



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 01:31 AM EST

PDB ID : 6U59
EMDB ID : EMD-20642
Title : HIV-1 B41 SOSIP.664 in complex with rabbit antibody 13B
Authors : Yang, Y.R.; Ward, A.B.
Deposited on : 2019-08-27
Resolution : 3.86 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:

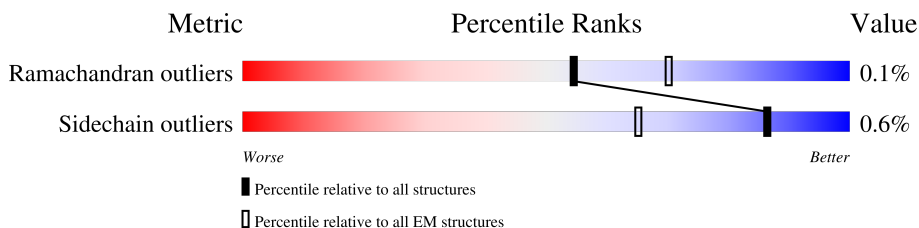
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.86 Å.

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



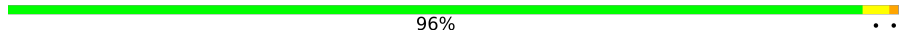
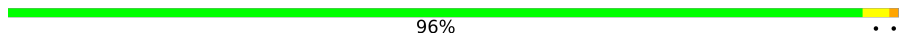
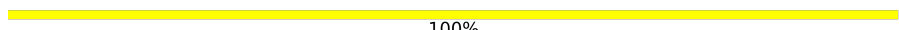
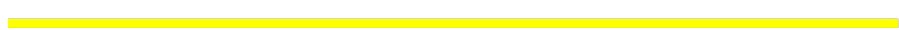

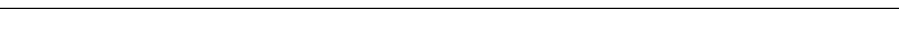
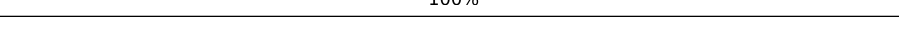
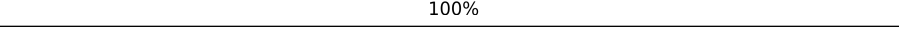
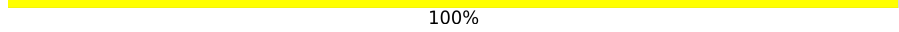
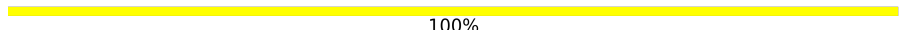
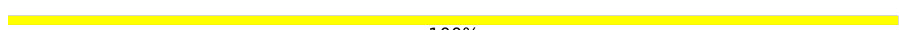


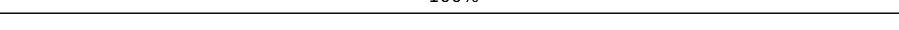
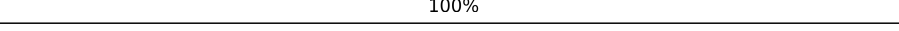
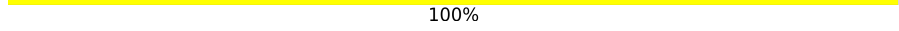
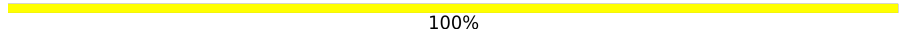
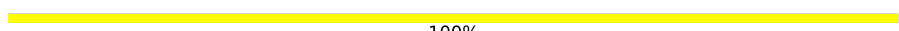



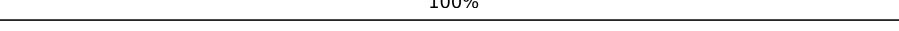
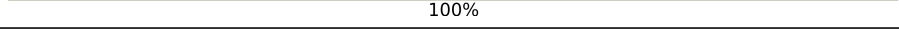
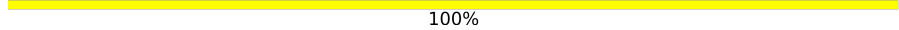
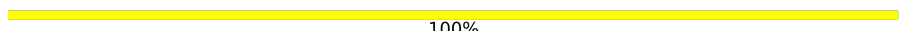
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	524	84% 13%
1	C	524	84% 13%
1	G	524	84% 13%
2	B	153	73% 5% 22%
2	D	153	73% 5% 22%
2	I	153	74% 5% 22%
3	E	112	96% .
3	J	112	96% .
3	L	112	95% 5%
4	F	119	96% . . .

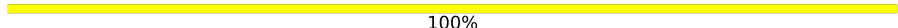
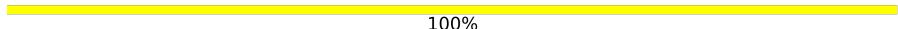
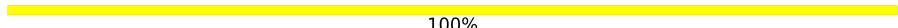
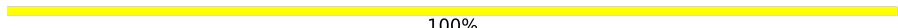
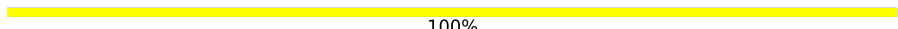
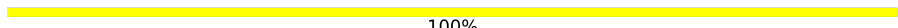
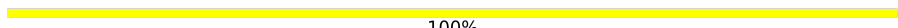
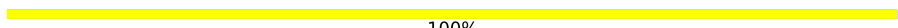
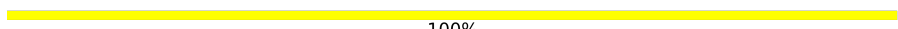

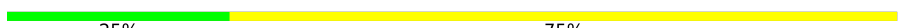
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Mol	Chain	Length	Quality of chain
4	H	119	 96%
4	K	119	 96%
5	M	2	 100%
5	N	2	 100%
5	O	2	 100%
5	P	2	 100%
5	Q	2	 100%
5	S	2	 100%
5	T	2	 100%
5	U	2	 100%
5	V	2	 100%
5	X	2	 100%
5	Y	2	 100%
5	Z	2	 100%
5	a	2	 100%
5	b	2	 100%
5	c	2	 100%
5	d	2	 100%
5	f	2	 100%
5	g	2	 100%
5	h	2	 100%
5	i	2	 100%
5	k	2	 100%
5	l	2	 100%
5	m	2	 100%

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Mol	Chain	Length	Quality of chain
5	n	2	 100%
5	o	2	 100%
5	p	2	 100%
5	q	2	 100%
5	s	2	 100%
5	t	2	 100%
5	u	2	 100%
5	v	2	 100%
5	x	2	 100%
5	y	2	 100%
6	R	3	 100%
6	e	3	 100%
6	r	3	 100%
7	W	4	 25% 75%
7	j	4	 25% 75%
7	w	4	 25% 75%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20439 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 SOSIP.664 gp120,SOSIP.664 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	454	3562	2234	629	672	27	0	0
1	C	454	3562	2234	629	672	27	0	0
1	G	454	3562	2234	629	672	27	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	501	CYS	ALA	engineered mutation	UNP B3UES2
A	509	ARG	GLU	engineered mutation	UNP B3UES2
A	510	ARG	LYS	engineered mutation	UNP B3UES2
A	512	ARG	ALA	engineered mutation	UNP B3UES2
A	513	ARG	VAL	engineered mutation	UNP B3UES2
C	501	CYS	ALA	engineered mutation	UNP B3UES2
C	509	ARG	GLU	engineered mutation	UNP B3UES2
C	510	ARG	LYS	engineered mutation	UNP B3UES2
C	512	ARG	ALA	engineered mutation	UNP B3UES2
C	513	ARG	VAL	engineered mutation	UNP B3UES2
G	501	CYS	ALA	engineered mutation	UNP B3UES2
G	509	ARG	GLU	engineered mutation	UNP B3UES2
G	510	ARG	LYS	engineered mutation	UNP B3UES2
G	512	ARG	ALA	engineered mutation	UNP B3UES2
G	513	ARG	VAL	engineered mutation	UNP B3UES2

- Molecule 2 is a protein called SOSIP.664 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	120	975	616	167	184	8	0	0
2	D	120	975	616	167	184	8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I	120	975	616	167	184	8	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP B3UEZ6
B	605	CYS	THR	engineered mutation	UNP B3UEZ6
D	559	PRO	ILE	engineered mutation	UNP B3UEZ6
D	605	CYS	THR	engineered mutation	UNP B3UEZ6
I	559	PRO	ILE	engineered mutation	UNP B3UEZ6
I	605	CYS	THR	engineered mutation	UNP B3UEZ6

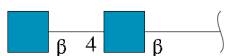
- Molecule 3 is a protein called rabbit antibody 13B Fragment antigen binding light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	112	842	527	139	172	4	0	0
3	E	112	842	527	139	172	4	0	0
3	J	112	842	527	139	172	4	0	0

- Molecule 4 is a protein called rabbit antibody 13B Fragment antigen binding heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	118	897	577	143	174	3	0	0
4	F	118	897	577	143	174	3	0	0
4	K	118	897	577	143	174	3	0	0

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



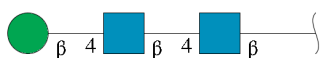
Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		
5	S	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		
5	V	2	Total	C	N	O	0	0
			28	16	2	10		
5	X	2	Total	C	N	O	0	0
			28	16	2	10		
5	Y	2	Total	C	N	O	0	0
			28	16	2	10		
5	Z	2	Total	C	N	O	0	0
			28	16	2	10		
5	a	2	Total	C	N	O	0	0
			28	16	2	10		
5	b	2	Total	C	N	O	0	0
			28	16	2	10		
5	c	2	Total	C	N	O	0	0
			28	16	2	10		
5	d	2	Total	C	N	O	0	0
			28	16	2	10		
5	f	2	Total	C	N	O	0	0
			28	16	2	10		
5	g	2	Total	C	N	O	0	0
			28	16	2	10		
5	h	2	Total	C	N	O	0	0
			28	16	2	10		
5	i	2	Total	C	N	O	0	0
			28	16	2	10		
5	k	2	Total	C	N	O	0	0
			28	16	2	10		
5	l	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	m	2	28	16	2	10	0	0
5	n	2	28	16	2	10	0	0
5	o	2	28	16	2	10	0	0
5	p	2	28	16	2	10	0	0
5	q	2	28	16	2	10	0	0
5	s	2	28	16	2	10	0	0
5	t	2	28	16	2	10	0	0
5	u	2	28	16	2	10	0	0
5	v	2	28	16	2	10	0	0
5	x	2	28	16	2	10	0	0
5	y	2	28	16	2	10	0	0

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



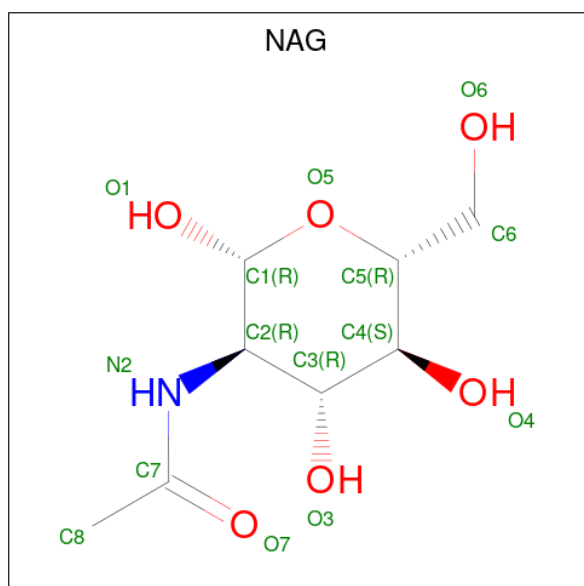
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	R	3	39	22	2	15	0	0
6	e	3	39	22	2	15	0	0
6	r	3	39	22	2	15	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
7	W	4	50	28	2	20	0	0
7	j	4	50	28	2	20	0	0
7	w	4	50	28	2	20	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
8	A	1	84	48	6	30	0
8	A	1	84	48	6	30	0
8	A	1	84	48	6	30	0
8	A	1	84	48	6	30	0
8	A	1	84	48	6	30	0
8	A	1	84	48	6	30	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
8	B	1	Total 56	C 32	N 4	O 20	0
8	B	1	Total 56	C 32	N 4	O 20	0
8	B	1	Total 56	C 32	N 4	O 20	0
8	B	1	Total 56	C 32	N 4	O 20	0
8	C	1	Total 84	C 48	N 6	O 30	0
8	C	1	Total 84	C 48	N 6	O 30	0
8	C	1	Total 84	C 48	N 6	O 30	0
8	C	1	Total 84	C 48	N 6	O 30	0
8	C	1	Total 84	C 48	N 6	O 30	0
8	C	1	Total 84	C 48	N 6	O 30	0
8	C	1	Total 84	C 48	N 6	O 30	0
8	D	1	Total 56	C 32	N 4	O 20	0
8	D	1	Total 56	C 32	N 4	O 20	0
8	D	1	Total 56	C 32	N 4	O 20	0
8	D	1	Total 56	C 32	N 4	O 20	0
8	G	1	Total 84	C 48	N 6	O 30	0
8	G	1	Total 84	C 48	N 6	O 30	0
8	G	1	Total 84	C 48	N 6	O 30	0
8	G	1	Total 84	C 48	N 6	O 30	0
8	G	1	Total 84	C 48	N 6	O 30	0
8	G	1	Total 84	C 48	N 6	O 30	0
8	I	1	Total 56	C 32	N 4	O 20	0

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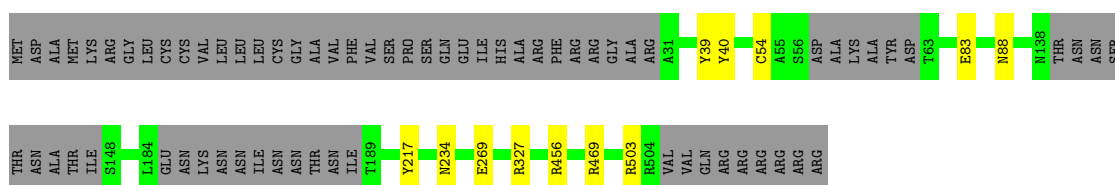
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
8	I	1	Total 56	32	4	20	0
8	I	1	Total 56	32	4	20	0
8	I	1	Total 56	32	4	20	0

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. 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. 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.

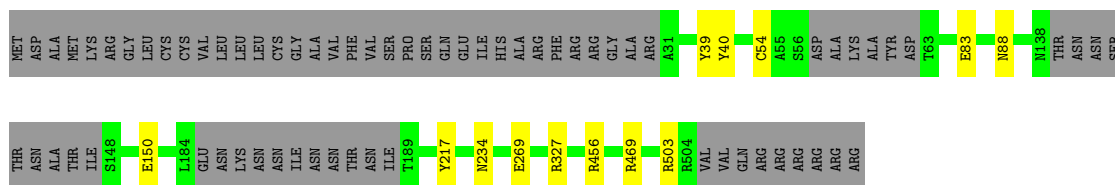
- Molecule 1: SOSIP.664 gp120,SOSIP.664 gp120

Chain A:  84% 13%




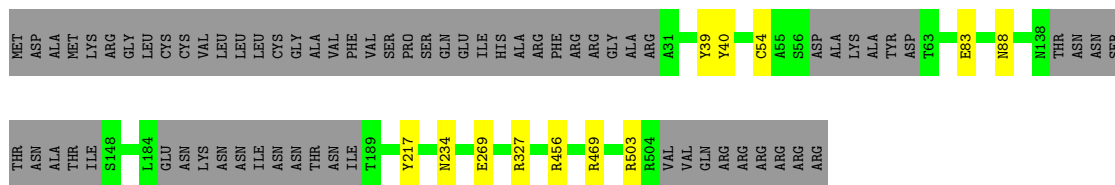
- Molecule 1: SOSIP.664 gp120,SOSIP.664 gp120

Chain C:  84% 13%



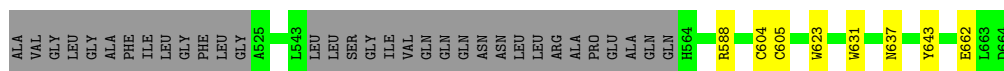
- Molecule 1: SOSIP.664 gp120,SOSIP.664 gp120

Chain G:  84% 13%

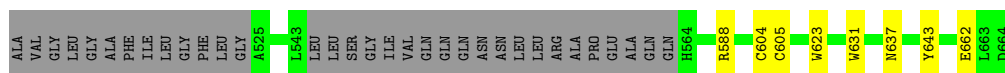


- Molecule 2: SOSIP.664 gp41

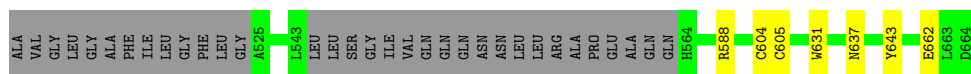
Chain B:  73% 5% 22%



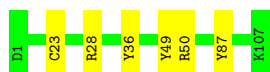
- Molecule 2: SOSIP.664 gp41



- Molecule 2: SOSIP.664 gp41



- Molecule 3: rabbit antibody 13B Fragment antigen binding light chain



- Molecule 3: rabbit antibody 13B Fragment antigen binding light chain



- Molecule 3: rabbit antibody 13B Fragment antigen binding light chain



- Molecule 4: rabbit antibody 13B Fragment antigen binding heavy chain



- Molecule 4: rabbit antibody 13B Fragment antigen binding heavy chain



- Molecule 4: rabbit antibody 13B Fragment antigen binding heavy chain

Chain K:  96% ...



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

Chain M:  100%



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

Chain N:  100%



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

Chain O:  100%



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

Chain P:  100%



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

Chain Q:  100%




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

Chain S:  100%

MAG1
MAG2

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

Chain T:  100%MAG1
MAG2


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

Chain U:  100%MAG1
MAG2


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

Chain V:  100%MAG1
MAG2

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

Chain X:  100%MAG1
MAG2

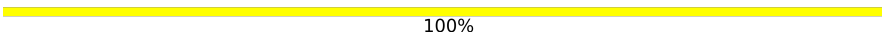
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  100%MAG1
MAG2

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

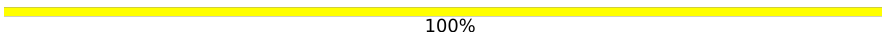
Chain Z:  100%MAG1
MAG2

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

Chain a:  100%

MAG1
MAG2

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

Chain b:  100%

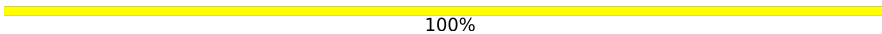
MAG1
MAG2

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

Chain c:  100%

MAG1
MAG2

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

Chain d:  100%

MAG1
MAG2

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

Chain f:  100%

MAG1
MAG2

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

Chain g:  100%

MAG1
MAG2

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

Chain h:  100%

MAG1
MAG2


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

Chain i:  100%MAG1
MAG2

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

Chain k:  100%MAG1
MAG2


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

Chain l:  100%MAG1
MAG2

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

Chain m:  100%MAG1
MAG2


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

Chain n:  100%MAG1
MAG2

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

Chain o:  100%MAG1
MAG2

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

Chain p:  100%


MAG1
MAG2

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

Chain q:  100%


MAG1
MAG2

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

Chain s:  100%


MAG1
MAG2

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

Chain t:  100%


MAG1
MAG2

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

Chain u:  100%

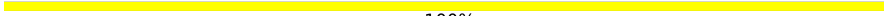
MAG1
MAG2

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

Chain v:  100%

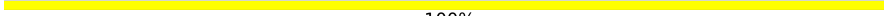
MAG1
MAG2

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

Chain x:  100%

MAG1
MAG2

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

Chain y:  100%

MAG1
MAG2

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

Chain R:  100%

MAG1
MAG2
BMA3

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

Chain e:  100%

MAG1
MAG2
BMA3

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

Chain r:  100%

MAG1
MAG2
BMA3

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

Chain W:  25% 75%

MAG1
MAG2
BMA3
MAIV4

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

Chain j:  25% 75%



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

Chain w:  25% 75%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	147520	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.03	4/3638 (0.1%)	0.89	7/4945 (0.1%)
1	C	1.03	5/3638 (0.1%)	0.89	8/4945 (0.2%)
1	G	1.03	4/3638 (0.1%)	0.89	7/4945 (0.1%)
2	B	1.12	6/993 (0.6%)	0.87	2/1347 (0.1%)
2	D	1.12	6/993 (0.6%)	0.87	2/1347 (0.1%)
2	I	1.11	5/993 (0.5%)	0.87	2/1347 (0.1%)
3	E	1.11	4/861 (0.5%)	1.03	1/1171 (0.1%)
3	J	1.11	4/861 (0.5%)	1.03	1/1171 (0.1%)
3	L	1.11	4/861 (0.5%)	1.03	2/1171 (0.2%)
4	F	1.10	4/922 (0.4%)	0.95	0/1257
4	H	1.10	4/922 (0.4%)	0.95	0/1257
4	K	1.10	4/922 (0.4%)	0.95	0/1257
All	All	1.06	54/19242 (0.3%)	0.92	32/26160 (0.1%)

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	100(G)	PHE	CB-CG	-7.24	1.39	1.51
4	H	100(G)	PHE	CB-CG	-7.24	1.39	1.51
4	F	100(G)	PHE	CB-CG	-7.18	1.39	1.51
2	B	605	CYS	CB-SG	-7.11	1.70	1.82
2	D	605	CYS	CB-SG	-7.10	1.70	1.82
2	I	605	CYS	CB-SG	-7.10	1.70	1.82
3	J	49	TYR	CB-CG	-6.87	1.41	1.51
3	L	49	TYR	CB-CG	-6.82	1.41	1.51
3	E	49	TYR	CB-CG	-6.81	1.41	1.51
4	H	100(C)	TYR	CE1-CZ	-6.59	1.29	1.38
4	K	100(C)	TYR	CE1-CZ	-6.58	1.30	1.38
1	G	54	CYS	CB-SG	-6.57	1.71	1.82
4	F	100(C)	TYR	CE1-CZ	-6.57	1.30	1.38
1	A	54	CYS	CB-SG	-6.52	1.71	1.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	54	CYS	CB-SG	-6.52	1.71	1.82
3	L	87	TYR	CB-CG	-6.08	1.42	1.51
3	E	87	TYR	CB-CG	-6.05	1.42	1.51
3	J	87	TYR	CB-CG	-6.02	1.42	1.51
3	J	23	CYS	CB-SG	-5.85	1.72	1.81
3	E	23	CYS	CB-SG	-5.84	1.72	1.81
4	F	47	PHE	CB-CG	-5.80	1.41	1.51
3	L	23	CYS	CB-SG	-5.80	1.72	1.81
4	H	47	PHE	CB-CG	-5.79	1.41	1.51
4	K	47	PHE	CB-CG	-5.78	1.41	1.51
4	K	100(C)	TYR	CD1-CE1	-5.62	1.30	1.39
4	F	100(C)	TYR	CD1-CE1	-5.60	1.30	1.39
4	H	100(C)	TYR	CD1-CE1	-5.56	1.31	1.39
2	I	604	CYS	CB-SG	-5.54	1.72	1.81
2	D	604	CYS	CB-SG	-5.53	1.72	1.81
2	B	604	CYS	CB-SG	-5.48	1.72	1.81
2	B	631	TRP	CD2-CE2	-5.42	1.34	1.41
2	B	662	GLU	CD-OE1	-5.41	1.19	1.25
2	D	631	TRP	CB-CG	-5.37	1.40	1.50
2	I	631	TRP	CB-CG	-5.37	1.40	1.50
2	D	662	GLU	CD-OE1	-5.37	1.19	1.25
2	I	631	TRP	CD2-CE2	-5.36	1.34	1.41
2	D	631	TRP	CD2-CE2	-5.34	1.34	1.41
2	B	631	TRP	CB-CG	-5.33	1.40	1.50
2	I	662	GLU	CD-OE1	-5.32	1.19	1.25
1	A	83	GLU	CD-OE2	-5.18	1.20	1.25
3	J	36	TYR	CB-CG	-5.16	1.44	1.51
3	L	36	TYR	CB-CG	-5.12	1.44	1.51
1	C	217	TYR	CB-CG	-5.12	1.44	1.51
1	C	83	GLU	CD-OE2	-5.11	1.20	1.25
1	A	269	GLU	CD-OE1	-5.10	1.20	1.25
1	G	83	GLU	CD-OE2	-5.10	1.20	1.25
1	C	269	GLU	CD-OE1	-5.10	1.20	1.25
1	G	269	GLU	CD-OE1	-5.10	1.20	1.25
3	E	36	TYR	CB-CG	-5.08	1.44	1.51
1	G	217	TYR	CB-CG	-5.05	1.44	1.51
1	A	217	TYR	CB-CG	-5.05	1.44	1.51
2	B	623	TRP	CB-CG	-5.02	1.41	1.50
2	D	623	TRP	CB-CG	-5.00	1.41	1.50
1	C	150	GLU	CD-OE1	-5.00	1.20	1.25

