



wwPDB EM Validation Summary Report ⓘ

Oct 26, 2024 – 11:04 AM EDT

PDB ID : 5V8M
EMDB ID : EMD-8644
Title : BG505 SOSIP.664 trimer in complex with broadly neutralizing HIV antibody 3BNC117
Authors : Lee, J.H.; Cottrell, C.A.; Ward, A.B.
Deposited on : 2017-03-22
Resolution : 4.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

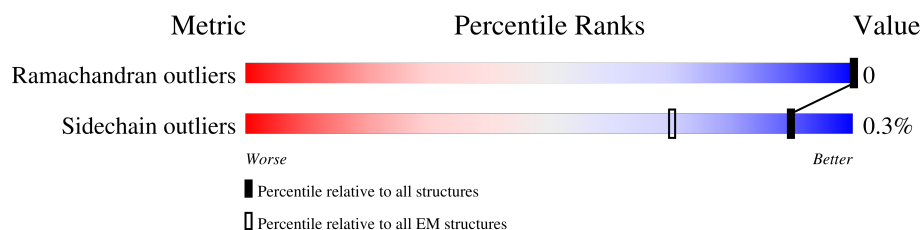
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance

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

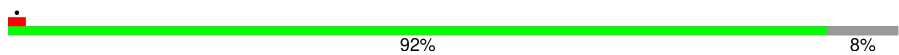
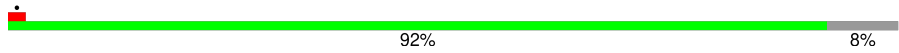
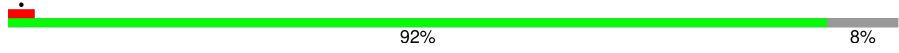
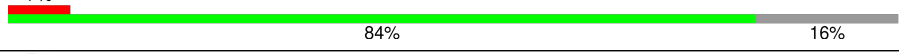

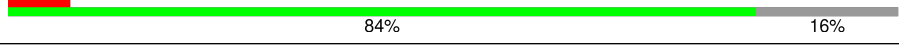



The reported resolution of this entry is 4.40 Å.

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





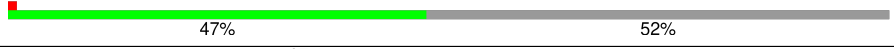
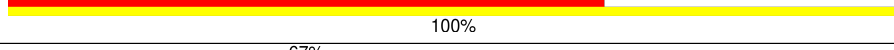
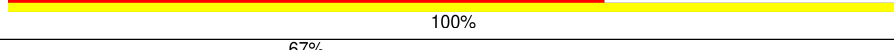
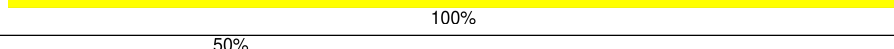

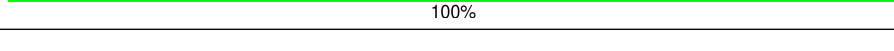


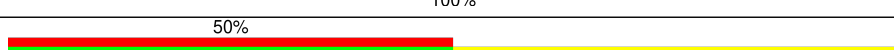



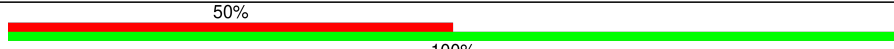
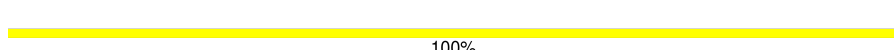
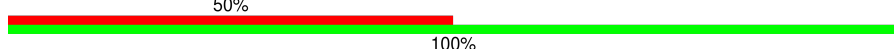



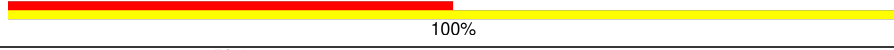

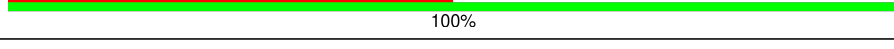
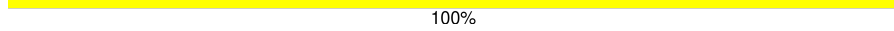

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	481	 92% 8%
1	F	481	 92% 8%
1	G	481	 92% 8%
2	B	153	 7% 84% 16%
2	I	153	 7% 84% 16%
2	J	153	 7% 84% 16%
3	H	226	 52% 46%
3	R	226	 53% 46%
3	S	226	 53% 46%

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Mol	Chain	Length	Quality of chain
4	L	206	
4	T	206	
4	U	206	
5	C	3	
5	Z	3	
5	m	3	
6	D	2	
6	E	2	
6	K	2	
6	O	2	
6	P	2	
6	Q	2	
6	X	2	
6	Y	2	
6	a	2	
6	b	2	
6	c	2	
6	f	2	
6	g	2	
6	h	2	
6	k	2	
6	l	2	
6	n	2	
6	o	2	
6	p	2	

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Mol	Chain	Length	Quality of chain
6	s	2	<div> <div>50%</div> <div>100%</div> </div>
6	t	2	<div> <div>50%</div> <div>100%</div> </div>
6	u	2	<div> <div>50%</div> <div>50%</div> </div>
6	x	2	<div> <div>100%</div> </div>
6	y	2	<div> <div>50%</div> <div>100%</div> </div>
7	M	7	<div> <div>43%</div> <div>100%</div> </div>
7	d	7	<div> <div>43%</div> <div>100%</div> </div>
7	q	7	<div> <div>43%</div> <div>100%</div> </div>
8	N	8	<div> <div>25%</div> <div>12%</div> <div>88%</div> </div>
8	e	8	<div> <div>25%</div> <div>12%</div> <div>88%</div> </div>
8	r	8	<div> <div>25%</div> <div>12%</div> <div>88%</div> </div>
9	V	6	<div> <div>50%</div> <div>17%</div> <div>83%</div> </div>
9	i	6	<div> <div>50%</div> <div>17%</div> <div>83%</div> </div>
9	v	6	<div> <div>50%</div> <div>17%</div> <div>83%</div> </div>
10	W	4	<div> <div>25%</div> <div>25%</div> <div>75%</div> </div>
10	j	4	<div> <div>25%</div> <div>25%</div> <div>75%</div> </div>
10	w	4	<div> <div>25%</div> <div>25%</div> <div>75%</div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 20835 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 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	444	Total	C	N	O	S	0	0
			3493	2192	617	656	28		
1	F	444	Total	C	N	O	S	0	0
			3493	2192	617	656	28		
1	G	444	Total	C	N	O	S	0	0
			3493	2192	617	656	28		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
A	509	ARG	-	expression tag	UNP Q2N0S6
A	510	ARG	-	expression tag	UNP Q2N0S6
A	511	ARG	-	expression tag	UNP Q2N0S6
A	512	ARG	-	expression tag	UNP Q2N0S6
A	513	ARG	-	expression tag	UNP Q2N0S6
F	332	ASN	THR	conflict	UNP Q2N0S6
F	501	CYS	ALA	conflict	UNP Q2N0S6
F	509	ARG	-	expression tag	UNP Q2N0S6
F	510	ARG	-	expression tag	UNP Q2N0S6
F	511	ARG	-	expression tag	UNP Q2N0S6
F	512	ARG	-	expression tag	UNP Q2N0S6
F	513	ARG	-	expression tag	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	129	Total	C	N	O	S	0	0
			1024	646	177	195	6		
2	I	129	Total	C	N	O	S	0	0
			1024	646	177	195	6		
2	J	129	Total	C	N	O	S	0	0
			1024	646	177	195	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6
I	559	PRO	ILE	conflict	UNP Q2N0S6
I	605	CYS	THR	conflict	UNP Q2N0S6
J	559	PRO	ILE	conflict	UNP Q2N0S6
J	605	CYS	THR	conflict	UNP Q2N0S6

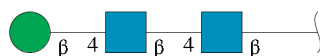
- Molecule 3 is a protein called antibody 3BNC117, heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	121	Total	C	N	O	S	0	0
			985	626	177	179	3		
3	R	121	Total	C	N	O	S	0	0
			985	626	177	179	3		
3	S	121	Total	C	N	O	S	0	0
			985	626	177	179	3		

- Molecule 4 is a protein called antibody 3BNC117, light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	98	Total	C	N	O	S	0	0
			783	493	137	150	3		
4	T	98	Total	C	N	O	S	0	0
			783	493	137	150	3		
4	U	98	Total	C	N	O	S	0	0
			783	493	137	150	3		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
5	C	3	Total	C	N	O	0	0
			39	22	2	15		
5	Z	3	Total	C	N	O	0	0
			39	22	2	15		
5	m	3	Total	C	N	O	0	0
			39	22	2	15		

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



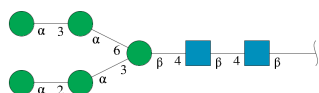
Mol	Chain	Residues	Atoms				AltConf	Trace
6	D	2	Total	C	N	O	0	0
			28	16	2	10		
6	E	2	Total	C	N	O	0	0
			28	16	2	10		
6	K	2	Total	C	N	O	0	0
			28	16	2	10		
6	O	2	Total	C	N	O	0	0
			28	16	2	10		
6	P	2	Total	C	N	O	0	0
			28	16	2	10		
6	Q	2	Total	C	N	O	0	0
			28	16	2	10		
6	X	2	Total	C	N	O	0	0
			28	16	2	10		
6	Y	2	Total	C	N	O	0	0
			28	16	2	10		
6	a	2	Total	C	N	O	0	0
			28	16	2	10		
6	b	2	Total	C	N	O	0	0
			28	16	2	10		
6	c	2	Total	C	N	O	0	0
			28	16	2	10		
6	f	2	Total	C	N	O	0	0
			28	16	2	10		
6	g	2	Total	C	N	O	0	0
			28	16	2	10		
6	h	2	Total	C	N	O	0	0
			28	16	2	10		

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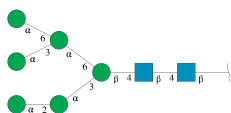
Mol	Chain	Residues	Atoms				AltConf	Trace
6	k	2	Total	C	N	O	0	0
			28	16	2	10		
6	l	2	Total	C	N	O	0	0
			28	16	2	10		
6	n	2	Total	C	N	O	0	0
			28	16	2	10		
6	o	2	Total	C	N	O	0	0
			28	16	2	10		
6	p	2	Total	C	N	O	0	0
			28	16	2	10		
6	s	2	Total	C	N	O	0	0
			28	16	2	10		
6	t	2	Total	C	N	O	0	0
			28	16	2	10		
6	u	2	Total	C	N	O	0	0
			28	16	2	10		
6	x	2	Total	C	N	O	0	0
			28	16	2	10		
6	y	2	Total	C	N	O	0	0
			28	16	2	10		

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



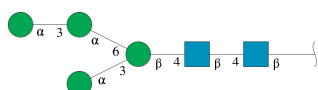
Mol	Chain	Residues	Atoms				AltConf	Trace
7	M	7	Total	C	N	O	0	0
			83	46	2	35		
7	d	7	Total	C	N	O	0	0
			83	46	2	35		
7	q	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 8 is an oligosaccharide called 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
8	N	8	Total	C	N	O	0	0
			94	52	2	40		
8	e	8	Total	C	N	O	0	0
			94	52	2	40		
8	r	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
9	V	6	Total	C	N	O	0	0
			72	40	2	30		
9	i	6	Total	C	N	O	0	0
			72	40	2	30		
9	v	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 10 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
10	W	4	Total	C	N	O	0	0
			50	28	2	20		
10	j	4	Total	C	N	O	0	0
			50	28	2	20		
10	w	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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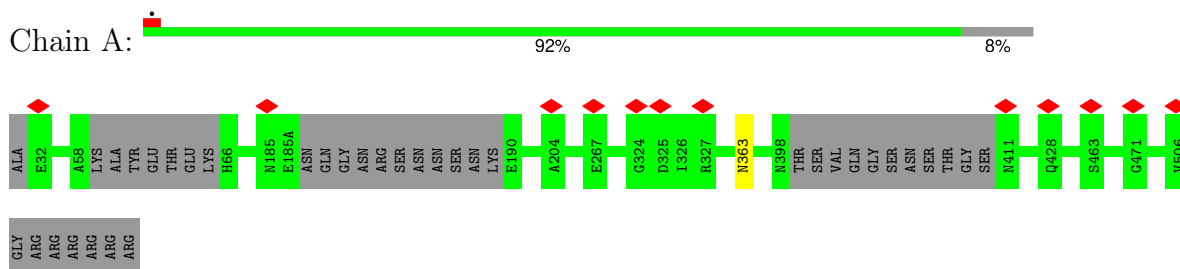
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Mol	Chain	Residues	Atoms				AltConf
11	I	1	Total 14	C 8	N 1	O 5	0
11	I	1	Total 14	C 8	N 1	O 5	0
11	G	1	Total 14	C 8	N 1	O 5	0
11	G	1	Total 14	C 8	N 1	O 5	0
11	G	1	Total 14	C 8	N 1	O 5	0
11	G	1	Total 14	C 8	N 1	O 5	0
11	G	1	Total 14	C 8	N 1	O 5	0
11	J	1	Total 14	C 8	N 1	O 5	0
11	J	1	Total 14	C 8	N 1	O 5	0

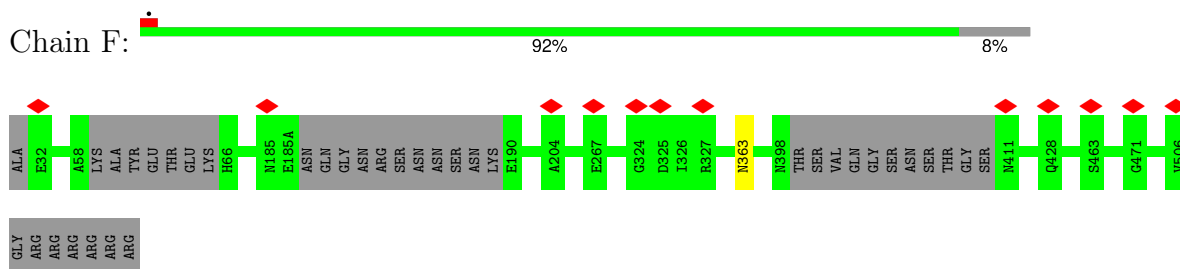
3 Residue-property plots [i](#)

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.

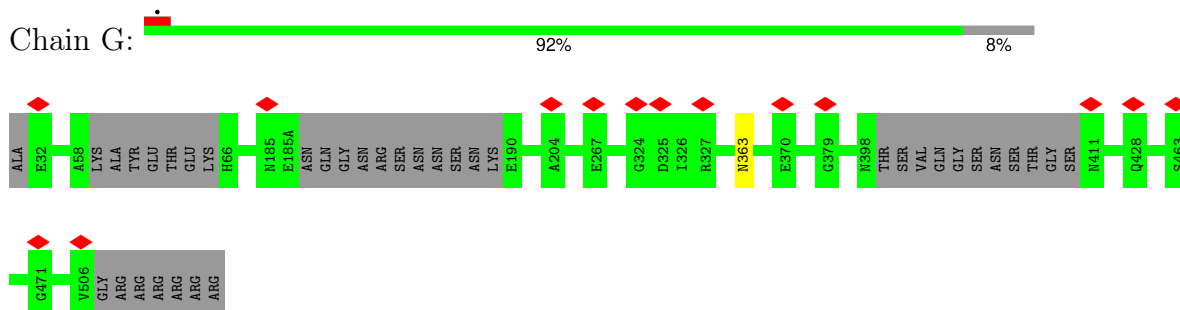
- Molecule 1: gp120



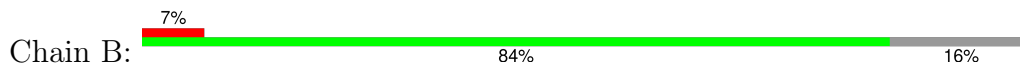
- Molecule 1: gp120

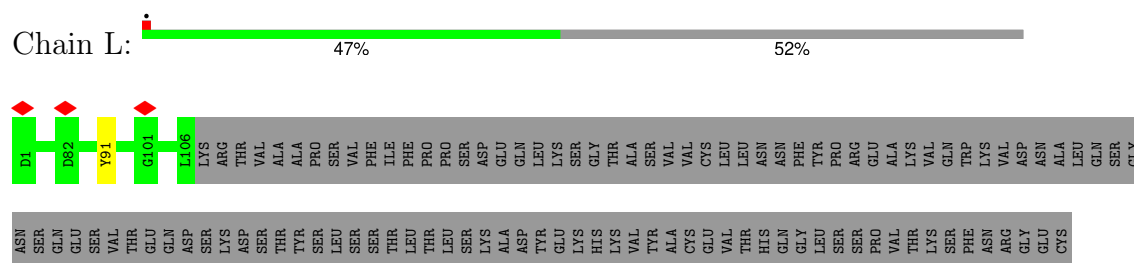


- Molecule 1: gp120

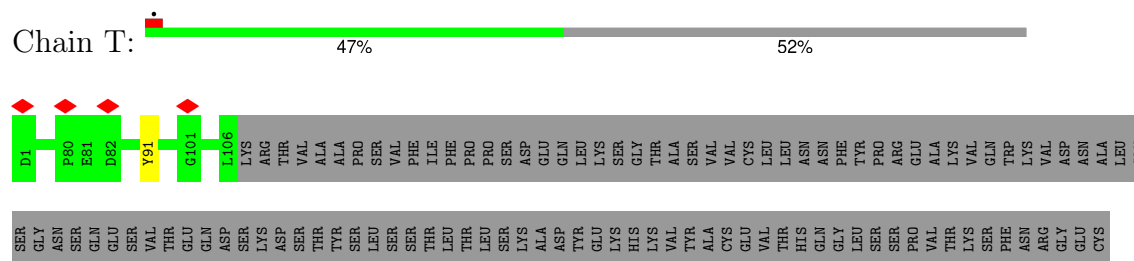


- Molecule 2: gp41

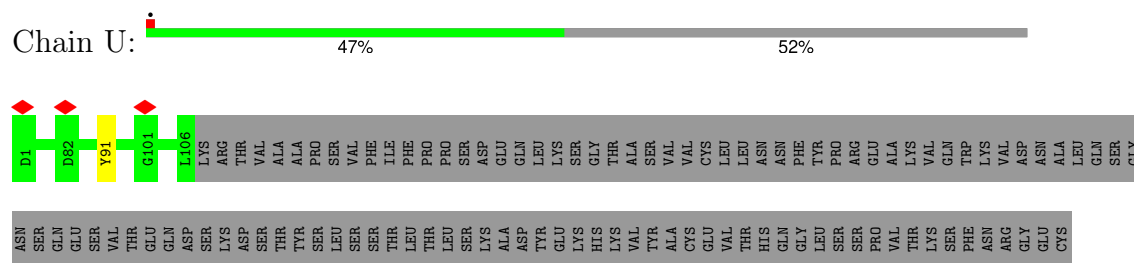




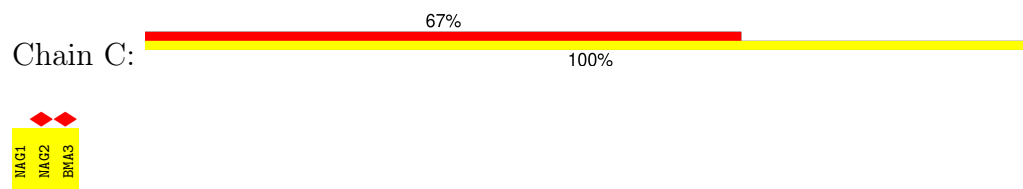
- Molecule 4: antibody 3BNC117, light chain



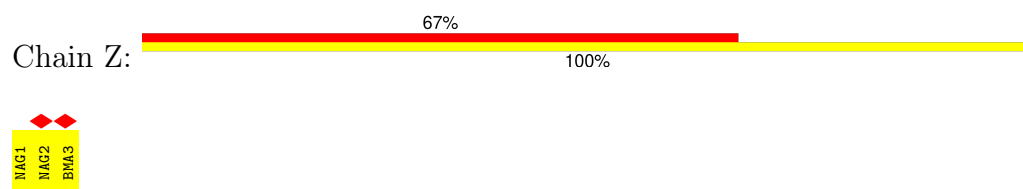
- Molecule 4: antibody 3BNC117, light chain



