



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 12:23 pm GMT

PDB ID : 5ACO
EMDB ID : EMD-3121
Title : Cryo-EM structure of PGT128 Fab in complex with BG505 SOSIP.664 Env trimer
Authors : Lee, J.H.; Ward, A.B.
Deposited on : 2015-08-17
Resolution : 4.36 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

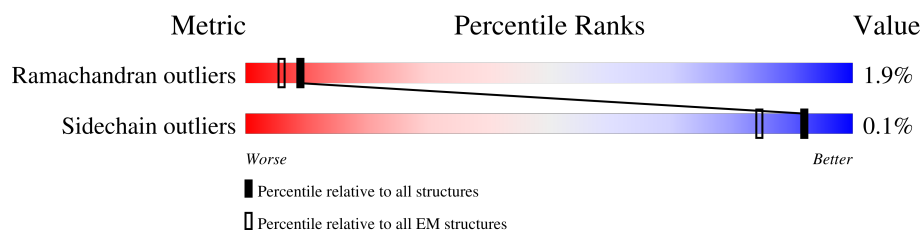
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 4.36 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	207382	16835
Sidechain outliers	206894	16415

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	476	 7% 89% .. 8%
1	C	476	 7% 89% .. 8%
1	D	476	 7% 89% .. 8%
2	B	153	 14% 82% 5% 14%
2	E	153	 14% 82% 5% 14%
2	F	153	 14% 82% 5% 14%
3	G	239	 8% 55% 45%
3	H	239	 8% 55% 45%
3	I	239	 8% 55% 45%

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Mol	Chain	Length	Quality of chain
4	J	211	
4	K	211	
4	L	211	
5	0	3	
5	5	3	
5	6	3	
5	M	3	
5	O	3	
5	P	3	
5	T	3	
5	Y	3	
5	Z	3	
5	d	3	
5	f	3	
5	g	3	
5	k	3	
5	p	3	
5	q	3	
5	t	3	
5	v	3	
5	w	3	
6	4	2	
6	7	2	
6	8	2	
6	9	2	

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Mol	Chain	Length	Quality of chain
6	AA	2	100%
6	N	2	50% 100%
6	Q	2	50% 100%
6	R	2	50% 100%
6	X	2	100% 100%
6	a	2	100% 100%
6	b	2	50% 100%
6	c	2	100% 100%
6	e	2	50% 100%
6	h	2	50% 100%
6	i	2	50% 100%
6	o	2	100% 100% 100%
6	r	2	100% 100%
6	s	2	50% 100%
6	u	2	50% 100%
6	x	2	50% 100%
6	y	2	50% 100%
7	2	7	29% 100%
7	S	7	57% 86% 14%
7	V	7	29% 100%
7	j	7	57% 86% 14%
7	m	7	29% 100%
7	z	7	57% 86% 14%
8	1	5	60% 100%
8	U	5	60% 100%

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Mol	Chain	Length	Quality of chain
8	1	5	<div><div></div><div>60%100%</div></div>
9	3	10	<div><div></div><div>10%20%80%</div></div>
9	W	10	<div><div></div><div>10%20%80%</div></div>
9	n	10	<div><div></div><div>20%80%</div></div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 21297 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 HIV-1 ENVELOPE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	438	Total	C	N	O	S	0	0
			3453	2170	610	645	28		
1	C	438	Total	C	N	O	S	0	0
			3453	2170	610	645	28		
1	D	438	Total	C	N	O	S	0	0
			3453	2170	610	645	28		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	engineered mutation	UNP Q2N0S6
A	501	CYS	ALA	engineered mutation	UNP Q2N0S6
C	332	ASN	THR	engineered mutation	UNP Q2N0S6
C	501	CYS	ALA	engineered mutation	UNP Q2N0S6
D	332	ASN	THR	engineered mutation	UNP Q2N0S6
D	501	CYS	ALA	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called HIV-1 ENVELOPE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	132	Total	C	N	O	S	0	0
			1051	667	180	198	6		
2	E	132	Total	C	N	O	S	0	0
			1051	667	180	198	6		
2	F	132	Total	C	N	O	S	0	0
			1051	667	180	198	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6
E	559	PRO	ILE	engineered mutation	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	605	CYS	THR	engineered mutation	UNP Q2N0S6
F	559	PRO	ILE	engineered mutation	UNP Q2N0S6
F	605	CYS	THR	engineered mutation	UNP Q2N0S6

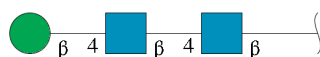
- Molecule 3 is a protein called PGT128 FAB.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	132	Total	C	N	O	S	0	0
			1028	659	175	190	4		
3	H	132	Total	C	N	O	S	0	0
			1028	659	175	190	4		
3	I	132	Total	C	N	O	S	0	0
			1028	659	175	190	4		

- Molecule 4 is a protein called PGT128 FAB.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	103	Total	C	N	O	S	0	0
			752	469	128	153	2		
4	K	103	Total	C	N	O	S	0	0
			752	469	128	153	2		
4	L	103	Total	C	N	O	S	0	0
			752	469	128	153	2		

- Molecule 5 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
5	M	3	Total	C	N	O	0	0
			39	22	2	15		
5	O	3	Total	C	N	O	0	0
			39	22	2	15		
5	P	3	Total	C	N	O	0	0
			39	22	2	15		
5	T	3	Total	C	N	O	0	0
			39	22	2	15		
5	Y	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	Z	3	Total	C	N	O	0	0
			39	22	2	15		
5	d	3	Total	C	N	O	0	0
			39	22	2	15		
5	f	3	Total	C	N	O	0	0
			39	22	2	15		
5	g	3	Total	C	N	O	0	0
			39	22	2	15		
5	k	3	Total	C	N	O	0	0
			39	22	2	15		
5	p	3	Total	C	N	O	0	0
			39	22	2	15		
5	q	3	Total	C	N	O	0	0
			39	22	2	15		
5	t	3	Total	C	N	O	0	0
			39	22	2	15		
5	v	3	Total	C	N	O	0	0
			39	22	2	15		
5	w	3	Total	C	N	O	0	0
			39	22	2	15		
5	0	3	Total	C	N	O	0	0
			39	22	2	15		
5	5	3	Total	C	N	O	0	0
			39	22	2	15		
5	6	3	Total	C	N	O	0	0
			39	22	2	15		

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



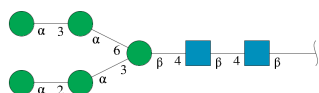
Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	2	Total	C	N	O	0	0
			28	16	2	10		
6	Q	2	Total	C	N	O	0	0
			28	16	2	10		
6	R	2	Total	C	N	O	0	0
			28	16	2	10		
6	X	2	Total	C	N	O	0	0
			28	16	2	10		

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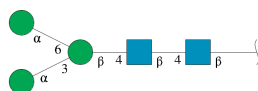
Mol	Chain	Residues	Atoms				AltConf	Trace
6	a	2	Total	C	N	O	0	0
			28	16	2	10		
6	b	2	Total	C	N	O	0	0
			28	16	2	10		
6	c	2	Total	C	N	O	0	0
			28	16	2	10		
6	e	2	Total	C	N	O	0	0
			28	16	2	10		
6	h	2	Total	C	N	O	0	0
			28	16	2	10		
6	i	2	Total	C	N	O	0	0
			28	16	2	10		
6	o	2	Total	C	N	O	0	0
			28	16	2	10		
6	r	2	Total	C	N	O	0	0
			28	16	2	10		
6	s	2	Total	C	N	O	0	0
			28	16	2	10		
6	u	2	Total	C	N	O	0	0
			28	16	2	10		
6	x	2	Total	C	N	O	0	0
			28	16	2	10		
6	y	2	Total	C	N	O	0	0
			28	16	2	10		
6	4	2	Total	C	N	O	0	0
			28	16	2	10		
6	7	2	Total	C	N	O	0	0
			28	16	2	10		
6	8	2	Total	C	N	O	0	0
			28	16	2	10		
6	9	2	Total	C	N	O	0	0
			28	16	2	10		
6	AA	2	Total	C	N	O	0	0
			28	16	2	10		

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



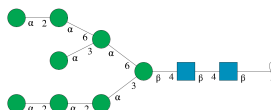
Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	7	Total	C	N	O	0	0
			83	46	2	35		
7	V	7	Total	C	N	O	0	0
			83	46	2	35		
7	j	7	Total	C	N	O	0	0
			83	46	2	35		
7	m	7	Total	C	N	O	0	0
			83	46	2	35		
7	z	7	Total	C	N	O	0	0
			83	46	2	35		
7	2	7	Total	C	N	O	0	0
			83	46	2	35		

- 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	U	5	Total	C	N	O	0	0
			61	34	2	25		
8	l	5	Total	C	N	O	0	0
			61	34	2	25		
8	1	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-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.



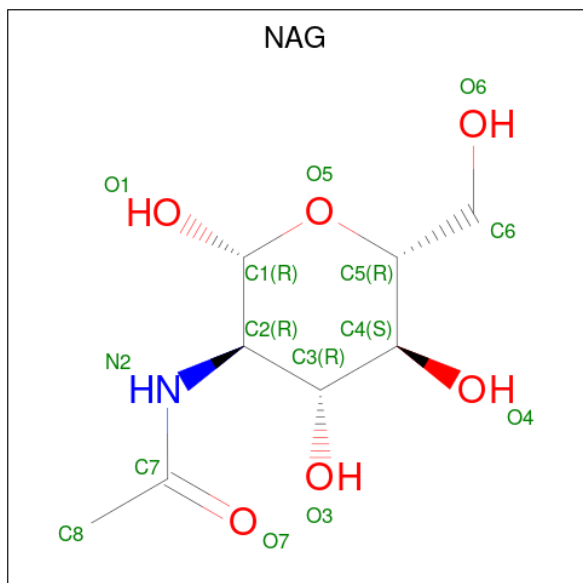
Mol	Chain	Residues	Atoms				AltConf	Trace
9	W	10	Total	C	N	O	0	0
			116	64	2	50		

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	n	10	Total	C	N	O	0	0
			116	64	2	50		
9	3	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

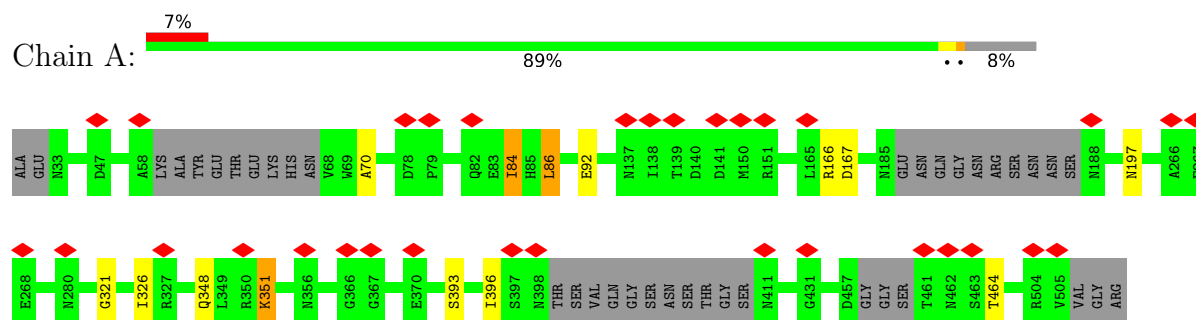


Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	B	1	Total	C	N	O	0
			14	8	1	5	
10	B	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	D	1	Total	C	N	O	0
			14	8	1	5	
10	E	1	Total	C	N	O	0
			14	8	1	5	
10	E	1	Total	C	N	O	0
			14	8	1	5	
10	F	1	Total	C	N	O	0
			14	8	1	5	
10	F	1	Total	C	N	O	0
			14	8	1	5	

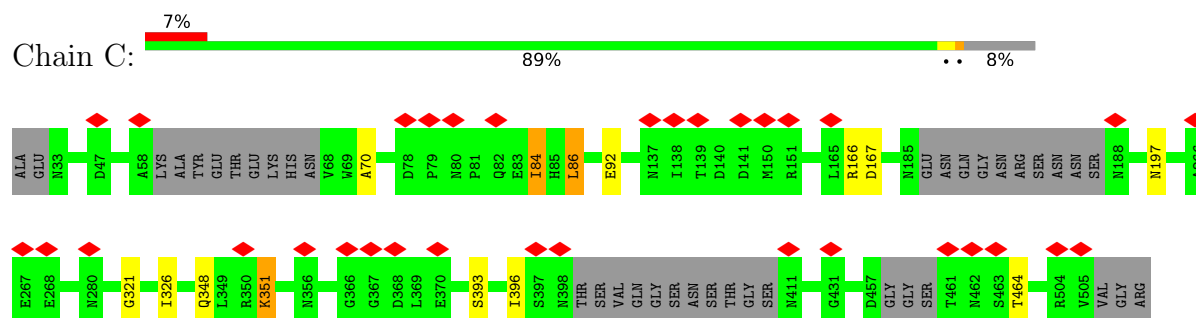
3 Residue-property plots [i](#)

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

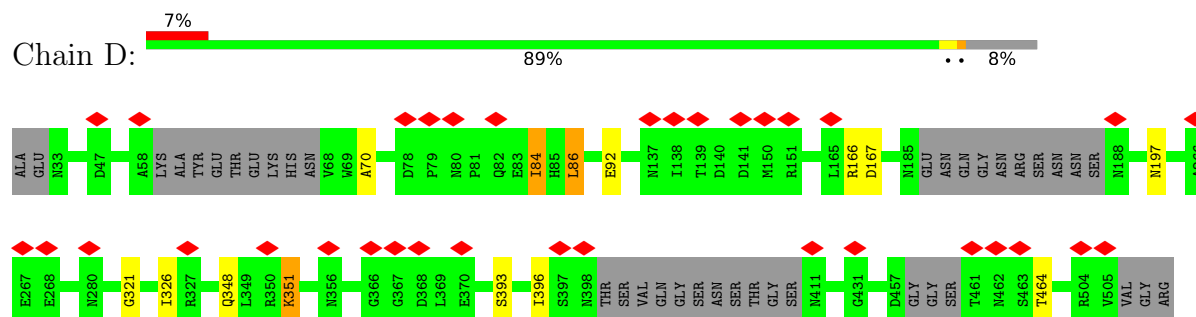
• Molecule 1: HIV-1 ENVELOPE GLYCOPROTEIN



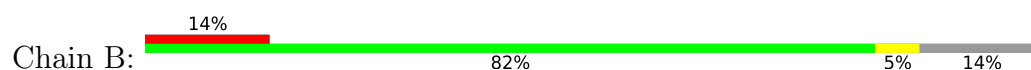
• Molecule 1: HIV-1 ENVELOPE GLYCOPROTEIN

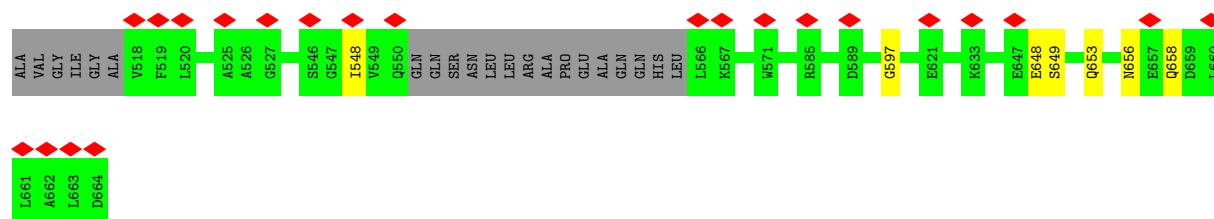


• Molecule 1: HIV-1 ENVELOPE GLYCOPROTEIN

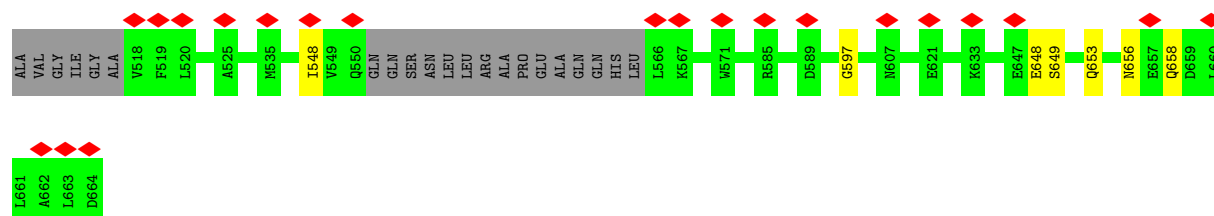
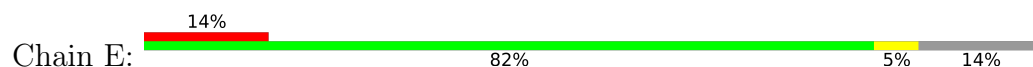


• Molecule 2: HIV-1 ENVELOPE GLYCOPROTEIN

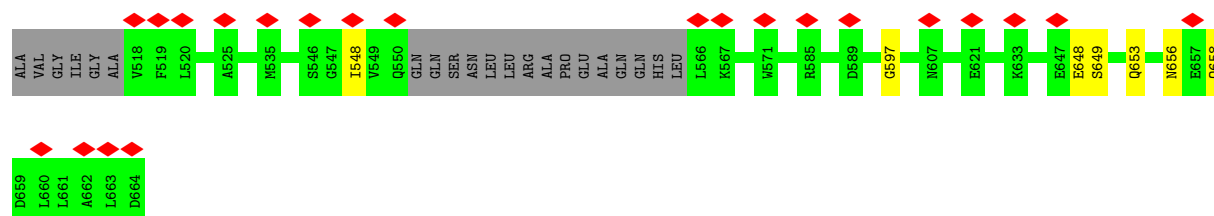
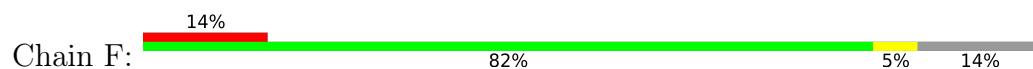




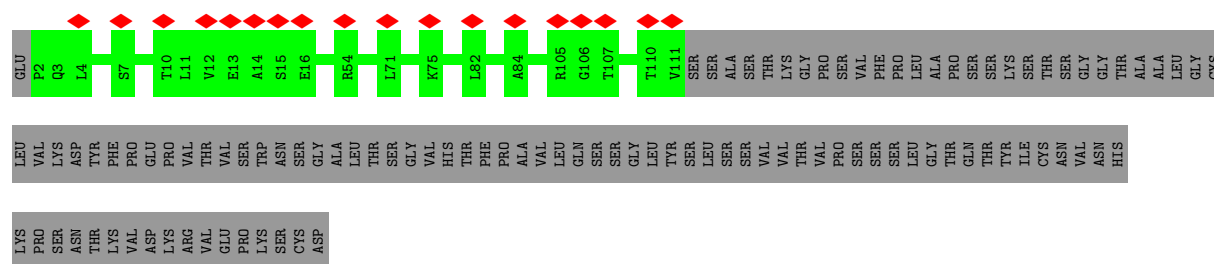
- Molecule 2: HIV-1 ENVELOPE GLYCOPROTEIN



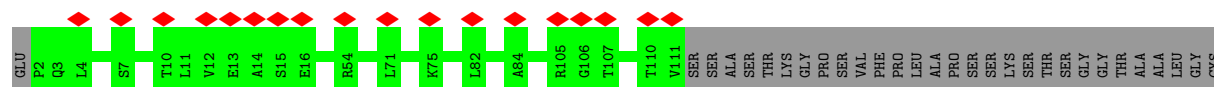
- Molecule 2: HIV-1 ENVELOPE GLYCOPROTEIN



- Molecule 3: PGT128 FAB



- Molecule 3: PGT128 FAB



LYS
ALA
THR
LEU
VAL
CYS
VAL
LEU
ILE
SER
ASP
PHE
TYR
PRO
GLY
ALA
VAL
THR
VAL
ALA
TRP
LYS
ASP
SER
SER
PRO
VAL
LYS
ALA
GLY
VAL
GLU
THR
THR
PRO
SER
LYS
GLN
SER
ASN
LYS
TYR
ALA
ALA
SER
SER
TYR
LEU
SER
LEU
THR
PRO
GLN
TRP
LYS
SER
HIS

ARG
SER
TYR
SER
CYS
GLN
VAL
THR
HIS
SER
GLY
SER
THR
VAL
GLU
LYS
THR
VAL
ALA
PRO
THR
GLU
CYS
SER

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

Chain M: 

 
MAG1
MAG2
BMA3

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

Chain O: 

 
MAG1
MAG2
BMA3

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

Chain P: 

 
MAG1
MAG2
BMA3

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

Chain T: 

 
MAG1
MAG2
BMA3

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

Chain Y: 

 
MAG1
MAG2
BMA3

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



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



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



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

Chain q:  33% 100%



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

Chain t:  100% 100%



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

Chain v:  67% 100%



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

Chain w:  67% 100%



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

Chain 0:  100% 100%



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

Chain 5:  67% 100%



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



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



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



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



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



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



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



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



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



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



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



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

Chain o:  100%
100%



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

Chain r:  100%
100%



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

Chain s:  50%
100%



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

Chain u:  50%
100%



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

Chain x:  50%
100%



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

Chain y:  50%
100%



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



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



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



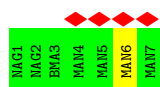
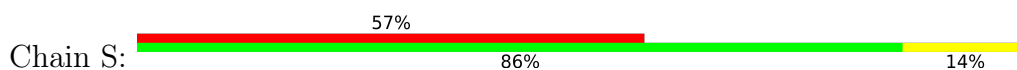
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



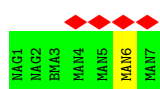
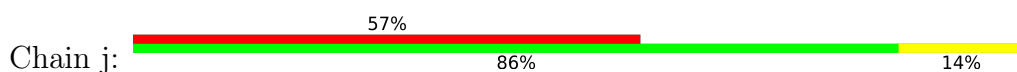
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 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



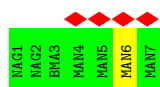
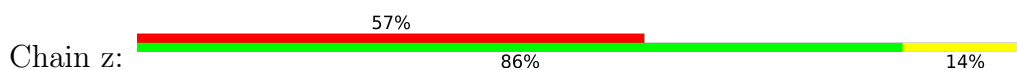
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 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 7: 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 7: 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 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-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

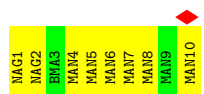


- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	92095	Depositor
Resolution determination method	Not provided	
CTF correction method	WHOLE MICROGRAPH	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.041	Depositor
Map size (\AA)	335.36, 335.36, 335.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.31, 1.31, 1.31	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: BMA, MAN, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.64	2/3523 (0.1%)	0.73	15/4783 (0.3%)
1	C	0.64	2/3523 (0.1%)	0.73	15/4783 (0.3%)
1	D	0.64	2/3523 (0.1%)	0.73	15/4783 (0.3%)
2	B	0.72	1/1069 (0.1%)	0.81	5/1448 (0.3%)
2	E	0.72	1/1069 (0.1%)	0.81	5/1448 (0.3%)
2	F	0.72	1/1069 (0.1%)	0.81	5/1448 (0.3%)
3	G	0.66	0/1061	0.72	0/1455
3	H	0.65	0/1061	0.72	0/1455
3	I	0.65	0/1061	0.72	0/1455
4	J	0.75	2/769 (0.3%)	0.92	3/1048 (0.3%)
4	K	0.75	2/769 (0.3%)	0.92	3/1048 (0.3%)
4	L	0.75	2/769 (0.3%)	0.92	3/1048 (0.3%)
All	All	0.67	15/19266 (0.1%)	0.77	69/26202 (0.3%)

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	1
1	C	0	1
1	D	0	1
All	All	0	3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	658	GLN	C-N	12.04	1.61	1.34
2	F	658	GLN	C-N	12.04	1.61	1.34
2	E	658	GLN	C-N	12.00	1.61	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	8	PRO	C-N	10.79	1.58	1.34
4	J	8	PRO	C-N	10.77	1.58	1.34

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	648	GLU	N-CA-C	14.16	149.23	111.00
2	B	648	GLU	N-CA-C	14.16	149.22	111.00
2	F	648	GLU	N-CA-C	14.14	149.18	111.00
1	C	84	ILE	O-C-N	12.71	143.04	122.70
1	D	84	ILE	O-C-N	12.70	143.01	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	86	LEU	Mainchain
1	C	86	LEU	Mainchain
1	D	86	LEU	Mainchain

5.2 Too-close contacts [i](#)

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	428/476 (90%)	386 (90%)	33 (8%)	9 (2%)	5	30
1	C	428/476 (90%)	386 (90%)	33 (8%)	9 (2%)	5	30
1	D	428/476 (90%)	386 (90%)	33 (8%)	9 (2%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	128/153 (84%)	102 (80%)	22 (17%)	4 (3%)	3	23
2	E	128/153 (84%)	102 (80%)	22 (17%)	4 (3%)	3	23
2	F	128/153 (84%)	102 (80%)	22 (17%)	4 (3%)	3	23
3	G	130/239 (54%)	121 (93%)	9 (7%)	0	100	100
3	H	130/239 (54%)	121 (93%)	9 (7%)	0	100	100
3	I	130/239 (54%)	121 (93%)	9 (7%)	0	100	100
4	J	101/211 (48%)	91 (90%)	8 (8%)	2 (2%)	6	32
4	K	101/211 (48%)	91 (90%)	8 (8%)	2 (2%)	6	32
4	L	101/211 (48%)	91 (90%)	8 (8%)	2 (2%)	6	32
All	All	2361/3237 (73%)	2100 (89%)	216 (9%)	45 (2%)	9	33

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	ASP
1	A	396	ILE
1	C	167	ASP
1	C	396	ILE
1	D	167	ASP

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	393/423 (93%)	392 (100%)	1 (0%)	91	92
1	C	393/423 (93%)	392 (100%)	1 (0%)	91	92
1	D	393/423 (93%)	392 (100%)	1 (0%)	91	92
2	B	114/129 (88%)	114 (100%)	0	100	100
2	E	114/129 (88%)	114 (100%)	0	100	100
2	F	114/129 (88%)	114 (100%)	0	100	100
3	G	110/203 (54%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	110/203 (54%)	110 (100%)	0	100	100
3	I	110/203 (54%)	110 (100%)	0	100	100
4	J	84/177 (48%)	84 (100%)	0	100	100
4	K	84/177 (48%)	84 (100%)	0	100	100
4	L	84/177 (48%)	84 (100%)	0	100	100
All	All	2103/2796 (75%)	2100 (100%)	3 (0%)	92	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	C	197	ASN
1	D	197	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	59	HIS
3	H	59	HIS
3	I	59	HIS
1	C	279	ASN
1	A	279	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](#)

