19,21	0.61	0
3	NAG	mA	2	3	14,14,15	0.44	0	17,19,21	1.43	2 (11%)
3	BMA	mA	3	3	11,11,12	0.87	1 (9%)	15,15,17	0.95	0
3	MAN	mA	4	3	11,11,12	0.69	0	15,15,17	1.05	2 (13%)
3	MAN	mA	5	3	11,11,12	0.69	0	15,15,17	1.22	2 (13%)
3	MAN	mA	6	3	11,11,12	0.60	0	15,15,17	0.94	2 (13%)
3	MAN	mA	7	3	11,11,12	0.67	0	15,15,17	1.12	2 (13%)
9	NAG	n	1	9,1	14,14,15	0.92	1 (7%)	17,19,21	1.62	4 (23%)
9	NAG	n	2	9	14,14,15	0.34	0	17,19,21	0.38	0
2	NAG	nA	1	2,1	14,14,15	0.21	0	17,19,21	0.55	0
2	NAG	nA	2	2	14,14,15	0.20	0	17,19,21	0.46	0
2	BMA	nA	3	2	11,11,12	0.62	0	15,15,17	0.78	0
2	MAN	nA	4	2	11,11,12	0.61	0	15,15,17	0.92	2 (13%)
2	MAN	nA	5	2	11,11,12	0.63	0	15,15,17	0.96	2 (13%)
2	MAN	nA	6	2	11,11,12	0.68	0	15,15,17	1.07	2 (13%)
2	MAN	nA	7	2	11,11,12	0.63	0	15,15,17	0.94	2 (13%)
2	NAG	o	1	2,1	14,14,15	0.24	0	17,19,21	0.45	0
2	NAG	o	2	2	14,14,15	0.22	0	17,19,21	0.45	0
2	BMA	o	3	2	11,11,12	0.58	0	15,15,17	0.86	0
2	MAN	o	4	2	11,11,12	0.61	0	15,15,17	0.90	2 (13%)
2	MAN	o	5	2	11,11,12	0.62	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
2	MAN	o	6	2	11,11,12	0.66	0	15,15,17	0.99	2 (13%)
2	MAN	o	7	2	11,11,12	1.54	2 (18%)	15,15,17	2.13	4 (26%)
3	NAG	oA	1	3,1	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	oA	2	3	14,14,15	0.31	0	17,19,21	0.67	0
3	BMA	oA	3	3	11,11,12	0.59	0	15,15,17	1.02	1 (6%)
3	MAN	oA	4	3	11,11,12	0.73	0	15,15,17	1.21	2 (13%)
3	MAN	oA	5	3	11,11,12	0.65	0	15,15,17	0.97	2 (13%)
3	MAN	oA	6	3	11,11,12	0.61	0	15,15,17	0.99	2 (13%)
3	MAN	oA	7	3	11,11,12	0.63	0	15,15,17	0.99	2 (13%)
3	NAG	p	1	3,1	14,14,15	0.67	1 (7%)	17,19,21	0.81	1 (5%)
3	NAG	p	2	3	14,14,15	0.28	0	17,19,21	0.60	0
3	BMA	p	3	3	11,11,12	0.55	0	15,15,17	0.79	0
3	MAN	p	4	3	11,11,12	0.98	0	15,15,17	1.02	1 (6%)
3	MAN	p	5	3	11,11,12	0.67	0	15,15,17	0.98	2 (13%)
3	MAN	p	6	3	11,11,12	0.62	0	15,15,17	1.01	2 (13%)
3	MAN	p	7	3	11,11,12	0.63	0	15,15,17	0.92	2 (13%)
7	NAG	pA	1	7,1	14,14,15	0.61	1 (7%)	17,19,21	0.73	1 (5%)
7	NAG	pA	10	7	14,14,15	0.22	0	17,19,21	0.43	0
7	GAL	pA	11	7	11,11,12	0.51	0	15,15,17	0.90	0
7	FUC	pA	12	7	10,10,11	1.58	2 (20%)	14,14,16	1.62	3 (21%)
7	NAG	pA	2	7	14,14,15	0.68	1 (7%)	17,19,21	0.61	0
7	BMA	pA	3	7	11,11,12	0.76	0	15,15,17	0.98	1 (6%)
7	MAN	pA	4	7	11,11,12	1.07	1 (9%)	15,15,17	0.96	0
7	NAG	pA	5	7	14,14,15	0.19	0	17,19,21	0.44	0
7	GAL	pA	6	7	11,11,12	0.72	0	15,15,17	1.38	2 (13%)
7	NAG	pA	7	7	14,14,15	0.30	0	17,19,21	0.57	0
7	GAL	pA	8	7	11,11,12	0.51	0	15,15,17	0.87	0
7	MAN	pA	9	7	11,11,12	0.74	1 (9%)	15,15,17	1.19	2 (13%)
4	NAG	q	1	4,1	14,14,15	0.20	0	17,19,21	0.50	0
4	NAG	q	2	4	14,14,15	0.20	0	17,19,21	0.51	0
4	BMA	q	3	4	11,11,12	1.06	1 (9%)	15,15,17	1.25	2 (13%)
4	MAN	q	4	4	11,11,12	0.66	0	15,15,17	1.20	2 (13%)
4	MAN	q	5	4	11,11,12	0.97	1 (9%)	15,15,17	1.23	2 (13%)
4	MAN	q	6	4	11,11,12	0.62	0	15,15,17	0.91	2 (13%)
4	MAN	q	7	4	11,11,12	0.67	0	15,15,17	1.14	2 (13%)
4	MAN	q	8	4	11,11,12	0.61	0	15,15,17	1.20	2 (13%)
4	MAN	q	9	4	11,11,12	0.70	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
2	NAG	qA	1	2,1	14,14,15	0.25	0	17,19,21	0.44	0
2	NAG	qA	2	2	14,14,15	0.20	0	17,19,21	0.41	0
2	BMA	qA	3	2	11,11,12	1.19	1 (9%)	15,15,17	1.20	2 (13%)
2	MAN	qA	4	2	11,11,12	0.66	0	15,15,17	1.08	2 (13%)
2	MAN	qA	5	2	11,11,12	0.66	0	15,15,17	1.02	2 (13%)
2	MAN	qA	6	2	11,11,12	0.67	0	15,15,17	0.99	2 (13%)
2	MAN	qA	7	2	11,11,12	0.65	0	15,15,17	0.95	2 (13%)
5	NAG	r	1	1,5	14,14,15	0.64	1 (7%)	17,19,21	0.59	0
5	NAG	r	2	5	14,14,15	0.42	0	17,19,21	1.35	2 (11%)
5	BMA	r	3	5	11,11,12	0.51	0	15,15,17	0.84	0
5	MAN	r	4	5	11,11,12	0.73	1 (9%)	15,15,17	1.16	1 (6%)
5	NAG	r	5	5	14,14,15	0.22	0	17,19,21	0.77	1 (5%)
5	GAL	r	6	5	11,11,12	0.49	0	15,15,17	1.05	1 (6%)
5	MAN	r	7	5	11,11,12	0.59	0	15,15,17	0.99	2 (13%)
5	NAG	r	8	5	14,14,15	0.26	0	17,19,21	0.51	0
5	GAL	r	9	5	11,11,12	0.50	0	15,15,17	0.86	0
3	NAG	rA	1	3,1	14,14,15	0.33	0	17,19,21	0.49	0
3	NAG	rA	2	3	14,14,15	0.46	0	17,19,21	0.55	0
3	BMA	rA	3	3	11,11,12	0.86	0	15,15,17	0.83	0
3	MAN	rA	4	3	11,11,12	1.25	2 (18%)	15,15,17	0.96	0
3	MAN	rA	5	3	11,11,12	0.67	0	15,15,17	1.00	2 (13%)
3	MAN	rA	6	3	11,11,12	0.67	0	15,15,17	1.03	2 (13%)
3	MAN	rA	7	3	11,11,12	0.67	0	15,15,17	1.17	2 (13%)
3	NAG	s	1	3,1	14,14,15	0.25	0	17,19,21	0.48	0
3	NAG	s	2	3	14,14,15	0.29	0	17,19,21	0.77	1 (5%)
3	BMA	s	3	3	11,11,12	0.56	0	15,15,17	1.04	1 (6%)
3	MAN	s	4	3	11,11,12	1.19	1 (9%)	15,15,17	1.04	0
3	MAN	s	5	3	11,11,12	0.71	1 (9%)	15,15,17	1.06	2 (13%)
3	MAN	s	6	3	11,11,12	0.65	0	15,15,17	1.03	2 (13%)
3	MAN	s	7	3	11,11,12	0.62	0	15,15,17	0.97	2 (13%)
3	NAG	sA	1	3,1	14,14,15	0.24	0	17,19,21	0.40	0
3	NAG	sA	2	3	14,14,15	0.25	0	17,19,21	0.40	0
3	BMA	sA	3	3	11,11,12	0.55	0	15,15,17	0.73	0
3	MAN	sA	4	3	11,11,12	1.14	1 (9%)	15,15,17	0.97	0
3	MAN	sA	5	3	11,11,12	0.64	0	15,15,17	0.97	2 (13%)
3	MAN	sA	6	3	11,11,12	0.66	0	15,15,17	1.03	2 (13%)
3	MAN	sA	7	3	11,11,12	0.66	0	15,15,17	1.08	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	t	1	3,1	14,14,15	0.29	0	17,19,21	0.53	0
3	NAG	t	2	3	14,14,15	0.21	0	17,19,21	0.44	0
3	BMA	t	3	3	11,11,12	0.51	0	15,15,17	0.74	0
3	MAN	t	4	3	11,11,12	0.93	1 (9%)	15,15,17	1.50	2 (13%)
3	MAN	t	5	3	11,11,12	0.74	0	15,15,17	0.88	1 (6%)
3	MAN	t	6	3	11,11,12	0.68	0	15,15,17	0.88	1 (6%)
3	MAN	t	7	3	11,11,12	0.64	0	15,15,17	0.91	2 (13%)
3	NAG	tA	1	3,1	14,14,15	0.40	0	17,19,21	0.65	0
3	NAG	tA	2	3	14,14,15	0.24	0	17,19,21	0.41	0
3	BMA	tA	3	3	11,11,12	0.51	0	15,15,17	0.80	0
3	MAN	tA	4	3	11,11,12	1.05	0	15,15,17	1.26	1 (6%)
3	MAN	tA	5	3	11,11,12	0.62	0	15,15,17	0.96	2 (13%)
3	MAN	tA	6	3	11,11,12	0.63	0	15,15,17	1.02	2 (13%)
3	MAN	tA	7	3	11,11,12	0.65	0	15,15,17	0.89	1 (6%)
3	NAG	u	1	3,1	14,14,15	0.20	0	17,19,21	0.46	0
3	NAG	u	2	3	14,14,15	0.24	0	17,19,21	0.50	0
3	BMA	u	3	3	11,11,12	1.05	1 (9%)	15,15,17	1.11	1 (6%)
3	MAN	u	4	3	11,11,12	0.78	0	15,15,17	1.01	2 (13%)
3	MAN	u	5	3	11,11,12	0.74	1 (9%)	15,15,17	1.19	2 (13%)
3	MAN	u	6	3	11,11,12	0.67	0	15,15,17	0.90	1 (6%)
3	MAN	u	7	3	11,11,12	0.63	0	15,15,17	1.02	2 (13%)
2	NAG	uA	1	2,1	14,14,15	0.91	1 (7%)	17,19,21	0.84	1 (5%)
2	NAG	uA	2	2	14,14,15	0.30	0	17,19,21	0.69	1 (5%)
2	BMA	uA	3	2	11,11,12	0.68	0	15,15,17	0.71	0
2	MAN	uA	4	2	11,11,12	0.83	1 (9%)	15,15,17	1.12	2 (13%)
2	MAN	uA	5	2	11,11,12	0.62	0	15,15,17	1.00	2 (13%)
2	MAN	uA	6	2	11,11,12	0.62	0	15,15,17	1.06	2 (13%)
2	MAN	uA	7	2	11,11,12	0.65	0	15,15,17	1.01	2 (13%)
3	NAG	v	1	3,1	14,14,15	0.92	1 (7%)	17,19,21	1.61	3 (17%)
3	NAG	v	2	3	14,14,15	0.30	0	17,19,21	0.45	0
3	BMA	v	3	3	11,11,12	0.98	1 (9%)	15,15,17	0.78	0
3	MAN	v	4	3	11,11,12	0.72	0	15,15,17	0.94	1 (6%)
3	MAN	v	5	3	11,11,12	0.63	0	15,15,17	0.96	2 (13%)
3	MAN	v	6	3	11,11,12	1.50	2 (18%)	15,15,17	2.08	4 (26%)
3	MAN	v	7	3	11,11,12	0.60	0	15,15,17	0.99	2 (13%)
8	NAG	vA	1	8,1	14,14,15	0.36	0	17,19,21	1.65	2 (11%)
8	NAG	vA	2	8	14,14,15	0.27	0	17,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BMA	vA	3	8	11,11,12	1.47	3 (27%)	15,15,17	1.04	1 (6%)
8	MAN	vA	4	8	11,11,12	0.69	0	15,15,17	0.95	1 (6%)
8	MAN	vA	5	8	11,11,12	0.67	0	15,15,17	0.87	1 (6%)
2	NAG	w	1	2,1	14,14,15	0.22	0	17,19,21	0.45	0
2	NAG	w	2	2	14,14,15	0.32	0	17,19,21	0.43	0
2	BMA	w	3	2	11,11,12	0.54	0	15,15,17	0.74	0
2	MAN	w	4	2	11,11,12	0.59	0	15,15,17	1.00	2 (13%)
2	MAN	w	5	2	11,11,12	0.61	0	15,15,17	0.99	2 (13%)
2	MAN	w	6	2	11,11,12	0.69	0	15,15,17	1.10	2 (13%)
2	MAN	w	7	2	11,11,12	0.61	0	15,15,17	0.96	2 (13%)
2	NAG	wA	1	2,1	14,14,15	0.21	0	17,19,21	0.43	0
2	NAG	wA	2	2	14,14,15	0.24	0	17,19,21	0.40	0
2	BMA	wA	3	2	11,11,12	0.98	1 (9%)	15,15,17	0.85	0
2	MAN	wA	4	2	11,11,12	0.76	0	15,15,17	0.94	1 (6%)
2	MAN	wA	5	2	11,11,12	0.60	0	15,15,17	0.98	2 (13%)
2	MAN	wA	6	2	11,11,12	0.73	0	15,15,17	1.05	2 (13%)
2	MAN	wA	7	2	11,11,12	0.63	0	15,15,17	0.96	2 (13%)
6	NAG	x	1	1,6	14,14,15	0.27	0	17,19,21	0.44	0
6	NAG	x	2	6	14,14,15	0.19	0	17,19,21	0.52	0
6	BMA	x	3	6	11,11,12	0.86	0	15,15,17	1.01	1 (6%)
6	MAN	x	4	6	11,11,12	0.86	0	15,15,17	1.21	2 (13%)
6	MAN	x	5	6	11,11,12	0.73	0	15,15,17	0.98	1 (6%)
6	MAN	x	6	6	11,11,12	0.67	0	15,15,17	0.91	1 (6%)
6	MAN	x	7	6	11,11,12	0.99	1 (9%)	15,15,17	1.67	2 (13%)
6	MAN	x	8	6	11,11,12	0.63	0	15,15,17	1.07	2 (13%)
3	NAG	xA	1	3,1	14,14,15	0.37	0	17,19,21	0.60	0
3	NAG	xA	2	3	14,14,15	0.24	0	17,19,21	0.59	0
3	BMA	xA	3	3	11,11,12	0.74	0	15,15,17	0.85	0
3	MAN	xA	4	3	11,11,12	0.75	1 (9%)	15,15,17	1.04	2 (13%)
3	MAN	xA	5	3	11,11,12	0.63	0	15,15,17	0.94	2 (13%)
3	MAN	xA	6	3	11,11,12	0.62	0	15,15,17	1.03	2 (13%)
3	MAN	xA	7	3	11,11,12	0.66	0	15,15,17	1.08	2 (13%)
3	NAG	y	1	3,1	14,14,15	0.47	0	17,19,21	0.67	1 (5%)
3	NAG	y	2	3	14,14,15	0.27	0	17,19,21	0.43	0
3	BMA	y	3	3	11,11,12	0.61	0	15,15,17	0.92	0
3	MAN	y	4	3	11,11,12	0.62	0	15,15,17	0.96	2 (13%)
3	MAN	y	5	3	11,11,12	0.62	0	15,15,17	0.96	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	y	6	3	11,11,12	0.62	0	15,15,17	0.98	2 (13%)
3	MAN	y	7	3	11,11,12	0.62	0	15,15,17	0.99	2 (13%)
2	NAG	yA	1	2,1	14,14,15	0.34	0	17,19,21	0.64	0
2	NAG	yA	2	2	14,14,15	0.21	0	17,19,21	0.47	0
2	BMA	yA	3	2	11,11,12	1.03	1 (9%)	15,15,17	0.89	0
2	MAN	yA	4	2	11,11,12	1.08	0	15,15,17	0.94	0
2	MAN	yA	5	2	11,11,12	0.71	0	15,15,17	0.99	2 (13%)
2	MAN	yA	6	2	11,11,12	0.67	0	15,15,17	0.97	2 (13%)
2	MAN	yA	7	2	11,11,12	0.66	0	15,15,17	1.02	2 (13%)
3	NAG	z	1	3,1	14,14,15	0.22	0	17,19,21	0.48	0
3	NAG	z	2	3	14,14,15	0.21	0	17,19,21	0.45	0
3	BMA	z	3	3	11,11,12	0.56	0	15,15,17	0.78	0
3	MAN	z	4	3	11,11,12	0.60	0	15,15,17	0.95	2 (13%)
3	MAN	z	5	3	11,11,12	0.62	0	15,15,17	0.98	2 (13%)
3	MAN	z	6	3	11,11,12	0.70	0	15,15,17	1.09	2 (13%)
3	MAN	z	7	3	11,11,12	0.71	0	15,15,17	0.98	2 (13%)
9	NAG	zA	1	9,1	14,14,15	0.95	1 (7%)	17,19,21	1.68	4 (23%)
9	NAG	zA	2	9	14,14,15	0.30	0	17,19,21	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	0	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	0	2	3	-	2/6/23/26	0/1/1/1
3	BMA	0	3	3	-	2/2/19/22	0/1/1/1
3	MAN	0	4	3	-	0/2/19/22	0/1/1/1
3	MAN	0	5	3	-	0/2/19/22	0/1/1/1
3	MAN	0	6	3	-	0/2/19/22	0/1/1/1
3	MAN	0	7	3	-	0/2/19/22	0/1/1/1
10	NAG	0A	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	0A	2	10	-	0/6/23/26	0/1/1/1
10	BMA	0A	3	10	-	2/2/19/22	0/1/1/1
10	MAN	0A	4	10	-	0/2/19/22	0/1/1/1
10	MAN	0A	5	10	-	0/2/19/22	0/1/1/1
10	MAN	0A	6	10	-	0/2/19/22	0/1/1/1
10	MAN	0A	7	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	1	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	1	2	3	-	4/6/23/26	0/1/1/1
3	BMA	1	3	3	-	0/2/19/22	0/1/1/1
3	MAN	1	4	3	-	2/2/19/22	0/1/1/1
3	MAN	1	5	3	-	0/2/19/22	0/1/1/1
3	MAN	1	6	3	-	0/2/19/22	0/1/1/1
3	MAN	1	7	3	-	0/2/19/22	0/1/1/1
10	NAG	1A	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	1A	2	10	-	2/6/23/26	0/1/1/1
10	BMA	1A	3	10	-	1/2/19/22	0/1/1/1
10	MAN	1A	4	10	-	0/2/19/22	0/1/1/1
10	MAN	1A	5	10	-	0/2/19/22	0/1/1/1
10	MAN	1A	6	10	-	0/2/19/22	0/1/1/1
10	MAN	1A	7	10	-	0/2/19/22	0/1/1/1
2	NAG	2	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	2	2	2	-	0/6/23/26	0/1/1/1
2	BMA	2	3	2	-	0/2/19/22	0/1/1/1
2	MAN	2	4	2	-	2/2/19/22	0/1/1/1
2	MAN	2	5	2	-	0/2/19/22	0/1/1/1
2	MAN	2	6	2	-	0/2/19/22	0/1/1/1
2	MAN	2	7	2	-	0/2/19/22	0/1/1/1
10	NAG	2A	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	2A	2	10	-	2/6/23/26	0/1/1/1
10	BMA	2A	3	10	-	2/2/19/22	0/1/1/1
10	MAN	2A	4	10	-	0/2/19/22	0/1/1/1
10	MAN	2A	5	10	-	0/2/19/22	0/1/1/1
10	MAN	2A	6	10	-	0/2/19/22	0/1/1/1
10	MAN	2A	7	10	-	0/2/19/22	0/1/1/1
2	NAG	3	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	3	2	2	-	0/6/23/26	0/1/1/1
2	BMA	3	3	2	-	1/2/19/22	0/1/1/1
2	MAN	3	4	2	-	0/2/19/22	0/1/1/1
2	MAN	3	5	2	-	0/2/19/22	0/1/1/1
2	MAN	3	6	2	-	0/2/19/22	0/1/1/1
2	MAN	3	7	2	-	1/2/19/22	0/1/1/1
10	NAG	3A	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	3A	2	10	-	2/6/23/26	0/1/1/1
10	BMA	3A	3	10	-	2/2/19/22	0/1/1/1
10	MAN	3A	4	10	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	3A	5	10	-	0/2/19/22	0/1/1/1
10	MAN	3A	6	10	-	0/2/19/22	0/1/1/1
10	MAN	3A	7	10	-	0/2/19/22	0/1/1/1
2	NAG	4	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	4	2	2	-	2/6/23/26	0/1/1/1
2	BMA	4	3	2	-	0/2/19/22	0/1/1/1
2	MAN	4	4	2	-	1/2/19/22	0/1/1/1
2	MAN	4	5	2	-	0/2/19/22	0/1/1/1
2	MAN	4	6	2	-	0/2/19/22	0/1/1/1
2	MAN	4	7	2	-	0/2/19/22	0/1/1/1
10	NAG	4A	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	4A	2	10	-	1/6/23/26	0/1/1/1
10	BMA	4A	3	10	-	1/2/19/22	0/1/1/1
10	MAN	4A	4	10	-	0/2/19/22	0/1/1/1
10	MAN	4A	5	10	-	0/2/19/22	0/1/1/1
10	MAN	4A	6	10	-	0/2/19/22	0/1/1/1
10	MAN	4A	7	10	-	0/2/19/22	0/1/1/1
3	NAG	5	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	5	2	3	-	2/6/23/26	0/1/1/1
3	BMA	5	3	3	-	1/2/19/22	0/1/1/1
3	MAN	5	4	3	-	1/2/19/22	0/1/1/1
3	MAN	5	5	3	-	0/2/19/22	0/1/1/1
3	MAN	5	6	3	-	0/2/19/22	0/1/1/1
3	MAN	5	7	3	-	0/2/19/22	0/1/1/1
10	NAG	5A	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	5A	2	10	-	0/6/23/26	0/1/1/1
10	BMA	5A	3	10	-	2/2/19/22	0/1/1/1
10	MAN	5A	4	10	-	2/2/19/22	0/1/1/1
10	MAN	5A	5	10	-	0/2/19/22	0/1/1/1
10	MAN	5A	6	10	-	0/2/19/22	0/1/1/1
10	MAN	5A	7	10	-	0/2/19/22	0/1/1/1
3	NAG	6	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	6	2	3	-	0/6/23/26	0/1/1/1
3	BMA	6	3	3	-	0/2/19/22	0/1/1/1
3	MAN	6	4	3	-	1/2/19/22	0/1/1/1
3	MAN	6	5	3	-	0/2/19/22	0/1/1/1
3	MAN	6	6	3	-	0/2/19/22	0/1/1/1
3	MAN	6	7	3	-	0/2/19/22	0/1/1/1
10	NAG	6A	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	6A	2	10	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BMA	6A	3	10	-	2/2/19/22	0/1/1/1
10	MAN	6A	4	10	-	0/2/19/22	0/1/1/1
10	MAN	6A	5	10	-	0/2/19/22	0/1/1/1
10	MAN	6A	6	10	-	0/2/19/22	0/1/1/1
10	MAN	6A	7	10	-	0/2/19/22	0/1/1/1
2	NAG	7	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	7	2	2	-	3/6/23/26	0/1/1/1
2	BMA	7	3	2	-	0/2/19/22	0/1/1/1
2	MAN	7	4	2	-	1/2/19/22	0/1/1/1
2	MAN	7	5	2	-	0/2/19/22	0/1/1/1
2	MAN	7	6	2	-	0/2/19/22	0/1/1/1
2	MAN	7	7	2	-	0/2/19/22	0/1/1/1
10	NAG	7A	1	10,1	-	3/6/23/26	0/1/1/1
10	NAG	7A	2	10	-	0/6/23/26	0/1/1/1
10	BMA	7A	3	10	-	2/2/19/22	0/1/1/1
10	MAN	7A	4	10	-	0/2/19/22	0/1/1/1
10	MAN	7A	5	10	-	0/2/19/22	0/1/1/1
10	MAN	7A	6	10	-	0/2/19/22	0/1/1/1
10	MAN	7A	7	10	-	0/2/19/22	0/1/1/1
3	NAG	8	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	8	2	3	-	2/6/23/26	0/1/1/1
3	BMA	8	3	3	-	0/2/19/22	0/1/1/1
3	MAN	8	4	3	-	0/2/19/22	0/1/1/1
3	MAN	8	5	3	-	0/2/19/22	0/1/1/1
3	MAN	8	6	3	-	0/2/19/22	0/1/1/1
3	MAN	8	7	3	-	0/2/19/22	0/1/1/1
3	NAG	9	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	9	2	3	-	2/6/23/26	0/1/1/1
3	BMA	9	3	3	-	2/2/19/22	0/1/1/1
3	MAN	9	4	3	-	0/2/19/22	0/1/1/1
3	MAN	9	5	3	-	0/2/19/22	0/1/1/1
3	MAN	9	6	3	-	0/2/19/22	0/1/1/1
3	MAN	9	7	3	-	0/2/19/22	0/1/1/1
2	NAG	AA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	AA	2	2	-	4/6/23/26	0/1/1/1
2	BMA	AA	3	2	-	0/2/19/22	0/1/1/1
2	MAN	AA	4	2	-	1/2/19/22	0/1/1/1
2	MAN	AA	5	2	-	0/2/19/22	0/1/1/1
2	MAN	AA	6	2	-	0/2/19/22	0/1/1/1
2	MAN	AA	7	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	BA	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	BA	2	3	-	4/6/23/26	0/1/1/1
3	BMA	BA	3	3	-	2/2/19/22	0/1/1/1
3	MAN	BA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	BA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	BA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	BA	7	3	-	0/2/19/22	0/1/1/1
2	NAG	CA	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	CA	2	2	-	2/6/23/26	0/1/1/1
2	BMA	CA	3	2	-	1/2/19/22	0/1/1/1
2	MAN	CA	4	2	-	1/2/19/22	0/1/1/1
2	MAN	CA	5	2	-	0/2/19/22	0/1/1/1
2	MAN	CA	6	2	-	2/2/19/22	0/1/1/1
2	MAN	CA	7	2	-	2/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	MAN	D	4	2	-	2/2/19/22	0/1/1/1
2	MAN	D	5	2	-	0/2/19/22	0/1/1/1
2	MAN	D	6	2	-	0/2/19/22	0/1/1/1
2	MAN	D	7	2	-	0/2/19/22	0/1/1/1
3	NAG	DA	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	DA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	DA	3	3	-	2/2/19/22	0/1/1/1
3	MAN	DA	4	3	-	1/2/19/22	0/1/1/1
3	MAN	DA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	DA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	DA	7	3	-	0/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1
3	MAN	E	6	3	-	0/2/19/22	0/1/1/1
3	MAN	E	7	3	-	0/2/19/22	0/1/1/1
7	NAG	EA	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	EA	10	7	-	0/6/23/26	0/1/1/1
7	GAL	EA	11	7	-	2/2/19/22	0/1/1/1
7	FUC	EA	12	7	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	EA	2	7	-	2/6/23/26	0/1/1/1
7	BMA	EA	3	7	-	0/2/19/22	0/1/1/1
7	MAN	EA	4	7	-	2/2/19/22	0/1/1/1
7	NAG	EA	5	7	-	0/6/23/26	0/1/1/1
7	GAL	EA	6	7	-	2/2/19/22	0/1/1/1
7	NAG	EA	7	7	-	2/6/23/26	0/1/1/1
7	GAL	EA	8	7	-	0/2/19/22	0/1/1/1
7	MAN	EA	9	7	-	0/2/19/22	0/1/1/1
4	NAG	F	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
4	MAN	F	4	4	-	2/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	MAN	F	6	4	-	0/2/19/22	0/1/1/1
4	MAN	F	7	4	-	1/2/19/22	0/1/1/1
4	MAN	F	8	4	-	2/2/19/22	0/1/1/1
4	MAN	F	9	4	-	1/2/19/22	0/1/1/1
2	NAG	FA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	FA	2	2	-	0/6/23/26	0/1/1/1
2	BMA	FA	3	2	-	1/2/19/22	0/1/1/1
2	MAN	FA	4	2	-	2/2/19/22	0/1/1/1
2	MAN	FA	5	2	-	0/2/19/22	0/1/1/1
2	MAN	FA	6	2	-	0/2/19/22	0/1/1/1
2	MAN	FA	7	2	-	0/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	NAG	G	5	5	-	2/6/23/26	0/1/1/1
5	GAL	G	6	5	-	1/2/19/22	0/1/1/1
5	MAN	G	7	5	-	0/2/19/22	0/1/1/1
5	NAG	G	8	5	-	0/6/23/26	0/1/1/1
5	GAL	G	9	5	-	0/2/19/22	0/1/1/1
3	NAG	GA	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	GA	2	3	-	0/6/23/26	0/1/1/1
3	BMA	GA	3	3	-	2/2/19/22	0/1/1/1
3	MAN	GA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	GA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	GA	6	3	-	0/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	JA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	JA	5	2	-	0/2/19/22	0/1/1/1
2	MAN	JA	6	2	-	0/2/19/22	0/1/1/1
2	MAN	JA	7	2	-	0/2/19/22	0/1/1/1
3	NAG	K	1	3,1	-	6/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
3	MAN	K	4	3	-	1/2/19/22	0/1/1/1
3	MAN	K	5	3	-	0/2/19/22	0/1/1/1
3	MAN	K	6	3	-	0/2/19/22	0/1/1/1
3	MAN	K	7	3	-	0/2/19/22	0/1/1/1
8	NAG	KA	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	KA	2	8	-	2/6/23/26	0/1/1/1
8	BMA	KA	3	8	-	2/2/19/22	0/1/1/1
8	MAN	KA	4	8	-	0/2/19/22	0/1/1/1
8	MAN	KA	5	8	-	2/2/19/22	0/1/1/1
2	NAG	L	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	BMA	L	3	2	-	1/2/19/22	0/1/1/1
2	MAN	L	4	2	-	2/2/19/22	0/1/1/1
2	MAN	L	5	2	-	0/2/19/22	0/1/1/1
2	MAN	L	6	2	-	0/2/19/22	0/1/1/1
2	MAN	L	7	2	-	0/2/19/22	0/1/1/1
2	NAG	LA	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	LA	2	2	-	2/6/23/26	0/1/1/1
2	BMA	LA	3	2	-	1/2/19/22	0/1/1/1
2	MAN	LA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	LA	5	2	-	0/2/19/22	0/1/1/1
2	MAN	LA	6	2	-	0/2/19/22	0/1/1/1
2	MAN	LA	7	2	-	0/2/19/22	0/1/1/1
6	NAG	M	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	2/6/23/26	0/1/1/1
6	BMA	M	3	6	-	2/2/19/22	0/1/1/1
6	MAN	M	4	6	-	0/2/19/22	0/1/1/1
6	MAN	M	5	6	-	2/2/19/22	0/1/1/1
6	MAN	M	6	6	-	0/2/19/22	0/1/1/1
6	MAN	M	7	6	-	0/2/19/22	0/1/1/1
6	MAN	M	8	6	-	2/2/19/22	0/1/1/1
3	NAG	MA	1	3,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	MA	2	3	-	4/6/23/26	0/1/1/1
3	BMA	MA	3	3	-	1/2/19/22	0/1/1/1
3	MAN	MA	4	3	-	1/2/19/22	0/1/1/1
3	MAN	MA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	MA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	MA	7	3	-	0/2/19/22	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	BMA	N	3	3	-	0/2/19/22	0/1/1/1
3	MAN	N	4	3	-	2/2/19/22	0/1/1/1
3	MAN	N	5	3	-	0/2/19/22	0/1/1/1
3	MAN	N	6	3	-	0/2/19/22	0/1/1/1
3	MAN	N	7	3	-	0/2/19/22	0/1/1/1
2	NAG	NA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	NA	2	2	-	2/6/23/26	0/1/1/1
2	BMA	NA	3	2	-	0/2/19/22	0/1/1/1
2	MAN	NA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	NA	5	2	-	0/2/19/22	0/1/1/1
2	MAN	NA	6	2	-	0/2/19/22	0/1/1/1
2	MAN	NA	7	2	-	0/2/19/22	0/1/1/1
3	NAG	O	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	1/6/23/26	0/1/1/1
3	BMA	O	3	3	-	2/2/19/22	0/1/1/1
3	MAN	O	4	3	-	0/2/19/22	0/1/1/1
3	MAN	O	5	3	-	0/2/19/22	0/1/1/1
3	MAN	O	6	3	-	0/2/19/22	0/1/1/1
3	MAN	O	7	3	-	0/2/19/22	0/1/1/1
9	NAG	OA	1	9,1	-	6/6/23/26	0/1/1/1
9	NAG	OA	2	9	-	2/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
3	BMA	P	3	3	-	2/2/19/22	0/1/1/1
3	MAN	P	4	3	-	0/2/19/22	0/1/1/1
3	MAN	P	5	3	-	0/2/19/22	0/1/1/1
3	MAN	P	6	3	-	0/2/19/22	0/1/1/1
3	MAN	P	7	3	-	0/2/19/22	0/1/1/1
2	NAG	PA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	PA	2	2	-	0/6/23/26	0/1/1/1
2	BMA	PA	3	2	-	2/2/19/22	0/1/1/1
2	MAN	PA	4	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	PA	5	2	-	0/2/19/22	0/1/1/1
2	MAN	PA	6	2	-	0/2/19/22	0/1/1/1
2	MAN	PA	7	2	-	0/2/19/22	0/1/1/1
3	NAG	Q	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	4/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	0/2/19/22	0/1/1/1
3	MAN	Q	4	3	-	2/2/19/22	0/1/1/1
3	MAN	Q	5	3	-	0/2/19/22	0/1/1/1
3	MAN	Q	6	3	-	0/2/19/22	0/1/1/1
3	MAN	Q	7	3	-	0/2/19/22	0/1/1/1
3	NAG	QA	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	QA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	QA	3	3	-	0/2/19/22	0/1/1/1
3	MAN	QA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	QA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	QA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	QA	7	3	-	0/2/19/22	0/1/1/1
2	NAG	R	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
2	BMA	R	3	2	-	0/2/19/22	0/1/1/1
2	MAN	R	4	2	-	2/2/19/22	0/1/1/1
2	MAN	R	5	2	-	0/2/19/22	0/1/1/1
2	MAN	R	6	2	-	0/2/19/22	0/1/1/1
2	MAN	R	7	2	-	0/2/19/22	0/1/1/1
4	NAG	RA	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	RA	2	4	-	2/6/23/26	0/1/1/1
4	BMA	RA	3	4	-	2/2/19/22	0/1/1/1
4	MAN	RA	4	4	-	2/2/19/22	0/1/1/1
4	MAN	RA	5	4	-	0/2/19/22	0/1/1/1
4	MAN	RA	6	4	-	0/2/19/22	0/1/1/1
4	MAN	RA	7	4	-	1/2/19/22	0/1/1/1
4	MAN	RA	8	4	-	2/2/19/22	0/1/1/1
4	MAN	RA	9	4	-	1/2/19/22	0/1/1/1
2	NAG	S	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1
2	BMA	S	3	2	-	1/2/19/22	0/1/1/1
2	MAN	S	4	2	-	0/2/19/22	0/1/1/1
2	MAN	S	5	2	-	0/2/19/22	0/1/1/1
2	MAN	S	6	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	S	7	2	-	1/2/19/22	0/1/1/1
5	NAG	SA	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	SA	2	5	-	2/6/23/26	0/1/1/1
5	BMA	SA	3	5	-	2/2/19/22	0/1/1/1
5	MAN	SA	4	5	-	0/2/19/22	0/1/1/1
5	NAG	SA	5	5	-	2/6/23/26	0/1/1/1
5	GAL	SA	6	5	-	0/2/19/22	0/1/1/1
5	MAN	SA	7	5	-	0/2/19/22	0/1/1/1
5	NAG	SA	8	5	-	0/6/23/26	0/1/1/1
5	GAL	SA	9	5	-	0/2/19/22	0/1/1/1
2	NAG	T	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	0/1/1/1
2	BMA	T	3	2	-	0/2/19/22	0/1/1/1
2	MAN	T	4	2	-	1/2/19/22	0/1/1/1
2	MAN	T	5	2	-	0/2/19/22	0/1/1/1
2	MAN	T	6	2	-	0/2/19/22	0/1/1/1
2	MAN	T	7	2	-	0/2/19/22	0/1/1/1
3	NAG	TA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	TA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	TA	3	3	-	2/2/19/22	0/1/1/1
3	MAN	TA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	TA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	TA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	TA	7	3	-	0/2/19/22	0/1/1/1
3	NAG	U	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	BMA	U	3	3	-	1/2/19/22	0/1/1/1
3	MAN	U	4	3	-	1/2/19/22	0/1/1/1
3	MAN	U	5	3	-	0/2/19/22	0/1/1/1
3	MAN	U	6	3	-	0/2/19/22	0/1/1/1
3	MAN	U	7	3	-	0/2/19/22	0/1/1/1
3	NAG	UA	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	UA	2	3	-	4/6/23/26	0/1/1/1
3	BMA	UA	3	3	-	0/2/19/22	0/1/1/1
3	MAN	UA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	UA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	UA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	UA	7	3	-	0/2/19/22	0/1/1/1
3	NAG	V	1	3,1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	V	2	3	-	1/6/23/26	0/1/1/1
3	BMA	V	3	3	-	0/2/19/22	0/1/1/1
3	MAN	V	4	3	-	0/2/19/22	0/1/1/1
3	MAN	V	5	3	-	0/2/19/22	0/1/1/1
3	MAN	V	6	3	-	0/2/19/22	0/1/1/1
3	MAN	V	7	3	-	0/2/19/22	0/1/1/1
3	NAG	VA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	VA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	VA	3	3	-	2/2/19/22	0/1/1/1
3	MAN	VA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	VA	5	3	-	2/2/19/22	0/1/1/1
3	MAN	VA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	VA	7	3	-	0/2/19/22	0/1/1/1
2	NAG	W	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	W	2	2	-	2/6/23/26	0/1/1/1
2	BMA	W	3	2	-	0/2/19/22	0/1/1/1
2	MAN	W	4	2	-	1/2/19/22	0/1/1/1
2	MAN	W	5	2	-	0/2/19/22	0/1/1/1
2	MAN	W	6	2	-	0/2/19/22	0/1/1/1
2	MAN	W	7	2	-	0/2/19/22	0/1/1/1
3	NAG	WA	1	3,1	-	6/6/23/26	0/1/1/1
3	NAG	WA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	WA	3	3	-	0/2/19/22	0/1/1/1
3	MAN	WA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	WA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	WA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	WA	7	3	-	0/2/19/22	0/1/1/1
3	NAG	X	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	X	2	3	-	2/6/23/26	0/1/1/1
3	BMA	X	3	3	-	0/2/19/22	0/1/1/1
3	MAN	X	4	3	-	0/2/19/22	0/1/1/1
3	MAN	X	5	3	-	0/2/19/22	0/1/1/1
3	MAN	X	6	3	-	0/2/19/22	0/1/1/1
3	MAN	X	7	3	-	0/2/19/22	0/1/1/1
2	NAG	XA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	XA	2	2	-	2/6/23/26	0/1/1/1
2	BMA	XA	3	2	-	1/2/19/22	0/1/1/1
2	MAN	XA	4	2	-	2/2/19/22	0/1/1/1
2	MAN	XA	5	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	XA	6	2	-	0/2/19/22	0/1/1/1
2	MAN	XA	7	2	-	0/2/19/22	0/1/1/1
3	NAG	Y	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Y	3	3	-	2/2/19/22	0/1/1/1
3	MAN	Y	4	3	-	0/2/19/22	0/1/1/1
3	MAN	Y	5	3	-	0/2/19/22	0/1/1/1
3	MAN	Y	6	3	-	0/2/19/22	0/1/1/1
3	MAN	Y	7	3	-	0/2/19/22	0/1/1/1
6	NAG	YA	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	YA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	YA	3	6	-	2/2/19/22	0/1/1/1
6	MAN	YA	4	6	-	0/2/19/22	0/1/1/1
6	MAN	YA	5	6	-	0/2/19/22	0/1/1/1
6	MAN	YA	6	6	-	0/2/19/22	0/1/1/1
6	MAN	YA	7	6	-	0/2/19/22	0/1/1/1
6	MAN	YA	8	6	-	2/2/19/22	0/1/1/1
2	NAG	Z	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	4/6/23/26	0/1/1/1
2	BMA	Z	3	2	-	0/2/19/22	0/1/1/1
2	MAN	Z	4	2	-	1/2/19/22	0/1/1/1
2	MAN	Z	5	2	-	0/2/19/22	0/1/1/1
2	MAN	Z	6	2	-	0/2/19/22	0/1/1/1
2	MAN	Z	7	2	-	0/2/19/22	0/1/1/1
3	NAG	ZA	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	ZA	2	3	-	0/6/23/26	0/1/1/1
3	BMA	ZA	3	3	-	0/2/19/22	0/1/1/1
3	MAN	ZA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	ZA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	ZA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	ZA	7	3	-	0/2/19/22	0/1/1/1
3	NAG	a	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	4/6/23/26	0/1/1/1
3	BMA	a	3	3	-	2/2/19/22	0/1/1/1
3	MAN	a	4	3	-	1/2/19/22	0/1/1/1
3	MAN	a	5	3	-	0/2/19/22	0/1/1/1
3	MAN	a	6	3	-	0/2/19/22	0/1/1/1
3	MAN	a	7	3	-	0/2/19/22	0/1/1/1
3	NAG	aA	1	3,1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	aA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	aA	3	3	-	2/2/19/22	0/1/1/1
3	MAN	aA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	aA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	aA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	aA	7	3	-	0/2/19/22	0/1/1/1
2	NAG	b	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	b	2	2	-	2/6/23/26	0/1/1/1
2	BMA	b	3	2	-	1/2/19/22	0/1/1/1
2	MAN	b	4	2	-	1/2/19/22	0/1/1/1
2	MAN	b	5	2	-	0/2/19/22	0/1/1/1
2	MAN	b	6	2	-	2/2/19/22	0/1/1/1
2	MAN	b	7	2	-	2/2/19/22	0/1/1/1
3	NAG	bA	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	bA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	bA	3	3	-	2/2/19/22	0/1/1/1
3	MAN	bA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	bA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	bA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	bA	7	3	-	0/2/19/22	0/1/1/1
3	NAG	c	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	c	2	3	-	2/6/23/26	0/1/1/1
3	BMA	c	3	3	-	2/2/19/22	0/1/1/1
3	MAN	c	4	3	-	1/2/19/22	0/1/1/1
3	MAN	c	5	3	-	0/2/19/22	0/1/1/1
3	MAN	c	6	3	-	0/2/19/22	0/1/1/1
3	MAN	c	7	3	-	0/2/19/22	0/1/1/1
3	NAG	cA	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	cA	2	3	-	4/6/23/26	0/1/1/1
3	BMA	cA	3	3	-	0/2/19/22	0/1/1/1
3	MAN	cA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	cA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	cA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	cA	7	3	-	0/2/19/22	0/1/1/1
7	NAG	d	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	d	10	7	-	0/6/23/26	0/1/1/1
7	GAL	d	11	7	-	2/2/19/22	0/1/1/1
7	FUC	d	12	7	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	d	2	7	-	2/6/23/26	0/1/1/1
7	BMA	d	3	7	-	0/2/19/22	0/1/1/1
7	MAN	d	4	7	-	2/2/19/22	0/1/1/1
7	NAG	d	5	7	-	0/6/23/26	0/1/1/1
7	GAL	d	6	7	-	2/2/19/22	0/1/1/1
7	NAG	d	7	7	-	2/6/23/26	0/1/1/1
7	GAL	d	8	7	-	0/2/19/22	0/1/1/1
7	MAN	d	9	7	-	1/2/19/22	0/1/1/1
2	NAG	dA	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	dA	2	2	-	0/6/23/26	0/1/1/1
2	BMA	dA	3	2	-	0/2/19/22	0/1/1/1
2	MAN	dA	4	2	-	2/2/19/22	0/1/1/1
2	MAN	dA	5	2	-	0/2/19/22	0/1/1/1
2	MAN	dA	6	2	-	0/2/19/22	0/1/1/1
2	MAN	dA	7	2	-	0/2/19/22	0/1/1/1
2	NAG	e	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	e	2	2	-	0/6/23/26	0/1/1/1
2	BMA	e	3	2	-	1/2/19/22	0/1/1/1
2	MAN	e	4	2	-	2/2/19/22	0/1/1/1
2	MAN	e	5	2	-	0/2/19/22	0/1/1/1
2	MAN	e	6	2	-	0/2/19/22	0/1/1/1
2	MAN	e	7	2	-	0/2/19/22	0/1/1/1
2	NAG	eA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	eA	2	2	-	0/6/23/26	0/1/1/1
2	BMA	eA	3	2	-	1/2/19/22	0/1/1/1
2	MAN	eA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	eA	5	2	-	0/2/19/22	0/1/1/1
2	MAN	eA	6	2	-	0/2/19/22	0/1/1/1
2	MAN	eA	7	2	-	1/2/19/22	0/1/1/1
3	NAG	f	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	f	2	3	-	0/6/23/26	0/1/1/1
3	BMA	f	3	3	-	2/2/19/22	0/1/1/1
3	MAN	f	4	3	-	2/2/19/22	0/1/1/1
3	MAN	f	5	3	-	1/2/19/22	0/1/1/1
3	MAN	f	6	3	-	0/2/19/22	0/1/1/1
3	MAN	f	7	3	-	1/2/19/22	0/1/1/1
2	NAG	fA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	fA	2	2	-	2/6/23/26	0/1/1/1
2	BMA	fA	3	2	-	0/2/19/22	0/1/1/1
2	MAN	fA	4	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	fA	5	2	-	1/2/19/22	0/1/1/1
2	MAN	fA	6	2	-	0/2/19/22	0/1/1/1
2	MAN	fA	7	2	-	0/2/19/22	0/1/1/1
3	NAG	g	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	g	2	3	-	0/6/23/26	0/1/1/1
3	BMA	g	3	3	-	2/2/19/22	0/1/1/1
3	MAN	g	4	3	-	2/2/19/22	0/1/1/1
3	MAN	g	5	3	-	0/2/19/22	0/1/1/1
3	MAN	g	6	3	-	0/2/19/22	0/1/1/1
3	MAN	g	7	3	-	0/2/19/22	0/1/1/1
3	NAG	gA	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	gA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	gA	3	3	-	1/2/19/22	0/1/1/1
3	MAN	gA	4	3	-	1/2/19/22	0/1/1/1
3	MAN	gA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	gA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	gA	7	3	-	0/2/19/22	0/1/1/1
3	NAG	h	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	h	2	3	-	4/6/23/26	0/1/1/1
3	BMA	h	3	3	-	0/2/19/22	0/1/1/1
3	MAN	h	4	3	-	0/2/19/22	0/1/1/1
3	MAN	h	5	3	-	0/2/19/22	0/1/1/1
3	MAN	h	6	3	-	0/2/19/22	0/1/1/1
3	MAN	h	7	3	-	0/2/19/22	0/1/1/1
3	NAG	hA	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	hA	2	3	-	1/6/23/26	0/1/1/1
3	BMA	hA	3	3	-	0/2/19/22	0/1/1/1
3	MAN	hA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	hA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	hA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	hA	7	3	-	0/2/19/22	0/1/1/1
2	NAG	i	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	i	2	2	-	0/6/23/26	0/1/1/1
2	BMA	i	3	2	-	2/2/19/22	0/1/1/1
2	MAN	i	4	2	-	0/2/19/22	0/1/1/1
2	MAN	i	5	2	-	0/2/19/22	0/1/1/1
2	MAN	i	6	2	-	0/2/19/22	0/1/1/1
2	MAN	i	7	2	-	0/2/19/22	0/1/1/1
2	NAG	iA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	iA	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	iA	3	2	-	0/2/19/22	0/1/1/1
2	MAN	iA	4	2	-	1/2/19/22	0/1/1/1
2	MAN	iA	5	2	-	0/2/19/22	0/1/1/1
2	MAN	iA	6	2	-	0/2/19/22	0/1/1/1
2	MAN	iA	7	2	-	0/2/19/22	0/1/1/1
8	NAG	j	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	j	2	8	-	2/6/23/26	0/1/1/1
8	BMA	j	3	8	-	2/2/19/22	0/1/1/1
8	MAN	j	4	8	-	0/2/19/22	0/1/1/1
8	MAN	j	5	8	-	2/2/19/22	0/1/1/1
3	NAG	jA	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	jA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	jA	3	3	-	0/2/19/22	0/1/1/1
3	MAN	jA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	jA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	jA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	jA	7	3	-	0/2/19/22	0/1/1/1
2	NAG	k	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	k	2	2	-	2/6/23/26	0/1/1/1
2	BMA	k	3	2	-	1/2/19/22	0/1/1/1
2	MAN	k	4	2	-	0/2/19/22	0/1/1/1
2	MAN	k	5	2	-	0/2/19/22	0/1/1/1
2	MAN	k	6	2	-	0/2/19/22	0/1/1/1
2	MAN	k	7	2	-	0/2/19/22	0/1/1/1
3	NAG	kA	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	kA	2	3	-	3/6/23/26	0/1/1/1
3	BMA	kA	3	3	-	2/2/19/22	0/1/1/1
3	MAN	kA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	kA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	kA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	kA	7	3	-	0/2/19/22	0/1/1/1
3	NAG	l	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	l	2	3	-	4/6/23/26	0/1/1/1
3	BMA	l	3	3	-	1/2/19/22	0/1/1/1
3	MAN	l	4	3	-	2/2/19/22	0/1/1/1
3	MAN	l	5	3	-	0/2/19/22	0/1/1/1
3	MAN	l	6	3	-	0/2/19/22	0/1/1/1
3	MAN	l	7	3	-	0/2/19/22	0/1/1/1
2	NAG	lA	1	2,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	lA	2	2	-	4/6/23/26	0/1/1/1
2	BMA	lA	3	2	-	0/2/19/22	0/1/1/1
2	MAN	lA	4	2	-	1/2/19/22	0/1/1/1
2	MAN	lA	5	2	-	0/2/19/22	0/1/1/1
2	MAN	lA	6	2	-	0/2/19/22	0/1/1/1
2	MAN	lA	7	2	-	0/2/19/22	0/1/1/1
2	NAG	m	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	m	2	2	-	2/6/23/26	0/1/1/1
2	BMA	m	3	2	-	0/2/19/22	0/1/1/1
2	MAN	m	4	2	-	0/2/19/22	0/1/1/1
2	MAN	m	5	2	-	0/2/19/22	0/1/1/1
2	MAN	m	6	2	-	0/2/19/22	0/1/1/1
2	MAN	m	7	2	-	0/2/19/22	0/1/1/1
3	NAG	mA	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	mA	2	3	-	4/6/23/26	0/1/1/1
3	BMA	mA	3	3	-	2/2/19/22	0/1/1/1
3	MAN	mA	4	3	-	1/2/19/22	0/1/1/1
3	MAN	mA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	mA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	mA	7	3	-	0/2/19/22	0/1/1/1
9	NAG	n	1	9,1	-	6/6/23/26	0/1/1/1
9	NAG	n	2	9	-	2/6/23/26	0/1/1/1
2	NAG	nA	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	nA	2	2	-	2/6/23/26	0/1/1/1
2	BMA	nA	3	2	-	1/2/19/22	0/1/1/1
2	MAN	nA	4	2	-	1/2/19/22	0/1/1/1
2	MAN	nA	5	2	-	0/2/19/22	0/1/1/1
2	MAN	nA	6	2	-	2/2/19/22	0/1/1/1
2	MAN	nA	7	2	-	2/2/19/22	0/1/1/1
2	NAG	o	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	o	2	2	-	0/6/23/26	0/1/1/1
2	BMA	o	3	2	-	2/2/19/22	0/1/1/1
2	MAN	o	4	2	-	2/2/19/22	0/1/1/1
2	MAN	o	5	2	-	0/2/19/22	0/1/1/1
2	MAN	o	6	2	-	0/2/19/22	0/1/1/1
2	MAN	o	7	2	-	0/2/19/22	0/1/1/1
3	NAG	oA	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	oA	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	oA	3	3	-	2/2/19/22	0/1/1/1
3	MAN	oA	4	3	-	1/2/19/22	0/1/1/1
3	MAN	oA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	oA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	oA	7	3	-	0/2/19/22	0/1/1/1
3	NAG	p	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	p	2	3	-	2/6/23/26	0/1/1/1
3	BMA	p	3	3	-	0/2/19/22	0/1/1/1
3	MAN	p	4	3	-	0/2/19/22	0/1/1/1
3	MAN	p	5	3	-	0/2/19/22	0/1/1/1
3	MAN	p	6	3	-	0/2/19/22	0/1/1/1
3	MAN	p	7	3	-	0/2/19/22	0/1/1/1
7	NAG	pA	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	pA	10	7	-	0/6/23/26	0/1/1/1
7	GAL	pA	11	7	-	2/2/19/22	0/1/1/1
7	FUC	pA	12	7	-	-	0/1/1/1
7	NAG	pA	2	7	-	1/6/23/26	0/1/1/1
7	BMA	pA	3	7	-	0/2/19/22	0/1/1/1
7	MAN	pA	4	7	-	2/2/19/22	0/1/1/1
7	NAG	pA	5	7	-	0/6/23/26	0/1/1/1
7	GAL	pA	6	7	-	2/2/19/22	0/1/1/1
7	NAG	pA	7	7	-	2/6/23/26	0/1/1/1
7	GAL	pA	8	7	-	0/2/19/22	0/1/1/1
7	MAN	pA	9	7	-	0/2/19/22	0/1/1/1
4	NAG	q	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	q	2	4	-	2/6/23/26	0/1/1/1
4	BMA	q	3	4	-	2/2/19/22	0/1/1/1
4	MAN	q	4	4	-	2/2/19/22	0/1/1/1
4	MAN	q	5	4	-	0/2/19/22	0/1/1/1
4	MAN	q	6	4	-	0/2/19/22	0/1/1/1
4	MAN	q	7	4	-	1/2/19/22	0/1/1/1
4	MAN	q	8	4	-	2/2/19/22	0/1/1/1
4	MAN	q	9	4	-	1/2/19/22	0/1/1/1
2	NAG	qA	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	qA	2	2	-	0/6/23/26	0/1/1/1
2	BMA	qA	3	2	-	1/2/19/22	0/1/1/1
2	MAN	qA	4	2	-	2/2/19/22	0/1/1/1
2	MAN	qA	5	2	-	0/2/19/22	0/1/1/1
2	MAN	qA	6	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	qA	7	2	-	0/2/19/22	0/1/1/1
5	NAG	r	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	r	2	5	-	6/6/23/26	0/1/1/1
5	BMA	r	3	5	-	2/2/19/22	0/1/1/1
5	MAN	r	4	5	-	0/2/19/22	0/1/1/1
5	NAG	r	5	5	-	2/6/23/26	0/1/1/1
5	GAL	r	6	5	-	1/2/19/22	0/1/1/1
5	MAN	r	7	5	-	0/2/19/22	0/1/1/1
5	NAG	r	8	5	-	0/6/23/26	0/1/1/1
5	GAL	r	9	5	-	0/2/19/22	0/1/1/1
3	NAG	rA	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	rA	2	3	-	0/6/23/26	0/1/1/1
3	BMA	rA	3	3	-	2/2/19/22	0/1/1/1
3	MAN	rA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	rA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	rA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	rA	7	3	-	0/2/19/22	0/1/1/1
3	NAG	s	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	s	2	3	-	2/6/23/26	0/1/1/1
3	BMA	s	3	3	-	2/2/19/22	0/1/1/1
3	MAN	s	4	3	-	2/2/19/22	0/1/1/1
3	MAN	s	5	3	-	0/2/19/22	0/1/1/1
3	MAN	s	6	3	-	0/2/19/22	0/1/1/1
3	MAN	s	7	3	-	0/2/19/22	0/1/1/1
3	NAG	sA	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	sA	2	3	-	0/6/23/26	0/1/1/1
3	BMA	sA	3	3	-	2/2/19/22	0/1/1/1
3	MAN	sA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	sA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	sA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	sA	7	3	-	0/2/19/22	0/1/1/1
3	NAG	t	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	t	2	3	-	4/6/23/26	0/1/1/1
3	BMA	t	3	3	-	0/2/19/22	0/1/1/1
3	MAN	t	4	3	-	0/2/19/22	0/1/1/1
3	MAN	t	5	3	-	0/2/19/22	0/1/1/1
3	MAN	t	6	3	-	0/2/19/22	0/1/1/1
3	MAN	t	7	3	-	0/2/19/22	0/1/1/1
3	NAG	tA	1	3,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	tA	2	3	-	4/6/23/26	0/1/1/1
3	BMA	tA	3	3	-	0/2/19/22	0/1/1/1
3	MAN	tA	4	3	-	0/2/19/22	0/1/1/1
3	MAN	tA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	tA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	tA	7	3	-	0/2/19/22	0/1/1/1
3	NAG	u	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	u	2	3	-	2/6/23/26	0/1/1/1
3	BMA	u	3	3	-	2/2/19/22	0/1/1/1
3	MAN	u	4	3	-	0/2/19/22	0/1/1/1
3	MAN	u	5	3	-	2/2/19/22	0/1/1/1
3	MAN	u	6	3	-	0/2/19/22	0/1/1/1
3	MAN	u	7	3	-	0/2/19/22	0/1/1/1
2	NAG	uA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	uA	2	2	-	0/6/23/26	0/1/1/1
2	BMA	uA	3	2	-	2/2/19/22	0/1/1/1
2	MAN	uA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	uA	5	2	-	0/2/19/22	0/1/1/1
2	MAN	uA	6	2	-	0/2/19/22	0/1/1/1
2	MAN	uA	7	2	-	0/2/19/22	0/1/1/1
3	NAG	v	1	3,1	-	6/6/23/26	0/1/1/1
3	NAG	v	2	3	-	2/6/23/26	0/1/1/1
3	BMA	v	3	3	-	0/2/19/22	0/1/1/1
3	MAN	v	4	3	-	2/2/19/22	0/1/1/1
3	MAN	v	5	3	-	0/2/19/22	0/1/1/1
3	MAN	v	6	3	-	0/2/19/22	0/1/1/1
3	MAN	v	7	3	-	0/2/19/22	0/1/1/1
8	NAG	vA	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	vA	2	8	-	4/6/23/26	0/1/1/1
8	BMA	vA	3	8	-	2/2/19/22	0/1/1/1
8	MAN	vA	4	8	-	0/2/19/22	0/1/1/1
8	MAN	vA	5	8	-	2/2/19/22	0/1/1/1
2	NAG	w	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	w	2	2	-	2/6/23/26	0/1/1/1
2	BMA	w	3	2	-	1/2/19/22	0/1/1/1
2	MAN	w	4	2	-	2/2/19/22	0/1/1/1
2	MAN	w	5	2	-	0/2/19/22	0/1/1/1
2	MAN	w	6	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	w	7	2	-	0/2/19/22	0/1/1/1
2	NAG	wA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	wA	2	2	-	2/6/23/26	0/1/1/1
2	BMA	wA	3	2	-	1/2/19/22	0/1/1/1
2	MAN	wA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	wA	5	2	-	0/2/19/22	0/1/1/1
2	MAN	wA	6	2	-	0/2/19/22	0/1/1/1
2	MAN	wA	7	2	-	0/2/19/22	0/1/1/1
6	NAG	x	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	x	2	6	-	2/6/23/26	0/1/1/1
6	BMA	x	3	6	-	2/2/19/22	0/1/1/1
6	MAN	x	4	6	-	0/2/19/22	0/1/1/1
6	MAN	x	5	6	-	0/2/19/22	0/1/1/1
6	MAN	x	6	6	-	0/2/19/22	0/1/1/1
6	MAN	x	7	6	-	0/2/19/22	0/1/1/1
6	MAN	x	8	6	-	2/2/19/22	0/1/1/1
3	NAG	xA	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	xA	2	3	-	4/6/23/26	0/1/1/1
3	BMA	xA	3	3	-	1/2/19/22	0/1/1/1
3	MAN	xA	4	3	-	2/2/19/22	0/1/1/1
3	MAN	xA	5	3	-	0/2/19/22	0/1/1/1
3	MAN	xA	6	3	-	0/2/19/22	0/1/1/1
3	MAN	xA	7	3	-	0/2/19/22	0/1/1/1
3	NAG	y	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	y	2	3	-	1/6/23/26	0/1/1/1
3	BMA	y	3	3	-	0/2/19/22	0/1/1/1
3	MAN	y	4	3	-	2/2/19/22	0/1/1/1
3	MAN	y	5	3	-	0/2/19/22	0/1/1/1
3	MAN	y	6	3	-	0/2/19/22	0/1/1/1
3	MAN	y	7	3	-	0/2/19/22	0/1/1/1
2	NAG	yA	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	yA	2	2	-	2/6/23/26	0/1/1/1
2	BMA	yA	3	2	-	0/2/19/22	0/1/1/1
2	MAN	yA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	yA	5	2	-	0/2/19/22	0/1/1/1
2	MAN	yA	6	2	-	0/2/19/22	0/1/1/1
2	MAN	yA	7	2	-	0/2/19/22	0/1/1/1
3	NAG	z	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	z	2	3	-	2/6/23/26	0/1/1/1
3	BMA	z	3	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	z	4	3	-	0/2/19/22	0/1/1/1
3	MAN	z	5	3	-	0/2/19/22	0/1/1/1
3	MAN	z	6	3	-	0/2/19/22	0/1/1/1
3	MAN	z	7	3	-	0/2/19/22	0/1/1/1
9	NAG	zA	1	9,1	-	6/6/23/26	0/1/1/1
9	NAG	zA	2	9	-	2/6/23/26	0/1/1/1

All (145) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	iA	6	MAN	C1-C2	3.98	1.61	1.52
2	7	6	MAN	C1-C2	3.90	1.61	1.52
2	W	6	MAN	C1-C2	3.89	1.61	1.52
3	v	6	MAN	C1-C2	3.84	1.61	1.52
3	WA	6	MAN	C1-C2	3.83	1.61	1.52
2	i	1	NAG	O5-C1	3.82	1.50	1.43
3	K	6	MAN	C1-C2	3.81	1.61	1.52
2	JA	1	NAG	O5-C1	3.77	1.50	1.43
2	o	7	MAN	C1-C2	3.73	1.61	1.52
2	PA	7	MAN	C1-C2	3.73	1.61	1.52
2	D	7	MAN	C1-C2	3.71	1.61	1.52
7	pA	12	FUC	C1-C2	3.60	1.60	1.52
7	d	12	FUC	C1-C2	3.58	1.60	1.52
7	EA	12	FUC	C1-C2	3.53	1.60	1.52
9	zA	1	NAG	O5-C1	-3.34	1.38	1.43
9	n	1	NAG	O5-C1	-3.24	1.38	1.43
3	0	4	MAN	C2-C3	3.06	1.57	1.52
3	P	4	MAN	C2-C3	3.05	1.57	1.52
3	bA	4	MAN	C2-C3	3.04	1.57	1.52
2	PA	7	MAN	O5-C1	3.00	1.48	1.43
9	OA	1	NAG	O5-C1	-2.99	1.38	1.43
2	D	7	MAN	O5-C1	2.98	1.48	1.43
3	WA	1	NAG	C1-C2	2.88	1.56	1.52
2	o	7	MAN	O5-C1	2.87	1.48	1.43
4	RA	3	BMA	C1-C2	2.85	1.59	1.52
3	K	1	NAG	C1-C2	2.85	1.56	1.52
4	q	3	BMA	C1-C2	2.84	1.59	1.52
3	v	1	NAG	C1-C2	2.80	1.56	1.52
8	KA	3	BMA	C2-C3	2.80	1.56	1.52
7	pA	12	FUC	O5-C1	2.76	1.48	1.43
3	K	6	MAN	O5-C1	2.76	1.48	1.43
3	WA	6	MAN	O5-C1	2.76	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	3	BMA	C1-C2	2.75	1.58	1.52
3	bA	4	MAN	C1-C2	2.74	1.58	1.52
2	uA	1	NAG	O5-C1	2.73	1.48	1.43
7	d	12	FUC	O5-C1	2.73	1.48	1.43
3	P	4	MAN	C1-C2	2.72	1.58	1.52
3	0	4	MAN	C1-C2	2.70	1.58	1.52
8	j	3	BMA	C2-C3	2.70	1.56	1.52
7	EA	12	FUC	O5-C1	2.68	1.48	1.43
8	vA	3	BMA	C4-C3	2.67	1.59	1.52
3	v	6	MAN	O5-C1	2.66	1.48	1.43
2	W	6	MAN	O5-C1	2.63	1.48	1.43
8	KA	3	BMA	C4-C3	2.63	1.59	1.52
8	j	3	BMA	C4-C3	2.62	1.59	1.52
3	6	3	BMA	C2-C3	2.60	1.56	1.52
3	U	4	MAN	C1-C2	2.58	1.58	1.52
3	VA	3	BMA	C1-C2	2.56	1.58	1.52
3	hA	3	BMA	C2-C3	2.56	1.56	1.52
2	eA	3	BMA	C1-C2	2.56	1.58	1.52
2	7	6	MAN	O5-C1	2.54	1.48	1.43
3	V	3	BMA	C2-C3	2.53	1.56	1.52
3	u	3	BMA	C1-C2	2.52	1.58	1.52
3	5	4	MAN	C1-C2	2.52	1.58	1.52
2	S	3	BMA	C1-C2	2.52	1.58	1.52
3	J	3	BMA	C1-C2	2.50	1.58	1.52
3	gA	4	MAN	C1-C2	2.49	1.58	1.52
2	3	3	BMA	C1-C2	2.48	1.58	1.52
2	i	4	MAN	C1-C2	2.42	1.58	1.52
2	iA	6	MAN	O5-C1	2.42	1.47	1.43
7	EA	4	MAN	C4-C3	2.39	1.58	1.52
2	JA	4	MAN	C1-C2	2.37	1.57	1.52
2	uA	4	MAN	C1-C2	2.36	1.57	1.52
7	d	4	MAN	C4-C3	2.35	1.58	1.52
8	KA	3	BMA	O5-C1	-2.35	1.39	1.43
2	NA	3	BMA	C2-C3	2.32	1.56	1.52
8	vA	3	BMA	C2-C3	2.32	1.56	1.52
2	yA	3	BMA	C2-C3	2.31	1.56	1.52
8	j	3	BMA	O5-C1	-2.31	1.39	1.43
3	E	1	NAG	C1-C2	2.29	1.55	1.52
6	x	7	MAN	C1-C2	2.28	1.57	1.52
3	QA	1	NAG	C1-C2	2.27	1.55	1.52
5	r	1	NAG	O5-C1	-2.26	1.39	1.43
3	p	1	NAG	C1-C2	2.26	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	pA	2	NAG	O5-C1	-2.26	1.39	1.43
2	m	3	BMA	C2-C3	2.26	1.55	1.52
2	qA	3	BMA	C4-C3	2.23	1.58	1.52
3	rA	4	MAN	C4-C3	2.22	1.58	1.52
7	EA	4	MAN	O5-C1	-2.21	1.40	1.43
6	M	7	MAN	C1-C2	2.20	1.57	1.52
3	f	4	MAN	C4-C3	2.20	1.58	1.52
3	K	3	BMA	C2-C3	2.20	1.55	1.52
2	e	3	BMA	C4-C3	2.20	1.58	1.52
3	HA	4	MAN	C4-C3	2.19	1.58	1.52
3	GA	4	MAN	C4-C3	2.19	1.58	1.52
3	sA	4	MAN	C4-C3	2.19	1.58	1.52
10	7A	1	NAG	C1-C2	2.18	1.55	1.52
7	d	4	MAN	O5-C1	-2.17	1.40	1.43
2	wA	3	BMA	C4-C3	2.17	1.58	1.52
3	H	4	MAN	C4-C3	2.17	1.58	1.52
3	J	5	MAN	C1-C2	2.17	1.57	1.52
6	YA	7	MAN	C1-C2	2.17	1.57	1.52
3	P	5	MAN	C1-C2	2.16	1.57	1.52
7	pA	4	MAN	C4-C3	2.16	1.57	1.52
3	bA	5	MAN	C1-C2	2.16	1.57	1.52
3	u	5	MAN	C1-C2	2.16	1.57	1.52
4	F	5	MAN	C1-C2	2.15	1.57	1.52
3	xA	4	MAN	C1-C2	2.15	1.57	1.52
2	k	3	BMA	C4-C3	2.15	1.57	1.52
3	g	4	MAN	C4-C3	2.15	1.57	1.52
3	TA	4	MAN	C4-C3	2.14	1.57	1.52
2	FA	3	BMA	C4-C3	2.13	1.57	1.52
3	hA	4	MAN	C1-C2	2.13	1.57	1.52
4	q	5	MAN	C1-C2	2.13	1.57	1.52
3	0	5	MAN	C1-C2	2.13	1.57	1.52
3	v	3	BMA	C2-C3	2.13	1.55	1.52
2	LA	3	BMA	C4-C3	2.13	1.57	1.52
3	VA	5	MAN	C1-C2	2.13	1.57	1.52
3	l	4	MAN	C1-C2	2.13	1.57	1.52
4	RA	5	MAN	C1-C2	2.13	1.57	1.52
7	pA	9	MAN	C1-C2	2.12	1.57	1.52
3	WA	3	BMA	C2-C3	2.12	1.55	1.52
3	s	4	MAN	C4-C3	2.12	1.57	1.52
5	G	4	MAN	C1-C2	2.12	1.57	1.52
3	8	4	MAN	C1-C2	2.11	1.57	1.52
3	X	6	MAN	C1-C2	2.10	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	5	MAN	C1-C2	2.09	1.57	1.52
3	MA	4	MAN	C1-C2	2.09	1.57	1.52
3	TA	5	MAN	C1-C2	2.09	1.57	1.52
3	X	4	MAN	C1-C2	2.09	1.57	1.52
3	rA	4	MAN	O5-C1	-2.09	1.40	1.43
3	s	5	MAN	C1-C2	2.09	1.57	1.52
3	8	6	MAN	C1-C2	2.09	1.57	1.52
3	jA	6	MAN	C1-C2	2.09	1.57	1.52
5	SA	4	MAN	C1-C2	2.08	1.57	1.52
3	I	4	MAN	C1-C2	2.08	1.57	1.52
7	pA	1	NAG	O5-C1	2.08	1.47	1.43
3	a	7	MAN	C1-C2	2.08	1.57	1.52
3	jA	4	MAN	C1-C2	2.07	1.57	1.52
3	UA	4	MAN	C1-C2	2.07	1.57	1.52
3	a	3	BMA	C1-C2	2.06	1.57	1.52
3	t	4	MAN	C1-C2	2.06	1.57	1.52
3	GA	4	MAN	O5-C1	-2.05	1.40	1.43
3	GA	7	MAN	C1-C2	2.04	1.57	1.52
3	mA	3	BMA	C1-C2	2.04	1.57	1.52
2	e	3	BMA	O5-C1	-2.03	1.40	1.43
3	6	4	MAN	C1-C2	2.02	1.57	1.52
3	V	4	MAN	C1-C2	2.02	1.57	1.52
2	FA	3	BMA	C2-C3	2.02	1.55	1.52
8	vA	3	BMA	O5-C1	-2.02	1.40	1.43
3	GA	4	MAN	C2-C3	2.02	1.55	1.52
5	r	4	MAN	C1-C2	2.01	1.57	1.52
3	BA	3	BMA	C1-C2	2.01	1.57	1.52
2	FA	3	BMA	O5-C1	-2.01	1.40	1.43
3	f	4	MAN	C2-C3	2.00	1.55	1.52