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	503	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	C	503	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	A	503	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	G	503	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	503	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	C	503	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	G	327	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	A	327	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	C	327	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	C	469	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	469	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	G	469	ARG	NE-CZ-NH2	-7.12	116.74	120.30
3	J	28	ARG	NE-CZ-NH2	-6.66	116.97	120.30
3	E	28	ARG	NE-CZ-NH2	-6.64	116.98	120.30
3	L	28	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	A	40	TYR	CB-CG-CD1	-6.61	117.03	121.00
1	C	40	TYR	CB-CG-CD1	-6.60	117.04	121.00
2	D	588	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	G	40	TYR	CB-CG-CD1	-6.55	117.07	121.00
2	B	588	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	I	588	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	G	456	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	A	456	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	C	456	ARG	NE-CZ-NH1	6.05	123.32	120.30
2	B	643	TYR	CB-CG-CD2	-5.23	117.86	121.00
2	I	643	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	A	39	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	C	39	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	G	39	TYR	CB-CG-CD2	-5.16	117.90	121.00
2	D	643	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	C	469	ARG	NE-CZ-NH1	5.08	122.84	120.30
3	L	50	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/524 (85%)	435 (98%)	11 (2%)	0	100	100
1	C	446/524 (85%)	435 (98%)	11 (2%)	0	100	100
1	G	446/524 (85%)	435 (98%)	11 (2%)	0	100	100
2	B	116/153 (76%)	113 (97%)	3 (3%)	0	100	100
2	D	116/153 (76%)	113 (97%)	3 (3%)	0	100	100
2	I	116/153 (76%)	113 (97%)	3 (3%)	0	100	100
3	E	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
3	J	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
3	L	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
4	F	116/119 (98%)	111 (96%)	4 (3%)	1 (1%)	17	53
4	H	116/119 (98%)	111 (96%)	4 (3%)	1 (1%)	17	53
4	K	116/119 (98%)	111 (96%)	4 (3%)	1 (1%)	17	53
All	All	2364/2724 (87%)	2301 (97%)	60 (2%)	3 (0%)	54	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	100(A)	ALA
4	F	100(A)	ALA
4	K	100(A)	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	401/461 (87%)	399 (100%)	2 (0%)	88	93
1	C	401/461 (87%)	399 (100%)	2 (0%)	88	93
1	G	401/461 (87%)	399 (100%)	2 (0%)	88	93
2	B	106/130 (82%)	105 (99%)	1 (1%)	78	88
2	D	106/130 (82%)	105 (99%)	1 (1%)	78	88
2	I	106/130 (82%)	105 (99%)	1 (1%)	78	88
3	E	93/93 (100%)	93 (100%)	0	100	100
3	J	93/93 (100%)	93 (100%)	0	100	100
3	L	93/93 (100%)	93 (100%)	0	100	100
4	F	92/93 (99%)	91 (99%)	1 (1%)	73	84
4	H	92/93 (99%)	91 (99%)	1 (1%)	73	84
4	K	92/93 (99%)	91 (99%)	1 (1%)	73	84
All	All	2076/2331 (89%)	2064 (99%)	12 (1%)	86	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	234	ASN
2	B	637	ASN
4	H	100(C)	TYR
1	C	88	ASN
1	C	234	ASN
2	D	637	ASN
4	F	100(C)	TYR
1	G	88	ASN
1	G	234	ASN
2	I	637	ASN
4	K	100(C)	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	575	GLN
2	D	575	GLN
4	F	35	GLN
2	I	575	GLN

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](#)

87 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
5	NAG	M	1	5,1	14,14,15	0.70	0	17,19,21	1.22	3 (17%)
5	NAG	M	2	5	14,14,15	0.77	1 (7%)	17,19,21	0.93	1 (5%)
5	NAG	N	1	5,1	14,14,15	0.72	1 (7%)	17,19,21	0.87	1 (5%)
5	NAG	N	2	5	14,14,15	0.68	0	17,19,21	1.02	1 (5%)
5	NAG	O	1	5,1	14,14,15	0.66	0	17,19,21	1.10	1 (5%)
5	NAG	O	2	5	14,14,15	0.72	1 (7%)	17,19,21	0.87	1 (5%)
5	NAG	P	1	5,1	14,14,15	0.69	0	17,19,21	0.92	1 (5%)
5	NAG	P	2	5	14,14,15	0.72	1 (7%)	17,19,21	0.77	1 (5%)
5	NAG	Q	1	5,1	14,14,15	0.78	1 (7%)	17,19,21	0.91	1 (5%)
5	NAG	Q	2	5	14,14,15	0.66	0	17,19,21	0.97	1 (5%)
6	NAG	R	1	6,1	14,14,15	0.87	1 (7%)	17,19,21	1.80	4 (23%)
6	NAG	R	2	6	14,14,15	0.70	0	17,19,21	1.16	1 (5%)
6	BMA	R	3	6	11,11,12	0.70	0	15,15,17	0.98	1 (6%)
5	NAG	S	1	5,1	14,14,15	0.66	0	17,19,21	0.81	1 (5%)
5	NAG	S	2	5	14,14,15	0.75	1 (7%)	17,19,21	0.98	1 (5%)
5	NAG	T	1	5,1	14,14,15	0.65	0	17,19,21	1.21	2 (11%)
5	NAG	T	2	5	14,14,15	0.77	1 (7%)	17,19,21	1.01	1 (5%)
5	NAG	U	1	5,1	14,14,15	0.79	0	17,19,21	1.44	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	U	2	5	14,14,15	0.69	1 (7%)	17,19,21	0.98	1 (5%)
5	NAG	V	1	5,1	14,14,15	0.79	1 (7%)	17,19,21	1.00	1 (5%)
5	NAG	V	2	5	14,14,15	0.66	0	17,19,21	0.97	1 (5%)
7	NAG	W	1	1,7	14,14,15	0.70	0	17,19,21	0.90	1 (5%)
7	NAG	W	2	7	14,14,15	0.72	0	17,19,21	0.79	0
7	BMA	W	3	7	11,11,12	0.61	0	15,15,17	0.96	1 (6%)
7	MAN	W	4	7	11,11,12	0.58	0	15,15,17	0.95	1 (6%)
5	NAG	X	1	5,1	14,14,15	0.79	0	17,19,21	1.52	4 (23%)
5	NAG	X	2	5	14,14,15	0.75	1 (7%)	17,19,21	0.96	1 (5%)
5	NAG	Y	1	5,1	14,14,15	0.67	0	17,19,21	0.99	1 (5%)
5	NAG	Y	2	5	14,14,15	0.77	1 (7%)	17,19,21	0.88	1 (5%)
5	NAG	Z	1	5,1	14,14,15	0.70	0	17,19,21	1.22	3 (17%)
5	NAG	Z	2	5	14,14,15	0.78	1 (7%)	17,19,21	0.93	1 (5%)
5	NAG	a	1	5,1	14,14,15	0.72	1 (7%)	17,19,21	0.87	1 (5%)
5	NAG	a	2	5	14,14,15	0.67	0	17,19,21	1.02	1 (5%)
5	NAG	b	1	5,1	14,14,15	0.68	0	17,19,21	1.09	1 (5%)
5	NAG	b	2	5	14,14,15	0.74	1 (7%)	17,19,21	0.87	1 (5%)
5	NAG	c	1	5,1	14,14,15	0.68	0	17,19,21	0.92	1 (5%)
5	NAG	c	2	5	14,14,15	0.73	1 (7%)	17,19,21	0.77	1 (5%)
5	NAG	d	1	5,1	14,14,15	0.77	1 (7%)	17,19,21	0.91	1 (5%)
5	NAG	d	2	5	14,14,15	0.65	0	17,19,21	0.97	1 (5%)
6	NAG	e	1	6,1	14,14,15	0.87	1 (7%)	17,19,21	1.81	4 (23%)
6	NAG	e	2	6	14,14,15	0.70	0	17,19,21	1.16	1 (5%)
6	BMA	e	3	6	11,11,12	0.69	0	15,15,17	0.98	1 (6%)
5	NAG	f	1	5,1	14,14,15	0.66	0	17,19,21	0.82	1 (5%)
5	NAG	f	2	5	14,14,15	0.75	1 (7%)	17,19,21	0.99	1 (5%)
5	NAG	g	1	5,1	14,14,15	0.64	0	17,19,21	1.22	2 (11%)
5	NAG	g	2	5	14,14,15	0.78	1 (7%)	17,19,21	1.01	1 (5%)
5	NAG	h	1	5,1	14,14,15	0.78	0	17,19,21	1.45	3 (17%)
5	NAG	h	2	5	14,14,15	0.68	0	17,19,21	0.98	1 (5%)
5	NAG	i	1	5,1	14,14,15	0.78	1 (7%)	17,19,21	1.00	1 (5%)
5	NAG	i	2	5	14,14,15	0.68	0	17,19,21	0.98	1 (5%)
7	NAG	j	1	1,7	14,14,15	0.71	0	17,19,21	0.91	1 (5%)
7	NAG	j	2	7	14,14,15	0.71	0	17,19,21	0.80	0
7	BMA	j	3	7	11,11,12	0.59	0	15,15,17	0.96	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	j	4	7	11,11,12	0.59	0	15,15,17	0.95	1 (6%)
5	NAG	k	1	5,1	14,14,15	0.78	0	17,19,21	1.52	4 (23%)
5	NAG	k	2	5	14,14,15	0.75	1 (7%)	17,19,21	0.96	1 (5%)
5	NAG	l	1	5,1	14,14,15	0.66	0	17,19,21	0.99	1 (5%)
5	NAG	l	2	5	14,14,15	0.79	1 (7%)	17,19,21	0.89	1 (5%)
5	NAG	m	1	5,1	14,14,15	0.70	0	17,19,21	1.22	3 (17%)
5	NAG	m	2	5	14,14,15	0.78	1 (7%)	17,19,21	0.93	1 (5%)
5	NAG	n	1	5,1	14,14,15	0.72	1 (7%)	17,19,21	0.86	1 (5%)
5	NAG	n	2	5	14,14,15	0.68	0	17,19,21	1.02	1 (5%)
5	NAG	o	1	5,1	14,14,15	0.66	0	17,19,21	1.10	1 (5%)
5	NAG	o	2	5	14,14,15	0.72	1 (7%)	17,19,21	0.87	1 (5%)
5	NAG	p	1	5,1	14,14,15	0.68	0	17,19,21	0.92	1 (5%)
5	NAG	p	2	5	14,14,15	0.72	1 (7%)	17,19,21	0.77	1 (5%)
5	NAG	q	1	5,1	14,14,15	0.76	1 (7%)	17,19,21	0.91	1 (5%)
5	NAG	q	2	5	14,14,15	0.65	0	17,19,21	0.97	1 (5%)
6	NAG	r	1	6,1	14,14,15	0.85	1 (7%)	17,19,21	1.81	4 (23%)
6	NAG	r	2	6	14,14,15	0.69	0	17,19,21	1.16	1 (5%)
6	BMA	r	3	6	11,11,12	0.72	0	15,15,17	0.98	1 (6%)
5	NAG	s	1	5,1	14,14,15	0.67	0	17,19,21	0.81	1 (5%)
5	NAG	s	2	5	14,14,15	0.75	1 (7%)	17,19,21	0.99	1 (5%)
5	NAG	t	1	5,1	14,14,15	0.64	0	17,19,21	1.21	2 (11%)
5	NAG	t	2	5	14,14,15	0.79	1 (7%)	17,19,21	1.01	1 (5%)
5	NAG	u	1	5,1	14,14,15	0.79	0	17,19,21	1.44	3 (17%)
5	NAG	u	2	5	14,14,15	0.67	0	17,19,21	0.98	1 (5%)
5	NAG	v	1	5,1	14,14,15	0.78	1 (7%)	17,19,21	1.00	1 (5%)
5	NAG	v	2	5	14,14,15	0.68	0	17,19,21	0.98	1 (5%)
7	NAG	w	1	1,7	14,14,15	0.70	0	17,19,21	0.90	1 (5%)
7	NAG	w	2	7	14,14,15	0.70	0	17,19,21	0.80	0
7	BMA	w	3	7	11,11,12	0.60	0	15,15,17	0.96	1 (6%)
7	MAN	w	4	7	11,11,12	0.60	0	15,15,17	0.95	1 (6%)
5	NAG	x	1	5,1	14,14,15	0.78	0	17,19,21	1.52	4 (23%)
5	NAG	x	2	5	14,14,15	0.74	1 (7%)	17,19,21	0.95	1 (5%)
5	NAG	y	1	5,1	14,14,15	0.65	0	17,19,21	0.99	1 (5%)
5	NAG	y	2	5	14,14,15	0.78	1 (7%)	17,19,21	0.88	1 (5%)

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
5	NAG	M	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	1/6/23/26	0/1/1/1
5	NAG	N	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	2/6/23/26	0/1/1/1
5	NAG	O	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	1/6/23/26	0/1/1/1
5	NAG	P	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	1/6/23/26	0/1/1/1
5	NAG	Q	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1
6	NAG	R	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	R	2	6	-	0/6/23/26	0/1/1/1
6	BMA	R	3	6	-	1/2/19/22	0/1/1/1
5	NAG	S	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	S	2	5	-	2/6/23/26	0/1/1/1
5	NAG	T	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	NAG	U	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	U	2	5	-	2/6/23/26	0/1/1/1
5	NAG	V	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	V	2	5	-	1/6/23/26	0/1/1/1
7	NAG	W	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	W	2	7	-	1/6/23/26	0/1/1/1
7	BMA	W	3	7	-	1/2/19/22	0/1/1/1
7	MAN	W	4	7	-	1/2/19/22	0/1/1/1
5	NAG	X	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	2/6/23/26	0/1/1/1
5	NAG	Y	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	1/6/23/26	0/1/1/1
5	NAG	Z	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	1/6/23/26	0/1/1/1
5	NAG	a	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	a	2	5	-	2/6/23/26	0/1/1/1
5	NAG	b	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	1/6/23/26	0/1/1/1
5	NAG	c	1	5,1	-	0/6/23/26	0/1/1/1

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

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

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	1	NAG	C1-C2	2.82	1.56	1.52
6	e	1	NAG	C1-C2	2.81	1.56	1.52
6	r	1	NAG	C1-C2	2.76	1.56	1.52
5	Z	2	NAG	C1-C2	2.50	1.56	1.52
5	V	1	NAG	C1-C2	2.47	1.56	1.52
5	t	2	NAG	C1-C2	2.46	1.56	1.52
5	m	2	NAG	C1-C2	2.46	1.56	1.52
5	g	2	NAG	C1-C2	2.45	1.56	1.52
5	v	1	NAG	C1-C2	2.44	1.56	1.52
5	M	2	NAG	C1-C2	2.43	1.56	1.52
5	l	2	NAG	C1-C2	2.42	1.56	1.52
5	T	2	NAG	C1-C2	2.42	1.55	1.52
5	i	1	NAG	C1-C2	2.42	1.55	1.52
5	k	2	NAG	C1-C2	2.39	1.55	1.52
5	X	2	NAG	C1-C2	2.38	1.55	1.52
5	x	2	NAG	C1-C2	2.38	1.55	1.52
5	y	2	NAG	C1-C2	2.37	1.55	1.52
5	b	2	NAG	C1-C2	2.37	1.55	1.52
5	Y	2	NAG	C1-C2	2.32	1.55	1.52
5	S	2	NAG	C1-C2	2.30	1.55	1.52
5	O	2	NAG	C1-C2	2.29	1.55	1.52
5	s	2	NAG	C1-C2	2.29	1.55	1.52
5	f	2	NAG	C1-C2	2.28	1.55	1.52
5	o	2	NAG	C1-C2	2.28	1.55	1.52
5	c	2	NAG	C1-C2	2.21	1.55	1.52
5	P	2	NAG	C1-C2	2.19	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	p	2	NAG	C1-C2	2.18	1.55	1.52
5	n	1	NAG	C1-C2	2.17	1.55	1.52
5	N	1	NAG	C1-C2	2.17	1.55	1.52
5	a	1	NAG	C1-C2	2.14	1.55	1.52
5	Q	1	NAG	C1-C2	2.11	1.55	1.52
5	q	1	NAG	C1-C2	2.06	1.55	1.52
5	d	1	NAG	C1-C2	2.06	1.55	1.52
5	U	2	NAG	C1-C2	2.06	1.55	1.52

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	e	1	NAG	C2-N2-C7	4.40	129.17	122.90
6	r	1	NAG	C2-N2-C7	4.39	129.15	122.90
6	R	1	NAG	C2-N2-C7	4.37	129.12	122.90
6	R	1	NAG	C1-C2-N2	4.03	117.37	110.49
6	e	1	NAG	C1-C2-N2	4.02	117.36	110.49
6	r	1	NAG	C1-C2-N2	4.02	117.35	110.49
5	Y	1	NAG	C3-C4-C5	-3.51	103.98	110.24
5	l	1	NAG	C3-C4-C5	-3.51	103.98	110.24
5	h	1	NAG	C4-C3-C2	-3.50	105.89	111.02
5	y	1	NAG	C3-C4-C5	-3.49	104.01	110.24
5	k	1	NAG	O5-C5-C6	-3.48	101.75	107.20
5	U	1	NAG	C4-C3-C2	-3.48	105.92	111.02
5	X	1	NAG	O5-C5-C6	-3.47	101.76	107.20
5	u	1	NAG	C4-C3-C2	-3.46	105.95	111.02
5	x	1	NAG	O5-C5-C6	-3.45	101.79	107.20
6	R	2	NAG	C3-C4-C5	-3.24	104.45	110.24
6	e	2	NAG	C3-C4-C5	-3.24	104.45	110.24
6	r	2	NAG	C3-C4-C5	-3.23	104.47	110.24
5	g	1	NAG	C3-C4-C5	-3.10	104.71	110.24
5	t	1	NAG	C3-C4-C5	-3.09	104.72	110.24
5	T	1	NAG	C3-C4-C5	-3.09	104.72	110.24
5	V	1	NAG	C4-C3-C2	-2.96	106.68	111.02
5	v	1	NAG	C4-C3-C2	-2.95	106.69	111.02
5	i	1	NAG	C4-C3-C2	-2.94	106.71	111.02
5	g	2	NAG	C4-C3-C2	-2.92	106.73	111.02
5	a	2	NAG	C4-C3-C2	-2.91	106.75	111.02
5	n	2	NAG	C4-C3-C2	-2.91	106.75	111.02
5	t	2	NAG	C4-C3-C2	-2.91	106.76	111.02
5	T	2	NAG	C4-C3-C2	-2.90	106.76	111.02
5	N	2	NAG	C4-C3-C2	-2.90	106.76	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	j	3	BMA	C2-C3-C4	-2.89	105.89	110.89
7	w	3	BMA	C2-C3-C4	-2.89	105.89	110.89
7	W	3	BMA	C2-C3-C4	-2.86	105.94	110.89
7	w	1	NAG	C3-C4-C5	-2.82	105.21	110.24
7	j	1	NAG	C3-C4-C5	-2.81	105.22	110.24
7	W	1	NAG	C3-C4-C5	-2.80	105.24	110.24
5	P	1	NAG	C3-C4-C5	-2.73	105.37	110.24
5	p	1	NAG	C3-C4-C5	-2.72	105.39	110.24
5	c	1	NAG	C3-C4-C5	-2.71	105.40	110.24
7	w	4	MAN	C2-C3-C4	-2.69	106.24	110.89
7	W	4	MAN	C2-C3-C4	-2.68	106.26	110.89
5	f	2	NAG	C4-C3-C2	-2.68	107.09	111.02
5	N	1	NAG	C3-C4-C5	-2.68	105.46	110.24
5	V	2	NAG	C4-C3-C2	-2.68	107.10	111.02
5	a	1	NAG	C3-C4-C5	-2.67	105.47	110.24
5	i	2	NAG	C4-C3-C2	-2.67	107.10	111.02
5	v	2	NAG	C4-C3-C2	-2.67	107.11	111.02
7	j	4	MAN	C2-C3-C4	-2.66	106.28	110.89
5	S	2	NAG	C4-C3-C2	-2.66	107.12	111.02
5	n	1	NAG	C3-C4-C5	-2.66	105.50	110.24
5	u	2	NAG	C4-C3-C2	-2.64	107.15	111.02
5	U	2	NAG	C4-C3-C2	-2.64	107.15	111.02
5	s	2	NAG	C4-C3-C2	-2.64	107.15	111.02
5	h	2	NAG	C4-C3-C2	-2.63	107.17	111.02
5	Q	2	NAG	C4-C3-C2	-2.62	107.18	111.02
5	d	2	NAG	C4-C3-C2	-2.61	107.19	111.02
5	q	2	NAG	C4-C3-C2	-2.61	107.19	111.02
5	Z	1	NAG	O5-C5-C6	-2.60	103.13	107.20
5	O	1	NAG	C4-C3-C2	-2.60	107.21	111.02
5	m	1	NAG	O5-C5-C6	-2.60	103.13	107.20
5	o	1	NAG	C4-C3-C2	-2.60	107.21	111.02
5	M	1	NAG	O5-C5-C6	-2.59	103.14	107.20
5	b	1	NAG	C4-C3-C2	-2.59	107.22	111.02
5	d	1	NAG	C3-C4-C5	-2.57	105.65	110.24
5	k	2	NAG	C4-C3-C2	-2.56	107.26	111.02
5	Q	1	NAG	C3-C4-C5	-2.56	105.67	110.24
5	x	2	NAG	C4-C3-C2	-2.56	107.27	111.02
5	m	1	NAG	C4-C3-C2	-2.55	107.27	111.02
5	q	1	NAG	C3-C4-C5	-2.55	105.70	110.24
5	X	2	NAG	C4-C3-C2	-2.54	107.29	111.02
5	Z	1	NAG	C4-C3-C2	-2.54	107.29	111.02
5	f	1	NAG	C3-C4-C5	-2.54	105.72	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	s	1	NAG	C3-C4-C5	-2.54	105.72	110.24
5	S	1	NAG	C3-C4-C5	-2.54	105.72	110.24
5	M	1	NAG	C4-C3-C2	-2.53	107.31	111.02
5	X	1	NAG	C4-C3-C2	-2.51	107.34	111.02
5	x	1	NAG	C4-C3-C2	-2.50	107.35	111.02
5	k	1	NAG	C4-C3-C2	-2.50	107.35	111.02
5	M	2	NAG	C4-C3-C2	-2.43	107.45	111.02
5	Z	2	NAG	C4-C3-C2	-2.42	107.47	111.02
5	m	2	NAG	C4-C3-C2	-2.41	107.48	111.02
6	R	1	NAG	C3-C4-C5	-2.38	105.99	110.24
6	r	1	NAG	C3-C4-C5	-2.36	106.02	110.24
6	e	1	NAG	C3-C4-C5	-2.35	106.04	110.24
5	c	2	NAG	C4-C3-C2	-2.33	107.61	111.02
5	P	2	NAG	C4-C3-C2	-2.32	107.62	111.02
5	p	2	NAG	C4-C3-C2	-2.31	107.63	111.02
5	u	1	NAG	C2-N2-C7	-2.31	119.62	122.90
5	U	1	NAG	C2-N2-C7	-2.31	119.62	122.90
5	h	1	NAG	C2-N2-C7	-2.29	119.65	122.90
6	R	1	NAG	O5-C1-C2	-2.28	107.69	111.29
6	e	1	NAG	O5-C1-C2	-2.28	107.69	111.29
6	r	1	NAG	O5-C1-C2	-2.27	107.71	111.29
5	k	1	NAG	C3-C4-C5	-2.26	106.20	110.24
5	O	2	NAG	C4-C3-C2	-2.26	107.70	111.02
5	o	2	NAG	C4-C3-C2	-2.26	107.71	111.02
5	t	1	NAG	O4-C4-C3	-2.25	105.14	110.35
5	X	1	NAG	C3-C4-C5	-2.25	106.22	110.24
5	x	1	NAG	C3-C4-C5	-2.25	106.23	110.24
5	b	2	NAG	C4-C3-C2	-2.24	107.73	111.02
5	y	2	NAG	C4-C3-C2	-2.24	107.74	111.02
5	T	1	NAG	O4-C4-C3	-2.24	105.18	110.35
5	g	1	NAG	O4-C4-C3	-2.24	105.18	110.35
5	Y	2	NAG	C4-C3-C2	-2.23	107.75	111.02
5	Z	1	NAG	C3-C4-C5	-2.23	106.26	110.24
5	m	1	NAG	C3-C4-C5	-2.23	106.27	110.24
5	l	2	NAG	C4-C3-C2	-2.22	107.76	111.02
5	M	1	NAG	C3-C4-C5	-2.21	106.30	110.24
6	r	3	BMA	C2-C3-C4	-2.18	107.13	110.89
5	x	1	NAG	C1-O5-C5	2.15	115.11	112.19
6	e	3	BMA	C2-C3-C4	-2.14	107.19	110.89
6	R	3	BMA	C2-C3-C4	-2.14	107.19	110.89
5	k	1	NAG	C1-O5-C5	2.13	115.08	112.19
5	X	1	NAG	C1-O5-C5	2.13	115.07	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	1	NAG	C3-C4-C5	-2.11	106.47	110.24
5	u	1	NAG	C3-C4-C5	-2.10	106.50	110.24
5	h	1	NAG	C3-C4-C5	-2.09	106.51	110.24