183 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	0	1	1,5	14,14,15	0.49	0	17,19,21	2.24	3 (17%)
5	NAG	0	2	5	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
5	BMA	0	3	5	11,11,12	0.63	0	15,15,17	1.47	3 (20%)
8	NAG	1	1	8,1	14,14,15	0.49	0	17,19,21	2.24	3 (17%)
8	NAG	1	2	8	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
8	BMA	1	3	8	11,11,12	0.64	0	15,15,17	1.46	3 (20%)
8	MAN	1	4	8	11,11,12	0.55	0	15,15,17	1.72	4 (26%)
8	MAN	1	5	8	11,11,12	0.63	0	15,15,17	2.53	4 (26%)
7	NAG	2	1	1,7	14,14,15	0.31	0	17,19,21	0.87	1 (5%)
7	NAG	2	2	7	14,14,15	0.32	0	17,19,21	2.40	4 (23%)
7	BMA	2	3	7	11,11,12	0.44	0	15,15,17	1.22	2 (13%)
7	MAN	2	4	7	11,11,12	0.44	0	15,15,17	0.90	1 (6%)
7	MAN	2	5	7	11,11,12	0.44	0	15,15,17	0.88	1 (6%)
7	MAN	2	6	7	11,11,12	0.49	0	15,15,17	0.82	1 (6%)
7	MAN	2	7	7	11,11,12	0.34	0	15,15,17	1.31	2 (13%)
9	NAG	3	1	1,9	14,14,15	0.32	0	17,19,21	0.89	1 (5%)
9	MAN	3	10	9	11,11,12	0.34	0	15,15,17	0.92	2 (13%)
9	NAG	3	2	9	14,14,15	0.33	0	17,19,21	0.90	1 (5%)
9	BMA	3	3	9	11,11,12	0.42	0	15,15,17	0.63	0
9	MAN	3	4	9	11,11,12	0.43	0	15,15,17	1.07	1 (6%)
9	MAN	3	5	9	11,11,12	0.47	0	15,15,17	1.05	2 (13%)
9	MAN	3	6	9	11,11,12	0.49	0	15,15,17	1.19	1 (6%)
9	MAN	3	7	9	11,11,12	0.29	0	15,15,17	1.12	1 (6%)
9	MAN	3	8	9	11,11,12	0.38	0	15,15,17	1.26	1 (6%)
9	MAN	3	9	9	11,11,12	0.34	0	15,15,17	0.78	0
6	NAG	4	1	1,6	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
6	NAG	4	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
5	NAG	5	1	1,5	14,14,15	0.49	0	17,19,21	2.24	3 (17%)
5	NAG	5	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
5	BMA	5	3	5	11,11,12	0.65	0	15,15,17	1.47	3 (20%)
5	NAG	6	1	1,5	14,14,15	0.50	0	17,19,21	2.23	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	6	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
5	BMA	6	3	5	11,11,12	0.66	0	15,15,17	1.47	3 (20%)
6	NAG	7	1	1,6	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
6	NAG	7	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
6	NAG	8	1	1,6	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
6	NAG	8	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
6	NAG	9	1	2,6	14,14,15	0.52	0	17,19,21	2.23	3 (17%)
6	NAG	9	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
6	NAG	AA	1	2,6	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
6	NAG	AA	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
5	NAG	M	1	1,5	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	M	2	5	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
5	BMA	M	3	5	11,11,12	0.64	0	15,15,17	1.47	3 (20%)
6	NAG	N	1	1,6	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
6	NAG	N	2	6	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
5	NAG	O	1	1,5	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	O	2	5	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
5	BMA	O	3	5	11,11,12	0.64	0	15,15,17	1.46	3 (20%)
5	NAG	P	1	1,5	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	P	2	5	14,14,15	0.51	0	17,19,21	1.37	3 (17%)
5	BMA	P	3	5	11,11,12	0.66	0	15,15,17	1.47	3 (20%)
6	NAG	Q	1	1,6	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
6	NAG	Q	2	6	14,14,15	0.53	0	17,19,21	1.38	3 (17%)
6	NAG	R	1	1,6	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
6	NAG	R	2	6	14,14,15	0.50	0	17,19,21	1.39	3 (17%)
7	NAG	S	1	1,7	14,14,15	0.60	0	17,19,21	0.68	0
7	NAG	S	2	7	14,14,15	0.58	0	17,19,21	0.89	0
7	BMA	S	3	7	11,11,12	0.66	0	15,15,17	0.86	0
7	MAN	S	4	7	11,11,12	0.62	0	15,15,17	0.67	0
7	MAN	S	5	7	11,11,12	0.53	0	15,15,17	0.74	0
7	MAN	S	6	7	11,11,12	0.66	0	15,15,17	1.10	2 (13%)
7	MAN	S	7	7	11,11,12	0.62	0	15,15,17	0.62	0
5	NAG	T	1	1,5	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	T	2	5	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
5	BMA	T	3	5	11,11,12	0.64	0	15,15,17	1.47	3 (20%)
8	NAG	U	1	8,1	14,14,15	0.50	0	17,19,21	2.23	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	U	2	8	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
8	BMA	U	3	8	11,11,12	0.64	0	15,15,17	1.46	3 (20%)
8	MAN	U	4	8	11,11,12	0.55	0	15,15,17	1.72	4 (26%)
8	MAN	U	5	8	11,11,12	0.62	0	15,15,17	2.53	4 (26%)
7	NAG	V	1	1,7	14,14,15	0.31	0	17,19,21	0.87	1 (5%)
7	NAG	V	2	7	14,14,15	0.32	0	17,19,21	2.40	4 (23%)
7	BMA	V	3	7	11,11,12	0.44	0	15,15,17	1.22	2 (13%)
7	MAN	V	4	7	11,11,12	0.44	0	15,15,17	0.90	1 (6%)
7	MAN	V	5	7	11,11,12	0.45	0	15,15,17	0.87	1 (6%)
7	MAN	V	6	7	11,11,12	0.48	0	15,15,17	0.82	1 (6%)
7	MAN	V	7	7	11,11,12	0.33	0	15,15,17	1.30	2 (13%)
9	NAG	W	1	1,9	14,14,15	0.31	0	17,19,21	0.89	1 (5%)
9	MAN	W	10	9	11,11,12	0.34	0	15,15,17	0.92	2 (13%)
9	NAG	W	2	9	14,14,15	0.33	0	17,19,21	0.89	1 (5%)
9	BMA	W	3	9	11,11,12	0.42	0	15,15,17	0.62	0
9	MAN	W	4	9	11,11,12	0.43	0	15,15,17	1.07	1 (6%)
9	MAN	W	5	9	11,11,12	0.47	0	15,15,17	1.04	2 (13%)
9	MAN	W	6	9	11,11,12	0.49	0	15,15,17	1.20	1 (6%)
9	MAN	W	7	9	11,11,12	0.28	0	15,15,17	1.12	1 (6%)
9	MAN	W	8	9	11,11,12	0.38	0	15,15,17	1.26	1 (6%)
9	MAN	W	9	9	11,11,12	0.33	0	15,15,17	0.77	0
6	NAG	X	1	1,6	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
6	NAG	X	2	6	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
5	NAG	Y	1	1,5	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
5	NAG	Y	2	5	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
5	BMA	Y	3	5	11,11,12	0.64	0	15,15,17	1.47	3 (20%)
5	NAG	Z	1	1,5	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
5	NAG	Z	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
5	BMA	Z	3	5	11,11,12	0.65	0	15,15,17	1.47	3 (20%)
6	NAG	a	1	1,6	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
6	NAG	a	2	6	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
6	NAG	b	1	1,6	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
6	NAG	b	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
6	NAG	c	1	2,6	14,14,15	0.52	0	17,19,21	2.23	3 (17%)
6	NAG	c	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	d	1	1,5	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	d	2	5	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
5	BMA	d	3	5	11,11,12	0.64	0	15,15,17	1.47	3 (20%)
6	NAG	e	1	1,6	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
6	NAG	e	2	6	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
5	NAG	f	1	1,5	14,14,15	0.52	0	17,19,21	2.24	3 (17%)
5	NAG	f	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
5	BMA	f	3	5	11,11,12	0.64	0	15,15,17	1.46	3 (20%)
5	NAG	g	1	1,5	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	g	2	5	14,14,15	0.52	0	17,19,21	1.37	3 (17%)
5	BMA	g	3	5	11,11,12	0.65	0	15,15,17	1.46	3 (20%)
6	NAG	h	1	1,6	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
6	NAG	h	2	6	14,14,15	0.54	0	17,19,21	1.38	3 (17%)
6	NAG	i	1	1,6	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
6	NAG	i	2	6	14,14,15	0.50	0	17,19,21	1.39	3 (17%)
7	NAG	j	1	1,7	14,14,15	0.60	0	17,19,21	0.67	0
7	NAG	j	2	7	14,14,15	0.57	0	17,19,21	0.90	0
7	BMA	j	3	7	11,11,12	0.66	0	15,15,17	0.87	0
7	MAN	j	4	7	11,11,12	0.61	0	15,15,17	0.67	0
7	MAN	j	5	7	11,11,12	0.53	0	15,15,17	0.74	0
7	MAN	j	6	7	11,11,12	0.66	0	15,15,17	1.10	2 (13%)
7	MAN	j	7	7	11,11,12	0.63	0	15,15,17	0.63	0
5	NAG	k	1	1,5	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
5	NAG	k	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
5	BMA	k	3	5	11,11,12	0.64	0	15,15,17	1.46	3 (20%)
8	NAG	l	1	8,1	14,14,15	0.49	0	17,19,21	2.23	3 (17%)
8	NAG	l	2	8	14,14,15	0.52	0	17,19,21	1.37	3 (17%)
8	BMA	l	3	8	11,11,12	0.65	0	15,15,17	1.46	3 (20%)
8	MAN	l	4	8	11,11,12	0.55	0	15,15,17	1.72	4 (26%)
8	MAN	l	5	8	11,11,12	0.64	0	15,15,17	2.52	4 (26%)
7	NAG	m	1	1,7	14,14,15	0.32	0	17,19,21	0.87	1 (5%)
7	NAG	m	2	7	14,14,15	0.32	0	17,19,21	2.39	4 (23%)
7	BMA	m	3	7	11,11,12	0.44	0	15,15,17	1.22	2 (13%)
7	MAN	m	4	7	11,11,12	0.44	0	15,15,17	0.90	1 (6%)
7	MAN	m	5	7	11,11,12	0.45	0	15,15,17	0.86	1 (6%)
7	MAN	m	6	7	11,11,12	0.48	0	15,15,17	0.82	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	m	7	7	11,11,12	0.33	0	15,15,17	1.31	2 (13%)
9	NAG	n	1	1,9	14,14,15	0.32	0	17,19,21	0.90	1 (5%)
9	MAN	n	10	9	11,11,12	0.33	0	15,15,17	0.93	2 (13%)
9	NAG	n	2	9	14,14,15	0.33	0	17,19,21	0.89	1 (5%)
9	BMA	n	3	9	11,11,12	0.41	0	15,15,17	0.62	0
9	MAN	n	4	9	11,11,12	0.44	0	15,15,17	1.07	1 (6%)
9	MAN	n	5	9	11,11,12	0.47	0	15,15,17	1.04	2 (13%)
9	MAN	n	6	9	11,11,12	0.49	0	15,15,17	1.19	1 (6%)
9	MAN	n	7	9	11,11,12	0.29	0	15,15,17	1.13	1 (6%)
9	MAN	n	8	9	11,11,12	0.39	0	15,15,17	1.27	1 (6%)
9	MAN	n	9	9	11,11,12	0.33	0	15,15,17	0.78	0
6	NAG	o	1	1,6	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
6	NAG	o	2	6	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
5	NAG	p	1	1,5	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
5	NAG	p	2	5	14,14,15	0.53	0	17,19,21	1.39	3 (17%)
5	BMA	p	3	5	11,11,12	0.64	0	15,15,17	1.47	3 (20%)
5	NAG	q	1	1,5	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
5	NAG	q	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
5	BMA	q	3	5	11,11,12	0.65	0	15,15,17	1.48	3 (20%)
6	NAG	r	1	1,6	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
6	NAG	r	2	6	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
6	NAG	s	1	1,6	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
6	NAG	s	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
5	NAG	t	1	1,5	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	t	2	5	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
5	BMA	t	3	5	11,11,12	0.63	0	15,15,17	1.47	3 (20%)
6	NAG	u	1	1,6	14,14,15	0.49	0	17,19,21	2.24	3 (17%)
6	NAG	u	2	6	14,14,15	0.51	0	17,19,21	1.37	3 (17%)
5	NAG	v	1	1,5	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
5	NAG	v	2	5	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
5	BMA	v	3	5	11,11,12	0.64	0	15,15,17	1.46	3 (20%)
5	NAG	w	1	1,5	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
5	NAG	w	2	5	14,14,15	0.51	0	17,19,21	1.37	3 (17%)
5	BMA	w	3	5	11,11,12	0.66	0	15,15,17	1.47	3 (20%)
6	NAG	x	1	1,6	14,14,15	0.50	0	17,19,21	2.24	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	x	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
6	NAG	y	1	1,6	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
6	NAG	y	2	6	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
7	NAG	z	1	1,7	14,14,15	0.60	0	17,19,21	0.68	0
7	NAG	z	2	7	14,14,15	0.58	0	17,19,21	0.89	0
7	BMA	z	3	7	11,11,12	0.67	0	15,15,17	0.86	0
7	MAN	z	4	7	11,11,12	0.60	0	15,15,17	0.68	0
7	MAN	z	5	7	11,11,12	0.53	0	15,15,17	0.74	0
7	MAN	z	6	7	11,11,12	0.67	0	15,15,17	1.10	1 (6%)
7	MAN	z	7	7	11,11,12	0.62	0	15,15,17	0.63	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
5	NAG	0	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	0	2	5	-	0/6/23/26	0/1/1/1
5	BMA	0	3	5	-	2/2/19/22	0/1/1/1
8	NAG	1	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	1	2	8	-	0/6/23/26	0/1/1/1
8	BMA	1	3	8	-	2/2/19/22	0/1/1/1
8	MAN	1	4	8	-	0/2/19/22	0/1/1/1
8	MAN	1	5	8	-	0/2/19/22	0/1/1/1
7	NAG	2	1	1,7	-	3/6/23/26	0/1/1/1
7	NAG	2	2	7	-	1/6/23/26	0/1/1/1
7	BMA	2	3	7	-	0/2/19/22	0/1/1/1
7	MAN	2	4	7	-	2/2/19/22	0/1/1/1
7	MAN	2	5	7	-	0/2/19/22	0/1/1/1
7	MAN	2	6	7	-	2/2/19/22	0/1/1/1
7	MAN	2	7	7	-	1/2/19/22	0/1/1/1
9	NAG	3	1	1,9	-	0/6/23/26	0/1/1/1
9	MAN	3	10	9	-	1/2/19/22	0/1/1/1
9	NAG	3	2	9	-	1/6/23/26	0/1/1/1
9	BMA	3	3	9	-	0/2/19/22	0/1/1/1
9	MAN	3	4	9	-	1/2/19/22	0/1/1/1
9	MAN	3	5	9	-	0/2/19/22	0/1/1/1
9	MAN	3	6	9	-	0/2/19/22	0/1/1/1
9	MAN	3	7	9	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	3	8	9	-	0/2/19/22	0/1/1/1
9	MAN	3	9	9	-	1/2/19/22	0/1/1/1
6	NAG	4	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	4	2	6	-	0/6/23/26	0/1/1/1
5	NAG	5	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	5	2	5	-	0/6/23/26	0/1/1/1
5	BMA	5	3	5	-	2/2/19/22	0/1/1/1
5	NAG	6	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	6	2	5	-	0/6/23/26	0/1/1/1
5	BMA	6	3	5	-	2/2/19/22	0/1/1/1
6	NAG	7	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	7	2	6	-	0/6/23/26	0/1/1/1
6	NAG	8	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	8	2	6	-	0/6/23/26	0/1/1/1
6	NAG	9	1	2,6	-	1/6/23/26	0/1/1/1
6	NAG	9	2	6	-	0/6/23/26	0/1/1/1
6	NAG	AA	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	AA	2	6	-	0/6/23/26	0/1/1/1
5	NAG	M	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	2/2/19/22	0/1/1/1
6	NAG	N	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
5	NAG	O	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	BMA	O	3	5	-	2/2/19/22	0/1/1/1
5	NAG	P	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	BMA	P	3	5	-	2/2/19/22	0/1/1/1
6	NAG	Q	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	0/6/23/26	0/1/1/1
6	NAG	R	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	R	2	6	-	0/6/23/26	0/1/1/1
7	NAG	S	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	S	2	7	-	2/6/23/26	0/1/1/1
7	BMA	S	3	7	-	2/2/19/22	0/1/1/1
7	MAN	S	4	7	-	0/2/19/22	0/1/1/1
7	MAN	S	5	7	-	2/2/19/22	0/1/1/1
7	MAN	S	6	7	-	2/2/19/22	0/1/1/1
7	MAN	S	7	7	-	0/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	d	2	5	-	0/6/23/26	0/1/1/1
5	BMA	d	3	5	-	2/2/19/22	0/1/1/1
6	NAG	e	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	e	2	6	-	0/6/23/26	0/1/1/1
5	NAG	f	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	f	2	5	-	0/6/23/26	0/1/1/1
5	BMA	f	3	5	-	2/2/19/22	0/1/1/1
5	NAG	g	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	g	2	5	-	0/6/23/26	0/1/1/1
5	BMA	g	3	5	-	2/2/19/22	0/1/1/1
6	NAG	h	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	h	2	6	-	0/6/23/26	0/1/1/1
6	NAG	i	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	i	2	6	-	0/6/23/26	0/1/1/1
7	NAG	j	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	j	2	7	-	2/6/23/26	0/1/1/1
7	BMA	j	3	7	-	2/2/19/22	0/1/1/1
7	MAN	j	4	7	-	0/2/19/22	0/1/1/1
7	MAN	j	5	7	-	2/2/19/22	0/1/1/1
7	MAN	j	6	7	-	2/2/19/22	0/1/1/1
7	MAN	j	7	7	-	0/2/19/22	0/1/1/1
5	NAG	k	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	k	2	5	-	0/6/23/26	0/1/1/1
5	BMA	k	3	5	-	2/2/19/22	0/1/1/1
8	NAG	l	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	l	2	8	-	0/6/23/26	0/1/1/1
8	BMA	l	3	8	-	2/2/19/22	0/1/1/1
8	MAN	l	4	8	-	0/2/19/22	0/1/1/1
8	MAN	l	5	8	-	0/2/19/22	0/1/1/1
7	NAG	m	1	1,7	-	3/6/23/26	0/1/1/1
7	NAG	m	2	7	-	1/6/23/26	0/1/1/1
7	BMA	m	3	7	-	0/2/19/22	0/1/1/1
7	MAN	m	4	7	-	2/2/19/22	0/1/1/1
7	MAN	m	5	7	-	0/2/19/22	0/1/1/1
7	MAN	m	6	7	-	2/2/19/22	0/1/1/1
7	MAN	m	7	7	-	1/2/19/22	0/1/1/1
9	NAG	n	1	1,9	-	0/6/23/26	0/1/1/1
9	MAN	n	10	9	-	1/2/19/22	0/1/1/1
9	NAG	n	2	9	-	1/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	z	7	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 410 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	2	2	NAG	C1-C2-N2	8.39	124.82	110.49
7	V	2	NAG	C1-C2-N2	8.39	124.81	110.49
7	m	2	NAG	C1-C2-N2	8.38	124.80	110.49
6	u	1	NAG	O5-C1-C2	-7.40	99.60	111.29
5	q	1	NAG	O5-C1-C2	-7.39	99.62	111.29

There are no chirality outliers.

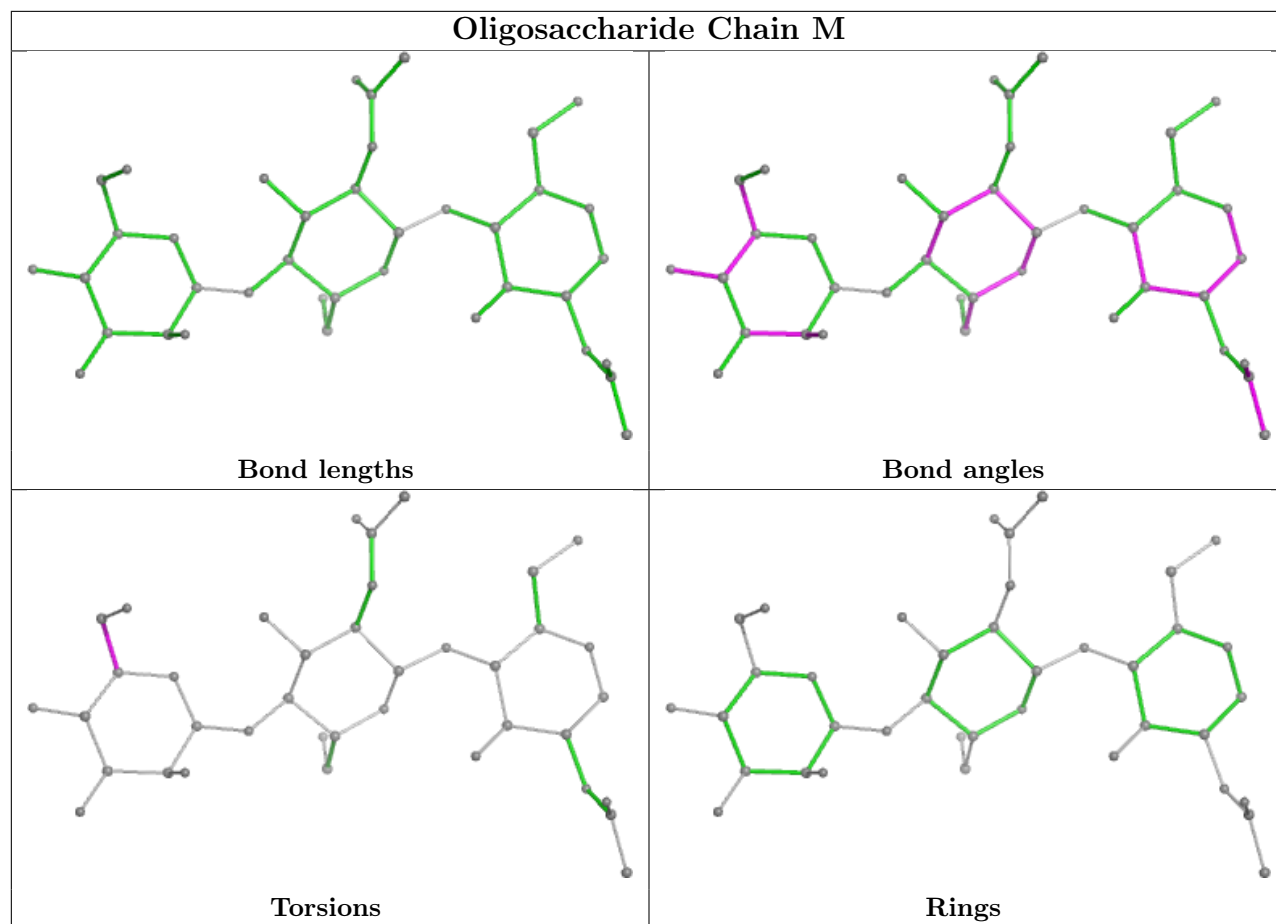
5 of 128 torsion outliers are listed below:

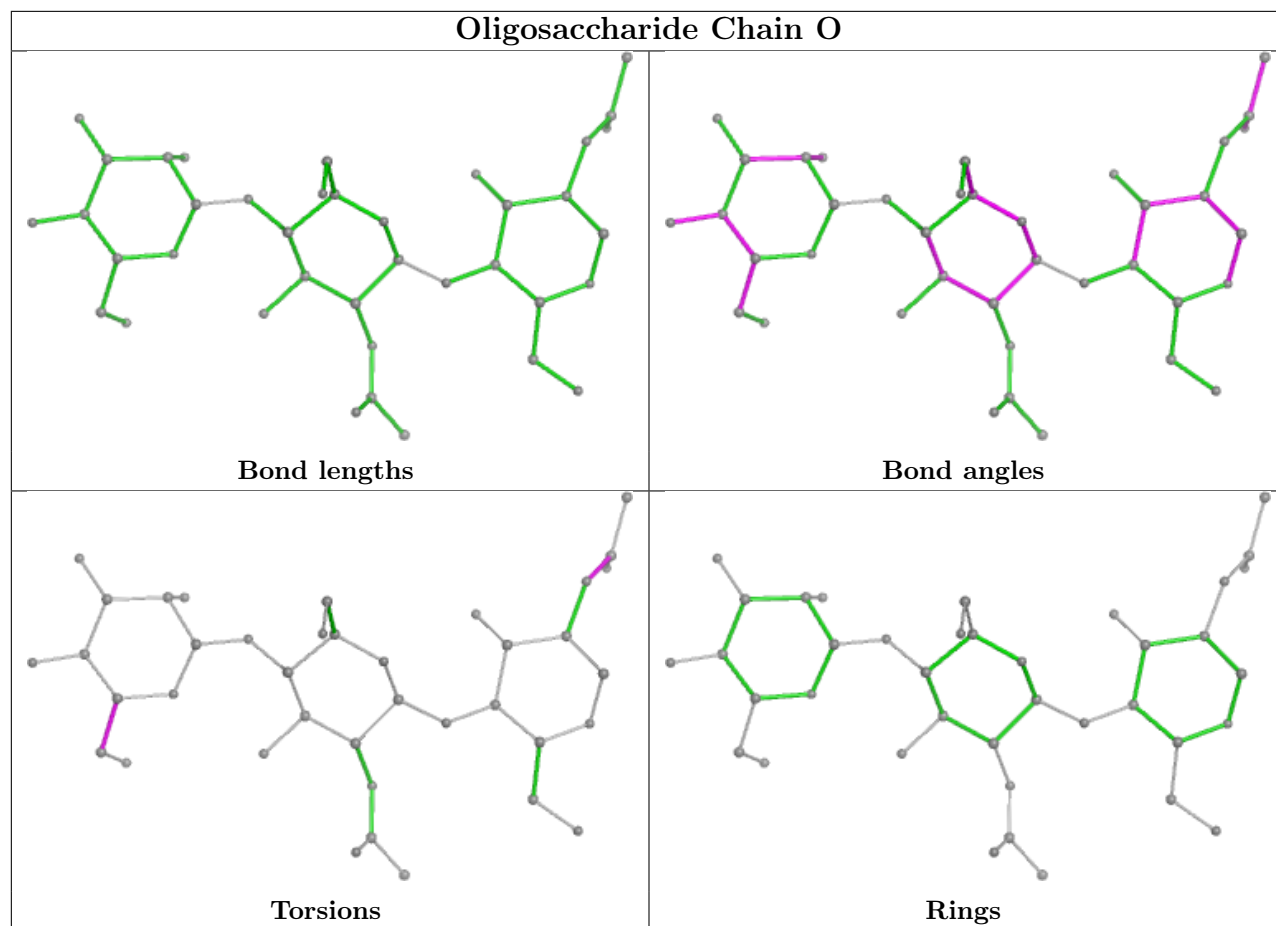
Mol	Chain	Res	Type	Atoms
5	T	1	NAG	O5-C5-C6-O6
5	k	1	NAG	O5-C5-C6-O6
5	0	1	NAG	O5-C5-C6-O6
7	V	1	NAG	C8-C7-N2-C2
7	V	1	NAG	O7-C7-N2-C2

There are no ring outliers.

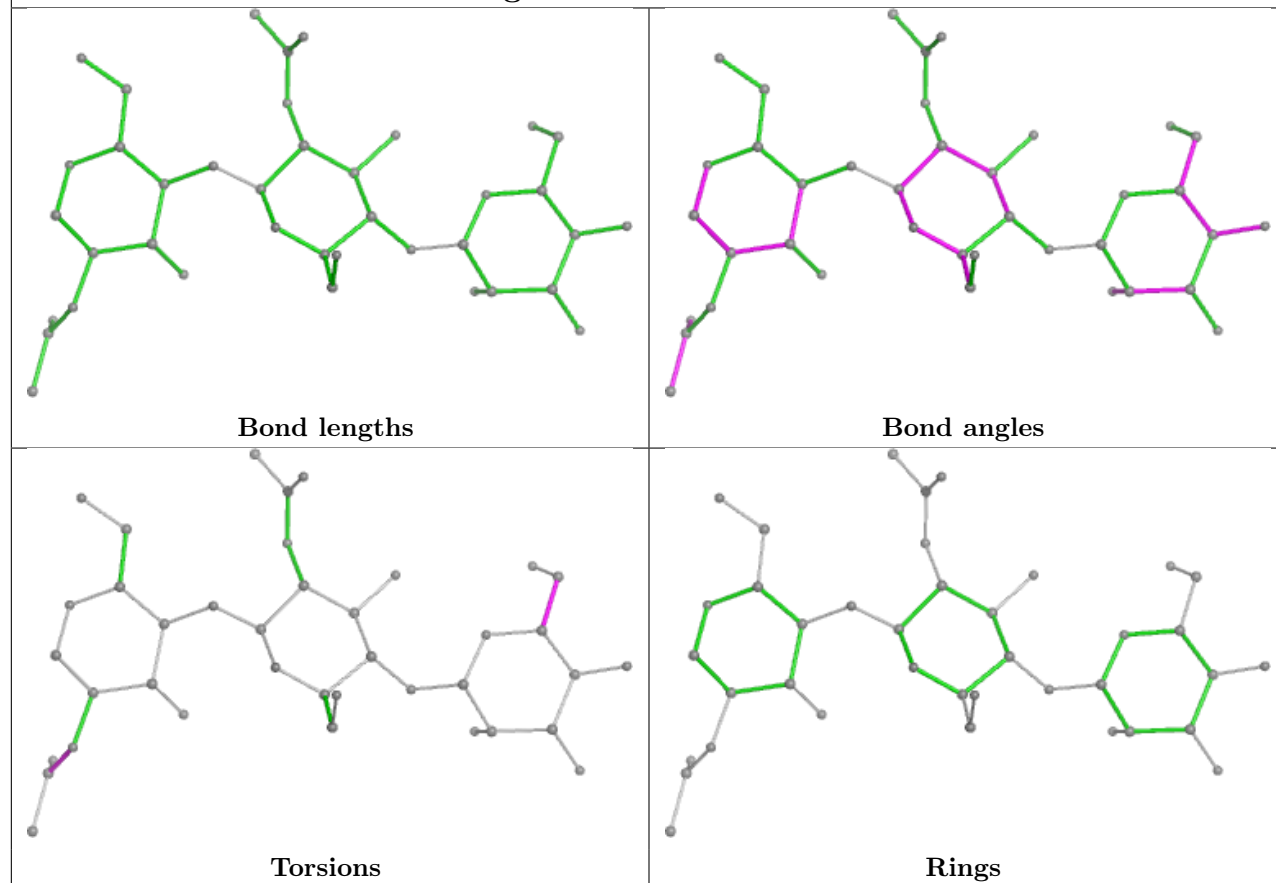
No monomer is involved in short contacts.

