



## wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 11:45 PM EST

PDB ID : 7LXN  
EMDB ID : EMD-23572  
Title : Cryo-EM structure of EDC-crosslinked ConM SOSIP.v7 (ConM-EDC) in complex with bNAbs PGT122  
Authors : Martin, G.M.; Ward, A.B.; Sattentau, Q.J.  
Deposited on : 2021-03-04  
Resolution : 3.85 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](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:

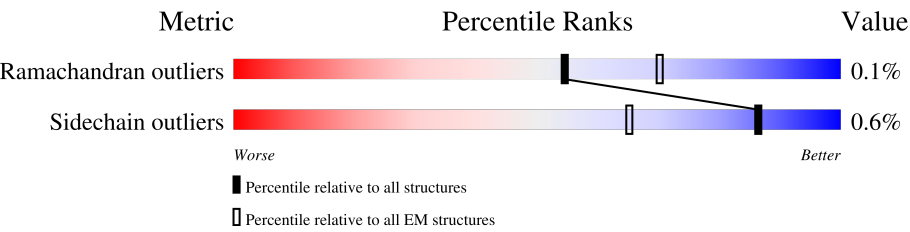
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.85 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	A	492	<div><div>6%</div><div>86%</div><div>12%</div></div>
1	C	492	<div><div>6%</div><div>86%</div><div>12%</div></div>
1	E	492	<div><div>6%</div><div>86%</div><div>12%</div></div>
2	B	153	<div><div>76%</div><div>23%</div></div>
2	D	153	<div><div>76%</div><div>23%</div></div>
2	F	153	<div><div>76%</div><div>23%</div></div>
3	H	235	<div><div>52%</div><div>44%</div></div>
3	I	235	<div><div>53%</div><div>44%</div></div>
3	J	235	<div><div>53%</div><div>44%</div></div>

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Mol	Chain	Length	Quality of chain
4	L	213	
4	M	213	
4	N	213	
5	G	8	
5	a	8	
5	o	8	
6	0	2	
6	1	2	
6	K	2	
6	O	2	
6	P	2	
6	Q	2	
6	R	2	
6	T	2	
6	Y	2	
6	Z	2	
6	b	2	
6	c	2	
6	d	2	
6	e	2	
6	f	2	
6	h	2	
6	m	2	
6	n	2	
6	p	2	

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Mol	Chain	Length	Quality of chain
6	q	2	<div>50%</div> <div>100%</div>
6	r	2	<div>50%</div> <div>100%</div>
6	s	2	<div>100%</div> <div>100%</div>
6	t	2	<div>50%</div> <div>100%</div>
6	v	2	<div>50%</div> <div>100%</div>
7	S	7	<div>57%</div> <div>100%</div>
7	g	7	<div>14%</div> <div>57%</div> <div>86%</div>
7	u	7	<div>57%</div> <div>100%</div>
8	U	4	<div>25%</div> <div>75%</div> <div>75%</div>
8	i	4	<div>25%</div> <div>75%</div> <div>75%</div>
8	w	4	<div>25%</div> <div>75%</div> <div>75%</div>
9	V	9	<div>11%</div> <div>33%</div> <div>89%</div>
9	j	9	<div>11%</div> <div>33%</div> <div>89%</div>
9	x	9	<div>11%</div> <div>33%</div> <div>89%</div>
10	W	3	<div>67%</div> <div>100%</div>
10	X	3	<div>67%</div> <div>100%</div>
10	k	3	<div>67%</div> <div>100%</div>
10	l	3	<div>67%</div> <div>100%</div>
10	y	3	<div>67%</div> <div>100%</div>
10	z	3	<div>67%</div> <div>100%</div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 20820 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 Env glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	434	Total	C	N	O	S	0	0
			3450	2170	605	649	26		
1	C	434	Total	C	N	O	S	0	0
			3450	2170	605	649	26		
1	E	434	Total	C	N	O	S	0	0
			3450	2170	605	649	26		

- Molecule 2 is a protein called HIV-1 Env glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	118	Total	C	N	O	S	0	0
			950	598	160	185	7		
2	D	118	Total	C	N	O	S	0	0
			950	598	160	185	7		
2	F	118	Total	C	N	O	S	0	0
			950	598	160	185	7		

- Molecule 3 is a protein called PGT122 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	131	Total	C	N	O	S	0	0
			1041	666	179	193	3		
3	I	131	Total	C	N	O	S	0	0
			1041	666	179	193	3		
3	J	131	Total	C	N	O	S	0	0
			1041	666	179	193	3		

- Molecule 4 is a protein called PGT122 Fab light chain.

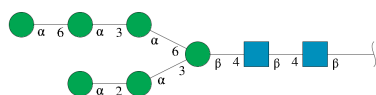
Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	108	Total	C	N	O	S	0	0
			823	515	142	164	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	108	Total	C	N	O	S	0	0
			823	515	142	164	2		
4	N	108	Total	C	N	O	S	0	0
			823	515	142	164	2		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	8	Total	C	N	O		0	0
			94	52	2	40			
5	a	8	Total	C	N	O		0	0
			94	52	2	40			
5	o	8	Total	C	N	O		0	0
			94	52	2	40			

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



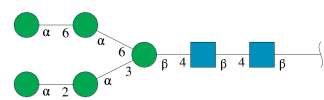
Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	2	Total	C	N	O		0	0
			28	16	2	10			
6	O	2	Total	C	N	O		0	0
			28	16	2	10			
6	P	2	Total	C	N	O		0	0
			28	16	2	10			
6	Q	2	Total	C	N	O		0	0
			28	16	2	10			
6	R	2	Total	C	N	O		0	0
			28	16	2	10			
6	T	2	Total	C	N	O		0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	Y	2	Total	C	N	O	0	0
			28	16	2	10		
6	Z	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	d	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	f	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	m	2	Total	C	N	O	0	0
			28	16	2	10		
6	n	2	Total	C	N	O	0	0
			28	16	2	10		
6	p	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	s	2	Total	C	N	O	0	0
			28	16	2	10		
6	t	2	Total	C	N	O	0	0
			28	16	2	10		
6	v	2	Total	C	N	O	0	0
			28	16	2	10		
6	0	2	Total	C	N	O	0	0
			28	16	2	10		
6	1	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-(1-6)-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.



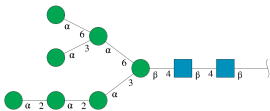
Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	7	Total	C	N	O	0	0
			83	46	2	35		
7	g	7	Total	C	N	O	0	0
			83	46	2	35		
7	u	7	Total	C	N	O	0	0
			83	46	2	35		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
8	U	4	Total	C	N	O	0	0
			50	28	2	20		
8	i	4	Total	C	N	O	0	0
			50	28	2	20		
8	w	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[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
9	V	9	Total	C	N	O	0	0
			105	58	2	45		
9	j	9	Total	C	N	O	0	0
			105	58	2	45		

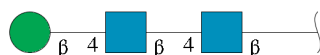
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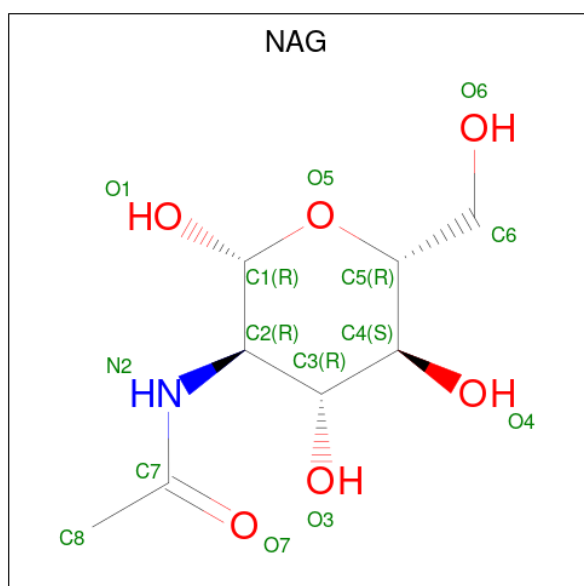
Mol	Chain	Residues	Atoms				AltConf	Trace
9	x	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 10 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.



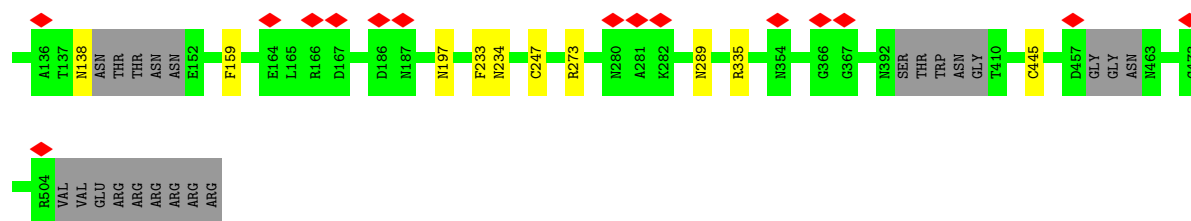
Mol	Chain	Residues	Atoms				AltConf	Trace
10	W	3	Total	C	N	O	0	0
			39	22	2	15		
10	X	3	Total	C	N	O	0	0
			39	22	2	15		
10	k	3	Total	C	N	O	0	0
			39	22	2	15		
10	l	3	Total	C	N	O	0	0
			39	22	2	15		
10	y	3	Total	C	N	O	0	0
			39	22	2	15		
10	z	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 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>).

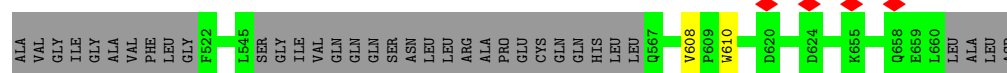
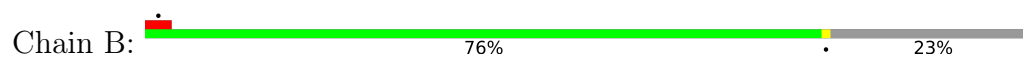


Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total 28	C 16	N 2	O 10	0
11	A	1	Total 28	C 16	N 2	O 10	0
11	B	1	Total 14	C 8	N 1	O 5	0
11	C	1	Total 28	C 16	N 2	O 10	0
11	C	1	Total 28	C 16	N 2	O 10	0
11	D	1	Total 14	C 8	N 1	O 5	0
11	E	1	Total 28	C 16	N 2	O 10	0
11	E	1	Total 28	C 16	N 2	O 10	0
11	F	1	Total 14	C 8	N 1	O 5	0

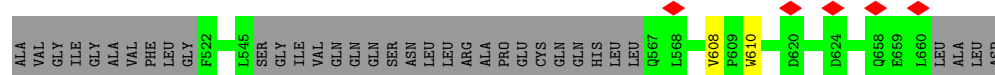
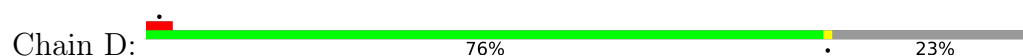




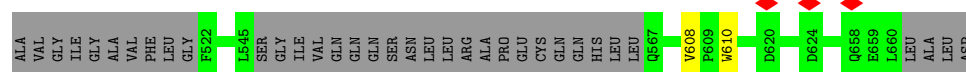
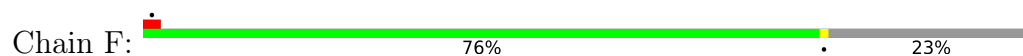
• Molecule 2: HIV-1 Env glycoprotein gp41



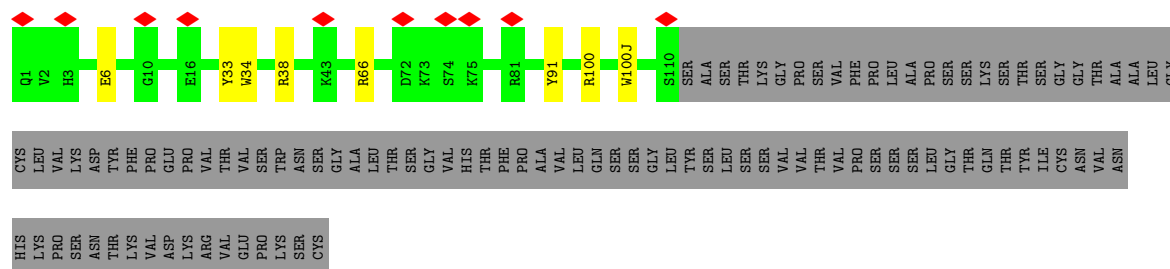
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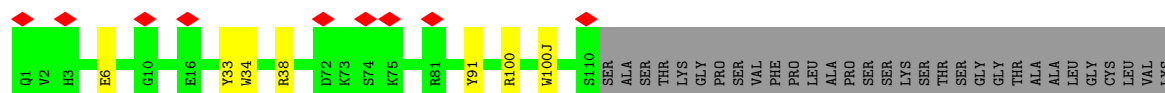
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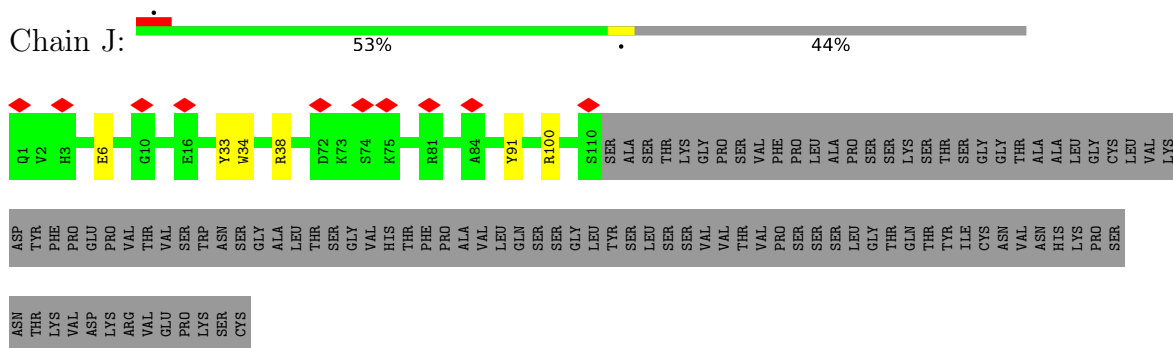
• Molecule 3: PGT122 Fab heavy chain



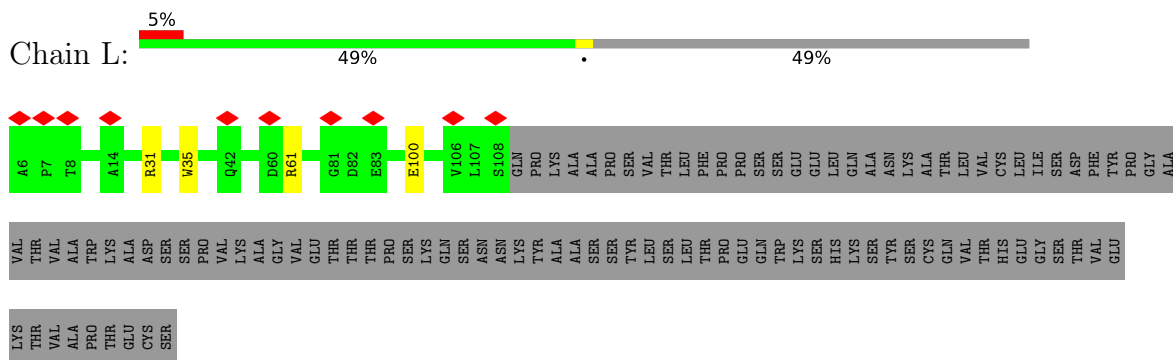
• Molecule 3: PGT122 Fab heavy chain



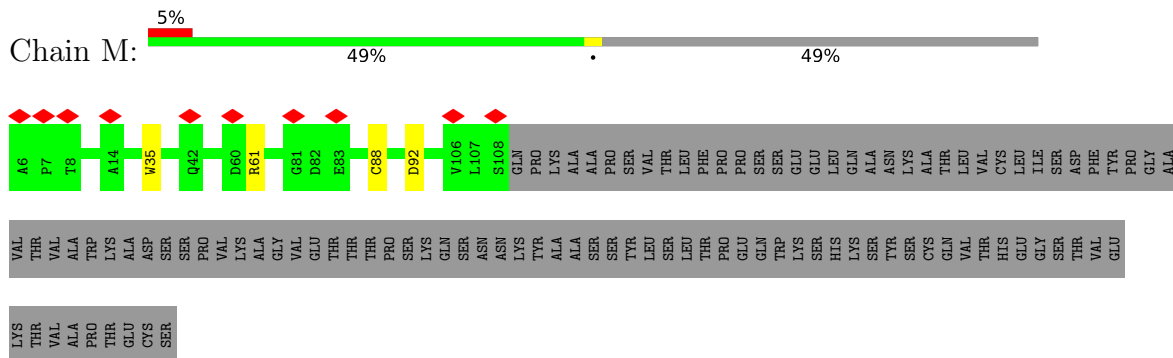
- Molecule 3: PGT122 Fab heavy chain



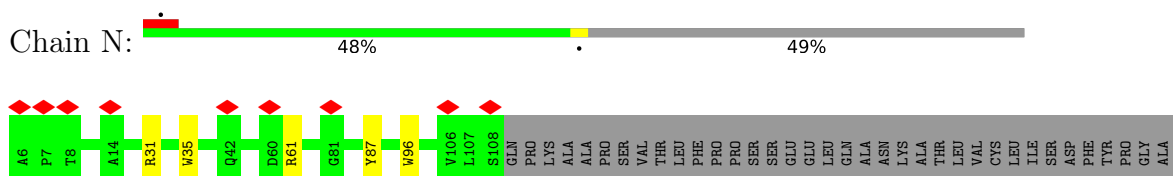
- Molecule 4: PGT122 Fab light chain



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



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- 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-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



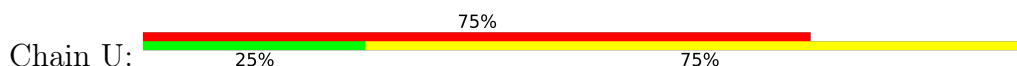
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



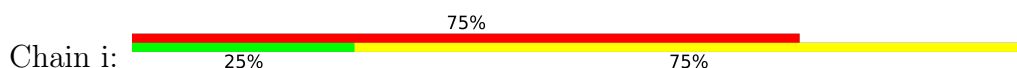
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



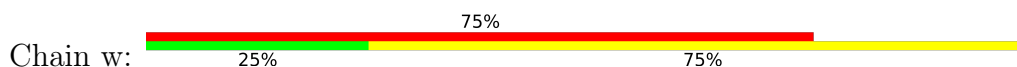
- Molecule 8: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

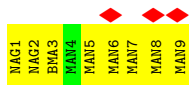


- Molecule 8: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

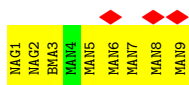




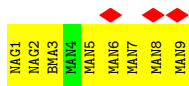
- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 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 9: 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 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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





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



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



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



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91987	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 ( $e^-/\text{\AA}^2$ )	50	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	2.223	Depositor
Minimum map value	-1.280	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	225.72, 225.72, 225.72	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.026, 1.026, 1.026	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: MAN, BMA, 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	1.08	5/3520 (0.1%)	0.89	6/4779 (0.1%)
1	C	1.08	6/3520 (0.2%)	0.89	7/4779 (0.1%)
1	E	1.08	5/3520 (0.1%)	0.89	6/4779 (0.1%)
2	B	1.21	3/967 (0.3%)	0.83	0/1310
2	D	1.19	3/967 (0.3%)	0.81	0/1310
2	F	1.17	3/967 (0.3%)	0.83	0/1310
3	H	1.22	6/1070 (0.6%)	0.93	3/1457 (0.2%)
3	I	1.22	6/1070 (0.6%)	0.92	2/1457 (0.1%)
3	J	1.21	4/1070 (0.4%)	0.91	2/1457 (0.1%)
4	L	1.17	2/845 (0.2%)	0.95	2/1157 (0.2%)
4	M	1.25	3/845 (0.4%)	0.91	1/1157 (0.1%)
4	N	1.19	3/845 (0.4%)	0.94	2/1157 (0.2%)
All	All	1.14	49/19206 (0.3%)	0.89	31/26109 (0.1%)

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	88	CYS	CB-SG	-11.40	1.62	1.82
1	E	247	CYS	CB-SG	-10.30	1.64	1.82
1	A	247	CYS	CB-SG	-9.99	1.65	1.82
1	C	247	CYS	CB-SG	-9.95	1.65	1.82
2	B	610	TRP	CB-CG	-8.30	1.35	1.50

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	335	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	A	335	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	E	335	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	C	217	TYR	CB-CG-CD2	-7.65	116.41	121.00
1	A	95	MET	CG-SD-CE	7.13	111.61	100.20

There are no chirality outliers.

There are no planarity outliers.

## 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	426/492 (87%)	420 (99%)	6 (1%)	0	100	100
1	C	426/492 (87%)	418 (98%)	8 (2%)	0	100	100
1	E	426/492 (87%)	422 (99%)	4 (1%)	0	100	100
2	B	114/153 (74%)	110 (96%)	3 (3%)	1 (1%)	17	53
2	D	114/153 (74%)	112 (98%)	1 (1%)	1 (1%)	17	53
2	F	114/153 (74%)	112 (98%)	1 (1%)	1 (1%)	17	53
3	H	129/235 (55%)	127 (98%)	2 (2%)	0	100	100
3	I	129/235 (55%)	128 (99%)	1 (1%)	0	100	100
3	J	129/235 (55%)	128 (99%)	1 (1%)	0	100	100
4	L	106/213 (50%)	105 (99%)	1 (1%)	0	100	100
4	M	106/213 (50%)	105 (99%)	1 (1%)	0	100	100
4	N	106/213 (50%)	105 (99%)	1 (1%)	0	100	100
All	All	2325/3279 (71%)	2292 (99%)	30 (1%)	3 (0%)	54	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	608	VAL
2	D	608	VAL
2	F	608	VAL



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/440 (89%)	389 (99%)	4 (1%)	76	85
1	C	393/440 (89%)	390 (99%)	3 (1%)	81	89
1	E	393/440 (89%)	389 (99%)	4 (1%)	76	85
2	B	104/131 (79%)	104 (100%)	0	100	100
2	D	104/131 (79%)	104 (100%)	0	100	100
2	F	104/131 (79%)	104 (100%)	0	100	100
3	H	115/205 (56%)	115 (100%)	0	100	100
3	I	115/205 (56%)	115 (100%)	0	100	100
3	J	115/205 (56%)	114 (99%)	1 (1%)	78	88
4	L	90/181 (50%)	90 (100%)	0	100	100
4	M	90/181 (50%)	90 (100%)	0	100	100
4	N	90/181 (50%)	90 (100%)	0	100	100
All	All	2106/2871 (73%)	2094 (99%)	12 (1%)	86	91

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	138	ASN
1	E	197	ASN
3	J	100	ARG
1	E	234	ASN
1	A	289	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

