



## Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 05:04 AM EST

PDB ID : 6MPG  
EMDB ID : EMD-8977  
Title : Cryo-EM structure at 3.2 Å resolution of HIV-1 fusion peptide-directed antibody, A12V163-b.01, elicited by vaccination of Rhesus macaques, in complex with stabilized HIV-1 Env BG505 DS-SOSIP, which was also bound to antibodies VRC03 and PGT122  
Authors : Acharya, P.; Kwong, P.D.  
Deposited on : 2018-10-06  
Resolution : 3.20 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](mailto: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>.

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

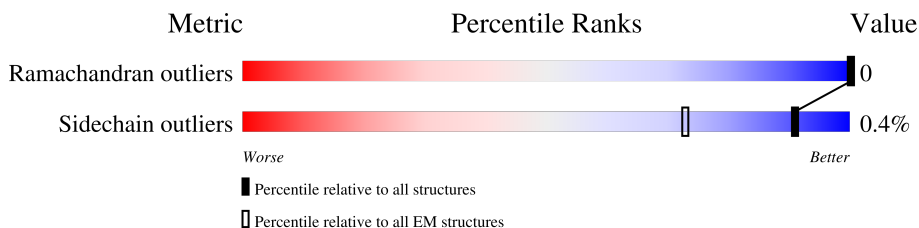
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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  $\geq 3$ , 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	4	113	21% 100%
1	B	113	20% 100%
1	Y	113	20% 100%
2	A	153	7% 86% 14%
2	D	153	6% 86% 14%
2	U	153	7% 86% 14%
3	2	473	10% 96%
3	C	473	10% 96%
3	V	473	11% 96%

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Mol	Chain	Length	Quality of chain	
4	3	117	11%	98%
4	W	117	12%	98%
4	X	117	11%	98%
5	5	132	30%	100%
5	M	132	30%	100%
5	m	132	30%	100%
6	6	107	29%	98%
6	N	107	27%	98%
6	n	107	29%	98%
7	8	227	56%	44%
7	Q	227	56%	44%
7	q	227	56%	44%
8	7	102	9%	98%
8	R	102	9%	98%
8	r	102	10%	98%
9	0	2	50%	100%
9	BA	2	50%	50%
9	E	2	50%	50%
9	G	2	100%	
9	H	2	50%	50%
9	I	2	50%	100%
9	K	2	50%	100%
9	L	2	50%	100%
9	T	2	50%	50%
9	b	2	50%	50%




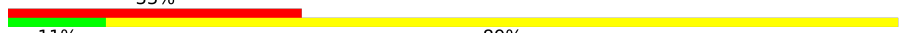
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Mol	Chain	Length	Quality of chain
9	d	2	100%
9	e	2	50% 50%
9	f	2	50% 100%
9	h	2	50% 100%
9	i	2	50% 100%
9	o	2	50% 50%
9	t	2	50% 50%
9	v	2	100%
9	w	2	50% 50%
9	x	2	50% 100%
9	z	2	50% 100%
10	9	4	50% 100%
10	CA	4	75% 25% 75%
10	F	4	75% 25% 75%
10	P	4	50% 100%
10	Z	4	75% 25% 75%
10	c	4	75% 25% 75%
10	k	4	50% 100%
10	p	4	75% 25% 75%
10	u	4	75% 25% 75%
11	J	5	60% 20% 80%
11	g	5	60% 20% 80%
11	y	5	60% 20% 80%
12	1	3	33% 67% 33%
12	DA	3	33% 67%

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Mol	Chain	Length	Quality of chain
12	O	3	
12	a	3	
12	j	3	
12	s	3	
13	AA	9	
13	S	9	
13	l	9	

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 32085 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 A12V163-b.01 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	113	868	549	142	174	3	0	0
1	4	113	868	549	142	174	3	0	0
1	Y	113	868	549	142	174	3	0	0

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	U	132	1034	654	178	196	6	0	0
2	A	132	1034	654	178	196	6	0	0
2	D	132	1034	654	178	196	6	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	605	CYS	THR	conflict	UNP Q2N0S7
A	605	CYS	THR	conflict	UNP Q2N0S7
D	605	CYS	THR	conflict	UNP Q2N0S7

- Molecule 3 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	V	453	3564	2233	630	671	30	0	0
3	2	453	3564	2233	630	671	30	0	0
3	C	453	3564	2233	630	671	30	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	201	CYS	ILE	conflict	UNP Q2N0S6
V	332	ASN	THR	conflict	UNP Q2N0S6
V	433	CYS	ALA	conflict	UNP Q2N0S6
V	501	CYS	ALA	conflict	UNP Q2N0S6
2	201	CYS	ILE	conflict	UNP Q2N0S6
2	332	ASN	THR	conflict	UNP Q2N0S6
2	433	CYS	ALA	conflict	UNP Q2N0S6
2	501	CYS	ALA	conflict	UNP Q2N0S6
C	201	CYS	ILE	conflict	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	433	CYS	ALA	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 4 is a protein called A12V163-b.01 Heavy Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
4	W	117	906	572	156	174	4	0	0
4	3	117	906	572	156	174	4	0	0
4	X	117	906	572	156	174	4	0	0

- Molecule 5 is a protein called PGT122 Heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
5	m	132	1047	669	180	195	3	0	0
5	5	132	1047	669	180	195	3	0	0
5	M	132	1047	669	180	195	3	0	0

- Molecule 6 is a protein called PGT122 Light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
6	n	105	805	504	139	160	2	0	0
6	6	105	805	504	139	160	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	N	105	805	504	139	160	2	0	0

- Molecule 7 is a protein called VRC03 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	q	128	1023	657	175	185	6	0	0
7	8	128	1023	657	175	185	6	0	0
7	Q	128	1023	657	175	185	6	0	0

- Molecule 8 is a protein called VRC03 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	r	102	802	510	137	152	3	0	0
8	7	102	802	510	137	152	3	0	0
8	R	102	802	510	137	152	3	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	E	2	28	16	2	10	0	0
9	G	2	28	16	2	10	0	0
9	H	2	28	16	2	10	0	0
9	I	2	28	16	2	10	0	0
9	K	2	28	16	2	10	0	0

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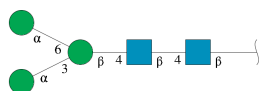
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	L	2	28	16	2	10	0	0
9	T	2	28	16	2	10	0	0
9	b	2	28	16	2	10	0	0
9	d	2	28	16	2	10	0	0
9	e	2	28	16	2	10	0	0
9	f	2	28	16	2	10	0	0
9	h	2	28	16	2	10	0	0
9	i	2	28	16	2	10	0	0
9	o	2	28	16	2	10	0	0
9	t	2	28	16	2	10	0	0
9	v	2	28	16	2	10	0	0
9	w	2	28	16	2	10	0	0
9	x	2	28	16	2	10	0	0
9	z	2	28	16	2	10	0	0
9	0	2	28	16	2	10	0	0
9	BA	2	28	16	2	10	0	0

- Molecule 10 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.



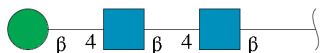
Mol	Chain	Residues	Atoms				AltConf	Trace
10	F	4	Total	C	N	O	0	0
			50	28	2	20		
10	P	4	Total	C	N	O	0	0
			50	28	2	20		
10	Z	4	Total	C	N	O	0	0
			50	28	2	20		
10	c	4	Total	C	N	O	0	0
			50	28	2	20		
10	k	4	Total	C	N	O	0	0
			50	28	2	20		
10	p	4	Total	C	N	O	0	0
			50	28	2	20		
10	u	4	Total	C	N	O	0	0
			50	28	2	20		
10	9	4	Total	C	N	O	0	0
			50	28	2	20		
10	CA	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 11 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.



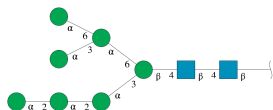
Mol	Chain	Residues	Atoms				AltConf	Trace
11	J	5	Total	C	N	O	0	0
			61	34	2	25		
11	g	5	Total	C	N	O	0	0
			61	34	2	25		
11	y	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 12 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
12	O	3	Total	C	N	O	0	0
			39	22	2	15		
12	a	3	Total	C	N	O	0	0
			39	22	2	15		
12	j	3	Total	C	N	O	0	0
			39	22	2	15		
12	s	3	Total	C	N	O	0	0
			39	22	2	15		
12	1	3	Total	C	N	O	0	0
			39	22	2	15		
12	DA	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
13	S	9	Total	C	N	O	0	0
			105	58	2	45		
13	1	9	Total	C	N	O	0	0
			105	58	2	45		
13	AA	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

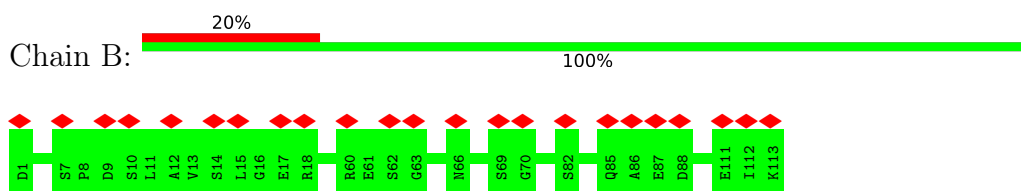


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
14	U	1	Total 14	8	1	5	0
14	V	1	Total 42	24	3	15	0
14	V	1	Total 42	24	3	15	0
14	V	1	Total 42	24	3	15	0
14	2	1	Total 42	24	3	15	0
14	2	1	Total 42	24	3	15	0
14	2	1	Total 42	24	3	15	0
14	A	1	Total 14	8	1	5	0
14	C	1	Total 42	24	3	15	0
14	C	1	Total 42	24	3	15	0
14	C	1	Total 42	24	3	15	0
14	D	1	Total 14	8	1	5	0

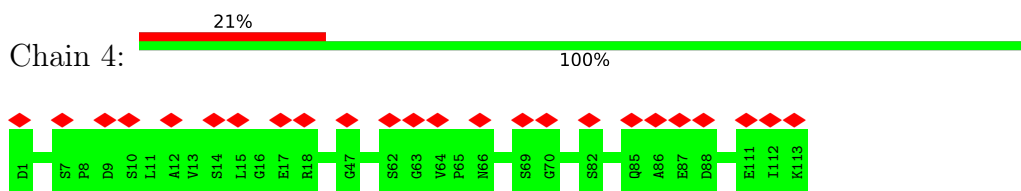
### 3 Residue-property plots [i](#)

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

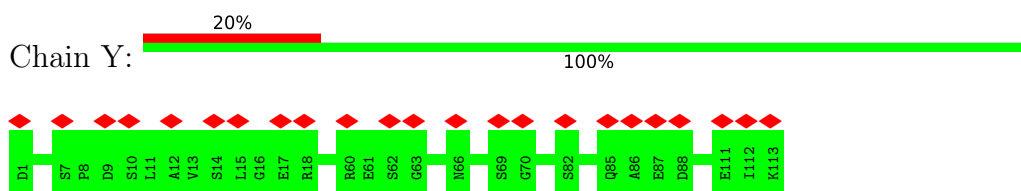
- Molecule 1: A12V163-b.01 Light Chain



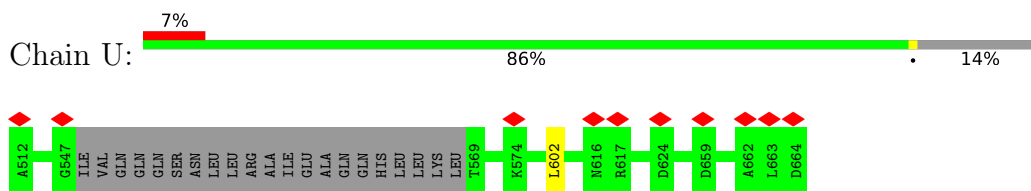
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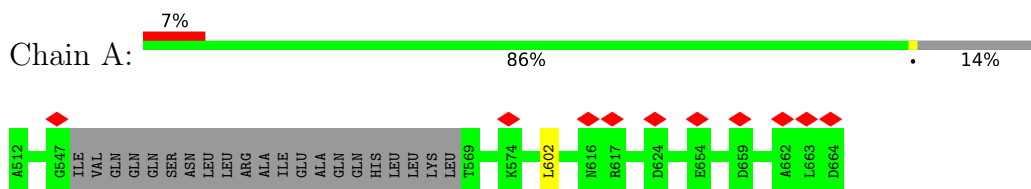
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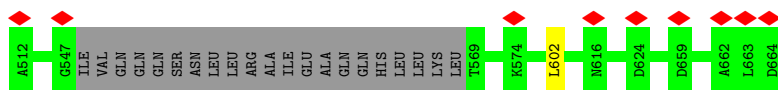
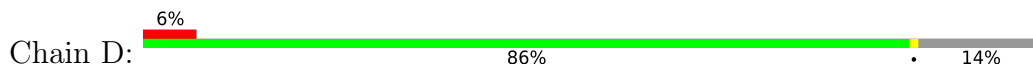
- Molecule 2: Envelope glycoprotein gp41



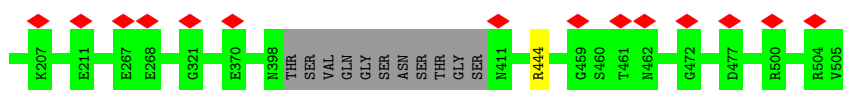
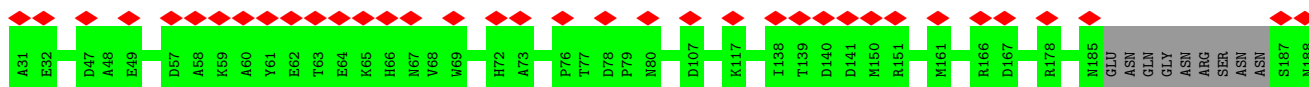
- Molecule 2: Envelope glycoprotein gp41



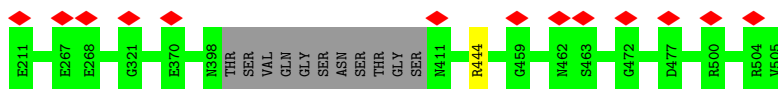
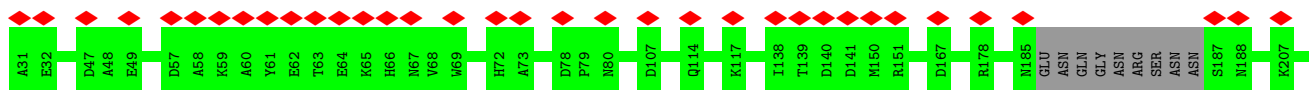
• Molecule 2: Envelope glycoprotein gp41



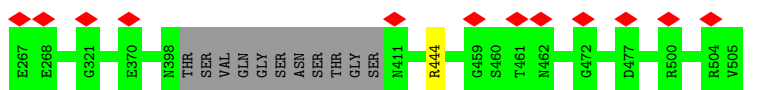
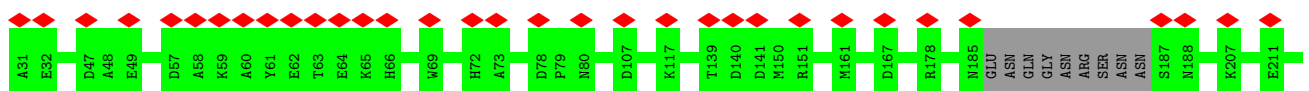
• Molecule 3: Envelope glycoprotein gp120



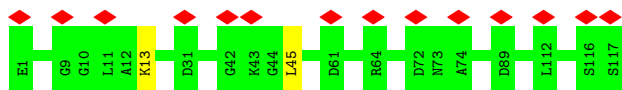
• Molecule 3: Envelope glycoprotein gp120



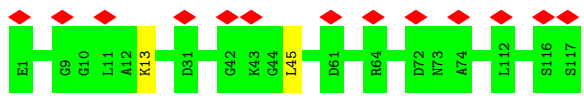
• Molecule 3: Envelope glycoprotein gp120



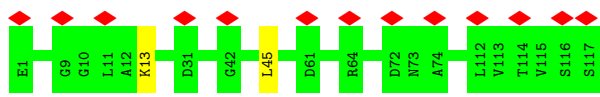
• Molecule 4: A12V163-b.01 Heavy Chain



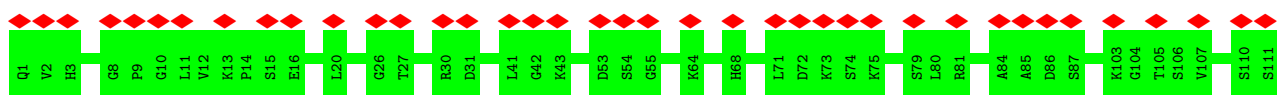
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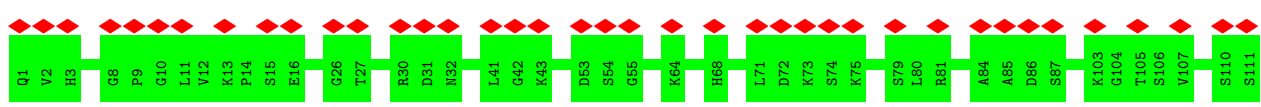
• Molecule 4: A12V163-b.01 Heavy Chain



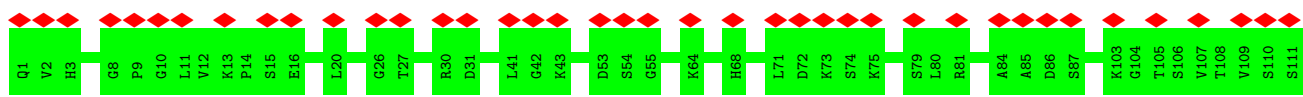
• Molecule 5: PGT122 Heavy chain



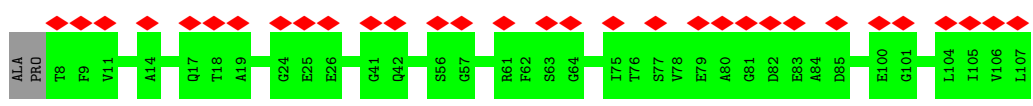
• Molecule 5: PGT122 Heavy chain



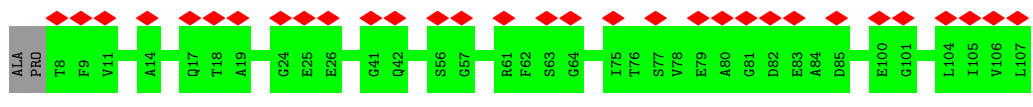
• Molecule 5: PGT122 Heavy chain



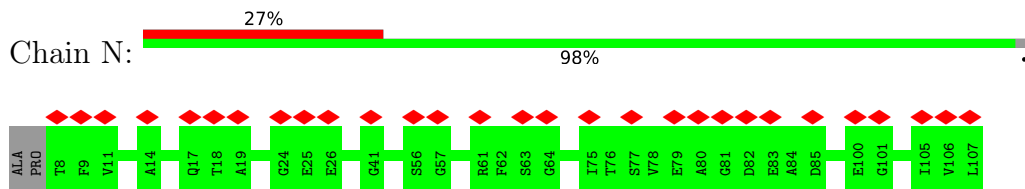
• Molecule 6: PGT122 Light chain



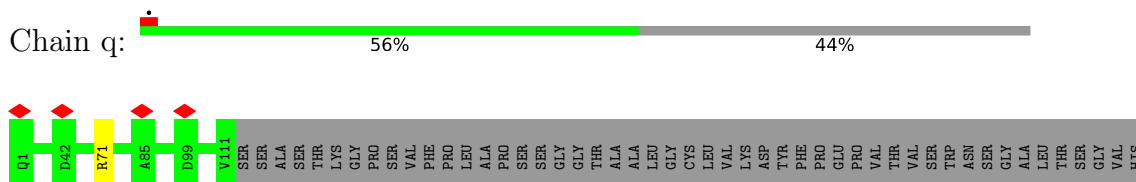
• Molecule 6: PGT122 Light chain



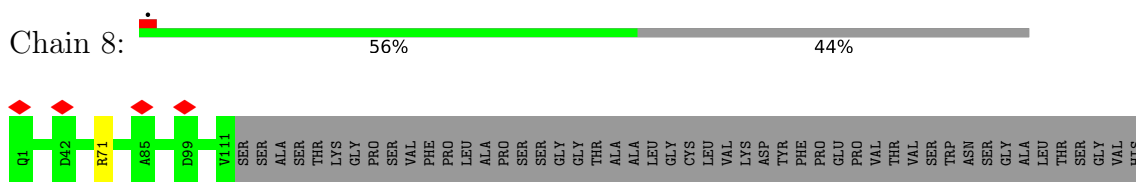
• Molecule 6: PGT122 Light chain



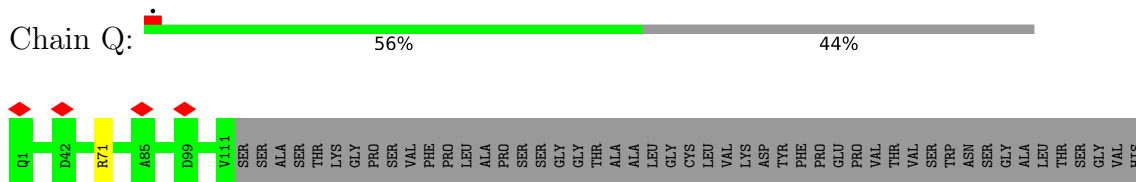
• Molecule 7: VRC03 heavy chain



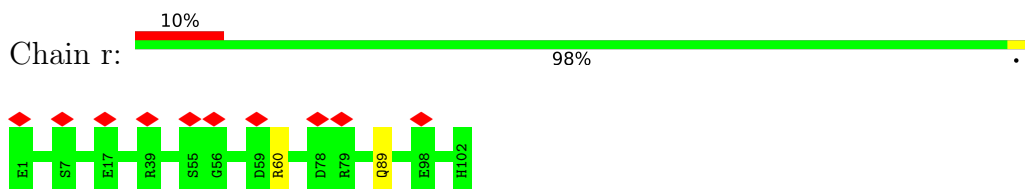
• Molecule 7: VRC03 heavy chain



• Molecule 7: VRC03 heavy chain



• Molecule 8: VRC03 Light chain



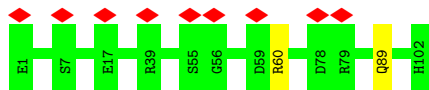
• Molecule 8: VRC03 Light chain







- Molecule 8: VRC03 Light chain



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



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



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



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



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





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



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



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



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



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



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





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



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



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



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



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



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





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



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



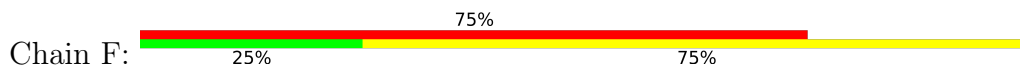
- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



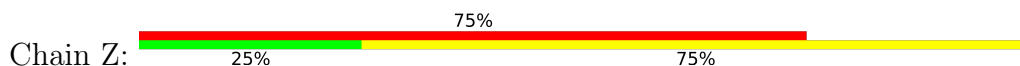
- Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



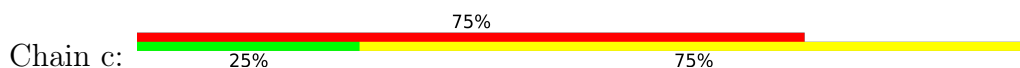
- Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



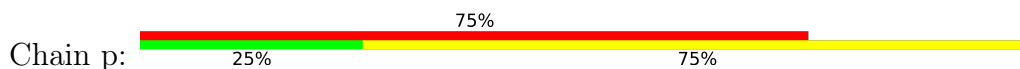
- Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



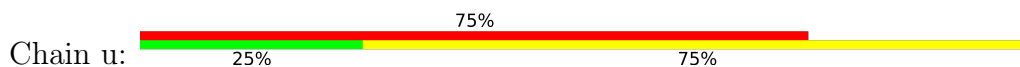
- Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



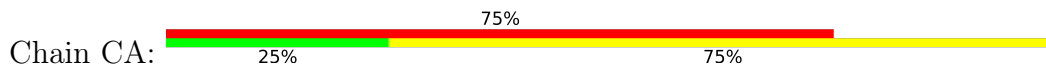
- Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



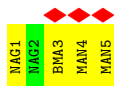
- Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



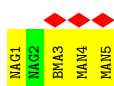
- Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



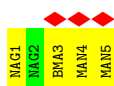
- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: 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 11: 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 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





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



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



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



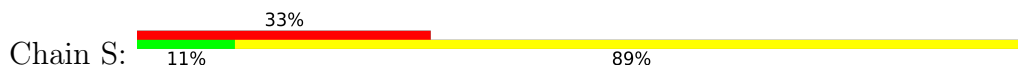
- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



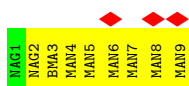
- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



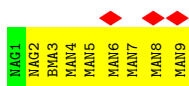
- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	138170	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.75	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.317	Depositor
Minimum map value	-2.860	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.126	Depositor
Recommended contour level	1.19	Depositor
Map size (Å)	410.88, 410.88, 410.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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, BMA, MAN

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	4	0.31	0/887	0.59	0/1204
1	B	0.31	0/887	0.59	0/1204
1	Y	0.31	0/887	0.59	0/1204
2	A	0.31	0/1052	0.59	1/1427 (0.1%)
2	D	0.30	0/1052	0.59	1/1427 (0.1%)
2	U	0.30	0/1052	0.59	1/1427 (0.1%)
3	2	0.31	0/3638	0.56	0/4939
3	C	0.31	0/3638	0.56	0/4939
3	V	0.31	0/3638	0.56	0/4939
4	3	0.31	0/927	0.61	1/1255 (0.1%)
4	W	0.31	0/927	0.61	1/1255 (0.1%)
4	X	0.31	0/927	0.61	1/1255 (0.1%)
5	5	0.28	0/1076	0.62	0/1465
5	M	0.28	0/1076	0.62	0/1465
5	m	0.28	0/1076	0.62	0/1465
6	6	0.27	0/826	0.55	0/1130
6	N	0.27	0/826	0.55	0/1130
6	n	0.27	0/826	0.55	0/1130
7	8	0.31	0/1056	0.53	0/1439
7	Q	0.31	0/1056	0.53	0/1439
7	q	0.31	0/1056	0.53	0/1439
8	7	0.31	0/820	0.55	0/1107
8	R	0.31	0/820	0.55	0/1107
8	r	0.31	0/820	0.55	0/1107
All	All	0.30	0/30846	0.57	6/41898 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	7	0	1
8	R	0	1
8	r	0	1
All	All	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	U	602	LEU	CA-CB-CG	5.48	127.90	115.30
2	D	602	LEU	CA-CB-CG	5.47	127.88	115.30
2	A	602	LEU	CA-CB-CG	5.46	127.86	115.30
4	3	45	LEU	CA-CB-CG	5.22	127.32	115.30
4	X	45	LEU	CA-CB-CG	5.22	127.31	115.30
4	W	45	LEU	CA-CB-CG	5.20	127.26	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	7	89	GLN	Peptide
8	R	89	GLN	Peptide
8	r	89	GLN	Peptide

## 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	4	111/113 (98%)	107 (96%)	4 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
1	Y	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
2	A	128/153 (84%)	122 (95%)	6 (5%)	0	100	100
2	D	128/153 (84%)	122 (95%)	6 (5%)	0	100	100
2	U	128/153 (84%)	122 (95%)	6 (5%)	0	100	100
3	2	447/473 (94%)	422 (94%)	25 (6%)	0	100	100
3	C	447/473 (94%)	422 (94%)	25 (6%)	0	100	100
3	V	447/473 (94%)	422 (94%)	25 (6%)	0	100	100
4	3	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
4	W	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
4	X	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
5	5	130/132 (98%)	120 (92%)	10 (8%)	0	100	100
5	M	130/132 (98%)	120 (92%)	10 (8%)	0	100	100
5	m	130/132 (98%)	120 (92%)	10 (8%)	0	100	100
6	6	103/107 (96%)	93 (90%)	10 (10%)	0	100	100
6	N	103/107 (96%)	93 (90%)	10 (10%)	0	100	100
6	n	103/107 (96%)	93 (90%)	10 (10%)	0	100	100
7	8	126/227 (56%)	123 (98%)	3 (2%)	0	100	100
7	Q	126/227 (56%)	123 (98%)	3 (2%)	0	100	100
7	q	126/227 (56%)	123 (98%)	3 (2%)	0	100	100
8	7	100/102 (98%)	92 (92%)	8 (8%)	0	100	100
8	R	100/102 (98%)	92 (92%)	8 (8%)	0	100	100
8	r	100/102 (98%)	92 (92%)	8 (8%)	0	100	100
All	All	3780/4272 (88%)	3573 (94%)	207 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	4	96/96 (100%)	96 (100%)	0	100	100
1	B	96/96 (100%)	96 (100%)	0	100	100
1	Y	96/96 (100%)	96 (100%)	0	100	100
2	A	110/129 (85%)	110 (100%)	0	100	100
2	D	110/129 (85%)	110 (100%)	0	100	100
2	U	110/129 (85%)	110 (100%)	0	100	100
3	2	405/422 (96%)	404 (100%)	1 (0%)	93	98
3	C	405/422 (96%)	404 (100%)	1 (0%)	93	98
3	V	405/422 (96%)	404 (100%)	1 (0%)	93	98
4	3	94/94 (100%)	93 (99%)	1 (1%)	73	88
4	W	94/94 (100%)	93 (99%)	1 (1%)	73	88
4	X	94/94 (100%)	93 (99%)	1 (1%)	73	88
5	5	116/116 (100%)	116 (100%)	0	100	100
5	M	116/116 (100%)	116 (100%)	0	100	100
5	m	116/116 (100%)	116 (100%)	0	100	100
6	6	88/89 (99%)	88 (100%)	0	100	100
6	N	88/89 (99%)	88 (100%)	0	100	100
6	n	88/89 (99%)	88 (100%)	0	100	100
7	8	108/193 (56%)	107 (99%)	1 (1%)	78	91
7	Q	108/193 (56%)	107 (99%)	1 (1%)	78	91
7	q	108/193 (56%)	107 (99%)	1 (1%)	78	91
8	7	86/86 (100%)	85 (99%)	1 (1%)	71	88
8	R	86/86 (100%)	85 (99%)	1 (1%)	71	88
8	r	86/86 (100%)	85 (99%)	1 (1%)	71	88
All	All	3309/3675 (90%)	3297 (100%)	12 (0%)	91	95

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

Mol	Chain	Res	Type
3	V	444	ARG
4	W	13	LYS
7	q	71	ARG
8	r	60	ARG
3	2	444	ARG
4	3	13	LYS