All (968) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	7	MAN	C1-O5-C5	6.68	121.14	112.19
2	PA	7	MAN	C1-O5-C5	6.66	121.11	112.19
2	o	7	MAN	C1-O5-C5	6.56	120.97	112.19
3	K	6	MAN	C1-O5-C5	6.29	120.61	112.19
3	WA	6	MAN	C1-O5-C5	6.20	120.50	112.19
2	W	6	MAN	C1-O5-C5	6.09	120.35	112.19
2	7	6	MAN	C1-O5-C5	6.04	120.29	112.19
3	v	6	MAN	C1-O5-C5	6.03	120.27	112.19
8	vA	1	NAG	C1-O5-C5	5.87	120.05	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	iA	6	MAN	C1-O5-C5	5.81	119.98	112.19
8	KA	1	NAG	C1-O5-C5	5.55	119.62	112.19
8	j	1	NAG	C1-O5-C5	5.50	119.55	112.19
6	x	7	MAN	C1-O5-C5	5.35	119.36	112.19
6	M	7	MAN	C1-O5-C5	5.30	119.29	112.19
6	YA	7	MAN	C1-O5-C5	5.29	119.27	112.19
3	t	4	MAN	C1-O5-C5	4.79	118.60	112.19
9	zA	1	NAG	C2-N2-C7	4.76	129.28	122.90
3	UA	4	MAN	C1-O5-C5	4.72	118.52	112.19
3	I	4	MAN	C1-O5-C5	4.72	118.51	112.19
2	JA	1	NAG	C1-O5-C5	4.71	118.50	112.19
9	n	1	NAG	C2-N2-C7	4.66	129.15	122.90
9	OA	1	NAG	C2-N2-C7	4.65	129.13	122.90
2	i	1	NAG	C1-O5-C5	4.63	118.39	112.19
5	r	2	NAG	C2-N2-C7	4.59	129.06	122.90
3	mA	2	NAG	C2-N2-C7	4.58	129.04	122.90
3	BA	2	NAG	C2-N2-C7	4.56	129.01	122.90
3	a	2	NAG	C2-N2-C7	4.51	128.95	122.90
3	K	1	NAG	C2-N2-C7	4.43	128.84	122.90
3	WA	1	NAG	C2-N2-C7	4.43	128.84	122.90
3	v	1	NAG	C2-N2-C7	4.43	128.83	122.90
3	h	4	MAN	C1-O5-C5	3.97	117.51	112.19
3	tA	4	MAN	C1-O5-C5	3.93	117.45	112.19
3	IA	4	MAN	C1-O5-C5	3.92	117.44	112.19
7	pA	12	FUC	C1-O5-C5	3.79	121.91	112.97
7	EA	12	FUC	C1-O5-C5	3.76	121.84	112.97
7	d	12	FUC	C1-O5-C5	3.74	121.78	112.97
3	6	4	MAN	C1-O5-C5	3.73	117.19	112.19
3	hA	4	MAN	C1-O5-C5	3.66	117.09	112.19
3	V	4	MAN	C1-O5-C5	3.65	117.07	112.19
3	a	5	MAN	C1-O5-C5	3.62	117.03	112.19
3	BA	5	MAN	C1-O5-C5	3.61	117.03	112.19
3	mA	5	MAN	C1-O5-C5	3.60	117.02	112.19
2	iA	6	MAN	C1-C2-C3	3.52	114.78	109.64
3	oA	4	MAN	C1-O5-C5	3.51	116.89	112.19
3	DA	4	MAN	C1-O5-C5	3.51	116.89	112.19
3	c	4	MAN	C1-O5-C5	3.50	116.87	112.19
3	v	1	NAG	C1-O5-C5	3.48	116.85	112.19
5	G	4	MAN	C1-O5-C5	3.44	116.79	112.19
2	7	6	MAN	C1-C2-C3	3.44	114.65	109.64
3	K	1	NAG	C1-O5-C5	3.43	116.79	112.19
5	SA	4	MAN	C1-O5-C5	3.42	116.78	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	d	9	MAN	C1-O5-C5	3.42	116.76	112.19
3	WA	1	NAG	C1-O5-C5	3.38	116.72	112.19
3	v	6	MAN	C1-C2-C3	3.37	114.55	109.64
3	rA	7	MAN	C1-O5-C5	3.36	116.69	112.19
7	EA	9	MAN	C1-O5-C5	3.36	116.69	112.19
3	8	6	MAN	C1-O5-C5	3.35	116.68	112.19
3	jA	6	MAN	C1-O5-C5	3.35	116.67	112.19
3	X	6	MAN	C1-O5-C5	3.34	116.66	112.19
5	r	4	MAN	C1-O5-C5	3.34	116.66	112.19
3	GA	7	MAN	C1-O5-C5	3.33	116.65	112.19
2	W	6	MAN	C1-C2-C3	3.33	114.49	109.64
3	f	7	MAN	C1-O5-C5	3.32	116.64	112.19
4	q	8	MAN	C1-O5-C5	3.29	116.59	112.19
3	WA	6	MAN	C1-C2-C3	3.29	114.43	109.64
3	c	3	BMA	C1-O5-C5	3.28	116.58	112.19
3	oA	3	BMA	C1-O5-C5	3.25	116.55	112.19
3	TA	3	BMA	C1-O5-C5	3.25	116.55	112.19
3	DA	3	BMA	C1-O5-C5	3.25	116.54	112.19
7	pA	9	MAN	C1-O5-C5	3.25	116.54	112.19
3	8	4	MAN	C1-O5-C5	3.24	116.53	112.19
3	jA	4	MAN	C1-O5-C5	3.23	116.52	112.19
10	3A	5	MAN	C1-O5-C5	3.23	116.51	112.19
3	u	5	MAN	C1-O5-C5	3.23	116.51	112.19
6	M	4	MAN	O2-C2-C3	-3.22	103.48	110.15
6	YA	4	MAN	O2-C2-C3	-3.21	103.50	110.15
3	H	3	BMA	C1-O5-C5	3.21	116.49	112.19
3	s	3	BMA	C1-O5-C5	3.20	116.48	112.19
3	VA	5	MAN	C1-O5-C5	3.20	116.47	112.19
3	K	6	MAN	C1-C2-C3	3.20	114.30	109.64
7	pA	12	FUC	C1-C2-C3	3.20	114.30	109.64
4	RA	4	MAN	O2-C2-C3	-3.19	103.54	110.15
3	J	5	MAN	C1-O5-C5	3.19	116.46	112.19
4	q	4	MAN	O2-C2-C3	-3.19	103.55	110.15
3	X	4	MAN	C1-O5-C5	3.18	116.44	112.19
3	a	7	MAN	C1-O5-C5	3.17	116.44	112.19
7	d	12	FUC	C1-C2-C3	3.17	114.26	109.64
7	EA	12	FUC	C1-C2-C3	3.17	114.26	109.64
6	x	4	MAN	O2-C2-C3	-3.16	103.60	110.15
4	F	4	MAN	O2-C2-C3	-3.10	103.73	110.15
3	BA	7	MAN	C1-O5-C5	3.09	116.33	112.19
3	9	4	MAN	C1-O5-C5	3.07	116.30	112.19
3	mA	7	MAN	C1-O5-C5	3.06	116.28	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	XA	6	MAN	C1-O5-C5	3.05	116.27	112.19
2	o	7	MAN	C1-C2-C3	3.04	114.07	109.64
2	FA	4	MAN	C1-O5-C5	3.03	116.25	112.19
3	bA	4	MAN	C1-C2-C3	3.03	114.06	109.64
4	q	7	MAN	C1-O5-C5	3.03	116.24	112.19
4	RA	8	MAN	C1-O5-C5	3.03	116.24	112.19
2	D	7	MAN	C1-C2-C3	3.03	114.05	109.64
2	w	6	MAN	C1-O5-C5	3.02	116.24	112.19
4	F	8	MAN	C1-O5-C5	3.02	116.23	112.19
2	PA	7	MAN	C1-C2-C3	3.01	114.03	109.64
3	P	4	MAN	C1-C2-C3	3.01	114.02	109.64
2	L	6	MAN	C1-O5-C5	3.00	116.20	112.19
3	0	6	MAN	C1-O5-C5	3.00	116.20	112.19
3	0	4	MAN	C1-C2-C3	2.99	114.00	109.64
3	P	6	MAN	C1-O5-C5	2.98	116.18	112.19
3	aA	6	MAN	C1-O5-C5	2.97	116.17	112.19
3	u	3	BMA	O2-C2-C3	-2.97	103.99	110.15
4	RA	7	MAN	C1-O5-C5	2.97	116.17	112.19
2	i	6	MAN	C1-O5-C5	2.97	116.16	112.19
2	T	4	MAN	C1-O5-C5	2.96	116.16	112.19
2	4	4	MAN	C1-O5-C5	2.95	116.14	112.19
3	bA	6	MAN	C1-O5-C5	2.95	116.14	112.19
4	RA	5	MAN	O2-C2-C1	2.95	115.98	109.22
2	uA	6	MAN	C1-O5-C5	2.94	116.12	112.19
2	fA	5	MAN	C1-O5-C5	2.94	116.12	112.19
2	qA	4	MAN	C1-O5-C5	2.94	116.12	112.19
3	U	4	MAN	C1-O5-C5	2.94	116.12	112.19
3	J	3	BMA	O2-C2-C3	-2.94	104.07	110.15
3	kA	4	MAN	C1-O5-C5	2.93	116.12	112.19
3	bA	5	MAN	C1-O5-C5	2.93	116.11	112.19
2	T	5	MAN	C1-O5-C5	2.92	116.11	112.19
3	Y	4	MAN	C1-O5-C5	2.92	116.10	112.19
4	F	5	MAN	O2-C2-C1	2.92	115.91	109.22
3	gA	4	MAN	C1-O5-C5	2.92	116.10	112.19
3	z	6	MAN	C1-O5-C5	2.92	116.09	112.19
4	q	5	MAN	O2-C2-C1	2.92	115.90	109.22
3	xA	7	MAN	C1-O5-C5	2.91	116.09	112.19
3	O	6	MAN	C1-O5-C5	2.91	116.09	112.19
4	F	7	MAN	C1-O5-C5	2.91	116.09	112.19
3	VA	3	BMA	O2-C2-C3	-2.91	104.12	110.15
3	P	5	MAN	C1-O5-C5	2.91	116.08	112.19
2	4	5	MAN	C1-O5-C5	2.90	116.08	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	4	MAN	C1-O5-C5	2.90	116.07	112.19
2	JA	6	MAN	C1-O5-C5	2.89	116.06	112.19
3	HA	7	MAN	C1-O5-C5	2.89	116.05	112.19
2	eA	7	MAN	C1-O5-C5	2.88	116.05	112.19
3	0	5	MAN	C1-O5-C5	2.88	116.05	112.19
3	cA	4	MAN	C1-O5-C5	2.88	116.04	112.19
3	g	7	MAN	C1-O5-C5	2.86	116.02	112.19
3	P	7	MAN	C1-O5-C5	2.85	116.01	112.19
2	3	7	MAN	C1-O5-C5	2.85	116.01	112.19
2	S	7	MAN	C1-O5-C5	2.85	116.00	112.19
3	MA	7	MAN	C1-O5-C5	2.85	116.00	112.19
3	Q	6	MAN	C1-O5-C5	2.84	115.99	112.19
3	1	6	MAN	C1-O5-C5	2.83	115.98	112.19
2	lA	6	MAN	C1-O5-C5	2.83	115.98	112.19
3	5	4	MAN	C1-O5-C5	2.83	115.98	112.19
2	fA	4	MAN	C1-O5-C5	2.83	115.97	112.19
3	bA	7	MAN	C1-O5-C5	2.82	115.96	112.19
3	xA	6	MAN	C1-O5-C5	2.81	115.96	112.19
3	1	4	MAN	C1-O5-C5	2.81	115.95	112.19
3	cA	6	MAN	C1-O5-C5	2.81	115.95	112.19
3	0	7	MAN	C1-O5-C5	2.80	115.94	112.19
6	YA	8	MAN	C1-O5-C5	2.80	115.94	112.19
3	l	7	MAN	C1-O5-C5	2.80	115.94	112.19
4	RA	4	MAN	C1-O5-C5	2.80	115.94	112.19
3	sA	7	MAN	C1-O5-C5	2.80	115.93	112.19
3	l	6	MAN	C1-O5-C5	2.80	115.93	112.19
3	MA	6	MAN	C1-O5-C5	2.79	115.93	112.19
6	YA	5	MAN	O2-C2-C3	-2.79	104.38	110.15
6	x	5	MAN	O2-C2-C3	-2.79	104.38	110.15
6	M	8	MAN	C1-O5-C5	2.78	115.92	112.19
6	M	5	MAN	O2-C2-C3	-2.78	104.39	110.15
2	Z	6	MAN	C1-O5-C5	2.78	115.91	112.19
3	Q	4	MAN	C1-O5-C5	2.78	115.91	112.19
4	q	4	MAN	C1-O5-C5	2.77	115.90	112.19
3	6	6	MAN	C1-O5-C5	2.77	115.89	112.19
3	hA	6	MAN	C1-O5-C5	2.76	115.89	112.19
3	V	6	MAN	C1-O5-C5	2.76	115.88	112.19
4	F	4	MAN	C1-O5-C5	2.76	115.88	112.19
2	uA	4	MAN	C1-O5-C5	2.75	115.87	112.19
3	QA	4	MAN	C1-O5-C5	2.75	115.86	112.19
2	FA	3	BMA	C1-C2-C3	2.75	113.64	109.64
3	E	4	MAN	C1-O5-C5	2.74	115.86	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AA	6	MAN	C1-O5-C5	2.72	115.84	112.19
3	u	7	MAN	C1-O5-C5	2.71	115.82	112.19
6	x	8	MAN	C1-O5-C5	2.71	115.81	112.19
3	H	6	MAN	C1-O5-C5	2.70	115.81	112.19
10	3A	7	MAN	C1-O5-C5	2.70	115.81	112.19
3	H	5	MAN	C1-O5-C5	2.70	115.80	112.19
3	p	4	MAN	C1-O5-C5	2.69	115.79	112.19
3	E	6	MAN	C1-O5-C5	2.69	115.79	112.19
2	b	6	MAN	C1-O5-C5	2.68	115.78	112.19
3	ZA	7	MAN	C1-O5-C5	2.68	115.77	112.19
2	qA	3	BMA	C1-C2-C3	2.68	113.54	109.64
2	FA	5	MAN	C1-O5-C5	2.68	115.77	112.19
2	qA	5	MAN	C1-O5-C5	2.67	115.77	112.19
2	CA	6	MAN	C1-O5-C5	2.67	115.77	112.19
3	J	7	MAN	C1-O5-C5	2.67	115.76	112.19
3	hA	7	MAN	C1-O5-C5	2.67	115.76	112.19
3	VA	7	MAN	C1-O5-C5	2.66	115.75	112.19
3	TA	5	MAN	C1-O5-C5	2.66	115.75	112.19
2	nA	6	MAN	C1-O5-C5	2.66	115.75	112.19
2	e	3	BMA	C1-C2-C3	2.66	113.51	109.64
7	pA	6	GAL	C3-C4-C5	-2.65	105.43	110.23
3	TA	6	MAN	C1-O5-C5	2.64	115.73	112.19
10	5A	7	MAN	C1-O5-C5	2.64	115.73	112.19
2	w	4	MAN	C1-O5-C5	2.64	115.73	112.19
7	EA	6	GAL	C3-C4-C5	-2.64	105.44	110.23
2	R	6	MAN	C1-O5-C5	2.64	115.72	112.19
3	IA	6	MAN	C1-O5-C5	2.64	115.72	112.19
2	i	5	MAN	C1-O5-C5	2.64	115.72	112.19
3	tA	6	MAN	C1-O5-C5	2.64	115.72	112.19
3	N	7	MAN	C1-O5-C5	2.63	115.71	112.19
3	QA	6	MAN	C1-O5-C5	2.63	115.71	112.19
3	s	5	MAN	C1-O5-C5	2.63	115.71	112.19
5	G	6	GAL	C1-O5-C5	2.63	115.70	112.19
5	r	6	GAL	C1-O5-C5	2.63	115.70	112.19
2	T	7	MAN	C1-O5-C5	2.62	115.70	112.19
3	p	6	MAN	C1-O5-C5	2.62	115.70	112.19
7	d	6	GAL	C3-C4-C5	-2.62	105.47	110.23
2	JA	5	MAN	C1-O5-C5	2.62	115.70	112.19
3	f	6	MAN	C1-O5-C5	2.62	115.70	112.19
3	sA	6	MAN	C1-O5-C5	2.62	115.69	112.19
2	dA	6	MAN	C1-O5-C5	2.61	115.69	112.19
3	g	6	MAN	C1-O5-C5	2.61	115.68	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	5	MAN	C1-O5-C5	2.61	115.68	112.19
3	V	7	MAN	C1-O5-C5	2.61	115.68	112.19
10	2A	7	MAN	C1-O5-C5	2.61	115.68	112.19
3	s	6	MAN	C1-O5-C5	2.60	115.67	112.19
3	HA	6	MAN	C1-O5-C5	2.60	115.67	112.19
3	rA	6	MAN	C1-O5-C5	2.60	115.67	112.19
3	h	6	MAN	C1-O5-C5	2.60	115.67	112.19
2	2	6	MAN	C1-O5-C5	2.60	115.67	112.19
2	uA	5	MAN	C1-O5-C5	2.60	115.66	112.19
3	y	7	MAN	C1-O5-C5	2.59	115.66	112.19
3	GA	6	MAN	C1-O5-C5	2.59	115.66	112.19
3	6	7	MAN	C1-O5-C5	2.58	115.65	112.19
5	SA	6	GAL	C1-O5-C5	2.58	115.65	112.19
2	fA	7	MAN	C1-O5-C5	2.57	115.63	112.19
8	KA	4	MAN	C1-O5-C5	2.56	115.62	112.19
3	9	7	MAN	C1-O5-C5	2.56	115.61	112.19
2	m	7	MAN	C1-O5-C5	2.55	115.61	112.19
2	W	7	MAN	C1-O5-C5	2.55	115.60	112.19
2	4	7	MAN	C1-O5-C5	2.55	115.60	112.19
3	1	5	MAN	C1-O5-C5	2.54	115.59	112.19
2	i	4	MAN	C1-O5-C5	2.54	115.59	112.19
10	2A	5	MAN	C1-O5-C5	2.54	115.59	112.19
10	6A	7	MAN	C1-O5-C5	2.53	115.58	112.19
2	yA	7	MAN	C1-O5-C5	2.53	115.58	112.19
3	cA	5	MAN	C1-O5-C5	2.53	115.58	112.19
3	v	7	MAN	C1-O5-C5	2.52	115.56	112.19
3	gA	7	MAN	C1-O5-C5	2.52	115.56	112.19
5	r	7	MAN	C1-O5-C5	2.52	115.56	112.19
2	Z	7	MAN	C1-O5-C5	2.52	115.56	112.19
2	XA	4	MAN	C1-O5-C5	2.52	115.56	112.19
2	wA	6	MAN	C1-O5-C5	2.52	115.56	112.19
2	7	7	MAN	C1-O5-C5	2.51	115.56	112.19
2	L	4	MAN	C1-O5-C5	2.51	115.55	112.19
2	wA	5	MAN	C1-O5-C5	2.51	115.55	112.19
2	L	5	MAN	C1-O5-C5	2.51	115.55	112.19
3	5	7	MAN	C1-O5-C5	2.51	115.55	112.19
2	NA	7	MAN	C1-O5-C5	2.51	115.55	112.19
6	M	3	BMA	O3-C3-C2	2.51	115.17	110.05
2	T	4	MAN	O3-C3-C2	2.50	115.16	110.05
3	WA	7	MAN	C1-O5-C5	2.50	115.54	112.19
3	Q	5	MAN	C1-O5-C5	2.50	115.54	112.19
2	iA	7	MAN	C1-O5-C5	2.50	115.54	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	4	MAN	O3-C3-C2	2.50	115.15	110.05
3	K	7	MAN	C1-O5-C5	2.50	115.53	112.19
2	AA	7	MAN	C1-O5-C5	2.50	115.53	112.19
2	JA	4	MAN	C1-O5-C5	2.50	115.53	112.19
3	U	7	MAN	C1-O5-C5	2.50	115.53	112.19
2	LA	6	MAN	C1-O5-C5	2.49	115.53	112.19
2	k	5	MAN	C1-O5-C5	2.49	115.52	112.19
2	XA	5	MAN	C1-O5-C5	2.49	115.52	112.19
2	uA	7	MAN	C1-O5-C5	2.49	115.52	112.19
3	oA	6	MAN	C1-O5-C5	2.49	115.52	112.19
10	1A	4	MAN	C1-O5-C5	2.49	115.52	112.19
3	z	5	MAN	C1-O5-C5	2.48	115.51	112.19
2	PA	6	MAN	C1-O5-C5	2.48	115.50	112.19
3	mA	2	NAG	C1-C2-N2	2.48	114.33	110.43
3	oA	7	MAN	C1-O5-C5	2.47	115.50	112.19
2	T	6	MAN	C1-O5-C5	2.47	115.50	112.19
3	O	5	MAN	C1-O5-C5	2.47	115.50	112.19
3	c	6	MAN	C1-O5-C5	2.47	115.50	112.19
3	p	1	NAG	C1-O5-C5	2.47	115.50	112.19
2	k	6	MAN	C1-O5-C5	2.47	115.50	112.19
2	LA	5	MAN	C1-O5-C5	2.47	115.50	112.19
3	DA	6	MAN	C1-O5-C5	2.47	115.50	112.19
10	7A	6	MAN	C1-O5-C5	2.47	115.49	112.19
2	fA	4	MAN	O3-C3-C2	2.47	115.09	110.05
2	w	5	MAN	C1-O5-C5	2.46	115.49	112.19
2	lA	7	MAN	C1-O5-C5	2.46	115.49	112.19
2	4	6	MAN	C1-O5-C5	2.46	115.48	112.19
10	4A	6	MAN	C1-O5-C5	2.46	115.48	112.19
9	zA	1	NAG	C1-O5-C5	2.46	115.48	112.19
3	DA	7	MAN	C1-O5-C5	2.45	115.47	112.19
4	q	8	MAN	O2-C2-C3	-2.45	105.07	110.15
2	D	6	MAN	C1-O5-C5	2.45	115.47	112.19
10	2A	6	MAN	C1-O5-C5	2.45	115.47	112.19
4	RA	8	MAN	O2-C2-C3	-2.45	105.08	110.15
7	pA	3	BMA	C1-C2-C3	2.45	113.21	109.64
2	o	6	MAN	C1-O5-C5	2.45	115.47	112.19
3	gA	1	NAG	C1-O5-C5	2.45	115.47	112.19
10	7A	5	MAN	C1-O5-C5	2.45	115.47	112.19
3	c	7	MAN	C1-O5-C5	2.45	115.46	112.19
3	aA	4	MAN	C1-O5-C5	2.44	115.46	112.19
10	6A	5	MAN	C1-O5-C5	2.44	115.46	112.19
3	U	1	NAG	C1-O5-C5	2.44	115.46	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	x	3	BMA	O3-C3-C2	2.44	115.03	110.05
3	xA	4	MAN	C1-O5-C5	2.44	115.45	112.19
10	5A	4	MAN	C1-O5-C5	2.44	115.45	112.19
3	aA	5	MAN	C1-O5-C5	2.44	115.45	112.19
3	y	6	MAN	C1-O5-C5	2.43	115.45	112.19
3	1	7	MAN	C1-O5-C5	2.43	115.44	112.19
3	Q	7	MAN	C1-O5-C5	2.43	115.44	112.19
3	ZA	6	MAN	C1-O5-C5	2.42	115.43	112.19
3	N	6	MAN	C1-O5-C5	2.42	115.43	112.19
3	cA	7	MAN	C1-O5-C5	2.42	115.43	112.19
2	fA	6	MAN	C1-O5-C5	2.42	115.43	112.19
10	0A	6	MAN	C1-O5-C5	2.42	115.43	112.19
3	kA	7	MAN	C1-O5-C5	2.42	115.42	112.19
10	0A	7	MAN	C1-O5-C5	2.41	115.42	112.19
10	5A	5	MAN	C1-O5-C5	2.41	115.42	112.19
3	l	4	MAN	C1-O5-C5	2.41	115.42	112.19
3	y	5	MAN	C1-O5-C5	2.41	115.41	112.19
4	q	3	BMA	O2-C2-C3	-2.41	105.16	110.15
4	F	8	MAN	O2-C2-C3	-2.41	105.17	110.15
3	5	1	NAG	C1-O5-C5	2.41	115.41	112.19
3	8	7	MAN	C1-O5-C5	2.41	115.41	112.19
2	k	7	MAN	C1-O5-C5	2.41	115.41	112.19
8	j	4	MAN	C1-O5-C5	2.41	115.41	112.19
4	F	3	BMA	O2-C2-C3	-2.41	105.17	110.15
2	W	6	MAN	O5-C1-C2	2.41	116.53	110.79
3	Y	6	MAN	C1-O5-C5	2.40	115.41	112.19
2	uA	2	NAG	C1-O5-C5	2.40	115.40	112.19
3	E	1	NAG	C1-O5-C5	2.40	115.40	112.19
3	O	4	MAN	C1-O5-C5	2.40	115.40	112.19
10	1A	6	MAN	C1-O5-C5	2.40	115.40	112.19
10	7A	7	MAN	C1-O5-C5	2.40	115.40	112.19
3	MA	4	MAN	C1-O5-C5	2.40	115.40	112.19
3	rA	5	MAN	C1-O5-C5	2.40	115.40	112.19
7	d	6	GAL	C1-O5-C5	2.40	115.40	112.19
5	r	7	MAN	O2-C2-C3	-2.40	105.19	110.15
10	0A	5	MAN	C1-O5-C5	2.40	115.40	112.19
4	RA	3	BMA	C1-C2-C3	-2.39	106.16	109.64
3	f	5	MAN	C1-O5-C5	2.39	115.39	112.19
2	iA	6	MAN	O5-C1-C2	2.39	116.49	110.79
2	i	7	MAN	C1-O5-C5	2.39	115.39	112.19
2	LA	7	MAN	C1-O5-C5	2.39	115.39	112.19
2	wA	7	MAN	C1-O5-C5	2.39	115.39	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	6A	6	MAN	C1-O5-C5	2.39	115.39	112.19
2	e	6	MAN	C1-O5-C5	2.39	115.38	112.19
3	jA	7	MAN	C1-O5-C5	2.39	115.38	112.19
3	9	6	MAN	C1-O5-C5	2.38	115.38	112.19
10	1A	1	NAG	C1-O5-C5	2.38	115.38	112.19
2	7	6	MAN	O5-C1-C2	2.38	116.47	110.79
6	YA	3	BMA	O3-C3-C2	2.38	114.91	110.05
2	D	5	MAN	C1-O5-C5	2.38	115.38	112.19
3	xA	5	MAN	C1-O5-C5	2.38	115.37	112.19
7	EA	6	GAL	C1-O5-C5	2.38	115.37	112.19
3	GA	5	MAN	C1-O5-C5	2.37	115.37	112.19
6	x	4	MAN	C1-O5-C5	2.37	115.37	112.19
6	YA	4	MAN	C1-O5-C5	2.37	115.36	112.19
3	U	6	MAN	C1-O5-C5	2.37	115.36	112.19
8	j	3	BMA	C2-C3-C4	2.37	115.03	110.86
2	qA	7	MAN	C1-O5-C5	2.37	115.36	112.19
3	kA	6	MAN	C1-O5-C5	2.37	115.36	112.19
8	KA	3	BMA	C2-C3-C4	2.37	115.03	110.86
4	RA	3	BMA	O2-C2-C3	-2.37	105.25	110.15
2	JA	7	MAN	C1-O5-C5	2.36	115.36	112.19
8	KA	1	NAG	O4-C4-C5	2.36	115.15	109.32
3	K	5	MAN	C1-O5-C5	2.36	115.35	112.19
8	j	1	NAG	O4-C4-C5	2.36	115.14	109.32
3	z	4	MAN	C1-O5-C5	2.36	115.35	112.19
2	qA	6	MAN	C1-O5-C5	2.36	115.35	112.19
3	sA	5	MAN	C1-O5-C5	2.36	115.34	112.19
2	FA	6	MAN	C1-O5-C5	2.35	115.34	112.19
3	MA	5	MAN	C1-O5-C5	2.35	115.34	112.19
3	mA	6	MAN	C1-O5-C5	2.35	115.33	112.19
3	X	5	MAN	C1-O5-C5	2.35	115.33	112.19
10	4A	1	NAG	C1-O5-C5	2.34	115.33	112.19
3	s	7	MAN	C1-O5-C5	2.34	115.32	112.19
3	jA	5	MAN	C1-O5-C5	2.34	115.32	112.19
6	YA	7	MAN	O2-C2-C3	-2.34	105.31	110.15
2	o	5	MAN	C1-O5-C5	2.34	115.32	112.19
3	WA	5	MAN	C1-O5-C5	2.34	115.32	112.19
3	gA	6	MAN	C1-O5-C5	2.34	115.32	112.19
3	ZA	1	NAG	C1-O5-C5	2.34	115.32	112.19
6	x	7	MAN	O2-C2-C3	-2.34	105.31	110.15
10	4A	7	MAN	C1-O5-C5	2.33	115.31	112.19
2	m	6	MAN	C1-O5-C5	2.33	115.31	112.19
3	a	2	NAG	C1-C2-N2	2.33	114.11	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1	NAG	C1-O5-C5	2.33	115.31	112.19
3	QA	1	NAG	C1-O5-C5	2.33	115.31	112.19
2	FA	7	MAN	C1-O5-C5	2.33	115.31	112.19
7	pA	6	GAL	C1-O5-C5	2.33	115.31	112.19
2	o	7	MAN	O5-C1-C2	2.33	116.35	110.79
3	X	7	MAN	C1-O5-C5	2.33	115.31	112.19
3	l	5	MAN	C1-O5-C5	2.33	115.31	112.19
4	q	3	BMA	C1-C2-C3	-2.33	106.25	109.64
4	F	3	BMA	C1-C2-C3	-2.33	106.25	109.64
3	Y	7	MAN	C1-O5-C5	2.33	115.31	112.19
2	PA	5	MAN	C1-O5-C5	2.32	115.30	112.19
3	IA	5	MAN	C1-O5-C5	2.32	115.30	112.19
3	H	7	MAN	C1-O5-C5	2.32	115.29	112.19
10	7A	1	NAG	C1-O5-C5	2.32	115.29	112.19
6	M	7	MAN	O2-C2-C3	-2.32	105.35	110.15
3	TA	7	MAN	C1-O5-C5	2.32	115.29	112.19
4	F	5	MAN	C1-O5-C5	2.31	115.29	112.19
10	3A	6	MAN	C1-O5-C5	2.31	115.29	112.19
3	BA	2	NAG	C1-C2-N2	2.31	114.08	110.43
2	e	7	MAN	C1-O5-C5	2.31	115.29	112.19
3	5	6	MAN	C1-O5-C5	2.31	115.28	112.19
3	BA	6	MAN	C1-O5-C5	2.31	115.28	112.19
3	N	5	MAN	C1-O5-C5	2.31	115.28	112.19
2	R	7	MAN	C1-O5-C5	2.31	115.28	112.19
3	HA	5	MAN	C1-O5-C5	2.31	115.28	112.19
3	tA	5	MAN	C1-O5-C5	2.31	115.28	112.19
5	SA	7	MAN	C1-O5-C5	2.31	115.28	112.19
3	v	6	MAN	O5-C1-C2	2.31	116.29	110.79
2	yA	6	MAN	C1-O5-C5	2.30	115.28	112.19
2	dA	7	MAN	C1-O5-C5	2.30	115.27	112.19
3	N	4	MAN	C1-O5-C5	2.30	115.27	112.19
3	ZA	5	MAN	C1-O5-C5	2.30	115.27	112.19
3	DA	5	MAN	C1-O5-C5	2.30	115.27	112.19
3	bA	4	MAN	C1-O5-C5	2.30	115.27	112.19
6	M	4	MAN	C1-O5-C5	2.30	115.26	112.19
2	W	5	MAN	C1-O5-C5	2.30	115.26	112.19
2	CA	5	MAN	C1-O5-C5	2.30	115.26	112.19
5	G	7	MAN	C1-O5-C5	2.29	115.26	112.19
2	S	5	MAN	C1-O5-C5	2.29	115.26	112.19
3	v	5	MAN	C1-O5-C5	2.29	115.26	112.19
3	g	5	MAN	C1-O5-C5	2.29	115.26	112.19
3	oA	5	MAN	C1-O5-C5	2.29	115.26	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	zA	1	NAG	O4-C4-C3	-2.29	104.98	110.38
10	5A	6	MAN	C1-O5-C5	2.29	115.25	112.19
2	CA	7	MAN	C1-O5-C5	2.29	115.25	112.19
2	NA	6	MAN	C1-O5-C5	2.29	115.25	112.19
4	F	6	MAN	O2-C2-C3	-2.29	105.42	110.15
3	K	6	MAN	O5-C1-C2	2.29	116.24	110.79
5	G	7	MAN	O2-C2-C3	-2.29	105.42	110.15
2	7	5	MAN	C1-O5-C5	2.29	115.25	112.19
2	2	7	MAN	C1-O5-C5	2.28	115.25	112.19
3	h	5	MAN	C1-O5-C5	2.28	115.25	112.19
2	nA	5	MAN	C1-O5-C5	2.28	115.25	112.19
3	c	5	MAN	C1-O5-C5	2.28	115.25	112.19
3	y	4	MAN	C1-O5-C5	2.28	115.25	112.19
2	iA	4	MAN	C1-O5-C5	2.28	115.24	112.19
3	8	7	MAN	O2-C2-C3	-2.28	105.43	110.15
3	8	5	MAN	C1-O5-C5	2.28	115.24	112.19
2	PA	7	MAN	O5-C1-C2	2.28	116.22	110.79
3	y	1	NAG	C1-O5-C5	2.27	115.23	112.19
2	XA	7	MAN	C1-O5-C5	2.27	115.23	112.19
2	D	7	MAN	O5-C1-C2	2.27	116.20	110.79
3	ZA	4	MAN	C1-O5-C5	2.27	115.23	112.19
2	iA	5	MAN	C1-O5-C5	2.27	115.23	112.19
3	WA	6	MAN	O5-C1-C2	2.27	116.20	110.79
3	mA	4	MAN	C1-O5-C5	2.27	115.22	112.19
3	a	6	MAN	C1-O5-C5	2.27	115.22	112.19
2	L	7	MAN	C1-O5-C5	2.26	115.22	112.19
3	X	7	MAN	O2-C2-C3	-2.26	105.47	110.15
6	M	8	MAN	O2-C2-C3	-2.26	105.47	110.15
2	b	5	MAN	C1-O5-C5	2.26	115.21	112.19
2	w	7	MAN	C1-O5-C5	2.26	115.21	112.19
3	l	7	MAN	O2-C2-C3	-2.25	105.48	110.15
3	kA	4	MAN	O2-C2-C3	-2.25	105.49	110.15
2	3	5	MAN	C1-O5-C5	2.25	115.20	112.19
4	RA	6	MAN	O2-C2-C3	-2.25	105.49	110.15
9	n	1	NAG	O4-C4-C3	-2.25	105.07	110.38
3	v	6	MAN	O2-C2-C3	-2.25	105.50	110.15
2	eA	4	MAN	C1-O5-C5	2.25	115.20	112.19
3	jA	7	MAN	O2-C2-C3	-2.24	105.50	110.15
10	3A	1	NAG	C1-O5-C5	2.24	115.19	112.19
5	SA	7	MAN	O2-C2-C3	-2.24	105.51	110.15
9	zA	1	NAG	C1-C2-N2	2.24	113.96	110.43
6	x	8	MAN	O2-C2-C3	-2.24	105.51	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3A	4	MAN	C1-O5-C5	2.24	115.19	112.19
4	q	6	MAN	O2-C2-C3	-2.24	105.51	110.15
6	YA	8	MAN	O2-C2-C3	-2.24	105.52	110.15
2	7	4	MAN	C1-O5-C5	2.24	115.18	112.19
3	WA	6	MAN	O2-C2-C3	-2.23	105.52	110.15
3	K	6	MAN	O2-C2-C3	-2.23	105.53	110.15
3	P	4	MAN	C1-O5-C5	2.23	115.18	112.19
4	RA	5	MAN	C1-O5-C5	2.23	115.18	112.19
2	nA	7	MAN	C1-O5-C5	2.23	115.18	112.19
3	MA	7	MAN	O2-C2-C3	-2.23	105.53	110.15
3	Y	4	MAN	O2-C2-C3	-2.23	105.53	110.15
5	r	2	NAG	C1-C2-N2	2.23	113.95	110.43
2	b	7	MAN	C1-O5-C5	2.23	115.17	112.19
2	o	7	MAN	O2-C2-C3	-2.23	105.53	110.15
2	eA	5	MAN	C1-O5-C5	2.23	115.17	112.19
2	7	6	MAN	O2-C2-C3	-2.23	105.54	110.15
3	0	4	MAN	C1-O5-C5	2.23	115.17	112.19
10	4A	5	MAN	C1-O5-C5	2.22	115.17	112.19
3	UA	5	MAN	O2-C2-C3	-2.22	105.55	110.15
3	mA	4	MAN	O2-C2-C3	-2.22	105.55	110.15
3	t	5	MAN	O2-C2-C3	-2.22	105.55	110.15
4	q	5	MAN	C1-O5-C5	2.22	115.16	112.19
2	S	4	MAN	C1-O5-C5	2.22	115.16	112.19
3	5	5	MAN	C1-O5-C5	2.22	115.16	112.19
3	cA	4	MAN	O2-C2-C3	-2.22	105.56	110.15
3	tA	5	MAN	O2-C2-C3	-2.21	105.57	110.15
2	dA	5	MAN	C1-O5-C5	2.21	115.15	112.19
3	xA	7	MAN	O2-C2-C3	-2.21	105.57	110.15
3	aA	7	MAN	C1-O5-C5	2.21	115.15	112.19
5	SA	5	NAG	C1-O5-C5	2.21	115.15	112.19
3	E	5	MAN	O2-C2-C3	-2.21	105.58	110.15
3	BA	4	MAN	O2-C2-C3	-2.21	105.58	110.15
3	p	5	MAN	O2-C2-C3	-2.21	105.58	110.15
2	w	7	MAN	O2-C2-C3	-2.21	105.58	110.15
9	n	1	NAG	C1-C2-N2	2.21	113.91	110.43
2	uA	7	MAN	O2-C2-C3	-2.21	105.58	110.15
4	RA	9	MAN	O2-C2-C3	-2.21	105.58	110.15
2	L	7	MAN	O2-C2-C3	-2.21	105.58	110.15
2	eA	6	MAN	C1-O5-C5	2.21	115.14	112.19
3	xA	4	MAN	O2-C2-C3	-2.21	105.58	110.15
2	b	4	MAN	O2-C2-C3	-2.20	105.58	110.15
2	PA	7	MAN	O2-C2-C3	-2.20	105.58	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	iA	6	MAN	O2-C2-C3	-2.20	105.58	110.15
3	I	5	MAN	O2-C2-C3	-2.20	105.59	110.15
3	oA	4	MAN	O2-C2-C3	-2.20	105.59	110.15
3	l	4	MAN	O2-C2-C3	-2.20	105.59	110.15
2	D	7	MAN	O2-C2-C3	-2.20	105.59	110.15
3	X	5	MAN	O2-C2-C3	-2.20	105.59	110.15
3	1	4	MAN	O2-C2-C3	-2.20	105.59	110.15
3	BA	4	MAN	C1-O5-C5	2.20	115.14	112.19
2	w	6	MAN	O2-C2-C3	-2.20	105.59	110.15
2	XA	7	MAN	O2-C2-C3	-2.20	105.59	110.15
2	XA	6	MAN	O2-C2-C3	-2.20	105.59	110.15
3	QA	5	MAN	C1-O5-C5	2.20	115.13	112.19
2	eA	7	MAN	O2-C2-C3	-2.20	105.60	110.15
2	R	5	MAN	C1-O5-C5	2.20	115.13	112.19
2	CA	4	MAN	O2-C2-C3	-2.20	105.60	110.15
2	nA	4	MAN	O2-C2-C3	-2.20	105.60	110.15
3	jA	5	MAN	O2-C2-C3	-2.20	105.60	110.15
10	6A	4	MAN	C1-O5-C5	2.20	115.13	112.19
2	W	6	MAN	O2-C2-C3	-2.20	105.60	110.15
3	DA	6	MAN	O2-C2-C3	-2.20	105.60	110.15
3	DA	4	MAN	O2-C2-C3	-2.20	105.60	110.15
10	1A	4	MAN	O2-C2-C3	-2.19	105.61	110.15
10	2A	5	MAN	O2-C2-C3	-2.19	105.61	110.15
2	W	4	MAN	C1-O5-C5	2.19	115.13	112.19
3	IA	5	MAN	O2-C2-C3	-2.19	105.61	110.15
10	3A	4	MAN	O2-C2-C3	-2.19	105.61	110.15
3	E	5	MAN	C1-O5-C5	2.19	115.13	112.19
2	uA	4	MAN	O2-C2-C3	-2.19	105.61	110.15
3	c	7	MAN	O2-C2-C3	-2.19	105.61	110.15
3	DA	7	MAN	O2-C2-C3	-2.19	105.61	110.15
10	3A	5	MAN	O2-C2-C3	-2.19	105.61	110.15
3	5	4	MAN	O2-C2-C3	-2.19	105.61	110.15
3	gA	4	MAN	O2-C2-C3	-2.19	105.61	110.15
3	Q	4	MAN	O2-C2-C3	-2.19	105.61	110.15
3	oA	7	MAN	O2-C2-C3	-2.19	105.61	110.15
4	F	9	MAN	O2-C2-C3	-2.19	105.62	110.15
4	q	9	MAN	O2-C2-C3	-2.19	105.62	110.15
3	U	4	MAN	O2-C2-C3	-2.19	105.62	110.15
3	8	5	MAN	O2-C2-C3	-2.19	105.62	110.15
3	oA	6	MAN	O2-C2-C3	-2.19	105.62	110.15
3	c	4	MAN	O2-C2-C3	-2.19	105.62	110.15
2	L	6	MAN	O2-C2-C3	-2.19	105.62	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	eA	5	MAN	O2-C2-C3	-2.19	105.62	110.15
3	1	7	MAN	O2-C2-C3	-2.19	105.62	110.15
10	1A	7	MAN	C1-O5-C5	2.18	115.11	112.19
2	i	7	MAN	O2-C2-C3	-2.18	105.63	110.15
3	h	5	MAN	O2-C2-C3	-2.18	105.63	110.15
3	jA	4	MAN	O2-C2-C3	-2.18	105.63	110.15
3	Y	5	MAN	C1-O5-C5	2.18	115.11	112.19
2	o	4	MAN	O2-C2-C3	-2.18	105.63	110.15
3	H	7	MAN	O2-C2-C3	-2.18	105.63	110.15
2	dA	5	MAN	O2-C2-C3	-2.18	105.63	110.15
3	8	6	MAN	O2-C2-C3	-2.18	105.63	110.15
2	3	6	MAN	C1-O5-C5	2.18	115.11	112.19
3	9	4	MAN	O2-C2-C3	-2.18	105.63	110.15
2	PA	4	MAN	O2-C2-C3	-2.18	105.63	110.15
3	mA	6	MAN	O2-C2-C3	-2.18	105.63	110.15
2	Z	6	MAN	O2-C2-C3	-2.18	105.63	110.15
3	c	6	MAN	O2-C2-C3	-2.18	105.63	110.15
2	JA	7	MAN	O2-C2-C3	-2.18	105.64	110.15
2	R	5	MAN	O2-C2-C3	-2.18	105.64	110.15
2	JA	5	MAN	O2-C2-C3	-2.18	105.64	110.15
3	QA	5	MAN	O2-C2-C3	-2.18	105.64	110.15
2	3	4	MAN	C1-O5-C5	2.18	115.11	112.19
2	JA	4	MAN	O2-C2-C3	-2.18	105.64	110.15
3	0	5	MAN	O2-C2-C3	-2.18	105.64	110.15
3	P	5	MAN	O2-C2-C3	-2.18	105.64	110.15
3	a	6	MAN	O2-C2-C3	-2.18	105.64	110.15
10	3A	6	MAN	O2-C2-C3	-2.18	105.64	110.15
2	S	6	MAN	C1-O5-C5	2.18	115.10	112.19
2	eA	6	MAN	O2-C2-C3	-2.18	105.64	110.15
2	wA	5	MAN	O2-C2-C3	-2.18	105.64	110.15
3	h	6	MAN	O2-C2-C3	-2.18	105.64	110.15
3	u	7	MAN	O2-C2-C3	-2.18	105.64	110.15
3	J	7	MAN	O2-C2-C3	-2.18	105.65	110.15
2	S	5	MAN	O2-C2-C3	-2.17	105.65	110.15
2	S	6	MAN	O2-C2-C3	-2.17	105.65	110.15
3	X	6	MAN	O2-C2-C3	-2.17	105.65	110.15
3	DA	5	MAN	O2-C2-C3	-2.17	105.65	110.15
2	fA	6	MAN	O2-C2-C3	-2.17	105.65	110.15
3	tA	6	MAN	O2-C2-C3	-2.17	105.65	110.15
5	G	5	NAG	C1-O5-C5	2.17	115.10	112.19
2	CA	7	MAN	O2-C2-C3	-2.17	105.65	110.15
3	s	7	MAN	O2-C2-C3	-2.17	105.65	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	MA	4	MAN	O2-C2-C3	-2.17	105.65	110.15
3	cA	7	MAN	O2-C2-C3	-2.17	105.65	110.15
6	x	6	MAN	O2-C2-C3	-2.17	105.65	110.15
3	a	4	MAN	O2-C2-C3	-2.17	105.65	110.15
3	8	4	MAN	O2-C2-C3	-2.17	105.65	110.15
9	OA	1	NAG	C1-C2-N2	2.17	113.85	110.43
2	i	4	MAN	O2-C2-C3	-2.17	105.66	110.15
10	4A	5	MAN	O2-C2-C3	-2.17	105.66	110.15
2	4	6	MAN	O2-C2-C3	-2.17	105.66	110.15
3	TA	7	MAN	O2-C2-C3	-2.17	105.66	110.15
10	0A	5	MAN	O2-C2-C3	-2.17	105.66	110.15
2	b	7	MAN	O2-C2-C3	-2.17	105.66	110.15
2	3	5	MAN	O2-C2-C3	-2.17	105.66	110.15
3	X	4	MAN	O2-C2-C3	-2.17	105.66	110.15
2	3	7	MAN	O2-C2-C3	-2.17	105.66	110.15
6	YA	6	MAN	O2-C2-C3	-2.17	105.66	110.15
10	6A	4	MAN	O2-C2-C3	-2.17	105.66	110.15
3	tA	7	MAN	O2-C2-C3	-2.17	105.66	110.15
2	wA	4	MAN	O2-C2-C3	-2.17	105.66	110.15
3	bA	5	MAN	O2-C2-C3	-2.17	105.66	110.15
3	IA	6	MAN	O2-C2-C3	-2.17	105.66	110.15
2	LA	4	MAN	O2-C2-C3	-2.17	105.67	110.15
8	vA	5	MAN	O2-C2-C3	-2.17	105.67	110.15
2	3	6	MAN	O2-C2-C3	-2.17	105.67	110.15
3	jA	6	MAN	O2-C2-C3	-2.17	105.67	110.15
6	M	6	MAN	O2-C2-C3	-2.17	105.67	110.15
2	T	6	MAN	O2-C2-C3	-2.16	105.67	110.15
3	Q	7	MAN	O2-C2-C3	-2.16	105.67	110.15
2	nA	5	MAN	O2-C2-C3	-2.16	105.67	110.15
3	K	7	MAN	O2-C2-C3	-2.16	105.67	110.15
3	BA	6	MAN	O2-C2-C3	-2.16	105.67	110.15
3	VA	7	MAN	O2-C2-C3	-2.16	105.67	110.15
3	QA	7	MAN	O2-C2-C3	-2.16	105.67	110.15
3	v	4	MAN	O2-C2-C3	-2.16	105.67	110.15
3	sA	7	MAN	O2-C2-C3	-2.16	105.67	110.15
10	7A	6	MAN	O2-C2-C3	-2.16	105.67	110.15
3	p	5	MAN	C1-O5-C5	2.16	115.08	112.19
3	WA	7	MAN	O2-C2-C3	-2.16	105.68	110.15
2	S	7	MAN	O2-C2-C3	-2.16	105.68	110.15
2	W	7	MAN	O2-C2-C3	-2.16	105.68	110.15
7	pA	9	MAN	O2-C2-C3	-2.16	105.68	110.15
2	yA	5	MAN	C1-O5-C5	2.16	115.08	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	i	5	MAN	O2-C2-C3	-2.16	105.68	110.15
2	PA	5	MAN	O2-C2-C3	-2.16	105.68	110.15
2	qA	6	MAN	O2-C2-C3	-2.16	105.68	110.15
3	Y	7	MAN	O2-C2-C3	-2.16	105.68	110.15
3	HA	7	MAN	O2-C2-C3	-2.16	105.68	110.15
2	W	4	MAN	O2-C2-C3	-2.16	105.68	110.15
3	H	6	MAN	O2-C2-C3	-2.16	105.69	110.15
3	K	4	MAN	O2-C2-C3	-2.16	105.69	110.15
2	2	5	MAN	O2-C2-C3	-2.16	105.69	110.15
3	I	6	MAN	O2-C2-C3	-2.16	105.69	110.15
3	c	5	MAN	O2-C2-C3	-2.16	105.69	110.15
2	AA	6	MAN	O2-C2-C3	-2.16	105.69	110.15
3	h	7	MAN	O2-C2-C3	-2.16	105.69	110.15
3	kA	5	MAN	C1-O5-C5	2.15	115.07	112.19
2	i	6	MAN	O2-C2-C3	-2.15	105.69	110.15
3	IA	7	MAN	O2-C2-C3	-2.15	105.69	110.15
10	6A	5	MAN	O2-C2-C3	-2.15	105.69	110.15
2	NA	5	MAN	C1-O5-C5	2.15	115.07	112.19
3	H	5	MAN	O2-C2-C3	-2.15	105.69	110.15
3	gA	5	MAN	C1-O5-C5	2.15	115.07	112.19
7	EA	4	MAN	O2-C2-C3	-2.15	105.69	110.15
10	1A	5	MAN	O2-C2-C3	-2.15	105.69	110.15
2	lA	6	MAN	O2-C2-C3	-2.15	105.69	110.15
3	mA	7	MAN	O2-C2-C3	-2.15	105.69	110.15
2	D	4	MAN	O2-C2-C3	-2.15	105.69	110.15
3	kA	7	MAN	O2-C2-C3	-2.15	105.69	110.15
10	5A	5	MAN	O2-C2-C3	-2.15	105.69	110.15
2	k	5	MAN	O2-C2-C3	-2.15	105.69	110.15
2	uA	5	MAN	O2-C2-C3	-2.15	105.69	110.15
10	5A	7	MAN	O2-C2-C3	-2.15	105.69	110.15
3	a	4	MAN	C1-O5-C5	2.15	115.07	112.19
3	z	7	MAN	C1-O5-C5	2.15	115.07	112.19
2	FA	6	MAN	O2-C2-C3	-2.15	105.70	110.15
2	JA	6	MAN	O2-C2-C3	-2.15	105.70	110.15
3	p	7	MAN	C1-O5-C5	2.15	115.07	112.19
2	e	6	MAN	O2-C2-C3	-2.15	105.70	110.15
3	z	4	MAN	O2-C2-C3	-2.15	105.70	110.15
3	QA	6	MAN	O2-C2-C3	-2.15	105.70	110.15
2	NA	6	MAN	O2-C2-C3	-2.15	105.70	110.15
3	GA	6	MAN	O2-C2-C3	-2.15	105.70	110.15
10	2A	4	MAN	O2-C2-C3	-2.15	105.70	110.15
2	iA	7	MAN	O2-C2-C3	-2.15	105.70	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	0A	6	MAN	O2-C2-C3	-2.15	105.70	110.15
3	U	5	MAN	O2-C2-C3	-2.15	105.70	110.15
3	V	5	MAN	O2-C2-C3	-2.15	105.70	110.15
3	UA	6	MAN	O2-C2-C3	-2.15	105.70	110.15
2	iA	4	MAN	O2-C2-C3	-2.15	105.70	110.15
3	rA	7	MAN	O2-C2-C3	-2.15	105.70	110.15
2	CA	5	MAN	O2-C2-C3	-2.15	105.71	110.15
3	rA	6	MAN	O2-C2-C3	-2.15	105.71	110.15
2	LA	5	MAN	O2-C2-C3	-2.15	105.71	110.15
3	hA	4	MAN	O2-C2-C3	-2.15	105.71	110.15
10	7A	4	MAN	O2-C2-C3	-2.15	105.71	110.15
3	v	7	MAN	O2-C2-C3	-2.14	105.71	110.15
3	O	7	MAN	C1-O5-C5	2.14	115.06	112.19
3	u	6	MAN	O2-C2-C3	-2.14	105.71	110.15
4	q	7	MAN	O2-C2-C3	-2.14	105.71	110.15
3	9	7	MAN	O2-C2-C3	-2.14	105.71	110.15
3	TA	5	MAN	O2-C2-C3	-2.14	105.71	110.15
7	d	9	MAN	O2-C2-C3	-2.14	105.71	110.15
10	5A	4	MAN	O2-C2-C3	-2.14	105.71	110.15
3	K	5	MAN	O2-C2-C3	-2.14	105.72	110.15
3	g	7	MAN	O2-C2-C3	-2.14	105.72	110.15
3	ZA	7	MAN	O2-C2-C3	-2.14	105.72	110.15
2	2	6	MAN	O2-C2-C3	-2.14	105.72	110.15
3	s	6	MAN	O2-C2-C3	-2.14	105.72	110.15
2	m	5	MAN	O2-C2-C3	-2.14	105.72	110.15
2	uA	6	MAN	O2-C2-C3	-2.14	105.72	110.15
2	dA	6	MAN	O2-C2-C3	-2.14	105.72	110.15
3	MA	6	MAN	O2-C2-C3	-2.14	105.72	110.15
3	WA	4	MAN	O2-C2-C3	-2.14	105.72	110.15
10	7A	5	MAN	O2-C2-C3	-2.14	105.72	110.15
8	vA	3	BMA	C2-C3-C4	2.14	114.62	110.86
2	nA	7	MAN	O2-C2-C3	-2.14	105.72	110.15
2	wA	6	MAN	O2-C2-C3	-2.14	105.72	110.15
2	7	7	MAN	O2-C2-C3	-2.14	105.73	110.15
2	Z	5	MAN	C1-O5-C5	2.14	115.05	112.19
2	2	5	MAN	C1-O5-C5	2.14	115.05	112.19
2	7	4	MAN	O2-C2-C3	-2.14	105.73	110.15
2	LA	6	MAN	O2-C2-C3	-2.14	105.73	110.15
2	PA	6	MAN	O2-C2-C3	-2.14	105.73	110.15
3	N	7	MAN	O2-C2-C3	-2.14	105.73	110.15
7	EA	9	MAN	O2-C2-C3	-2.14	105.73	110.15
2	w	5	MAN	O2-C2-C3	-2.13	105.73	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	p	7	MAN	O2-C2-C3	-2.13	105.73	110.15
3	E	7	MAN	O2-C2-C3	-2.13	105.73	110.15
3	u	5	MAN	O2-C2-C3	-2.13	105.73	110.15
3	9	5	MAN	O2-C2-C3	-2.13	105.73	110.15
3	GA	7	MAN	O2-C2-C3	-2.13	105.73	110.15
2	4	5	MAN	O2-C2-C3	-2.13	105.73	110.15
3	t	6	MAN	O2-C2-C3	-2.13	105.73	110.15
3	TA	2	NAG	C1-O5-C5	2.13	115.05	112.19
2	NA	7	MAN	O2-C2-C3	-2.13	105.73	110.15
3	y	4	MAN	O2-C2-C3	-2.13	105.73	110.15
3	6	7	MAN	O2-C2-C3	-2.13	105.73	110.15
3	bA	7	MAN	O2-C2-C3	-2.13	105.73	110.15
3	rA	5	MAN	O2-C2-C3	-2.13	105.73	110.15
10	5A	6	MAN	O2-C2-C3	-2.13	105.73	110.15
3	V	4	MAN	O2-C2-C3	-2.13	105.73	110.15
3	gA	5	MAN	O2-C2-C3	-2.13	105.73	110.15
10	1A	6	MAN	O2-C2-C3	-2.13	105.73	110.15
2	m	7	MAN	O2-C2-C3	-2.13	105.73	110.15
2	NA	5	MAN	O2-C2-C3	-2.13	105.73	110.15
3	hA	7	MAN	O2-C2-C3	-2.13	105.73	110.15
2	LA	7	MAN	O2-C2-C3	-2.13	105.74	110.15
3	V	6	MAN	O2-C2-C3	-2.13	105.74	110.15
2	D	5	MAN	O2-C2-C3	-2.13	105.74	110.15
2	FA	7	MAN	O2-C2-C3	-2.13	105.74	110.15
3	5	5	MAN	O2-C2-C3	-2.13	105.74	110.15
3	kA	5	MAN	O2-C2-C3	-2.13	105.74	110.15
3	oA	5	MAN	O2-C2-C3	-2.13	105.74	110.15
10	2A	7	MAN	O2-C2-C3	-2.13	105.74	110.15
10	6A	6	MAN	O2-C2-C3	-2.13	105.74	110.15
2	yA	6	MAN	O2-C2-C3	-2.13	105.74	110.15
3	U	7	MAN	O2-C2-C3	-2.13	105.74	110.15
3	s	5	MAN	O2-C2-C3	-2.13	105.74	110.15
2	k	4	MAN	O2-C2-C3	-2.13	105.74	110.15
3	TA	6	MAN	O2-C2-C3	-2.13	105.74	110.15
3	f	6	MAN	O2-C2-C3	-2.13	105.74	110.15
7	d	4	MAN	O2-C2-C3	-2.13	105.74	110.15
10	3A	7	MAN	O2-C2-C3	-2.13	105.74	110.15
3	H	2	NAG	C1-O5-C5	2.13	115.04	112.19
2	iA	5	MAN	O2-C2-C3	-2.13	105.75	110.15
3	E	6	MAN	O2-C2-C3	-2.13	105.75	110.15
2	2	7	MAN	O2-C2-C3	-2.13	105.75	110.15
3	V	7	MAN	O2-C2-C3	-2.13	105.75	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	gA	7	MAN	O2-C2-C3	-2.13	105.75	110.15
2	e	7	MAN	O2-C2-C3	-2.13	105.75	110.15
3	HA	5	MAN	O2-C2-C3	-2.13	105.75	110.15
2	b	5	MAN	O2-C2-C3	-2.13	105.75	110.15
3	P	7	MAN	O2-C2-C3	-2.13	105.75	110.15
3	5	7	MAN	O2-C2-C3	-2.13	105.75	110.15
3	gA	6	MAN	O2-C2-C3	-2.13	105.75	110.15
3	f	7	MAN	O2-C2-C3	-2.12	105.75	110.15
10	7A	7	MAN	O2-C2-C3	-2.12	105.75	110.15
3	y	7	MAN	O2-C2-C3	-2.12	105.75	110.15
2	k	7	MAN	O2-C2-C3	-2.12	105.75	110.15
2	dA	7	MAN	O2-C2-C3	-2.12	105.75	110.15
3	bA	6	MAN	O2-C2-C3	-2.12	105.75	110.15
10	0A	7	MAN	O2-C2-C3	-2.12	105.75	110.15
2	W	5	MAN	O2-C2-C3	-2.12	105.75	110.15
3	6	5	MAN	O2-C2-C3	-2.12	105.75	110.15
3	aA	4	MAN	O2-C2-C3	-2.12	105.75	110.15
2	e	5	MAN	O2-C2-C3	-2.12	105.75	110.15
2	yA	5	MAN	O2-C2-C3	-2.12	105.75	110.15
3	g	6	MAN	O2-C2-C3	-2.12	105.76	110.15
3	t	7	MAN	O2-C2-C3	-2.12	105.76	110.15
3	VA	6	MAN	O2-C2-C3	-2.12	105.76	110.15
3	sA	6	MAN	O2-C2-C3	-2.12	105.76	110.15
3	UA	7	MAN	O2-C2-C3	-2.12	105.76	110.15
10	2A	6	MAN	O2-C2-C3	-2.12	105.76	110.15
10	4A	6	MAN	O2-C2-C3	-2.12	105.76	110.15
3	xA	6	MAN	O2-C2-C3	-2.12	105.76	110.15
3	O	4	MAN	O2-C2-C3	-2.12	105.76	110.15
2	o	6	MAN	O2-C2-C3	-2.12	105.76	110.15
8	KA	5	MAN	O2-C2-C3	-2.12	105.76	110.15
2	T	5	MAN	O2-C2-C3	-2.12	105.76	110.15
3	g	5	MAN	O2-C2-C3	-2.12	105.76	110.15
2	lA	4	MAN	O2-C2-C3	-2.12	105.76	110.15
3	0	7	MAN	O2-C2-C3	-2.12	105.76	110.15
2	b	6	MAN	O2-C2-C3	-2.12	105.76	110.15
3	VA	5	MAN	O2-C2-C3	-2.12	105.76	110.15
2	AA	5	MAN	O2-C2-C3	-2.12	105.77	110.15
3	hA	5	MAN	O2-C2-C3	-2.12	105.77	110.15
2	qA	5	MAN	O2-C2-C3	-2.12	105.77	110.15
3	p	6	MAN	O2-C2-C3	-2.12	105.77	110.15
2	k	6	MAN	O2-C2-C3	-2.12	105.77	110.15
2	FA	5	MAN	O2-C2-C3	-2.12	105.77	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	qA	7	MAN	O2-C2-C3	-2.12	105.77	110.15
3	l	6	MAN	O2-C2-C3	-2.12	105.77	110.15
3	sA	5	MAN	O2-C2-C3	-2.12	105.77	110.15
2	nA	6	MAN	O2-C2-C3	-2.12	105.77	110.15
3	z	5	MAN	O2-C2-C3	-2.12	105.77	110.15
2	R	4	MAN	C1-O5-C5	2.12	115.02	112.19
3	J	5	MAN	O2-C2-C3	-2.12	105.77	110.15
3	N	6	MAN	O2-C2-C3	-2.12	105.77	110.15
2	yA	7	MAN	O2-C2-C3	-2.11	105.77	110.15
2	o	5	MAN	O2-C2-C3	-2.11	105.77	110.15
3	aA	5	MAN	O2-C2-C3	-2.11	105.77	110.15
10	4A	4	MAN	O2-C2-C3	-2.11	105.77	110.15
2	uA	1	NAG	C1-O5-C5	2.11	115.02	112.19
3	J	6	MAN	O2-C2-C3	-2.11	105.77	110.15
10	1A	7	MAN	O2-C2-C3	-2.11	105.77	110.15
4	q	9	MAN	C1-O5-C5	2.11	115.02	112.19
2	Z	5	MAN	O2-C2-C3	-2.11	105.78	110.15
3	I	7	MAN	O2-C2-C3	-2.11	105.78	110.15
10	6A	7	MAN	O2-C2-C3	-2.11	105.78	110.15
3	E	7	MAN	C1-O5-C5	2.11	115.02	112.19
3	U	5	MAN	C1-O5-C5	2.11	115.02	112.19
2	R	6	MAN	O2-C2-C3	-2.11	105.78	110.15
3	N	4	MAN	O2-C2-C3	-2.11	105.78	110.15
3	Q	5	MAN	O2-C2-C3	-2.11	105.78	110.15
2	XA	4	MAN	O2-C2-C3	-2.11	105.78	110.15
2	fA	5	MAN	O2-C2-C3	-2.11	105.78	110.15
3	BA	7	MAN	O2-C2-C3	-2.11	105.78	110.15
3	ZA	4	MAN	O2-C2-C3	-2.11	105.78	110.15
10	4A	7	MAN	O2-C2-C3	-2.11	105.78	110.15
10	0A	4	MAN	O2-C2-C3	-2.11	105.78	110.15
7	pA	1	NAG	C1-O5-C5	2.11	115.02	112.19
3	Y	5	MAN	O2-C2-C3	-2.11	105.78	110.15
3	aA	6	MAN	O2-C2-C3	-2.11	105.78	110.15
3	xA	5	MAN	O2-C2-C3	-2.11	105.78	110.15
3	WA	5	MAN	O2-C2-C3	-2.11	105.78	110.15
9	n	1	NAG	C1-O5-C5	2.11	115.01	112.19
8	j	3	BMA	C1-C2-C3	2.11	112.72	109.64
2	Z	4	MAN	O2-C2-C3	-2.11	105.78	110.15
2	XA	5	MAN	O2-C2-C3	-2.11	105.78	110.15
3	N	5	MAN	O2-C2-C3	-2.11	105.78	110.15
3	0	6	MAN	O2-C2-C3	-2.11	105.78	110.15
2	L	5	MAN	O2-C2-C3	-2.11	105.78	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	j	5	MAN	O2-C2-C3	-2.11	105.78	110.15
2	D	6	MAN	O2-C2-C3	-2.11	105.79	110.15
2	fA	7	MAN	O2-C2-C3	-2.11	105.79	110.15
3	hA	6	MAN	O2-C2-C3	-2.11	105.79	110.15
2	lA	5	MAN	O2-C2-C3	-2.11	105.79	110.15
2	wA	7	MAN	O2-C2-C3	-2.11	105.79	110.15
3	Q	6	MAN	O2-C2-C3	-2.11	105.79	110.15
3	a	5	MAN	O2-C2-C3	-2.11	105.79	110.15
3	z	6	MAN	O2-C2-C3	-2.11	105.79	110.15
3	9	6	MAN	O2-C2-C3	-2.11	105.79	110.15
2	CA	6	MAN	O2-C2-C3	-2.10	105.79	110.15
2	m	5	MAN	C1-O5-C5	2.10	115.00	112.19
3	9	5	MAN	C1-O5-C5	2.10	115.00	112.19
3	l	5	MAN	O2-C2-C3	-2.10	105.80	110.15
3	QA	7	MAN	C1-O5-C5	2.10	115.00	112.19
3	f	5	MAN	O2-C2-C3	-2.10	105.80	110.15
2	lA	5	MAN	C1-O5-C5	2.10	115.00	112.19
3	I	7	MAN	C1-O5-C5	2.10	115.00	112.19
2	L	4	MAN	O2-C2-C3	-2.10	105.80	110.15
2	3	4	MAN	O2-C2-C3	-2.10	105.80	110.15
3	v	5	MAN	O2-C2-C3	-2.10	105.80	110.15
3	mA	5	MAN	O2-C2-C3	-2.10	105.80	110.15
2	m	6	MAN	O2-C2-C3	-2.10	105.80	110.15
3	y	6	MAN	O2-C2-C3	-2.10	105.80	110.15
3	GA	5	MAN	O2-C2-C3	-2.10	105.80	110.15
3	cA	6	MAN	O2-C2-C3	-2.10	105.80	110.15
3	v	1	NAG	C1-C2-N2	2.10	113.74	110.43
2	w	4	MAN	O2-C2-C3	-2.10	105.80	110.15
3	a	7	MAN	O2-C2-C3	-2.10	105.80	110.15
9	OA	1	NAG	O4-C4-C3	-2.10	105.43	110.38
2	T	7	MAN	O2-C2-C3	-2.10	105.80	110.15
3	O	5	MAN	O2-C2-C3	-2.10	105.80	110.15
3	U	6	MAN	O2-C2-C3	-2.10	105.81	110.15
2	7	5	MAN	O2-C2-C3	-2.10	105.81	110.15
2	Z	4	MAN	C1-O5-C5	2.10	115.00	112.19
2	R	7	MAN	O2-C2-C3	-2.10	105.81	110.15
3	6	6	MAN	O2-C2-C3	-2.10	105.81	110.15
3	BA	5	MAN	O2-C2-C3	-2.10	105.81	110.15
3	y	5	MAN	O2-C2-C3	-2.10	105.81	110.15
3	cA	5	MAN	O2-C2-C3	-2.09	105.81	110.15
3	t	7	MAN	C1-O5-C5	2.09	114.99	112.19
2	S	4	MAN	O2-C2-C3	-2.09	105.81	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6	4	MAN	O2-C2-C3	-2.09	105.81	110.15
5	r	5	NAG	C1-O5-C5	2.09	114.99	112.19
2	qA	3	BMA	C2-C3-C4	2.09	114.54	110.86
4	RA	7	MAN	O2-C2-C3	-2.09	105.81	110.15
3	HA	6	MAN	O2-C2-C3	-2.09	105.82	110.15
3	Y	6	MAN	O2-C2-C3	-2.09	105.82	110.15
2	AA	7	MAN	O2-C2-C3	-2.09	105.82	110.15
3	1	6	MAN	O2-C2-C3	-2.09	105.82	110.15
3	O	6	MAN	O2-C2-C3	-2.09	105.82	110.15
8	j	4	MAN	O2-C2-C3	-2.09	105.82	110.15
2	FA	4	MAN	O2-C2-C3	-2.09	105.82	110.15
3	kA	6	MAN	O2-C2-C3	-2.09	105.82	110.15
3	ZA	6	MAN	O2-C2-C3	-2.09	105.83	110.15
3	s	2	NAG	C1-O5-C5	2.09	114.98	112.19
2	AA	5	MAN	C1-O5-C5	2.09	114.98	112.19
2	qA	4	MAN	O2-C2-C3	-2.09	105.83	110.15
3	J	4	MAN	O2-C2-C3	-2.09	105.83	110.15
8	KA	4	MAN	O2-C2-C3	-2.09	105.83	110.15
3	5	6	MAN	O2-C2-C3	-2.09	105.83	110.15
2	Z	7	MAN	O2-C2-C3	-2.09	105.83	110.15
3	ZA	5	MAN	O2-C2-C3	-2.09	105.83	110.15
4	F	7	MAN	O2-C2-C3	-2.08	105.83	110.15
3	z	7	MAN	O2-C2-C3	-2.08	105.84	110.15
2	4	7	MAN	O2-C2-C3	-2.08	105.84	110.15
2	e	4	MAN	O2-C2-C3	-2.08	105.84	110.15
3	O	7	MAN	O2-C2-C3	-2.08	105.84	110.15
2	AA	4	MAN	O2-C2-C3	-2.08	105.84	110.15
8	vA	4	MAN	O2-C2-C3	-2.08	105.84	110.15
2	lA	7	MAN	O2-C2-C3	-2.08	105.84	110.15
3	MA	5	MAN	O2-C2-C3	-2.08	105.84	110.15
2	e	3	BMA	C2-C3-C4	2.08	114.52	110.86
3	P	6	MAN	O2-C2-C3	-2.08	105.84	110.15
2	lA	4	MAN	C1-O5-C5	2.08	114.97	112.19
3	K	1	NAG	C1-C2-N2	2.08	113.71	110.43
3	WA	1	NAG	C1-C2-N2	2.08	113.71	110.43
2	FA	3	BMA	C2-C3-C4	2.08	114.52	110.86
8	KA	3	BMA	C1-C2-C3	2.08	112.67	109.64
3	aA	7	MAN	O2-C2-C3	-2.07	105.85	110.15
2	JA	4	MAN	C1-C2-C3	2.07	112.66	109.64
2	lA	3	BMA	C1-O5-C5	2.07	114.96	112.19
3	1	5	MAN	O2-C2-C3	-2.07	105.86	110.15
2	CA	4	MAN	C1-O5-C5	2.07	114.96	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	eA	4	MAN	O2-C2-C3	-2.07	105.87	110.15
3	VA	4	MAN	O2-C2-C3	-2.07	105.87	110.15
2	i	4	MAN	C1-C2-C3	2.07	112.65	109.64
2	D	4	MAN	C1-O5-C5	2.07	114.95	112.19
8	vA	1	NAG	O4-C4-C5	2.06	114.41	109.32
2	nA	4	MAN	C1-O5-C5	2.06	114.95	112.19
3	u	4	MAN	C1-O5-C5	2.06	114.95	112.19
3	J	4	MAN	C1-O5-C5	2.06	114.95	112.19
2	Z	3	BMA	C1-O5-C5	2.06	114.95	112.19
2	dA	4	MAN	C1-O5-C5	2.06	114.95	112.19
2	2	4	MAN	C1-O5-C5	2.06	114.94	112.19
2	o	4	MAN	C1-O5-C5	2.06	114.94	112.19
3	UA	7	MAN	C1-O5-C5	2.05	114.94	112.19
2	AA	4	MAN	C1-O5-C5	2.05	114.94	112.19
4	RA	6	MAN	C1-O5-C5	2.05	114.93	112.19
3	u	4	MAN	O2-C2-C3	-2.04	105.92	110.15
2	AA	3	BMA	C1-O5-C5	2.04	114.92	112.19
3	VA	4	MAN	C1-O5-C5	2.04	114.92	112.19
2	PA	4	MAN	C1-O5-C5	2.04	114.92	112.19
4	F	9	MAN	C1-O5-C5	2.04	114.92	112.19
7	EA	12	FUC	O5-C5-C4	2.03	113.21	109.55
2	b	4	MAN	C1-O5-C5	2.03	114.91	112.19
7	d	12	FUC	O5-C5-C4	2.03	113.20	109.55
9	OA	1	NAG	C1-O5-C5	2.03	114.90	112.19
4	F	6	MAN	C1-O5-C5	2.02	114.90	112.19
2	eA	3	BMA	O2-C2-C3	-2.02	105.96	110.15
4	q	6	MAN	C1-O5-C5	2.01	114.89	112.19
3	U	4	MAN	C1-C2-C3	2.01	112.58	109.64
2	S	3	BMA	O2-C2-C3	-2.01	105.98	110.15
3	UA	4	MAN	O3-C3-C2	2.01	114.16	110.05
7	pA	12	FUC	O5-C5-C4	2.01	113.17	109.55
3	t	4	MAN	O2-C2-C3	-2.01	105.99	110.15
4	RA	9	MAN	C1-O5-C5	2.01	114.88	112.19
2	3	3	BMA	O2-C2-C3	-2.01	106.00	110.15
3	5	4	MAN	C1-C2-C3	2.00	112.56	109.64

There are no chirality outliers.

All (760) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	y	4	MAN	O5-C5-C6-O6
2	uA	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	RA	8	MAN	C4-C5-C6-O6
4	q	8	MAN	C4-C5-C6-O6
3	N	4	MAN	O5-C5-C6-O6
3	ZA	4	MAN	O5-C5-C6-O6
8	vA	5	MAN	O5-C5-C6-O6
10	2A	2	NAG	O5-C5-C6-O6
5	r	3	BMA	C4-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
2	Z	1	NAG	O5-C5-C6-O6
2	AA	1	NAG	O5-C5-C6-O6
3	TA	4	MAN	O5-C5-C6-O6
8	KA	3	BMA	O5-C5-C6-O6
9	n	1	NAG	O5-C5-C6-O6
9	zA	1	NAG	O5-C5-C6-O6
2	7	1	NAG	O5-C5-C6-O6
8	j	3	BMA	O5-C5-C6-O6
2	uA	3	BMA	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	c	3	BMA	O5-C5-C6-O6
3	s	4	MAN	O5-C5-C6-O6
3	v	1	NAG	O5-C5-C6-O6
3	DA	3	BMA	O5-C5-C6-O6
3	oA	3	BMA	O5-C5-C6-O6
4	RA	8	MAN	O5-C5-C6-O6
8	j	5	MAN	O5-C5-C6-O6
10	3A	1	NAG	O5-C5-C6-O6
2	b	7	MAN	O5-C5-C6-O6
2	iA	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	p	1	NAG	O5-C5-C6-O6
3	VA	2	NAG	O5-C5-C6-O6
4	q	8	MAN	O5-C5-C6-O6
10	0A	1	NAG	O5-C5-C6-O6
4	F	8	MAN	C4-C5-C6-O6
2	iA	1	NAG	O5-C5-C6-O6
2	qA	4	MAN	O5-C5-C6-O6
3	H	4	MAN	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
3	u	2	NAG	O5-C5-C6-O6
3	z	2	NAG	O5-C5-C6-O6
3	WA	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	EA	4	MAN	O5-C5-C6-O6
8	KA	5	MAN	O5-C5-C6-O6
9	OA	1	NAG	O5-C5-C6-O6
10	7A	1	NAG	O5-C5-C6-O6
9	zA	1	NAG	C4-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	e	4	MAN	O5-C5-C6-O6
2	7	2	NAG	O5-C5-C6-O6
2	FA	4	MAN	O5-C5-C6-O6
2	NA	2	NAG	O5-C5-C6-O6
2	XA	2	NAG	O5-C5-C6-O6
2	lA	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	f	3	BMA	O5-C5-C6-O6
3	cA	1	NAG	O5-C5-C6-O6
7	d	4	MAN	O5-C5-C6-O6
7	pA	1	NAG	O5-C5-C6-O6
7	pA	4	MAN	O5-C5-C6-O6
2	D	4	MAN	C4-C5-C6-O6
2	W	1	NAG	C4-C5-C6-O6
2	o	4	MAN	C4-C5-C6-O6
2	PA	4	MAN	C4-C5-C6-O6
2	iA	2	NAG	C4-C5-C6-O6
2	uA	3	BMA	C4-C5-C6-O6
3	H	4	MAN	C4-C5-C6-O6
3	DA	3	BMA	C4-C5-C6-O6
8	KA	5	MAN	C4-C5-C6-O6
10	0A	3	BMA	C4-C5-C6-O6
2	W	2	NAG	O5-C5-C6-O6
2	i	3	BMA	O5-C5-C6-O6
2	m	2	NAG	O5-C5-C6-O6
2	JA	3	BMA	O5-C5-C6-O6
2	LA	2	NAG	O5-C5-C6-O6
3	g	3	BMA	O5-C5-C6-O6
3	6	1	NAG	O5-C5-C6-O6
3	QA	1	NAG	O5-C5-C6-O6
3	aA	2	NAG	O5-C5-C6-O6
10	0A	3	BMA	O5-C5-C6-O6
2	7	1	NAG	C4-C5-C6-O6
3	J	3	BMA	C4-C5-C6-O6
3	N	4	MAN	C4-C5-C6-O6
3	TA	4	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	VA	3	BMA	C4-C5-C6-O6
3	ZA	4	MAN	C4-C5-C6-O6
8	j	5	MAN	C4-C5-C6-O6
10	0A	1	NAG	C4-C5-C6-O6
2	dA	1	NAG	O5-C5-C6-O6
2	uA	1	NAG	O5-C5-C6-O6
2	yA	2	NAG	O5-C5-C6-O6
3	9	2	NAG	O5-C5-C6-O6
3	GA	3	BMA	O5-C5-C6-O6
3	hA	1	NAG	O5-C5-C6-O6
3	rA	3	BMA	O5-C5-C6-O6
8	vA	1	NAG	O5-C5-C6-O6
9	zA	2	NAG	O5-C5-C6-O6
10	3A	2	NAG	O5-C5-C6-O6
2	i	3	BMA	C4-C5-C6-O6
3	c	3	BMA	C4-C5-C6-O6
3	u	3	BMA	C4-C5-C6-O6
3	y	4	MAN	C4-C5-C6-O6
3	oA	3	BMA	C4-C5-C6-O6
8	j	3	BMA	C4-C5-C6-O6
8	KA	3	BMA	C4-C5-C6-O6
9	n	1	NAG	C4-C5-C6-O6
2	k	2	NAG	O5-C5-C6-O6
2	wA	2	NAG	O5-C5-C6-O6
3	v	4	MAN	O5-C5-C6-O6
3	HA	3	BMA	O5-C5-C6-O6
3	gA	1	NAG	O5-C5-C6-O6
3	sA	3	BMA	O5-C5-C6-O6
8	vA	3	BMA	O5-C5-C6-O6
2	W	2	NAG	C4-C5-C6-O6
2	7	2	NAG	C4-C5-C6-O6
2	JA	3	BMA	C4-C5-C6-O6
2	iA	1	NAG	C4-C5-C6-O6
3	f	3	BMA	C4-C5-C6-O6
3	s	4	MAN	C4-C5-C6-O6
3	GA	3	BMA	C4-C5-C6-O6
3	rA	3	BMA	C4-C5-C6-O6
10	7A	1	NAG	C4-C5-C6-O6
3	1	1	NAG	O5-C5-C6-O6
4	RA	3	BMA	O5-C5-C6-O6
5	r	3	BMA	O5-C5-C6-O6
5	SA	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	M	2	NAG	O5-C5-C6-O6
7	EA	2	NAG	O5-C5-C6-O6
9	n	2	NAG	O5-C5-C6-O6
9	OA	2	NAG	O5-C5-C6-O6
2	Z	1	NAG	C4-C5-C6-O6
2	AA	1	NAG	C4-C5-C6-O6
2	CA	2	NAG	C4-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6
2	R	4	MAN	O5-C5-C6-O6
2	dA	4	MAN	O5-C5-C6-O6
7	d	7	NAG	O5-C5-C6-O6
2	XA	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	aA	2	NAG	C4-C5-C6-O6
8	vA	5	MAN	C4-C5-C6-O6
10	2A	2	NAG	C4-C5-C6-O6
2	w	2	NAG	O5-C5-C6-O6
2	2	4	MAN	O5-C5-C6-O6
3	0	3	BMA	O5-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
7	d	2	NAG	O5-C5-C6-O6
10	4A	1	NAG	O5-C5-C6-O6
10	5A	4	MAN	O5-C5-C6-O6
4	RA	2	NAG	C4-C5-C6-O6
5	SA	3	BMA	C4-C5-C6-O6
10	7A	3	BMA	C4-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
3	kA	2	NAG	O5-C5-C6-O6
6	x	2	NAG	O5-C5-C6-O6
6	YA	2	NAG	O5-C5-C6-O6
7	EA	7	NAG	O5-C5-C6-O6
3	p	1	NAG	C4-C5-C6-O6
3	z	2	NAG	C4-C5-C6-O6
7	EA	11	GAL	C4-C5-C6-O6
7	pA	11	GAL	C4-C5-C6-O6
10	5A	1	NAG	C4-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
3	kA	2	NAG	C4-C5-C6-O6
10	1A	2	NAG	C4-C5-C6-O6
2	AA	2	NAG	O5-C5-C6-O6
2	nA	7	MAN	O5-C5-C6-O6
3	WA	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	bA	3	BMA	O5-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6
3	0	3	BMA	C4-C5-C6-O6
3	HA	3	BMA	C4-C5-C6-O6
3	QA	1	NAG	C4-C5-C6-O6
3	gA	1	NAG	C4-C5-C6-O6
6	x	2	NAG	C4-C5-C6-O6
8	vA	3	BMA	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	m	2	NAG	C4-C5-C6-O6
3	WA	1	NAG	C4-C5-C6-O6
7	d	2	NAG	C4-C5-C6-O6
7	d	11	GAL	C4-C5-C6-O6
7	pA	7	NAG	O5-C5-C6-O6
2	b	7	MAN	C4-C5-C6-O6
2	LA	2	NAG	C4-C5-C6-O6
2	qA	4	MAN	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	u	2	NAG	C4-C5-C6-O6
3	v	1	NAG	C4-C5-C6-O6
3	VA	2	NAG	C4-C5-C6-O6
7	d	4	MAN	C4-C5-C6-O6
9	OA	1	NAG	C4-C5-C6-O6
10	3A	1	NAG	C4-C5-C6-O6
2	S	1	NAG	O5-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
2	lA	2	NAG	O5-C5-C6-O6
3	P	3	BMA	O5-C5-C6-O6
3	9	1	NAG	O5-C5-C6-O6
3	GA	4	MAN	O5-C5-C6-O6
3	rA	4	MAN	O5-C5-C6-O6
2	NA	2	NAG	C4-C5-C6-O6
3	1	1	NAG	C4-C5-C6-O6
3	bA	3	BMA	C4-C5-C6-O6
3	sA	3	BMA	C4-C5-C6-O6
7	EA	2	NAG	C4-C5-C6-O6
8	vA	1	NAG	C4-C5-C6-O6
10	4A	1	NAG	C4-C5-C6-O6
2	3	1	NAG	O5-C5-C6-O6
2	CA	2	NAG	O5-C5-C6-O6
3	f	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	s	3	BMA	O5-C5-C6-O6
4	F	8	MAN	O5-C5-C6-O6
4	q	3	BMA	O5-C5-C6-O6
10	7A	3	BMA	O5-C5-C6-O6
3	g	3	BMA	C4-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	eA	1	NAG	O5-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	5	1	NAG	O5-C5-C6-O6
10	1A	2	NAG	O5-C5-C6-O6
10	5A	1	NAG	O5-C5-C6-O6
10	6A	1	NAG	O5-C5-C6-O6
2	e	4	MAN	C4-C5-C6-O6
2	FA	4	MAN	C4-C5-C6-O6
2	lA	1	NAG	C4-C5-C6-O6
6	YA	2	NAG	C4-C5-C6-O6
7	EA	4	MAN	C4-C5-C6-O6
7	pA	1	NAG	C4-C5-C6-O6
7	pA	4	MAN	C4-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
6	M	2	NAG	C4-C5-C6-O6
3	hA	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	a	2	NAG	C8-C7-N2-C2
3	a	2	NAG	O7-C7-N2-C2
3	c	1	NAG	C8-C7-N2-C2
3	c	1	NAG	O7-C7-N2-C2
3	h	2	NAG	C8-C7-N2-C2
3	h	2	NAG	O7-C7-N2-C2
3	t	2	NAG	C8-C7-N2-C2
3	t	2	NAG	O7-C7-N2-C2
3	v	1	NAG	C8-C7-N2-C2
3	v	1	NAG	O7-C7-N2-C2
3	v	2	NAG	C8-C7-N2-C2
3	v	2	NAG	O7-C7-N2-C2
3	BA	2	NAG	C8-C7-N2-C2
3	BA	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	DA	1	NAG	C8-C7-N2-C2
3	DA	1	NAG	O7-C7-N2-C2
3	IA	2	NAG	C8-C7-N2-C2
3	IA	2	NAG	O7-C7-N2-C2
3	UA	2	NAG	C8-C7-N2-C2
3	UA	2	NAG	O7-C7-N2-C2
3	WA	1	NAG	C8-C7-N2-C2
3	WA	1	NAG	O7-C7-N2-C2
3	WA	2	NAG	C8-C7-N2-C2
3	WA	2	NAG	O7-C7-N2-C2
3	mA	2	NAG	C8-C7-N2-C2
3	mA	2	NAG	O7-C7-N2-C2
3	oA	1	NAG	C8-C7-N2-C2
3	oA	1	NAG	O7-C7-N2-C2
3	tA	2	NAG	C8-C7-N2-C2
3	tA	2	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
5	r	2	NAG	C8-C7-N2-C2
5	r	2	NAG	O7-C7-N2-C2
5	SA	2	NAG	C8-C7-N2-C2
5	SA	2	NAG	O7-C7-N2-C2
9	n	1	NAG	C8-C7-N2-C2
9	n	1	NAG	O7-C7-N2-C2
9	OA	1	NAG	C8-C7-N2-C2
9	OA	1	NAG	O7-C7-N2-C2
9	zA	1	NAG	C8-C7-N2-C2
9	zA	1	NAG	O7-C7-N2-C2
8	j	1	NAG	O5-C5-C6-O6
2	dA	1	NAG	C4-C5-C6-O6
2	nA	7	MAN	C4-C5-C6-O6
2	wA	2	NAG	C4-C5-C6-O6
3	P	3	BMA	C4-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
3	J	3	BMA	O5-C5-C6-O6
3	K	4	MAN	O5-C5-C6-O6
3	TA	3	BMA	O5-C5-C6-O6
3	VA	3	BMA	O5-C5-C6-O6
3	kA	1	NAG	O5-C5-C6-O6
4	q	7	MAN	O5-C5-C6-O6
7	EA	11	GAL	O5-C5-C6-O6
7	pA	11	GAL	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	b	2	NAG	C4-C5-C6-O6
2	yA	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	l	2	NAG	C4-C5-C6-O6
10	3A	2	NAG	C4-C5-C6-O6
2	PA	4	MAN	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	Y	1	NAG	O5-C5-C6-O6
3	u	3	BMA	O5-C5-C6-O6
4	RA	7	MAN	O5-C5-C6-O6
8	KA	1	NAG	O5-C5-C6-O6
3	V	1	NAG	C4-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6
2	o	4	MAN	O5-C5-C6-O6
3	gA	2	NAG	O5-C5-C6-O6
2	k	2	NAG	C4-C5-C6-O6
2	nA	2	NAG	C4-C5-C6-O6
3	s	2	NAG	C4-C5-C6-O6
3	9	3	BMA	C4-C5-C6-O6
3	TA	2	NAG	C4-C5-C6-O6
7	d	7	NAG	C4-C5-C6-O6
10	5A	4	MAN	C4-C5-C6-O6
2	w	1	NAG	O5-C5-C6-O6
2	XA	1	NAG	O5-C5-C6-O6
10	6A	1	NAG	C4-C5-C6-O6
4	F	7	MAN	O5-C5-C6-O6
2	dA	4	MAN	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	5	1	NAG	C4-C5-C6-O6
4	RA	2	NAG	O5-C5-C6-O6
7	d	11	GAL	O5-C5-C6-O6
2	R	4	MAN	C4-C5-C6-O6
2	w	2	NAG	C4-C5-C6-O6
7	EA	7	NAG	C4-C5-C6-O6
2	XA	1	NAG	C4-C5-C6-O6
3	6	1	NAG	C4-C5-C6-O6
3	gA	2	NAG	C4-C5-C6-O6
2	CA	7	MAN	O5-C5-C6-O6
3	5	2	NAG	O5-C5-C6-O6
2	w	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	oA	1	NAG	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	q	2	NAG	C4-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	w	4	MAN	C4-C5-C6-O6
3	5	2	NAG	C4-C5-C6-O6
3	DA	1	NAG	C4-C5-C6-O6
3	cA	1	NAG	C4-C5-C6-O6
10	3A	4	MAN	C4-C5-C6-O6
3	g	4	MAN	O5-C5-C6-O6
3	oA	1	NAG	O5-C5-C6-O6
2	L	4	MAN	C4-C5-C6-O6
3	DA	1	NAG	O5-C5-C6-O6
2	CA	7	MAN	C4-C5-C6-O6
2	2	4	MAN	C4-C5-C6-O6
4	F	9	MAN	O5-C5-C6-O6
2	XA	4	MAN	C4-C5-C6-O6
3	g	1	NAG	C4-C5-C6-O6
3	MA	2	NAG	C4-C5-C6-O6
3	sA	4	MAN	O5-C5-C6-O6
3	Y	3	BMA	C4-C5-C6-O6
3	9	2	NAG	C4-C5-C6-O6
3	kA	3	BMA	C4-C5-C6-O6
3	mA	3	BMA	O5-C5-C6-O6
4	q	9	MAN	O5-C5-C6-O6
3	c	1	NAG	C4-C5-C6-O6
3	s	2	NAG	O5-C5-C6-O6
3	cA	4	MAN	O5-C5-C6-O6
3	HA	1	NAG	C4-C5-C6-O6
3	sA	1	NAG	C4-C5-C6-O6
7	pA	7	NAG	C4-C5-C6-O6
2	AA	2	NAG	C4-C5-C6-O6
2	b	2	NAG	O5-C5-C6-O6
3	a	3	BMA	O5-C5-C6-O6
3	l	2	NAG	O5-C5-C6-O6
3	1	2	NAG	O5-C5-C6-O6
3	9	3	BMA	O5-C5-C6-O6
10	2A	1	NAG	C4-C5-C6-O6
3	HA	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	TA	2	NAG	O5-C5-C6-O6
2	o	3	BMA	C4-C5-C6-O6
2	nA	2	NAG	O5-C5-C6-O6
3	8	2	NAG	O5-C5-C6-O6
3	GA	4	MAN	C4-C5-C6-O6
3	rA	4	MAN	C4-C5-C6-O6
9	n	2	NAG	C4-C5-C6-O6
2	fA	2	NAG	O5-C5-C6-O6
3	c	1	NAG	O5-C5-C6-O6
3	jA	2	NAG	O5-C5-C6-O6
3	UA	2	NAG	C4-C5-C6-O6
3	0	2	NAG	O5-C5-C6-O6
3	BA	3	BMA	O5-C5-C6-O6
7	pA	2	NAG	O5-C5-C6-O6
10	1A	1	NAG	O5-C5-C6-O6
3	UA	1	NAG	O5-C5-C6-O6
3	UA	2	NAG	O5-C5-C6-O6
3	t	1	NAG	O5-C5-C6-O6
4	RA	9	MAN	O5-C5-C6-O6
2	fA	2	NAG	C4-C5-C6-O6
3	IA	2	NAG	C4-C5-C6-O6
2	4	2	NAG	O5-C5-C6-O6
3	Q	4	MAN	O5-C5-C6-O6
3	1	4	MAN	O5-C5-C6-O6
3	bA	2	NAG	O5-C5-C6-O6
3	8	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
2	iA	4	MAN	O5-C5-C6-O6
3	jA	2	NAG	C4-C5-C6-O6
2	i	1	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	f	4	MAN	C4-C5-C6-O6
2	S	3	BMA	O5-C5-C6-O6
2	o	3	BMA	O5-C5-C6-O6
3	cA	2	NAG	O5-C5-C6-O6
2	Z	2	NAG	C4-C5-C6-O6
3	Y	3	BMA	O5-C5-C6-O6
3	kA	3	BMA	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	q	2	NAG	O5-C5-C6-O6
2	4	2	NAG	C4-C5-C6-O6
2	lA	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	zA	2	NAG	C4-C5-C6-O6
3	t	2	NAG	C4-C5-C6-O6
6	x	3	BMA	C4-C5-C6-O6
10	1A	1	NAG	C4-C5-C6-O6
10	6A	3	BMA	C4-C5-C6-O6
2	3	3	BMA	O5-C5-C6-O6
10	3A	4	MAN	O5-C5-C6-O6
2	eA	3	BMA	O5-C5-C6-O6
2	w	4	MAN	O5-C5-C6-O6
8	j	1	NAG	C4-C5-C6-O6
10	2A	3	BMA	C4-C5-C6-O6
2	JA	1	NAG	O5-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
4	RA	3	BMA	C4-C5-C6-O6
6	YA	3	BMA	C4-C5-C6-O6
9	OA	2	NAG	C4-C5-C6-O6
3	g	1	NAG	O5-C5-C6-O6
3	s	1	NAG	O5-C5-C6-O6
4	RA	1	NAG	O5-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
7	d	6	GAL	C4-C5-C6-O6
2	eA	7	MAN	O5-C5-C6-O6
2	PA	3	BMA	C4-C5-C6-O6
7	EA	6	GAL	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	L	4	MAN	O5-C5-C6-O6
2	7	4	MAN	O5-C5-C6-O6
2	XA	4	MAN	O5-C5-C6-O6
2	nA	3	BMA	O5-C5-C6-O6
3	t	2	NAG	O5-C5-C6-O6
3	HA	1	NAG	O5-C5-C6-O6
3	MA	2	NAG	O5-C5-C6-O6
3	sA	1	NAG	O5-C5-C6-O6
7	pA	6	GAL	C4-C5-C6-O6
2	S	7	MAN	O5-C5-C6-O6
2	b	3	BMA	O5-C5-C6-O6
2	3	7	MAN	O5-C5-C6-O6
3	l	3	BMA	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	MA	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	TA	1	NAG	O5-C5-C6-O6
3	xA	3	BMA	O5-C5-C6-O6
2	CA	3	BMA	O5-C5-C6-O6
2	W	4	MAN	O5-C5-C6-O6
2	e	3	BMA	O5-C5-C6-O6
2	NA	1	NAG	C4-C5-C6-O6
3	xA	2	NAG	C4-C5-C6-O6
6	M	3	BMA	C4-C5-C6-O6
8	KA	1	NAG	C4-C5-C6-O6
10	5A	3	BMA	C4-C5-C6-O6
4	q	1	NAG	O5-C5-C6-O6
3	tA	2	NAG	C4-C5-C6-O6
2	FA	3	BMA	O5-C5-C6-O6
2	qA	3	BMA	O5-C5-C6-O6
3	z	3	BMA	C4-C5-C6-O6
2	b	4	MAN	O5-C5-C6-O6
2	CA	4	MAN	O5-C5-C6-O6
2	nA	4	MAN	O5-C5-C6-O6
10	2A	1	NAG	O5-C5-C6-O6
3	9	1	NAG	C4-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
2	PA	3	BMA	O5-C5-C6-O6
3	xA	4	MAN	O5-C5-C6-O6
2	S	1	NAG	C4-C5-C6-O6
2	FA	1	NAG	C4-C5-C6-O6
2	Z	4	MAN	O5-C5-C6-O6
2	3	1	NAG	C4-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
5	r	2	NAG	C4-C5-C6-O6
3	O	3	BMA	C4-C5-C6-O6
2	AA	4	MAN	O5-C5-C6-O6
2	fA	5	MAN	O5-C5-C6-O6
3	h	2	NAG	C4-C5-C6-O6
10	2A	3	BMA	O5-C5-C6-O6
3	aA	3	BMA	C4-C5-C6-O6
8	vA	2	NAG	C4-C5-C6-O6
10	6A	3	BMA	O5-C5-C6-O6
2	eA	1	NAG	C4-C5-C6-O6
3	l	4	MAN	O5-C5-C6-O6
3	IA	2	NAG	O5-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	lA	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	P	2	NAG	C4-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
3	MA	4	MAN	O5-C5-C6-O6
4	q	3	BMA	C4-C5-C6-O6
6	x	3	BMA	O5-C5-C6-O6
2	T	4	MAN	O5-C5-C6-O6
2	4	4	MAN	O5-C5-C6-O6
10	4A	2	NAG	O5-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
6	YA	3	BMA	O5-C5-C6-O6
2	m	1	NAG	C4-C5-C6-O6
2	2	1	NAG	C1-C2-N2-C7
2	dA	1	NAG	C1-C2-N2-C7
3	Q	1	NAG	C1-C2-N2-C7
3	Q	2	NAG	C1-C2-N2-C7
3	V	1	NAG	C1-C2-N2-C7
3	c	2	NAG	C1-C2-N2-C7
3	l	2	NAG	C1-C2-N2-C7
3	1	1	NAG	C1-C2-N2-C7
3	1	2	NAG	C1-C2-N2-C7
3	6	1	NAG	C1-C2-N2-C7
3	DA	2	NAG	C1-C2-N2-C7
3	MA	2	NAG	C1-C2-N2-C7
3	cA	1	NAG	C1-C2-N2-C7
3	cA	2	NAG	C1-C2-N2-C7
3	hA	1	NAG	C1-C2-N2-C7
3	mA	1	NAG	C1-C2-N2-C7
3	oA	2	NAG	C1-C2-N2-C7
5	G	5	NAG	C1-C2-N2-C7
5	r	5	NAG	C1-C2-N2-C7
5	SA	5	NAG	C1-C2-N2-C7
8	KA	2	NAG	C1-C2-N2-C7
8	vA	2	NAG	C1-C2-N2-C7
10	5A	3	BMA	O5-C5-C6-O6
2	qA	1	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	u	1	NAG	C4-C5-C6-O6
3	z	3	BMA	O5-C5-C6-O6
10	3A	3	BMA	C4-C5-C6-O6
2	2	1	NAG	O5-C5-C6-O6
3	VA	5	MAN	O5-C5-C6-O6
3	O	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	kA	1	NAG	C4-C5-C6-O6
2	wA	3	BMA	C4-C5-C6-O6
6	M	3	BMA	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	aA	3	BMA	O5-C5-C6-O6
3	v	4	MAN	C4-C5-C6-O6
3	Y	1	NAG	C4-C5-C6-O6
6	x	8	MAN	O5-C5-C6-O6
2	k	3	BMA	C4-C5-C6-O6
3	VA	5	MAN	C4-C5-C6-O6
3	5	3	BMA	O5-C5-C6-O6
5	r	2	NAG	O5-C5-C6-O6
6	x	8	MAN	C4-C5-C6-O6
3	u	5	MAN	O5-C5-C6-O6
2	fA	4	MAN	O5-C5-C6-O6
2	yA	1	NAG	C4-C5-C6-O6
2	LA	3	BMA	C4-C5-C6-O6
3	J	5	MAN	O5-C5-C6-O6
7	d	6	GAL	O5-C5-C6-O6
10	3A	3	BMA	O5-C5-C6-O6
3	gA	3	BMA	O5-C5-C6-O6
3	u	5	MAN	C4-C5-C6-O6
3	J	5	MAN	C4-C5-C6-O6
7	EA	6	GAL	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
2	CA	1	NAG	C4-C5-C6-O6
7	pA	6	GAL	O5-C5-C6-O6
3	cA	4	MAN	C4-C5-C6-O6
3	g	4	MAN	C4-C5-C6-O6
3	U	3	BMA	O5-C5-C6-O6
2	nA	1	NAG	C4-C5-C6-O6
3	oA	4	MAN	O5-C5-C6-O6
2	R	1	NAG	C3-C2-N2-C7
2	Z	2	NAG	C3-C2-N2-C7
2	b	1	NAG	C3-C2-N2-C7
2	2	1	NAG	C3-C2-N2-C7
2	AA	2	NAG	C3-C2-N2-C7
2	CA	1	NAG	C3-C2-N2-C7
2	dA	1	NAG	C3-C2-N2-C7
2	lA	2	NAG	C3-C2-N2-C7
2	nA	1	NAG	C3-C2-N2-C7
3	E	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	I	1	NAG	C3-C2-N2-C7
3	Q	1	NAG	C3-C2-N2-C7
3	U	1	NAG	C3-C2-N2-C7
3	V	1	NAG	C3-C2-N2-C7
3	a	1	NAG	C3-C2-N2-C7
3	c	2	NAG	C3-C2-N2-C7
3	h	1	NAG	C3-C2-N2-C7
3	p	2	NAG	C3-C2-N2-C7
3	t	1	NAG	C3-C2-N2-C7
3	1	1	NAG	C3-C2-N2-C7
3	1	2	NAG	C3-C2-N2-C7
3	5	1	NAG	C3-C2-N2-C7
3	6	1	NAG	C3-C2-N2-C7
3	BA	1	NAG	C3-C2-N2-C7
3	DA	2	NAG	C3-C2-N2-C7
3	IA	1	NAG	C3-C2-N2-C7
3	QA	2	NAG	C3-C2-N2-C7
3	UA	1	NAG	C3-C2-N2-C7
3	cA	1	NAG	C3-C2-N2-C7
3	cA	2	NAG	C3-C2-N2-C7
3	gA	1	NAG	C3-C2-N2-C7
3	hA	1	NAG	C3-C2-N2-C7
3	oA	2	NAG	C3-C2-N2-C7
3	tA	1	NAG	C3-C2-N2-C7
3	xA	2	NAG	C3-C2-N2-C7
5	r	5	NAG	C3-C2-N2-C7
8	j	1	NAG	C3-C2-N2-C7
8	j	2	NAG	C3-C2-N2-C7
8	KA	1	NAG	C3-C2-N2-C7
8	KA	2	NAG	C3-C2-N2-C7
8	vA	1	NAG	C3-C2-N2-C7
10	7A	1	NAG	C3-C2-N2-C7
2	nA	6	MAN	O5-C5-C6-O6
2	nA	6	MAN	C4-C5-C6-O6
2	CA	6	MAN	O5-C5-C6-O6
7	d	9	MAN	O5-C5-C6-O6
2	CA	6	MAN	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	xA	2	NAG	O5-C5-C6-O6
3	tA	2	NAG	O5-C5-C6-O6
3	DA	4	MAN	O5-C5-C6-O6
6	M	8	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	1	2	NAG	C4-C5-C6-O6
6	M	8	MAN	O5-C5-C6-O6
3	Q	4	MAN	C4-C5-C6-O6
2	b	6	MAN	O5-C5-C6-O6
3	f	7	MAN	O5-C5-C6-O6
5	r	6	GAL	O5-C5-C6-O6
6	YA	8	MAN	O5-C5-C6-O6
3	sA	4	MAN	C4-C5-C6-O6
4	q	4	MAN	C4-C5-C6-O6
6	YA	8	MAN	C4-C5-C6-O6
2	b	6	MAN	C4-C5-C6-O6
3	1	4	MAN	C4-C5-C6-O6
3	MA	1	NAG	O5-C5-C6-O6
4	q	4	MAN	O5-C5-C6-O6
3	h	2	NAG	O5-C5-C6-O6
3	xA	1	NAG	O5-C5-C6-O6
2	FA	1	NAG	O5-C5-C6-O6
3	hA	2	NAG	O5-C5-C6-O6
2	NA	1	NAG	O5-C5-C6-O6
3	c	4	MAN	O5-C5-C6-O6
2	L	3	BMA	C4-C5-C6-O6
8	vA	2	NAG	O5-C5-C6-O6
4	F	4	MAN	O5-C5-C6-O6
2	e	1	NAG	C4-C5-C6-O6
3	s	3	BMA	C4-C5-C6-O6
3	VA	1	NAG	C4-C5-C6-O6
3	WA	4	MAN	C4-C5-C6-O6
3	xA	1	NAG	C4-C5-C6-O6
3	HA	4	MAN	C4-C5-C6-O6
4	F	4	MAN	C4-C5-C6-O6
3	u	1	NAG	O5-C5-C6-O6
3	MA	1	NAG	C4-C5-C6-O6
3	0	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C1-C2-N2-C7
2	R	1	NAG	C1-C2-N2-C7
2	Z	2	NAG	C1-C2-N2-C7
2	b	1	NAG	C1-C2-N2-C7
2	7	2	NAG	C1-C2-N2-C7
2	AA	2	NAG	C1-C2-N2-C7
2	CA	1	NAG	C1-C2-N2-C7
2	lA	2	NAG	C1-C2-N2-C7
2	nA	1	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C1-C2-N2-C7
3	I	1	NAG	C1-C2-N2-C7
3	K	1	NAG	C1-C2-N2-C7
3	U	1	NAG	C1-C2-N2-C7
3	a	1	NAG	C1-C2-N2-C7
3	a	2	NAG	C1-C2-N2-C7
3	h	1	NAG	C1-C2-N2-C7
3	p	2	NAG	C1-C2-N2-C7
3	t	1	NAG	C1-C2-N2-C7
3	v	1	NAG	C1-C2-N2-C7
3	y	2	NAG	C1-C2-N2-C7
3	5	1	NAG	C1-C2-N2-C7
3	BA	1	NAG	C1-C2-N2-C7
3	BA	2	NAG	C1-C2-N2-C7
3	IA	1	NAG	C1-C2-N2-C7
3	QA	2	NAG	C1-C2-N2-C7
3	UA	1	NAG	C1-C2-N2-C7
3	WA	1	NAG	C1-C2-N2-C7
3	gA	1	NAG	C1-C2-N2-C7
3	kA	2	NAG	C1-C2-N2-C7
3	mA	2	NAG	C1-C2-N2-C7
3	tA	1	NAG	C1-C2-N2-C7
3	xA	2	NAG	C1-C2-N2-C7
5	r	2	NAG	C1-C2-N2-C7
8	j	1	NAG	C1-C2-N2-C7
8	j	2	NAG	C1-C2-N2-C7
8	KA	1	NAG	C1-C2-N2-C7
8	vA	1	NAG	C1-C2-N2-C7
9	n	1	NAG	C1-C2-N2-C7
9	OA	1	NAG	C1-C2-N2-C7
9	zA	1	NAG	C1-C2-N2-C7
6	M	5	MAN	C4-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7
3	K	1	NAG	C3-C2-N2-C7
3	Q	2	NAG	C3-C2-N2-C7
3	a	2	NAG	C3-C2-N2-C7
3	l	2	NAG	C3-C2-N2-C7
3	p	1	NAG	C3-C2-N2-C7
3	v	1	NAG	C3-C2-N2-C7
3	BA	2	NAG	C3-C2-N2-C7
3	MA	2	NAG	C3-C2-N2-C7
3	QA	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	WA	1	NAG	C3-C2-N2-C7
3	mA	1	NAG	C3-C2-N2-C7
3	mA	2	NAG	C3-C2-N2-C7
5	G	5	NAG	C3-C2-N2-C7
5	r	2	NAG	C3-C2-N2-C7
5	SA	5	NAG	C3-C2-N2-C7
8	vA	2	NAG	C3-C2-N2-C7
9	n	1	NAG	C3-C2-N2-C7
9	OA	1	NAG	C3-C2-N2-C7
9	zA	1	NAG	C3-C2-N2-C7
3	bA	2	NAG	C4-C5-C6-O6
2	w	3	BMA	C4-C5-C6-O6
2	XA	3	BMA	C4-C5-C6-O6
3	a	3	BMA	C4-C5-C6-O6
3	f	5	MAN	C4-C5-C6-O6
3	a	4	MAN	C4-C5-C6-O6
3	ZA	1	NAG	C4-C5-C6-O6
2	CA	1	NAG	O5-C5-C6-O6
2	nA	1	NAG	O5-C5-C6-O6
4	RA	4	MAN	O5-C5-C6-O6
4	RA	4	MAN	C4-C5-C6-O6
7	d	1	NAG	C4-C5-C6-O6
6	M	5	MAN	O5-C5-C6-O6
3	5	4	MAN	O5-C5-C6-O6
3	cA	2	NAG	C4-C5-C6-O6
3	gA	4	MAN	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	mA	3	BMA	C4-C5-C6-O6
3	BA	3	BMA	C4-C5-C6-O6
3	TA	3	BMA	C4-C5-C6-O6
3	aA	1	NAG	C4-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6
2	b	1	NAG	C4-C5-C6-O6
3	xA	4	MAN	C4-C5-C6-O6
10	4A	3	BMA	C4-C5-C6-O6
3	mA	4	MAN	C4-C5-C6-O6
2	LA	1	NAG	O5-C5-C6-O6
3	6	4	MAN	O5-C5-C6-O6
10	1A	3	BMA	C4-C5-C6-O6
7	d	1	NAG	O5-C5-C6-O6
3	l	4	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	G	6	GAL	O5-C5-C6-O6
3	U	4	MAN	O5-C5-C6-O6

There are no ring outliers.