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



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



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





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



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



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



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



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



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





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

Chain X:  100%



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

Chain Y:  50% 100%



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

Chain a:  50% 50% 100%



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

Chain b:  50% 100%



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

Chain c:  100%



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

Chain f:  50% 100%



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



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



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



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



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



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





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

Chain p:  100%



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

Chain s:  100%



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

Chain t:  100%



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

Chain u:  50%



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

Chain x:  100%



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

Chain y:  100%



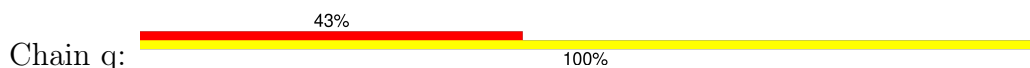
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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



- Molecule 10: 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: 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: 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	22625	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 ($e^-/\text{\AA}^2$)	32	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	0.119	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	335.36, 335.36, 335.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.84	0/3565	0.82	0/4842
1	F	0.84	0/3565	0.82	0/4842
1	G	0.84	0/3565	0.82	0/4842
2	B	0.88	0/1041	0.80	0/1412
2	I	0.87	0/1041	0.80	0/1412
2	J	0.88	0/1041	0.80	0/1412
3	H	0.81	0/1017	0.88	3/1386 (0.2%)
3	R	0.81	0/1017	0.88	2/1386 (0.1%)
3	S	0.81	0/1017	0.88	2/1386 (0.1%)
4	L	0.77	0/800	0.88	1/1086 (0.1%)
4	T	0.77	0/800	0.88	1/1086 (0.1%)
4	U	0.77	0/800	0.88	1/1086 (0.1%)
All	All	0.83	0/19269	0.84	10/26178 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	38	ARG	NE-CZ-NH2	-8.48	116.06	120.30
3	H	38	ARG	NE-CZ-NH2	-8.41	116.09	120.30
3	R	38	ARG	NE-CZ-NH2	-8.39	116.10	120.30
4	U	91	TYR	CB-CG-CD2	-6.80	116.92	121.00
4	L	91	TYR	CB-CG-CD2	-6.77	116.94	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/481 (91%)	427 (98%)	9 (2%)	0	100	100
1	F	436/481 (91%)	427 (98%)	9 (2%)	0	100	100
1	G	436/481 (91%)	427 (98%)	9 (2%)	0	100	100
2	B	125/153 (82%)	123 (98%)	2 (2%)	0	100	100
2	I	125/153 (82%)	123 (98%)	2 (2%)	0	100	100
2	J	125/153 (82%)	122 (98%)	3 (2%)	0	100	100
3	H	119/226 (53%)	117 (98%)	2 (2%)	0	100	100
3	R	119/226 (53%)	117 (98%)	2 (2%)	0	100	100
3	S	119/226 (53%)	117 (98%)	2 (2%)	0	100	100
4	L	96/206 (47%)	91 (95%)	5 (5%)	0	100	100
4	T	96/206 (47%)	91 (95%)	5 (5%)	0	100	100
4	U	96/206 (47%)	91 (95%)	5 (5%)	0	100	100
All	All	2328/3198 (73%)	2273 (98%)	55 (2%)	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	A	397/428 (93%)	396 (100%)	1 (0%)	91	92
1	F	397/428 (93%)	396 (100%)	1 (0%)	91	92
1	G	397/428 (93%)	396 (100%)	1 (0%)	91	92
2	B	111/129 (86%)	111 (100%)	0	100	100
2	I	111/129 (86%)	111 (100%)	0	100	100
2	J	111/129 (86%)	111 (100%)	0	100	100
3	H	102/193 (53%)	101 (99%)	1 (1%)	73	81
3	R	102/193 (53%)	101 (99%)	1 (1%)	73	81
3	S	102/193 (53%)	101 (99%)	1 (1%)	73	81
4	L	86/183 (47%)	86 (100%)	0	100	100
4	T	86/183 (47%)	86 (100%)	0	100	100
4	U	86/183 (47%)	86 (100%)	0	100	100
All	All	2088/2799 (75%)	2082 (100%)	6 (0%)	90	92

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	R	71	ARG
1	G	363	ASN
3	S	71	ARG
3	H	71	ARG
1	A	363	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	293	GLN
1	F	293	GLN
1	G	293	GLN

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 ⓘ

132 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	C	1	5,1	14,14,15	0.79	1 (7%)	17,19,21	0.92	1 (5%)
5	NAG	C	2	5	14,14,15	0.45	0	17,19,21	1.56	3 (17%)
5	BMA	C	3	5	11,11,12	1.15	1 (9%)	15,15,17	1.40	1 (6%)
6	NAG	D	1	6,1	14,14,15	0.26	0	17,19,21	0.55	0
6	NAG	D	2	6	14,14,15	0.32	0	17,19,21	0.67	1 (5%)
6	NAG	E	1	6,1	14,14,15	0.43	0	17,19,21	0.47	0
6	NAG	E	2	6	14,14,15	0.29	0	17,19,21	0.51	0
6	NAG	K	1	6,1	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
6	NAG	K	2	6	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
7	NAG	M	1	7,1	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
7	NAG	M	2	7	14,14,15	0.50	0	17,19,21	1.33	3 (17%)
7	BMA	M	3	7	11,11,12	0.66	0	15,15,17	1.43	3 (20%)
7	MAN	M	4	7	11,11,12	0.57	0	15,15,17	1.50	2 (13%)
7	MAN	M	5	7	11,11,12	0.59	0	15,15,17	2.30	5 (33%)
7	MAN	M	6	7	11,11,12	0.59	0	15,15,17	2.22	3 (20%)
7	MAN	M	7	7	11,11,12	0.55	0	15,15,17	1.92	5 (33%)
8	NAG	N	1	8,1	14,14,15	0.77	1 (7%)	17,19,21	0.69	0
8	NAG	N	2	8	14,14,15	0.41	0	17,19,21	0.47	0
8	BMA	N	3	8	11,11,12	1.65	4 (36%)	15,15,17	1.80	2 (13%)
8	MAN	N	4	8	11,11,12	1.66	3 (27%)	15,15,17	1.28	2 (13%)
8	MAN	N	5	8	11,11,12	2.28	4 (36%)	15,15,17	1.68	3 (20%)
8	MAN	N	6	8	11,11,12	0.60	0	15,15,17	2.21	3 (20%)
8	MAN	N	7	8	11,11,12	0.58	0	15,15,17	1.92	5 (33%)
8	MAN	N	8	8	11,11,12	0.61	0	15,15,17	2.26	7 (46%)
6	NAG	O	1	6,1	14,14,15	0.31	0	17,19,21	0.73	0
6	NAG	O	2	6	14,14,15	0.67	0	17,19,21	0.54	0
6	NAG	P	1	6,1	14,14,15	0.44	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	P	2	6	14,14,15	0.61	0	17,19,21	0.57	0
6	NAG	Q	1	6,1	14,14,15	0.40	0	17,19,21	0.76	1 (5%)
6	NAG	Q	2	6	14,14,15	0.54	0	17,19,21	0.55	0
9	NAG	V	1	9,1	14,14,15	0.34	0	17,19,21	0.59	0
9	NAG	V	2	9	14,14,15	0.36	0	17,19,21	0.84	1 (5%)
9	BMA	V	3	9	11,11,12	0.65	0	15,15,17	1.44	3 (20%)
9	MAN	V	4	9	11,11,12	0.61	0	15,15,17	2.20	3 (20%)
9	MAN	V	5	9	11,11,12	0.55	0	15,15,17	1.93	5 (33%)
9	MAN	V	6	9	11,11,12	0.54	0	15,15,17	1.47	2 (13%)
10	NAG	W	1	10,1	14,14,15	0.97	1 (7%)	17,19,21	1.06	1 (5%)
10	NAG	W	2	10	14,14,15	0.50	0	17,19,21	0.56	0
10	BMA	W	3	10	11,11,12	0.63	0	15,15,17	1.42	3 (20%)
10	MAN	W	4	10	11,11,12	0.60	0	15,15,17	2.22	3 (20%)
6	NAG	X	1	6,1	14,14,15	0.50	0	17,19,21	0.57	0
6	NAG	X	2	6	14,14,15	0.40	0	17,19,21	0.45	0
6	NAG	Y	1	4,6	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
6	NAG	Y	2	6	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
5	NAG	Z	1	5,1	14,14,15	0.79	1 (7%)	17,19,21	0.92	2 (11%)
5	NAG	Z	2	5	14,14,15	0.43	0	17,19,21	1.56	3 (17%)
5	BMA	Z	3	5	11,11,12	1.16	1 (9%)	15,15,17	1.40	1 (6%)
6	NAG	a	1	6,1	14,14,15	0.27	0	17,19,21	0.55	0
6	NAG	a	2	6	14,14,15	0.32	0	17,19,21	0.67	1 (5%)
6	NAG	b	1	6,1	14,14,15	0.44	0	17,19,21	0.48	0
6	NAG	b	2	6	14,14,15	0.28	0	17,19,21	0.51	0
6	NAG	c	1	6,1	14,14,15	0.49	0	17,19,21	2.27	3 (17%)
6	NAG	c	2	6	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
7	NAG	d	1	7,1	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
7	NAG	d	2	7	14,14,15	0.49	0	17,19,21	1.33	3 (17%)
7	BMA	d	3	7	11,11,12	0.66	0	15,15,17	1.43	3 (20%)
7	MAN	d	4	7	11,11,12	0.57	0	15,15,17	1.50	2 (13%)
7	MAN	d	5	7	11,11,12	0.59	0	15,15,17	2.30	5 (33%)
7	MAN	d	6	7	11,11,12	0.59	0	15,15,17	2.22	3 (20%)
7	MAN	d	7	7	11,11,12	0.57	0	15,15,17	1.93	5 (33%)
8	NAG	e	1	8,1	14,14,15	0.76	1 (7%)	17,19,21	0.68	0
8	NAG	e	2	8	14,14,15	0.41	0	17,19,21	0.47	0
8	BMA	e	3	8	11,11,12	1.66	4 (36%)	15,15,17	1.79	2 (13%)
8	MAN	e	4	8	11,11,12	1.66	3 (27%)	15,15,17	1.28	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	e	5	8	11,11,12	2.27	4 (36%)	15,15,17	1.68	3 (20%)
8	MAN	e	6	8	11,11,12	0.59	0	15,15,17	2.21	3 (20%)
8	MAN	e	7	8	11,11,12	0.58	0	15,15,17	1.92	5 (33%)
8	MAN	e	8	8	11,11,12	0.61	0	15,15,17	2.27	7 (46%)
6	NAG	f	1	6,1	14,14,15	0.30	0	17,19,21	0.73	0
6	NAG	f	2	6	14,14,15	0.68	0	17,19,21	0.55	0
6	NAG	g	1	6,1	14,14,15	0.45	0	17,19,21	0.43	0
6	NAG	g	2	6	14,14,15	0.62	0	17,19,21	0.57	0
6	NAG	h	1	6,1	14,14,15	0.41	0	17,19,21	0.75	1 (5%)
6	NAG	h	2	6	14,14,15	0.56	0	17,19,21	0.55	0
9	NAG	i	1	9,1	14,14,15	0.33	0	17,19,21	0.59	0
9	NAG	i	2	9	14,14,15	0.35	0	17,19,21	0.83	1 (5%)
9	BMA	i	3	9	11,11,12	0.66	0	15,15,17	1.45	3 (20%)
9	MAN	i	4	9	11,11,12	0.62	0	15,15,17	2.20	3 (20%)
9	MAN	i	5	9	11,11,12	0.54	0	15,15,17	1.93	5 (33%)
9	MAN	i	6	9	11,11,12	0.54	0	15,15,17	1.47	2 (13%)
10	NAG	j	1	10,1	14,14,15	0.97	1 (7%)	17,19,21	1.05	1 (5%)
10	NAG	j	2	10	14,14,15	0.49	0	17,19,21	0.56	0
10	BMA	j	3	10	11,11,12	0.64	0	15,15,17	1.42	3 (20%)
10	MAN	j	4	10	11,11,12	0.60	0	15,15,17	2.21	3 (20%)
6	NAG	k	1	6,1	14,14,15	0.49	0	17,19,21	0.57	0
6	NAG	k	2	6	14,14,15	0.40	0	17,19,21	0.45	0
6	NAG	l	1	4,6	14,14,15	0.49	0	17,19,21	2.28	3 (17%)
6	NAG	l	2	6	14,14,15	0.52	0	17,19,21	1.32	3 (17%)
5	NAG	m	1	5,1	14,14,15	0.79	1 (7%)	17,19,21	0.92	2 (11%)
5	NAG	m	2	5	14,14,15	0.45	0	17,19,21	1.55	3 (17%)
5	BMA	m	3	5	11,11,12	1.15	1 (9%)	15,15,17	1.40	1 (6%)
6	NAG	n	1	6,1	14,14,15	0.26	0	17,19,21	0.56	0
6	NAG	n	2	6	14,14,15	0.31	0	17,19,21	0.66	1 (5%)
6	NAG	o	1	6,1	14,14,15	0.43	0	17,19,21	0.47	0
6	NAG	o	2	6	14,14,15	0.28	0	17,19,21	0.51	0
6	NAG	p	1	6,1	14,14,15	0.49	0	17,19,21	2.27	3 (17%)
6	NAG	p	2	6	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
7	NAG	q	1	7,1	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
7	NAG	q	2	7	14,14,15	0.49	0	17,19,21	1.34	3 (17%)
7	BMA	q	3	7	11,11,12	0.66	0	15,15,17	1.43	3 (20%)
7	MAN	q	4	7	11,11,12	0.56	0	15,15,17	1.50	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	q	5	7	11,11,12	0.60	0	15,15,17	2.30	5 (33%)
7	MAN	q	6	7	11,11,12	0.59	0	15,15,17	2.21	3 (20%)
7	MAN	q	7	7	11,11,12	0.55	0	15,15,17	1.92	5 (33%)
8	NAG	r	1	8,1	14,14,15	0.77	1 (7%)	17,19,21	0.69	0
8	NAG	r	2	8	14,14,15	0.41	0	17,19,21	0.47	0
8	BMA	r	3	8	11,11,12	1.65	4 (36%)	15,15,17	1.79	2 (13%)
8	MAN	r	4	8	11,11,12	1.66	3 (27%)	15,15,17	1.27	2 (13%)
8	MAN	r	5	8	11,11,12	2.27	4 (36%)	15,15,17	1.68	3 (20%)
8	MAN	r	6	8	11,11,12	0.61	0	15,15,17	2.22	3 (20%)
8	MAN	r	7	8	11,11,12	0.58	0	15,15,17	1.93	5 (33%)
8	MAN	r	8	8	11,11,12	0.61	0	15,15,17	2.26	7 (46%)
6	NAG	s	1	6,1	14,14,15	0.32	0	17,19,21	0.73	0
6	NAG	s	2	6	14,14,15	0.67	0	17,19,21	0.54	0
6	NAG	t	1	6,1	14,14,15	0.45	0	17,19,21	0.43	0
6	NAG	t	2	6	14,14,15	0.62	0	17,19,21	0.57	0
6	NAG	u	1	6,1	14,14,15	0.41	0	17,19,21	0.76	1 (5%)
6	NAG	u	2	6	14,14,15	0.55	0	17,19,21	0.55	0
9	NAG	v	1	9,1	14,14,15	0.33	0	17,19,21	0.59	0
9	NAG	v	2	9	14,14,15	0.36	0	17,19,21	0.84	1 (5%)
9	BMA	v	3	9	11,11,12	0.65	0	15,15,17	1.45	3 (20%)
9	MAN	v	4	9	11,11,12	0.61	0	15,15,17	2.20	3 (20%)
9	MAN	v	5	9	11,11,12	0.56	0	15,15,17	1.93	5 (33%)
9	MAN	v	6	9	11,11,12	0.54	0	15,15,17	1.47	2 (13%)
10	NAG	w	1	10,1	14,14,15	0.96	1 (7%)	17,19,21	1.06	1 (5%)
10	NAG	w	2	10	14,14,15	0.50	0	17,19,21	0.56	0
10	BMA	w	3	10	11,11,12	0.65	0	15,15,17	1.42	3 (20%)
10	MAN	w	4	10	11,11,12	0.62	0	15,15,17	2.21	3 (20%)
6	NAG	x	1	6,1	14,14,15	0.50	0	17,19,21	0.57	0
6	NAG	x	2	6	14,14,15	0.40	0	17,19,21	0.45	0
6	NAG	y	1	4,6	14,14,15	0.49	0	17,19,21	2.29	3 (17%)
6	NAG	y	2	6	14,14,15	0.51	0	17,19,21	1.33	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	C	2	5	-	6/6/23/26	0/1/1/1
5	BMA	C	3	5	-	2/2/19/22	0/1/1/1
6	NAG	D	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1
6	NAG	E	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	E	2	6	-	2/6/23/26	0/1/1/1
6	NAG	K	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
7	NAG	M	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	M	2	7	-	0/6/23/26	0/1/1/1
7	BMA	M	3	7	-	0/2/19/22	0/1/1/1
7	MAN	M	4	7	-	0/2/19/22	0/1/1/1
7	MAN	M	5	7	-	0/2/19/22	0/1/1/1
7	MAN	M	6	7	-	0/2/19/22	0/1/1/1
7	MAN	M	7	7	-	0/2/19/22	0/1/1/1
8	NAG	N	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	N	2	8	-	2/6/23/26	0/1/1/1
8	BMA	N	3	8	-	0/2/19/22	0/1/1/1
8	MAN	N	4	8	-	2/2/19/22	0/1/1/1
8	MAN	N	5	8	-	0/2/19/22	0/1/1/1
8	MAN	N	6	8	-	0/2/19/22	0/1/1/1
8	MAN	N	7	8	-	0/2/19/22	0/1/1/1
8	MAN	N	8	8	-	0/2/19/22	0/1/1/1
6	NAG	O	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1
6	NAG	P	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Q	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1
9	NAG	V	1	9,1	-	3/6/23/26	0/1/1/1
9	NAG	V	2	9	-	2/6/23/26	0/1/1/1
9	BMA	V	3	9	-	2/2/19/22	0/1/1/1
9	MAN	V	4	9	-	0/2/19/22	0/1/1/1
9	MAN	V	5	9	-	0/2/19/22	0/1/1/1
9	MAN	V	6	9	-	0/2/19/22	0/1/1/1
10	NAG	W	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	W	2	10	-	2/6/23/26	0/1/1/1
10	BMA	W	3	10	-	2/2/19/22	0/1/1/1

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

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

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

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	5	MAN	C4-C5	4.34	1.62	1.53
8	r	5	MAN	C4-C5	4.33	1.62	1.53
8	e	5	MAN	C4-C5	4.32	1.62	1.53
8	e	5	MAN	C4-C3	3.69	1.61	1.52
8	N	5	MAN	C4-C3	3.69	1.61	1.52

The worst 5 of 260 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	q	1	NAG	O5-C1-C2	-7.52	99.65	111.29
6	y	1	NAG	O5-C1-C2	-7.52	99.65	111.29
7	M	1	NAG	O5-C1-C2	-7.51	99.68	111.29
7	d	1	NAG	O5-C1-C2	-7.50	99.68	111.29
6	c	1	NAG	O5-C1-C2	-7.50	99.68	111.29

There are no chirality outliers.