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Mol	Chain	Res	Type
8	7	60	ARG
7	8	71	ARG
3	C	444	ARG
7	Q	71	ARG
8	R	60	ARG
4	X	13	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	95	GLN
2	U	656	ASN
3	V	80	ASN
3	V	114	GLN
3	V	203	GLN
3	V	315	GLN
3	V	432	GLN
3	2	80	ASN
3	2	114	GLN
3	2	203	GLN
3	2	315	GLN
3	2	432	GLN
1	4	95	GLN
2	A	656	ASN
3	C	80	ASN
3	C	114	GLN
3	C	203	GLN
3	C	315	GLN
3	C	432	GLN
2	D	656	ASN
1	Y	95	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

138 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
9	NAG	0	1	3,9	14,14,15	0.27	0	17,19,21	0.53	0
9	NAG	0	2	9	14,14,15	0.31	0	17,19,21	0.46	0
12	NAG	1	1	3,12	14,14,15	0.20	0	17,19,21	0.46	0
12	NAG	1	2	12	14,14,15	0.21	0	17,19,21	0.51	0
12	BMA	1	3	12	11,11,12	0.83	1 (9%)	15,15,17	1.02	2 (13%)
10	NAG	9	1	3,10	14,14,15	0.33	0	17,19,21	0.67	1 (5%)
10	NAG	9	2	10	14,14,15	0.55	0	17,19,21	1.14	2 (11%)
10	BMA	9	3	10	11,11,12	0.85	1 (9%)	15,15,17	1.63	3 (20%)
10	MAN	9	4	10	11,11,12	0.76	0	15,15,17	1.13	2 (13%)
13	NAG	AA	1	3,13	14,14,15	0.27	0	17,19,21	0.55	0
13	NAG	AA	2	13	14,14,15	0.34	0	17,19,21	1.17	1 (5%)
13	BMA	AA	3	13	11,11,12	0.78	0	15,15,17	1.36	1 (6%)
13	MAN	AA	4	13	11,11,12	0.84	0	15,15,17	1.44	1 (6%)
13	MAN	AA	5	13	11,11,12	0.72	0	15,15,17	1.43	2 (13%)
13	MAN	AA	6	13	11,11,12	0.90	0	15,15,17	0.94	2 (13%)
13	MAN	AA	7	13	11,11,12	0.76	0	15,15,17	1.23	2 (13%)
13	MAN	AA	8	13	11,11,12	0.83	0	15,15,17	1.05	2 (13%)
13	MAN	AA	9	13	11,11,12	0.77	0	15,15,17	1.12	2 (13%)
9	NAG	BA	1	3,9	14,14,15	0.34	0	17,19,21	0.96	1 (5%)
9	NAG	BA	2	9	14,14,15	0.32	0	17,19,21	0.49	0
10	NAG	CA	1	3,10	14,14,15	0.42	0	17,19,21	0.81	1 (5%)
10	NAG	CA	2	10	14,14,15	0.46	0	17,19,21	0.87	1 (5%)
10	BMA	CA	3	10	11,11,12	0.90	0	15,15,17	0.72	0
10	MAN	CA	4	10	11,11,12	0.85	0	15,15,17	1.04	2 (13%)
12	NAG	DA	1	12	14,14,15	0.76	1 (7%)	17,19,21	1.08	1 (5%)
12	NAG	DA	2	12	14,14,15	0.29	0	17,19,21	0.55	0
12	BMA	DA	3	12	11,11,12	1.05	1 (9%)	15,15,17	1.33	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	E	1	3,9	14,14,15	0.39	0	17,19,21	0.95	1 (5%)
9	NAG	E	2	9	14,14,15	0.45	0	17,19,21	0.50	0
10	NAG	F	1	3,10	14,14,15	0.34	0	17,19,21	0.58	0
10	NAG	F	2	10	14,14,15	0.45	0	17,19,21	1.05	1 (5%)
10	BMA	F	3	10	11,11,12	0.67	0	15,15,17	1.52	3 (20%)
10	MAN	F	4	10	11,11,12	0.92	0	15,15,17	1.03	2 (13%)
9	NAG	G	1	3,9	14,14,15	0.39	0	17,19,21	0.61	0
9	NAG	G	2	9	14,14,15	0.32	0	17,19,21	0.44	0
9	NAG	H	1	3,9	14,14,15	0.72	1 (7%)	17,19,21	1.01	1 (5%)
9	NAG	H	2	9	14,14,15	0.27	0	17,19,21	0.53	0
9	NAG	I	1	3,9	14,14,15	0.43	0	17,19,21	0.60	0
9	NAG	I	2	9	14,14,15	0.37	0	17,19,21	0.47	0
11	NAG	J	1	3,11	14,14,15	0.32	0	17,19,21	0.60	1 (5%)
11	NAG	J	2	11	14,14,15	0.25	0	17,19,21	0.54	0
11	BMA	J	3	11	11,11,12	0.68	0	15,15,17	1.30	1 (6%)
11	MAN	J	4	11	11,11,12	0.78	0	15,15,17	1.14	2 (13%)
11	MAN	J	5	11	11,11,12	0.83	0	15,15,17	1.04	2 (13%)
9	NAG	K	1	3,9	14,14,15	0.23	0	17,19,21	0.51	0
9	NAG	K	2	9	14,14,15	0.35	0	17,19,21	0.45	0
9	NAG	L	1	3,9	14,14,15	0.28	0	17,19,21	0.54	0
9	NAG	L	2	9	14,14,15	0.32	0	17,19,21	0.46	0
12	NAG	O	1	3,12	14,14,15	0.21	0	17,19,21	0.47	0
12	NAG	O	2	12	14,14,15	0.21	0	17,19,21	0.52	0
12	BMA	O	3	12	11,11,12	0.82	0	15,15,17	1.02	2 (13%)
10	NAG	P	1	3,10	14,14,15	0.33	0	17,19,21	0.67	1 (5%)
10	NAG	P	2	10	14,14,15	0.56	0	17,19,21	1.14	2 (11%)
10	BMA	P	3	10	11,11,12	0.85	1 (9%)	15,15,17	1.63	3 (20%)
10	MAN	P	4	10	11,11,12	0.75	0	15,15,17	1.14	2 (13%)
13	NAG	S	1	3,13	14,14,15	0.27	0	17,19,21	0.54	0
13	NAG	S	2	13	14,14,15	0.34	0	17,19,21	1.17	1 (5%)
13	BMA	S	3	13	11,11,12	0.77	0	15,15,17	1.36	1 (6%)
13	MAN	S	4	13	11,11,12	0.84	0	15,15,17	1.45	1 (6%)
13	MAN	S	5	13	11,11,12	0.72	0	15,15,17	1.42	2 (13%)
13	MAN	S	6	13	11,11,12	0.90	0	15,15,17	0.93	2 (13%)
13	MAN	S	7	13	11,11,12	0.75	0	15,15,17	1.23	2 (13%)
13	MAN	S	8	13	11,11,12	0.82	0	15,15,17	1.05	2 (13%)
13	MAN	S	9	13	11,11,12	0.77	0	15,15,17	1.12	2 (13%)
9	NAG	T	1	3,9	14,14,15	0.34	0	17,19,21	0.96	1 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	T	2	9	14,14,15	0.32	0	17,19,21	0.50	0
10	NAG	Z	1	3,10	14,14,15	0.41	0	17,19,21	0.81	1 (5%)
10	NAG	Z	2	10	14,14,15	0.46	0	17,19,21	0.88	1 (5%)
10	BMA	Z	3	10	11,11,12	0.91	0	15,15,17	0.72	0
10	MAN	Z	4	10	11,11,12	0.85	0	15,15,17	1.04	2 (13%)
12	NAG	a	1	12	14,14,15	0.75	1 (7%)	17,19,21	1.09	1 (5%)
12	NAG	a	2	12	14,14,15	0.29	0	17,19,21	0.55	0
12	BMA	a	3	12	11,11,12	1.05	1 (9%)	15,15,17	1.34	2 (13%)
9	NAG	b	1	3,9	14,14,15	0.39	0	17,19,21	0.96	1 (5%)
9	NAG	b	2	9	14,14,15	0.45	0	17,19,21	0.51	0
10	NAG	c	1	3,10	14,14,15	0.33	0	17,19,21	0.58	0
10	NAG	c	2	10	14,14,15	0.43	0	17,19,21	1.05	1 (5%)
10	BMA	c	3	10	11,11,12	0.67	0	15,15,17	1.53	3 (20%)
10	MAN	c	4	10	11,11,12	0.92	0	15,15,17	1.04	2 (13%)
9	NAG	d	1	3,9	14,14,15	0.39	0	17,19,21	0.60	0
9	NAG	d	2	9	14,14,15	0.32	0	17,19,21	0.44	0
9	NAG	e	1	3,9	14,14,15	0.70	1 (7%)	17,19,21	1.01	1 (5%)
9	NAG	e	2	9	14,14,15	0.28	0	17,19,21	0.53	0
9	NAG	f	1	3,9	14,14,15	0.43	0	17,19,21	0.60	0
9	NAG	f	2	9	14,14,15	0.36	0	17,19,21	0.47	0
11	NAG	g	1	3,11	14,14,15	0.32	0	17,19,21	0.60	1 (5%)
11	NAG	g	2	11	14,14,15	0.27	0	17,19,21	0.54	0
11	BMA	g	3	11	11,11,12	0.67	0	15,15,17	1.30	1 (6%)
11	MAN	g	4	11	11,11,12	0.80	0	15,15,17	1.14	2 (13%)
11	MAN	g	5	11	11,11,12	0.84	0	15,15,17	1.04	2 (13%)
9	NAG	h	1	3,9	14,14,15	0.23	0	17,19,21	0.52	0
9	NAG	h	2	9	14,14,15	0.34	0	17,19,21	0.45	0
9	NAG	i	1	3,9	14,14,15	0.27	0	17,19,21	0.53	0
9	NAG	i	2	9	14,14,15	0.32	0	17,19,21	0.46	0
12	NAG	j	1	3,12	14,14,15	0.21	0	17,19,21	0.46	0
12	NAG	j	2	12	14,14,15	0.20	0	17,19,21	0.52	0
12	BMA	j	3	12	11,11,12	0.83	1 (9%)	15,15,17	1.01	2 (13%)
10	NAG	k	1	3,10	14,14,15	0.33	0	17,19,21	0.67	1 (5%)
10	NAG	k	2	10	14,14,15	0.55	0	17,19,21	1.14	2 (11%)
10	BMA	k	3	10	11,11,12	0.86	1 (9%)	15,15,17	1.63	3 (20%)
10	MAN	k	4	10	11,11,12	0.76	0	15,15,17	1.13	2 (13%)
13	NAG	l	1	3,13	14,14,15	0.27	0	17,19,21	0.54	0
13	NAG	l	2	13	14,14,15	0.34	0	17,19,21	1.17	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	BMA	l	3	13	11,11,12	0.76	0	15,15,17	1.36	1 (6%)
13	MAN	l	4	13	11,11,12	0.83	0	15,15,17	1.44	1 (6%)
13	MAN	l	5	13	11,11,12	0.71	0	15,15,17	1.43	2 (13%)
13	MAN	l	6	13	11,11,12	0.89	0	15,15,17	0.94	2 (13%)
13	MAN	l	7	13	11,11,12	0.75	0	15,15,17	1.24	2 (13%)
13	MAN	l	8	13	11,11,12	0.82	0	15,15,17	1.05	2 (13%)
13	MAN	l	9	13	11,11,12	0.77	0	15,15,17	1.13	2 (13%)
9	NAG	o	1	3,9	14,14,15	0.34	0	17,19,21	0.95	1 (5%)
9	NAG	o	2	9	14,14,15	0.31	0	17,19,21	0.49	0
10	NAG	p	1	3,10	14,14,15	0.41	0	17,19,21	0.80	1 (5%)
10	NAG	p	2	10	14,14,15	0.47	0	17,19,21	0.87	1 (5%)
10	BMA	p	3	10	11,11,12	0.91	0	15,15,17	0.72	0
10	MAN	p	4	10	11,11,12	0.84	0	15,15,17	1.04	2 (13%)
12	NAG	s	1	12	14,14,15	0.76	1 (7%)	17,19,21	1.08	1 (5%)
12	NAG	s	2	12	14,14,15	0.29	0	17,19,21	0.54	0
12	BMA	s	3	12	11,11,12	1.04	1 (9%)	15,15,17	1.34	2 (13%)
9	NAG	t	1	3,9	14,14,15	0.39	0	17,19,21	0.95	1 (5%)
9	NAG	t	2	9	14,14,15	0.45	0	17,19,21	0.51	0
10	NAG	u	1	3,10	14,14,15	0.33	0	17,19,21	0.58	0
10	NAG	u	2	10	14,14,15	0.44	0	17,19,21	1.05	1 (5%)
10	BMA	u	3	10	11,11,12	0.67	0	15,15,17	1.53	3 (20%)
10	MAN	u	4	10	11,11,12	0.91	0	15,15,17	1.03	2 (13%)
9	NAG	v	1	3,9	14,14,15	0.39	0	17,19,21	0.60	0
9	NAG	v	2	9	14,14,15	0.32	0	17,19,21	0.44	0
9	NAG	w	1	3,9	14,14,15	0.72	1 (7%)	17,19,21	1.01	1 (5%)
9	NAG	w	2	9	14,14,15	0.27	0	17,19,21	0.52	0
9	NAG	x	1	3,9	14,14,15	0.44	0	17,19,21	0.60	0
9	NAG	x	2	9	14,14,15	0.37	0	17,19,21	0.47	0
11	NAG	y	1	3,11	14,14,15	0.32	0	17,19,21	0.60	1 (5%)
11	NAG	y	2	11	14,14,15	0.26	0	17,19,21	0.53	0
11	BMA	y	3	11	11,11,12	0.67	0	15,15,17	1.30	1 (6%)
11	MAN	y	4	11	11,11,12	0.79	0	15,15,17	1.14	2 (13%)
11	MAN	y	5	11	11,11,12	0.84	0	15,15,17	1.04	2 (13%)
9	NAG	z	1	3,9	14,14,15	0.23	0	17,19,21	0.52	0
9	NAG	z	2	9	14,14,15	0.34	0	17,19,21	0.45	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
9	NAG	0	1	3,9	-	2/6/23/26	0/1/1/1
9	NAG	0	2	9	-	2/6/23/26	0/1/1/1
12	NAG	1	1	3,12	-	0/6/23/26	0/1/1/1
12	NAG	1	2	12	-	0/6/23/26	0/1/1/1
12	BMA	1	3	12	-	1/2/19/22	0/1/1/1
10	NAG	9	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	9	2	10	-	2/6/23/26	0/1/1/1
10	BMA	9	3	10	-	1/2/19/22	0/1/1/1
10	MAN	9	4	10	-	0/2/19/22	0/1/1/1
13	NAG	AA	1	3,13	-	2/6/23/26	0/1/1/1
13	NAG	AA	2	13	-	3/6/23/26	0/1/1/1
13	BMA	AA	3	13	-	0/2/19/22	0/1/1/1
13	MAN	AA	4	13	-	0/2/19/22	0/1/1/1
13	MAN	AA	5	13	-	2/2/19/22	0/1/1/1
13	MAN	AA	6	13	-	0/2/19/22	0/1/1/1
13	MAN	AA	7	13	-	2/2/19/22	0/1/1/1
13	MAN	AA	8	13	-	2/2/19/22	0/1/1/1
13	MAN	AA	9	13	-	2/2/19/22	0/1/1/1
9	NAG	BA	1	3,9	-	1/6/23/26	0/1/1/1
9	NAG	BA	2	9	-	2/6/23/26	0/1/1/1
10	NAG	CA	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	CA	2	10	-	0/6/23/26	0/1/1/1
10	BMA	CA	3	10	-	0/2/19/22	0/1/1/1
10	MAN	CA	4	10	-	2/2/19/22	0/1/1/1
12	NAG	DA	1	12	-	2/6/23/26	0/1/1/1
12	NAG	DA	2	12	-	2/6/23/26	0/1/1/1
12	BMA	DA	3	12	-	2/2/19/22	0/1/1/1
9	NAG	E	1	3,9	-	1/6/23/26	0/1/1/1
9	NAG	E	2	9	-	2/6/23/26	0/1/1/1
10	NAG	F	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	F	2	10	-	2/6/23/26	0/1/1/1
10	BMA	F	3	10	-	0/2/19/22	0/1/1/1
10	MAN	F	4	10	-	0/2/19/22	0/1/1/1
9	NAG	G	1	3,9	-	0/6/23/26	0/1/1/1
9	NAG	G	2	9	-	1/6/23/26	0/1/1/1
9	NAG	H	1	3,9	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	H	2	9	-	0/6/23/26	0/1/1/1
9	NAG	I	1	3,9	-	0/6/23/26	0/1/1/1
9	NAG	I	2	9	-	0/6/23/26	0/1/1/1
11	NAG	J	1	3,11	-	0/6/23/26	0/1/1/1
11	NAG	J	2	11	-	2/6/23/26	0/1/1/1
11	BMA	J	3	11	-	1/2/19/22	0/1/1/1
11	MAN	J	4	11	-	2/2/19/22	0/1/1/1
11	MAN	J	5	11	-	0/2/19/22	0/1/1/1
9	NAG	K	1	3,9	-	0/6/23/26	0/1/1/1
9	NAG	K	2	9	-	0/6/23/26	0/1/1/1
9	NAG	L	1	3,9	-	2/6/23/26	0/1/1/1
9	NAG	L	2	9	-	2/6/23/26	0/1/1/1
12	NAG	O	1	3,12	-	0/6/23/26	0/1/1/1
12	NAG	O	2	12	-	0/6/23/26	0/1/1/1
12	BMA	O	3	12	-	1/2/19/22	0/1/1/1
10	NAG	P	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	P	2	10	-	2/6/23/26	0/1/1/1
10	BMA	P	3	10	-	1/2/19/22	0/1/1/1
10	MAN	P	4	10	-	0/2/19/22	0/1/1/1
13	NAG	S	1	3,13	-	2/6/23/26	0/1/1/1
13	NAG	S	2	13	-	3/6/23/26	0/1/1/1
13	BMA	S	3	13	-	0/2/19/22	0/1/1/1
13	MAN	S	4	13	-	0/2/19/22	0/1/1/1
13	MAN	S	5	13	-	2/2/19/22	0/1/1/1
13	MAN	S	6	13	-	0/2/19/22	0/1/1/1
13	MAN	S	7	13	-	2/2/19/22	0/1/1/1
13	MAN	S	8	13	-	2/2/19/22	0/1/1/1
13	MAN	S	9	13	-	2/2/19/22	0/1/1/1
9	NAG	T	1	3,9	-	1/6/23/26	0/1/1/1
9	NAG	T	2	9	-	2/6/23/26	0/1/1/1
10	NAG	Z	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	Z	2	10	-	0/6/23/26	0/1/1/1
10	BMA	Z	3	10	-	0/2/19/22	0/1/1/1
10	MAN	Z	4	10	-	2/2/19/22	0/1/1/1
12	NAG	a	1	12	-	2/6/23/26	0/1/1/1
12	NAG	a	2	12	-	2/6/23/26	0/1/1/1
12	BMA	a	3	12	-	2/2/19/22	0/1/1/1
9	NAG	b	1	3,9	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	b	2	9	-	2/6/23/26	0/1/1/1
10	NAG	c	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	c	2	10	-	2/6/23/26	0/1/1/1
10	BMA	c	3	10	-	0/2/19/22	0/1/1/1
10	MAN	c	4	10	-	0/2/19/22	0/1/1/1
9	NAG	d	1	3,9	-	0/6/23/26	0/1/1/1
9	NAG	d	2	9	-	1/6/23/26	0/1/1/1
9	NAG	e	1	3,9	-	3/6/23/26	0/1/1/1
9	NAG	e	2	9	-	0/6/23/26	0/1/1/1
9	NAG	f	1	3,9	-	0/6/23/26	0/1/1/1
9	NAG	f	2	9	-	0/6/23/26	0/1/1/1
11	NAG	g	1	3,11	-	0/6/23/26	0/1/1/1
11	NAG	g	2	11	-	2/6/23/26	0/1/1/1
11	BMA	g	3	11	-	1/2/19/22	0/1/1/1
11	MAN	g	4	11	-	2/2/19/22	0/1/1/1
11	MAN	g	5	11	-	0/2/19/22	0/1/1/1
9	NAG	h	1	3,9	-	0/6/23/26	0/1/1/1
9	NAG	h	2	9	-	0/6/23/26	0/1/1/1
9	NAG	i	1	3,9	-	2/6/23/26	0/1/1/1
9	NAG	i	2	9	-	2/6/23/26	0/1/1/1
12	NAG	j	1	3,12	-	0/6/23/26	0/1/1/1
12	NAG	j	2	12	-	0/6/23/26	0/1/1/1
12	BMA	j	3	12	-	1/2/19/22	0/1/1/1
10	NAG	k	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	k	2	10	-	2/6/23/26	0/1/1/1
10	BMA	k	3	10	-	1/2/19/22	0/1/1/1
10	MAN	k	4	10	-	0/2/19/22	0/1/1/1
13	NAG	l	1	3,13	-	2/6/23/26	0/1/1/1
13	NAG	l	2	13	-	3/6/23/26	0/1/1/1
13	BMA	l	3	13	-	0/2/19/22	0/1/1/1
13	MAN	l	4	13	-	0/2/19/22	0/1/1/1
13	MAN	l	5	13	-	2/2/19/22	0/1/1/1
13	MAN	l	6	13	-	0/2/19/22	0/1/1/1
13	MAN	l	7	13	-	2/2/19/22	0/1/1/1
13	MAN	l	8	13	-	2/2/19/22	0/1/1/1
13	MAN	l	9	13	-	2/2/19/22	0/1/1/1
9	NAG	o	1	3,9	-	1/6/23/26	0/1/1/1
9	NAG	o	2	9	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	p	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	p	2	10	-	0/6/23/26	0/1/1/1
10	BMA	p	3	10	-	0/2/19/22	0/1/1/1
10	MAN	p	4	10	-	2/2/19/22	0/1/1/1
12	NAG	s	1	12	-	2/6/23/26	0/1/1/1
12	NAG	s	2	12	-	2/6/23/26	0/1/1/1
12	BMA	s	3	12	-	2/2/19/22	0/1/1/1
9	NAG	t	1	3,9	-	1/6/23/26	0/1/1/1
9	NAG	t	2	9	-	2/6/23/26	0/1/1/1
10	NAG	u	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	u	2	10	-	2/6/23/26	0/1/1/1
10	BMA	u	3	10	-	0/2/19/22	0/1/1/1
10	MAN	u	4	10	-	0/2/19/22	0/1/1/1
9	NAG	v	1	3,9	-	0/6/23/26	0/1/1/1
9	NAG	v	2	9	-	1/6/23/26	0/1/1/1
9	NAG	w	1	3,9	-	3/6/23/26	0/1/1/1
9	NAG	w	2	9	-	0/6/23/26	0/1/1/1
9	NAG	x	1	3,9	-	0/6/23/26	0/1/1/1
9	NAG	x	2	9	-	0/6/23/26	0/1/1/1
11	NAG	y	1	3,11	-	0/6/23/26	0/1/1/1
11	NAG	y	2	11	-	2/6/23/26	0/1/1/1
11	BMA	y	3	11	-	1/2/19/22	0/1/1/1
11	MAN	y	4	11	-	2/2/19/22	0/1/1/1
11	MAN	y	5	11	-	0/2/19/22	0/1/1/1
9	NAG	z	1	3,9	-	0/6/23/26	0/1/1/1
9	NAG	z	2	9	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	3	BMA	C2-C3	2.62	1.56	1.52
12	s	3	BMA	C2-C3	2.61	1.56	1.52
12	DA	3	BMA	C2-C3	2.61	1.56	1.52
10	k	3	BMA	C1-C2	2.44	1.57	1.52
10	9	3	BMA	C1-C2	2.41	1.57	1.52
10	P	3	BMA	C1-C2	2.38	1.57	1.52
12	s	1	NAG	O5-C1	2.25	1.47	1.43
12	DA	1	NAG	O5-C1	2.23	1.47	1.43
12	a	1	NAG	O5-C1	2.21	1.47	1.43
9	w	1	NAG	C1-C2	2.18	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	1	NAG	C1-C2	2.17	1.55	1.52
9	e	1	NAG	C1-C2	2.12	1.55	1.52
12	j	3	BMA	C1-C2	2.02	1.56	1.52
12	1	3	BMA	C1-C2	2.02	1.56	1.52

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	S	4	MAN	C1-O5-C5	4.75	118.63	112.19
13	AA	4	MAN	C1-O5-C5	4.73	118.59	112.19
13	l	4	MAN	C1-O5-C5	4.70	118.56	112.19
10	k	3	BMA	C1-O5-C5	4.29	118.00	112.19
10	9	3	BMA	C1-O5-C5	4.26	117.97	112.19
10	P	3	BMA	C1-O5-C5	4.26	117.96	112.19
12	a	1	NAG	C1-O5-C5	4.21	117.90	112.19
12	DA	1	NAG	C1-O5-C5	4.18	117.86	112.19
12	s	1	NAG	C1-O5-C5	4.16	117.83	112.19
13	l	5	MAN	C1-O5-C5	4.10	117.74	112.19
13	AA	5	MAN	C1-O5-C5	4.09	117.73	112.19
10	u	3	BMA	C1-O5-C5	4.07	117.71	112.19
10	c	3	BMA	C1-O5-C5	4.07	117.71	112.19
13	S	5	MAN	C1-O5-C5	4.06	117.70	112.19
10	F	3	BMA	C1-O5-C5	4.05	117.68	112.19
13	l	7	MAN	C1-O5-C5	3.85	117.41	112.19
13	S	7	MAN	C1-O5-C5	3.84	117.39	112.19
13	AA	7	MAN	C1-O5-C5	3.83	117.39	112.19
13	S	3	BMA	C1-O5-C5	3.47	116.90	112.19
13	AA	3	BMA	C1-O5-C5	3.45	116.87	112.19
13	l	3	BMA	C1-O5-C5	3.44	116.86	112.19
10	u	2	NAG	C1-O5-C5	3.41	116.81	112.19
10	F	2	NAG	C1-O5-C5	3.40	116.80	112.19
10	c	2	NAG	C1-O5-C5	3.40	116.80	112.19
11	J	3	BMA	C1-O5-C5	3.26	116.61	112.19
11	y	3	BMA	C1-O5-C5	3.24	116.58	112.19
11	J	4	MAN	C1-O5-C5	3.22	116.56	112.19
11	g	3	BMA	C1-O5-C5	3.22	116.56	112.19
11	y	4	MAN	C1-O5-C5	3.21	116.54	112.19
10	9	2	NAG	C1-O5-C5	3.21	116.54	112.19
11	g	4	MAN	C1-O5-C5	3.20	116.53	112.19
10	P	2	NAG	C1-O5-C5	3.19	116.51	112.19
10	k	2	NAG	C1-O5-C5	3.18	116.51	112.19
13	l	5	MAN	O2-C2-C3	-3.18	103.77	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AA	5	MAN	O2-C2-C3	-3.17	103.78	110.14
10	P	4	MAN	C1-O5-C5	3.17	116.48	112.19
10	9	4	MAN	C1-O5-C5	3.15	116.47	112.19
13	S	5	MAN	O2-C2-C3	-3.15	103.82	110.14
10	k	4	MAN	C1-O5-C5	3.14	116.44	112.19
9	b	1	NAG	C2-N2-C7	3.13	127.36	122.90
9	t	1	NAG	C2-N2-C7	3.11	127.33	122.90
9	E	1	NAG	C2-N2-C7	3.08	127.29	122.90
9	BA	1	NAG	C2-N2-C7	3.06	127.27	122.90
13	l	9	MAN	C1-O5-C5	3.06	116.34	112.19
13	l	2	NAG	C2-N2-C7	3.06	127.26	122.90
13	AA	2	NAG	C2-N2-C7	3.06	127.26	122.90
9	T	1	NAG	C2-N2-C7	3.05	127.25	122.90
13	S	9	MAN	C1-O5-C5	3.05	116.32	112.19
13	AA	9	MAN	C1-O5-C5	3.04	116.31	112.19
13	S	2	NAG	C2-N2-C7	3.04	127.23	122.90
9	o	1	NAG	C2-N2-C7	3.03	127.22	122.90
9	H	1	NAG	C2-N2-C7	2.90	127.03	122.90
9	e	1	NAG	C2-N2-C7	2.88	127.01	122.90
9	w	1	NAG	C2-N2-C7	2.88	127.00	122.90
10	9	3	BMA	C1-C2-C3	2.82	113.13	109.67
10	k	3	BMA	C1-C2-C3	2.81	113.12	109.67
10	P	3	BMA	C1-C2-C3	2.80	113.11	109.67
13	S	8	MAN	C1-O5-C5	2.79	115.97	112.19
13	AA	8	MAN	C1-O5-C5	2.78	115.96	112.19
13	l	8	MAN	C1-O5-C5	2.78	115.96	112.19
10	c	4	MAN	C1-O5-C5	2.77	115.94	112.19
10	F	4	MAN	C1-O5-C5	2.76	115.94	112.19
11	y	5	MAN	C1-O5-C5	2.75	115.91	112.19
11	g	5	MAN	C1-O5-C5	2.75	115.91	112.19
10	u	4	MAN	C1-O5-C5	2.74	115.91	112.19
11	J	5	MAN	C1-O5-C5	2.73	115.89	112.19
10	CA	1	NAG	C1-O5-C5	2.72	115.88	112.19
10	Z	1	NAG	C1-O5-C5	2.72	115.88	112.19
10	p	1	NAG	C1-O5-C5	2.69	115.83	112.19
12	a	3	BMA	C1-O5-C5	2.61	115.73	112.19
10	p	4	MAN	C1-O5-C5	2.60	115.71	112.19
12	s	3	BMA	C1-O5-C5	2.59	115.71	112.19
10	CA	4	MAN	C1-O5-C5	2.58	115.69	112.19
10	Z	2	NAG	C1-O5-C5	2.58	115.69	112.19
10	CA	2	NAG	C1-O5-C5	2.57	115.68	112.19
12	DA	3	BMA	C1-O5-C5	2.57	115.67	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	p	2	NAG	C1-O5-C5	2.57	115.67	112.19
10	Z	4	MAN	C1-O5-C5	2.55	115.65	112.19
12	a	3	BMA	C1-C2-C3	2.53	112.78	109.67
12	s	3	BMA	C1-C2-C3	2.50	112.75	109.67
12	DA	3	BMA	C1-C2-C3	2.48	112.71	109.67
10	c	3	BMA	C1-C2-C3	2.41	112.63	109.67
10	u	3	BMA	C1-C2-C3	2.41	112.63	109.67
12	O	3	BMA	C1-O5-C5	2.41	115.46	112.19
12	l	3	BMA	C1-O5-C5	2.41	115.46	112.19
10	F	3	BMA	C1-C2-C3	2.40	112.61	109.67
12	j	3	BMA	C1-O5-C5	2.39	115.43	112.19
10	P	3	BMA	O5-C1-C2	2.35	114.39	110.77
13	AA	7	MAN	O2-C2-C3	-2.34	105.44	110.14
13	S	7	MAN	O2-C2-C3	-2.34	105.44	110.14
12	j	3	BMA	O2-C2-C3	-2.34	105.45	110.14
12	O	3	BMA	O2-C2-C3	-2.34	105.45	110.14
13	l	7	MAN	O2-C2-C3	-2.34	105.45	110.14
12	l	3	BMA	O2-C2-C3	-2.34	105.45	110.14
10	9	1	NAG	C1-O5-C5	2.34	115.36	112.19
10	9	3	BMA	O5-C1-C2	2.33	114.37	110.77
10	k	3	BMA	O5-C1-C2	2.33	114.36	110.77
10	P	1	NAG	C1-O5-C5	2.32	115.33	112.19
10	k	1	NAG	C1-O5-C5	2.31	115.33	112.19
11	J	4	MAN	O2-C2-C3	-2.27	105.60	110.14
10	p	4	MAN	O2-C2-C3	-2.25	105.64	110.14
10	P	4	MAN	O2-C2-C3	-2.24	105.64	110.14
10	Z	4	MAN	O2-C2-C3	-2.24	105.64	110.14
11	y	4	MAN	O2-C2-C3	-2.24	105.65	110.14
10	k	4	MAN	O2-C2-C3	-2.24	105.66	110.14
10	9	4	MAN	O2-C2-C3	-2.24	105.66	110.14
11	g	4	MAN	O2-C2-C3	-2.24	105.66	110.14
10	CA	4	MAN	O2-C2-C3	-2.23	105.67	110.14
10	F	3	BMA	O5-C1-C2	2.23	114.21	110.77
10	c	3	BMA	O5-C1-C2	2.22	114.19	110.77
10	u	3	BMA	O5-C1-C2	2.21	114.19	110.77
13	AA	9	MAN	O2-C2-C3	-2.21	105.72	110.14
11	J	5	MAN	O2-C2-C3	-2.21	105.72	110.14
13	l	9	MAN	O2-C2-C3	-2.20	105.72	110.14
13	S	9	MAN	O2-C2-C3	-2.20	105.73	110.14
11	y	5	MAN	O2-C2-C3	-2.19	105.75	110.14
10	c	4	MAN	O2-C2-C3	-2.19	105.76	110.14
10	u	4	MAN	O2-C2-C3	-2.19	105.76	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	g	5	MAN	O2-C2-C3	-2.19	105.76	110.14
13	l	6	MAN	C1-O5-C5	2.18	115.14	112.19
13	AA	6	MAN	C1-O5-C5	2.16	115.12	112.19
10	F	4	MAN	O2-C2-C3	-2.16	105.81	110.14
13	AA	6	MAN	O2-C2-C3	-2.16	105.81	110.14
13	l	6	MAN	O2-C2-C3	-2.15	105.83	110.14
13	S	6	MAN	C1-O5-C5	2.15	115.11	112.19
13	S	6	MAN	O2-C2-C3	-2.14	105.84	110.14
13	AA	8	MAN	O2-C2-C3	-2.13	105.88	110.14
13	S	8	MAN	O2-C2-C3	-2.13	105.88	110.14
13	l	8	MAN	O2-C2-C3	-2.13	105.88	110.14
11	J	1	NAG	C1-O5-C5	2.06	114.98	112.19
11	y	1	NAG	C1-O5-C5	2.06	114.98	112.19
11	g	1	NAG	C1-O5-C5	2.05	114.98	112.19
10	9	2	NAG	O4-C4-C3	2.03	115.03	110.35
10	k	2	NAG	O4-C4-C3	2.01	114.99	110.35
10	P	2	NAG	O4-C4-C3	2.00	114.98	110.35

There are no chirality outliers.