85 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	f	2	NAG	1	0
3	z	4	MAN	1	0
3	rA	2	NAG	1	0
3	y	1	NAG	1	0
3	WA	3	BMA	1	0
4	q	8	MAN	1	0
3	p	1	NAG	3	0
2	D	2	NAG	1	0
5	SA	5	NAG	1	0
8	j	5	MAN	1	0
3	K	1	NAG	1	0
2	D	1	NAG	1	0
10	3A	4	MAN	1	0
4	q	2	NAG	1	0
3	O	4	MAN	1	0
4	RA	8	MAN	1	0
3	aA	3	BMA	1	0
9	n	1	NAG	2	0
2	m	4	MAN	1	0
3	J	2	NAG	1	0
3	J	3	BMA	1	0
5	r	2	NAG	1	0
8	j	4	MAN	1	0
5	SA	4	MAN	1	0
3	z	3	BMA	1	0
3	H	1	NAG	1	0
5	G	1	NAG	1	0
2	o	2	NAG	1	0
2	e	1	NAG	1	0
5	G	5	NAG	1	0
2	qA	1	NAG	1	0
2	lA	4	MAN	1	0
2	Z	3	BMA	1	0
3	E	1	NAG	1	0
2	NA	6	MAN	1	0

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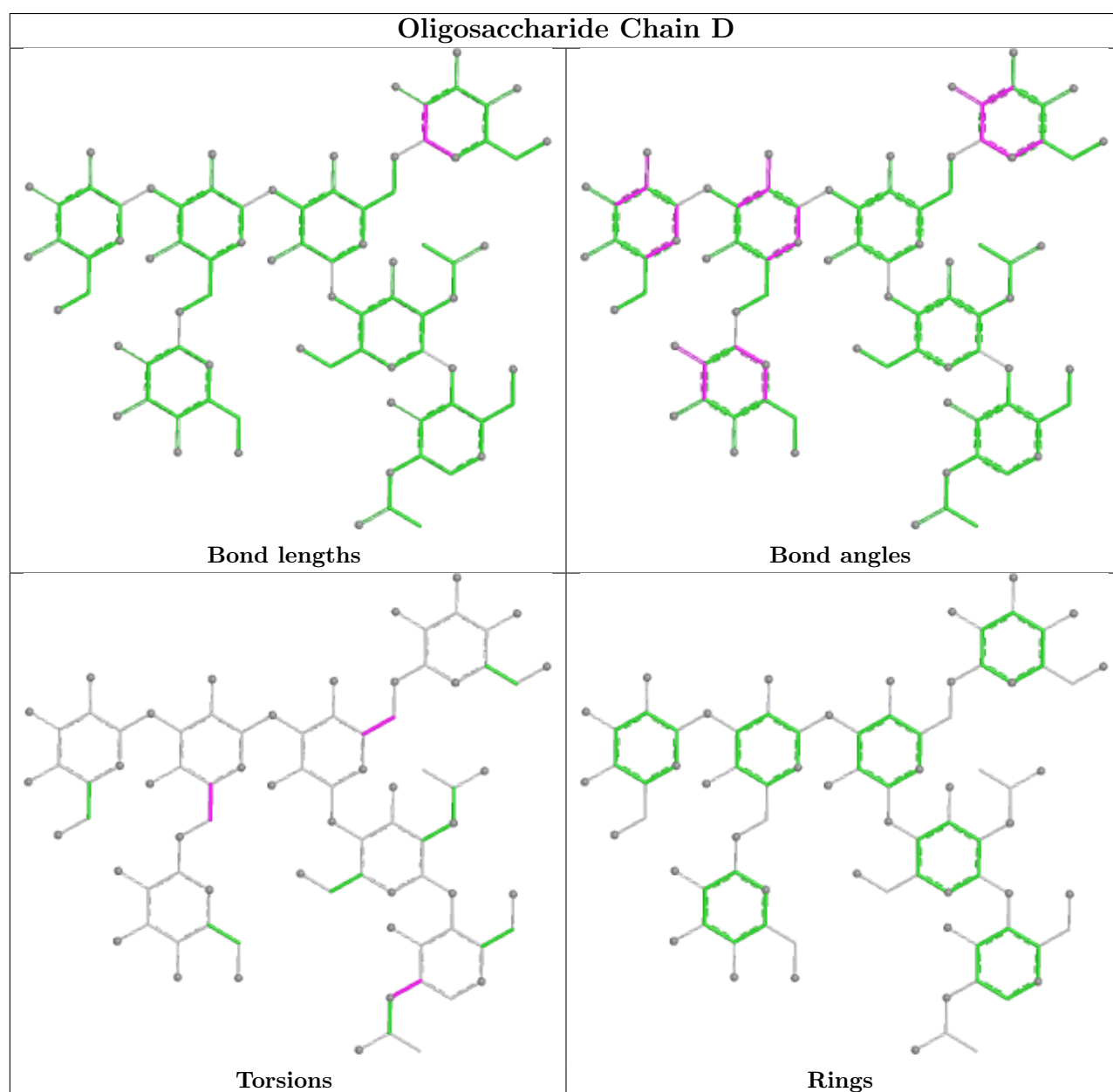
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	1	0
3	rA	1	NAG	1	0
3	u	2	NAG	1	0
2	Z	4	MAN	1	0
3	GA	1	NAG	1	0
9	OA	1	NAG	2	0
3	f	1	NAG	1	0
5	r	1	NAG	1	0
3	aA	4	MAN	1	0
2	PA	2	NAG	1	0
3	u	3	BMA	1	0
9	zA	1	NAG	1	0
3	a	2	NAG	1	0
4	q	1	NAG	1	0
3	K	3	BMA	1	0
5	G	4	MAN	1	0
4	RA	1	NAG	1	0
3	N	1	NAG	1	0
3	v	1	NAG	1	0
10	4A	1	NAG	1	0
4	F	1	NAG	1	0
7	pA	2	NAG	1	0
3	BA	2	NAG	1	0
2	m	6	MAN	1	0
3	WA	4	MAN	1	0
3	mA	2	NAG	1	0
9	OA	2	NAG	1	0
3	ZA	1	NAG	1	0
2	o	1	NAG	1	0
3	VA	2	NAG	1	0
3	s	1	NAG	1	0
5	SA	1	NAG	1	0
10	3A	1	NAG	2	0
3	E	2	NAG	1	0
3	TA	1	NAG	1	0
4	RA	2	NAG	1	0
3	O	3	BMA	1	0
8	j	3	BMA	1	0
3	K	4	MAN	1	0
2	lA	3	BMA	1	0
3	GA	2	NAG	1	0
2	FA	1	NAG	1	0

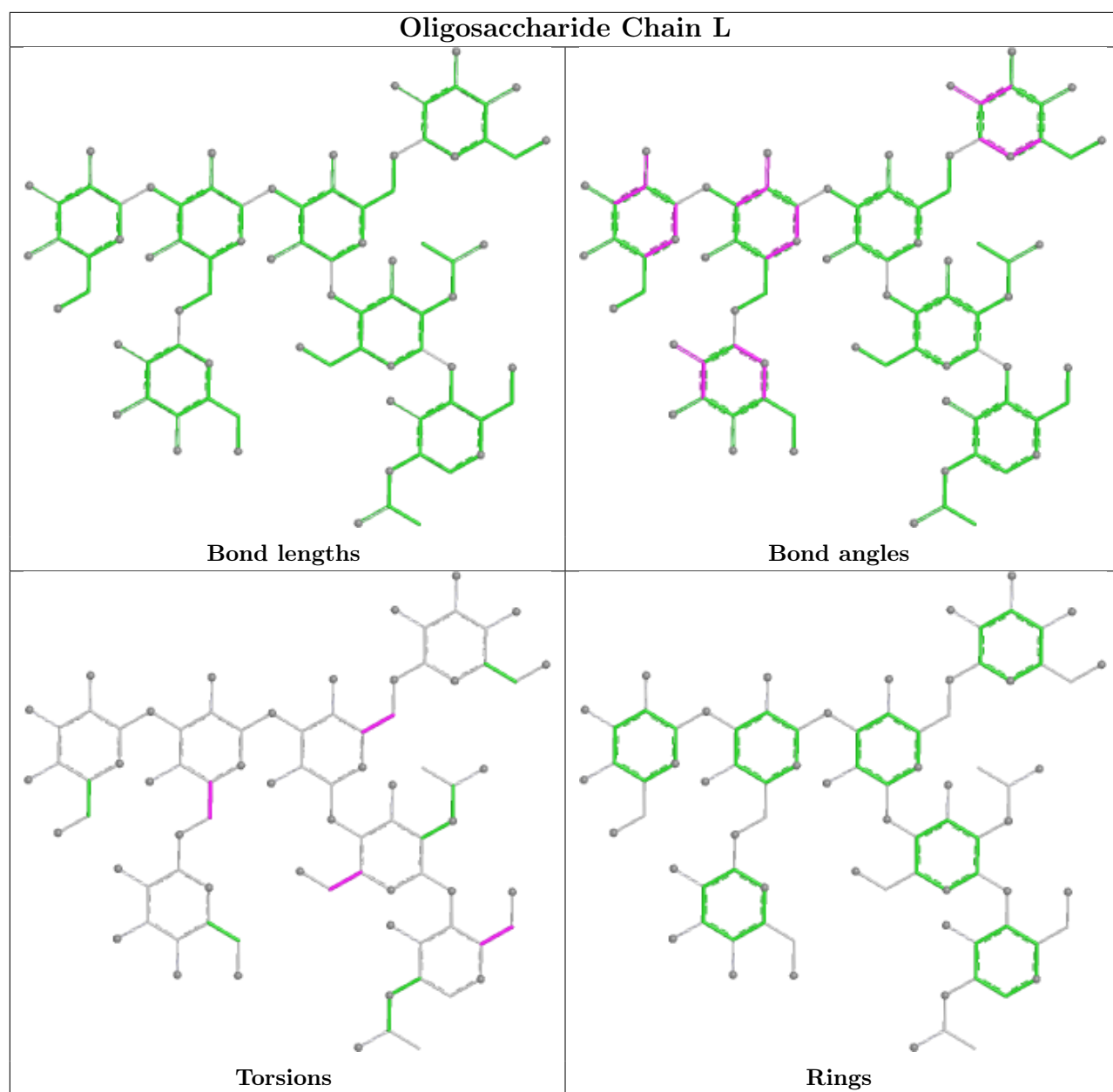
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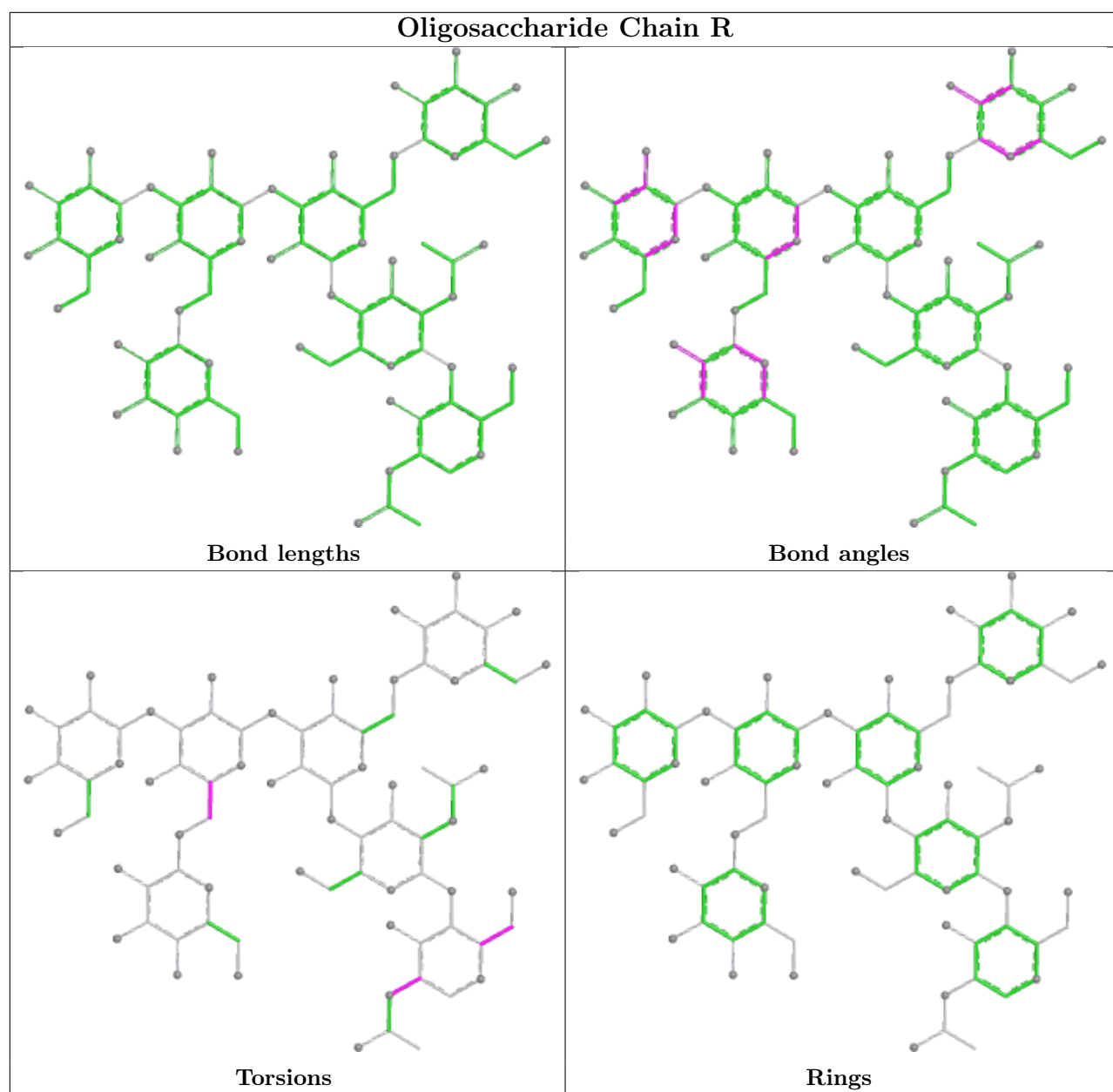
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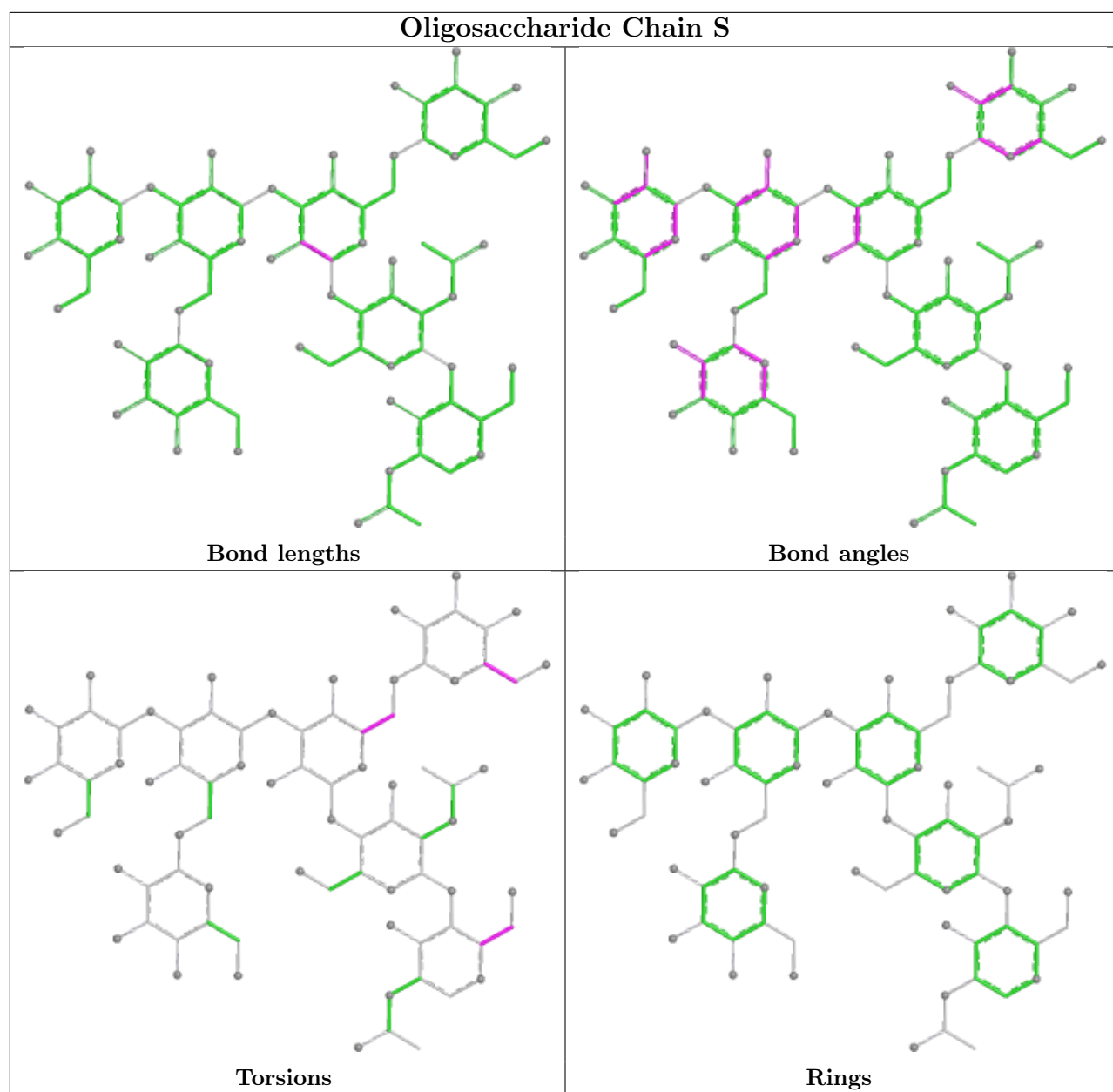
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	PA	1	NAG	1	0
4	q	9	MAN	1	0
2	NA	4	MAN	1	0
3	WA	1	NAG	1	0
8	vA	2	NAG	1	0
3	VA	3	BMA	1	0
10	3A	5	MAN	1	0
4	RA	9	MAN	1	0

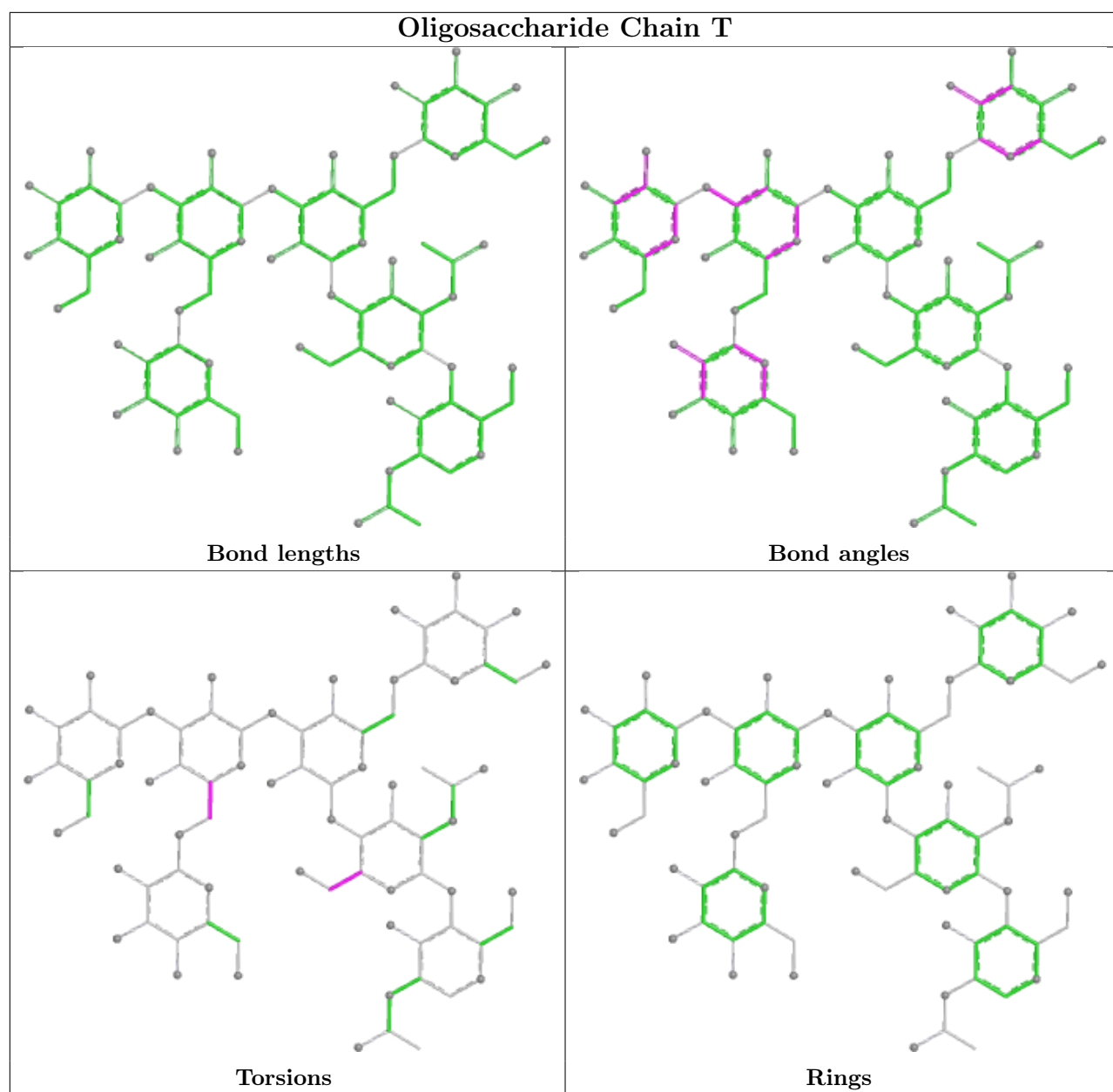
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