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

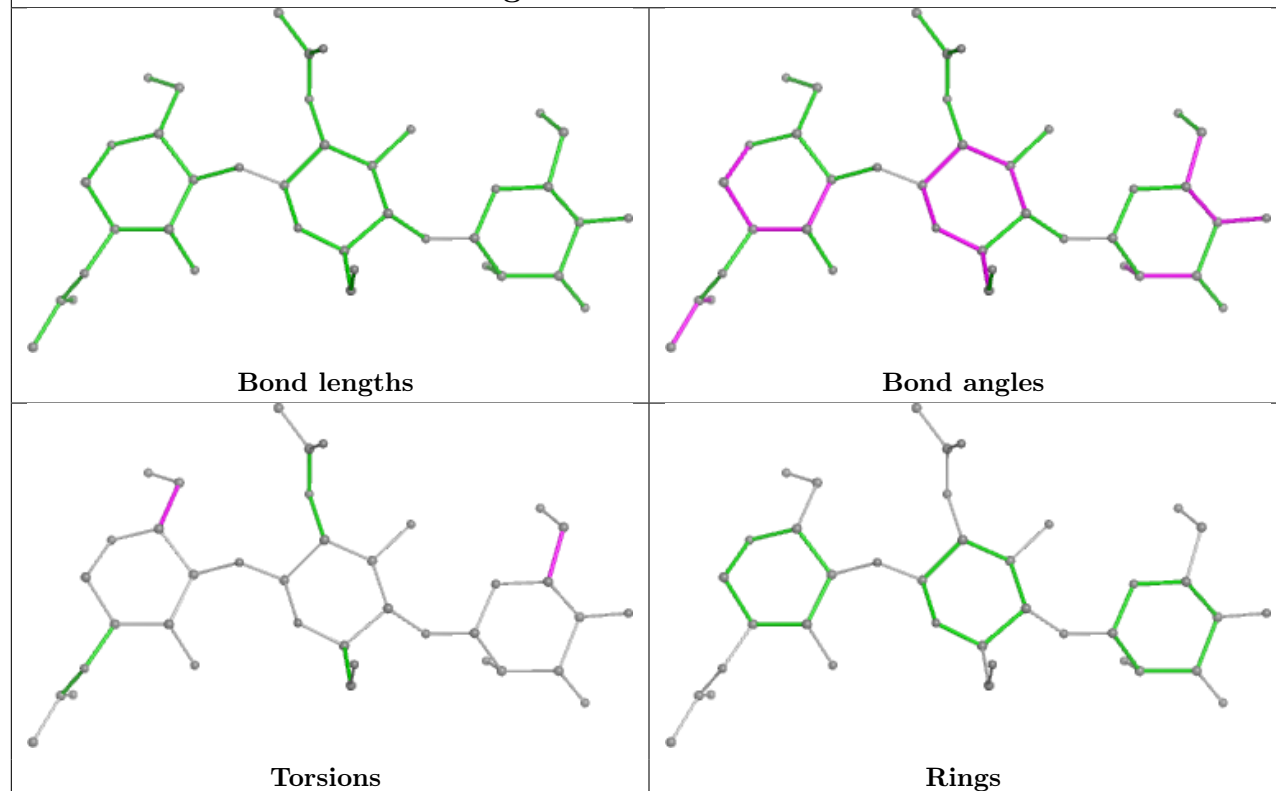


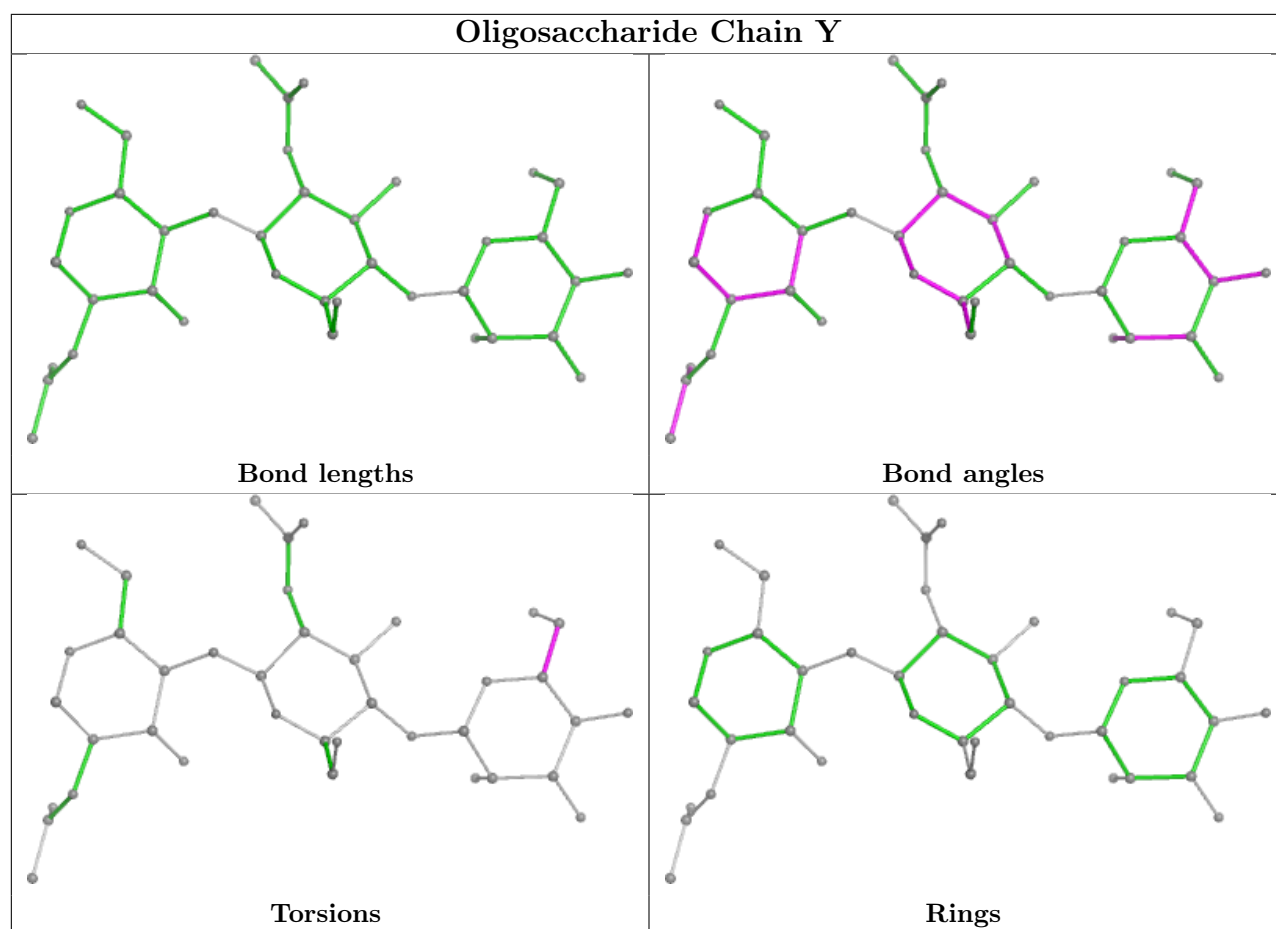


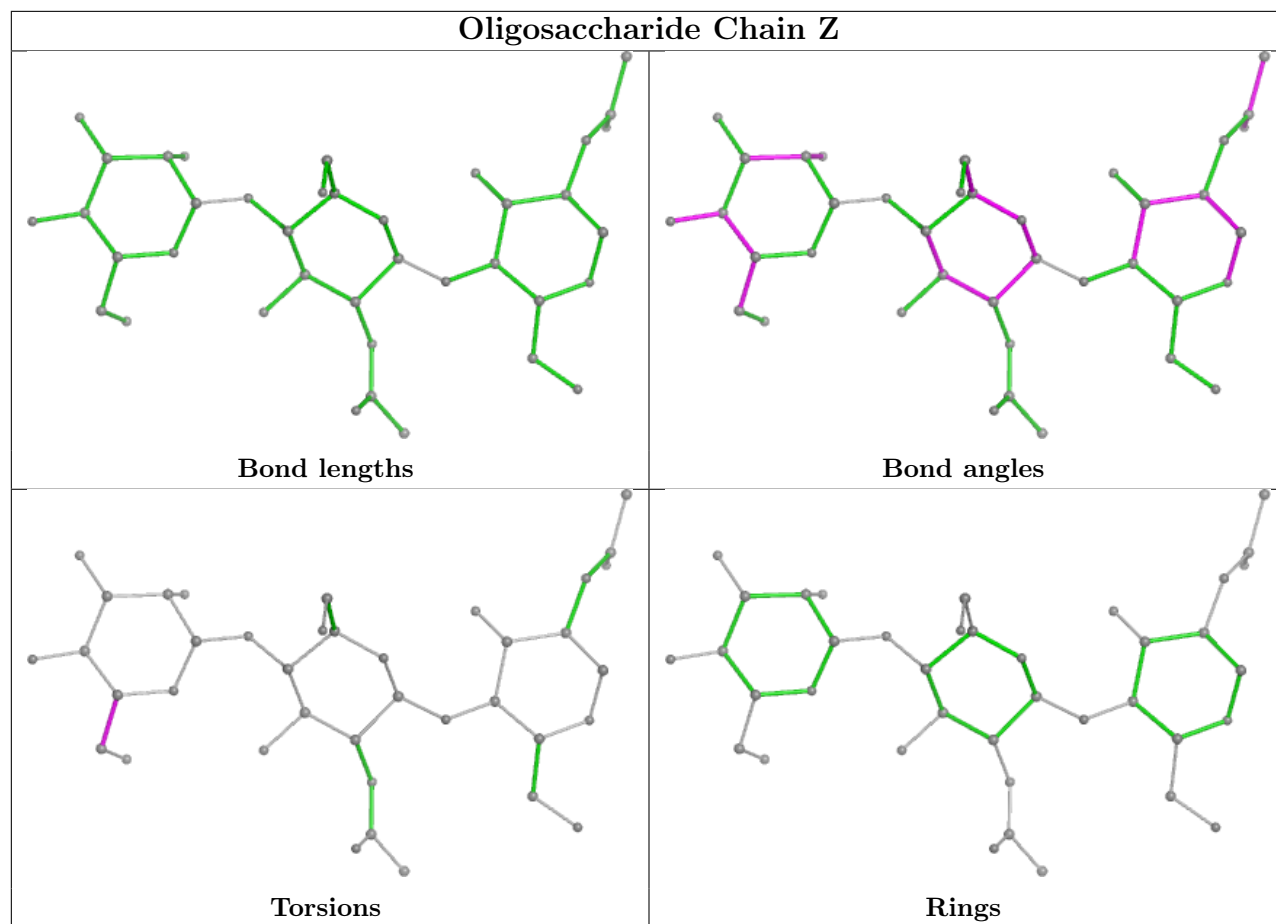
Oligosaccharide Chain P

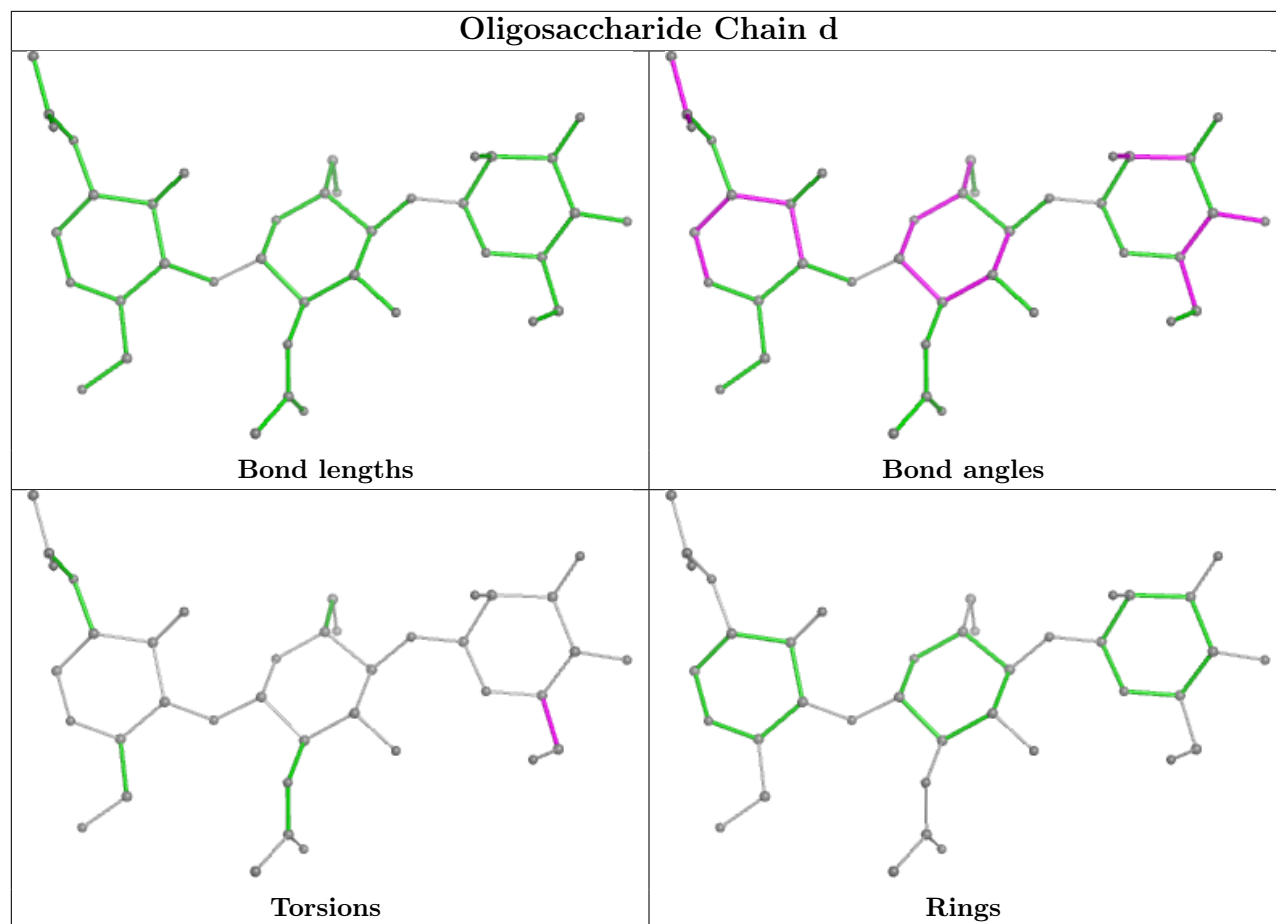


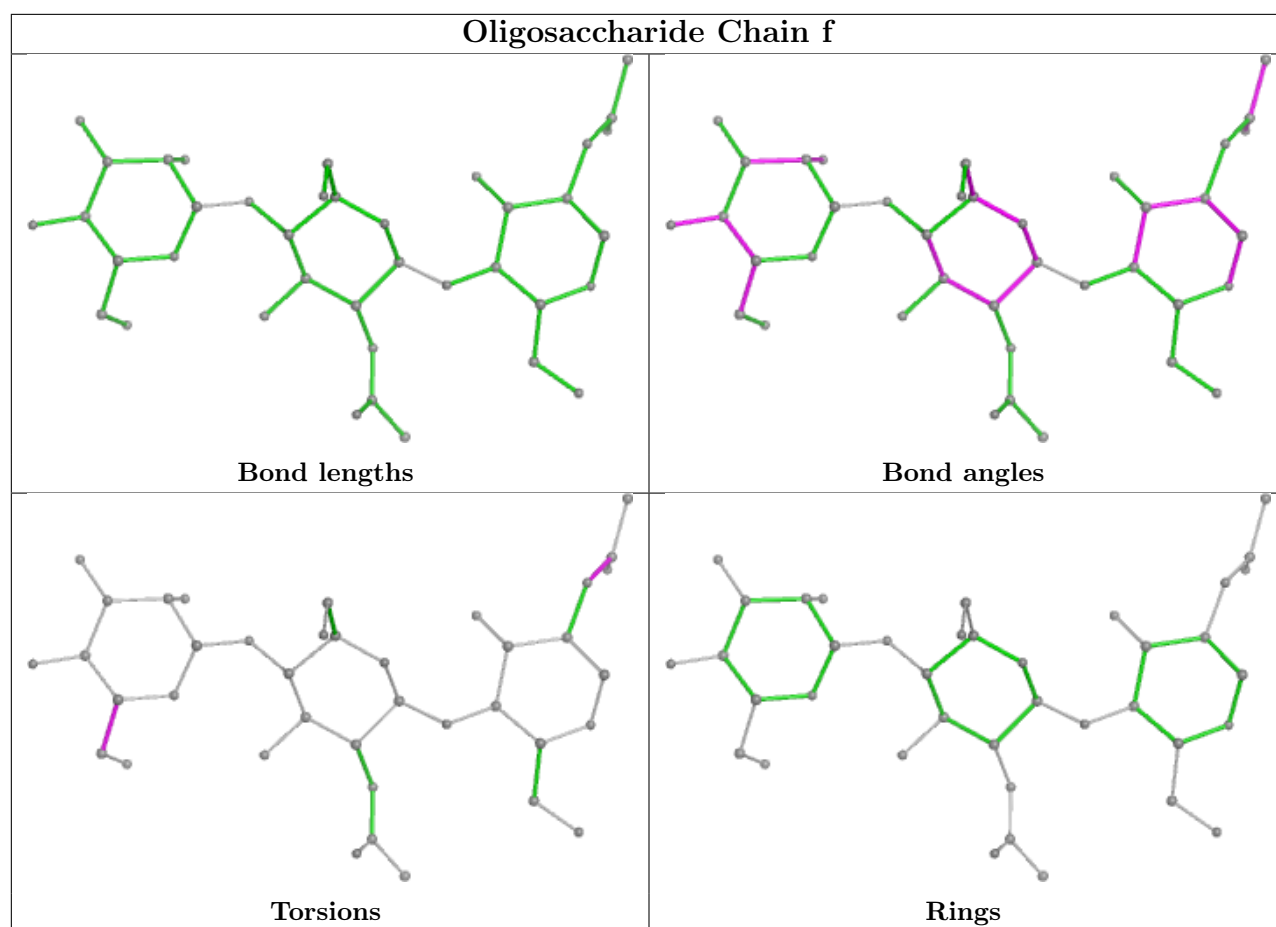
Oligosaccharide Chain T



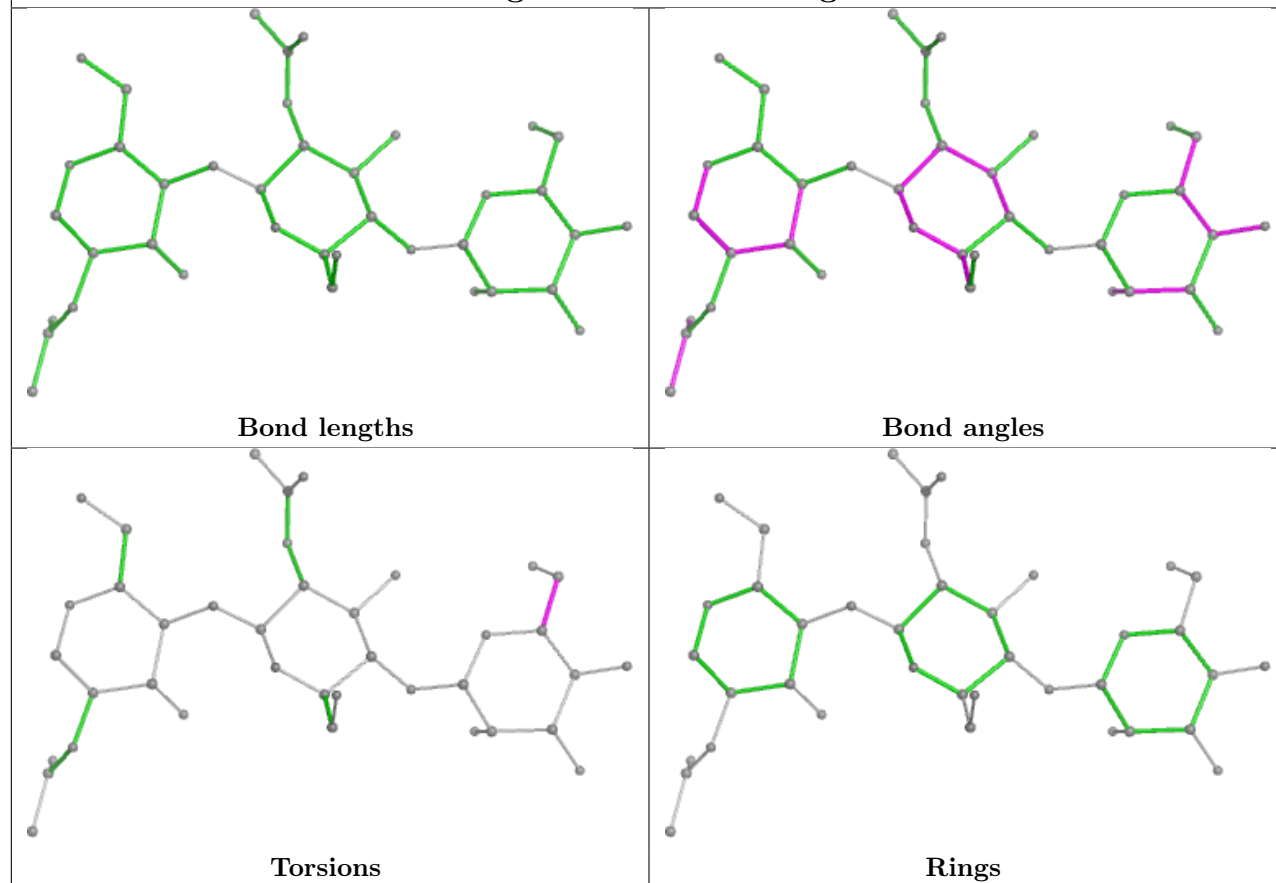




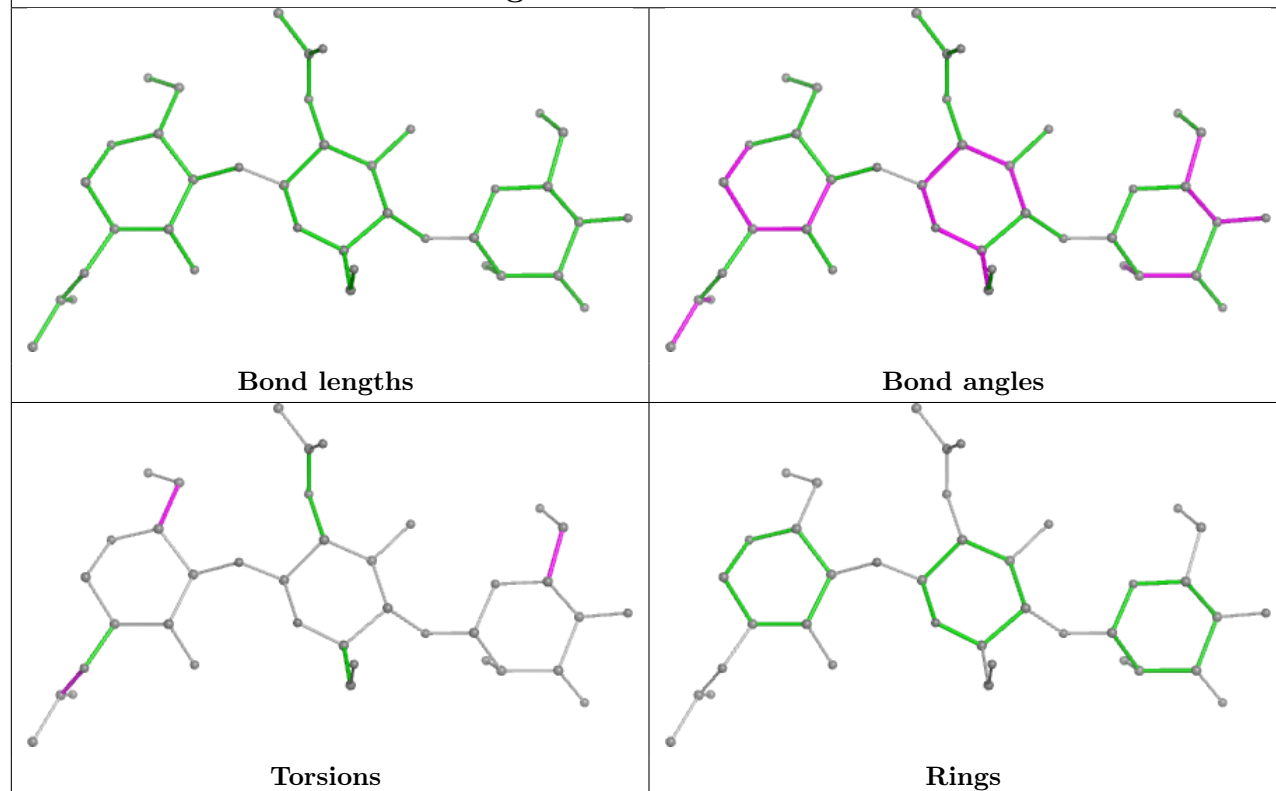


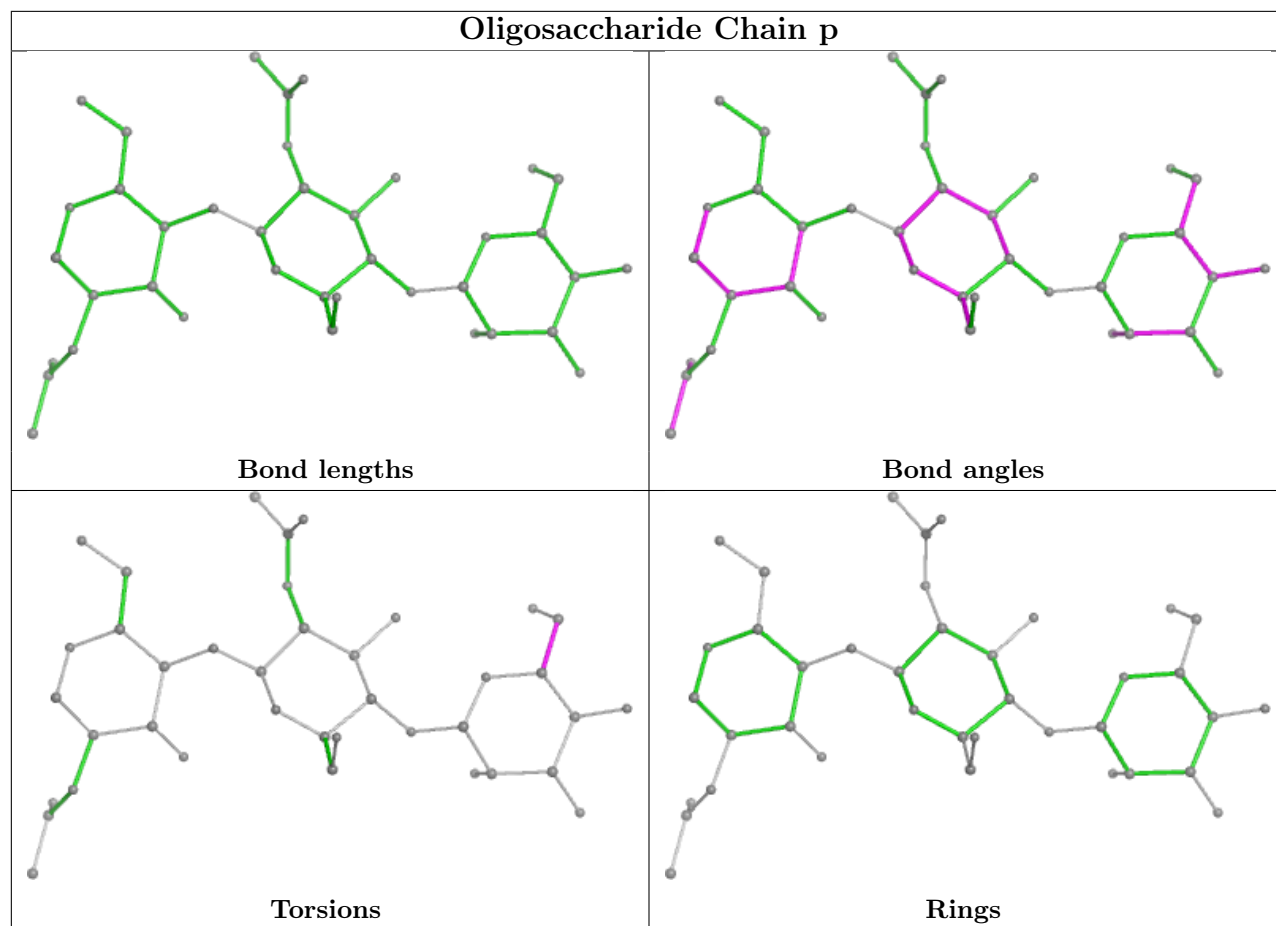


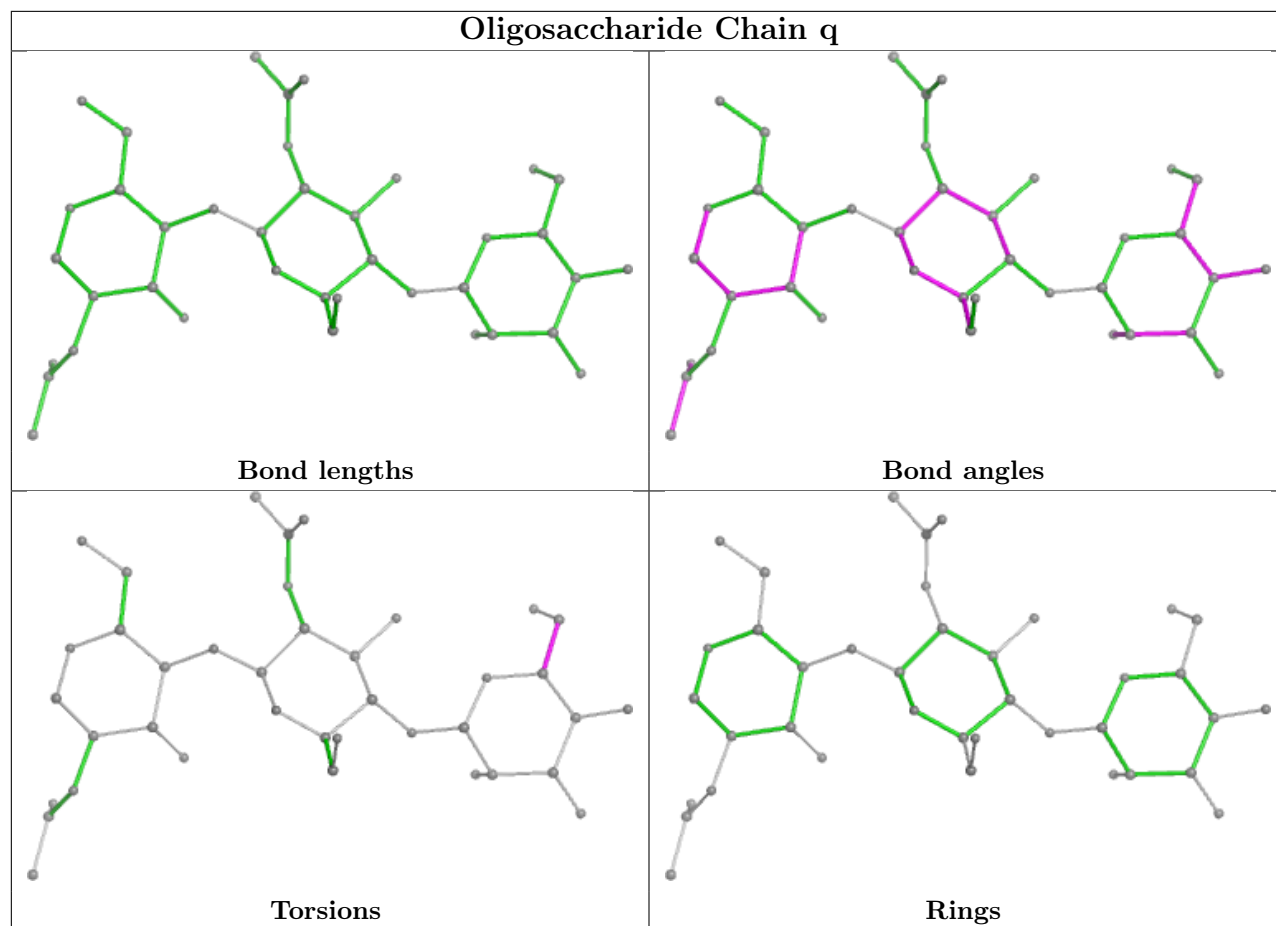
Oligosaccharide Chain g

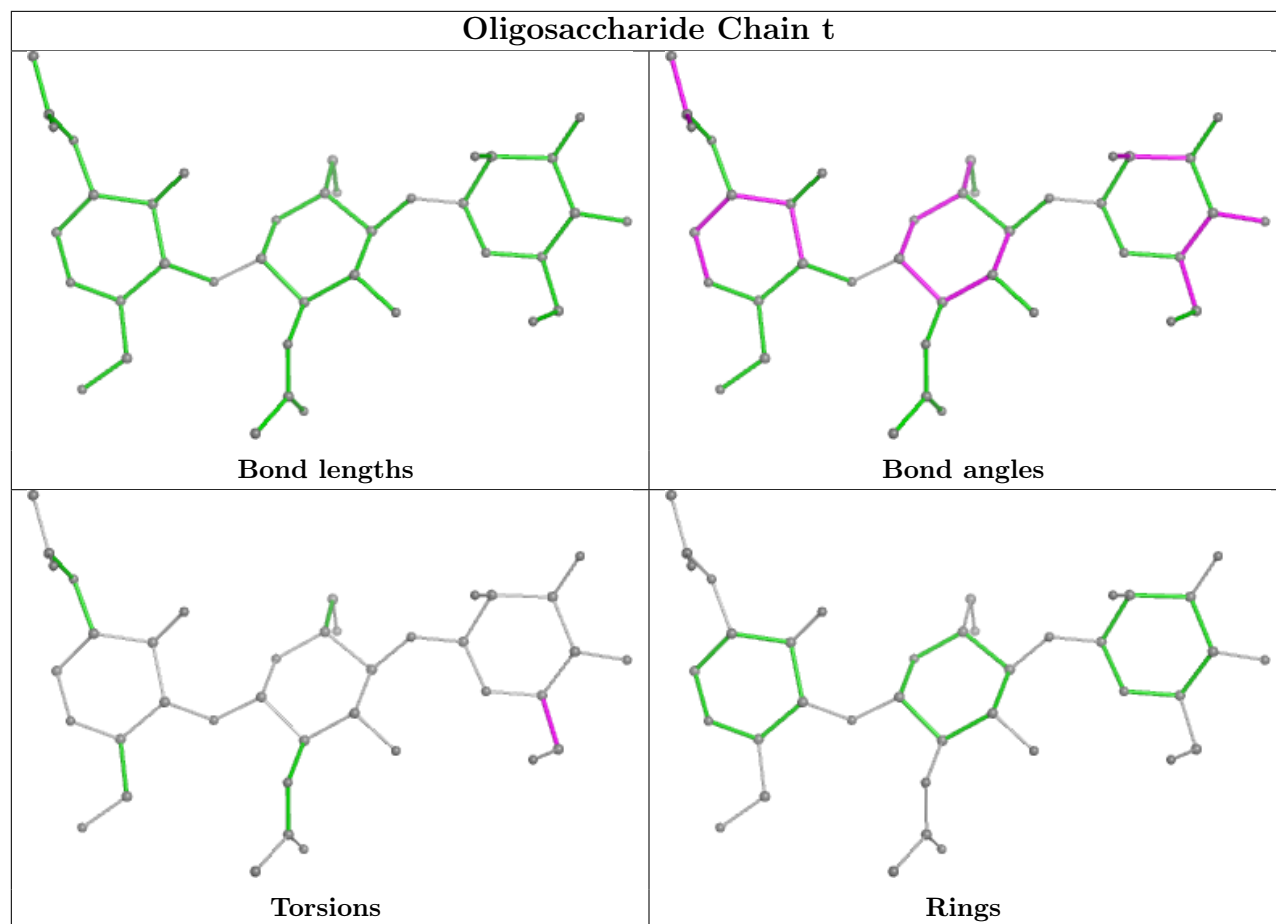


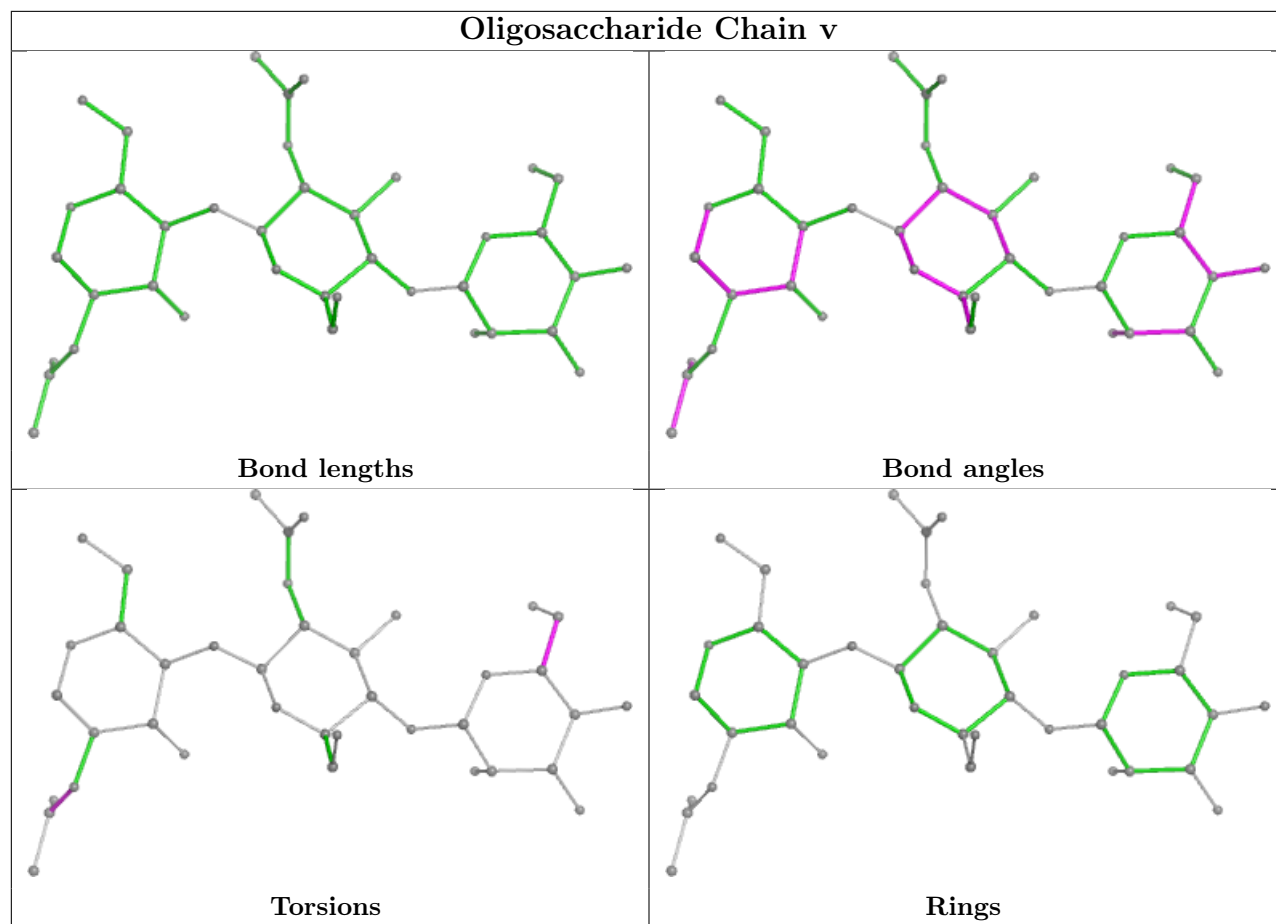
Oligosaccharide Chain k

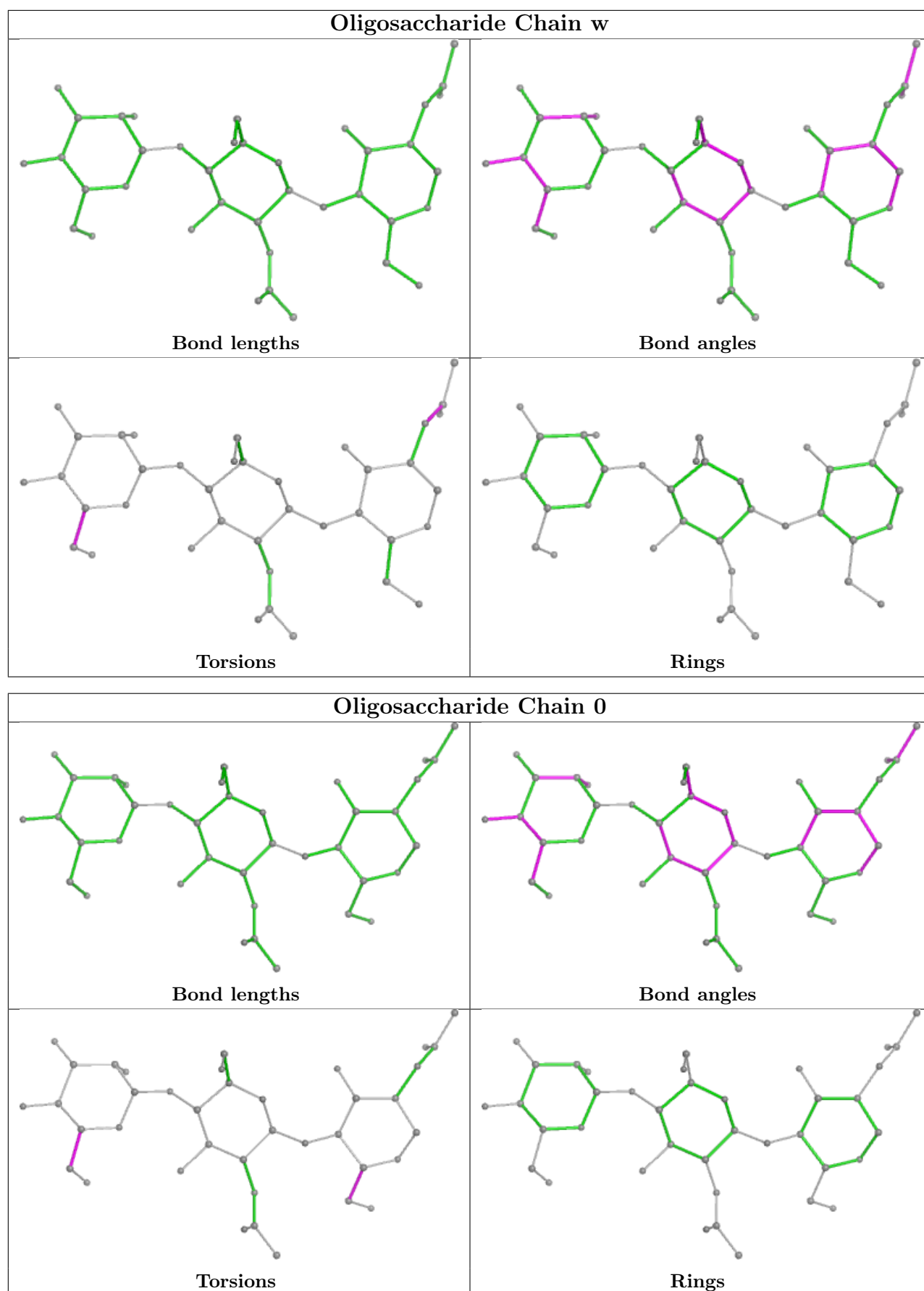


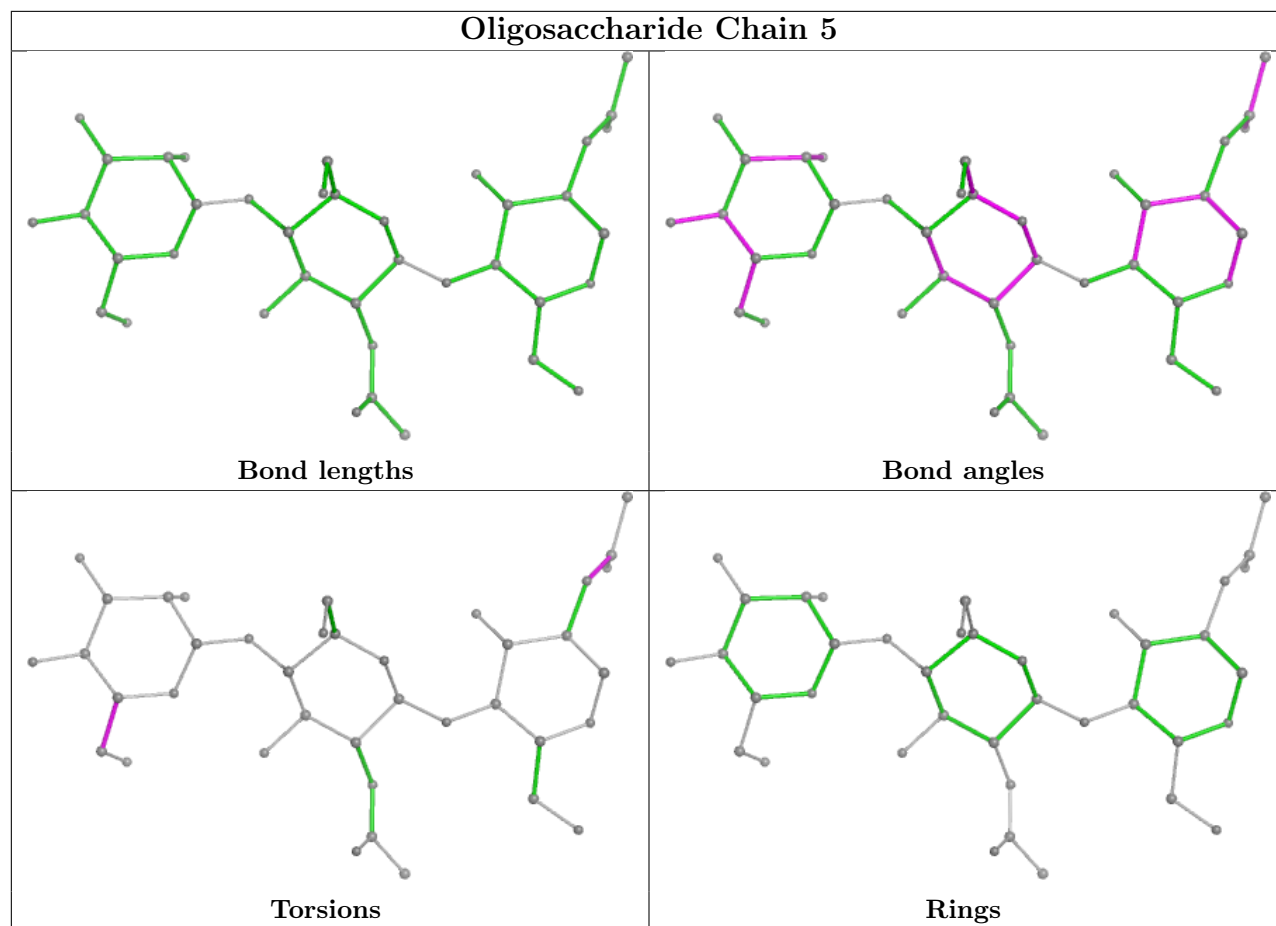


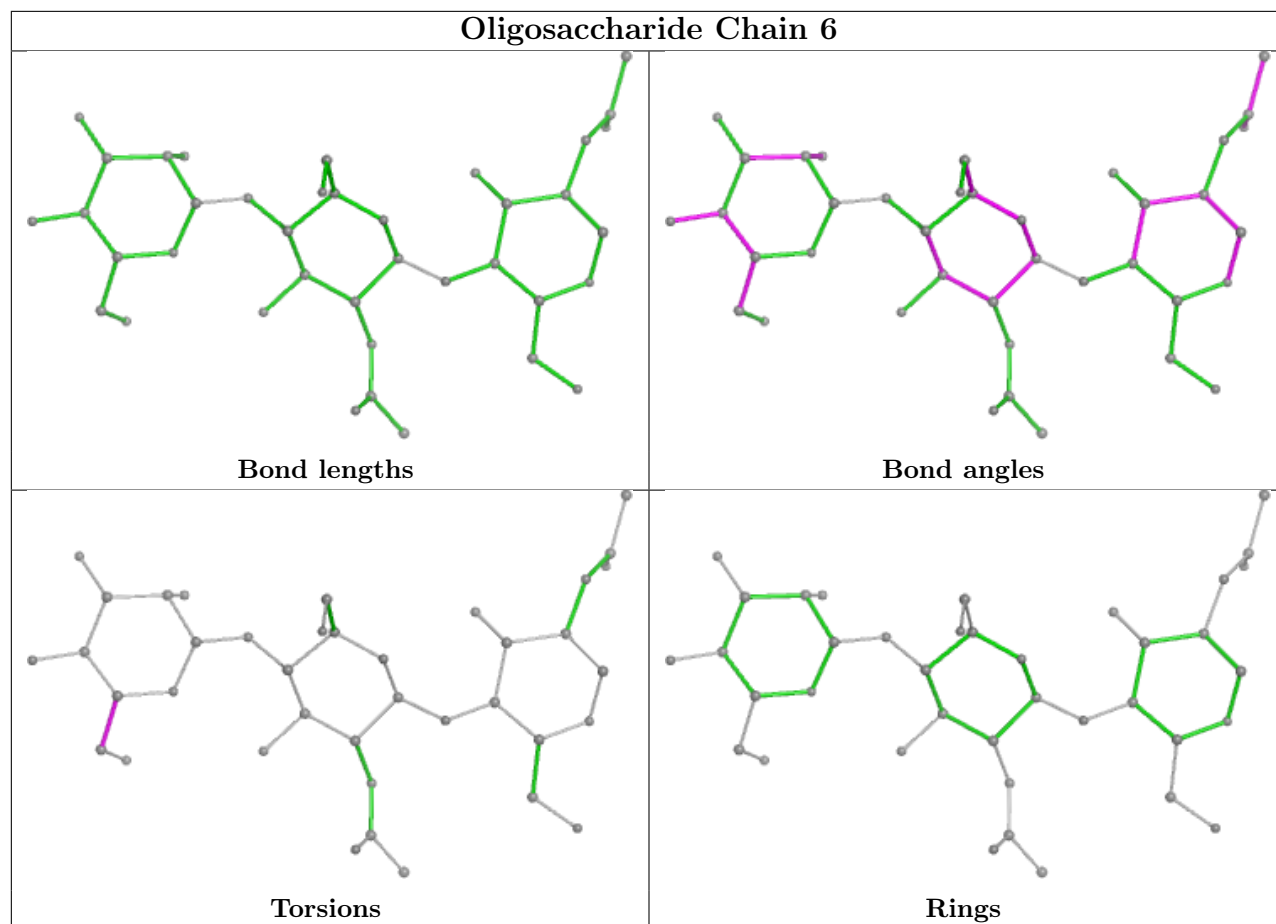


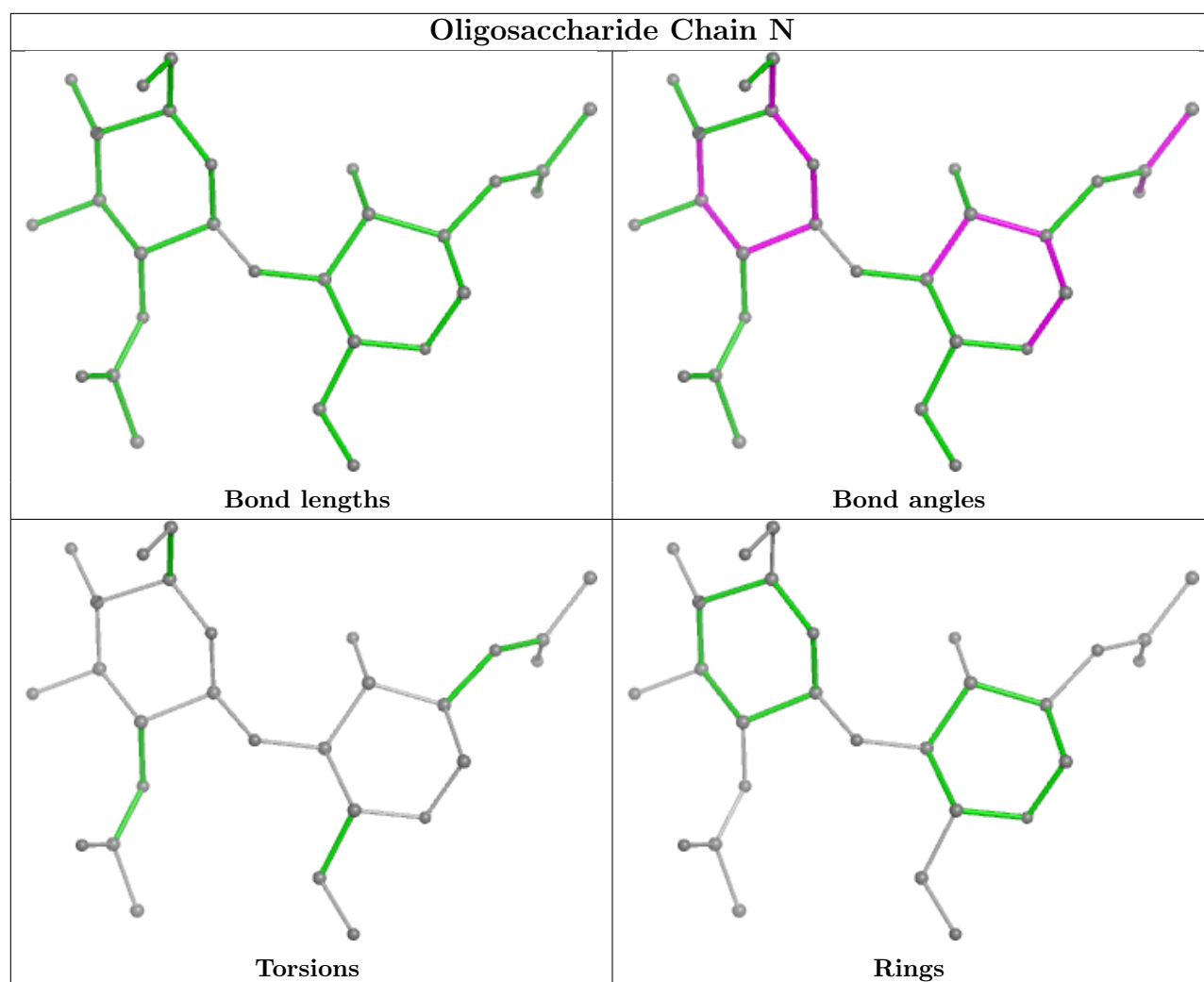


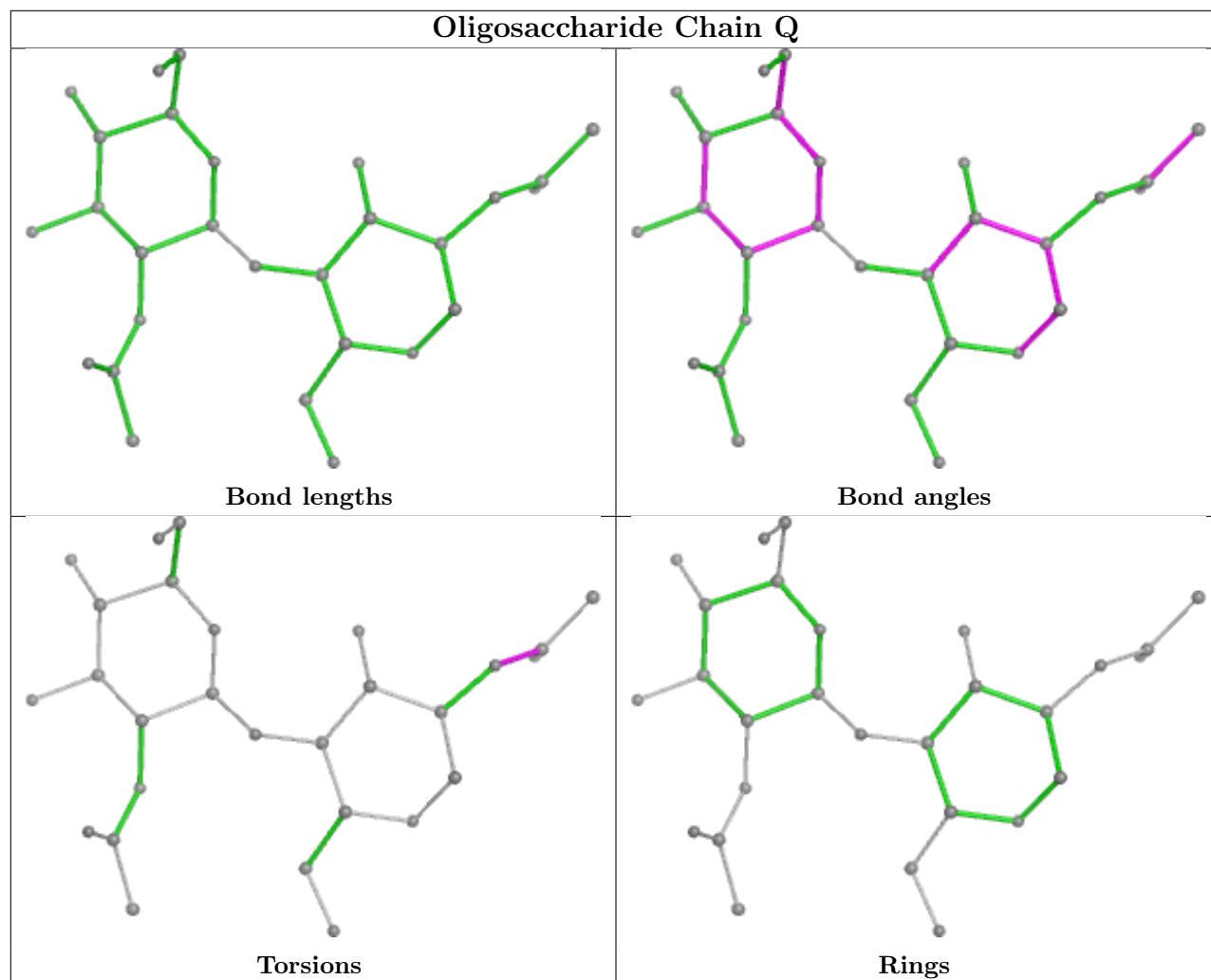