150 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
6	NAG	0	1	1,6	14,14,15	0.94	1 (7%)	17,19,21	1.13	1 (5%)
6	NAG	0	2	6	14,14,15	0.76	1 (7%)	17,19,21	1.06	1 (5%)
6	NAG	1	1	1,6	14,14,15	1.17	1 (7%)	17,19,21	1.75	4 (23%)
6	NAG	1	2	6	14,14,15	0.72	1 (7%)	17,19,21	0.90	1 (5%)
5	NAG	G	1	1,5	14,14,15	0.84	1 (7%)	17,19,21	2.05	4 (23%)
5	NAG	G	2	5	14,14,15	0.54	0	17,19,21	1.05	1 (5%)
5	BMA	G	3	5	11,11,12	0.72	0	15,15,17	1.81	3 (20%)
5	MAN	G	4	5	11,11,12	0.73	0	15,15,17	2.54	3 (20%)
5	MAN	G	5	5	11,11,12	0.63	0	15,15,17	0.91	1 (6%)
5	MAN	G	6	5	11,11,12	0.70	0	15,15,17	0.93	0
5	MAN	G	7	5	11,11,12	0.87	1 (9%)	15,15,17	1.61	4 (26%)
5	MAN	G	8	5	11,11,12	0.86	1 (9%)	15,15,17	1.53	5 (33%)
6	NAG	K	1	1,6	14,14,15	0.93	1 (7%)	17,19,21	1.52	3 (17%)
6	NAG	K	2	6	14,14,15	0.75	1 (7%)	17,19,21	0.77	1 (5%)
6	NAG	O	1	1,6	14,14,15	1.09	1 (7%)	17,19,21	1.80	3 (17%)
6	NAG	O	2	6	14,14,15	0.72	1 (7%)	17,19,21	0.92	1 (5%)
6	NAG	P	1	1,6	14,14,15	0.92	1 (7%)	17,19,21	1.31	2 (11%)
6	NAG	P	2	6	14,14,15	0.70	1 (7%)	17,19,21	1.00	1 (5%)
6	NAG	Q	1	1,6	14,14,15	1.29	1 (7%)	17,19,21	1.59	3 (17%)
6	NAG	Q	2	6	14,14,15	1.24	1 (7%)	17,19,21	0.91	0
6	NAG	R	1	1,6	14,14,15	0.91	1 (7%)	17,19,21	0.96	0
6	NAG	R	2	6	14,14,15	0.73	1 (7%)	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	S	1	1,7	14,14,15	0.88	1 (7%)	17,19,21	1.07	1 (5%)
7	NAG	S	2	7	14,14,15	0.59	0	17,19,21	1.08	1 (5%)
7	BMA	S	3	7	11,11,12	0.57	0	15,15,17	0.92	1 (6%)
7	MAN	S	4	7	11,11,12	0.72	0	15,15,17	1.01	1 (6%)
7	MAN	S	5	7	11,11,12	0.68	0	15,15,17	0.93	1 (6%)
7	MAN	S	6	7	11,11,12	0.66	0	15,15,17	0.98	1 (6%)
7	MAN	S	7	7	11,11,12	0.70	0	15,15,17	0.93	1 (6%)
6	NAG	T	1	1,6	14,14,15	0.78	1 (7%)	17,19,21	0.97	1 (5%)
6	NAG	T	2	6	14,14,15	0.61	0	17,19,21	0.83	1 (5%)
8	NAG	U	1	1,8	14,14,15	0.94	1 (7%)	17,19,21	0.86	1 (5%)
8	NAG	U	2	8	14,14,15	0.67	0	17,19,21	0.76	0
8	BMA	U	3	8	11,11,12	0.60	0	15,15,17	0.86	1 (6%)
8	MAN	U	4	8	11,11,12	0.69	0	15,15,17	1.04	1 (6%)
9	NAG	V	1	1,9	14,14,15	0.76	1 (7%)	17,19,21	1.22	1 (5%)
9	NAG	V	2	9	14,14,15	0.66	0	17,19,21	1.12	1 (5%)
9	BMA	V	3	9	11,11,12	0.44	0	15,15,17	0.92	1 (6%)
9	MAN	V	4	9	11,11,12	0.45	0	15,15,17	0.88	0
9	MAN	V	5	9	11,11,12	0.61	0	15,15,17	1.11	1 (6%)
9	MAN	V	6	9	11,11,12	0.52	0	15,15,17	0.81	1 (6%)
9	MAN	V	7	9	11,11,12	0.61	0	15,15,17	0.79	1 (6%)
9	MAN	V	8	9	11,11,12	0.64	0	15,15,17	0.93	1 (6%)
9	MAN	V	9	9	11,11,12	0.67	0	15,15,17	0.95	1 (6%)
10	NAG	W	1	1,10	14,14,15	1.00	1 (7%)	17,19,21	0.81	0
10	NAG	W	2	10	14,14,15	0.69	0	17,19,21	0.76	1 (5%)
10	BMA	W	3	10	11,11,12	0.58	0	15,15,17	0.85	1 (6%)
10	NAG	X	1	1,10	14,14,15	0.90	1 (7%)	17,19,21	1.07	2 (11%)
10	NAG	X	2	10	14,14,15	0.74	0	17,19,21	0.85	1 (5%)
10	BMA	X	3	10	11,11,12	0.63	0	15,15,17	0.84	1 (6%)
6	NAG	Y	1	1,6	14,14,15	0.96	1 (7%)	17,19,21	0.95	1 (5%)
6	NAG	Y	2	6	14,14,15	0.75	1 (7%)	17,19,21	1.03	1 (5%)
6	NAG	Z	1	1,6	14,14,15	1.16	1 (7%)	17,19,21	1.74	4 (23%)
6	NAG	Z	2	6	14,14,15	0.72	1 (7%)	17,19,21	0.89	1 (5%)
5	NAG	a	1	1,5	14,14,15	0.72	1 (7%)	17,19,21	1.41	3 (17%)
5	NAG	a	2	5	14,14,15	0.67	0	17,19,21	1.06	1 (5%)
5	BMA	a	3	5	11,11,12	0.79	1 (9%)	15,15,17	1.77	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MAN	a	4	5	11,11,12	0.67	0	15,15,17	2.88	4 (26%)
5	MAN	a	5	5	11,11,12	0.67	0	15,15,17	1.03	1 (6%)
5	MAN	a	6	5	11,11,12	0.68	0	15,15,17	0.88	1 (6%)
5	MAN	a	7	5	11,11,12	0.87	1 (9%)	15,15,17	1.56	4 (26%)
5	MAN	a	8	5	11,11,12	0.87	1 (9%)	15,15,17	1.60	5 (33%)
6	NAG	b	1	1,6	14,14,15	0.94	1 (7%)	17,19,21	1.49	3 (17%)
6	NAG	b	2	6	14,14,15	0.74	1 (7%)	17,19,21	0.77	1 (5%)
6	NAG	c	1	1,6	14,14,15	1.10	1 (7%)	17,19,21	1.77	3 (17%)
6	NAG	c	2	6	14,14,15	0.70	1 (7%)	17,19,21	0.92	1 (5%)
6	NAG	d	1	1,6	14,14,15	0.95	1 (7%)	17,19,21	1.30	2 (11%)
6	NAG	d	2	6	14,14,15	0.70	1 (7%)	17,19,21	1.00	1 (5%)
6	NAG	e	1	1,6	14,14,15	1.32	1 (7%)	17,19,21	1.56	3 (17%)
6	NAG	e	2	6	14,14,15	1.25	1 (7%)	17,19,21	0.87	0
6	NAG	f	1	1,6	14,14,15	0.94	1 (7%)	17,19,21	1.00	0
6	NAG	f	2	6	14,14,15	0.72	1 (7%)	17,19,21	0.73	0
7	NAG	g	1	1,7	14,14,15	0.86	1 (7%)	17,19,21	1.09	1 (5%)
7	NAG	g	2	7	14,14,15	0.60	0	17,19,21	1.01	0
7	BMA	g	3	7	11,11,12	0.55	0	15,15,17	0.91	1 (6%)
7	MAN	g	4	7	11,11,12	0.72	0	15,15,17	1.12	1 (6%)
7	MAN	g	5	7	11,11,12	0.67	0	15,15,17	0.91	1 (6%)
7	MAN	g	6	7	11,11,12	0.67	0	15,15,17	0.97	1 (6%)
7	MAN	g	7	7	11,11,12	0.70	0	15,15,17	0.93	1 (6%)
6	NAG	h	1	1,6	14,14,15	0.78	1 (7%)	17,19,21	0.94	1 (5%)
6	NAG	h	2	6	14,14,15	0.61	0	17,19,21	0.84	1 (5%)
8	NAG	i	1	1,8	14,14,15	0.94	1 (7%)	17,19,21	0.85	1 (5%)
8	NAG	i	2	8	14,14,15	0.67	0	17,19,21	0.76	0
8	BMA	i	3	8	11,11,12	0.60	0	15,15,17	0.86	1 (6%)
8	MAN	i	4	8	11,11,12	0.68	0	15,15,17	1.04	1 (6%)
9	NAG	j	1	1,9	14,14,15	0.82	1 (7%)	17,19,21	1.09	1 (5%)
9	NAG	j	2	9	14,14,15	0.65	0	17,19,21	1.25	1 (5%)
9	BMA	j	3	9	11,11,12	0.45	0	15,15,17	0.90	1 (6%)
9	MAN	j	4	9	11,11,12	0.40	0	15,15,17	0.90	0
9	MAN	j	5	9	11,11,12	0.58	0	15,15,17	1.10	2 (13%)
9	MAN	j	6	9	11,11,12	0.50	0	15,15,17	0.83	1 (6%)
9	MAN	j	7	9	11,11,12	0.61	0	15,15,17	0.78	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	MAN	j	8	9	11,11,12	0.66	0	15,15,17	0.94	1 (6%)
9	MAN	j	9	9	11,11,12	0.68	0	15,15,17	0.95	1 (6%)
10	NAG	k	1	1,10	14,14,15	0.98	1 (7%)	17,19,21	0.84	1 (5%)
10	NAG	k	2	10	14,14,15	0.70	0	17,19,21	0.75	1 (5%)
10	BMA	k	3	10	11,11,12	0.59	0	15,15,17	0.85	1 (6%)
10	NAG	l	1	1,10	14,14,15	0.89	1 (7%)	17,19,21	1.08	2 (11%)
10	NAG	l	2	10	14,14,15	0.75	1 (7%)	17,19,21	0.85	1 (5%)
10	BMA	l	3	10	11,11,12	0.63	0	15,15,17	0.84	1 (6%)
6	NAG	m	1	1,6	14,14,15	0.98	1 (7%)	17,19,21	0.98	1 (5%)
6	NAG	m	2	6	14,14,15	0.76	1 (7%)	17,19,21	1.04	1 (5%)
6	NAG	n	1	1,6	14,14,15	1.12	1 (7%)	17,19,21	1.51	3 (17%)
6	NAG	n	2	6	14,14,15	0.72	1 (7%)	17,19,21	0.88	1 (5%)
5	NAG	o	1	1,5	14,14,15	0.79	1 (7%)	17,19,21	2.07	4 (23%)
5	NAG	o	2	5	14,14,15	0.55	0	17,19,21	1.09	1 (5%)
5	BMA	o	3	5	11,11,12	0.77	0	15,15,17	1.88	4 (26%)
5	MAN	o	4	5	11,11,12	0.74	0	15,15,17	2.58	3 (20%)
5	MAN	o	5	5	11,11,12	0.67	0	15,15,17	0.83	1 (6%)
5	MAN	o	6	5	11,11,12	0.71	0	15,15,17	0.99	1 (6%)
5	MAN	o	7	5	11,11,12	0.88	1 (9%)	15,15,17	1.57	4 (26%)
5	MAN	o	8	5	11,11,12	0.87	1 (9%)	15,15,17	1.53	5 (33%)
6	NAG	p	1	1,6	14,14,15	0.95	1 (7%)	17,19,21	1.47	3 (17%)
6	NAG	p	2	6	14,14,15	0.78	1 (7%)	17,19,21	0.79	1 (5%)
6	NAG	q	1	1,6	14,14,15	1.09	1 (7%)	17,19,21	1.85	3 (17%)
6	NAG	q	2	6	14,14,15	0.71	1 (7%)	17,19,21	0.88	1 (5%)
6	NAG	r	1	1,6	14,14,15	0.92	1 (7%)	17,19,21	1.28	1 (5%)
6	NAG	r	2	6	14,14,15	0.71	1 (7%)	17,19,21	1.00	1 (5%)
6	NAG	s	1	1,6	14,14,15	1.28	1 (7%)	17,19,21	1.60	3 (17%)
6	NAG	s	2	6	14,14,15	1.27	1 (7%)	17,19,21	0.91	0
6	NAG	t	1	1,6	14,14,15	0.90	1 (7%)	17,19,21	0.90	0
6	NAG	t	2	6	14,14,15	0.71	1 (7%)	17,19,21	0.76	0
7	NAG	u	1	1,7	14,14,15	0.88	1 (7%)	17,19,21	1.09	1 (5%)
7	NAG	u	2	7	14,14,15	0.59	0	17,19,21	1.10	2 (11%)
7	BMA	u	3	7	11,11,12	0.57	0	15,15,17	0.94	1 (6%)
7	MAN	u	4	7	11,11,12	0.69	0	15,15,17	1.09	1 (6%)
7	MAN	u	5	7	11,11,12	0.65	0	15,15,17	0.92	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	MAN	u	6	7	11,11,12	0.65	0	15,15,17	0.98	1 (6%)
7	MAN	u	7	7	11,11,12	0.70	0	15,15,17	0.94	1 (6%)
6	NAG	v	1	1,6	14,14,15	0.79	1 (7%)	17,19,21	0.96	1 (5%)
6	NAG	v	2	6	14,14,15	0.62	0	17,19,21	0.83	1 (5%)
8	NAG	w	1	1,8	14,14,15	0.95	1 (7%)	17,19,21	0.86	1 (5%)
8	NAG	w	2	8	14,14,15	0.66	0	17,19,21	0.76	0
8	BMA	w	3	8	11,11,12	0.60	0	15,15,17	0.86	1 (6%)
8	MAN	w	4	8	11,11,12	0.69	0	15,15,17	1.03	1 (6%)
9	NAG	x	1	1,9	14,14,15	0.77	1 (7%)	17,19,21	1.24	1 (5%)
9	NAG	x	2	9	14,14,15	0.68	0	17,19,21	1.15	1 (5%)
9	BMA	x	3	9	11,11,12	0.43	0	15,15,17	0.88	1 (6%)
9	MAN	x	4	9	11,11,12	0.38	0	15,15,17	0.89	0
9	MAN	x	5	9	11,11,12	0.55	0	15,15,17	0.94	1 (6%)
9	MAN	x	6	9	11,11,12	0.49	0	15,15,17	0.83	1 (6%)
9	MAN	x	7	9	11,11,12	0.60	0	15,15,17	0.79	1 (6%)
9	MAN	x	8	9	11,11,12	0.66	0	15,15,17	0.94	1 (6%)
9	MAN	x	9	9	11,11,12	0.68	0	15,15,17	0.95	1 (6%)
10	NAG	y	1	1,10	14,14,15	1.00	1 (7%)	17,19,21	0.80	0
10	NAG	y	2	10	14,14,15	0.72	0	17,19,21	0.77	1 (5%)
10	BMA	y	3	10	11,11,12	0.59	0	15,15,17	0.85	1 (6%)
10	NAG	z	1	1,10	14,14,15	0.90	1 (7%)	17,19,21	1.07	2 (11%)
10	NAG	z	2	10	14,14,15	0.74	0	17,19,21	0.85	1 (5%)
10	BMA	z	3	10	11,11,12	0.63	0	15,15,17	0.84	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	0	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	0	2	6	-	2/6/23/26	0/1/1/1
6	NAG	1	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	1	2	6	-	1/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	G	4	5	-	1/2/19/22	0/1/1/1
5	MAN	G	5	5	-	2/2/19/22	0/1/1/1
5	MAN	G	6	5	-	0/2/19/22	0/1/1/1
5	MAN	G	7	5	-	1/2/19/22	0/1/1/1
5	MAN	G	8	5	-	1/2/19/22	0/1/1/1
6	NAG	K	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	1/6/23/26	0/1/1/1
6	NAG	O	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	O	2	6	-	1/6/23/26	0/1/1/1
6	NAG	P	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Q	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	1/6/23/26	0/1/1/1
6	NAG	R	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	R	2	6	-	1/6/23/26	0/1/1/1
7	NAG	S	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	S	2	7	-	0/6/23/26	0/1/1/1
7	BMA	S	3	7	-	2/2/19/22	0/1/1/1
7	MAN	S	4	7	-	1/2/19/22	0/1/1/1
7	MAN	S	5	7	-	2/2/19/22	0/1/1/1
7	MAN	S	6	7	-	1/2/19/22	0/1/1/1
7	MAN	S	7	7	-	2/2/19/22	0/1/1/1
6	NAG	T	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	T	2	6	-	2/6/23/26	0/1/1/1
8	NAG	U	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	U	2	8	-	1/6/23/26	0/1/1/1
8	BMA	U	3	8	-	0/2/19/22	0/1/1/1
8	MAN	U	4	8	-	1/2/19/22	0/1/1/1
9	NAG	V	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	V	2	9	-	2/6/23/26	0/1/1/1
9	BMA	V	3	9	-	0/2/19/22	0/1/1/1
9	MAN	V	4	9	-	1/2/19/22	0/1/1/1
9	MAN	V	5	9	-	1/2/19/22	0/1/1/1
9	MAN	V	6	9	-	1/2/19/22	0/1/1/1
9	MAN	V	7	9	-	0/2/19/22	0/1/1/1
9	MAN	V	8	9	-	1/2/19/22	0/1/1/1
9	MAN	V	9	9	-	1/2/19/22	0/1/1/1
10	NAG	W	1	1,10	-	1/6/23/26	0/1/1/1
10	NAG	W	2	10	-	1/6/23/26	0/1/1/1
10	BMA	W	3	10	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	X	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	X	2	10	-	1/6/23/26	0/1/1/1
10	BMA	X	3	10	-	1/2/19/22	0/1/1/1
6	NAG	Y	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Z	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	1/6/23/26	0/1/1/1
5	NAG	a	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	a	2	5	-	0/6/23/26	0/1/1/1
5	BMA	a	3	5	-	0/2/19/22	0/1/1/1
5	MAN	a	4	5	-	1/2/19/22	0/1/1/1
5	MAN	a	5	5	-	2/2/19/22	0/1/1/1
5	MAN	a	6	5	-	0/2/19/22	0/1/1/1
5	MAN	a	7	5	-	1/2/19/22	0/1/1/1
5	MAN	a	8	5	-	1/2/19/22	0/1/1/1
6	NAG	b	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	b	2	6	-	1/6/23/26	0/1/1/1
6	NAG	c	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	c	2	6	-	1/6/23/26	0/1/1/1
6	NAG	d	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	d	2	6	-	2/6/23/26	0/1/1/1
6	NAG	e	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	e	2	6	-	1/6/23/26	0/1/1/1
6	NAG	f	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	f	2	6	-	1/6/23/26	0/1/1/1
7	NAG	g	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	g	2	7	-	2/6/23/26	0/1/1/1
7	BMA	g	3	7	-	0/2/19/22	0/1/1/1
7	MAN	g	4	7	-	1/2/19/22	0/1/1/1
7	MAN	g	5	7	-	1/2/19/22	0/1/1/1
7	MAN	g	6	7	-	1/2/19/22	0/1/1/1
7	MAN	g	7	7	-	1/2/19/22	0/1/1/1
6	NAG	h	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	h	2	6	-	2/6/23/26	0/1/1/1
8	NAG	i	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	i	2	8	-	1/6/23/26	0/1/1/1
8	BMA	i	3	8	-	0/2/19/22	0/1/1/1
8	MAN	i	4	8	-	1/2/19/22	0/1/1/1
9	NAG	j	1	1,9	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	j	2	9	-	2/6/23/26	0/1/1/1
9	BMA	j	3	9	-	0/2/19/22	0/1/1/1
9	MAN	j	4	9	-	2/2/19/22	0/1/1/1
9	MAN	j	5	9	-	1/2/19/22	0/1/1/1
9	MAN	j	6	9	-	1/2/19/22	0/1/1/1
9	MAN	j	7	9	-	0/2/19/22	0/1/1/1
9	MAN	j	8	9	-	1/2/19/22	0/1/1/1
9	MAN	j	9	9	-	1/2/19/22	0/1/1/1
10	NAG	k	1	1,10	-	1/6/23/26	0/1/1/1
10	NAG	k	2	10	-	1/6/23/26	0/1/1/1
10	BMA	k	3	10	-	1/2/19/22	0/1/1/1
10	NAG	l	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	l	2	10	-	1/6/23/26	0/1/1/1
10	BMA	l	3	10	-	1/2/19/22	0/1/1/1
6	NAG	m	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	m	2	6	-	2/6/23/26	0/1/1/1
6	NAG	n	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	n	2	6	-	1/6/23/26	0/1/1/1
5	NAG	o	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	o	2	5	-	2/6/23/26	0/1/1/1
5	BMA	o	3	5	-	0/2/19/22	0/1/1/1
5	MAN	o	4	5	-	1/2/19/22	0/1/1/1
5	MAN	o	5	5	-	2/2/19/22	0/1/1/1
5	MAN	o	6	5	-	2/2/19/22	0/1/1/1
5	MAN	o	7	5	-	1/2/19/22	0/1/1/1
5	MAN	o	8	5	-	1/2/19/22	0/1/1/1
6	NAG	p	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	p	2	6	-	1/6/23/26	0/1/1/1
6	NAG	q	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	q	2	6	-	1/6/23/26	0/1/1/1
6	NAG	r	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	r	2	6	-	2/6/23/26	0/1/1/1
6	NAG	s	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	s	2	6	-	1/6/23/26	0/1/1/1
6	NAG	t	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	t	2	6	-	1/6/23/26	0/1/1/1
7	NAG	u	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	u	2	7	-	0/6/23/26	0/1/1/1
7	BMA	u	3	7	-	2/2/19/22	0/1/1/1
7	MAN	u	4	7	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	u	5	7	-	1/2/19/22	0/1/1/1
7	MAN	u	6	7	-	1/2/19/22	0/1/1/1
7	MAN	u	7	7	-	2/2/19/22	0/1/1/1
6	NAG	v	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	v	2	6	-	2/6/23/26	0/1/1/1
8	NAG	w	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	w	2	8	-	1/6/23/26	0/1/1/1
8	BMA	w	3	8	-	0/2/19/22	0/1/1/1
8	MAN	w	4	8	-	1/2/19/22	0/1/1/1
9	NAG	x	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	x	2	9	-	2/6/23/26	0/1/1/1
9	BMA	x	3	9	-	0/2/19/22	0/1/1/1
9	MAN	x	4	9	-	2/2/19/22	0/1/1/1
9	MAN	x	5	9	-	1/2/19/22	0/1/1/1
9	MAN	x	6	9	-	1/2/19/22	0/1/1/1
9	MAN	x	7	9	-	0/2/19/22	0/1/1/1
9	MAN	x	8	9	-	1/2/19/22	0/1/1/1
9	MAN	x	9	9	-	1/2/19/22	0/1/1/1
10	NAG	y	1	1,10	-	1/6/23/26	0/1/1/1
10	NAG	y	2	10	-	1/6/23/26	0/1/1/1
10	BMA	y	3	10	-	1/2/19/22	0/1/1/1
10	NAG	z	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	z	2	10	-	1/6/23/26	0/1/1/1
10	BMA	z	3	10	-	1/2/19/22	0/1/1/1

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	s	2	NAG	C1-C2	4.52	1.59	1.52
6	e	1	NAG	C1-C2	4.51	1.59	1.52
6	e	2	NAG	C1-C2	4.45	1.59	1.52
6	Q	2	NAG	C1-C2	4.45	1.59	1.52
6	Q	1	NAG	C1-C2	4.44	1.59	1.52

The worst 5 of 206 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	4	MAN	O3-C3-C2	-7.18	96.24	109.99
5	G	4	MAN	O3-C3-C2	-6.76	97.05	109.99
5	o	4	MAN	O3-C3-C2	-6.72	97.13	109.99
5	a	4	MAN	C1-C2-C3	5.87	116.89	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	o	4	MAN	C1-C2-C3	5.47	116.39	109.67

There are no chirality outliers.

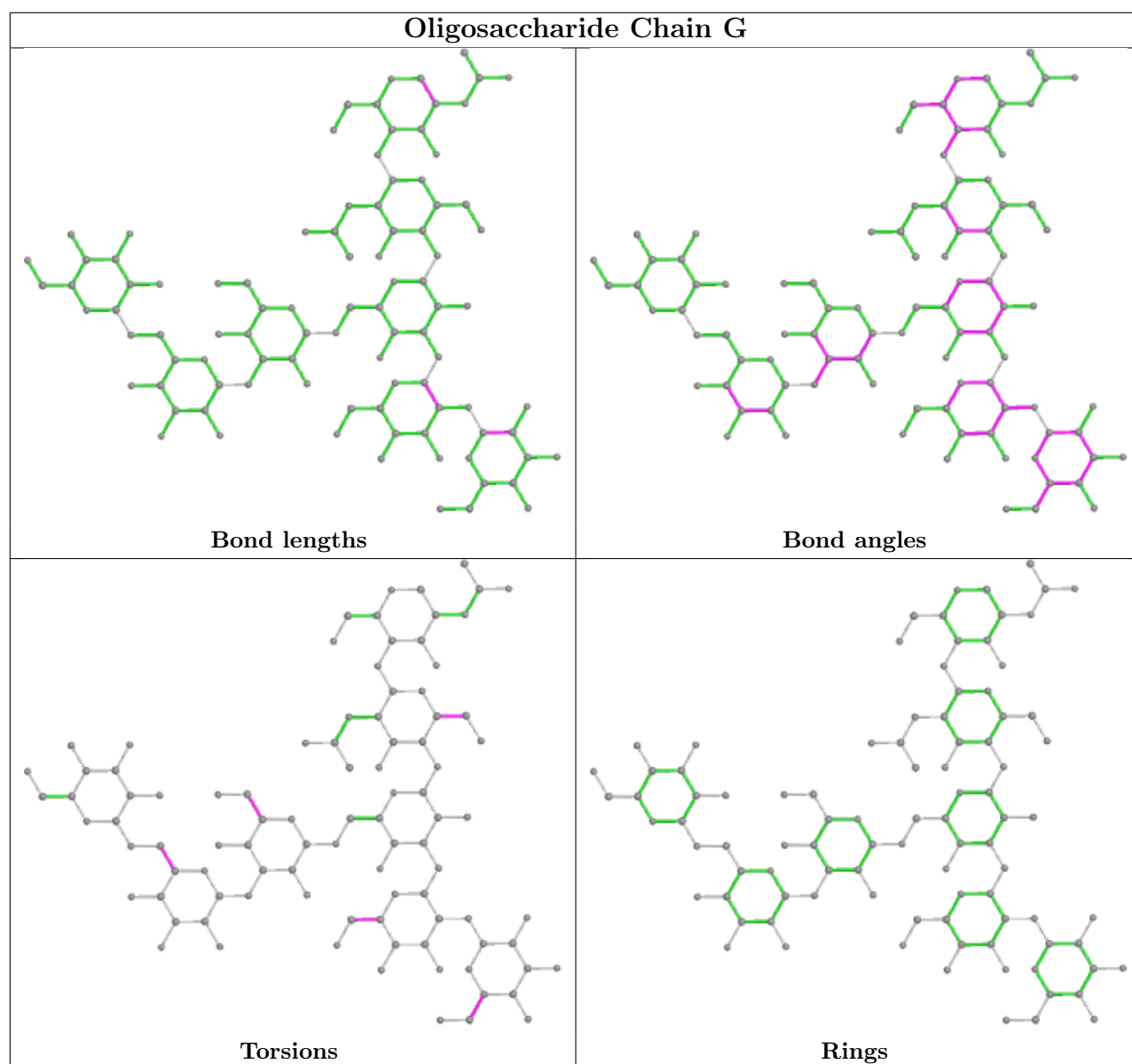
5 of 149 torsion outliers are listed below:

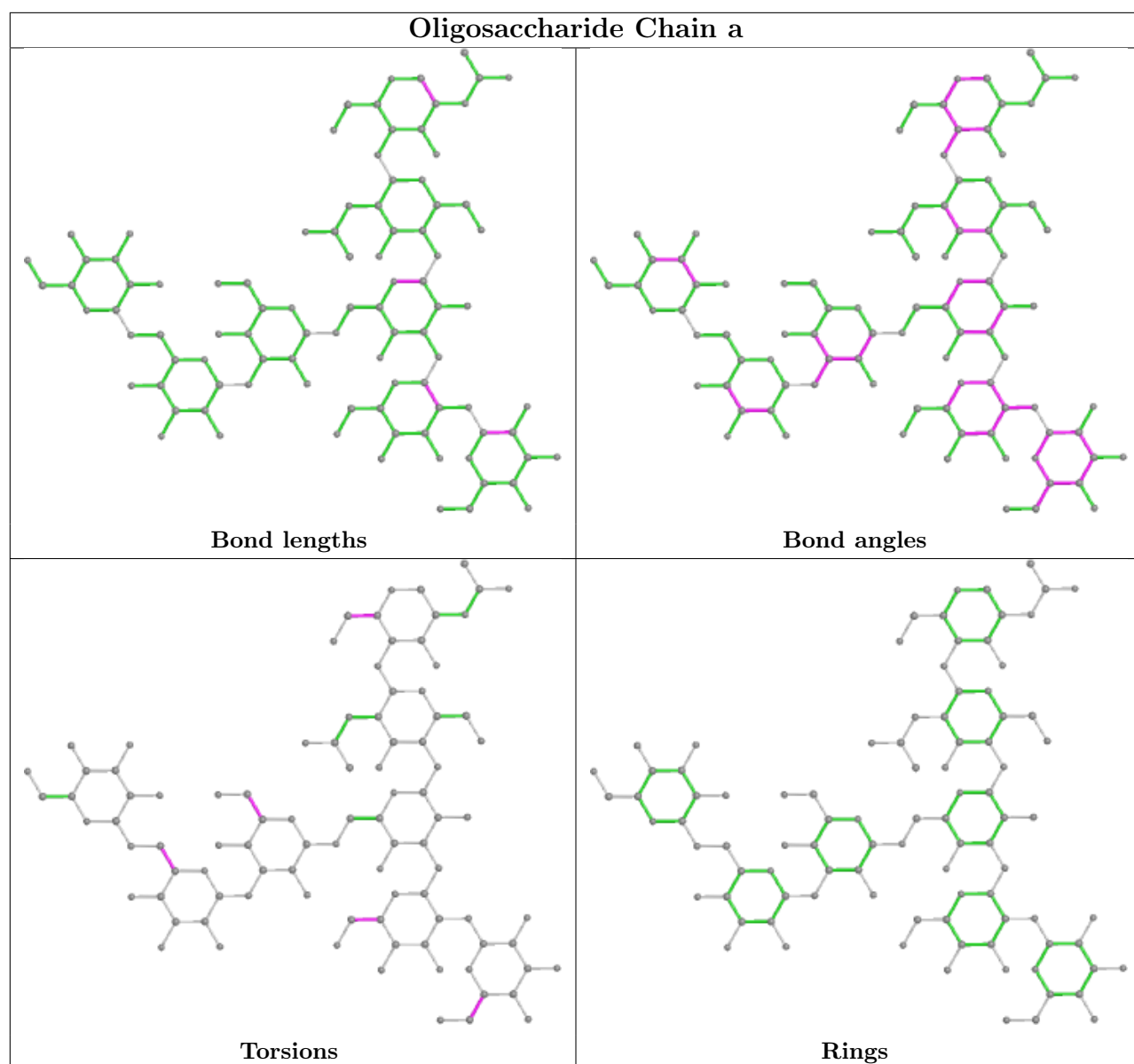
Mol	Chain	Res	Type	Atoms
6	O	1	NAG	C1-C2-N2-C7
6	q	1	NAG	C1-C2-N2-C7
6	c	1	NAG	C1-C2-N2-C7
5	G	5	MAN	C4-C5-C6-O6
9	x	4	MAN	O5-C5-C6-O6

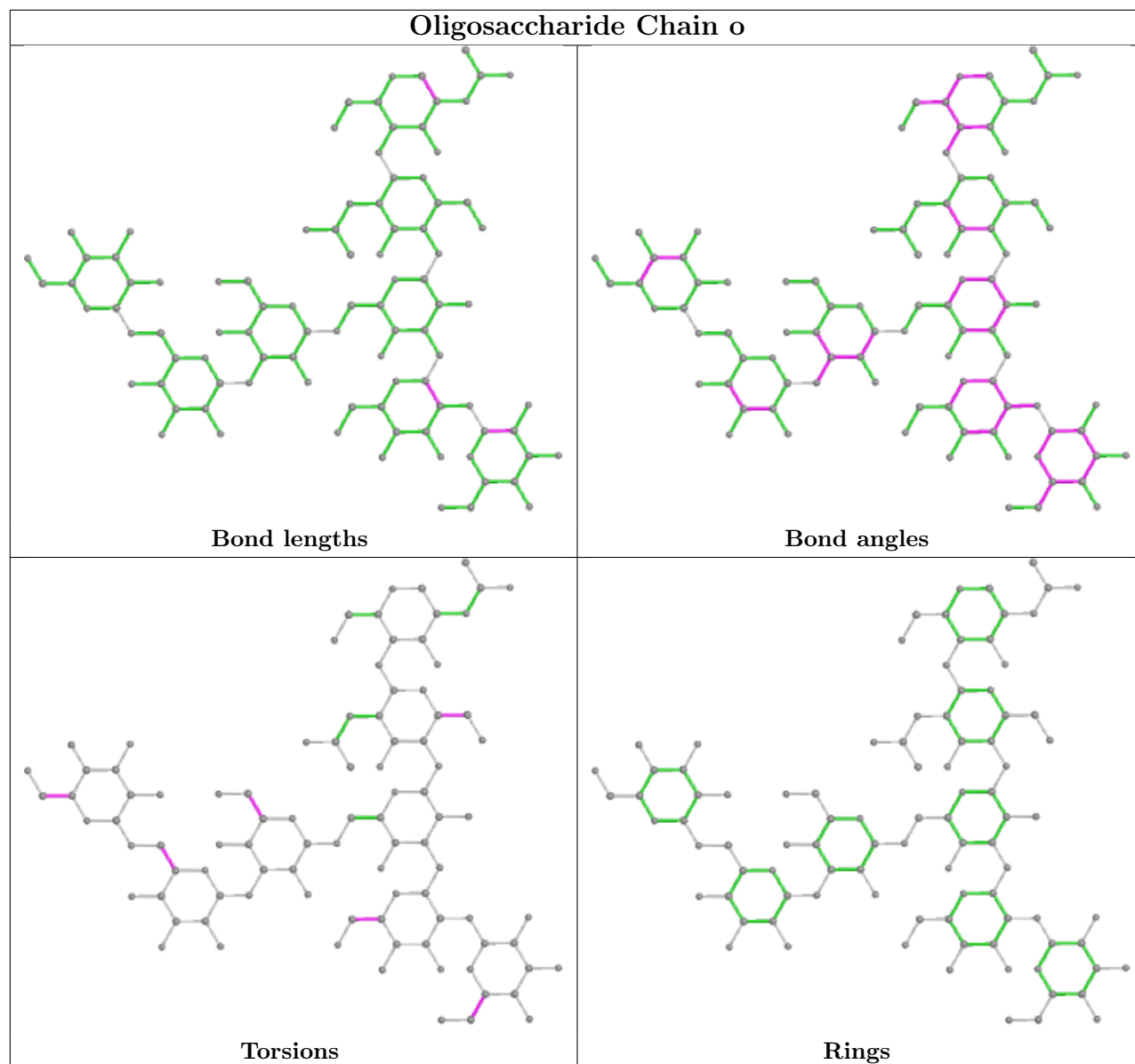
There are no ring outliers.