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	1	NAG	C1-C2-N2-C7
6	e	1	NAG	C1-C2-N2-C7
6	r	1	NAG	C1-C2-N2-C7
5	U	2	NAG	C4-C5-C6-O6
5	h	2	NAG	C4-C5-C6-O6
5	u	2	NAG	C4-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	Z	1	NAG	O5-C5-C6-O6
5	m	1	NAG	O5-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6
5	d	1	NAG	O5-C5-C6-O6
5	q	1	NAG	O5-C5-C6-O6
5	x	2	NAG	O5-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
5	k	2	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
5	h	2	NAG	O5-C5-C6-O6
5	u	2	NAG	O5-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	Z	1	NAG	C4-C5-C6-O6
5	m	1	NAG	C4-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
5	n	2	NAG	O5-C5-C6-O6
5	Q	2	NAG	O5-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
5	d	2	NAG	O5-C5-C6-O6
5	f	2	NAG	O5-C5-C6-O6
5	g	2	NAG	O5-C5-C6-O6
5	i	2	NAG	O5-C5-C6-O6
5	q	2	NAG	O5-C5-C6-O6
5	s	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	t	2	NAG	O5-C5-C6-O6
5	v	2	NAG	O5-C5-C6-O6
5	Q	1	NAG	C4-C5-C6-O6
5	d	1	NAG	C4-C5-C6-O6
5	q	1	NAG	C4-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6
5	o	2	NAG	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	m	2	NAG	O5-C5-C6-O6
7	W	3	BMA	O5-C5-C6-O6
7	j	3	BMA	O5-C5-C6-O6
7	w	3	BMA	O5-C5-C6-O6
6	R	3	BMA	O5-C5-C6-O6
6	e	3	BMA	O5-C5-C6-O6
6	r	3	BMA	O5-C5-C6-O6
7	W	4	MAN	O5-C5-C6-O6
7	j	4	MAN	O5-C5-C6-O6
7	w	4	MAN	O5-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6
5	l	2	NAG	O5-C5-C6-O6
5	y	2	NAG	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
5	p	2	NAG	O5-C5-C6-O6
5	X	2	NAG	C4-C5-C6-O6
5	k	2	NAG	C4-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6
7	j	2	NAG	O5-C5-C6-O6
7	w	2	NAG	O5-C5-C6-O6
5	x	2	NAG	C4-C5-C6-O6
5	X	1	NAG	O5-C5-C6-O6
5	i	1	NAG	O5-C5-C6-O6
5	v	1	NAG	O5-C5-C6-O6
5	x	1	NAG	O5-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
5	k	1	NAG	O5-C5-C6-O6
5	X	1	NAG	C4-C5-C6-O6
5	k	1	NAG	C4-C5-C6-O6
5	x	1	NAG	C4-C5-C6-O6
7	w	1	NAG	O5-C5-C6-O6

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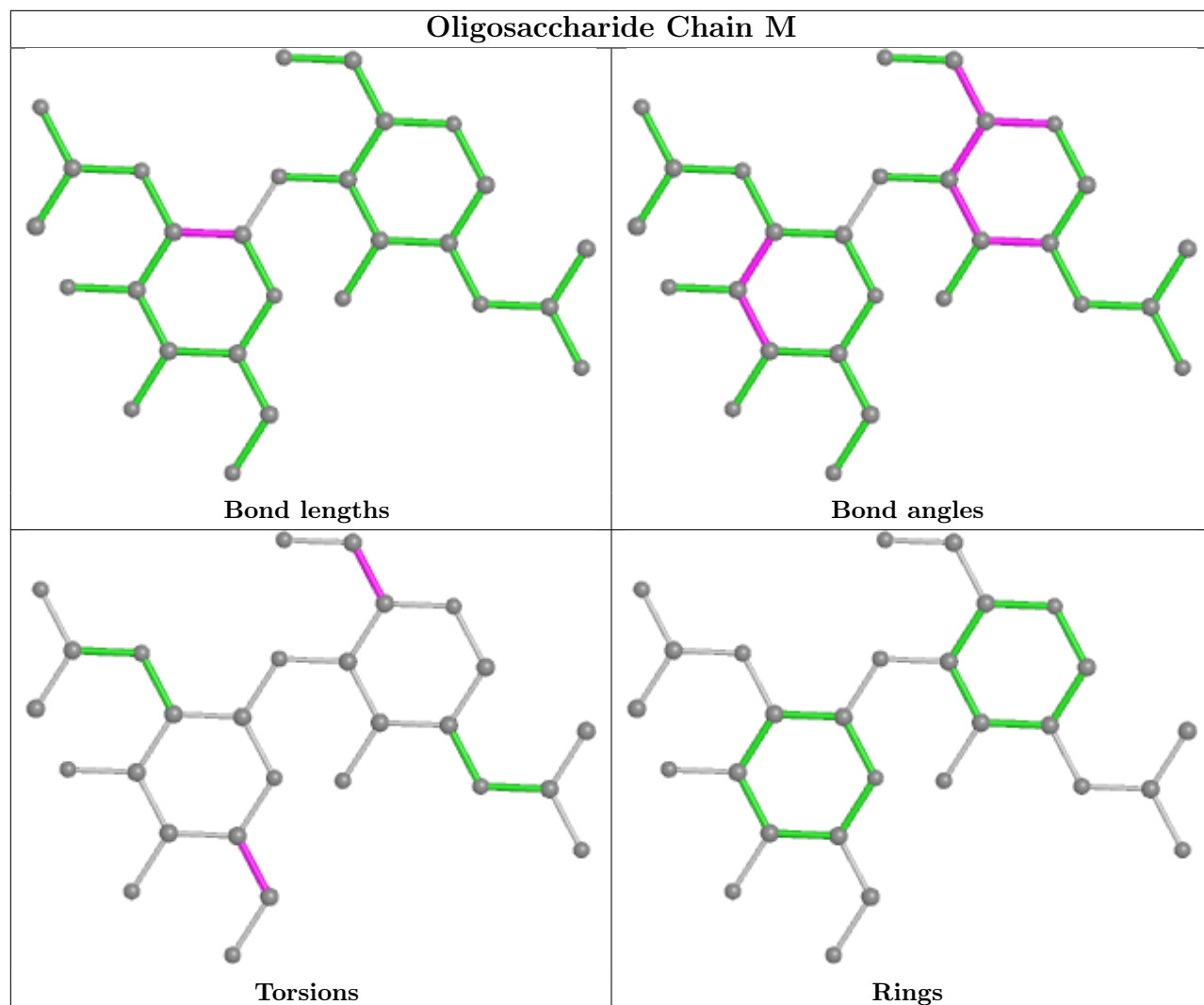
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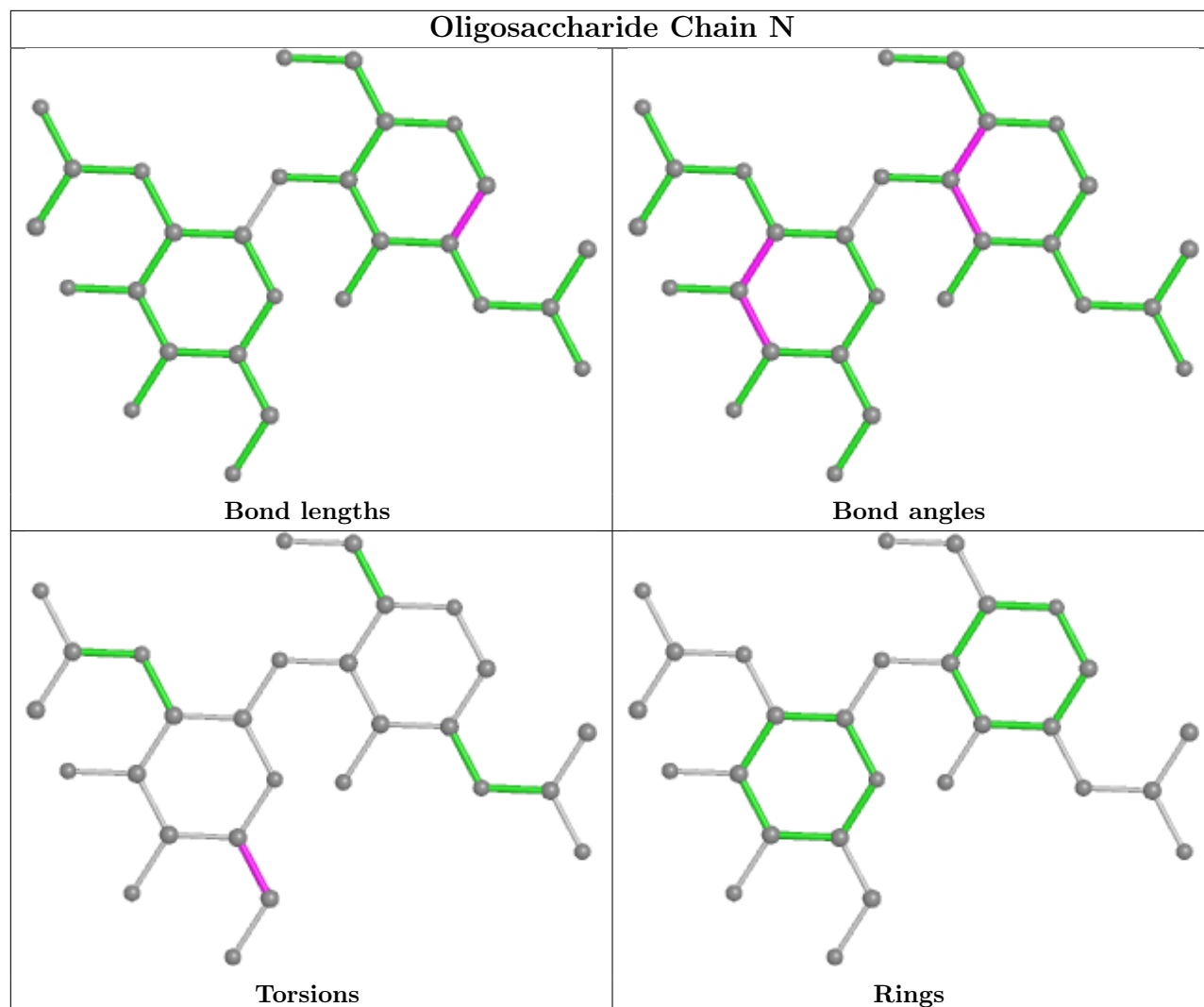
Mol	Chain	Res	Type	Atoms
7	W	1	NAG	O5-C5-C6-O6
7	j	1	NAG	O5-C5-C6-O6
5	g	2	NAG	C4-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
5	t	2	NAG	C4-C5-C6-O6
5	f	2	NAG	C4-C5-C6-O6
5	s	2	NAG	C4-C5-C6-O6
5	S	2	NAG	C4-C5-C6-O6
5	n	2	NAG	C4-C5-C6-O6
5	N	2	NAG	C4-C5-C6-O6
5	a	2	NAG	C4-C5-C6-O6
5	d	2	NAG	C4-C5-C6-O6
5	q	2	NAG	C4-C5-C6-O6
5	Q	2	NAG	C4-C5-C6-O6

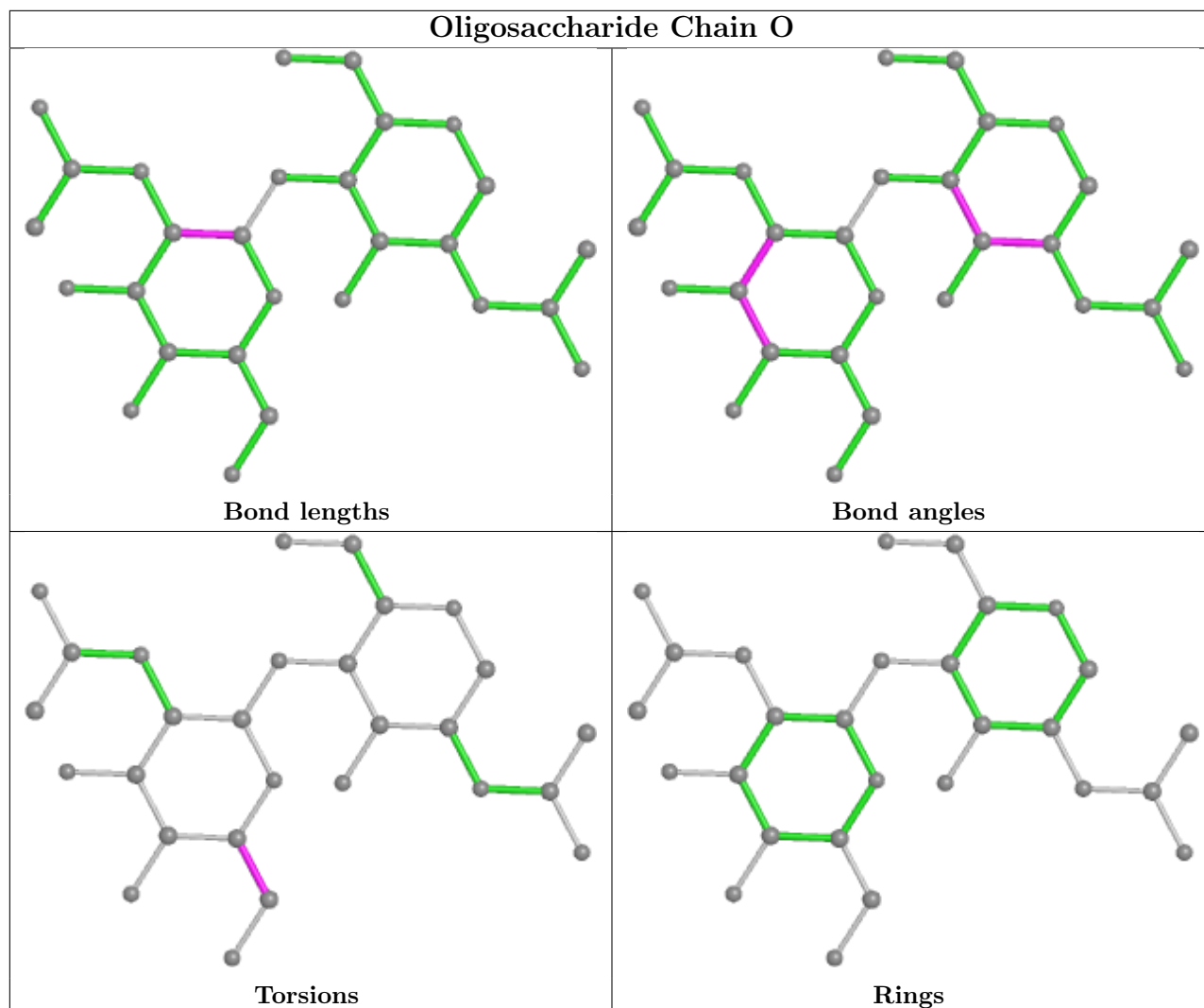
There are no ring outliers.

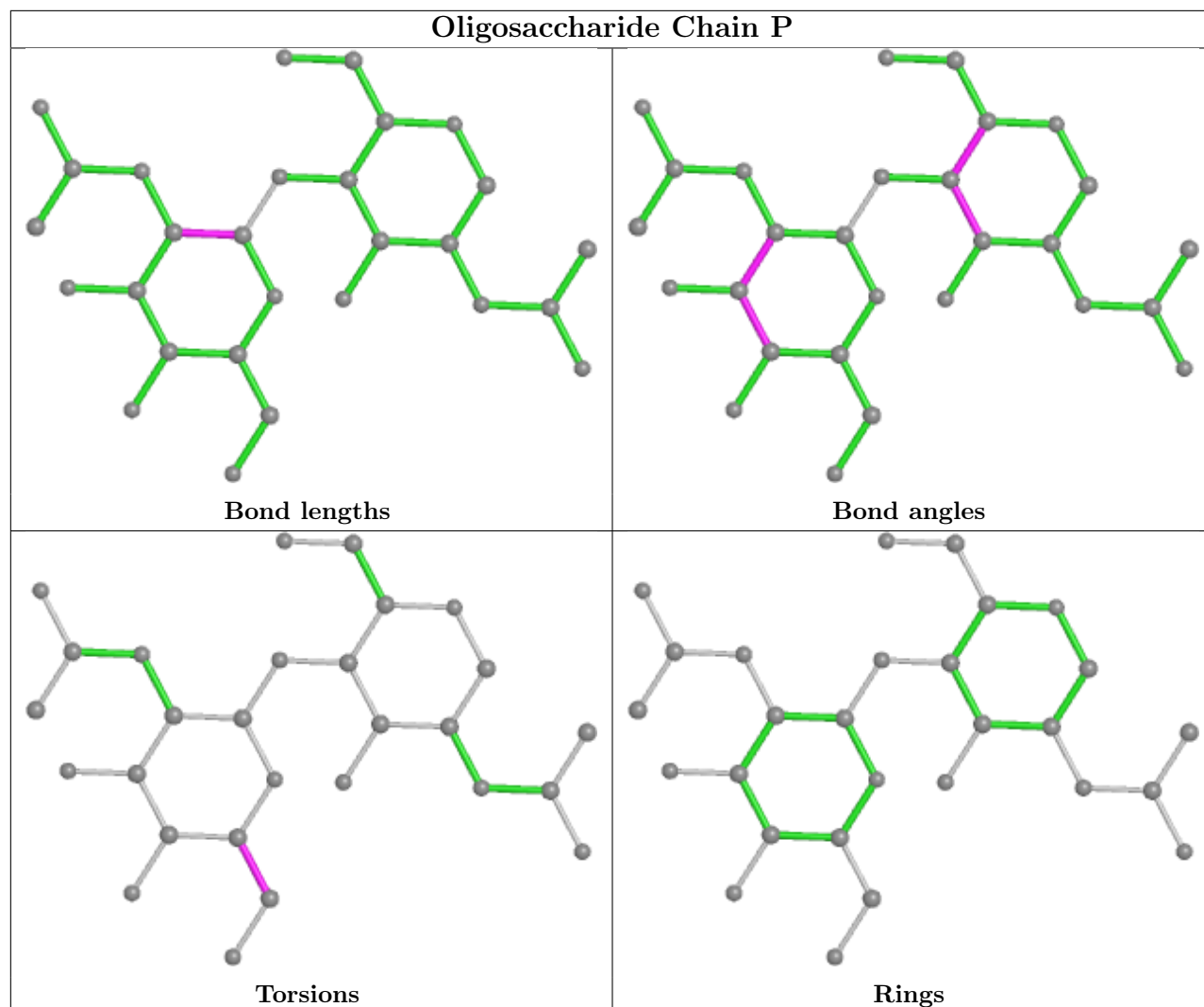
No monomer is involved in short contacts.

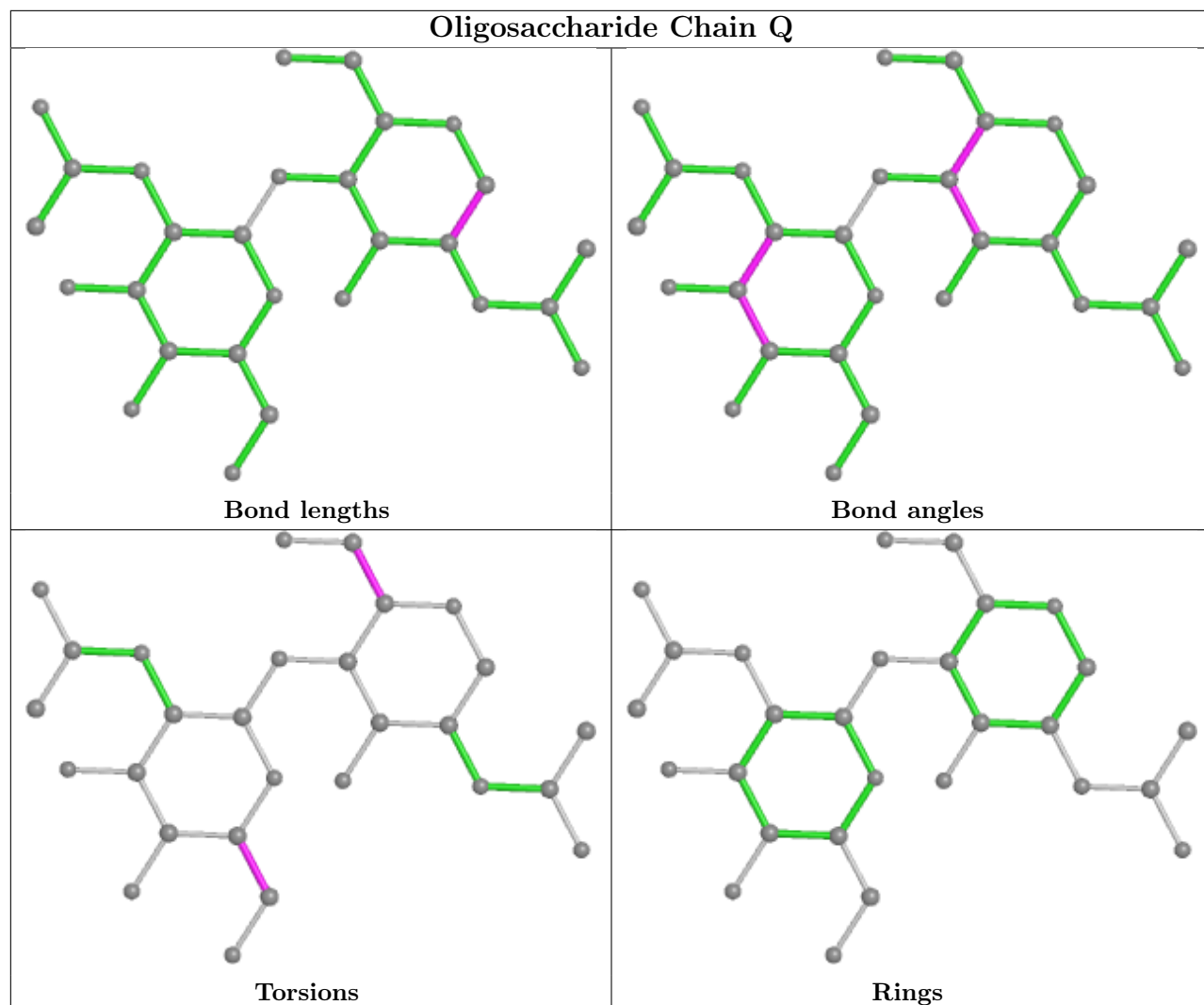
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