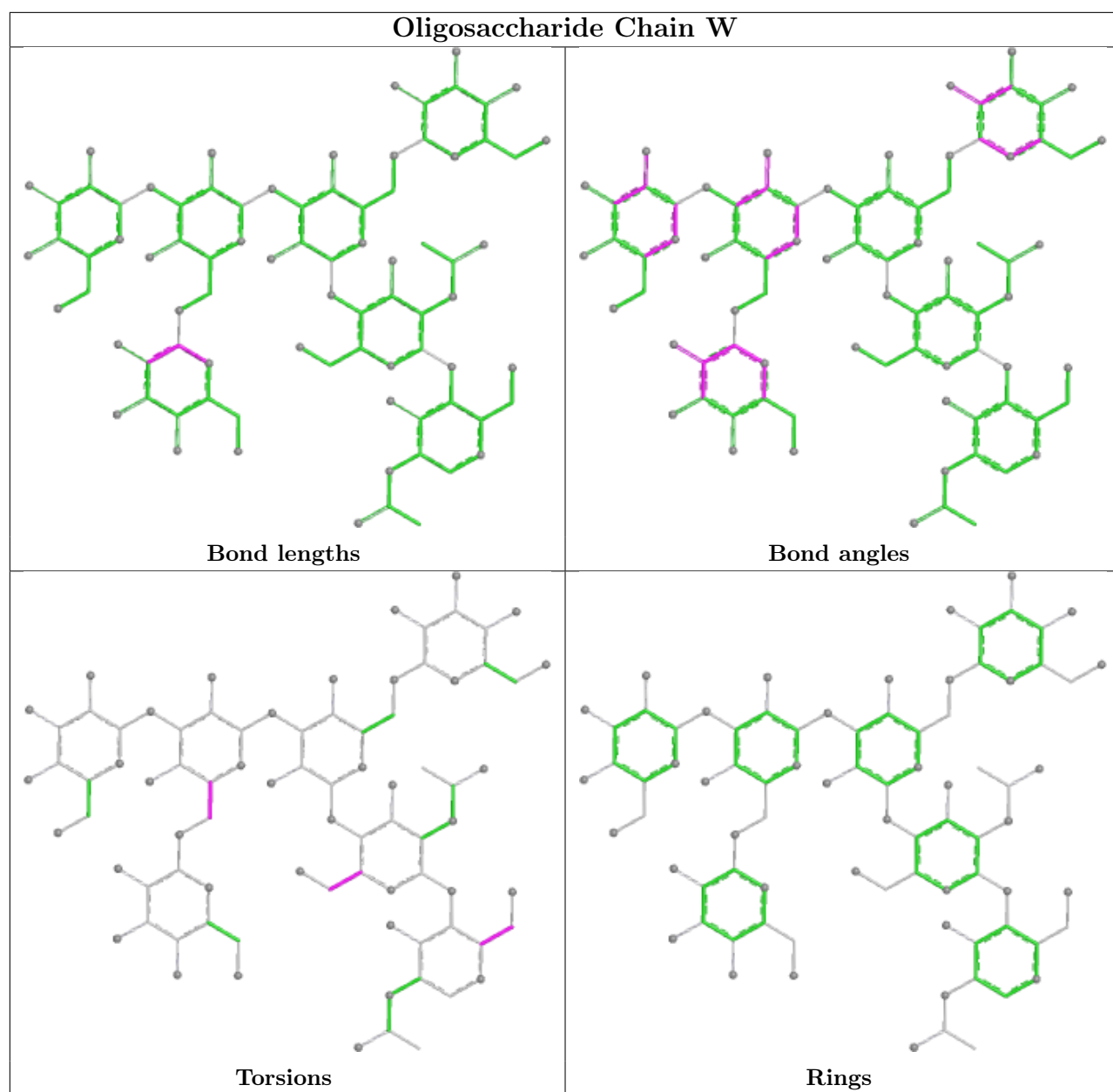


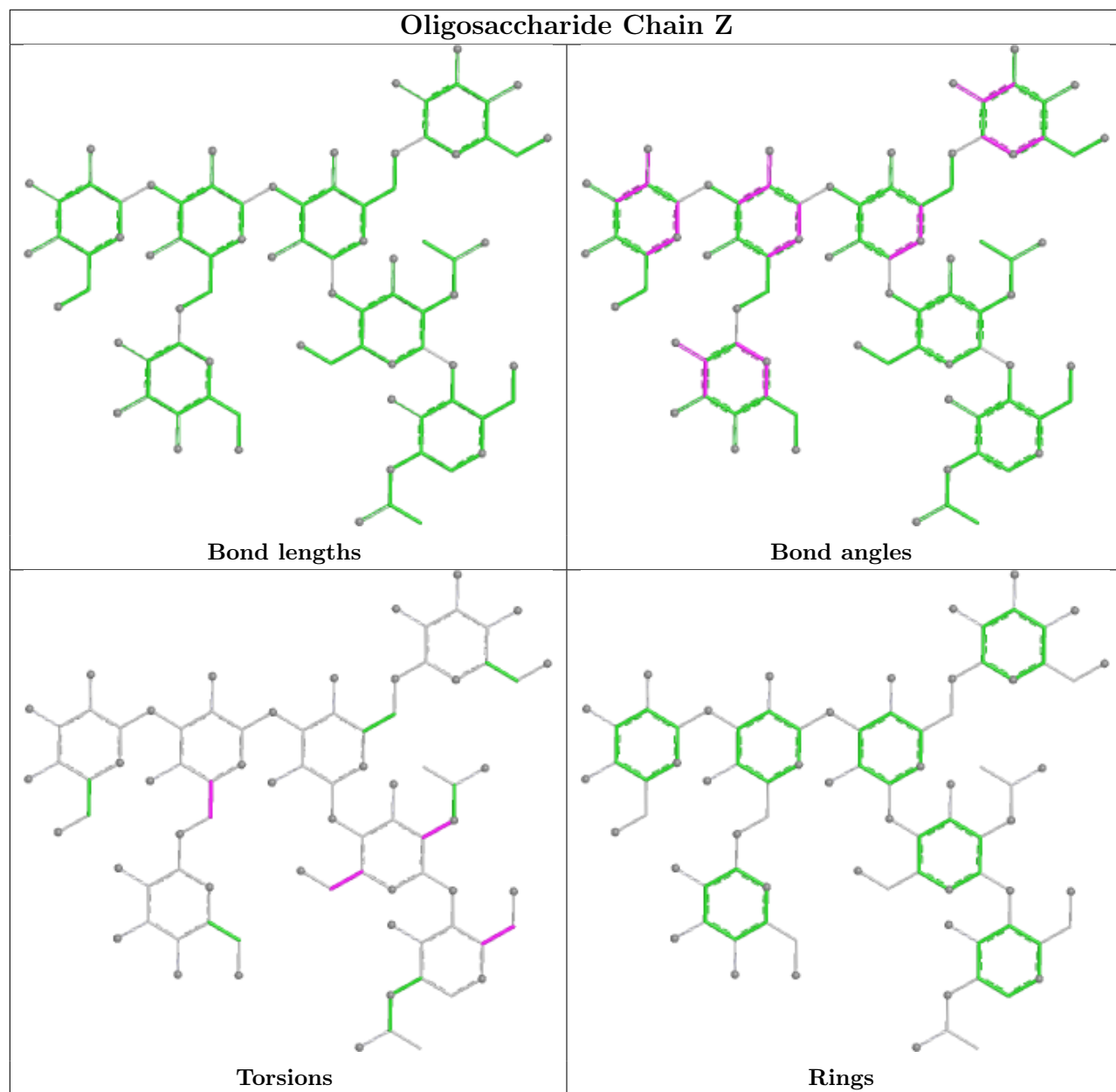


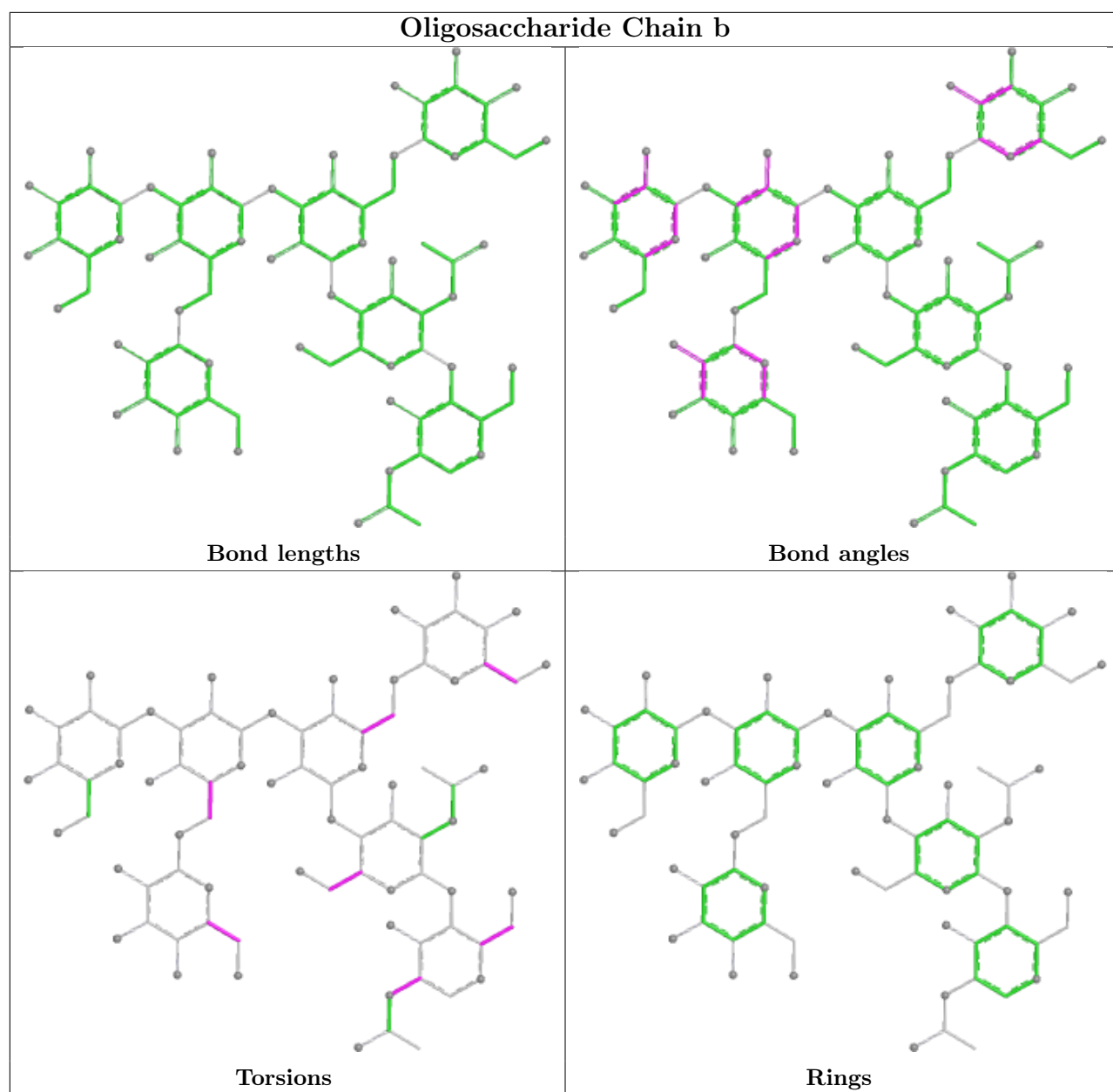


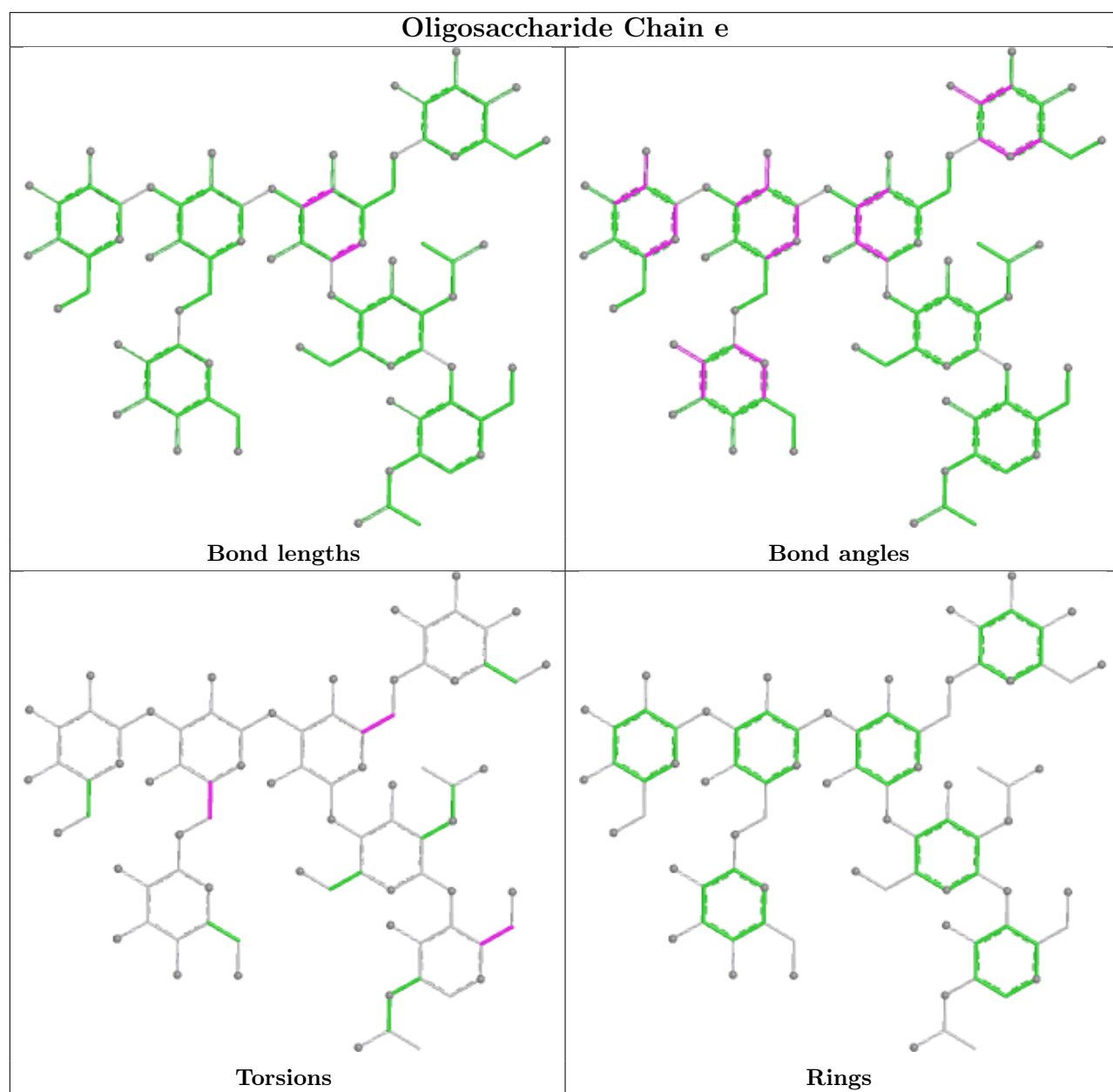


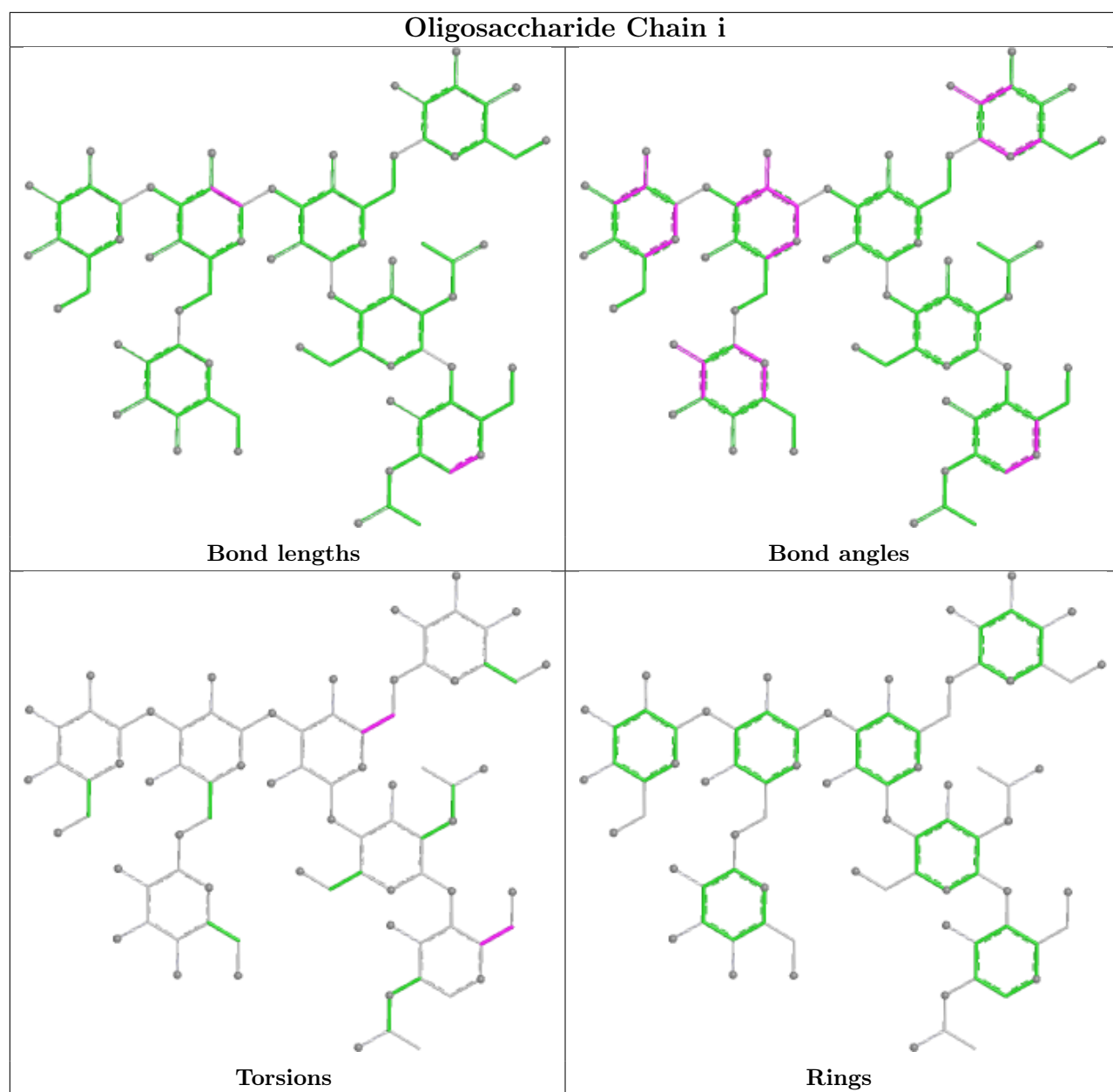


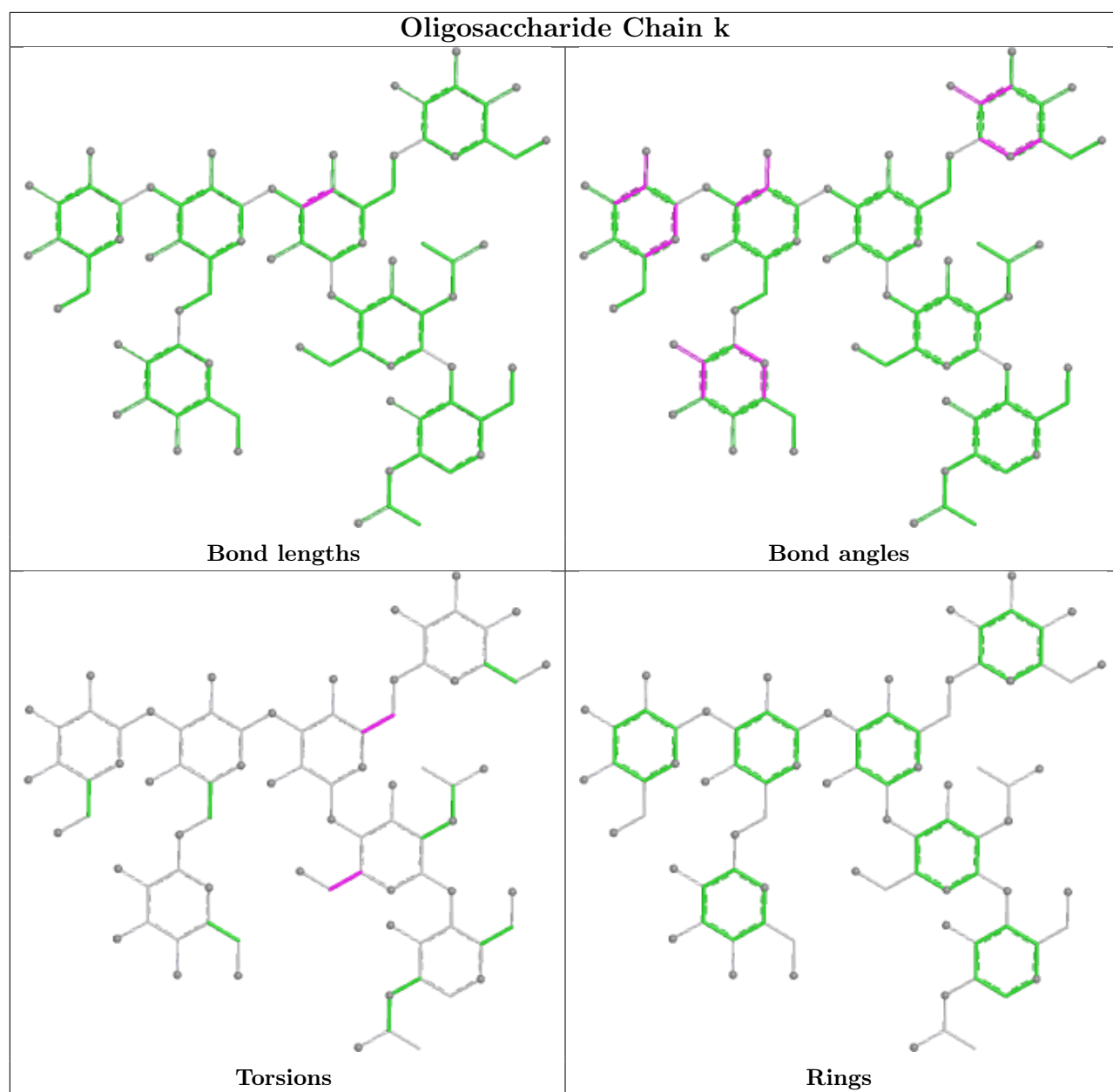


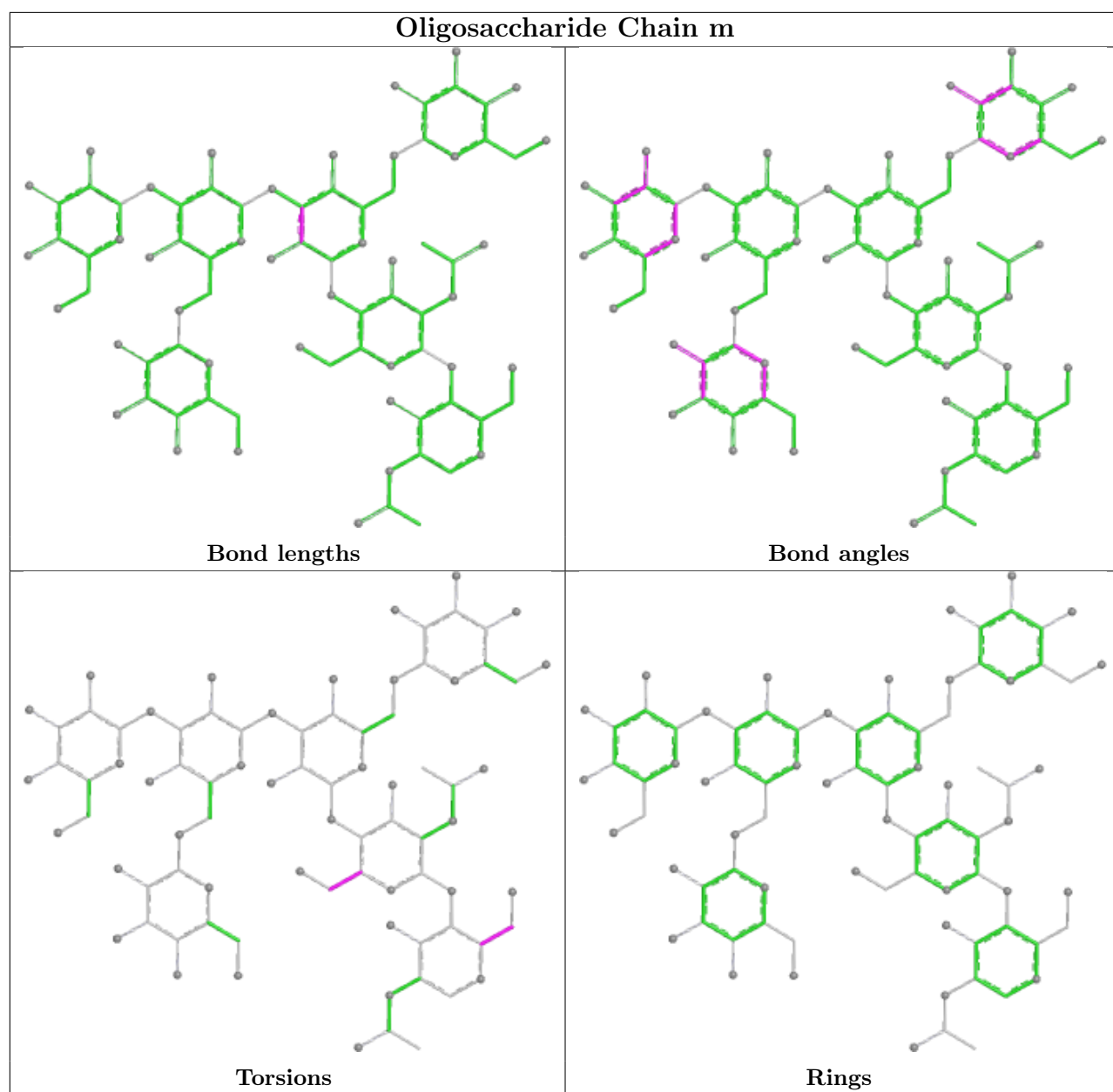


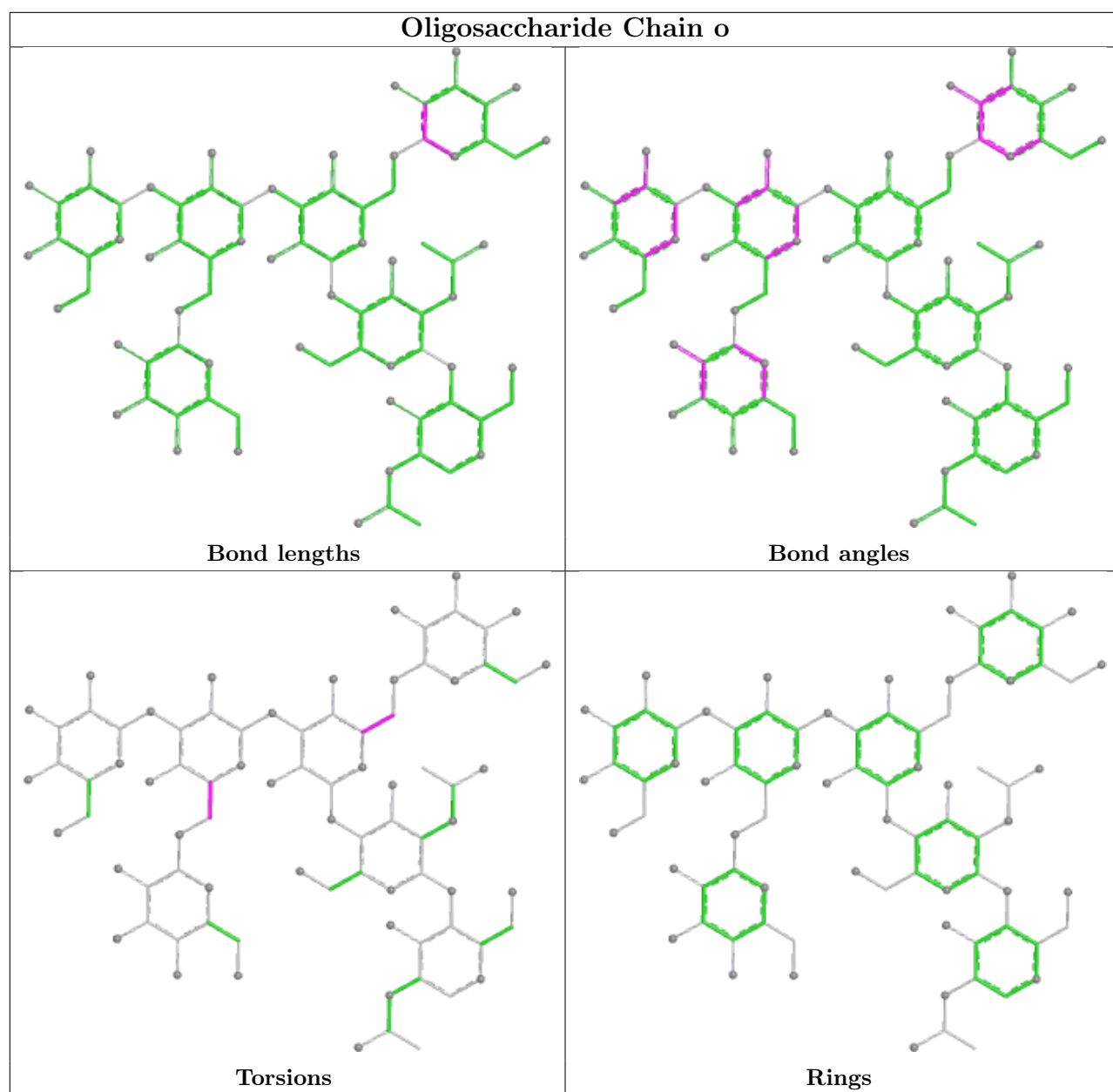


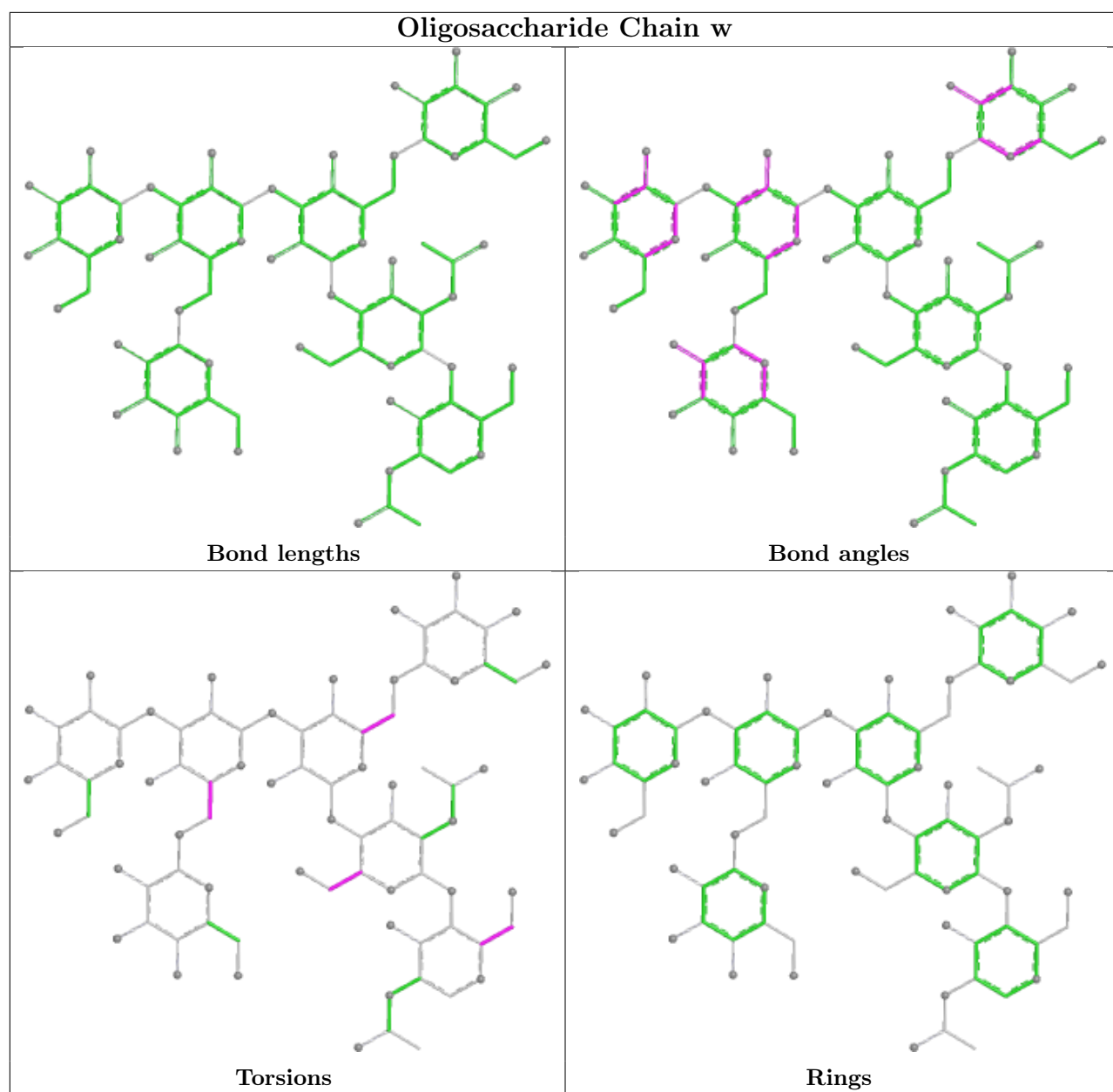


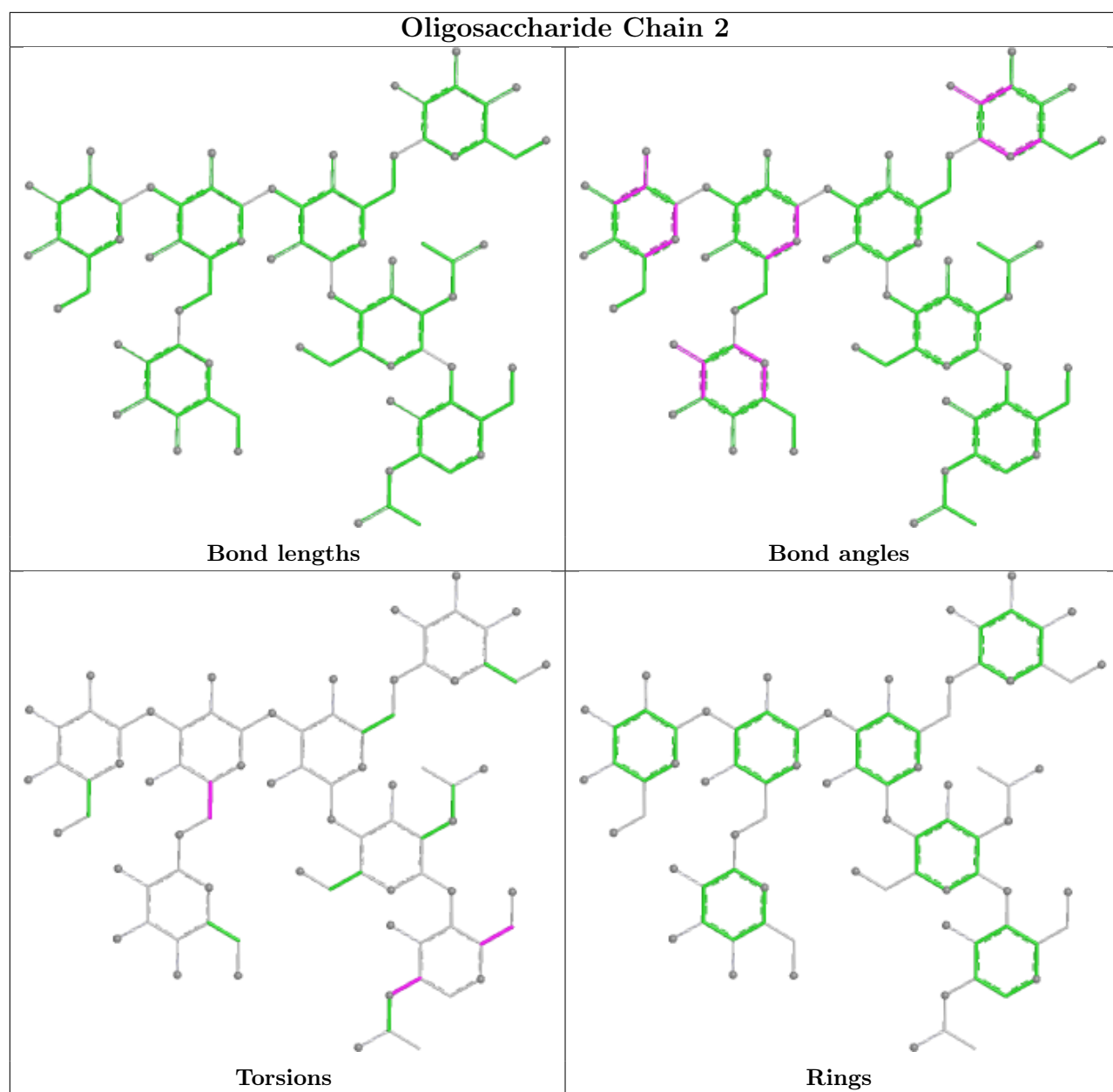


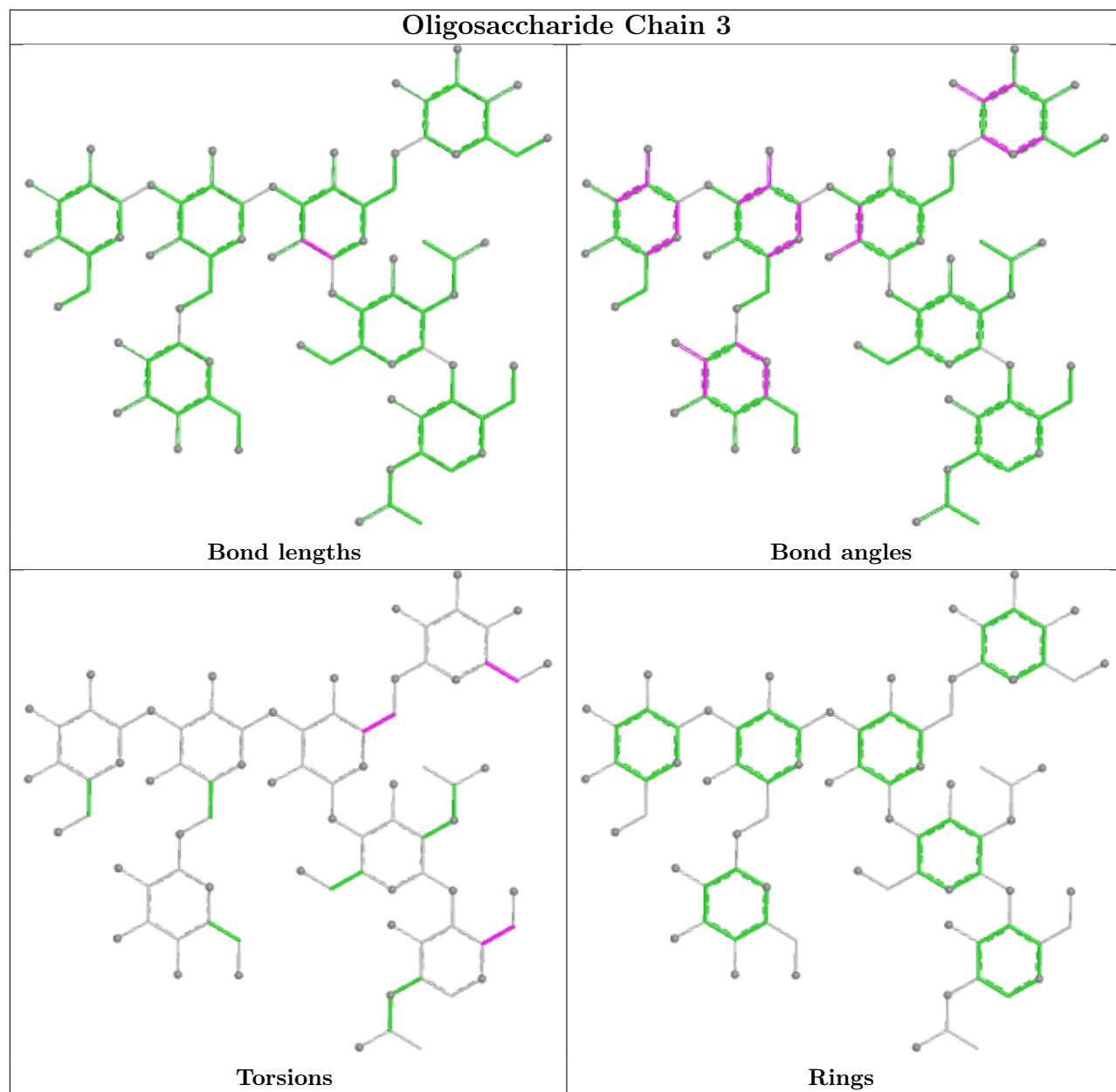


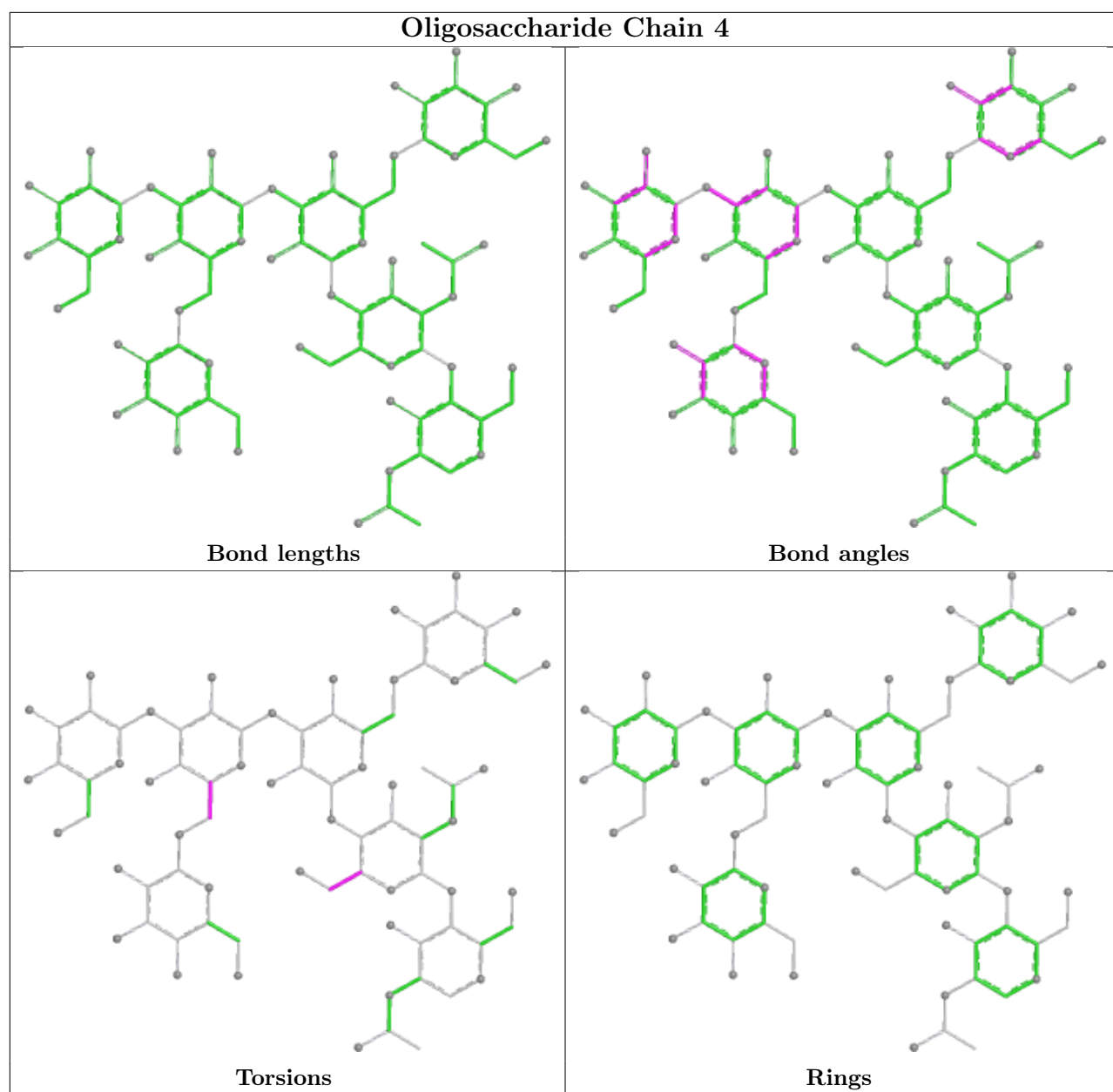


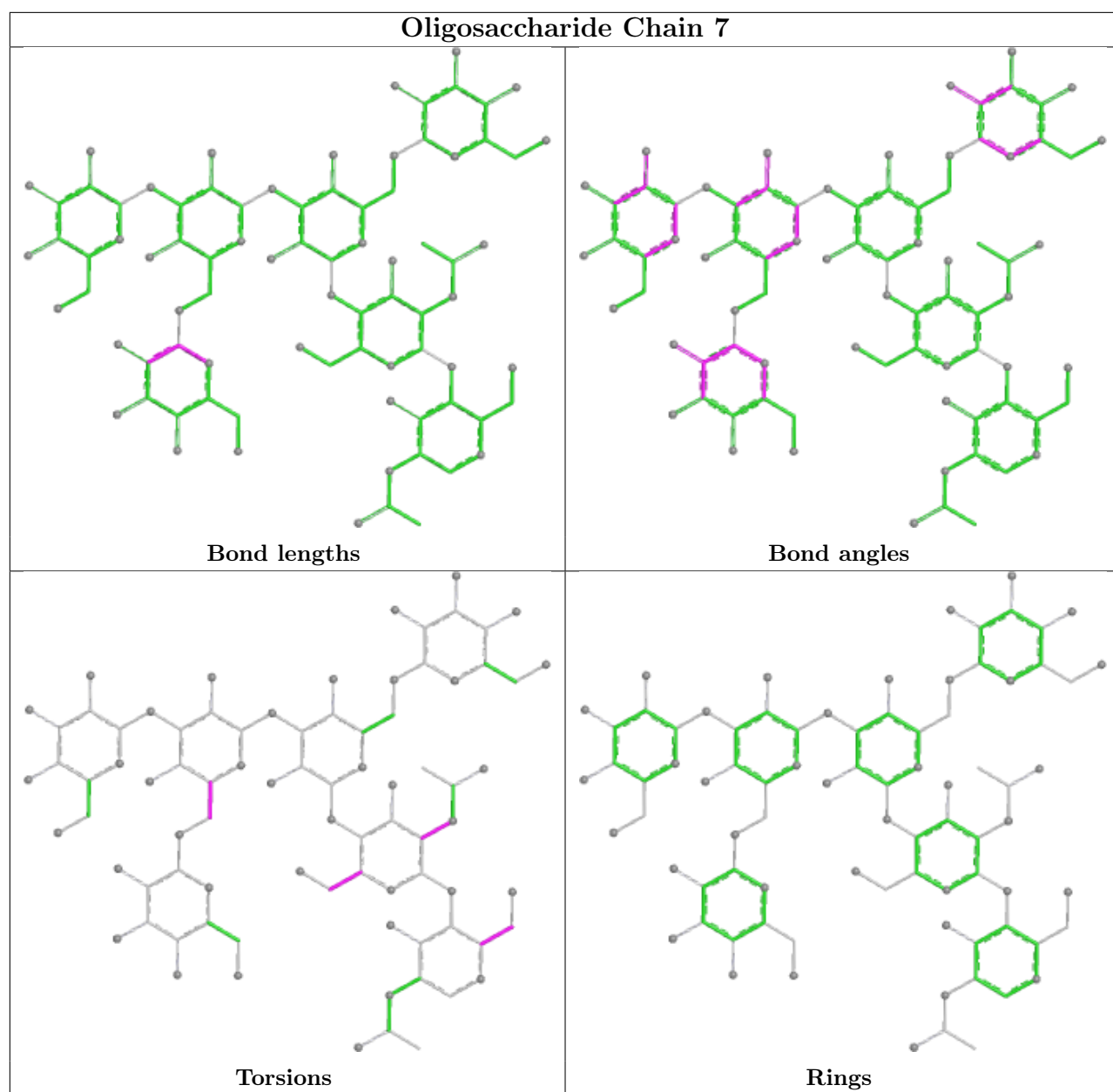


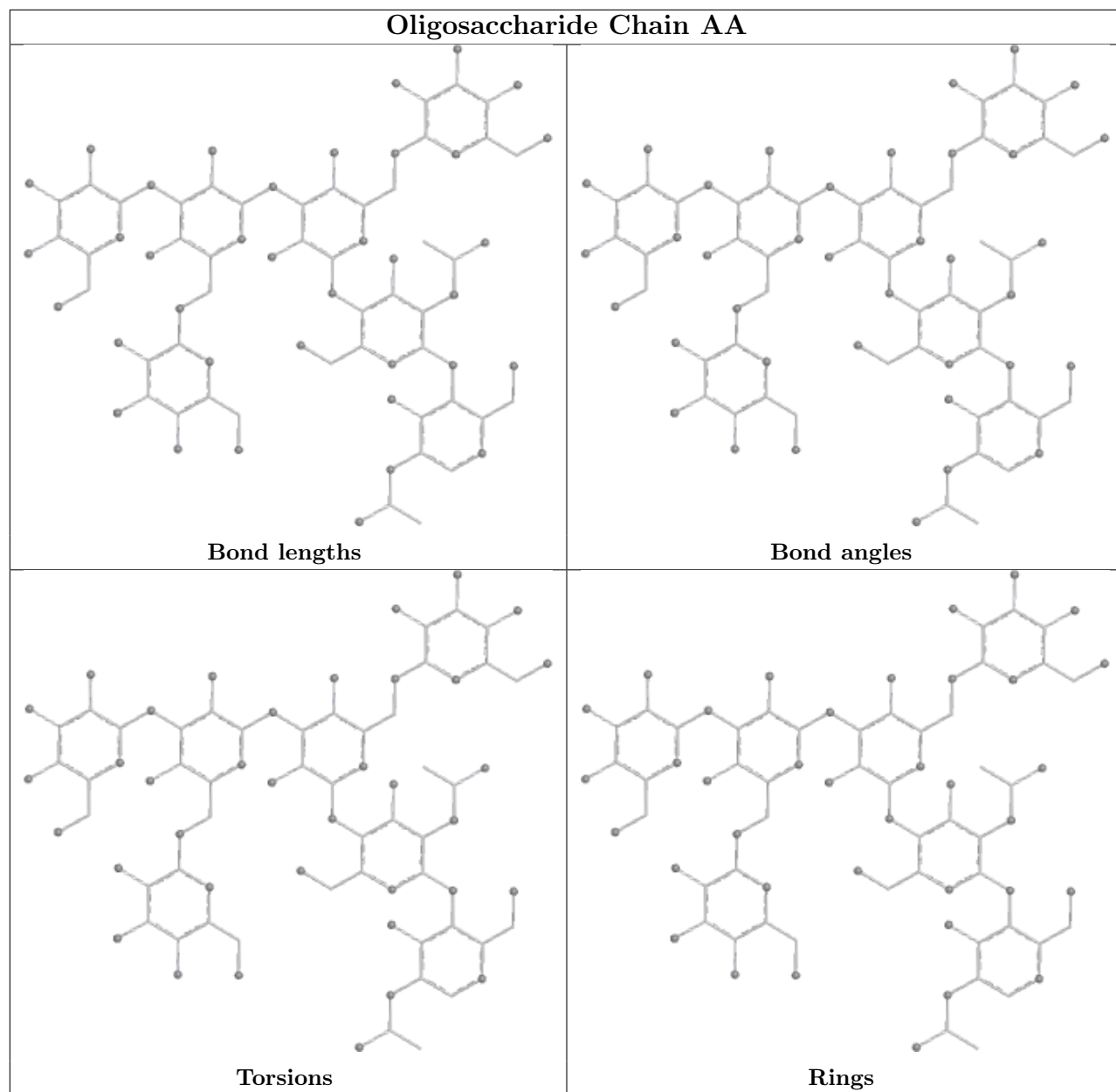


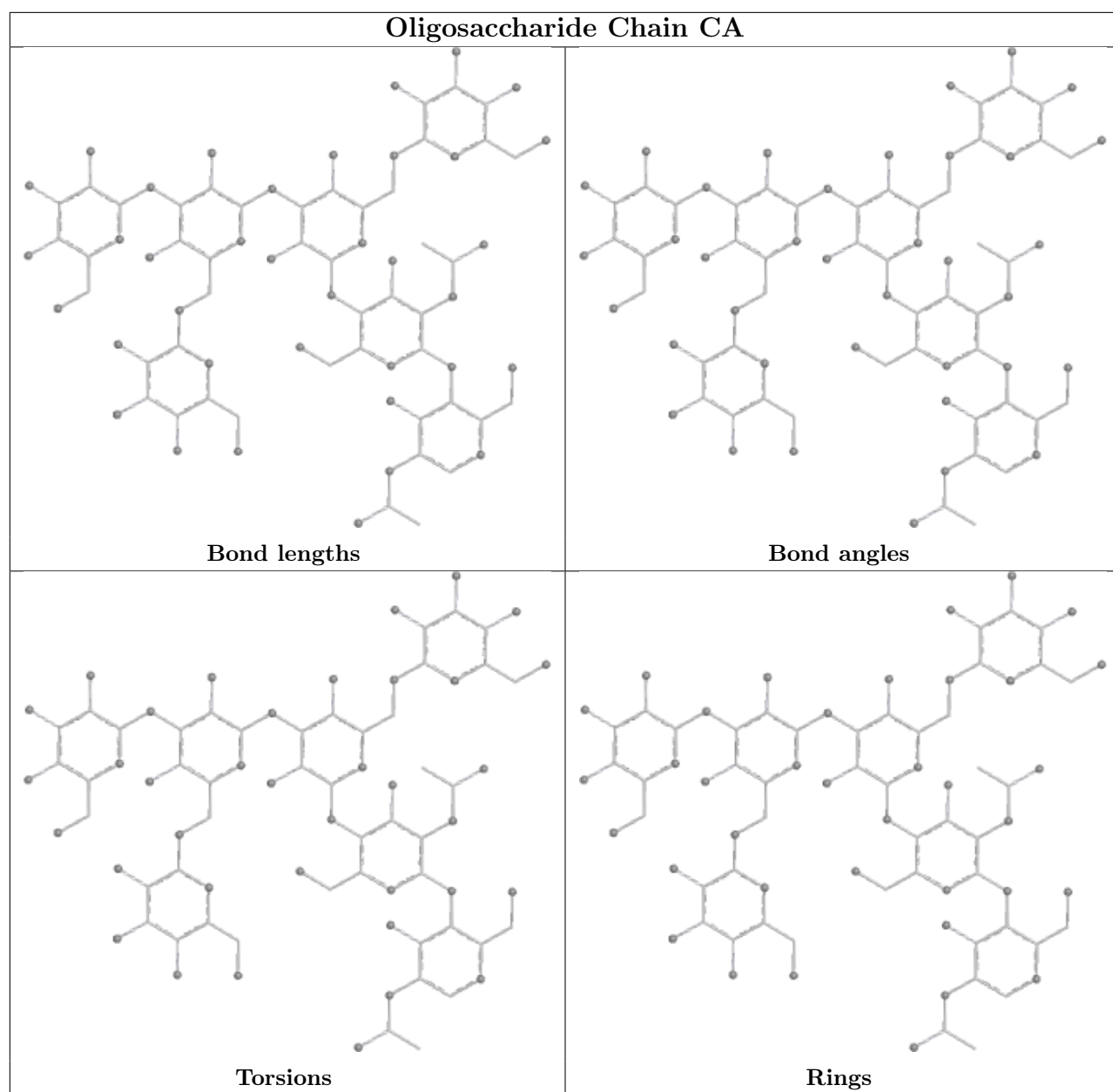


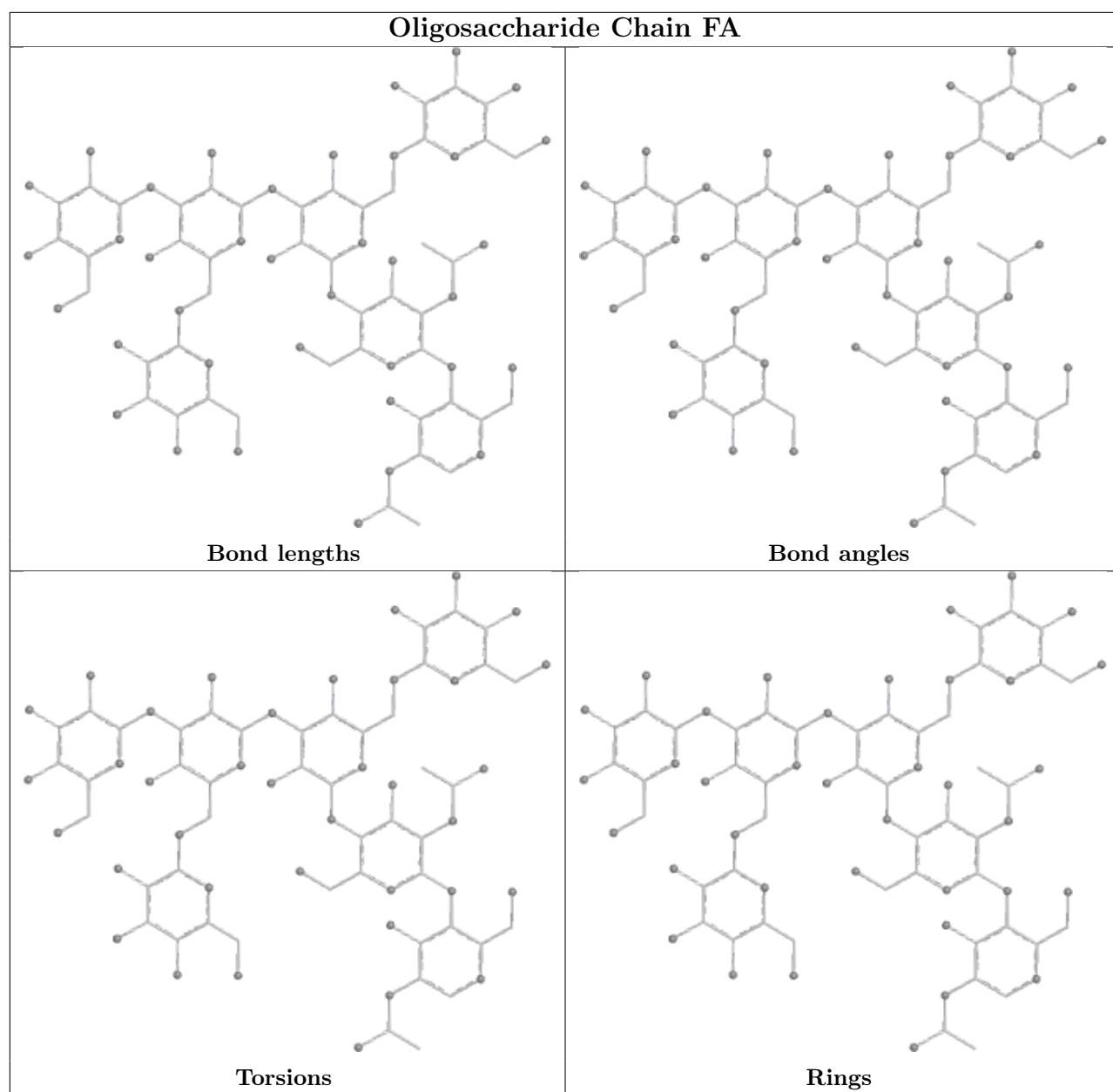


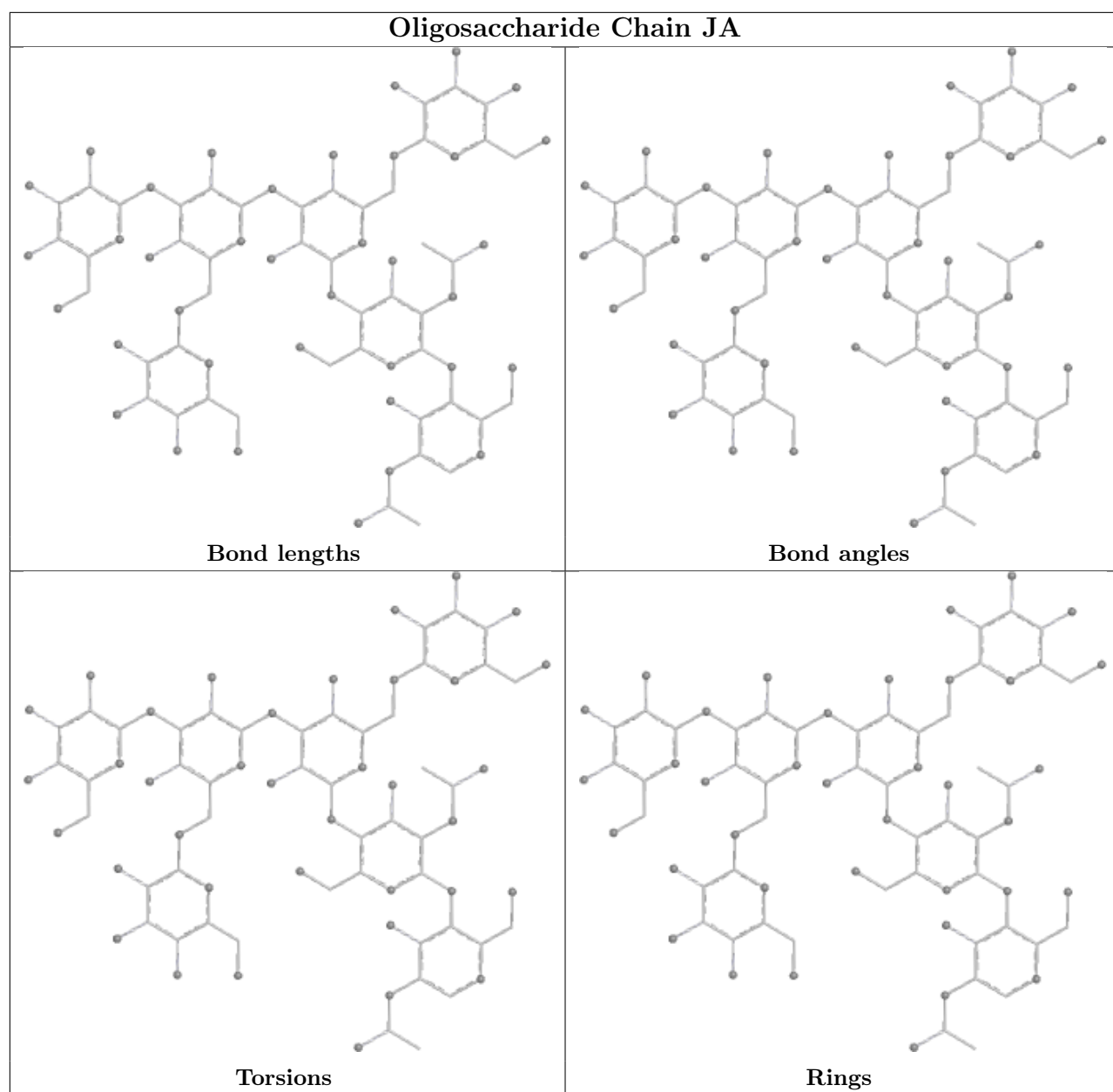


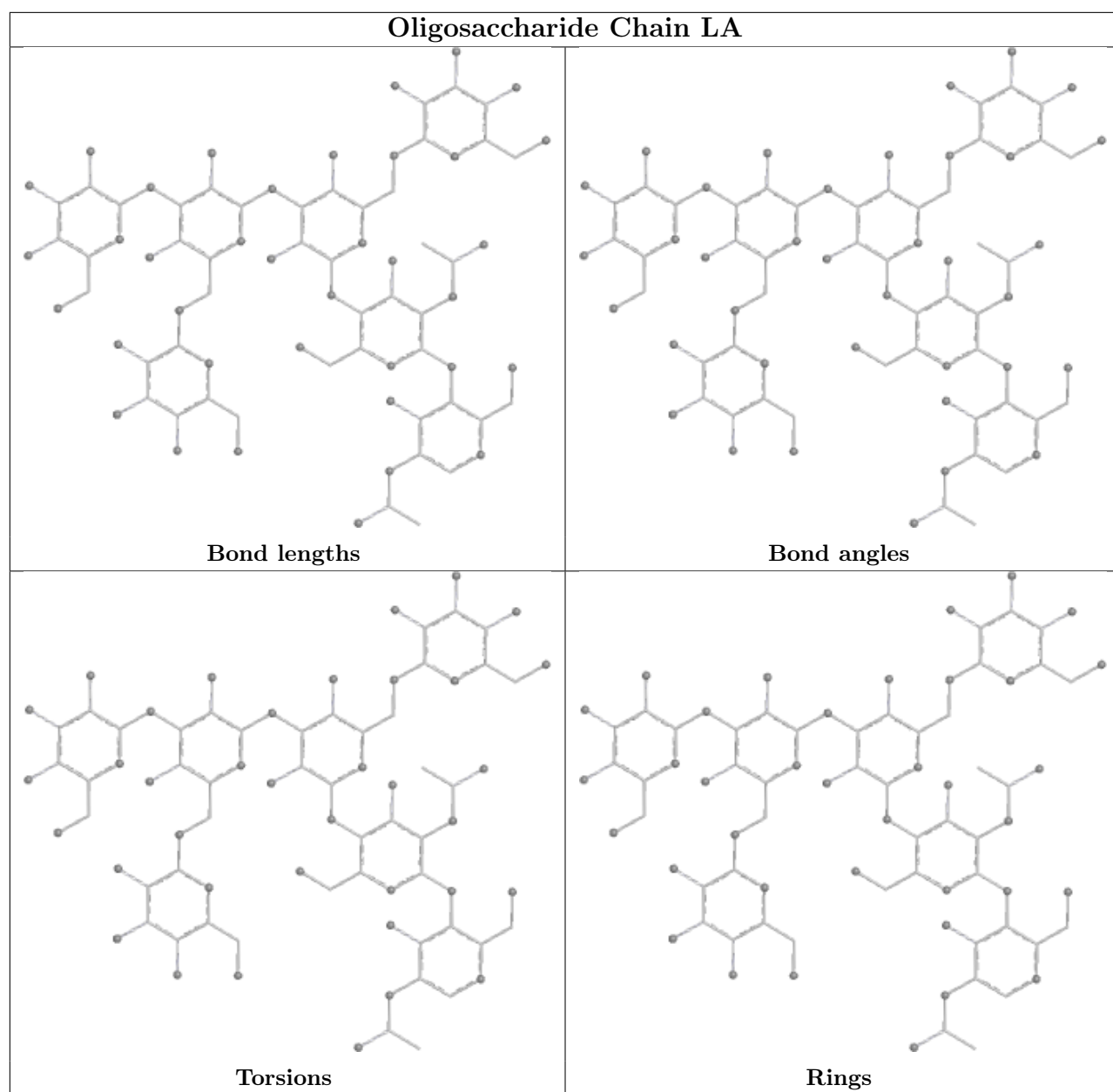


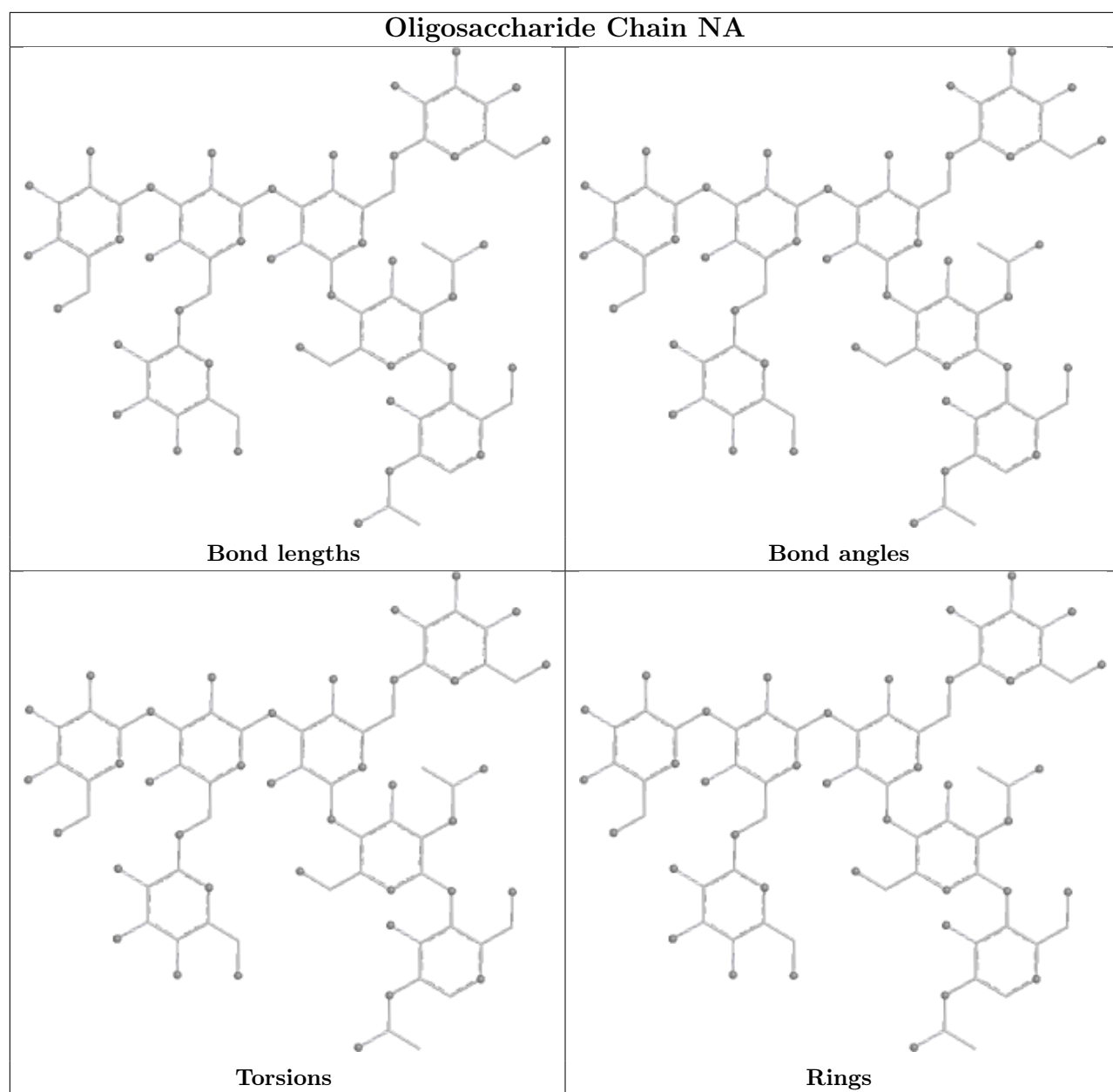


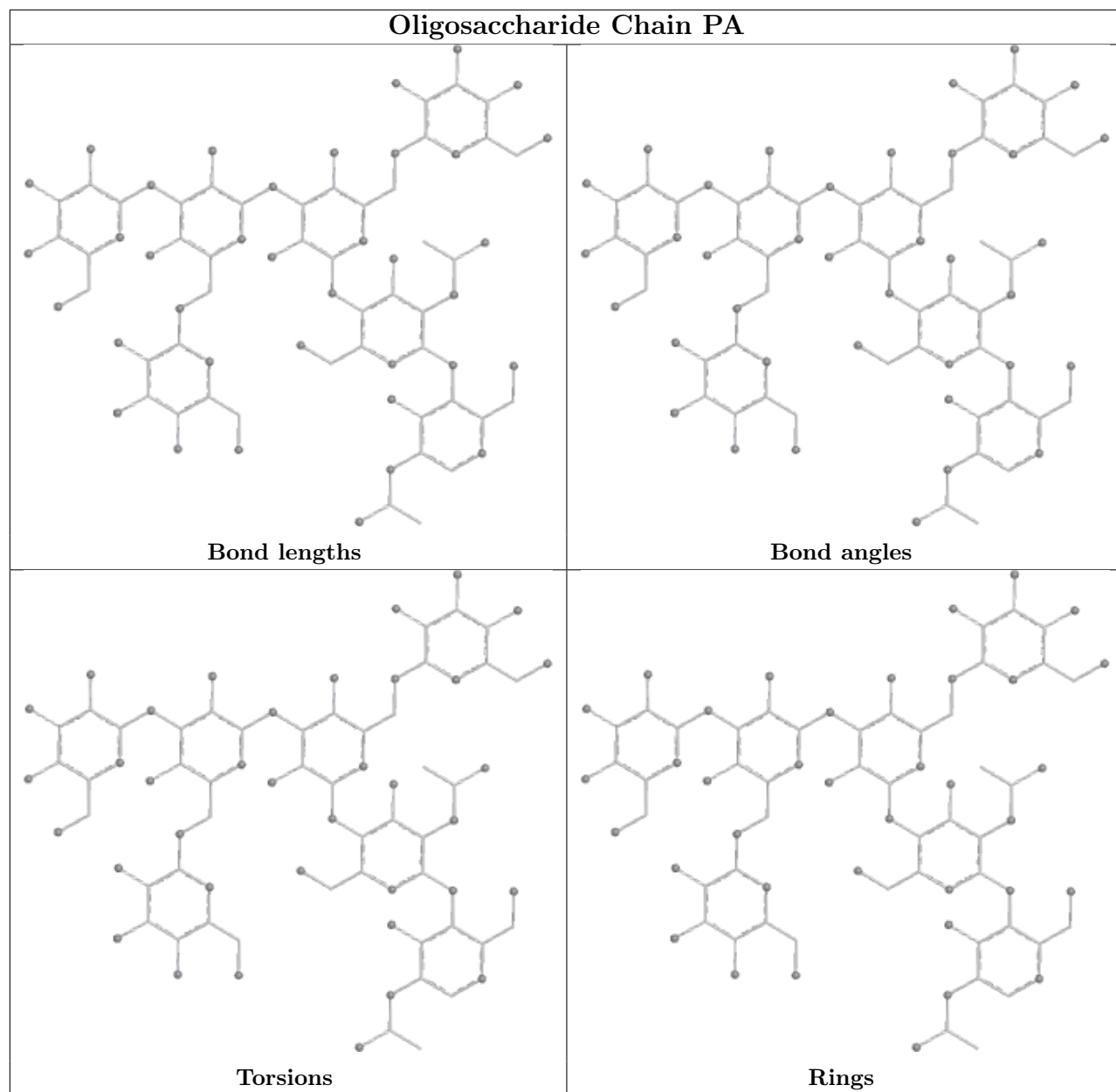


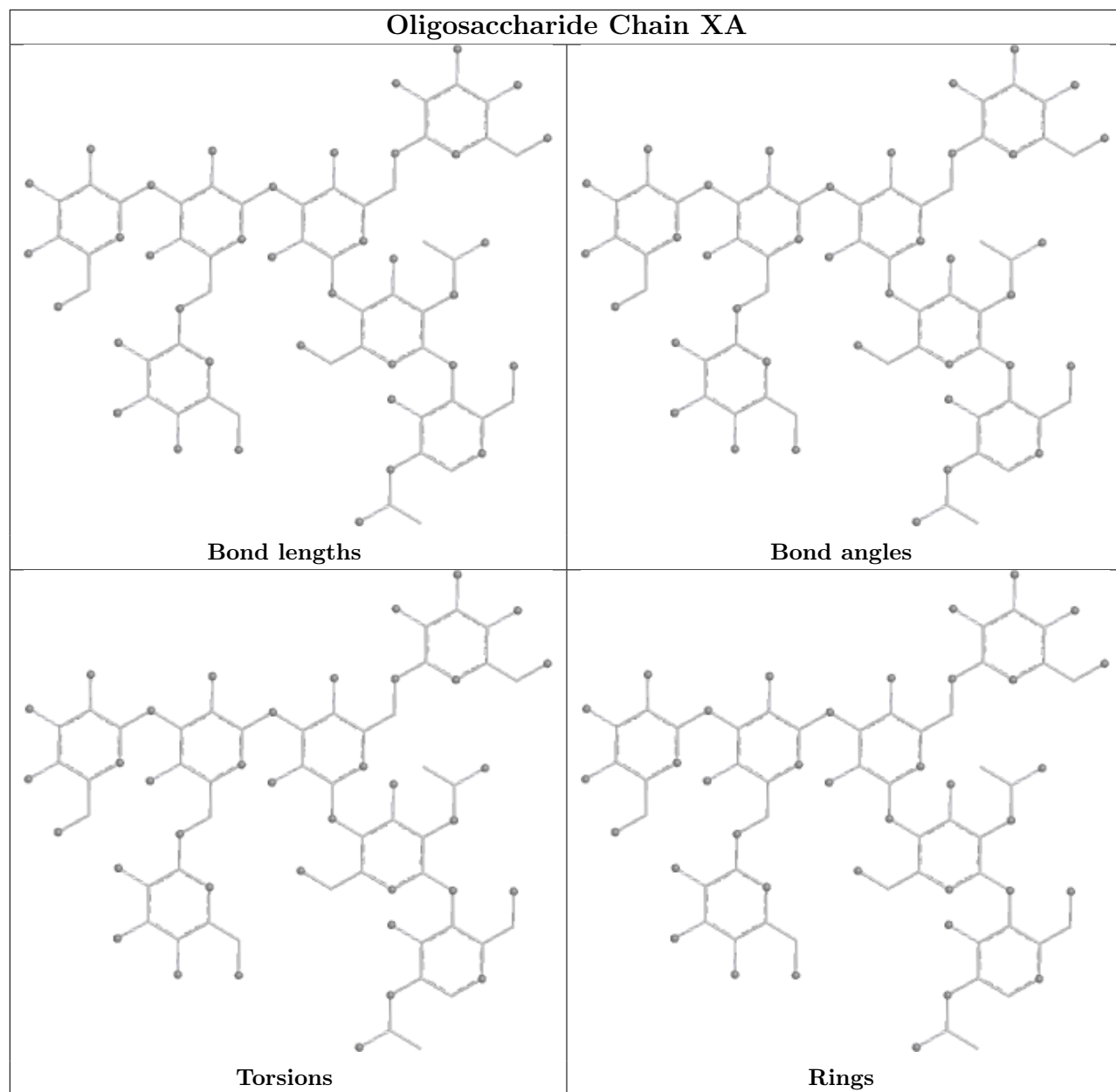


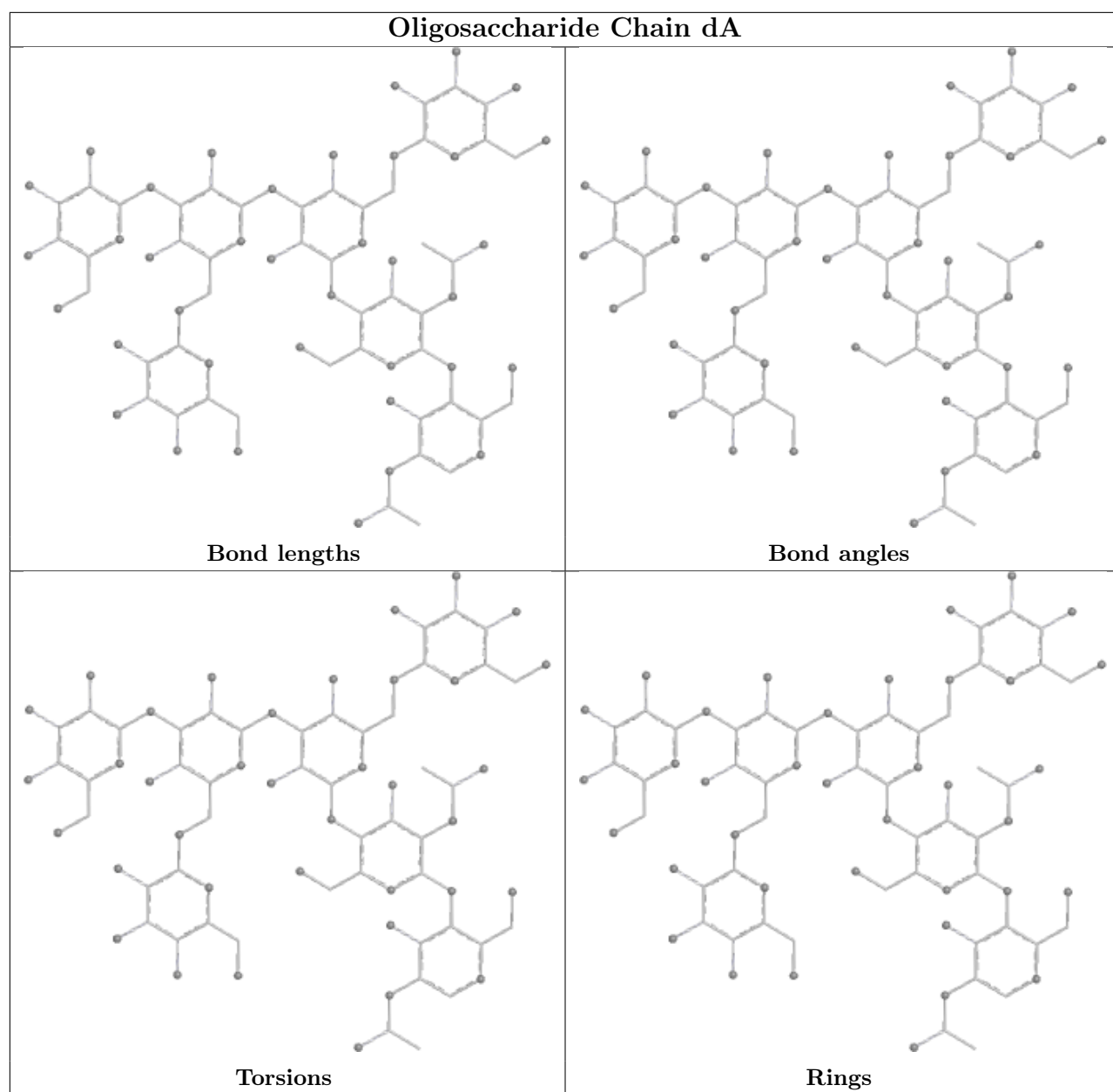


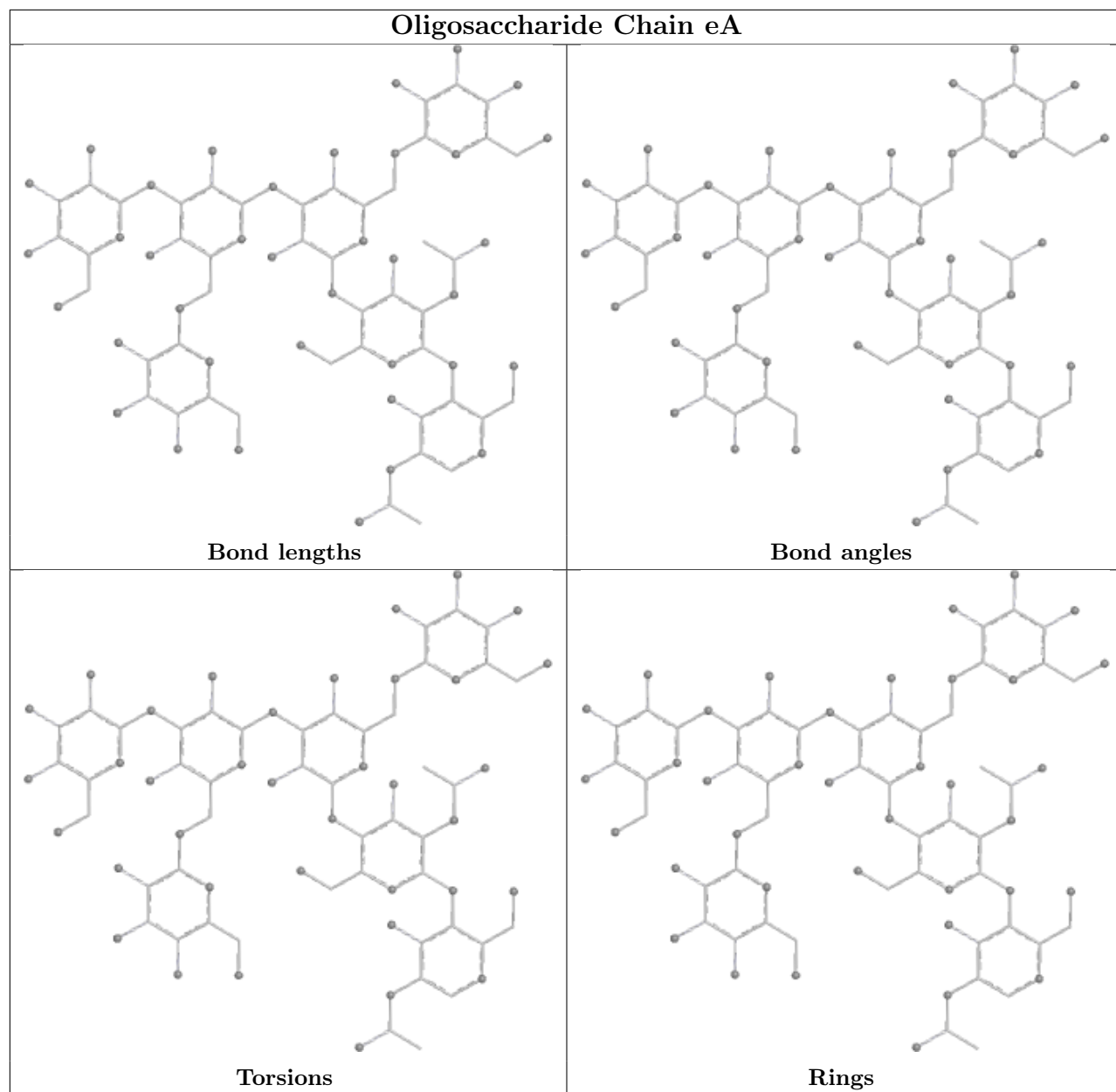


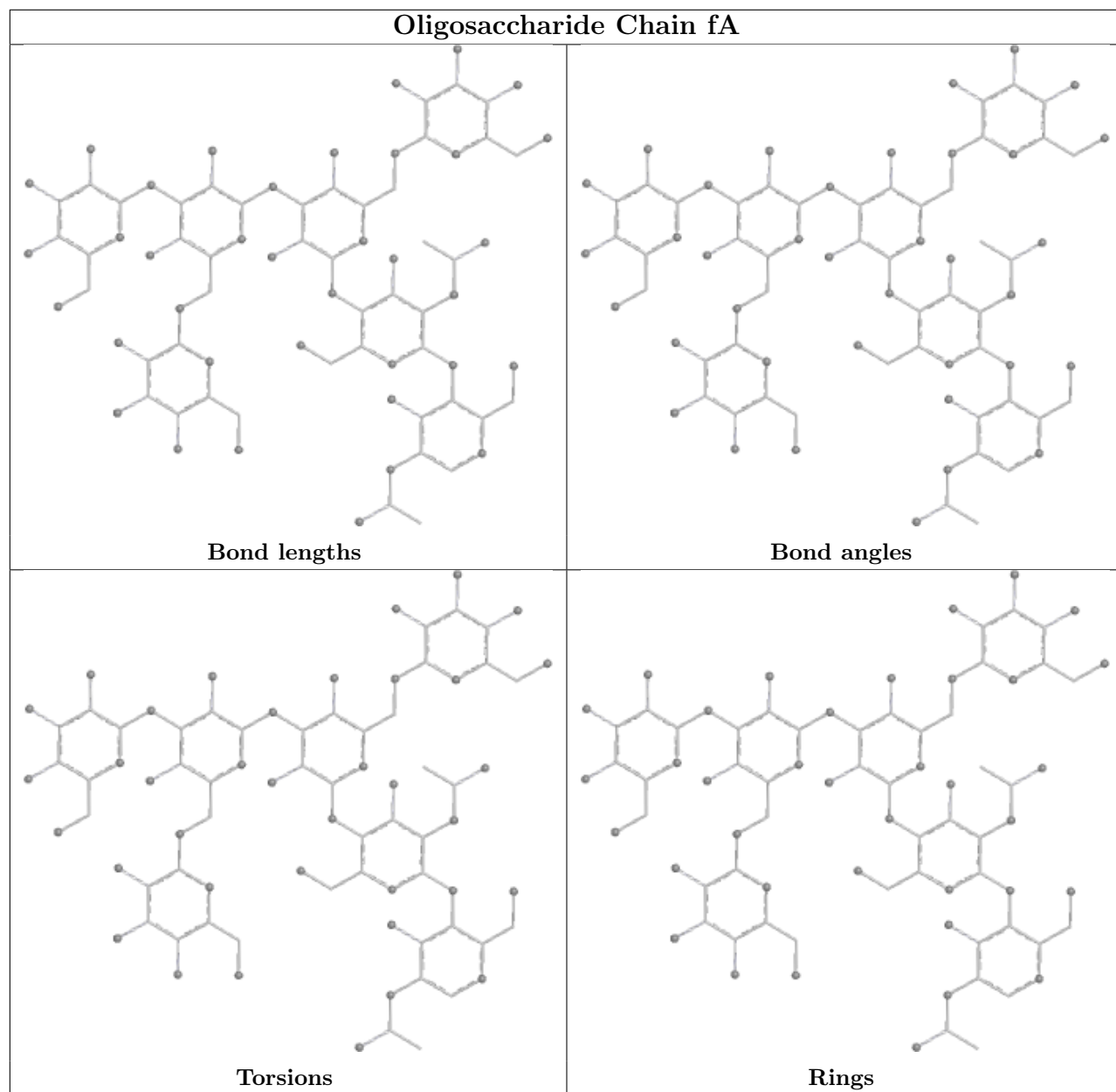


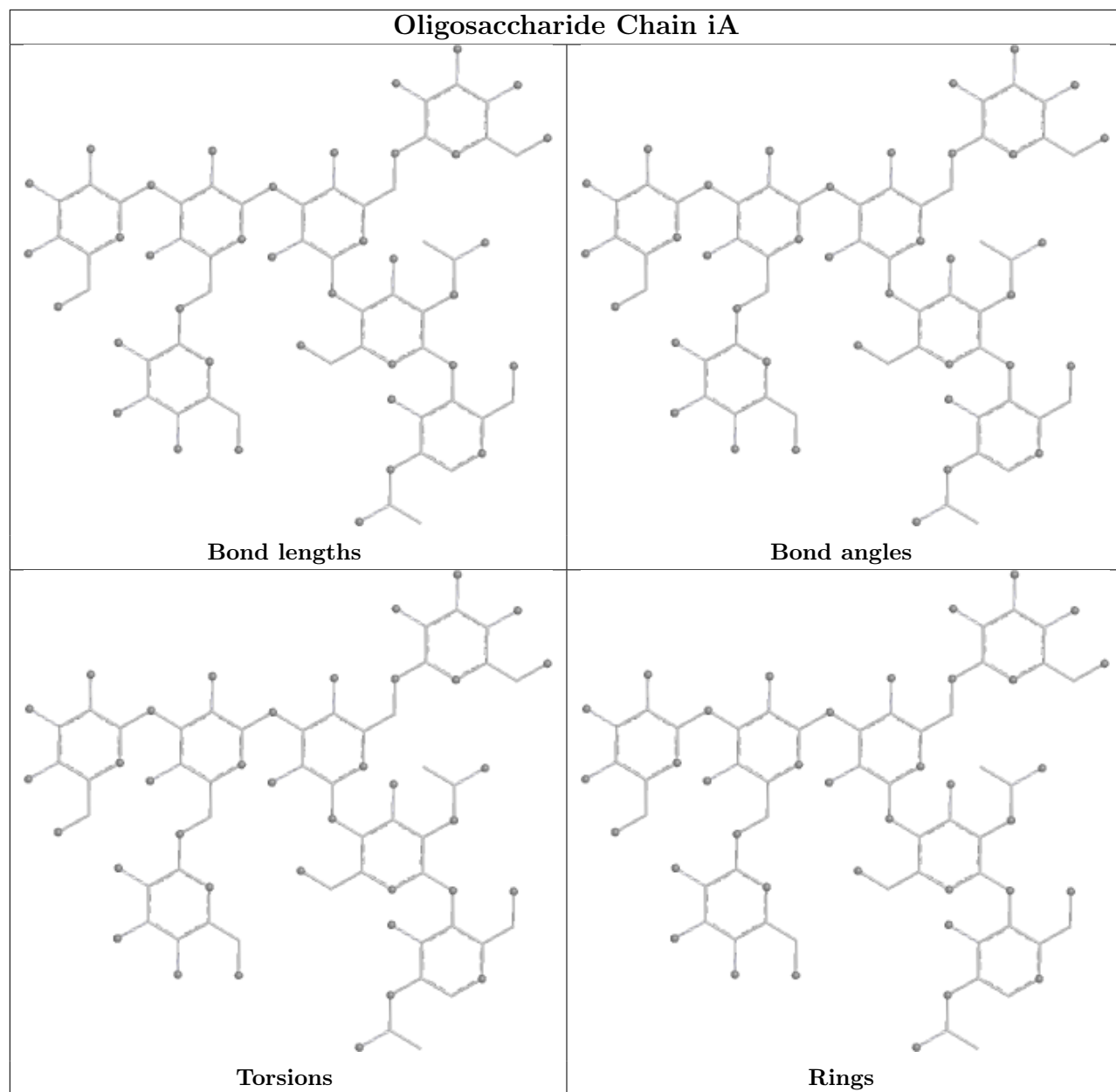


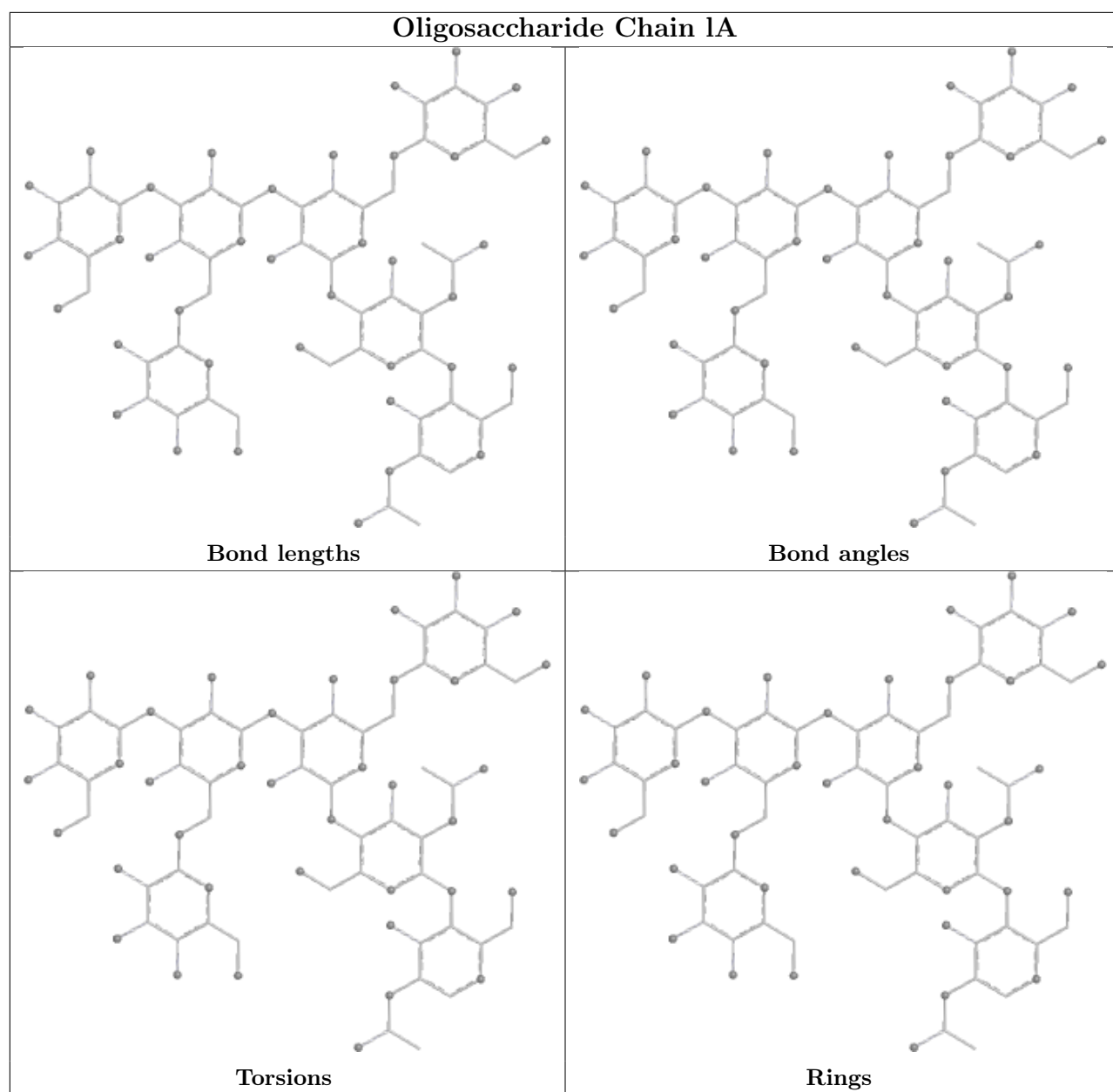


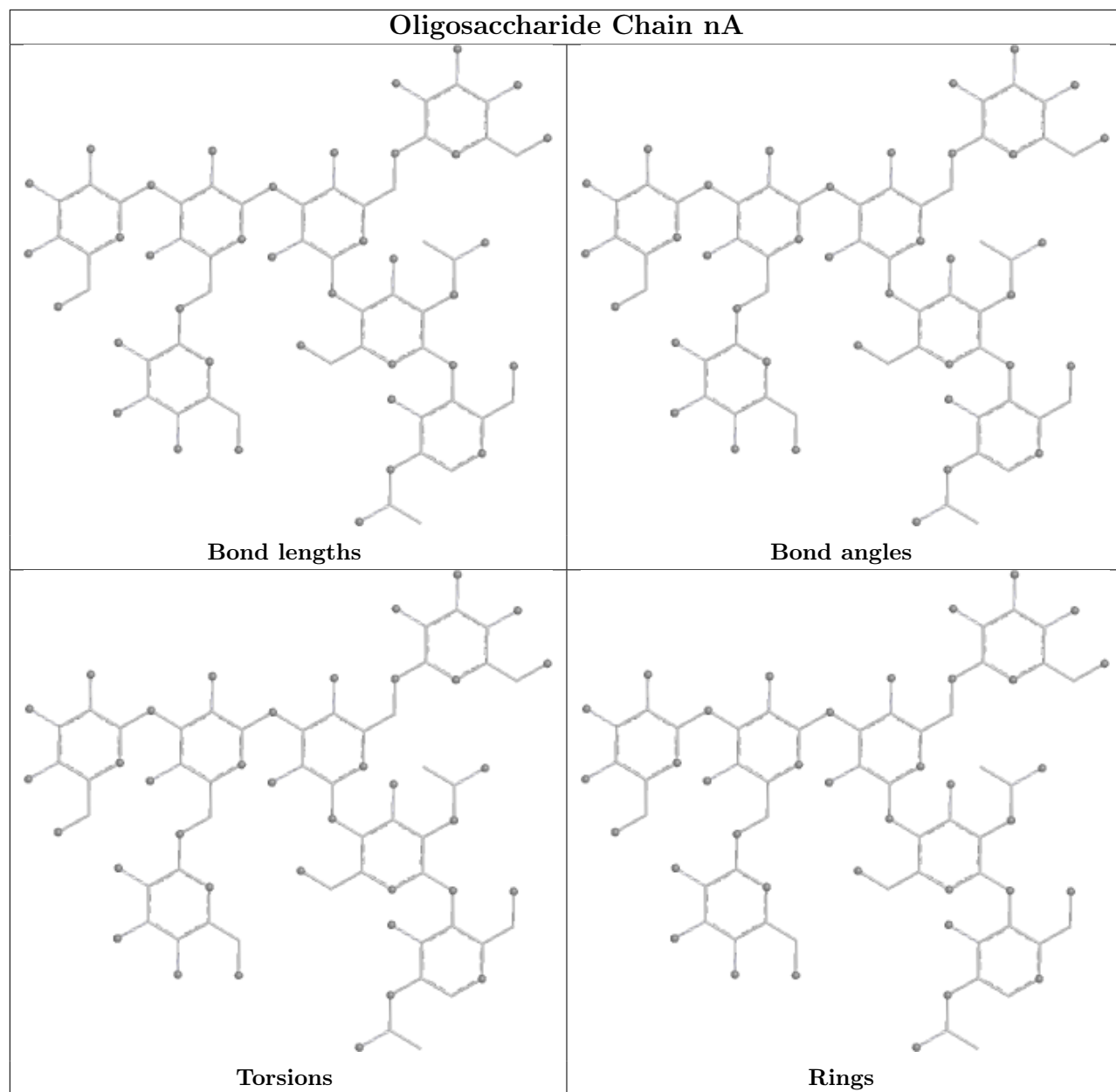


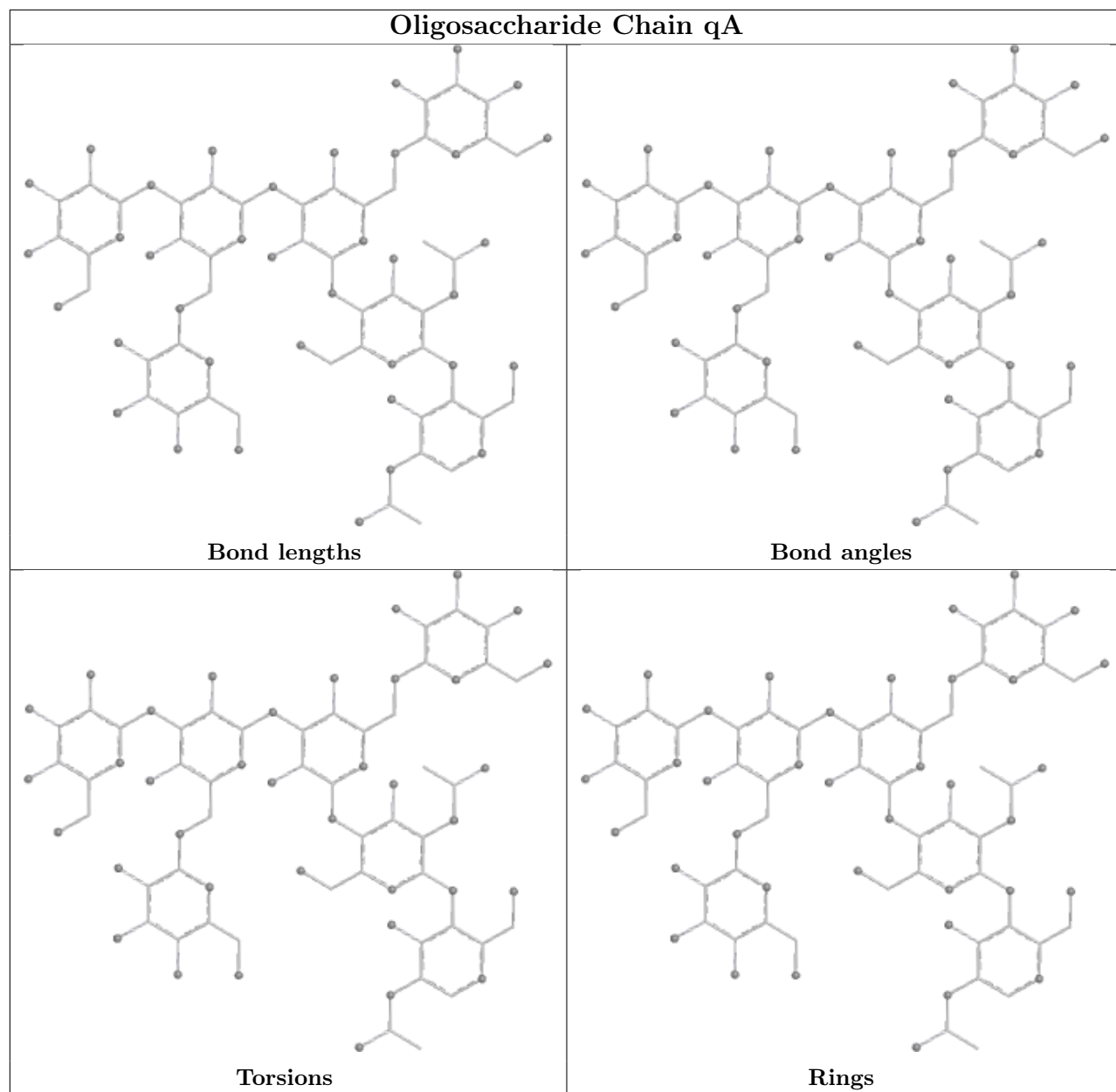


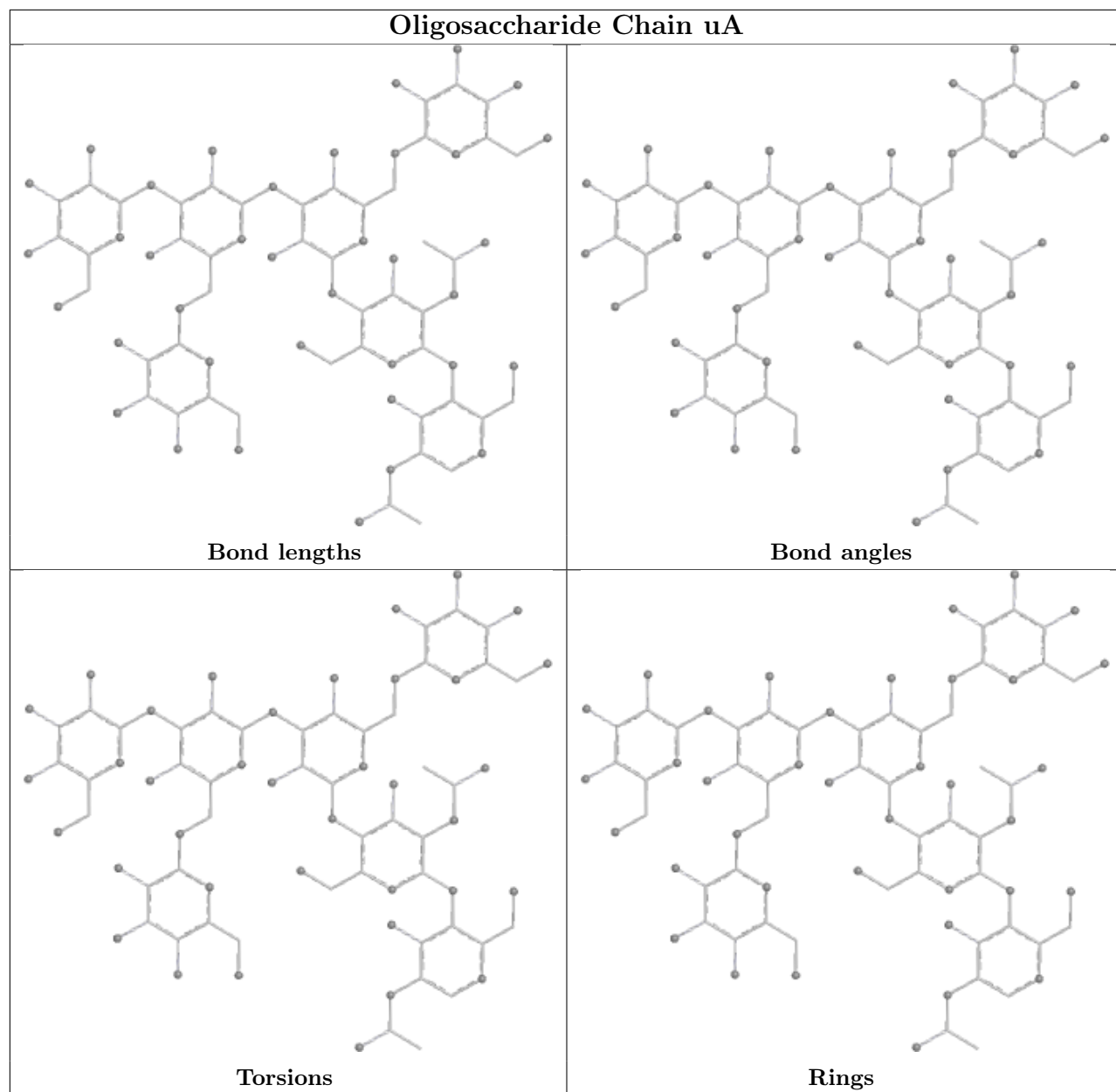


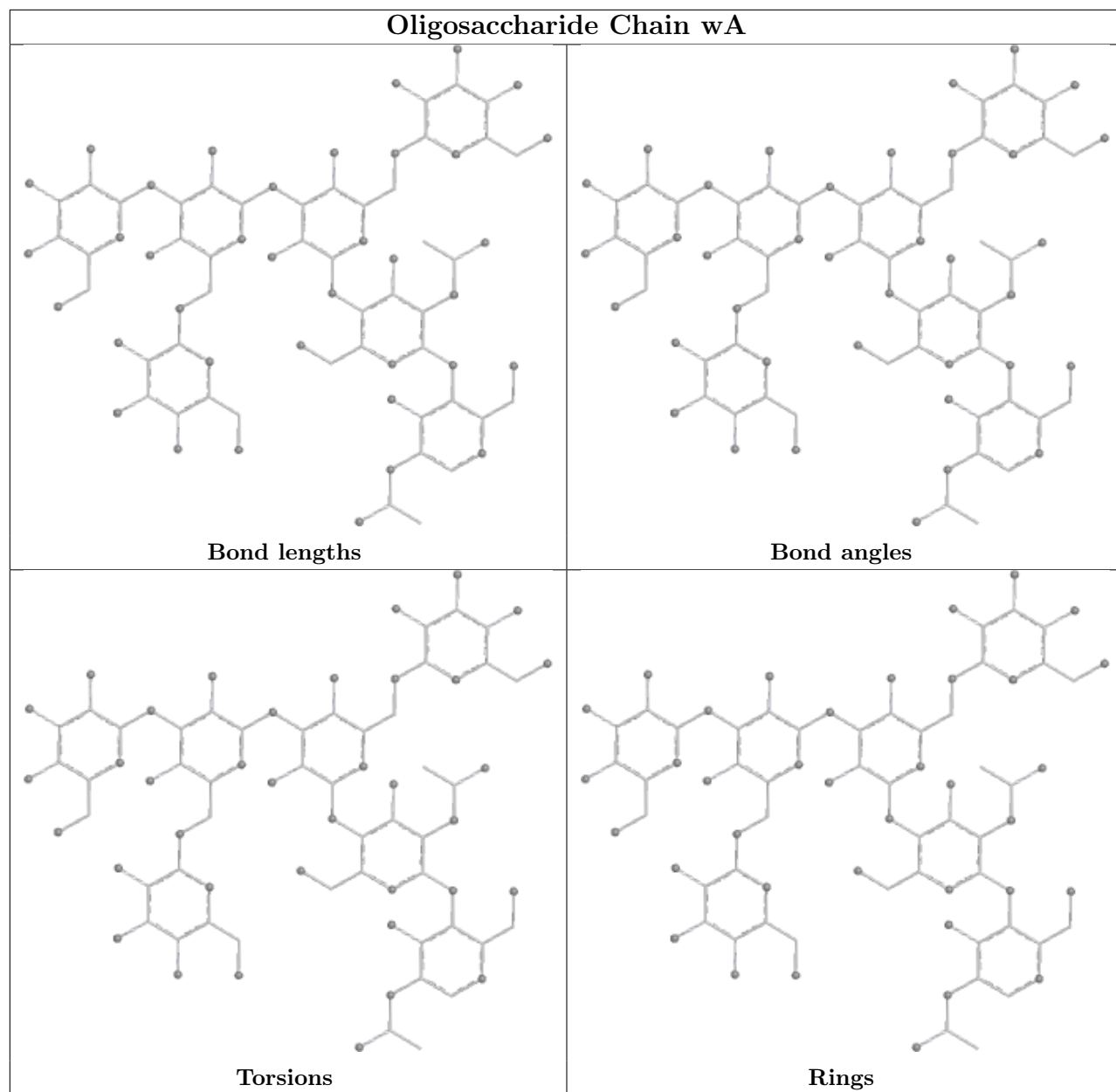


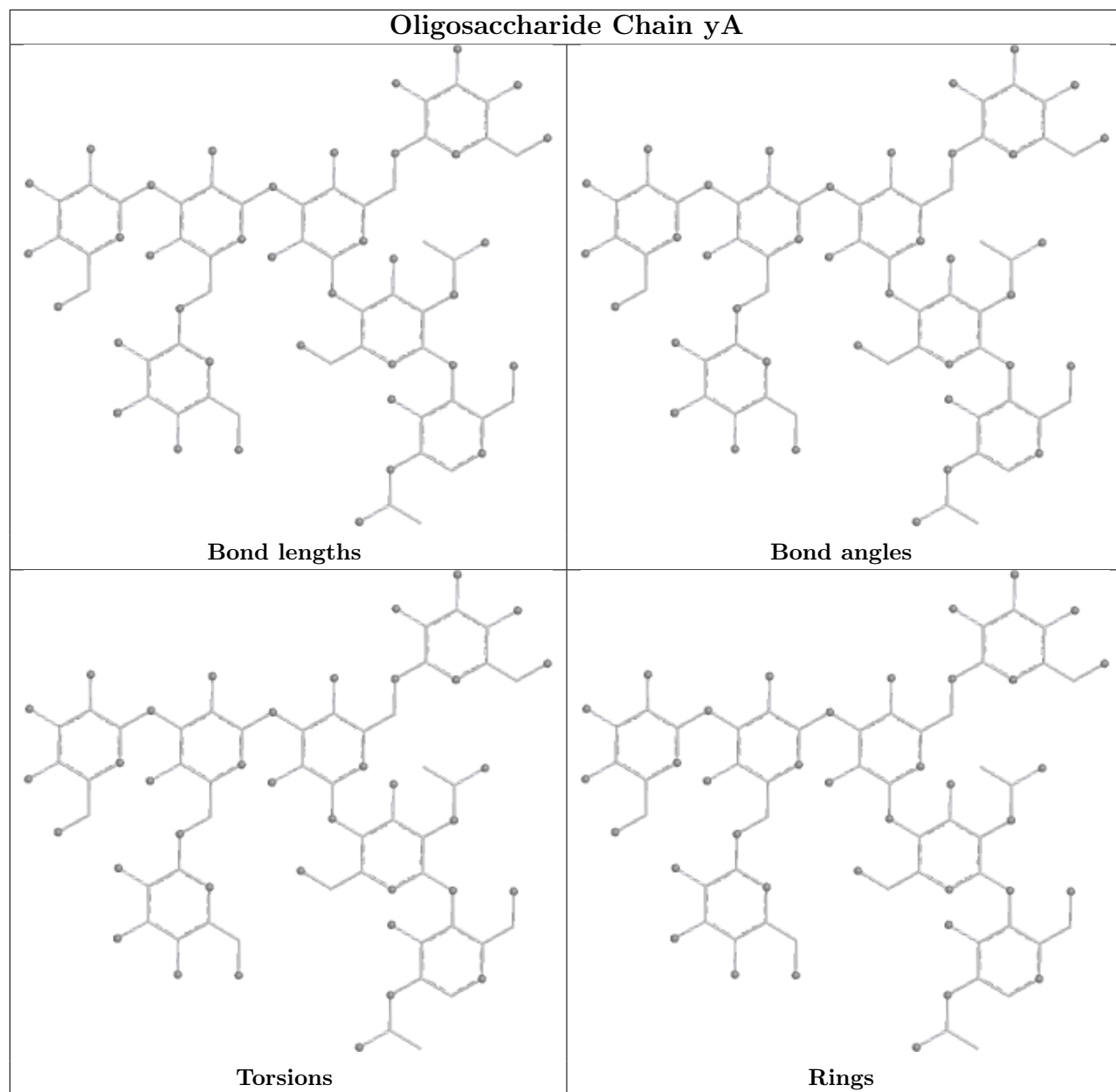


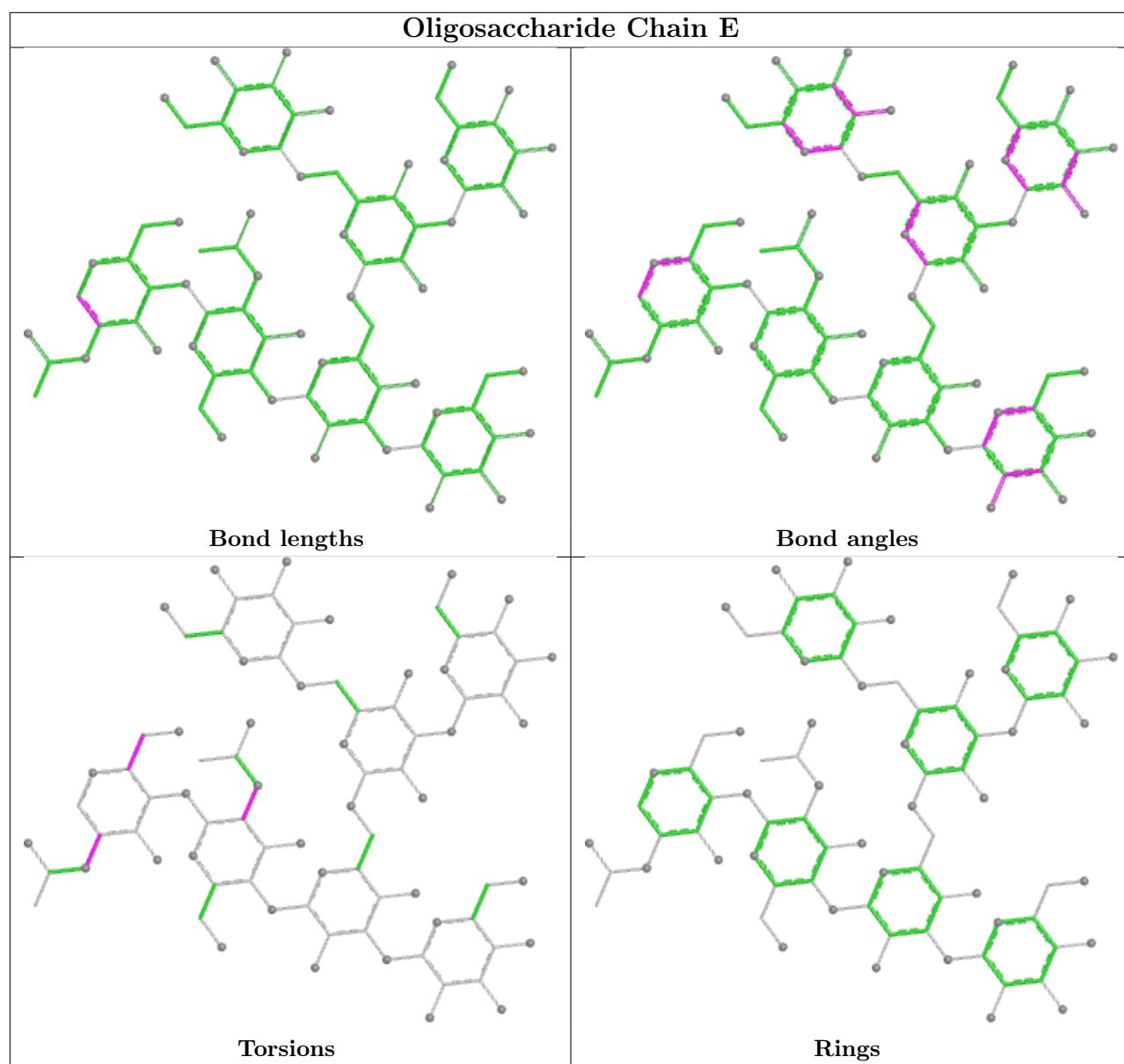


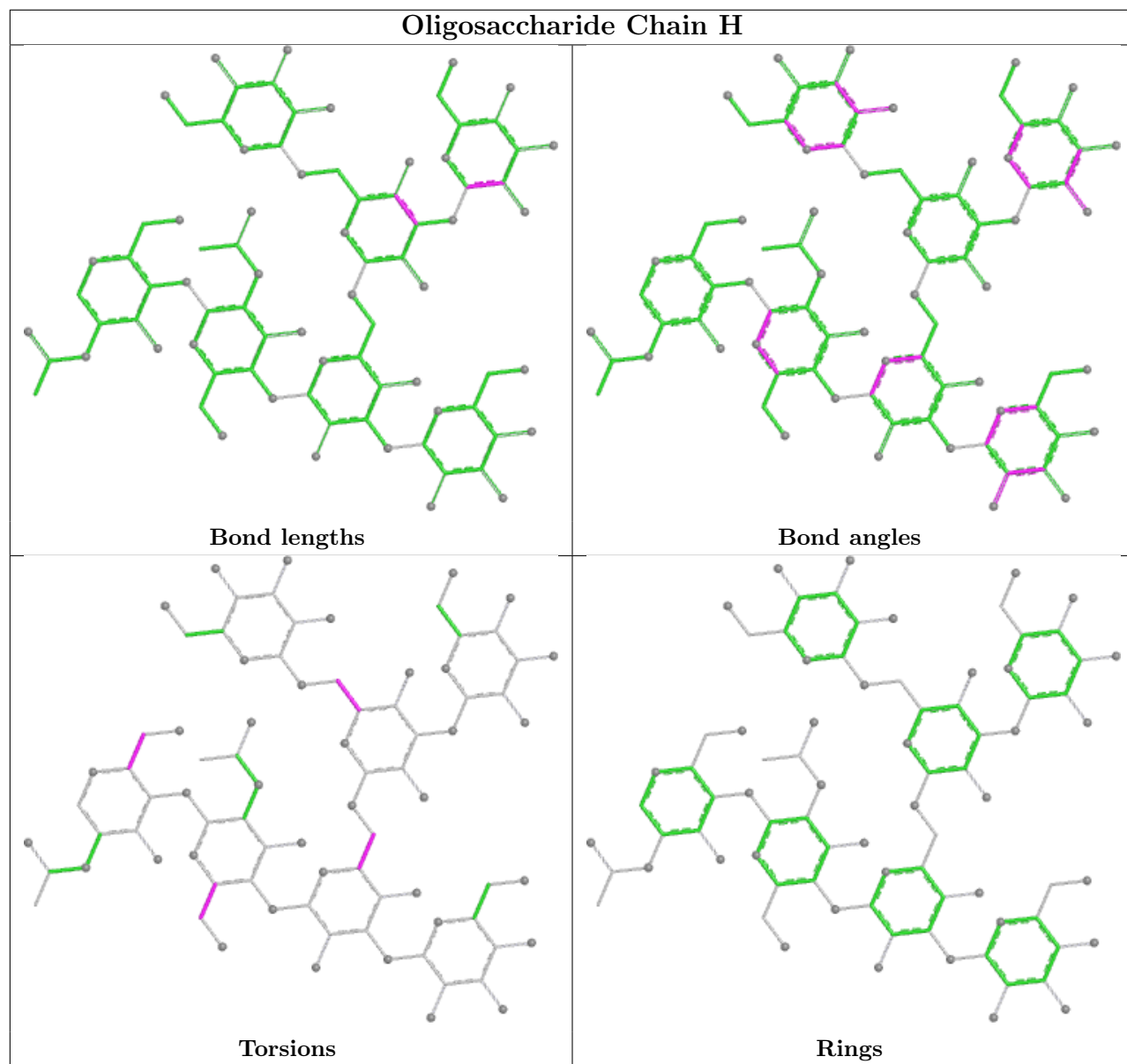


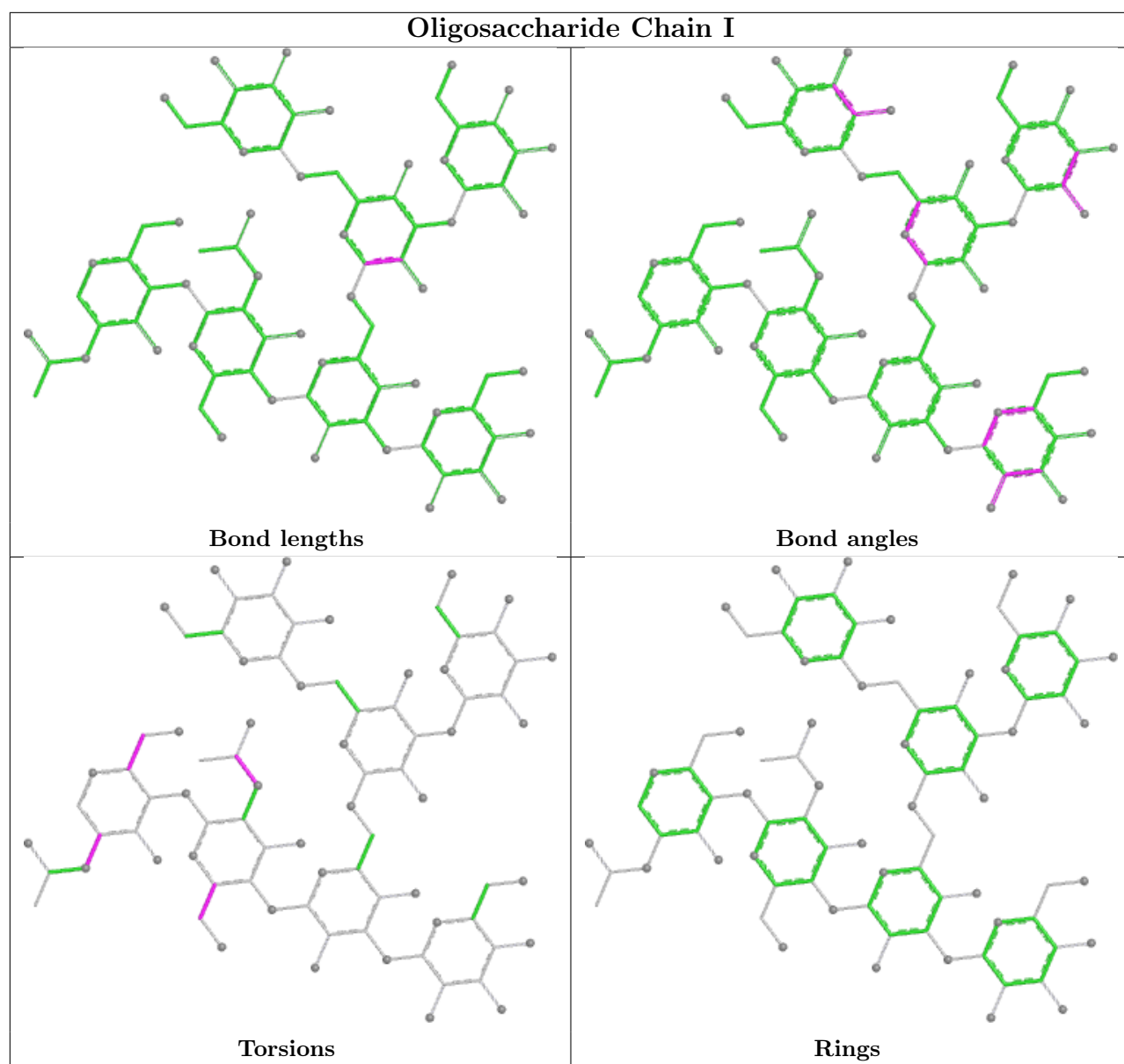


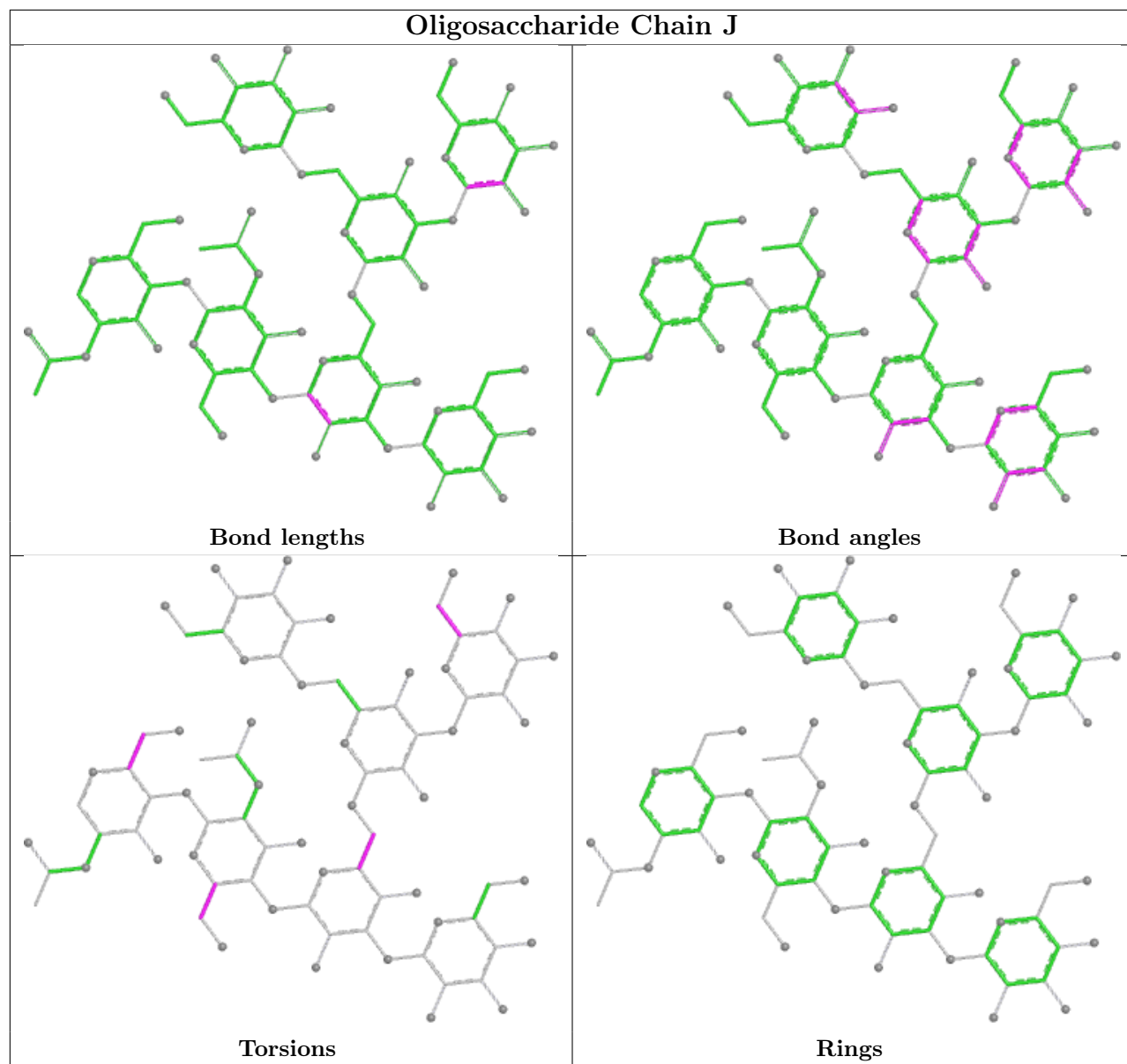


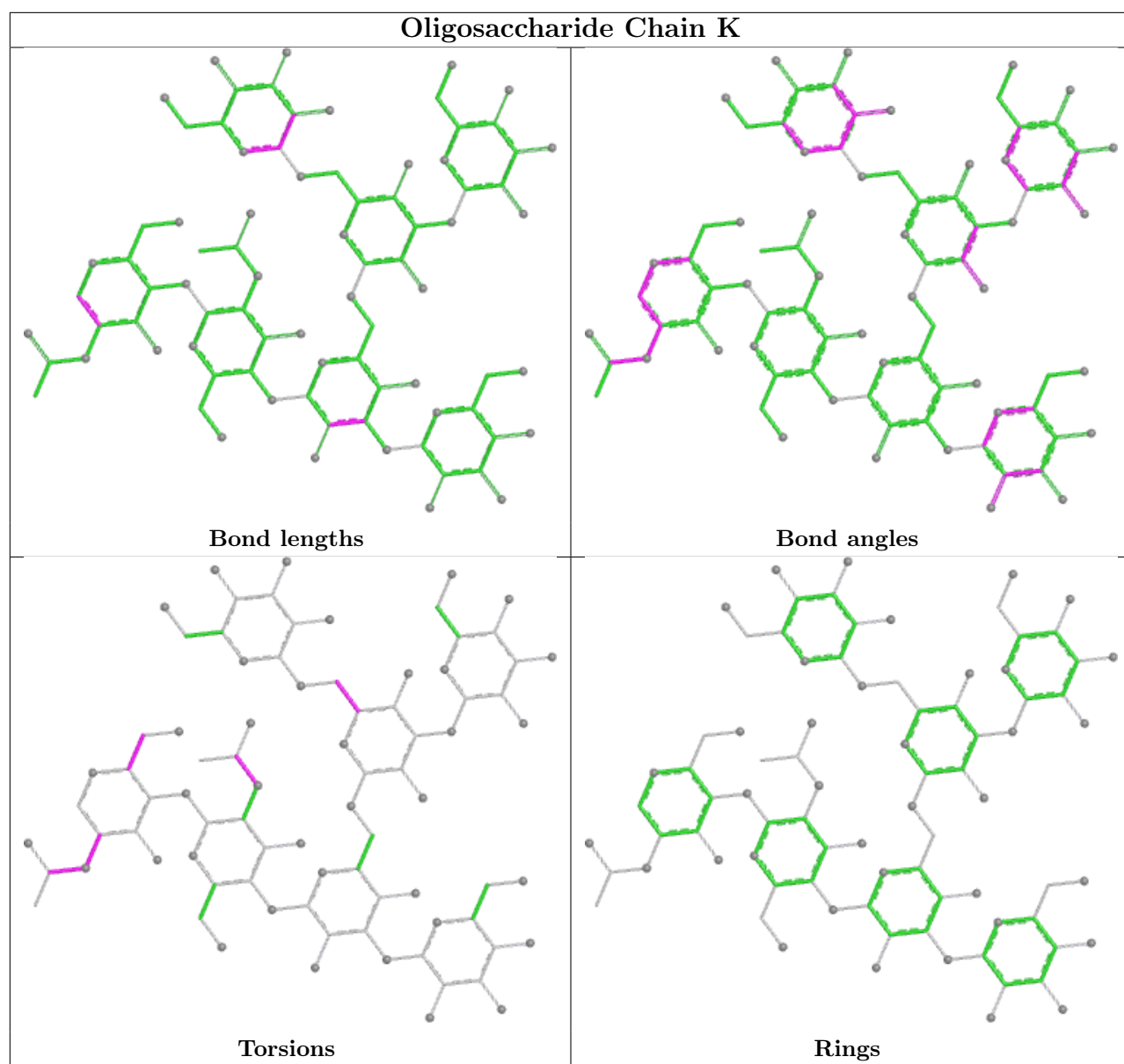


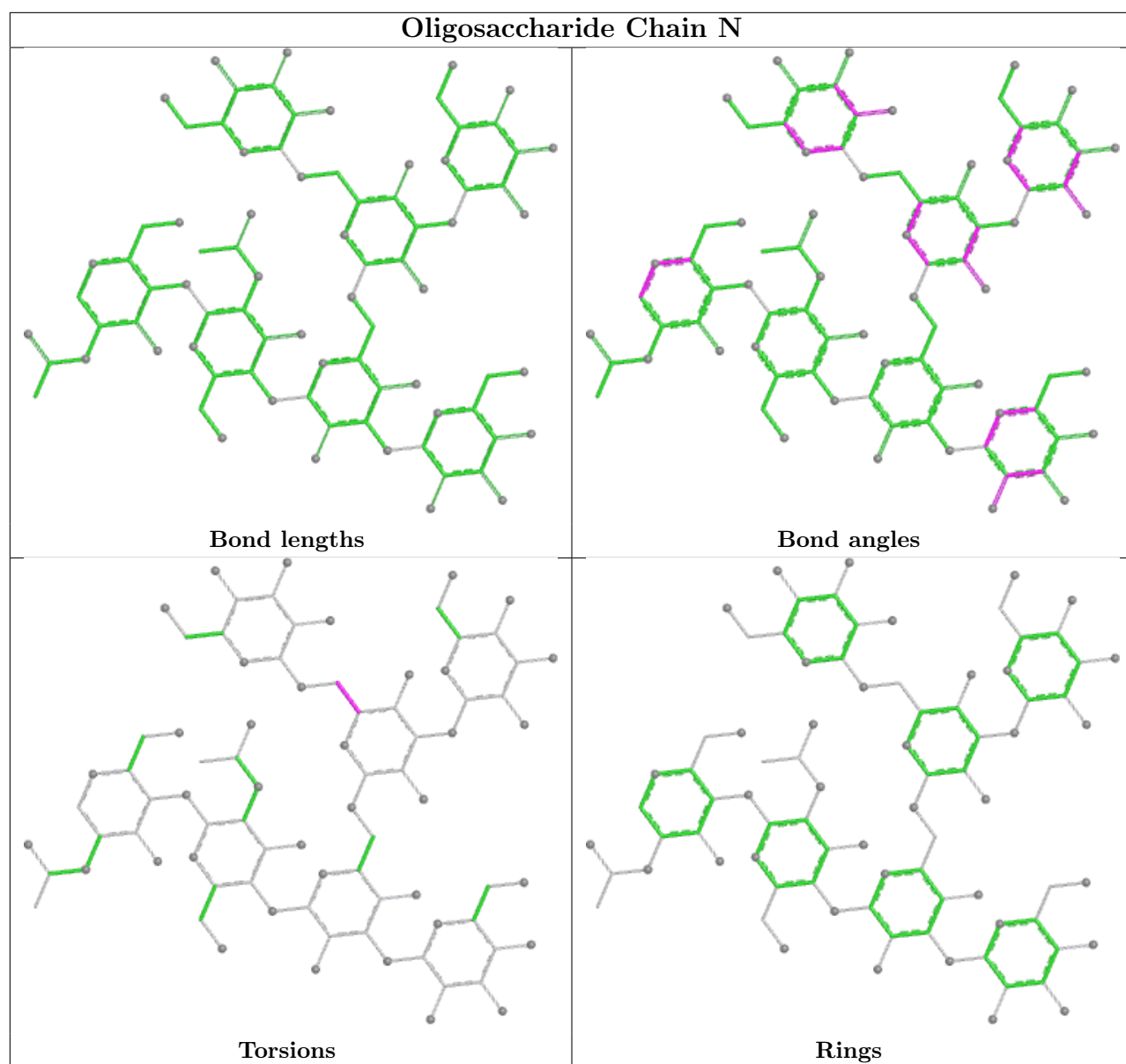