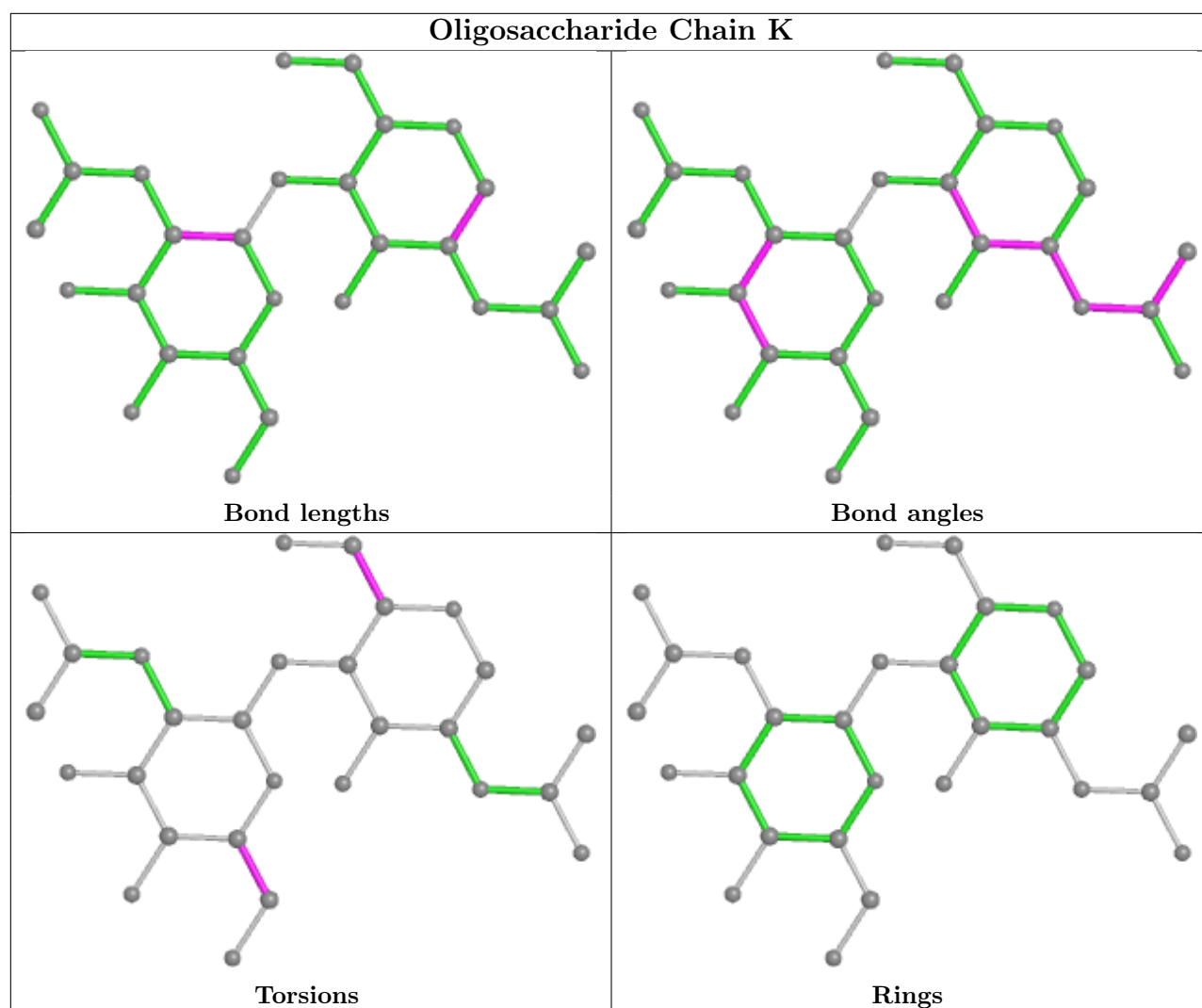
No monomer is involved in short contacts.

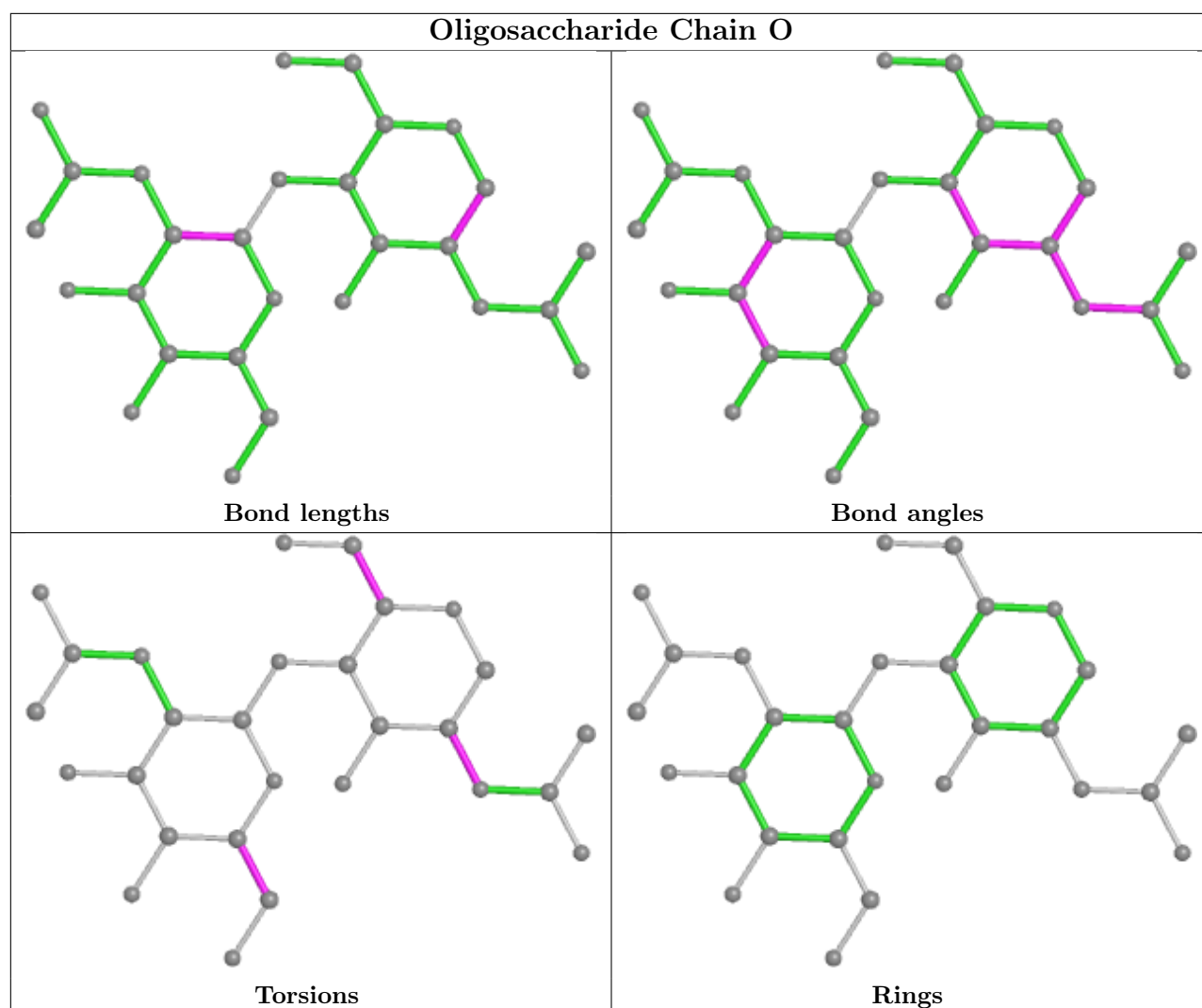
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