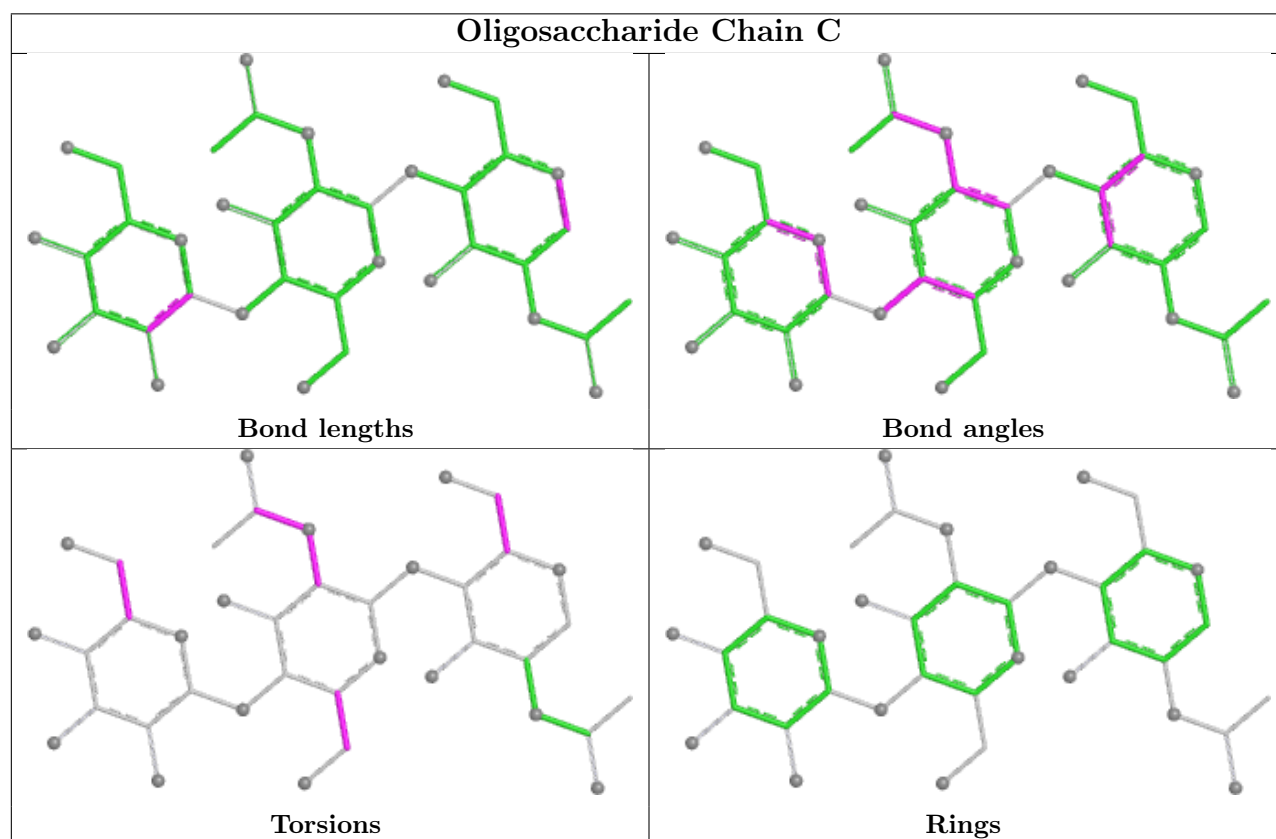
5 of 159 torsion outliers are listed below:

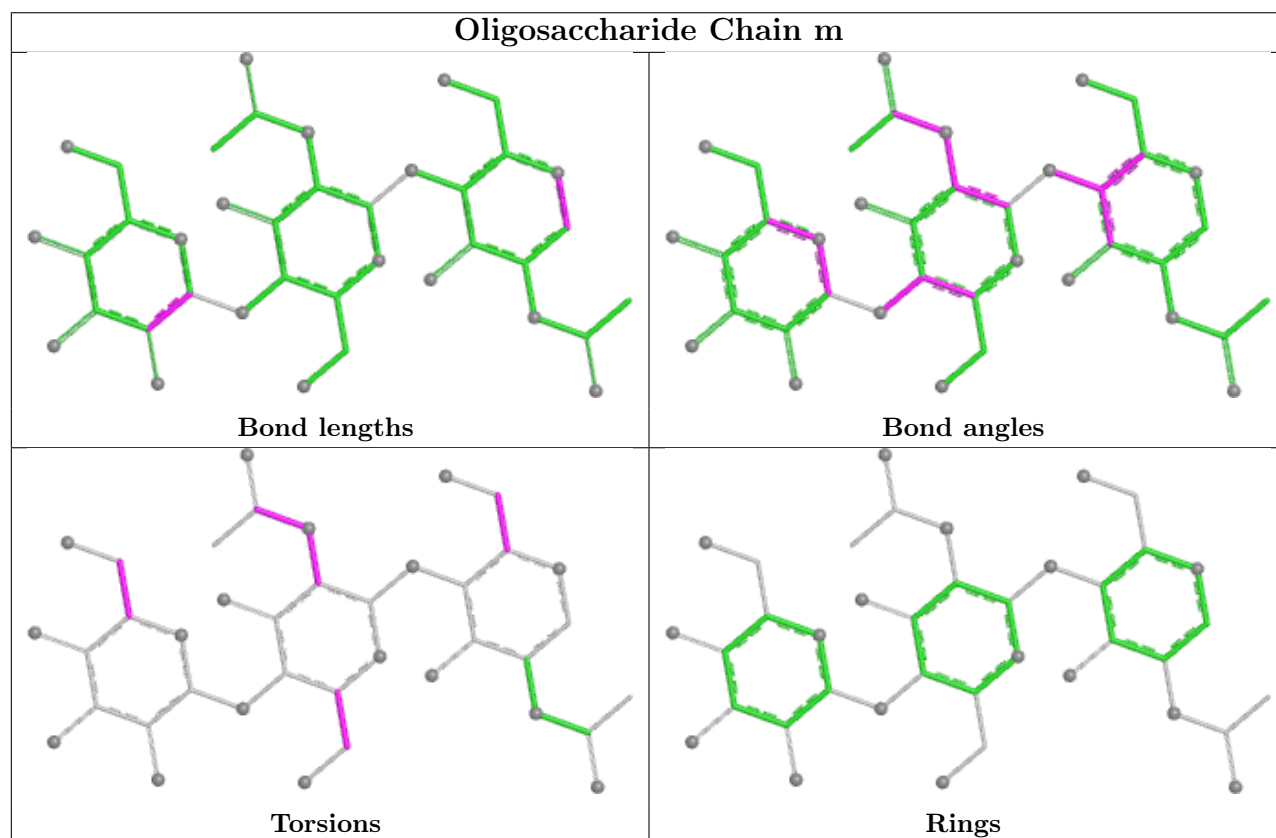
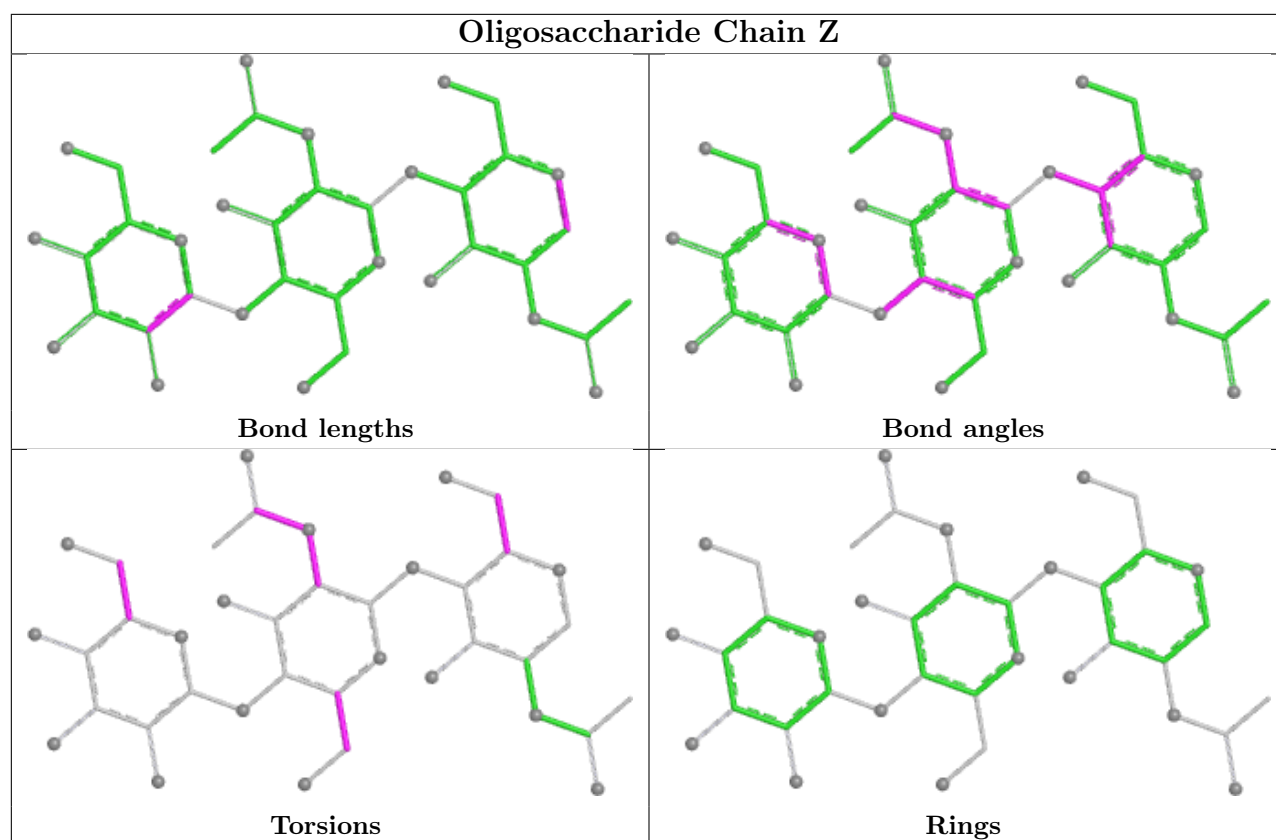
Mol	Chain	Res	Type	Atoms
5	C	3	BMA	C4-C5-C6-O6
5	Z	3	BMA	C4-C5-C6-O6
5	m	3	BMA	C4-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
6	f	1	NAG	O5-C5-C6-O6

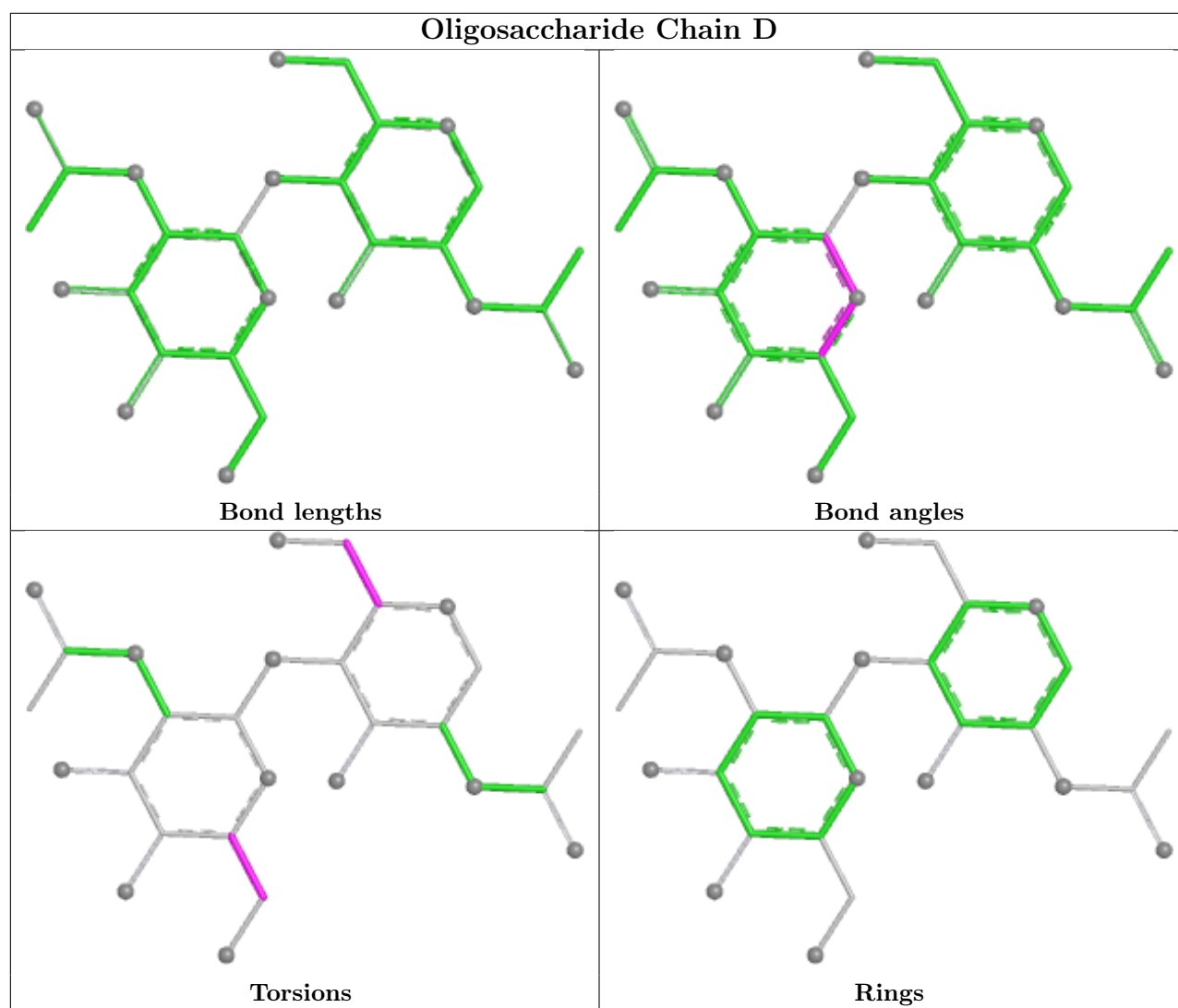
There are no ring outliers.

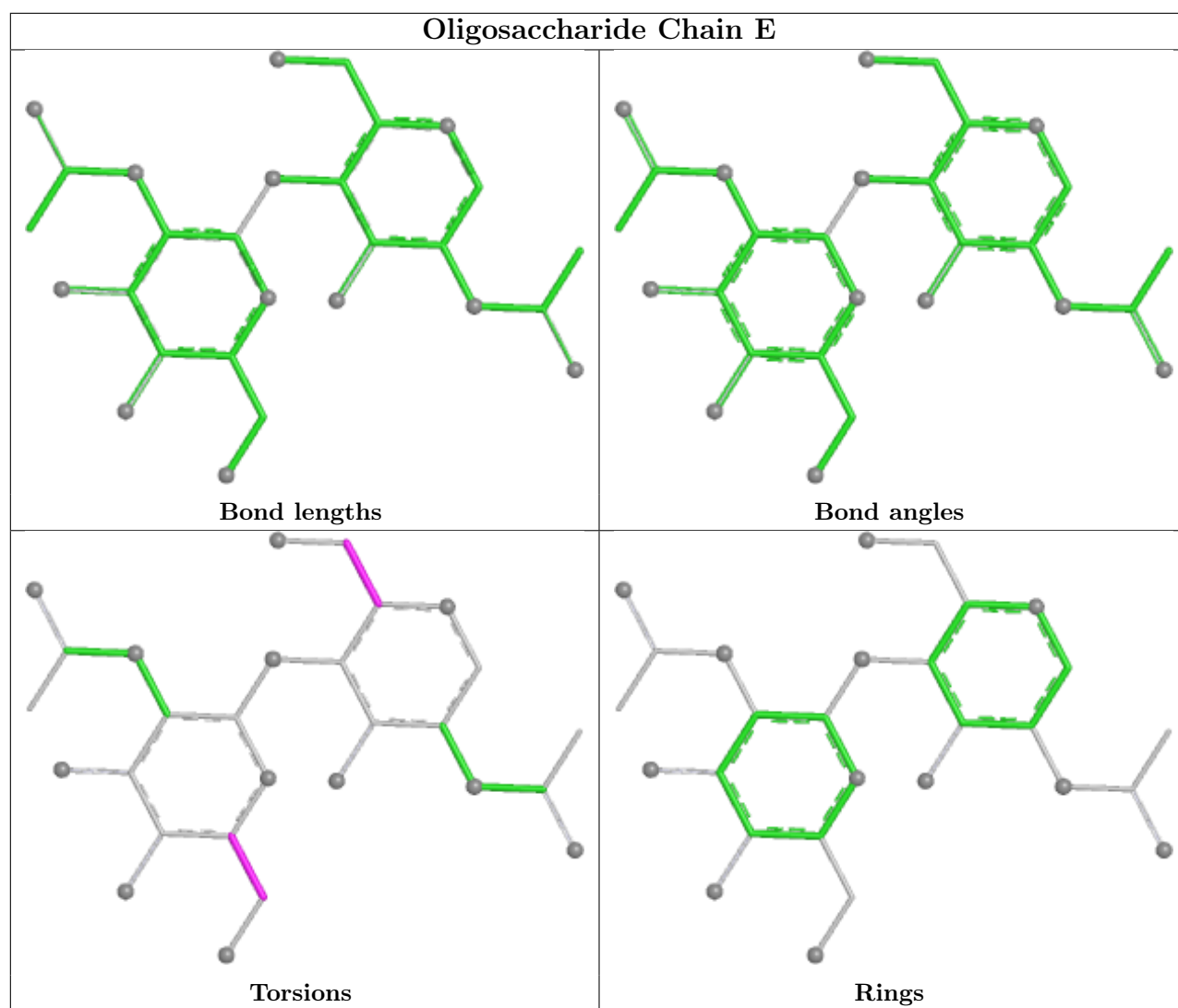
No monomer is involved in short contacts.