All (150) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	P	1	NAG	O5-C5-C6-O6
10	k	1	NAG	O5-C5-C6-O6
10	9	1	NAG	O5-C5-C6-O6
9	E	2	NAG	O5-C5-C6-O6
9	b	2	NAG	O5-C5-C6-O6
9	t	2	NAG	O5-C5-C6-O6
10	Z	4	MAN	O5-C5-C6-O6
10	p	4	MAN	O5-C5-C6-O6
10	CA	4	MAN	O5-C5-C6-O6
10	P	1	NAG	C4-C5-C6-O6
10	k	1	NAG	C4-C5-C6-O6
10	9	1	NAG	C4-C5-C6-O6
9	L	2	NAG	O5-C5-C6-O6
9	i	2	NAG	O5-C5-C6-O6
9	0	2	NAG	O5-C5-C6-O6
10	F	2	NAG	O5-C5-C6-O6
10	P	2	NAG	O5-C5-C6-O6
10	c	2	NAG	O5-C5-C6-O6
10	k	2	NAG	O5-C5-C6-O6
10	u	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	9	2	NAG	O5-C5-C6-O6
12	a	3	BMA	O5-C5-C6-O6
12	s	3	BMA	O5-C5-C6-O6
12	DA	3	BMA	O5-C5-C6-O6
13	S	2	NAG	O5-C5-C6-O6
13	l	2	NAG	O5-C5-C6-O6
13	AA	2	NAG	O5-C5-C6-O6
13	S	8	MAN	O5-C5-C6-O6
13	S	9	MAN	O5-C5-C6-O6
13	l	8	MAN	O5-C5-C6-O6
13	l	9	MAN	O5-C5-C6-O6
13	AA	8	MAN	O5-C5-C6-O6
13	AA	9	MAN	O5-C5-C6-O6
13	S	9	MAN	C4-C5-C6-O6
13	l	9	MAN	C4-C5-C6-O6
13	AA	9	MAN	C4-C5-C6-O6
9	T	2	NAG	O5-C5-C6-O6
9	o	2	NAG	O5-C5-C6-O6
9	BA	2	NAG	O5-C5-C6-O6
13	S	1	NAG	O5-C5-C6-O6
13	l	1	NAG	O5-C5-C6-O6
13	AA	1	NAG	O5-C5-C6-O6
10	F	1	NAG	C4-C5-C6-O6
10	P	2	NAG	C4-C5-C6-O6
10	c	1	NAG	C4-C5-C6-O6
10	k	2	NAG	C4-C5-C6-O6
10	u	1	NAG	C4-C5-C6-O6
10	9	2	NAG	C4-C5-C6-O6
10	F	2	NAG	C4-C5-C6-O6
10	c	2	NAG	C4-C5-C6-O6
10	u	2	NAG	C4-C5-C6-O6
9	L	2	NAG	C4-C5-C6-O6
9	i	2	NAG	C4-C5-C6-O6
9	0	2	NAG	C4-C5-C6-O6
9	L	1	NAG	C4-C5-C6-O6
9	i	1	NAG	C4-C5-C6-O6
9	0	1	NAG	C4-C5-C6-O6
12	a	1	NAG	C4-C5-C6-O6
12	s	1	NAG	C4-C5-C6-O6
12	DA	1	NAG	C4-C5-C6-O6
9	T	2	NAG	C4-C5-C6-O6
9	o	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	BA	2	NAG	C4-C5-C6-O6
13	S	5	MAN	O5-C5-C6-O6
13	l	5	MAN	O5-C5-C6-O6
13	AA	5	MAN	O5-C5-C6-O6
9	E	2	NAG	C4-C5-C6-O6
9	b	2	NAG	C4-C5-C6-O6
9	t	2	NAG	C4-C5-C6-O6
10	Z	4	MAN	C4-C5-C6-O6
10	p	4	MAN	C4-C5-C6-O6
10	CA	4	MAN	C4-C5-C6-O6
13	S	2	NAG	C4-C5-C6-O6
13	l	2	NAG	C4-C5-C6-O6
13	AA	2	NAG	C4-C5-C6-O6
10	F	1	NAG	O5-C5-C6-O6
10	c	1	NAG	O5-C5-C6-O6
10	u	1	NAG	O5-C5-C6-O6
11	J	2	NAG	O5-C5-C6-O6
11	g	2	NAG	O5-C5-C6-O6
11	y	2	NAG	O5-C5-C6-O6
13	S	1	NAG	C4-C5-C6-O6
13	l	1	NAG	C4-C5-C6-O6
13	AA	1	NAG	C4-C5-C6-O6
10	P	3	BMA	O5-C5-C6-O6
10	k	3	BMA	O5-C5-C6-O6
10	9	3	BMA	O5-C5-C6-O6
11	J	4	MAN	O5-C5-C6-O6
11	g	4	MAN	O5-C5-C6-O6
11	y	4	MAN	O5-C5-C6-O6
12	a	3	BMA	C4-C5-C6-O6
11	J	2	NAG	C4-C5-C6-O6
11	g	2	NAG	C4-C5-C6-O6
11	y	2	NAG	C4-C5-C6-O6
12	s	3	BMA	C4-C5-C6-O6
12	DA	3	BMA	C4-C5-C6-O6
13	S	8	MAN	C4-C5-C6-O6
13	l	8	MAN	C4-C5-C6-O6
13	AA	8	MAN	C4-C5-C6-O6
9	L	1	NAG	O5-C5-C6-O6
9	0	1	NAG	O5-C5-C6-O6
9	i	1	NAG	O5-C5-C6-O6
12	s	1	NAG	O5-C5-C6-O6
12	DA	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
12	O	3	BMA	O5-C5-C6-O6
12	a	1	NAG	O5-C5-C6-O6
12	j	3	BMA	O5-C5-C6-O6
12	l	3	BMA	O5-C5-C6-O6
12	s	2	NAG	O5-C5-C6-O6
12	a	2	NAG	O5-C5-C6-O6
12	DA	2	NAG	O5-C5-C6-O6
9	H	1	NAG	C4-C5-C6-O6
9	e	1	NAG	C4-C5-C6-O6
9	w	1	NAG	C4-C5-C6-O6
9	H	1	NAG	O5-C5-C6-O6
9	w	1	NAG	O5-C5-C6-O6
9	e	1	NAG	O5-C5-C6-O6
13	S	7	MAN	C4-C5-C6-O6
13	l	7	MAN	C4-C5-C6-O6
13	AA	7	MAN	C4-C5-C6-O6
13	l	7	MAN	O5-C5-C6-O6
13	AA	7	MAN	O5-C5-C6-O6
13	S	7	MAN	O5-C5-C6-O6
11	g	3	BMA	C4-C5-C6-O6
11	J	3	BMA	C4-C5-C6-O6
11	y	3	BMA	C4-C5-C6-O6
9	H	1	NAG	C3-C2-N2-C7
9	e	1	NAG	C3-C2-N2-C7
9	w	1	NAG	C3-C2-N2-C7
13	S	2	NAG	C3-C2-N2-C7
13	l	2	NAG	C3-C2-N2-C7
13	AA	2	NAG	C3-C2-N2-C7
13	l	5	MAN	C4-C5-C6-O6
13	AA	5	MAN	C4-C5-C6-O6
13	S	5	MAN	C4-C5-C6-O6
9	G	2	NAG	C4-C5-C6-O6
9	d	2	NAG	C4-C5-C6-O6
9	v	2	NAG	C4-C5-C6-O6
11	J	4	MAN	C4-C5-C6-O6
11	g	4	MAN	C4-C5-C6-O6
11	y	4	MAN	C4-C5-C6-O6
9	E	1	NAG	C3-C2-N2-C7
9	T	1	NAG	C3-C2-N2-C7
9	b	1	NAG	C3-C2-N2-C7
9	o	1	NAG	C3-C2-N2-C7
9	t	1	NAG	C3-C2-N2-C7

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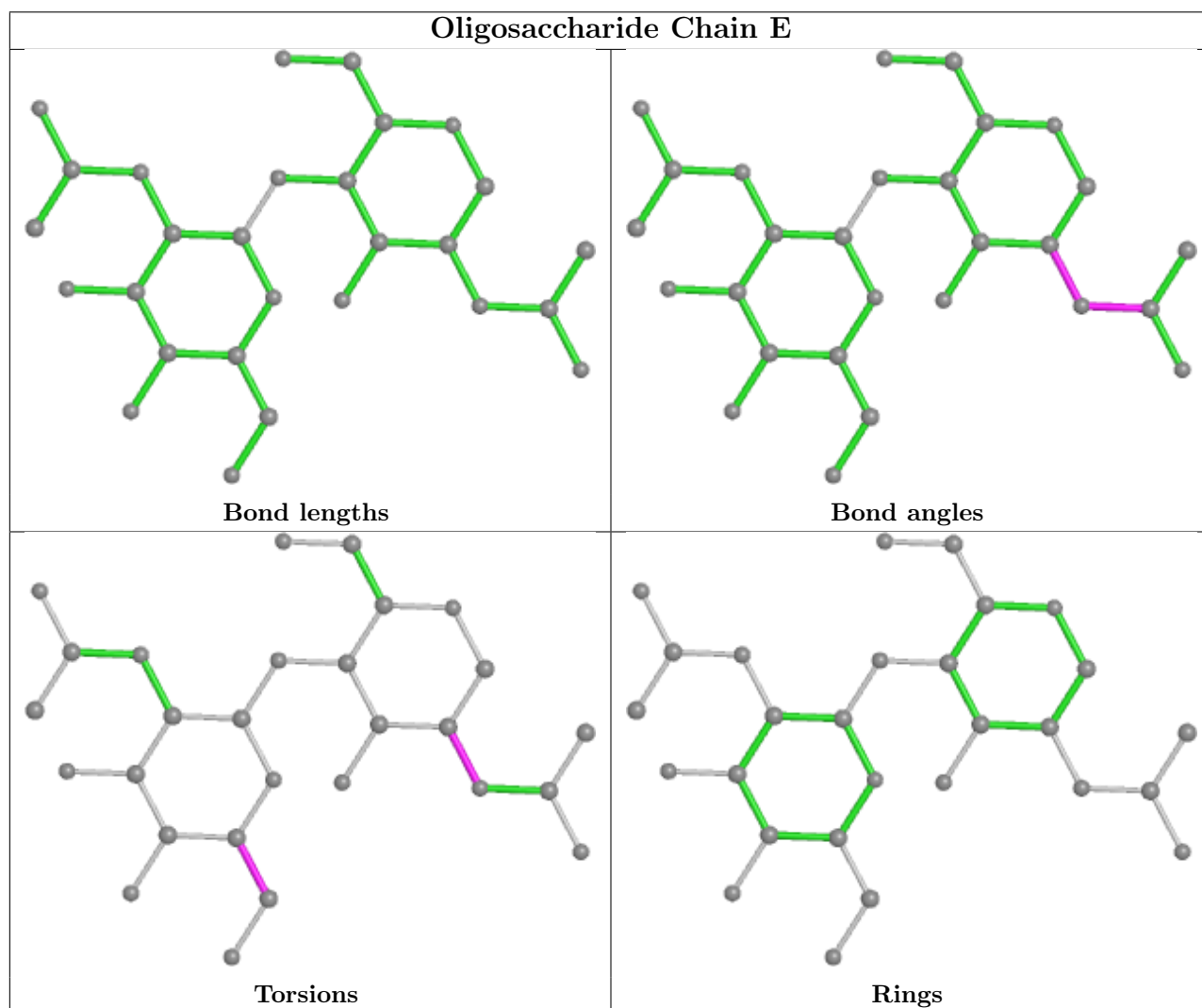
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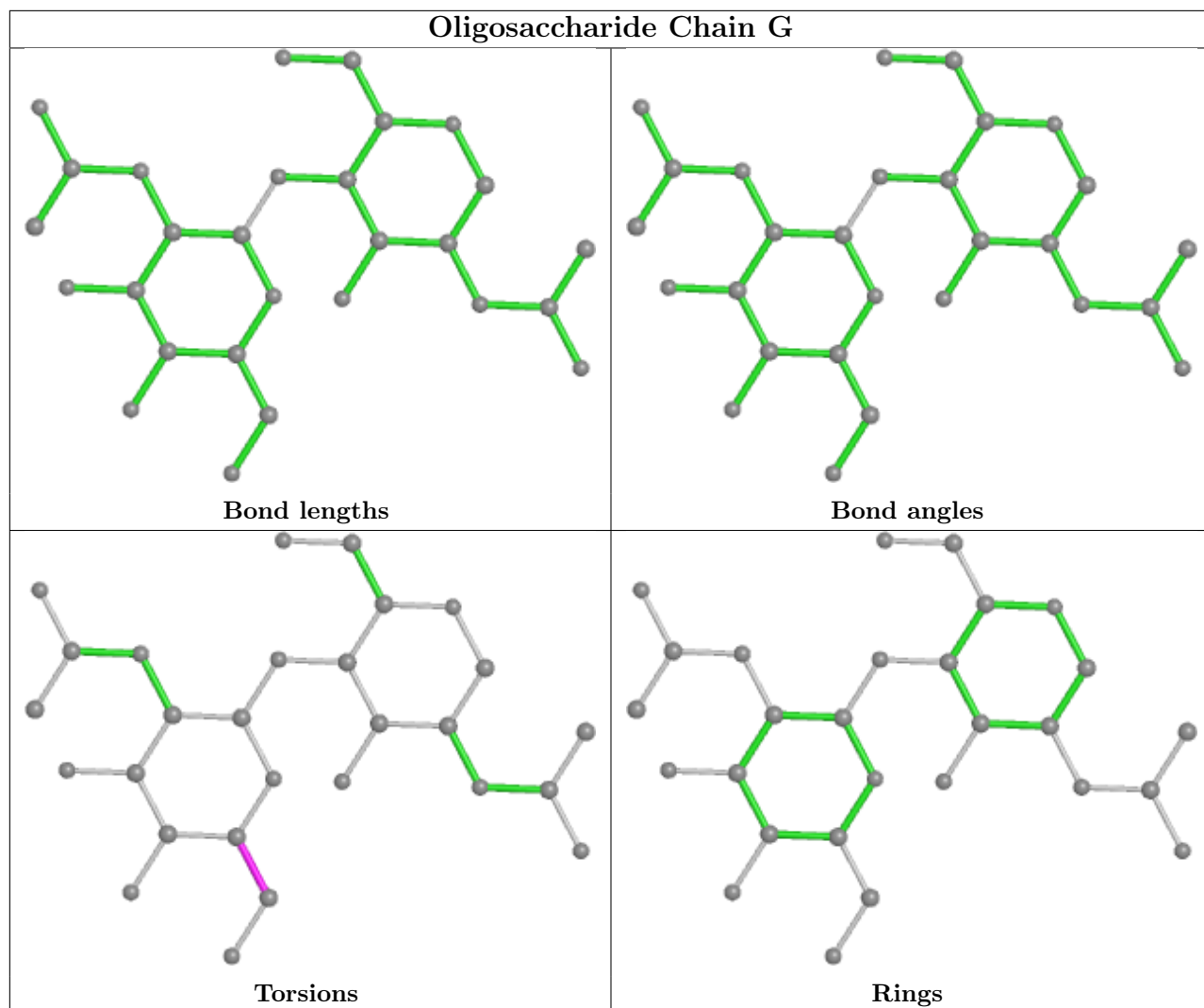
Mol	Chain	Res	Type	Atoms
9	BA	1	NAG	C3-C2-N2-C7
12	a	2	NAG	C4-C5-C6-O6
12	DA	2	NAG	C4-C5-C6-O6
12	s	2	NAG	C4-C5-C6-O6

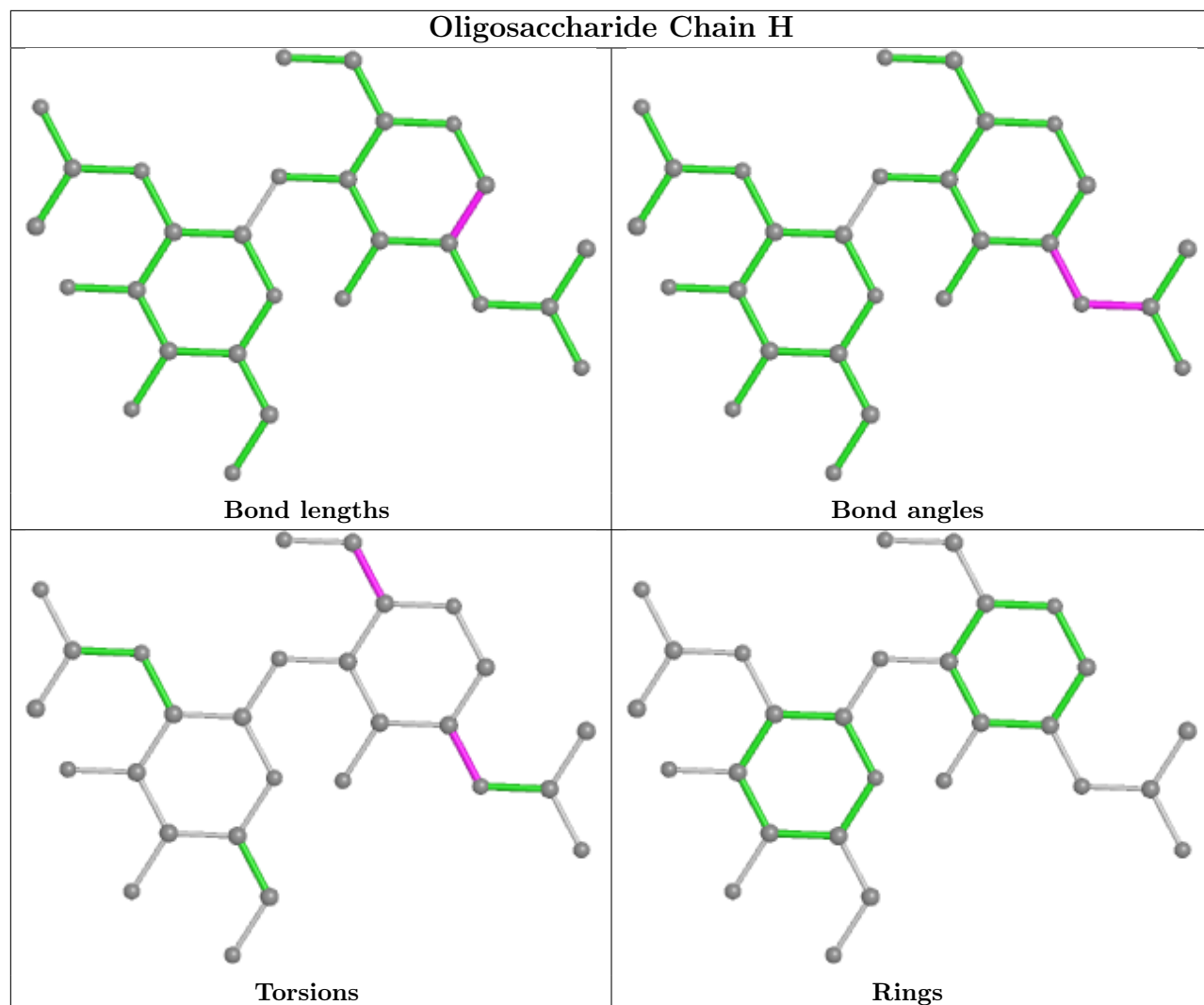
There are no ring outliers.

No monomer is involved in short contacts.

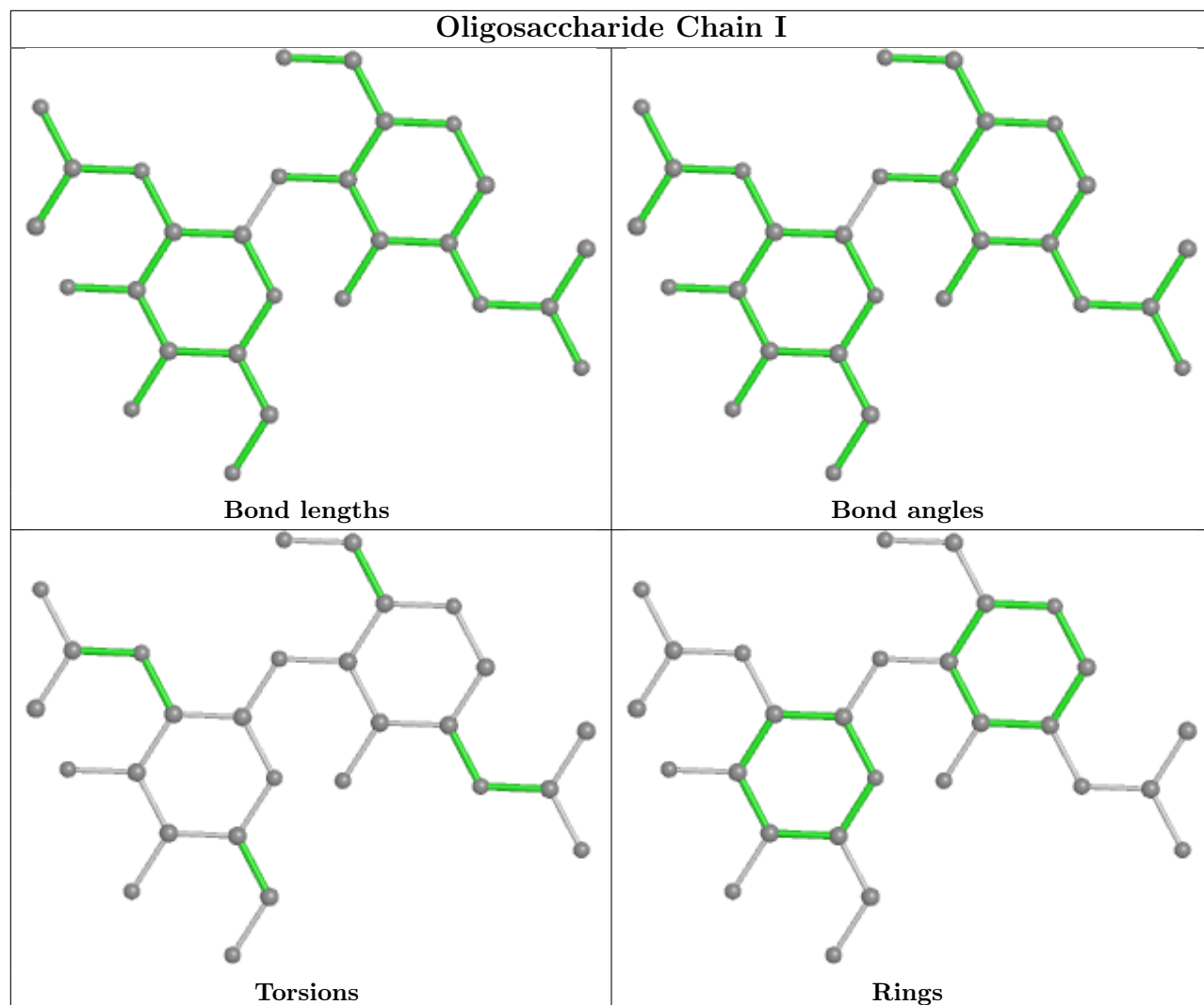
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