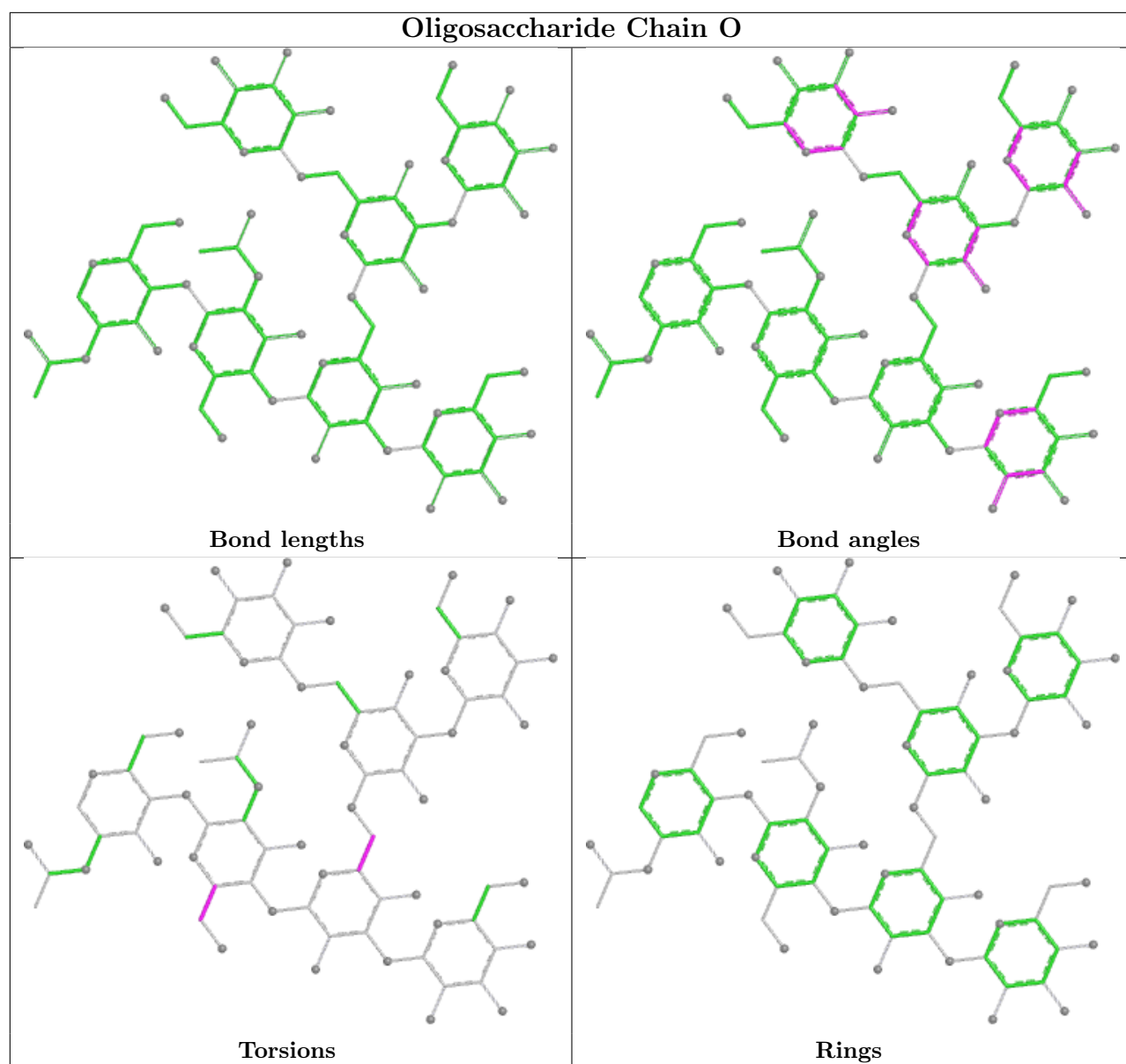


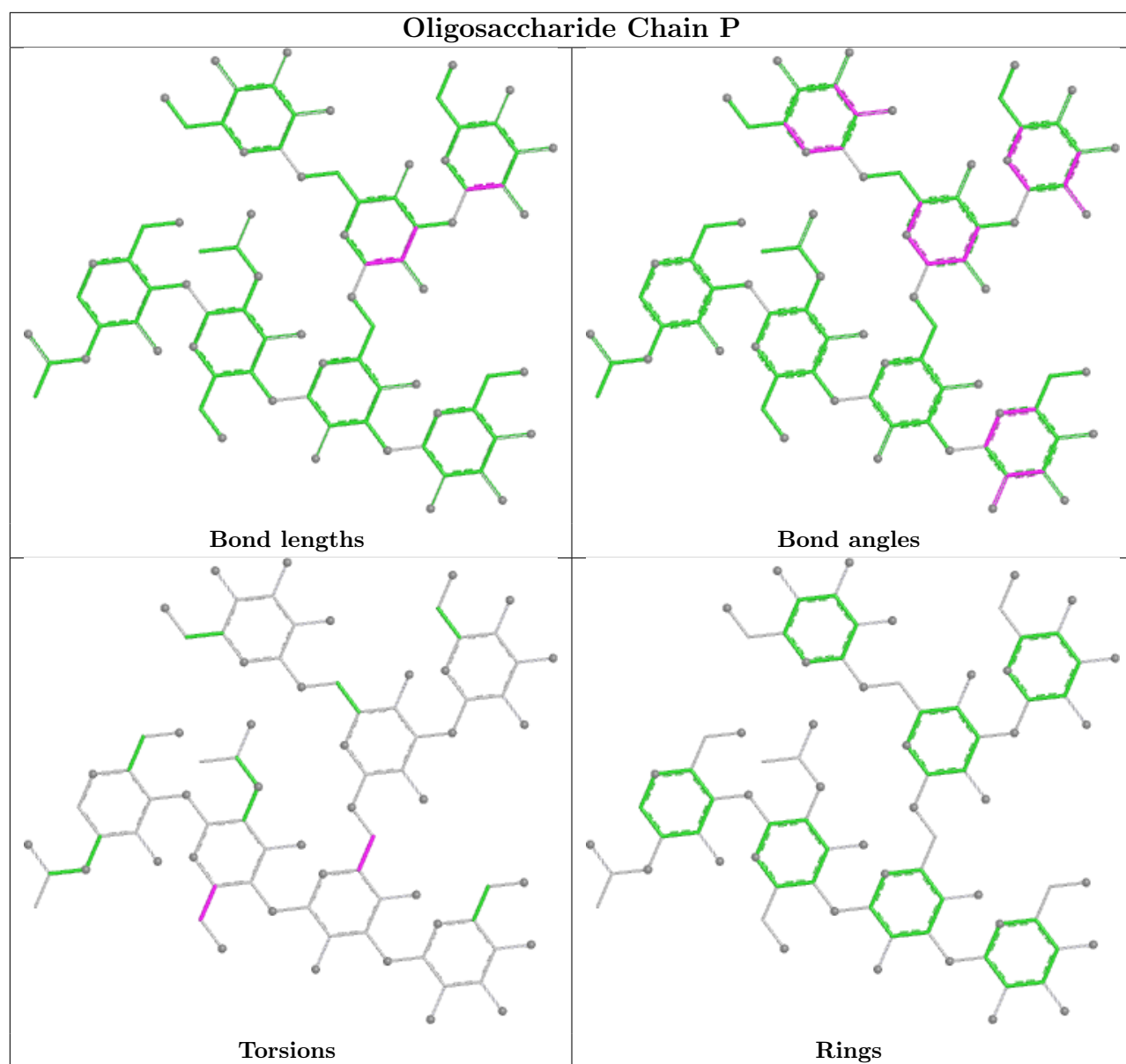


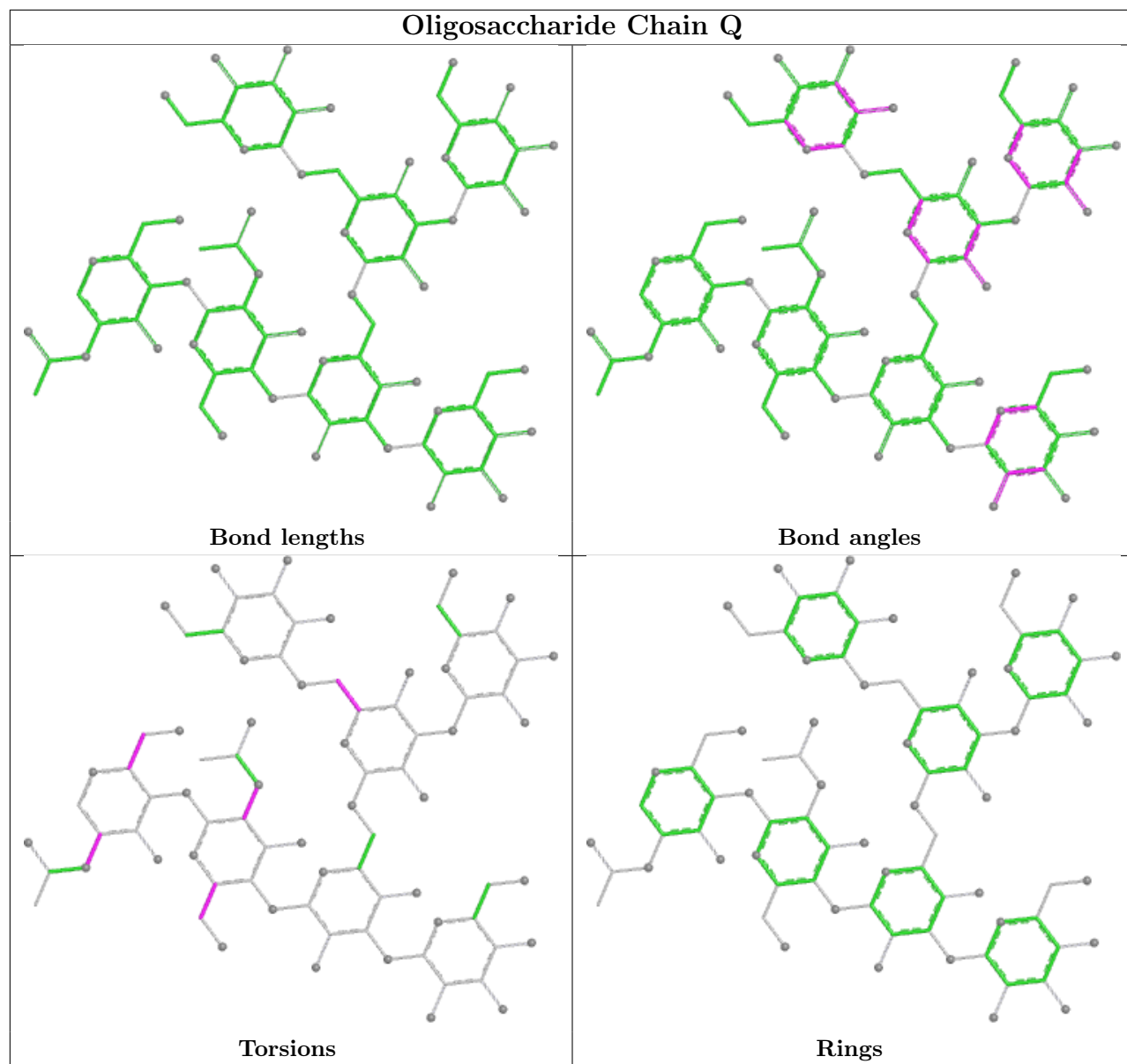


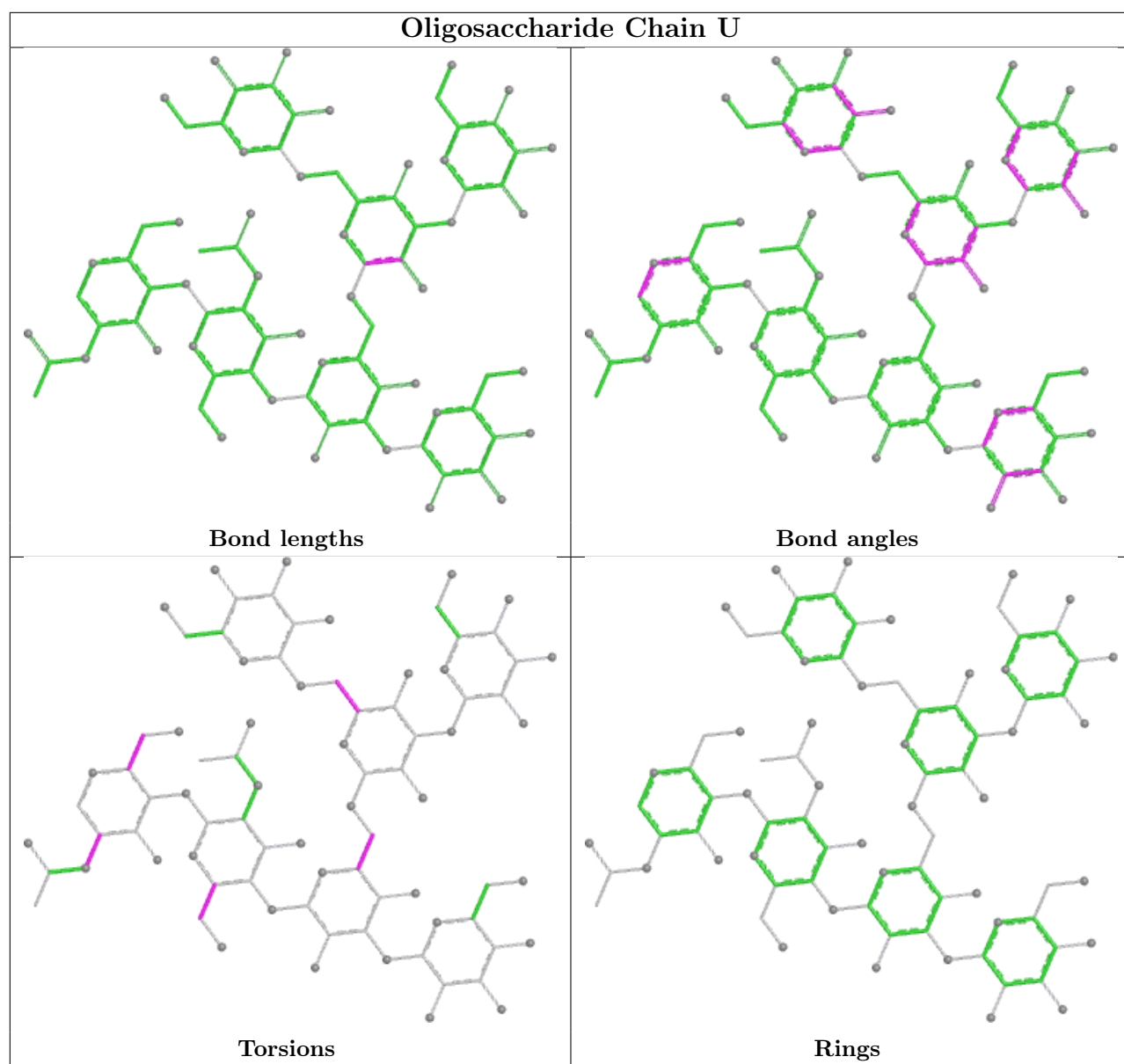


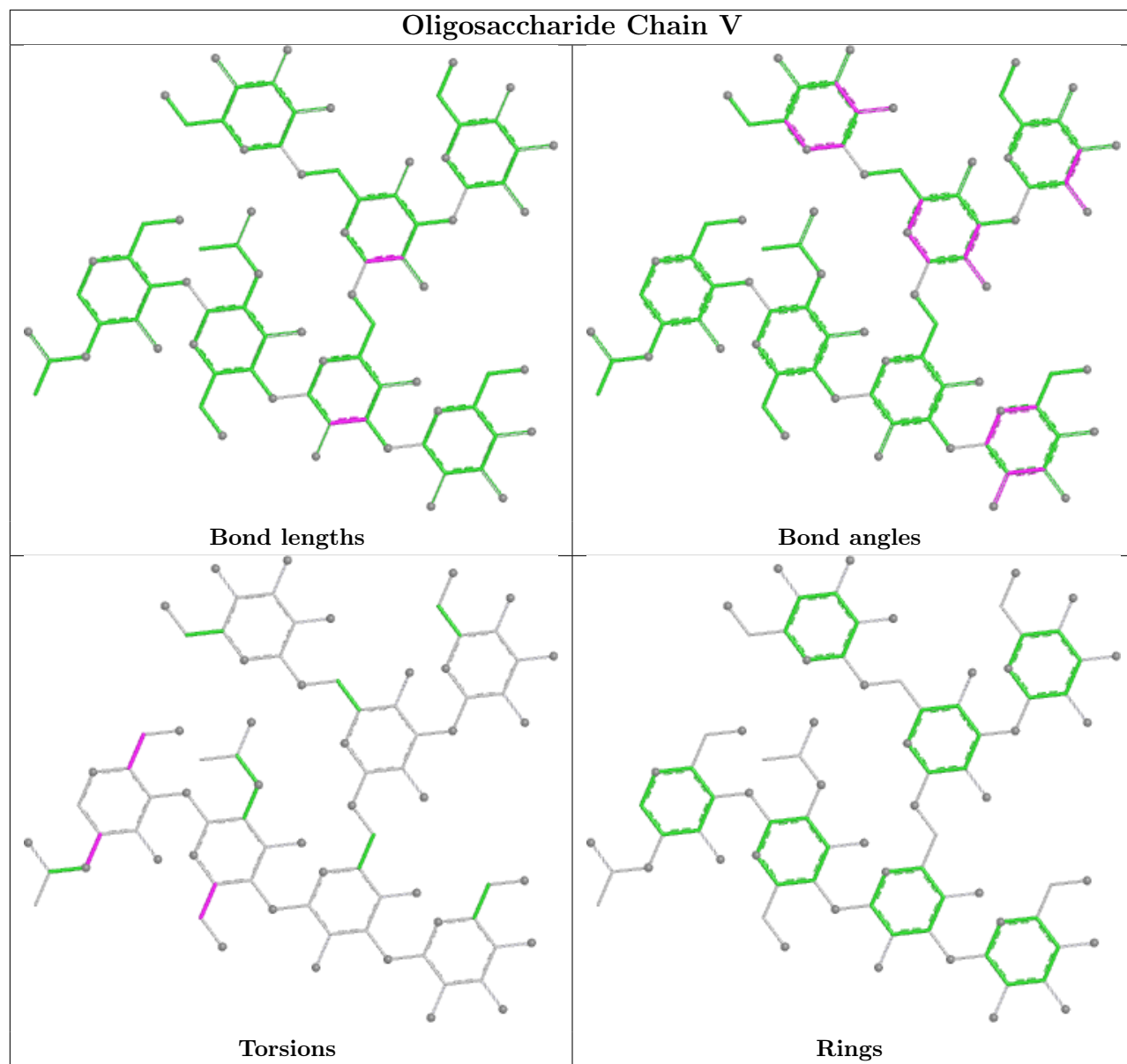


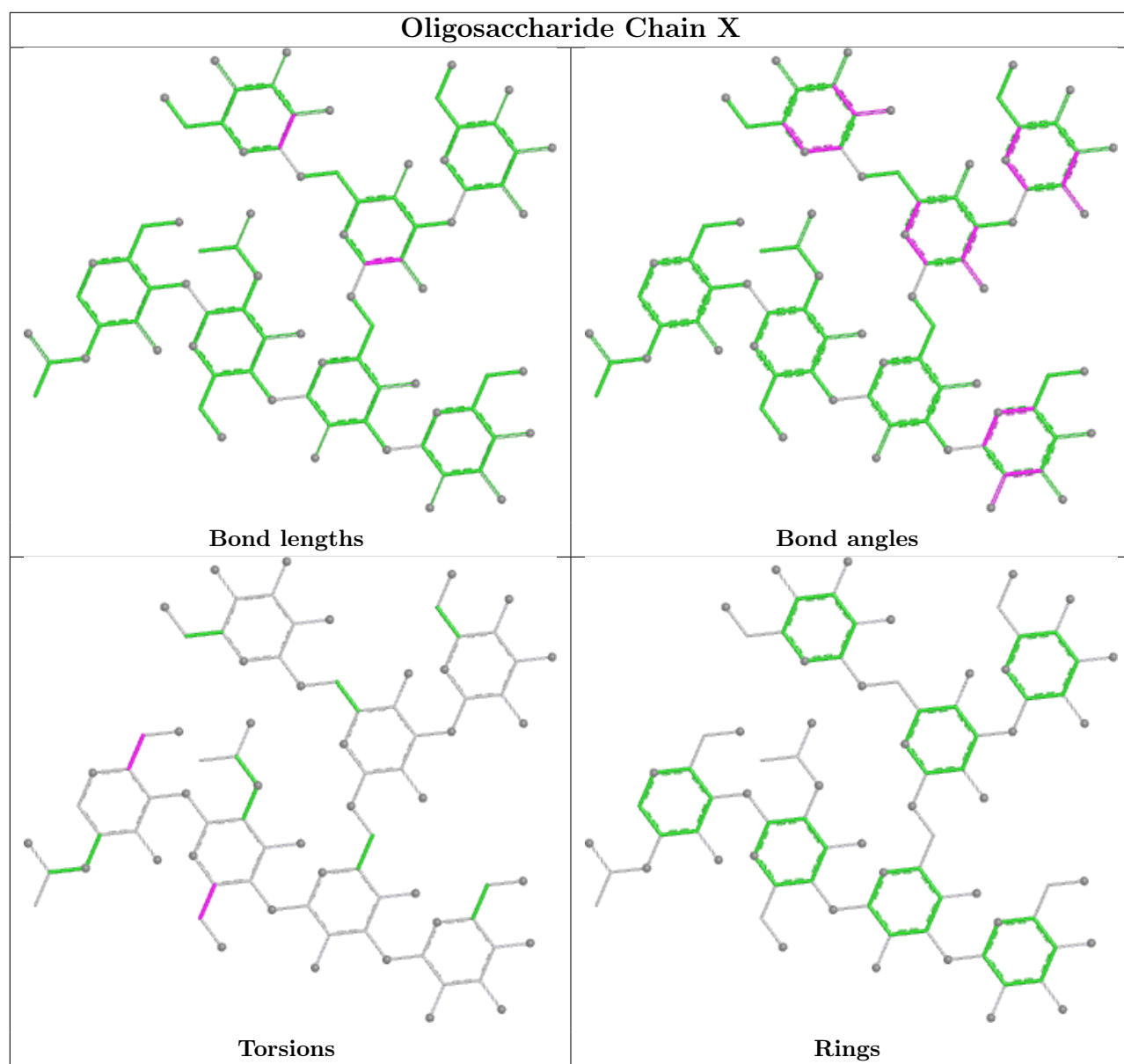


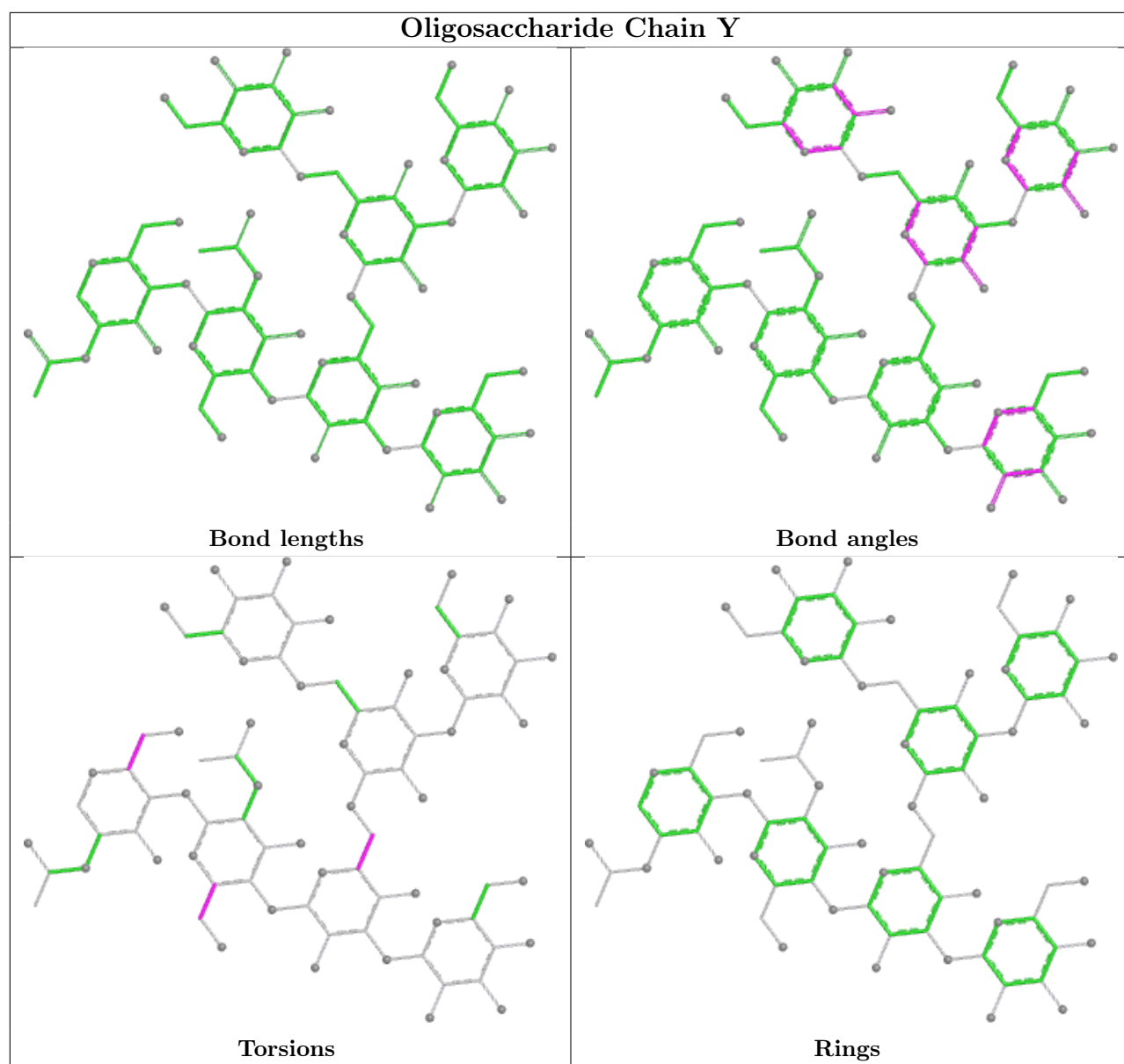


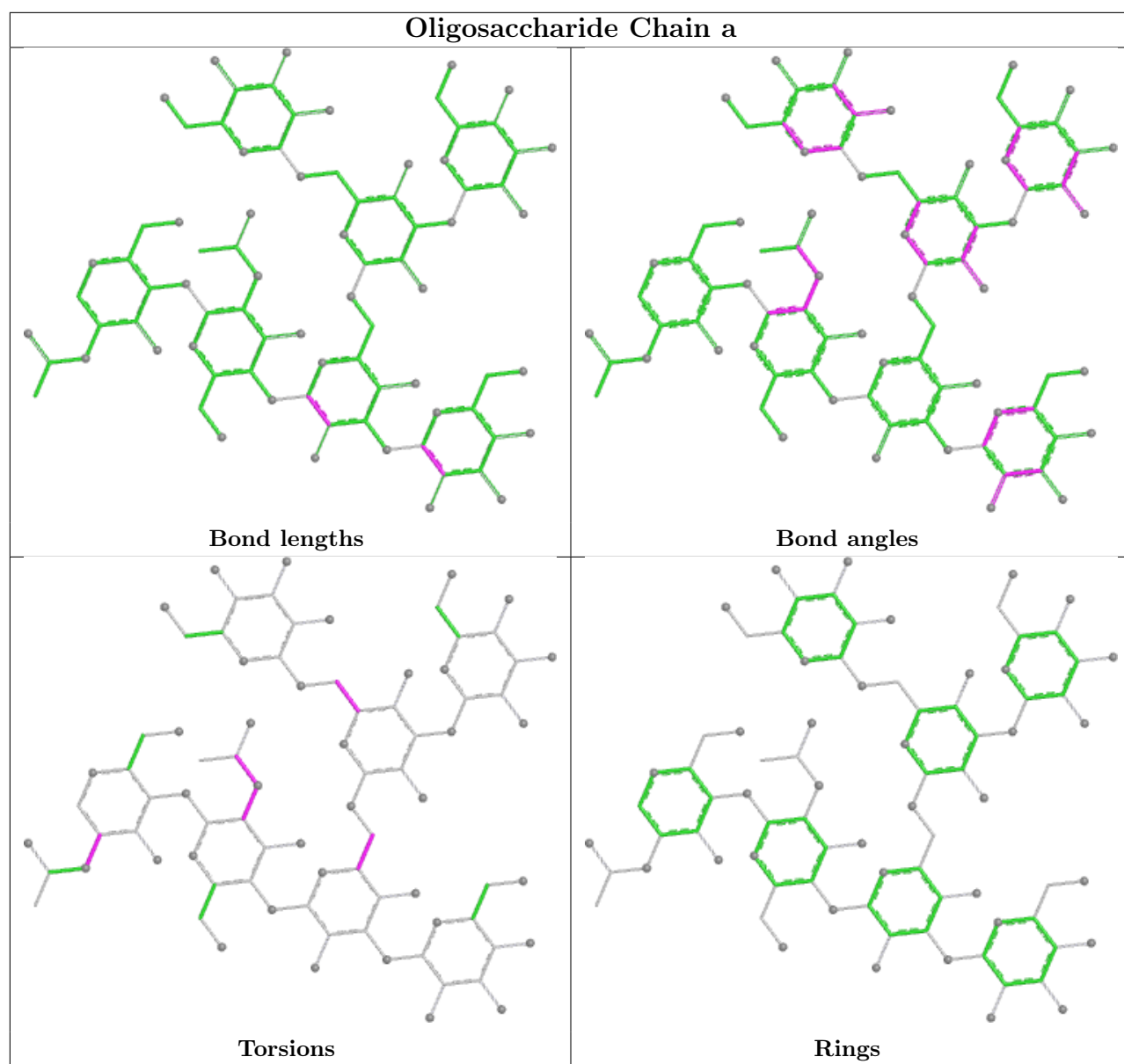


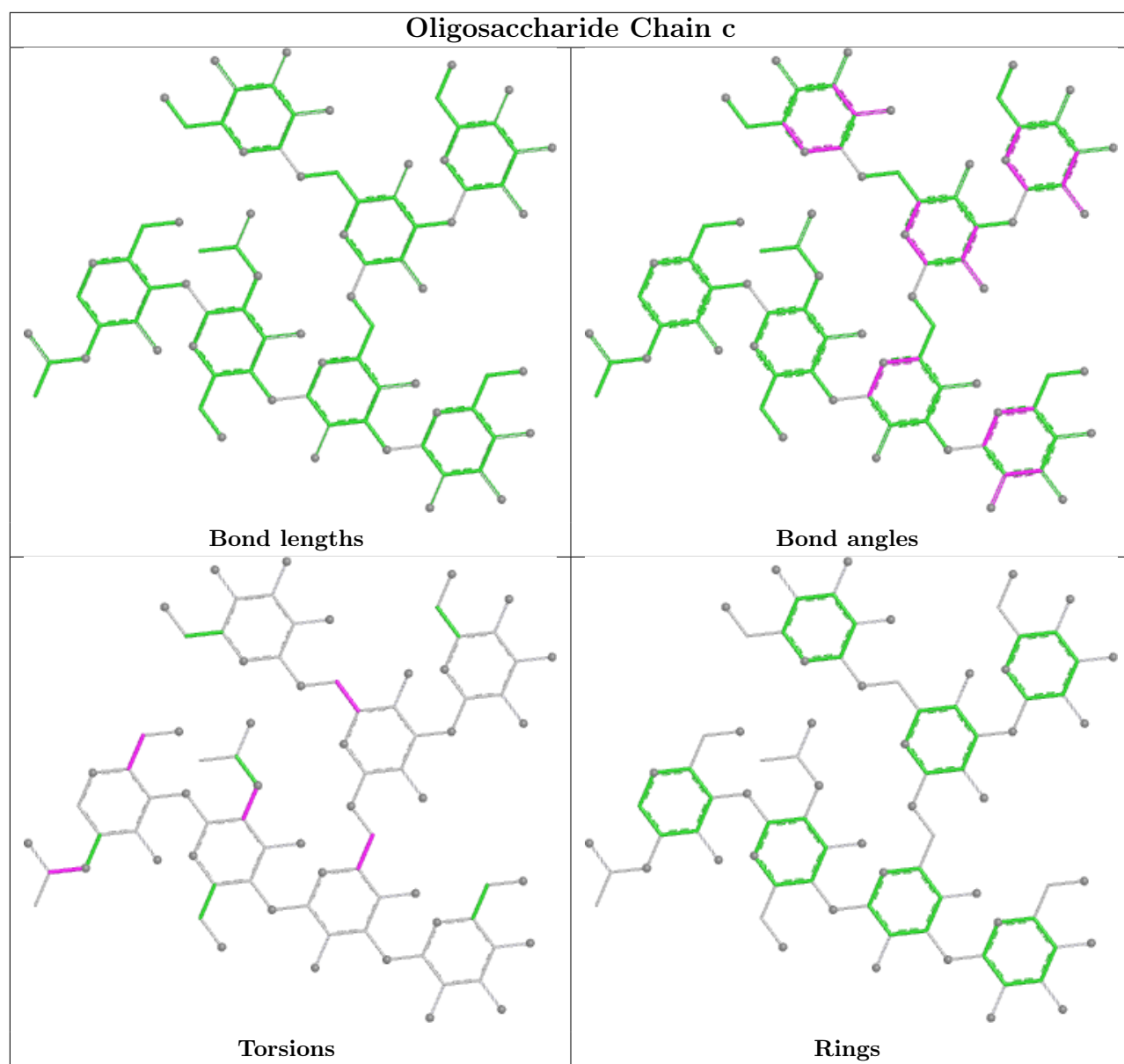


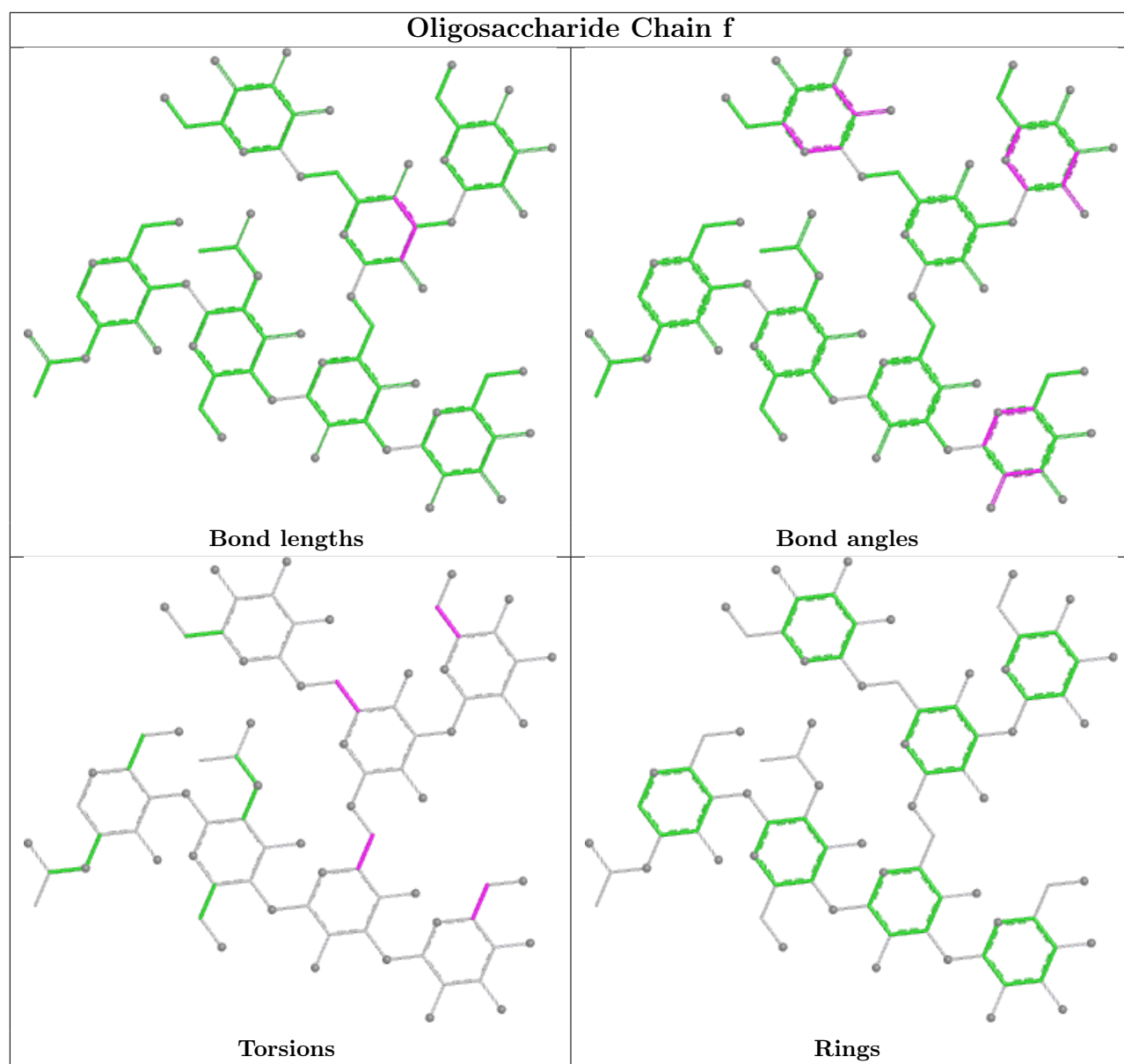


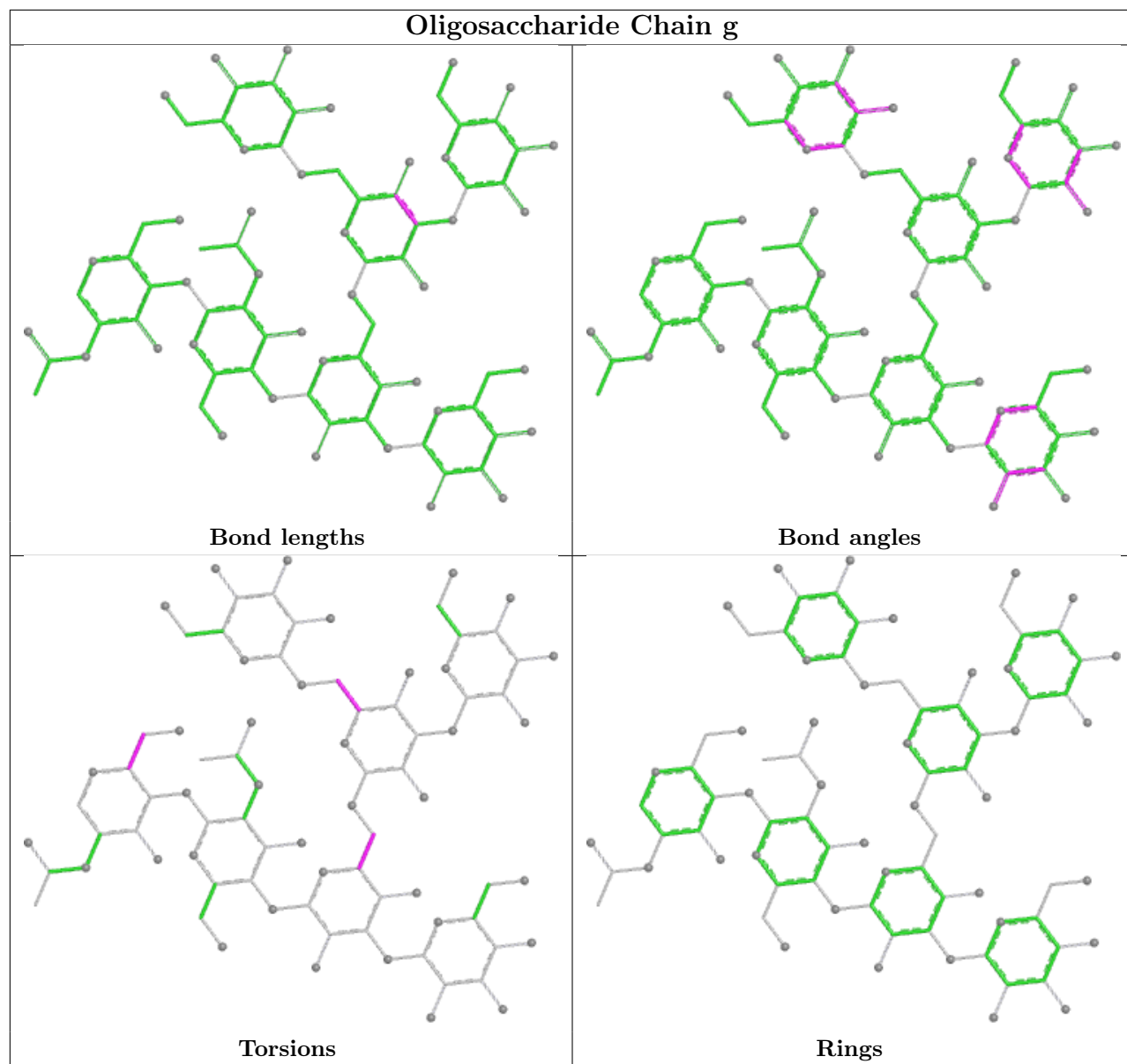


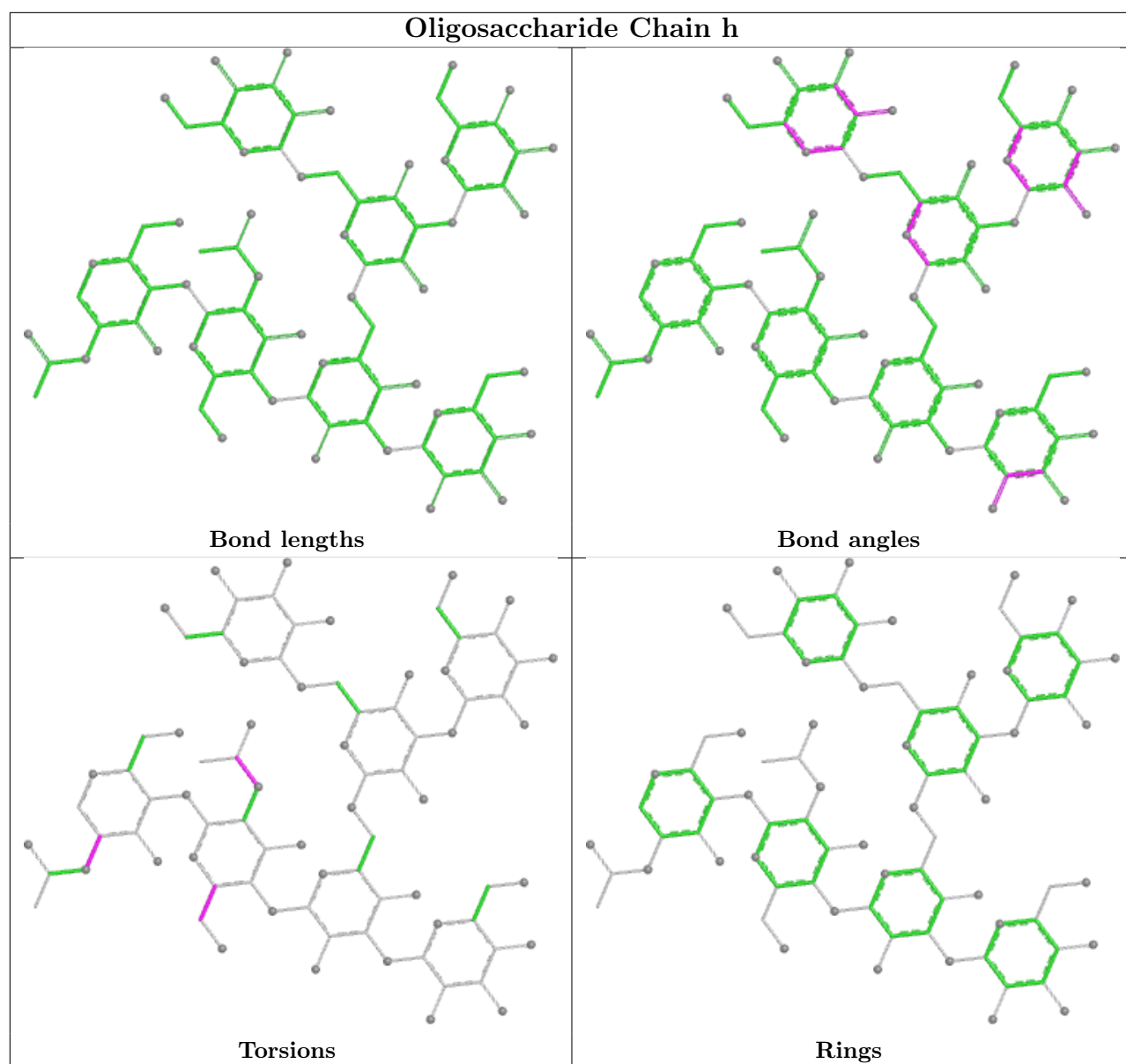


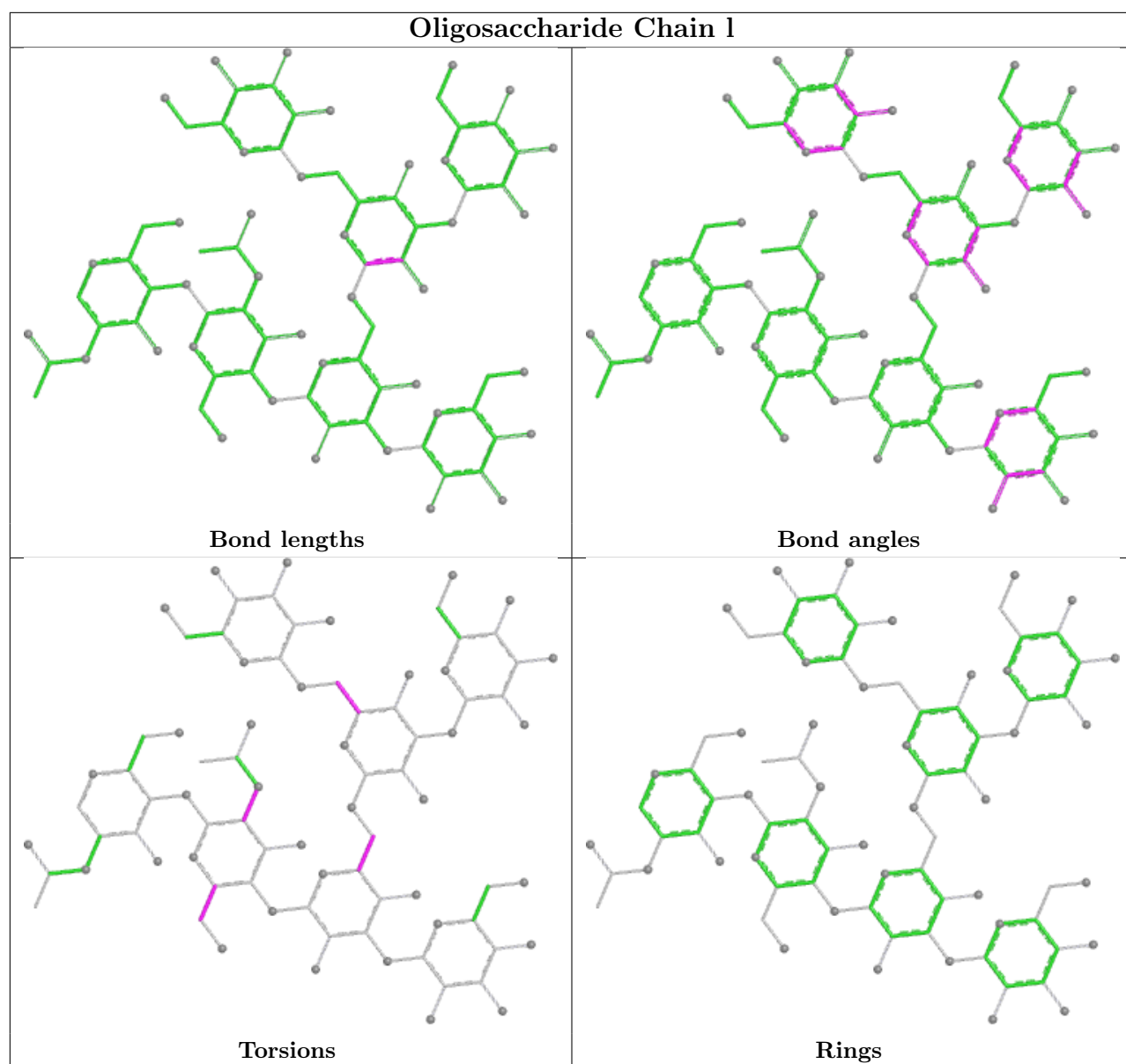


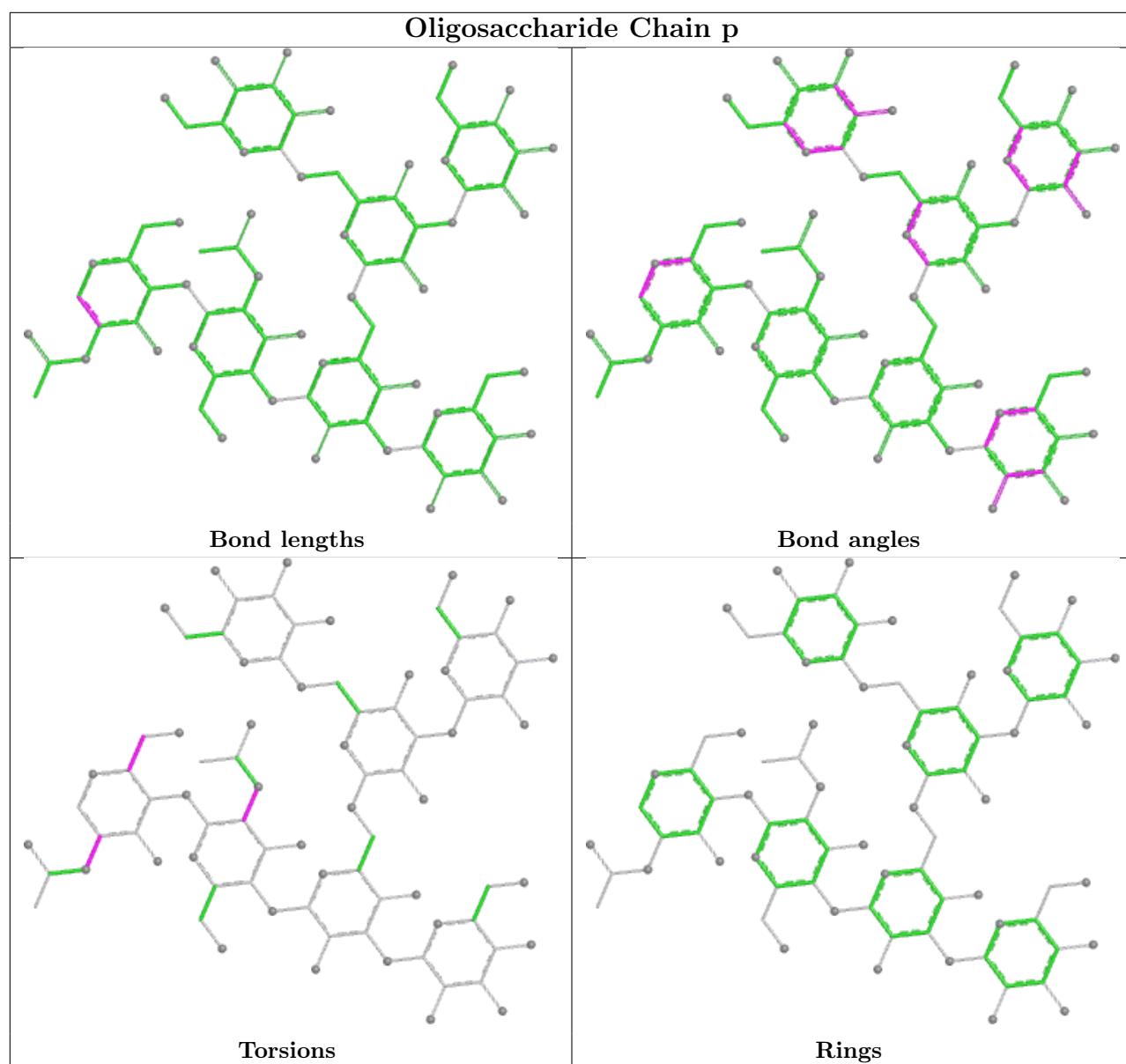


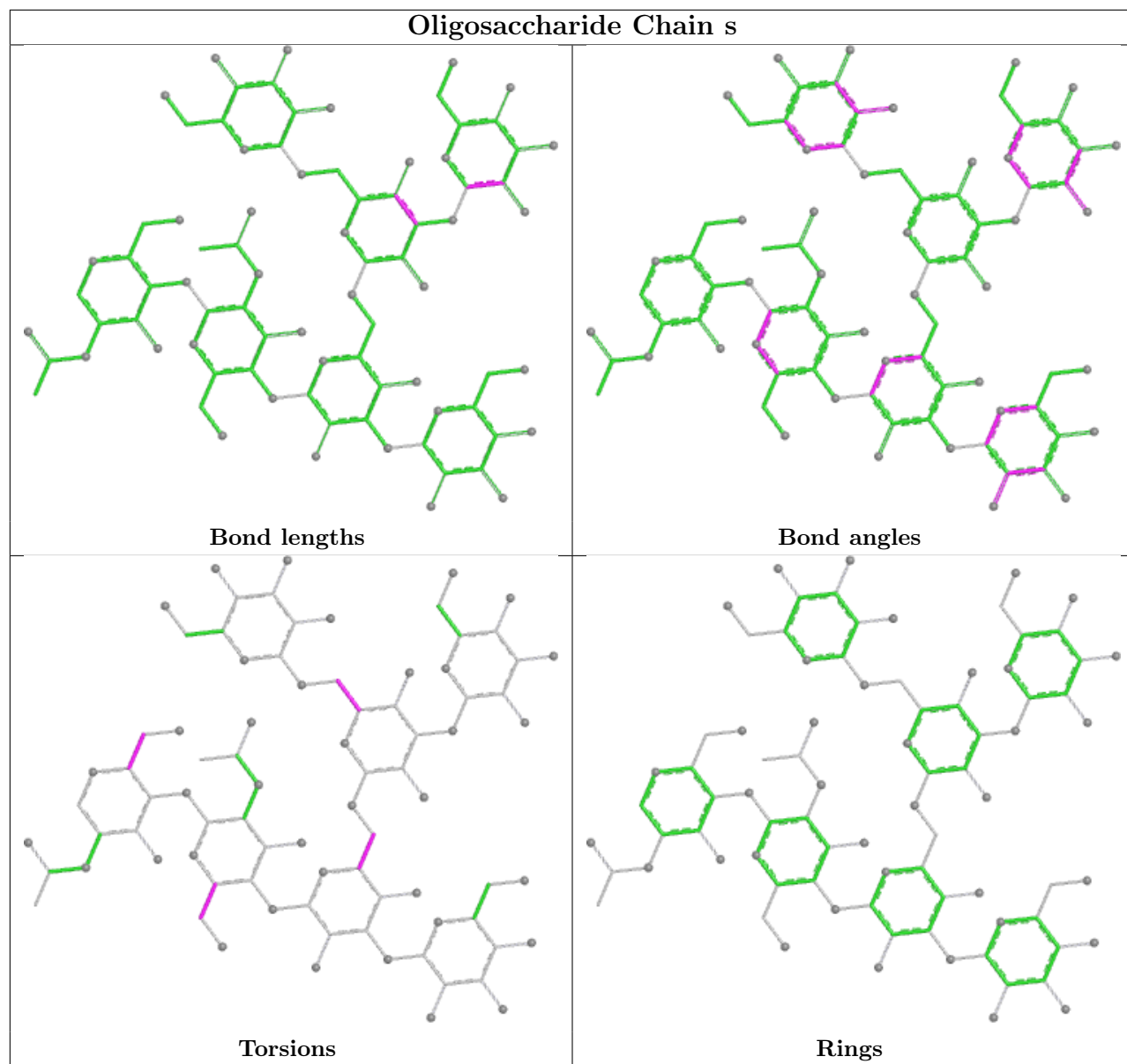


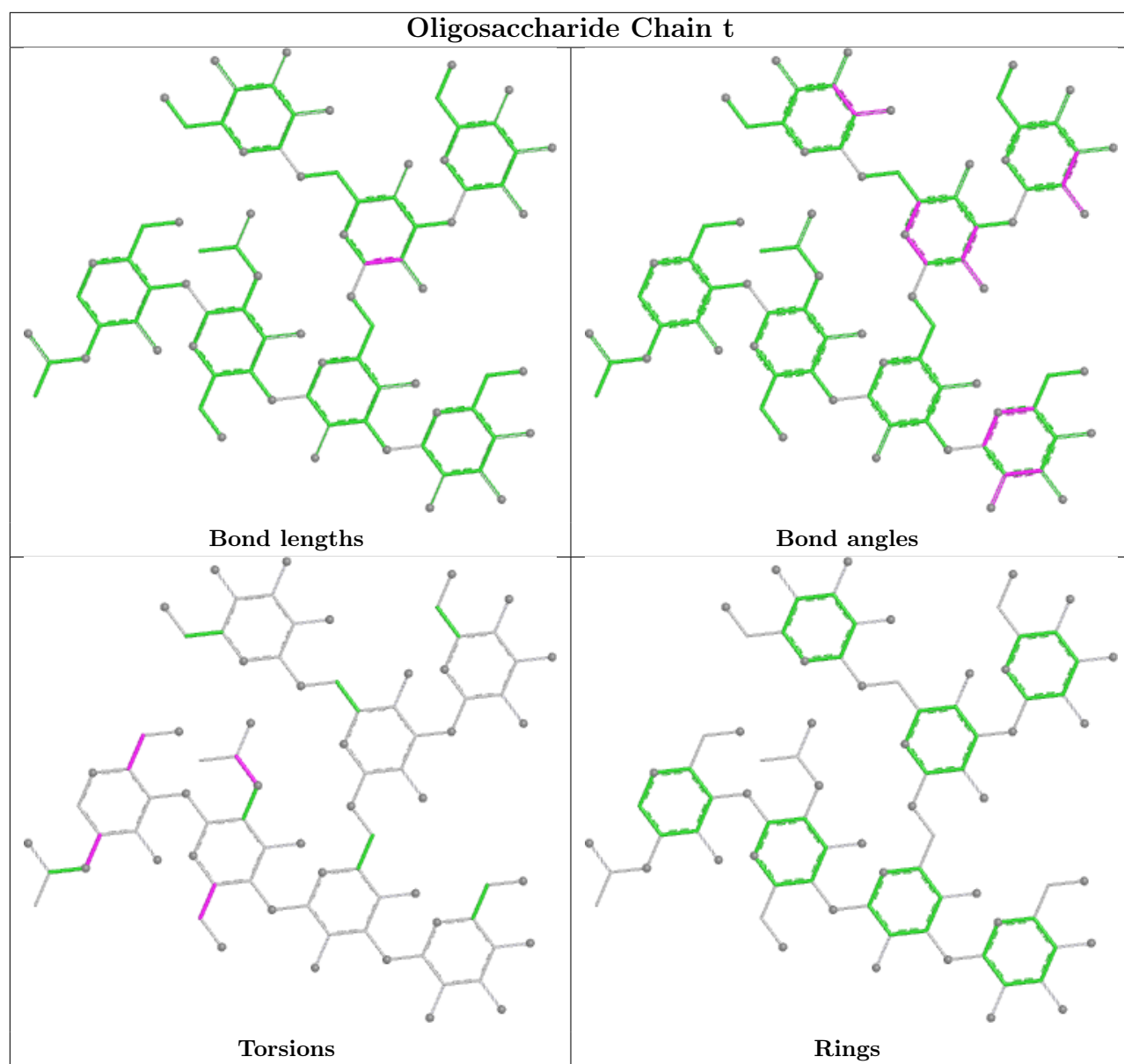


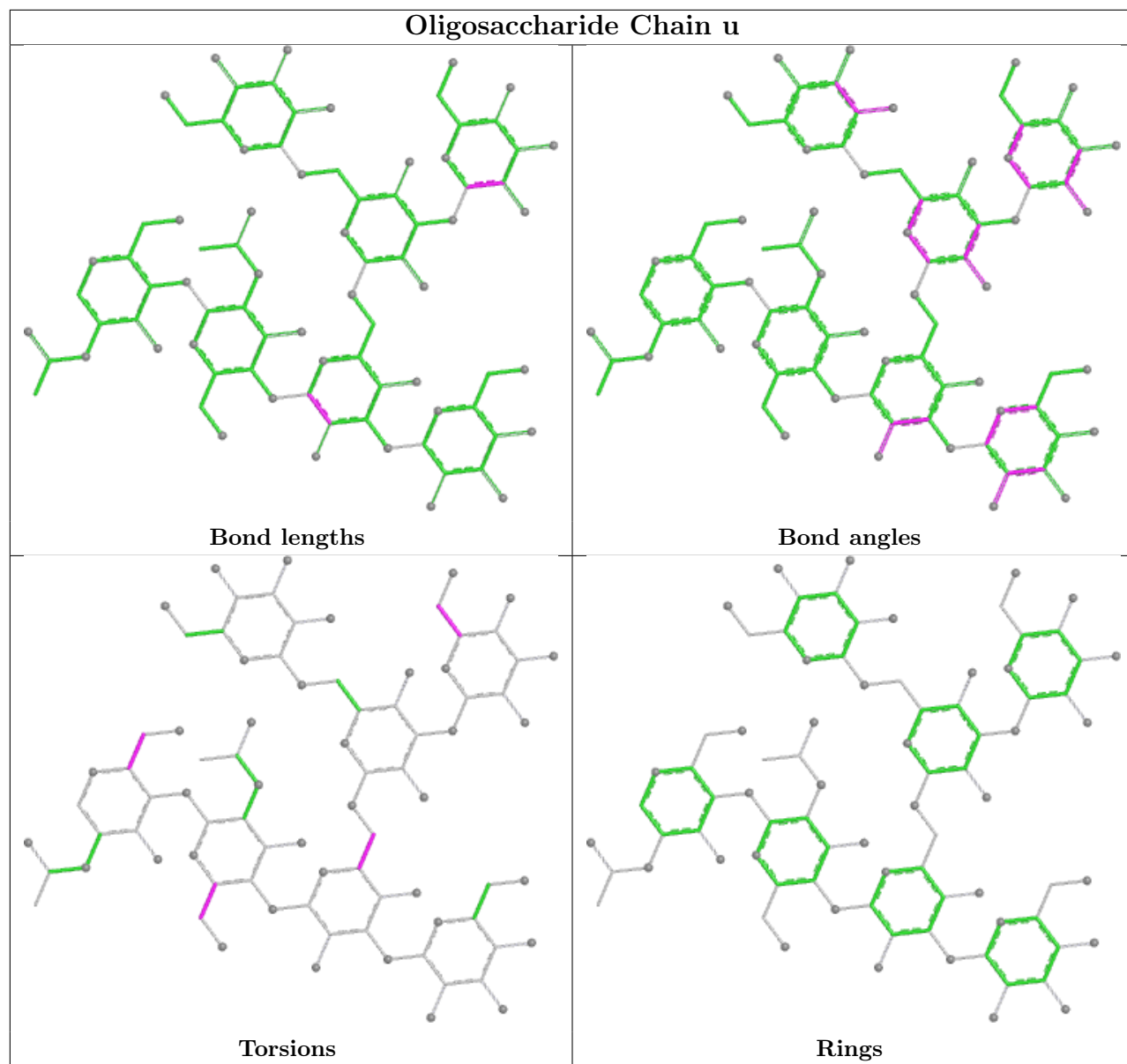


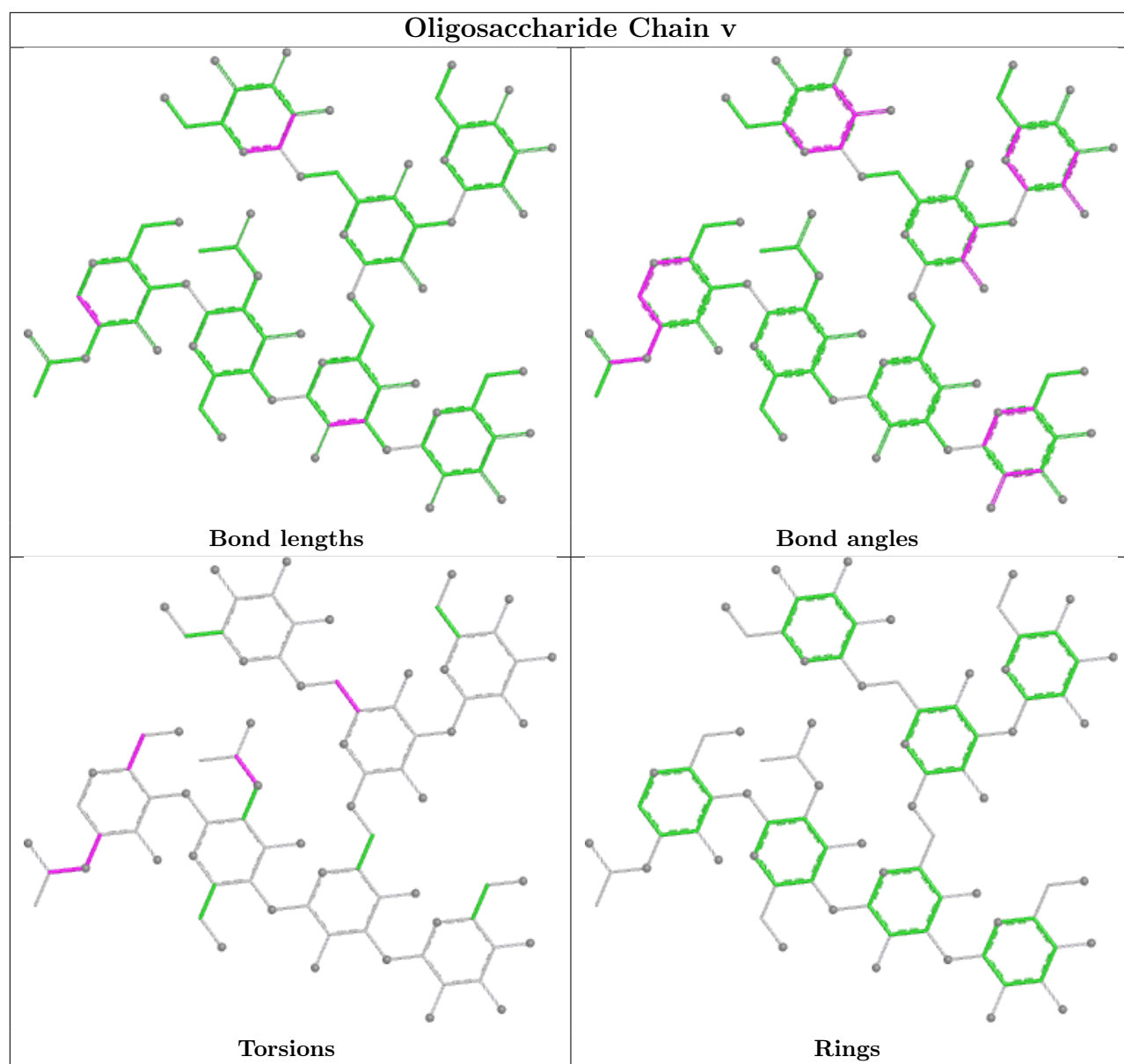


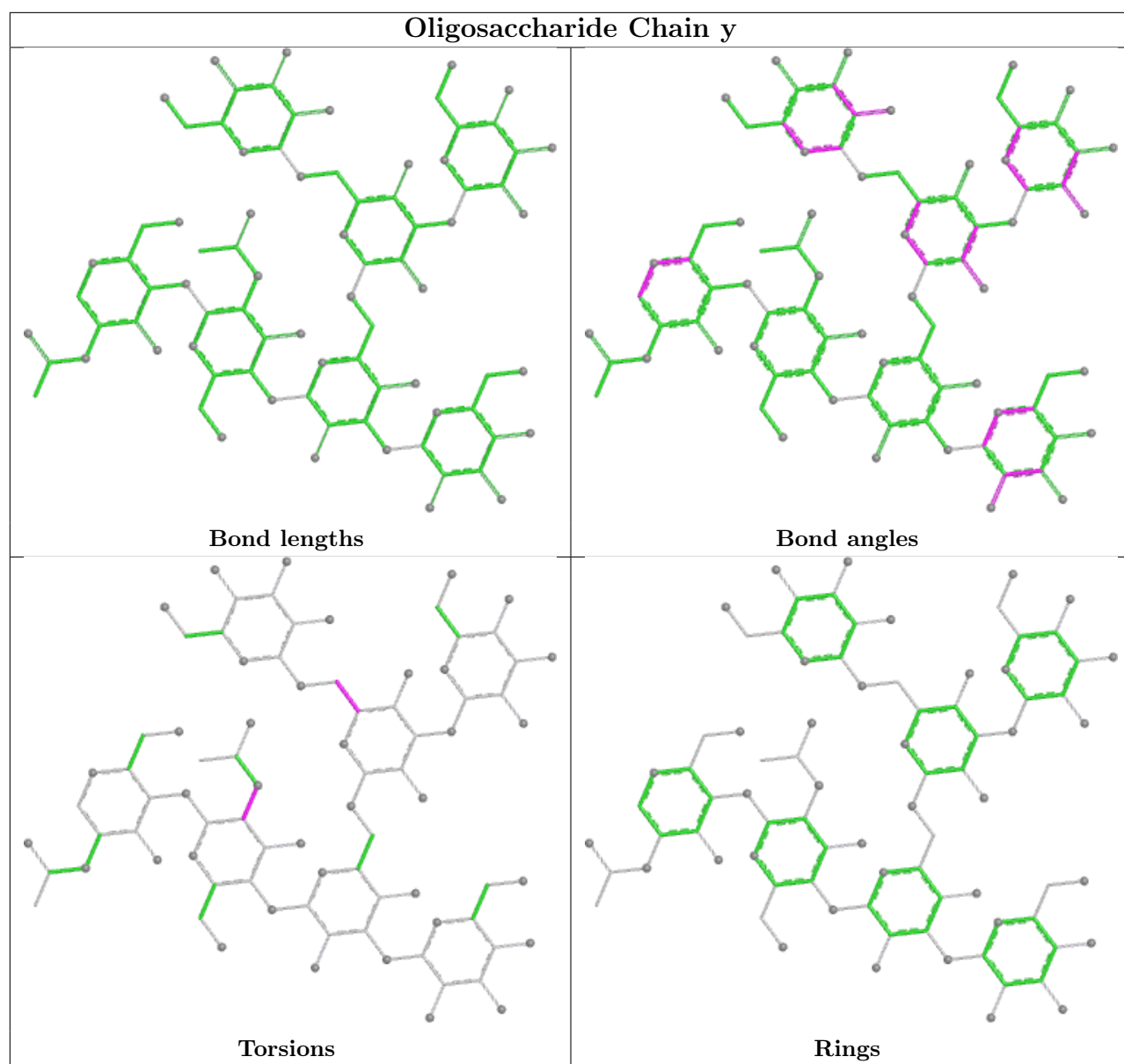


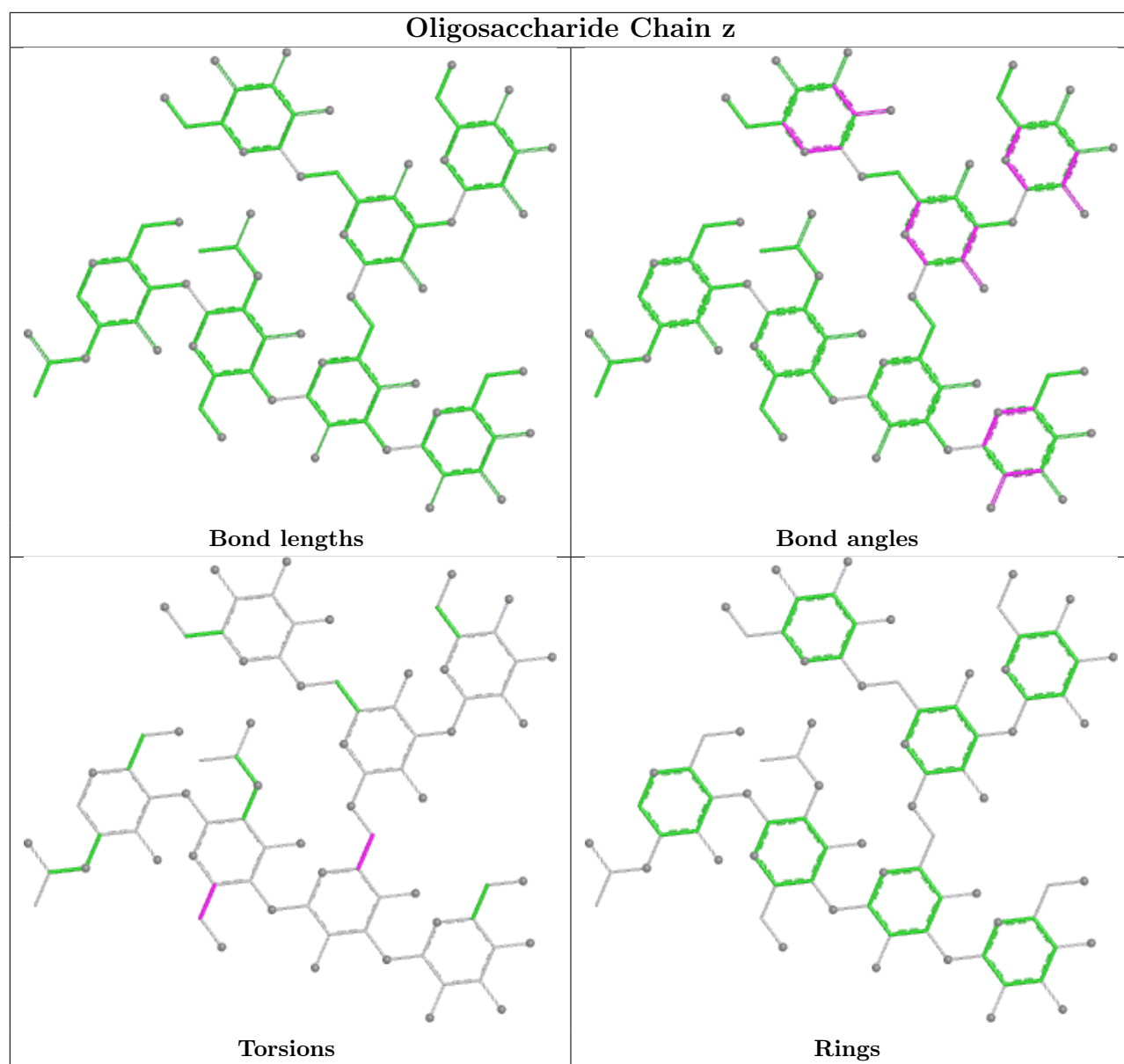


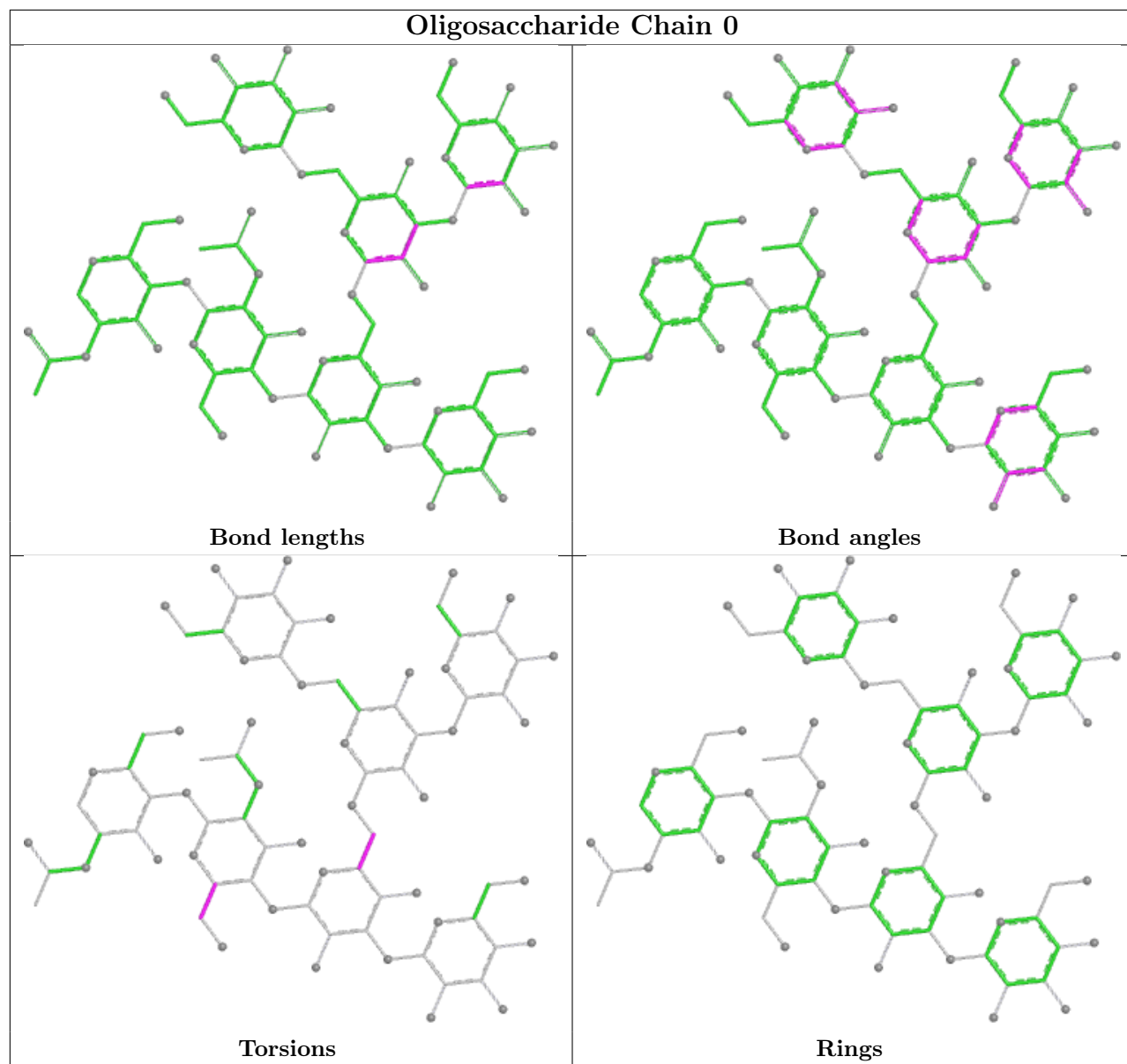


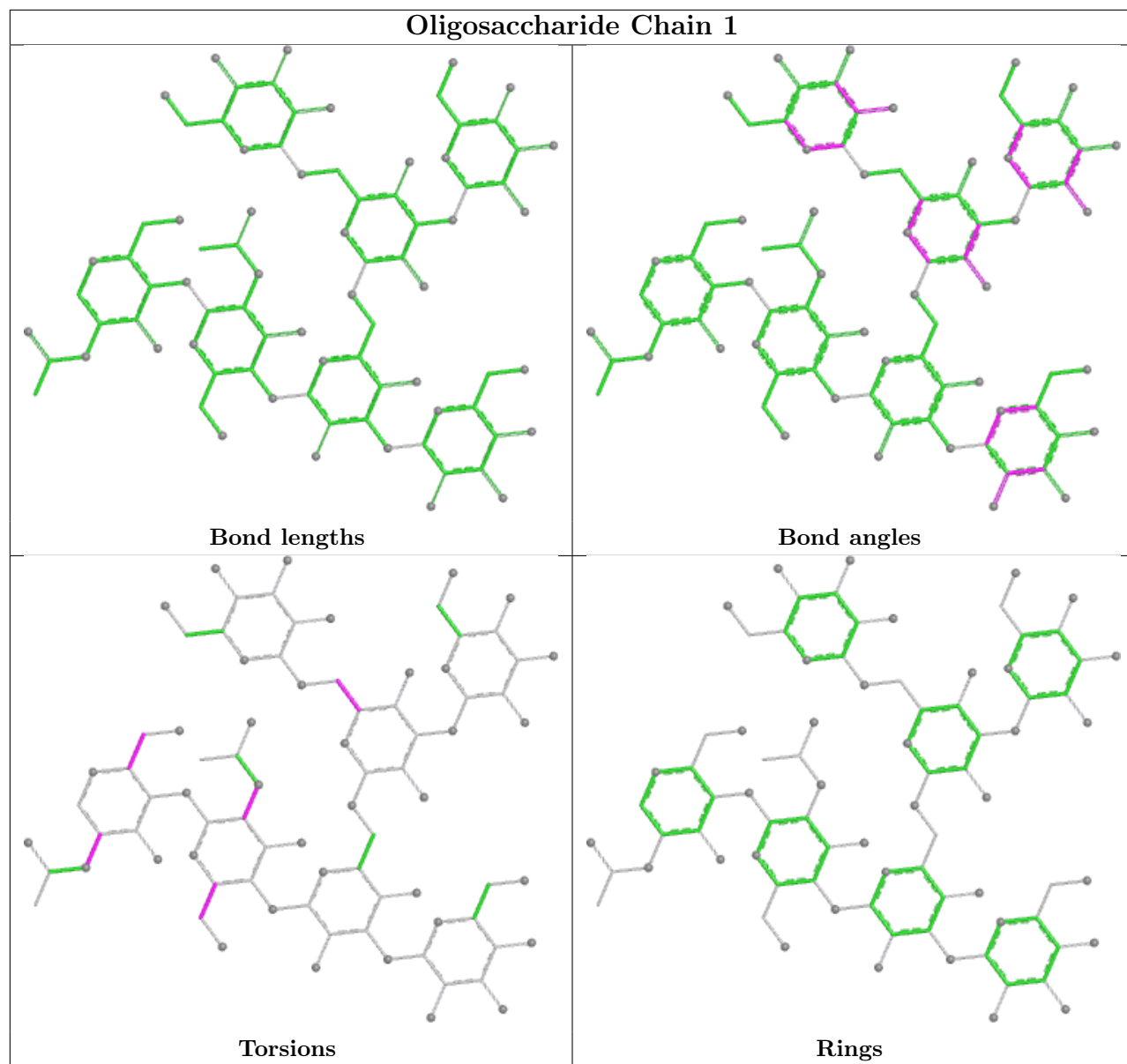


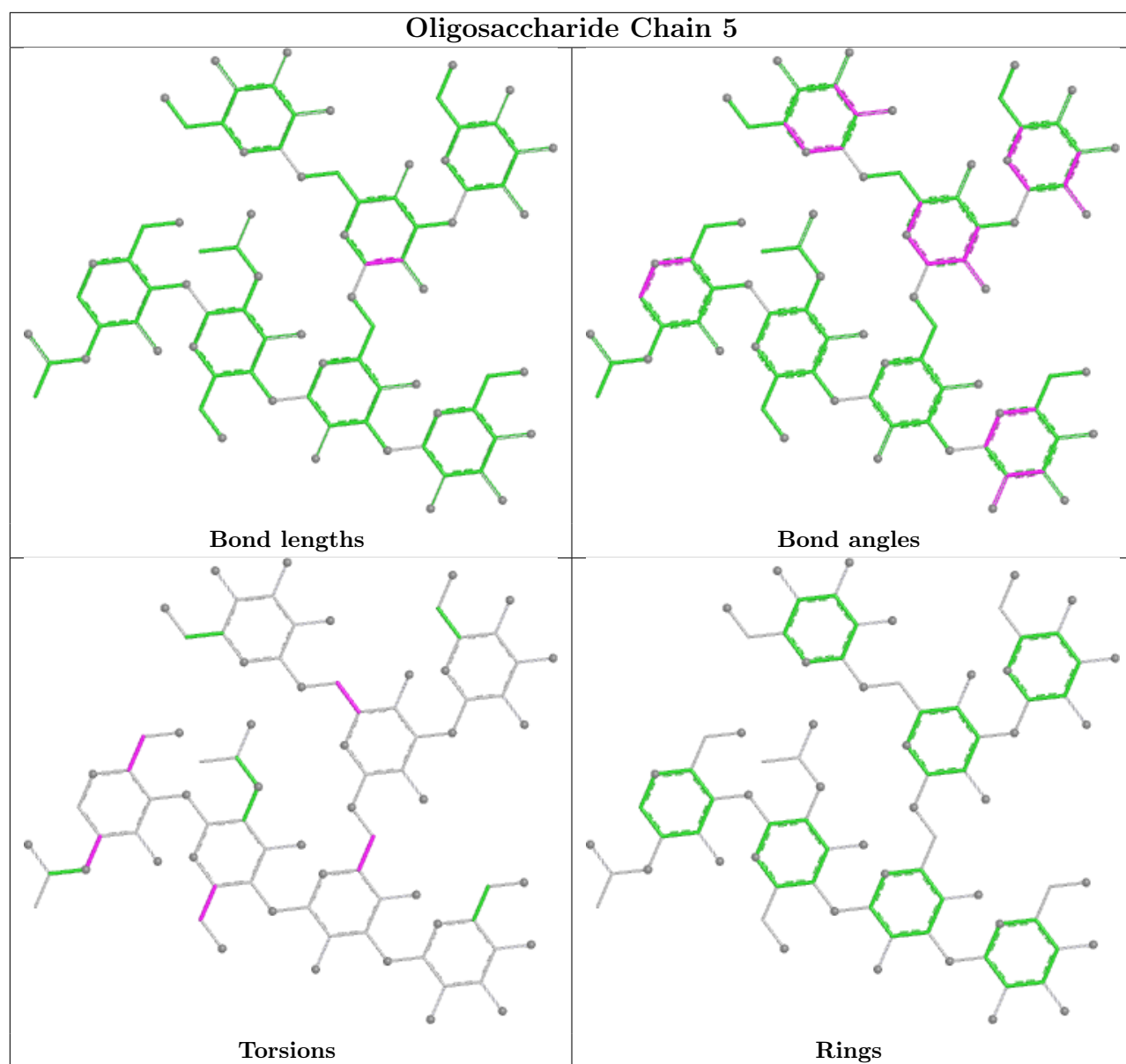


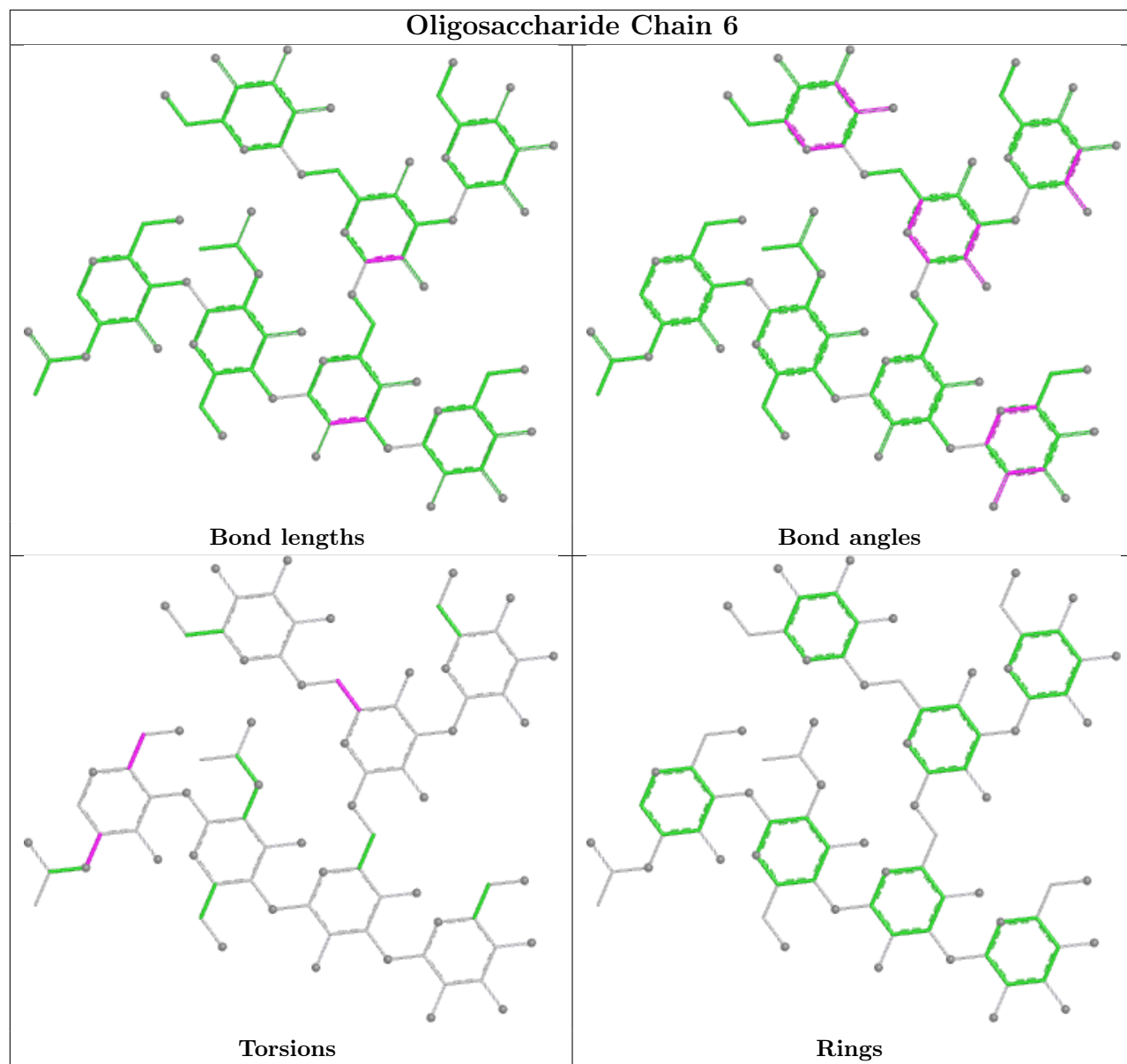


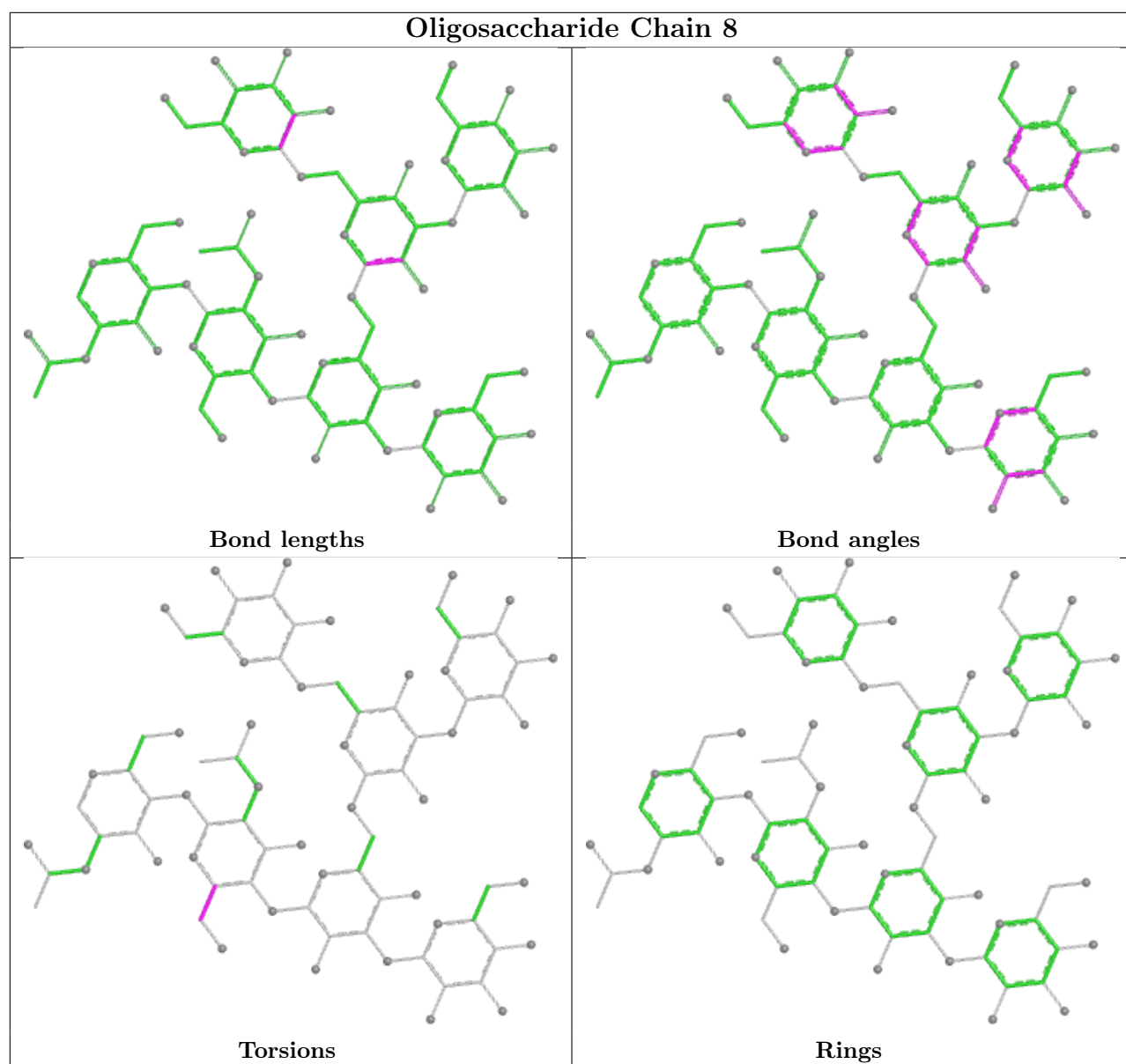


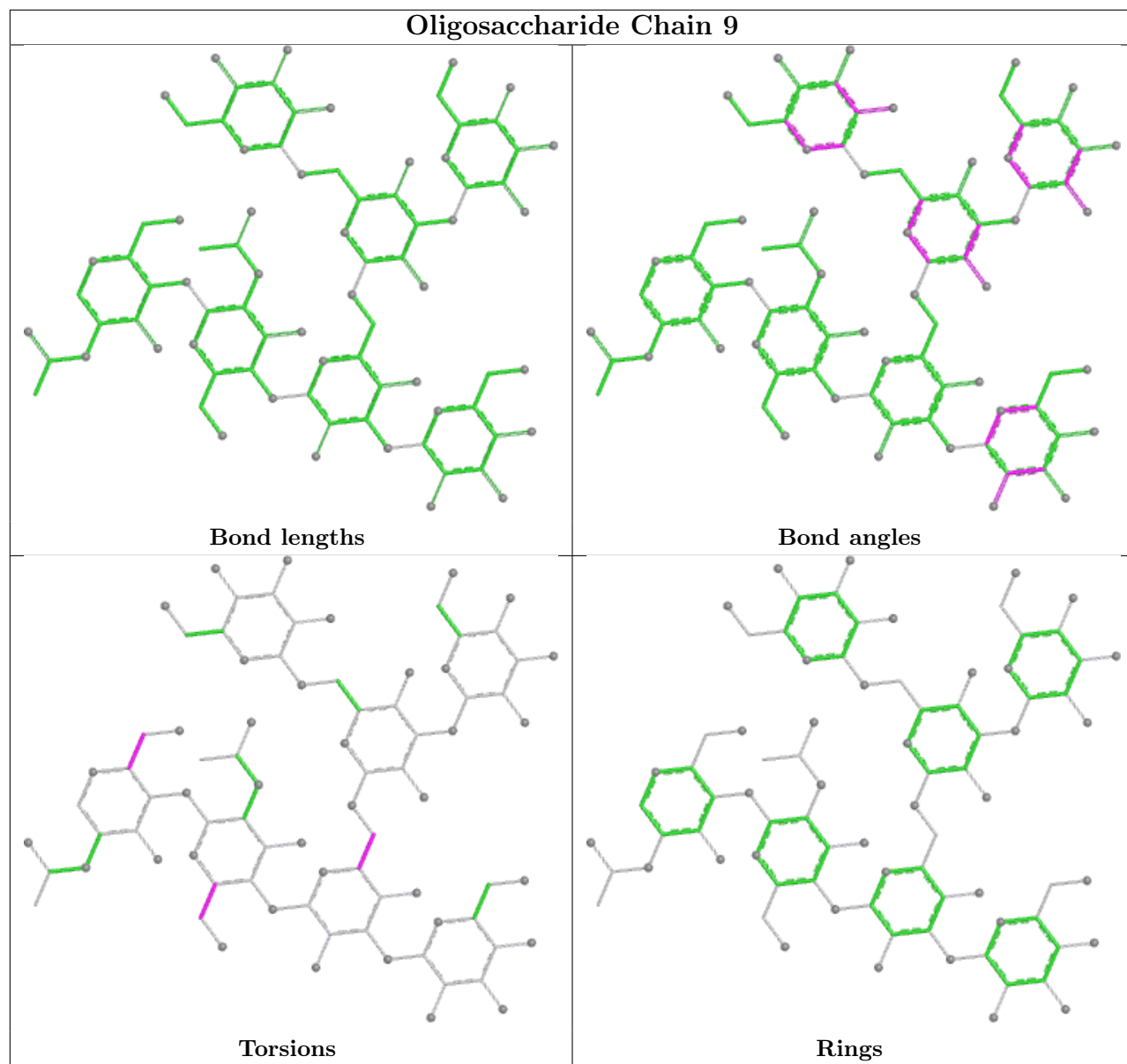


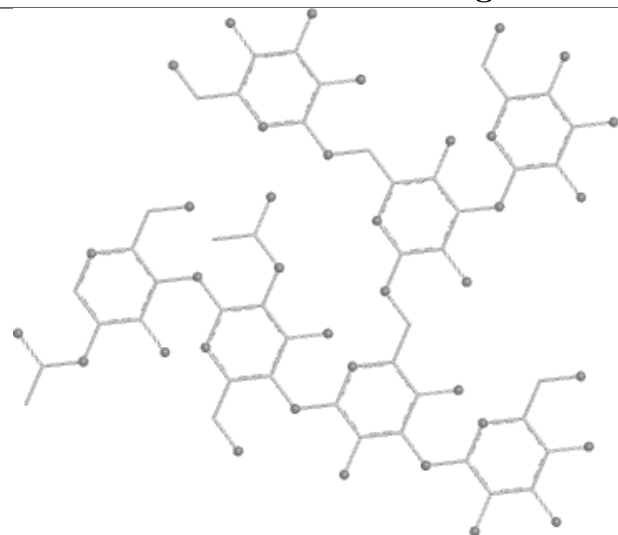
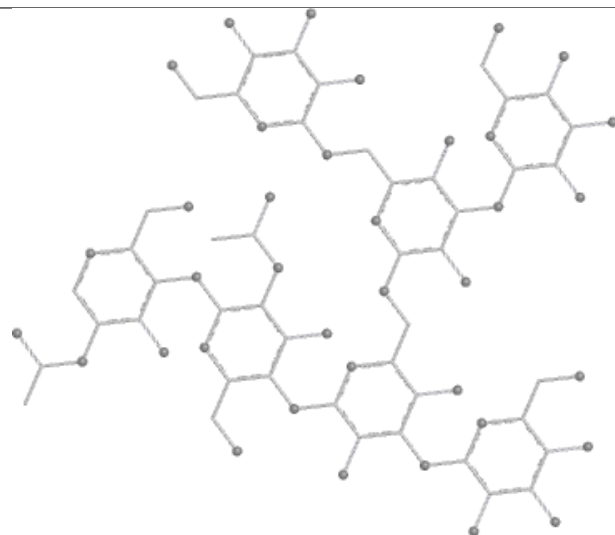
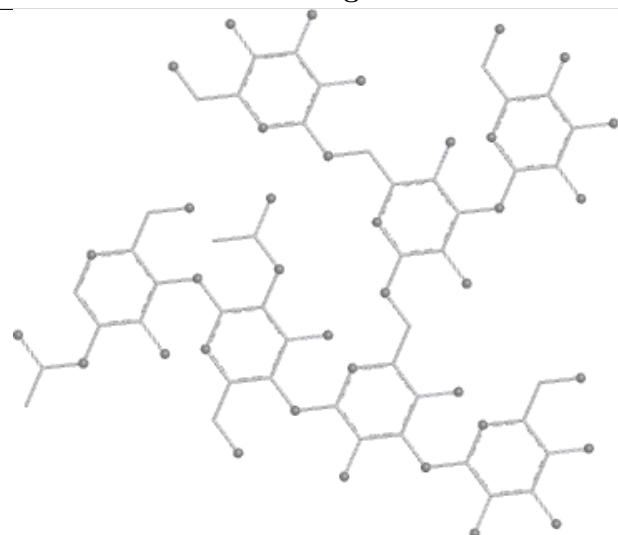
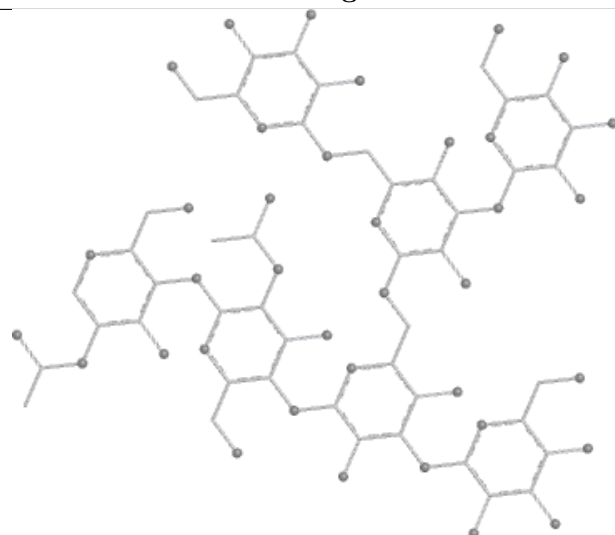


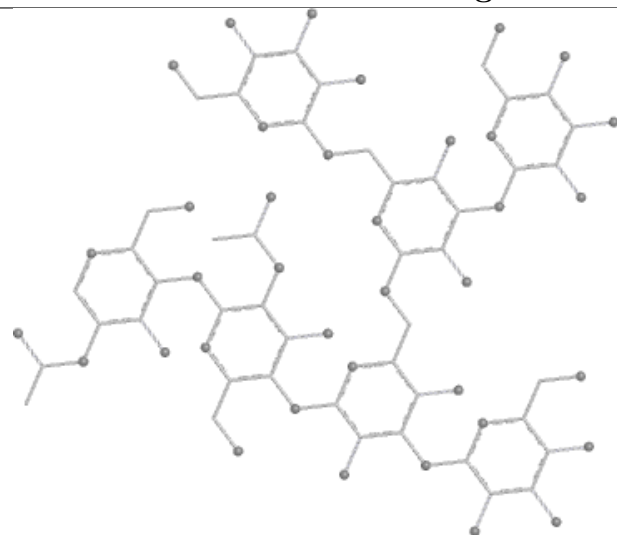
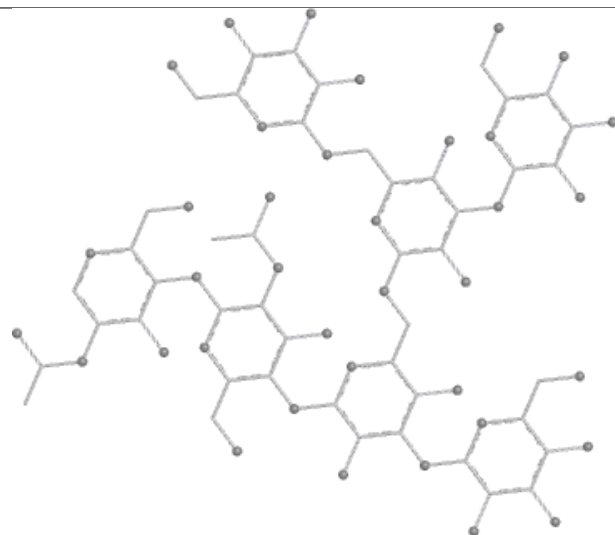
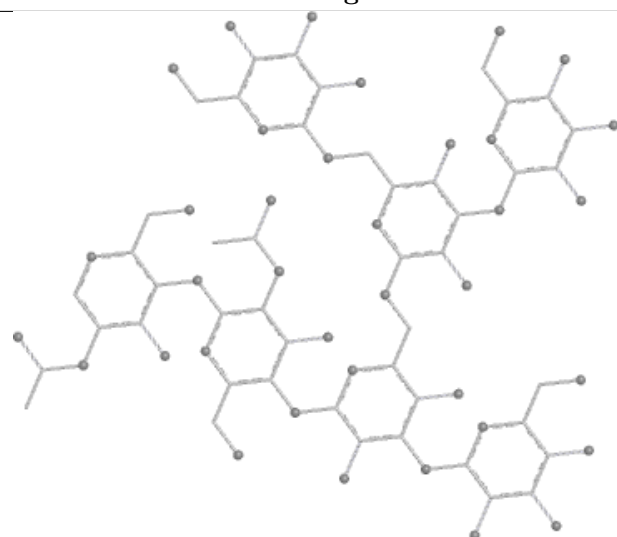
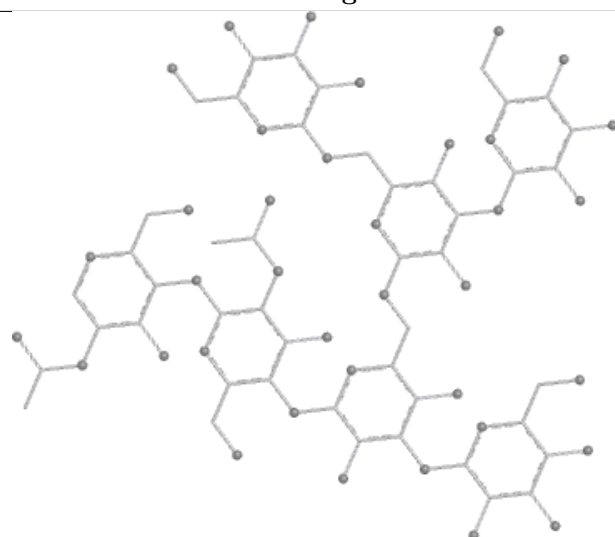


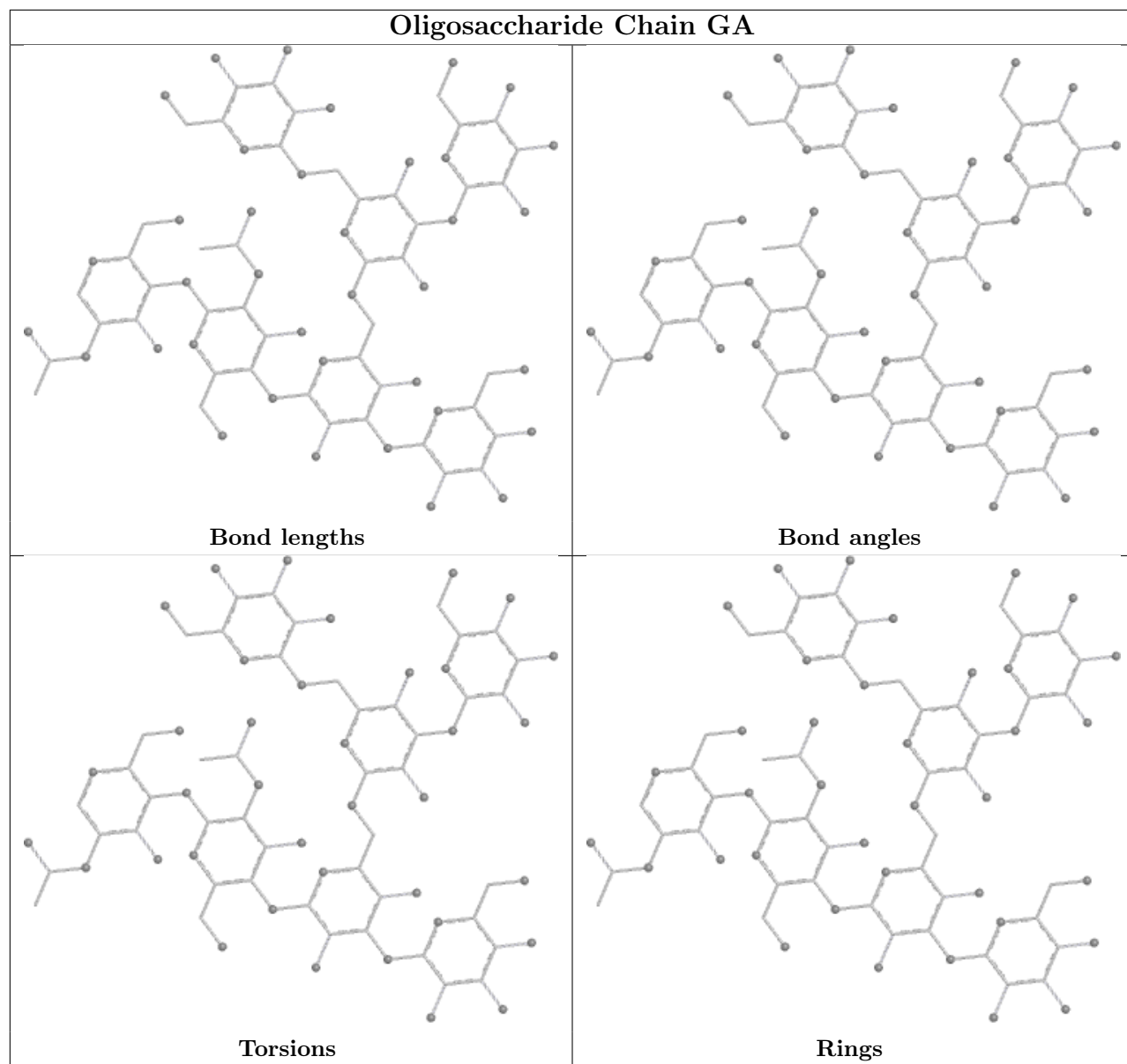


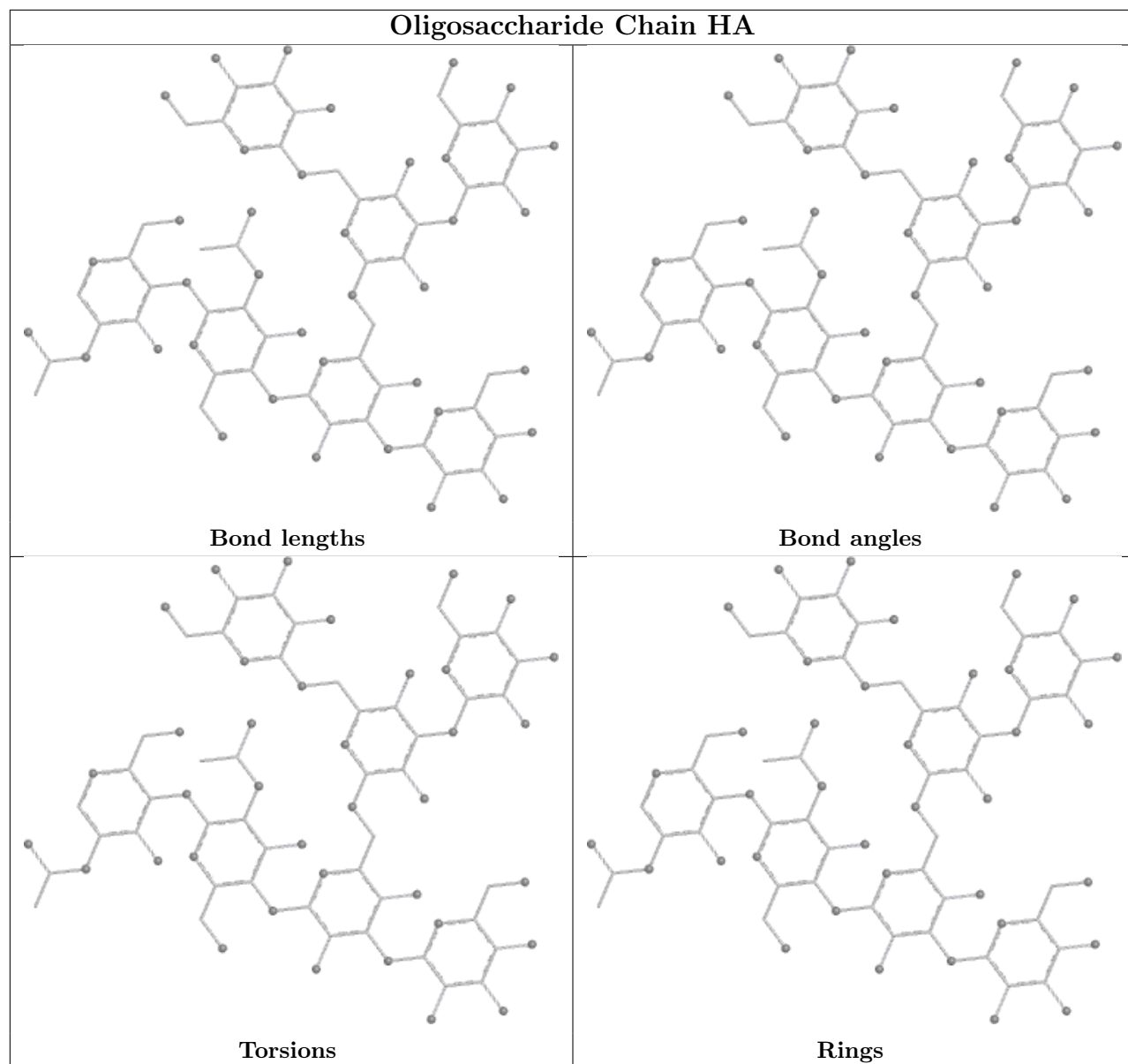