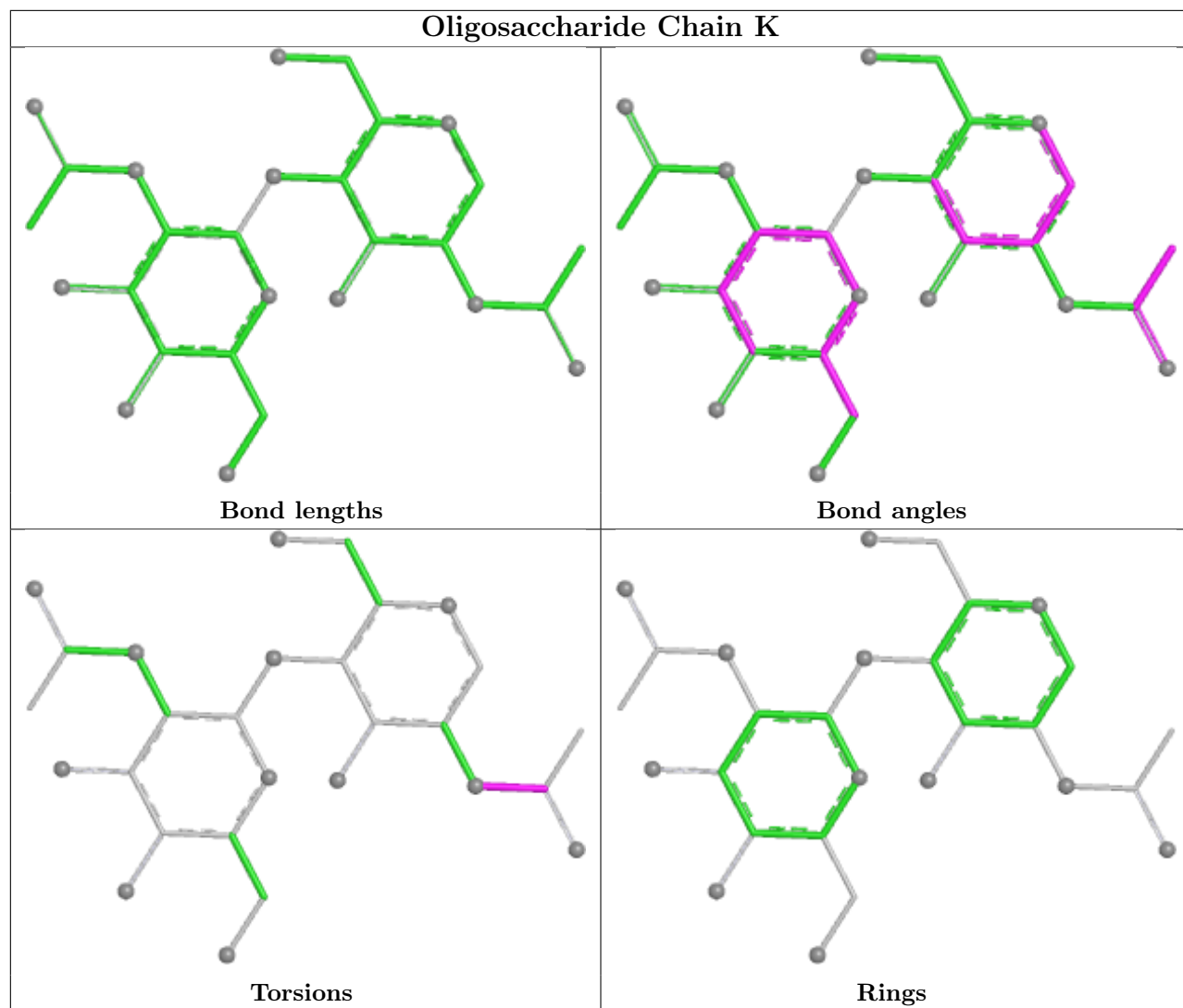
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