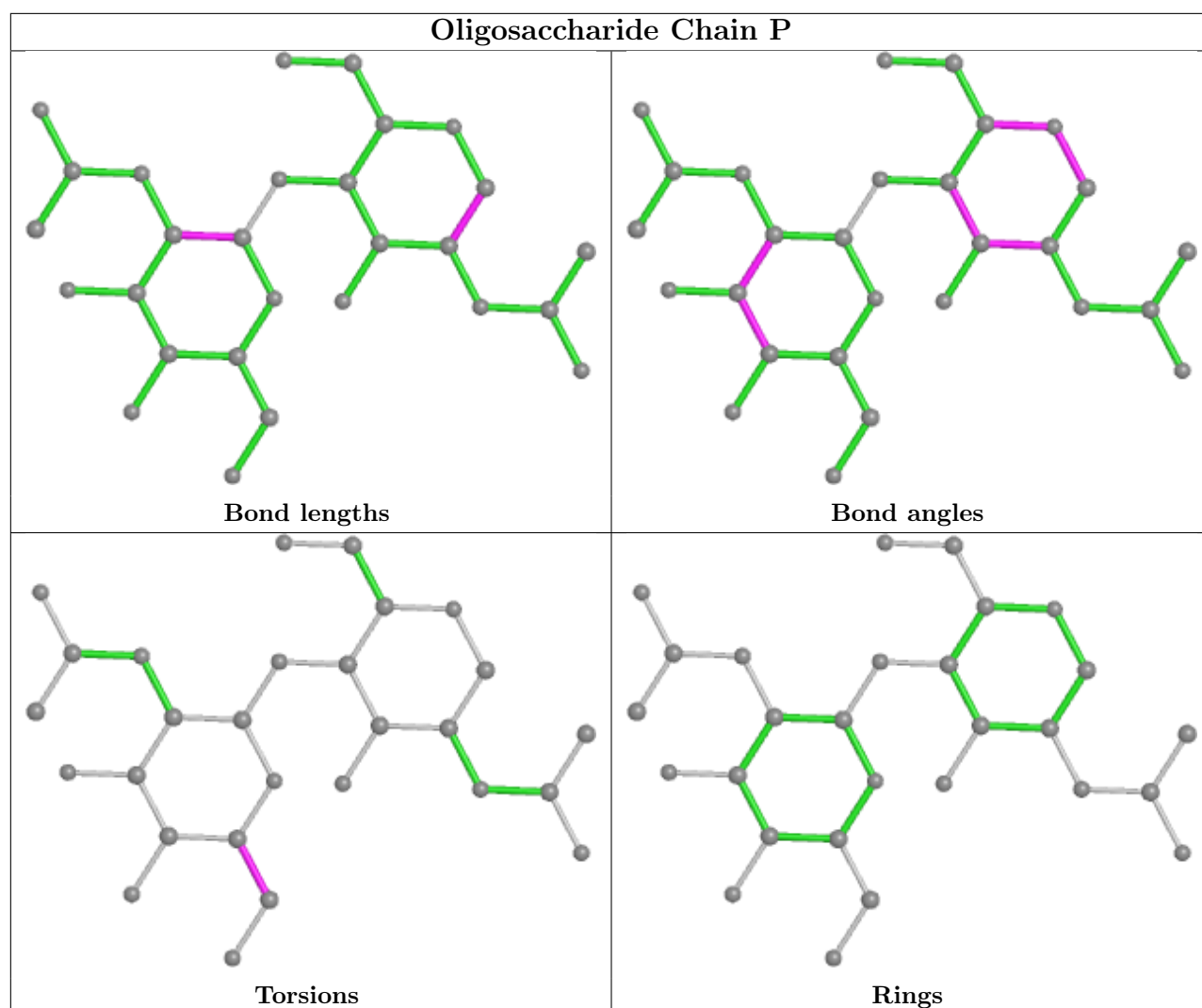


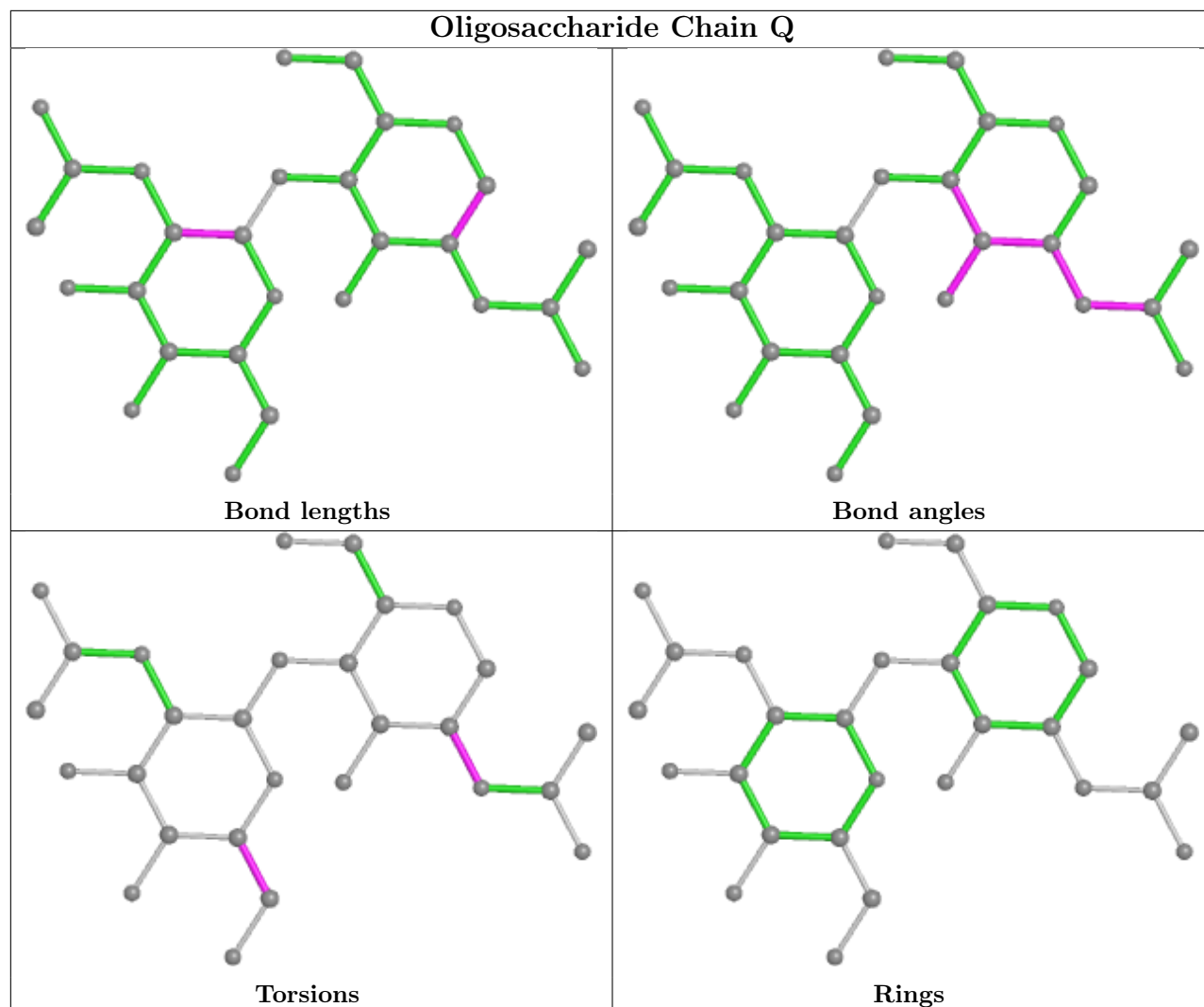


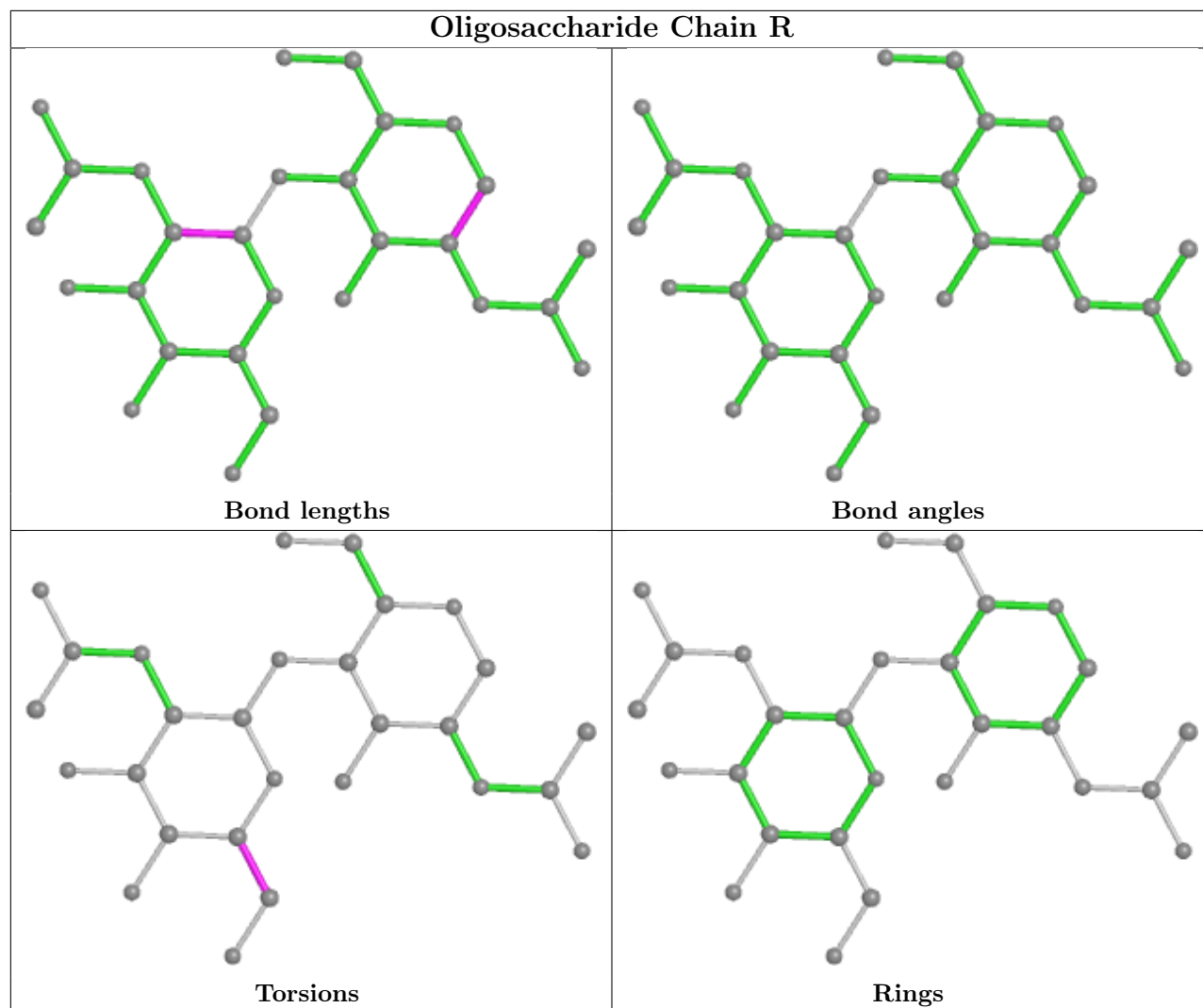


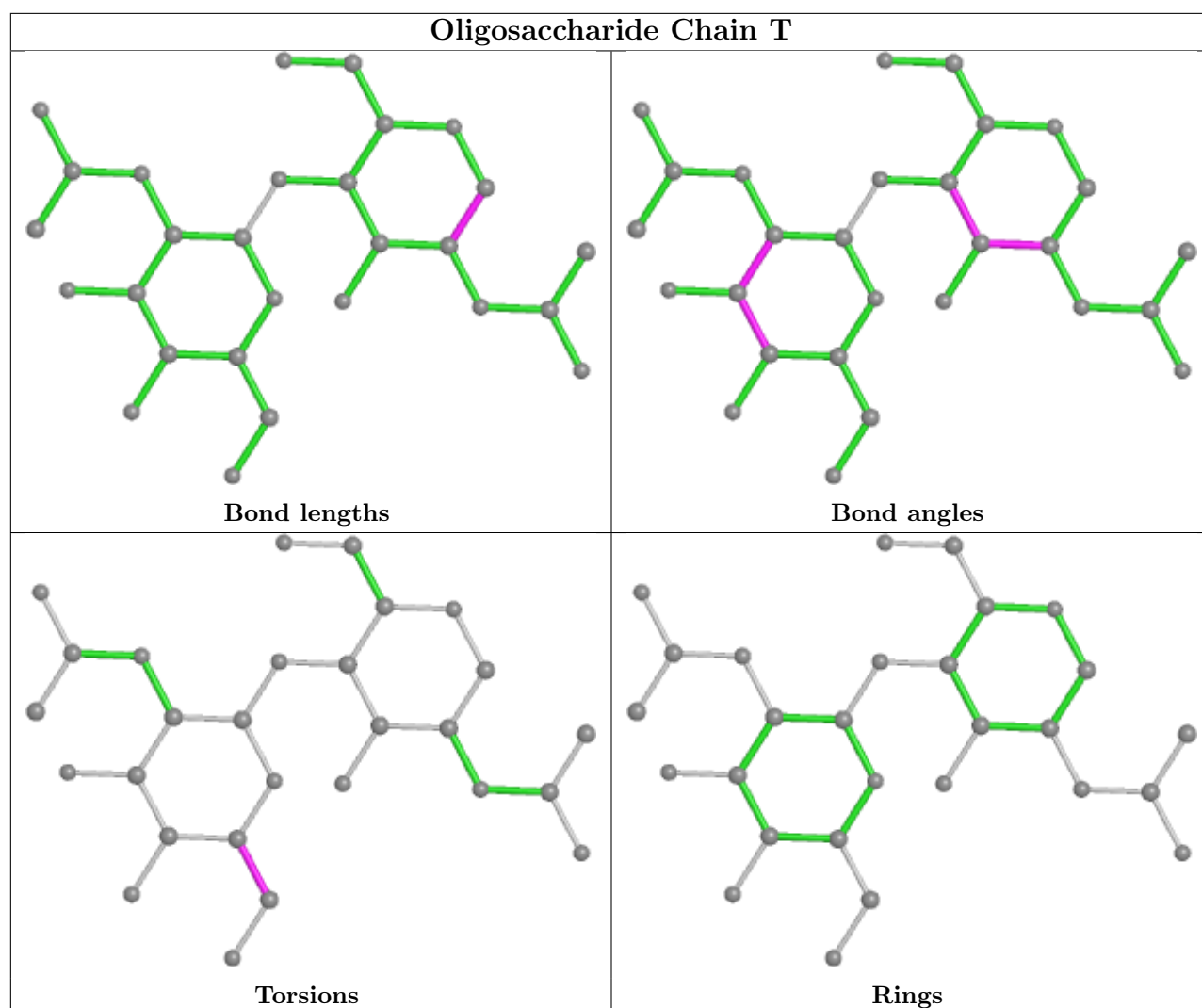


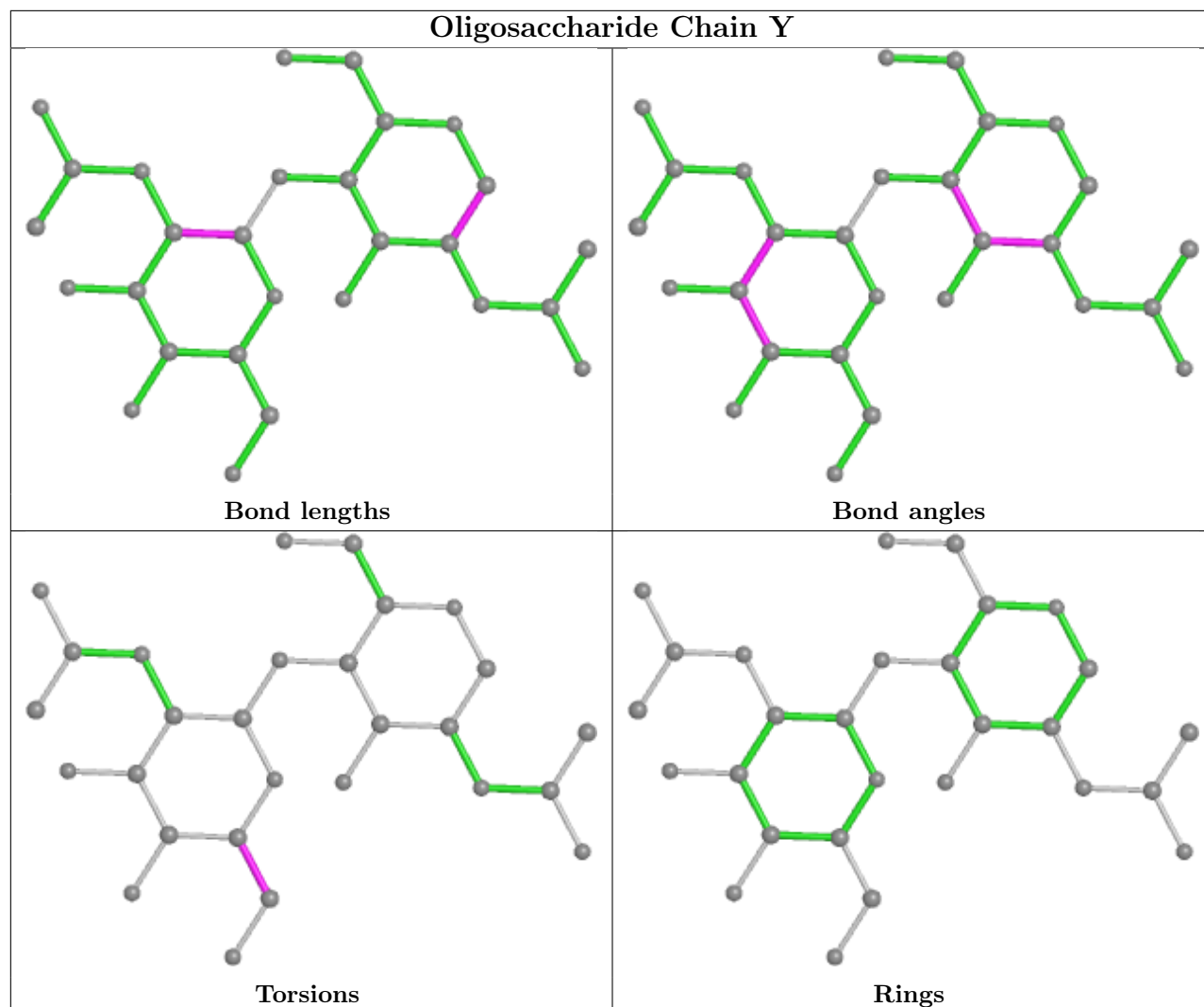


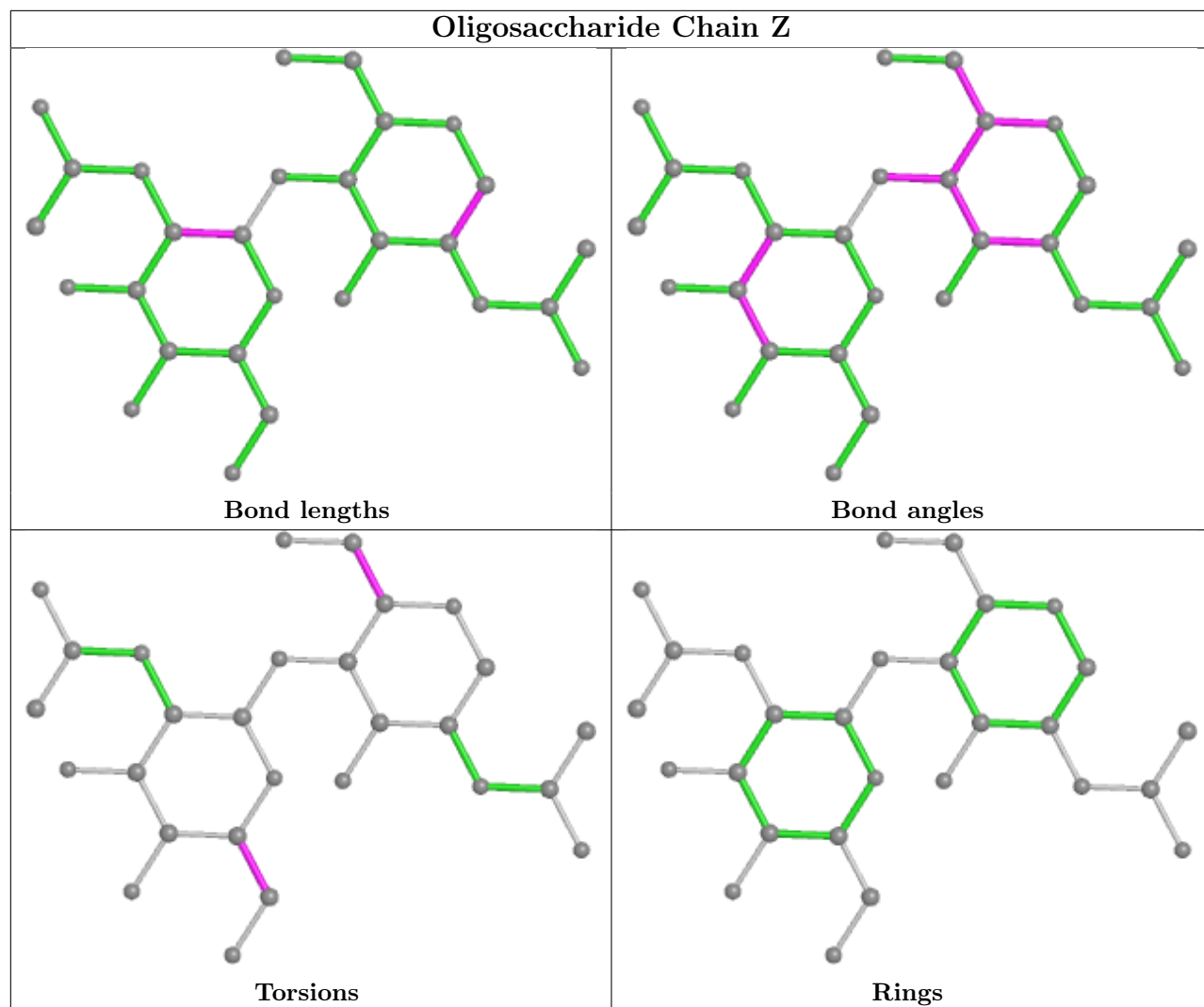


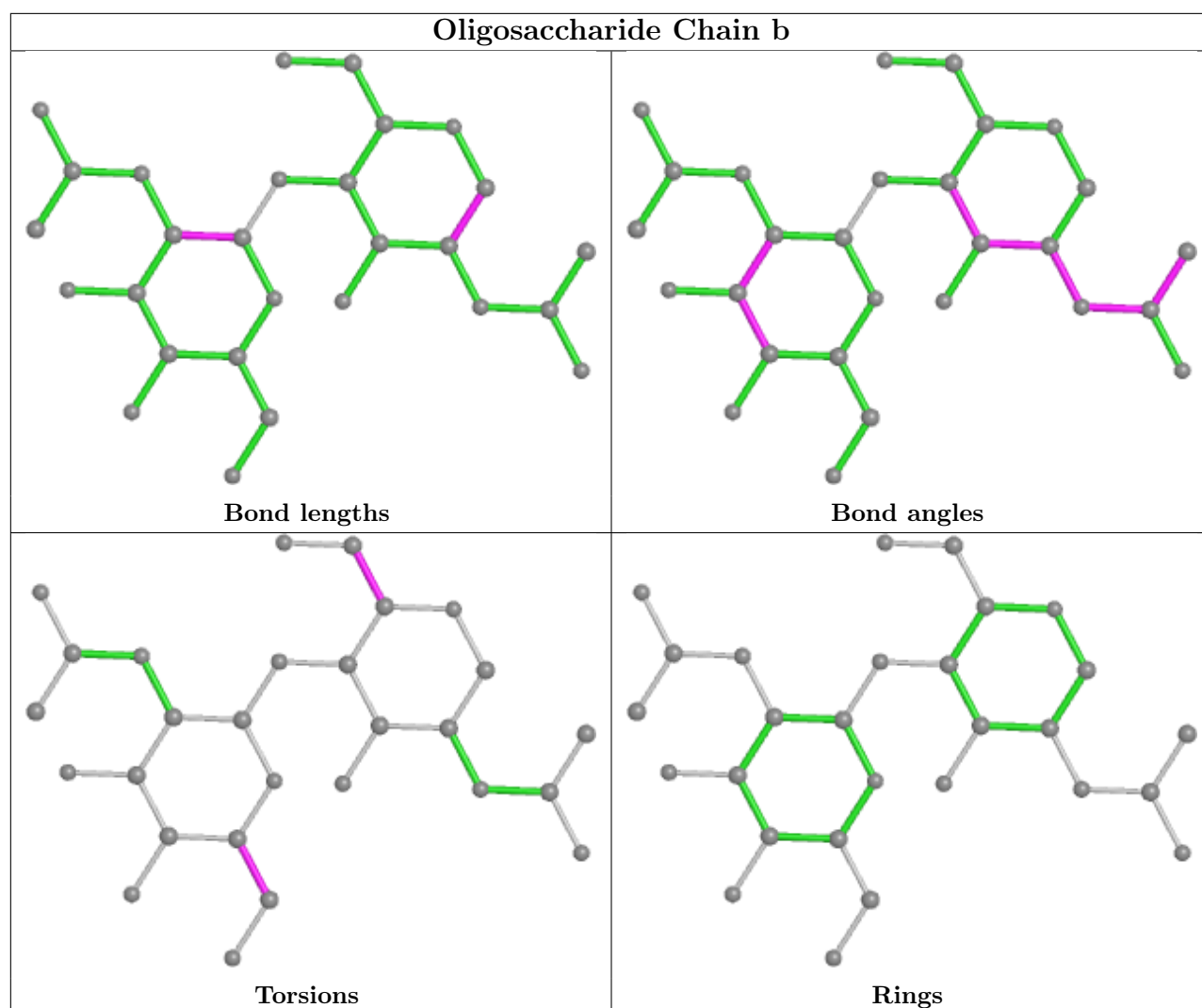


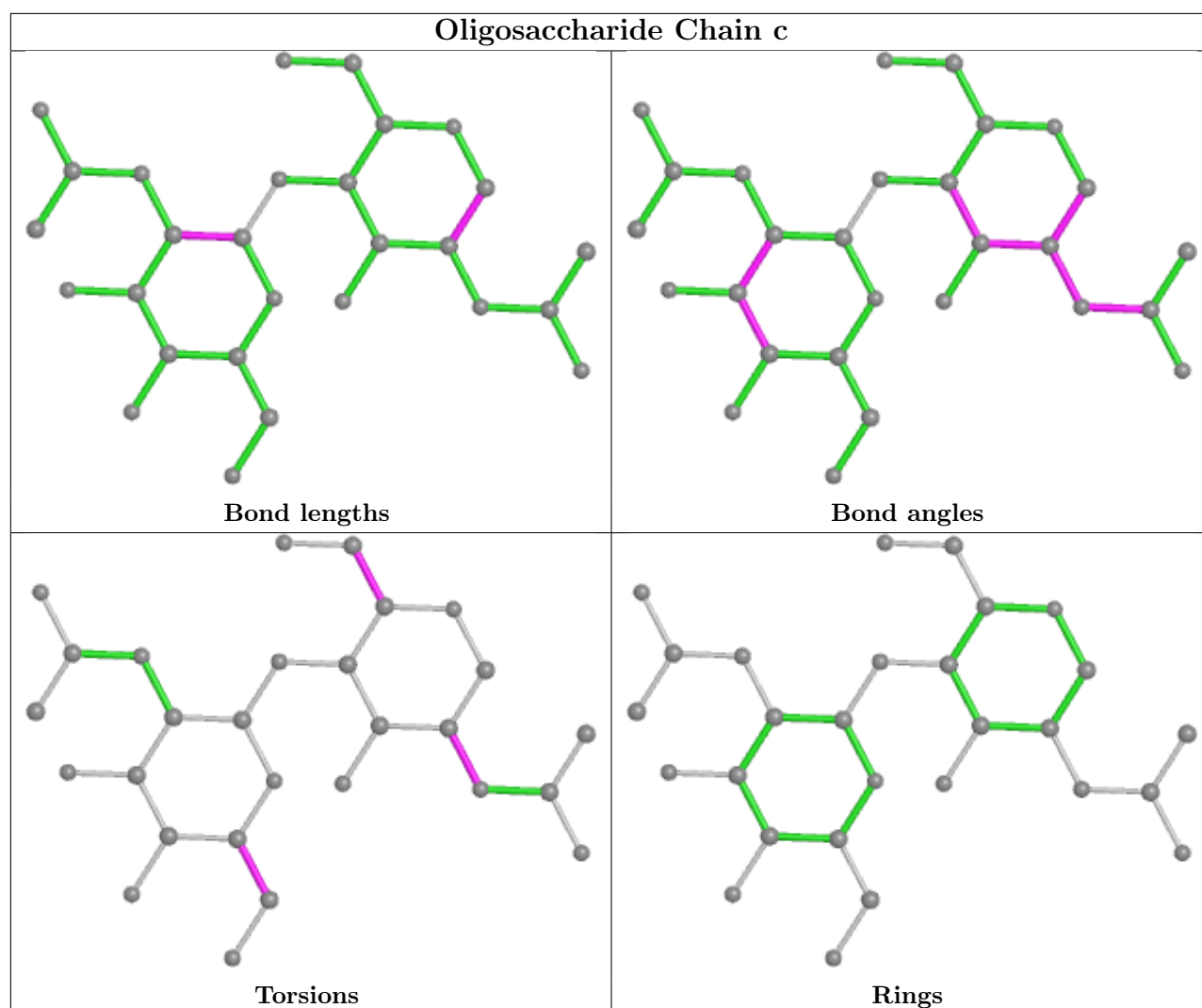




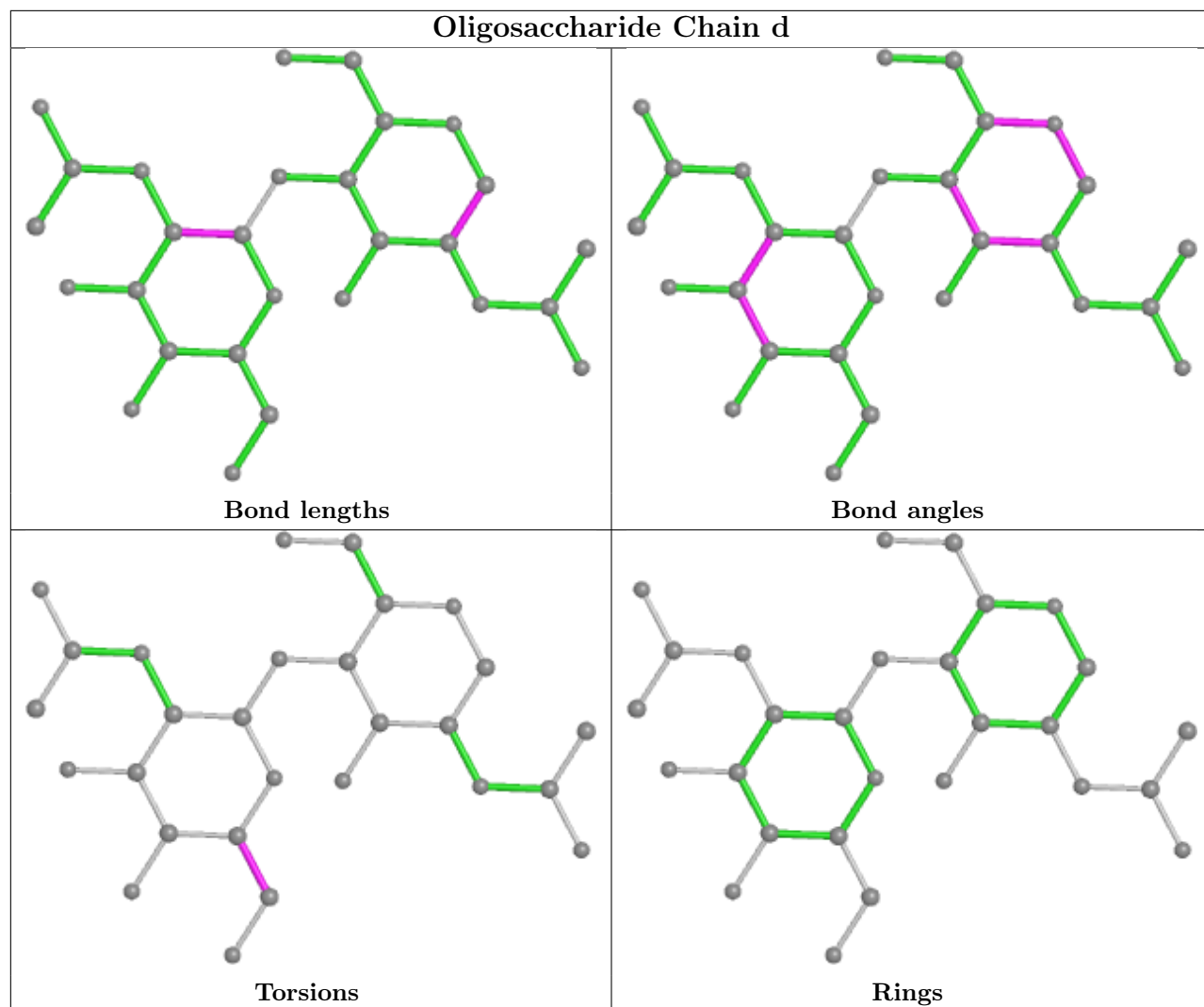