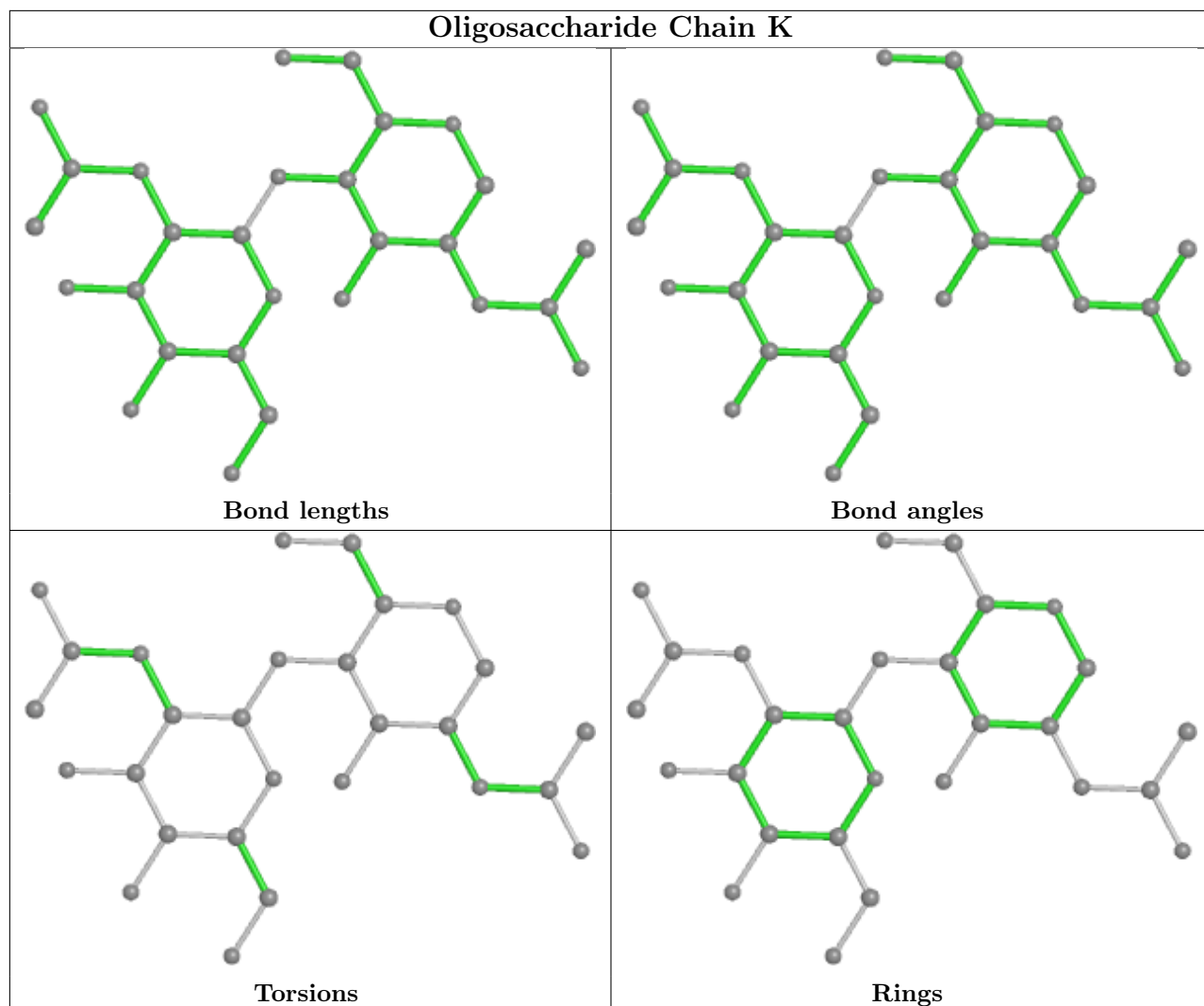


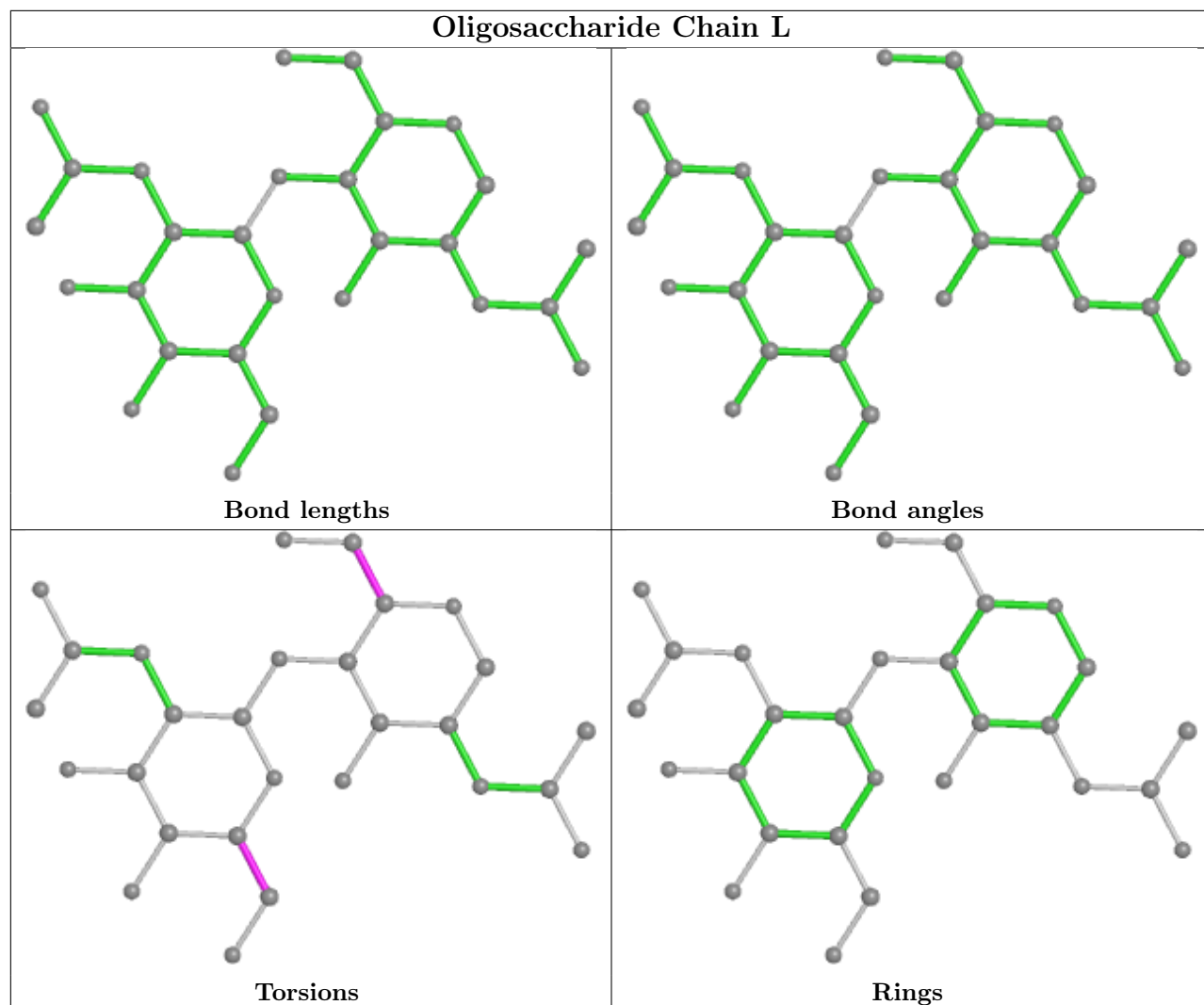


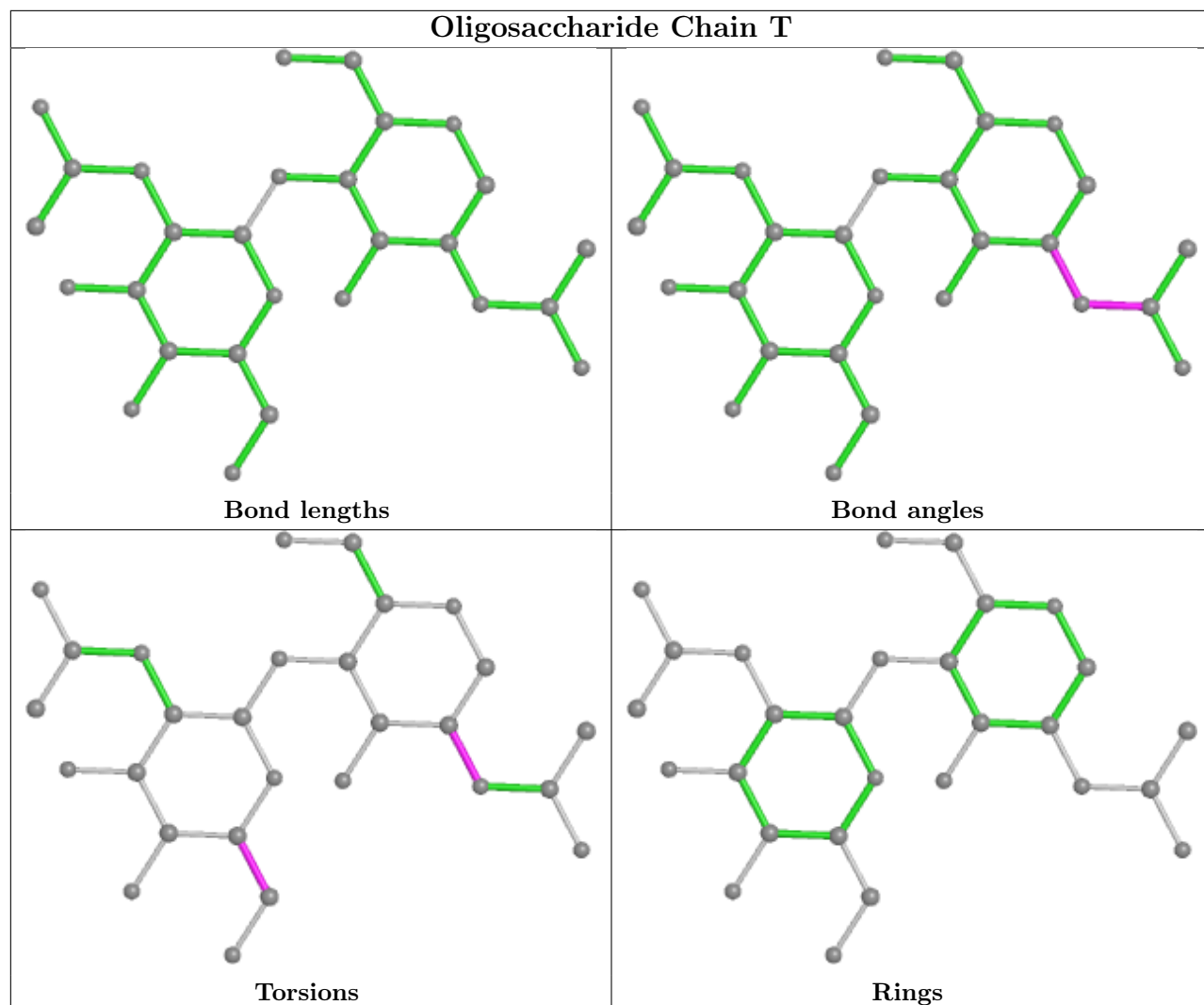


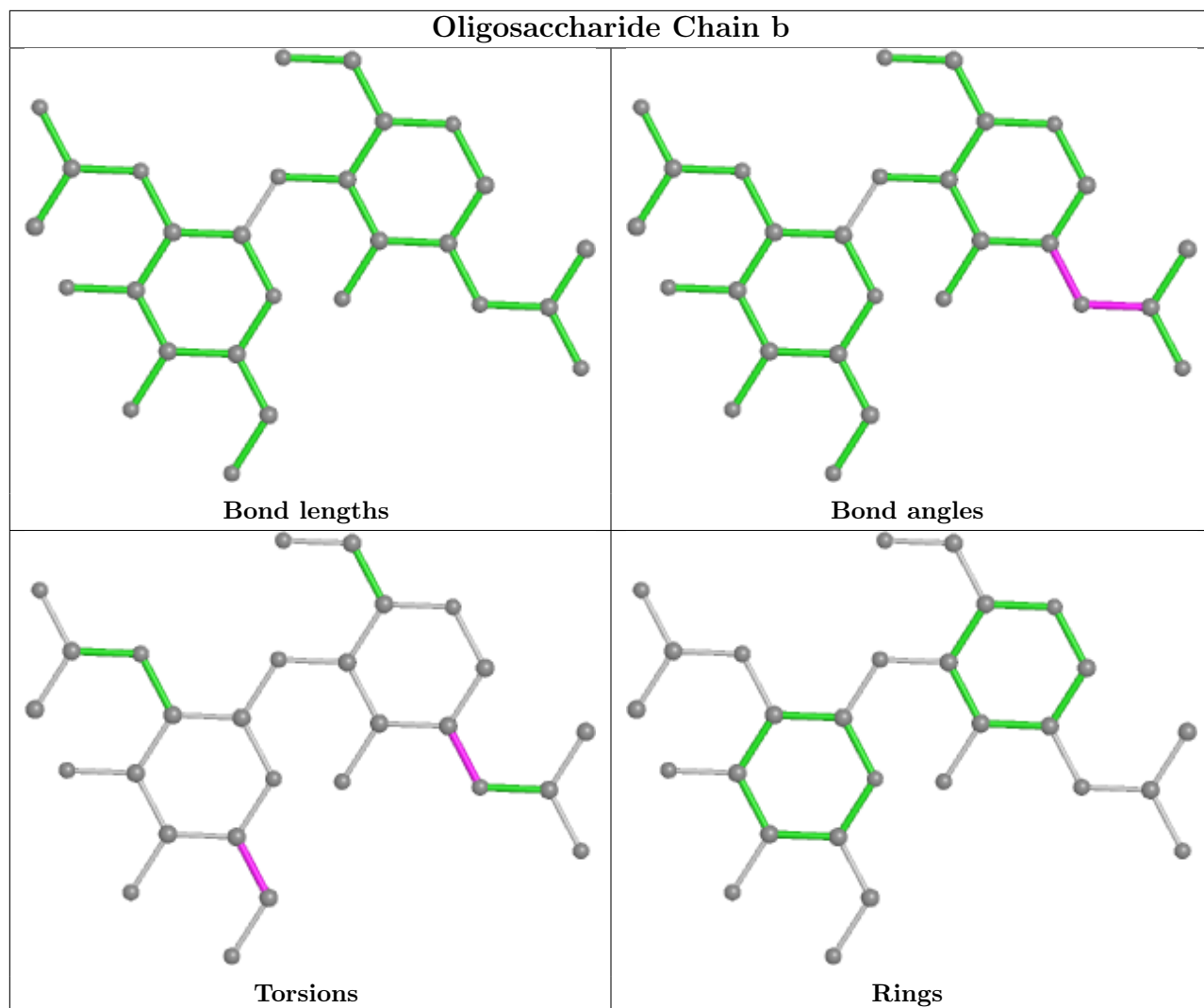


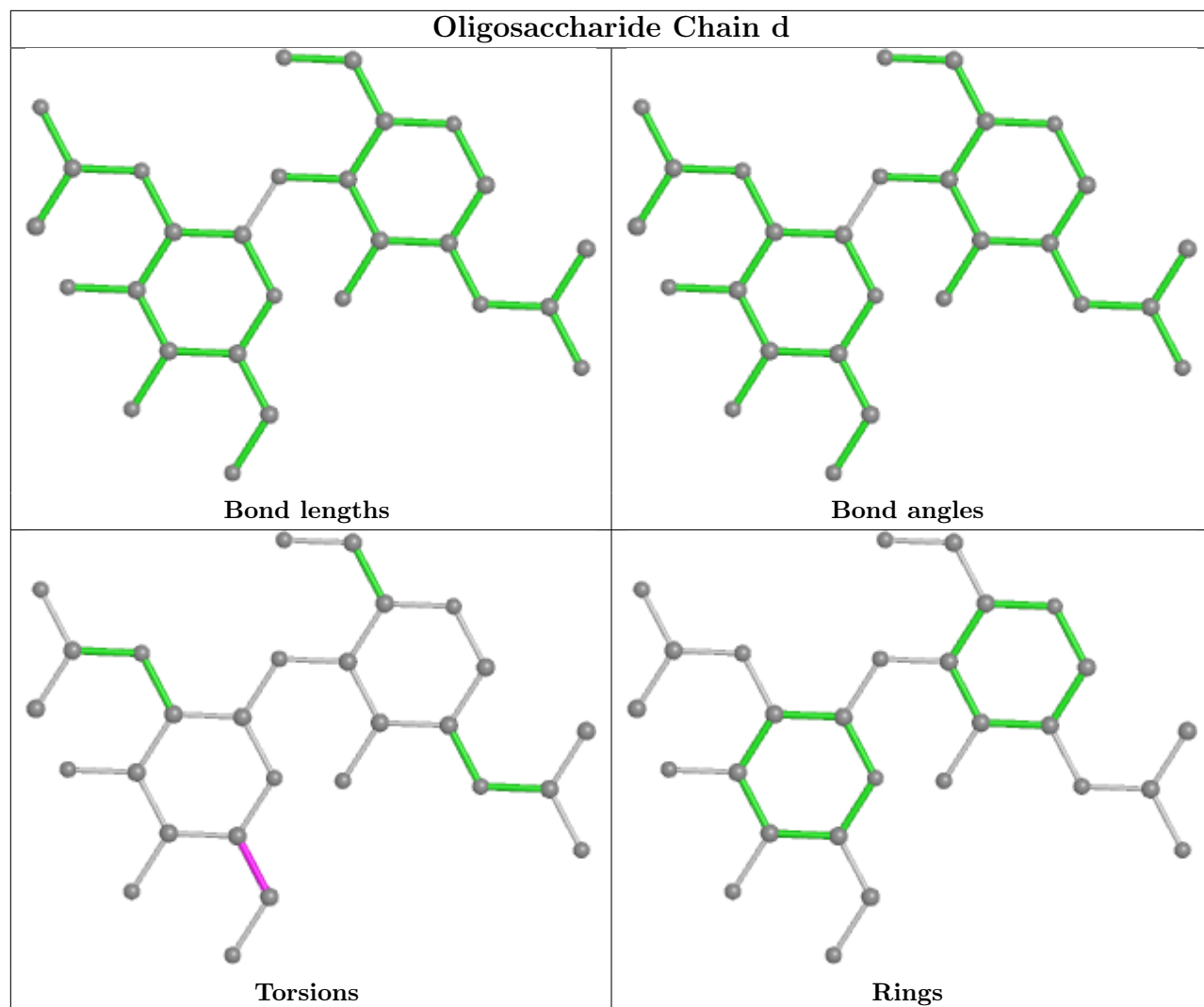


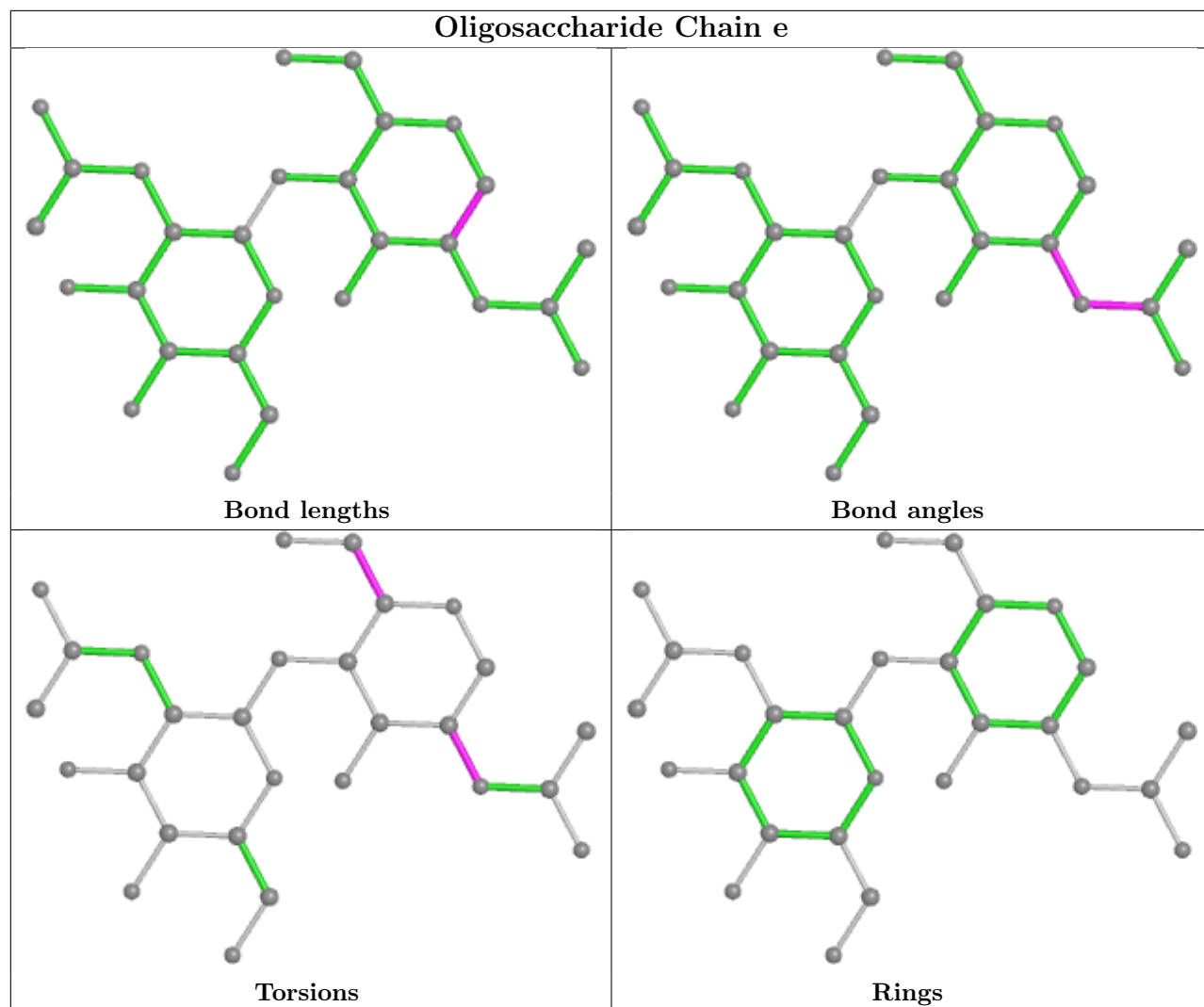


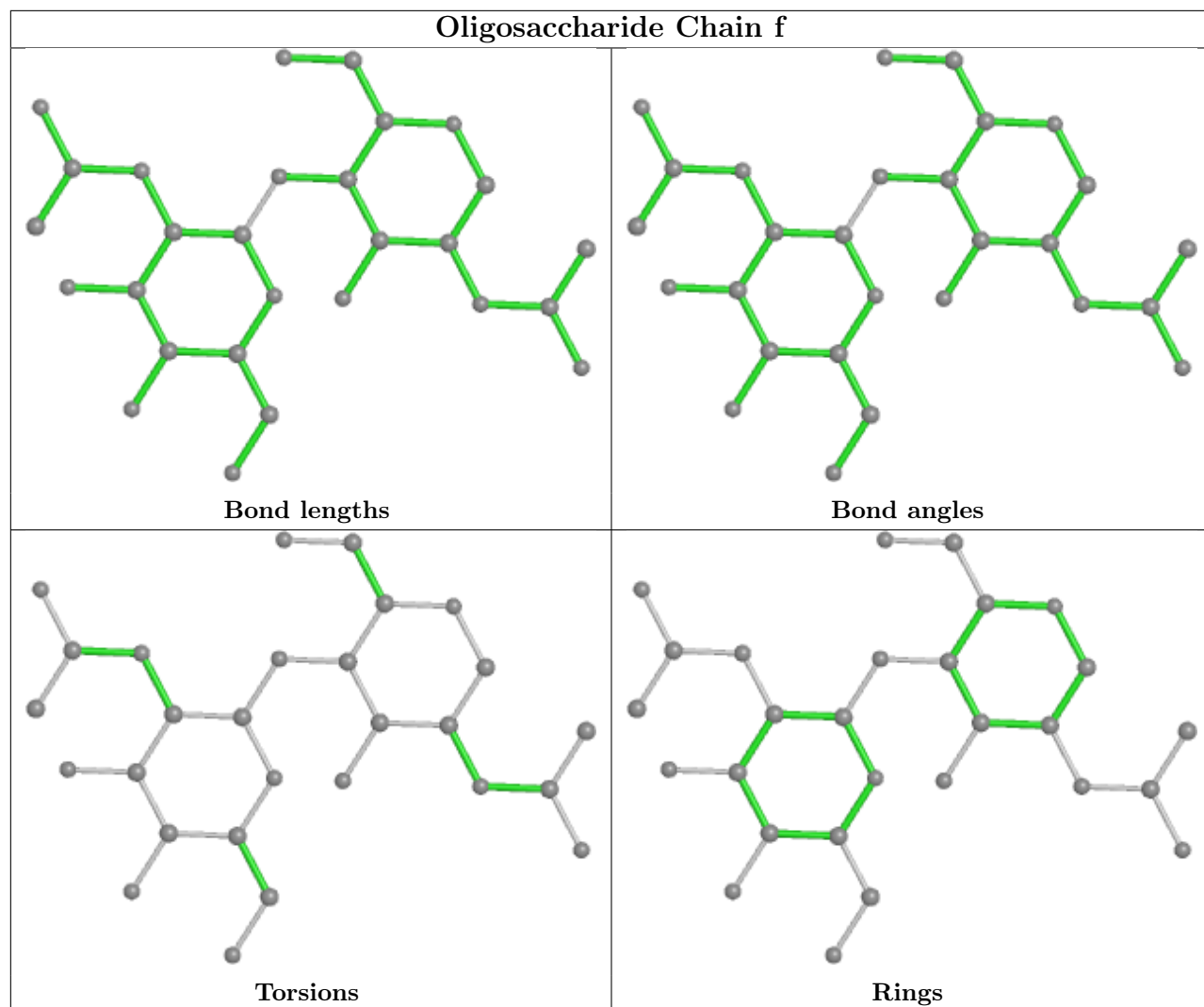




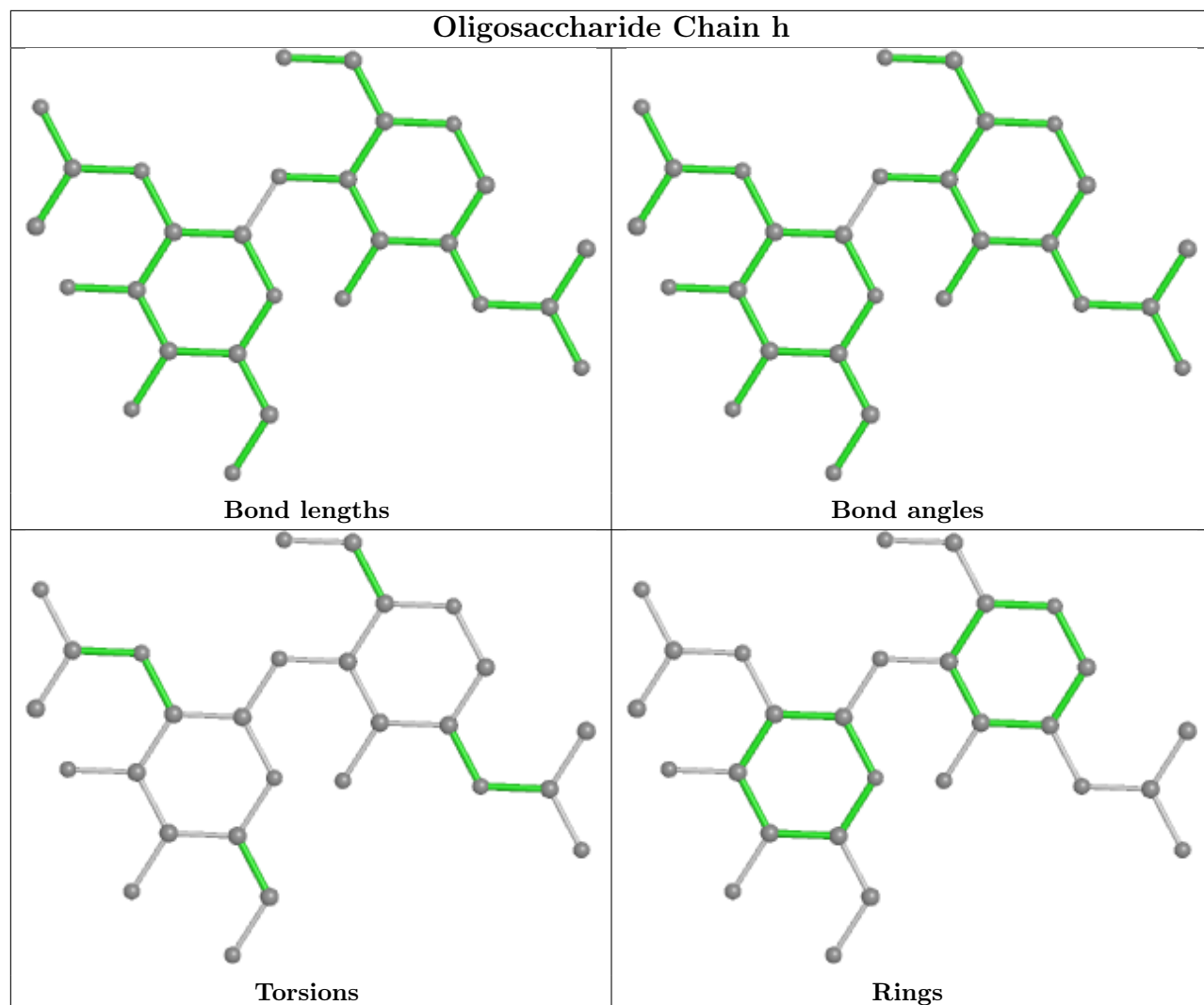


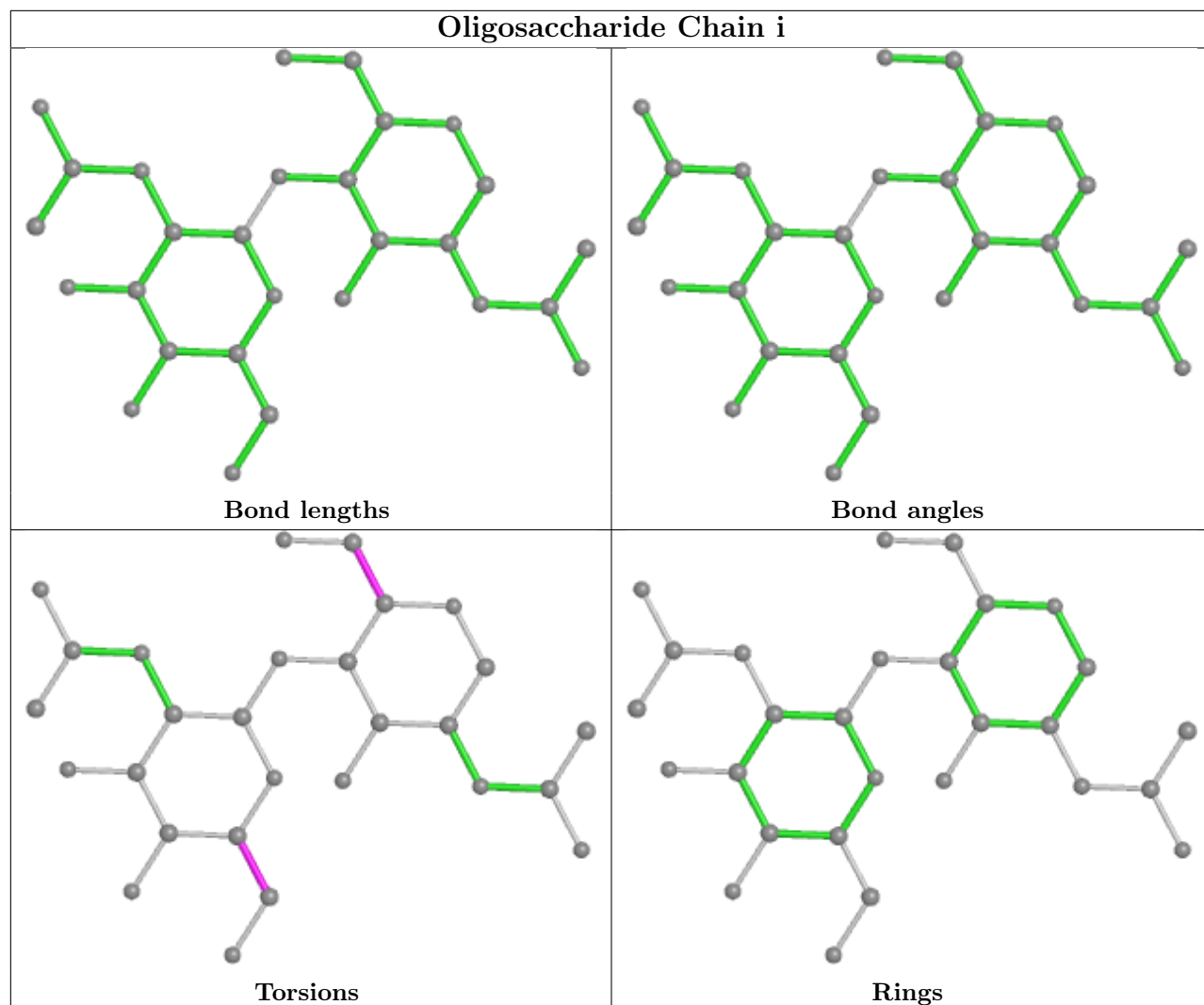