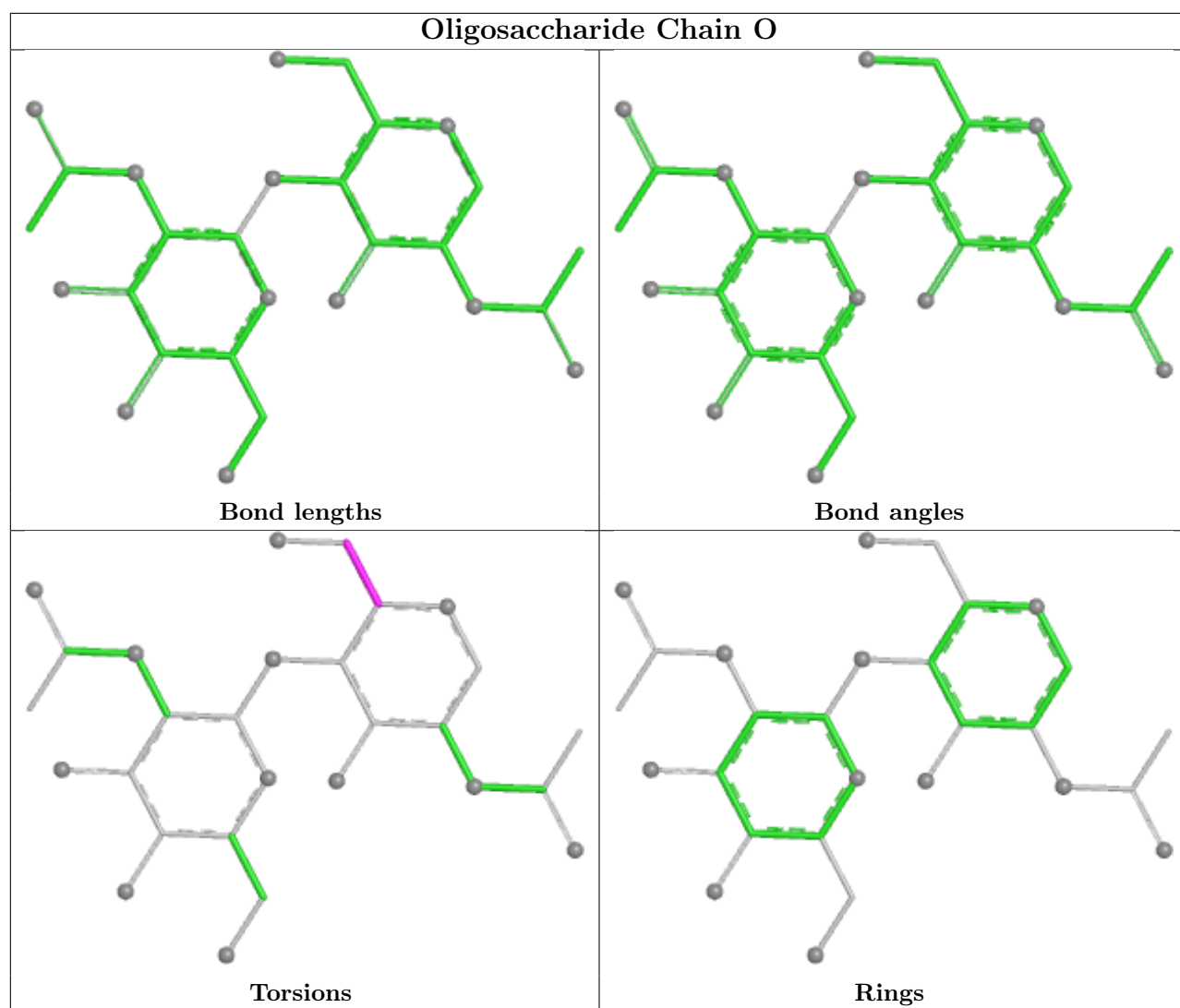


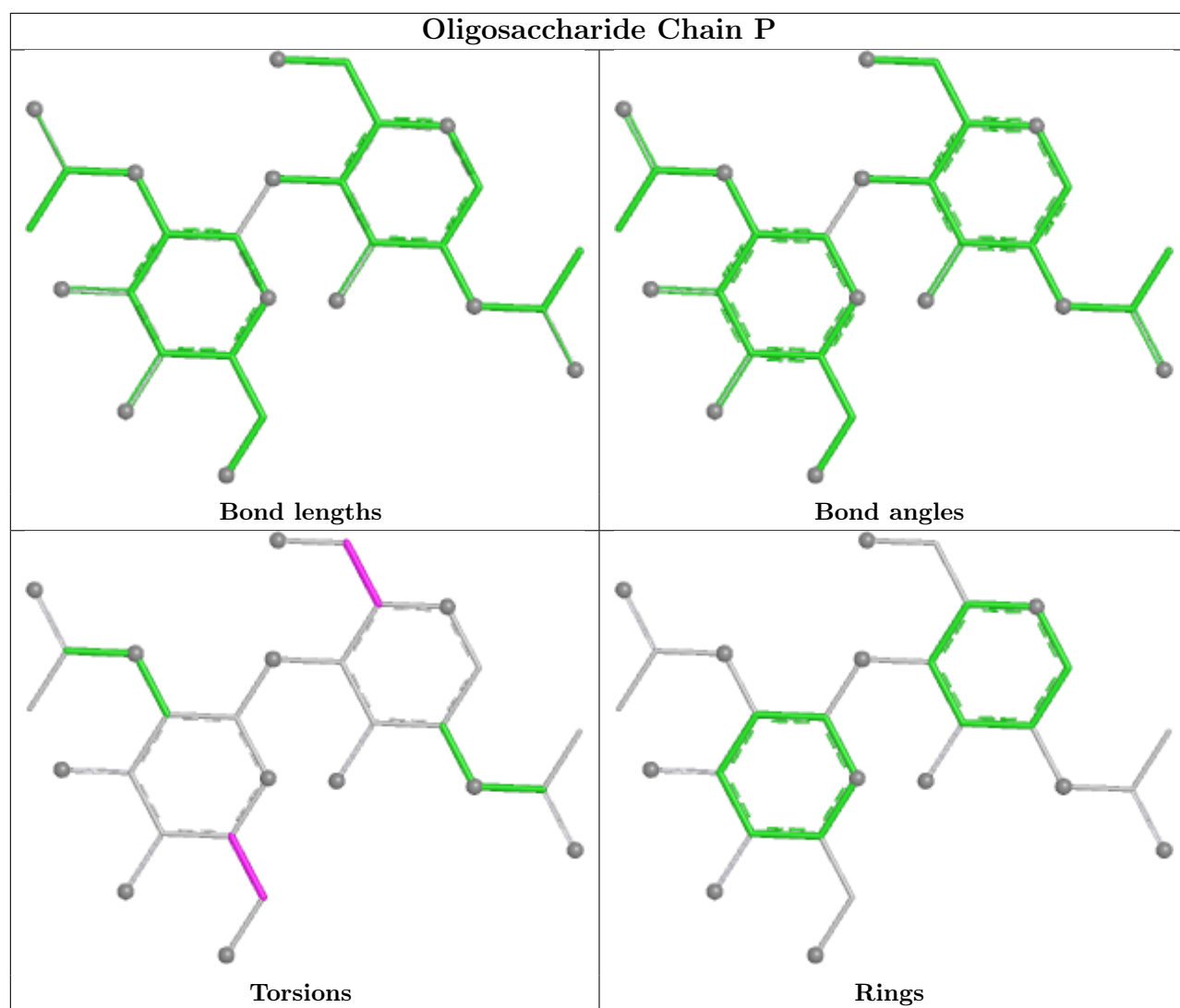


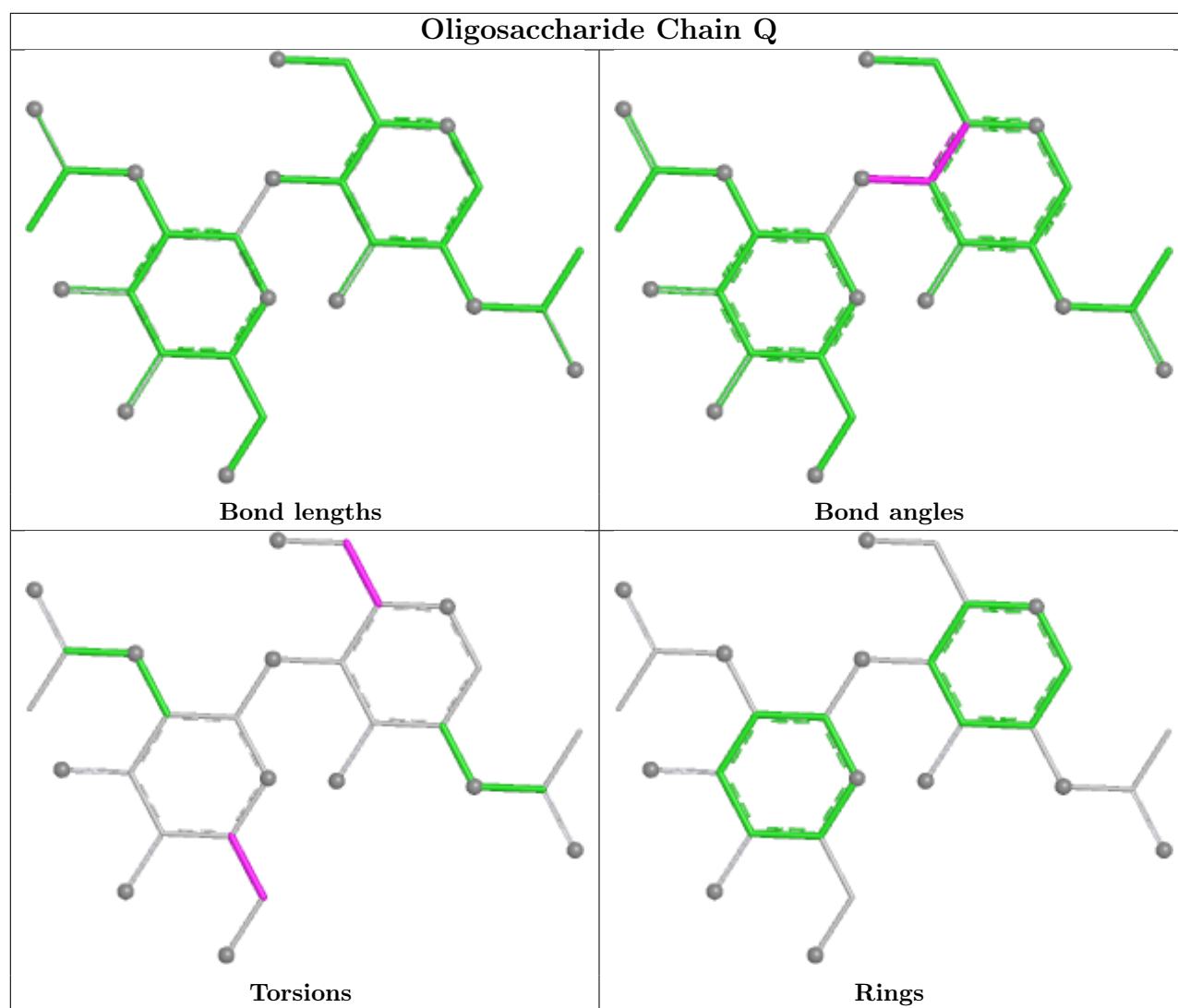


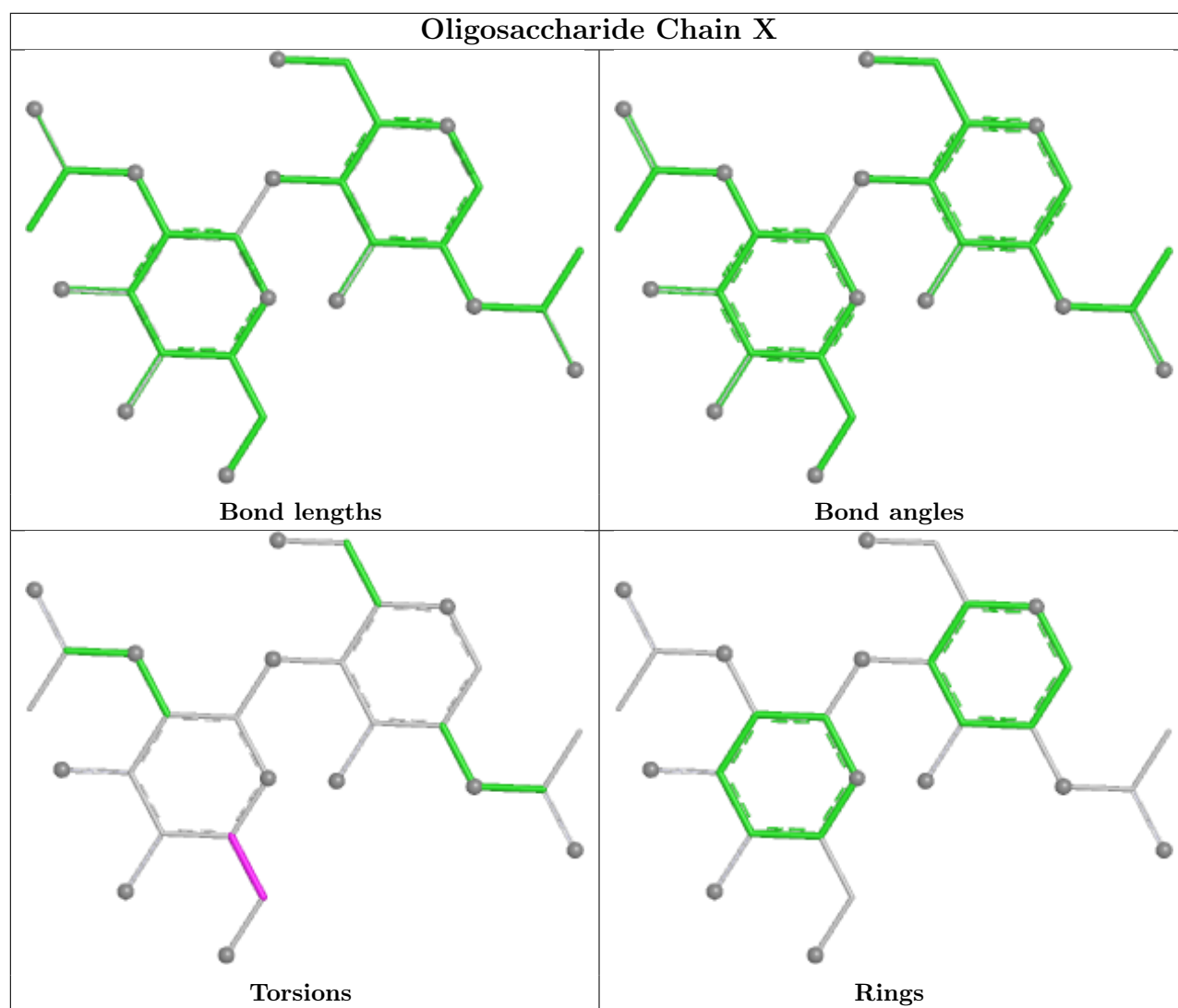


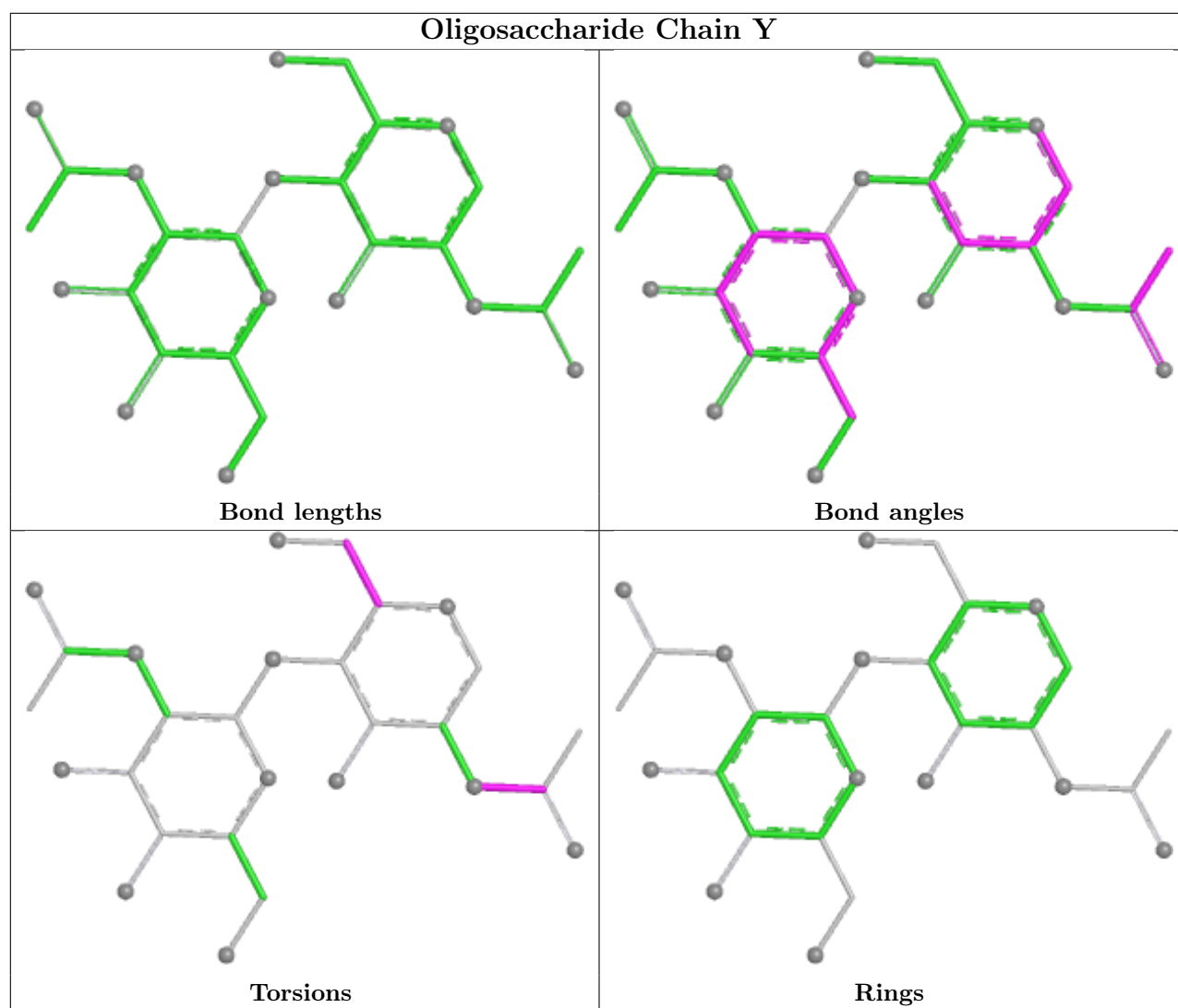


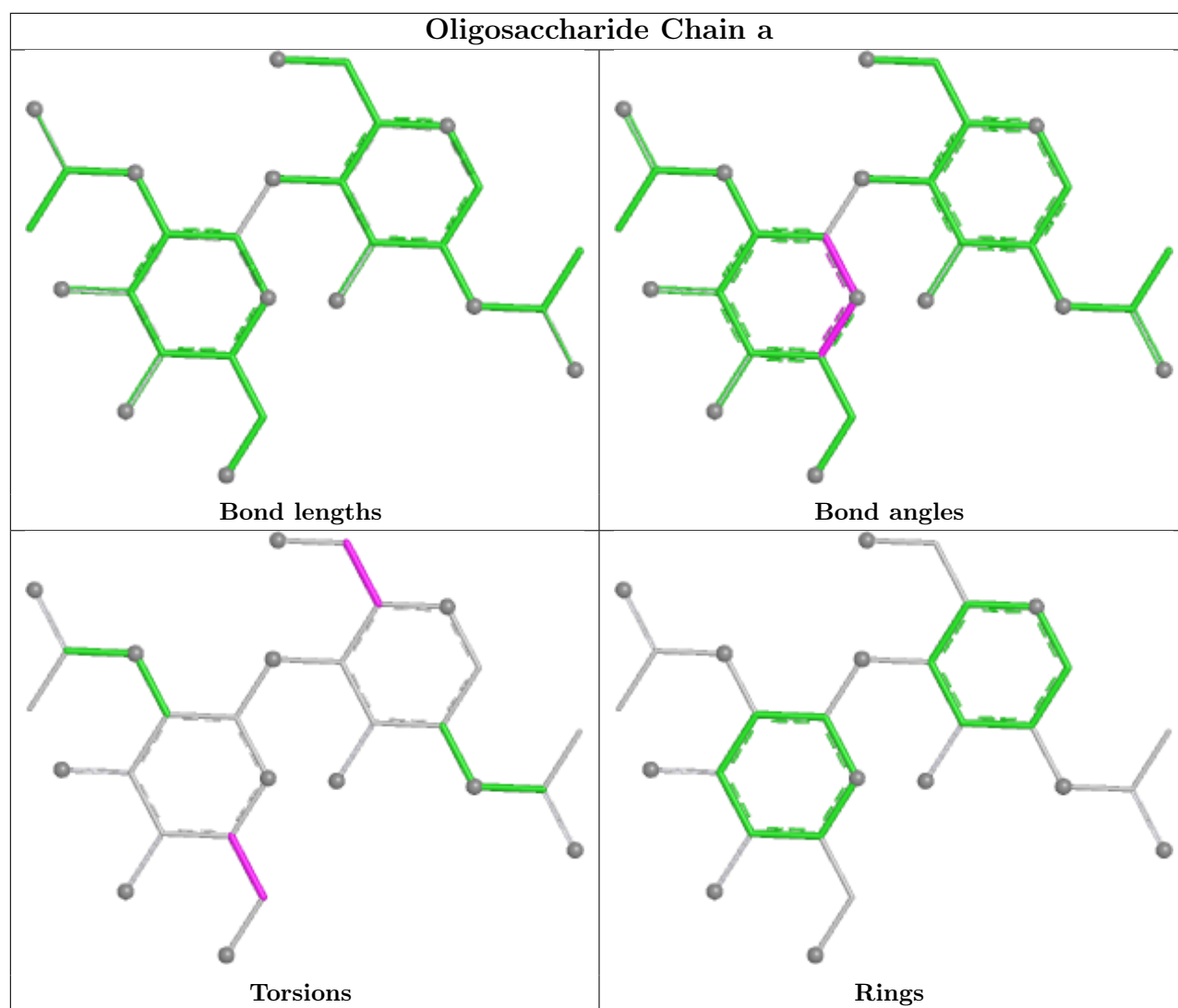