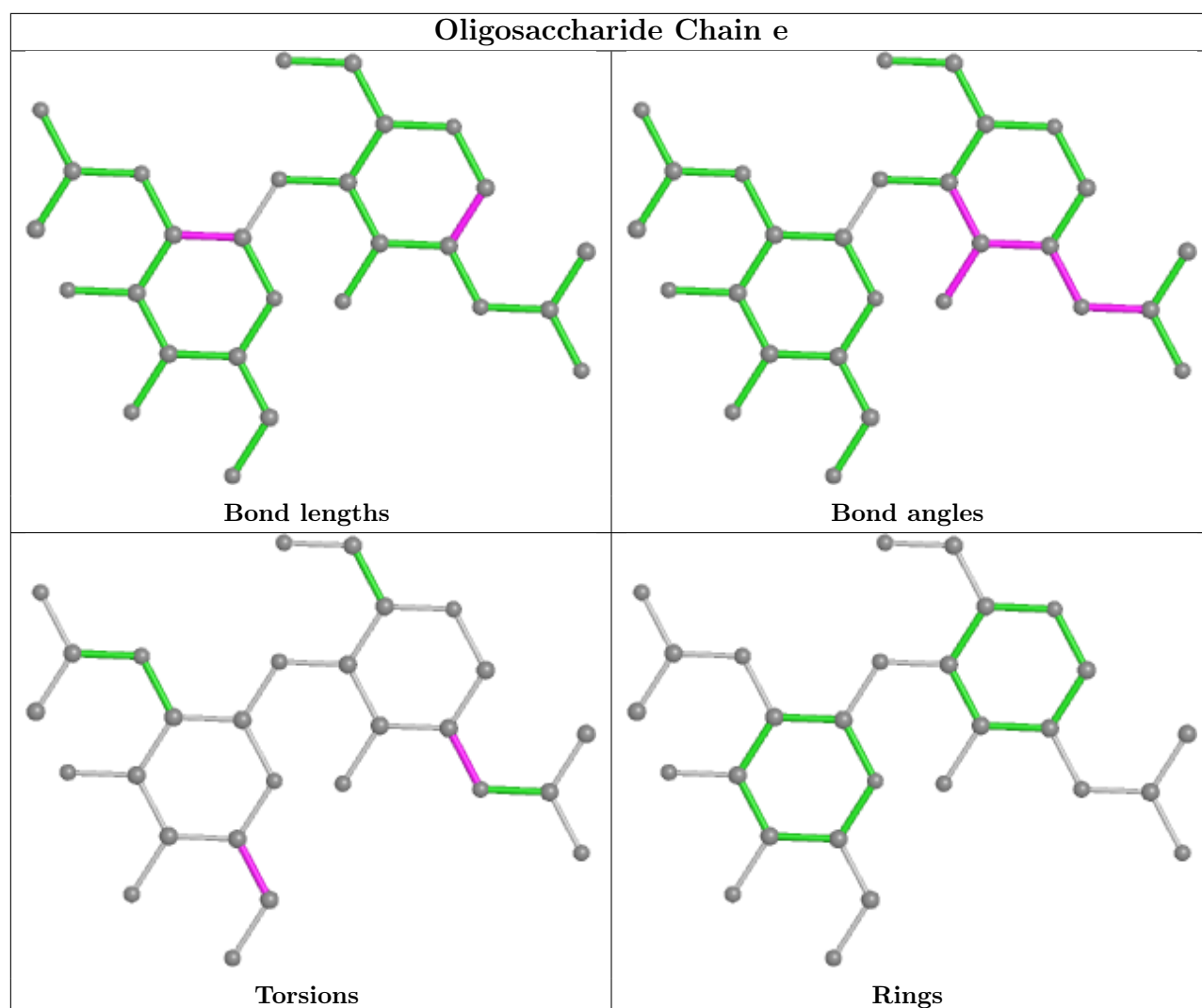


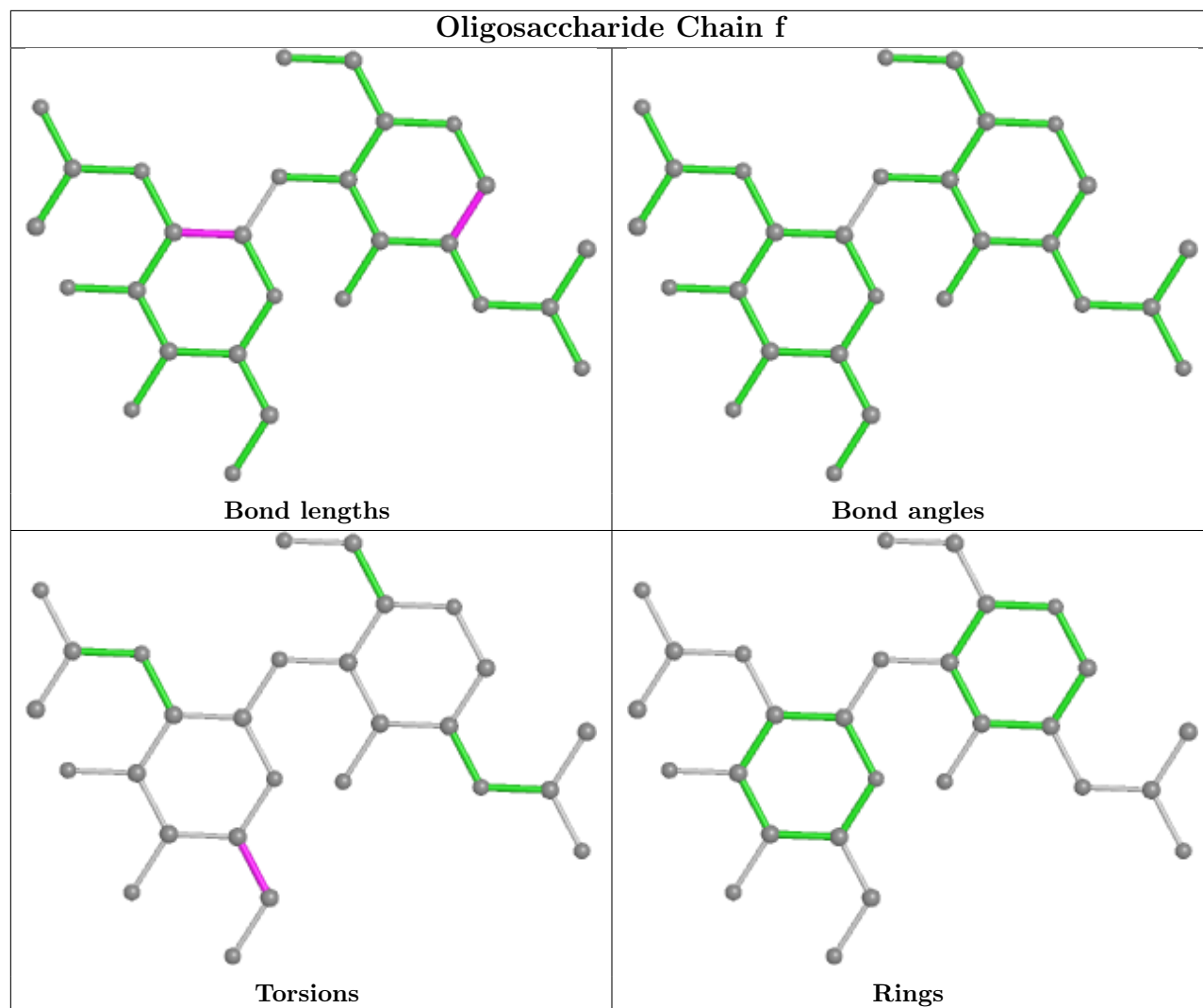


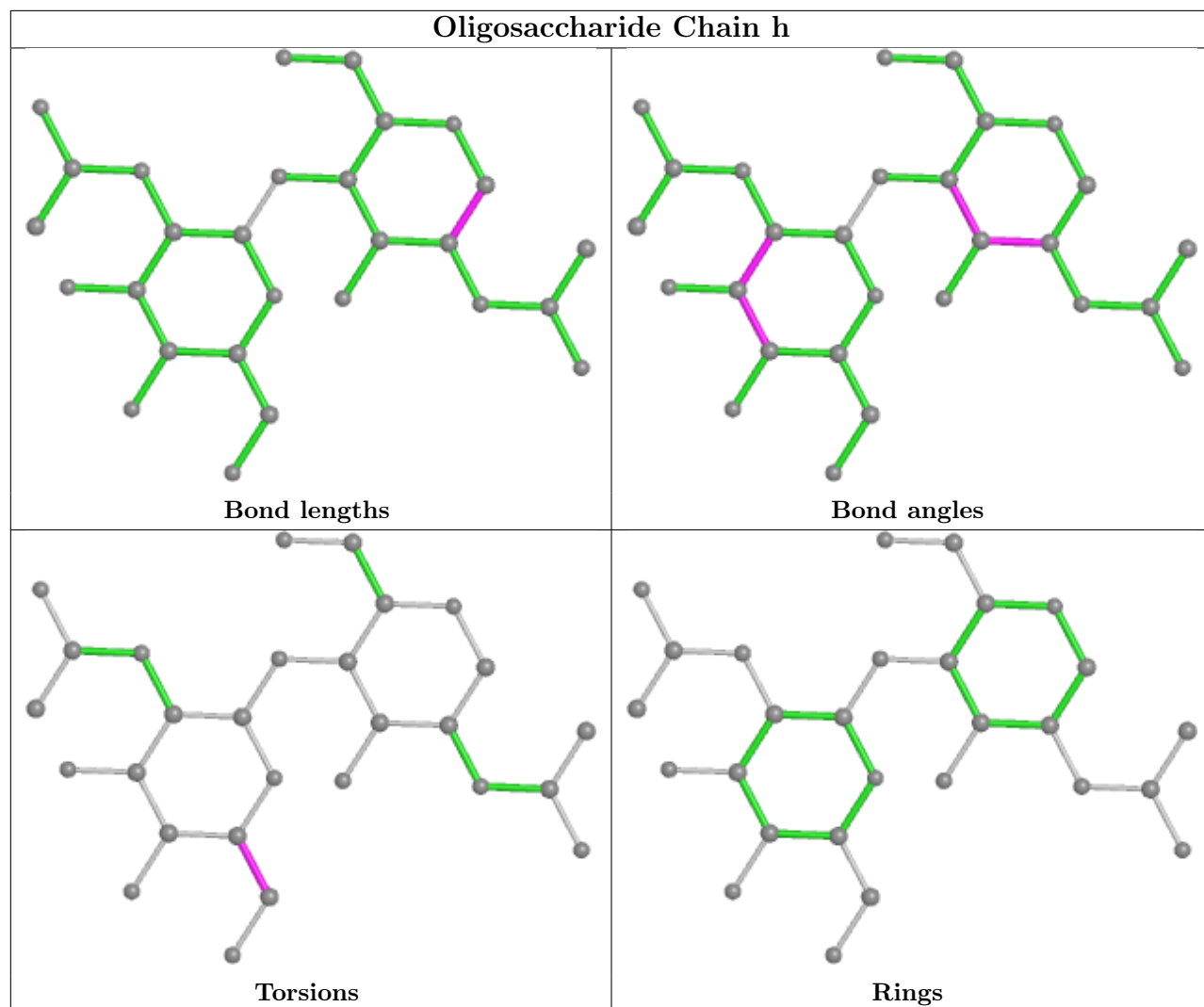


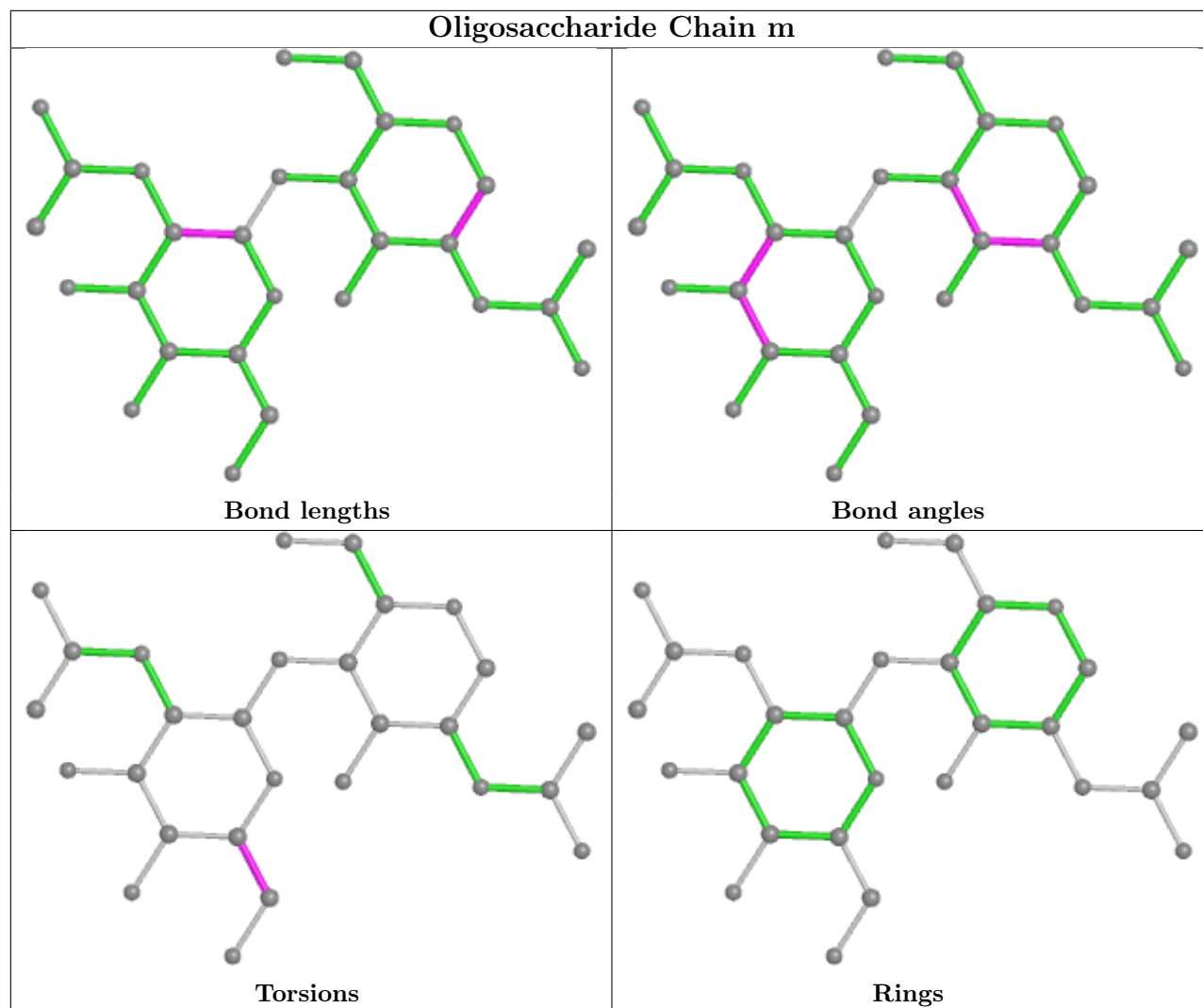


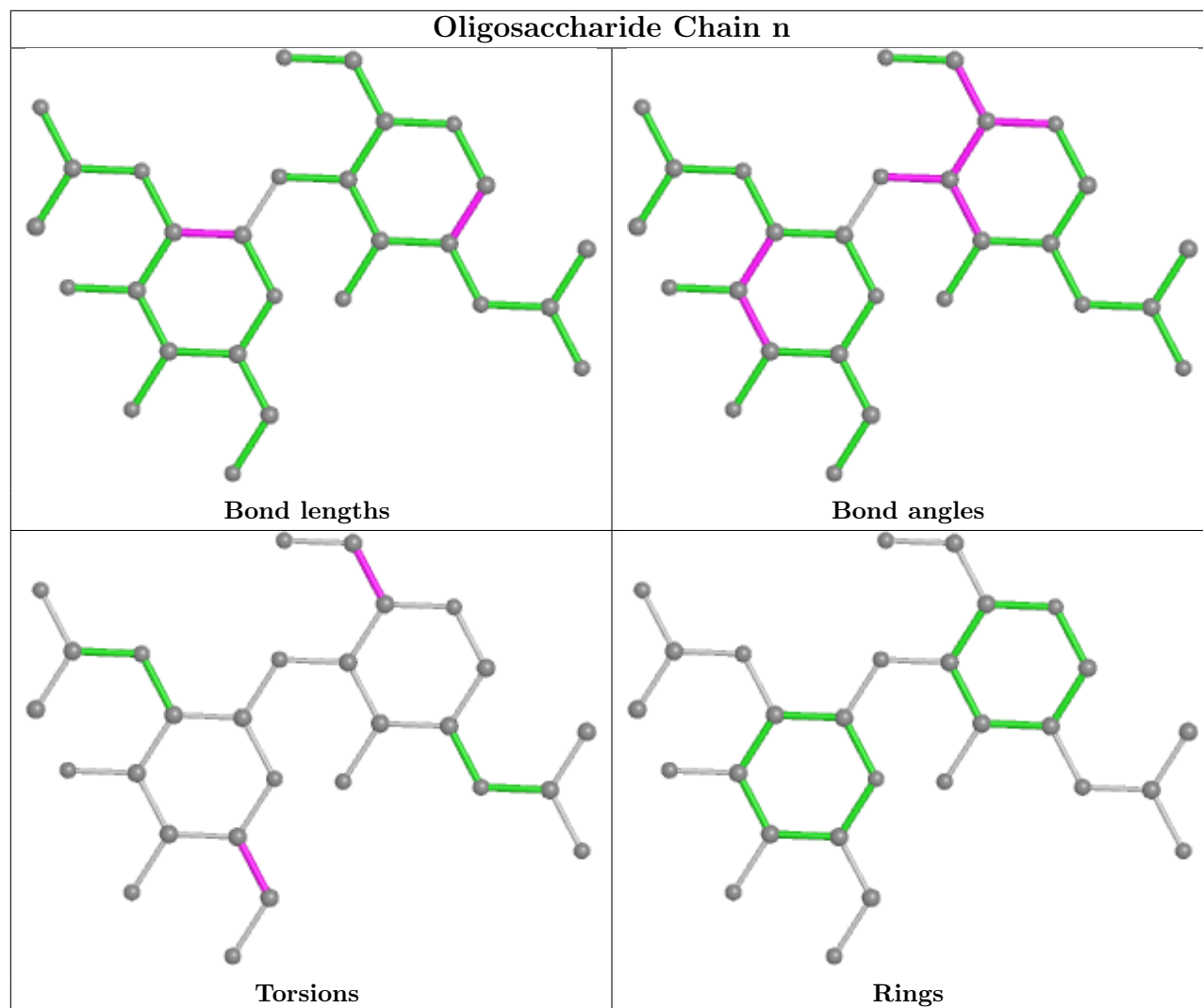


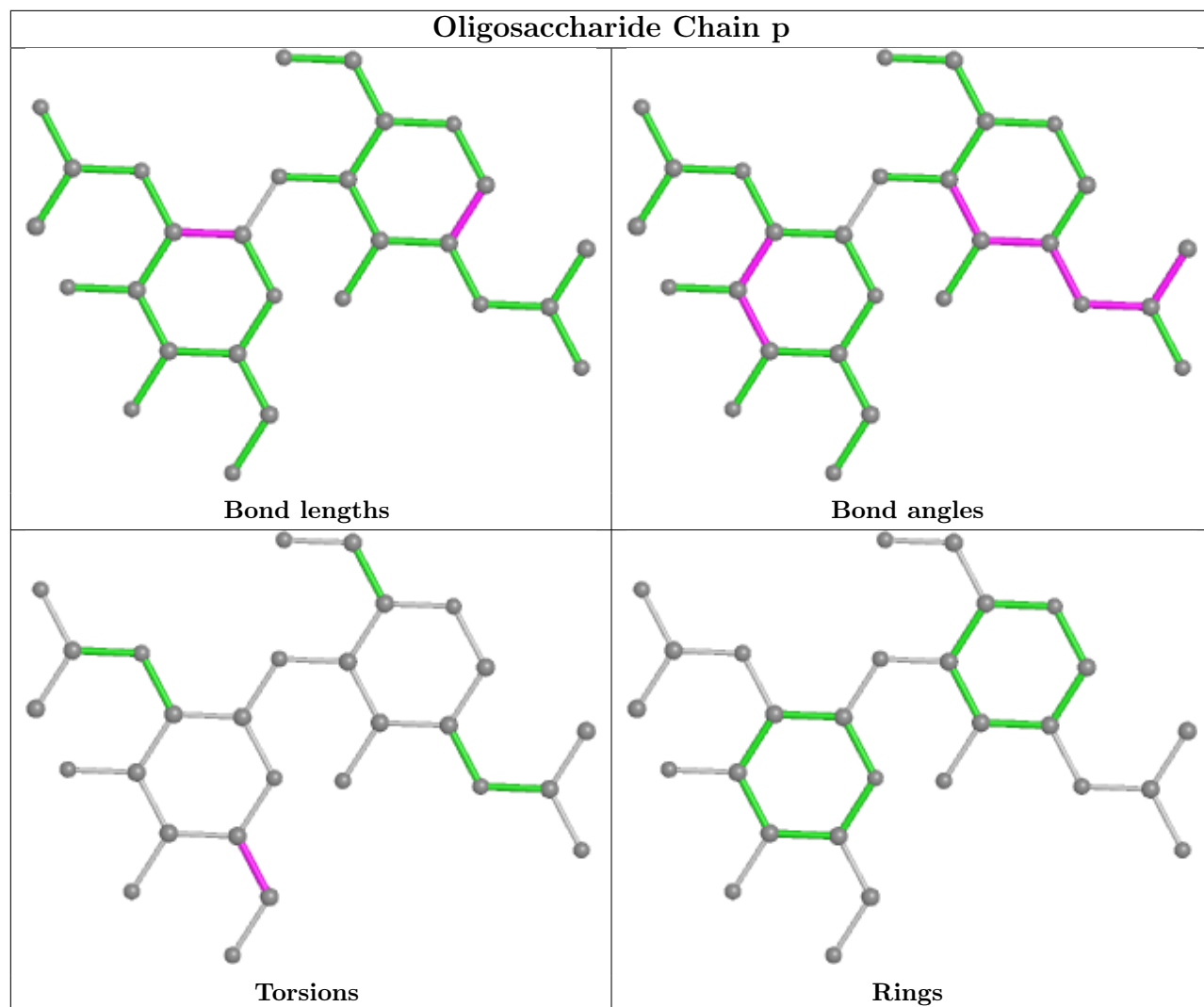


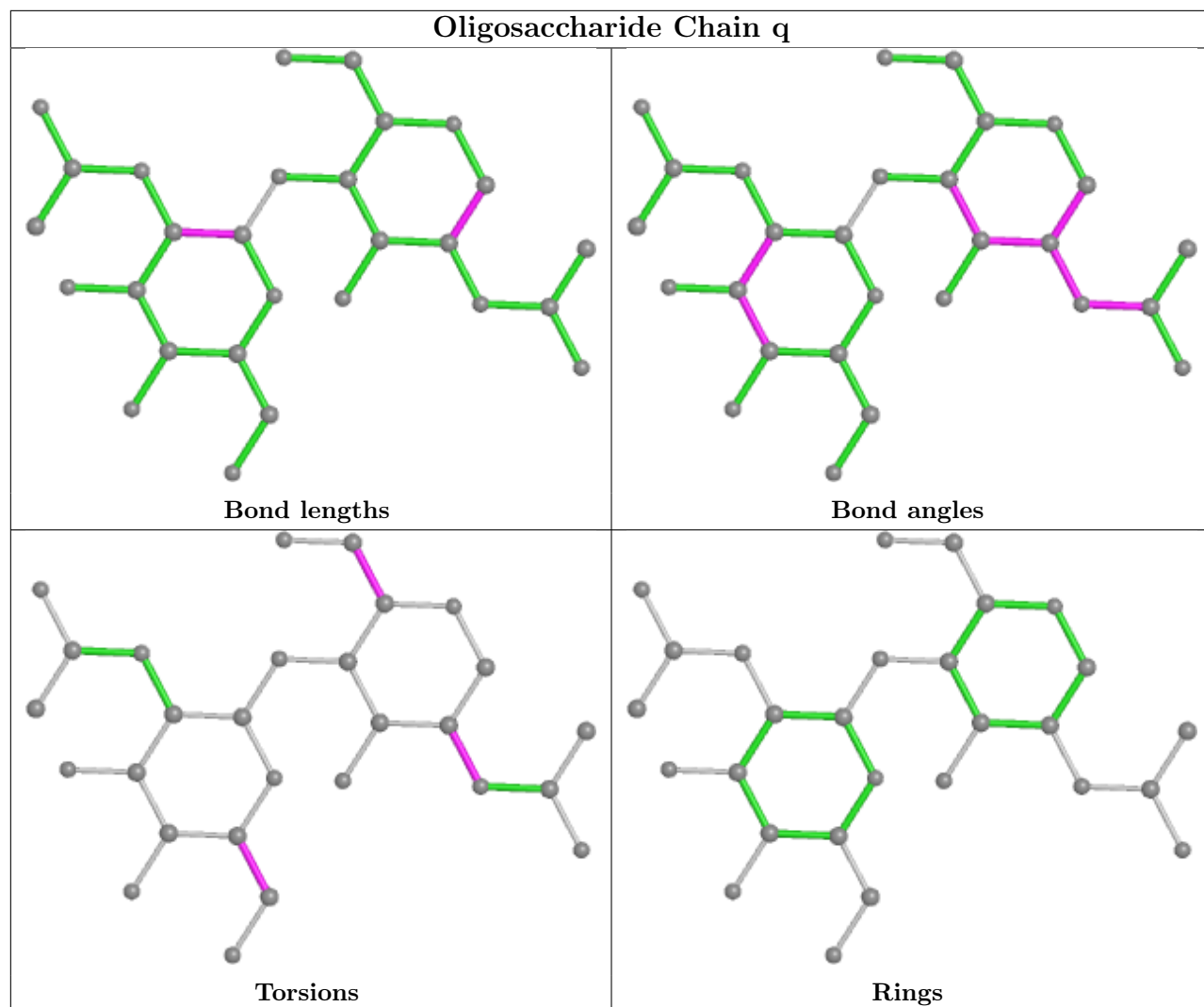




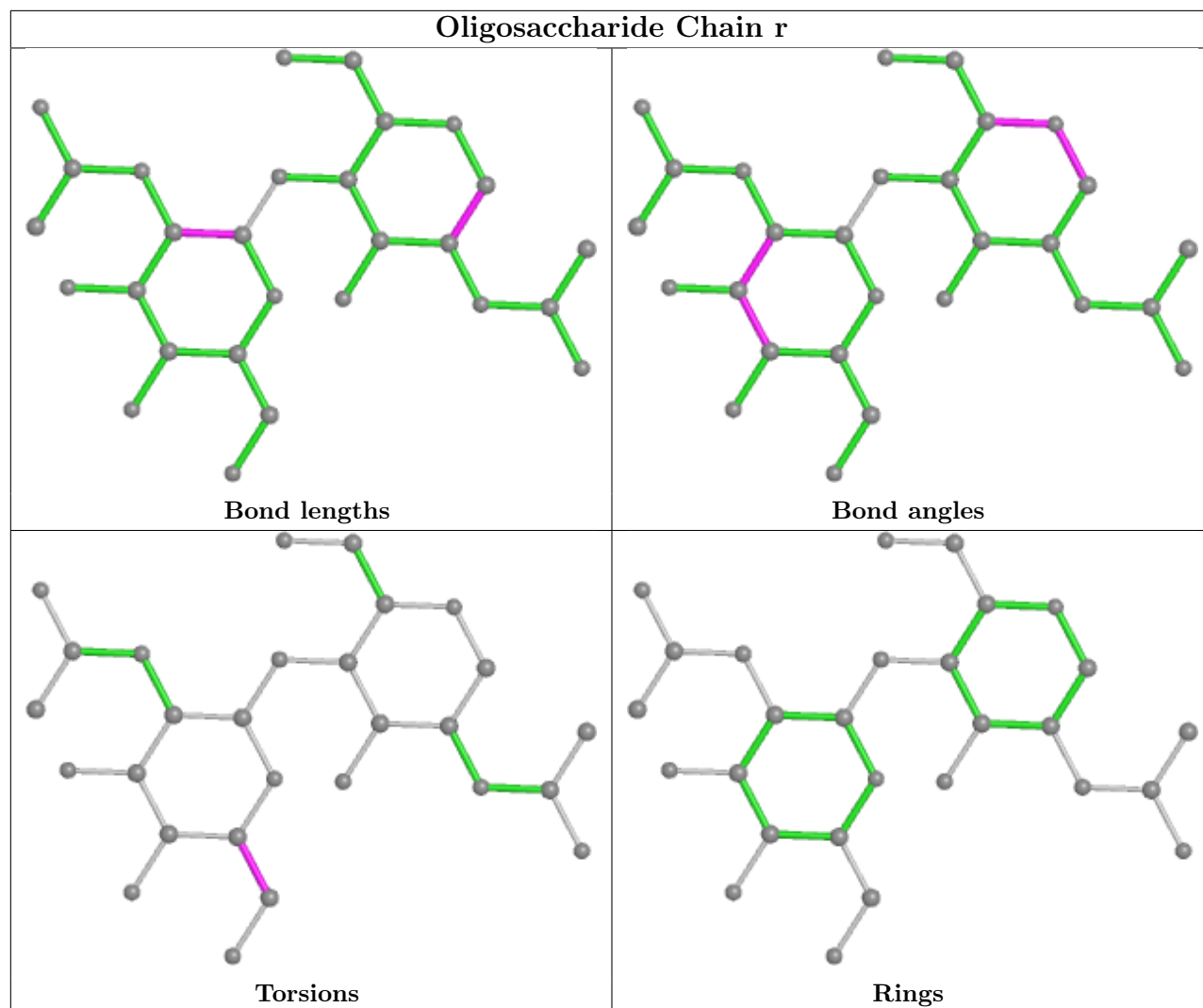


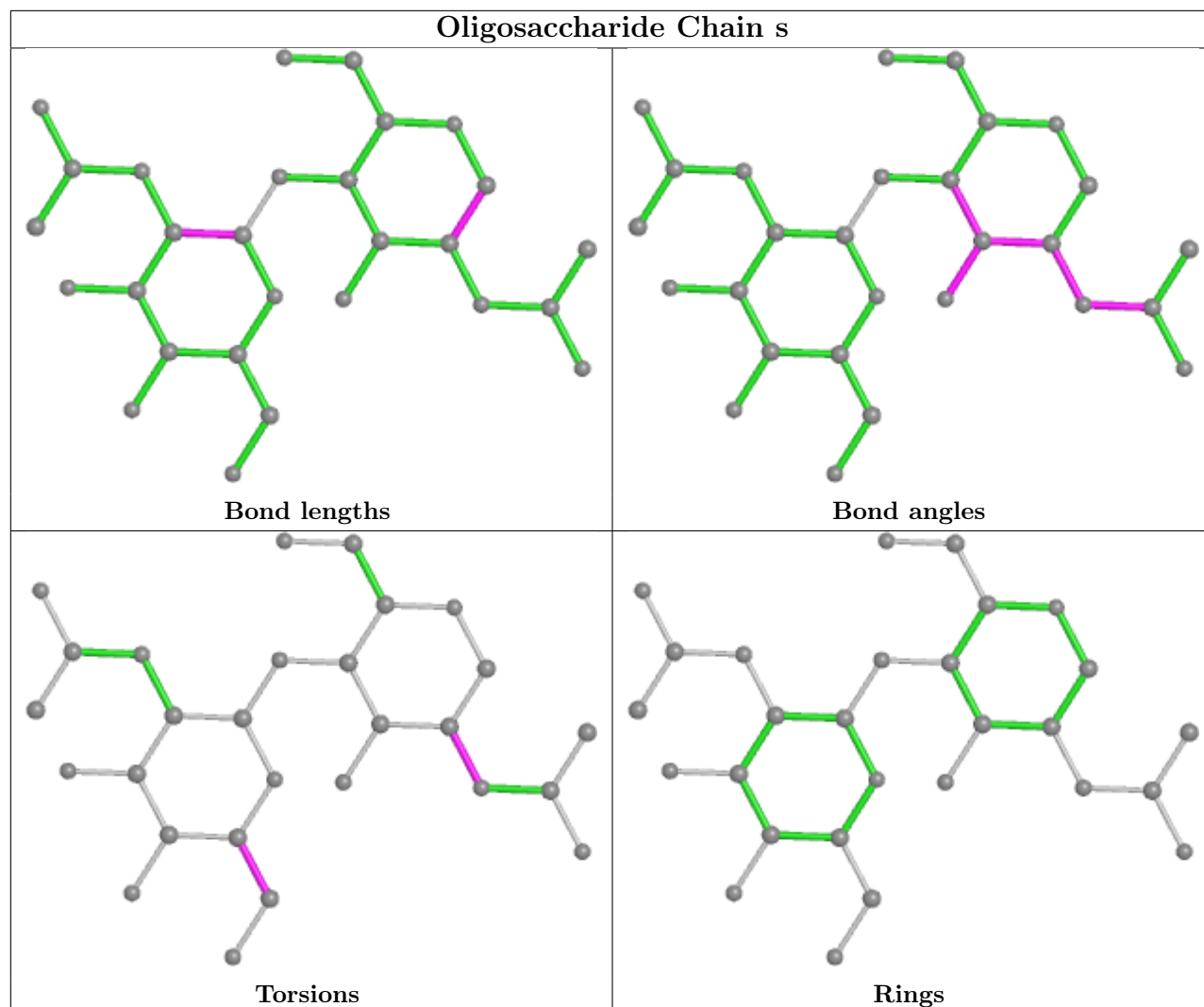