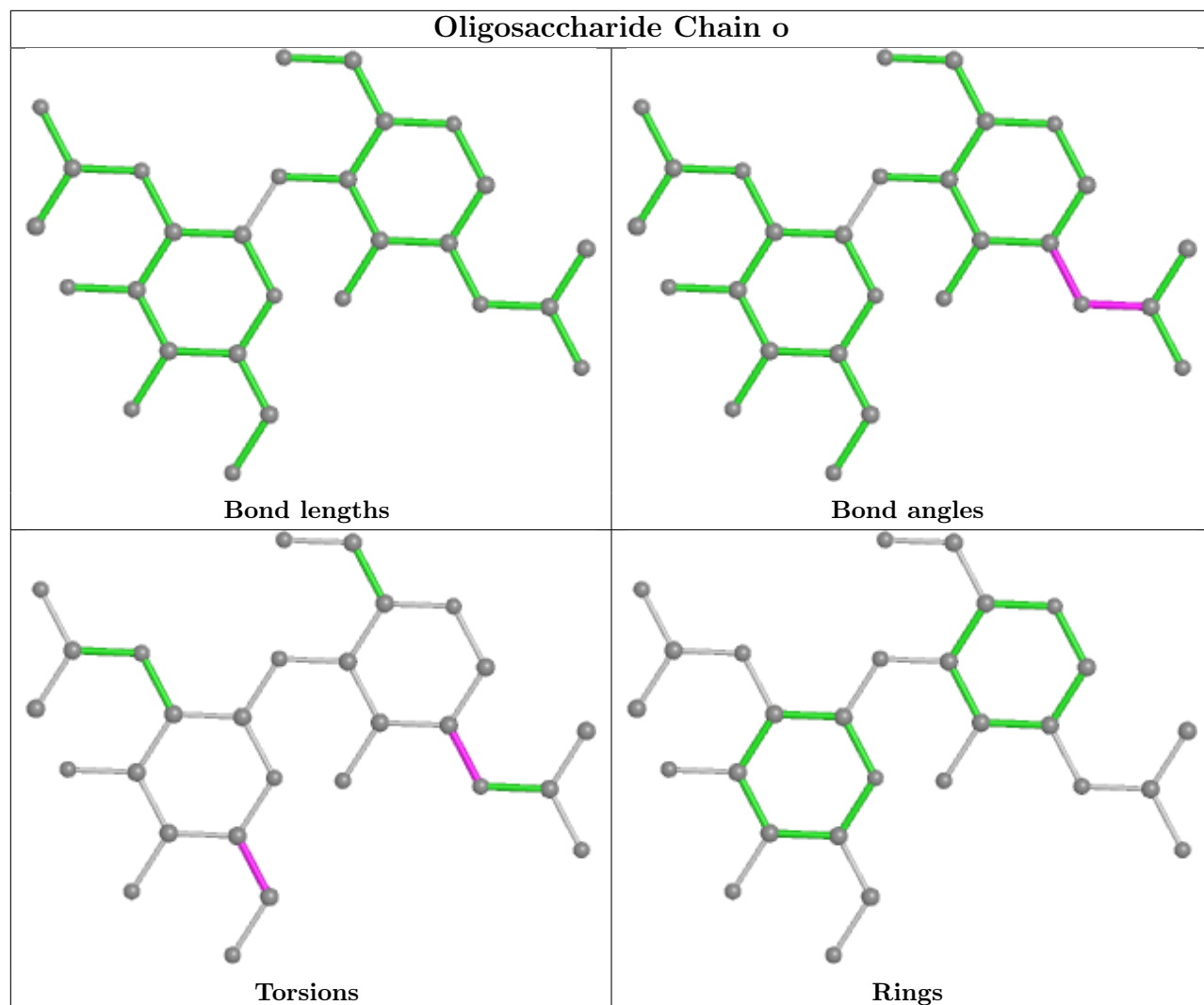


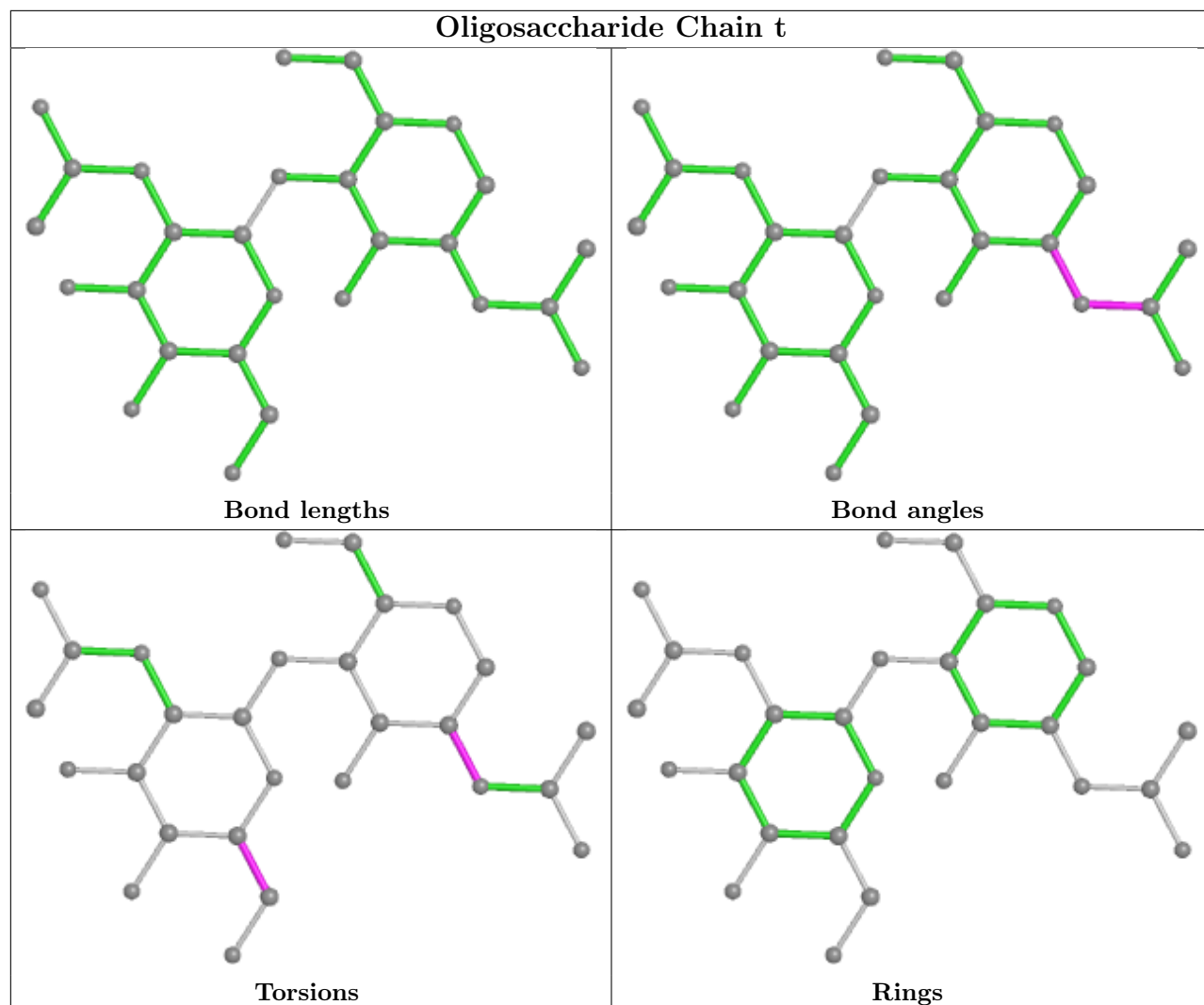


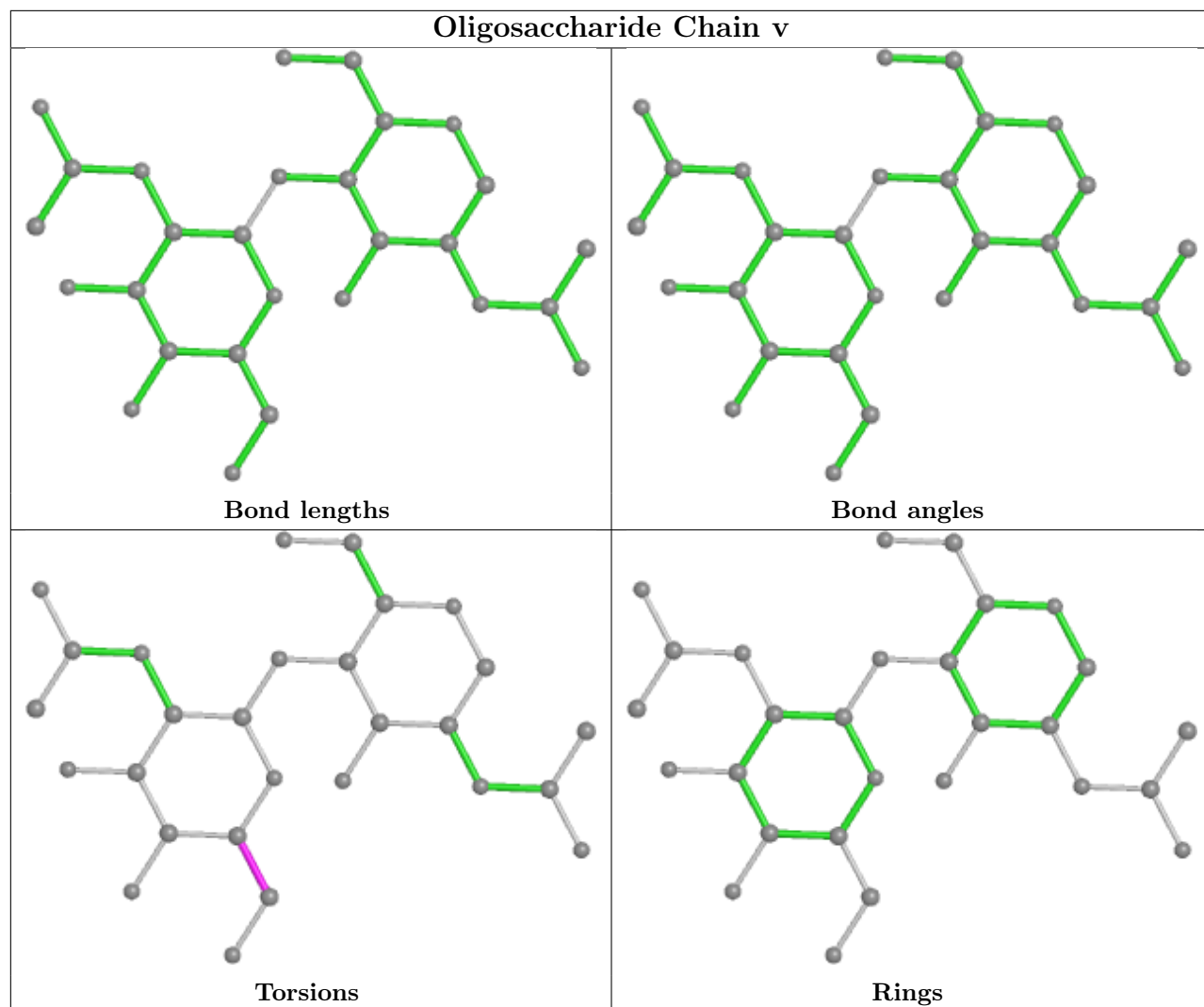


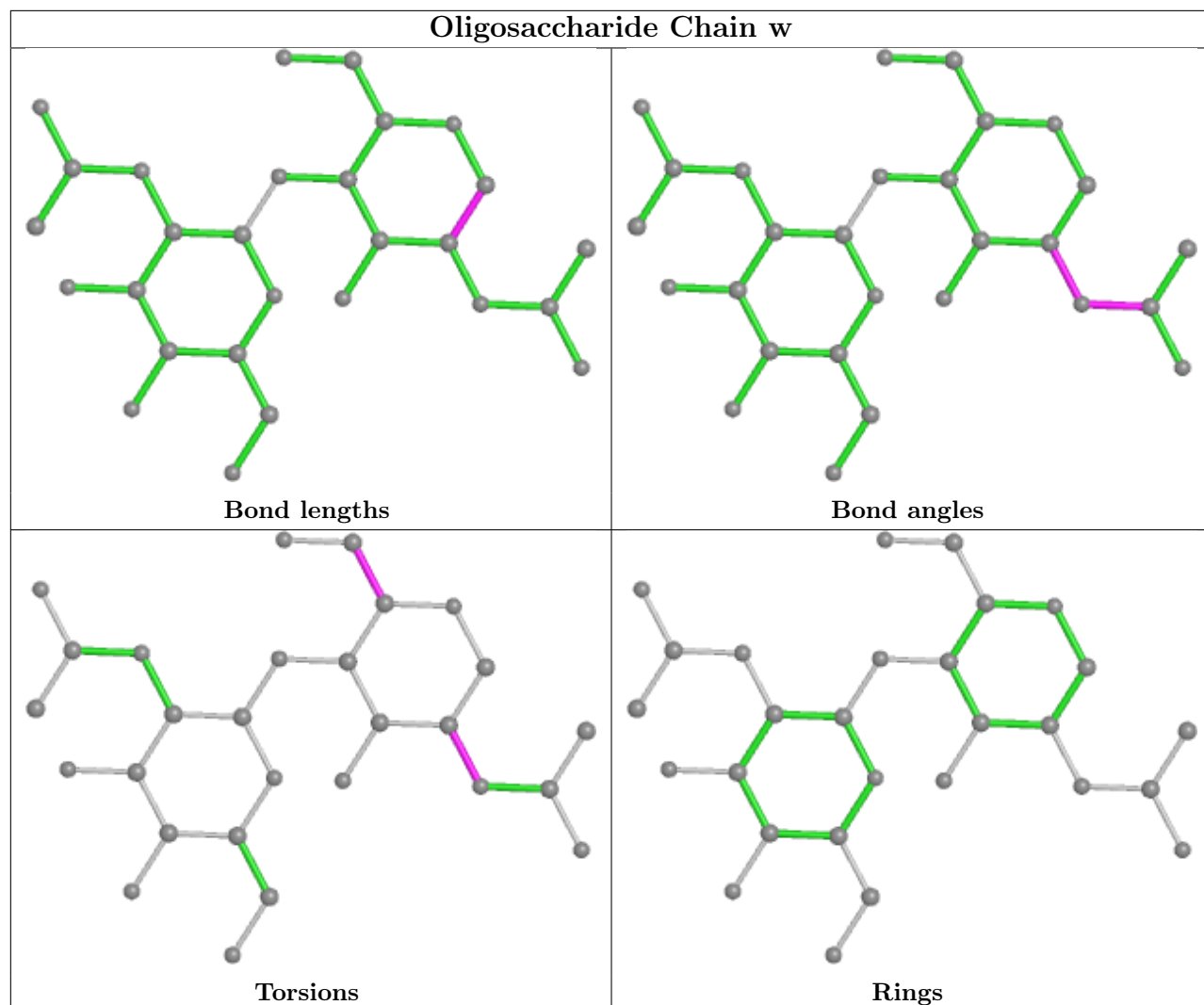


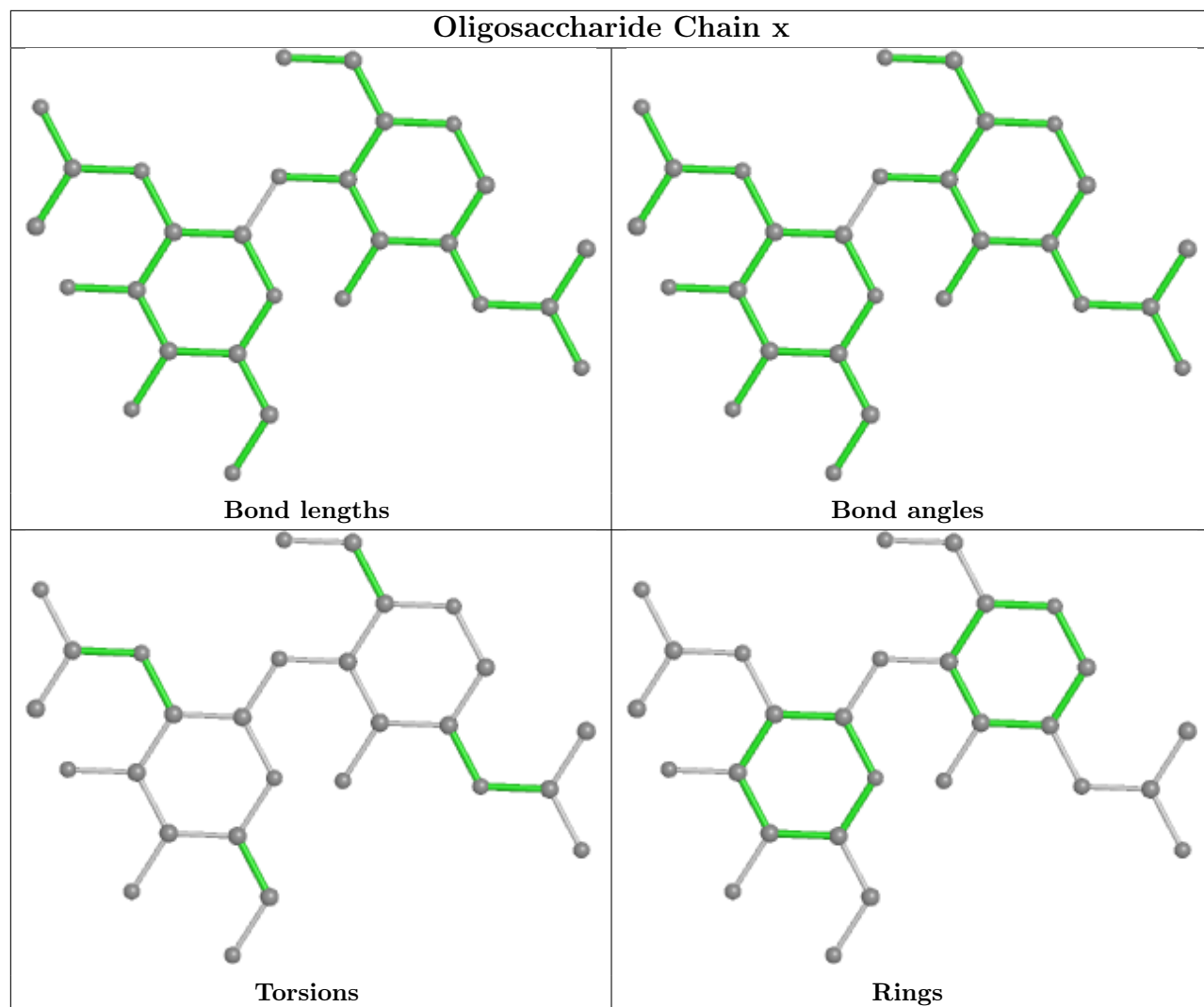


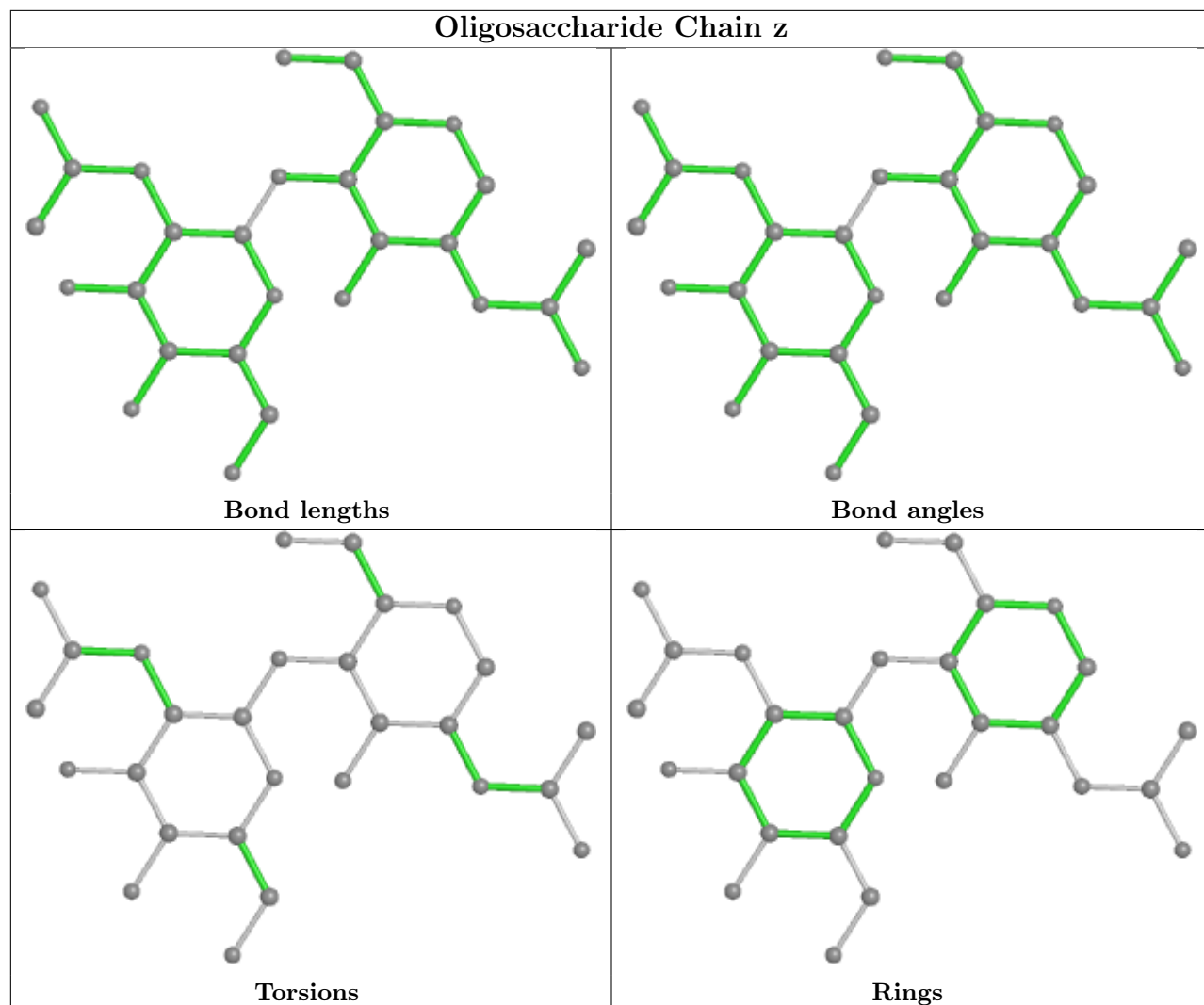




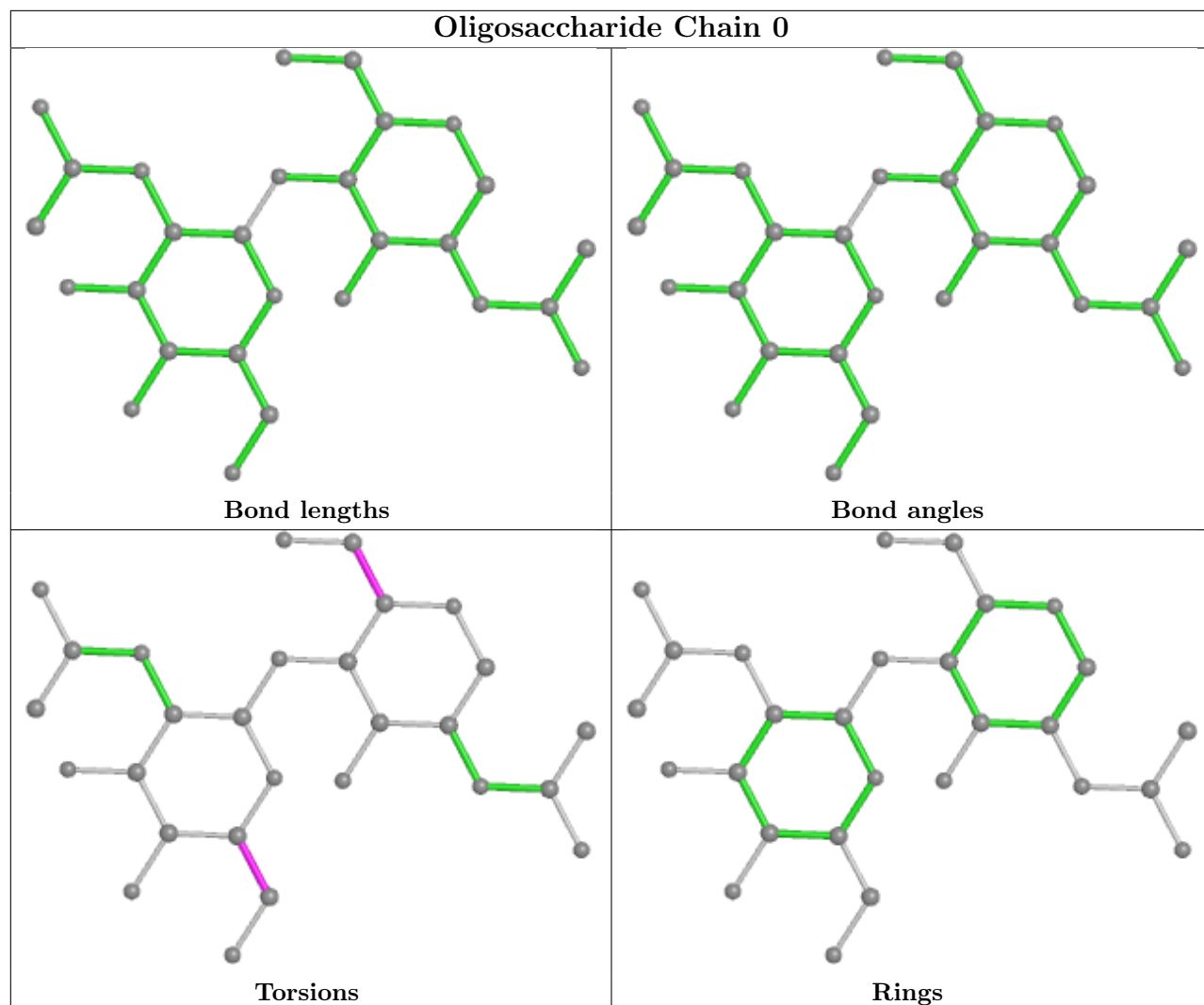


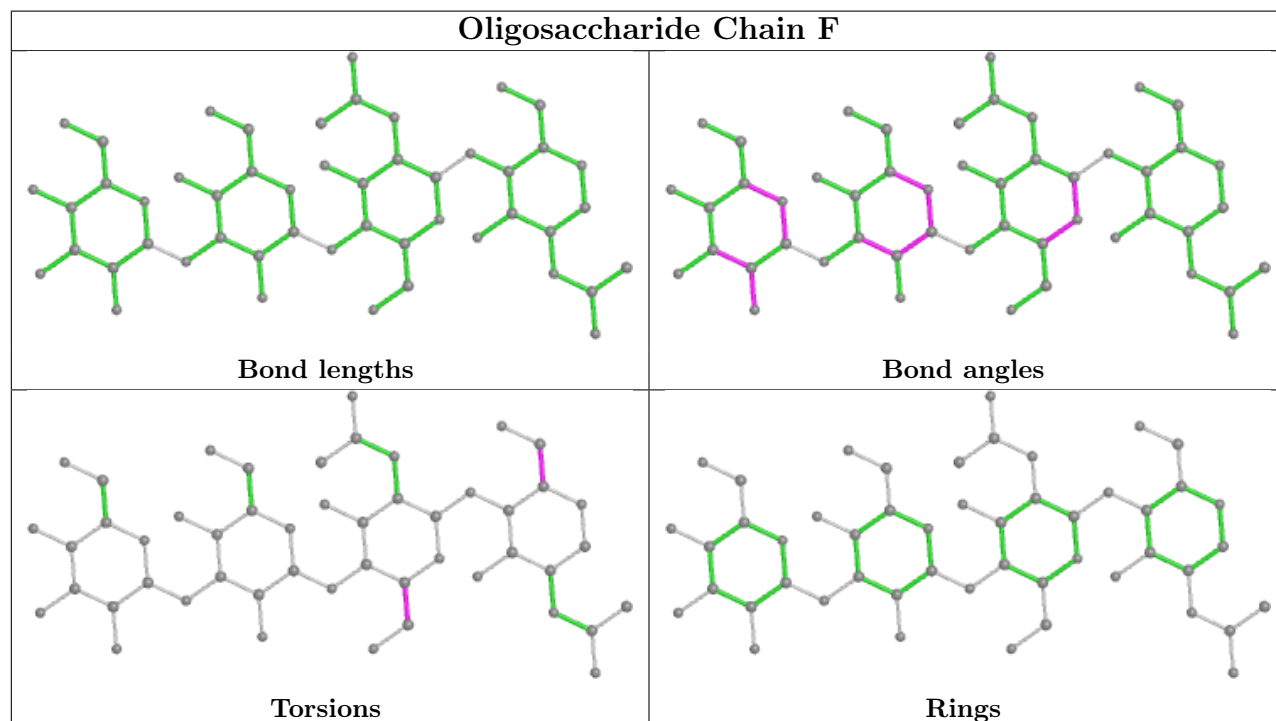
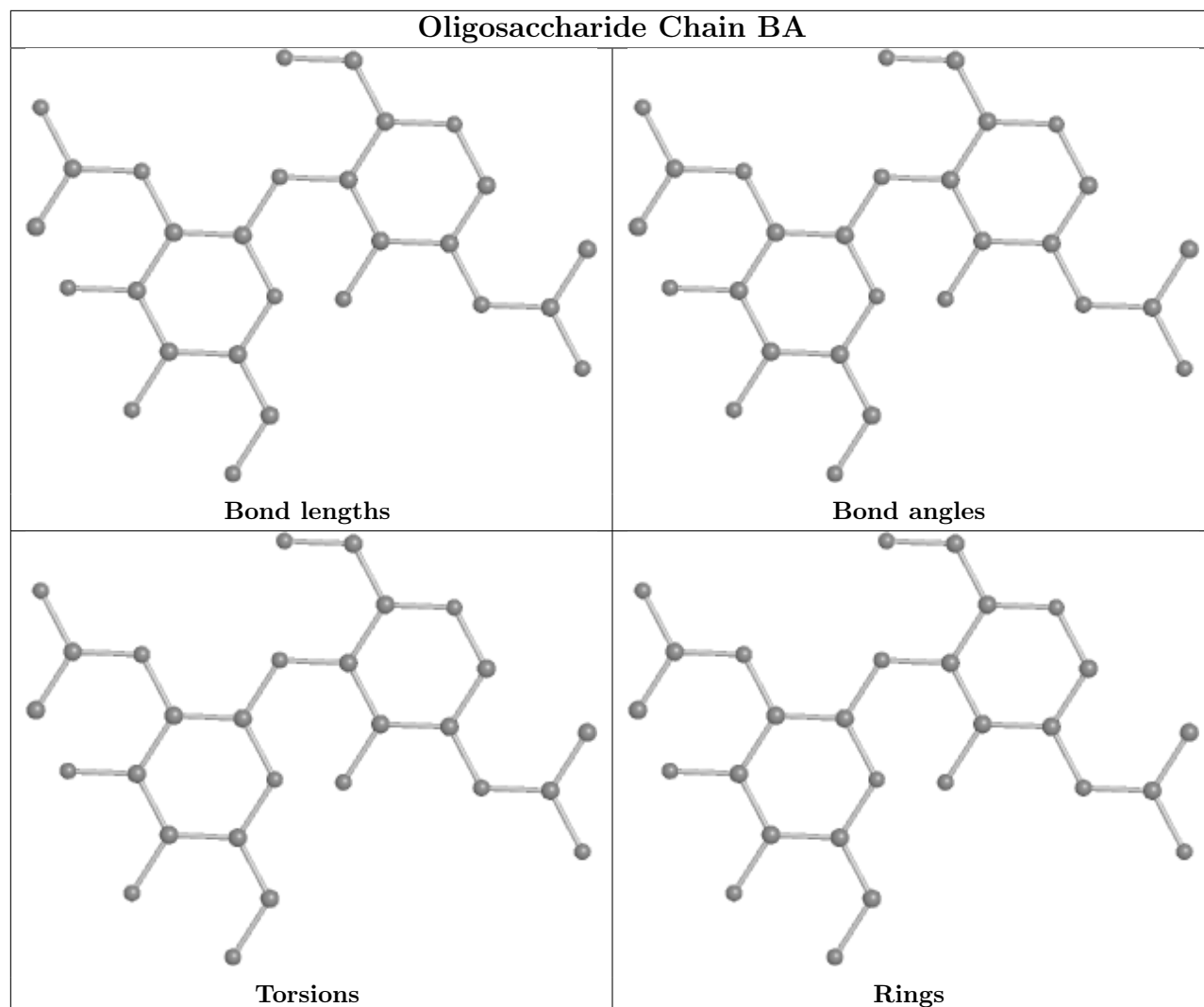