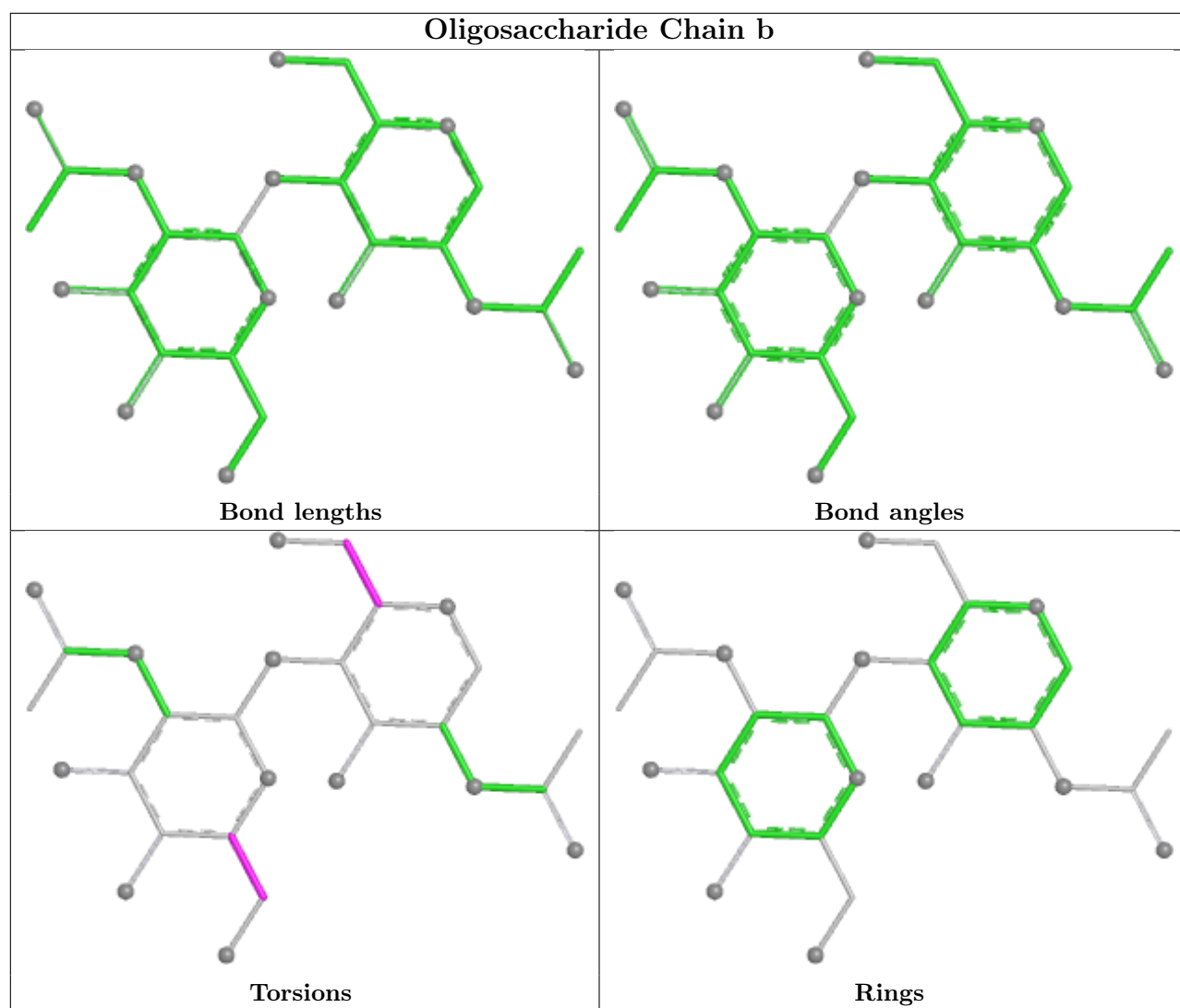


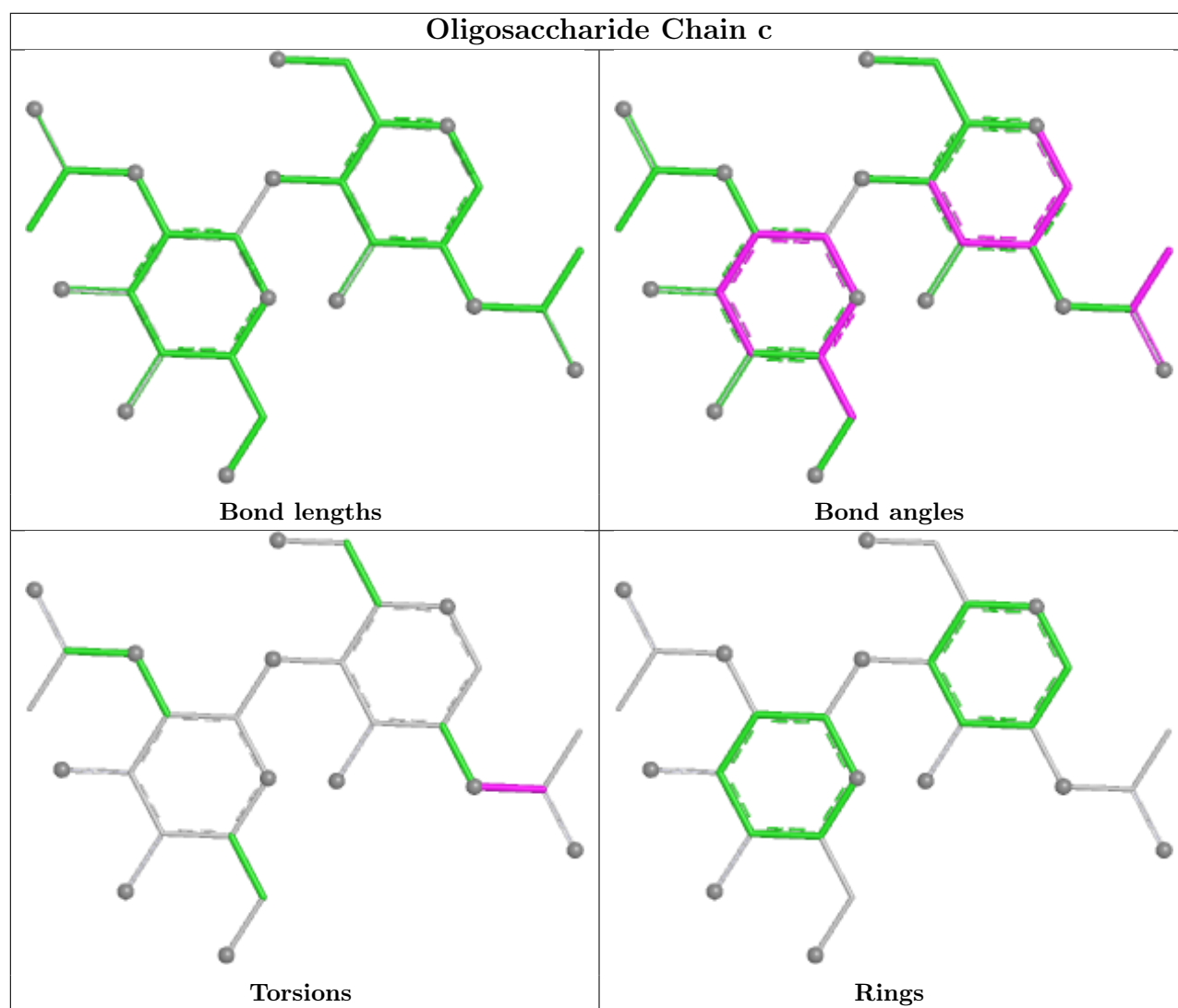


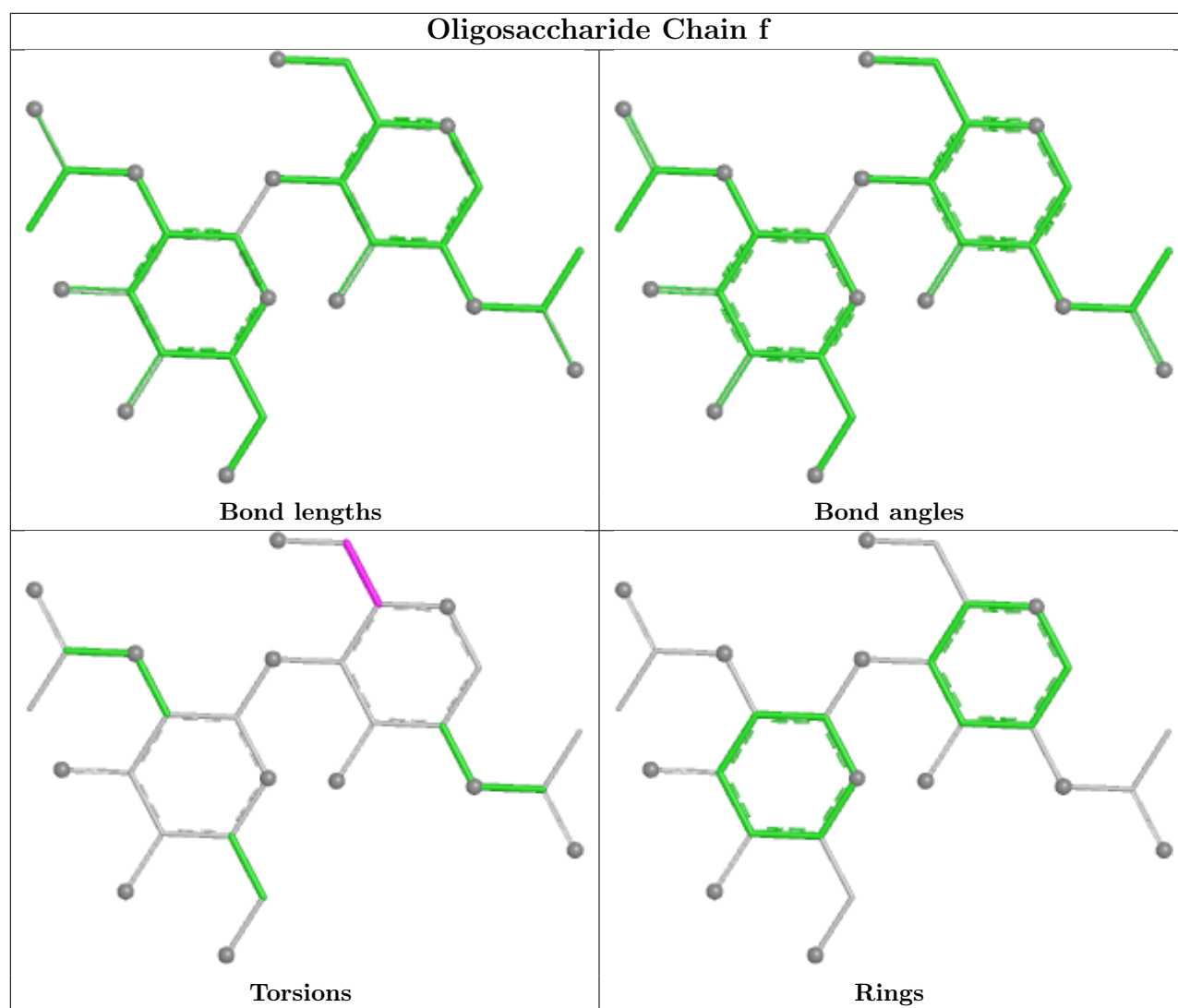


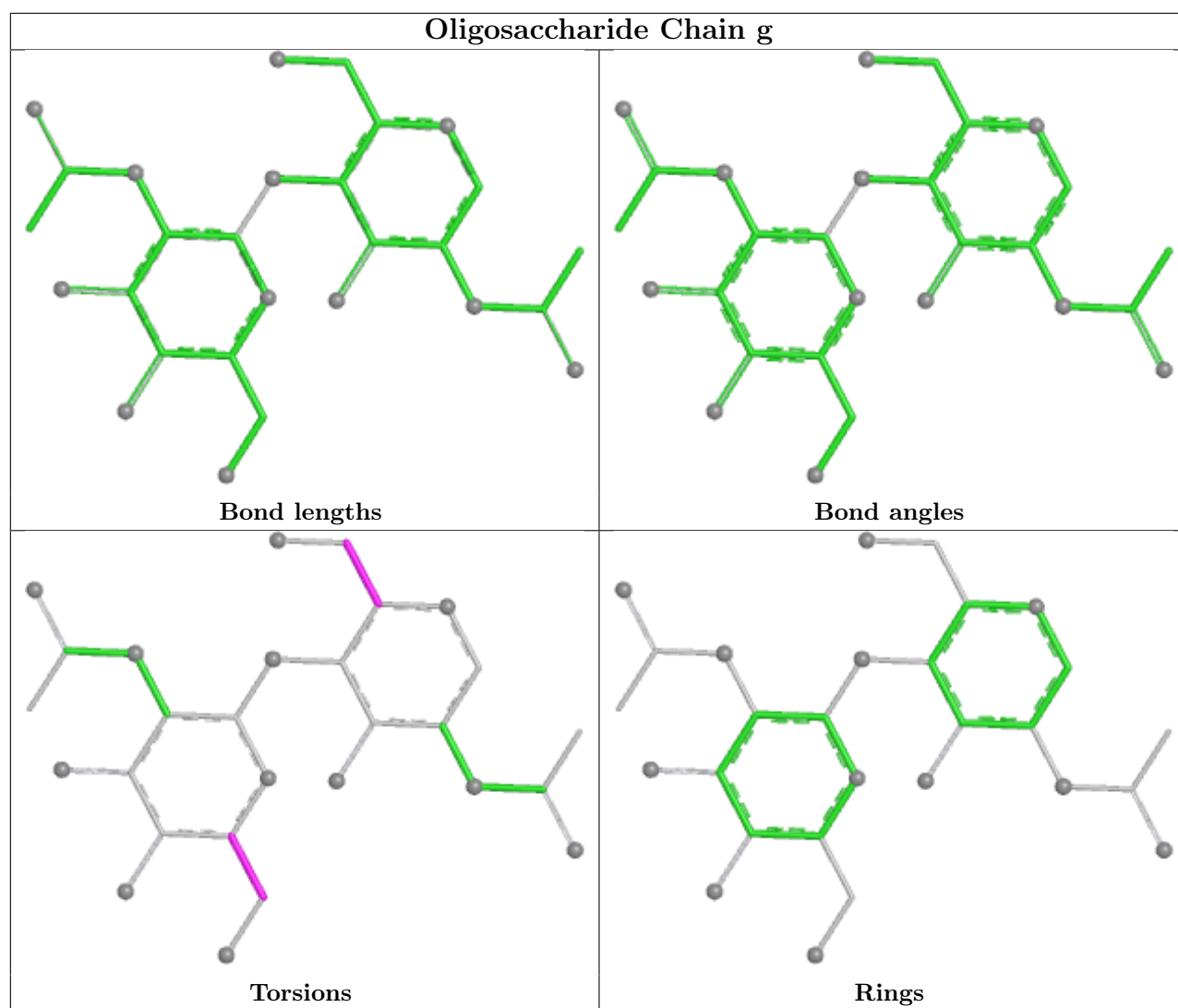


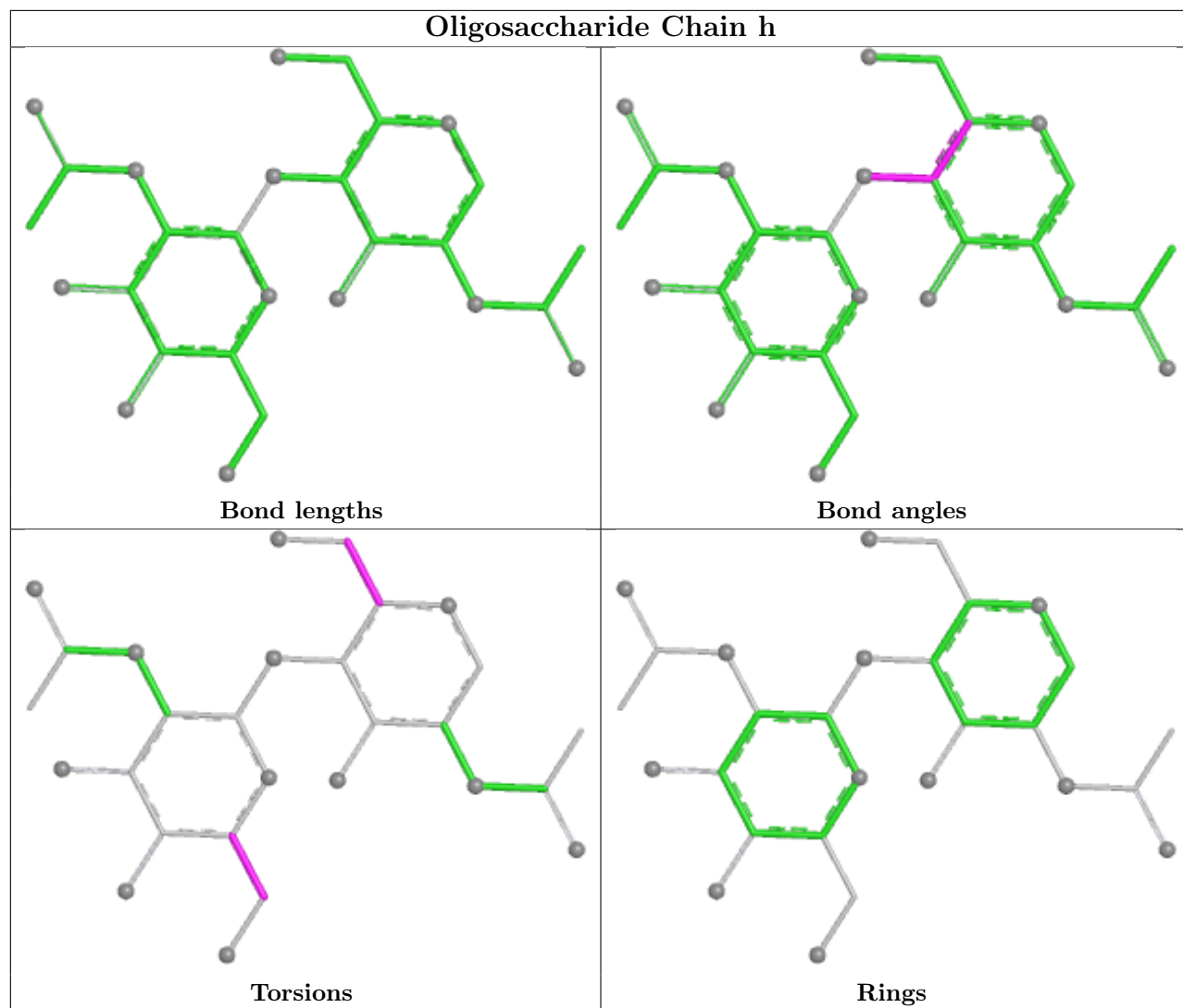


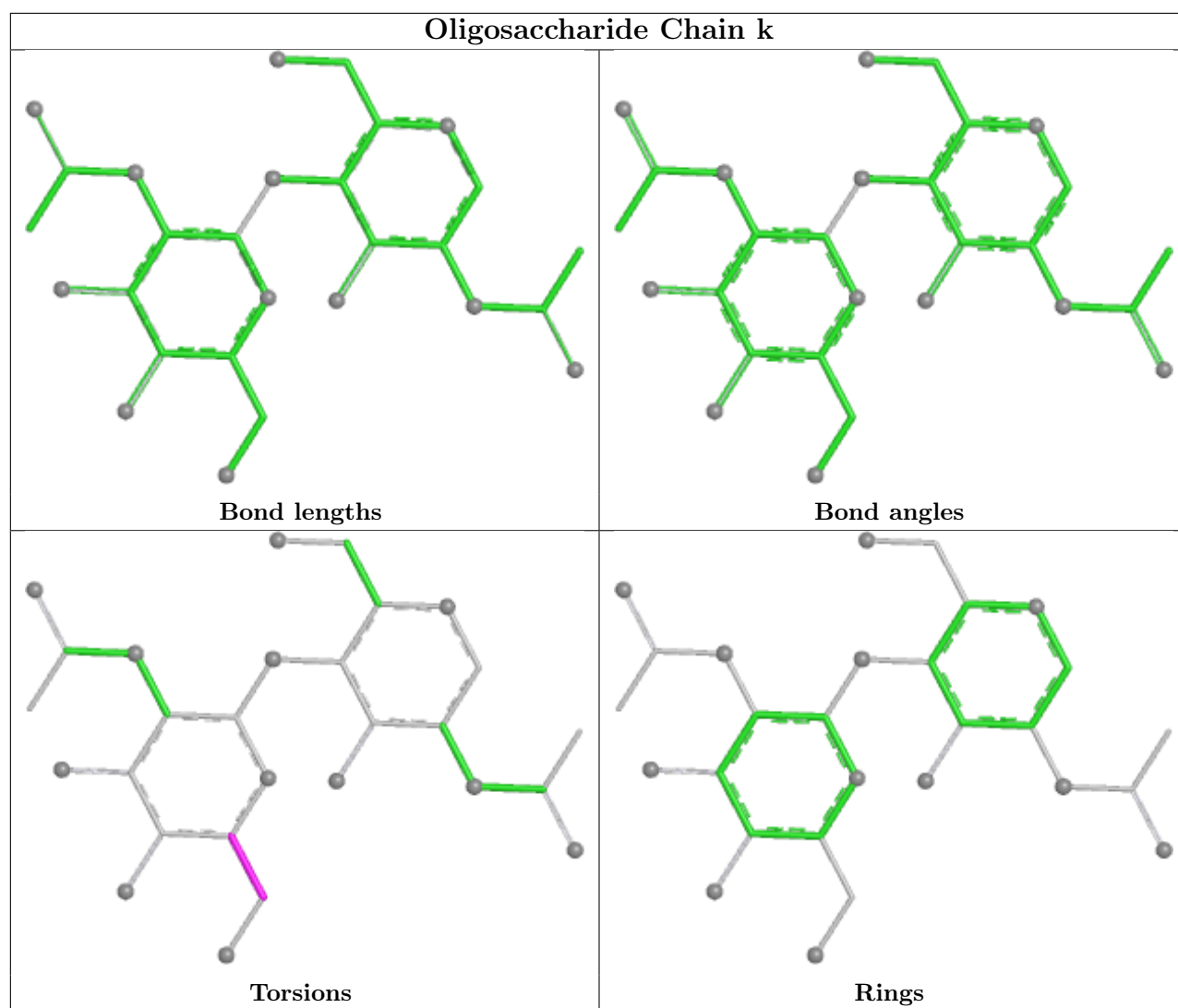


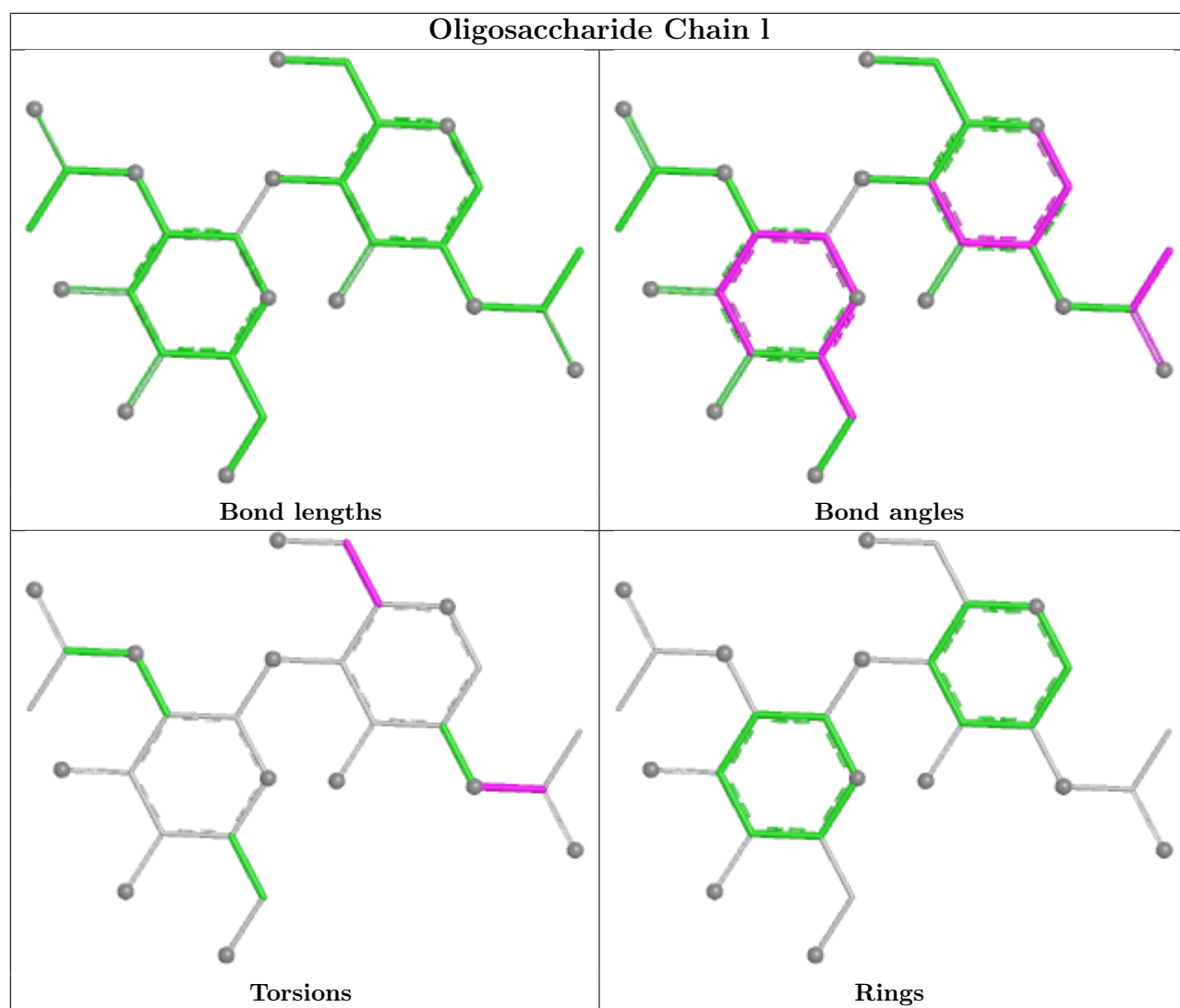