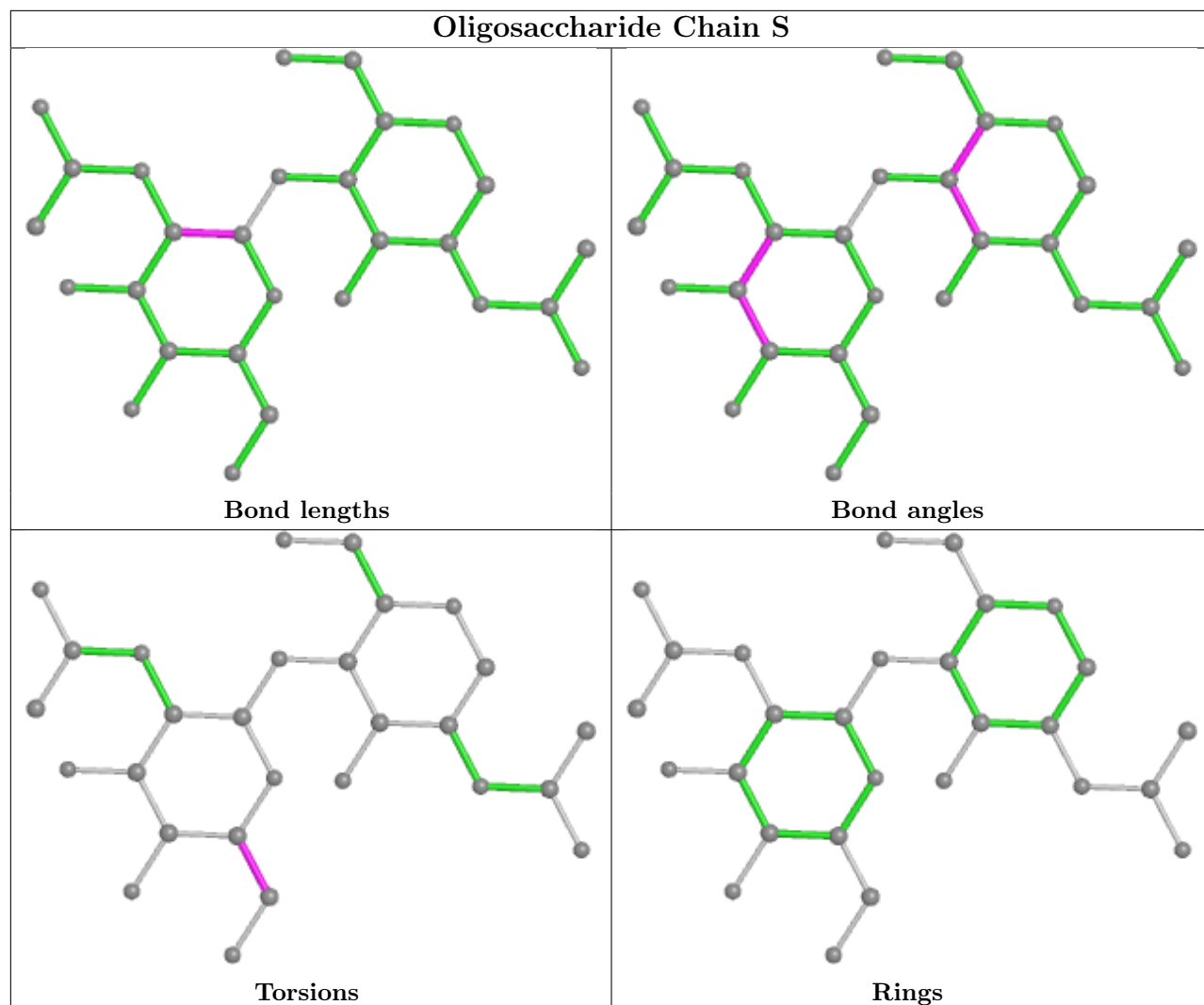


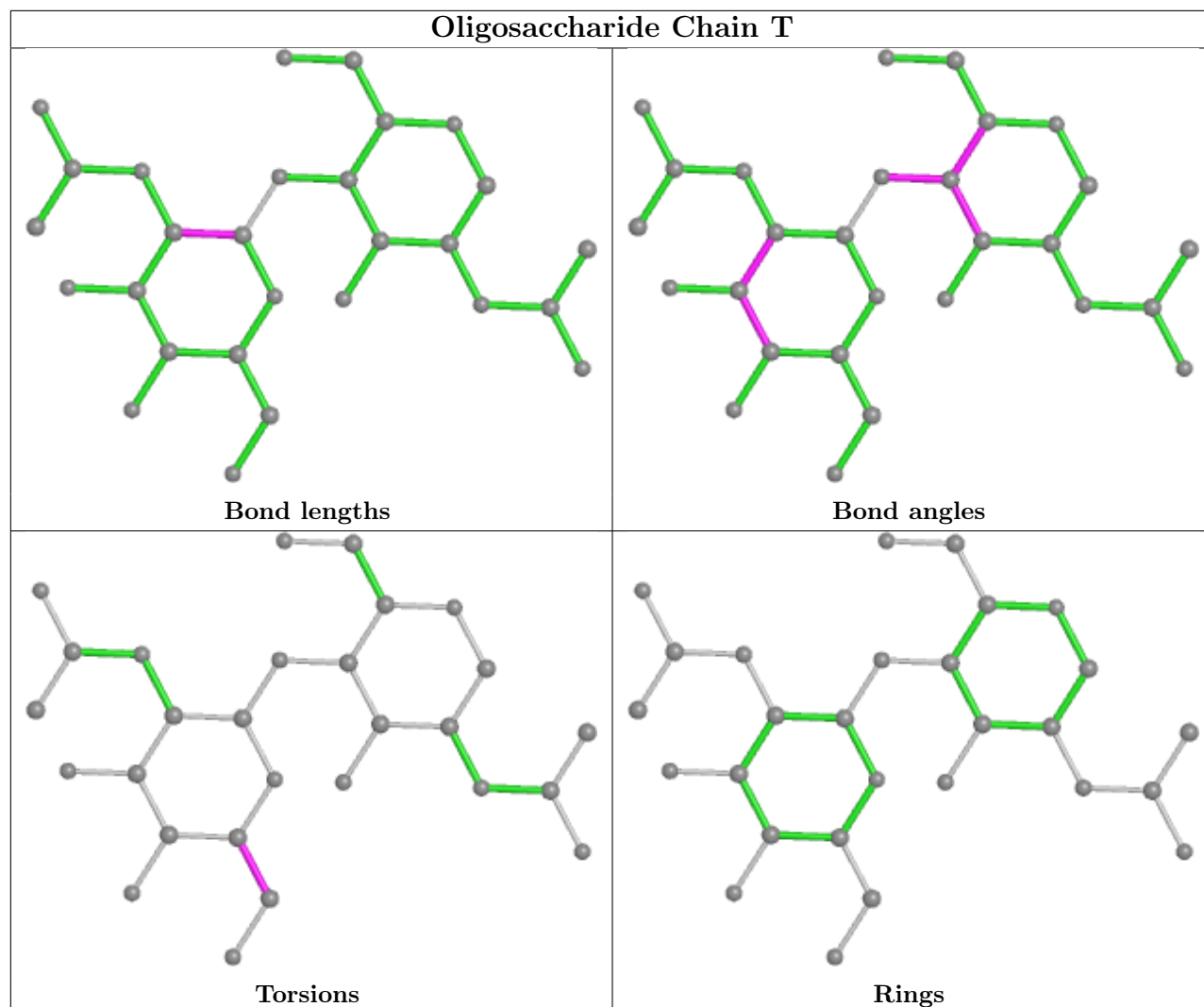


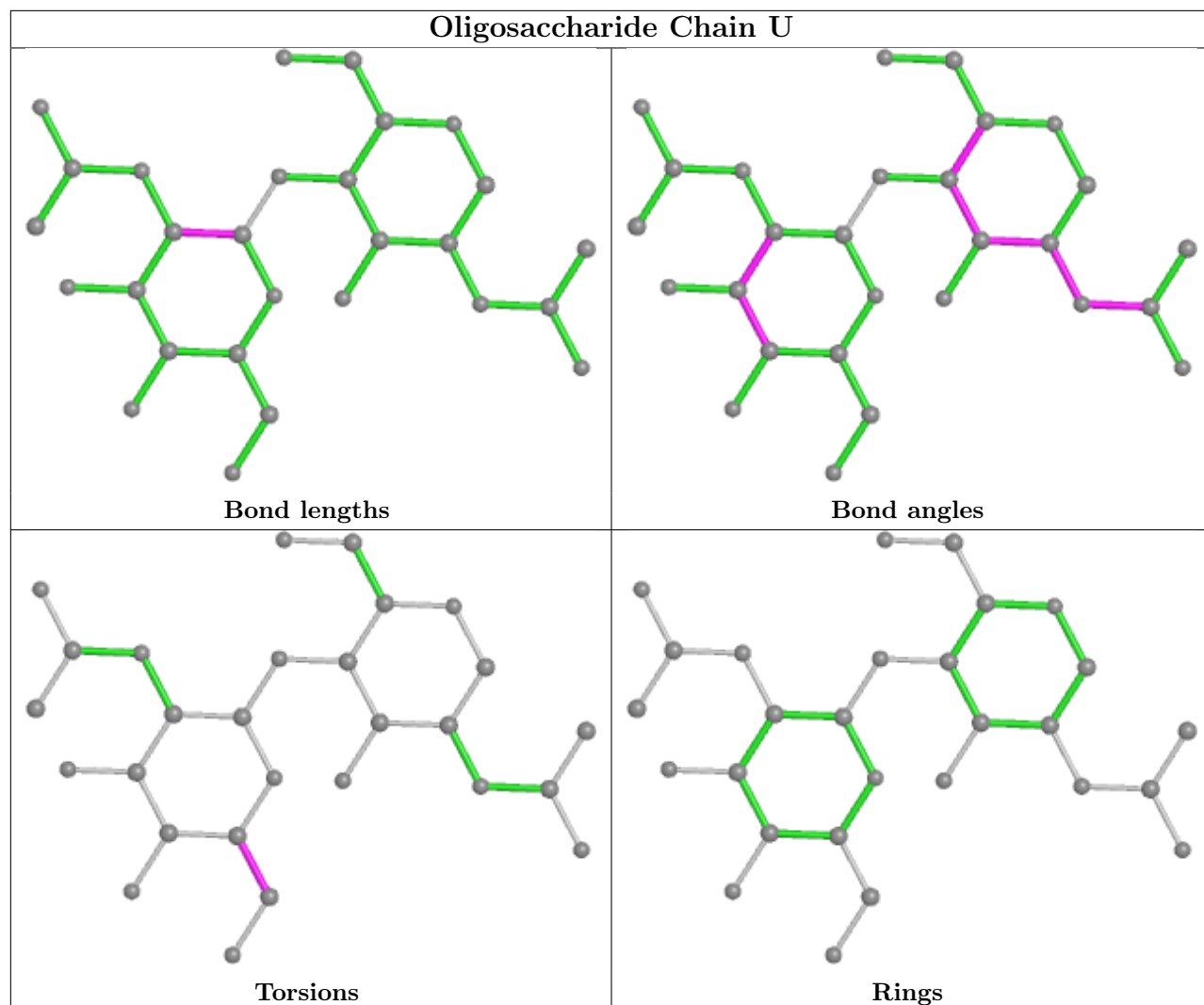


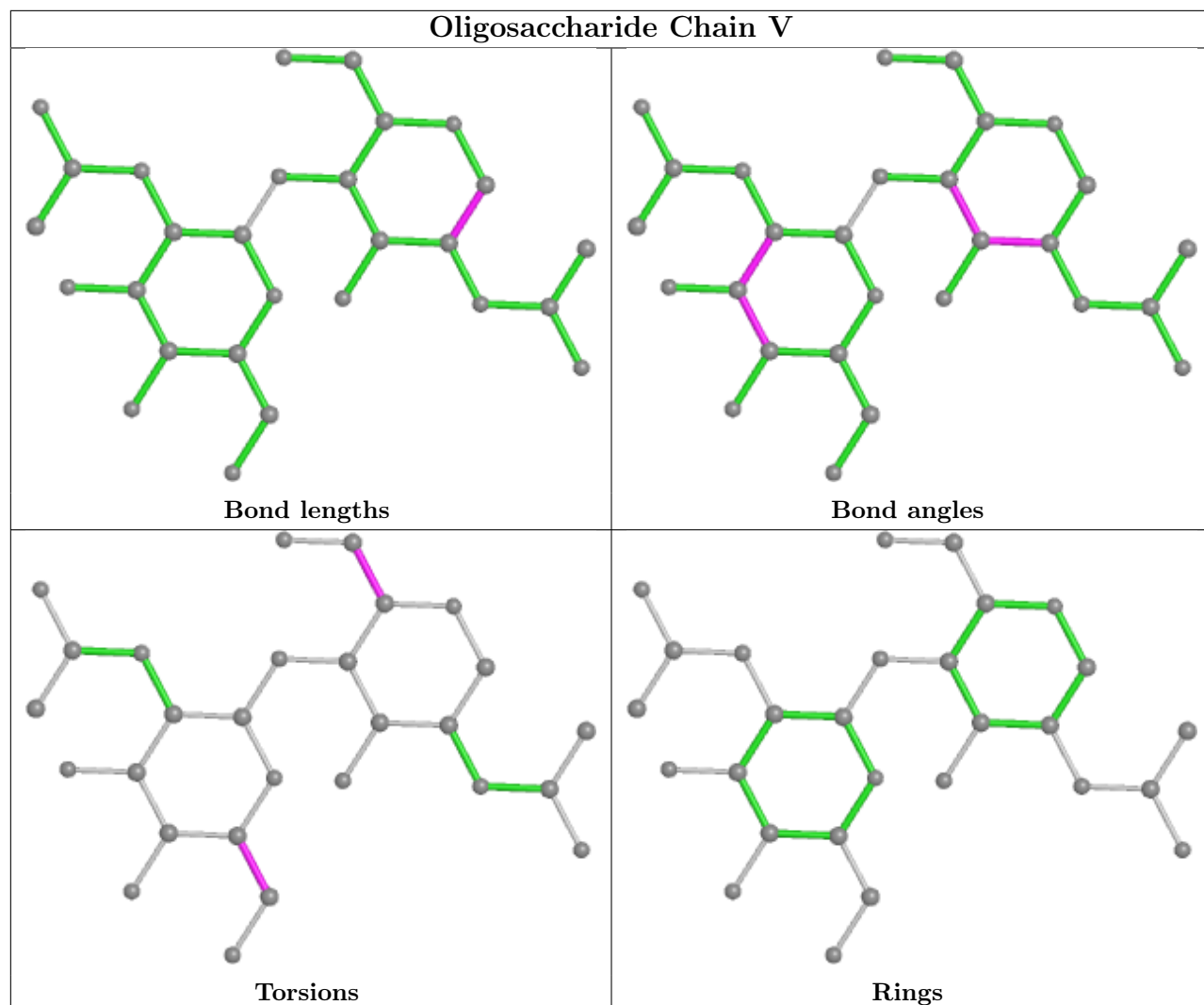


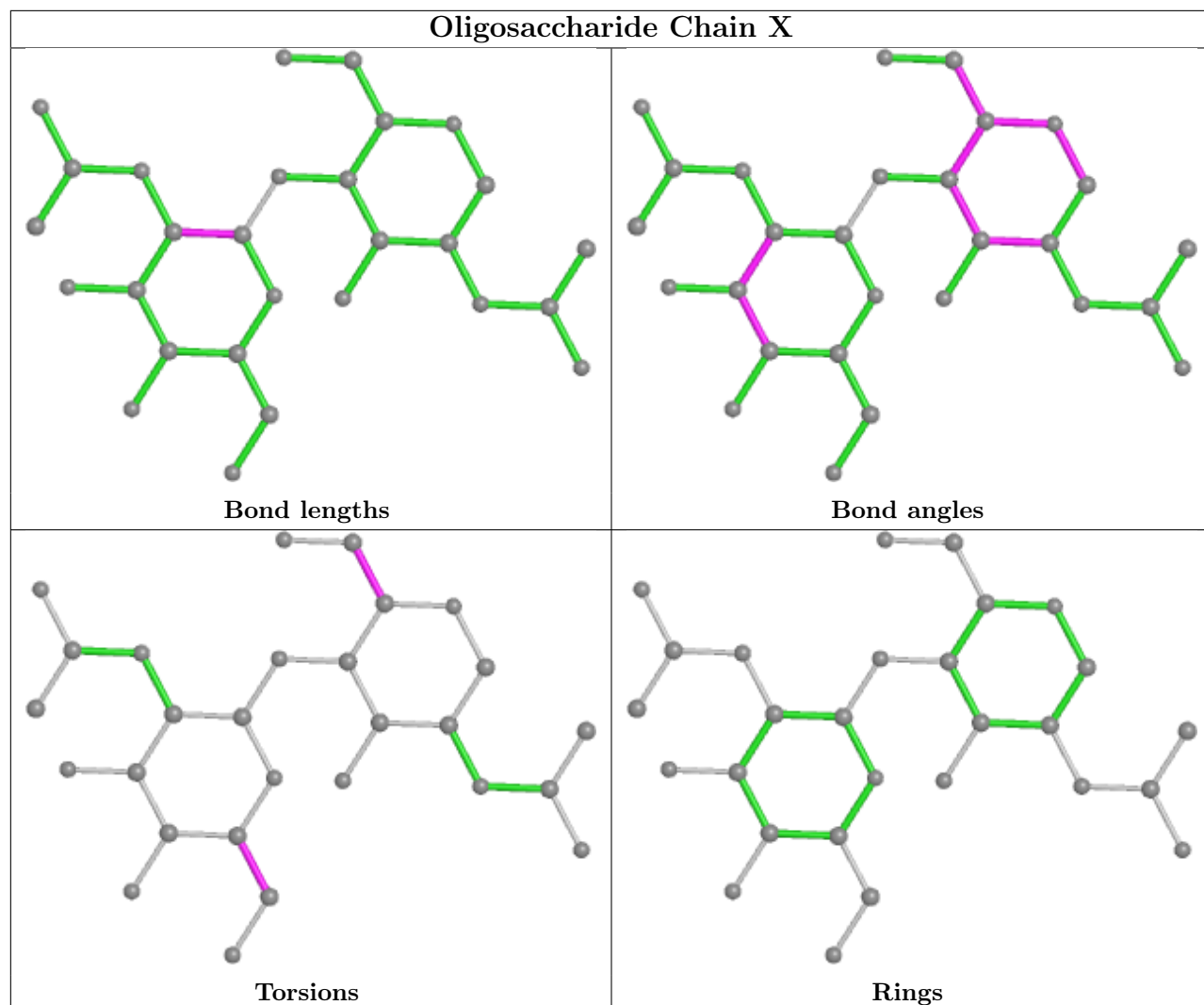


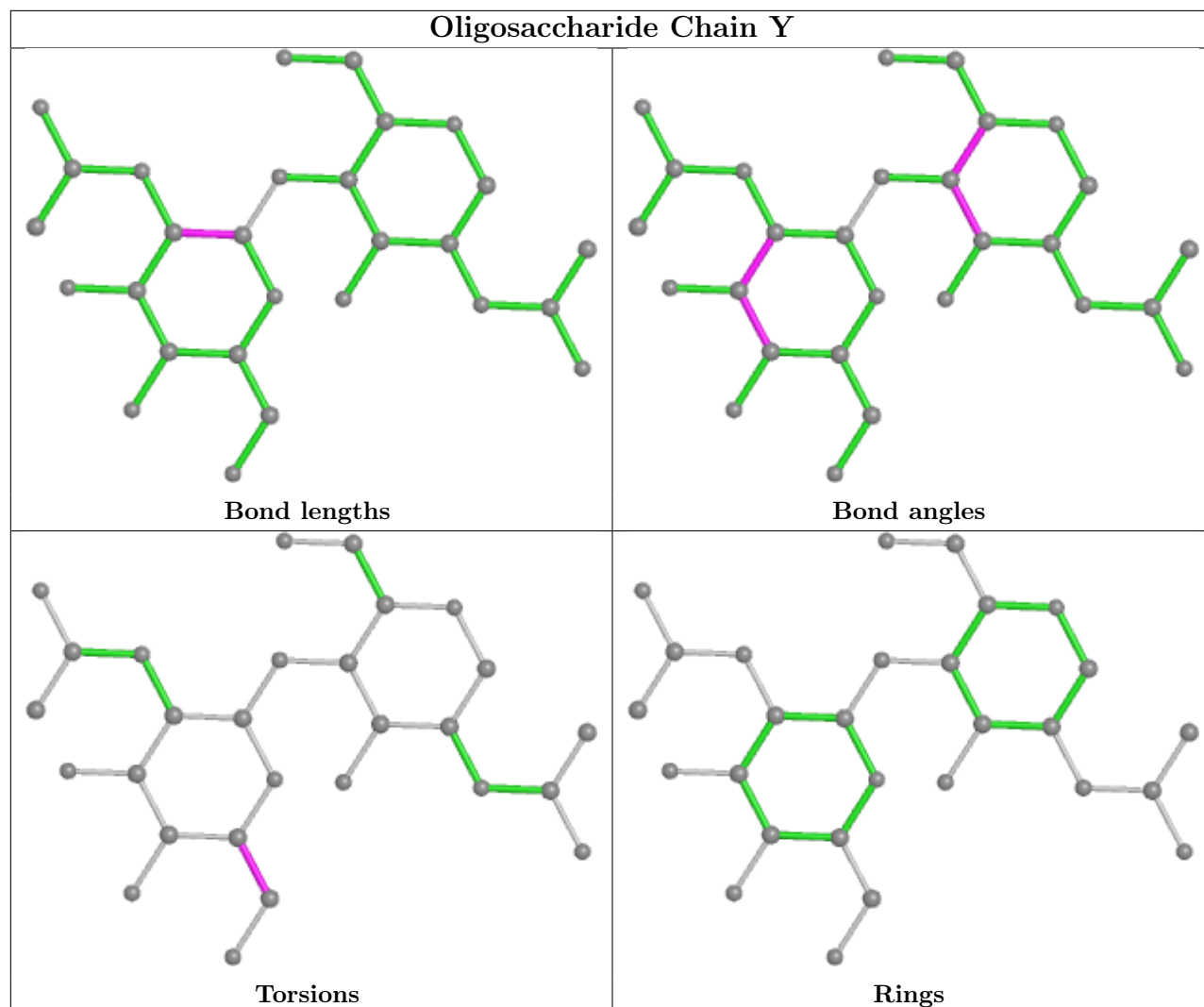


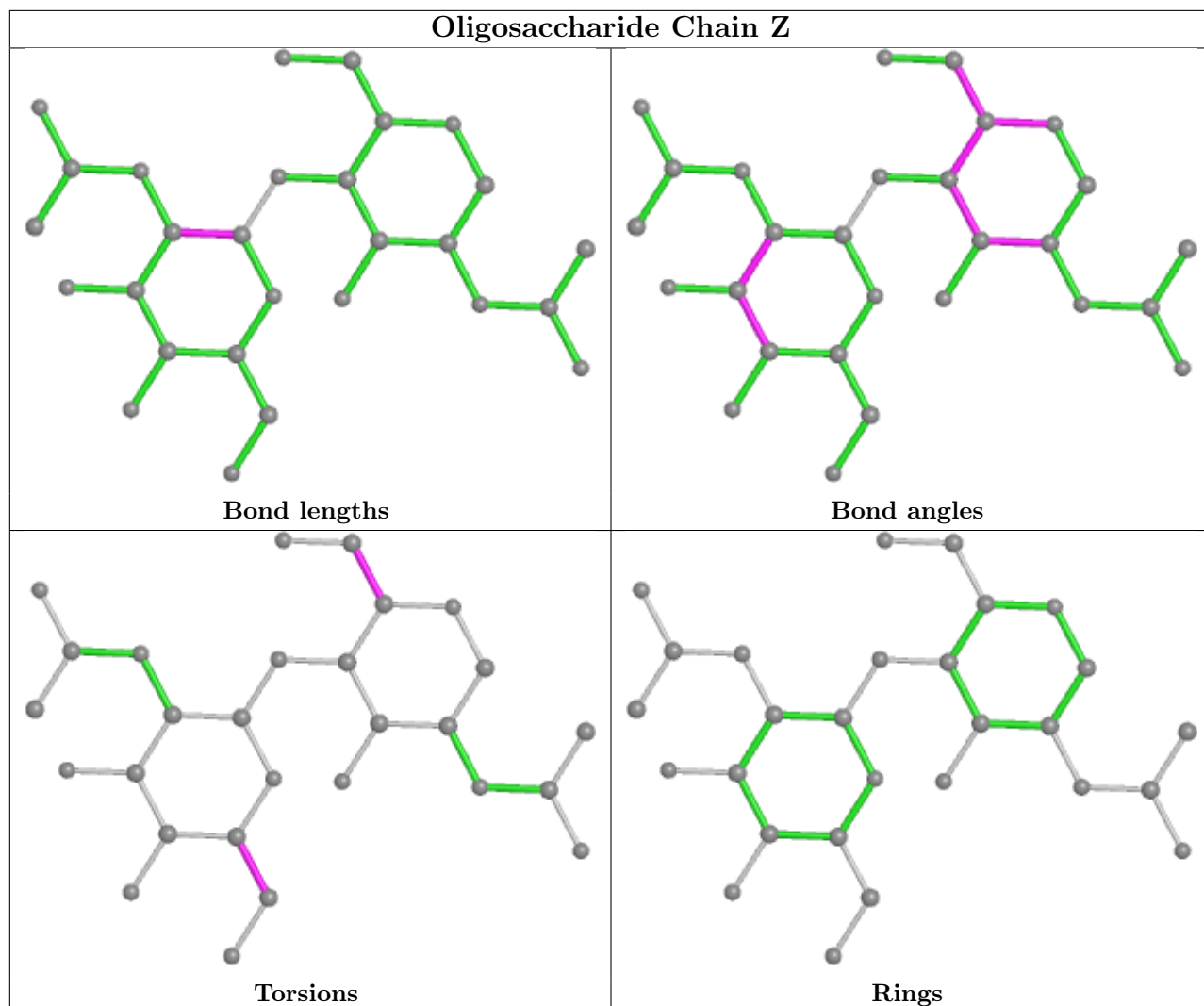


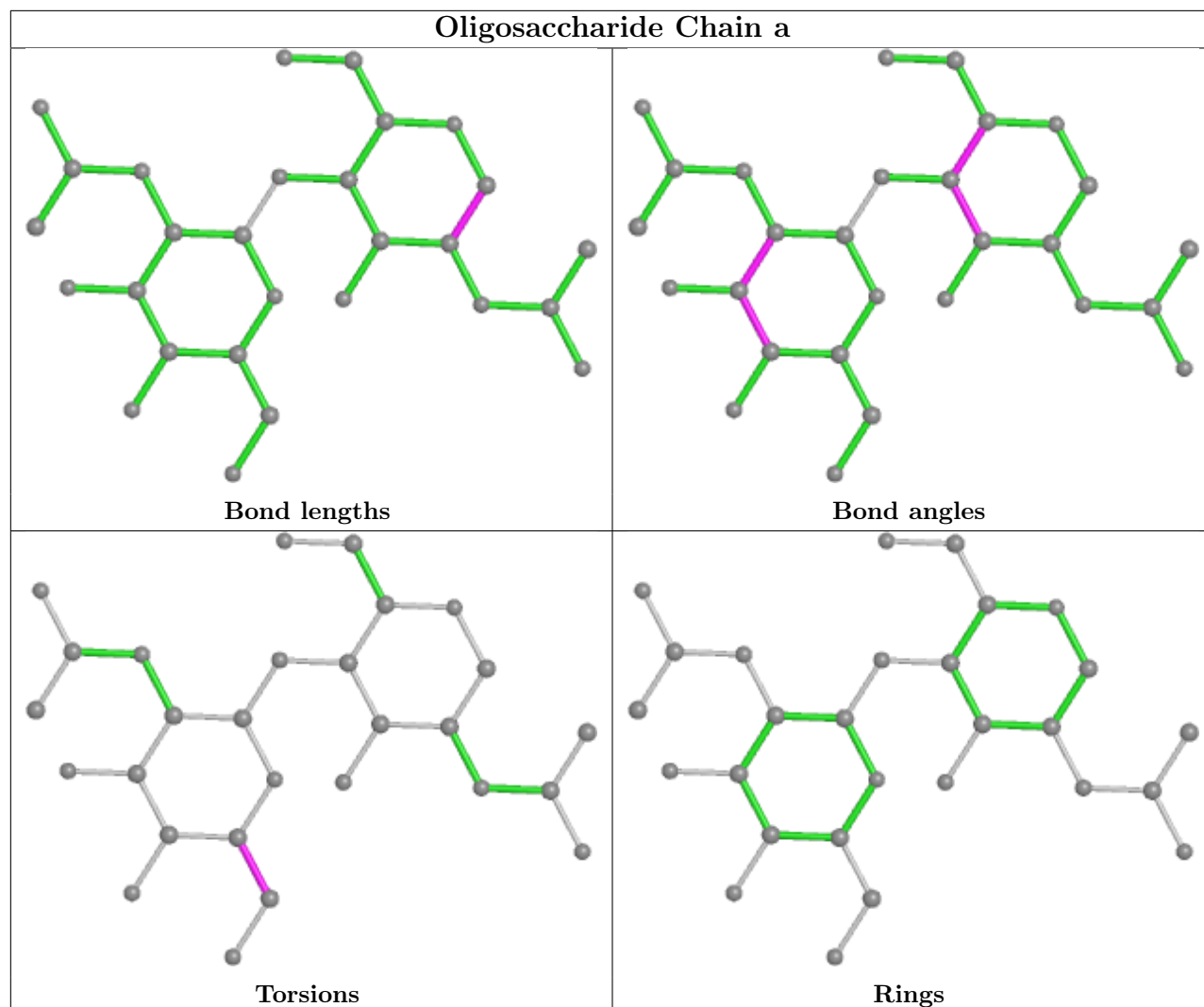


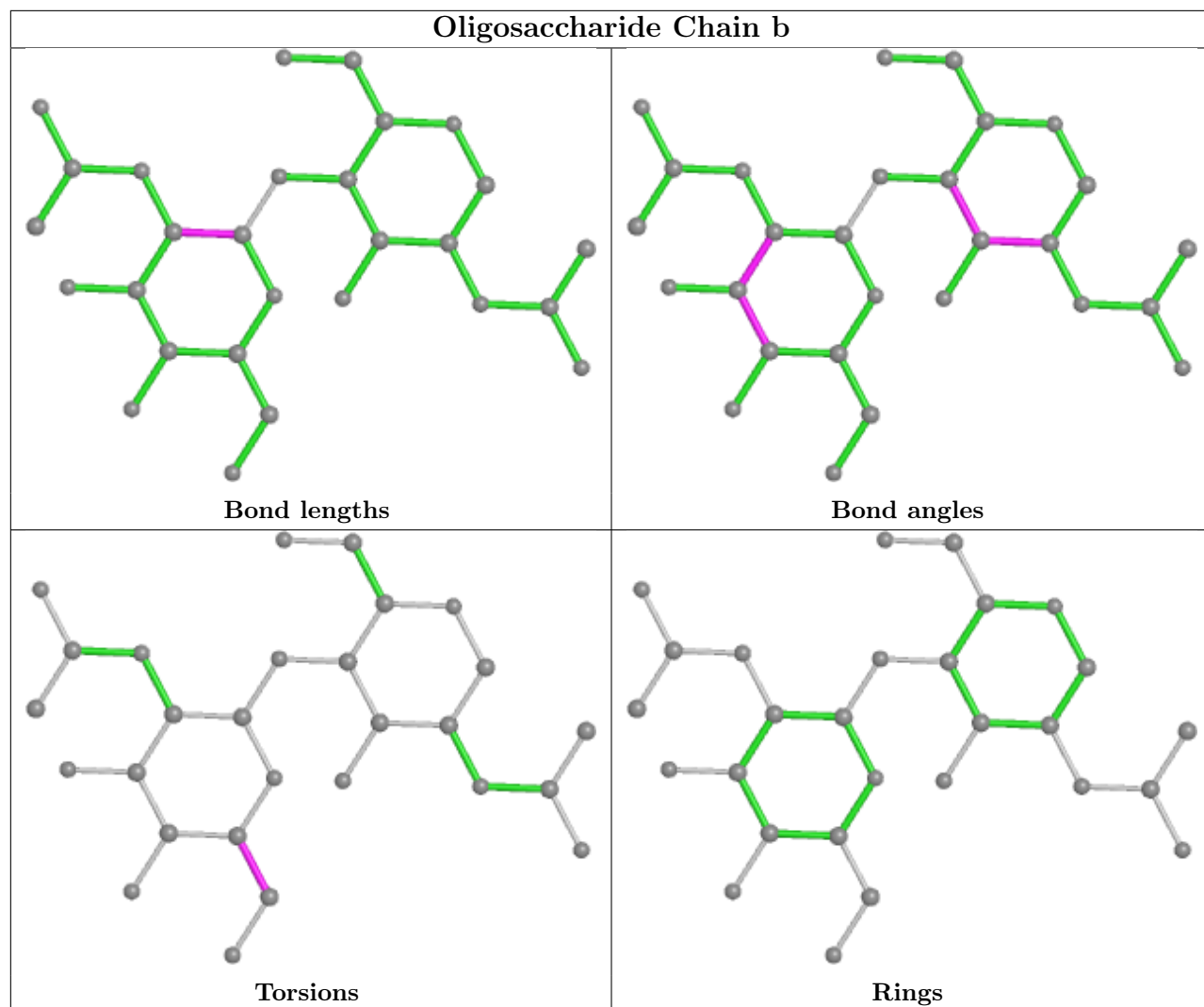


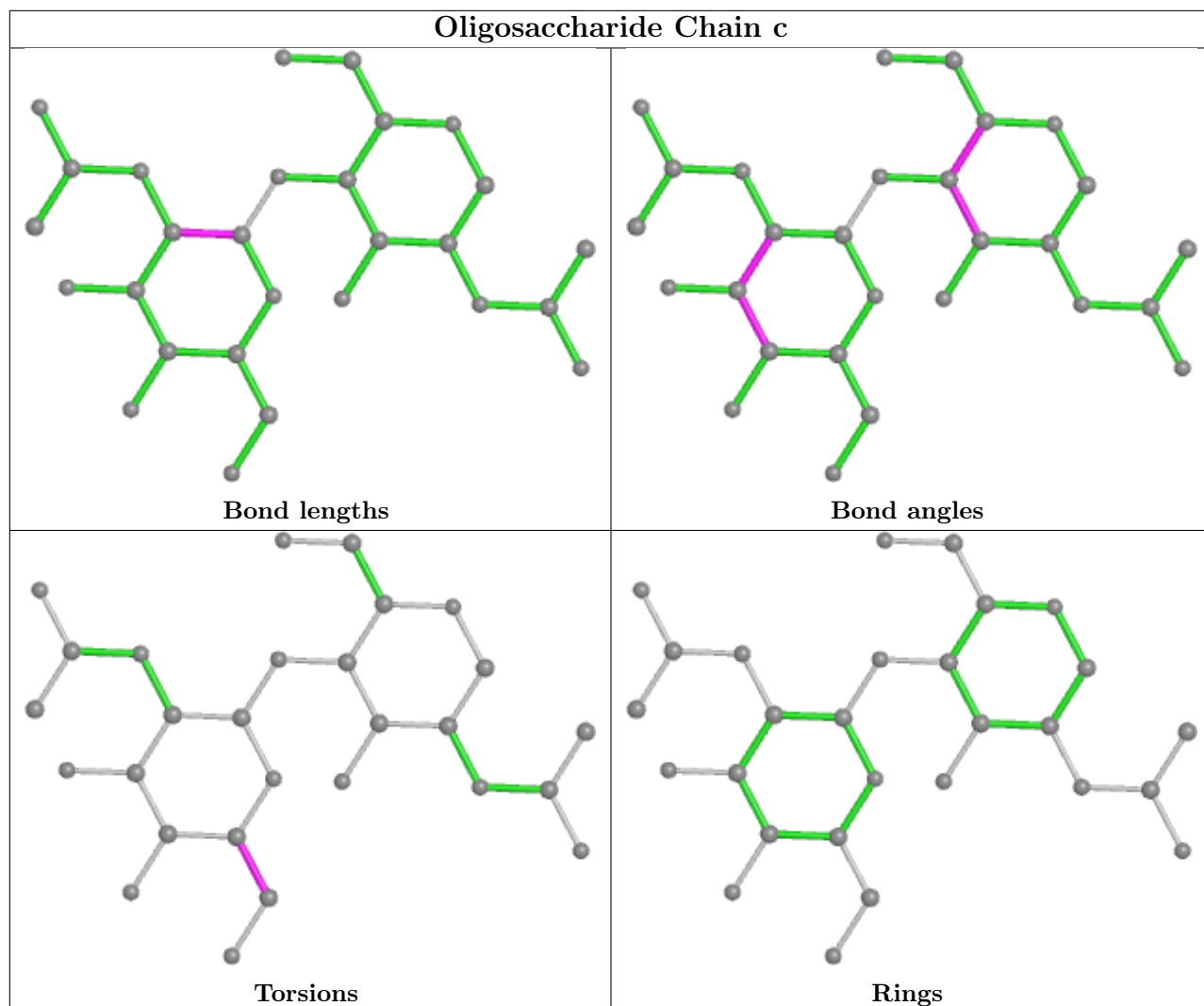


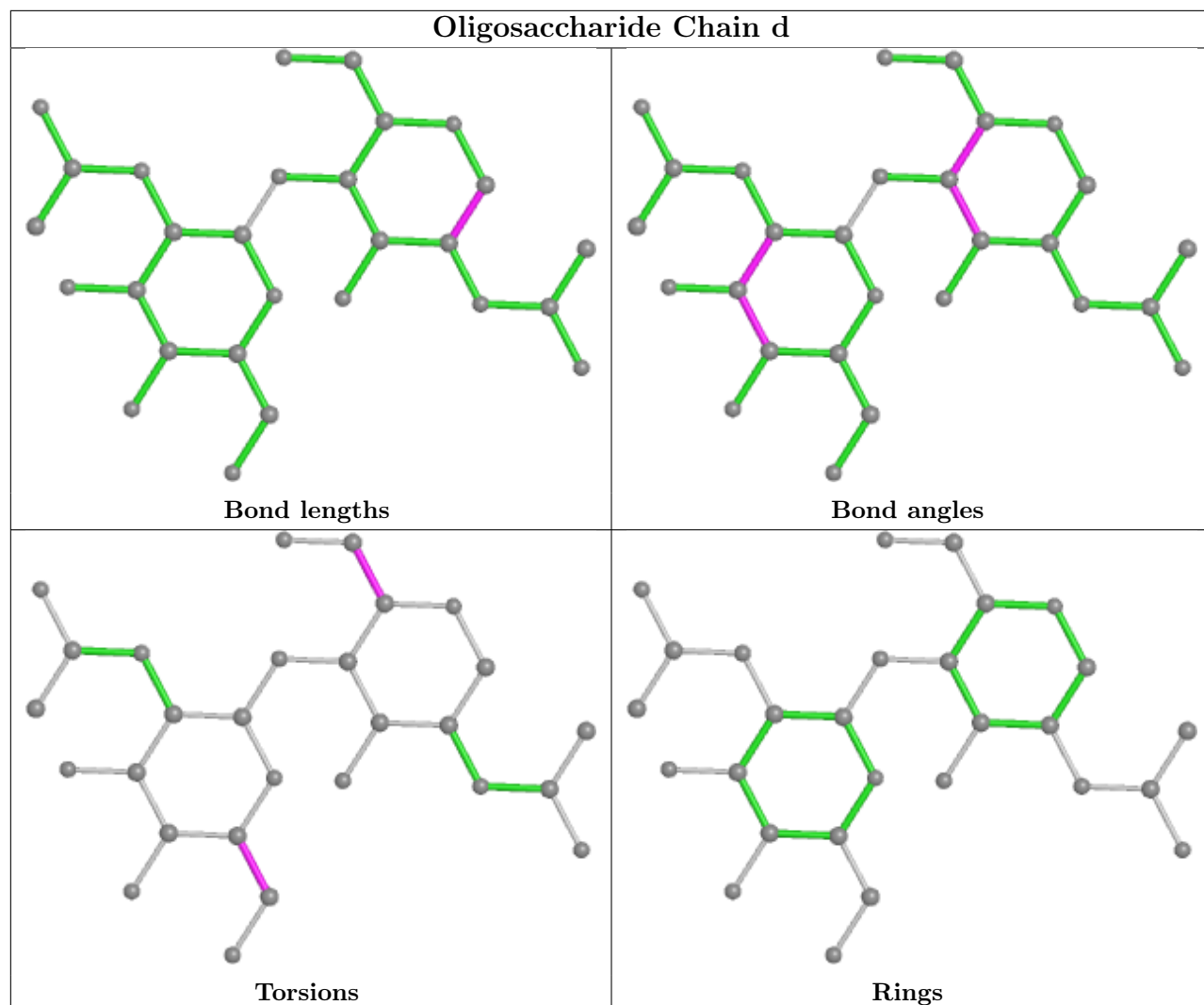


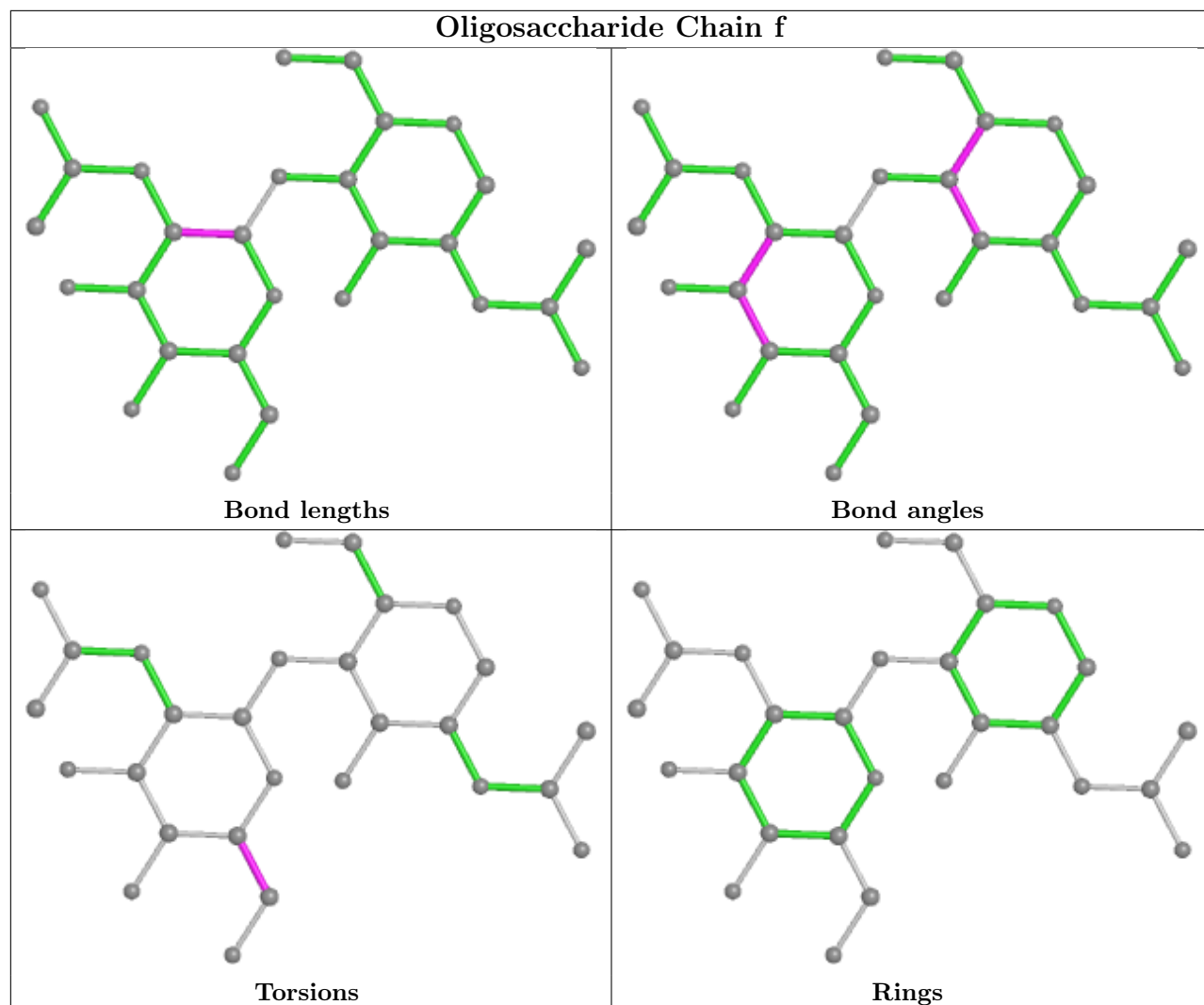


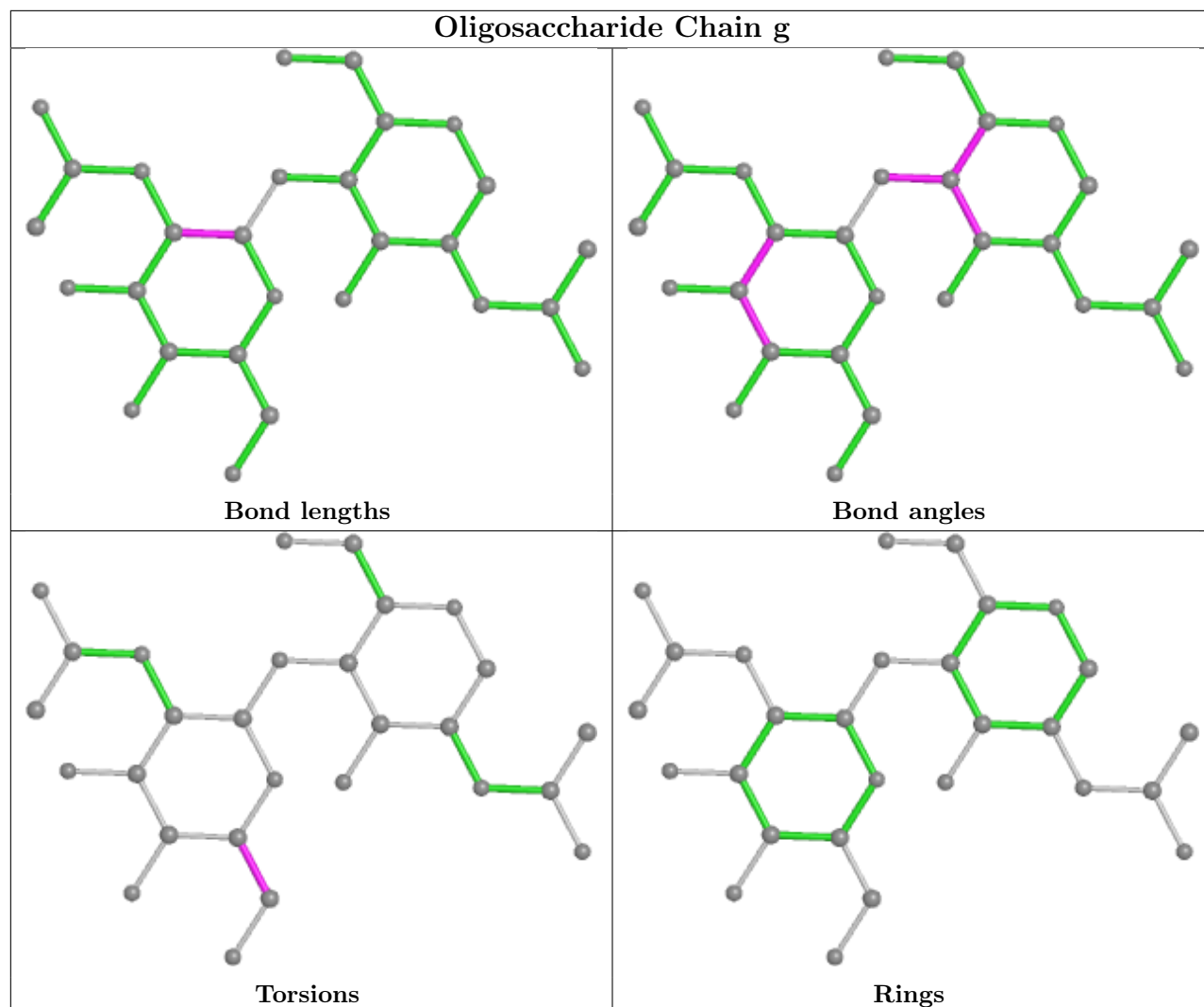


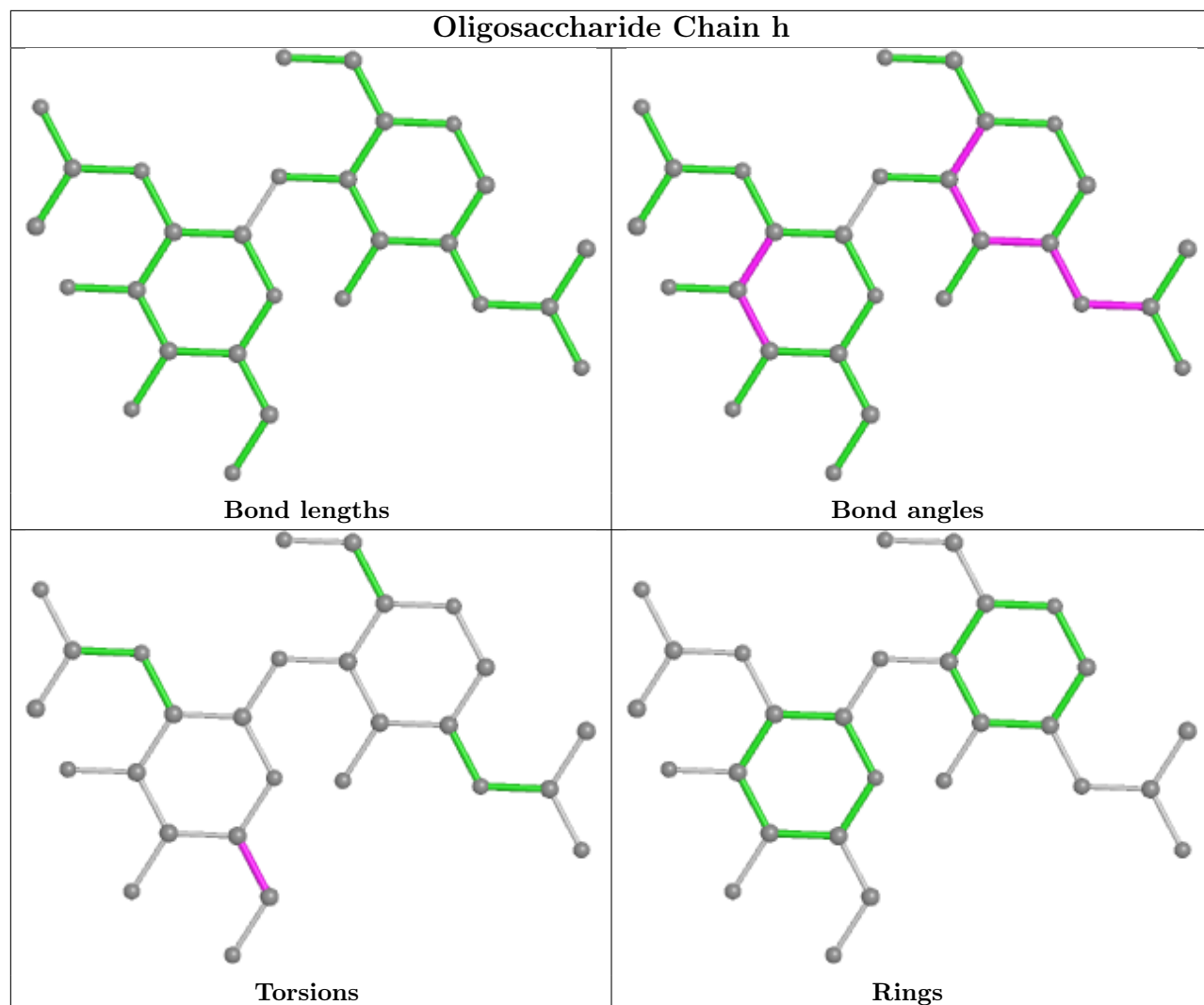


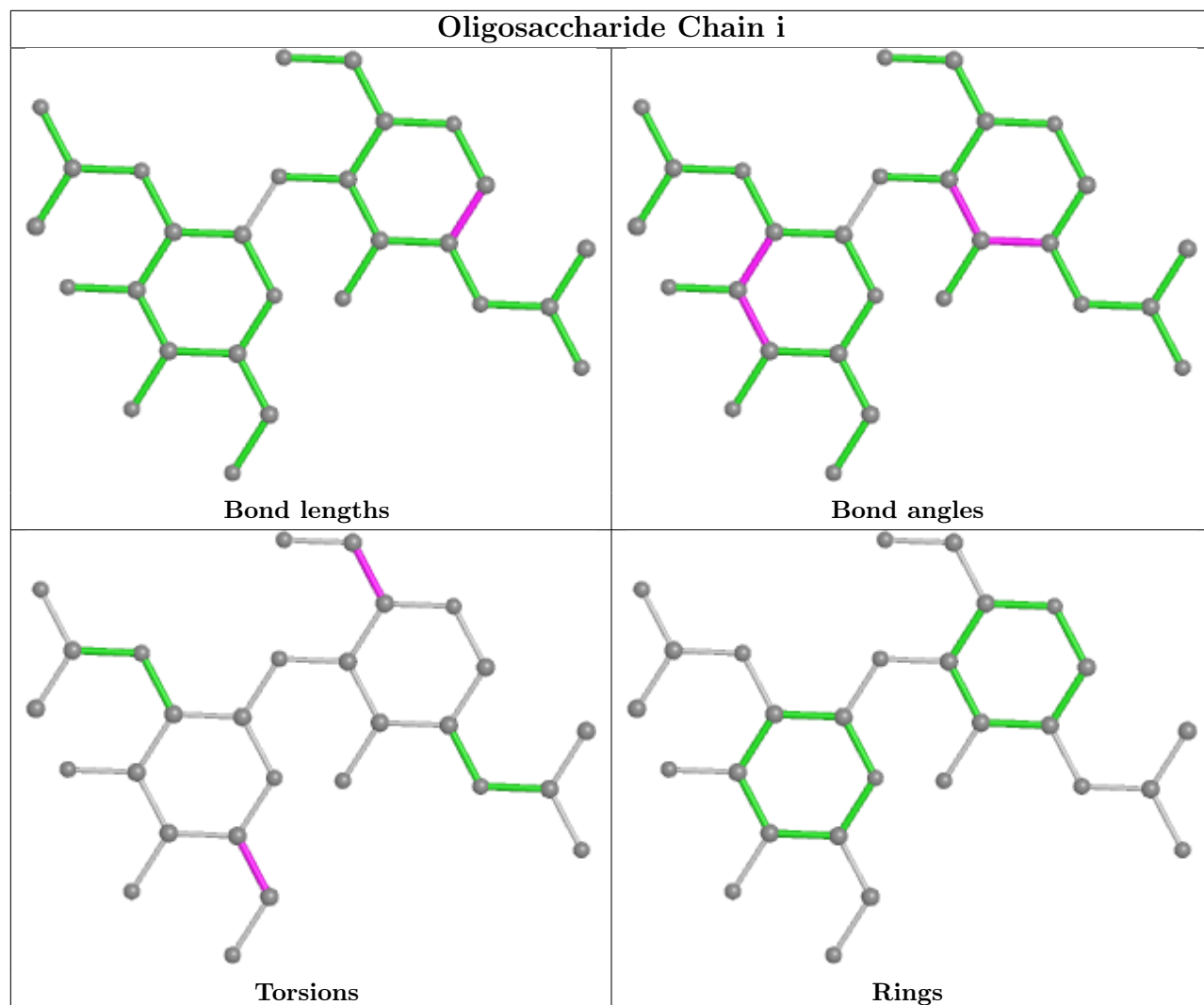


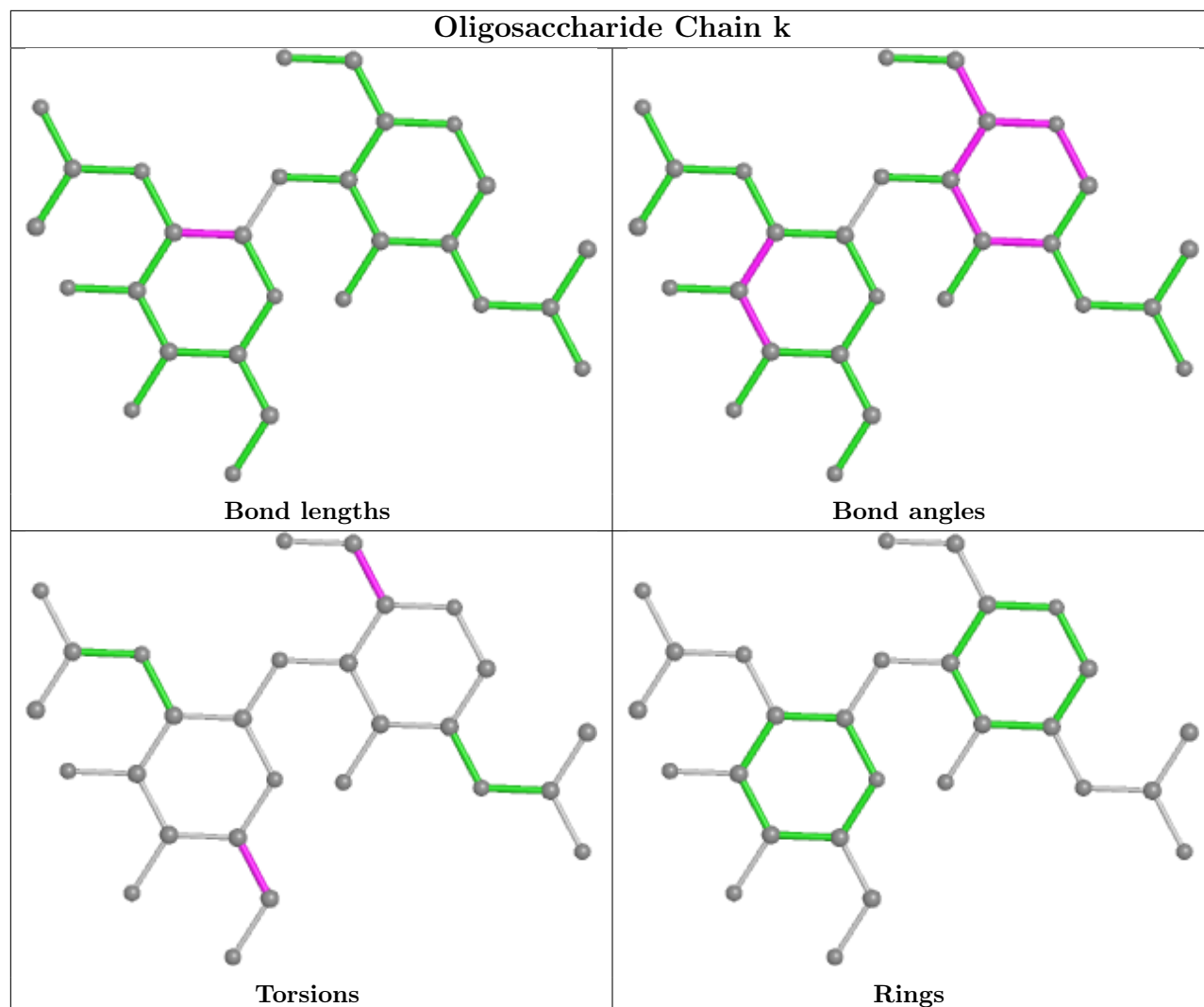


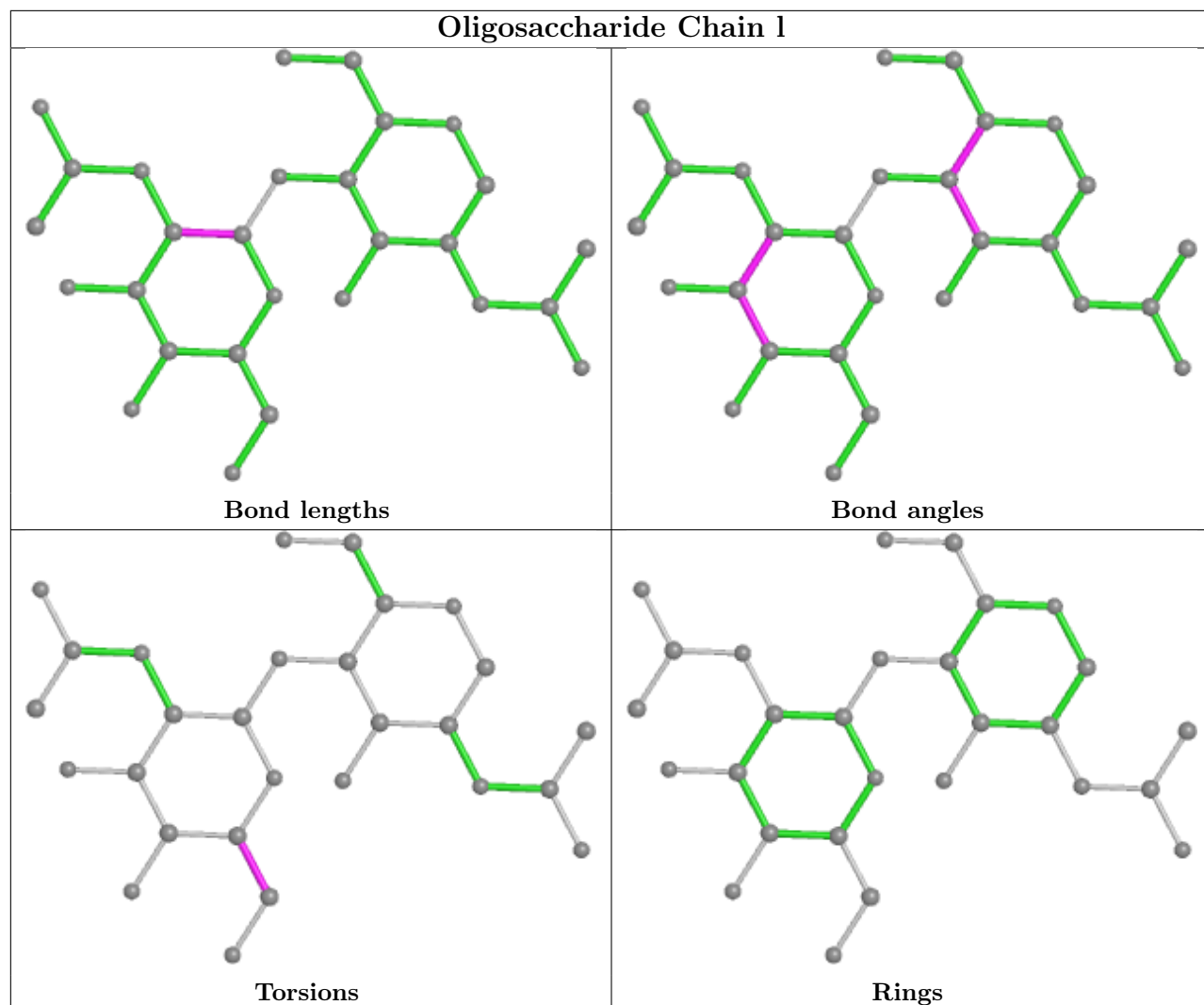


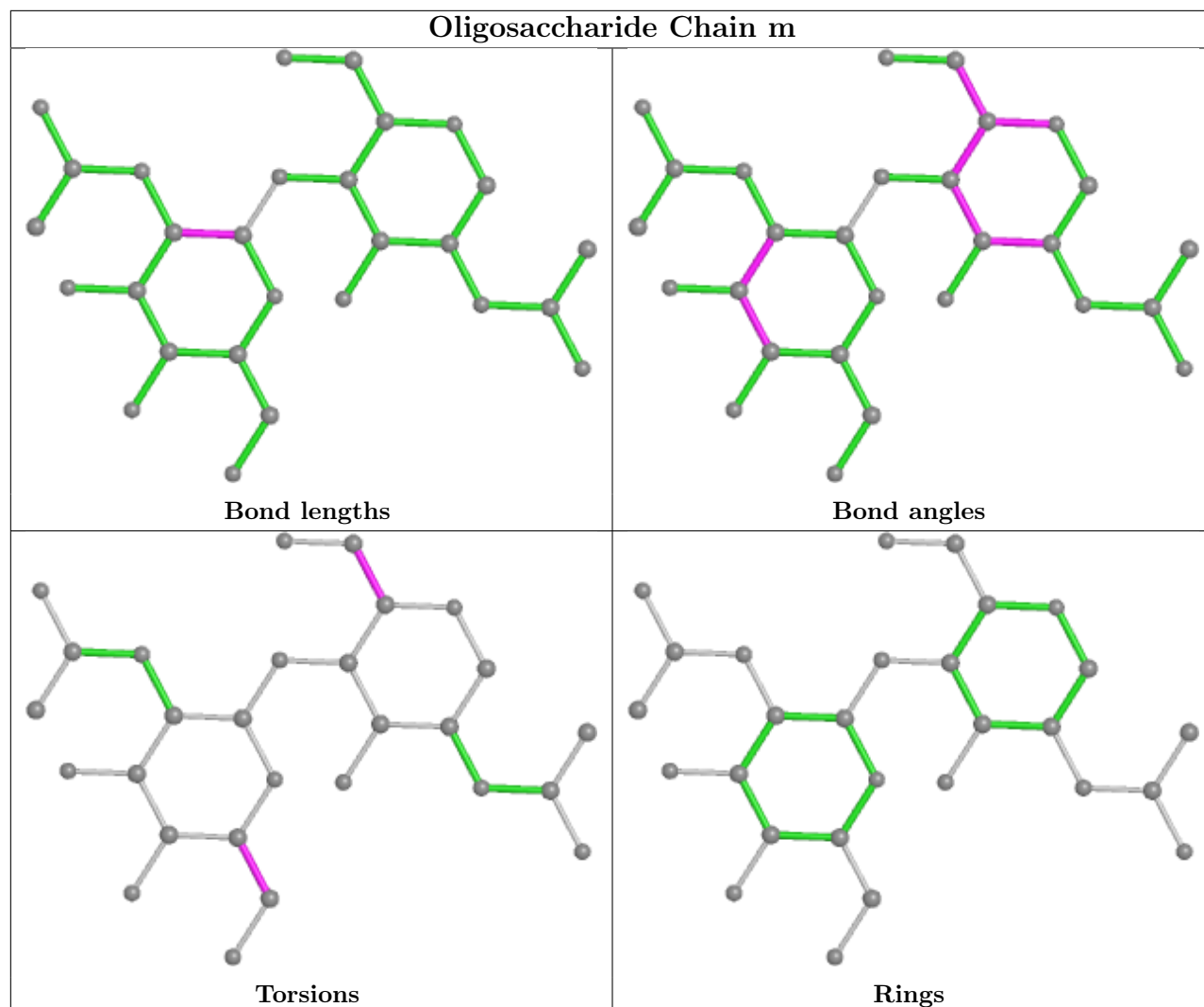


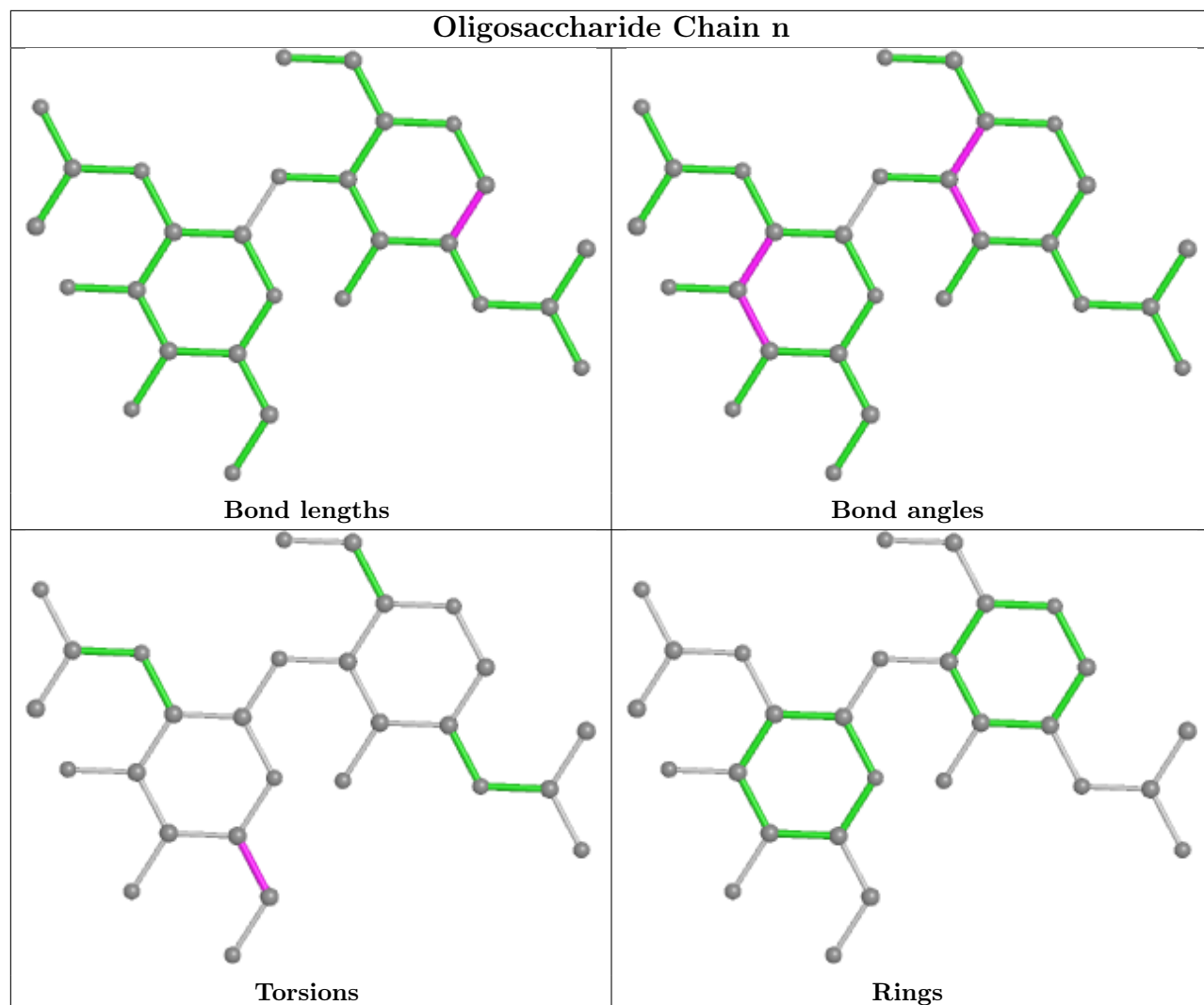


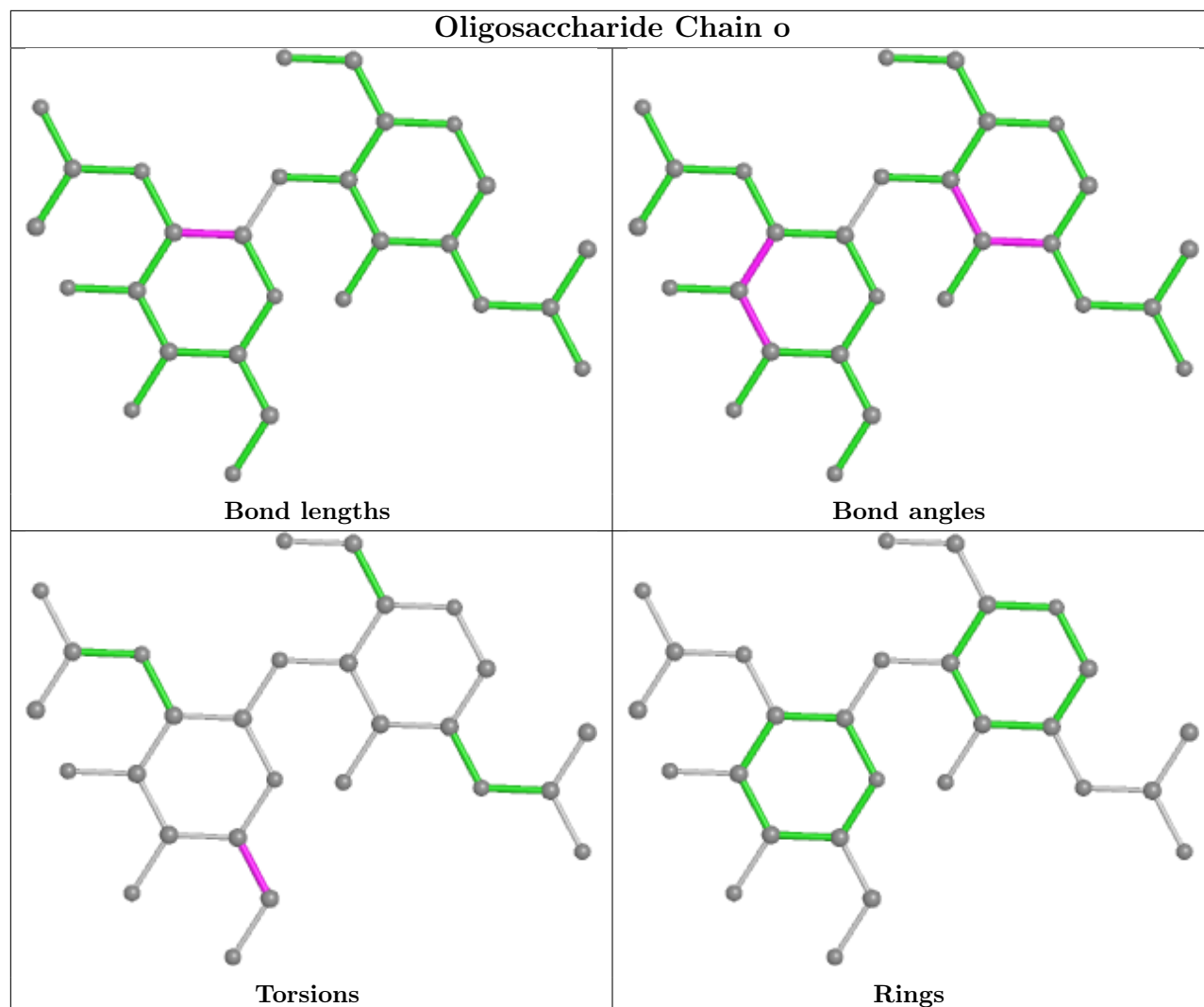


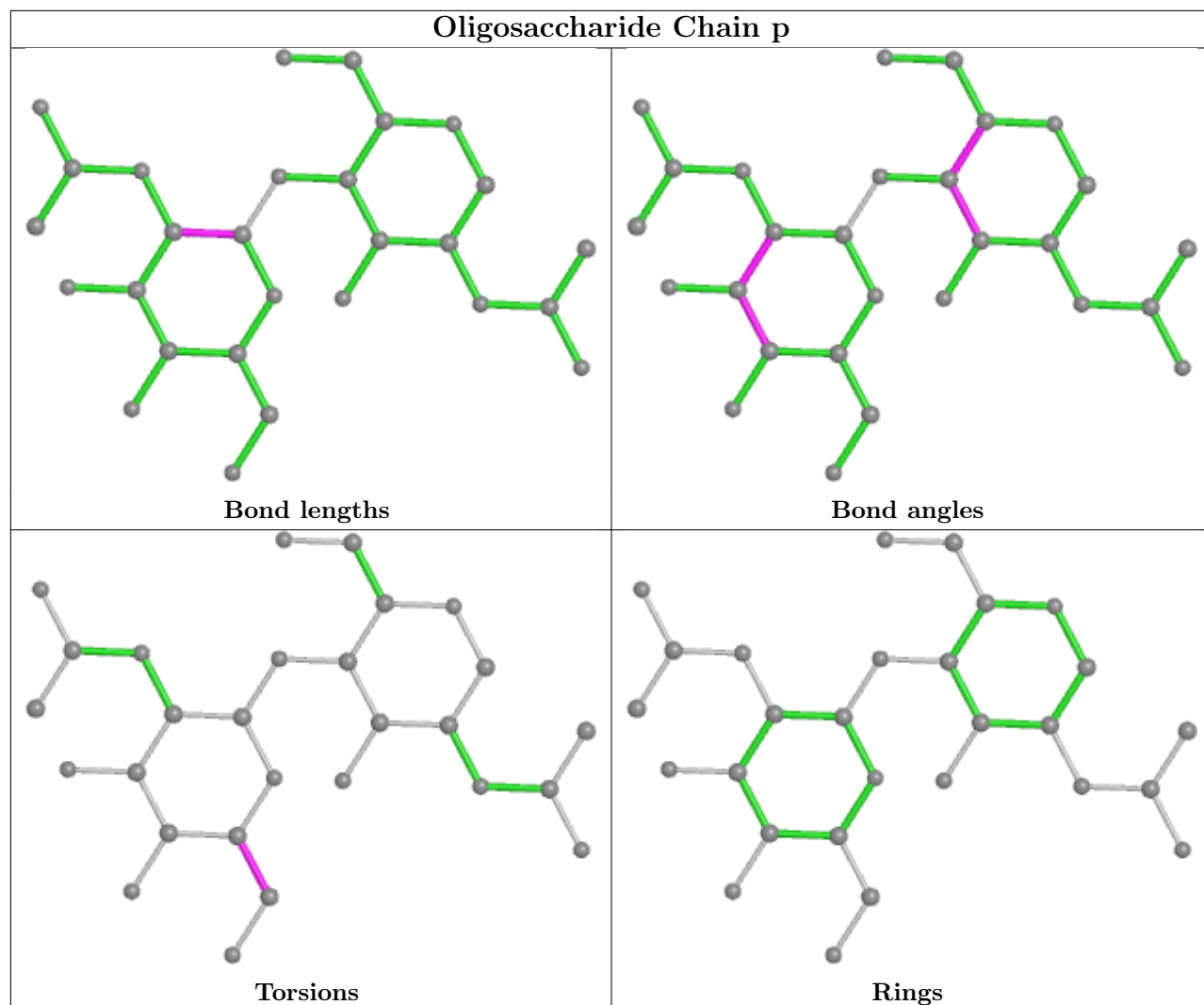


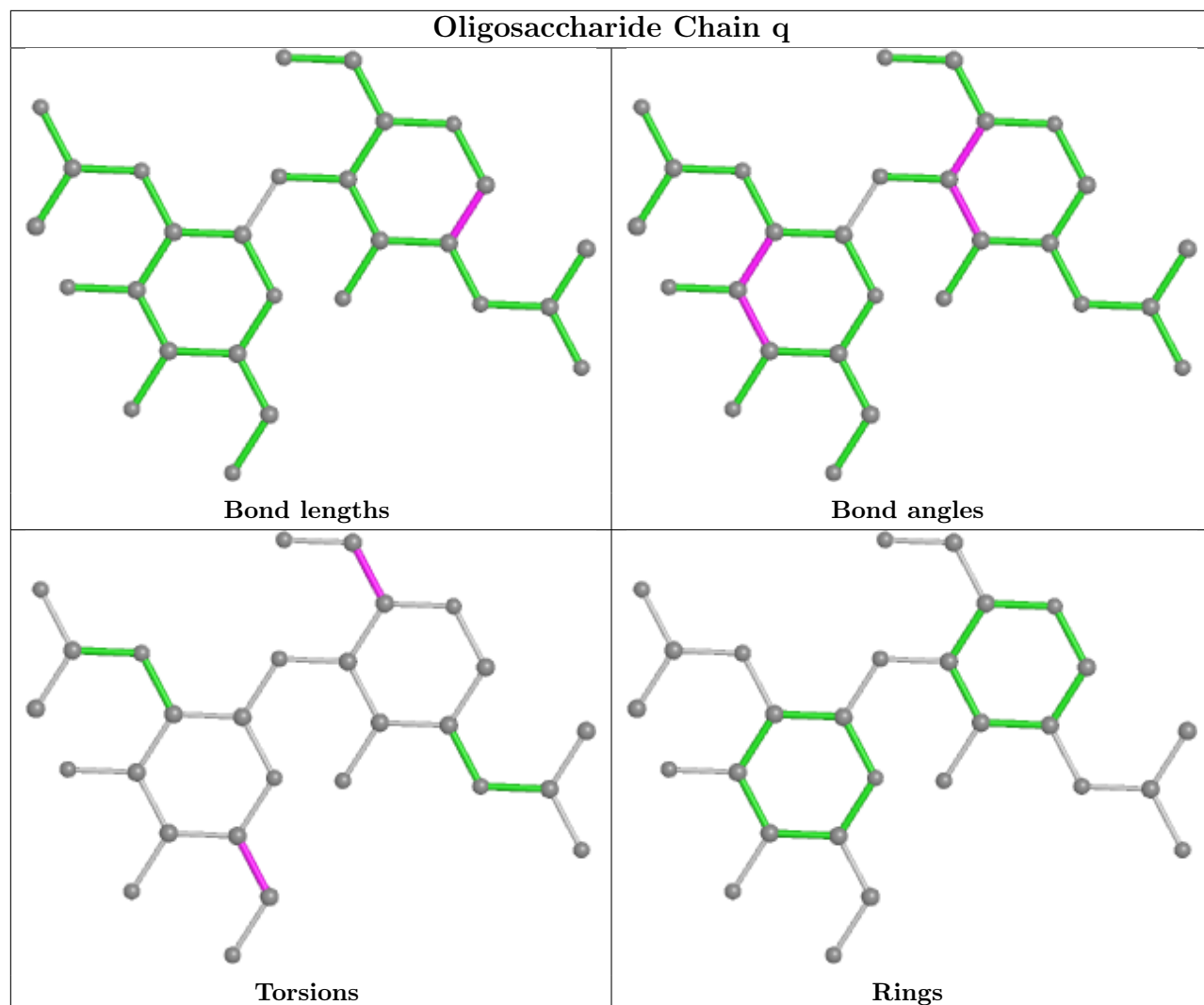


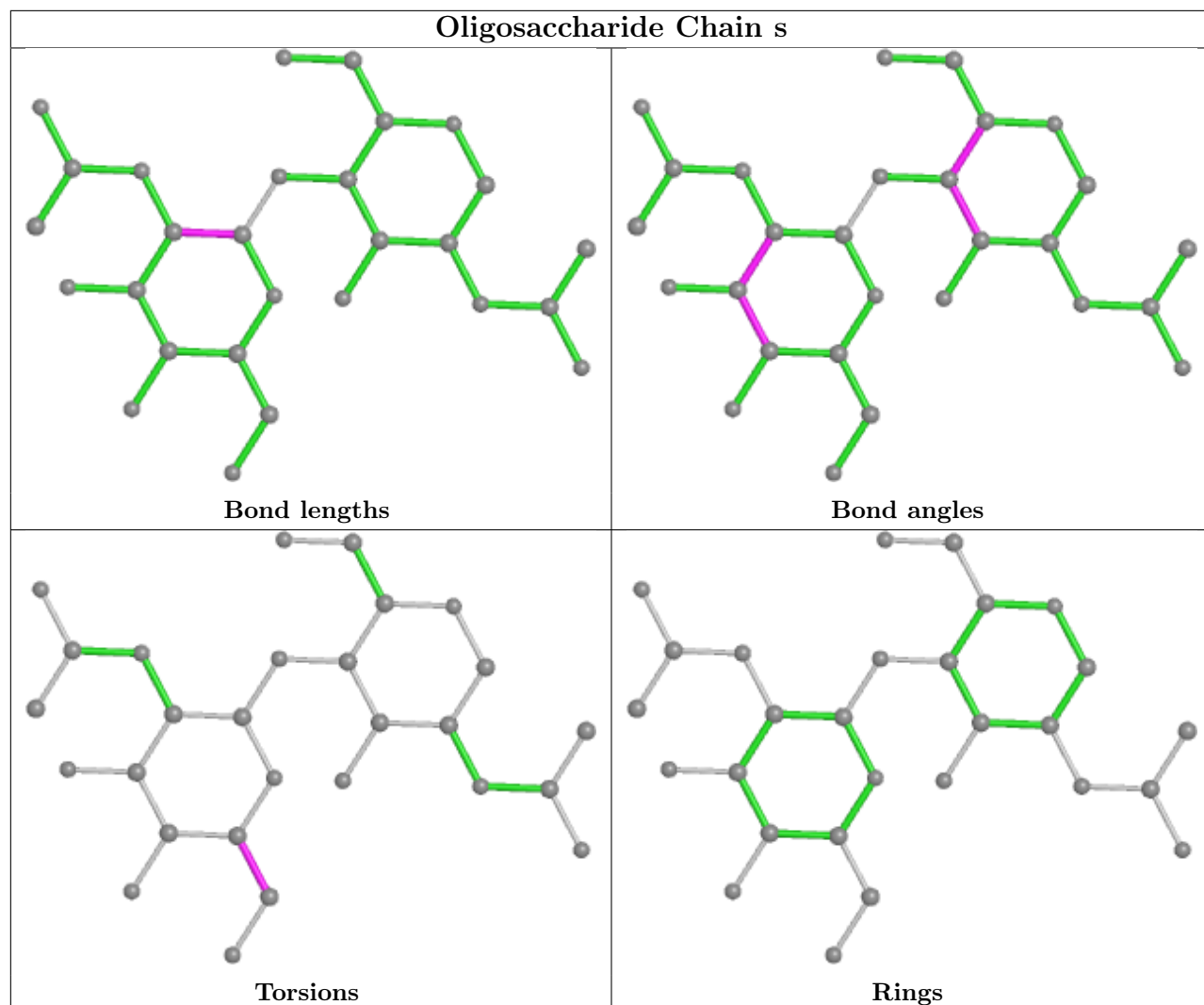


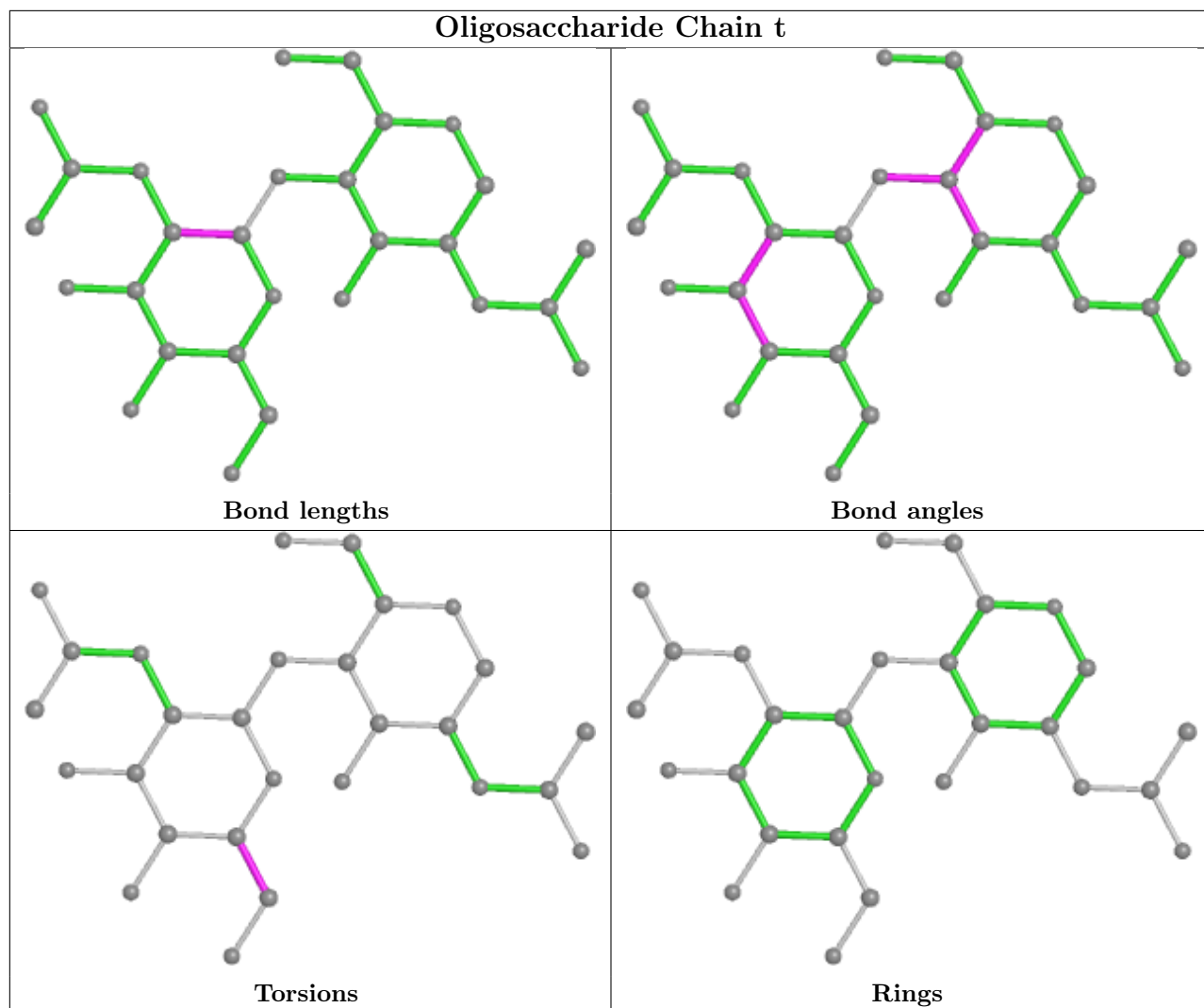


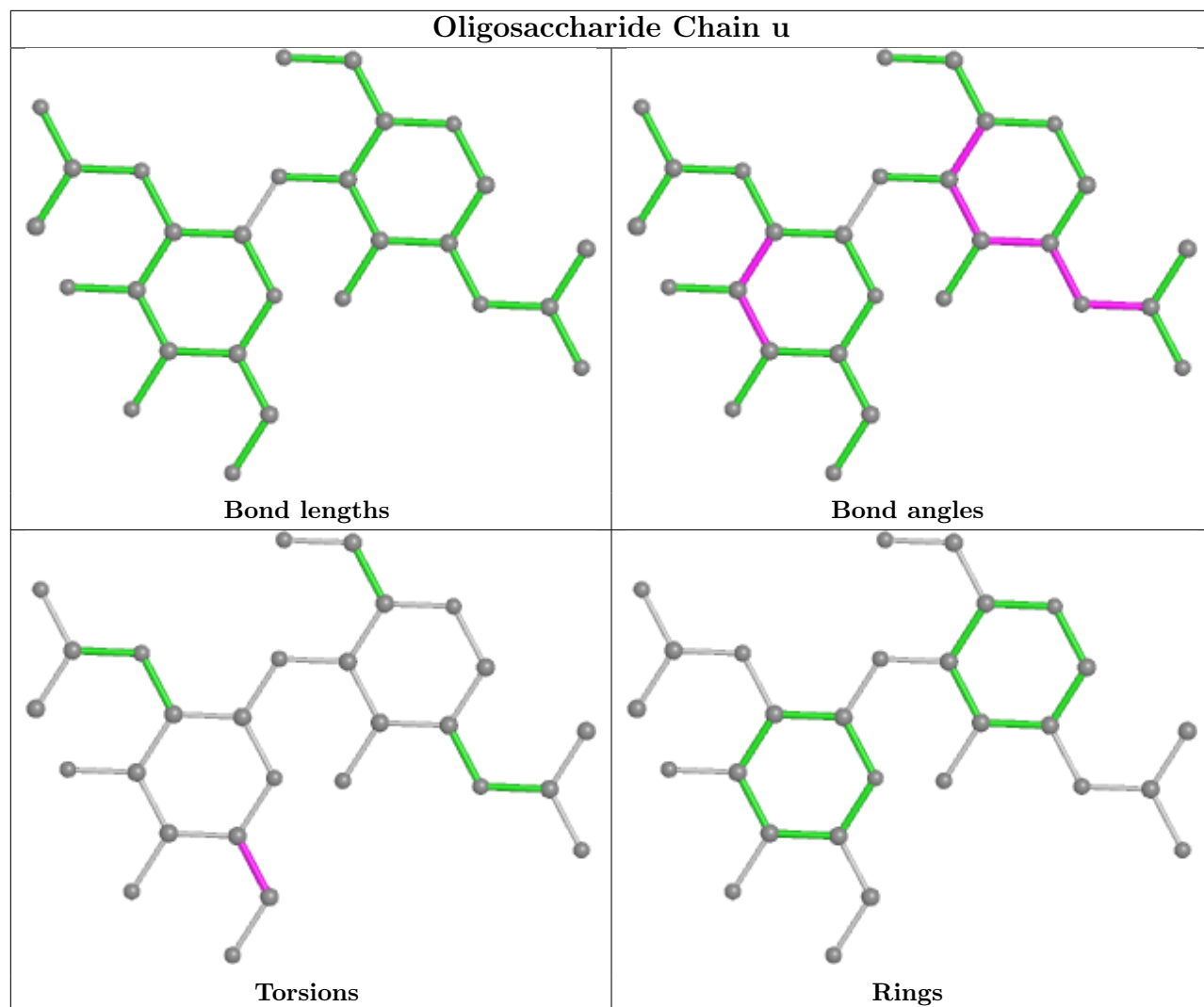


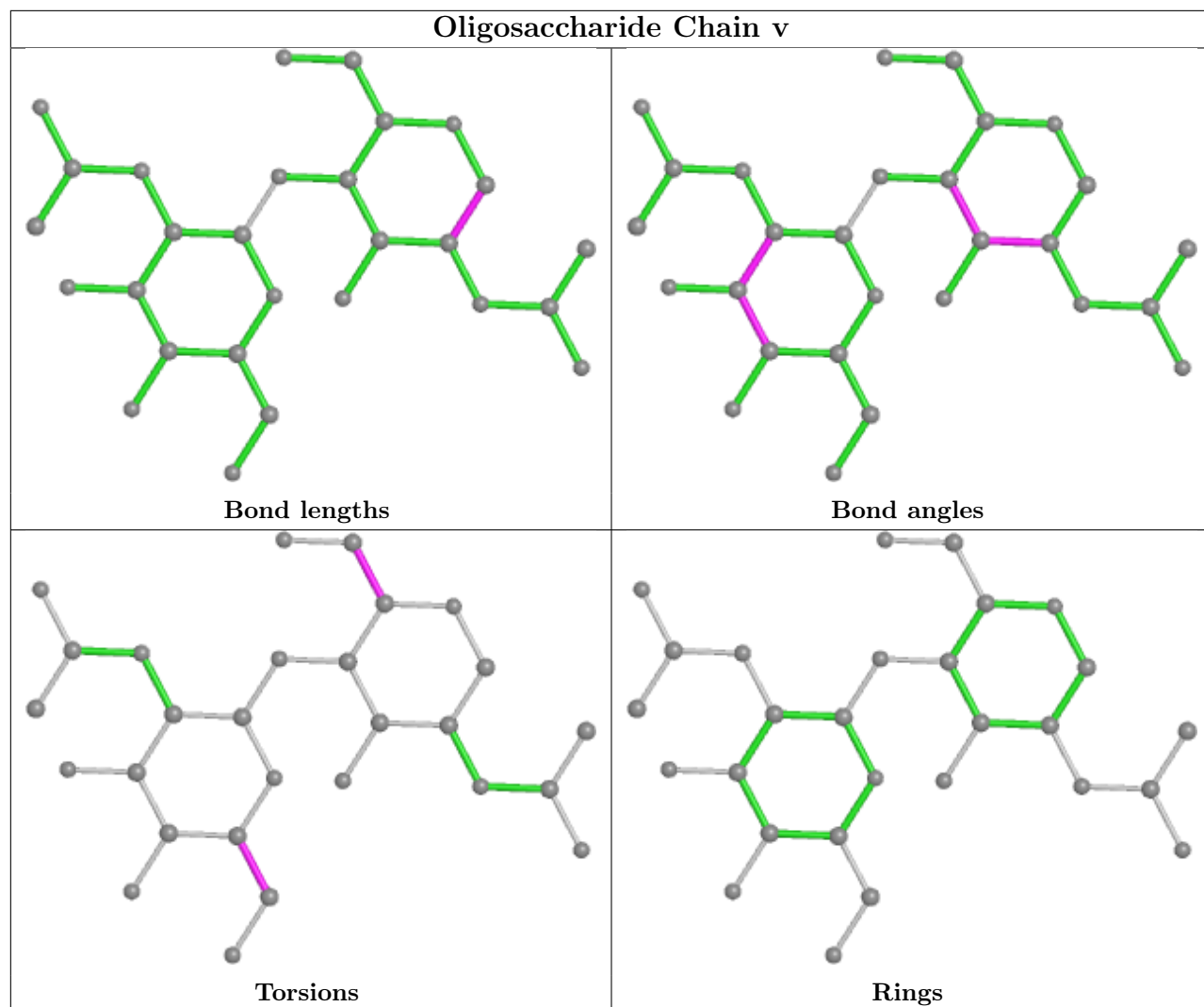


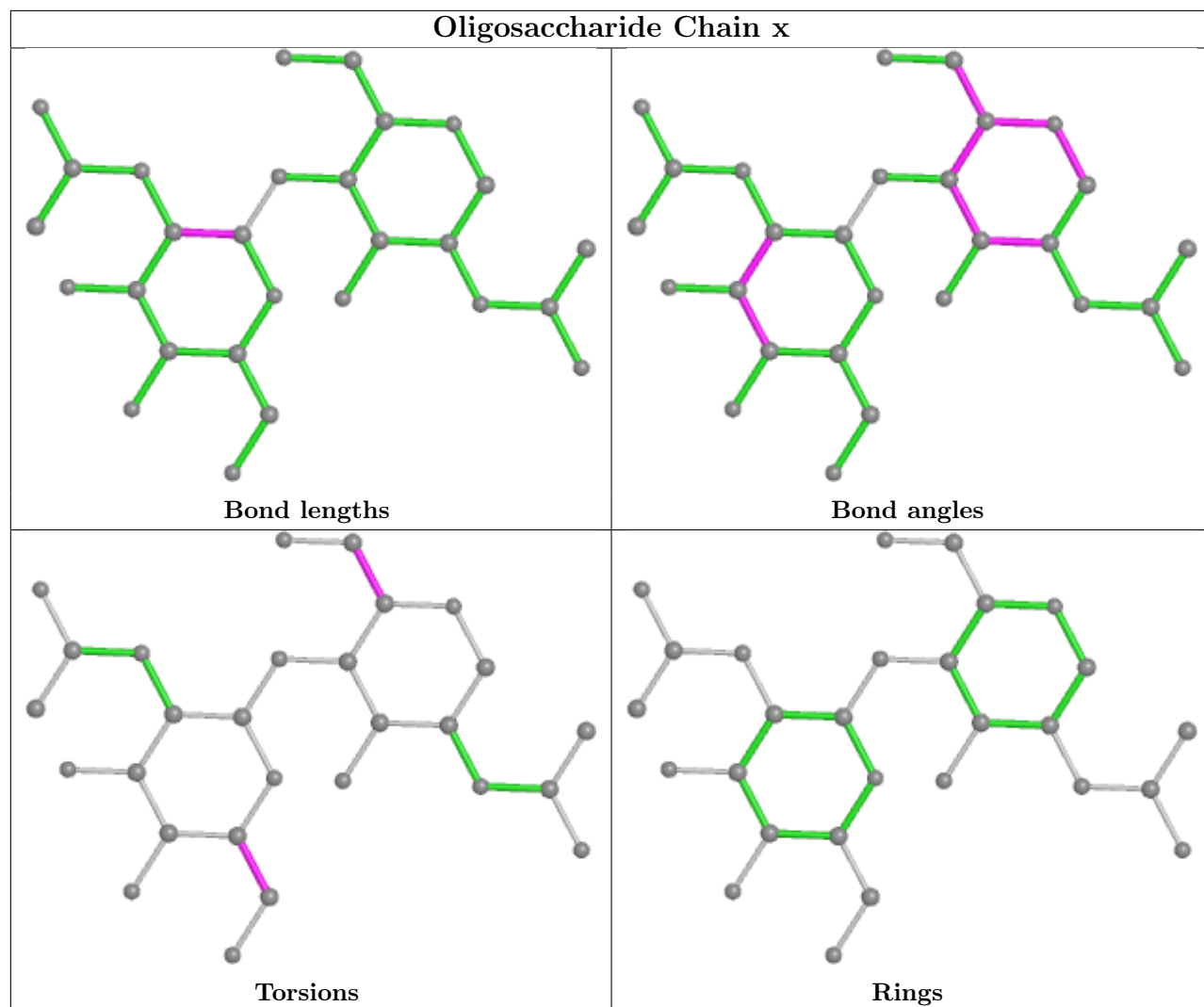


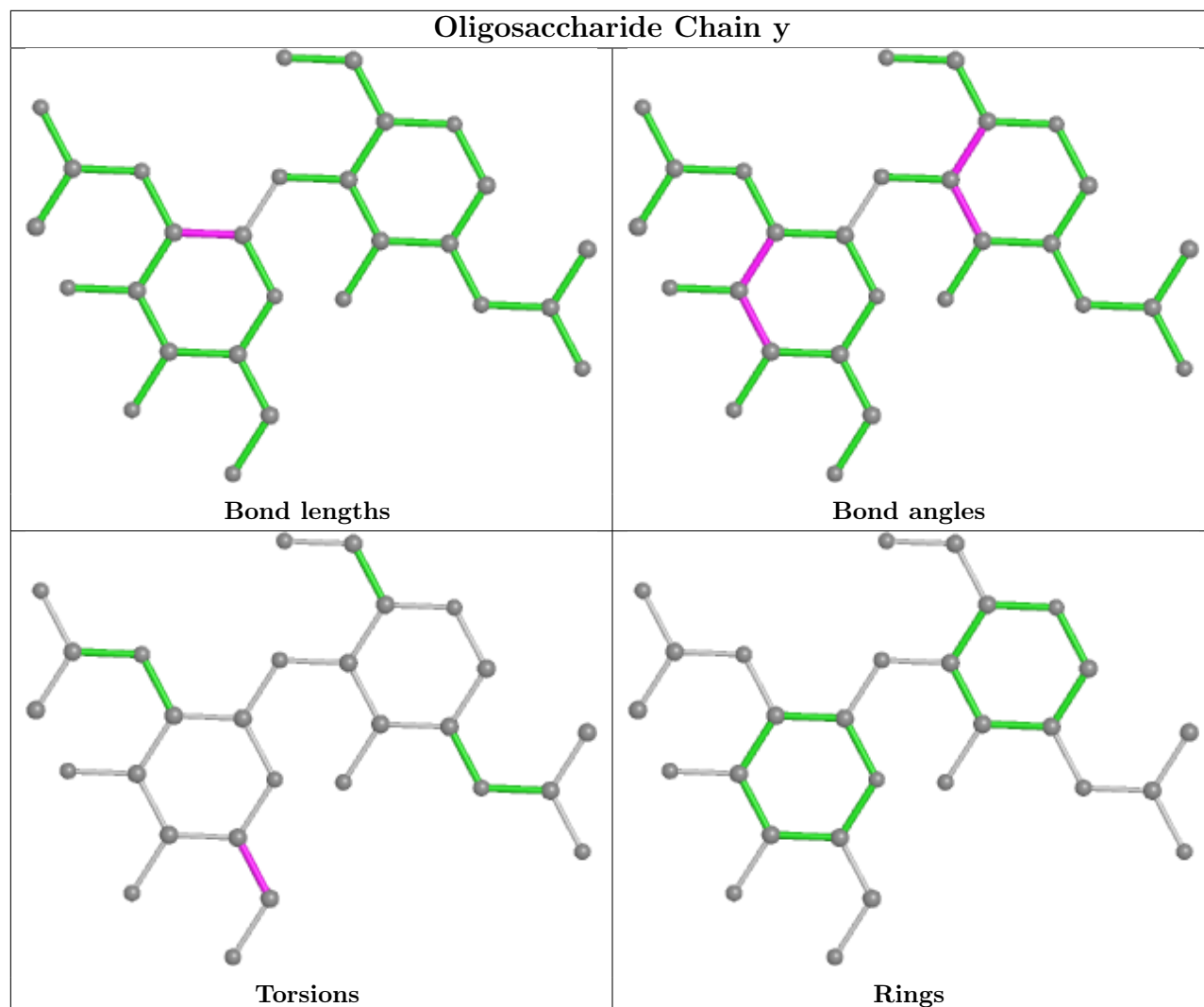


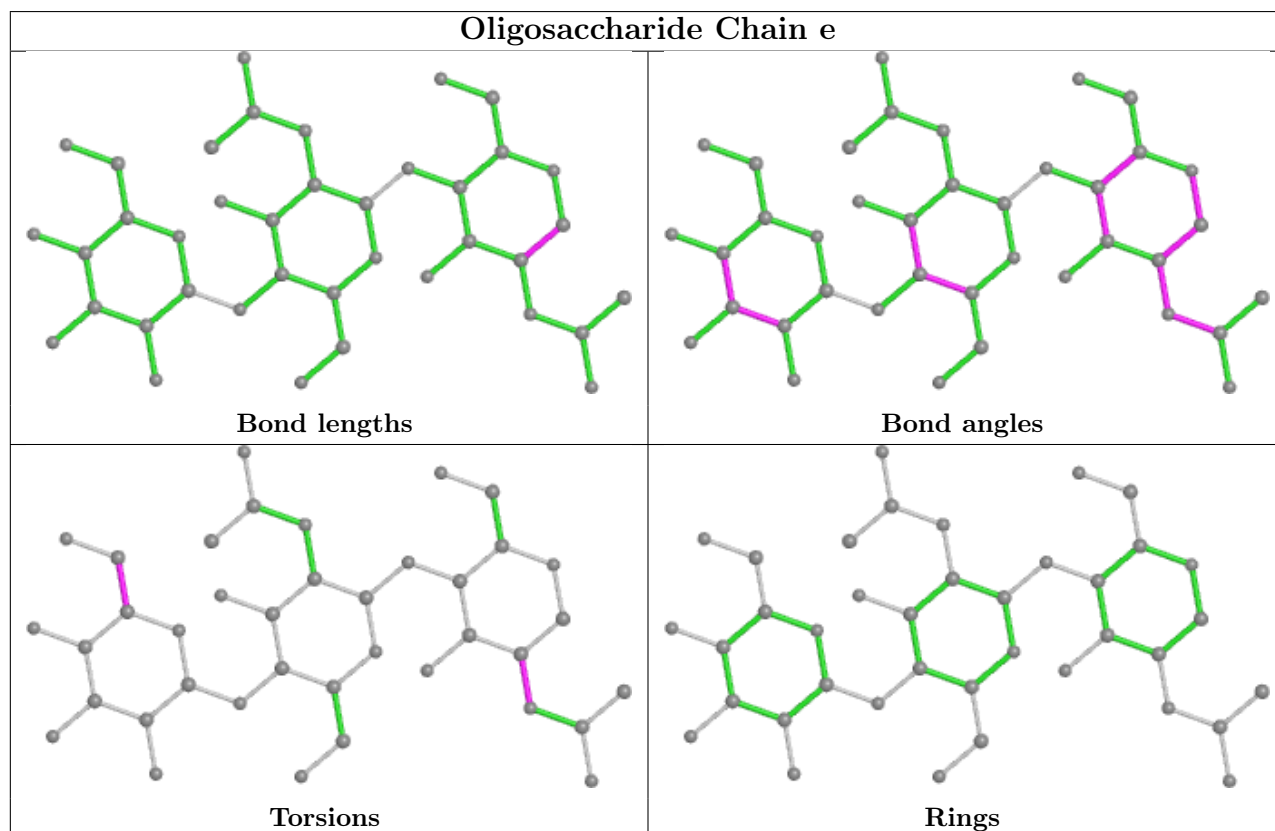
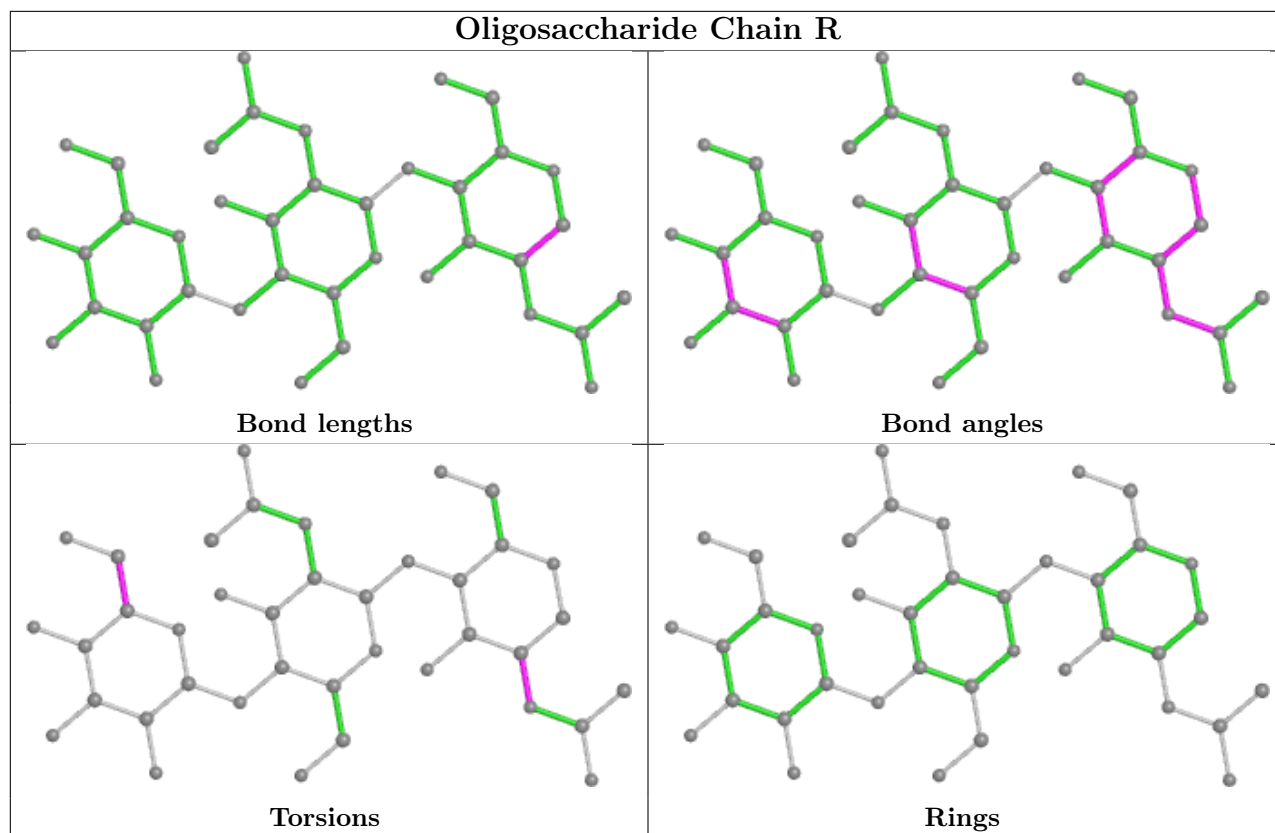


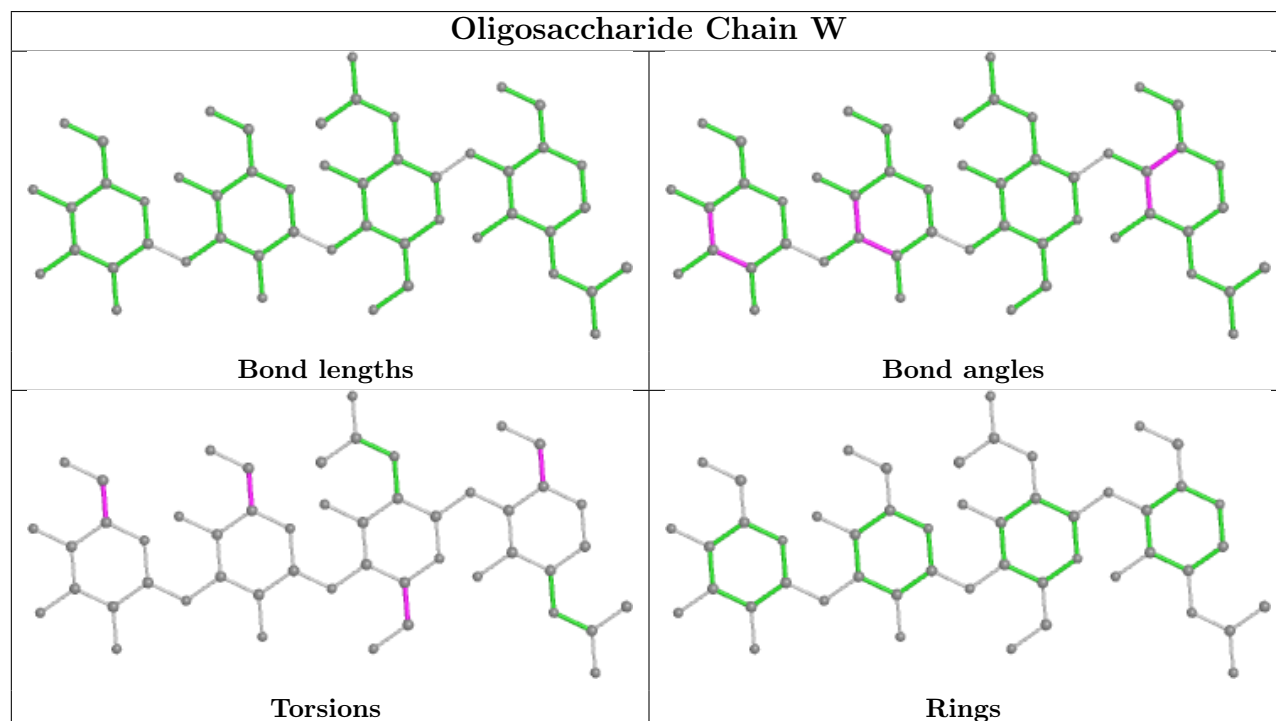
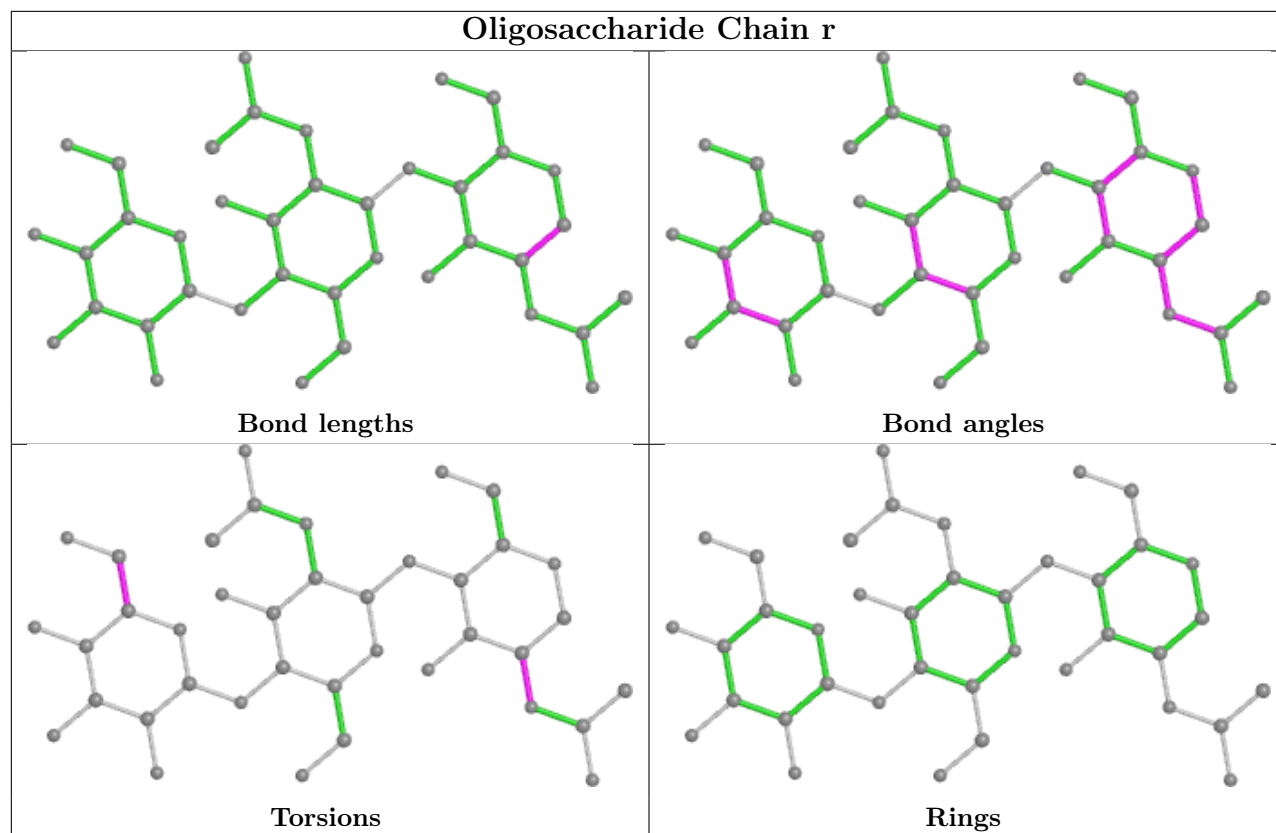


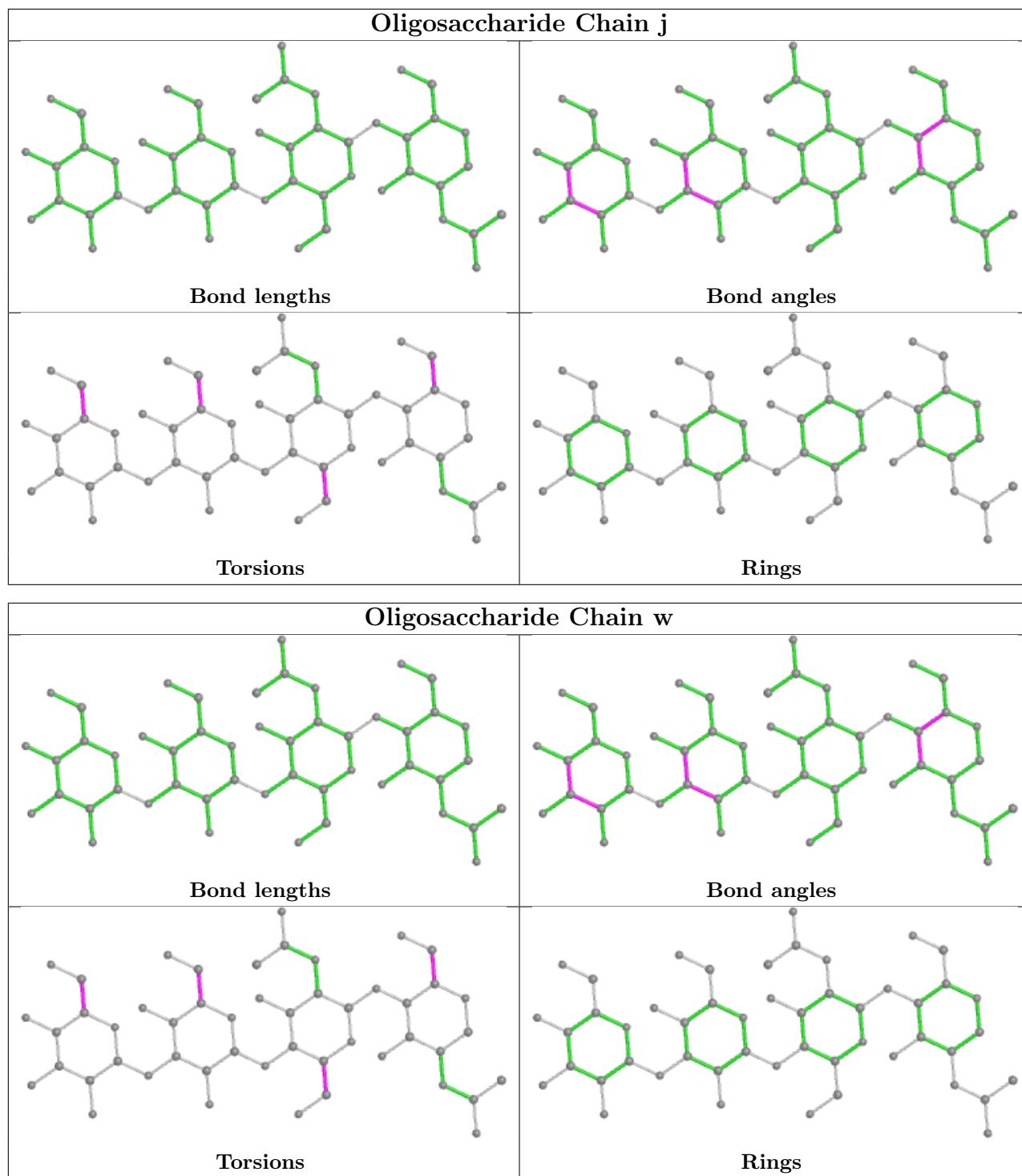












5.6 Ligand geometry [i](#)