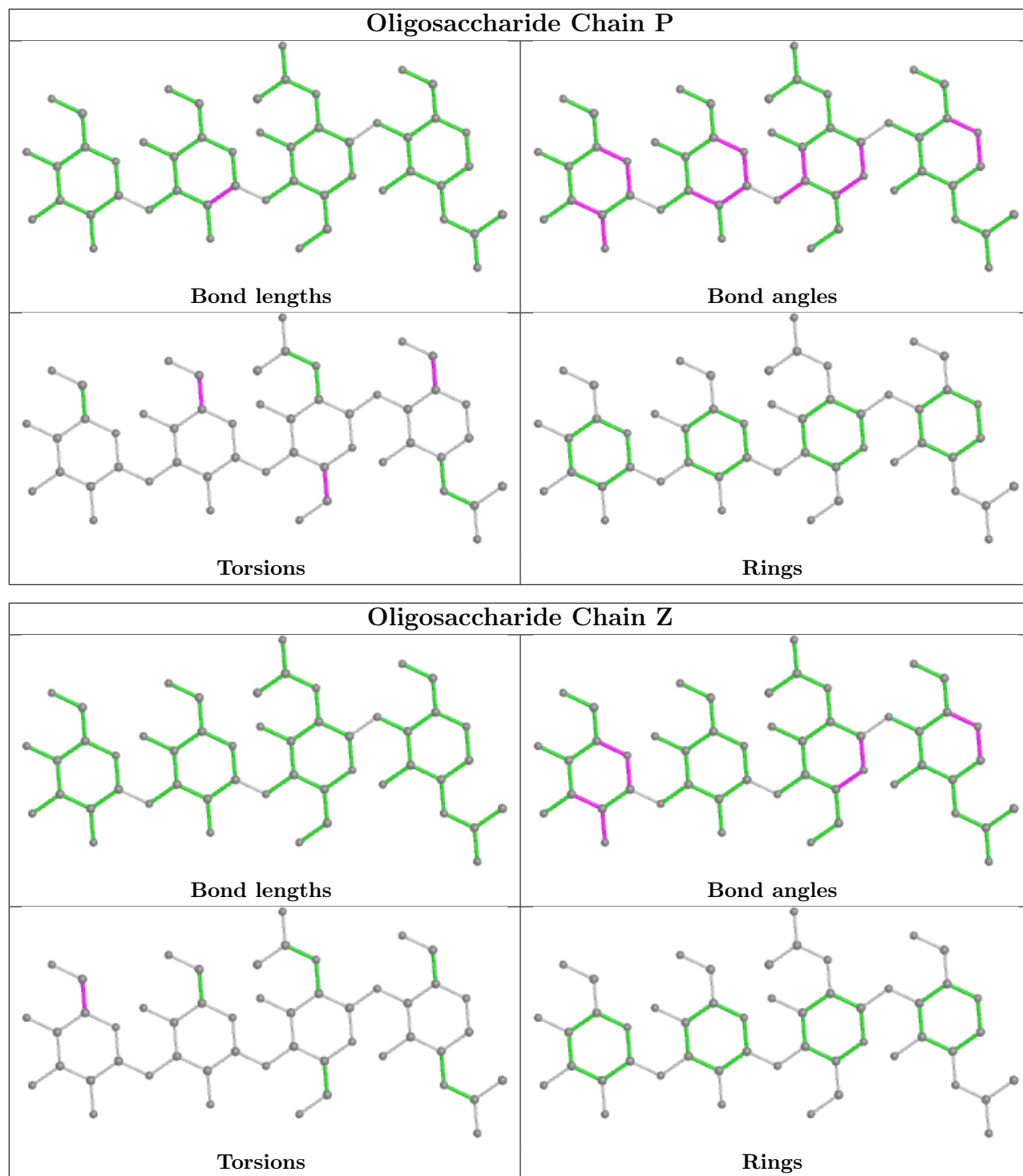


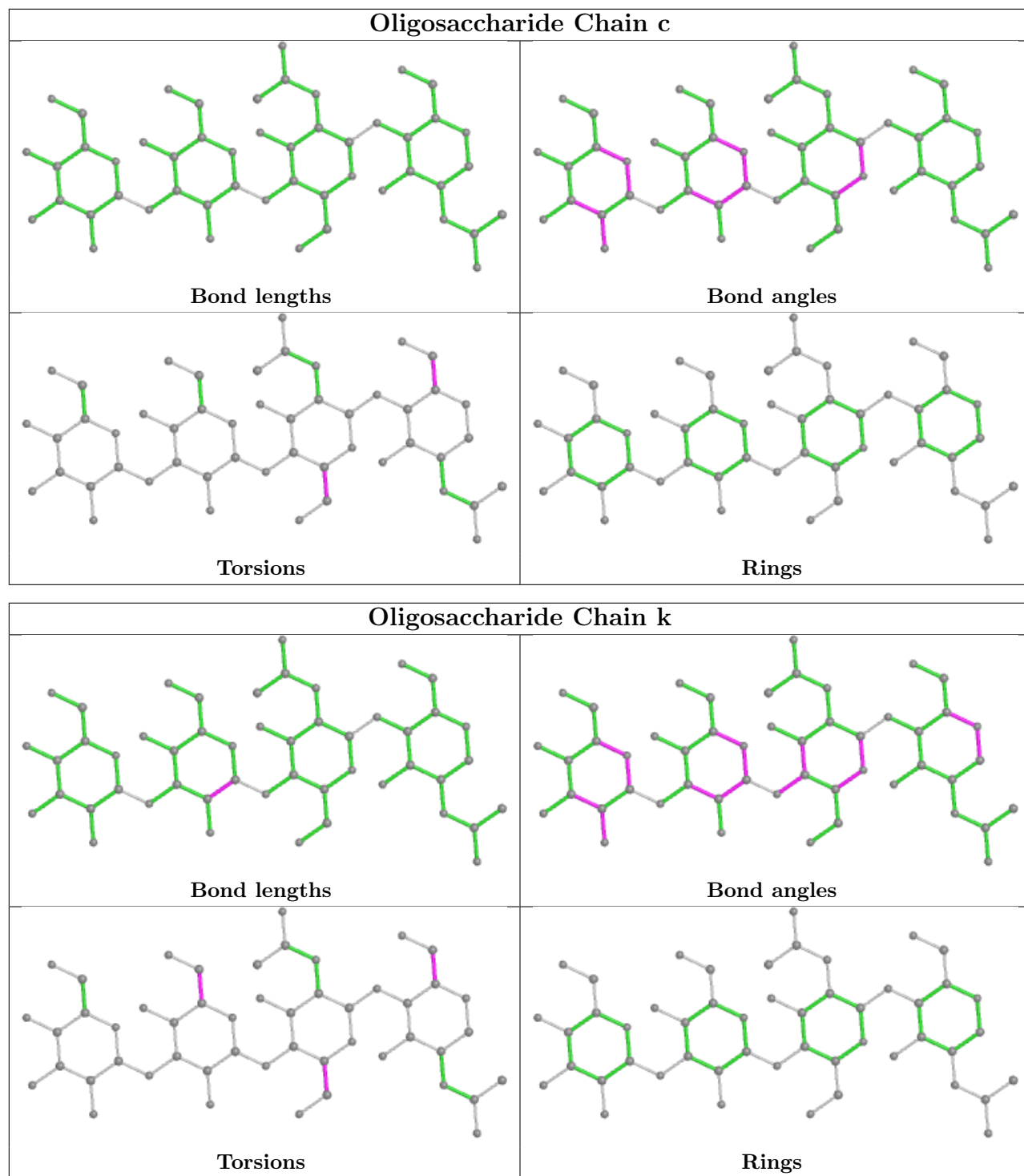


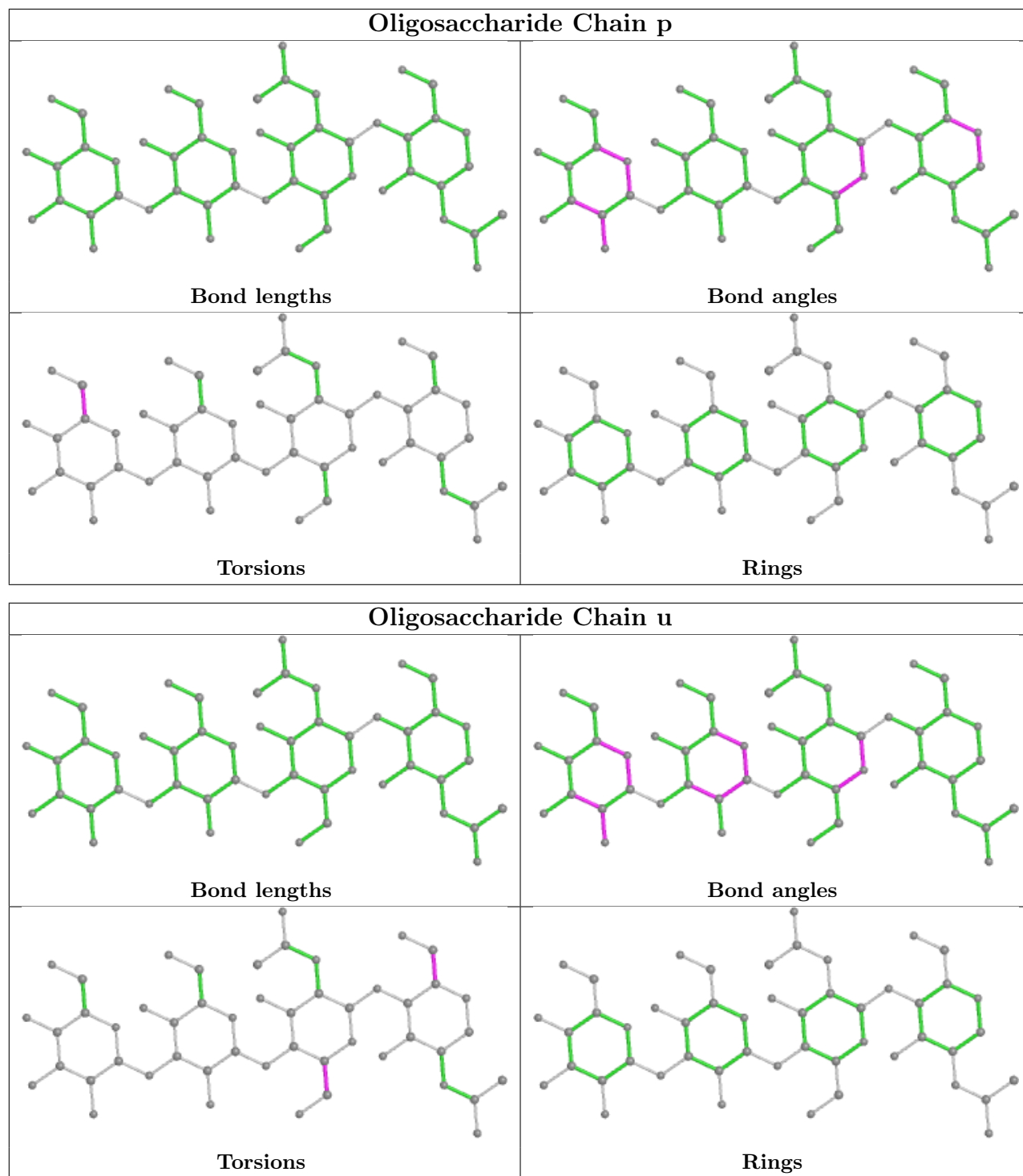


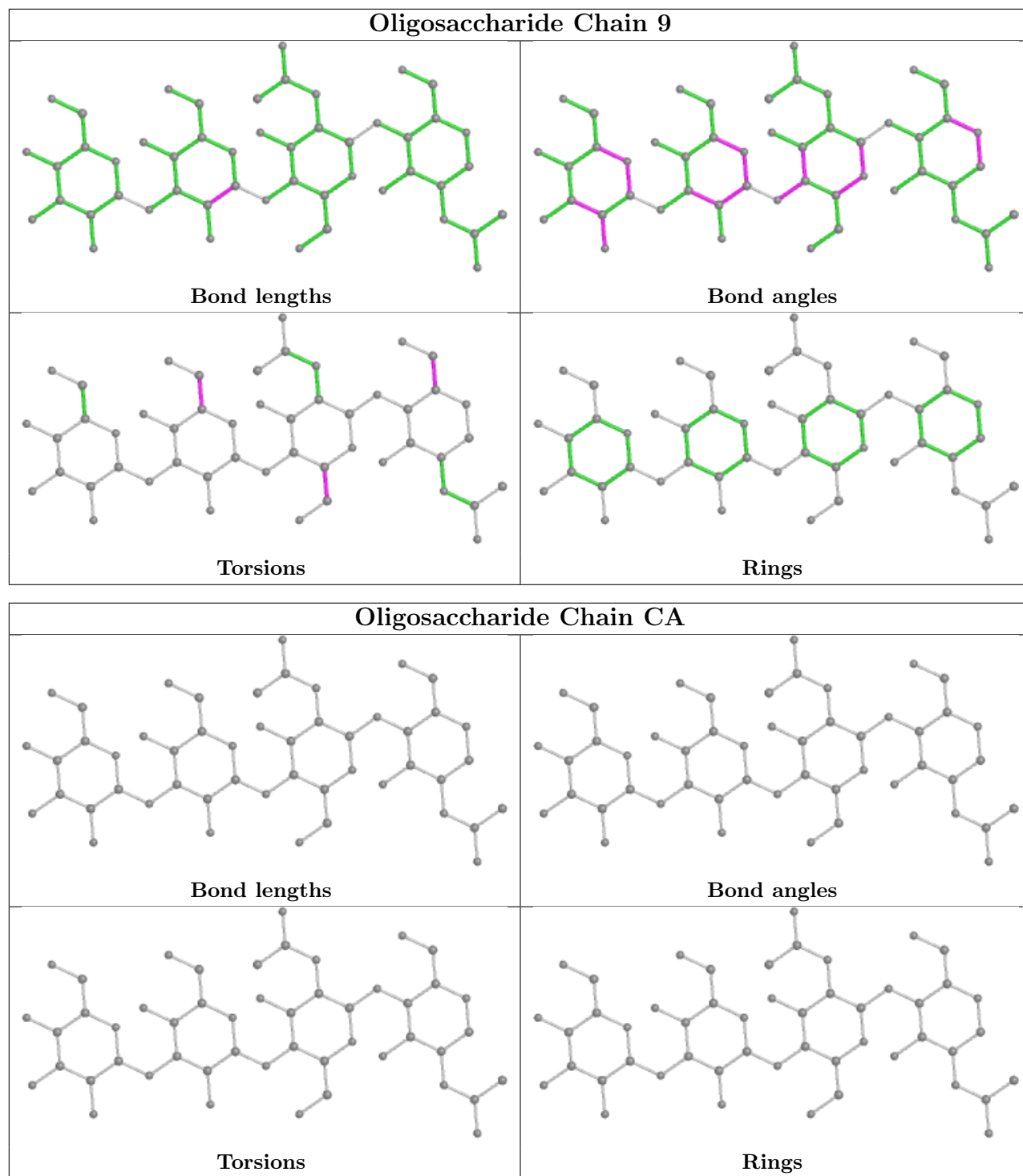


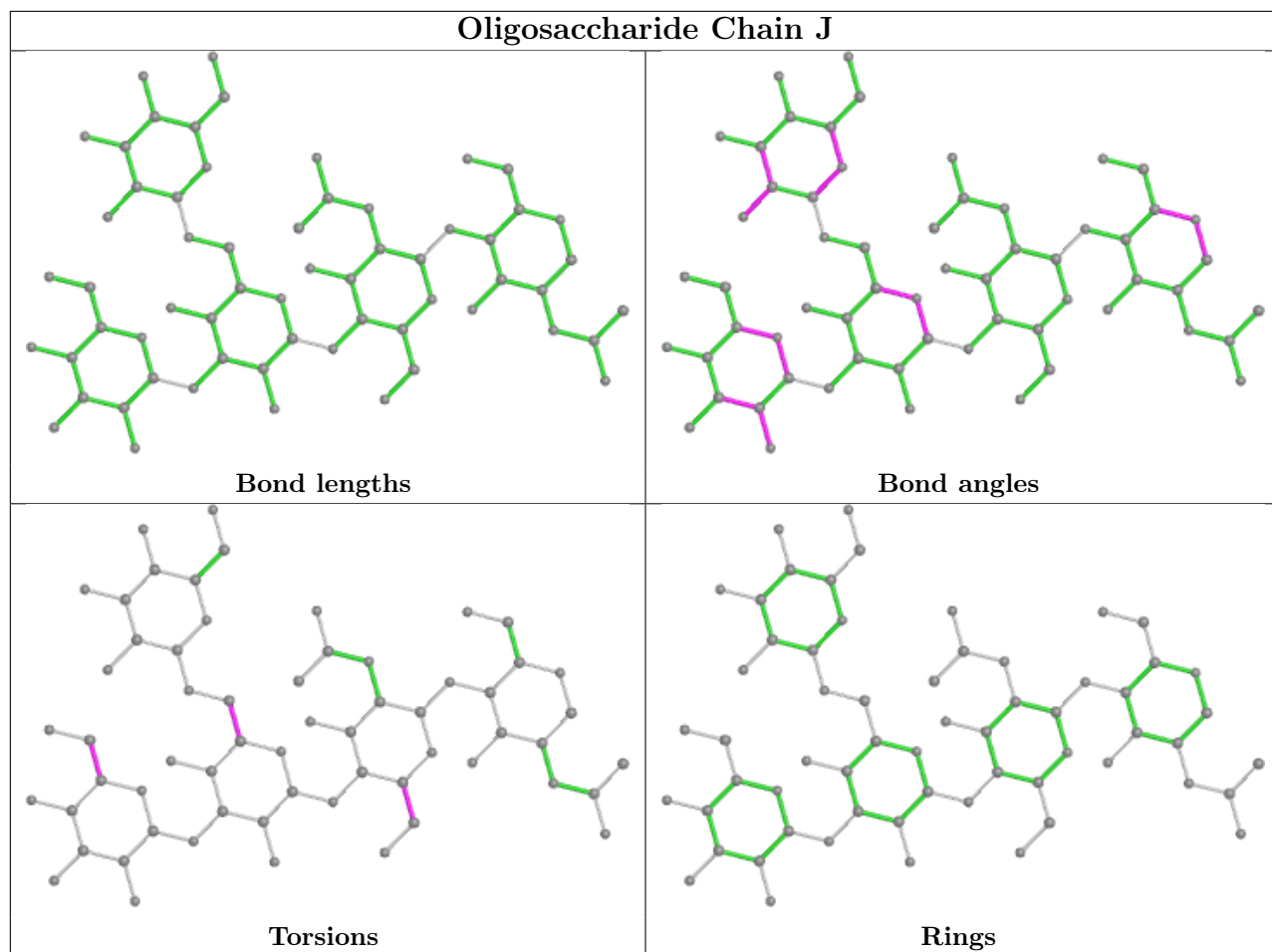


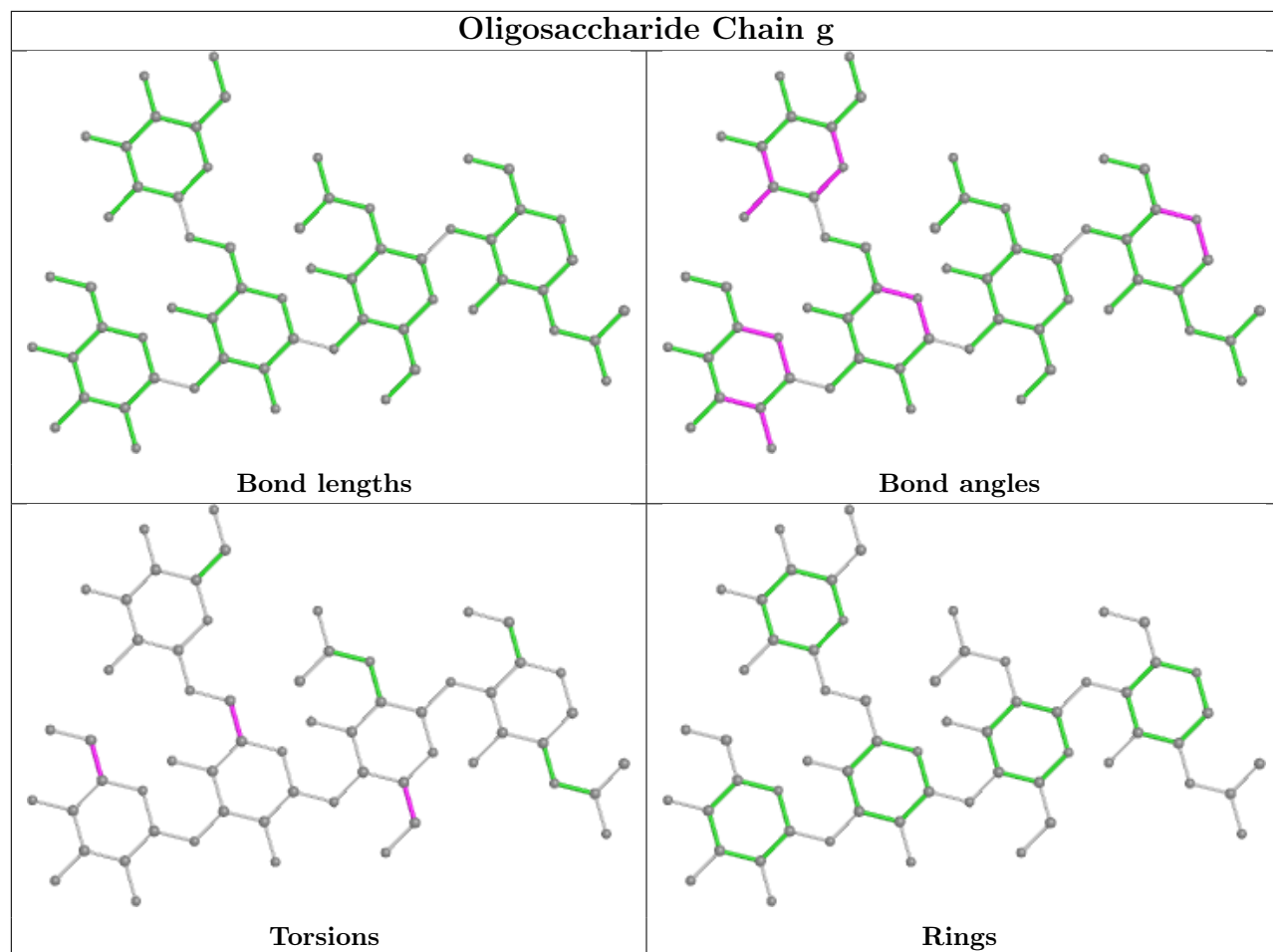




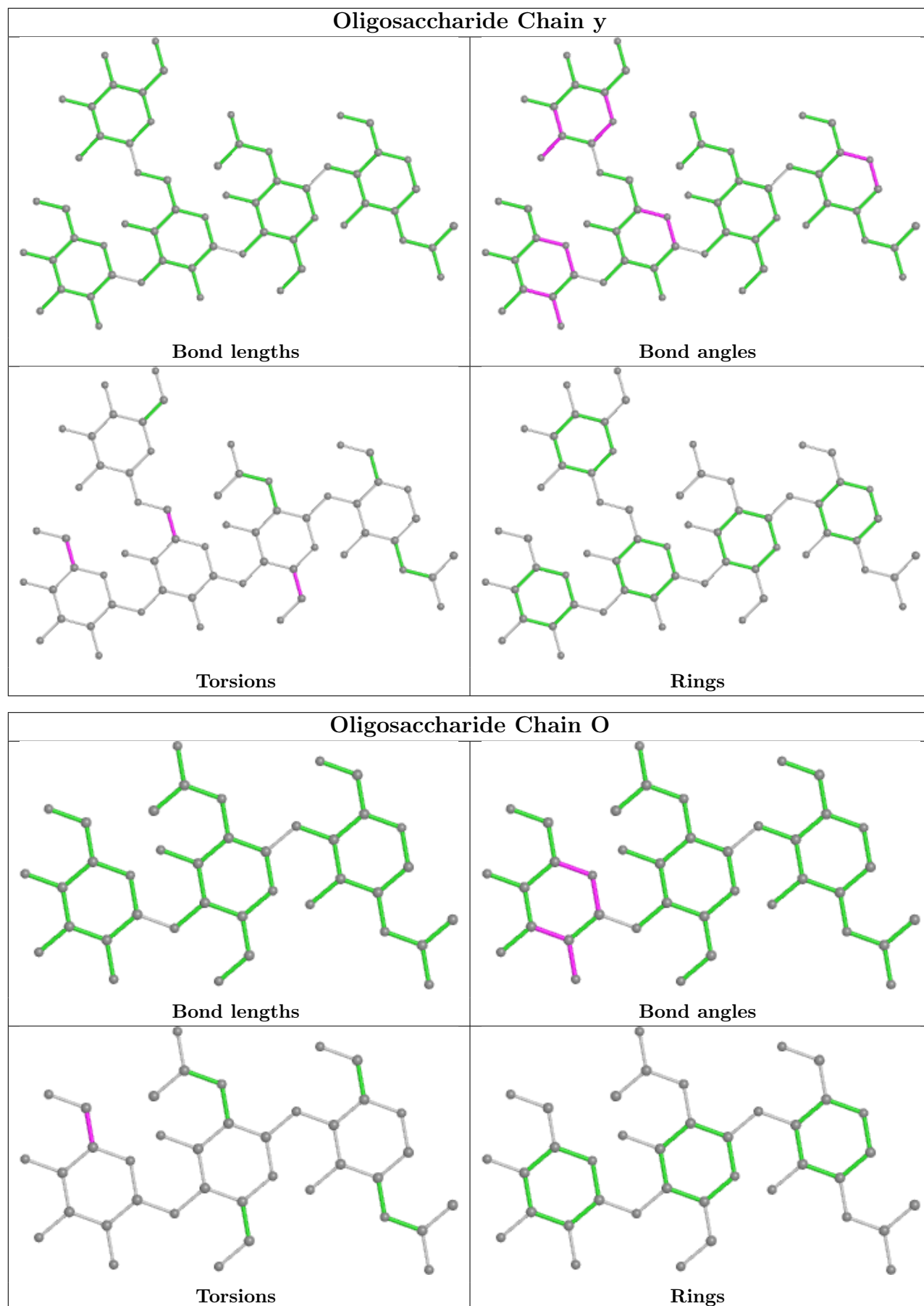


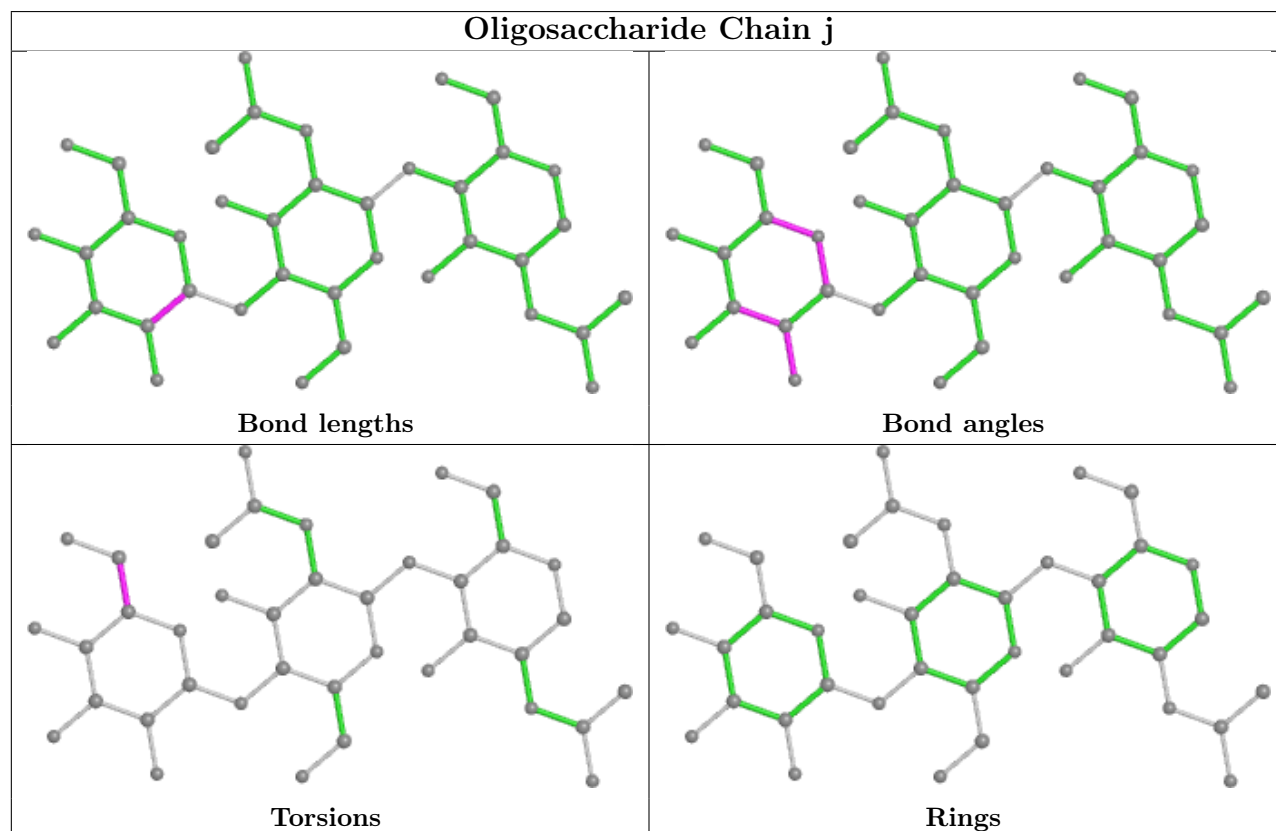
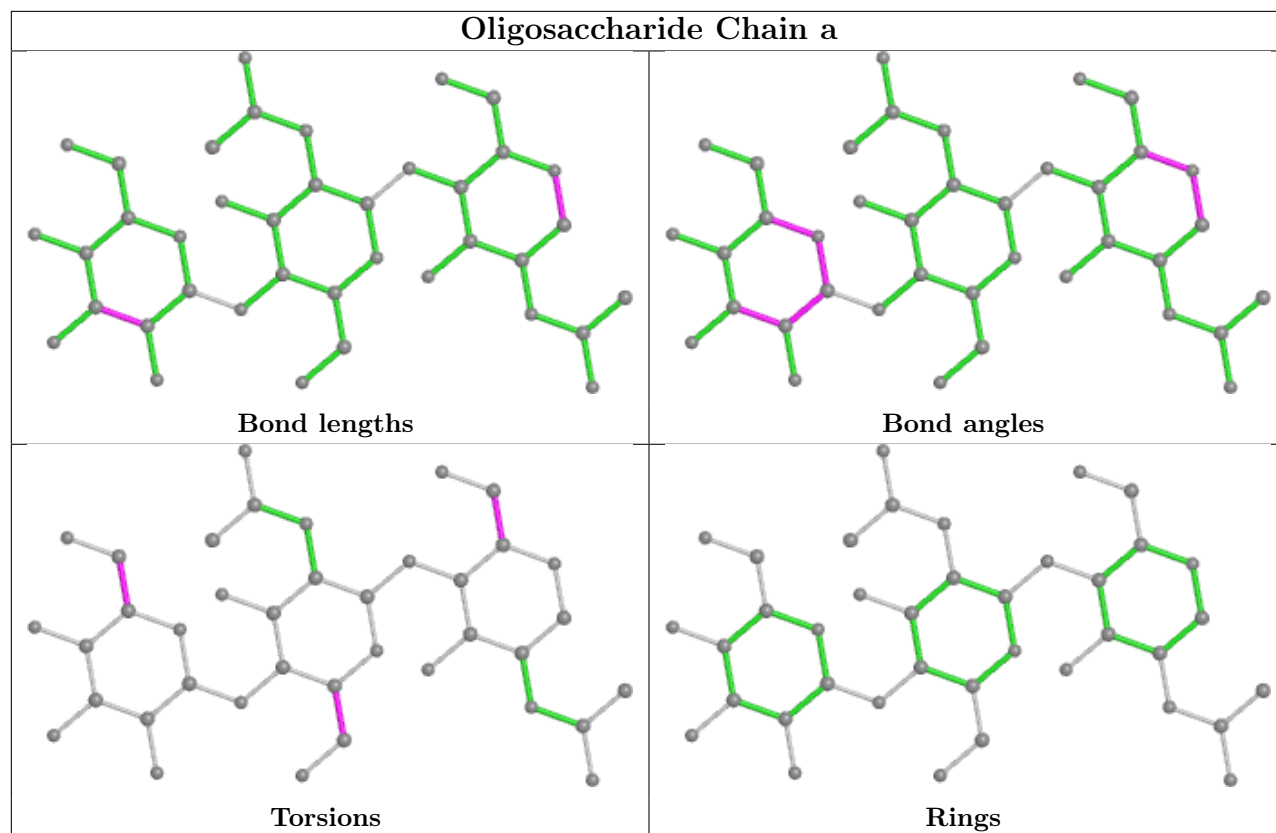