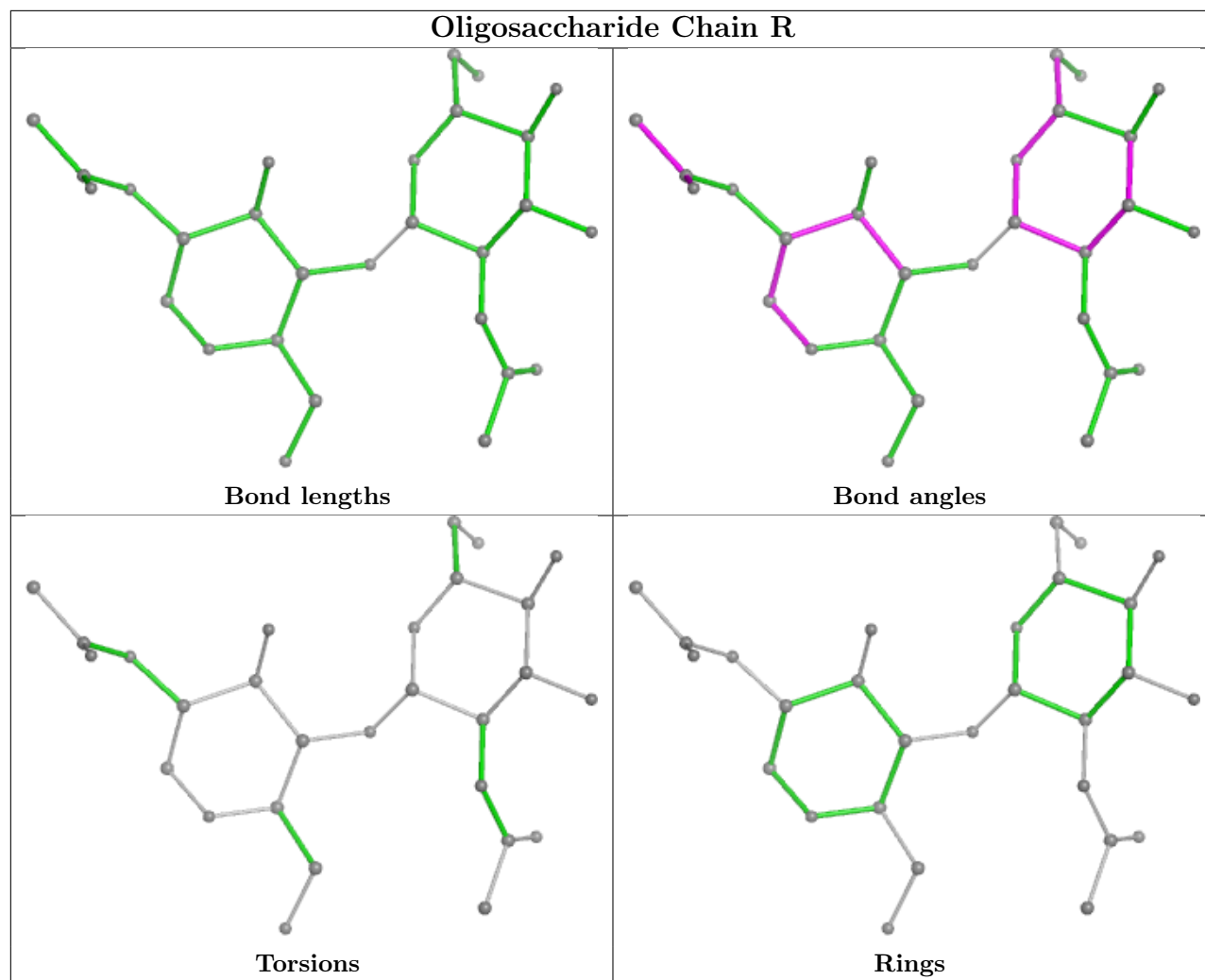


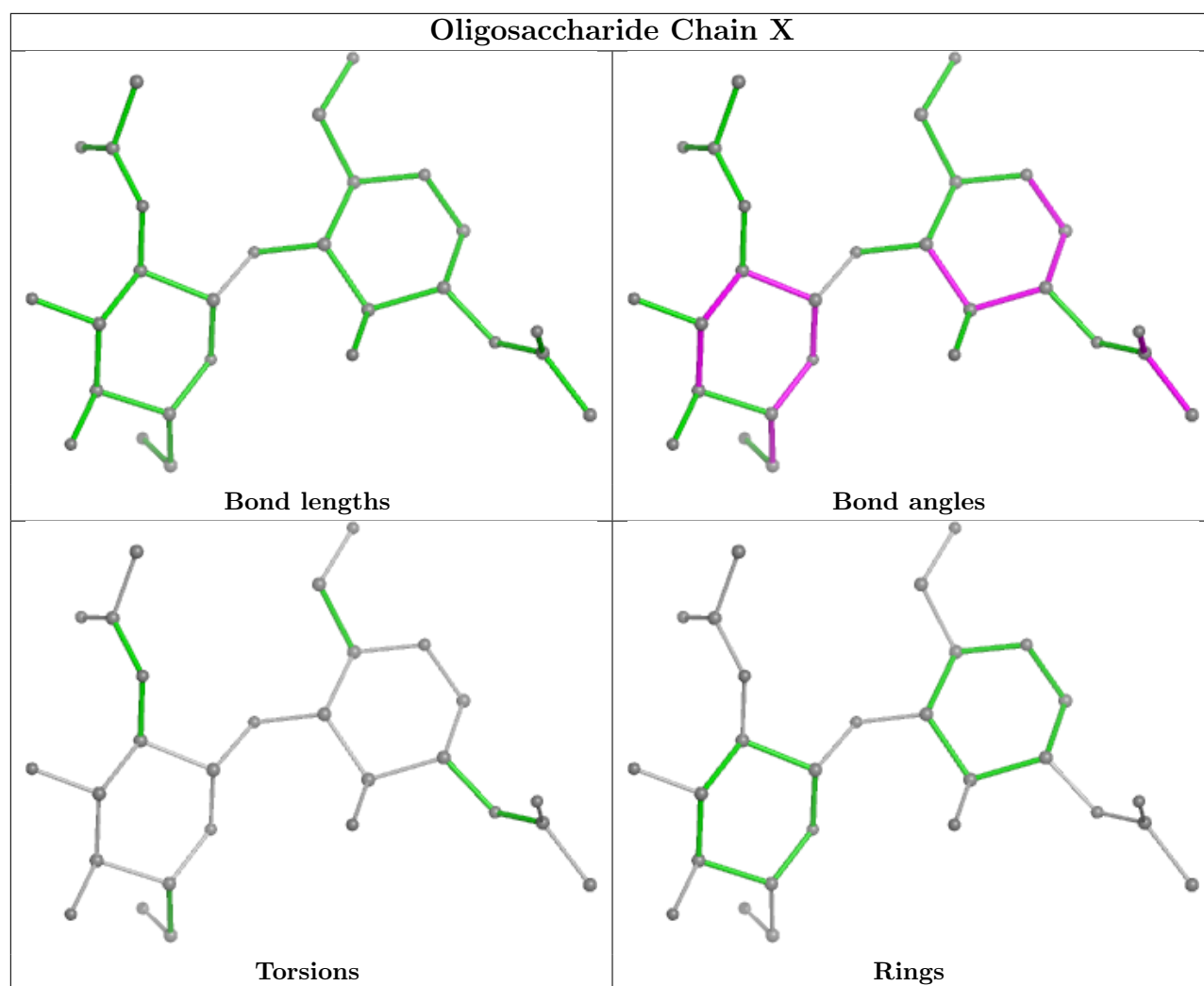


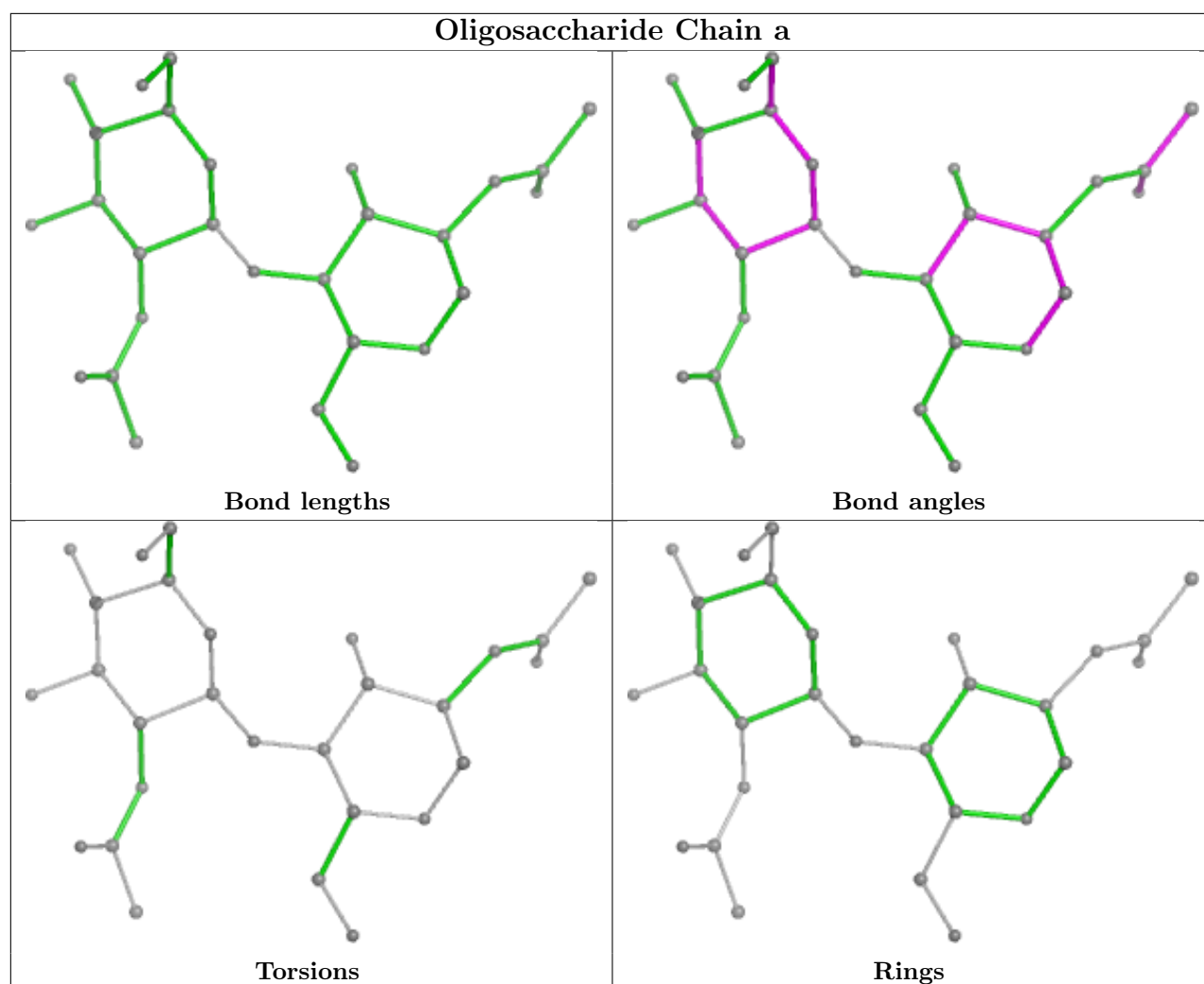


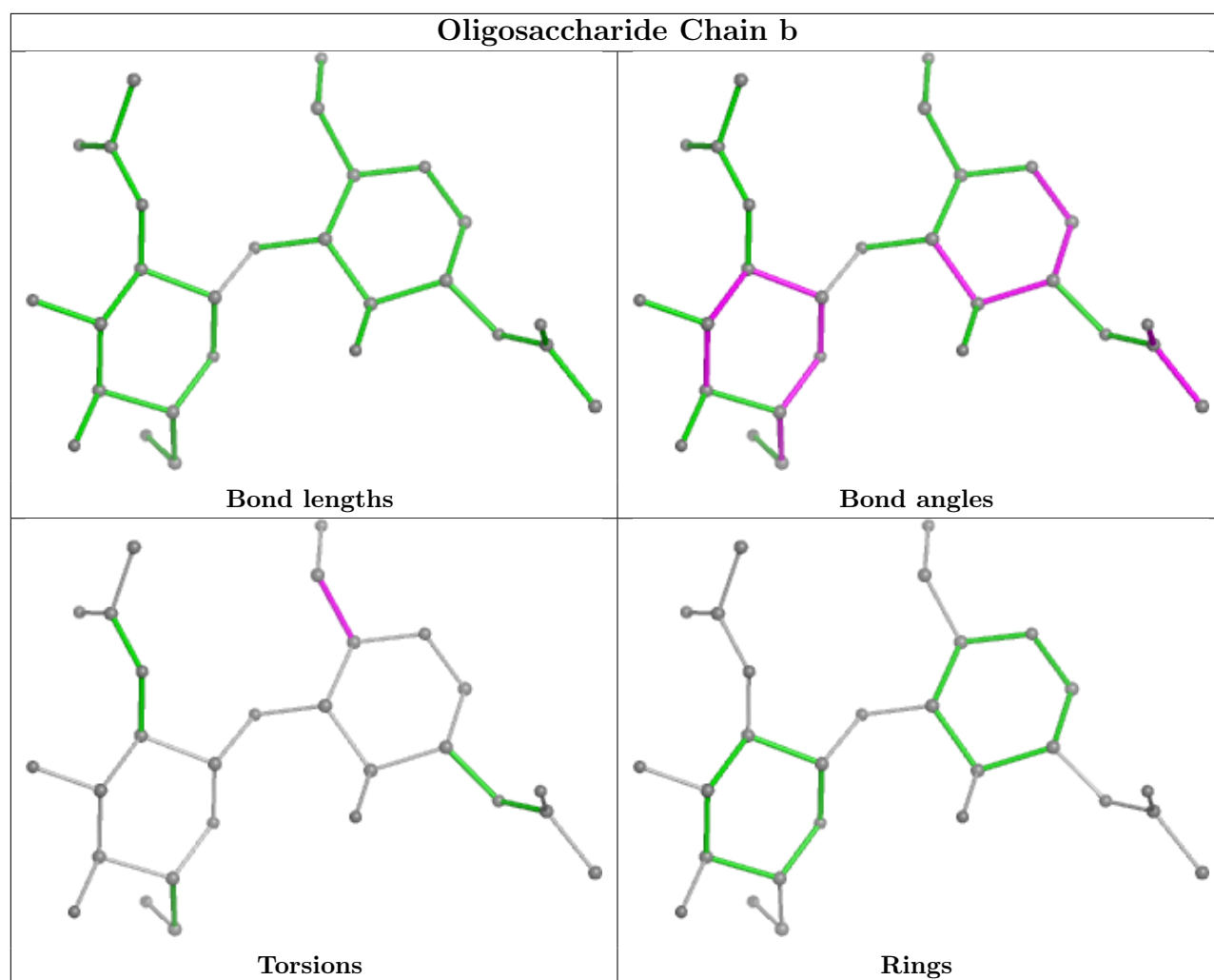


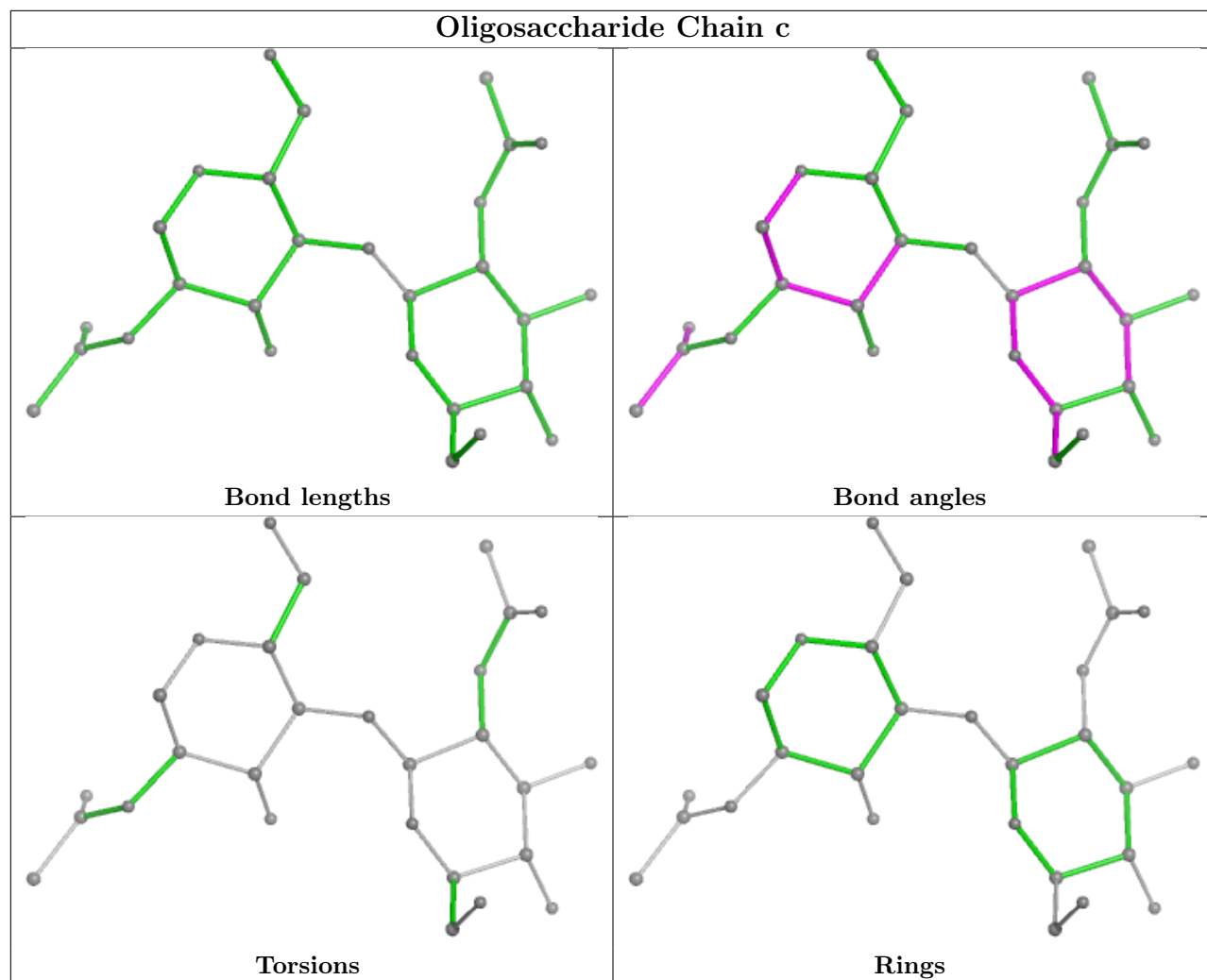


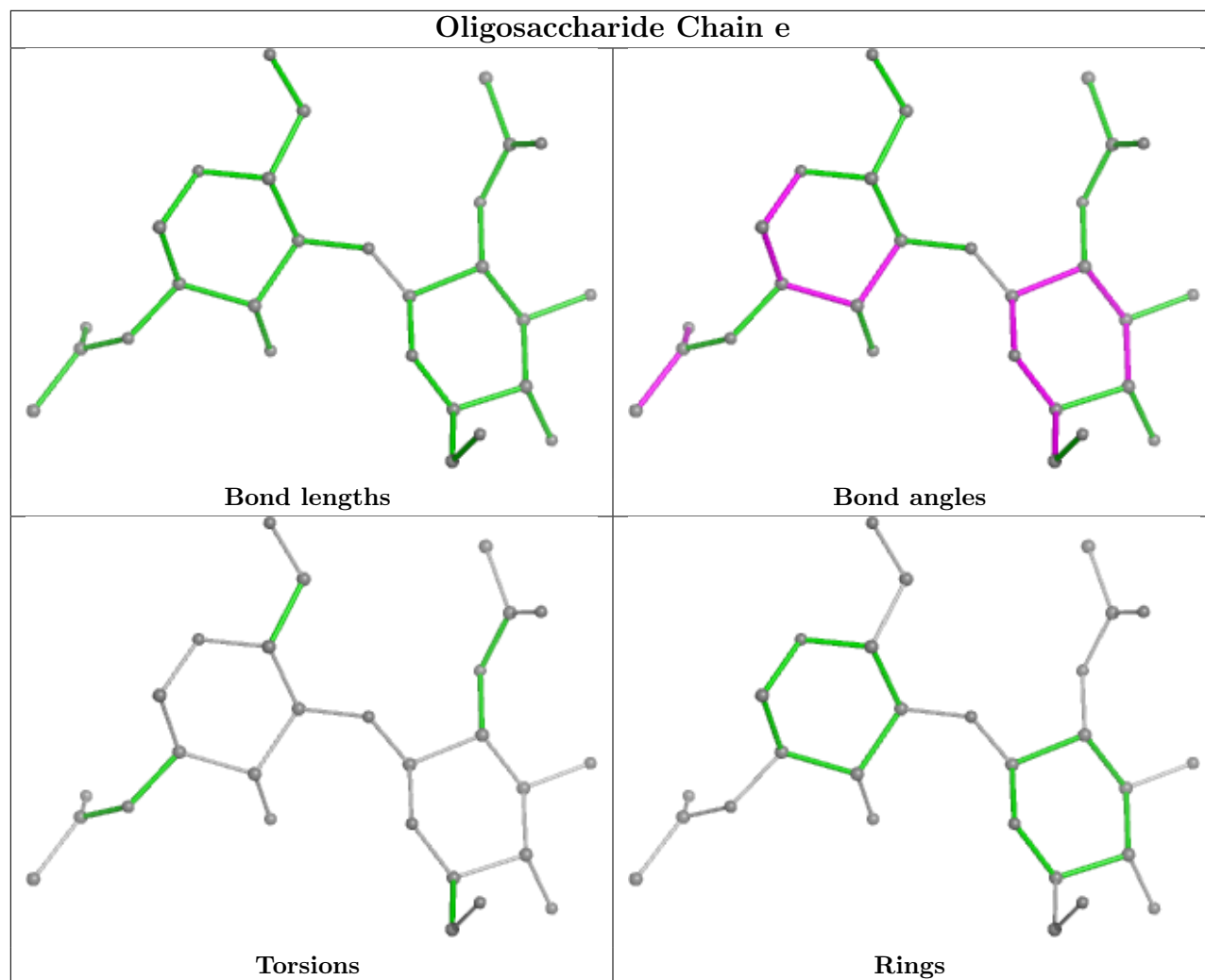


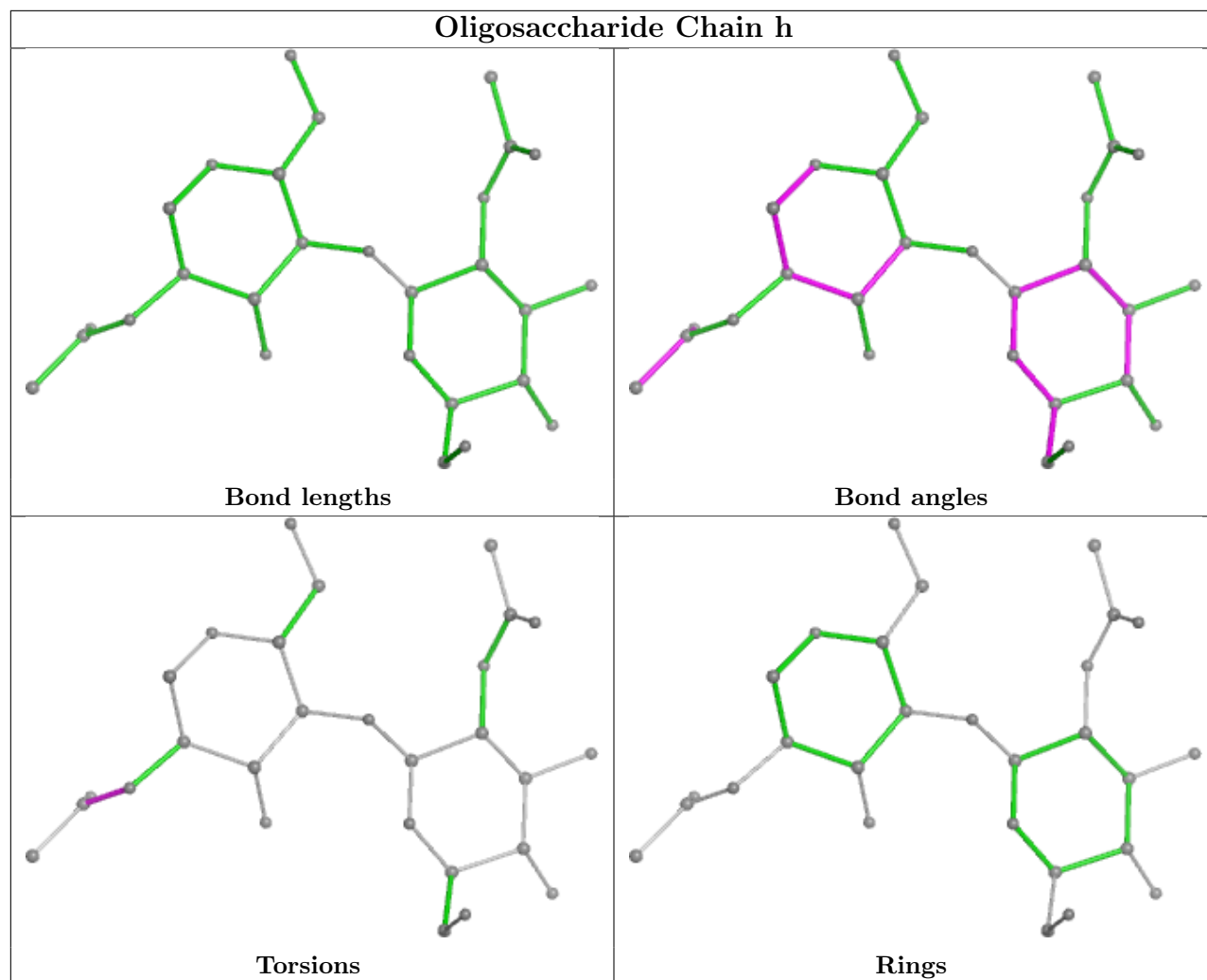


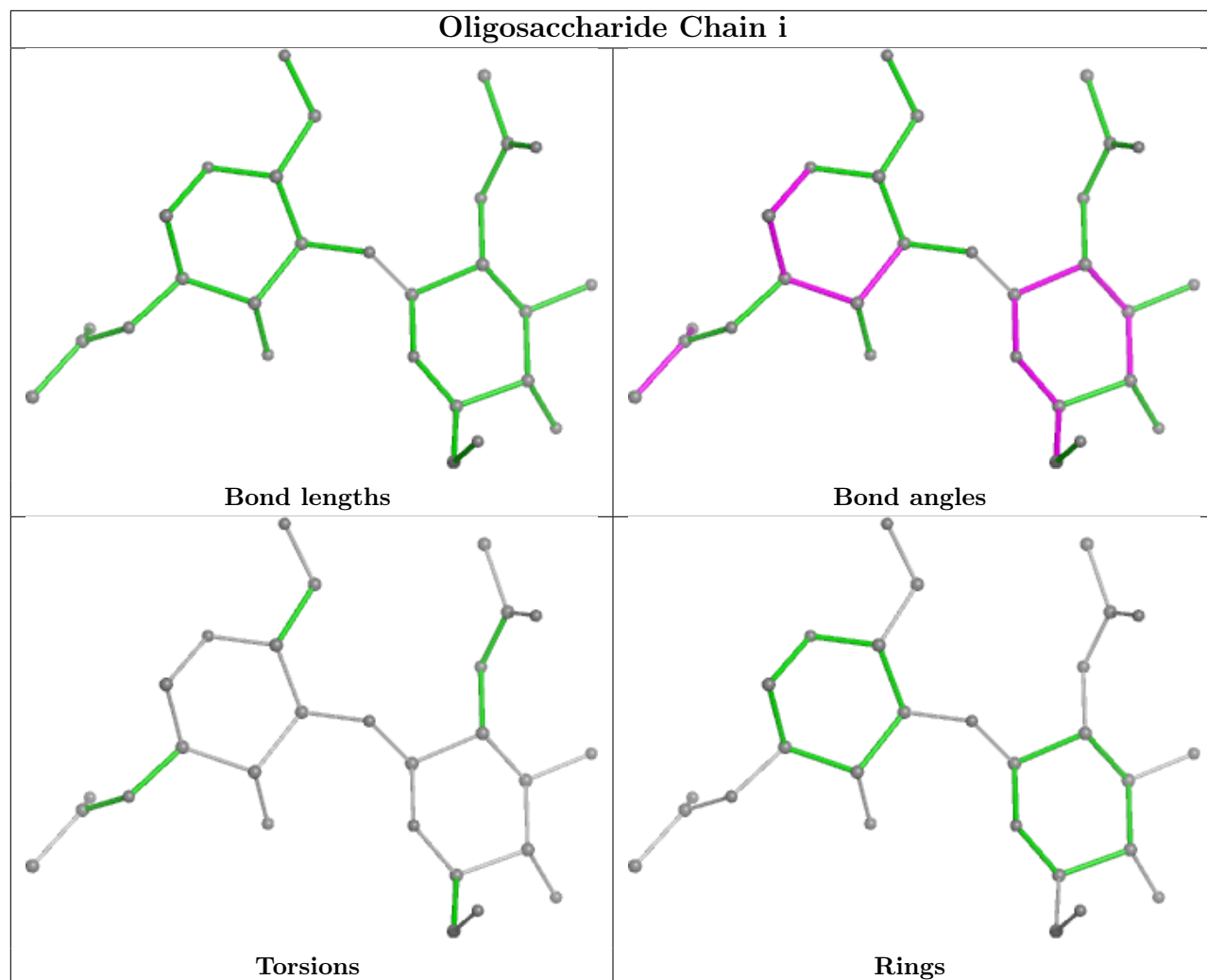


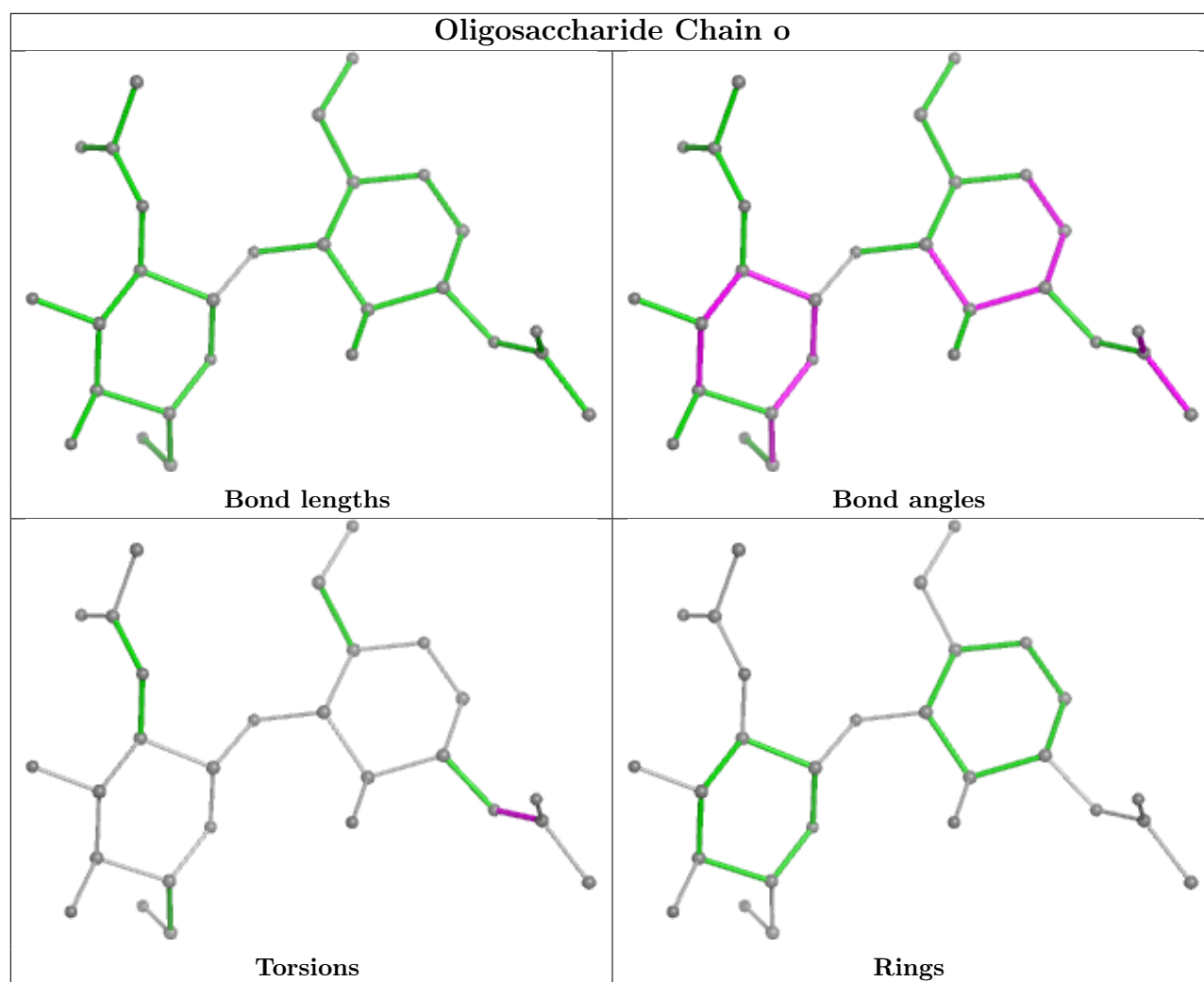


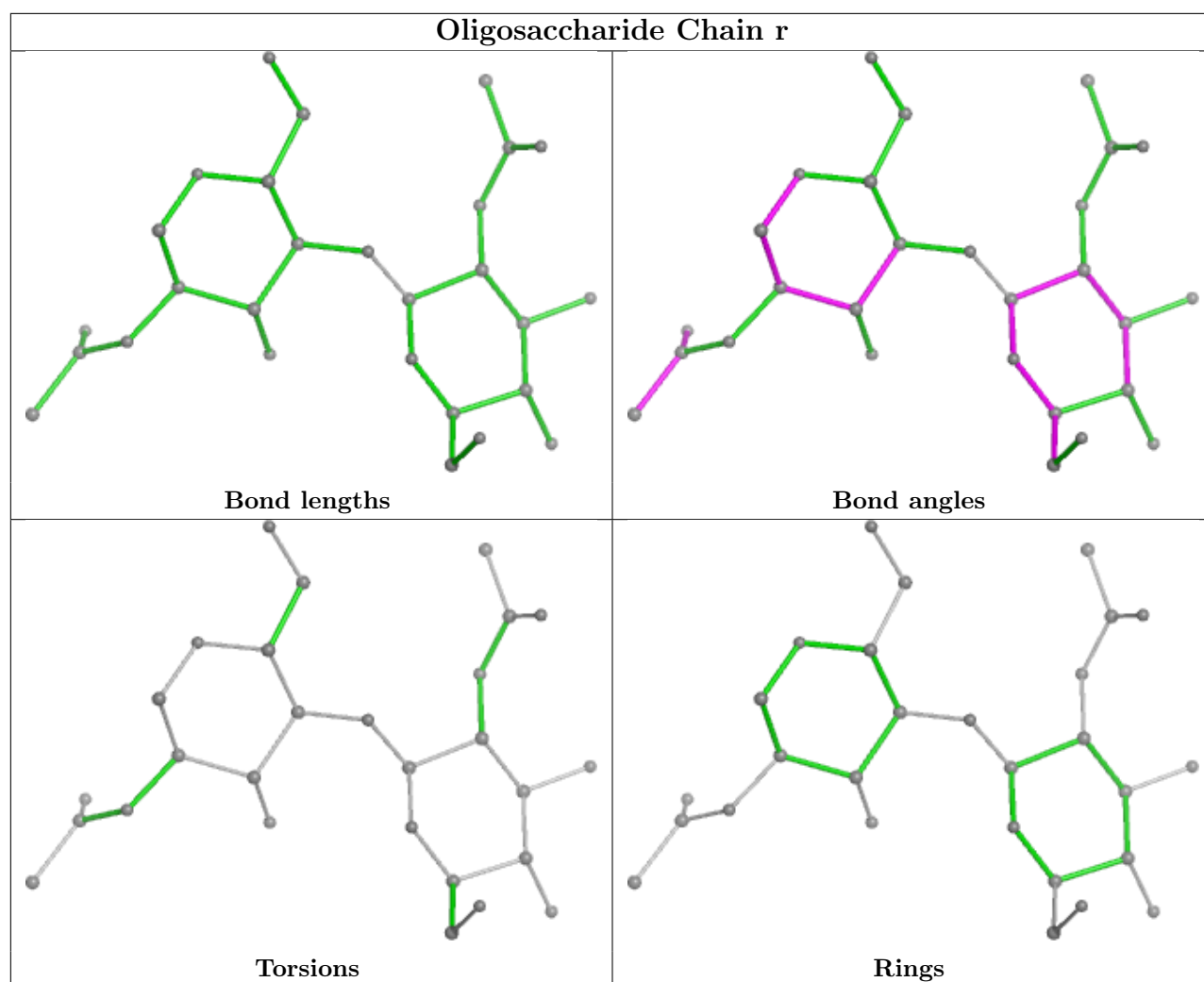


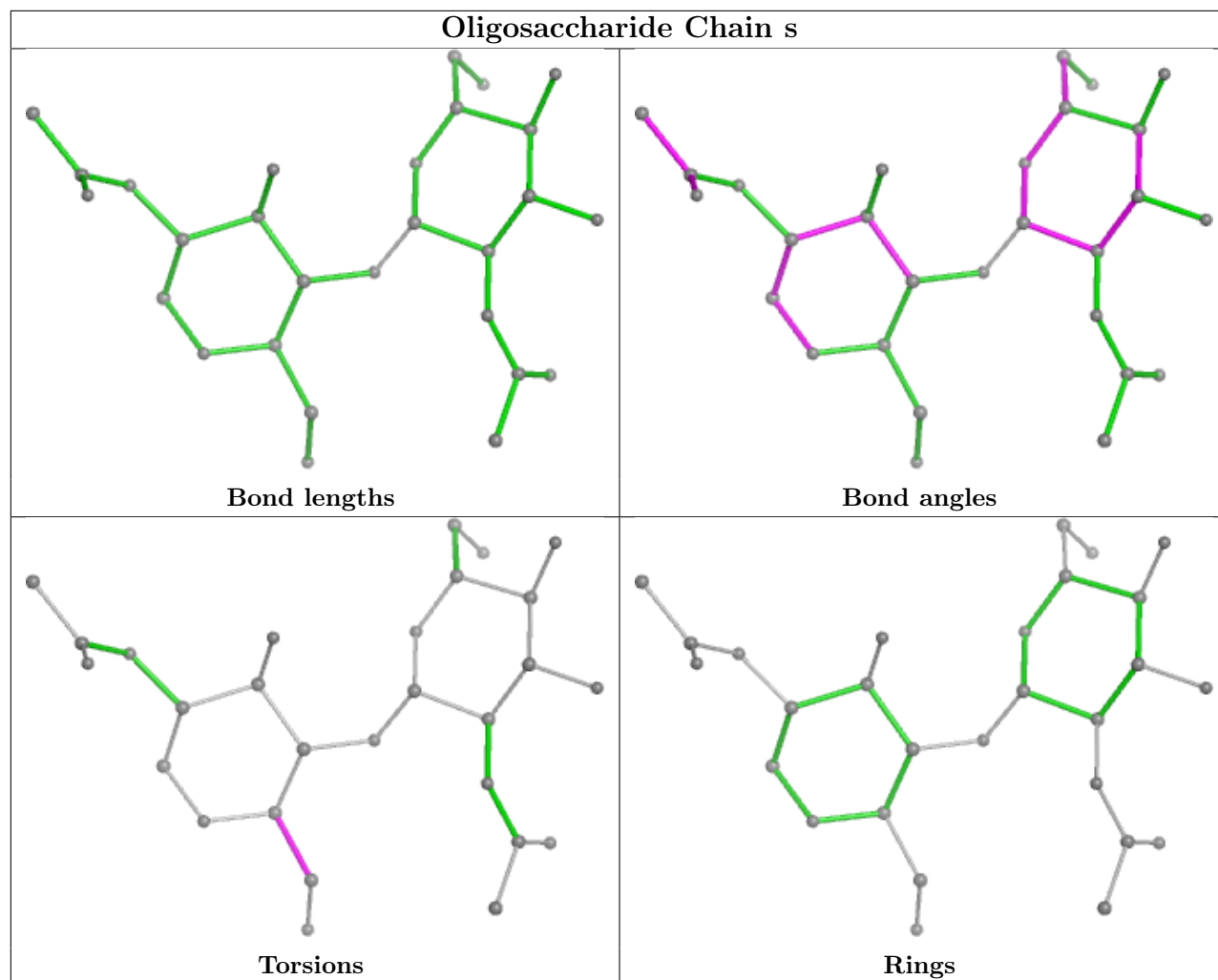


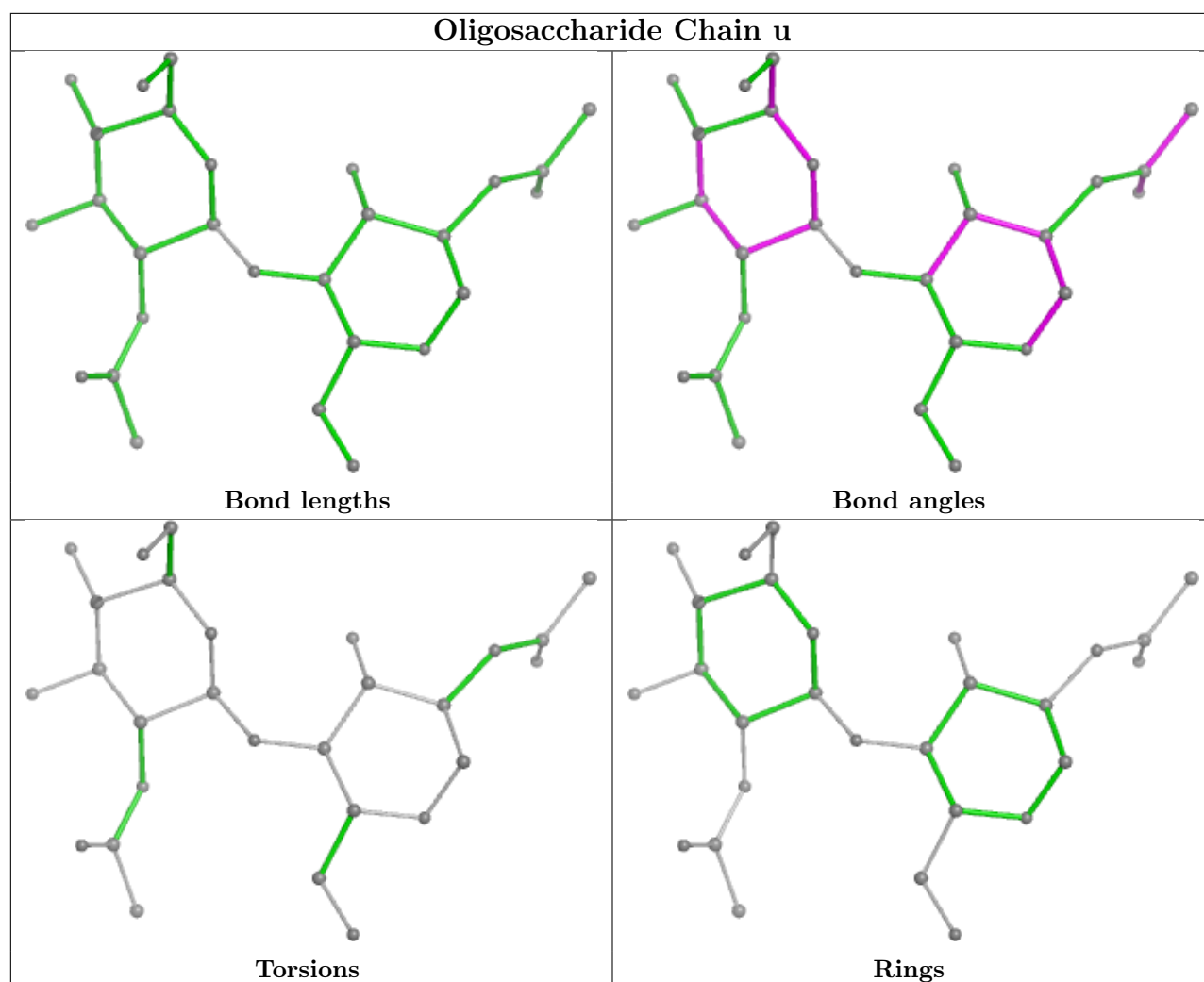


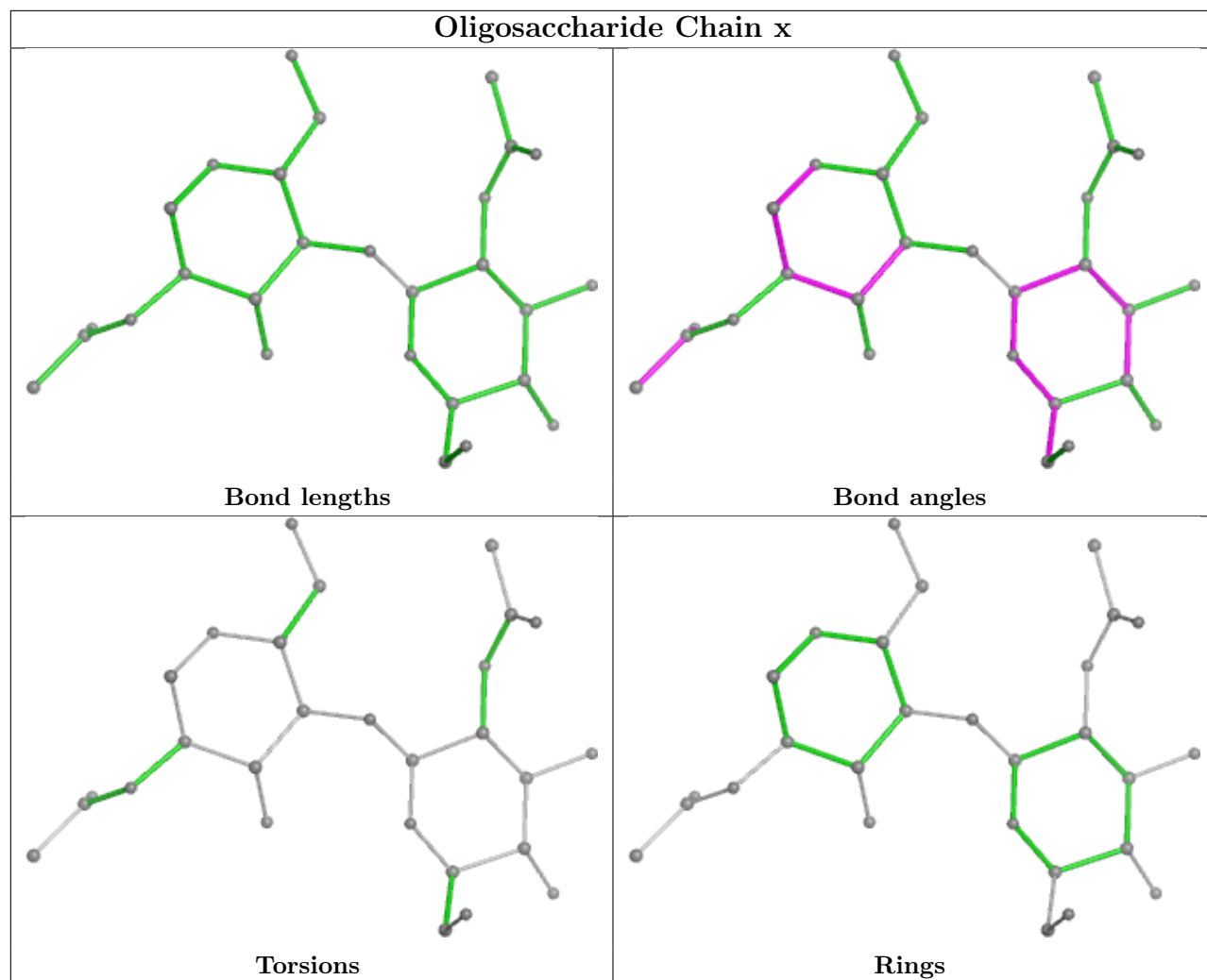


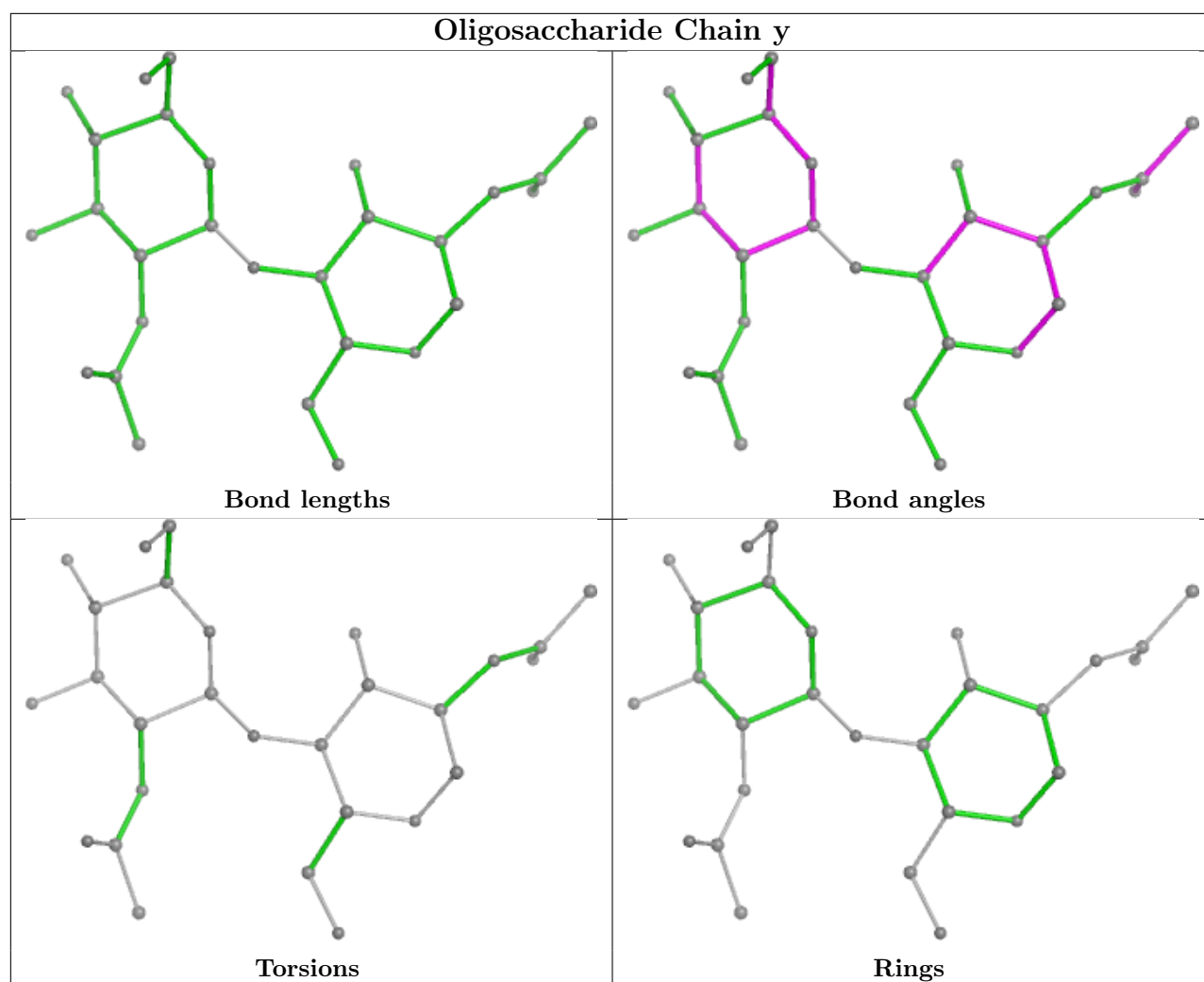


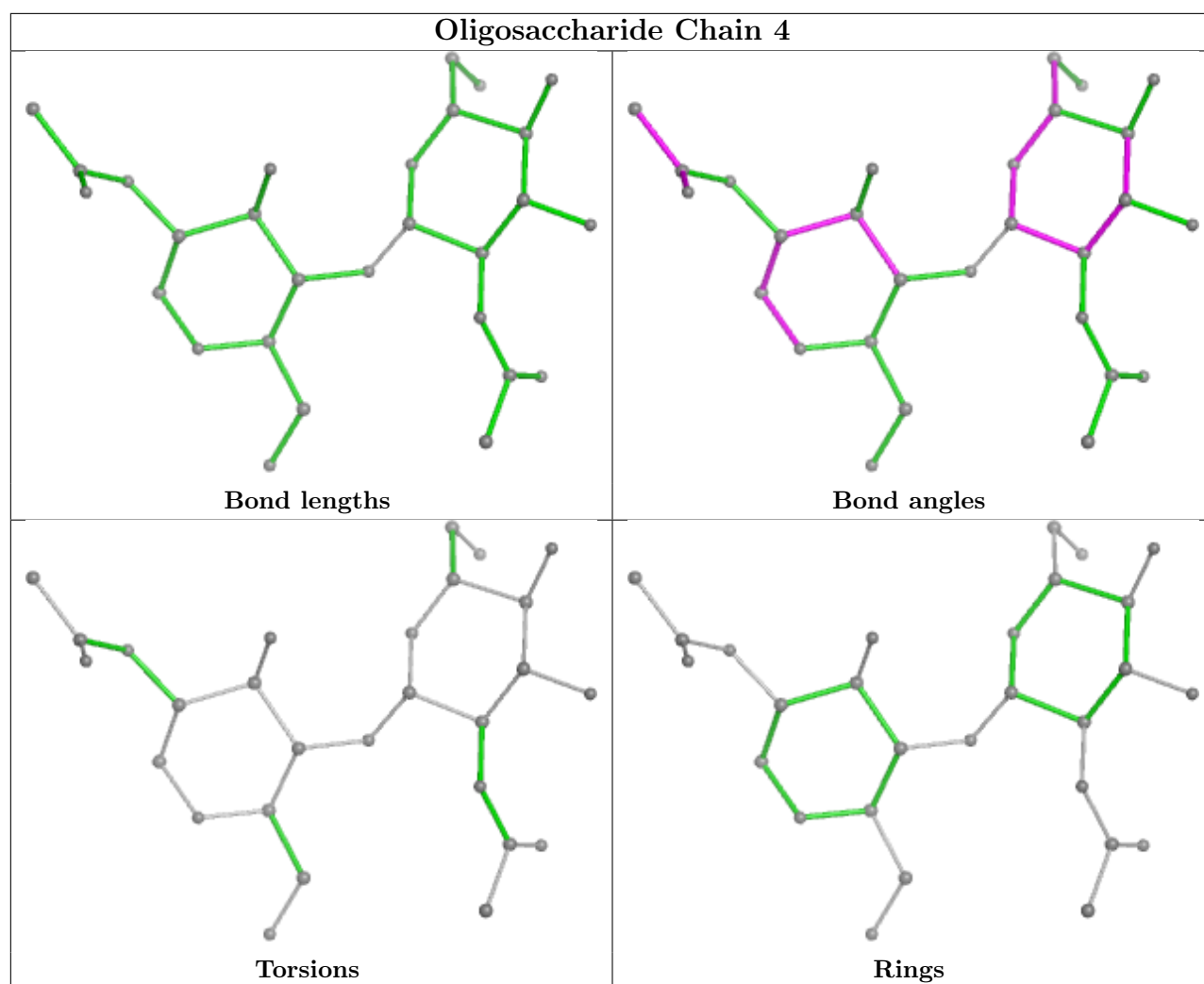


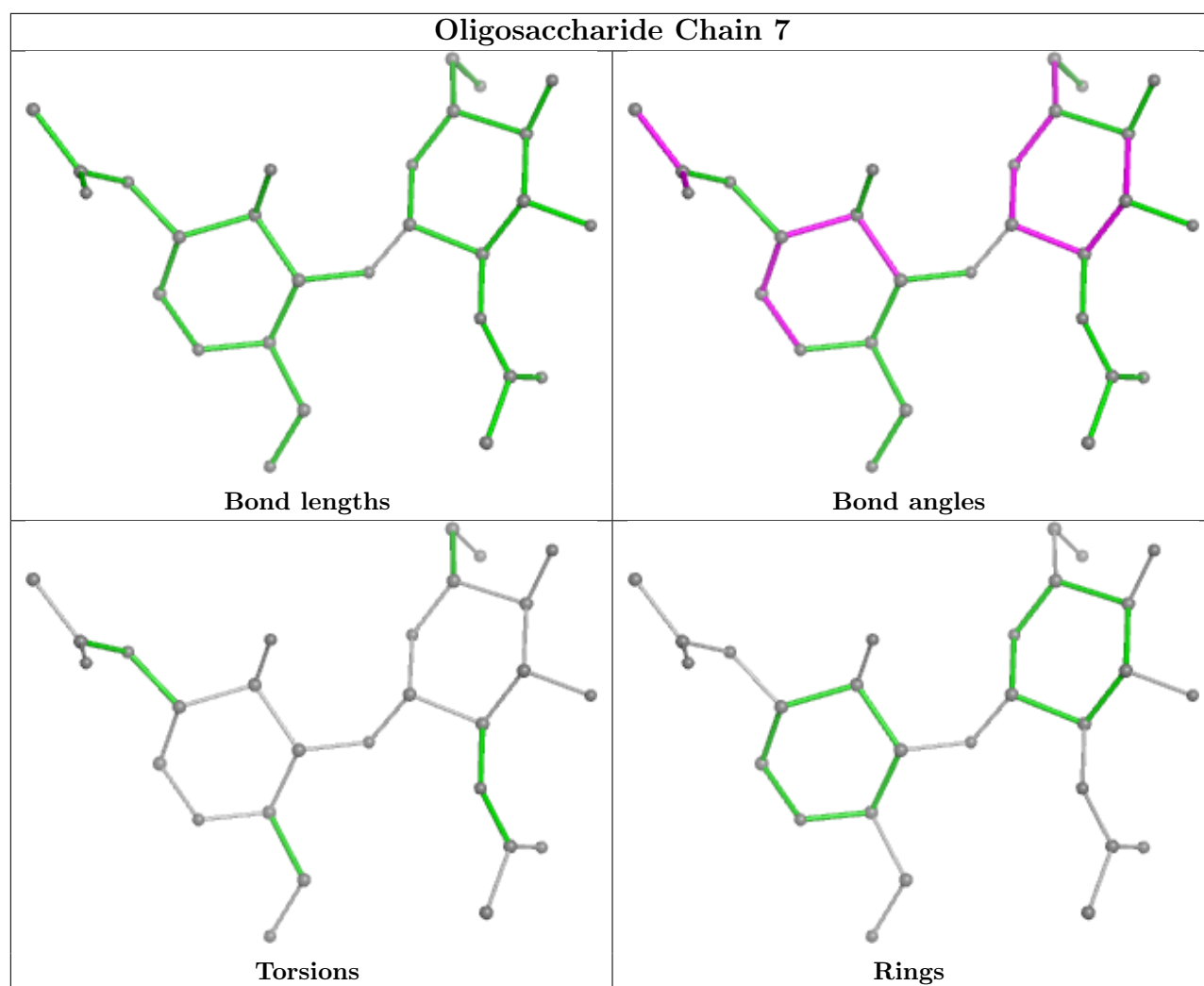


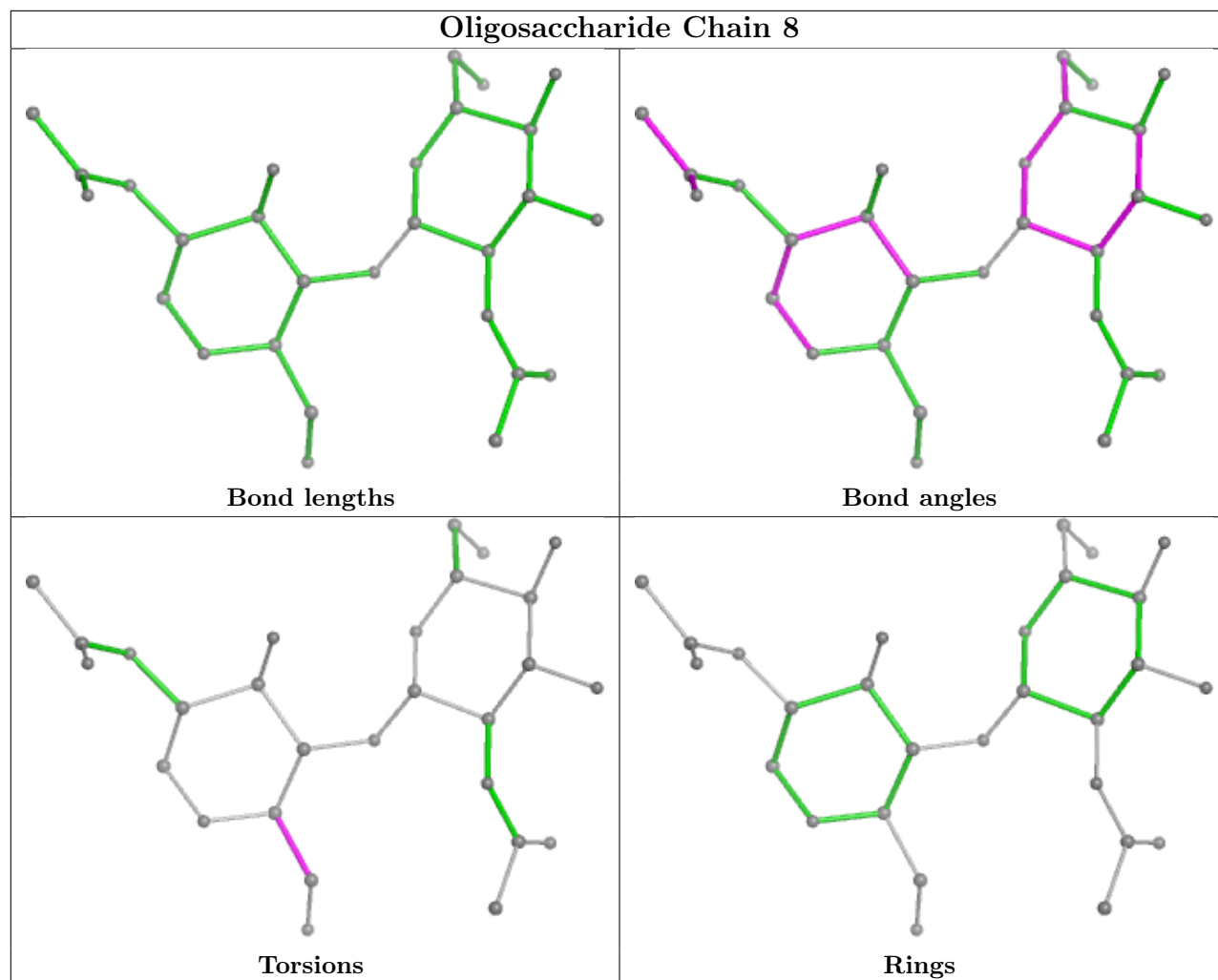


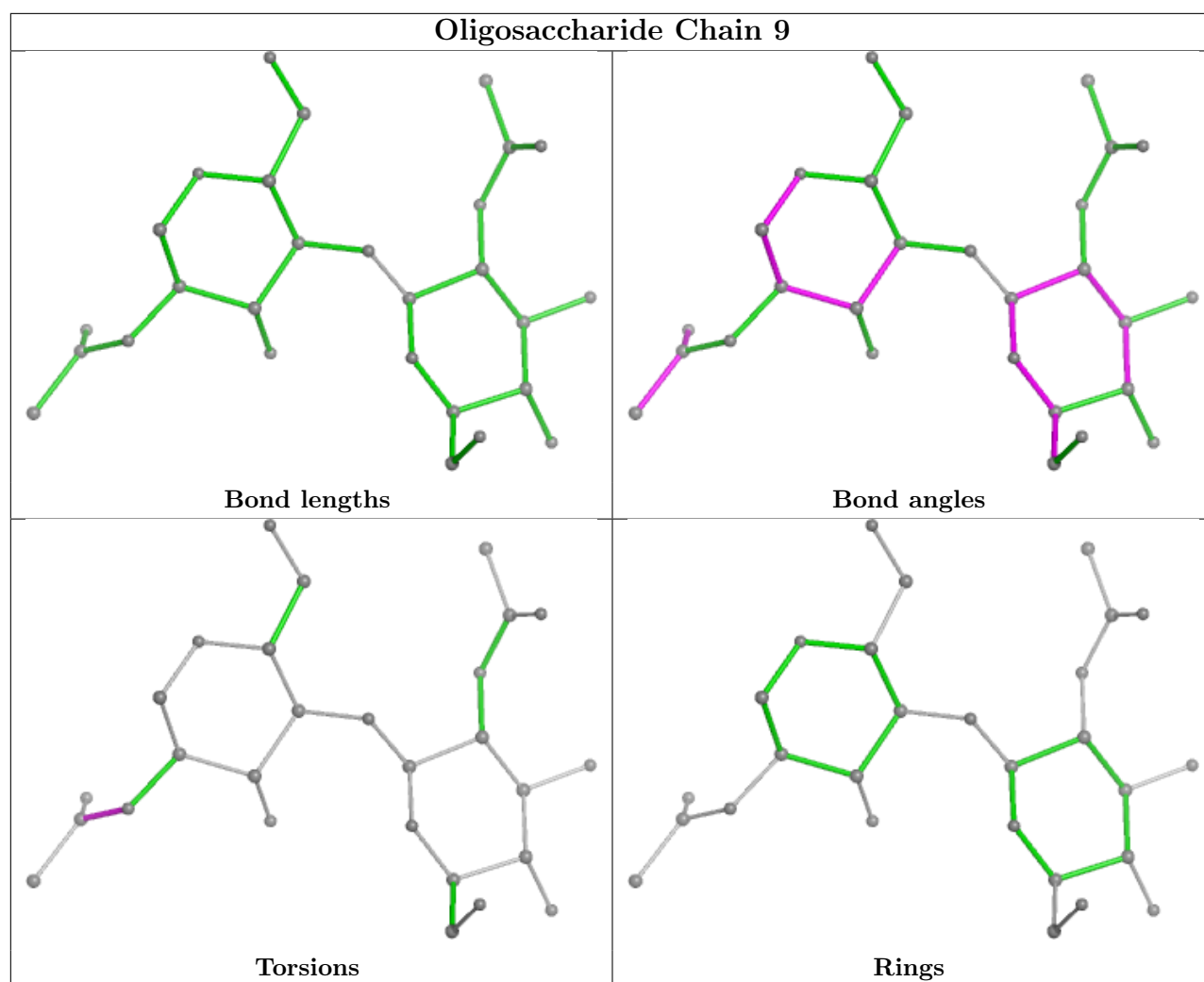


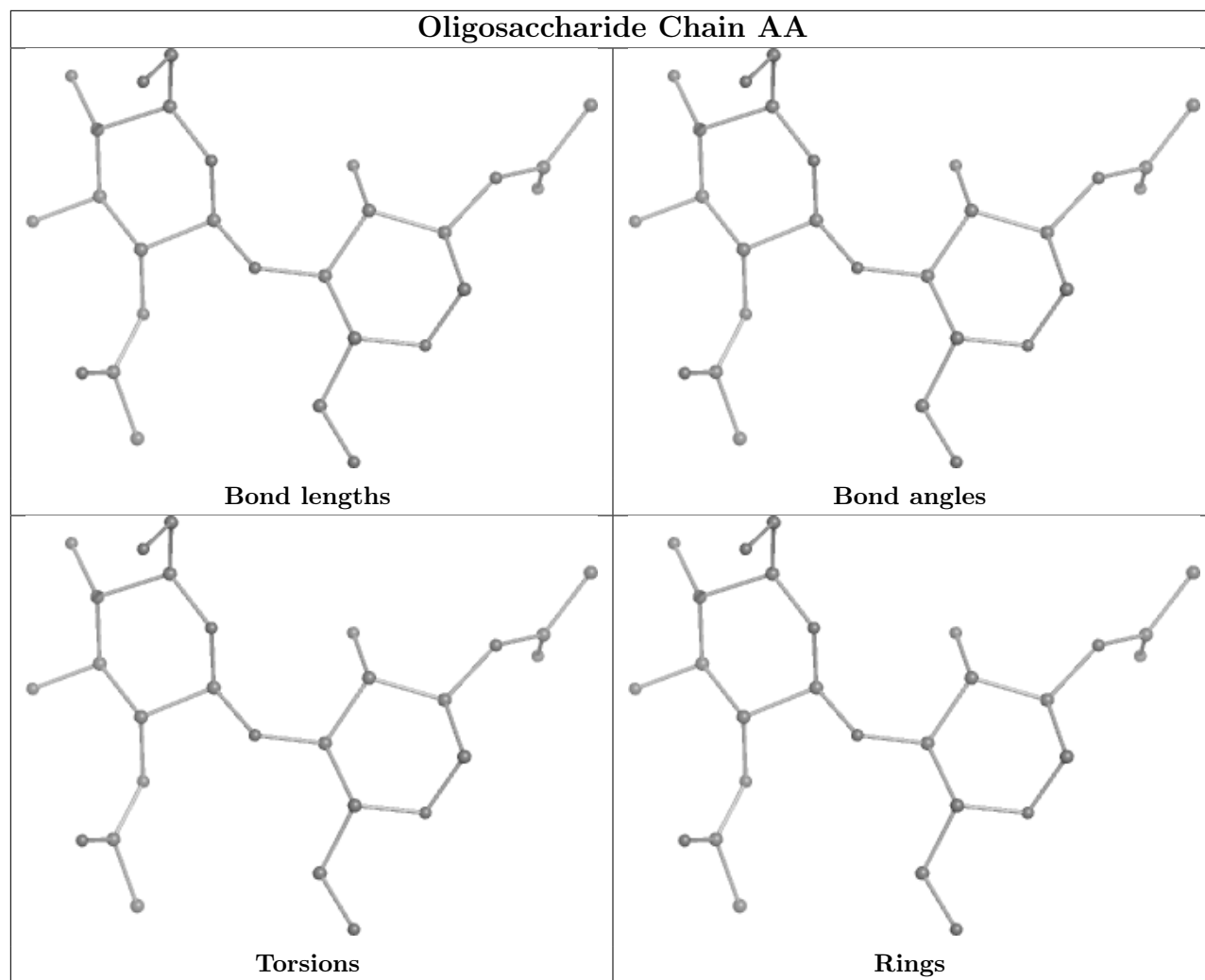