30 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	C	613	1	14,14,15	0.75	1 (7%)	17,19,21	0.98	1 (5%)
8	NAG	I	701	2	14,14,15	0.84	1 (7%)	17,19,21	0.98	1 (5%)
8	NAG	I	702	2	14,14,15	0.83	1 (7%)	17,19,21	0.79	1 (5%)
8	NAG	A	606	1	14,14,15	0.76	1 (7%)	17,19,21	1.06	1 (5%)
8	NAG	G	601	1	14,14,15	0.88	1 (7%)	17,19,21	0.75	0
8	NAG	B	701	2	14,14,15	0.83	1 (7%)	17,19,21	0.99	1 (5%)
8	NAG	C	606	1	14,14,15	0.75	1 (7%)	17,19,21	1.05	1 (5%)
8	NAG	A	613	1	14,14,15	0.73	1 (7%)	17,19,21	0.99	1 (5%)
8	NAG	B	703	2	14,14,15	0.71	1 (7%)	17,19,21	0.95	1 (5%)
8	NAG	B	702	2	14,14,15	0.83	1 (7%)	17,19,21	0.79	1 (5%)
8	NAG	C	601	1	14,14,15	0.89	1 (7%)	17,19,21	0.75	0
8	NAG	C	618	1	14,14,15	0.88	1 (7%)	17,19,21	1.09	1 (5%)
8	NAG	B	704	2	14,14,15	0.86	1 (7%)	17,19,21	0.83	0
8	NAG	I	703	2	14,14,15	0.71	1 (7%)	17,19,21	0.96	1 (5%)
8	NAG	G	635	1	14,14,15	0.89	1 (7%)	17,19,21	0.73	0
8	NAG	G	614	1	14,14,15	0.92	1 (7%)	17,19,21	1.18	1 (5%)
8	NAG	G	618	1	14,14,15	0.87	1 (7%)	17,19,21	1.10	1 (5%)
8	NAG	A	635	1	14,14,15	0.89	1 (7%)	17,19,21	0.73	0
8	NAG	A	601	1	14,14,15	0.88	1 (7%)	17,19,21	0.75	0
8	NAG	A	614	1	14,14,15	0.93	1 (7%)	17,19,21	1.18	1 (5%)
8	NAG	I	704	2	14,14,15	0.84	1 (7%)	17,19,21	0.82	0
8	NAG	D	701	2	14,14,15	0.84	1 (7%)	17,19,21	0.98	1 (5%)
8	NAG	G	613	1	14,14,15	0.73	1 (7%)	17,19,21	0.99	1 (5%)
8	NAG	A	618	1	14,14,15	0.88	1 (7%)	17,19,21	1.10	1 (5%)
8	NAG	D	702	2	14,14,15	0.84	1 (7%)	17,19,21	0.79	1 (5%)
8	NAG	D	703	2	14,14,15	0.69	1 (7%)	17,19,21	0.95	1 (5%)
8	NAG	G	606	1	14,14,15	0.75	1 (7%)	17,19,21	1.05	1 (5%)