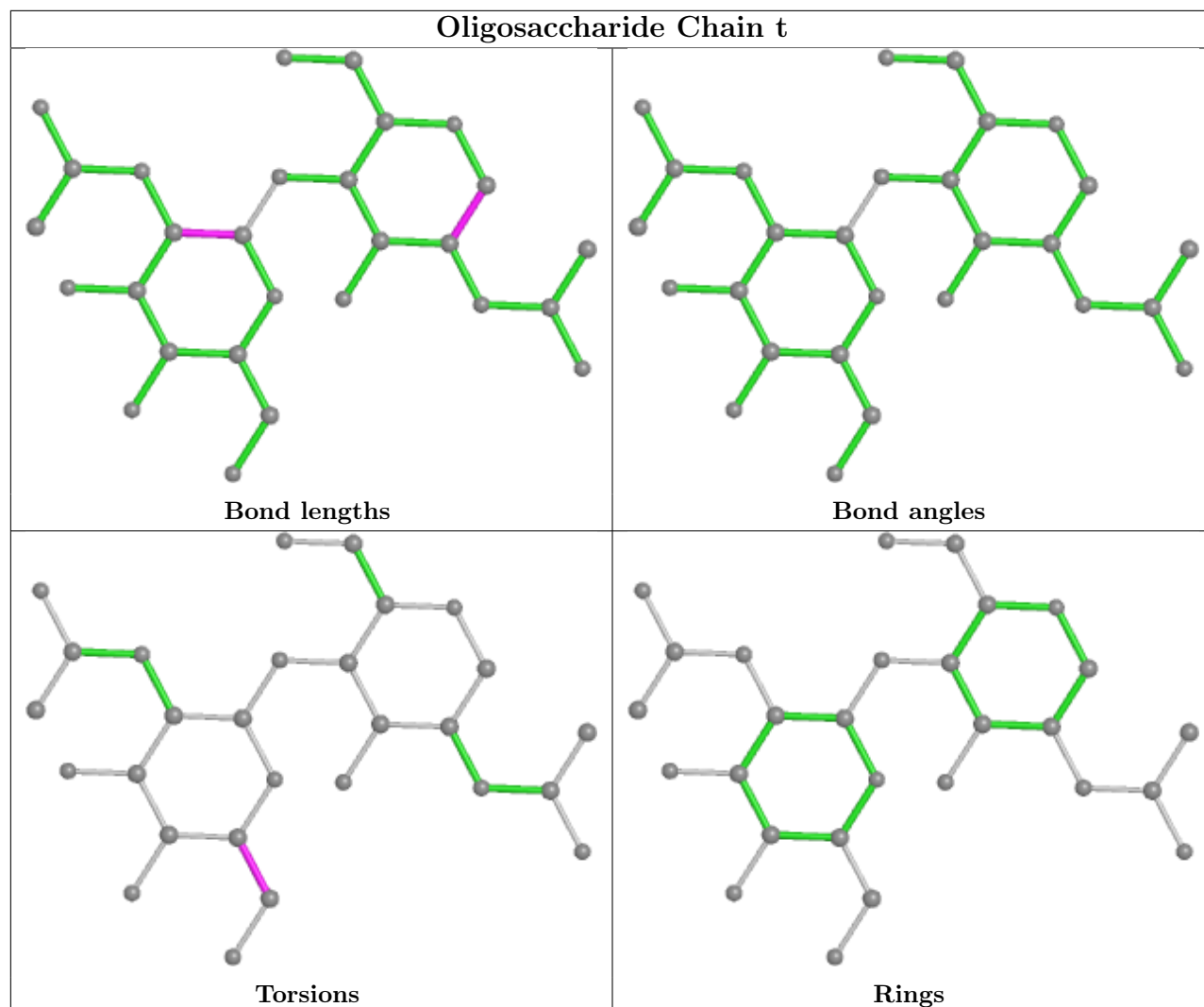


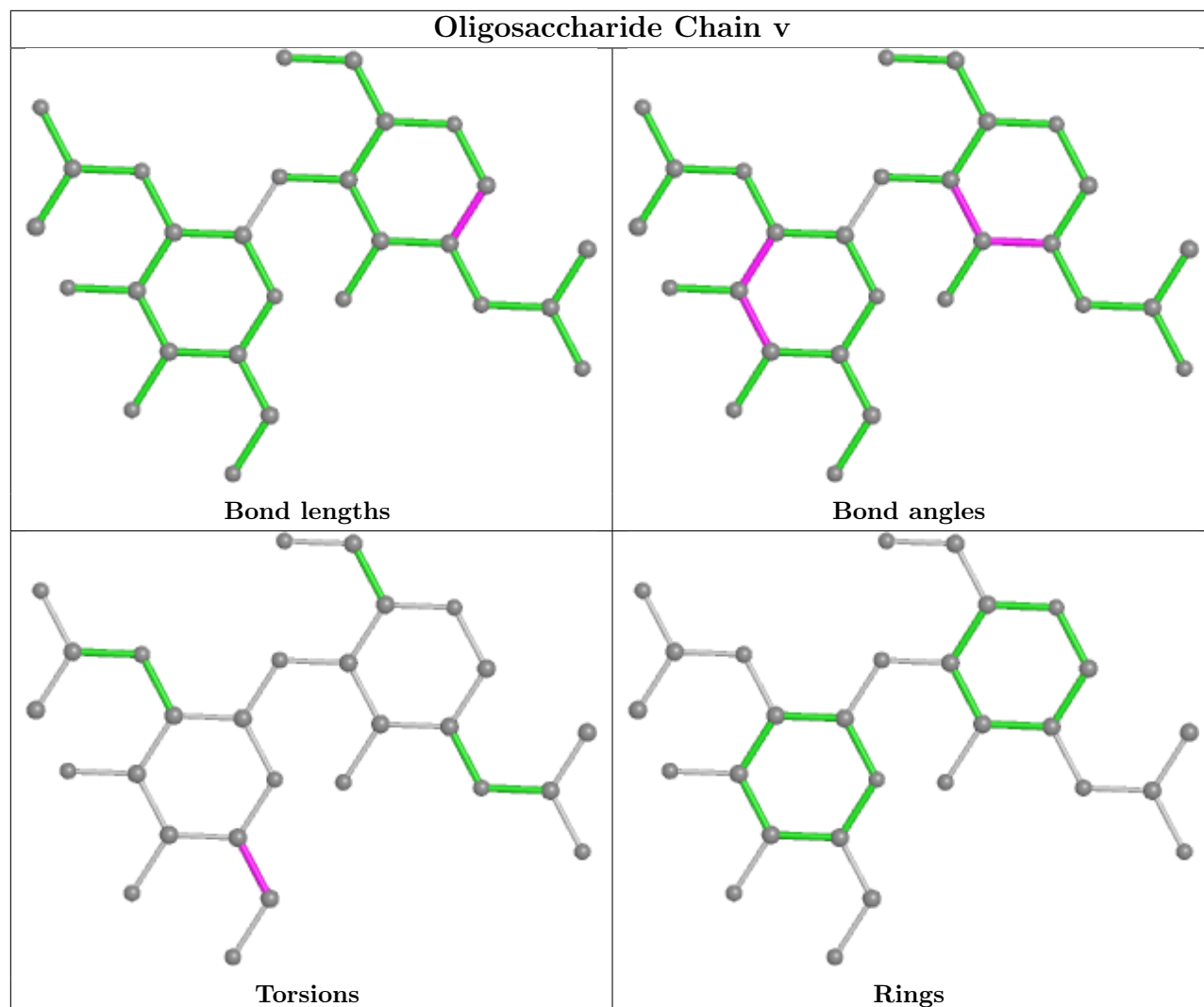


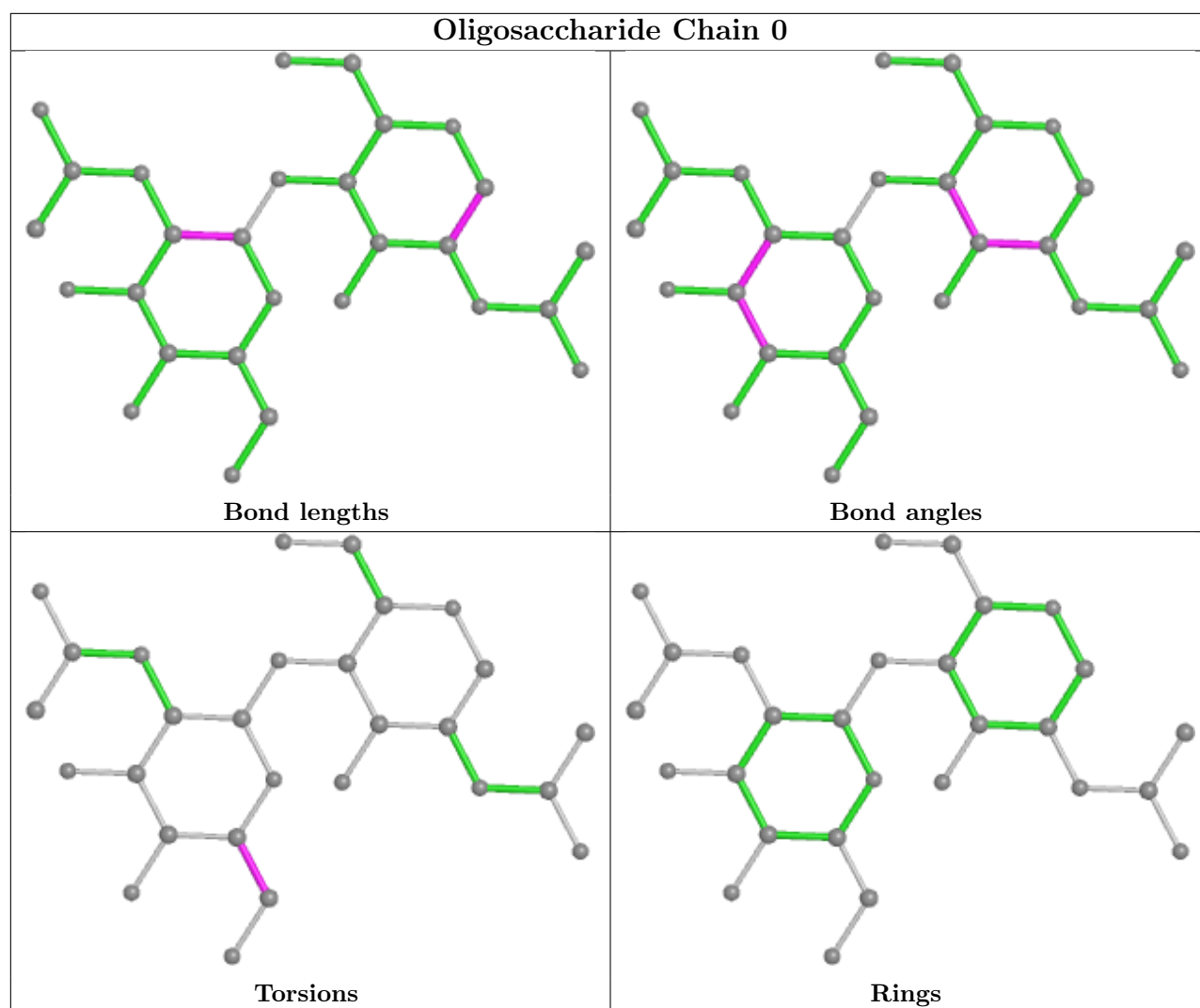


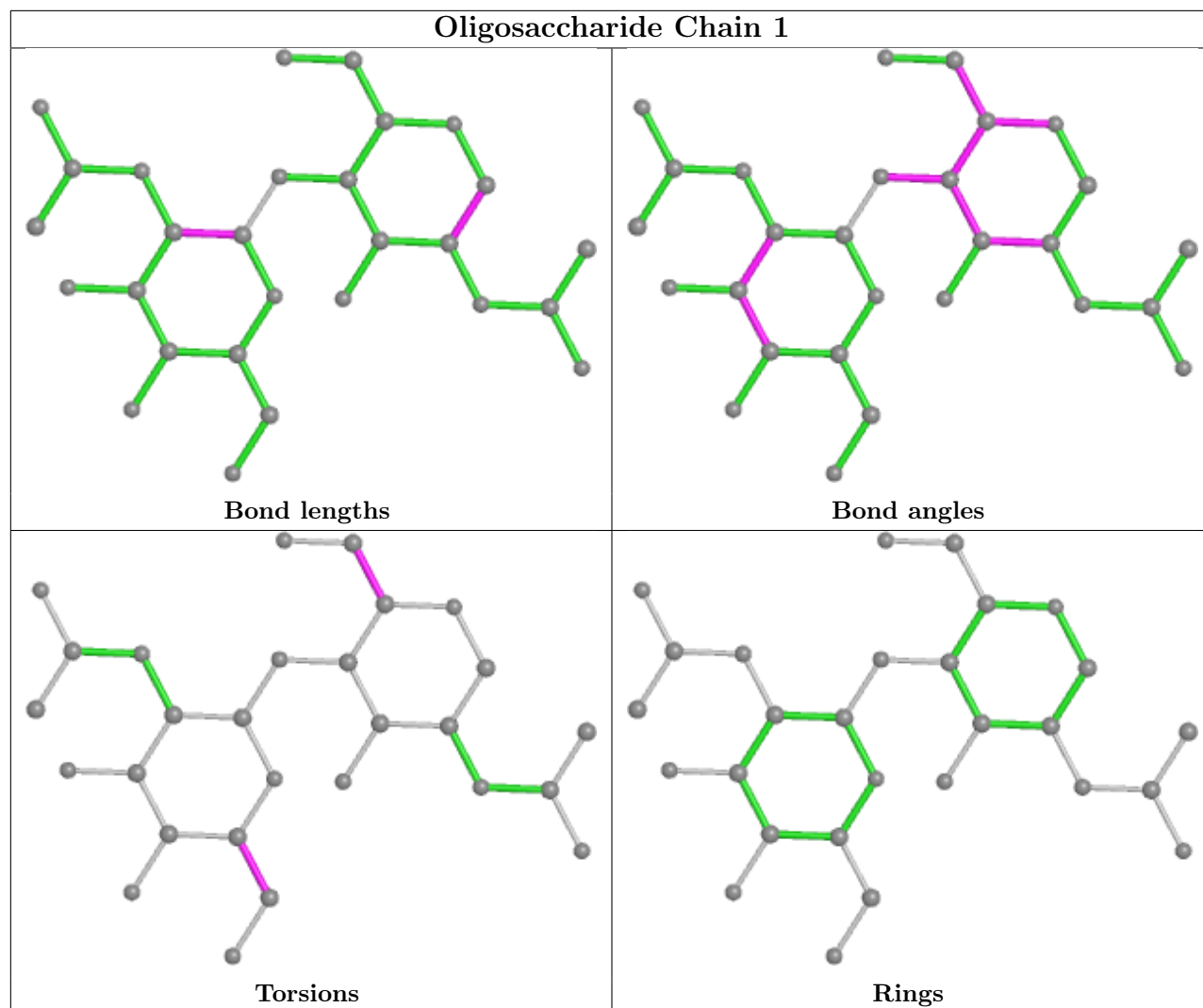


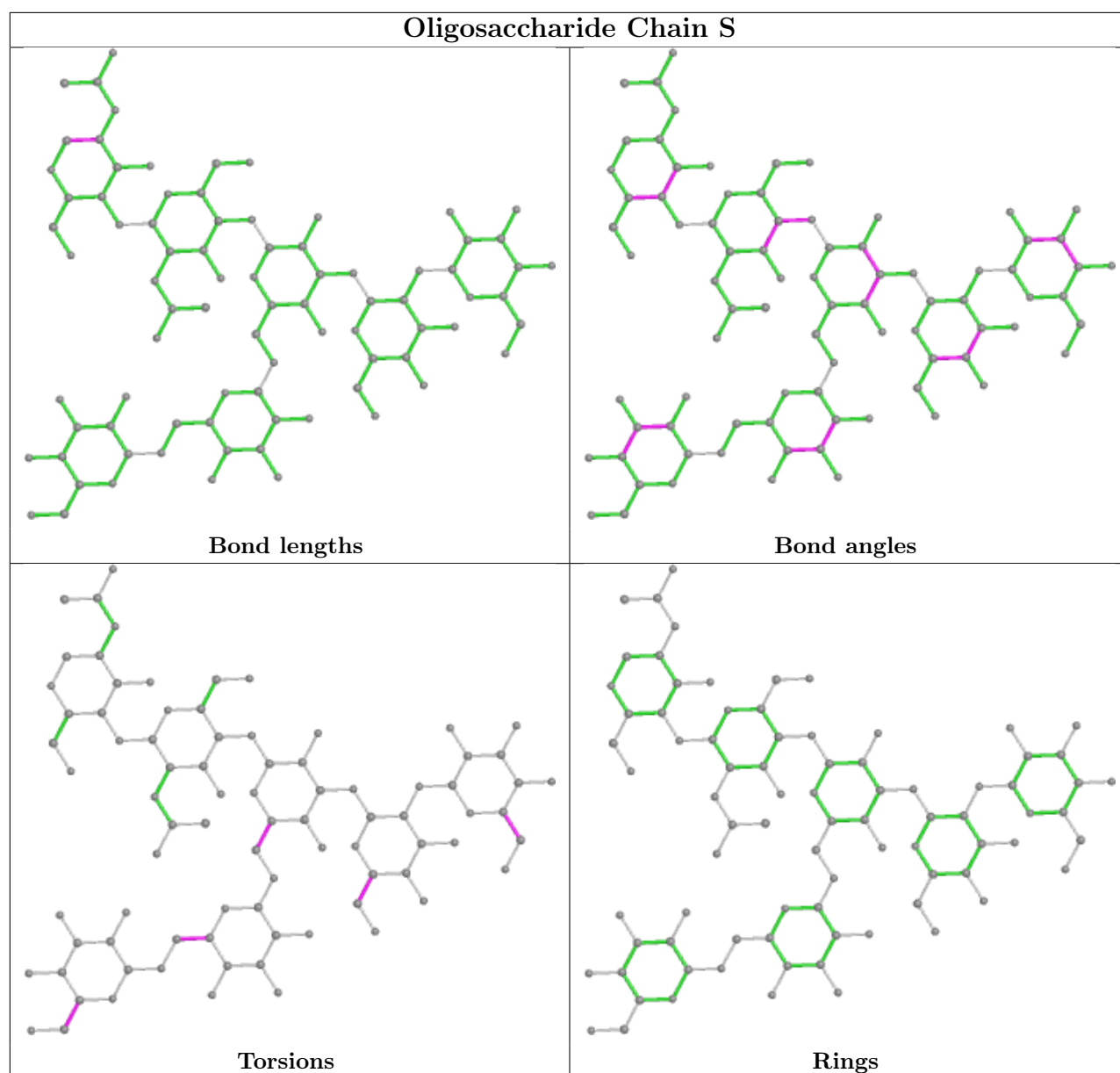


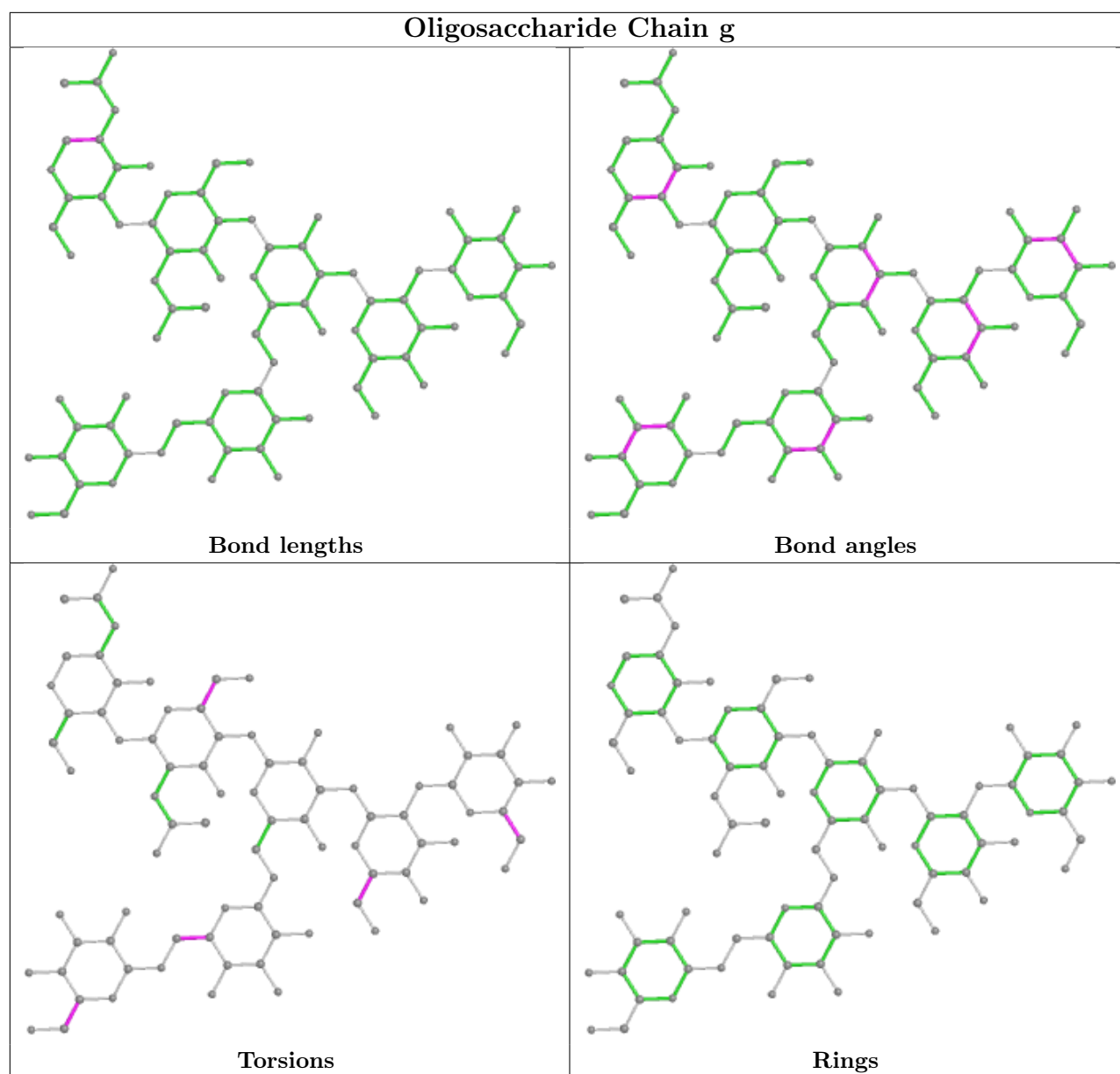




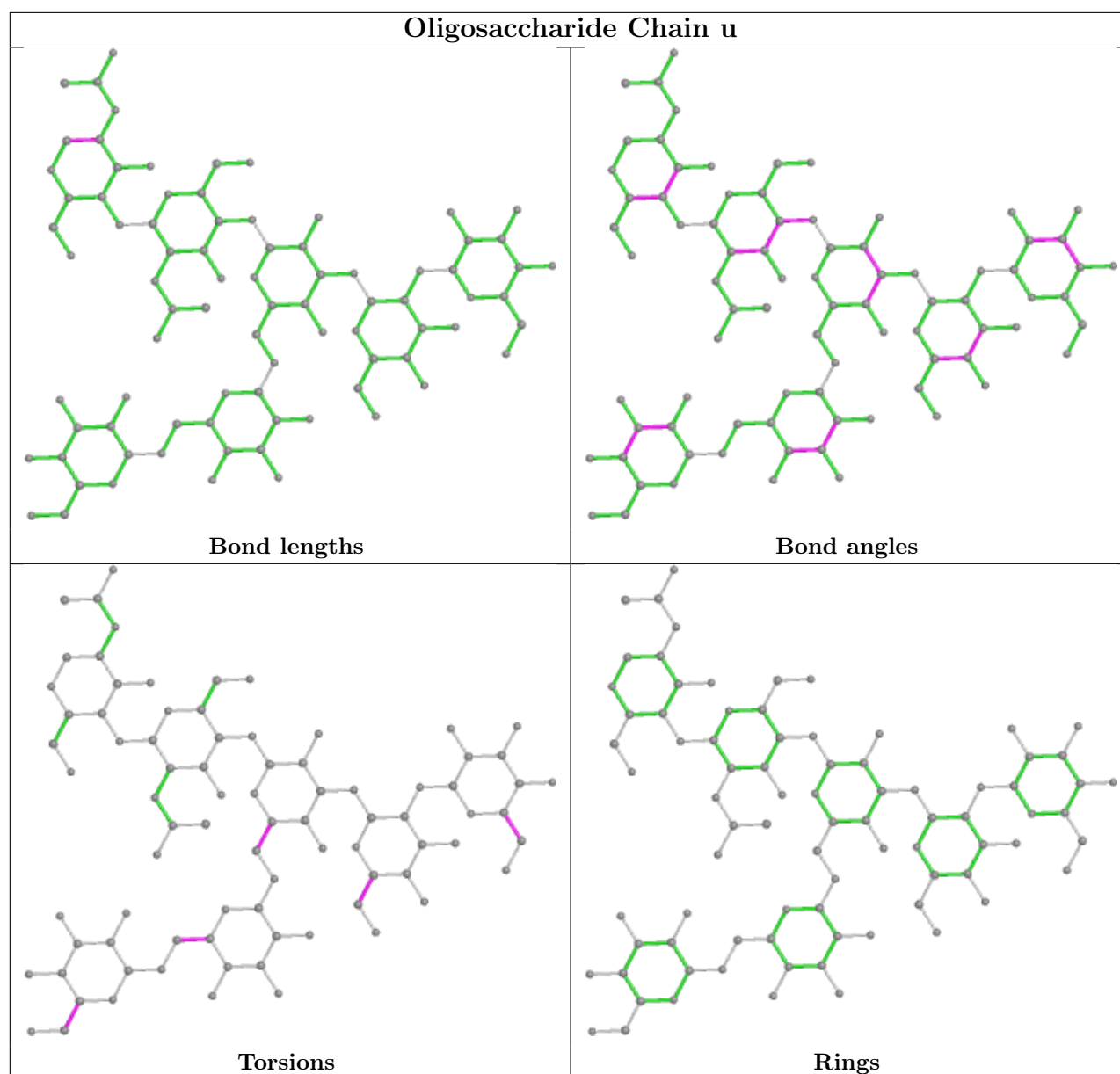


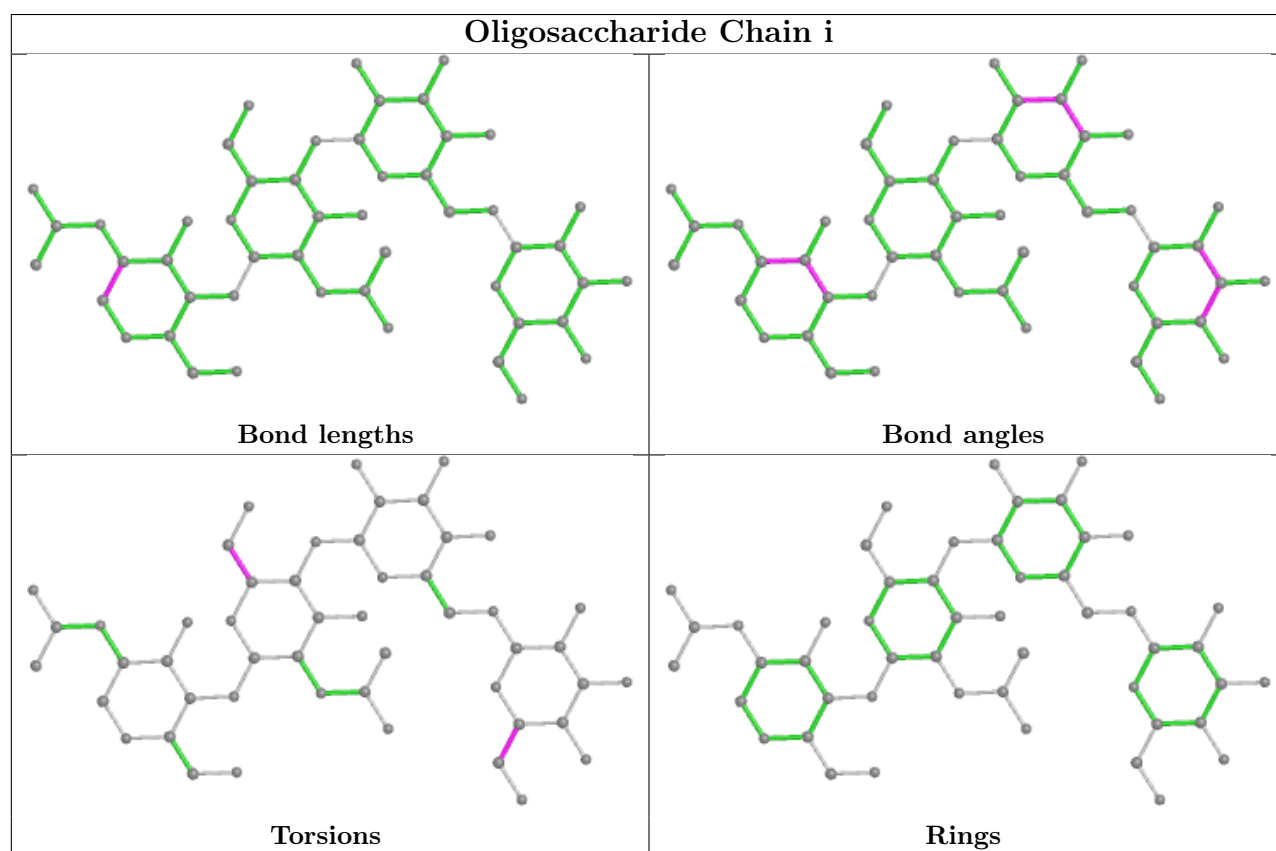
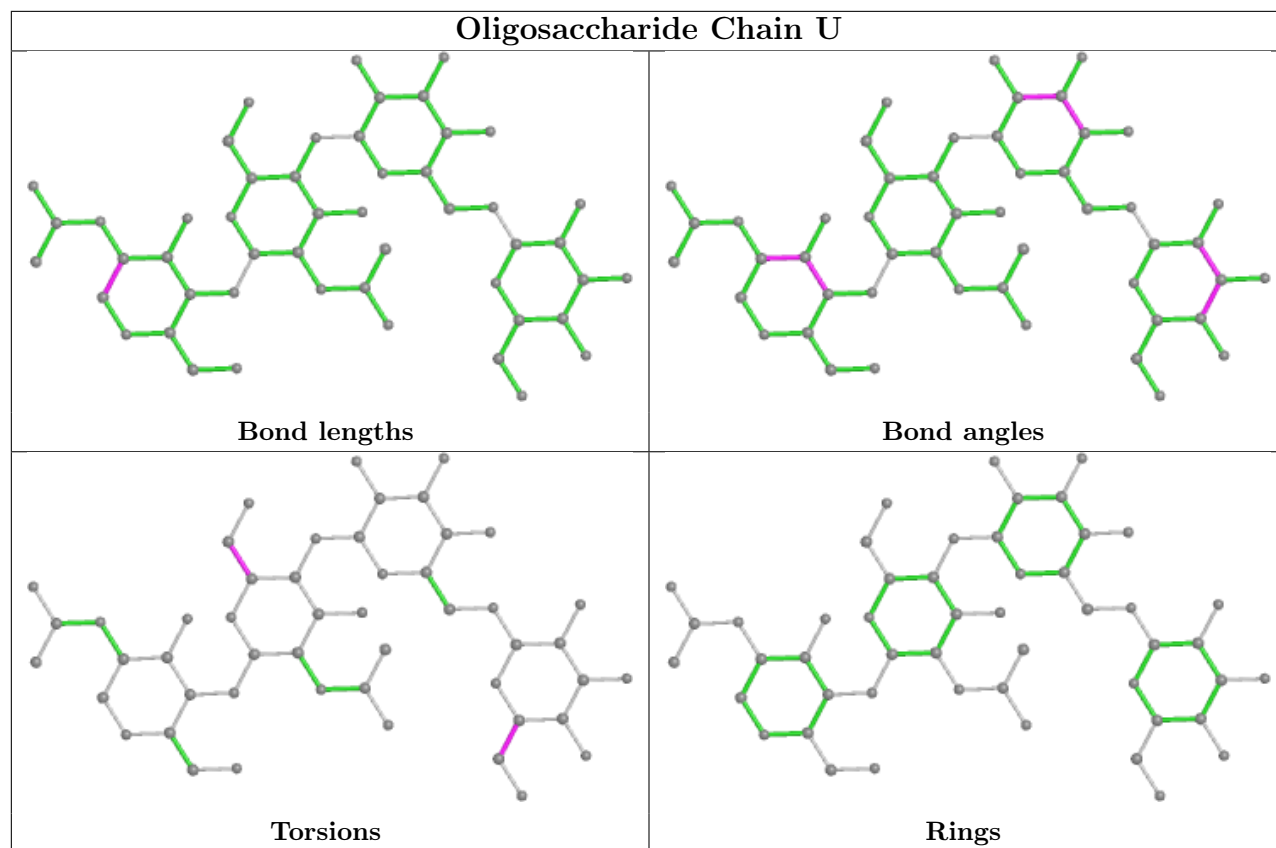