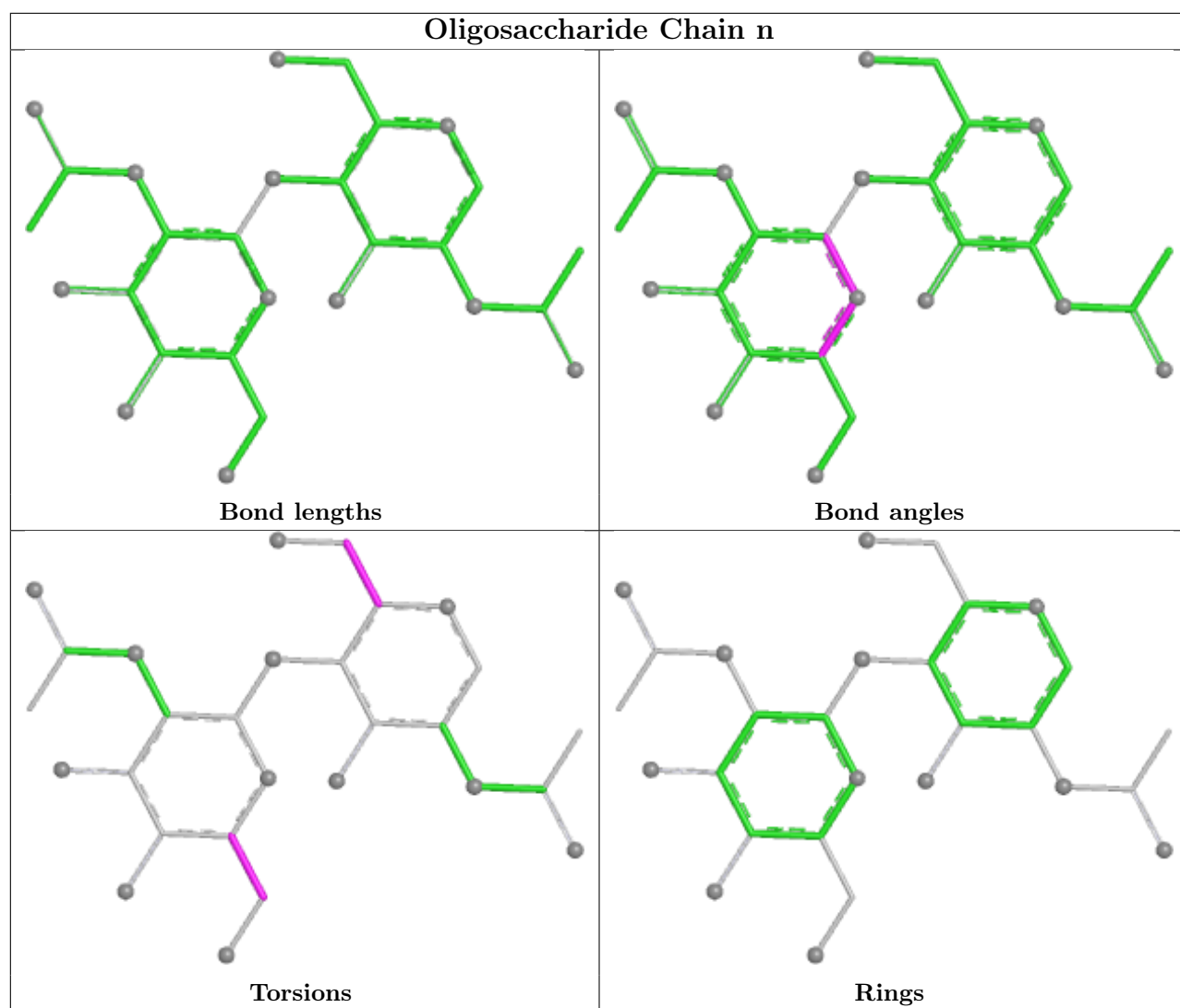


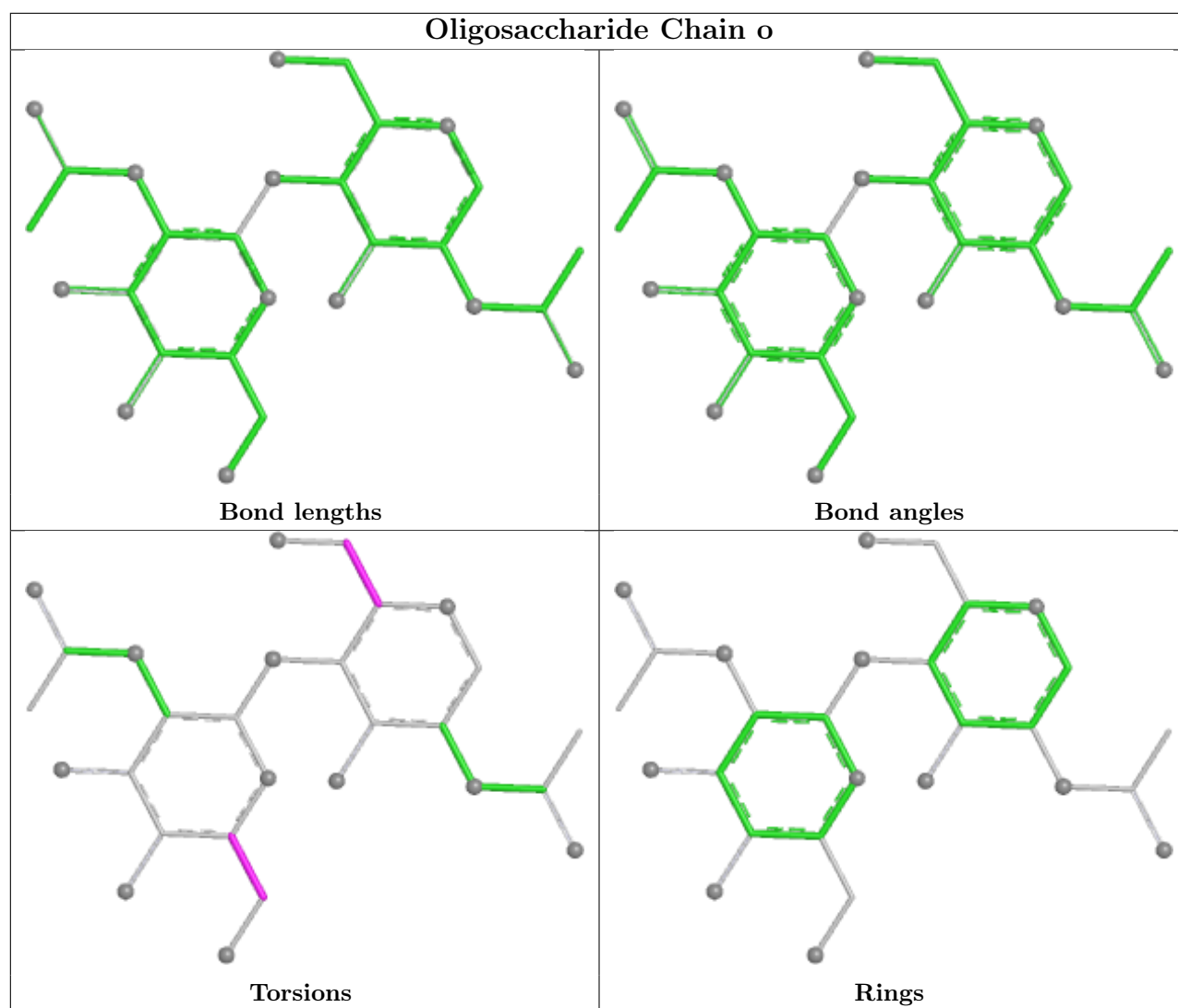


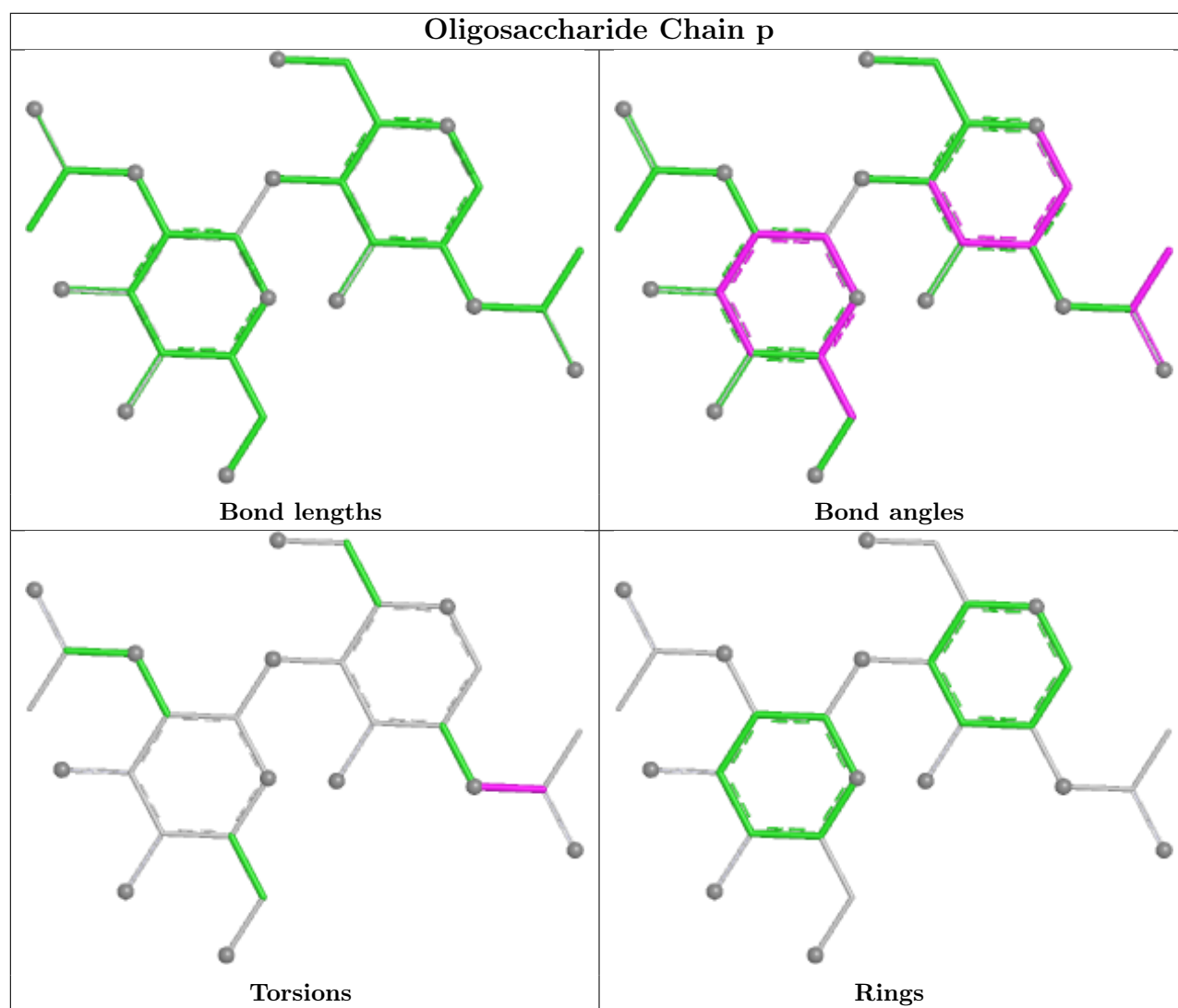


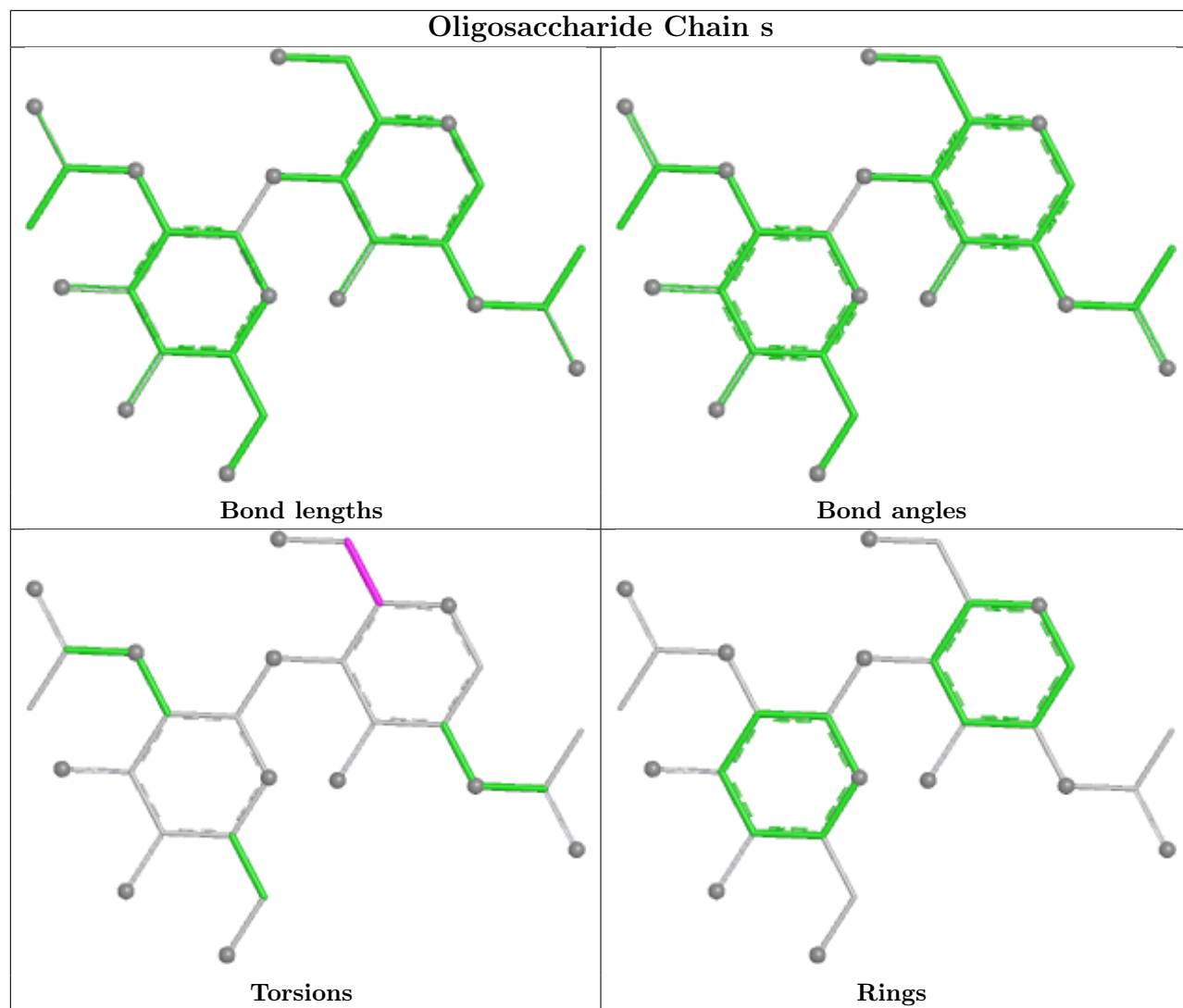


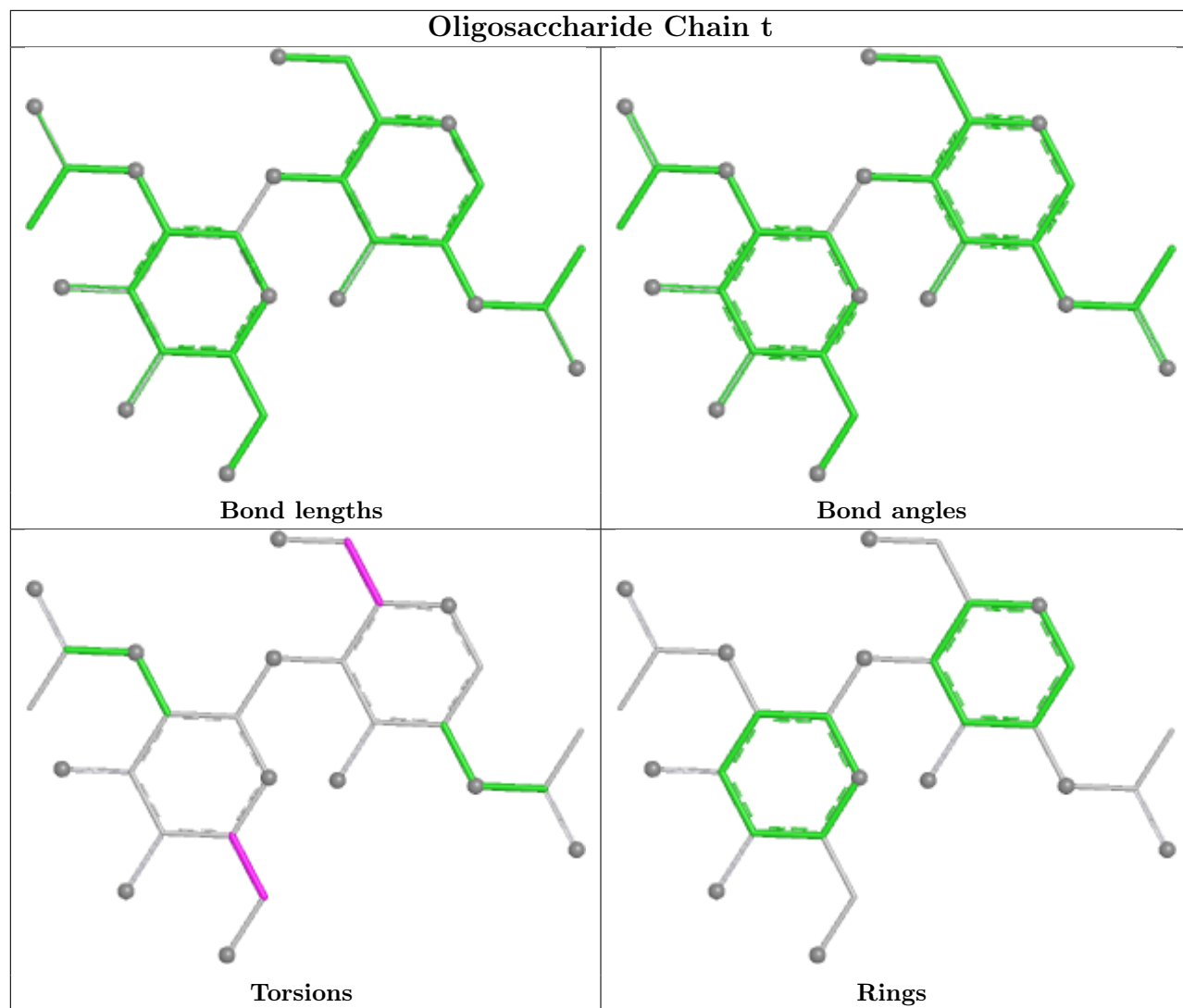


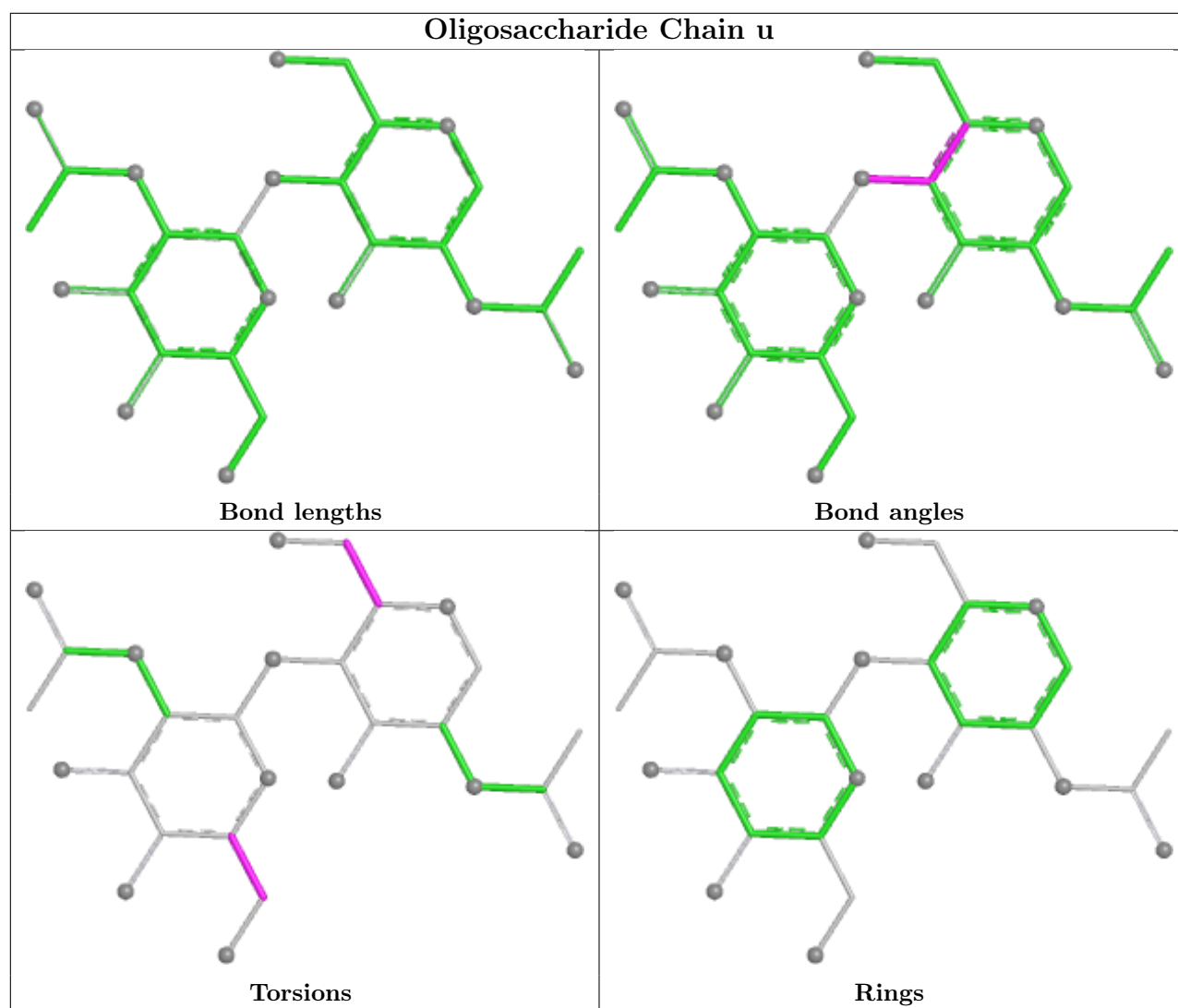