8	NAG	D	704	2	14,14,15	0.85	1 (7%)	17,19,21	0.82	0
8	NAG	C	635	1	14,14,15	0.89	1 (7%)	17,19,21	0.73	1 (5%)
8	NAG	C	614	1	14,14,15	0.92	1 (7%)	17,19,21	1.18	1 (5%)

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
8	NAG	C	613	1	-	1/6/23/26	0/1/1/1
8	NAG	I	701	2	-	1/6/23/26	0/1/1/1
8	NAG	I	702	2	-	1/6/23/26	0/1/1/1
8	NAG	A	606	1	-	2/6/23/26	0/1/1/1
8	NAG	G	601	1	-	2/6/23/26	0/1/1/1
8	NAG	B	701	2	-	1/6/23/26	0/1/1/1
8	NAG	C	606	1	-	2/6/23/26	0/1/1/1
8	NAG	A	613	1	-	1/6/23/26	0/1/1/1
8	NAG	B	703	2	-	1/6/23/26	0/1/1/1
8	NAG	B	702	2	-	1/6/23/26	0/1/1/1
8	NAG	C	601	1	-	2/6/23/26	0/1/1/1
8	NAG	C	618	1	-	2/6/23/26	0/1/1/1
8	NAG	B	704	2	-	1/6/23/26	0/1/1/1
8	NAG	I	703	2	-	1/6/23/26	0/1/1/1
8	NAG	G	635	1	-	1/6/23/26	0/1/1/1
8	NAG	G	614	1	-	1/6/23/26	0/1/1/1
8	NAG	G	618	1	-	2/6/23/26	0/1/1/1
8	NAG	A	635	1	-	1/6/23/26	0/1/1/1
8	NAG	A	601	1	-	2/6/23/26	0/1/1/1
8	NAG	A	614	1	-	1/6/23/26	0/1/1/1
8	NAG	I	704	2	-	1/6/23/26	0/1/1/1
8	NAG	D	701	2	-	1/6/23/26	0/1/1/1
8	NAG	G	613	1	-	1/6/23/26	0/1/1/1
8	NAG	A	618	1	-	2/6/23/26	0/1/1/1
8	NAG	D	702	2	-	1/6/23/26	0/1/1/1
8	NAG	D	703	2	-	1/6/23/26	0/1/1/1
8	NAG	G	606	1	-	2/6/23/26	0/1/1/1
8	NAG	D	704	2	-	1/6/23/26	0/1/1/1
8	NAG	C	635	1	-	1/6/23/26	0/1/1/1
8	NAG	C	614	1	-	1/6/23/26	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	635	NAG	C1-C2	2.98	1.56	1.52
8	G	635	NAG	C1-C2	2.97	1.56	1.52
8	A	635	NAG	C1-C2	2.94	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	618	NAG	C1-C2	2.86	1.56	1.52