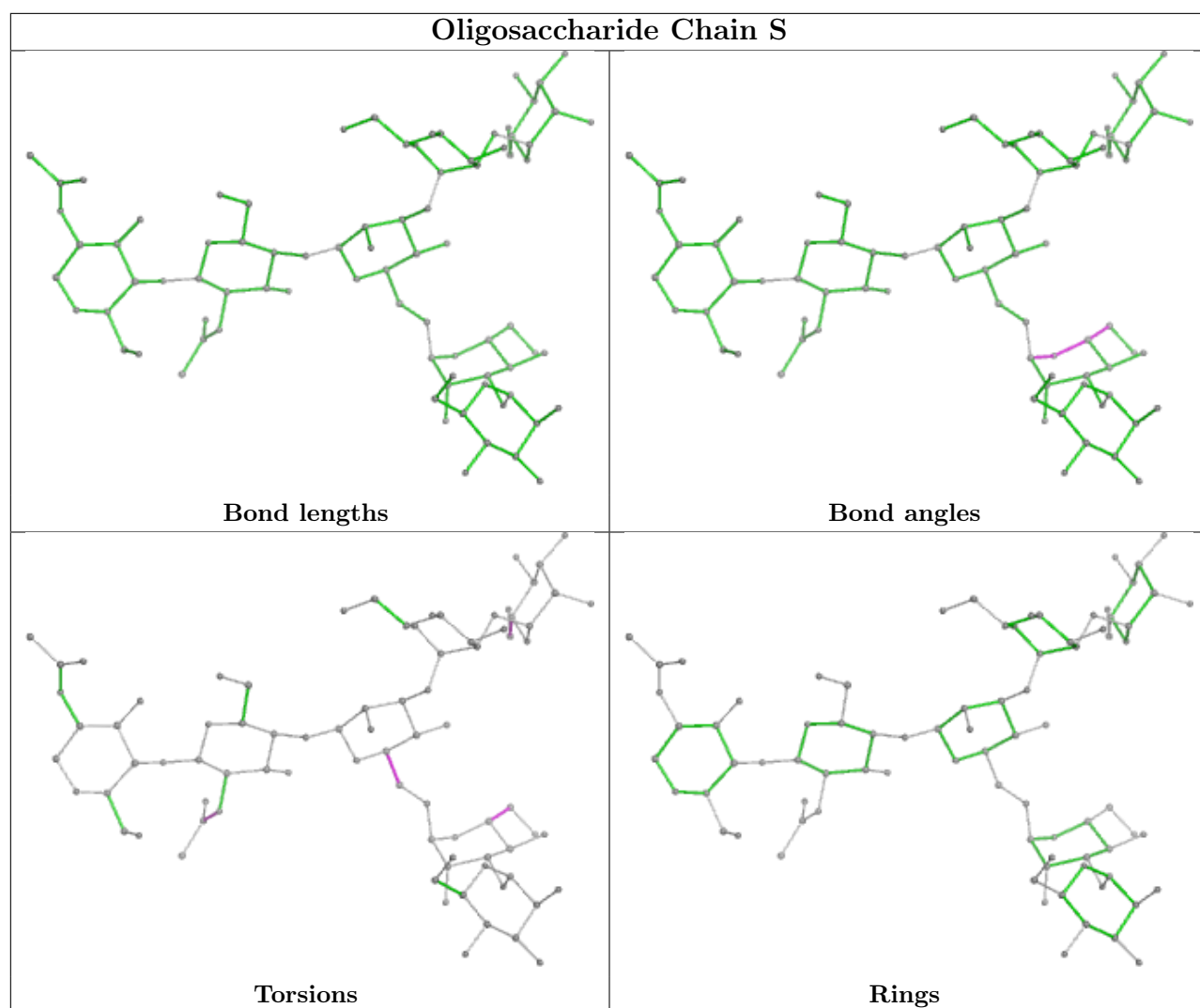


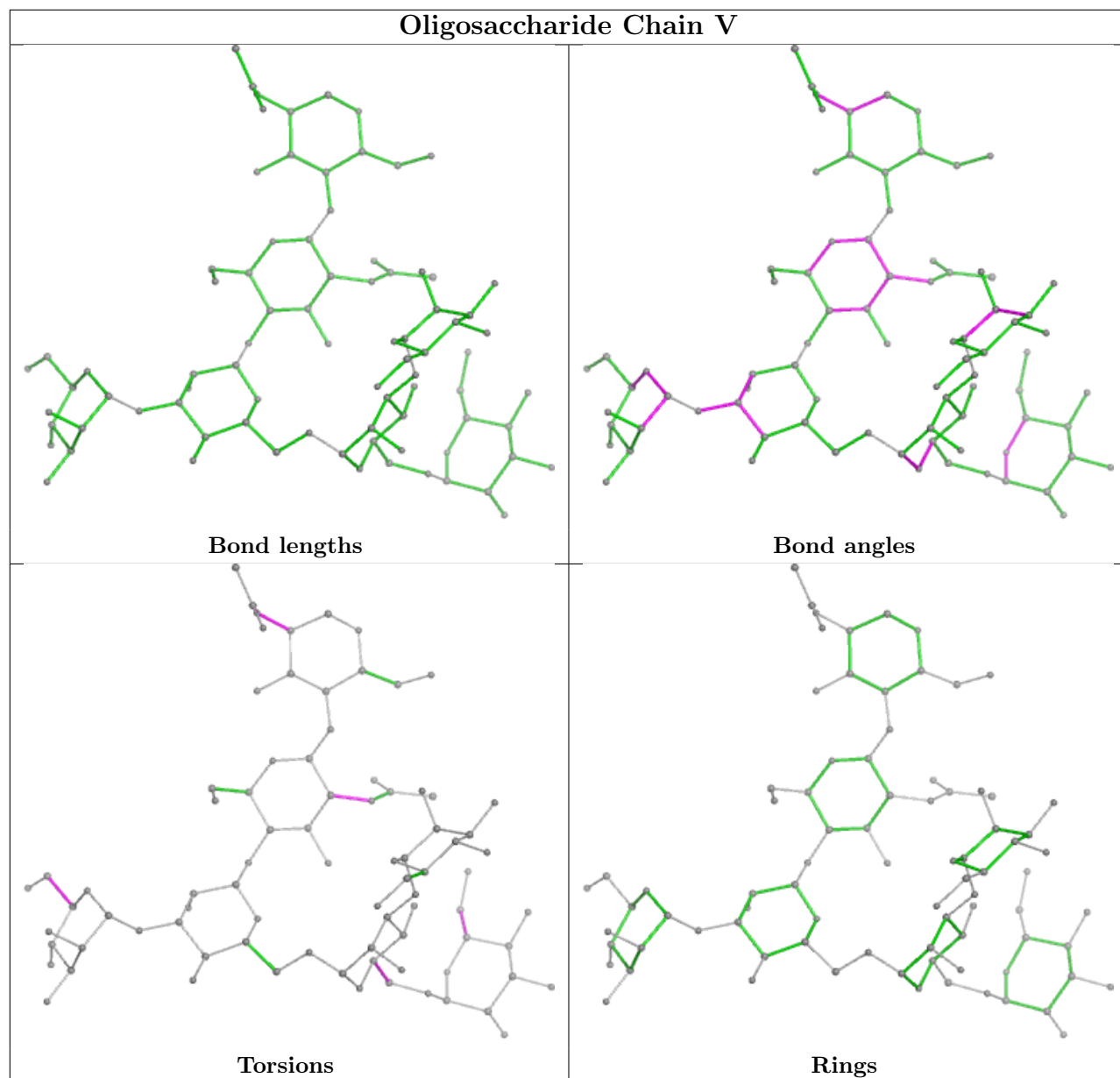


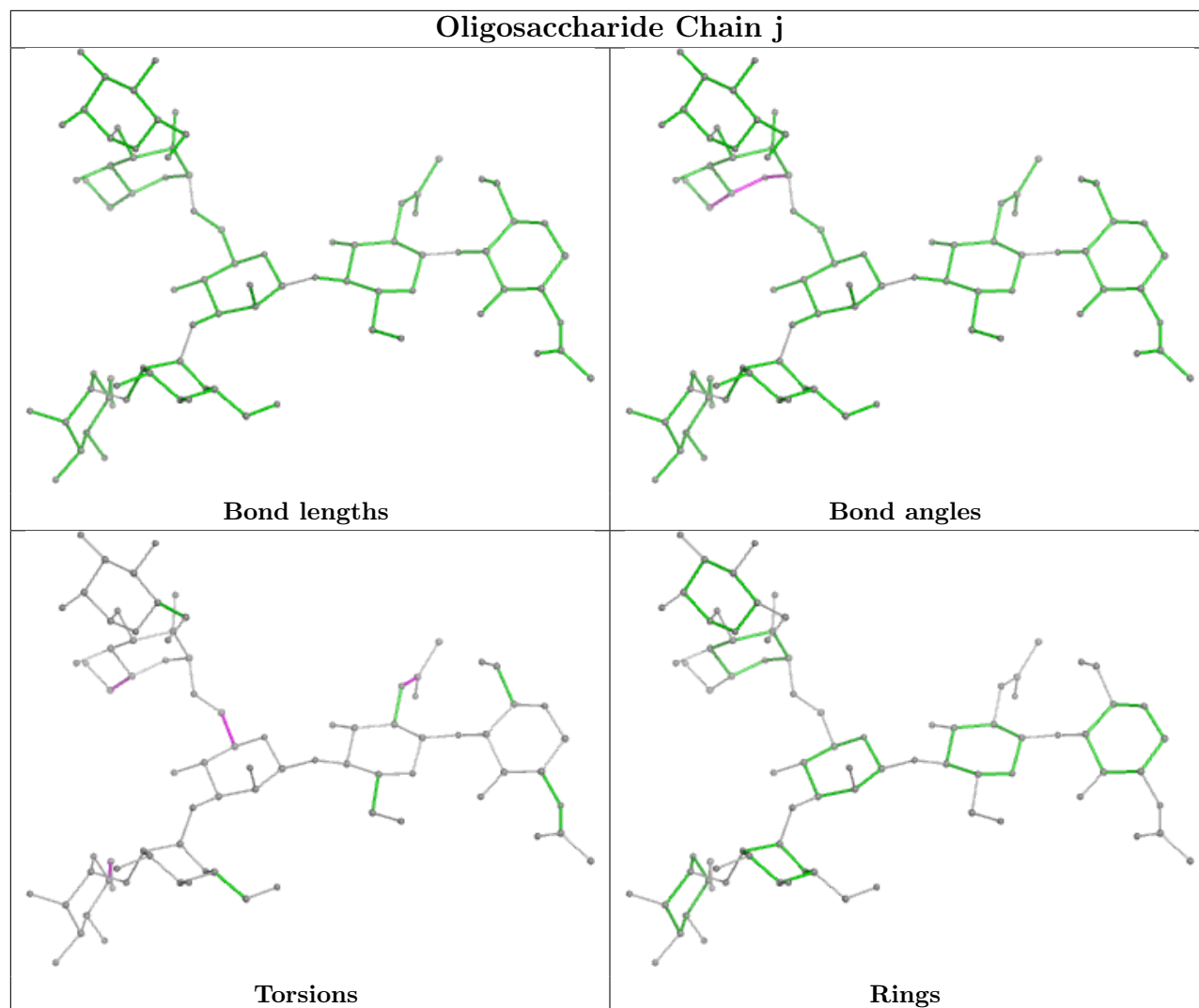


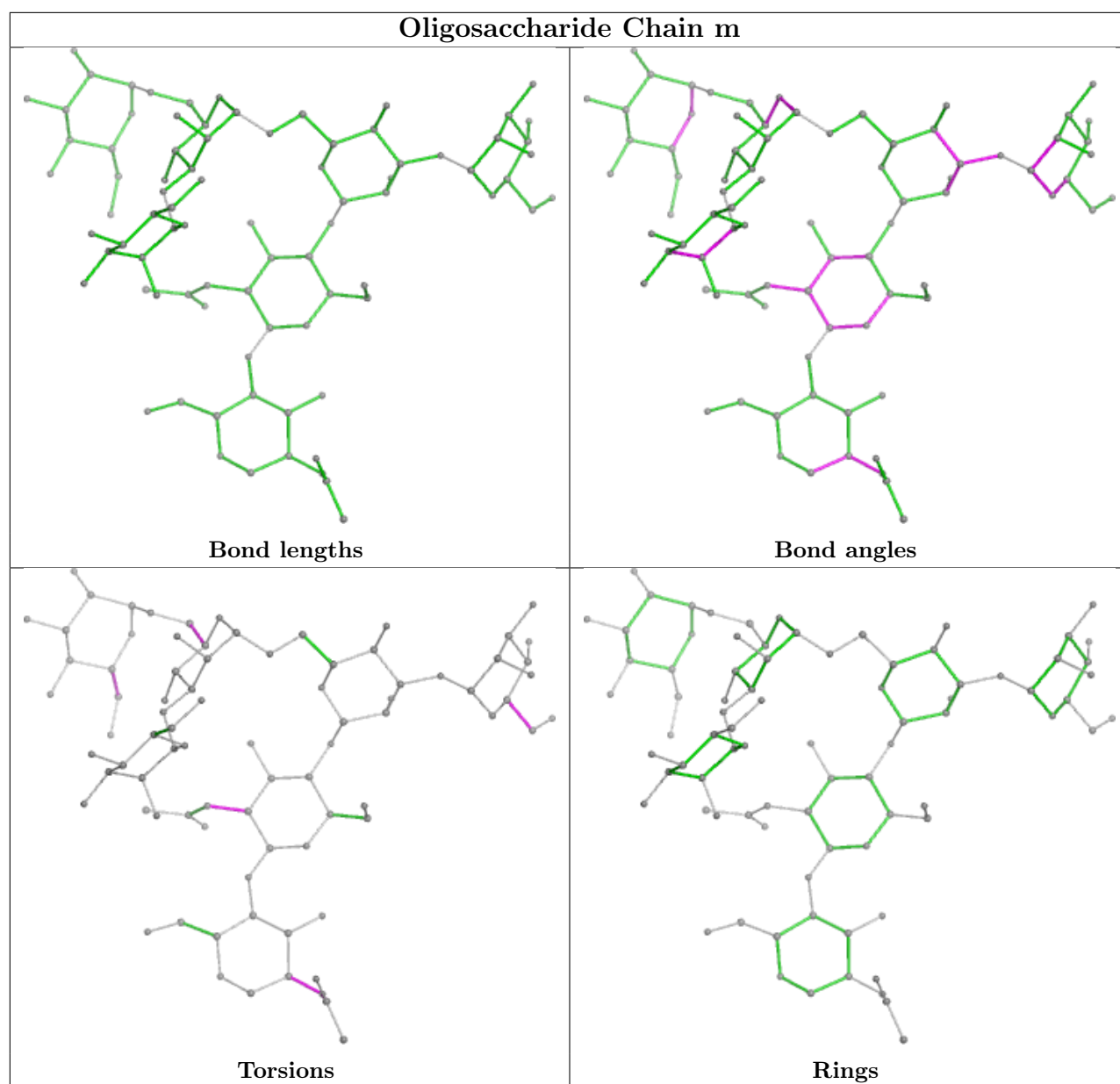


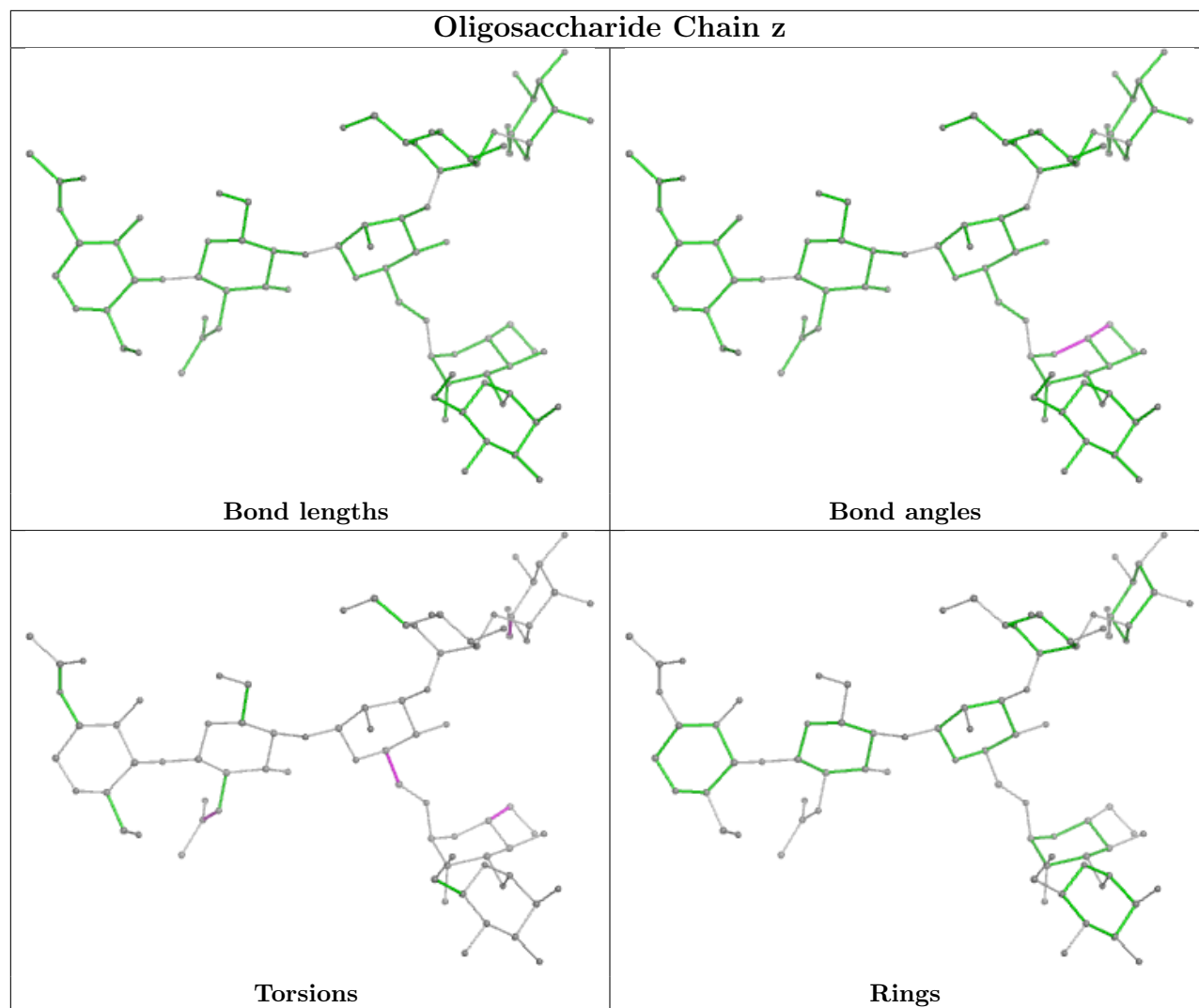


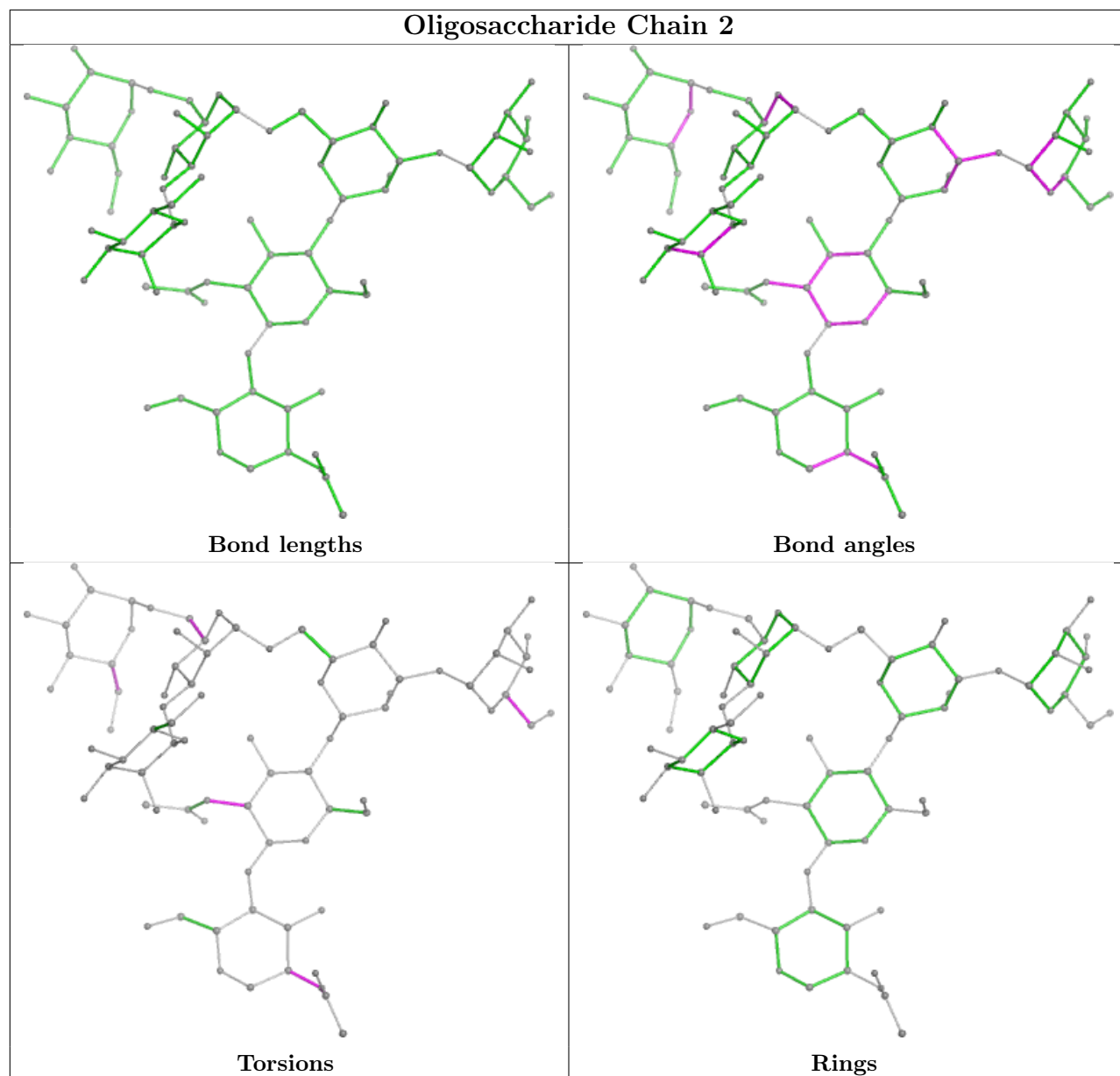


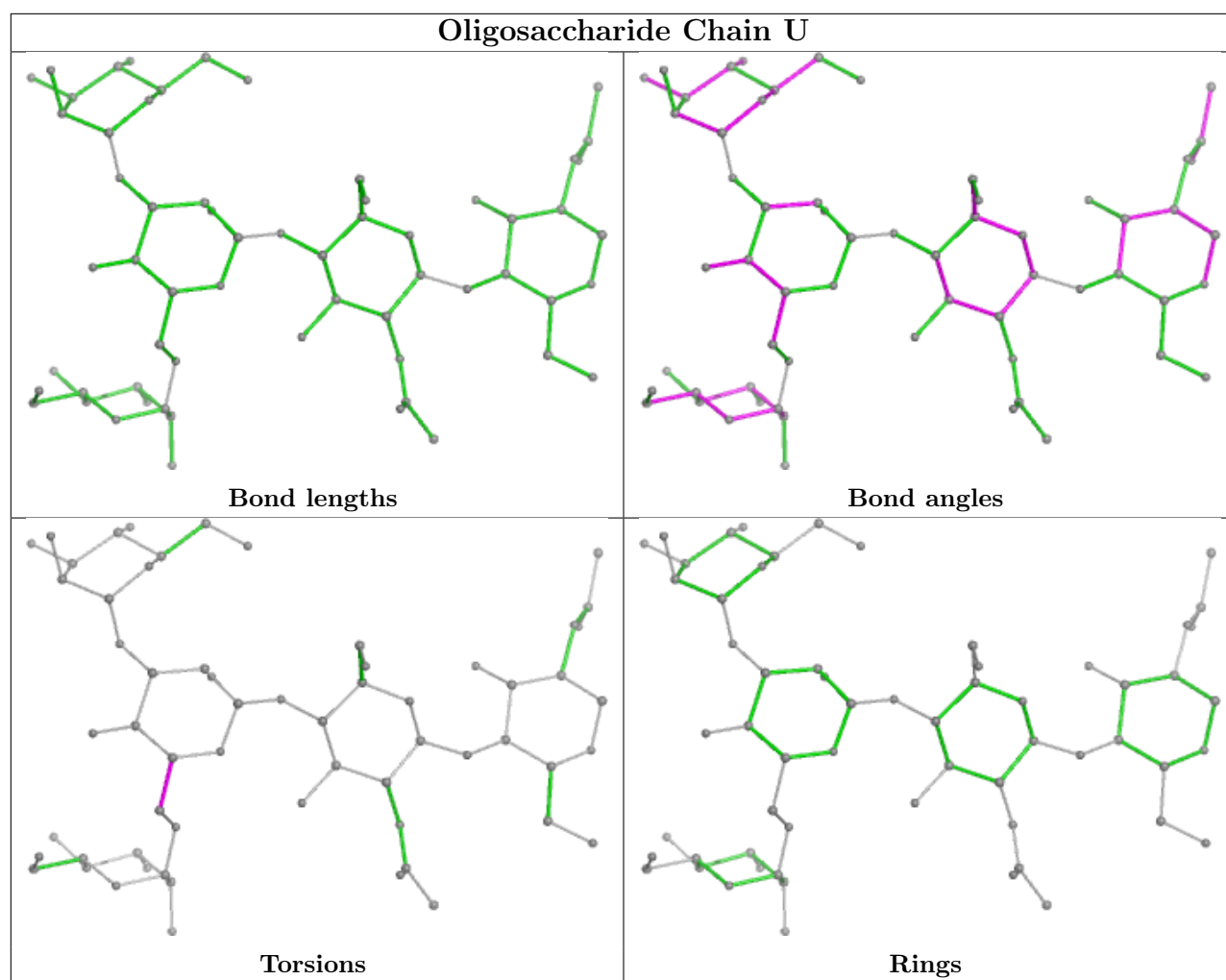


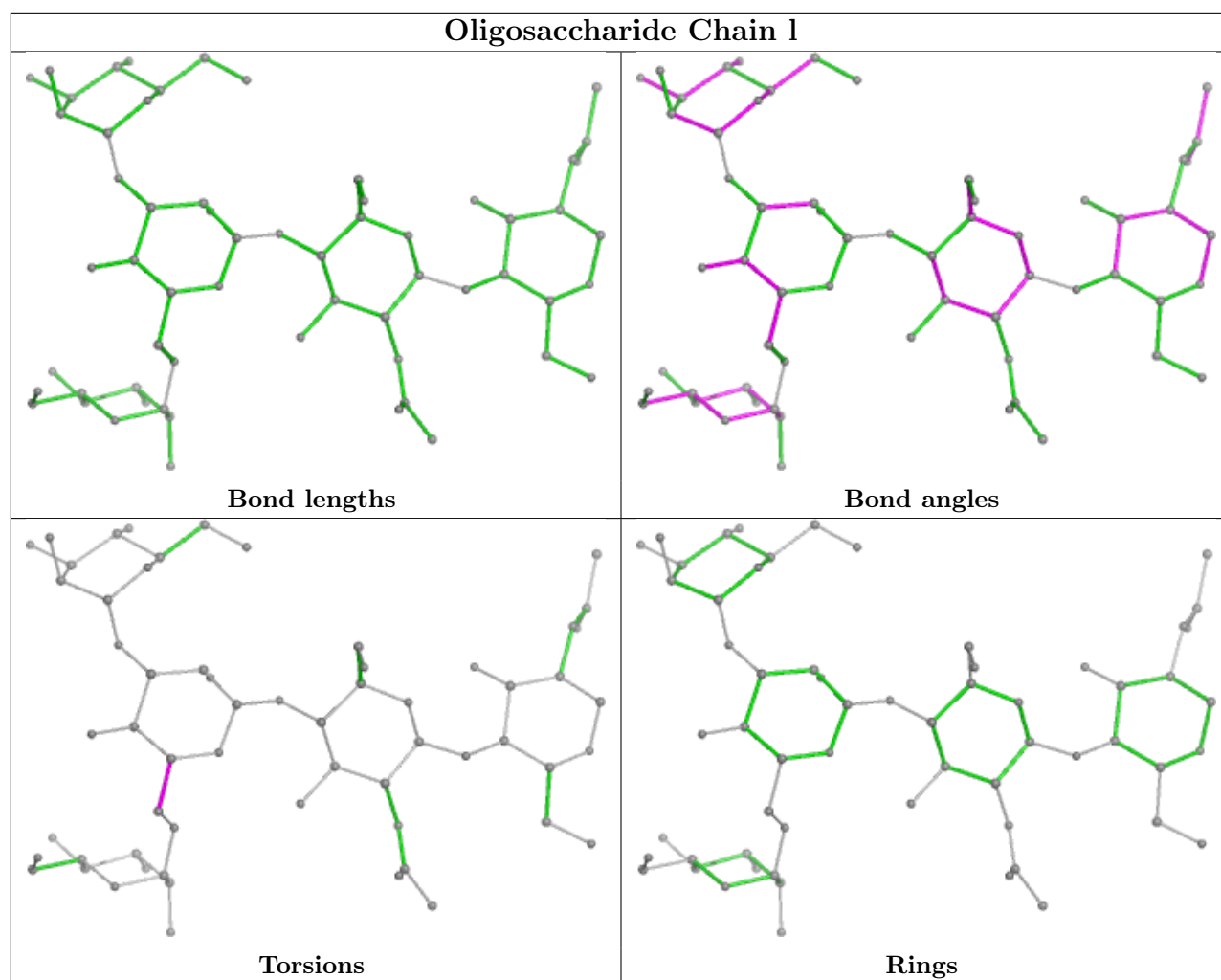


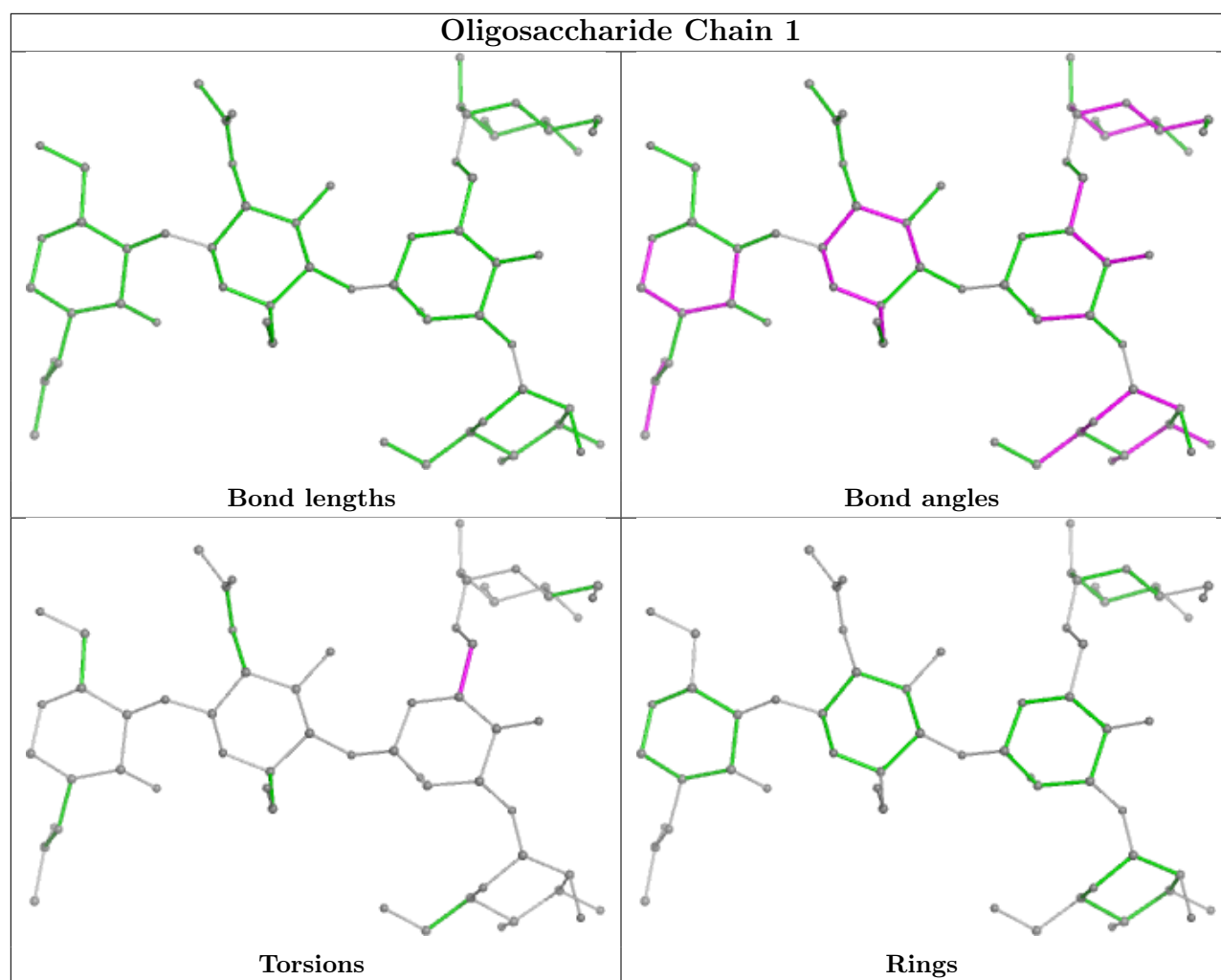


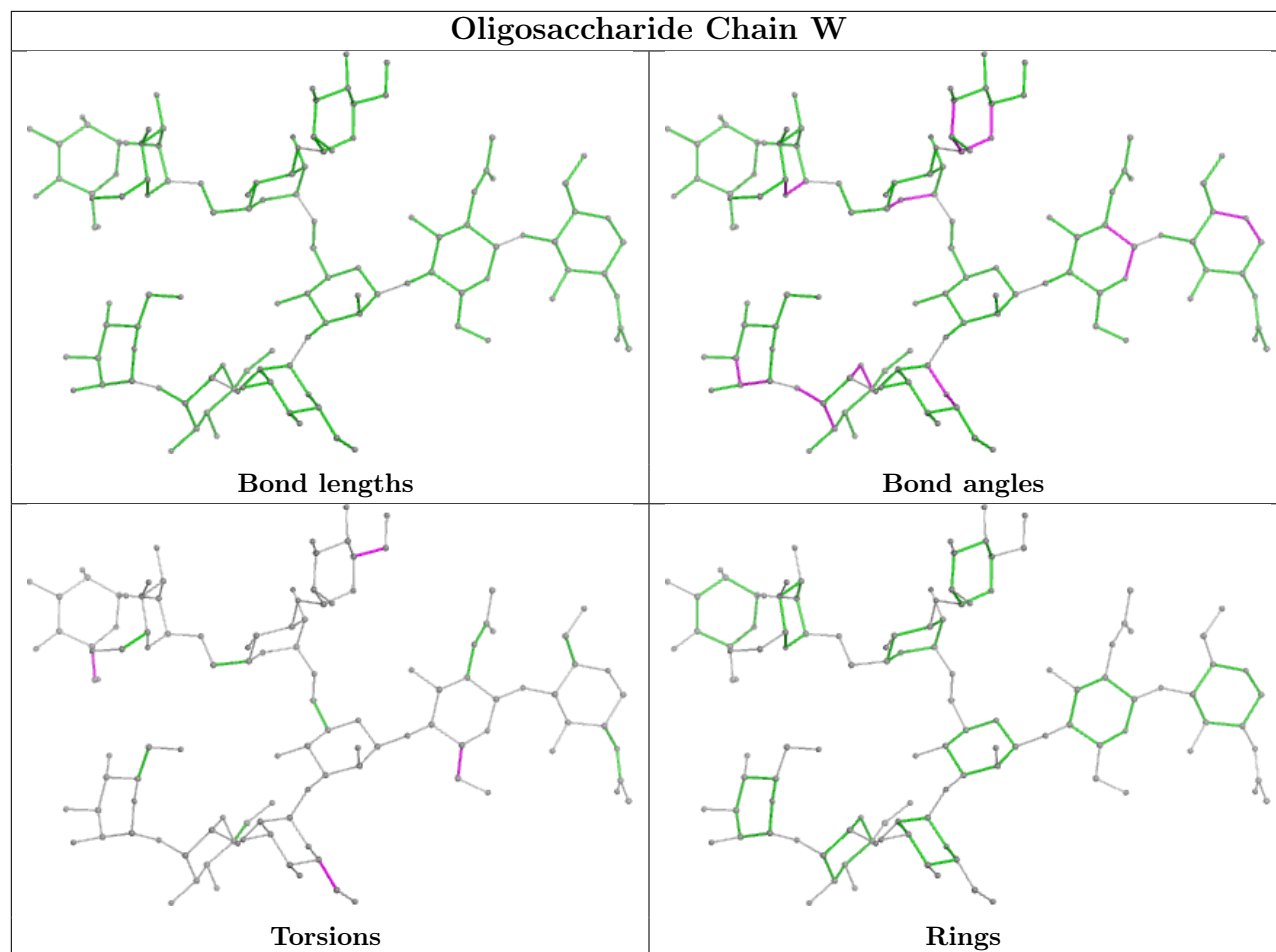


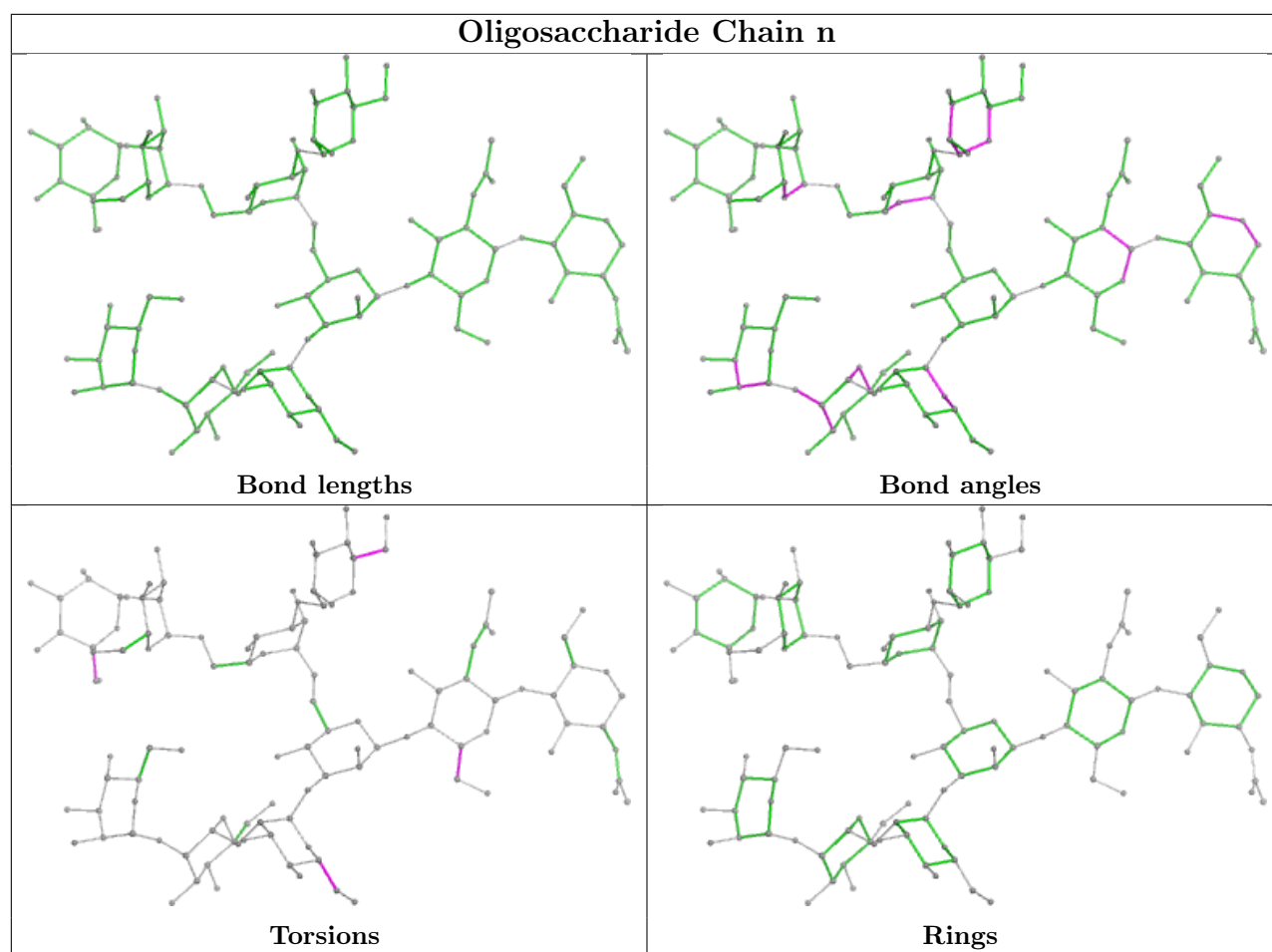


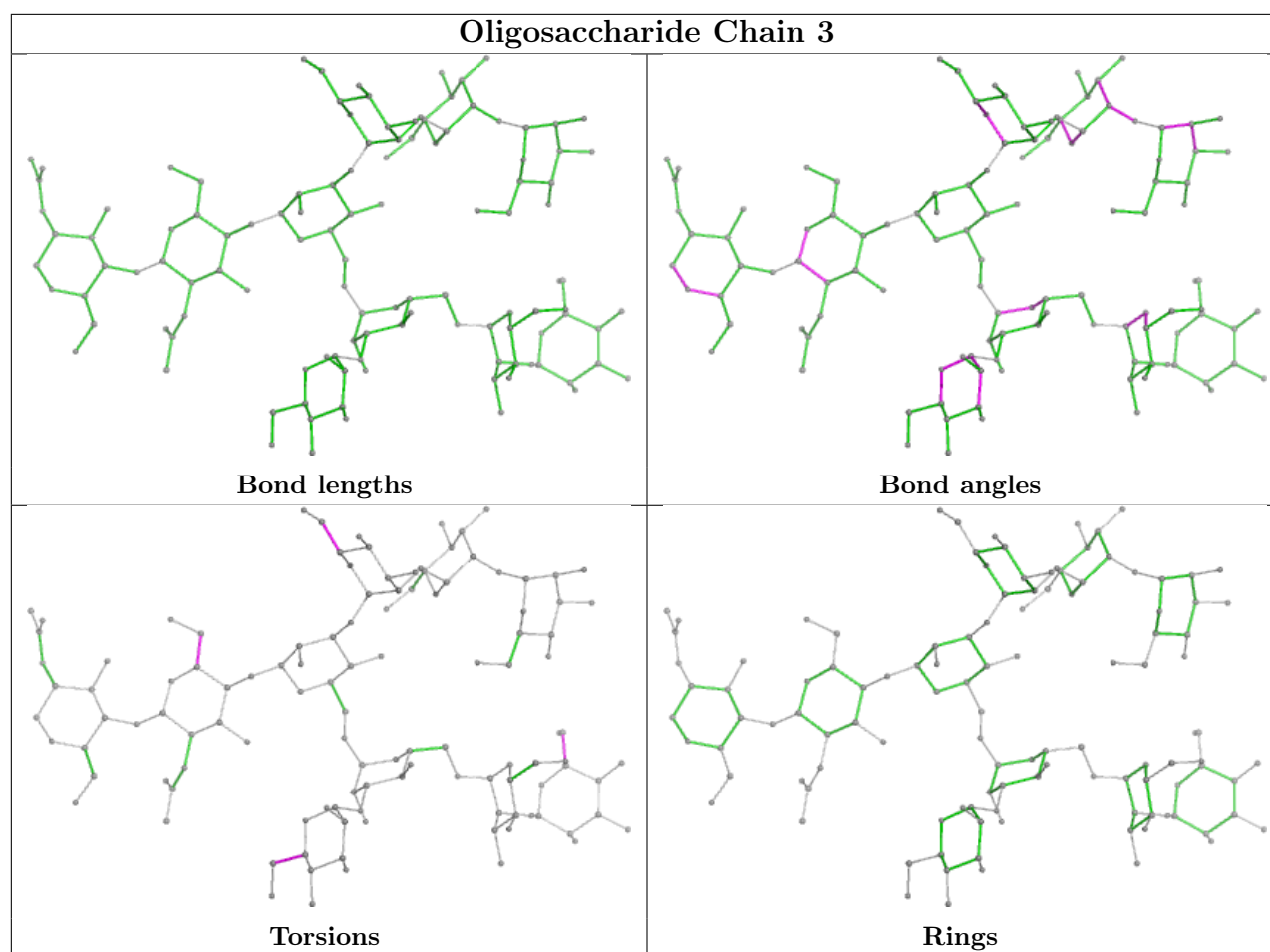












5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
10	NAG	F	1618	2	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
10	NAG	D	1343	1	14,14,15	0.53	0	17,19,21	2.23	3 (17%)
10	NAG	C	1343	1	14,14,15	0.50	0	17,19,21	2.25	3 (17%)
10	NAG	F	1637	2	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