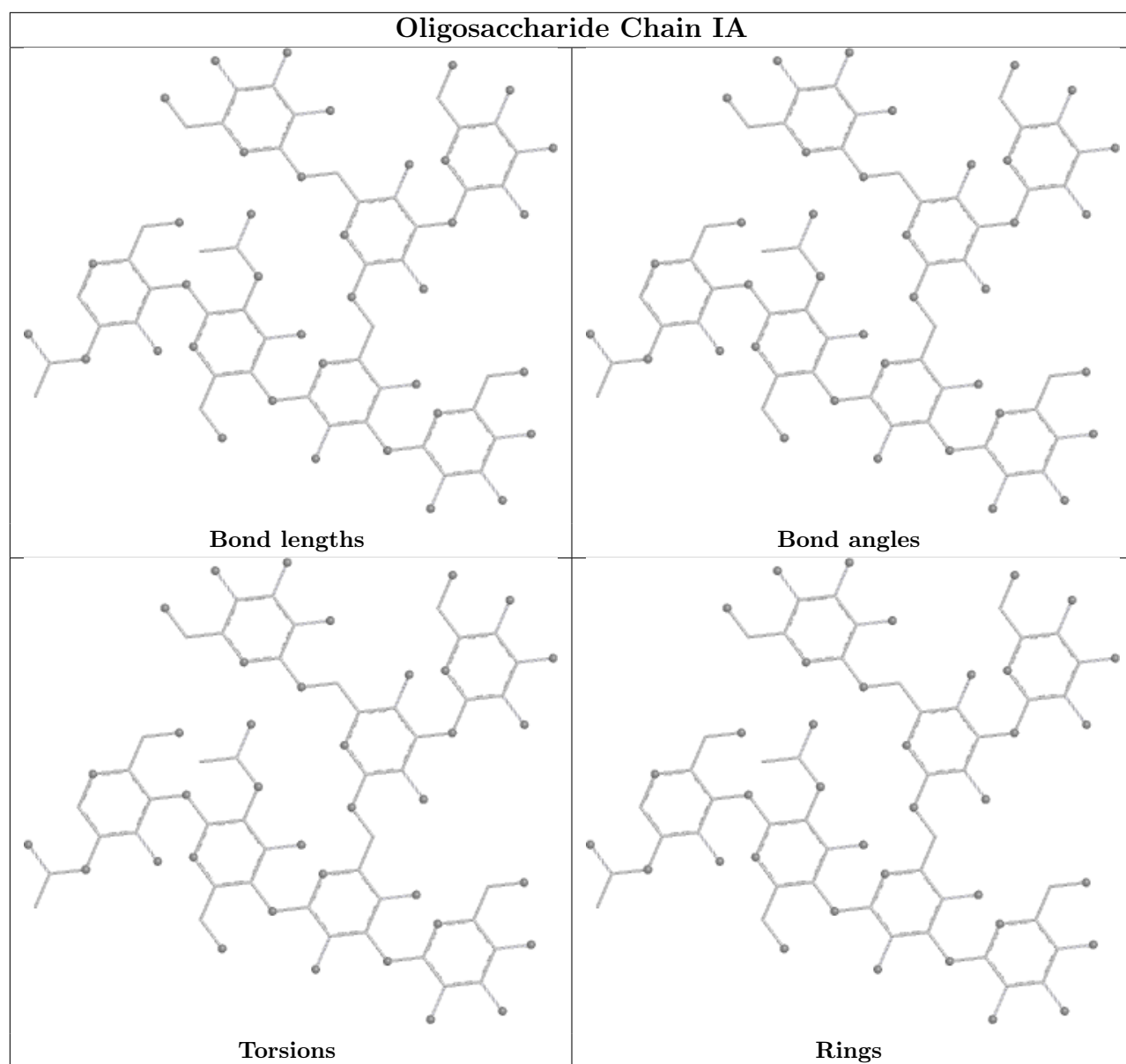


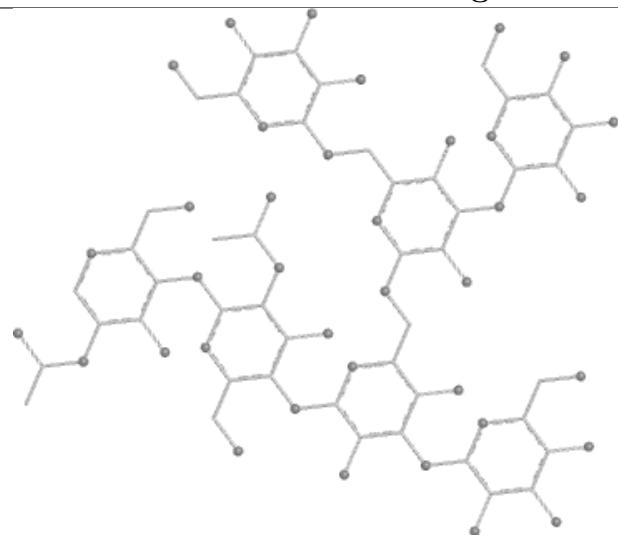
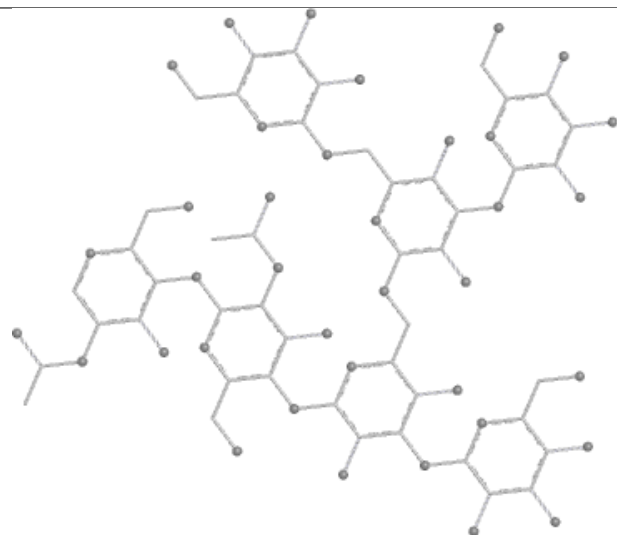
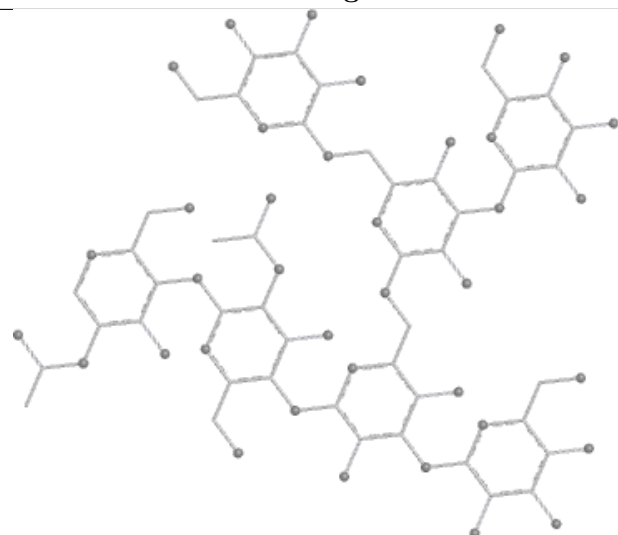
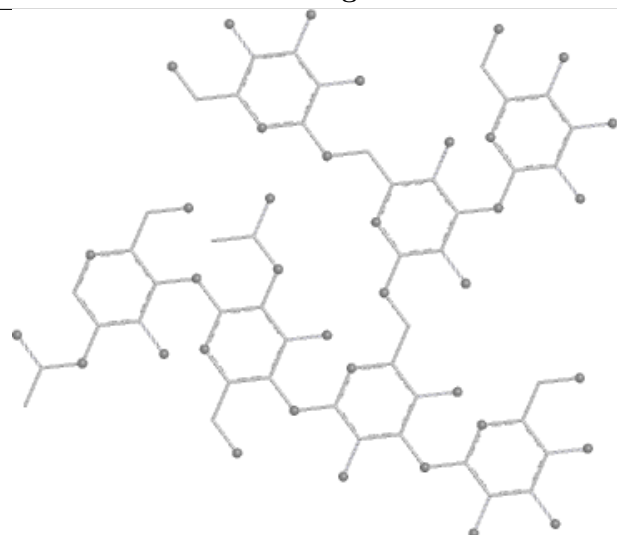
Oligosaccharide Chain BA**Bond lengths****Bond angles****Torsions****Rings**

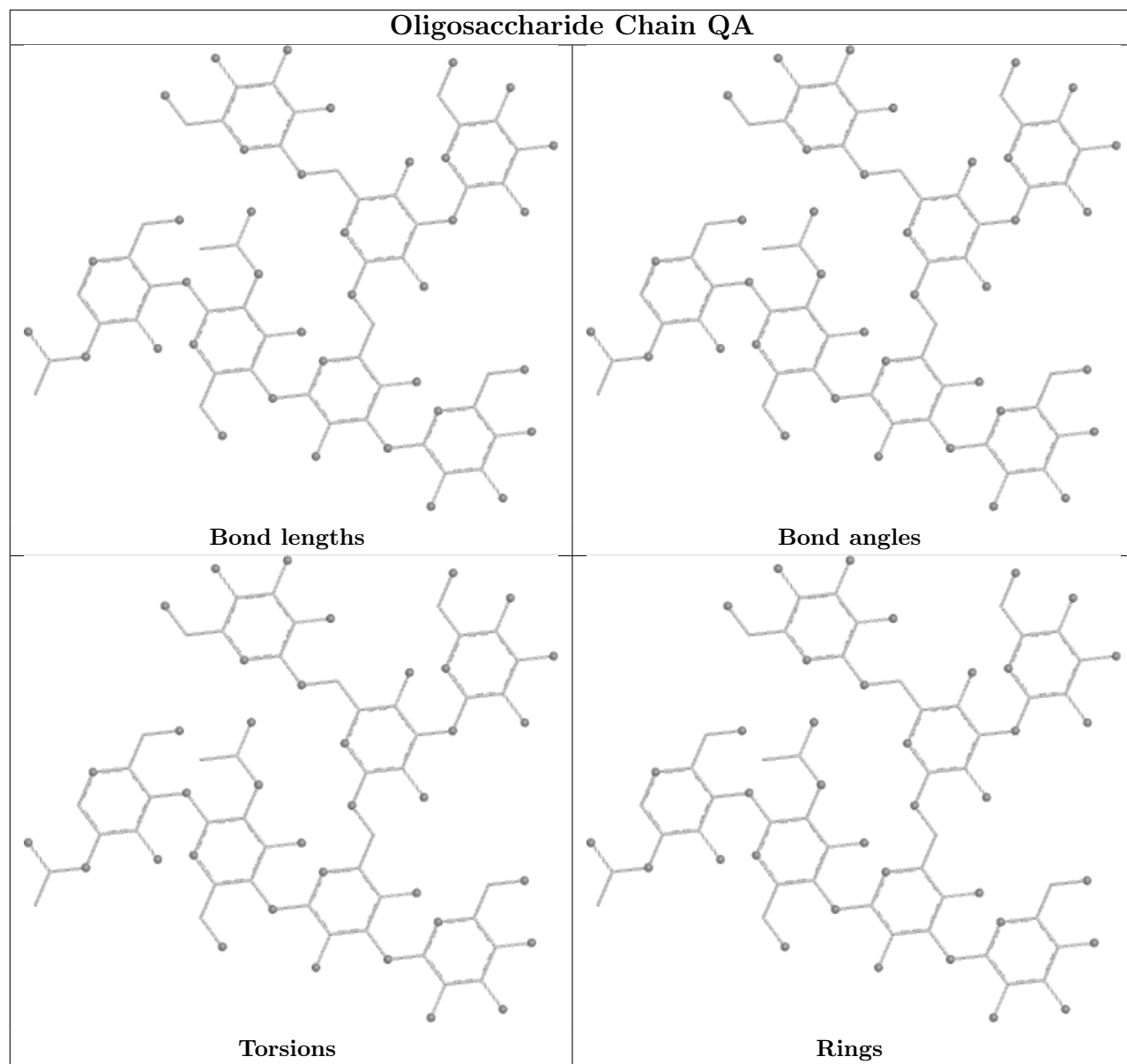
Oligosaccharide Chain DA**Bond lengths****Bond angles****Torsions****Rings**

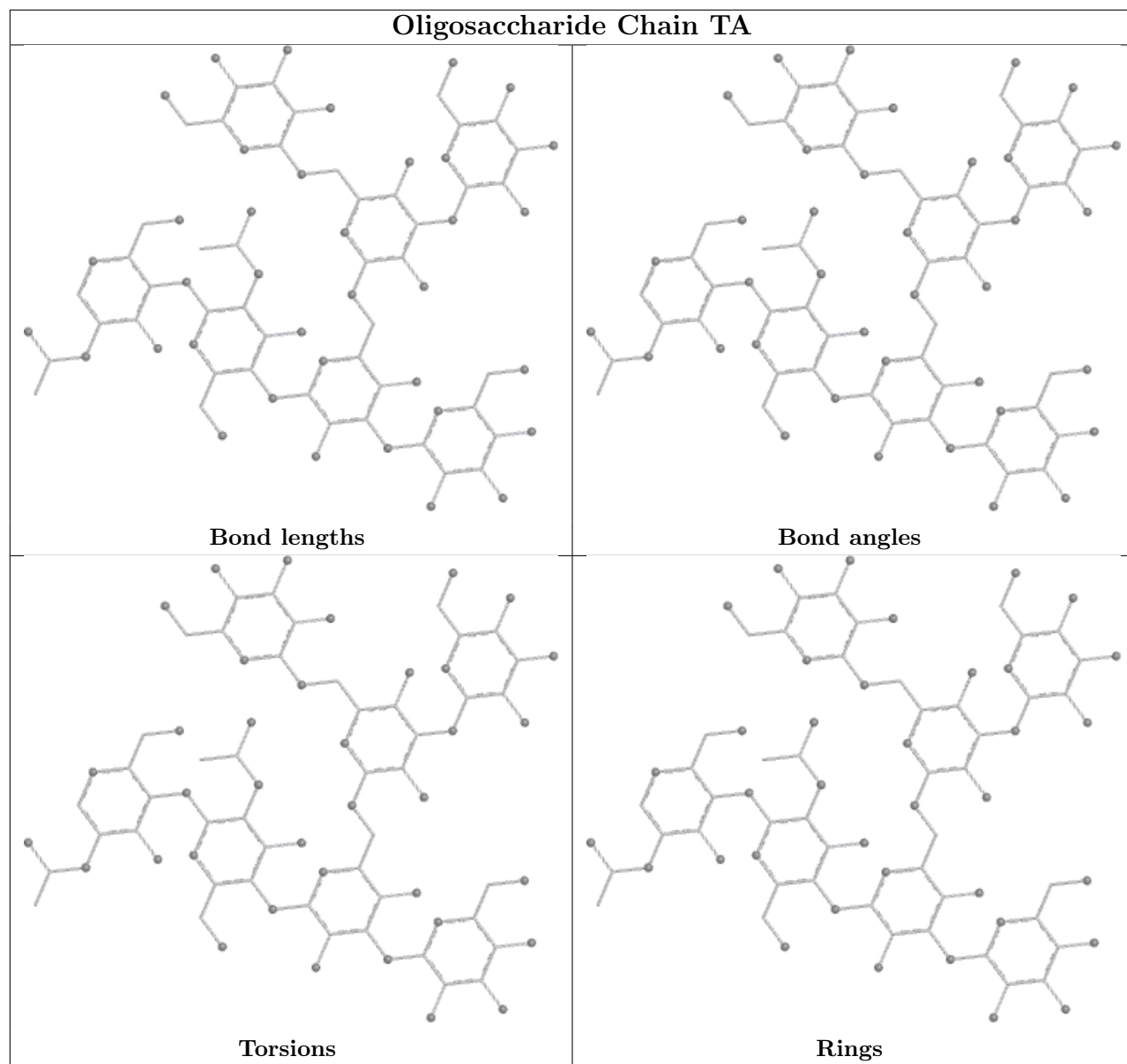


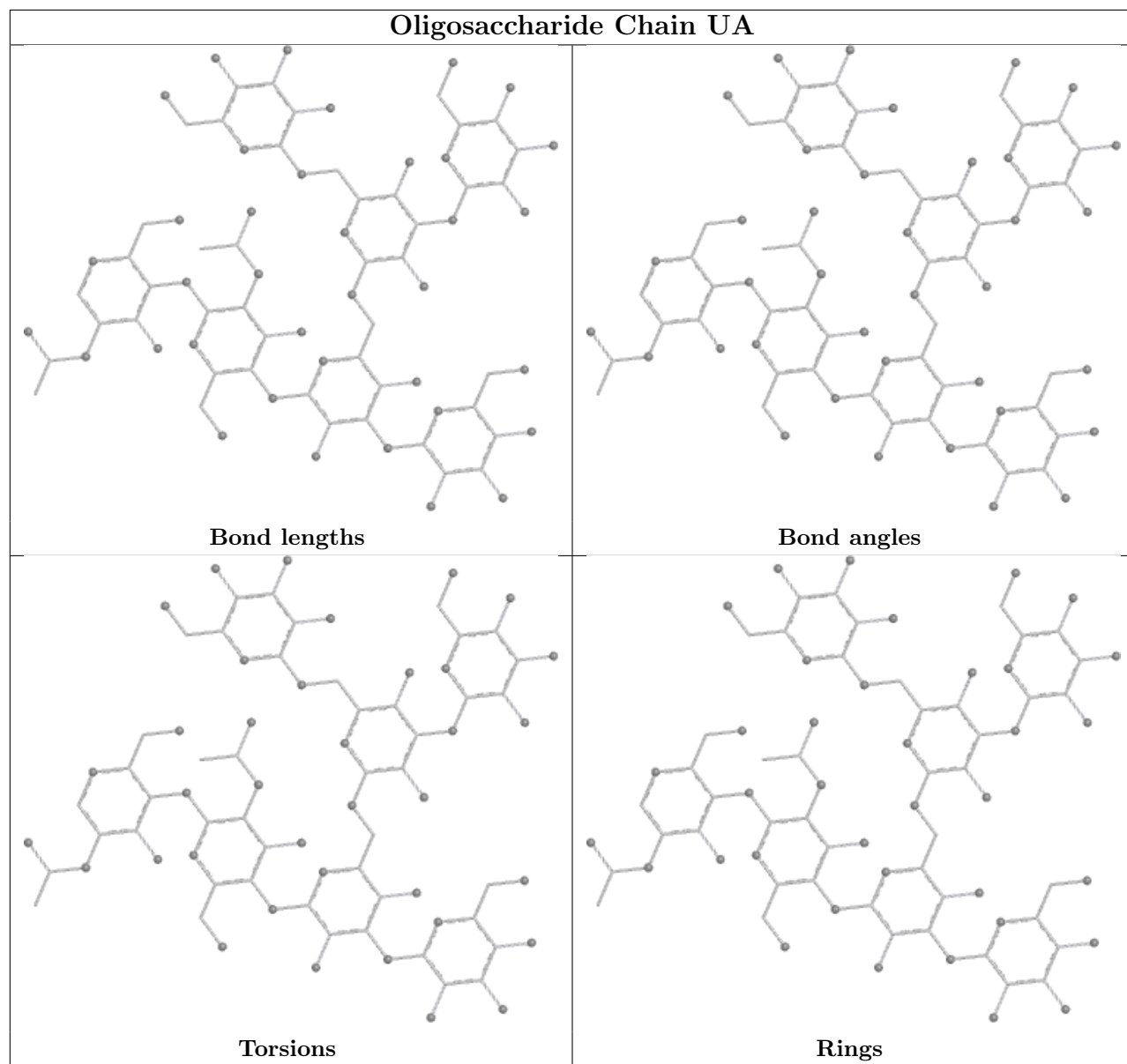


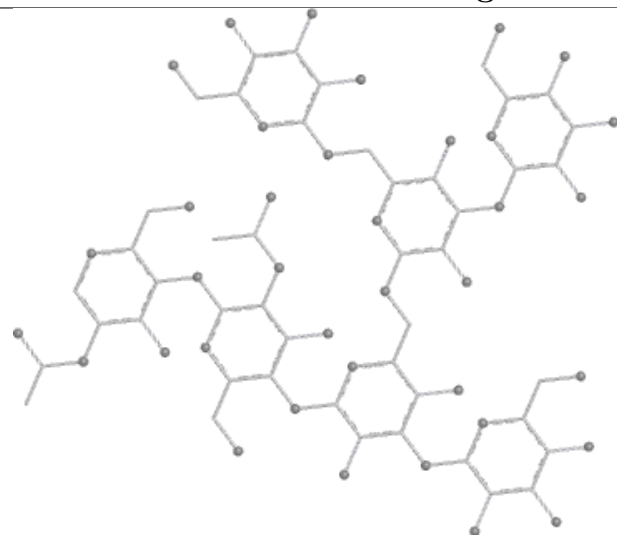
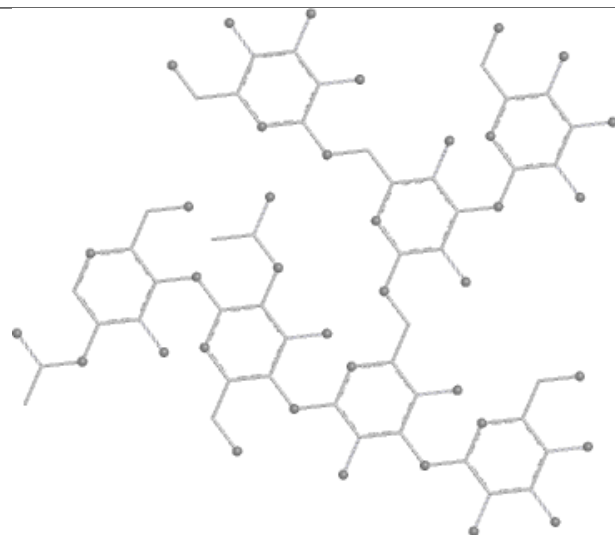
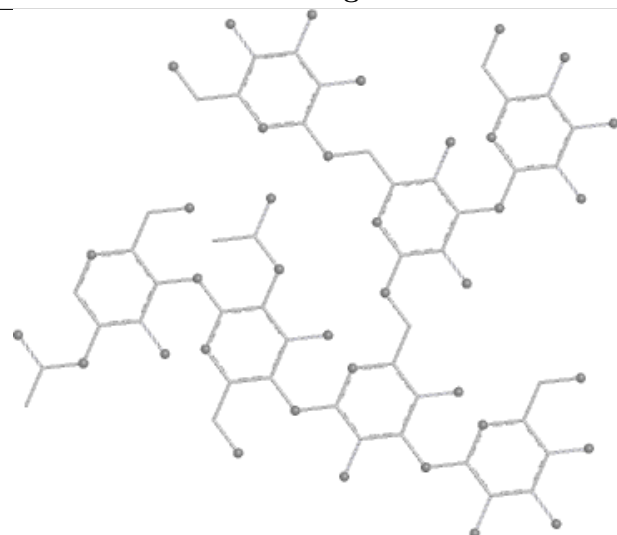
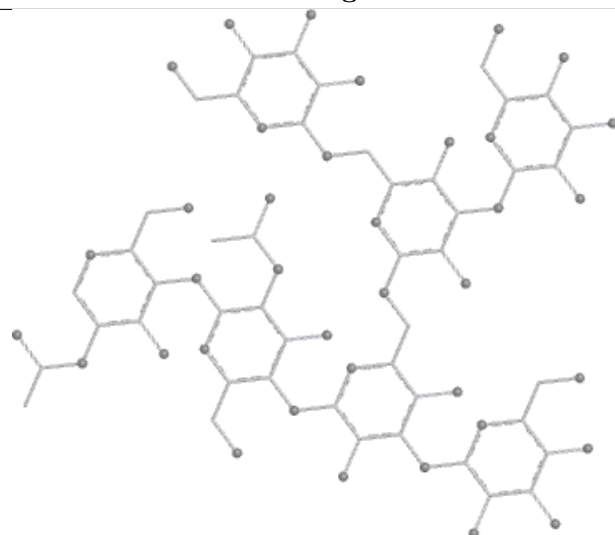


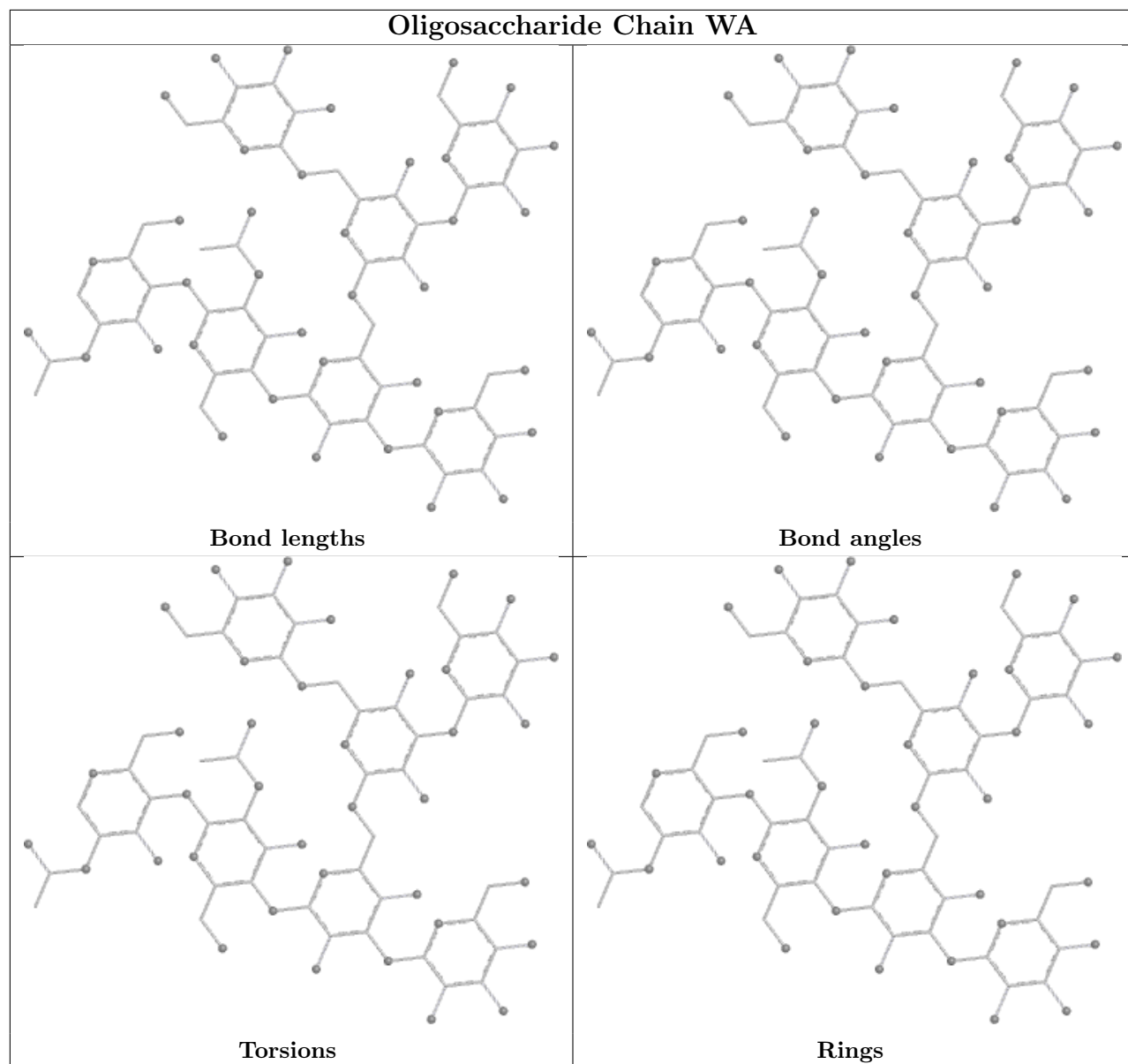
Oligosaccharide Chain MA**Bond lengths****Bond angles****Torsions****Rings**

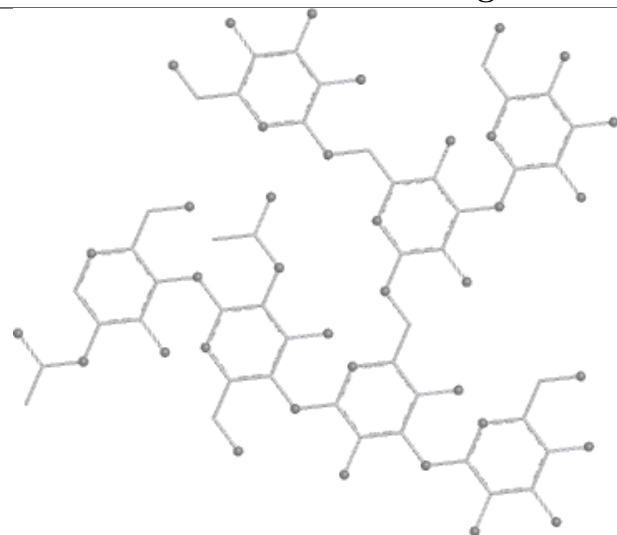
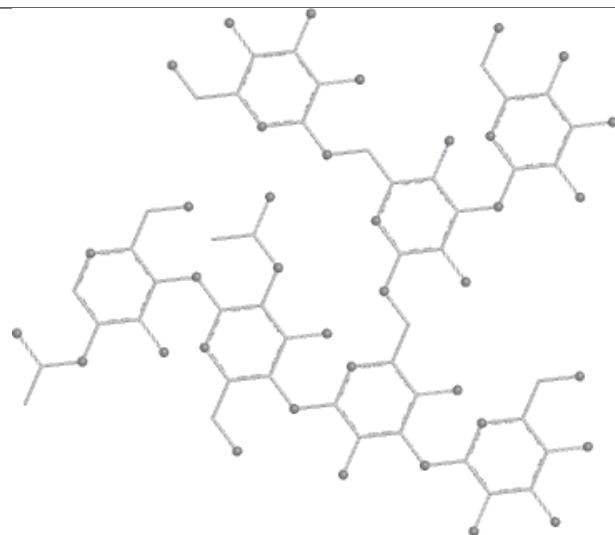
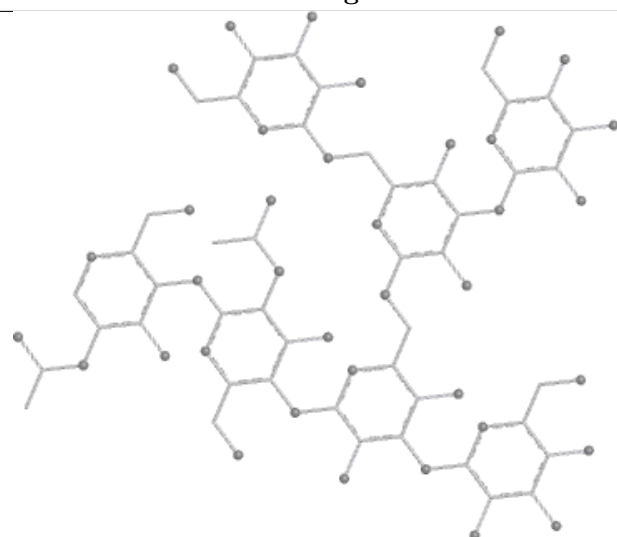
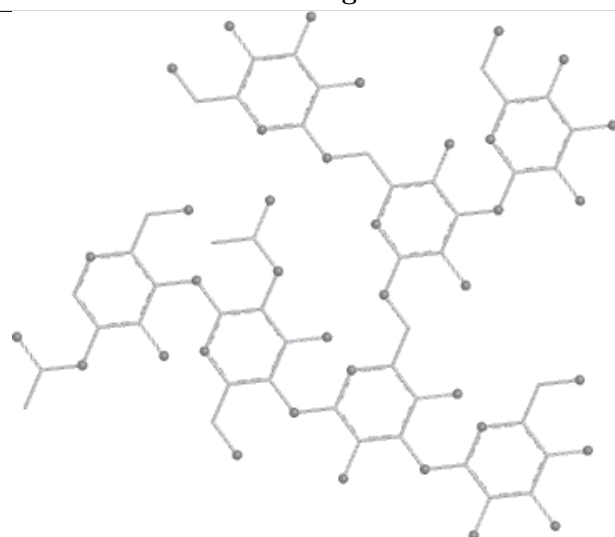


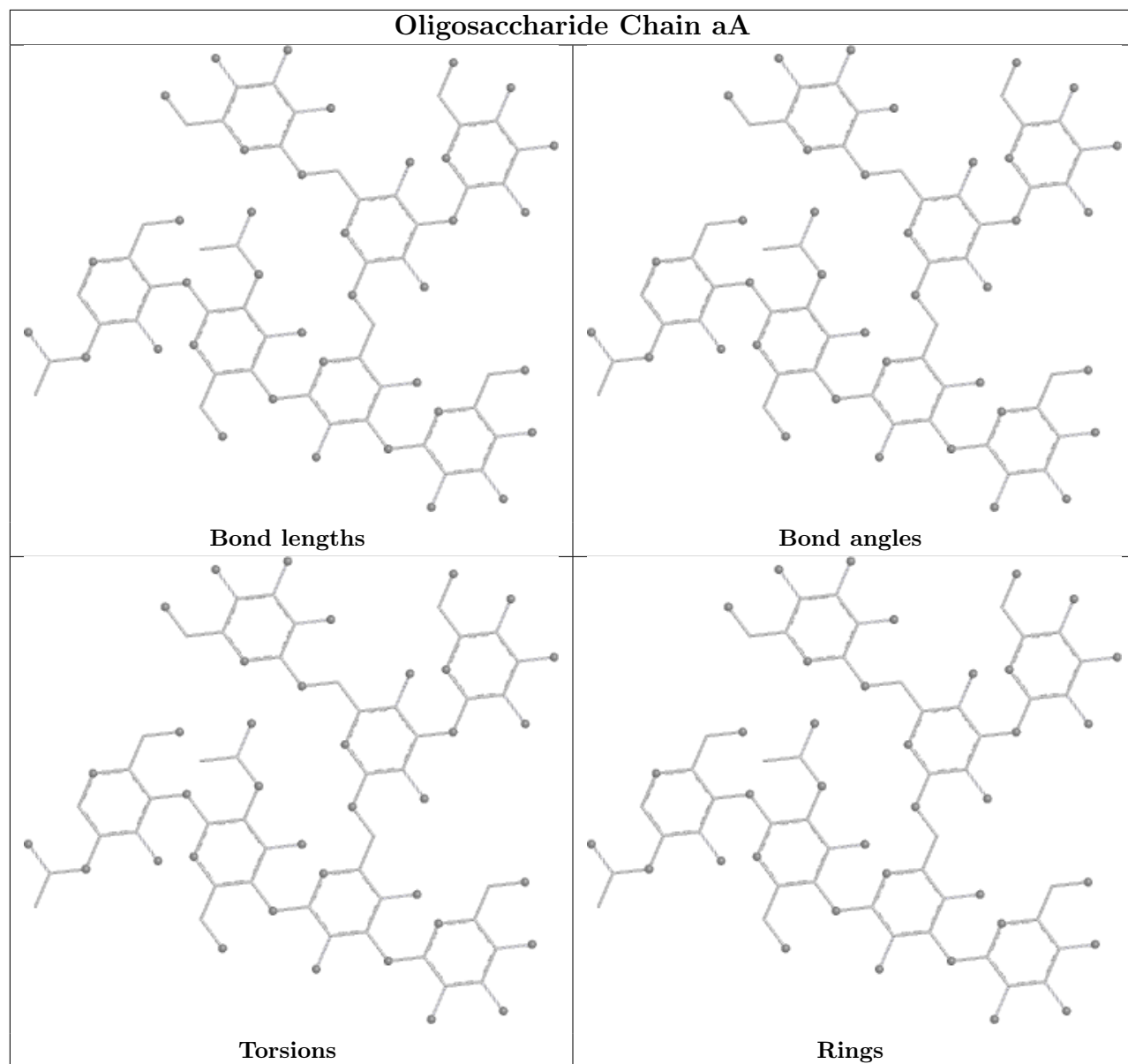


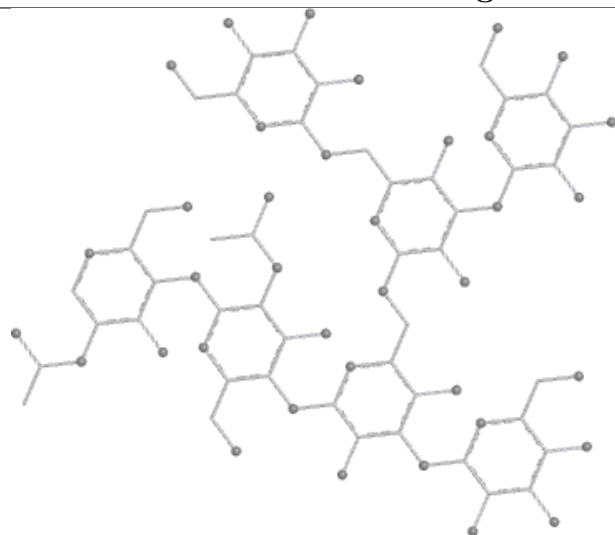
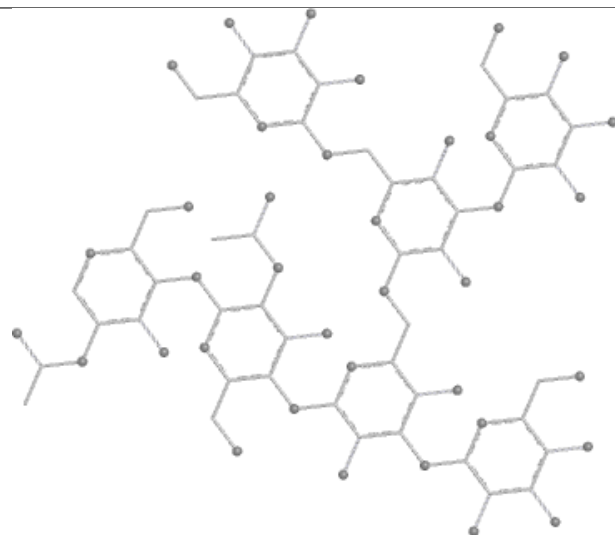
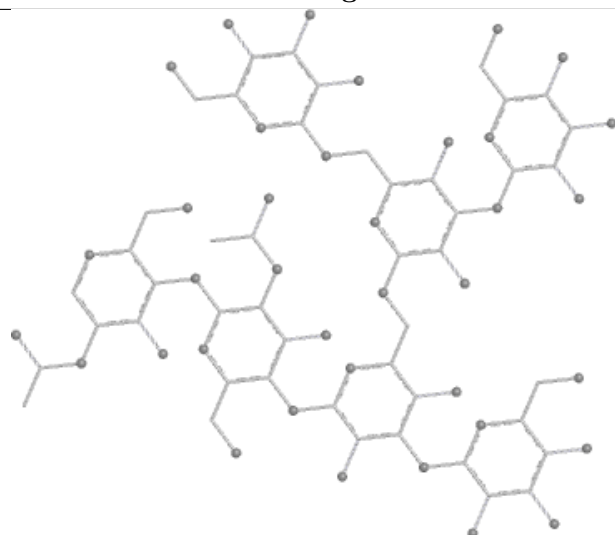
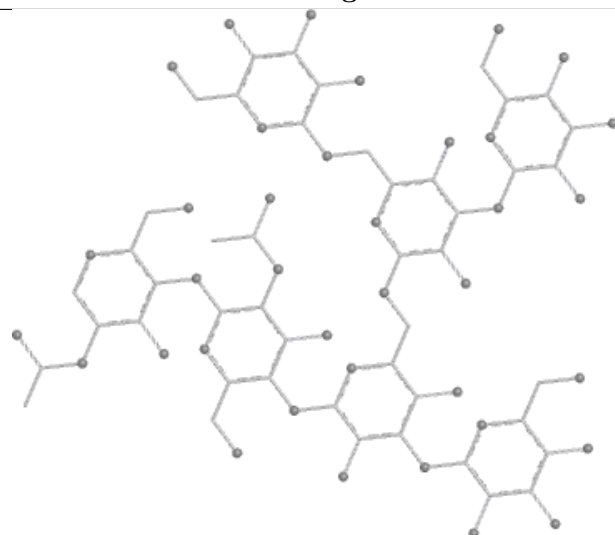


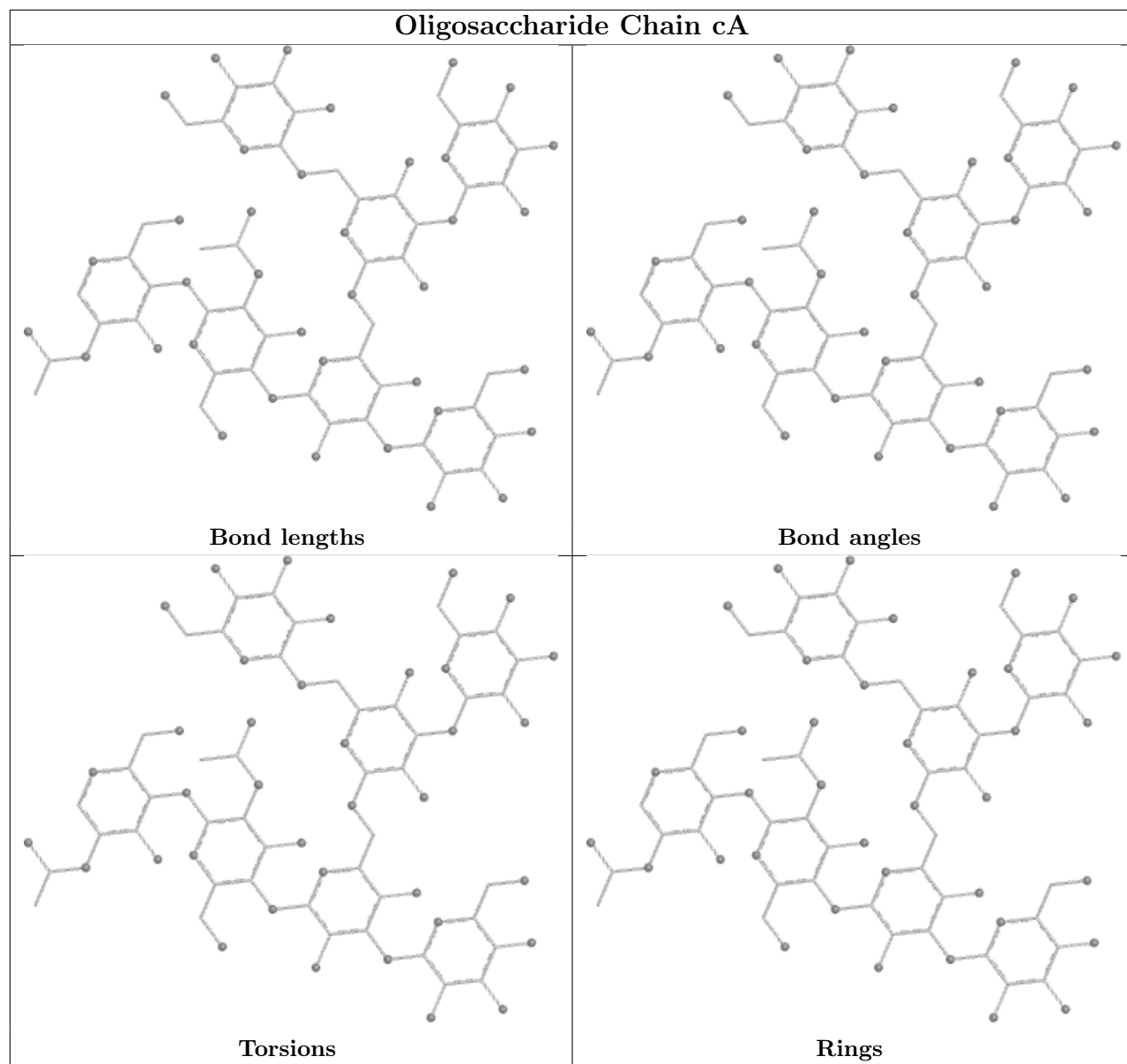
Oligosaccharide Chain VA**Bond lengths****Bond angles****Torsions****Rings**

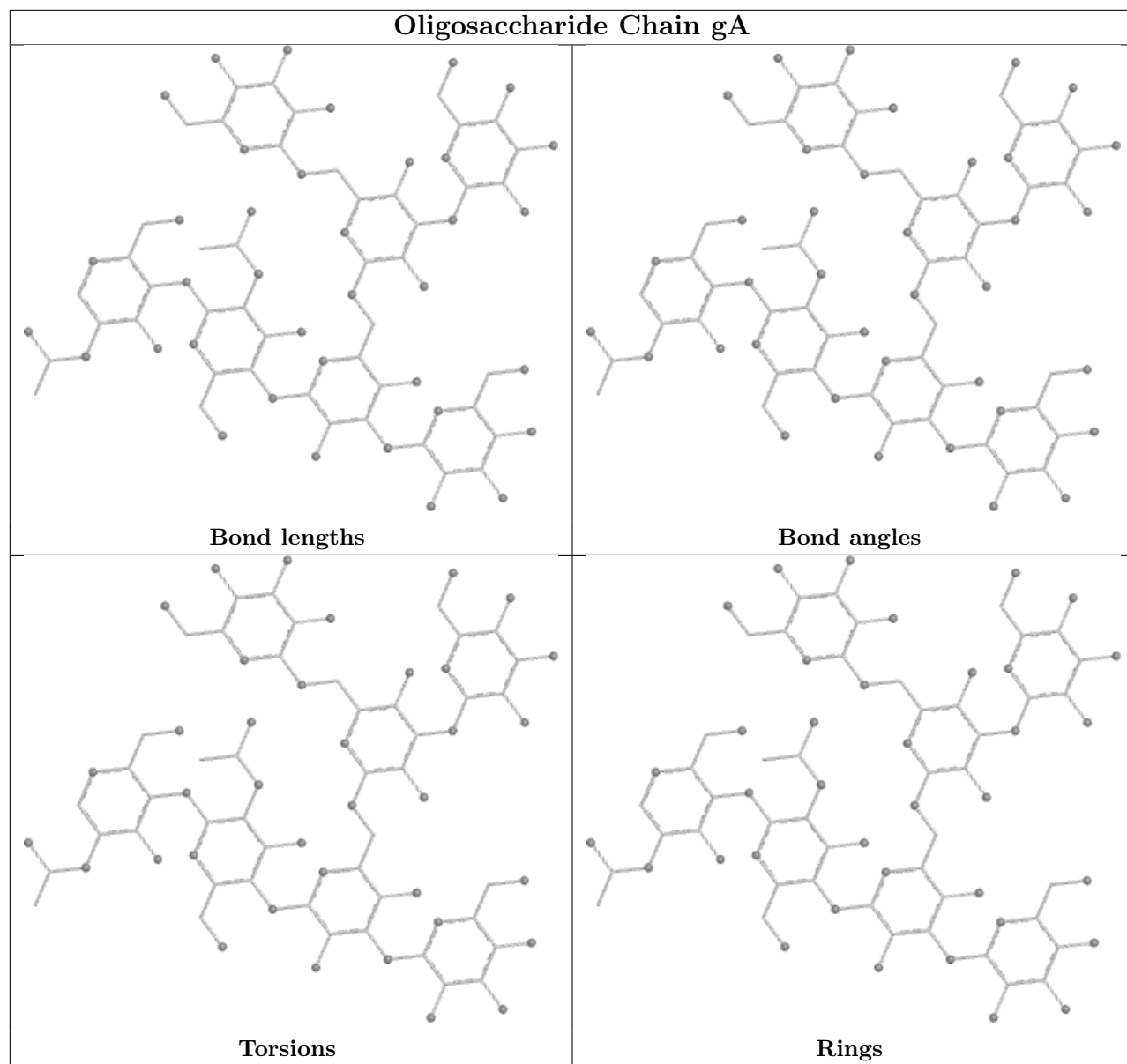


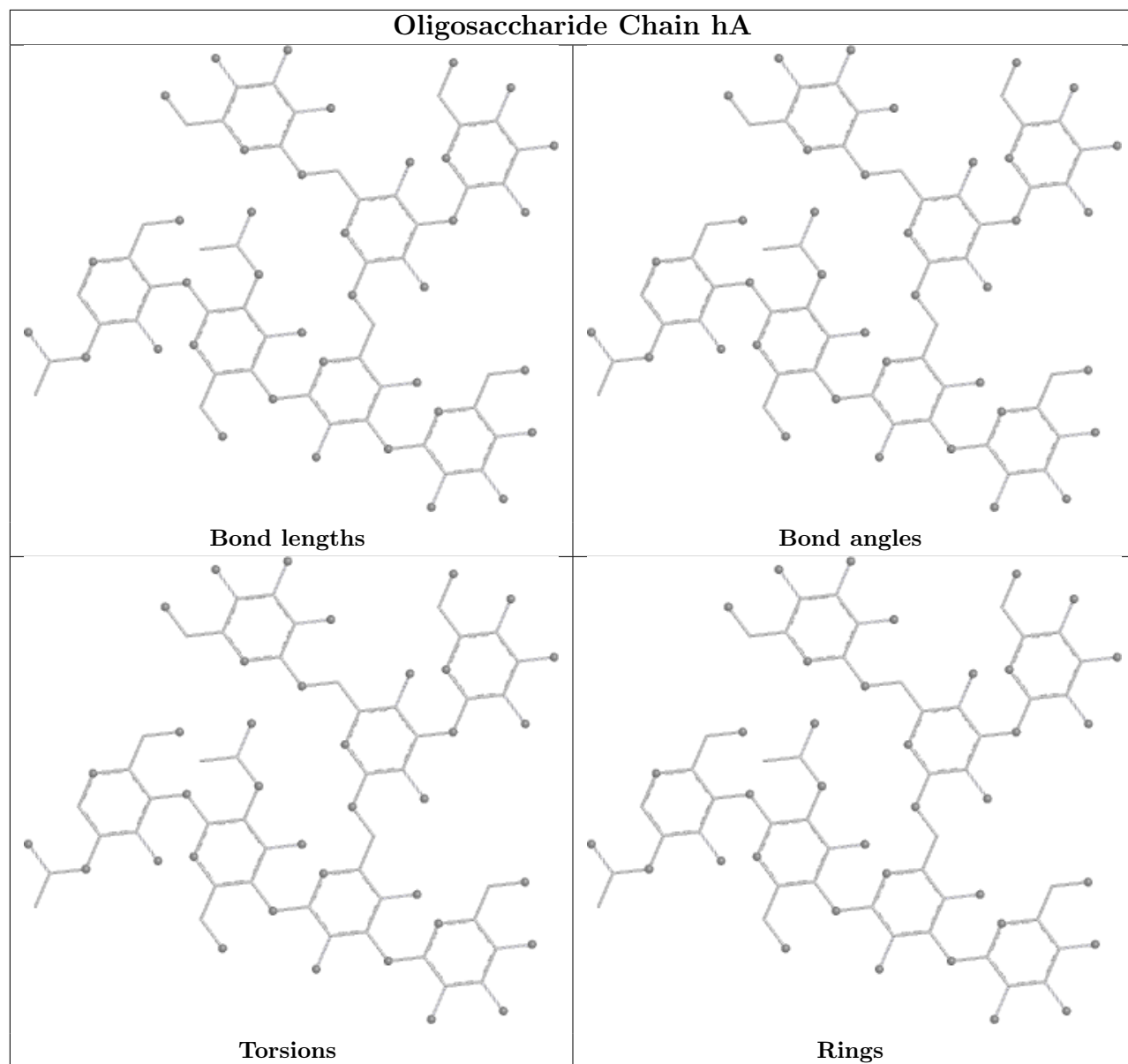
Oligosaccharide Chain ZA**Bond lengths****Bond angles****Torsions****Rings**

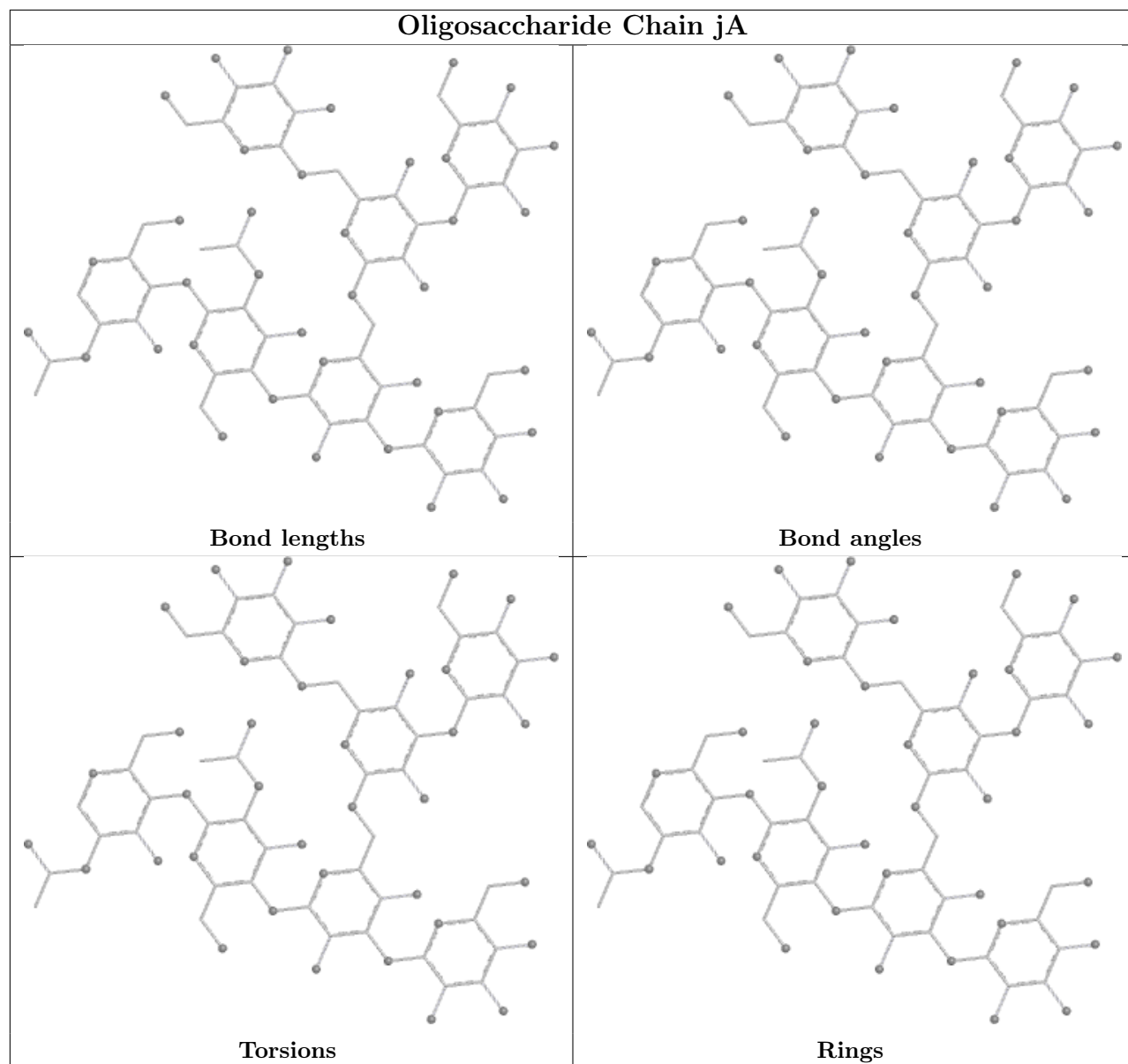


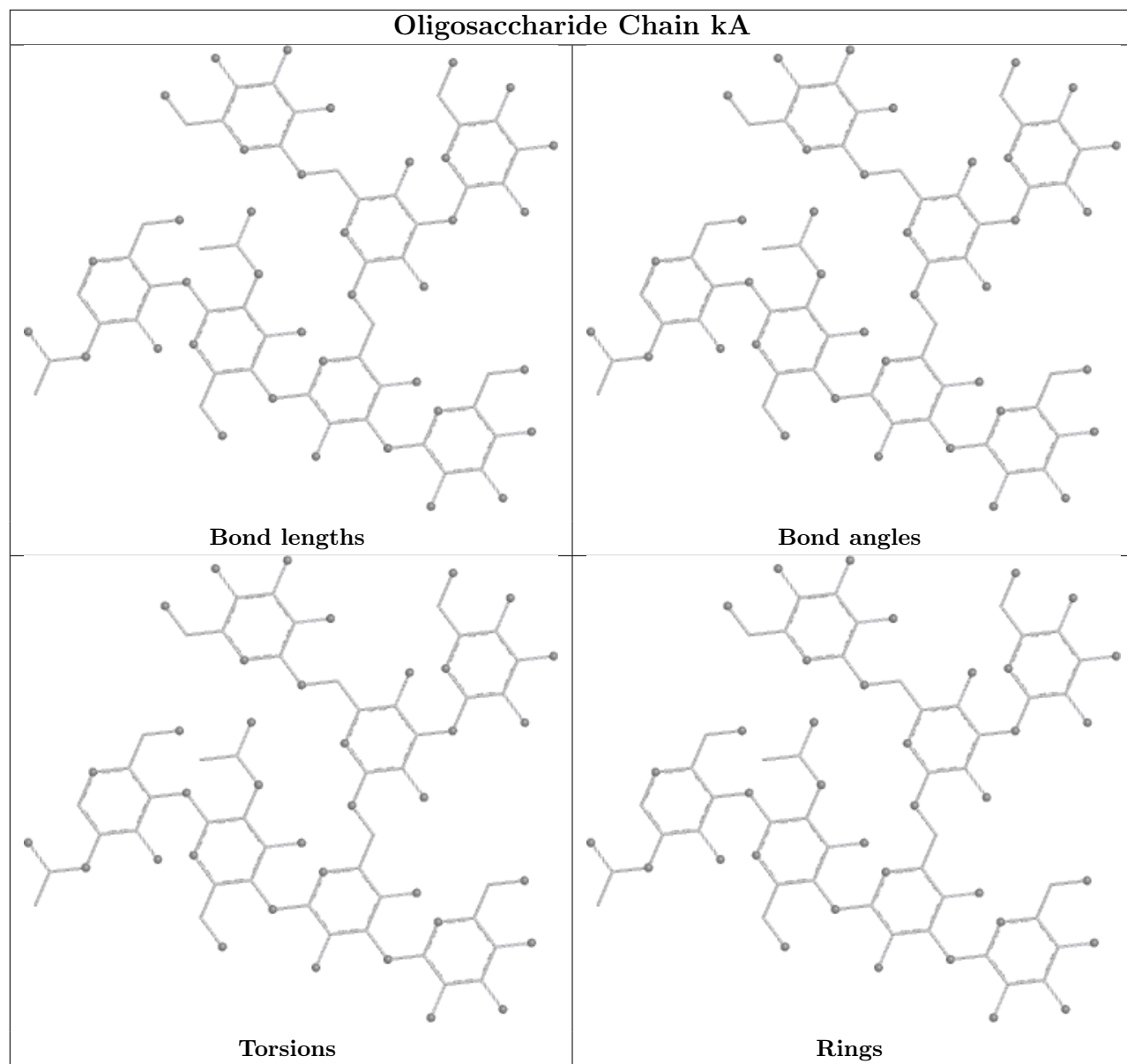
Oligosaccharide Chain bA**Bond lengths****Bond angles****Torsions****Rings**