8	A	618	NAG	C1-C2	2.85	1.56	1.52
8	G	618	NAG	C1-C2	2.82	1.56	1.52
8	C	601	NAG	C1-C2	2.81	1.56	1.52
8	A	601	NAG	C1-C2	2.75	1.56	1.52
8	D	702	NAG	C1-C2	2.73	1.56	1.52
8	G	601	NAG	C1-C2	2.72	1.56	1.52
8	I	702	NAG	C1-C2	2.72	1.56	1.52
8	B	702	NAG	C1-C2	2.71	1.56	1.52
8	I	701	NAG	C1-C2	2.69	1.56	1.52
8	D	701	NAG	C1-C2	2.69	1.56	1.52
8	B	704	NAG	C1-C2	2.67	1.56	1.52
8	D	704	NAG	C1-C2	2.64	1.56	1.52
8	B	701	NAG	C1-C2	2.64	1.56	1.52
8	I	704	NAG	C1-C2	2.64	1.56	1.52
8	A	614	NAG	C1-C2	2.33	1.55	1.52
8	A	606	NAG	C1-C2	2.32	1.55	1.52
8	C	614	NAG	C1-C2	2.29	1.55	1.52
8	G	614	NAG	C1-C2	2.29	1.55	1.52
8	C	606	NAG	C1-C2	2.27	1.55	1.52
8	B	703	NAG	C1-C2	2.27	1.55	1.52
8	G	606	NAG	C1-C2	2.26	1.55	1.52
8	I	703	NAG	C1-C2	2.26	1.55	1.52
8	C	613	NAG	C1-C2	2.25	1.55	1.52
8	D	703	NAG	C1-C2	2.19	1.55	1.52
8	A	613	NAG	C1-C2	2.19	1.55	1.52
8	G	613	NAG	C1-C2	2.16	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	618	NAG	C4-C3-C2	-3.37	106.07	111.02
8	A	618	NAG	C4-C3-C2	-3.33	106.14	111.02
8	C	618	NAG	C4-C3-C2	-3.33	106.14	111.02
8	C	614	NAG	C4-C3-C2	-3.27	106.22	111.02
8	G	614	NAG	C4-C3-C2	-3.26	106.25	111.02
8	A	614	NAG	C4-C3-C2	-3.24	106.26	111.02
8	D	703	NAG	C4-C3-C2	-2.96	106.67	111.02
8	I	703	NAG	C4-C3-C2	-2.96	106.68	111.02
8	B	703	NAG	C4-C3-C2	-2.95	106.69	111.02
8	A	613	NAG	C4-C3-C2	-2.83	106.86	111.02
8	G	613	NAG	C4-C3-C2	-2.81	106.90	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	613	NAG	C4-C3-C2	-2.78	106.94	111.02
8	A	606	NAG	C4-C3-C2	-2.68	107.10	111.02