10	NAG	E	1618	2	14,14,15	0.51	0	17,19,21	2.24	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	E	1637	2	14,14,15	0.49	0	17,19,21	2.24	3 (17%)
10	NAG	B	1618	2	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
10	NAG	A	1343	1	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
10	NAG	B	1637	2	14,14,15	0.50	0	17,19,21	2.23	3 (17%)

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
10	NAG	F	1618	2	-	3/6/23/26	0/1/1/1
10	NAG	D	1343	1	-	0/6/23/26	0/1/1/1
10	NAG	C	1343	1	-	0/6/23/26	0/1/1/1
10	NAG	F	1637	2	-	0/6/23/26	0/1/1/1
10	NAG	E	1618	2	-	3/6/23/26	0/1/1/1
10	NAG	E	1637	2	-	0/6/23/26	0/1/1/1
10	NAG	B	1618	2	-	3/6/23/26	0/1/1/1
10	NAG	A	1343	1	-	0/6/23/26	0/1/1/1
10	NAG	B	1637	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1343	NAG	O5-C1-C2	-7.39	99.61	111.29
10	B	1618	NAG	O5-C1-C2	-7.39	99.62	111.29
10	E	1637	NAG	O5-C1-C2	-7.38	99.63	111.29
10	F	1618	NAG	O5-C1-C2	-7.38	99.64	111.29
10	A	1343	NAG	O5-C1-C2	-7.38	99.64	111.29

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	1618	NAG	C1-C2-N2-C7
10	E	1618	NAG	C1-C2-N2-C7
10	F	1618	NAG	C1-C2-N2-C7
10	B	1618	NAG	C3-C2-N2-C7
10	E	1618	NAG	C3-C2-N2-C7

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
2	E	1
2	F	1
1	A	1
1	C	1
1	D	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	658:GLN	C	659:ASP	N	1.61
1	E	658:GLN	C	659:ASP	N	1.61
1	F	658:GLN	C	659:ASP	N	1.61
1	A	92:GLU	C	93:PHE	N	1.19
1	C	92:GLU	C	93:PHE	N	1.19

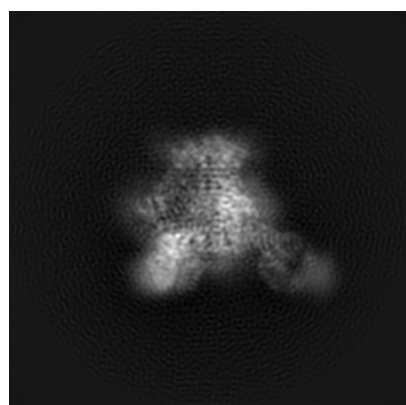
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3121. These allow visual inspection of the internal detail of the map and identification of artifacts.