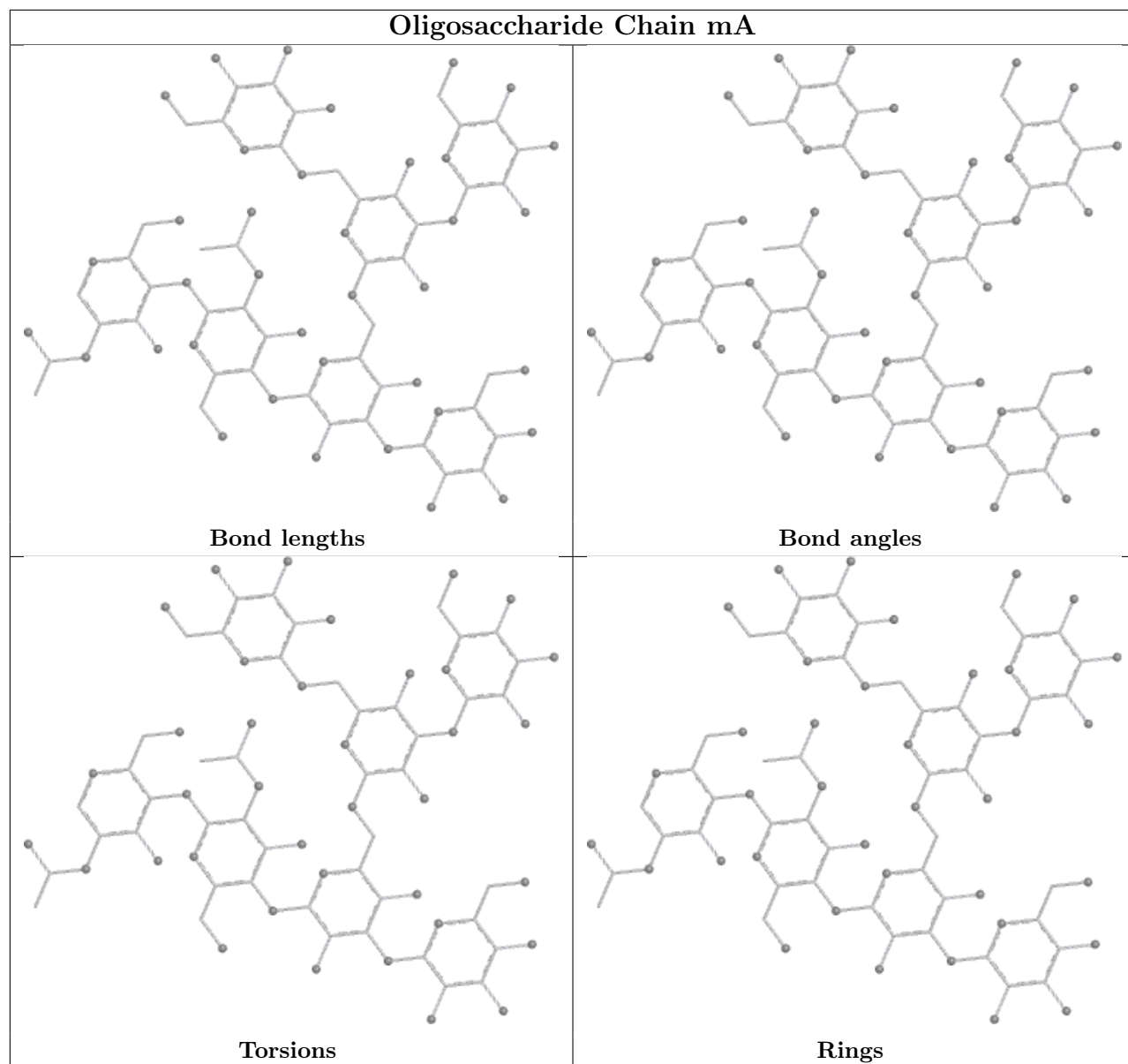


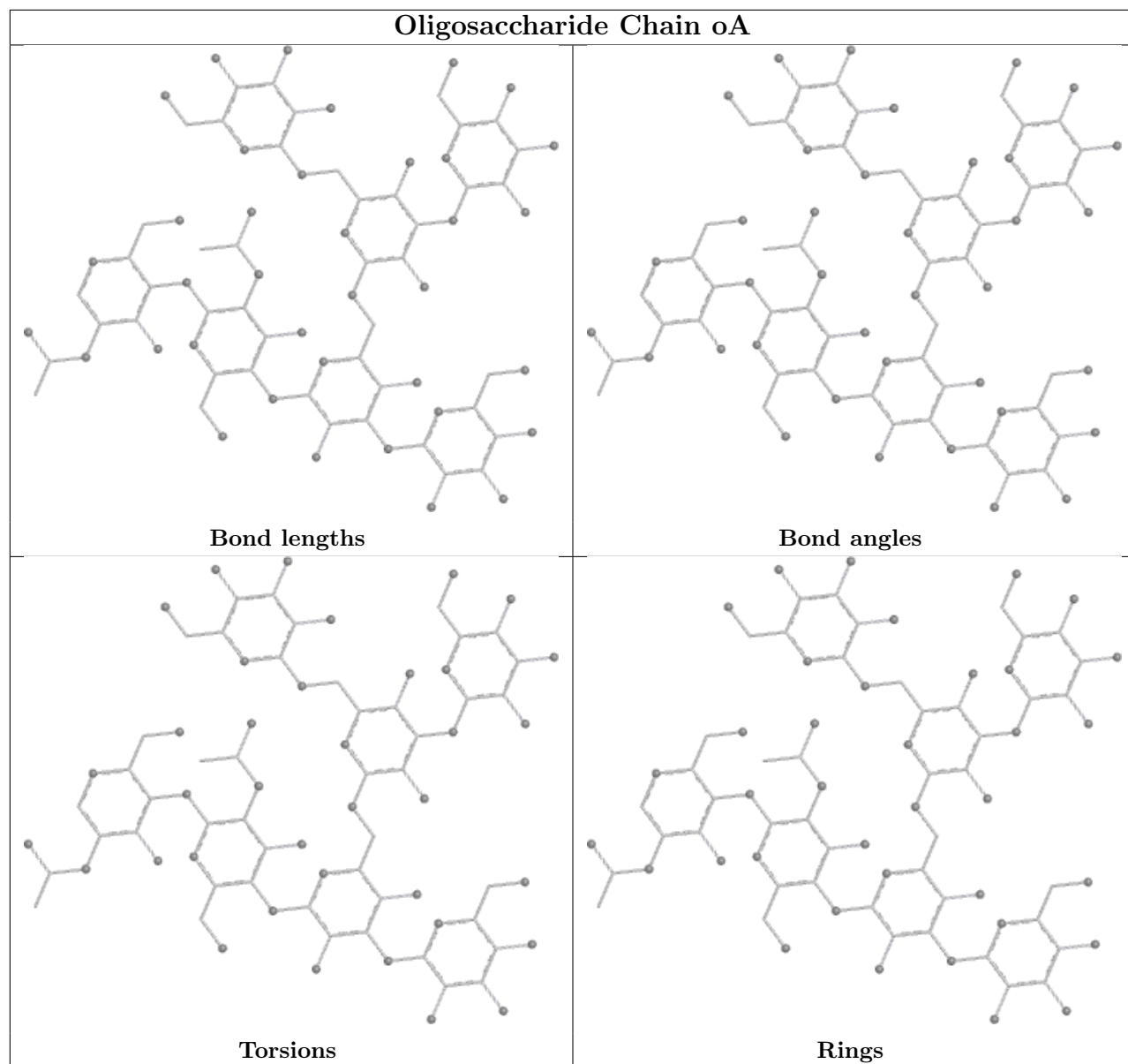


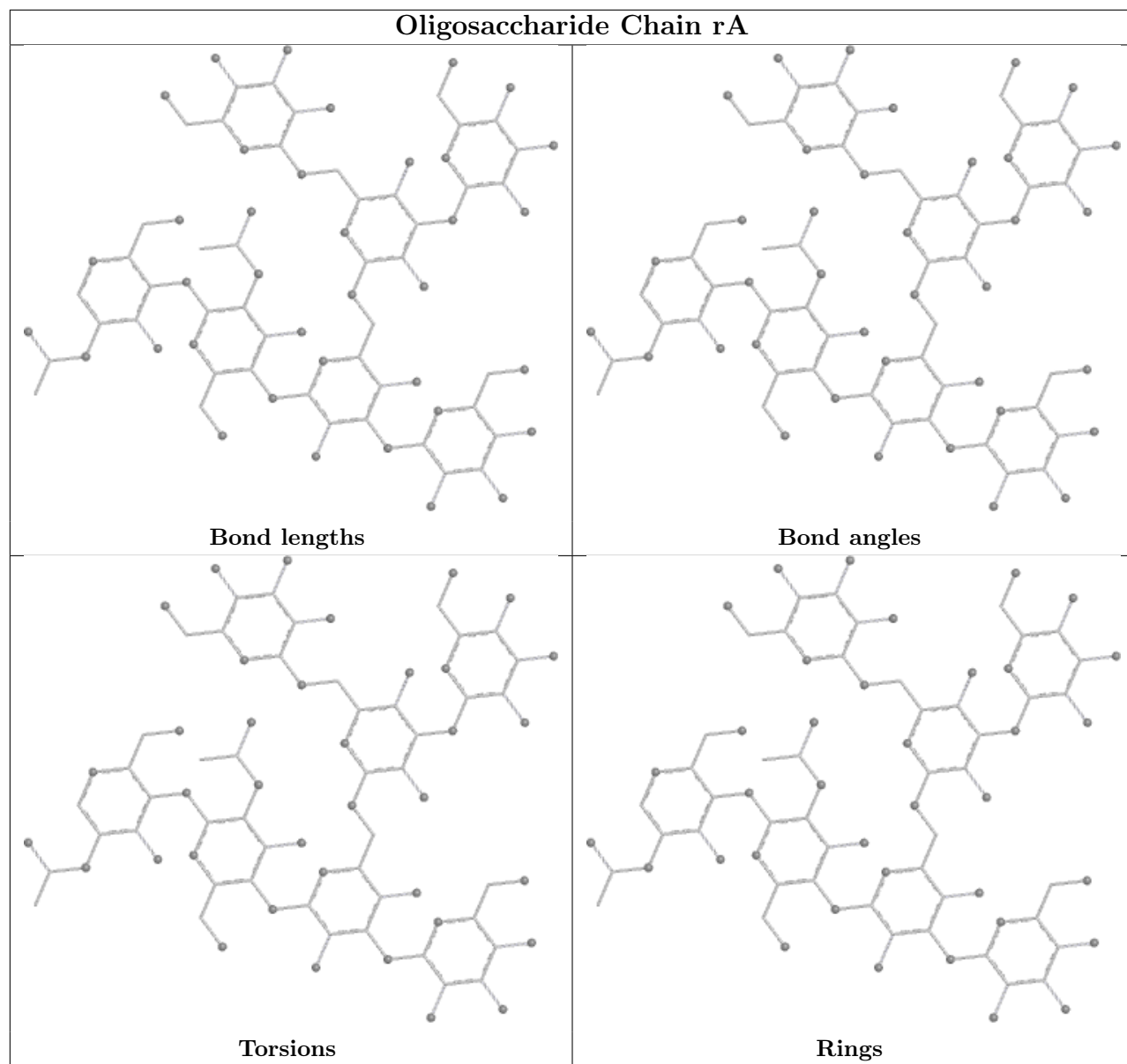


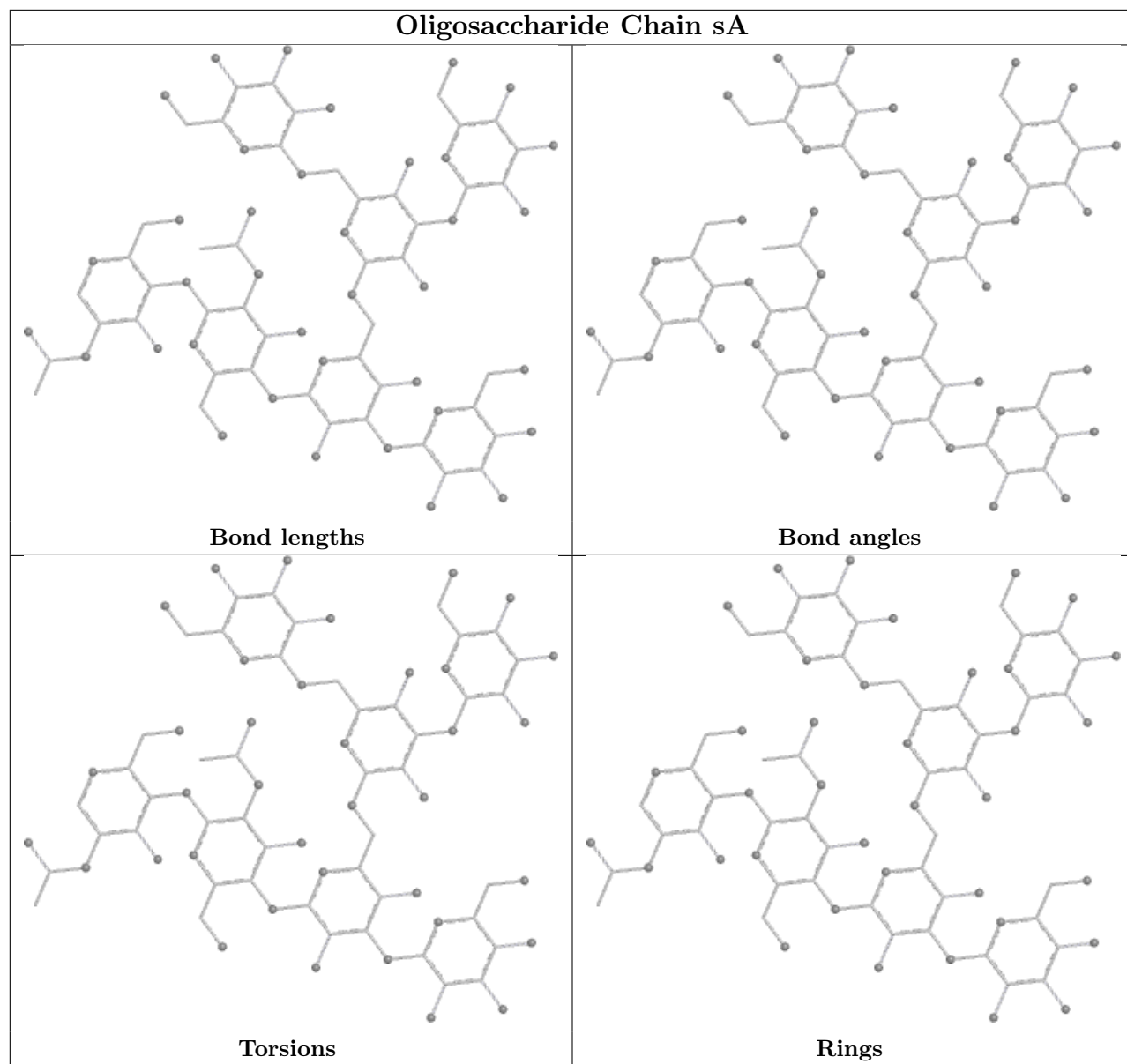


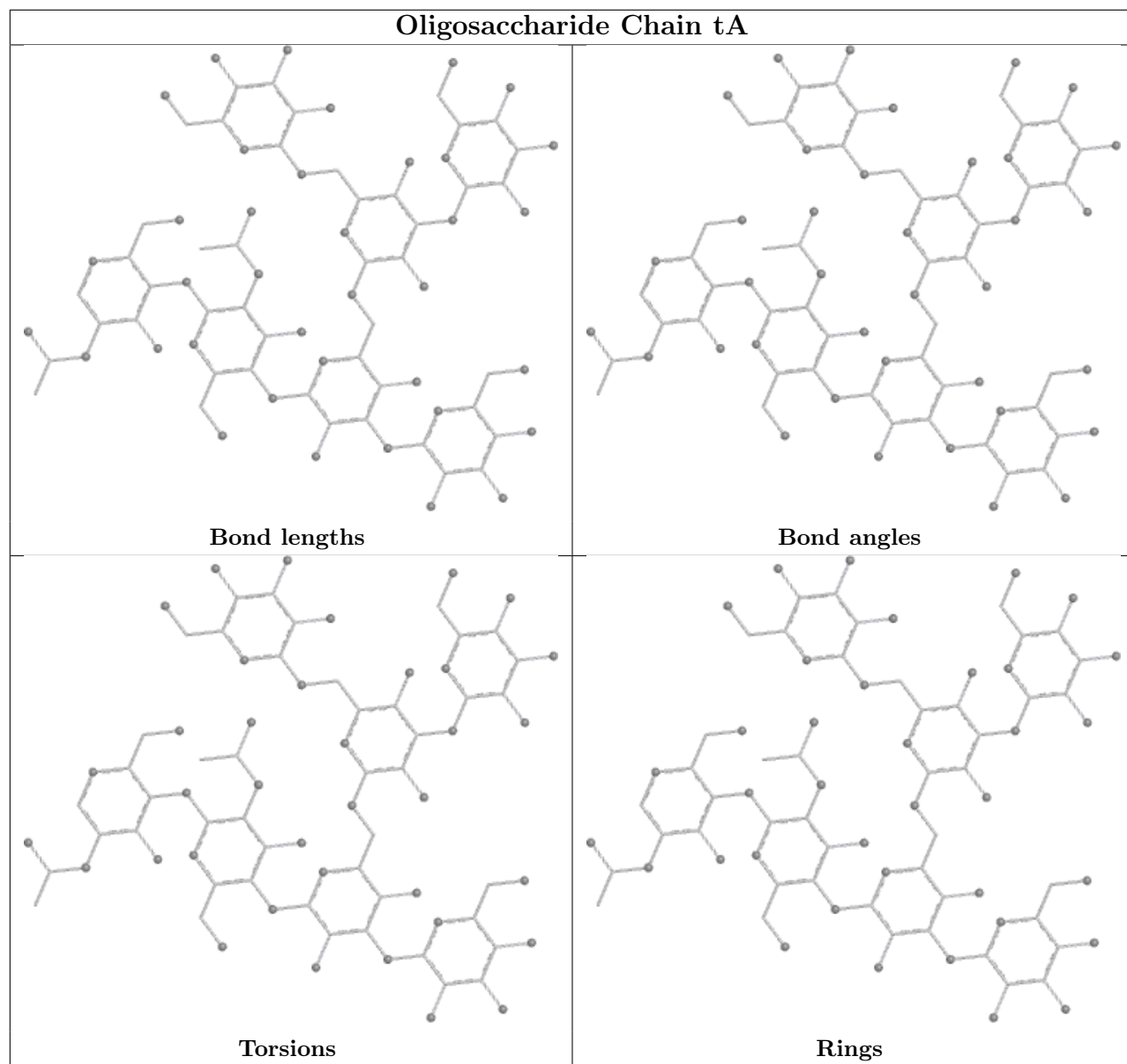


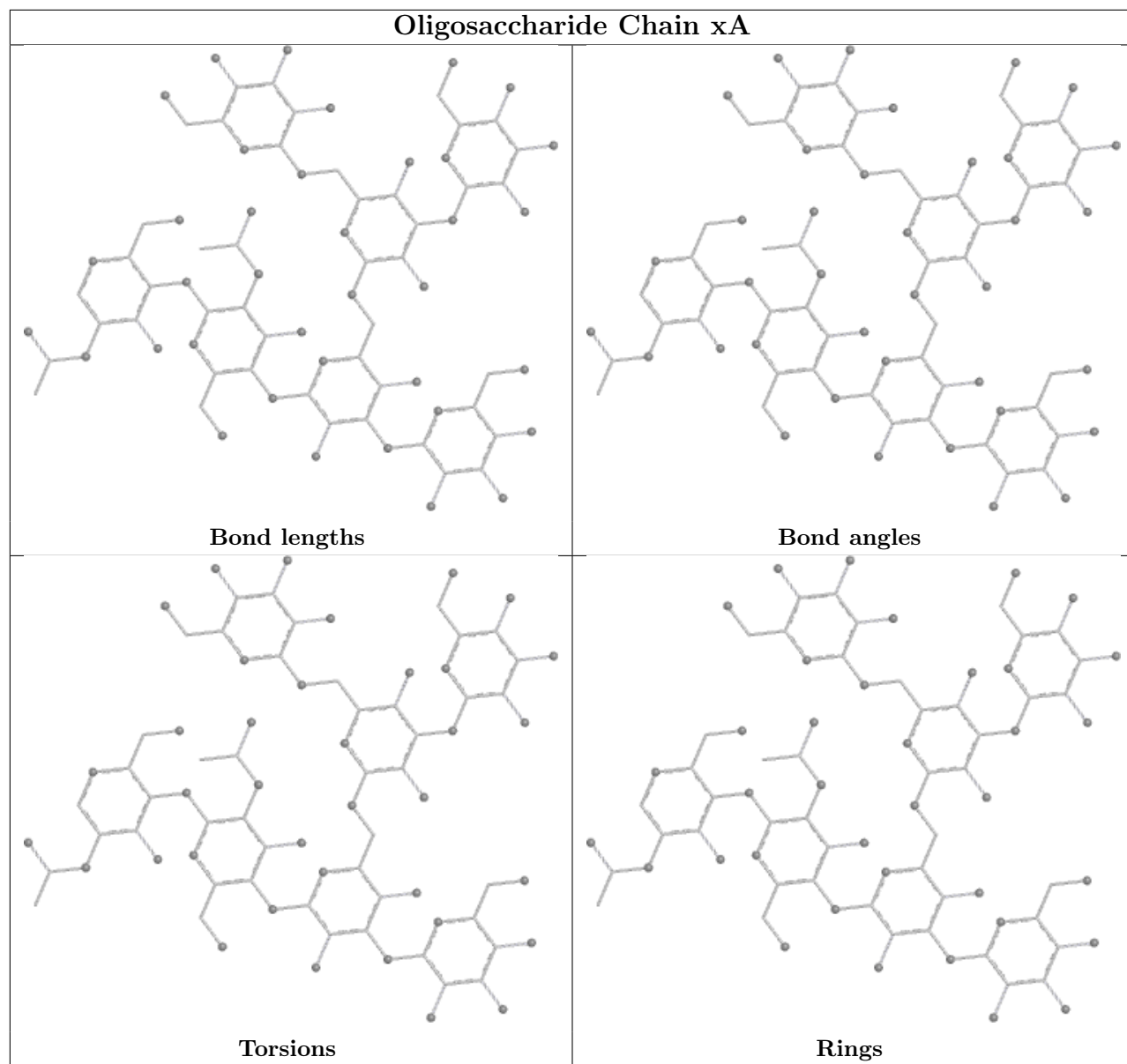


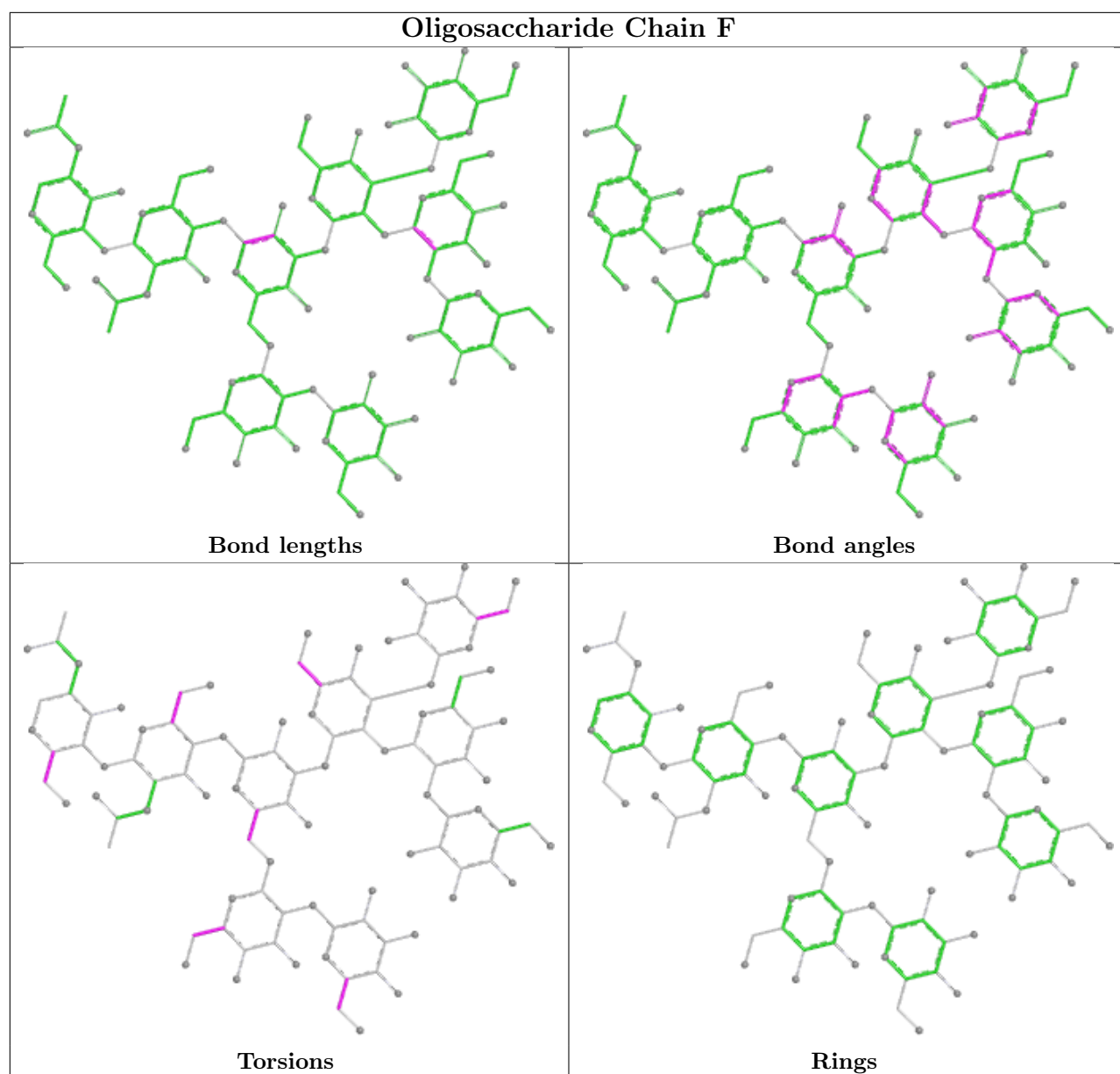


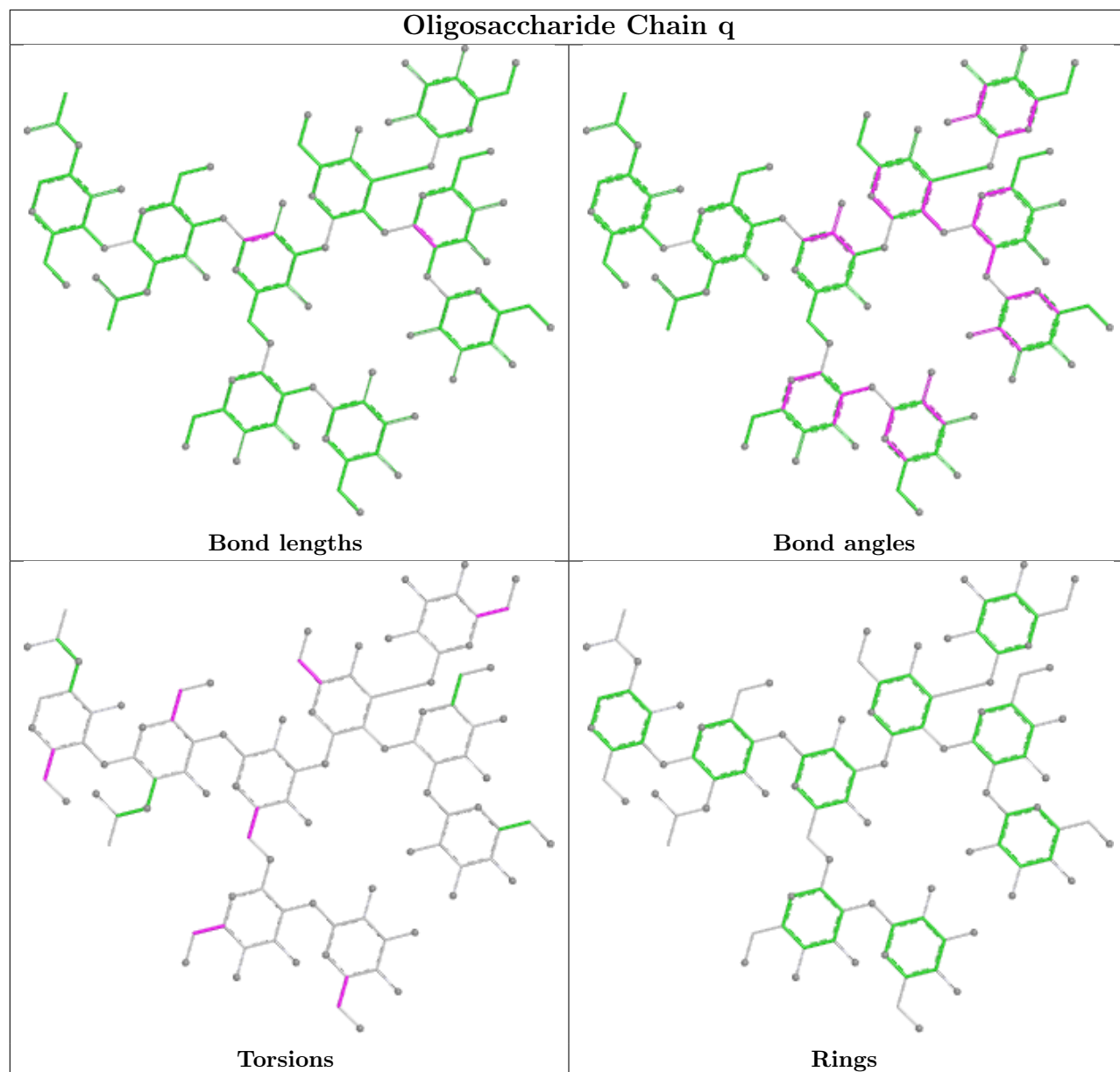


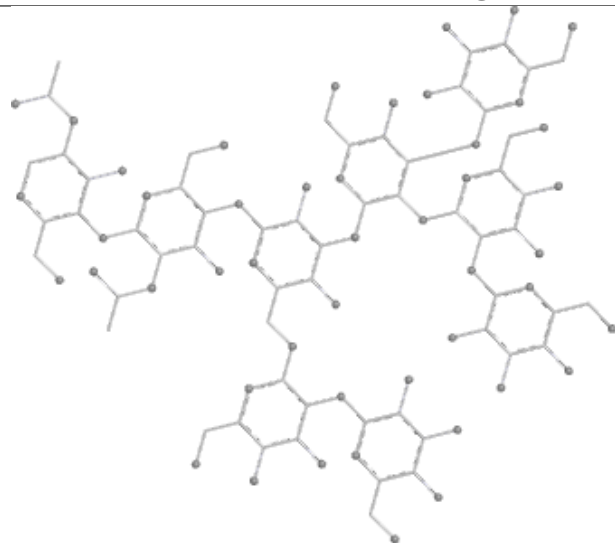
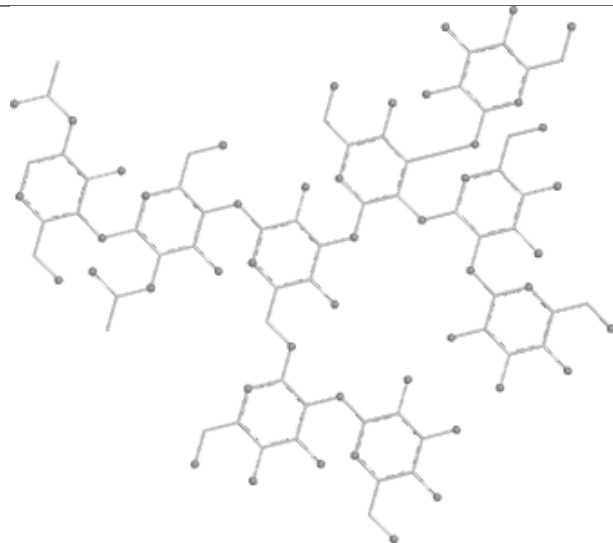
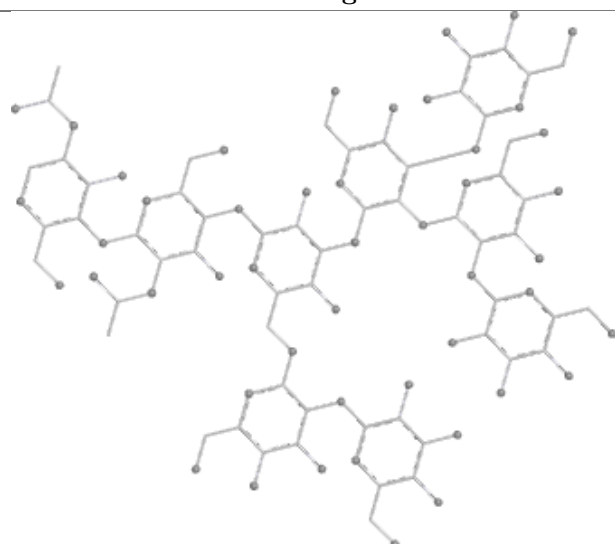
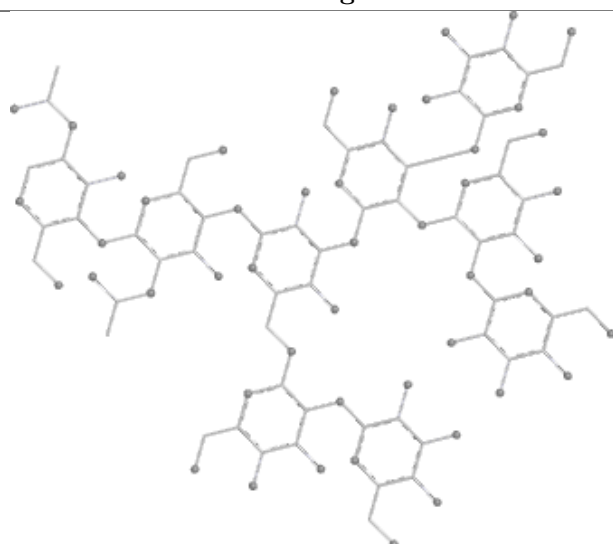


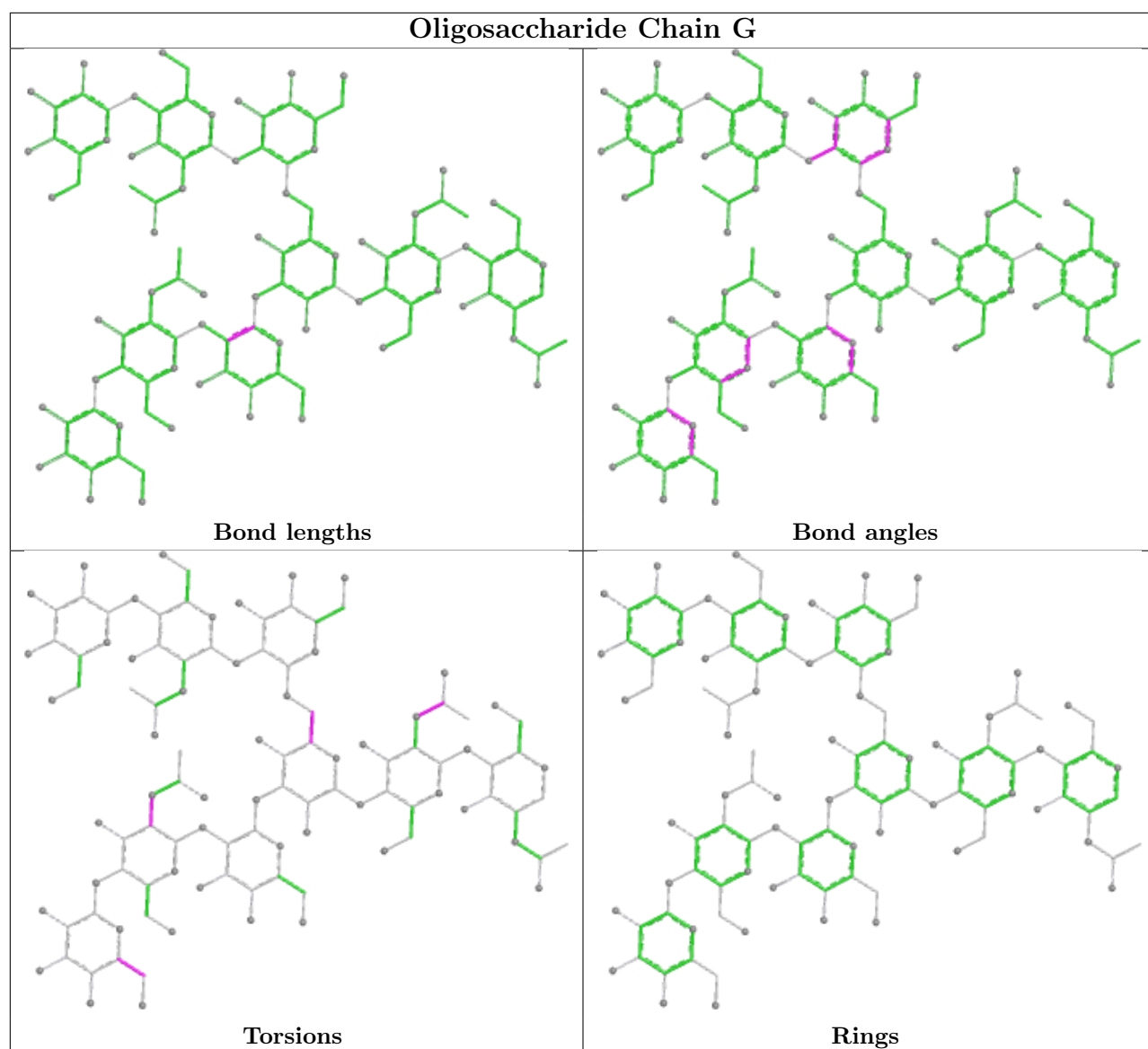


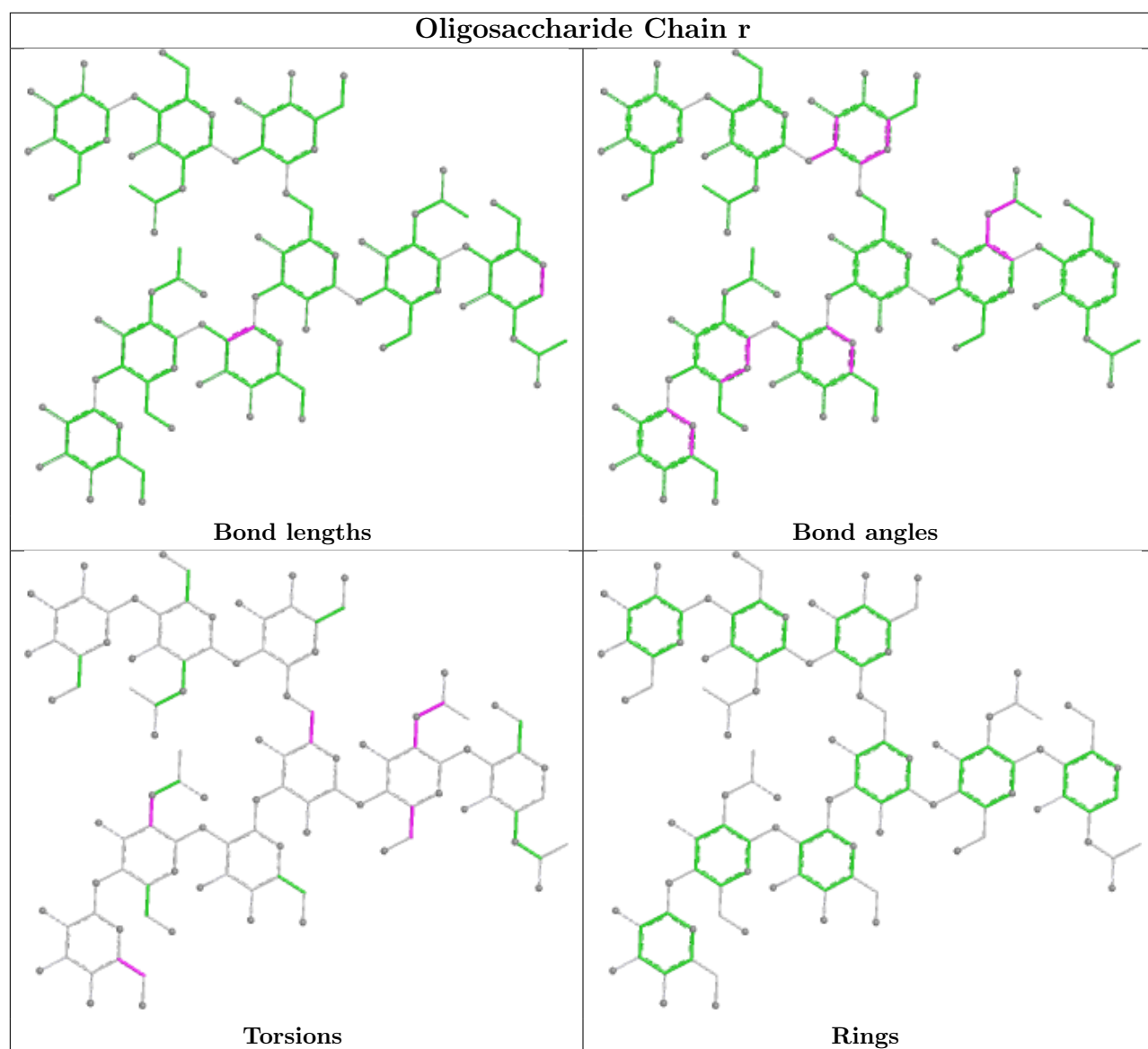


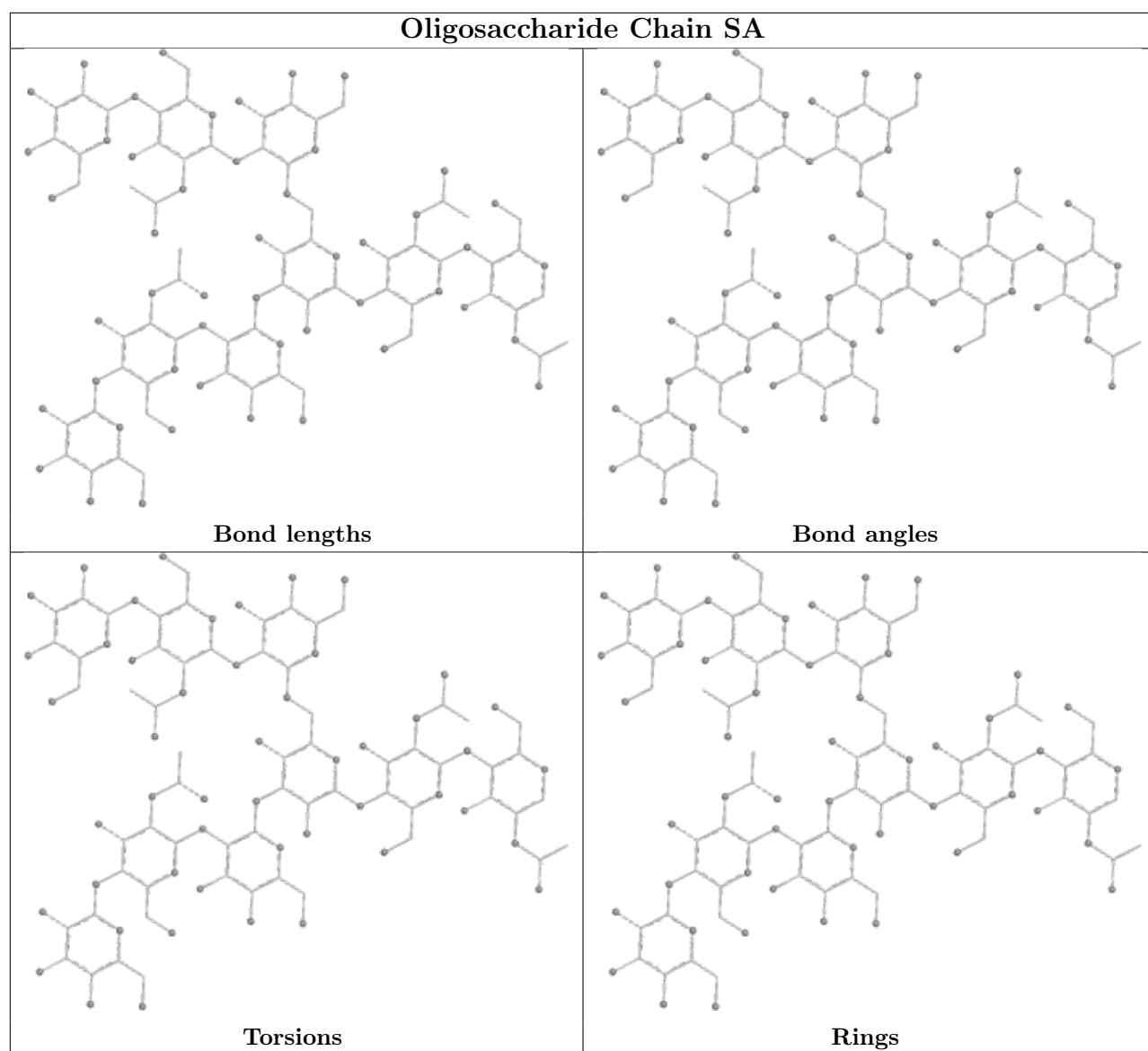


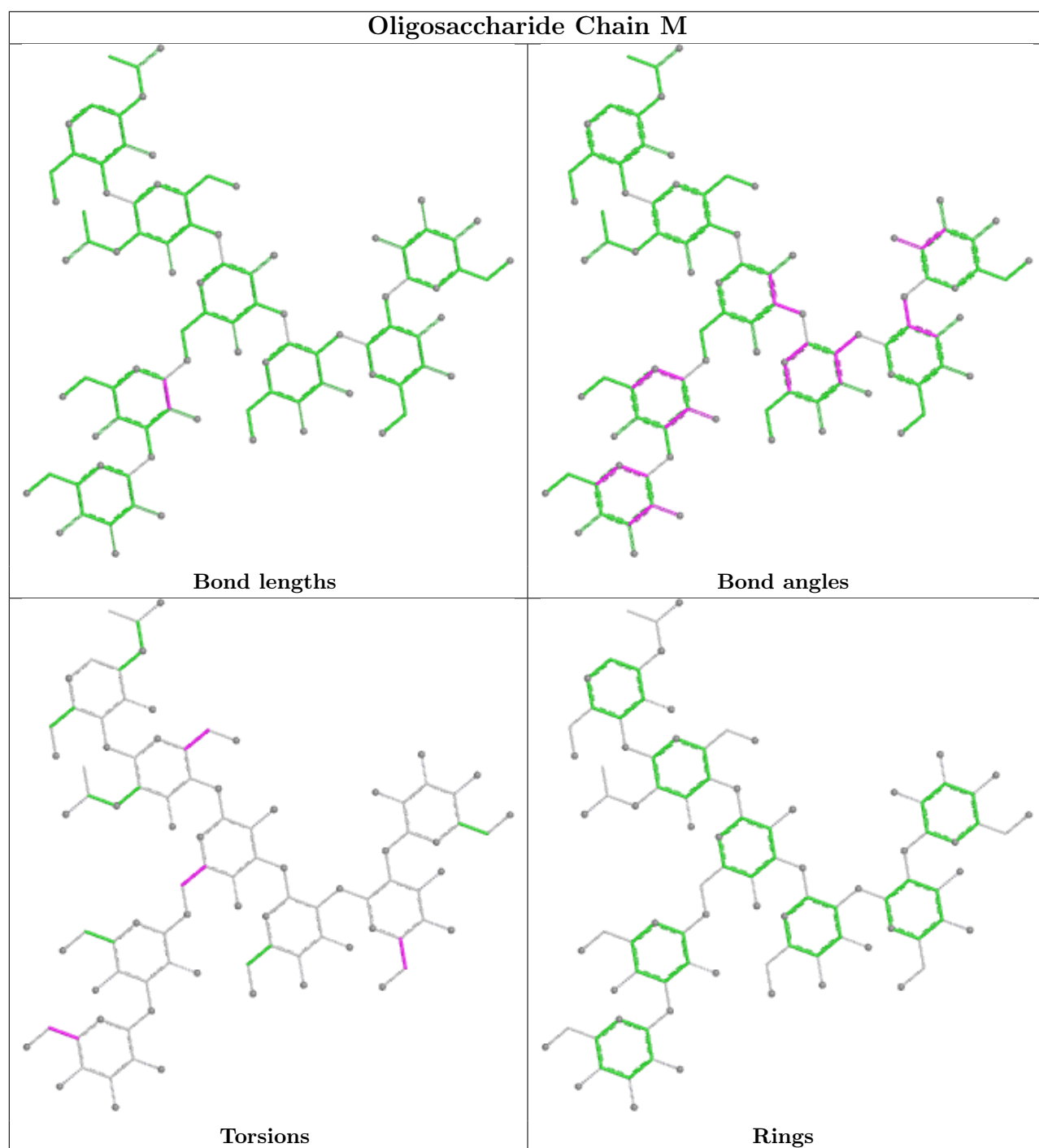


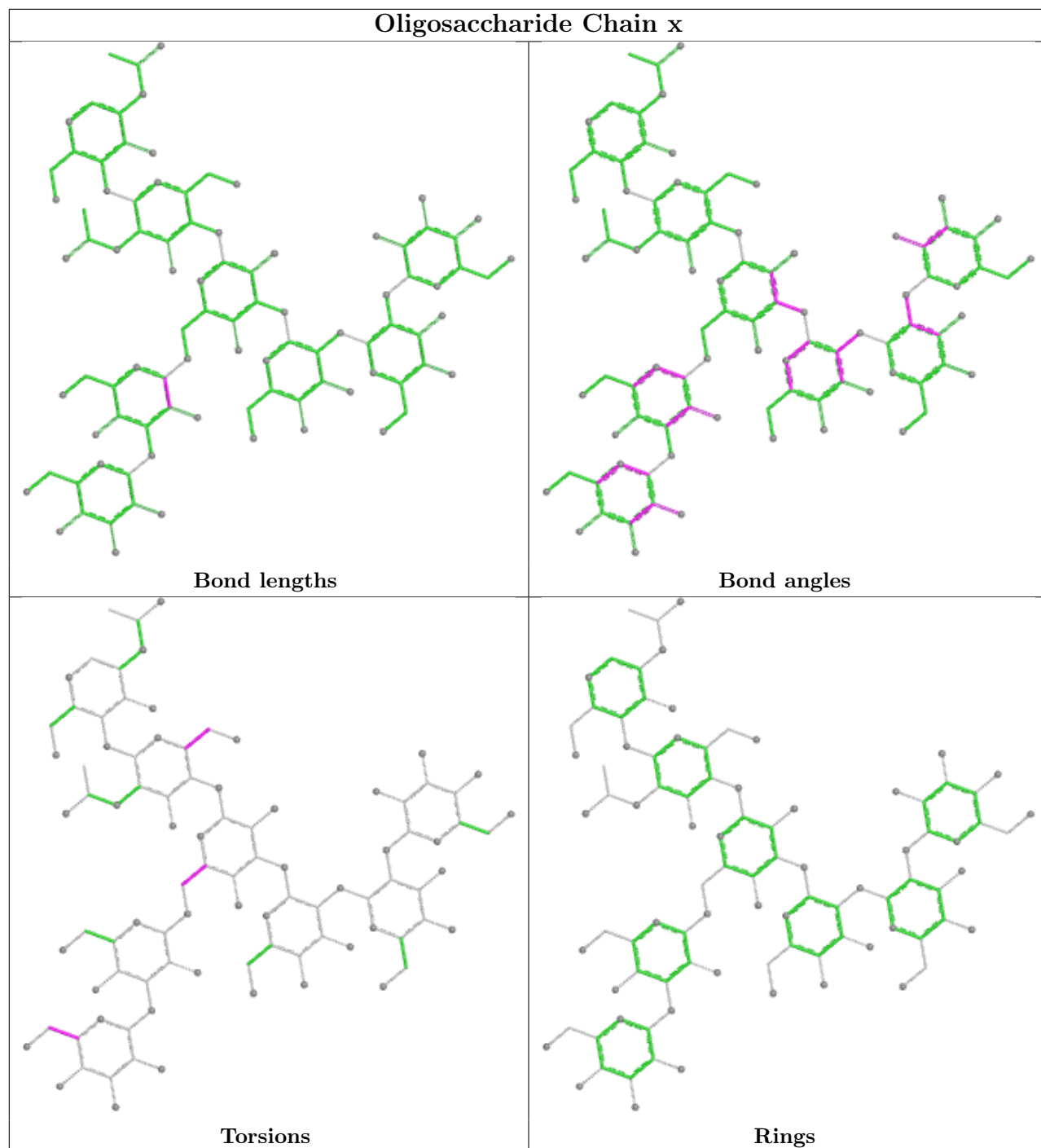
Oligosaccharide Chain RA**Bond lengths****Bond angles****Torsions****Rings**

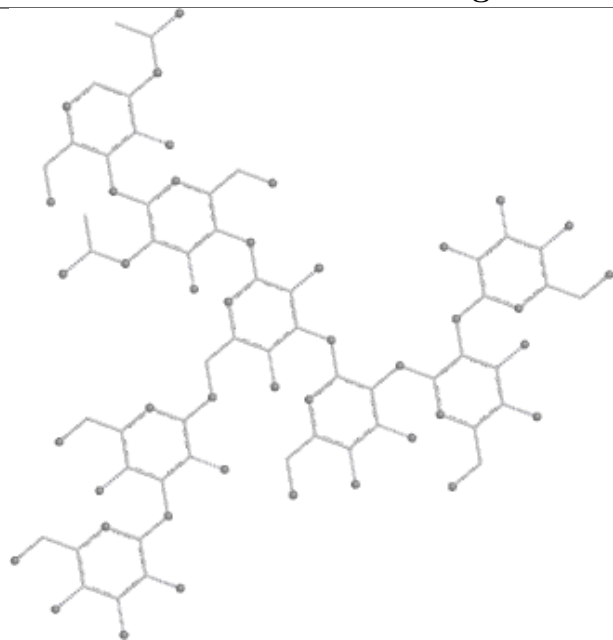
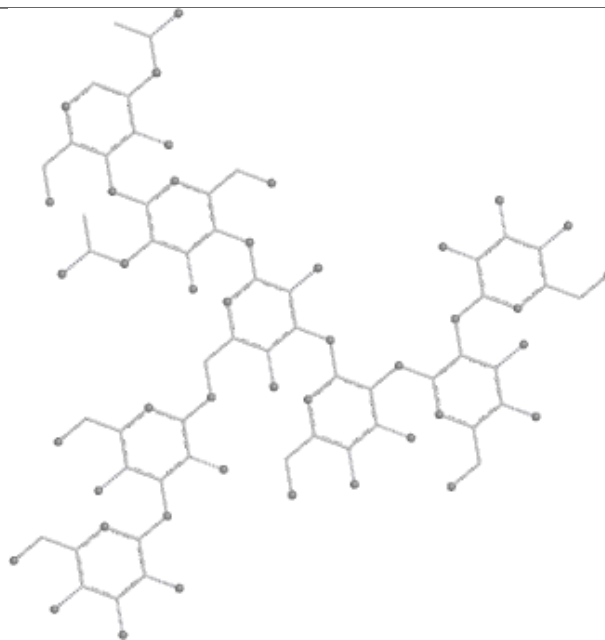
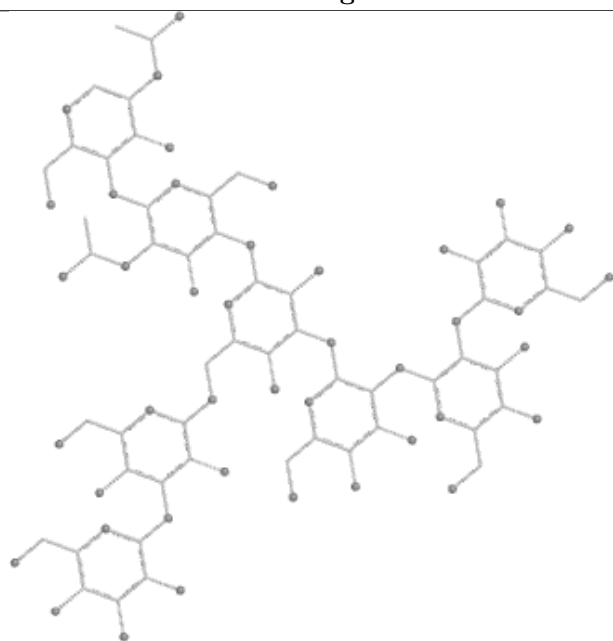
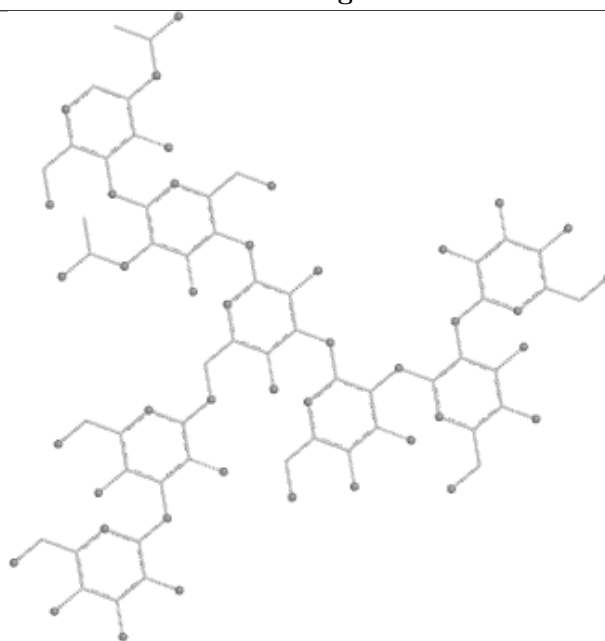


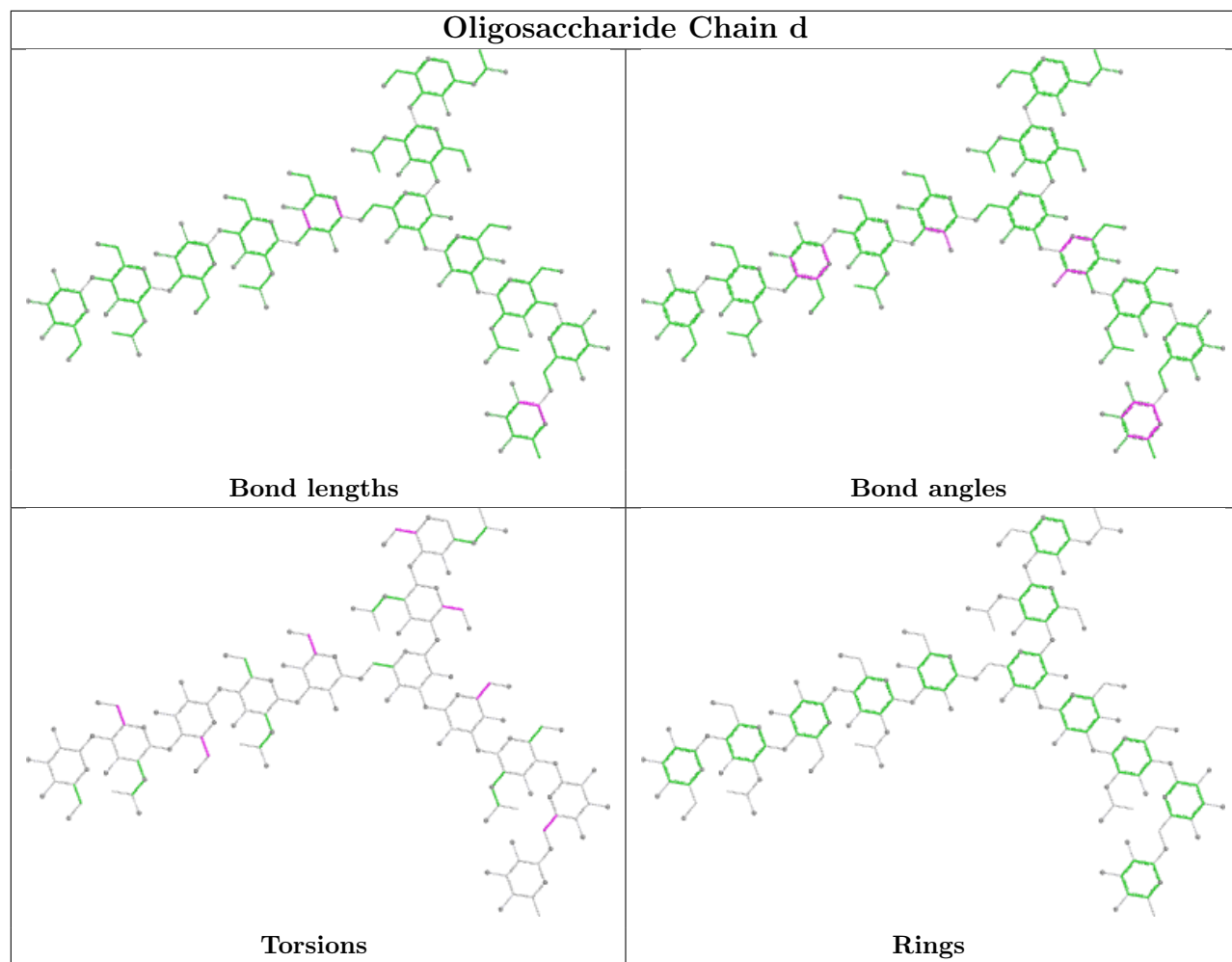


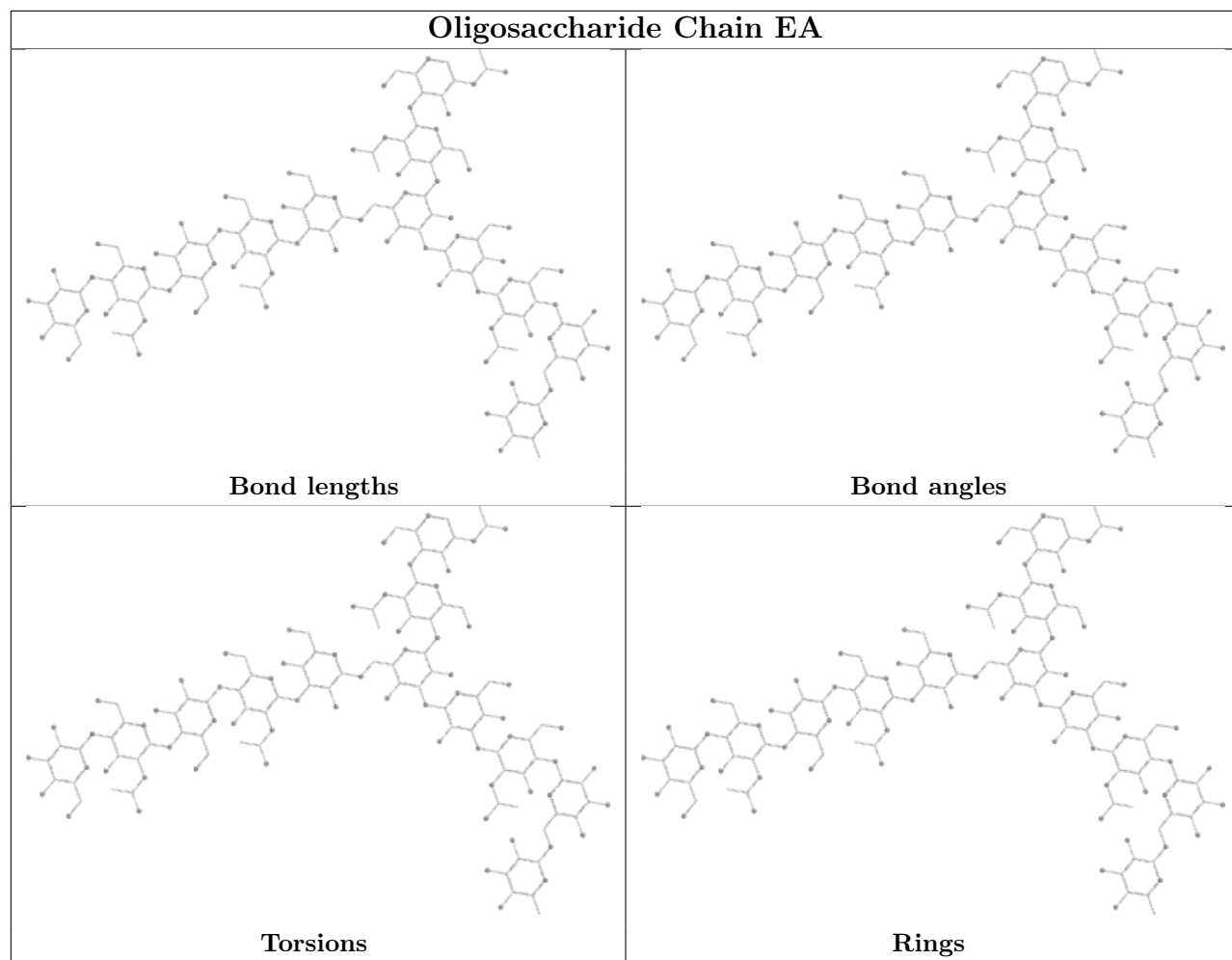


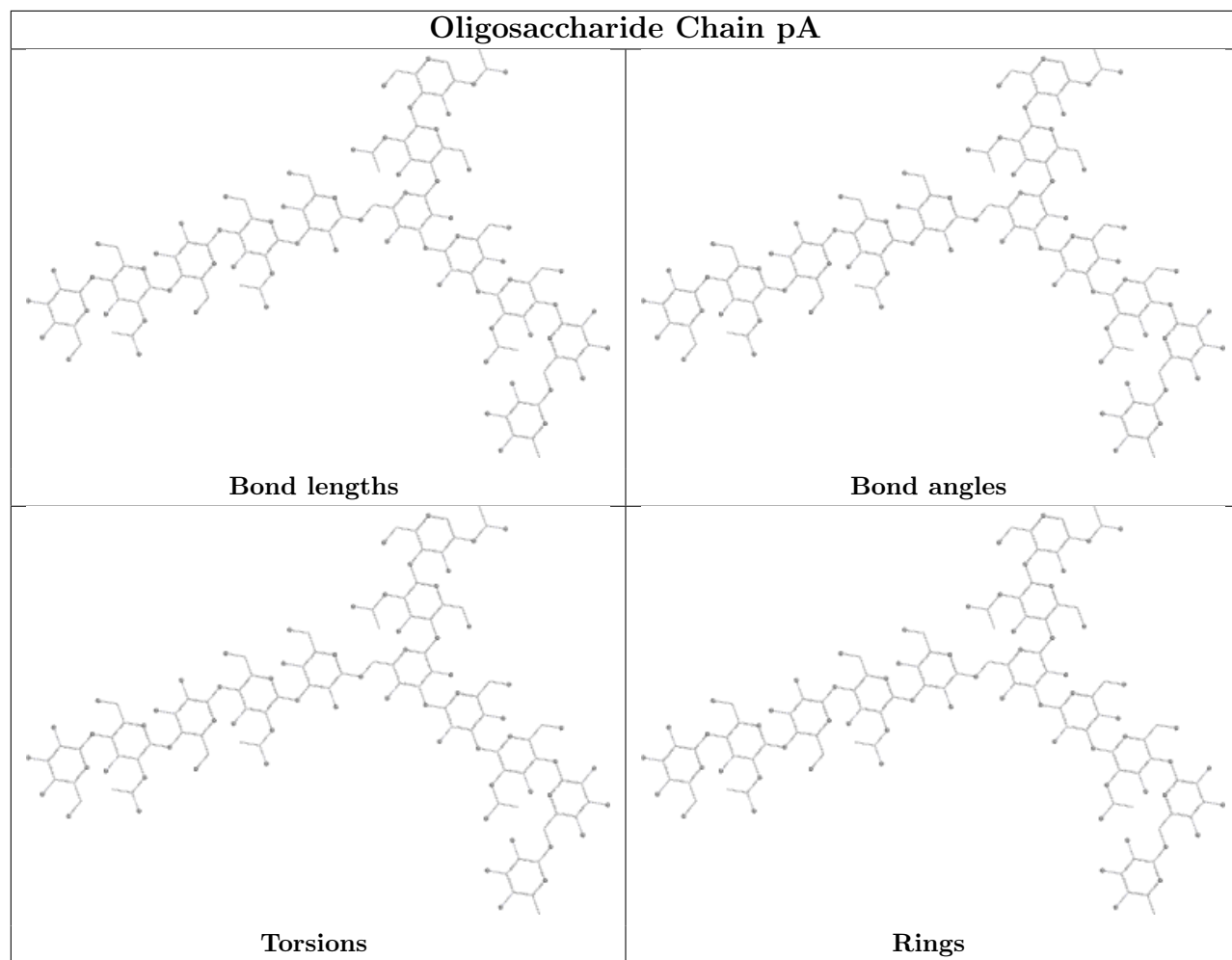


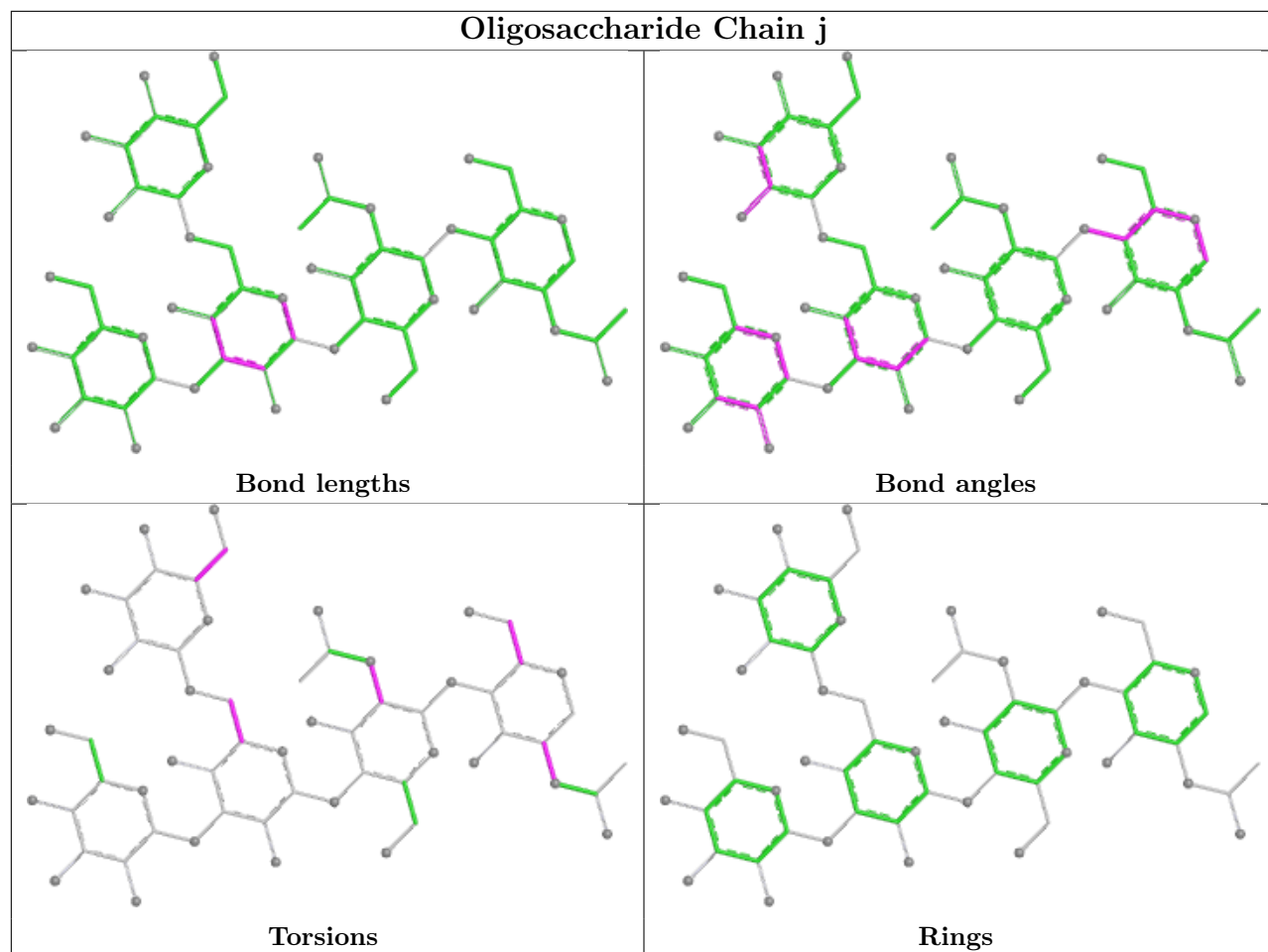


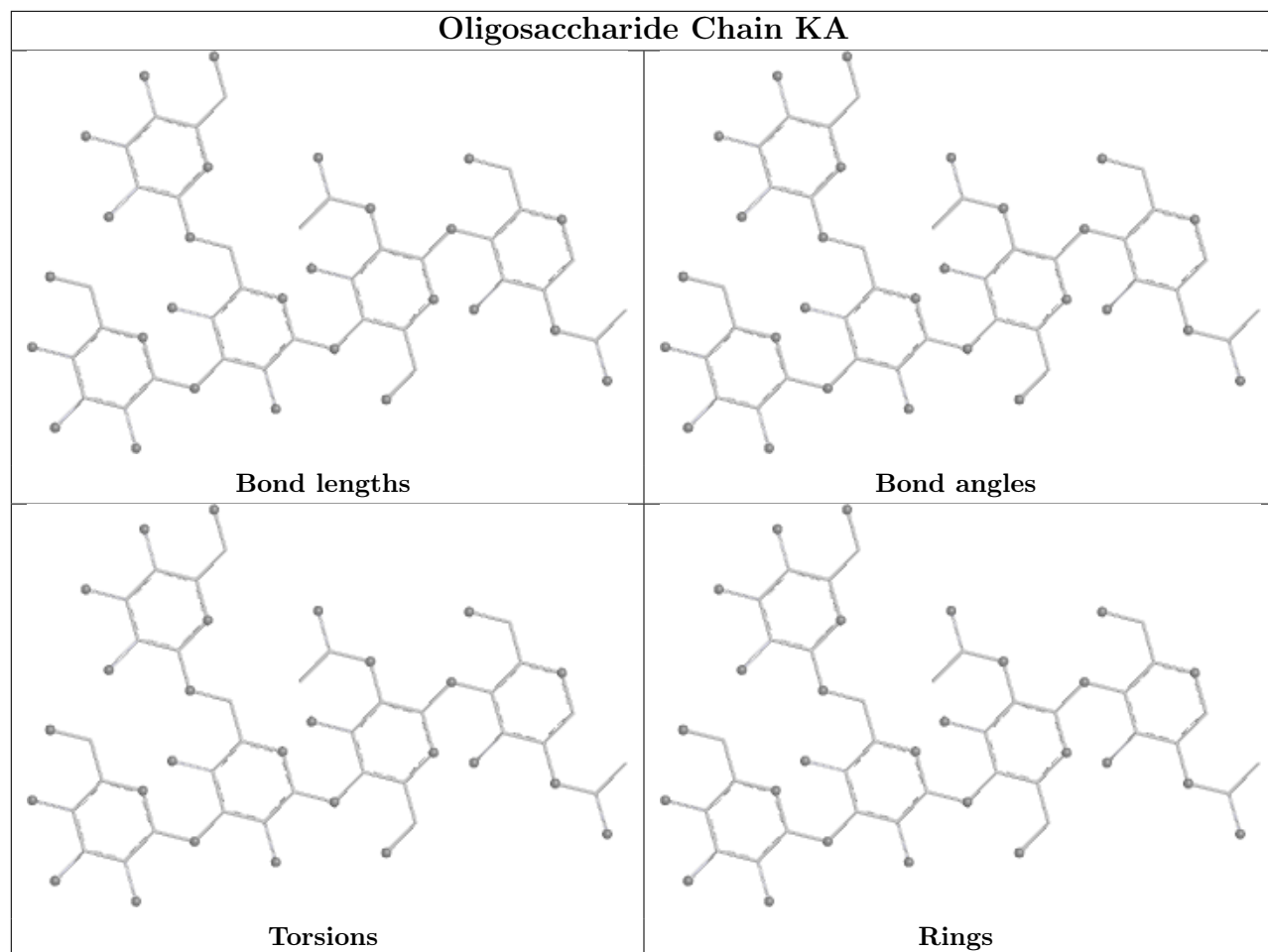
Oligosaccharide Chain YA**Bond lengths****Bond angles****Torsions****Rings**