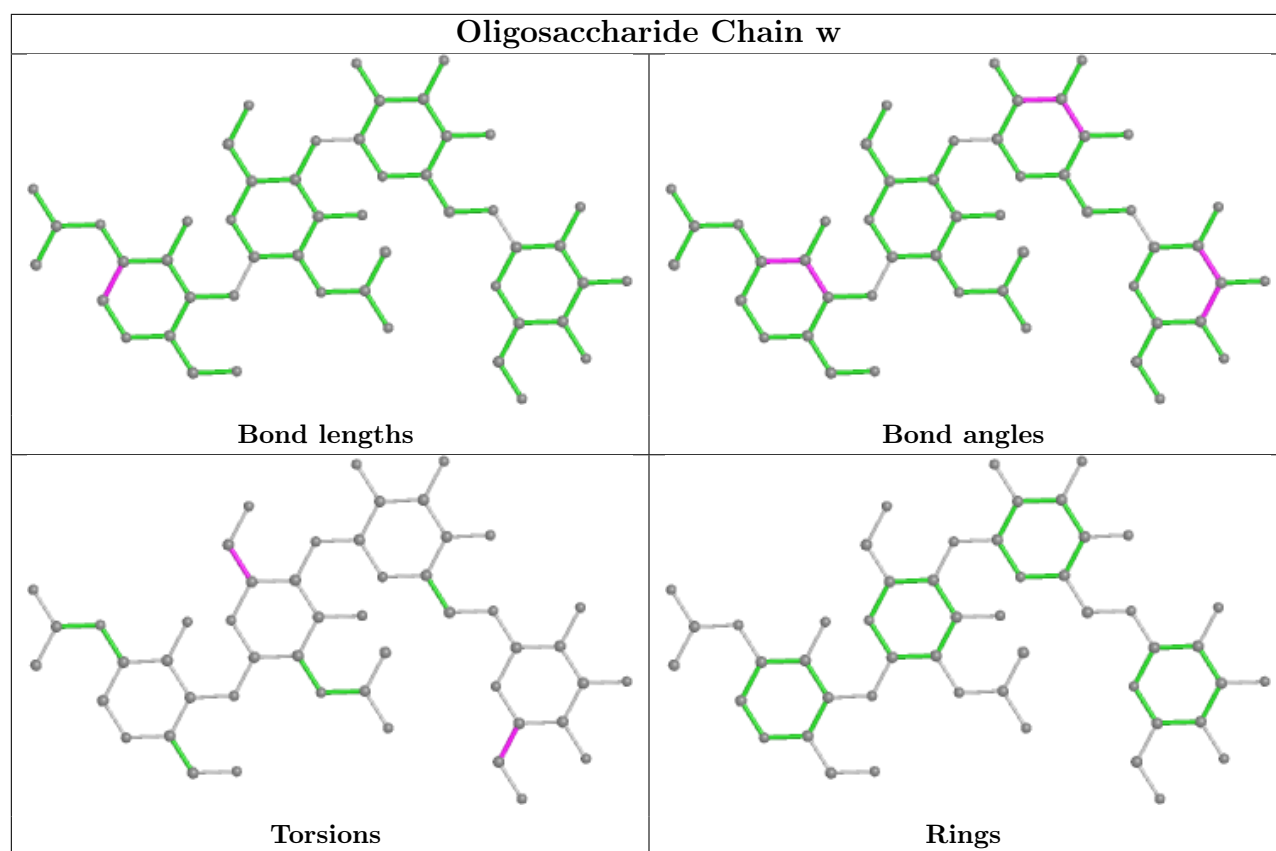


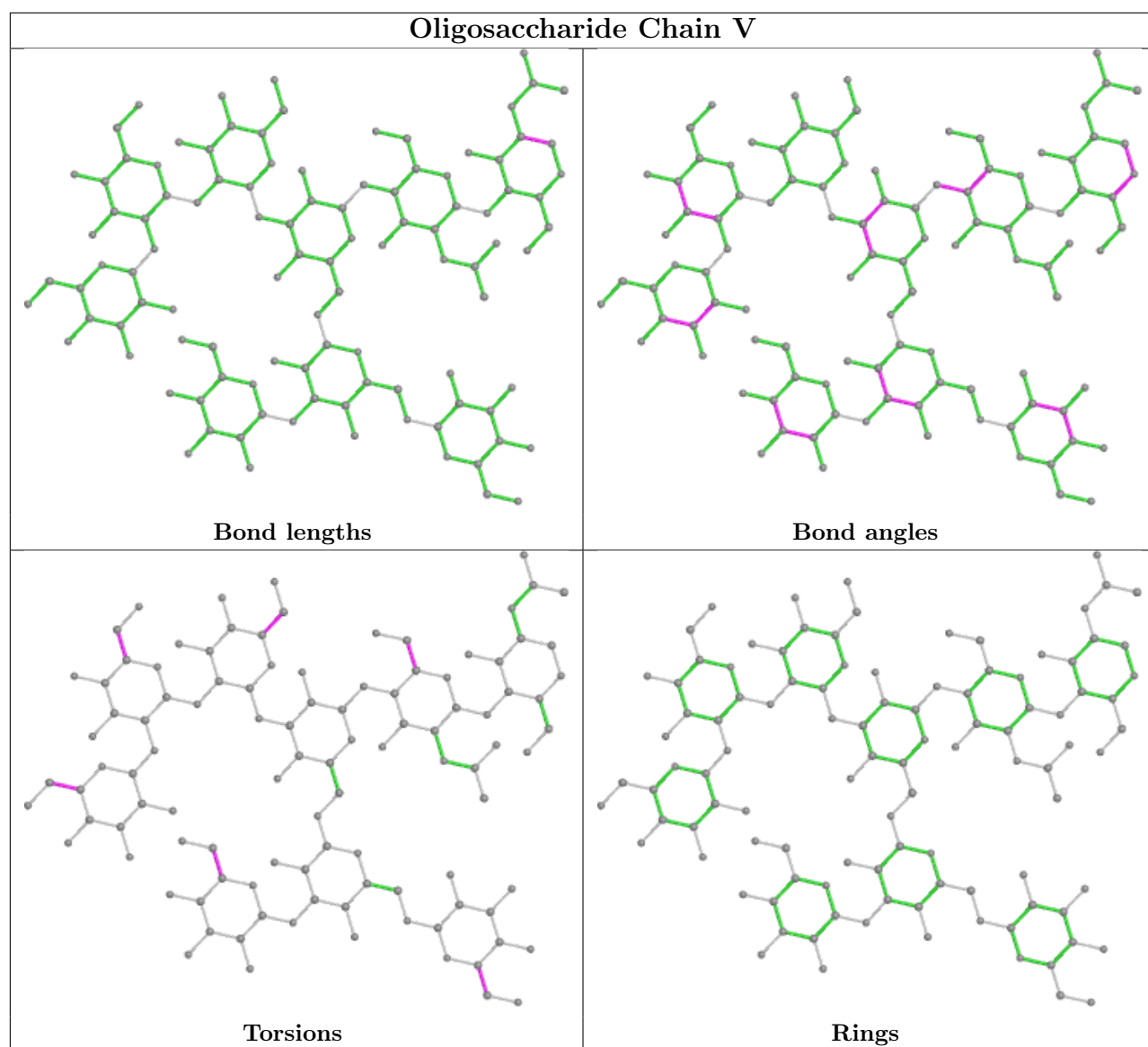


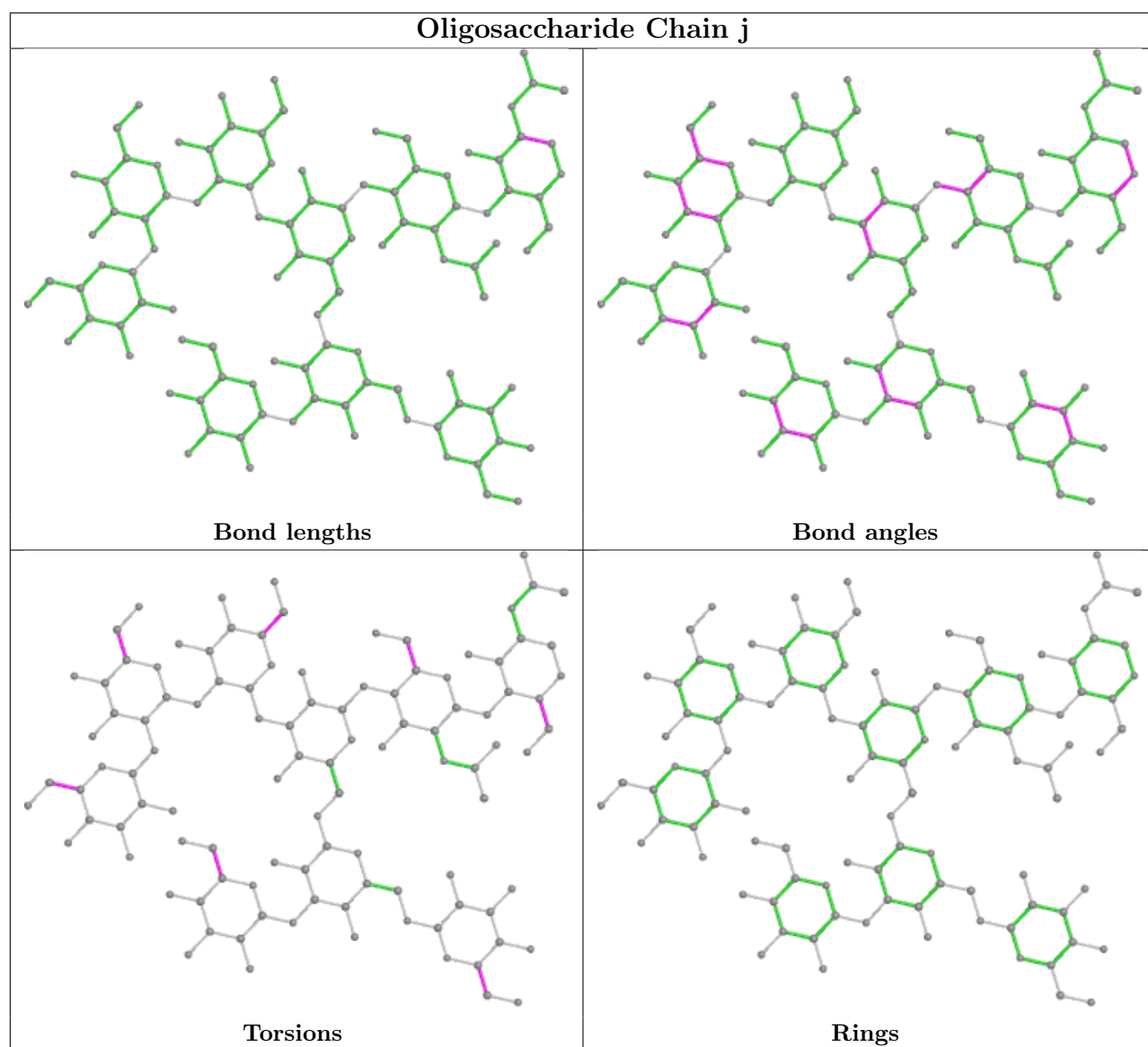


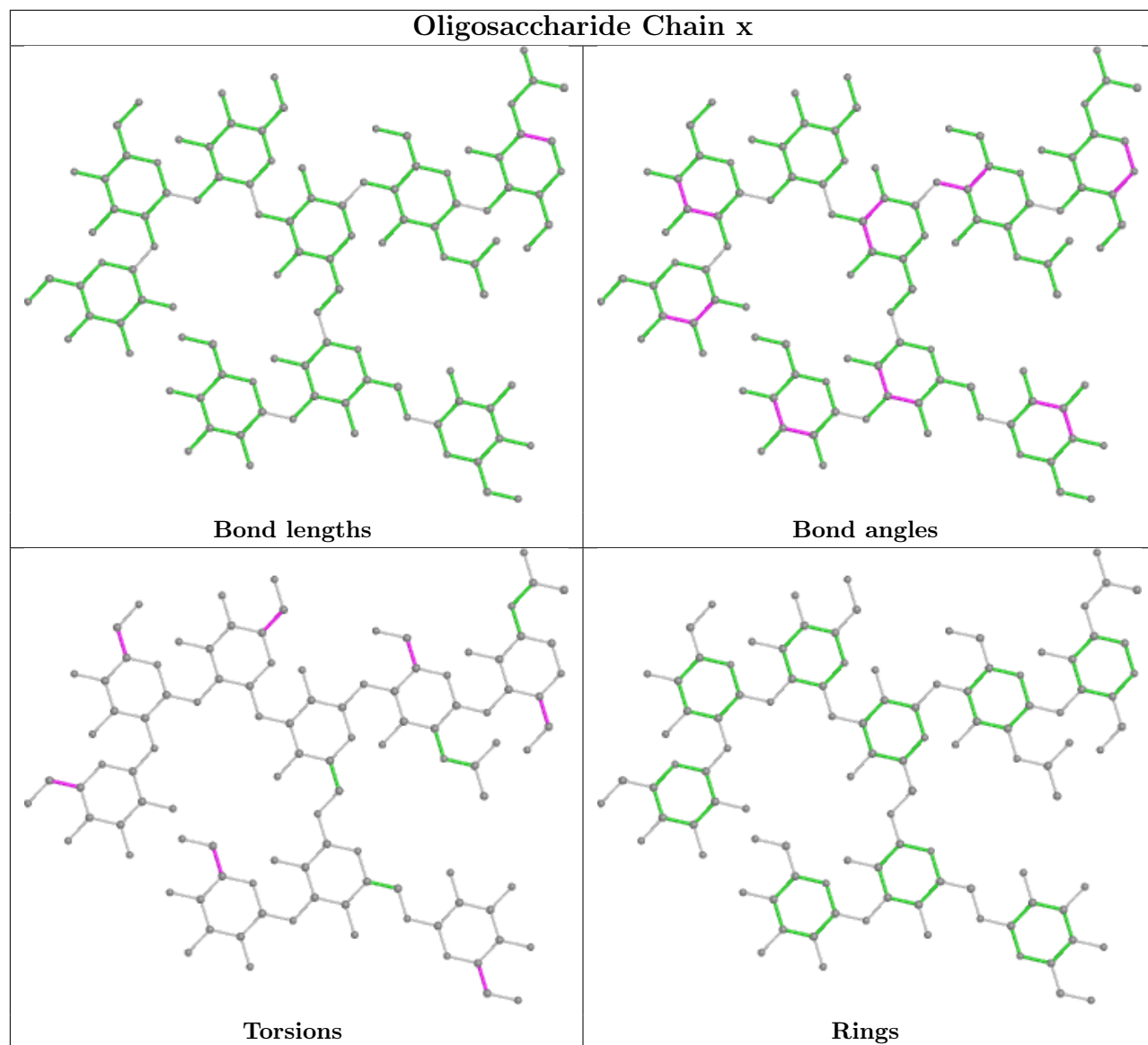


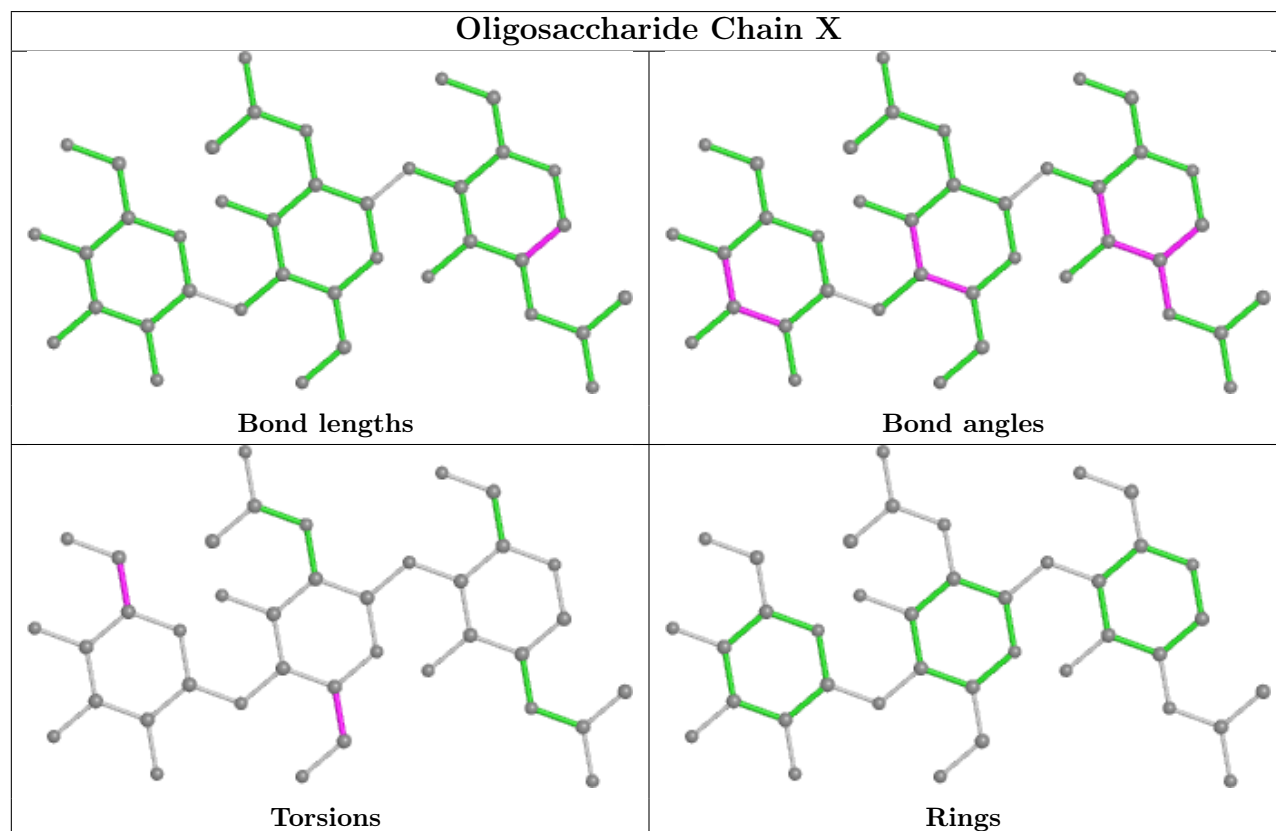
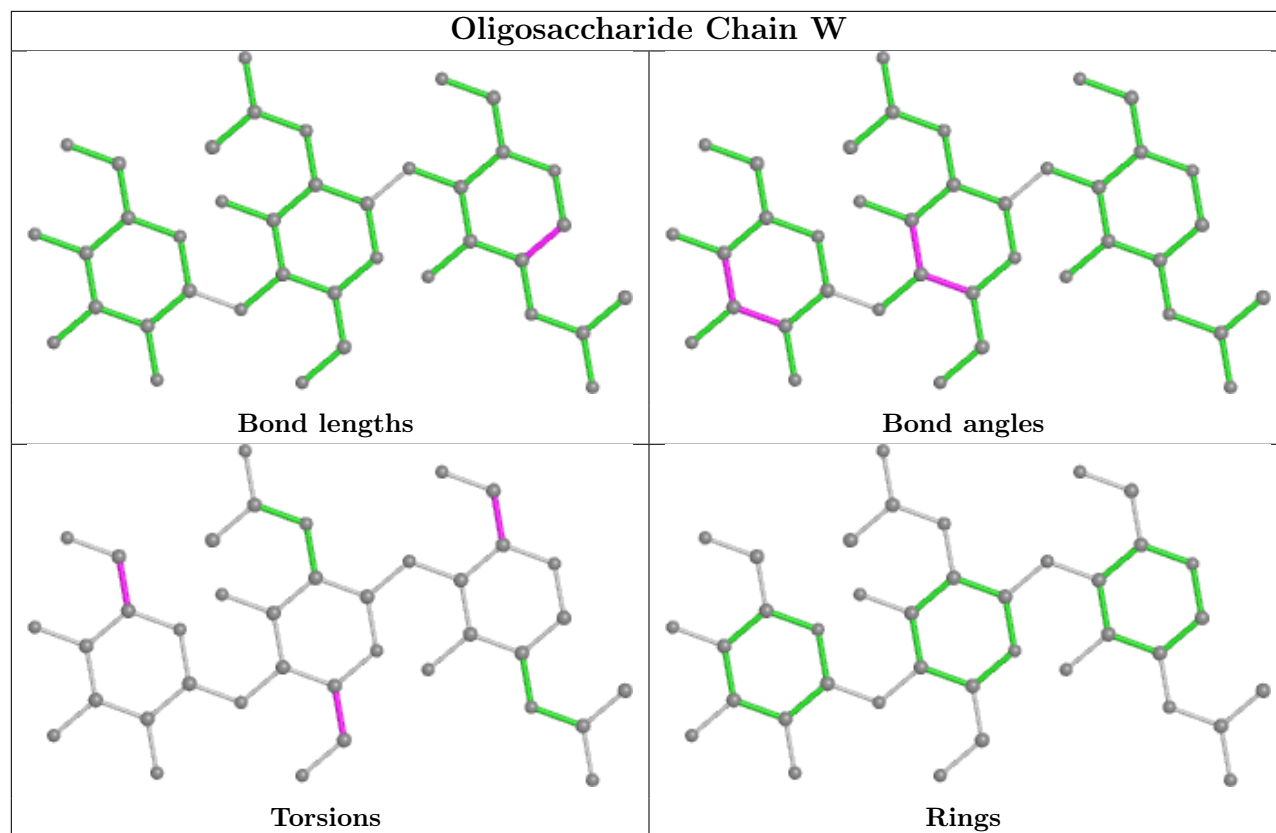


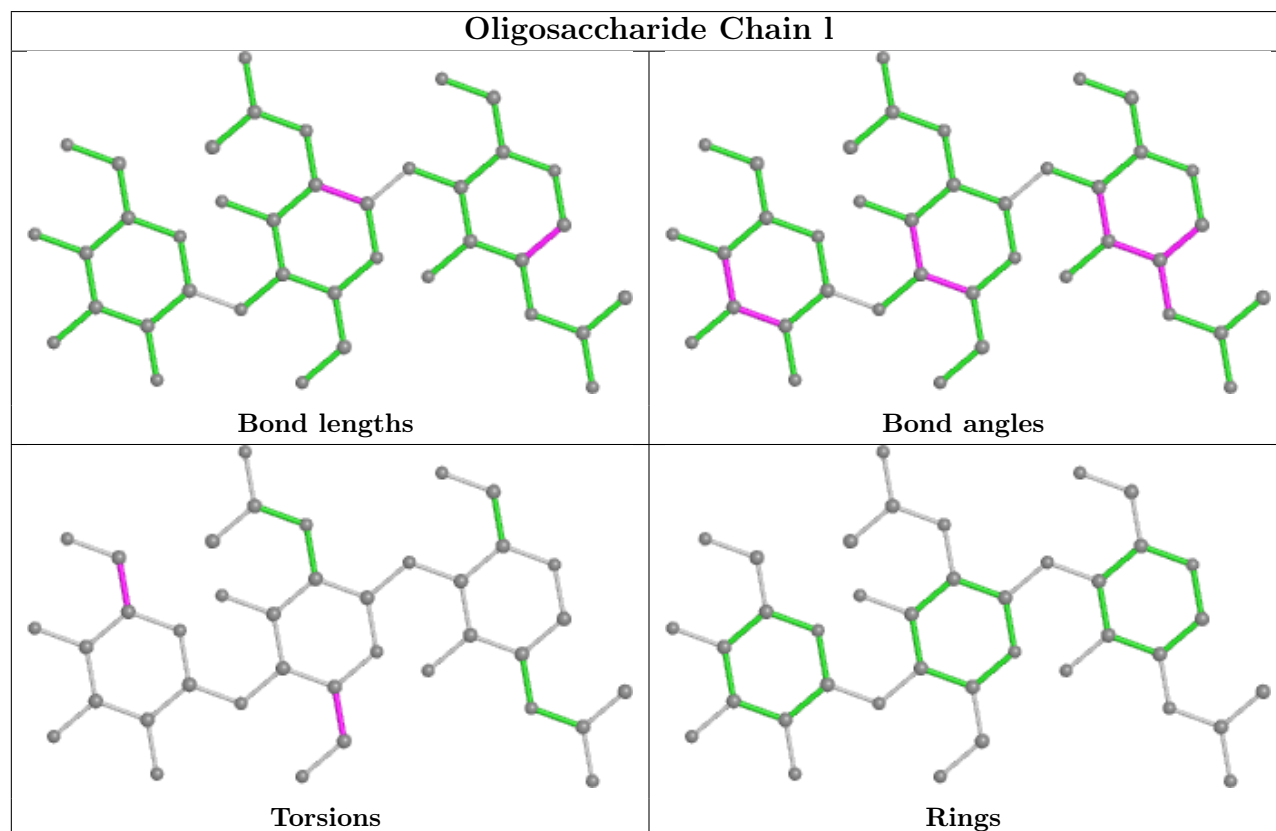
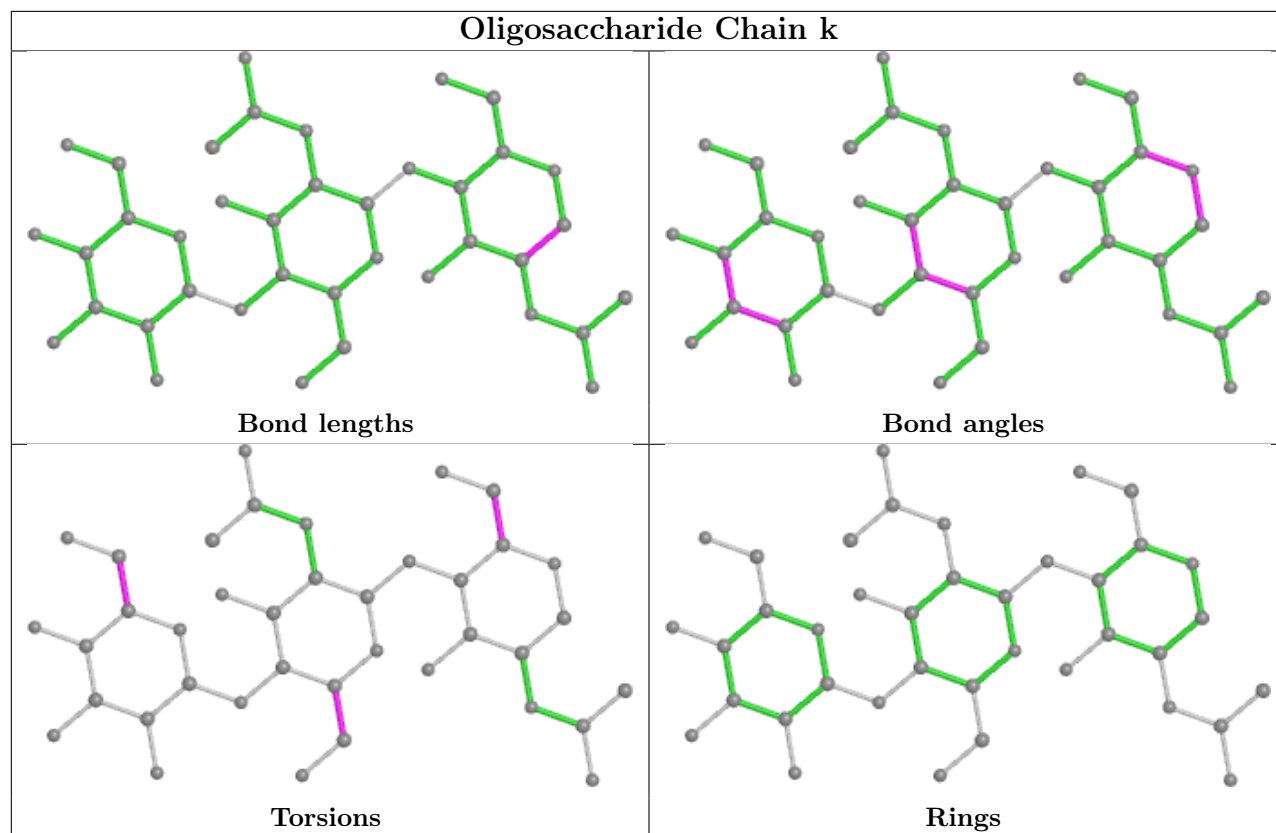




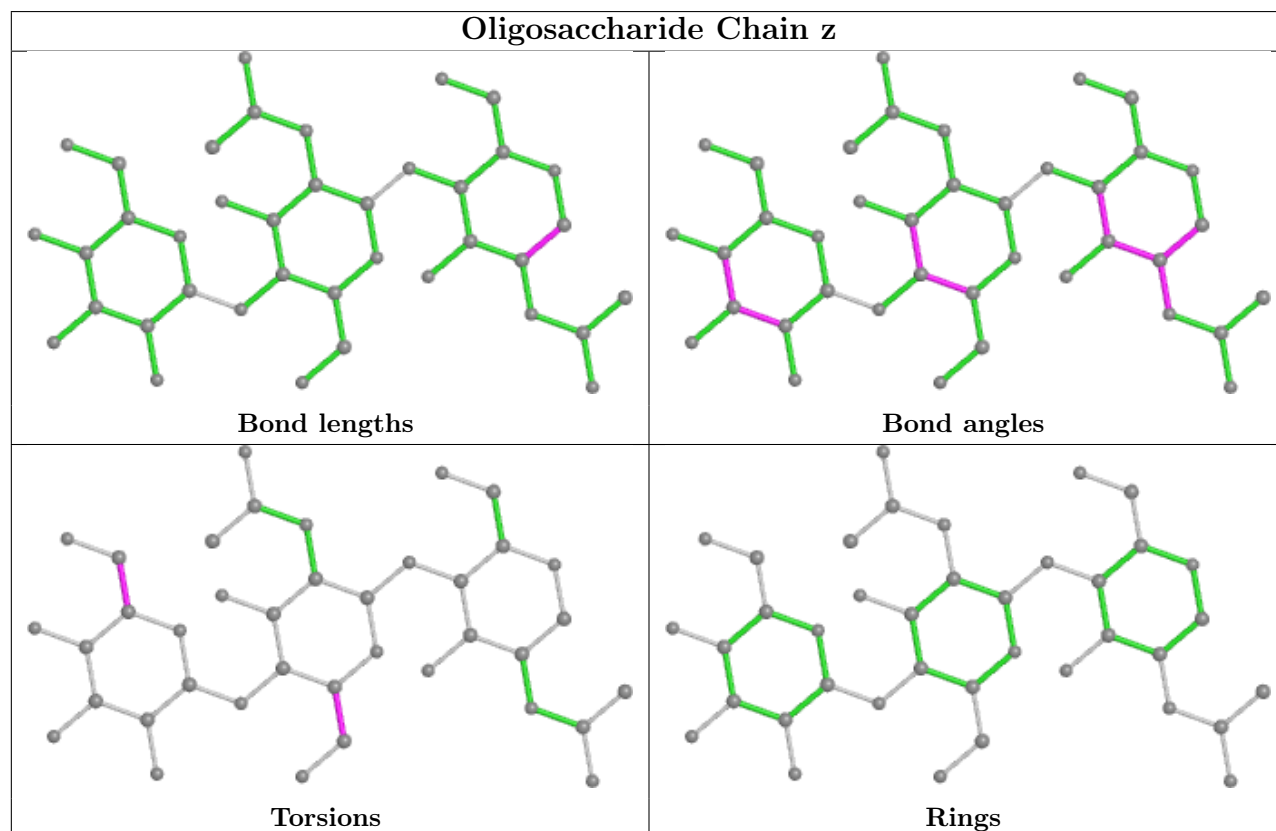
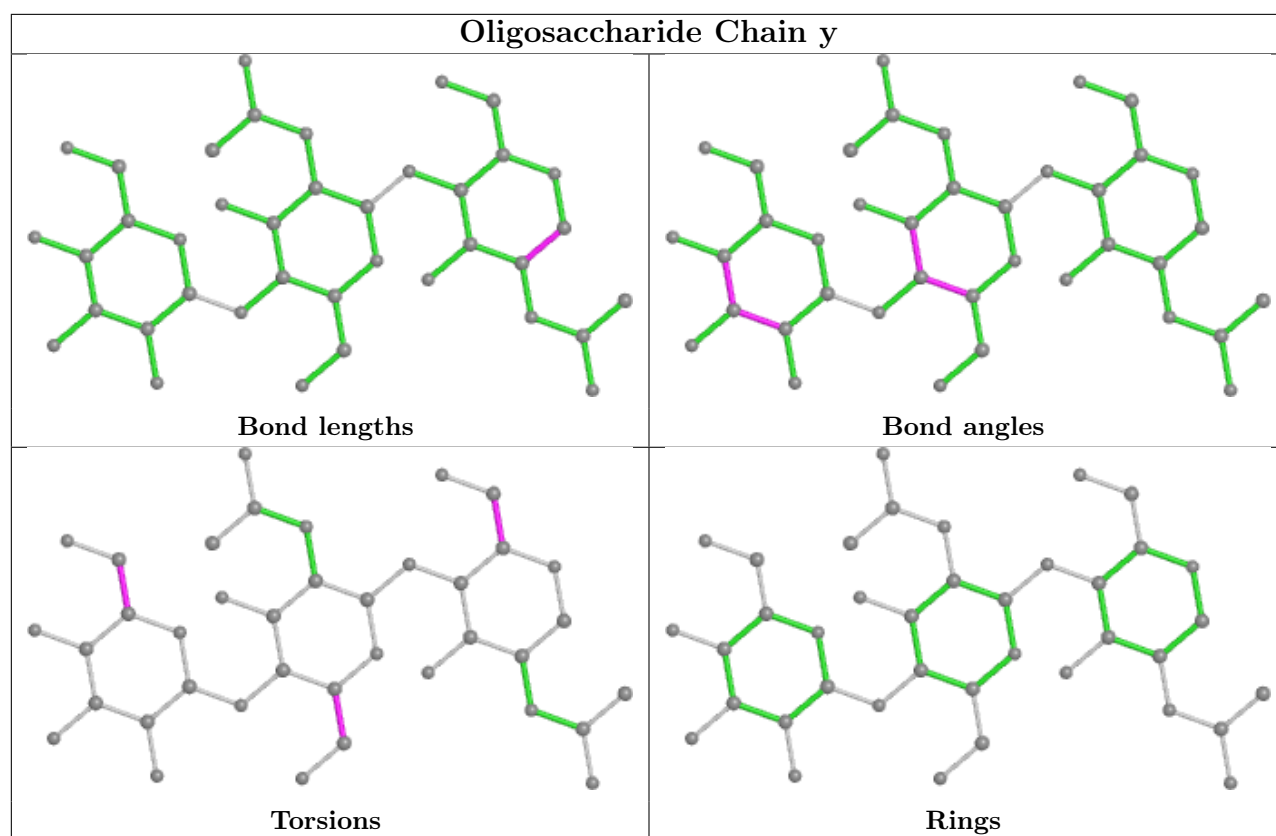












## 5.6 Ligand geometry

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
11	NAG	C	602	1	14,14,15	0.98	1 (7%)	17,19,21	0.93	1 (5%)
11	NAG	F	701	2	14,14,15	0.87	1 (7%)	17,19,21	1.09	1 (5%)
11	NAG	C	601	1	14,14,15	0.96	1 (7%)	17,19,21	0.78	1 (5%)
11	NAG	E	602	1	14,14,15	0.97	1 (7%)	17,19,21	0.93	1 (5%)
11	NAG	A	602	1	14,14,15	0.97	1 (7%)	17,19,21	0.93	1 (5%)
11	NAG	A	601	1	14,14,15	0.94	1 (7%)	17,19,21	0.84	1 (5%)
11	NAG	E	601	1	14,14,15	0.94	1 (7%)	17,19,21	0.84	1 (5%)
11	NAG	D	701	2	14,14,15	0.86	1 (7%)	17,19,21	1.38	1 (5%)
11	NAG	B	701	2	14,14,15	0.86	1 (7%)	17,19,21	1.35	2 (11%)

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
11	NAG	C	602	1	-	1/6/23/26	0/1/1/1
11	NAG	F	701	2	-	1/6/23/26	0/1/1/1
11	NAG	C	601	1	-	1/6/23/26	0/1/1/1
11	NAG	E	602	1	-	1/6/23/26	0/1/1/1
11	NAG	A	602	1	-	1/6/23/26	0/1/1/1
11	NAG	A	601	1	-	1/6/23/26	0/1/1/1
11	NAG	E	601	1	-	1/6/23/26	0/1/1/1
11	NAG	D	701	2	-	2/6/23/26	0/1/1/1
11	NAG	B	701	2	-	2/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	602	NAG	C1-C2	3.33	1.57	1.52
11	C	601	NAG	C1-C2	3.32	1.57	1.52
11	E	602	NAG	C1-C2	3.30	1.57	1.52
11	A	602	NAG	C1-C2	3.29	1.57	1.52
11	A	601	NAG	C1-C2	3.26	1.57	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	701	NAG	C4-C3-C2	-4.37	104.61	111.02
11	B	701	NAG	C4-C3-C2	-4.25	104.79	111.02
11	F	701	NAG	C4-C3-C2	-3.52	105.87	111.02
11	C	602	NAG	C4-C3-C2	-2.60	107.21	111.02
11	E	602	NAG	C4-C3-C2	-2.57	107.25	111.02

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	D	701	NAG	C4-C5-C6-O6
11	D	701	NAG	O5-C5-C6-O6
11	B	701	NAG	O5-C5-C6-O6
11	C	601	NAG	O5-C5-C6-O6
11	A	601	NAG	O5-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.