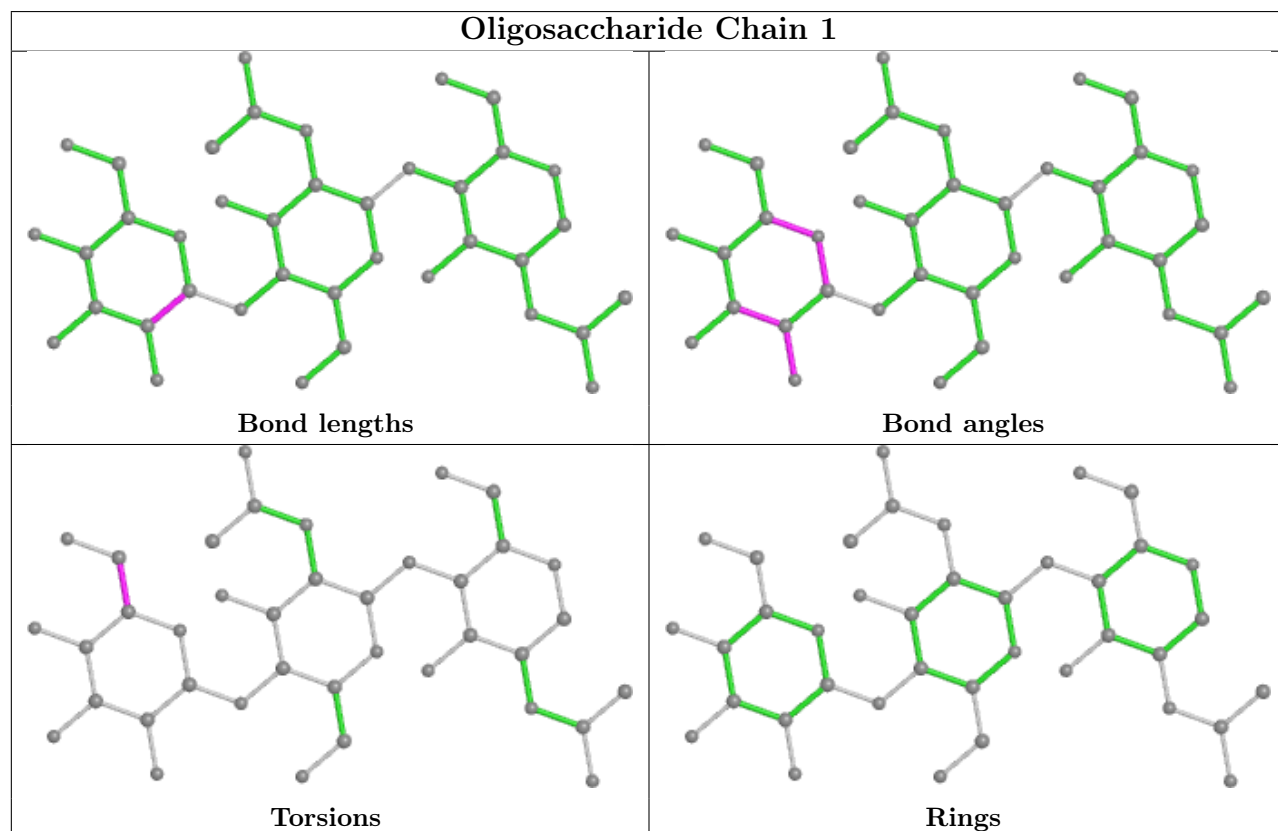
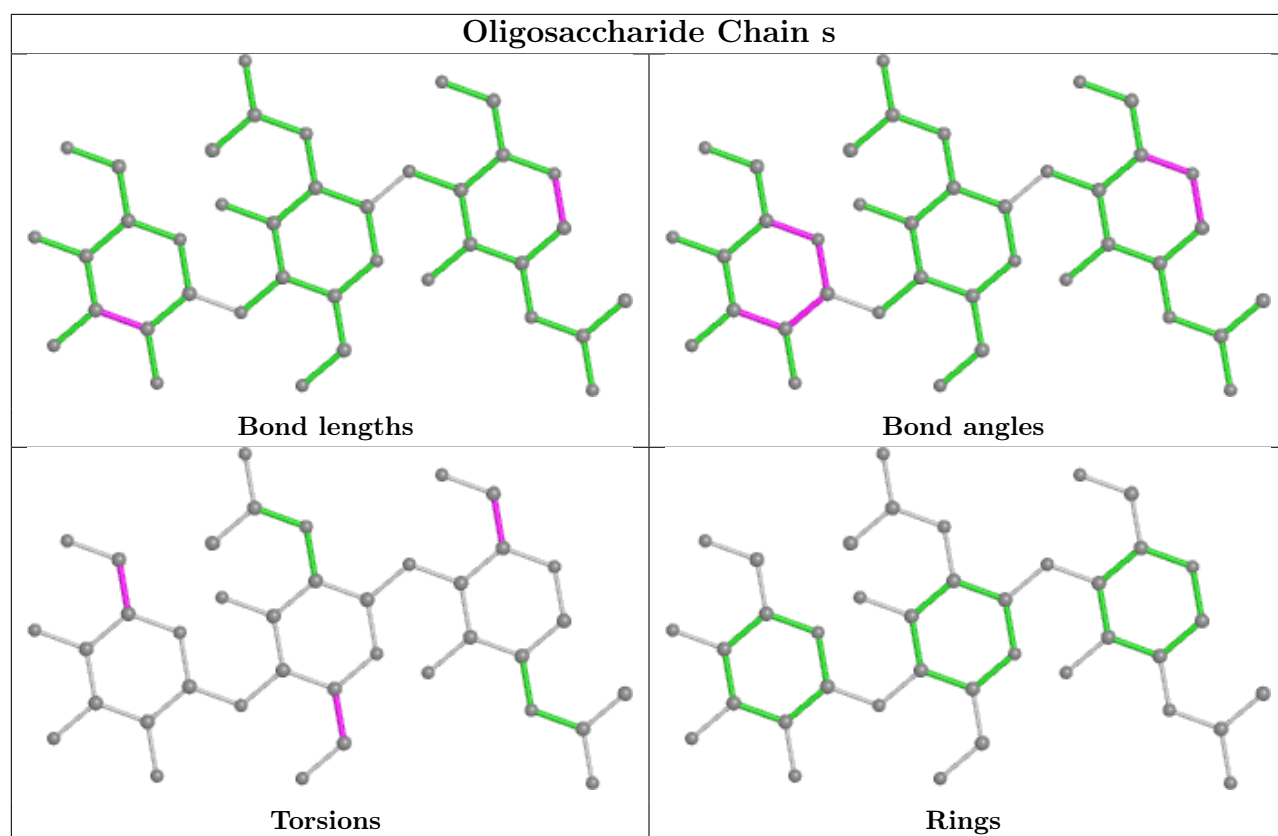


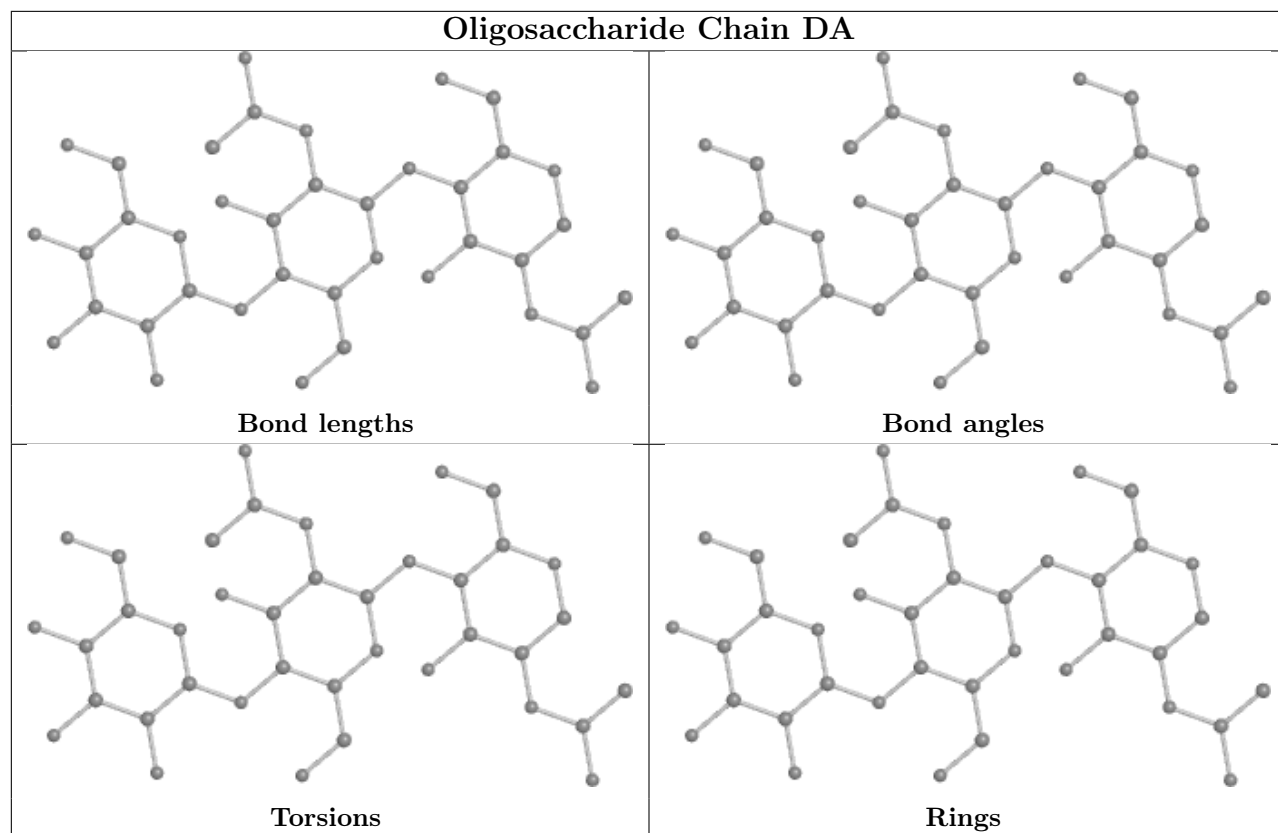


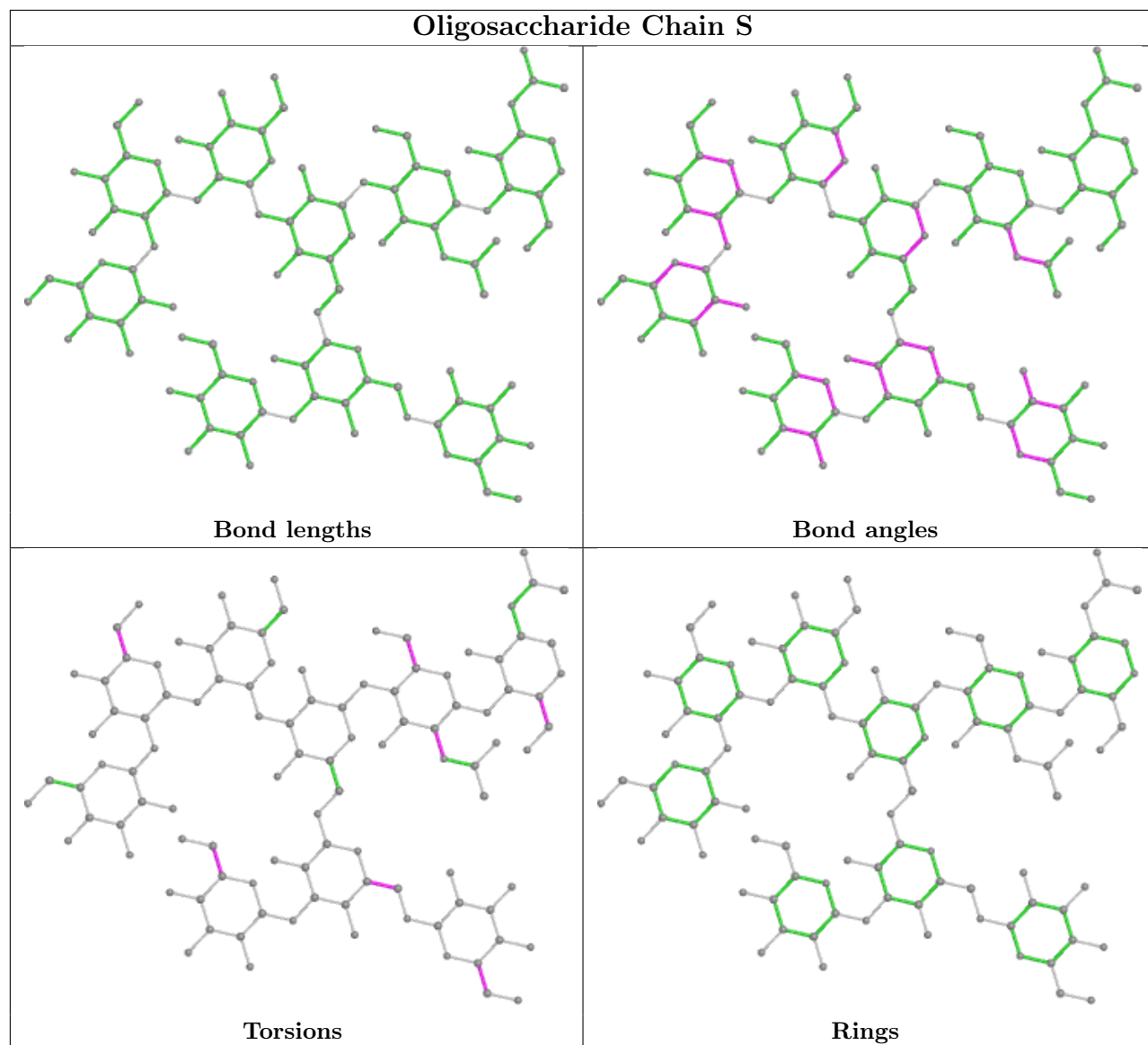


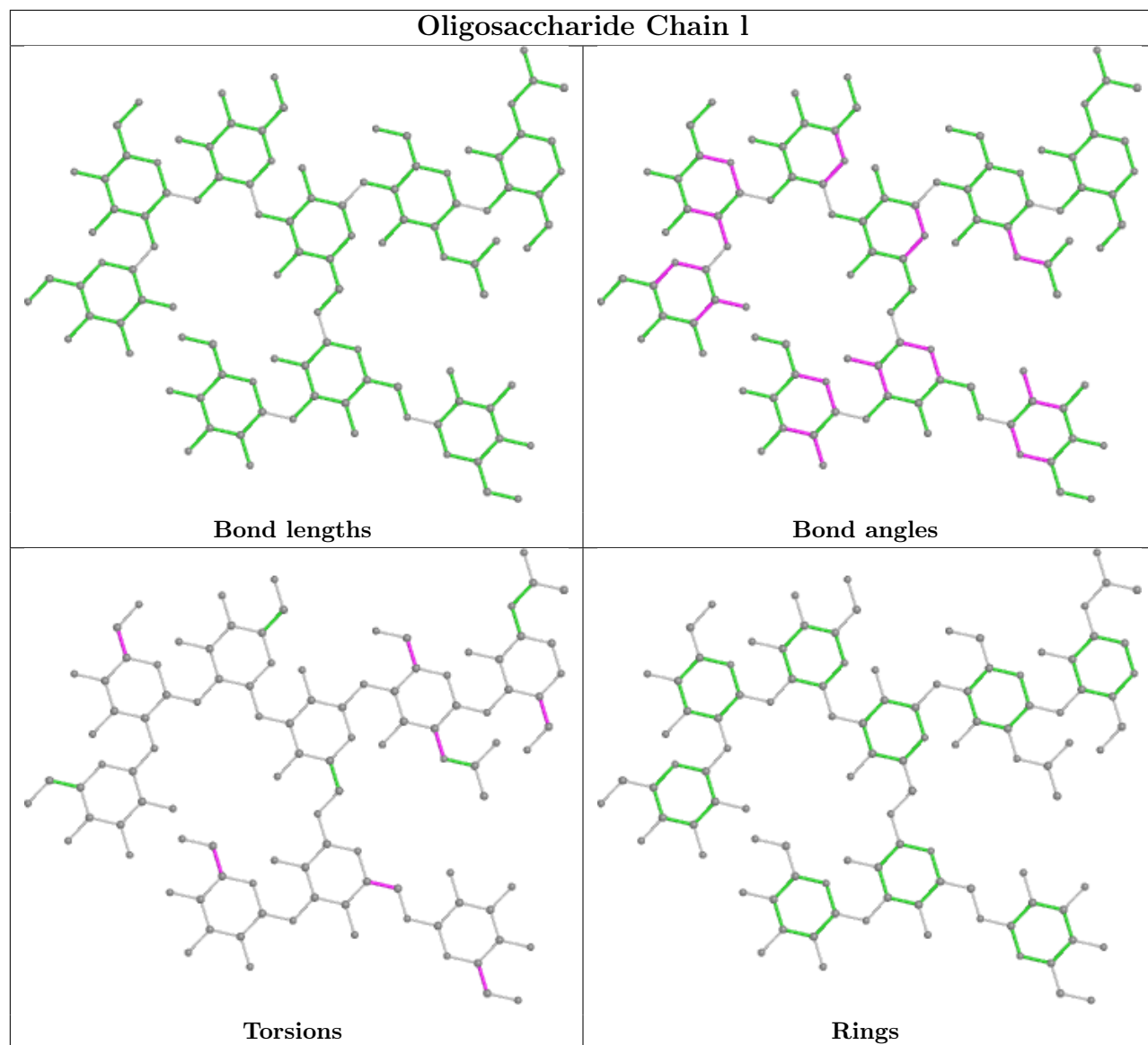


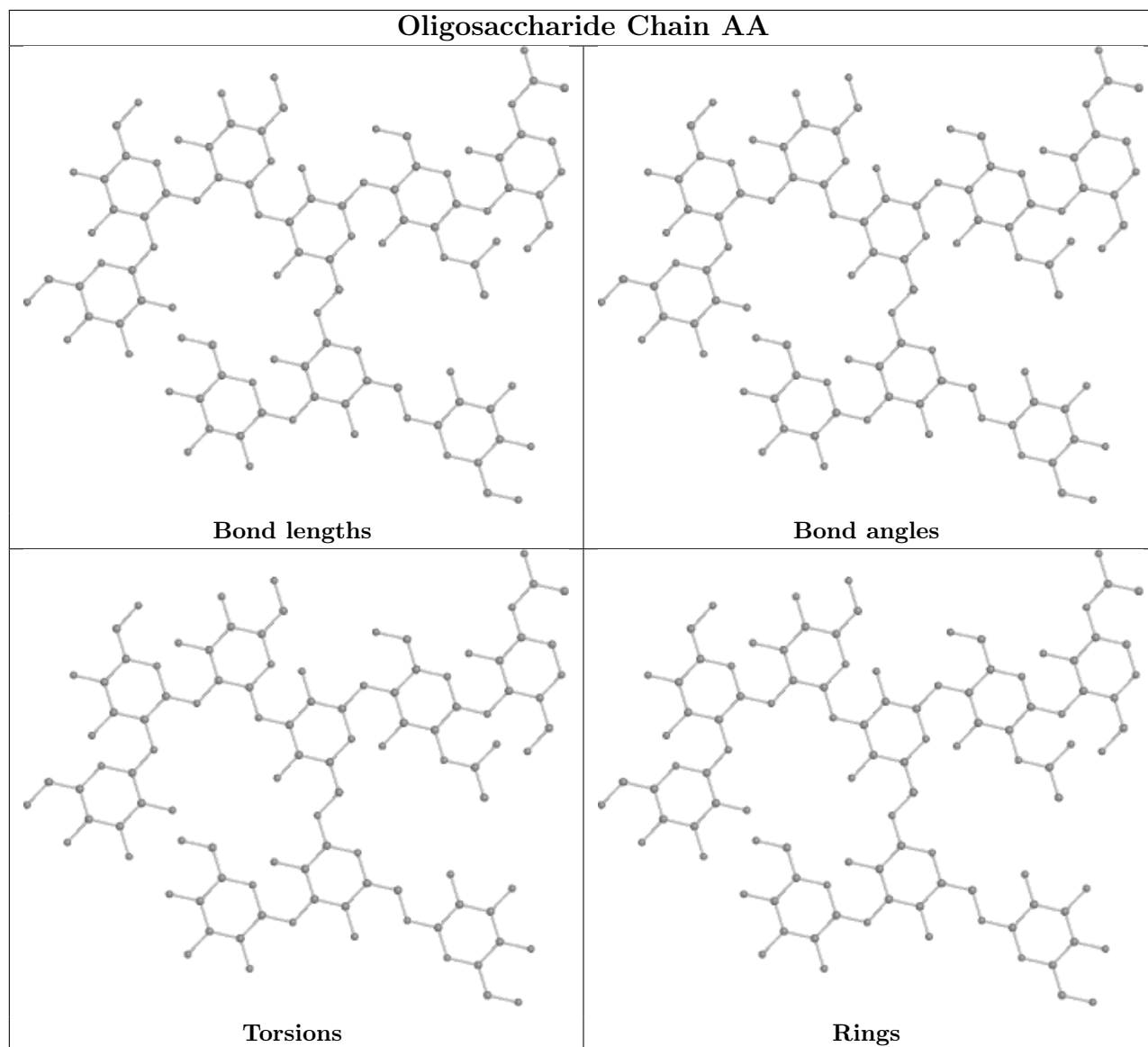












## 5.6 Ligand geometry [i](#)

12 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
14	NAG	C	631	3	14,14,15	0.42	0	17,19,21	0.76	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	NAG	V	623	3	14,14,15	0.26	0	17,19,21	0.39	0
14	NAG	C	611	3	14,14,15	0.30	0	17,19,21	0.49	0
14	NAG	2	611	3	14,14,15	0.30	0	17,19,21	0.49	0
14	NAG	U	701	2	14,14,15	0.63	0	17,19,21	0.82	1 (5%)
14	NAG	2	623	3	14,14,15	0.26	0	17,19,21	0.39	0
14	NAG	V	631	3	14,14,15	0.42	0	17,19,21	0.75	1 (5%)
14	NAG	2	631	3	14,14,15	0.41	0	17,19,21	0.75	1 (5%)
14	NAG	C	623	3	14,14,15	0.26	0	17,19,21	0.39	0
14	NAG	D	701	2	14,14,15	0.63	0	17,19,21	0.81	1 (5%)
14	NAG	V	611	3	14,14,15	0.30	0	17,19,21	0.49	0
14	NAG	A	701	2	14,14,15	0.64	0	17,19,21	0.81	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
14	NAG	C	631	3	-	2/6/23/26	0/1/1/1
14	NAG	V	623	3	-	2/6/23/26	0/1/1/1
14	NAG	C	611	3	-	0/6/23/26	0/1/1/1
14	NAG	2	611	3	-	0/6/23/26	0/1/1/1
14	NAG	U	701	2	-	0/6/23/26	0/1/1/1
14	NAG	2	623	3	-	2/6/23/26	0/1/1/1
14	NAG	V	631	3	-	2/6/23/26	0/1/1/1
14	NAG	2	631	3	-	2/6/23/26	0/1/1/1
14	NAG	C	623	3	-	2/6/23/26	0/1/1/1
14	NAG	D	701	2	-	0/6/23/26	0/1/1/1
14	NAG	V	611	3	-	0/6/23/26	0/1/1/1
14	NAG	A	701	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	U	701	NAG	C1-O5-C5	2.90	116.12	112.19
14	D	701	NAG	C1-O5-C5	2.89	116.11	112.19
14	A	701	NAG	C1-O5-C5	2.88	116.09	112.19
14	C	631	NAG	C1-O5-C5	2.61	115.73	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	V	631	NAG	C1-O5-C5	2.60	115.71	112.19
14	2	631	NAG	C1-O5-C5	2.59	115.70	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	V	623	NAG	O5-C5-C6-O6
14	2	623	NAG	O5-C5-C6-O6
14	C	623	NAG	O5-C5-C6-O6
14	V	623	NAG	C4-C5-C6-O6
14	2	623	NAG	C4-C5-C6-O6
14	C	623	NAG	C4-C5-C6-O6
14	V	631	NAG	O5-C5-C6-O6
14	2	631	NAG	O5-C5-C6-O6
14	C	631	NAG	O5-C5-C6-O6
14	V	631	NAG	C4-C5-C6-O6
14	2	631	NAG	C4-C5-C6-O6
14	C	631	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.

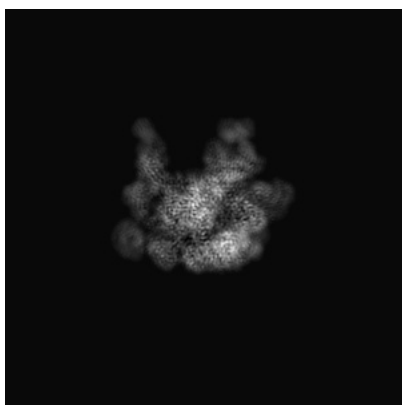
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8977. These allow visual inspection of the internal detail of the map and identification of artifacts.