8	B	701	NAG	C4-C3-C2	-2.64	107.15	111.02
8	C	606	NAG	C4-C3-C2	-2.62	107.17	111.02
8	I	701	NAG	C4-C3-C2	-2.62	107.18	111.02
8	G	606	NAG	C4-C3-C2	-2.62	107.19	111.02
8	D	701	NAG	C4-C3-C2	-2.61	107.20	111.02
8	I	702	NAG	C4-C3-C2	-2.30	107.64	111.02
8	B	702	NAG	C4-C3-C2	-2.30	107.65	111.02
8	D	702	NAG	C4-C3-C2	-2.28	107.67	111.02
8	C	635	NAG	C4-C3-C2	-2.00	108.09	111.02

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	606	NAG	O5-C5-C6-O6
8	C	606	NAG	O5-C5-C6-O6
8	G	606	NAG	O5-C5-C6-O6
8	A	618	NAG	O5-C5-C6-O6
8	C	618	NAG	O5-C5-C6-O6
8	G	618	NAG	O5-C5-C6-O6
8	A	614	NAG	O5-C5-C6-O6
8	B	701	NAG	O5-C5-C6-O6
8	C	614	NAG	O5-C5-C6-O6
8	D	701	NAG	O5-C5-C6-O6
8	G	614	NAG	O5-C5-C6-O6
8	I	701	NAG	O5-C5-C6-O6
8	D	703	NAG	O5-C5-C6-O6
8	I	703	NAG	O5-C5-C6-O6
8	B	703	NAG	O5-C5-C6-O6
8	B	704	NAG	O5-C5-C6-O6
8	D	704	NAG	O5-C5-C6-O6
8	I	704	NAG	O5-C5-C6-O6
8	A	613	NAG	O5-C5-C6-O6
8	C	613	NAG	O5-C5-C6-O6
8	G	613	NAG	O5-C5-C6-O6
8	A	606	NAG	C4-C5-C6-O6
8	C	606	NAG	C4-C5-C6-O6
8	B	702	NAG	O5-C5-C6-O6
8	D	702	NAG	O5-C5-C6-O6
8	I	702	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	G	606	NAG	C4-C5-C6-O6
8	A	601	NAG	C1-C2-N2-C7
8	C	601	NAG	C1-C2-N2-C7
8	G	601	NAG	C1-C2-N2-C7
8	A	635	NAG	O5-C5-C6-O6
8	C	635	NAG	O5-C5-C6-O6
8	G	635	NAG	O5-C5-C6-O6
8	A	601	NAG	O5-C5-C6-O6
8	C	601	NAG	O5-C5-C6-O6
8	G	601	NAG	O5-C5-C6-O6
8	C	618	NAG	C4-C5-C6-O6
8	A	618	NAG	C4-C5-C6-O6
8	G	618	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20642. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.