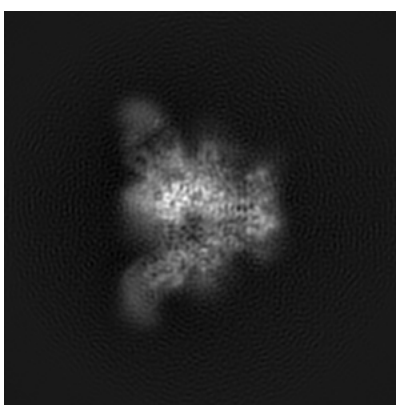
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

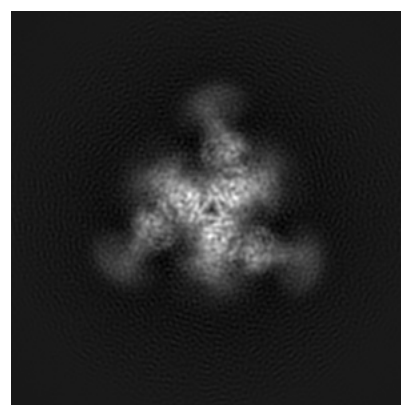
6.1.1 Primary map



X



Y

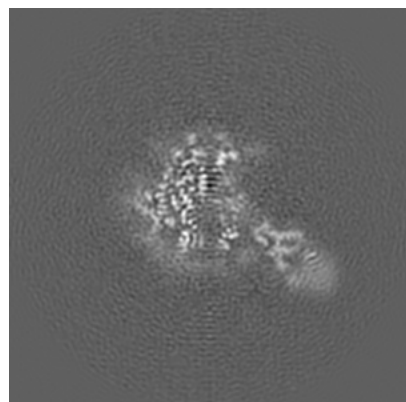


Z

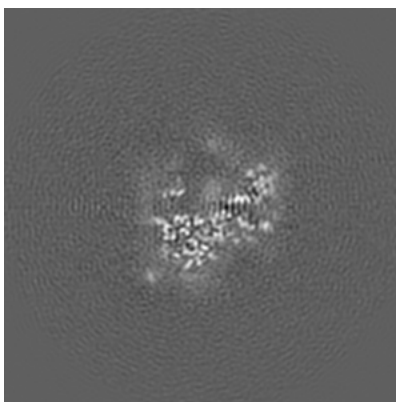
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

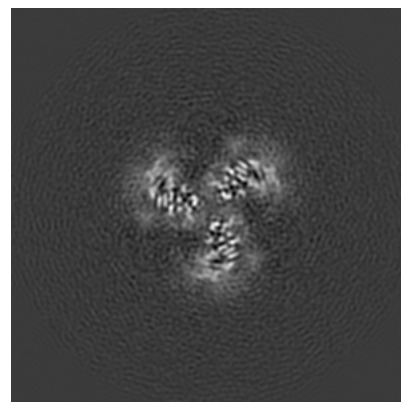
6.2.1 Primary map



X Index: 128



Y Index: 128

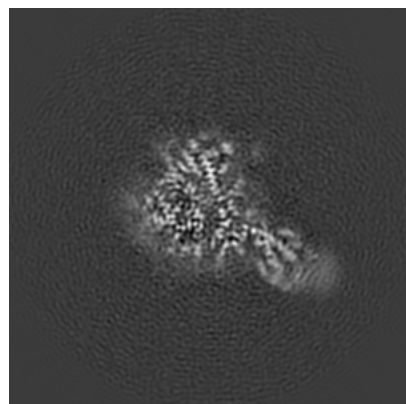


Z Index: 128

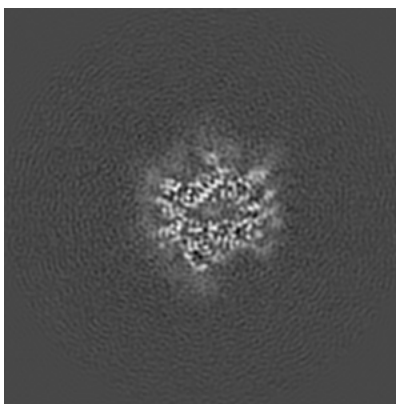
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

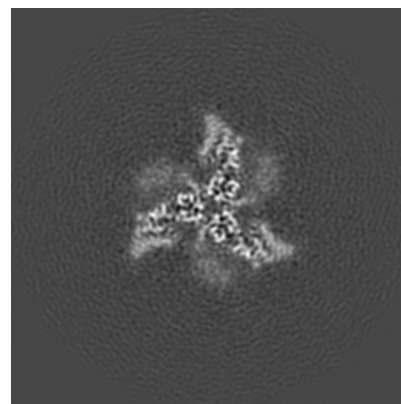
6.3.1 Primary map



X Index: 133



Y Index: 136

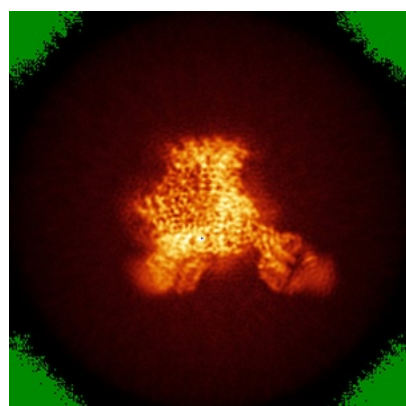


Z Index: 110

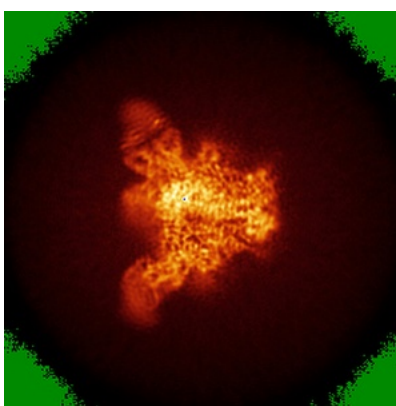
The images above show the largest variance slices of the map in three orthogonal directions.

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

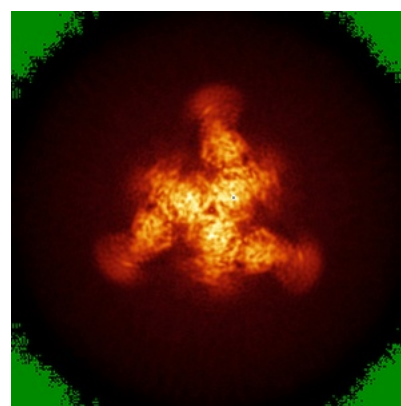
6.4.1 Primary map



X



Y



Z

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 0.041. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

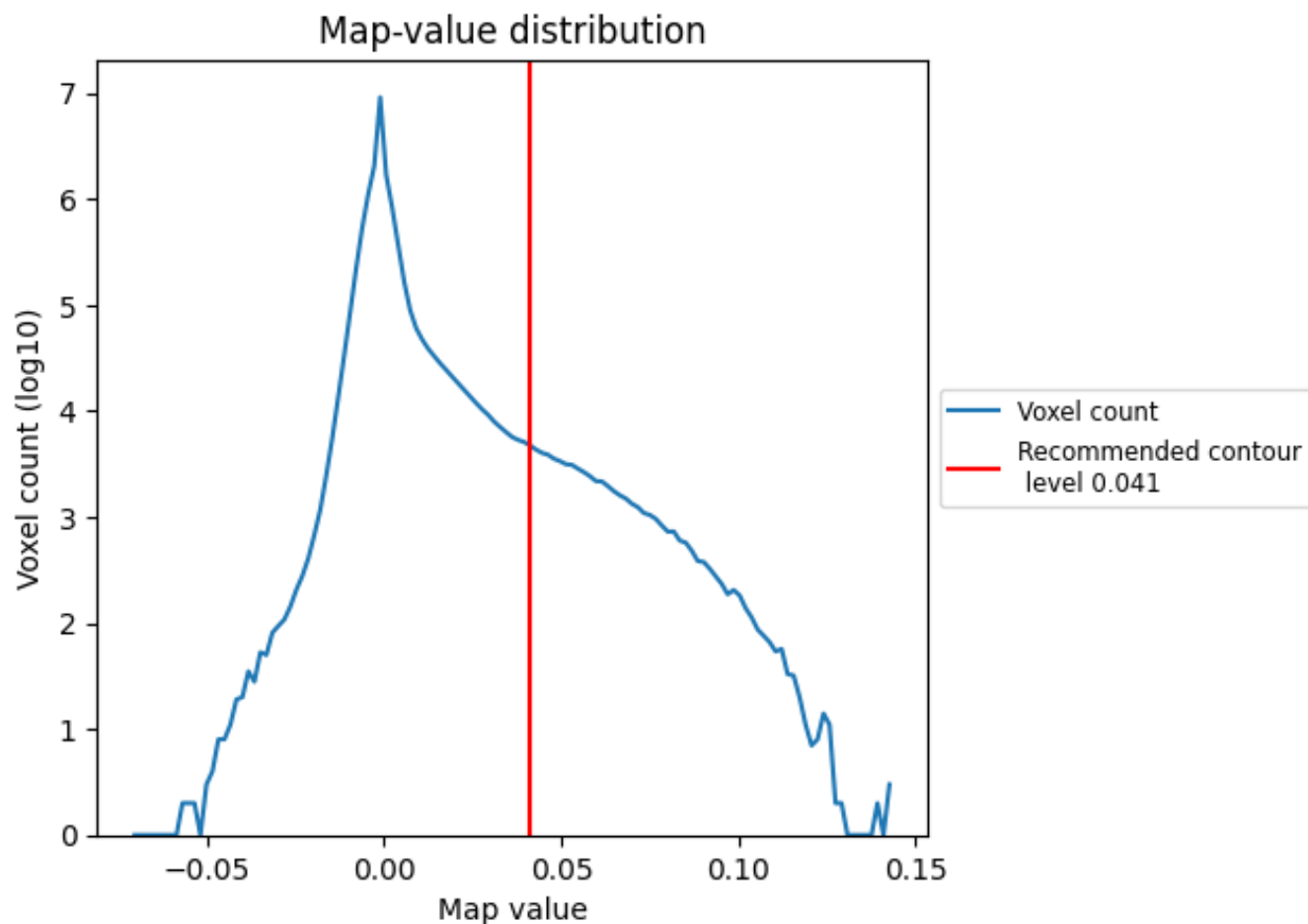
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

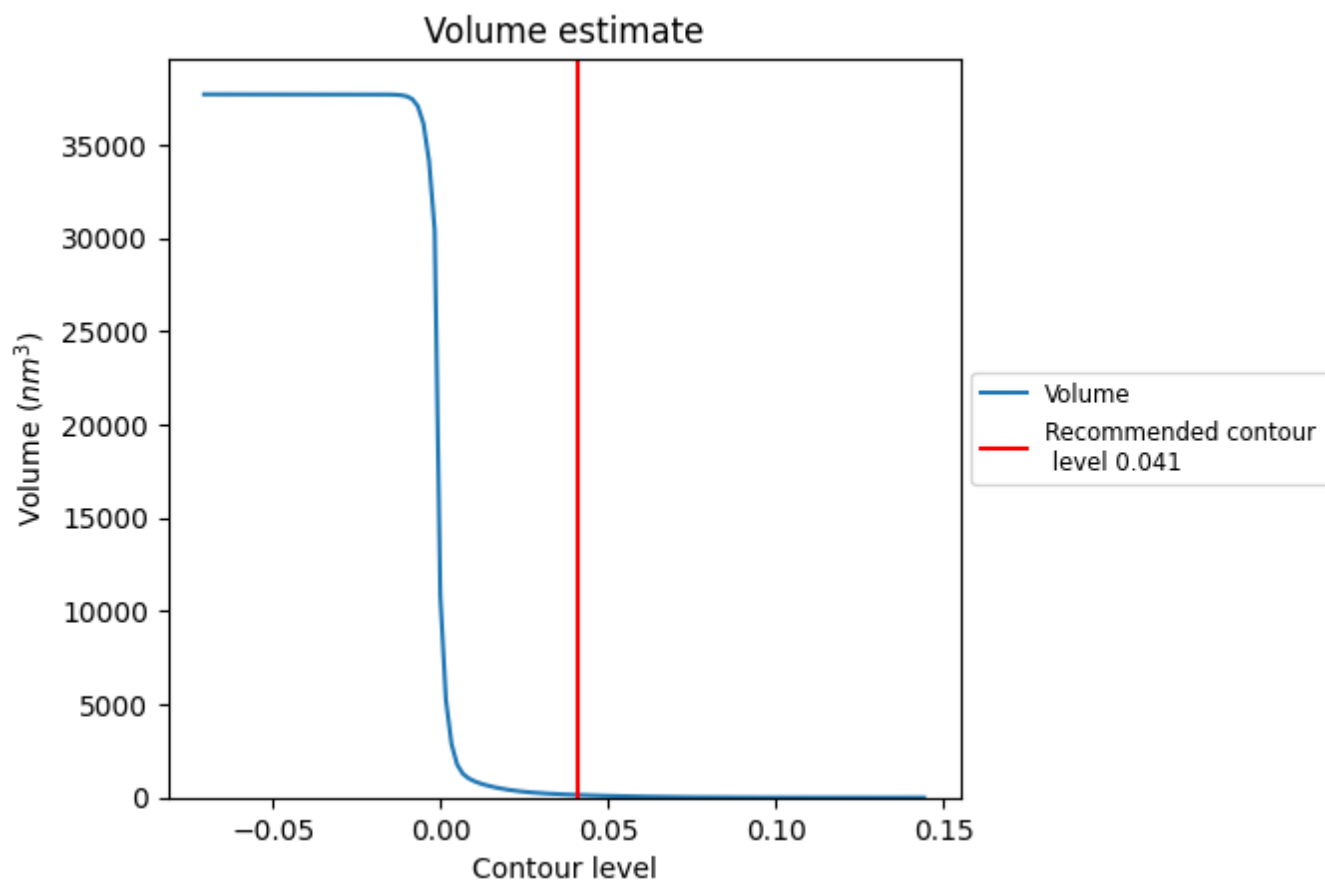
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

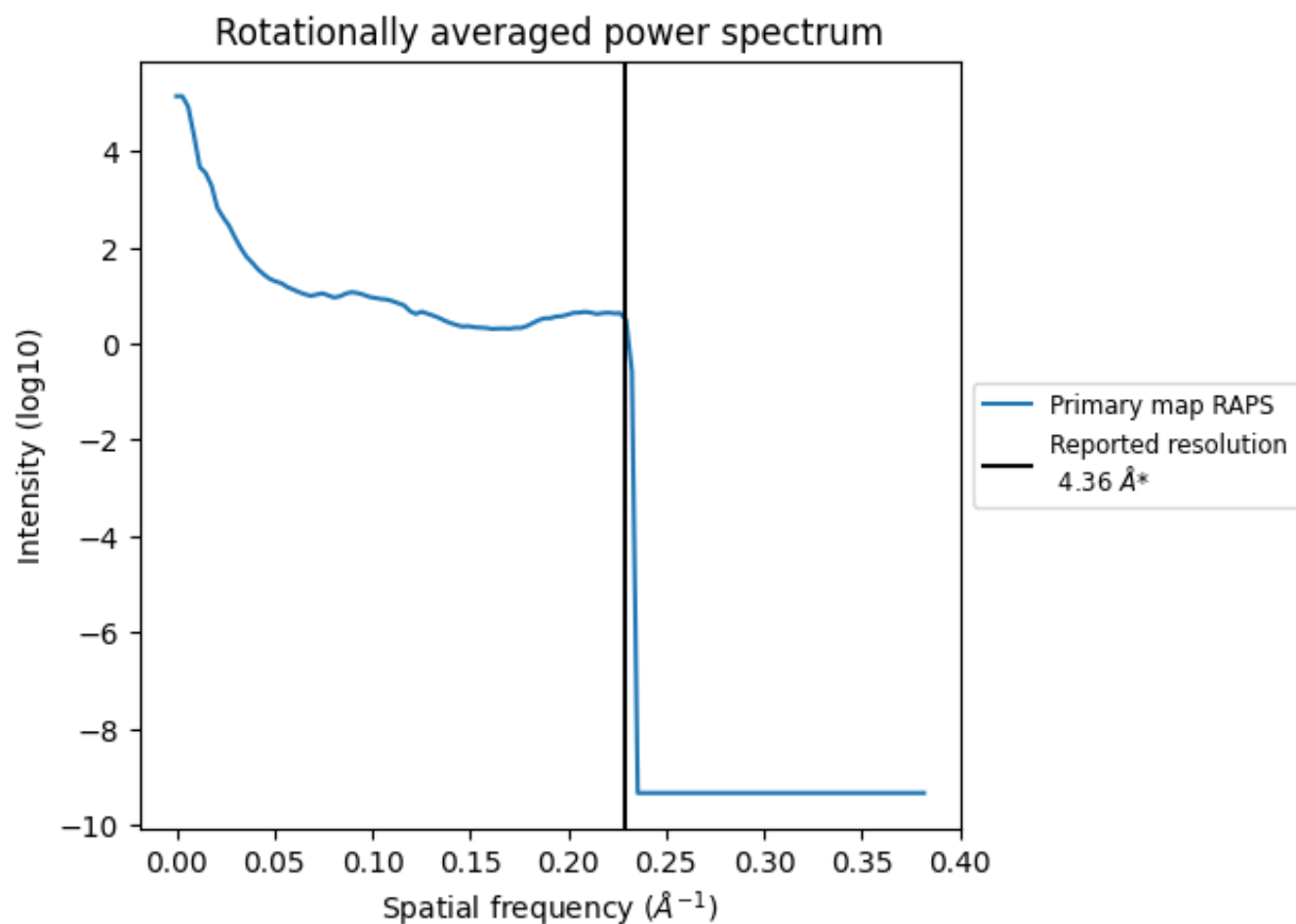
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 140 nm³; this corresponds to an approximate mass of 127 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 0.229 Å⁻¹

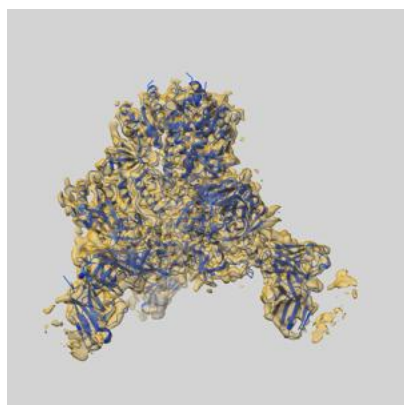
8 Fourier-Shell correlation

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

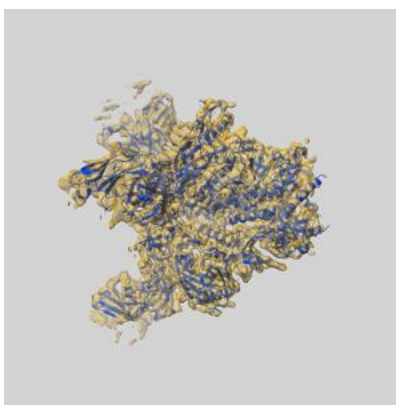
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3121 and PDB model 5ACO. Per-residue inclusion information can be found in section [3](#) on page [12](#).

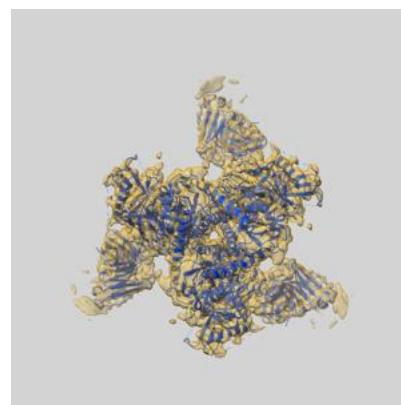
9.1 Map-model overlay [i](#)



X



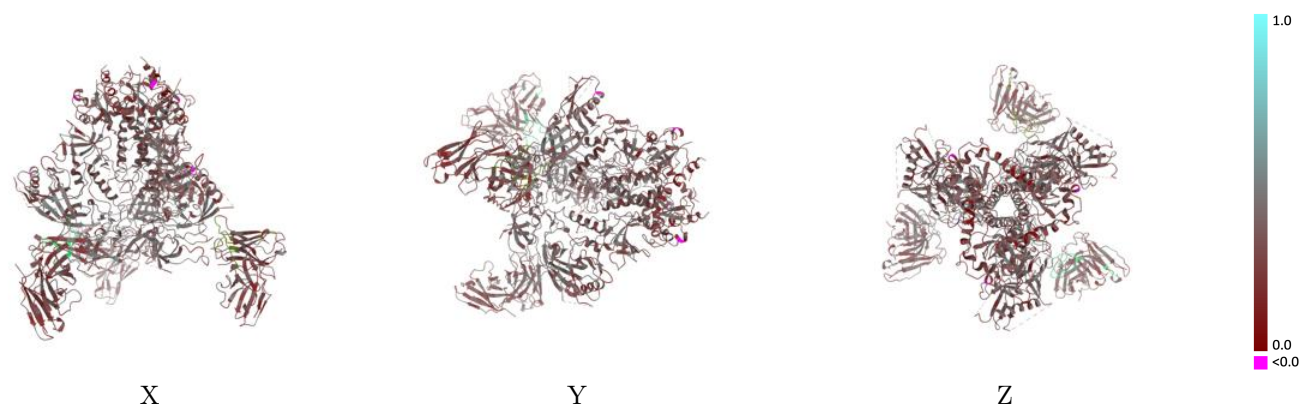
Y



Z

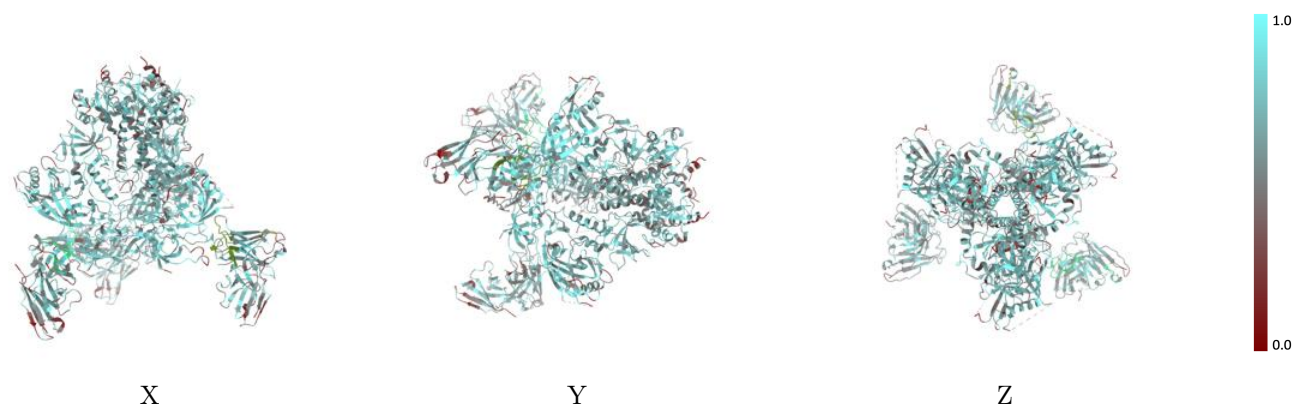
The images above show the 3D surface view of the map at the recommended contour level 0.041 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



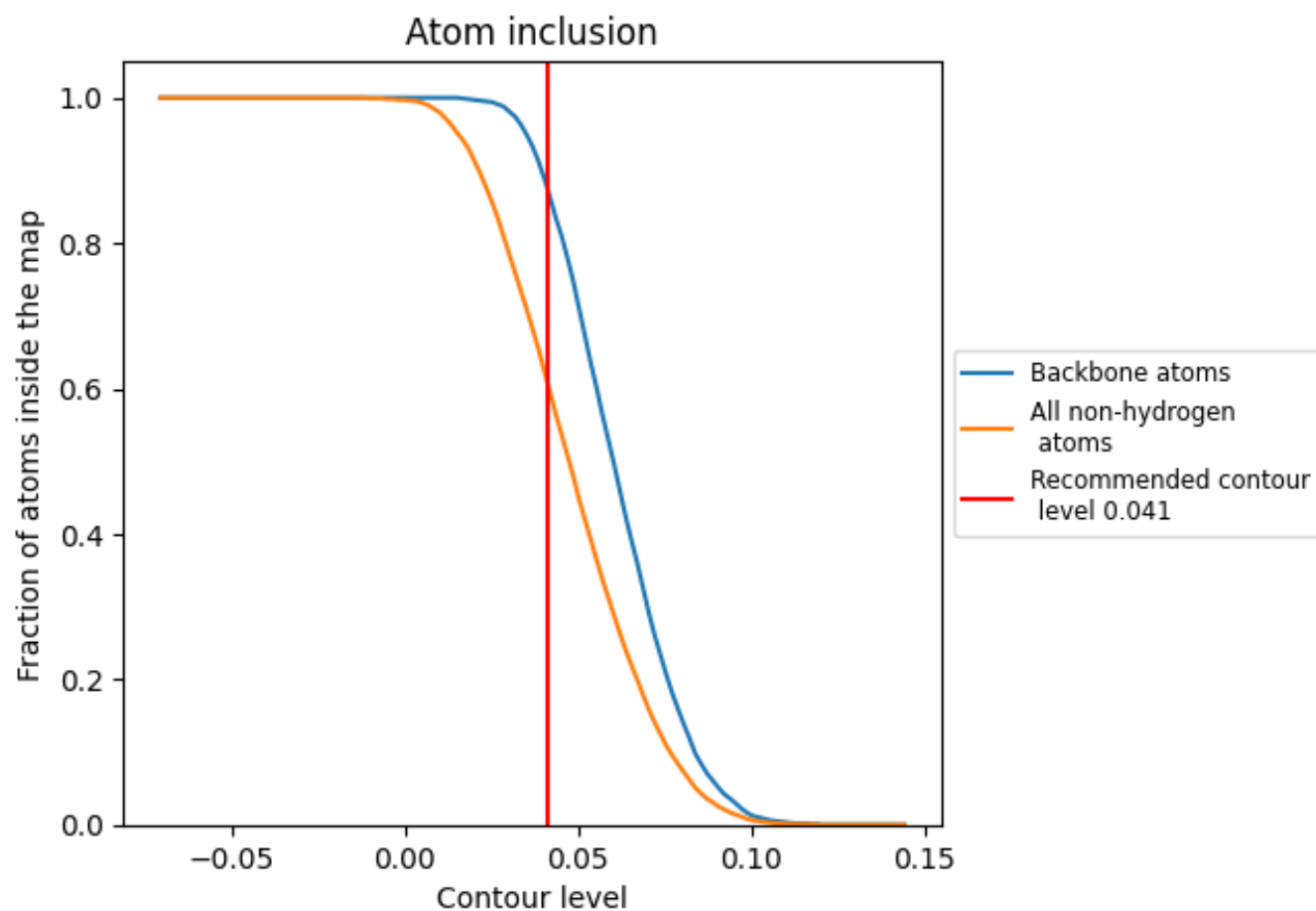
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.041).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 61% 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 (0.041) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6120	 0.3320
0	 0.1540	 0.2740
1	 0.2460	 0.2430
2	 0.4700	 0.3210
3	 0.6720	 0.3810
4	 0.0000	 0.2270
5	 0.2310	 0.1350
6	 0.3850	 0.1600
7	 0.0710	 0.2440
8	 0.3930	 0.2620
9	 0.1070	 0.2370
A	 0.6860	 0.3690
AA	 0.0710	 0.2290
B	 0.5840	 0.2980
C	 0.6860	 0.3690
D	 0.6840	 0.3690
E	 0.5900	 0.3000
F	 0.5880	 0.2990
G	 0.6290	 0.3150
H	 0.6320	 0.3160
I	 0.6320	 0.3170
J	 0.5780	 0.2900
K	 0.5770	 0.2850
L	 0.5760	 0.2890
M	 0.1280	 0.2900
N	 0.2140	 0.2910
O	 0.3330	 0.2100
P	 0.2560	 0.3290
Q	 0.3210	 0.2740
R	 0.2140	 0.2670
S	 0.3610	 0.2860
T	 0.1540	 0.2570
U	 0.2460	 0.2370
V	 0.4700	 0.3220
W	 0.6720	 0.3740



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Chain	Atom inclusion	Q-score
X	 0.0360	 0.2450
Y	 0.2310	 0.1310
Z	 0.3850	 0.1680
a	 0.0710	 0.2230
b	 0.3930	 0.2500
c	 0.0710	 0.2230
d	 0.1280	 0.2750
e	 0.2500	 0.3020
f	 0.3330	 0.2020
g	 0.2310	 0.3240
h	 0.3210	 0.2760
i	 0.2140	 0.2970
j	 0.3730	 0.2830
k	 0.1280	 0.2610
l	 0.2460	 0.2380
m	 0.4700	 0.3210
n	 0.6720	 0.3670
o	 0.0000	 0.2290
p	 0.2310	 0.1450
q	 0.4100	 0.1620
r	 0.0710	 0.2330
s	 0.3930	 0.2440
t	 0.1280	 0.2900
u	 0.2140	 0.2980
v	 0.3330	 0.2120
w	 0.2050	 0.3370
x	 0.3210	 0.2700
y	 0.2500	 0.2800
z	 0.3730	 0.2830