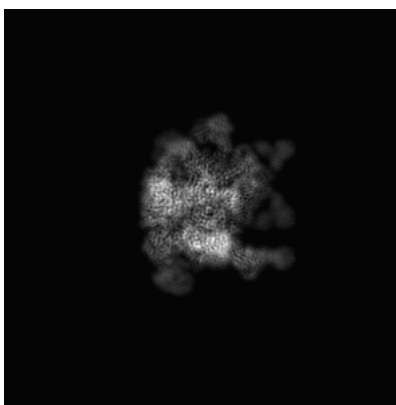
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

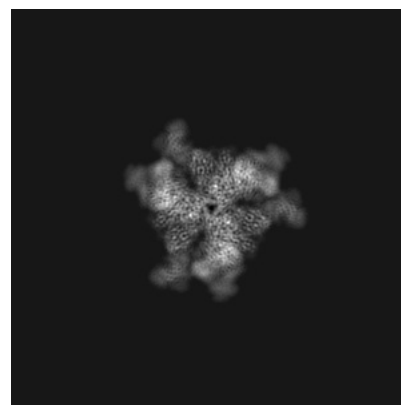
#### 6.1.1 Primary map



X



Y

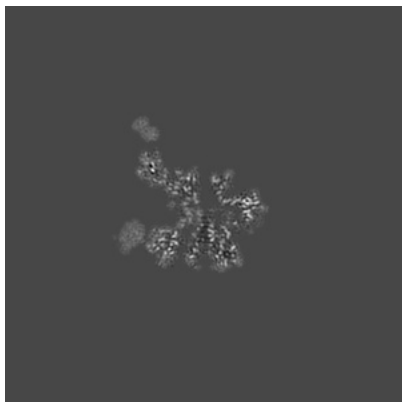


Z

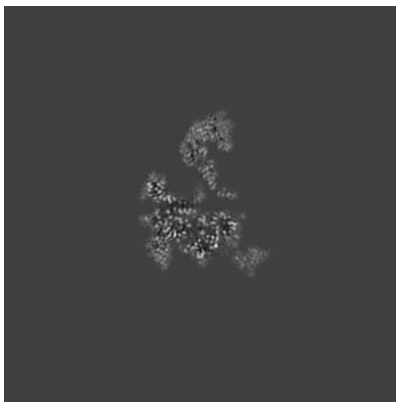
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

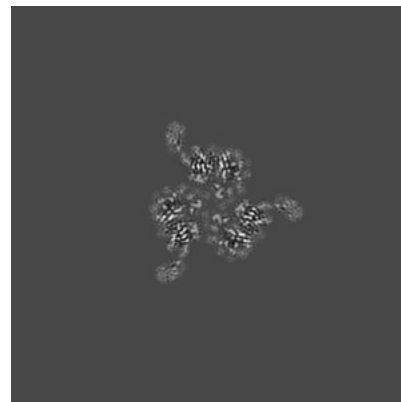
#### 6.2.1 Primary map



X Index: 192



Y Index: 192

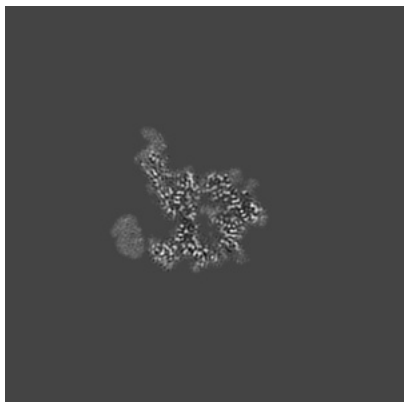


Z Index: 192

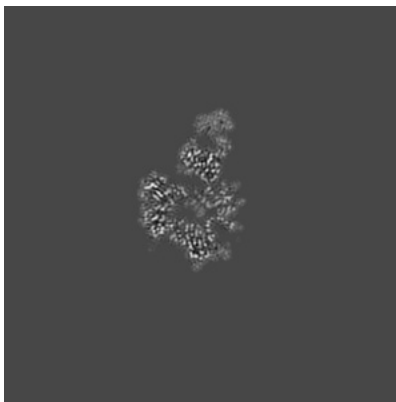
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

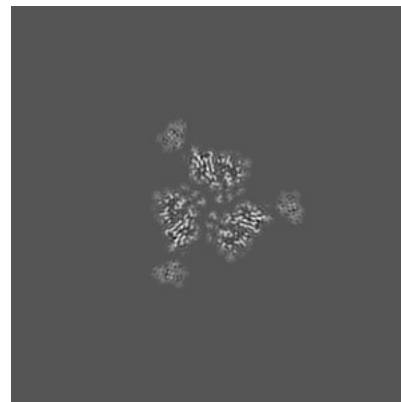
### 6.3.1 Primary map



X Index: 205



Y Index: 183

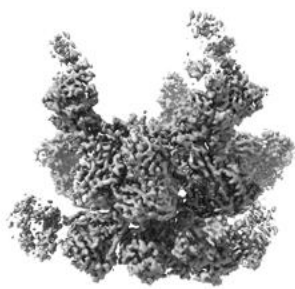


Z Index: 195

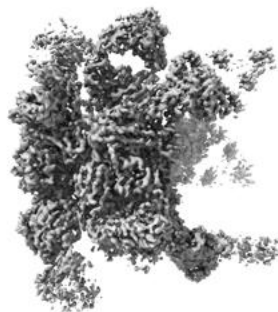
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

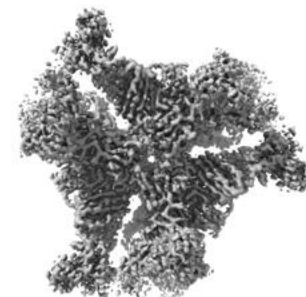
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

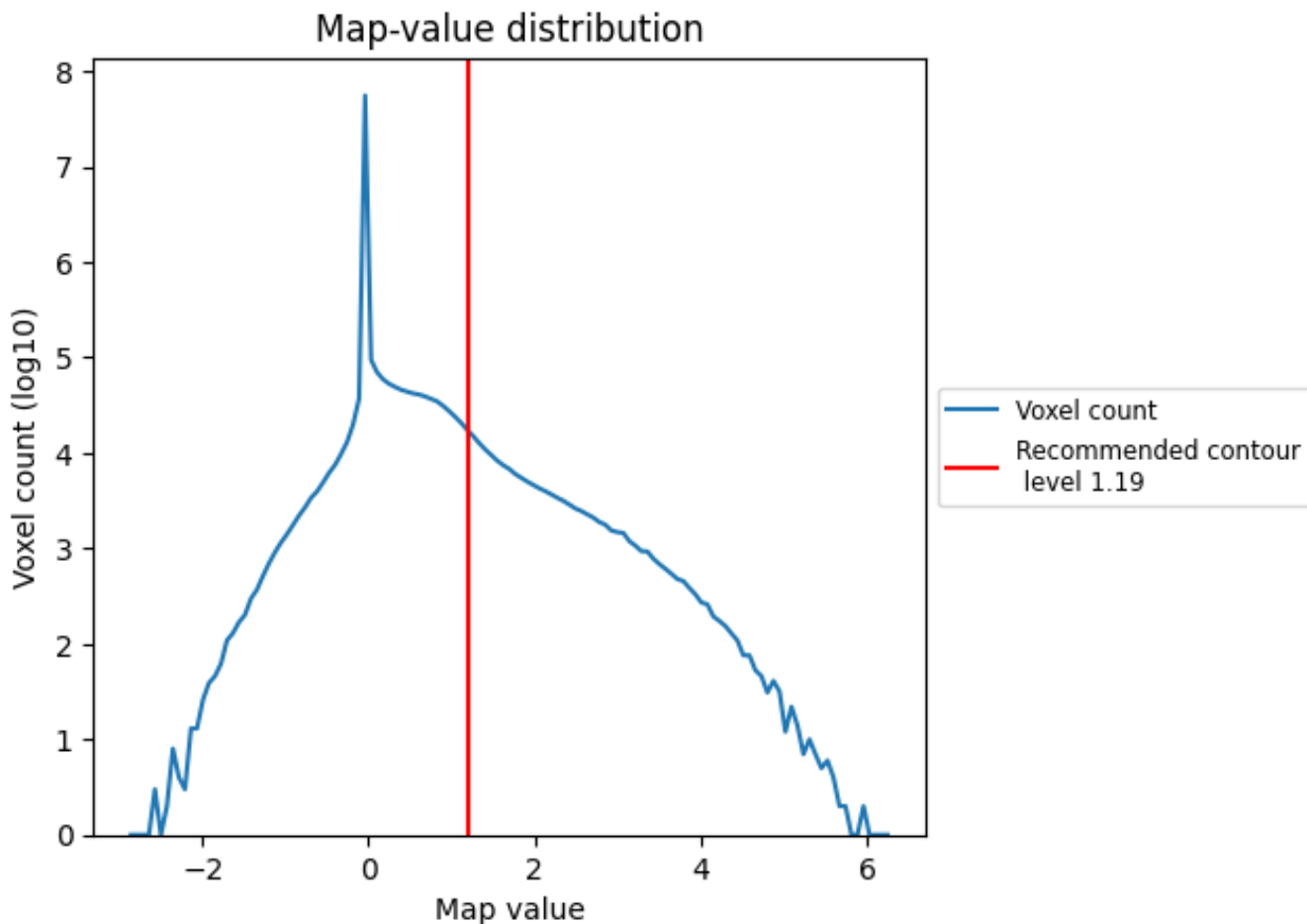
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

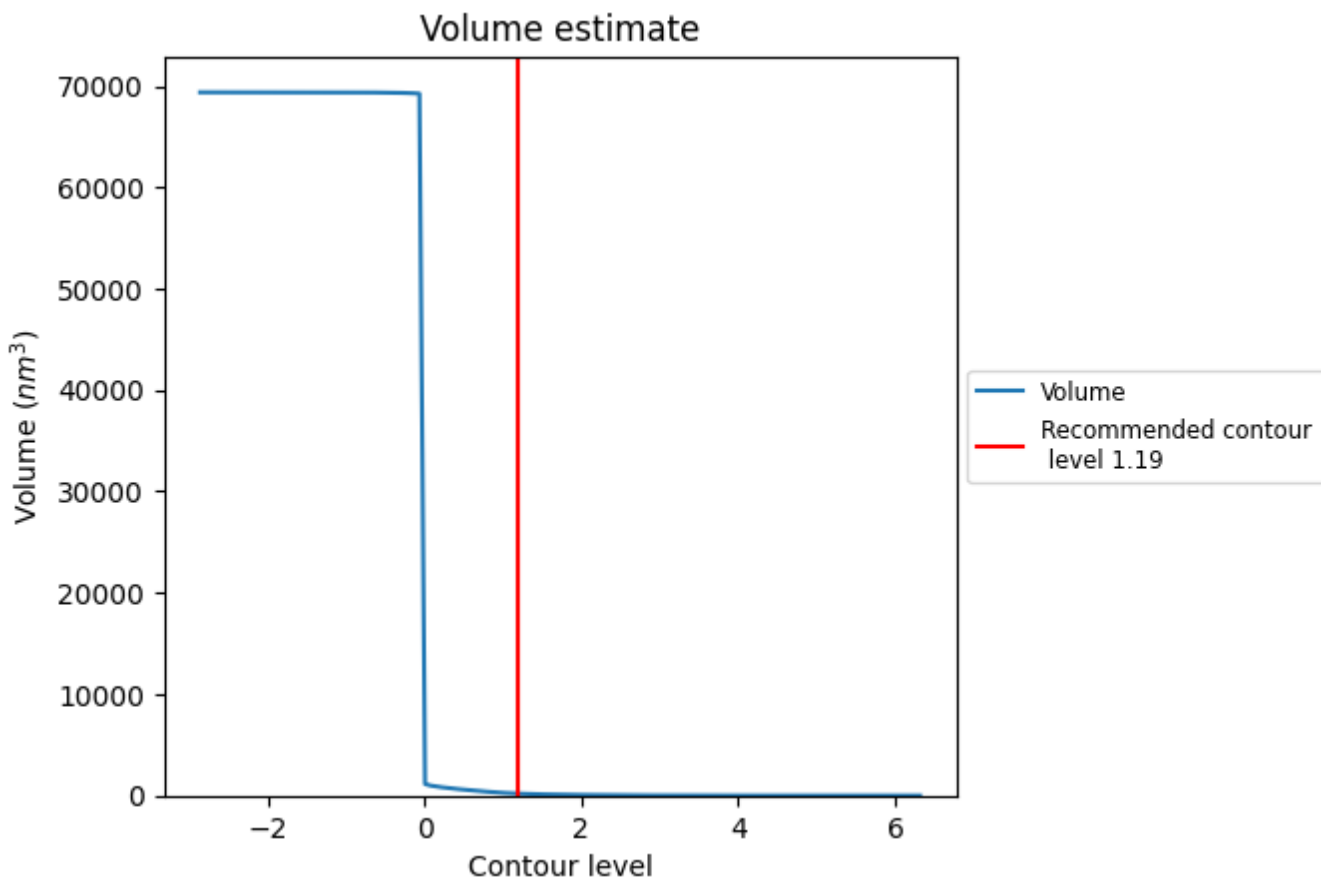
This section contains the results of statistical analysis of the map.

### 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.

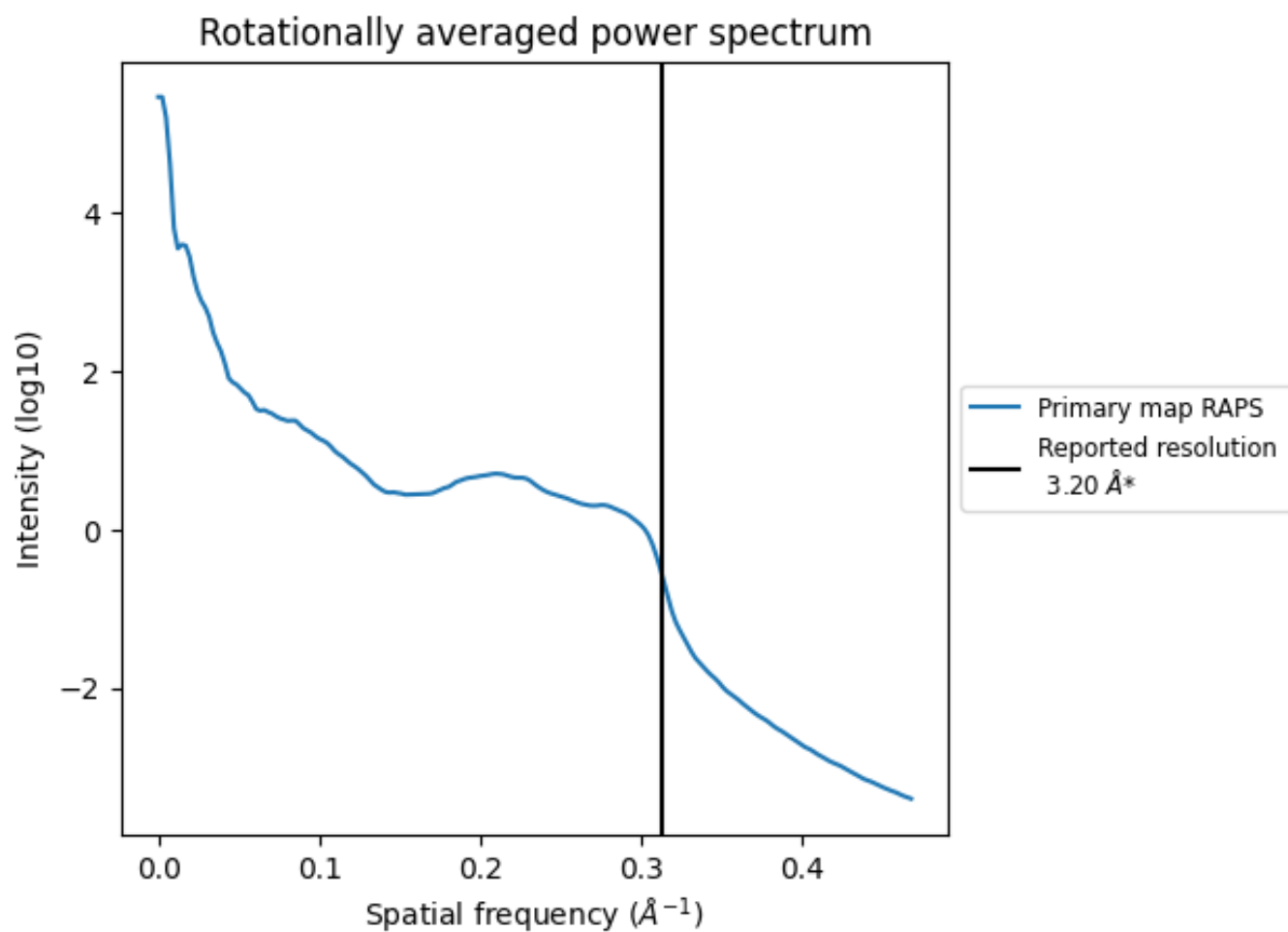
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 194 nm<sup>3</sup>; this corresponds to an approximate mass of 175 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 [i](#)

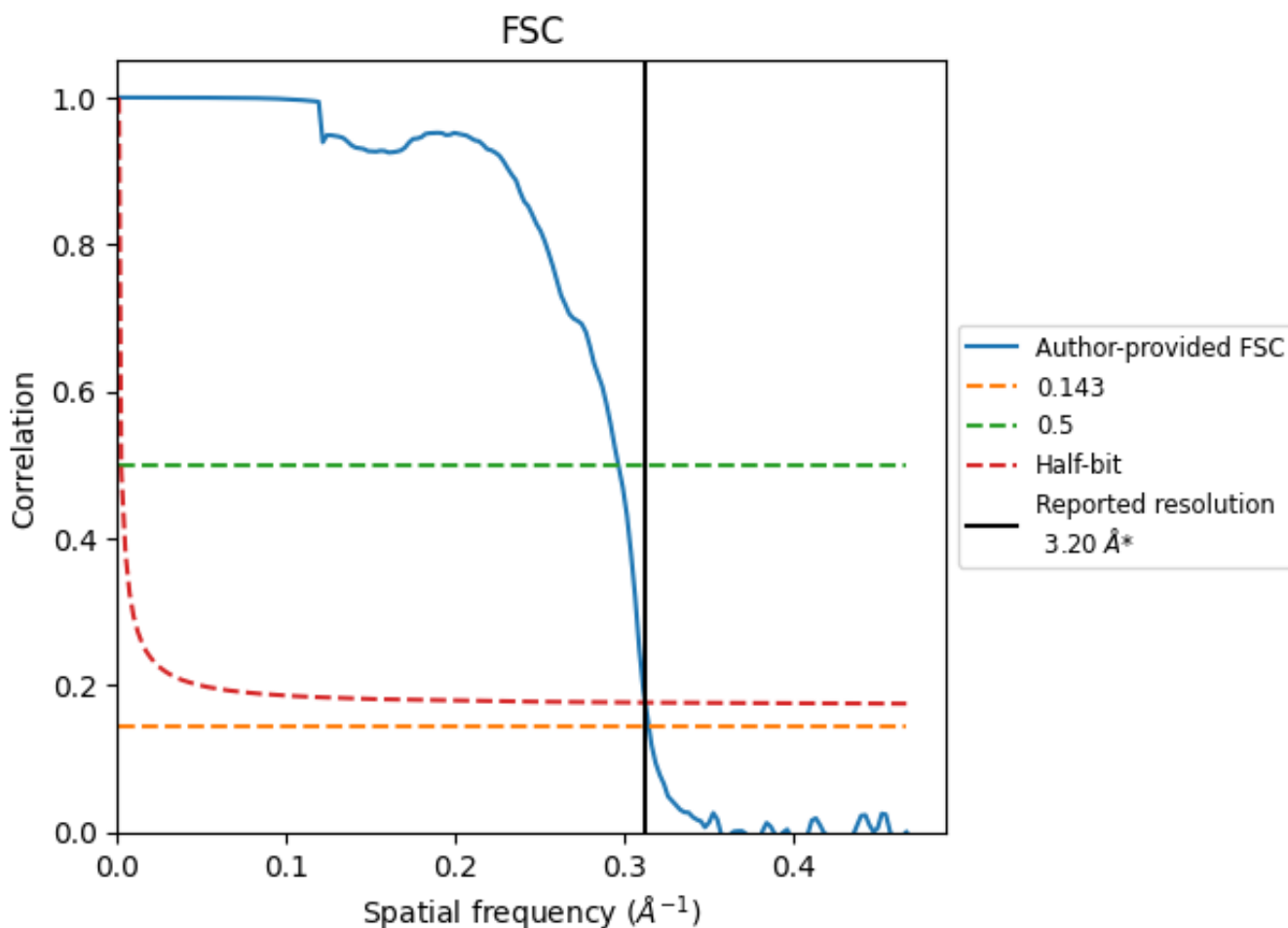


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [\(i\)](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

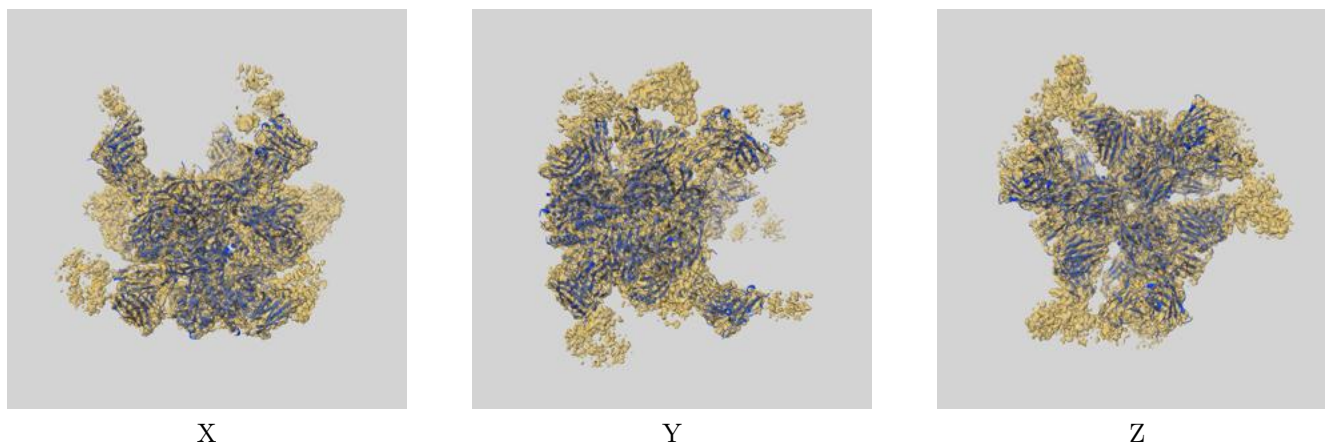
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.37	3.20
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

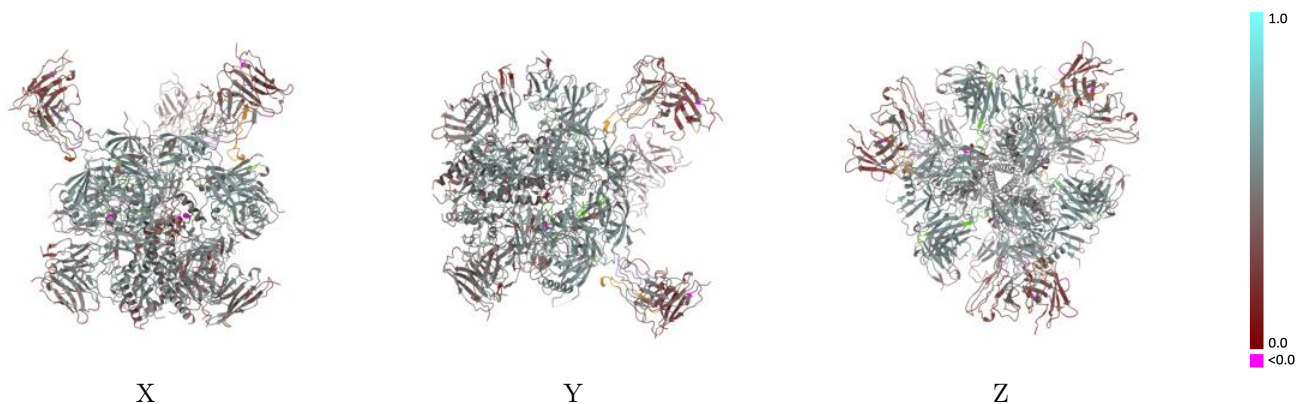
This section contains information regarding the fit between EMDB map EMD-8977 and PDB model 6MPG. Per-residue inclusion information can be found in section [3](#) on page [13](#).

### 9.1 Map-model overlay [i](#)



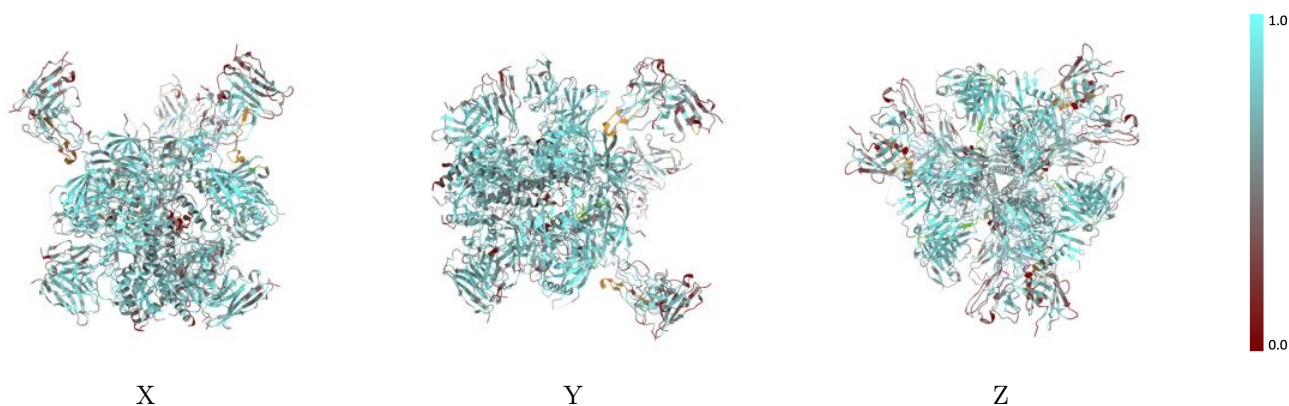
The images above show the 3D surface view of the map at the recommended contour level 1.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



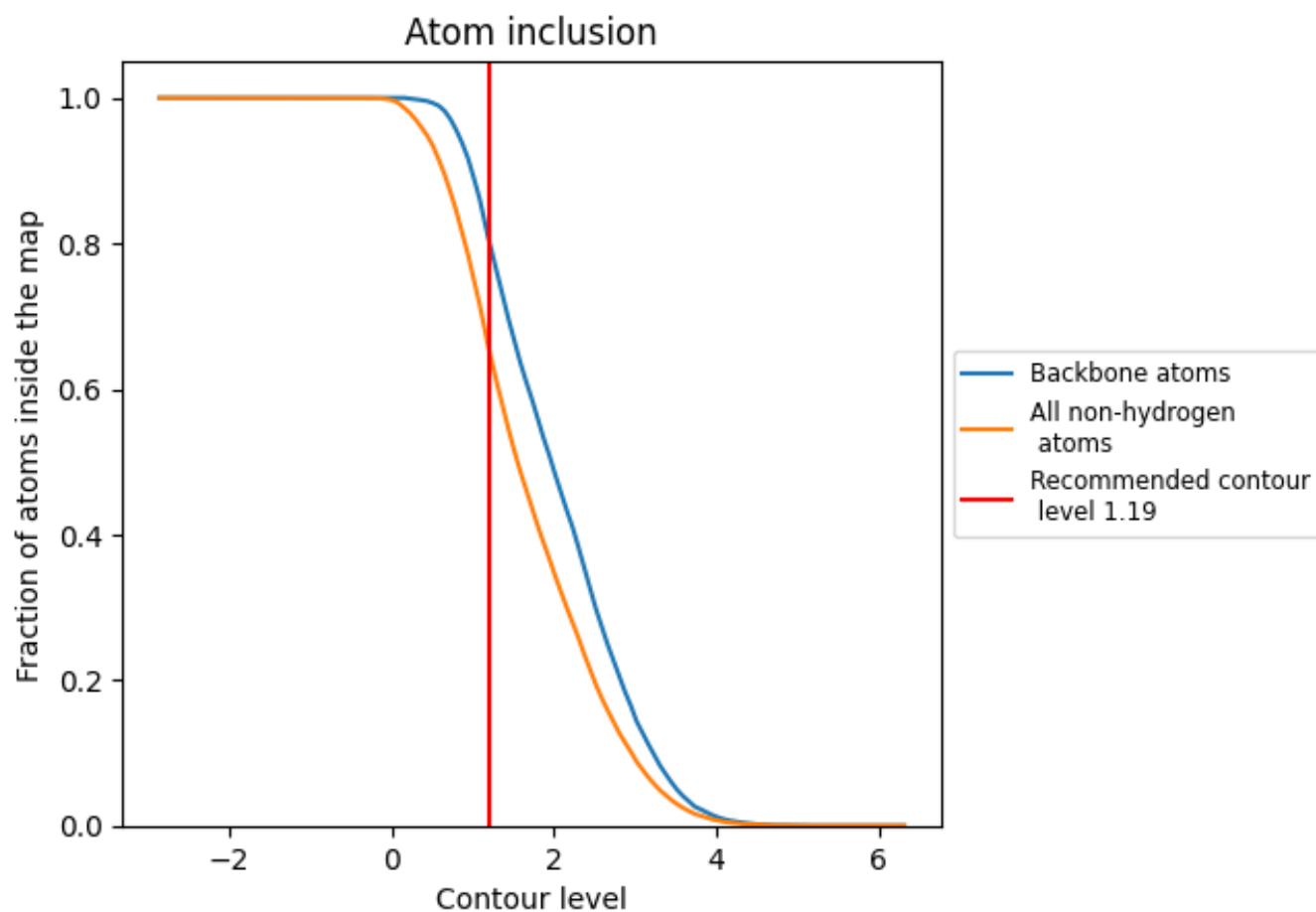
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.19).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

































































The table lists the average atom inclusion at the recommended contour level (1.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6583	 0.4590
0	 0.3929	 0.3780
1	 0.4872	 0.4230
2	 0.6960	 0.4910
3	 0.6992	 0.4360
4	 0.6056	 0.4280
5	 0.5646	 0.3560
6	 0.5867	 0.3970
7	 0.7088	 0.4800
8	 0.7523	 0.5230
9	 0.4200	 0.4510
A	 0.6868	 0.4730
AA	 0.5524	 0.4750
B	 0.5998	 0.4280
BA	 0.3214	 0.4170
C	 0.6969	 0.4940
CA	 0.3600	 0.4240
D	 0.6877	 0.4760
DA	 0.5897	 0.3560
E	 0.2500	 0.2950
F	 0.3600	 0.3930
G	 0.6786	 0.5210
H	 0.2500	 0.4280
I	 0.4286	 0.4500
J	 0.3115	 0.3880
K	 0.3929	 0.4290
L	 0.3929	 0.3840
M	 0.5626	 0.3600
N	 0.5855	 0.4000
O	 0.4872	 0.4430
P	 0.4000	 0.4430
Q	 0.7553	 0.5260
R	 0.7114	 0.4830
S	 0.5524	 0.4720
T	 0.3214	 0.4370



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Chain	Atom inclusion	Q-score
U	 0.6887	 0.4720
V	 0.6949	 0.4910
W	 0.6935	 0.4370
X	 0.7003	 0.4370
Y	 0.6150	 0.4290
Z	 0.3600	 0.4130
a	 0.5897	 0.3530
b	 0.2500	 0.3160
c	 0.3600	 0.3880
d	 0.6786	 0.5210
e	 0.2500	 0.4370
f	 0.3929	 0.4480
g	 0.3115	 0.3970
h	 0.3929	 0.4190
i	 0.3929	 0.4020
j	 0.4615	 0.4120
k	 0.4000	 0.4340
l	 0.5524	 0.4670
m	 0.5587	 0.3560
n	 0.5867	 0.4000
o	 0.3571	 0.4220
p	 0.3600	 0.4120
q	 0.7593	 0.5270
r	 0.7152	 0.4800
s	 0.4872	 0.3540
t	 0.2500	 0.3220
u	 0.3800	 0.4040
v	 0.6786	 0.5270
w	 0.2500	 0.4260
x	 0.3929	 0.4310
y	 0.3279	 0.4020
z	 0.4286	 0.4370