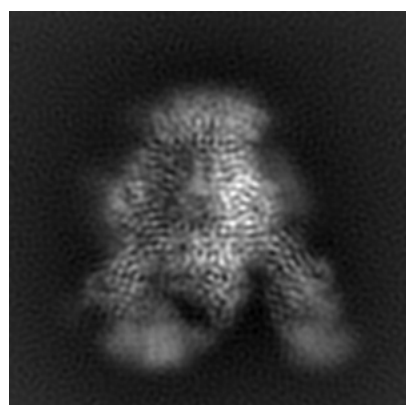
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23572. These allow visual inspection of the internal detail of the map and identification of artifacts.

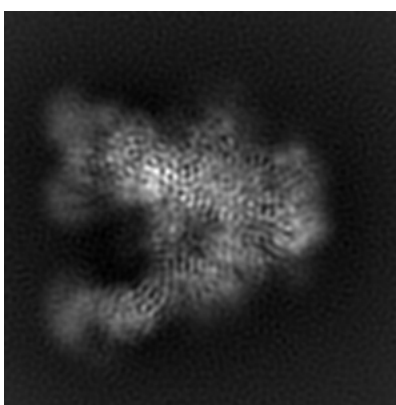
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

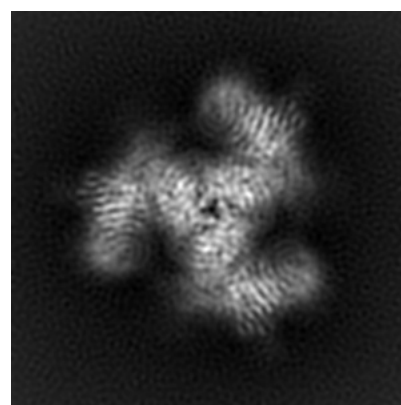
#### 6.1.1 Primary map



X



Y

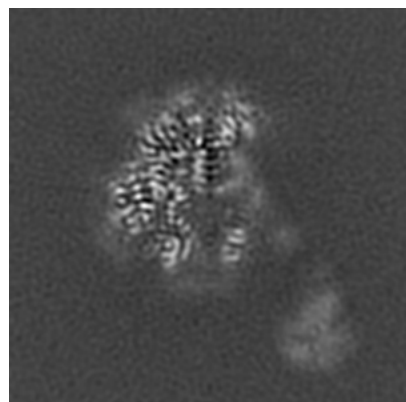


Z

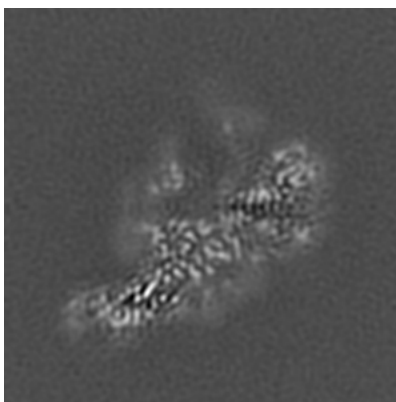
The images above show the map projected in three orthogonal directions.

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

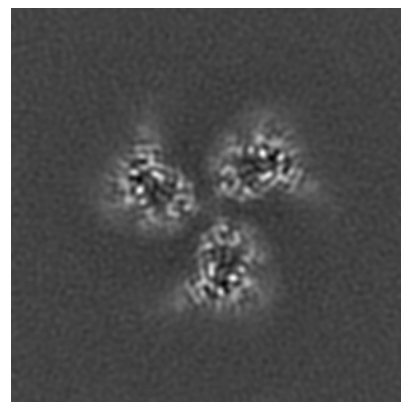
#### 6.2.1 Primary map



X Index: 110



Y Index: 110

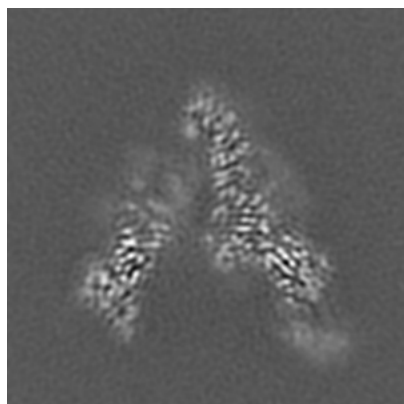


Z Index: 110

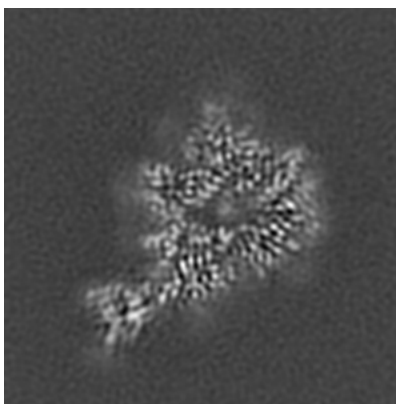
The images above show central slices of the map in three orthogonal directions.

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

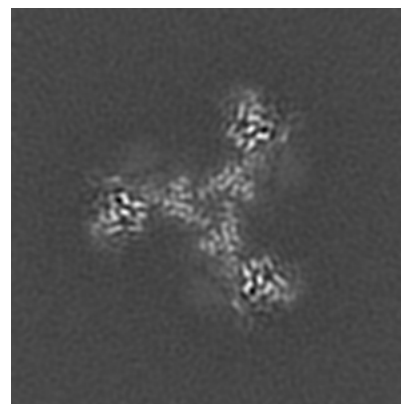
### 6.3.1 Primary map



X Index: 131



Y Index: 121

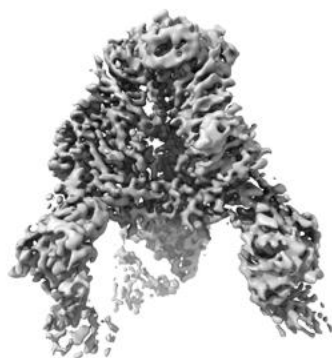


Z Index: 83

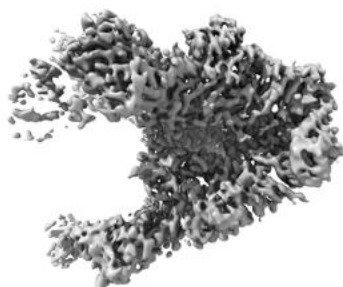
The images above show the largest variance slices of the map in three orthogonal directions.

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

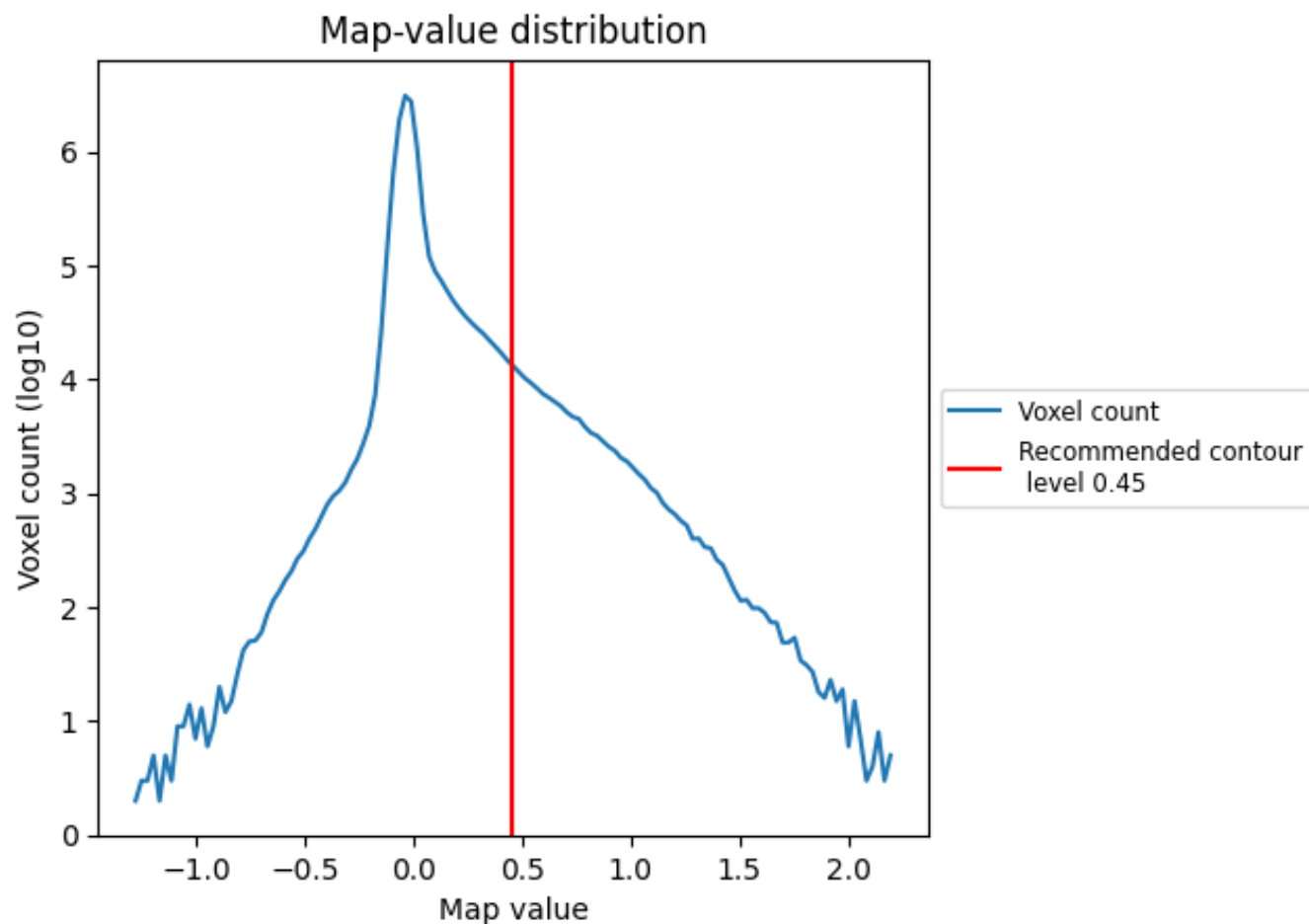
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

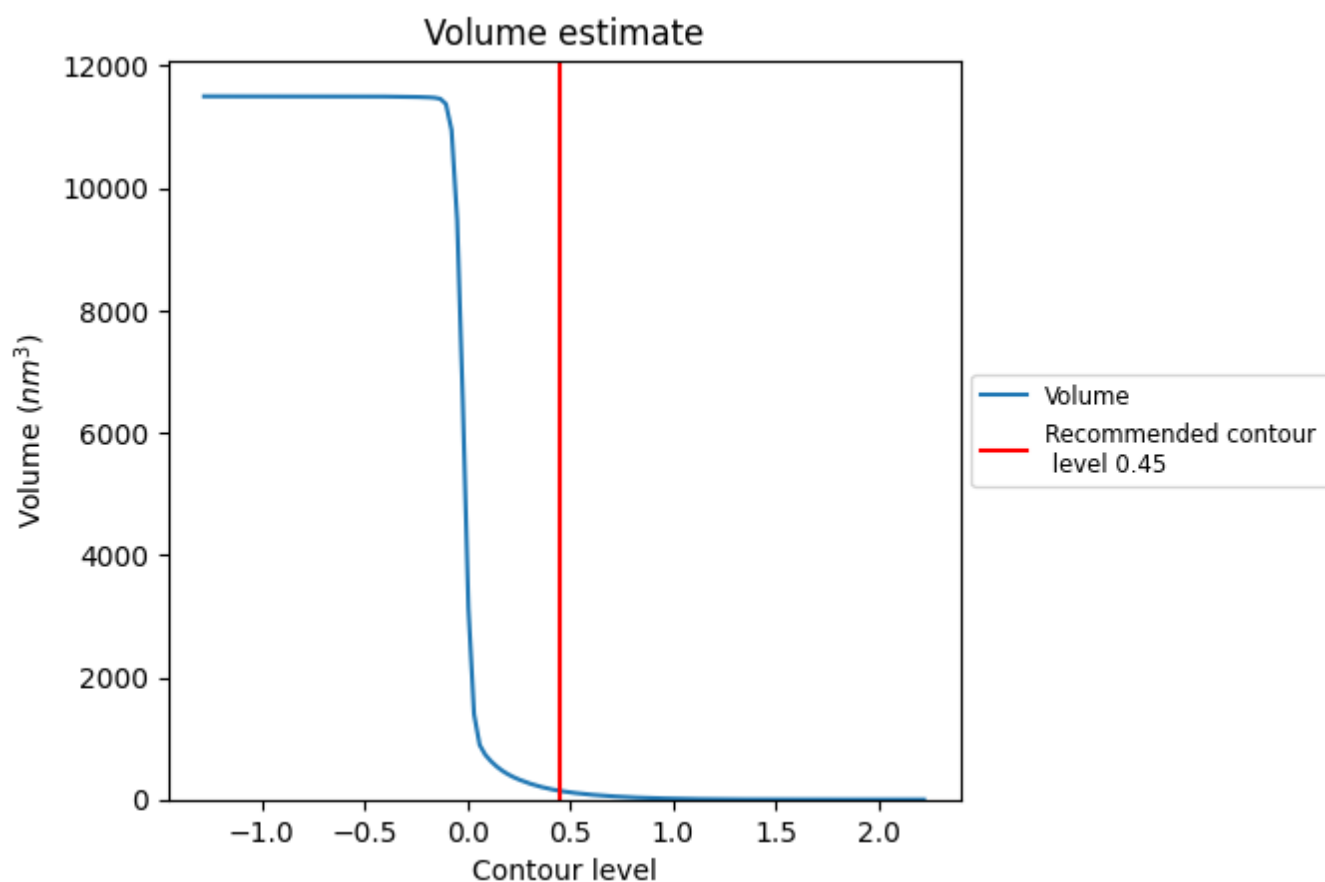
This section contains the results of statistical analysis of the map.

### 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](#)

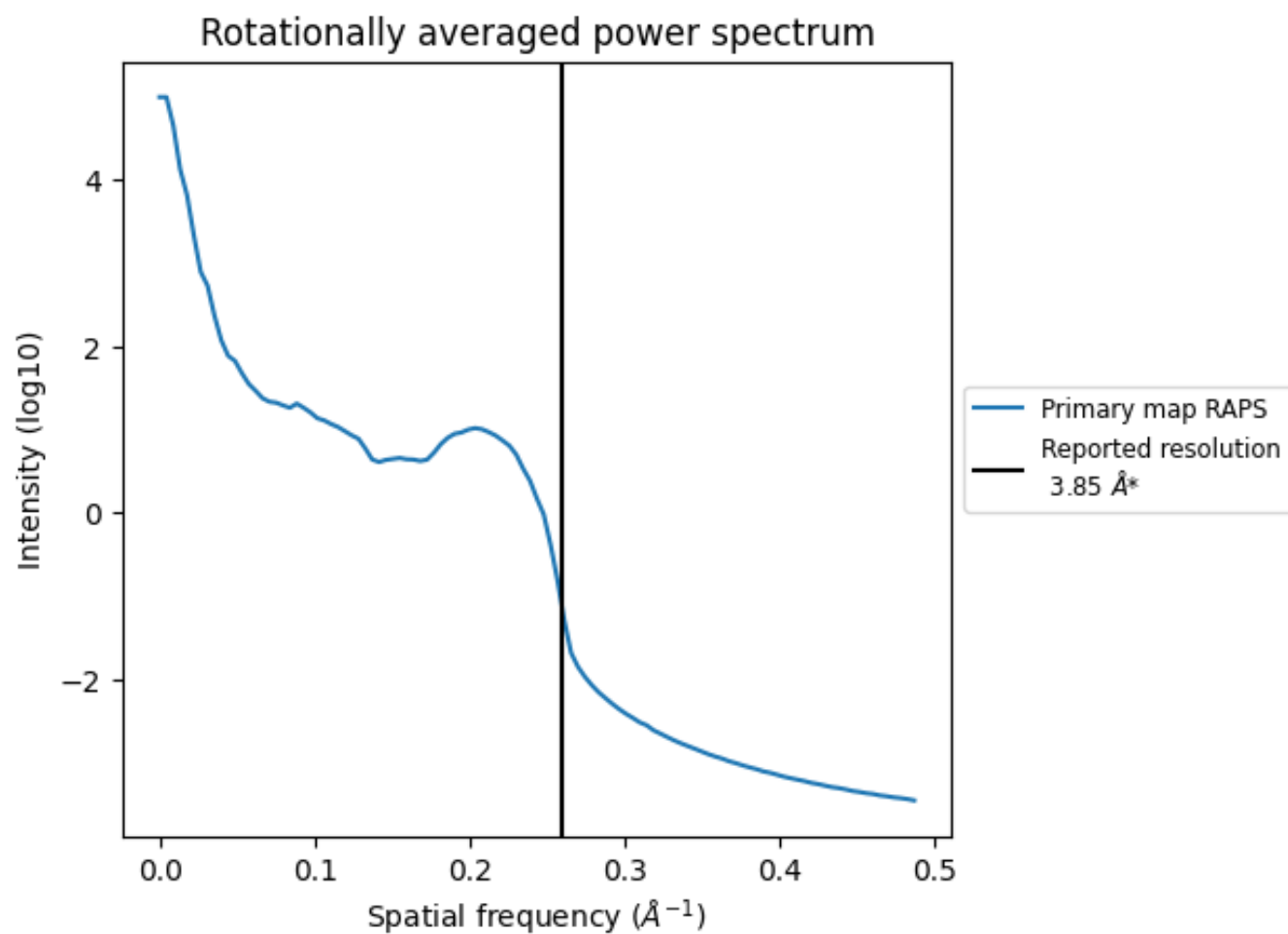


The volume at the recommended contour level is 144 nm<sup>3</sup>; this corresponds to an approximate mass of 130 kDa.

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 0.260 Å<sup>-1</sup>

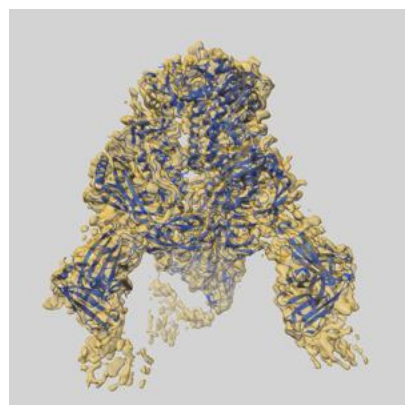
## 8 Fourier-Shell correlation

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

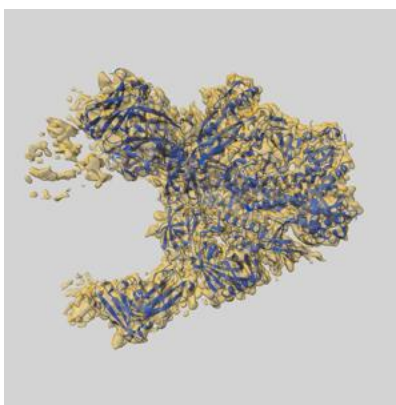
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23572 and PDB model 7LXN. Per-residue inclusion information can be found in section 3 on page 11.

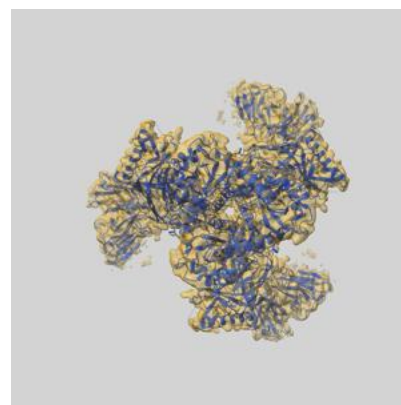
### 9.1 Map-model overlay [i](#)



X



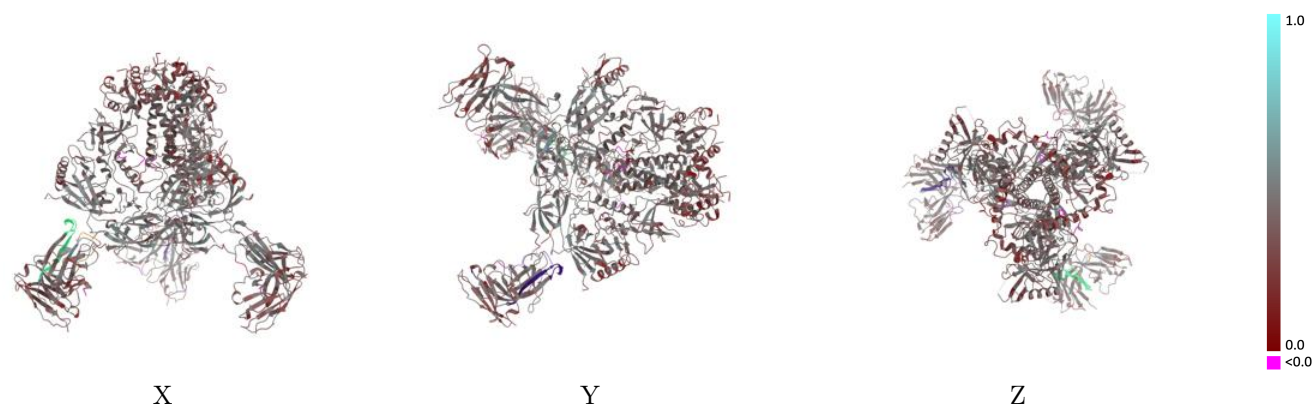
Y



Z

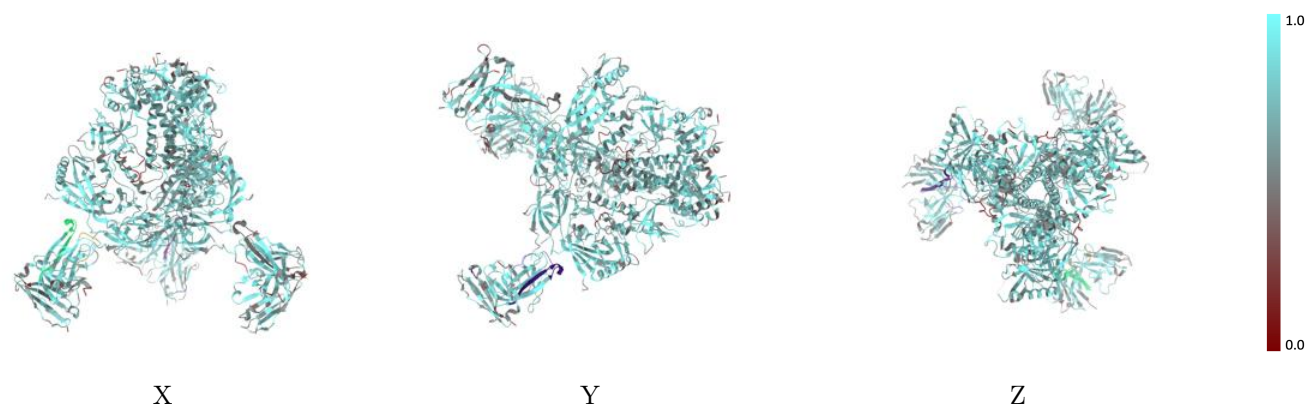
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



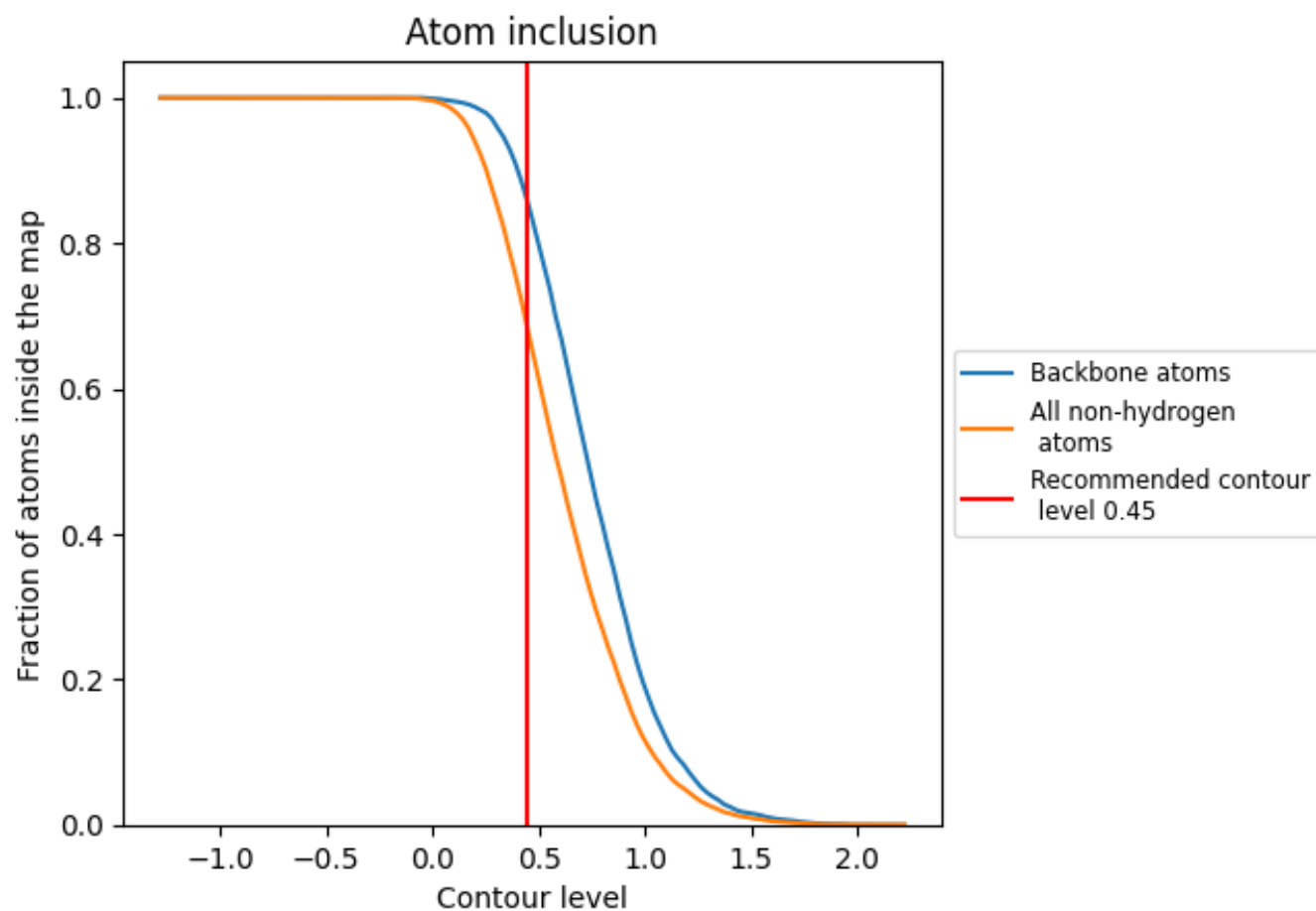
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 68% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6798	 0.3840
0	 0.3214	 0.3590
1	 0.1071	 0.3180
A	 0.7000	 0.3980
B	 0.6920	 0.3380
C	 0.7056	 0.3980
D	 0.6930	 0.3390
E	 0.7018	 0.4030
F	 0.7068	 0.3430
G	 0.5213	 0.2610
H	 0.7264	 0.3820
I	 0.7293	 0.3860
J	 0.7264	 0.3870
K	 0.2500	 0.3220
L	 0.7195	 0.3890
M	 0.7182	 0.3910
N	 0.7207	 0.3900
O	 0.3214	 0.2650
P	 0.2857	 0.3950
Q	 0.1786	 0.2630
R	 0.3929	 0.4160
S	 0.4458	 0.3980
T	 0.5714	 0.3740
U	 0.2400	 0.4040
V	 0.6476	 0.4230
W	 0.3590	 0.4000
X	 0.2308	 0.3140
Y	 0.3214	 0.3670
Z	 0.1071	 0.3080
a	 0.5532	 0.2760
b	 0.2857	 0.3220
c	 0.2857	 0.2710
d	 0.2857	 0.4060
e	 0.1786	 0.2620
f	 0.3929	 0.4250



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
g	 0.4458	 0.3800
h	 0.5714	 0.3600
i	 0.2400	 0.4020
j	 0.6476	 0.4180
k	 0.3333	 0.3880
l	 0.2308	 0.3180
m	 0.3214	 0.3650
n	 0.1071	 0.3270
o	 0.5106	 0.2580
p	 0.2500	 0.3110
q	 0.3214	 0.2720
r	 0.2857	 0.3920
s	 0.1786	 0.2690
t	 0.3929	 0.4270
u	 0.4337	 0.3920
v	 0.5714	 0.3780
w	 0.2200	 0.4130
x	 0.6476	 0.4170
y	 0.3590	 0.3900
z	 0.2308	 0.3200