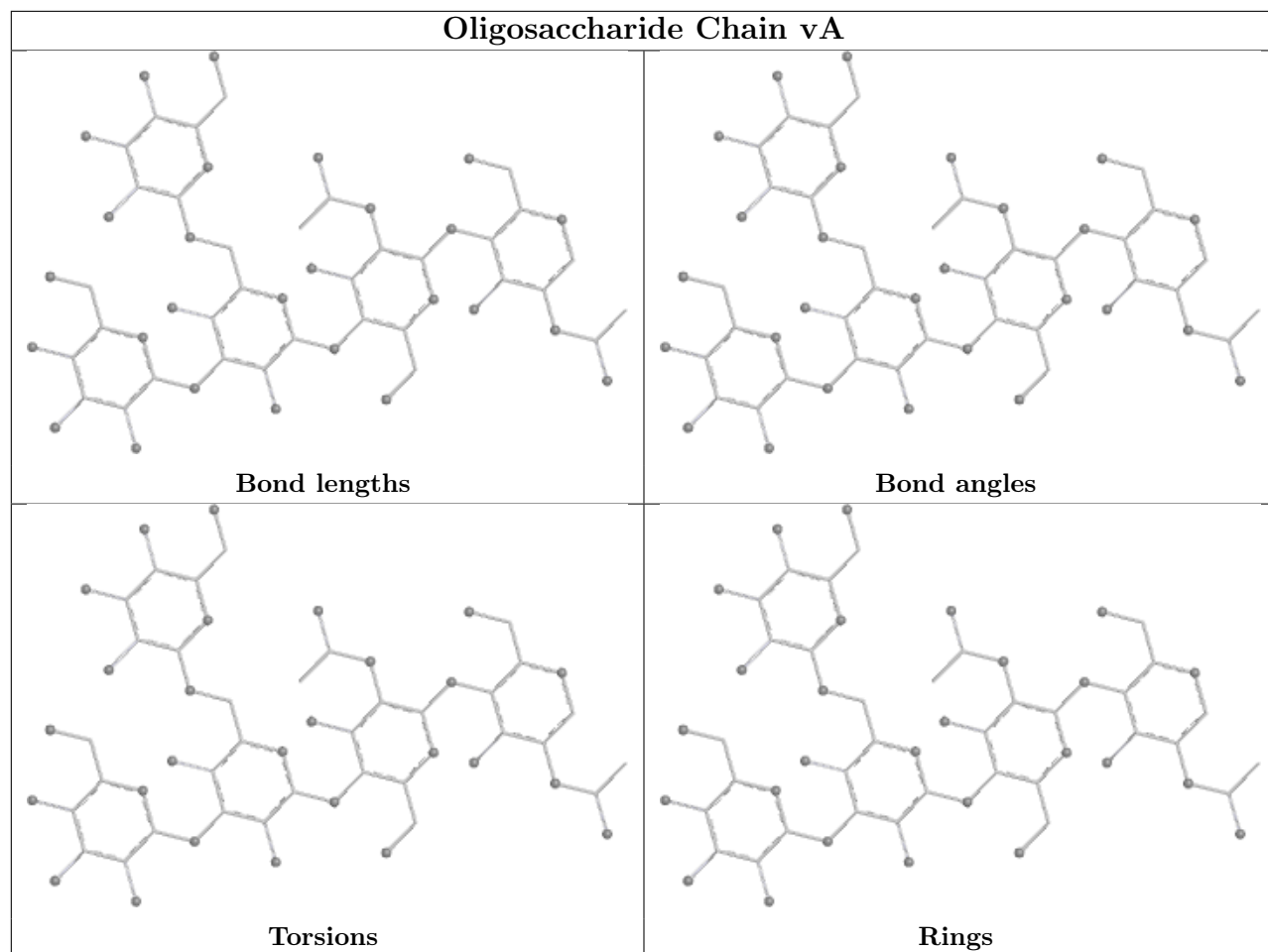


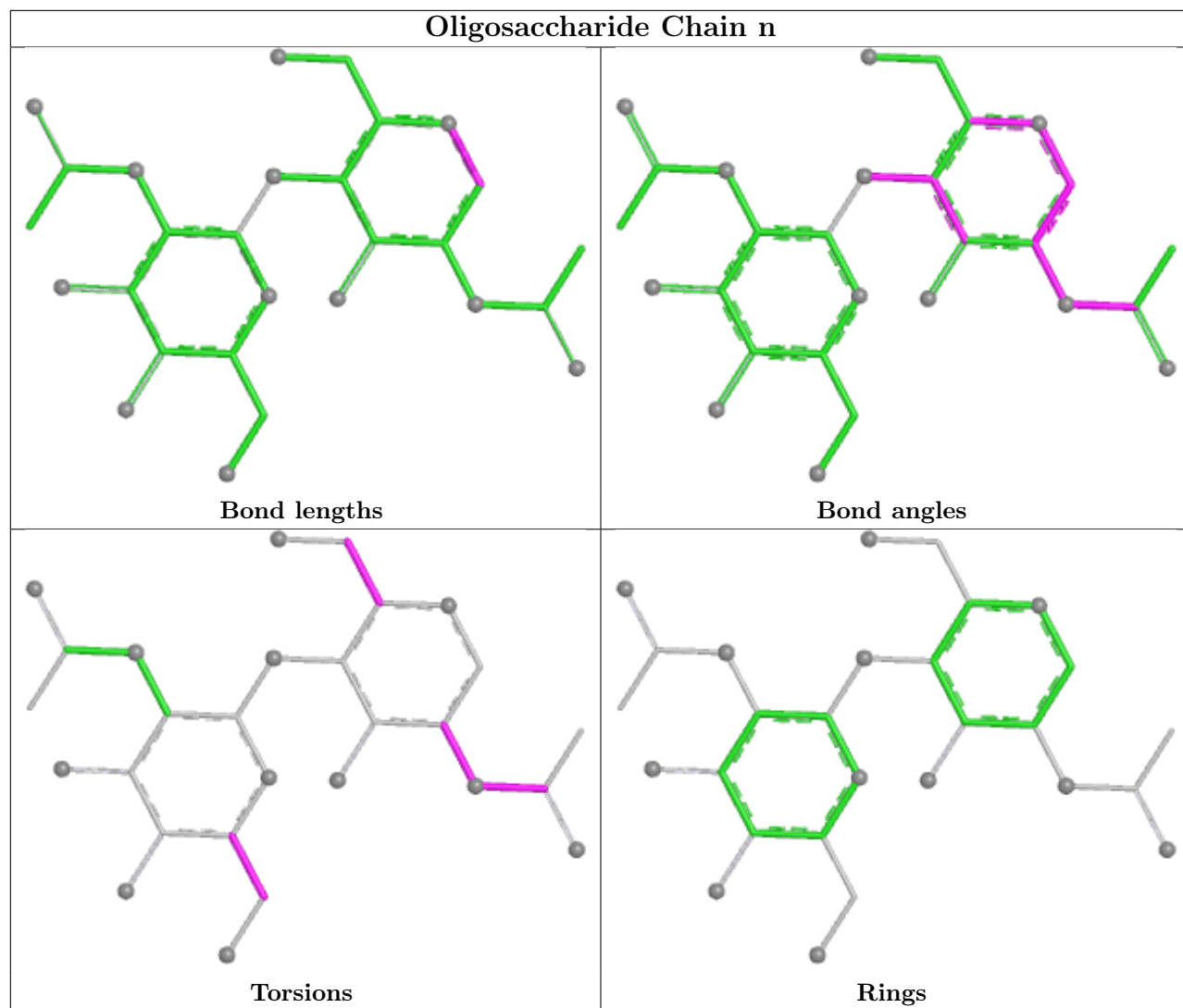


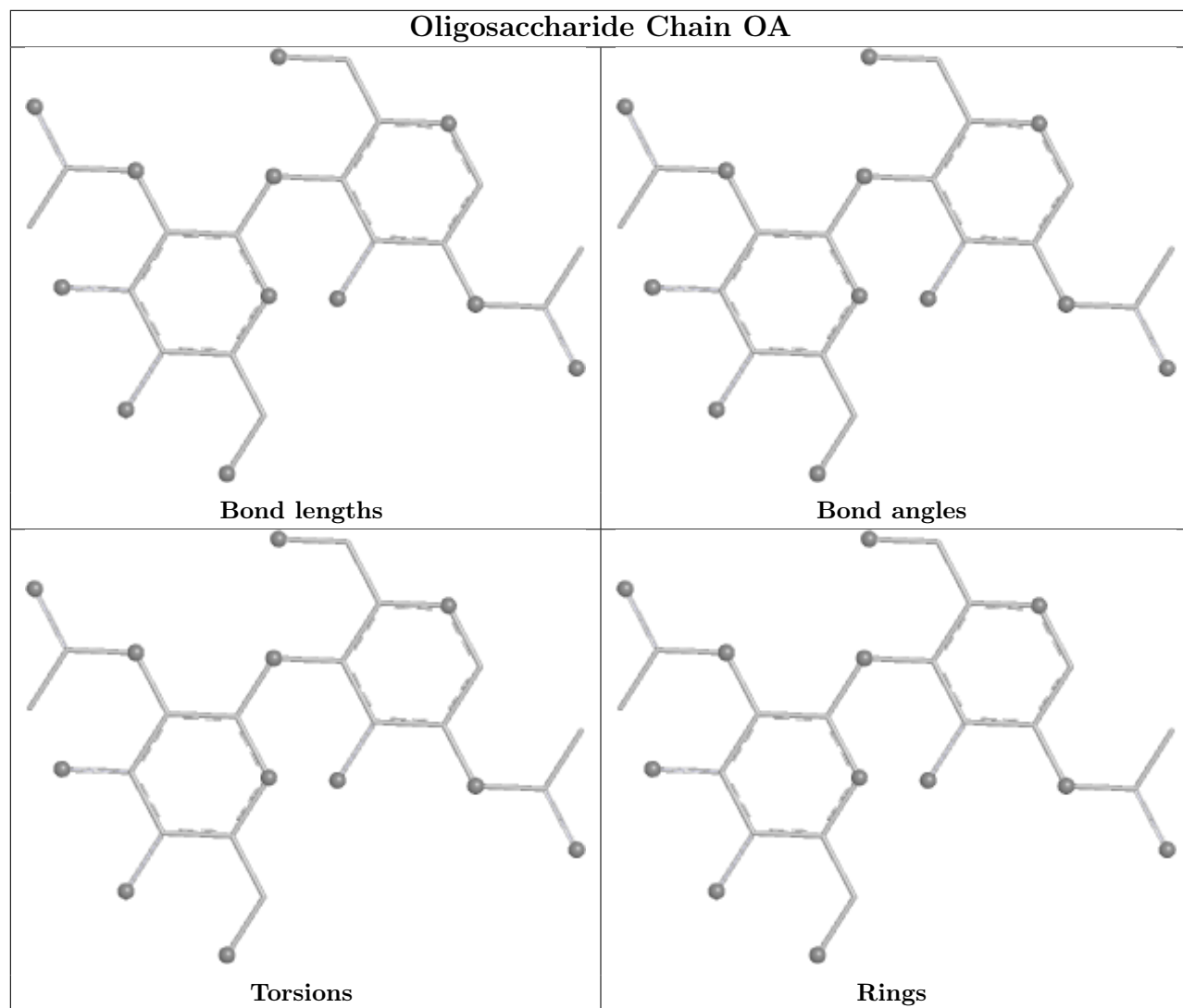


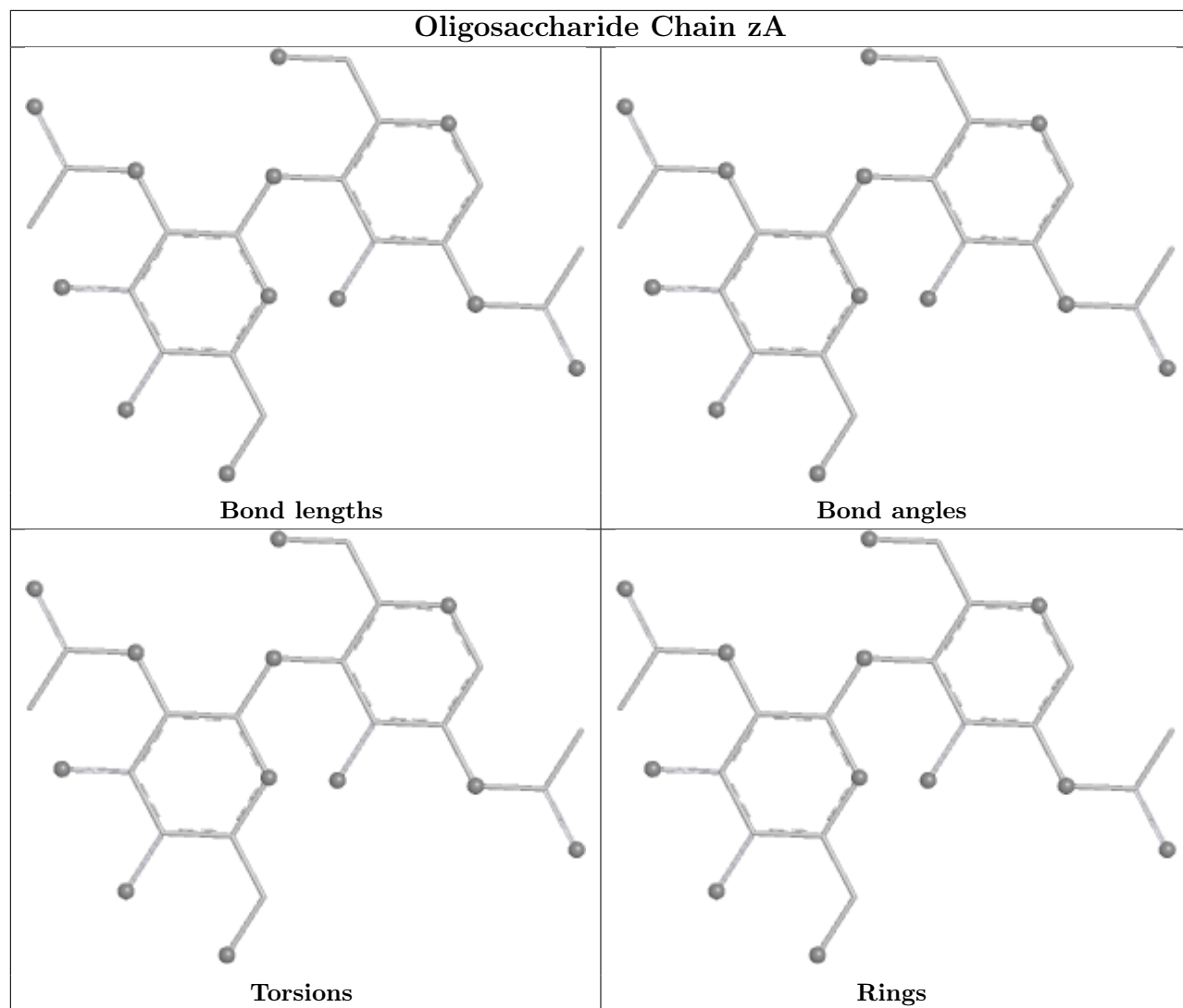


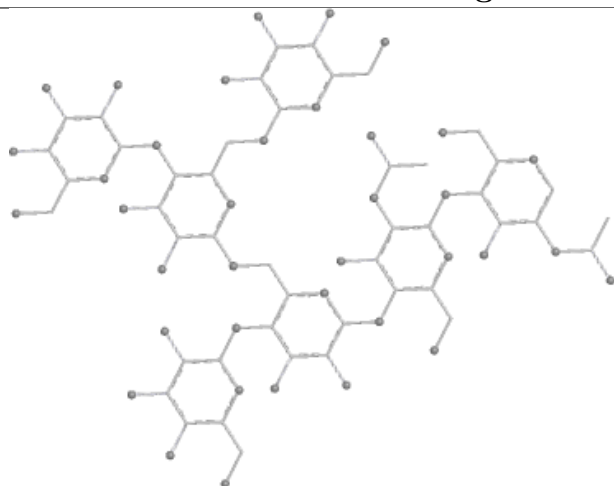
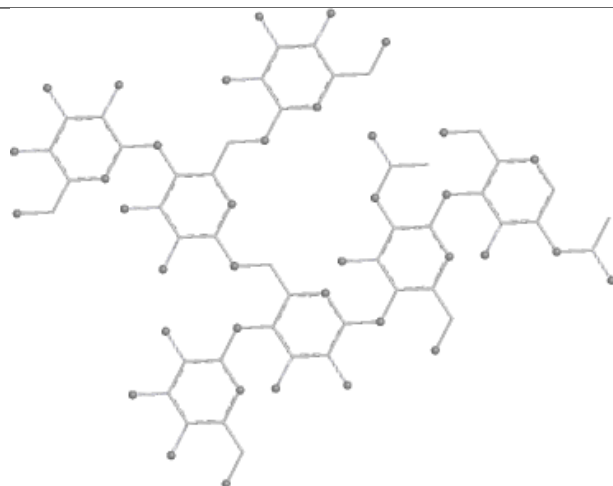
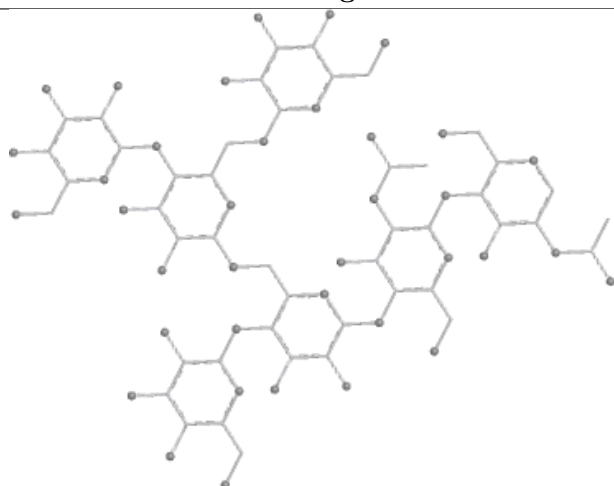
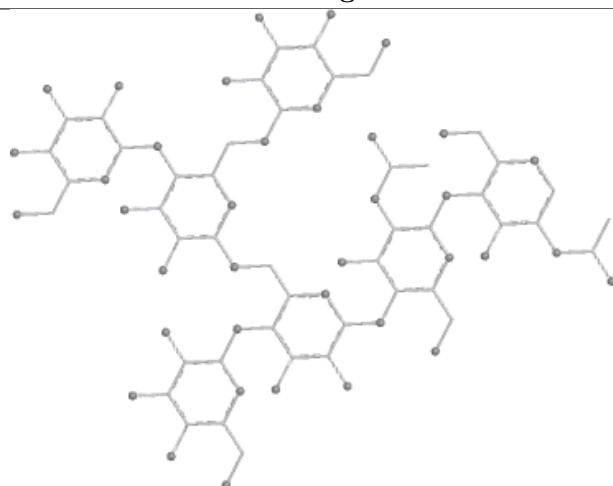


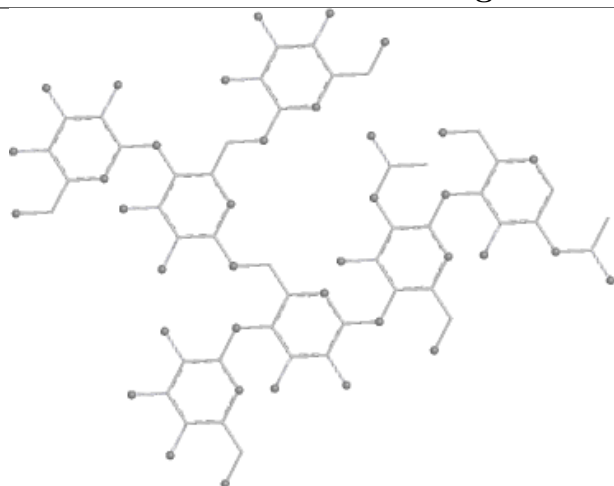
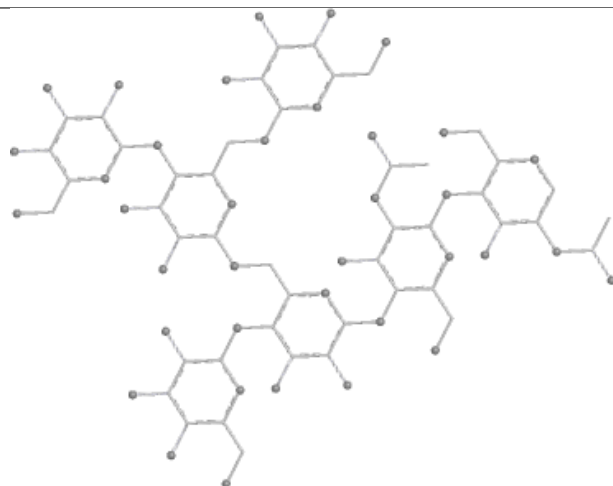
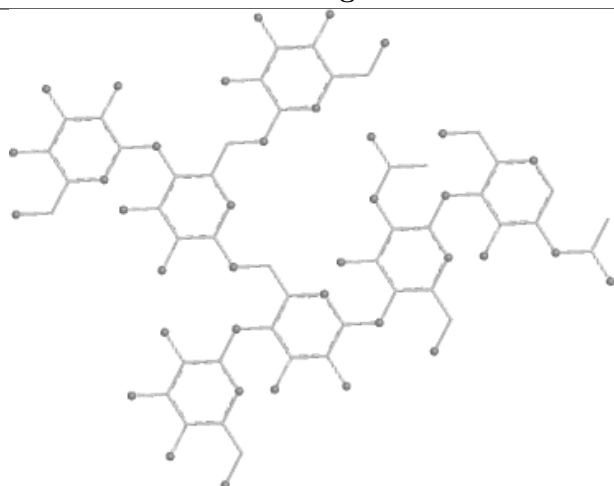
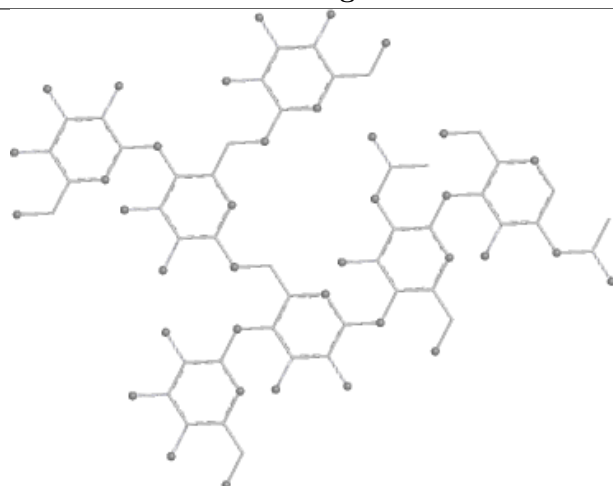


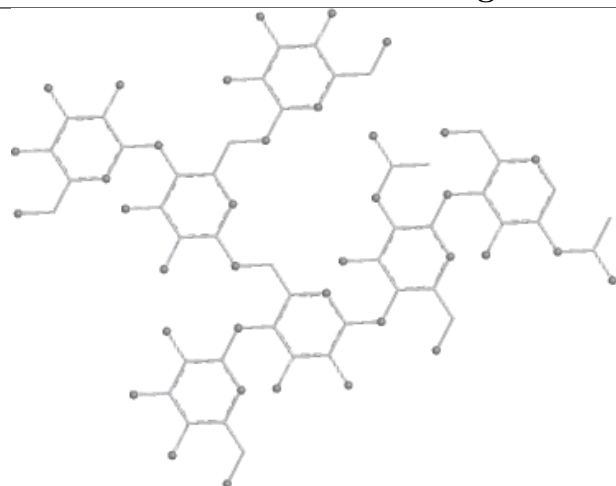
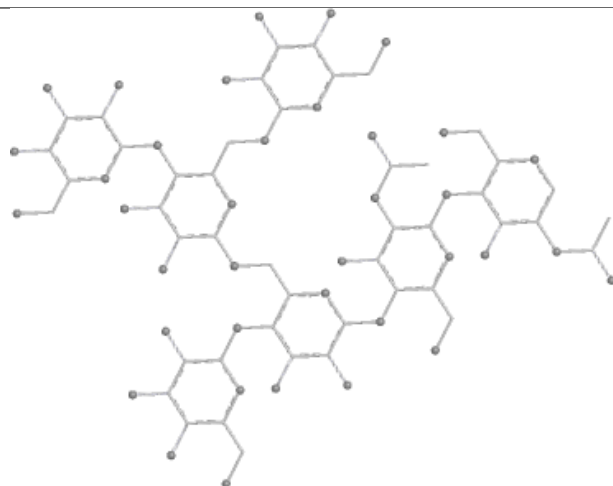
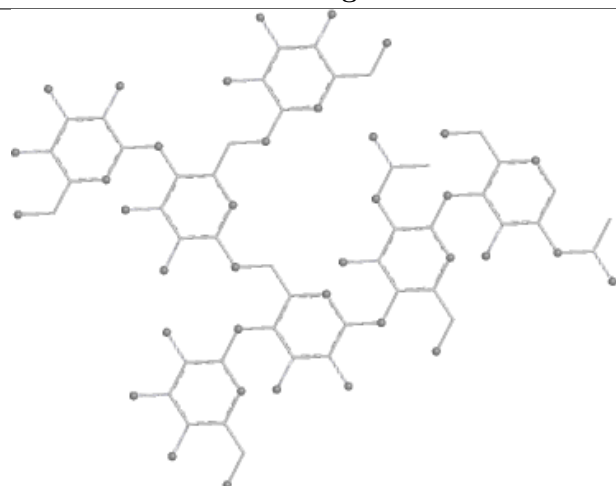
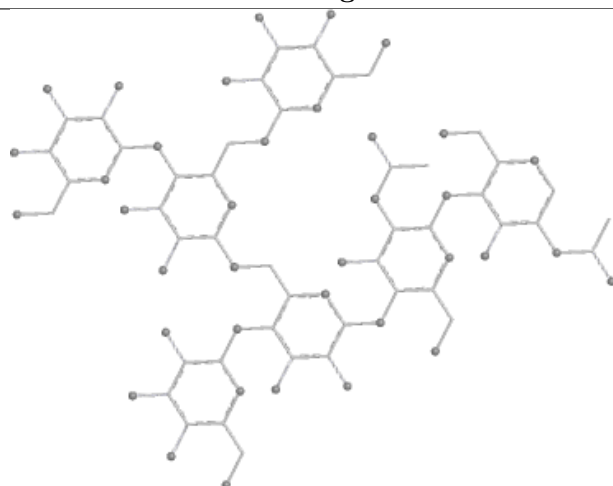


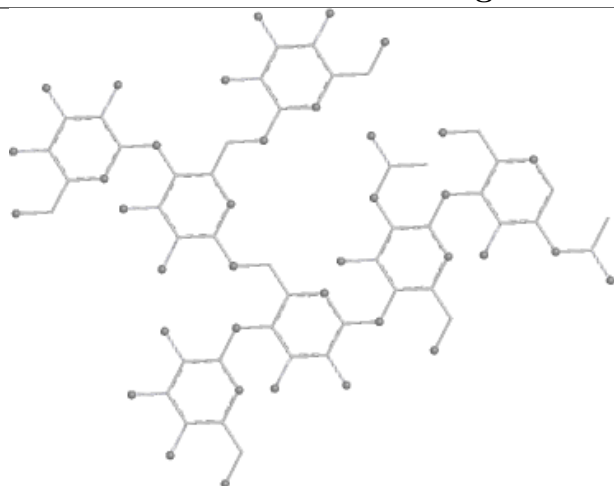
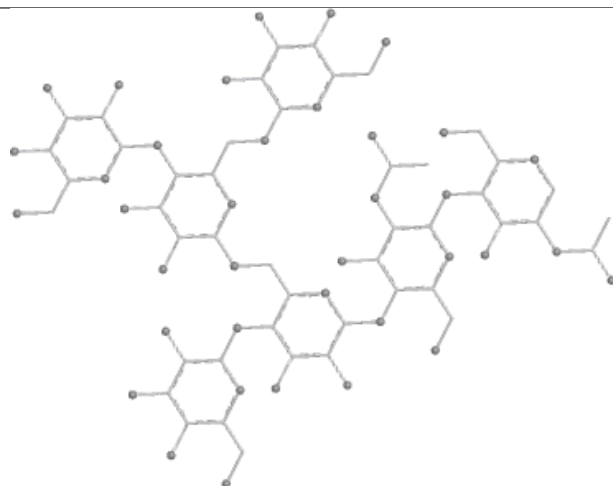
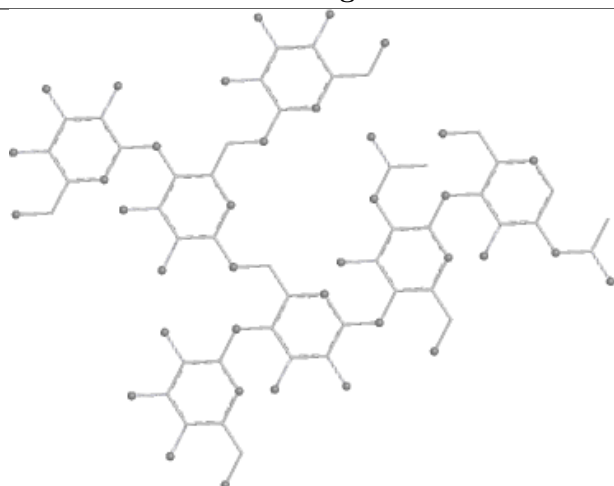
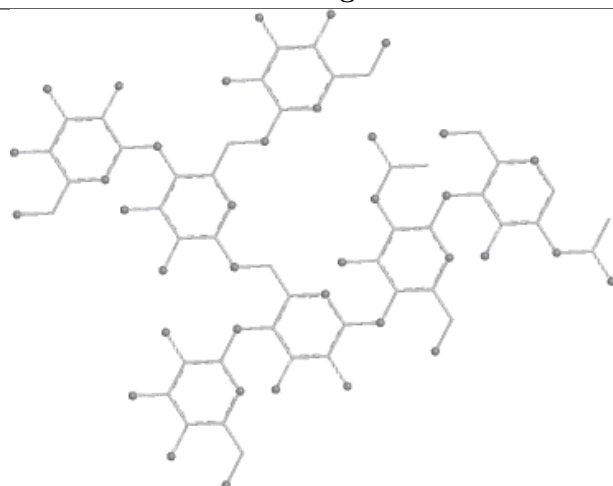


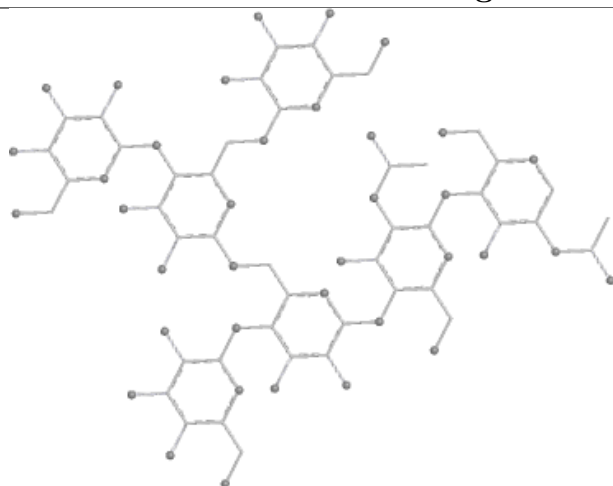
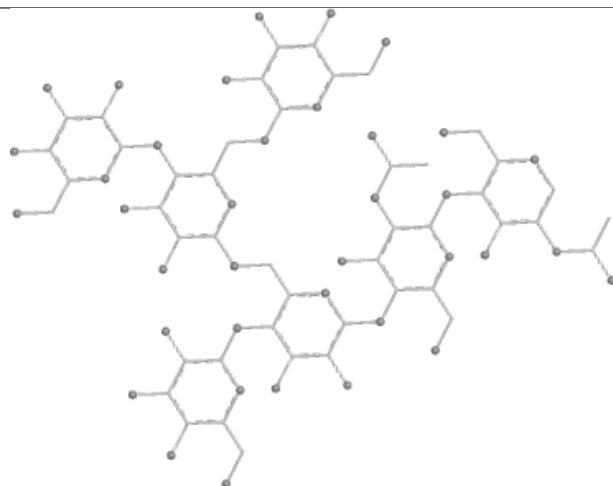
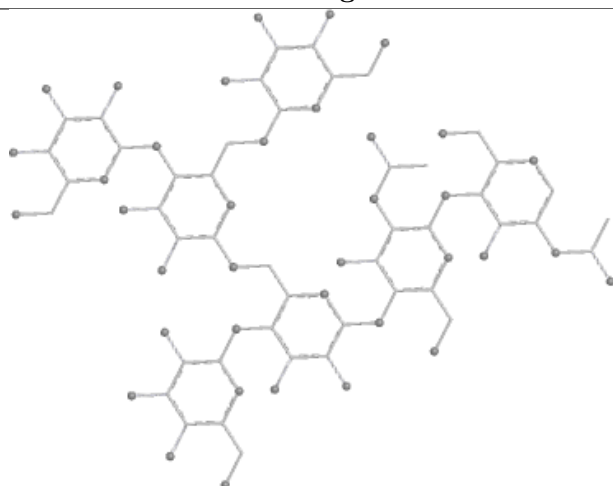
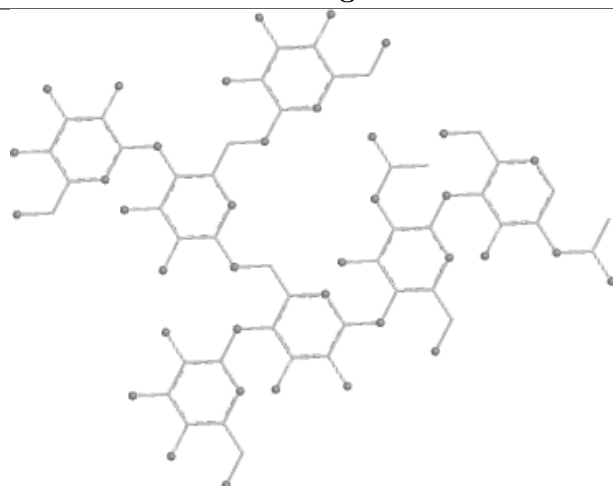


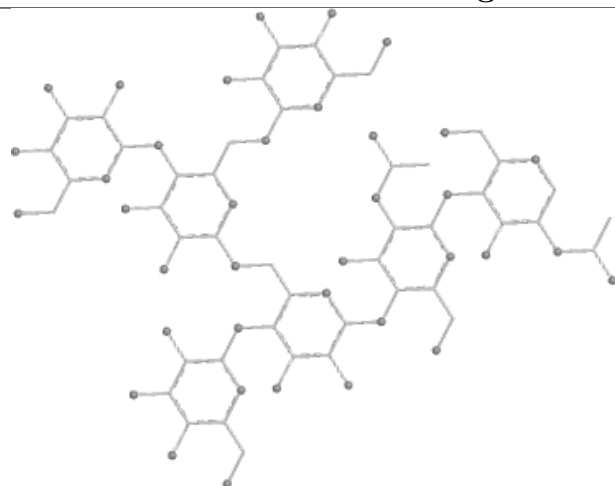
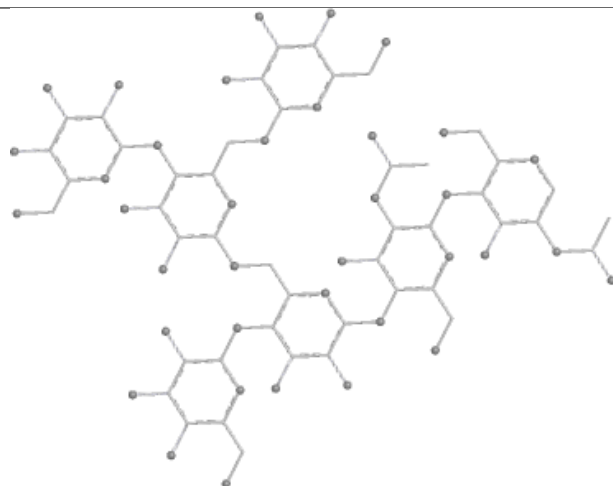
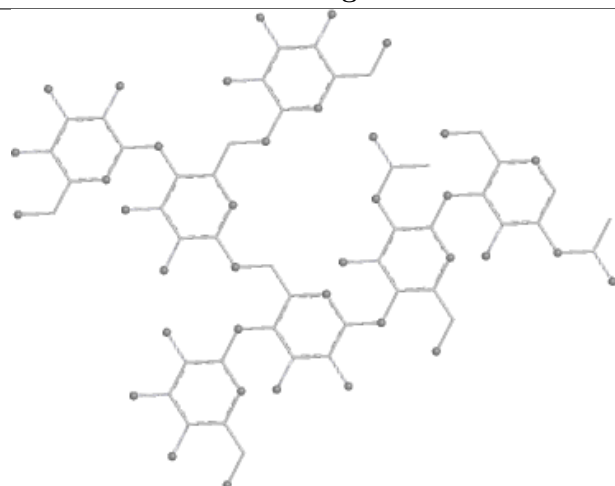
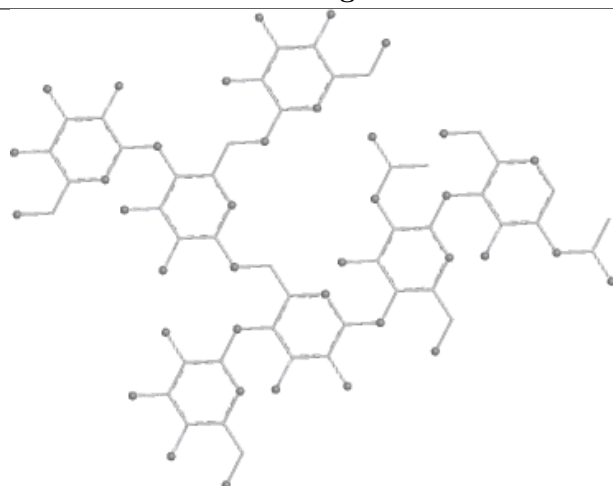
Oligosaccharide Chain 0A**Bond lengths****Bond angles****Torsions****Rings**

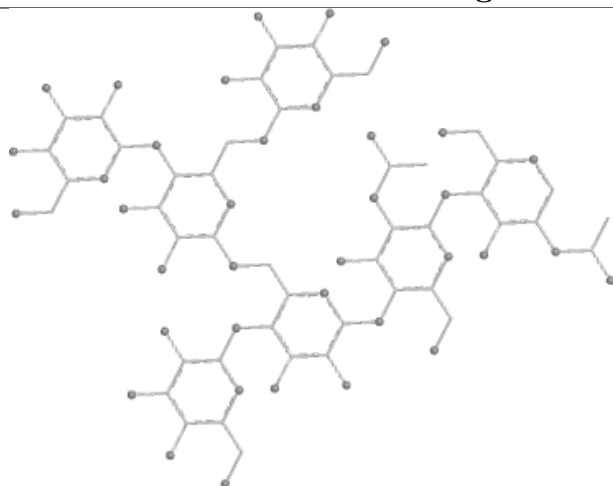
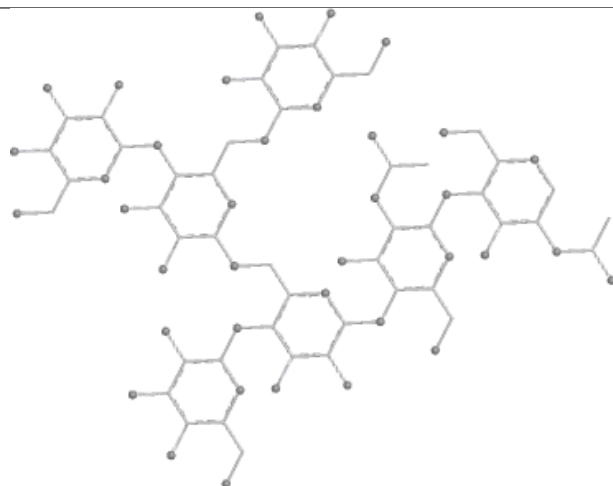
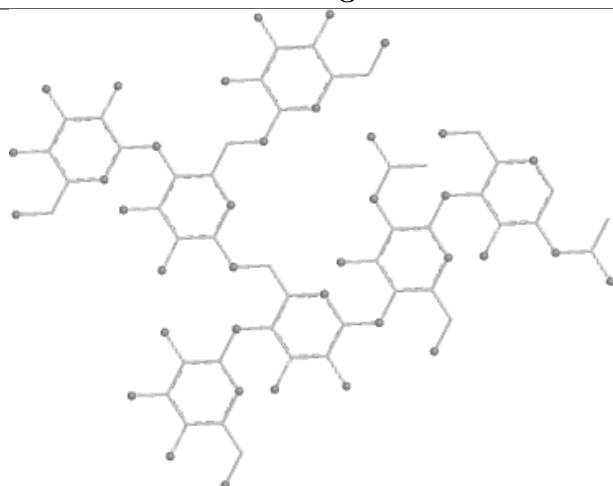
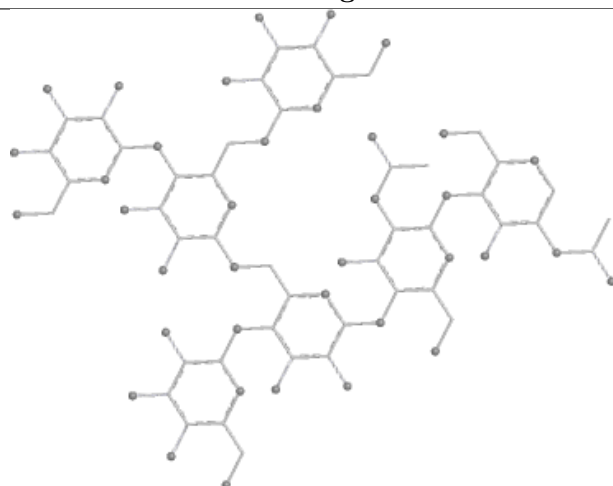
Oligosaccharide Chain 1A**Bond lengths****Bond angles****Torsions****Rings**

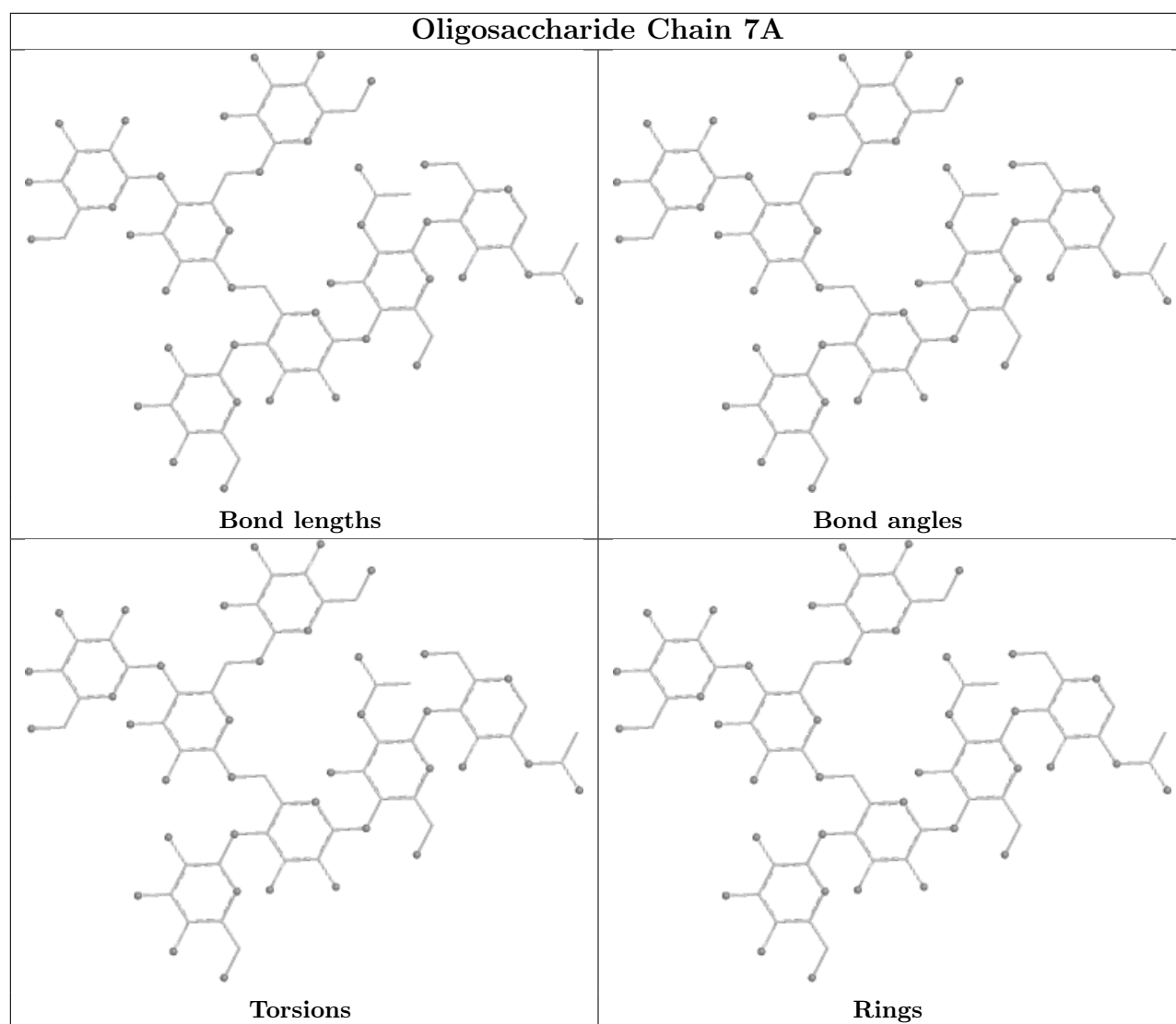
Oligosaccharide Chain 2A**Bond lengths****Bond angles****Torsions****Rings**

Oligosaccharide Chain 3A**Bond lengths****Bond angles****Torsions****Rings**

Oligosaccharide Chain 4A**Bond lengths****Bond angles****Torsions****Rings**

Oligosaccharide Chain 5A**Bond lengths****Bond angles****Torsions****Rings**

Oligosaccharide Chain 6A**Bond lengths****Bond angles****Torsions****Rings**



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

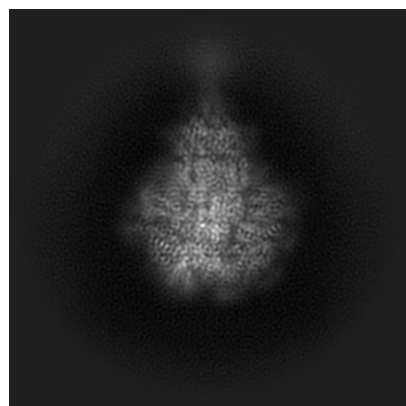
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22889. These allow visual inspection of the internal detail of the map and identification of artifacts.

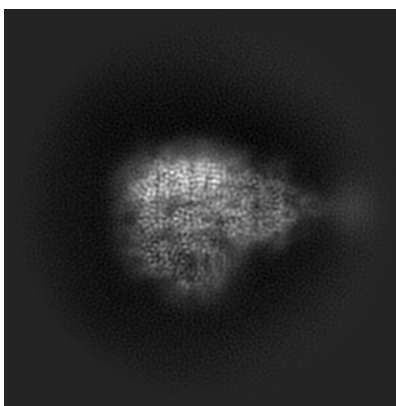
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

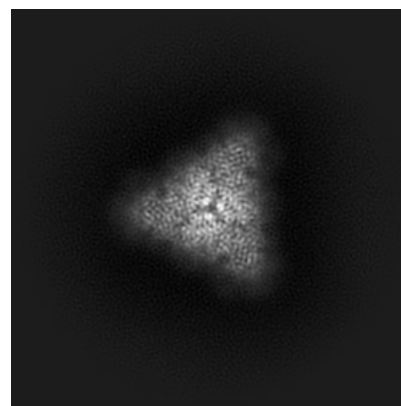
6.1.1 Primary map



X

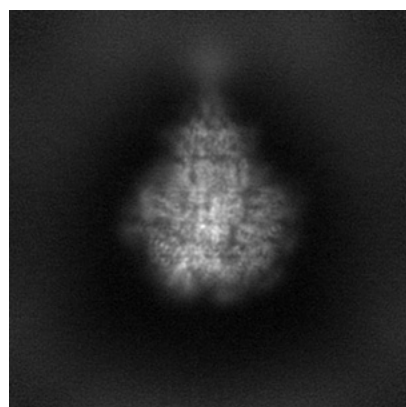


Y

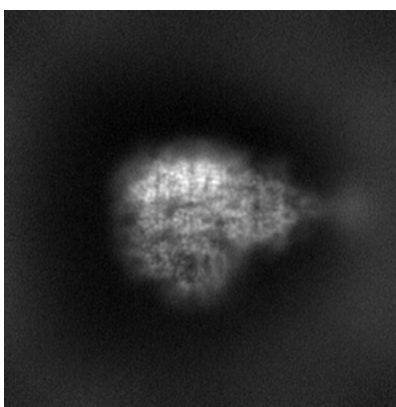


Z

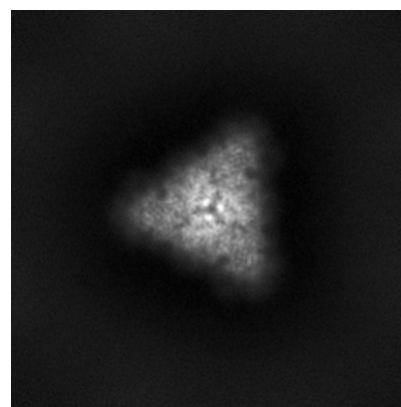
6.1.2 Raw map



X



Y

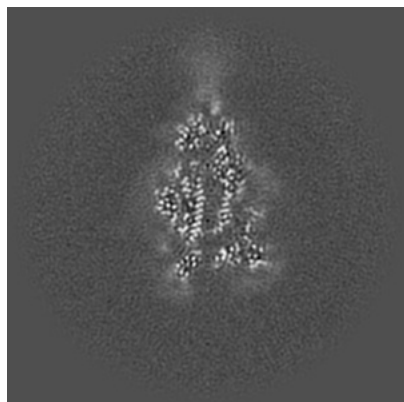


Z

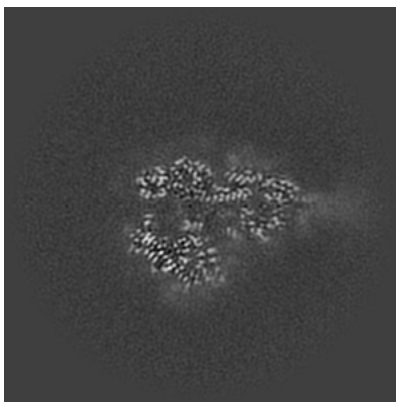
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

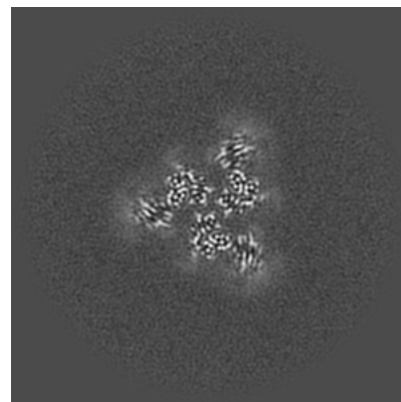
6.2.1 Primary map



X Index: 128

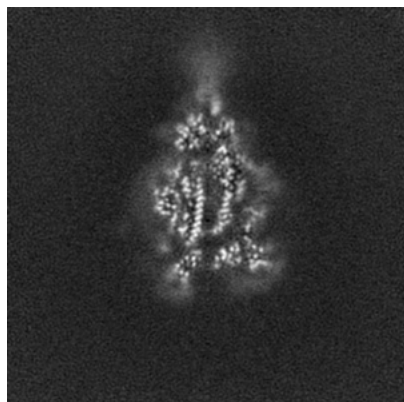


Y Index: 128

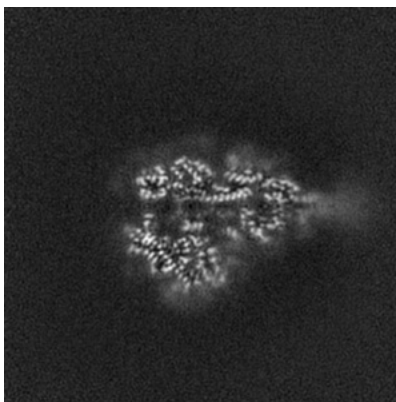


Z Index: 128

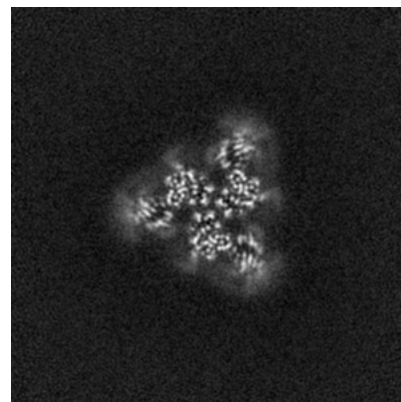
6.2.2 Raw map



X Index: 128



Y Index: 128

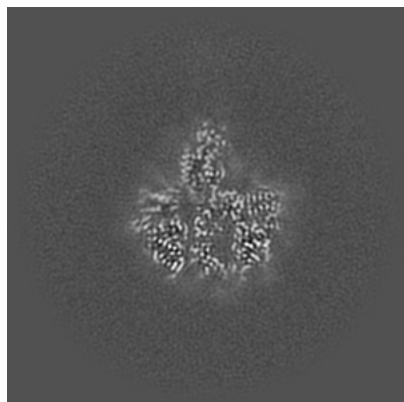


Z Index: 128

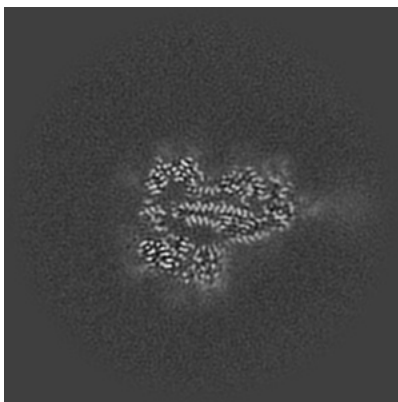
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

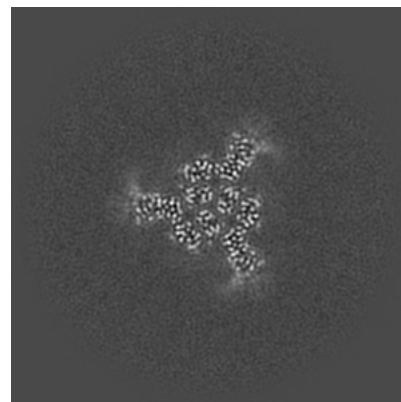
6.3.1 Primary map



X Index: 145

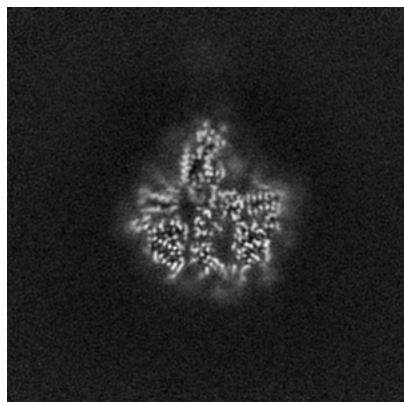


Y Index: 122

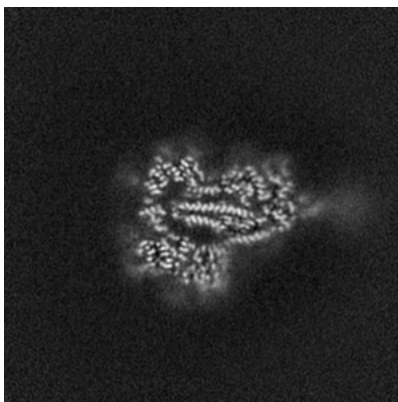


Z Index: 114

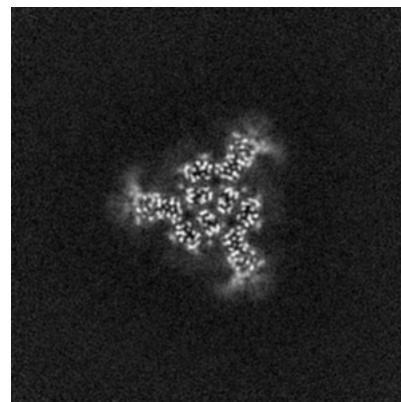
6.3.2 Raw map



X Index: 145



Y Index: 122

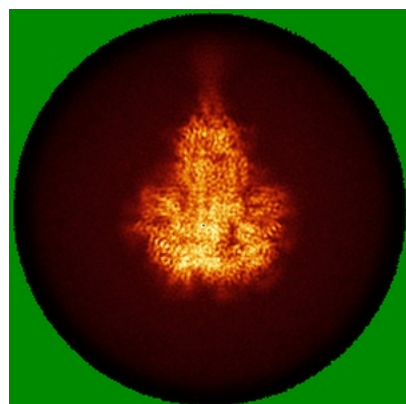


Z Index: 114

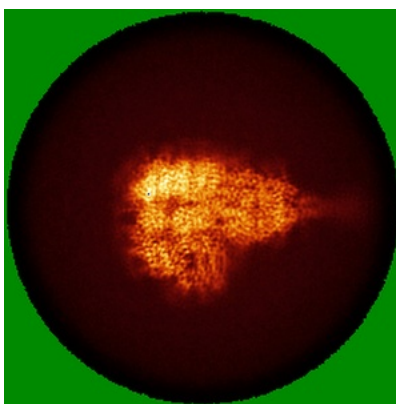
The images above show the largest variance slices of the map in three orthogonal directions.

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

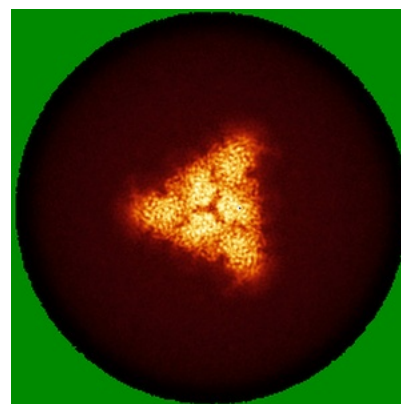
6.4.1 Primary map



X

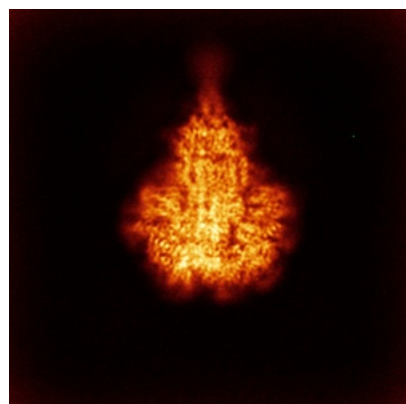


Y

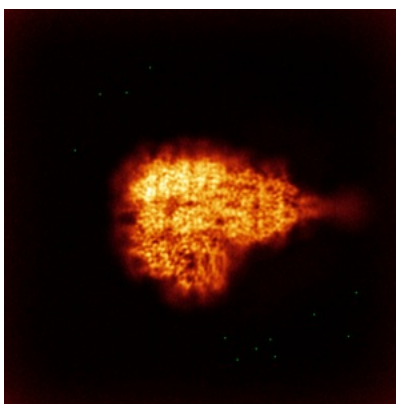


Z

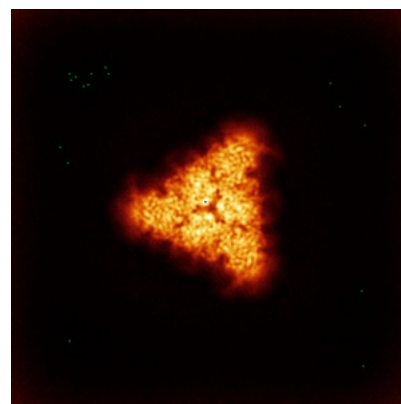
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.528. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

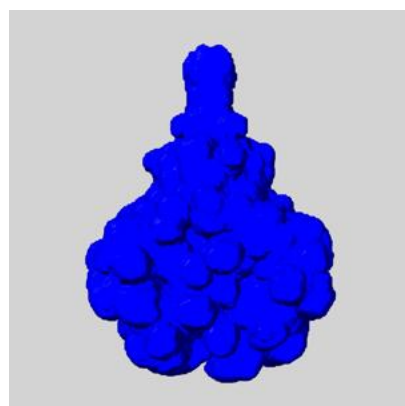
6.6 Mask visualisation [i](#)

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

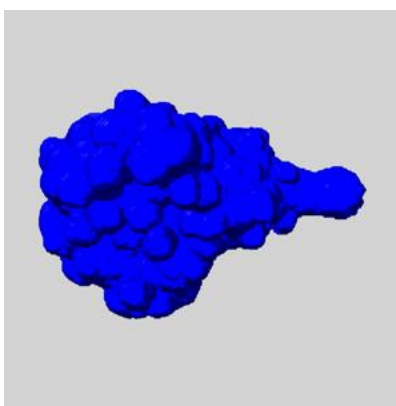
A mask typically either:

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

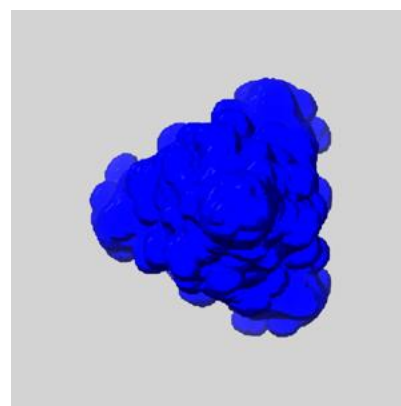
6.6.1 emd_22889_msk_1.map [i](#)



X



Y

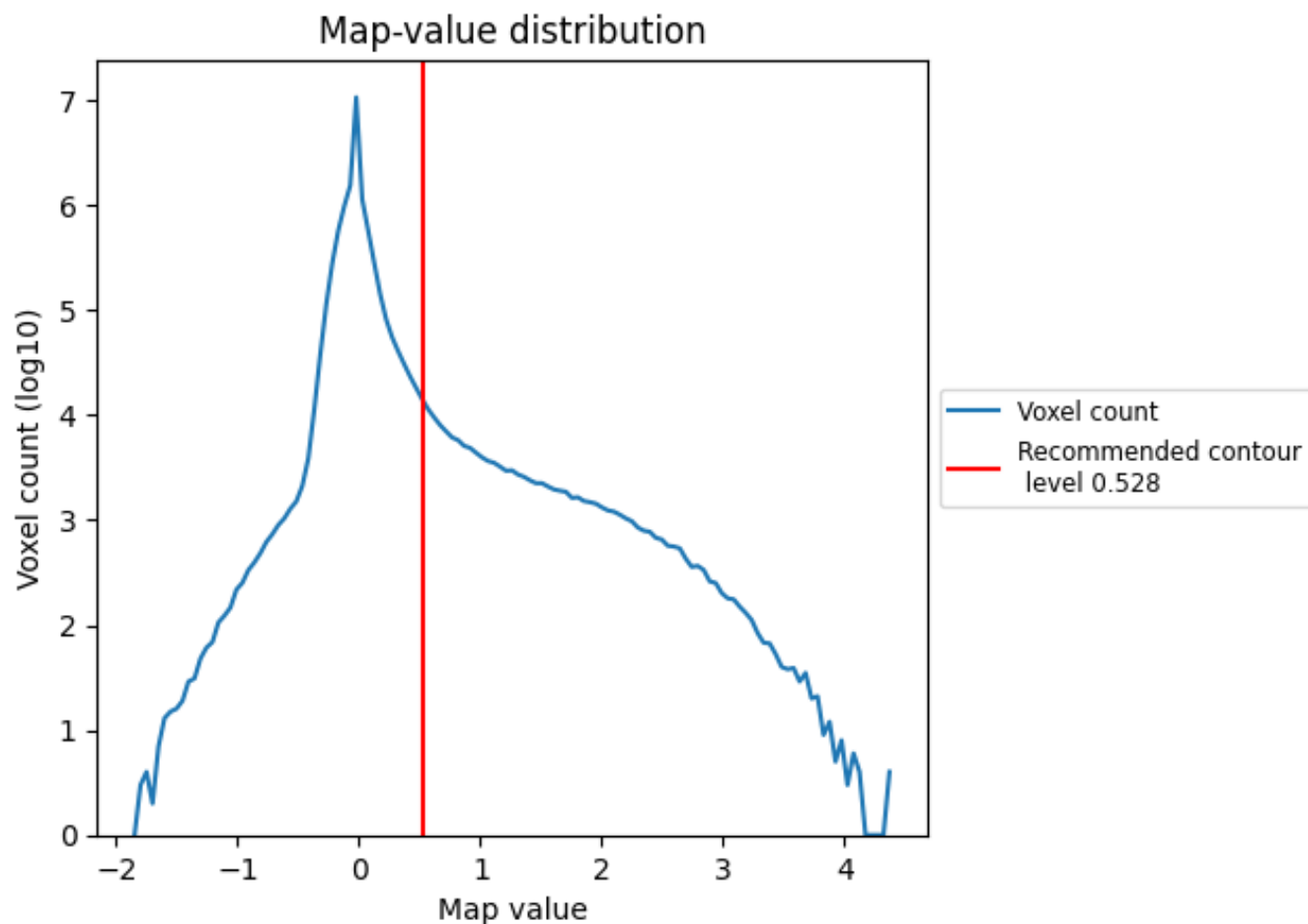


Z

7 Map analysis [i](#)

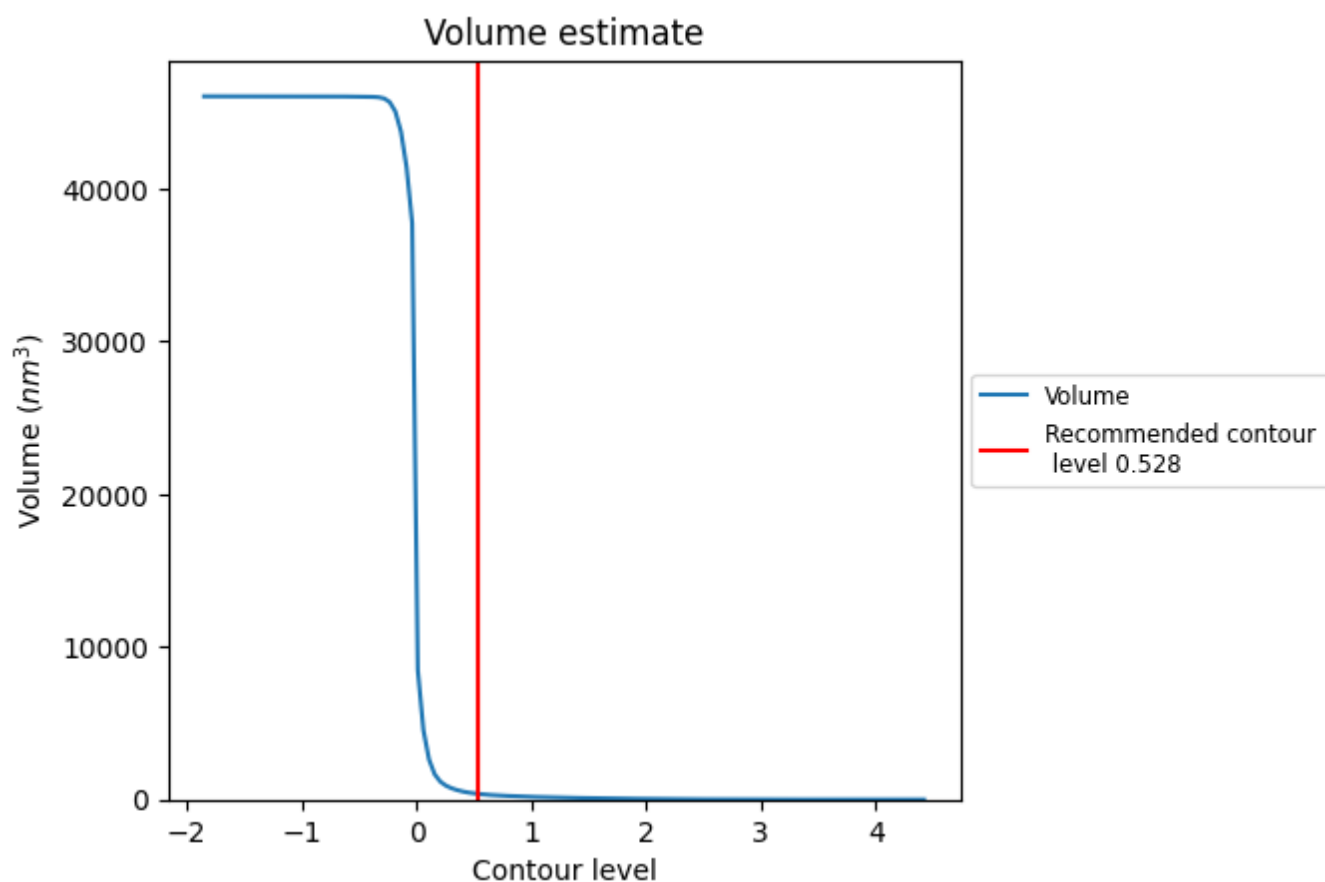
This section contains the results of statistical analysis of the map.

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.

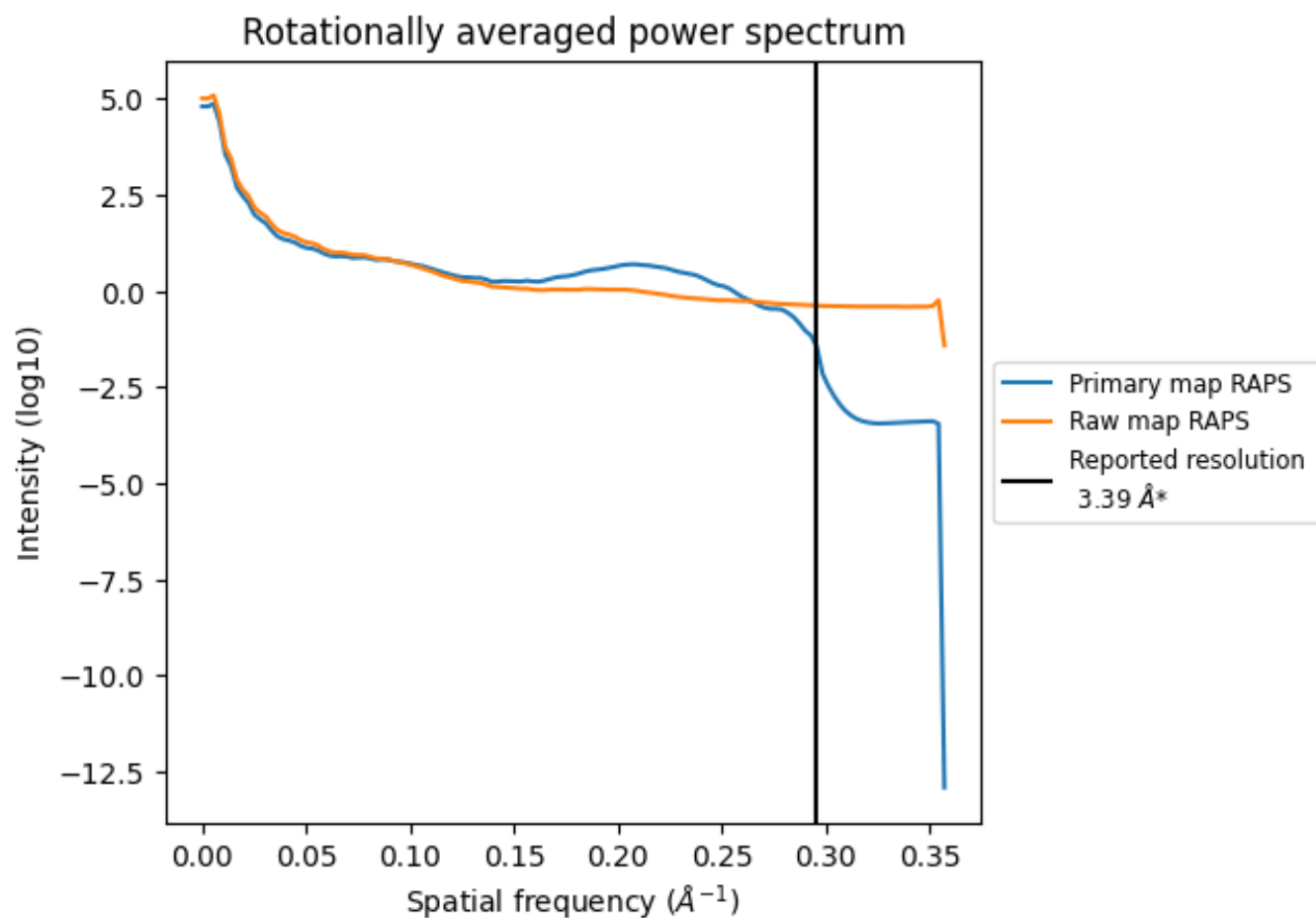
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 380 nm³; this corresponds to an approximate mass of 344 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 ⓘ

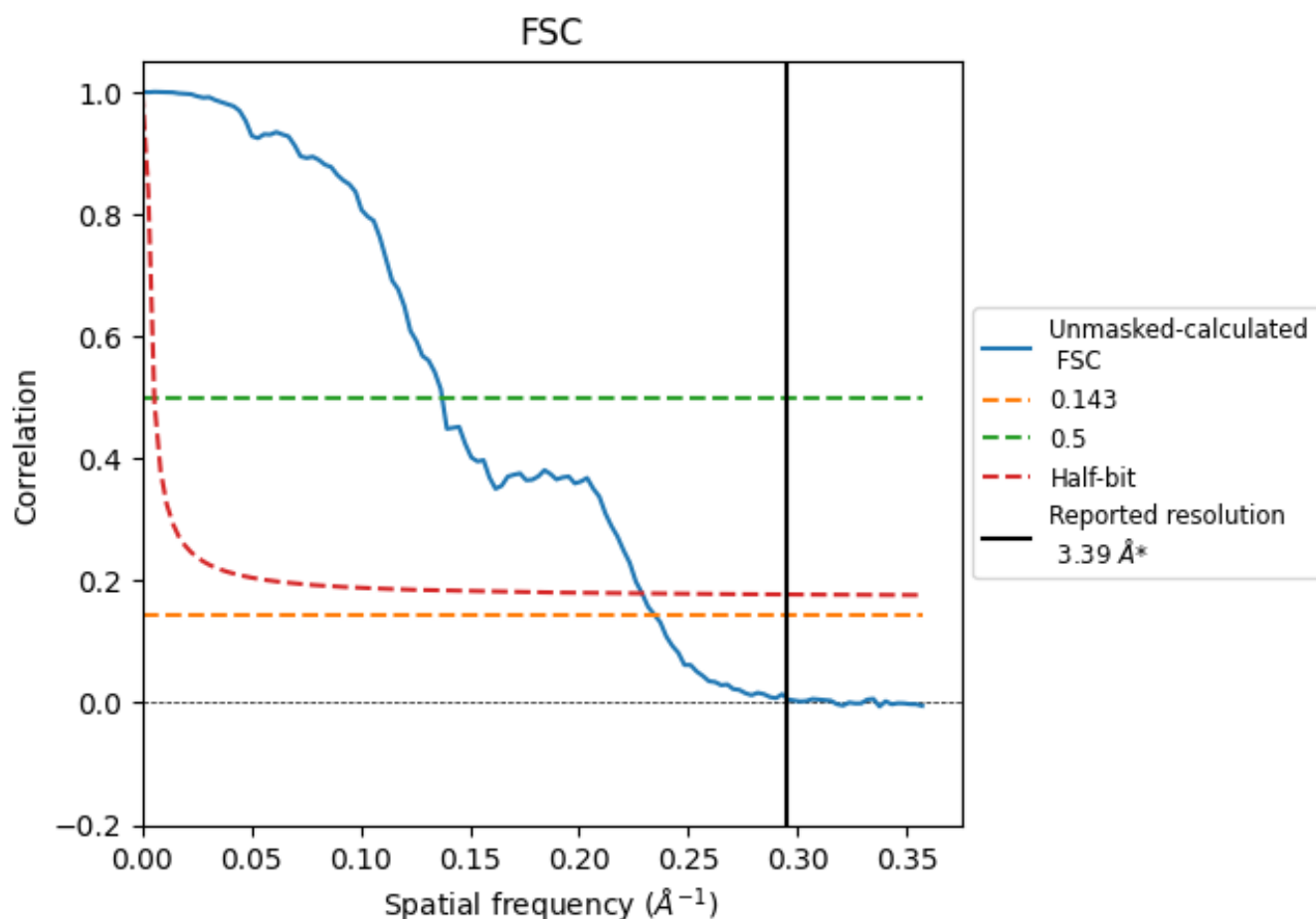


*Reported resolution corresponds to spatial frequency of 0.295 Å⁻¹

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 $0.295 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

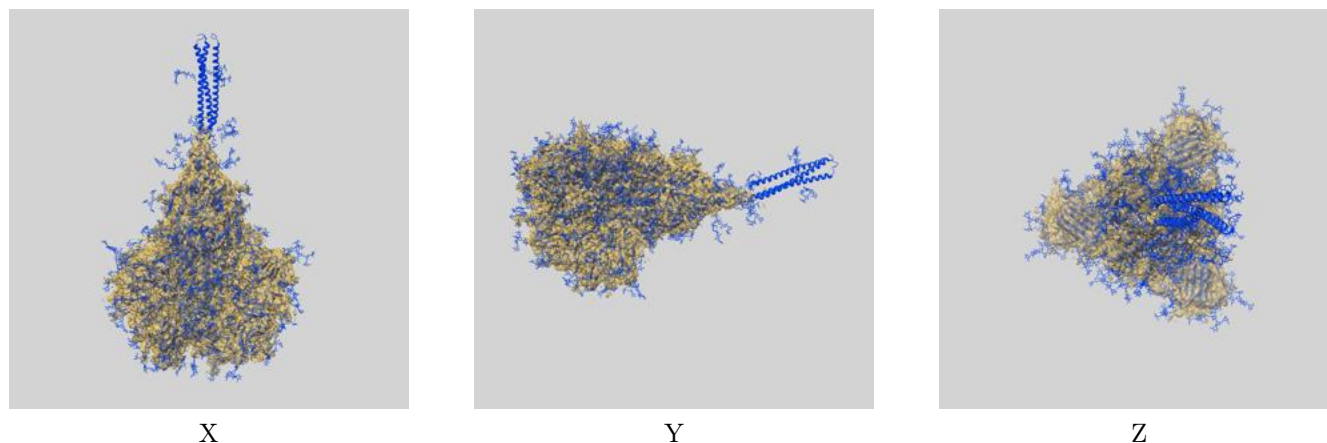
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.39	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.26	7.28	4.37

*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 4.26 differs from the reported value 3.39 by more than 10 %

9 Map-model fit [i](#)

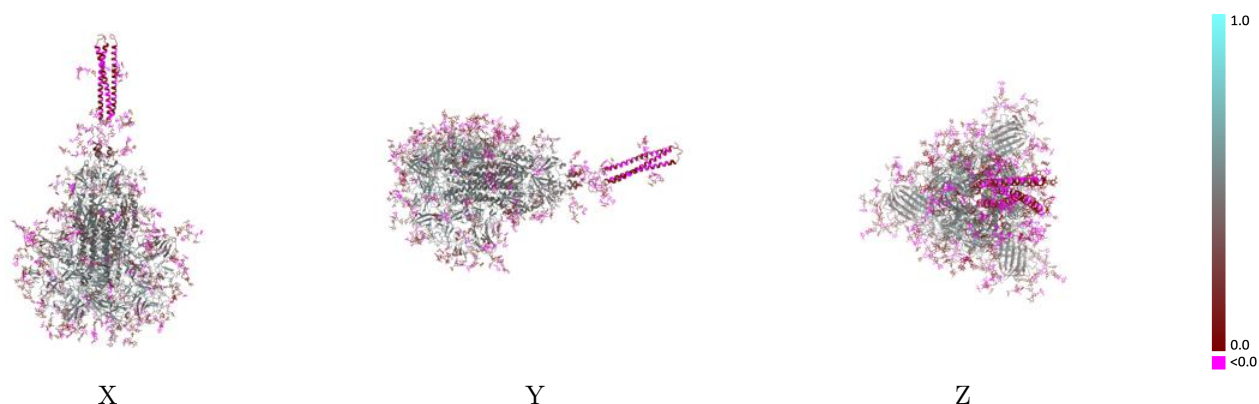
This section contains information regarding the fit between EMDB map EMD-22889 and PDB model 8FR7. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



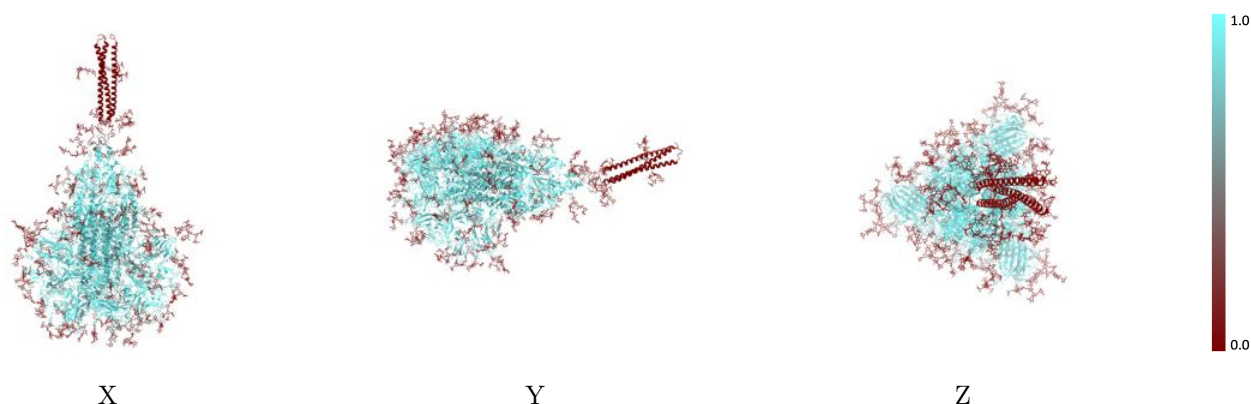
The images above show the 3D surface view of the map at the recommended contour level 0.528 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



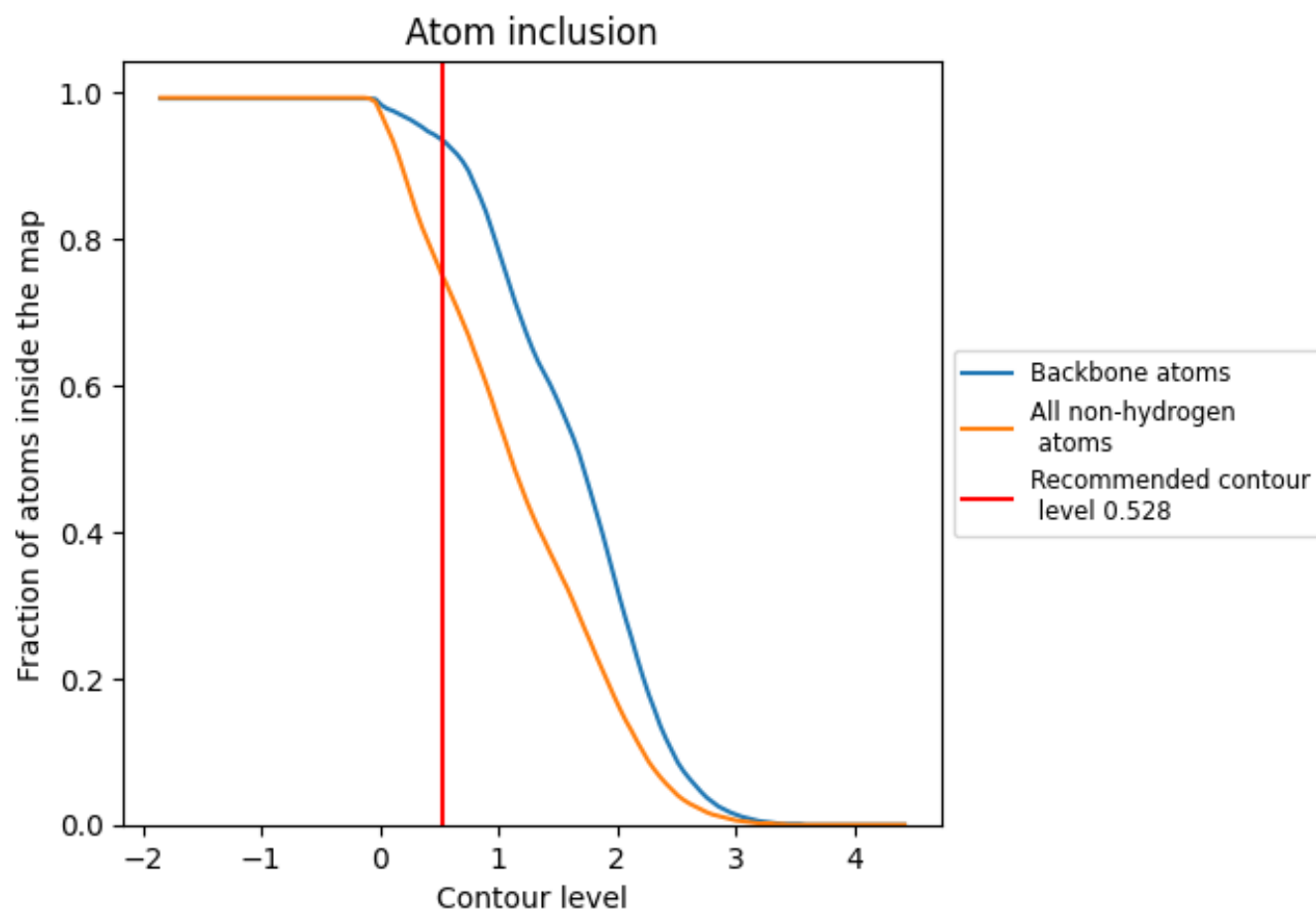
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.528).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 75% 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 (0.528) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7490	 0.3880
0	 0.1450	 0.0920
0A	 0.0000	 -0.0390
1	 0.1450	 0.0470
1A	 0.0000	 0.0230
2	 0.0240	 0.0400
2A	 0.0000	 0.0550
3	 0.3860	 0.1860
3A	 0.0240	 0.0950
4	 0.2410	 0.2050
4A	 0.0000	 0.0370
5	 0.1330	 0.0960
5A	 0.0000	 -0.0060
6	 0.2770	 0.0950
6A	 0.0000	 0.0480
7	 0.2170	 0.1790
7A	 0.0000	 0.0770
8	 0.1930	 0.0200
9	 0.2050	 0.0730
A	 0.9090	 0.4660
AA	 0.3980	 0.1810
B	 0.9100	 0.4650
BA	 0.5660	 0.2710
C	 0.9120	 0.4680
CA	 0.5060	 0.2700
D	 0.1200	 0.0930
DA	 0.4580	 0.3460
E	 0.2050	 0.0970
EA	 0.0960	 0.0640
F	 0.8950	 0.4260
FA	 0.3250	 0.0940
G	 0.2250	 0.1740
GA	 0.1450	 0.1550
H	 0.4580	 0.2370
HA	 0.0120	 0.0520



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Chain	Atom inclusion	Q-score
I	 0.3250	 0.2450
IA	 0.0480	 -0.0120
J	 0.4700	 0.2140
JA	 0.0480	 0.1050
K	 0.0840	 0.1600
KA	 0.4430	 0.1210
L	 0.3860	 0.1730
LA	 0.2170	 0.0770
M	 0.8830	 0.4410
MA	 0.2530	 0.0390
N	 0.2890	 0.1390
NA	 0.3130	 0.2560
O	 0.4700	 0.2890
OA	 0.5000	 0.2270
P	 0.1450	 0.1040
PA	 0.1200	 0.0920
Q	 0.1570	 0.0360
QA	 0.2170	 0.1040
R	 0.0120	 0.0520
RA	 0.8950	 0.4360
S	 0.3980	 0.1880
SA	 0.2250	 0.1780
T	 0.2530	 0.2240
TA	 0.4580	 0.2410
U	 0.1330	 0.0880
UA	 0.3370	 0.2410
V	 0.2650	 0.1110
VA	 0.4820	 0.2150
W	 0.2290	 0.1780
WA	 0.1080	 0.1830
X	 0.1930	 0.0120
XA	 0.3730	 0.1840
Y	 0.1930	 0.1000
YA	 0.8620	 0.4480
Z	 0.3980	 0.1710
ZA	 0.2890	 0.1530
a	 0.5660	 0.2750
aA	 0.4940	 0.2790
b	 0.5060	 0.2760
bA	 0.1570	 0.1040
c	 0.4340	 0.3480
cA	 0.1570	 0.0480

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Chain	Atom inclusion	Q-score
d	 0.0820	 0.0710
dA	 0.0360	 0.0530
e	 0.3130	 0.0970
eA	 0.3980	 0.1870
f	 0.1450	 0.1370
fA	 0.2650	 0.1980
g	 0.0120	 0.0290
gA	 0.1330	 0.0950
h	 0.0480	 -0.0140
hA	 0.2890	 0.1010
i	 0.0480	 0.1110
iA	 0.2170	 0.1840
j	 0.4430	 0.1210
jA	 0.1930	 0.0400
k	 0.2410	 0.0850
kA	 0.1930	 0.0970
l	 0.2530	 0.0390
lA	 0.3980	 0.1720
m	 0.3130	 0.2440
mA	 0.5540	 0.2600
n	 0.4640	 0.1740
nA	 0.5300	 0.2750
o	 0.1200	 0.0850
oA	 0.4580	 0.3500
p	 0.2050	 0.1070
pA	 0.0890	 0.0630
q	 0.8950	 0.4260
qA	 0.3010	 0.0870
r	 0.2340	 0.1750
rA	 0.1450	 0.1430
s	 0.4580	 0.2430
sA	 0.0120	 0.0410
t	 0.3370	 0.2300
tA	 0.0480	 -0.0030
u	 0.4820	 0.2200
uA	 0.0360	 0.1270
v	 0.0960	 0.1690
vA	 0.4260	 0.1230
w	 0.3980	 0.1760
wA	 0.2170	 0.0920
x	 0.8720	 0.4450
xA	 0.2530	 0.0340

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Chain	Atom inclusion	Q-score
y	 0.3010	 0.1520
yA	 0.3250	 0.2380
z	 0.4820	 0.2920
zA	 0.4640	 0.2300