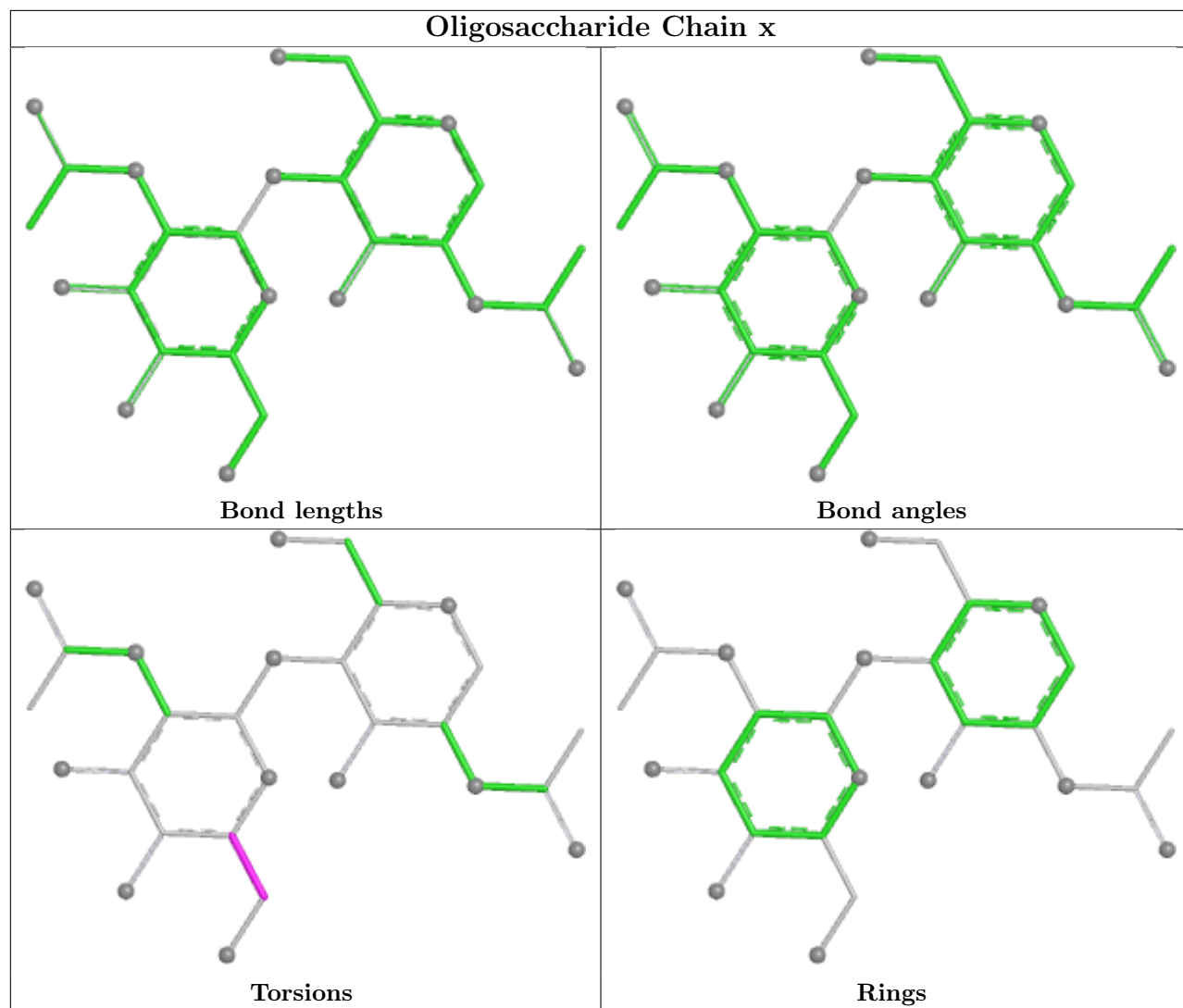


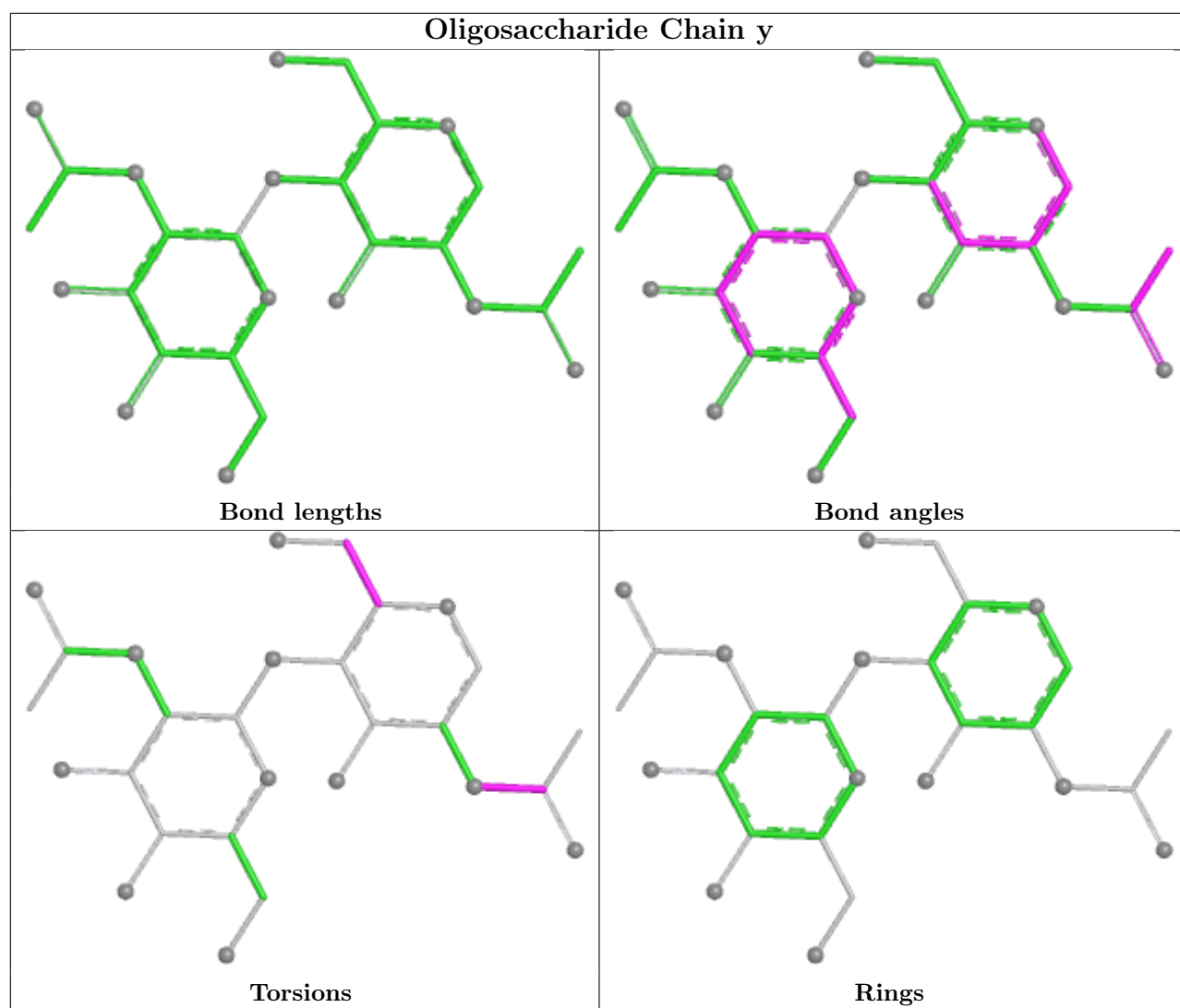


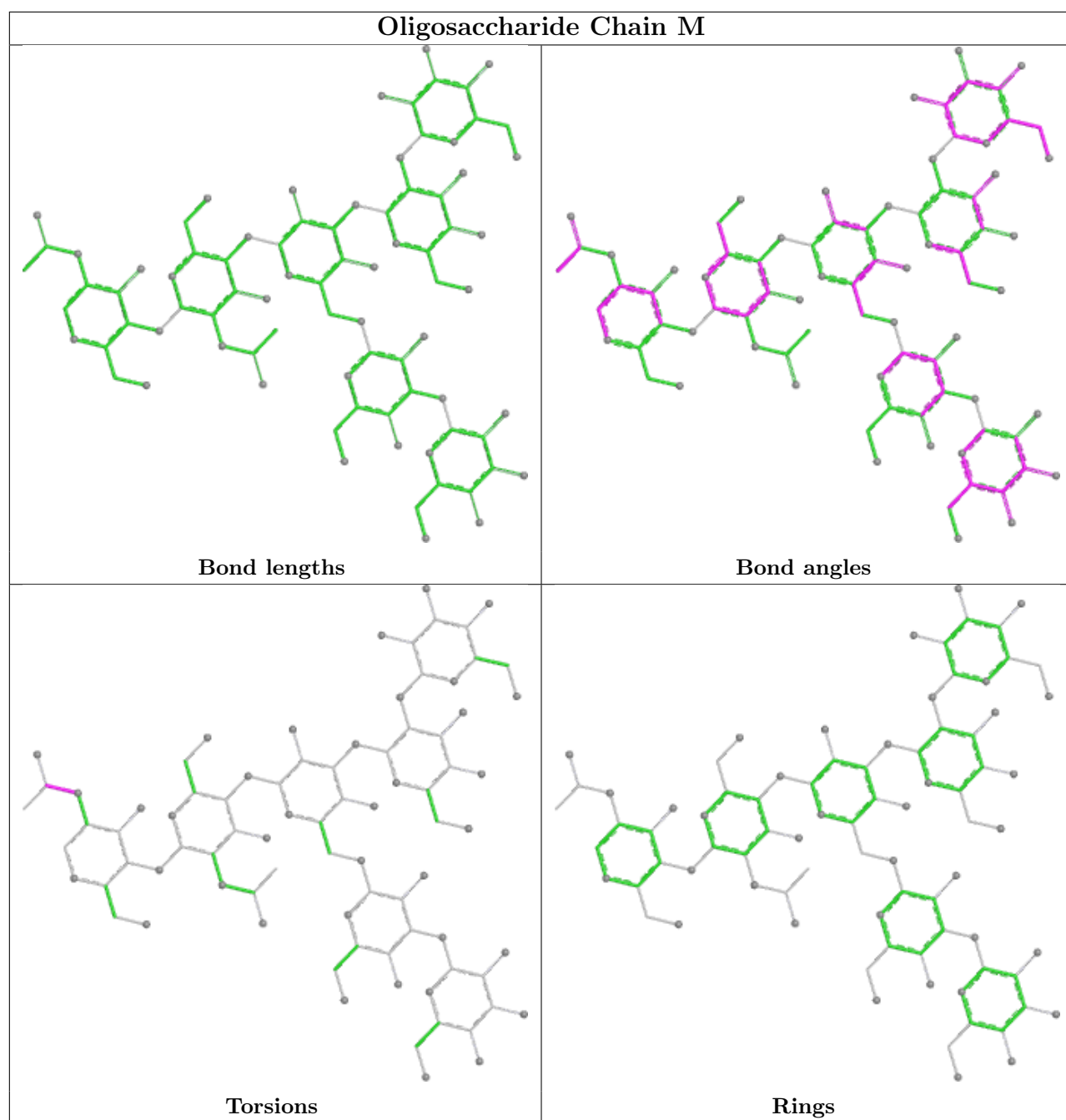


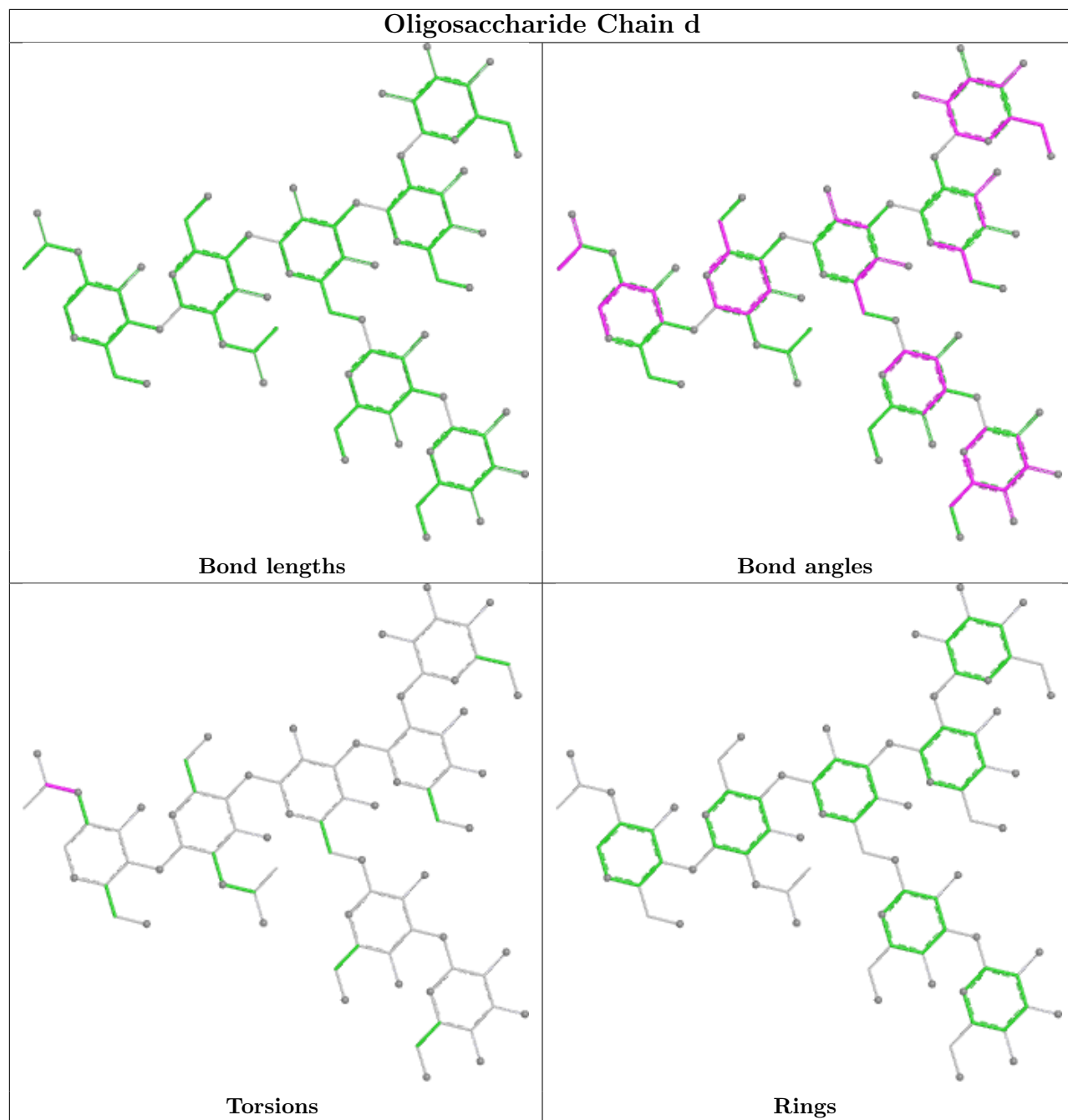


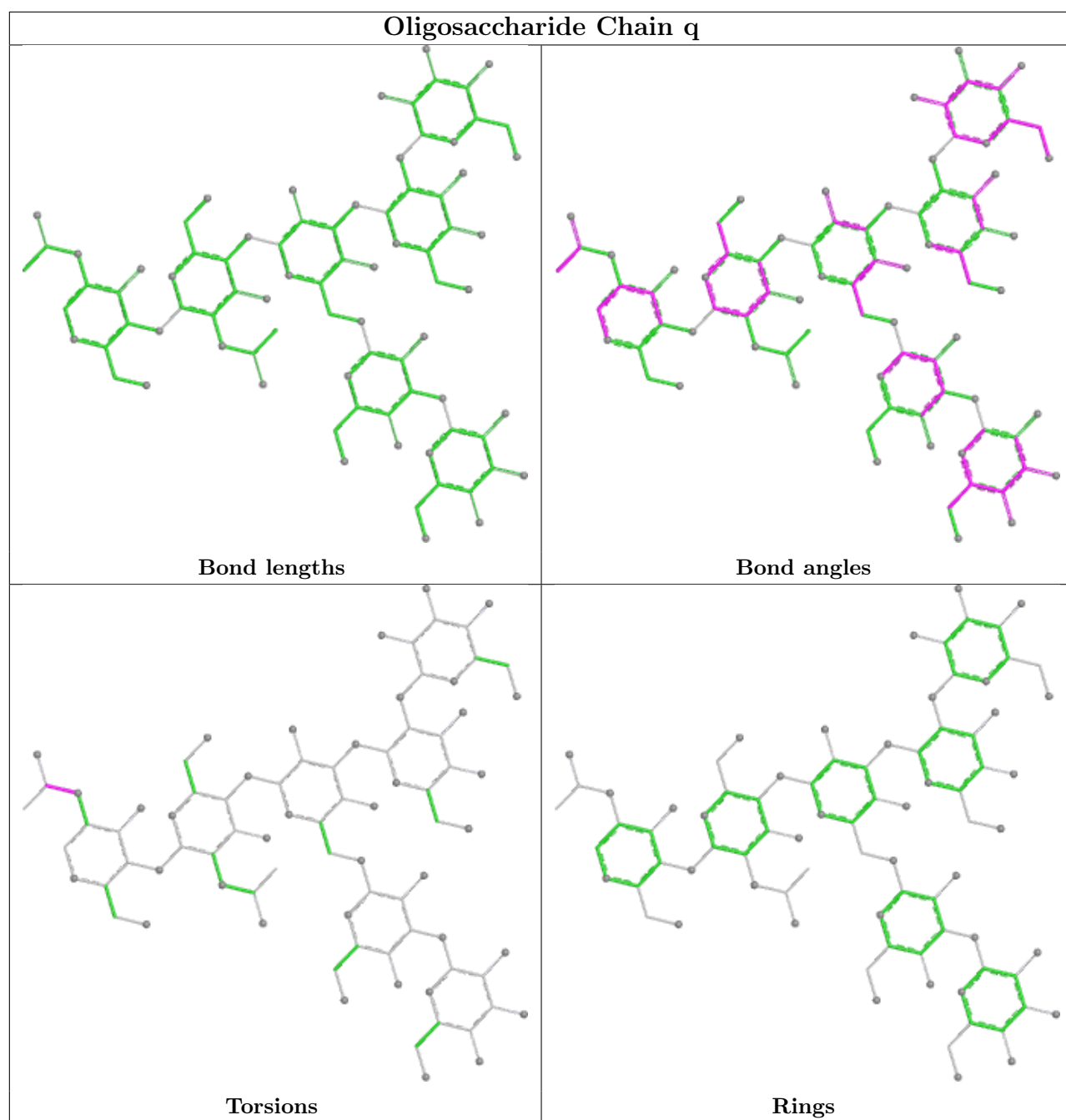


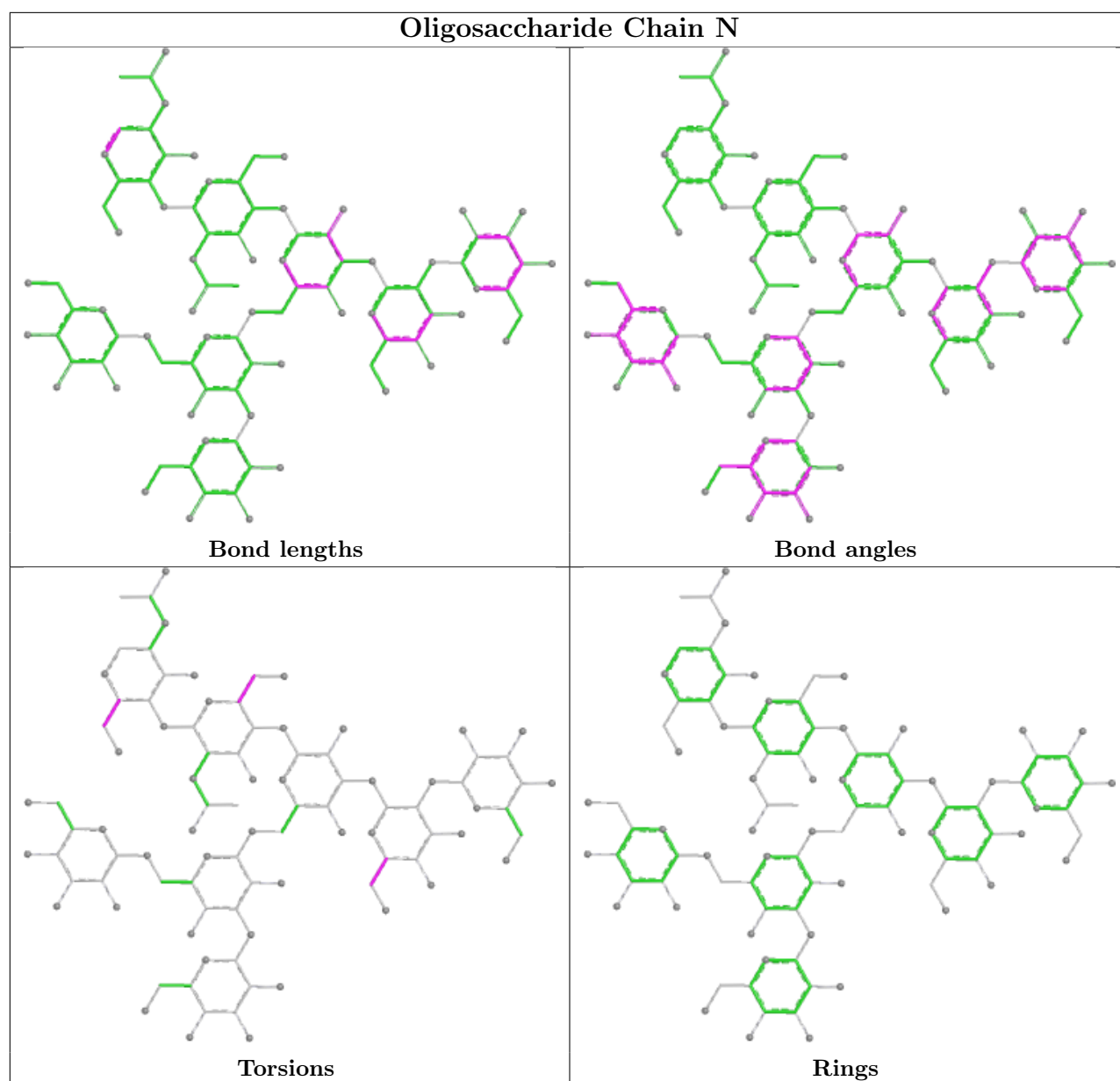


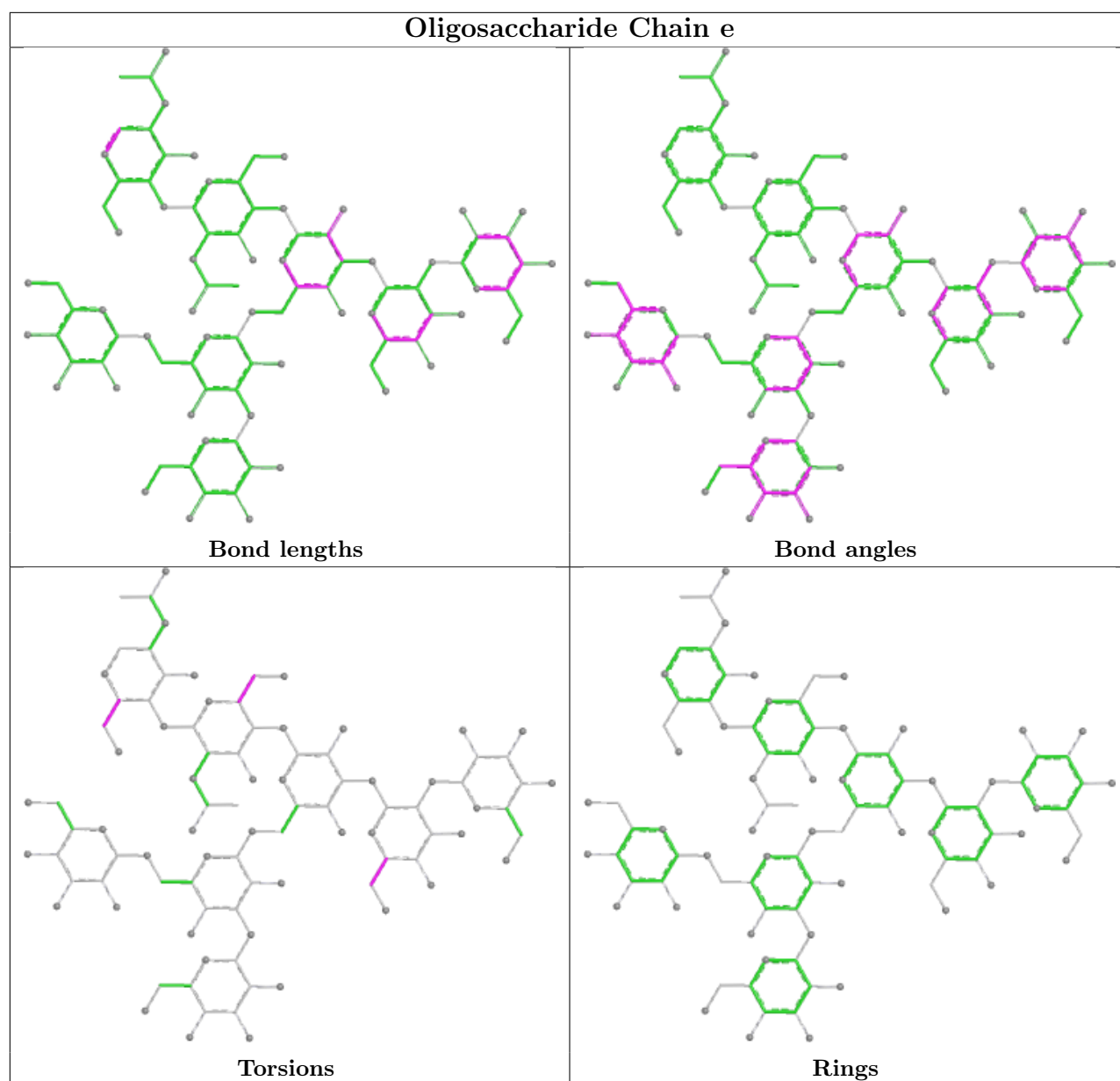


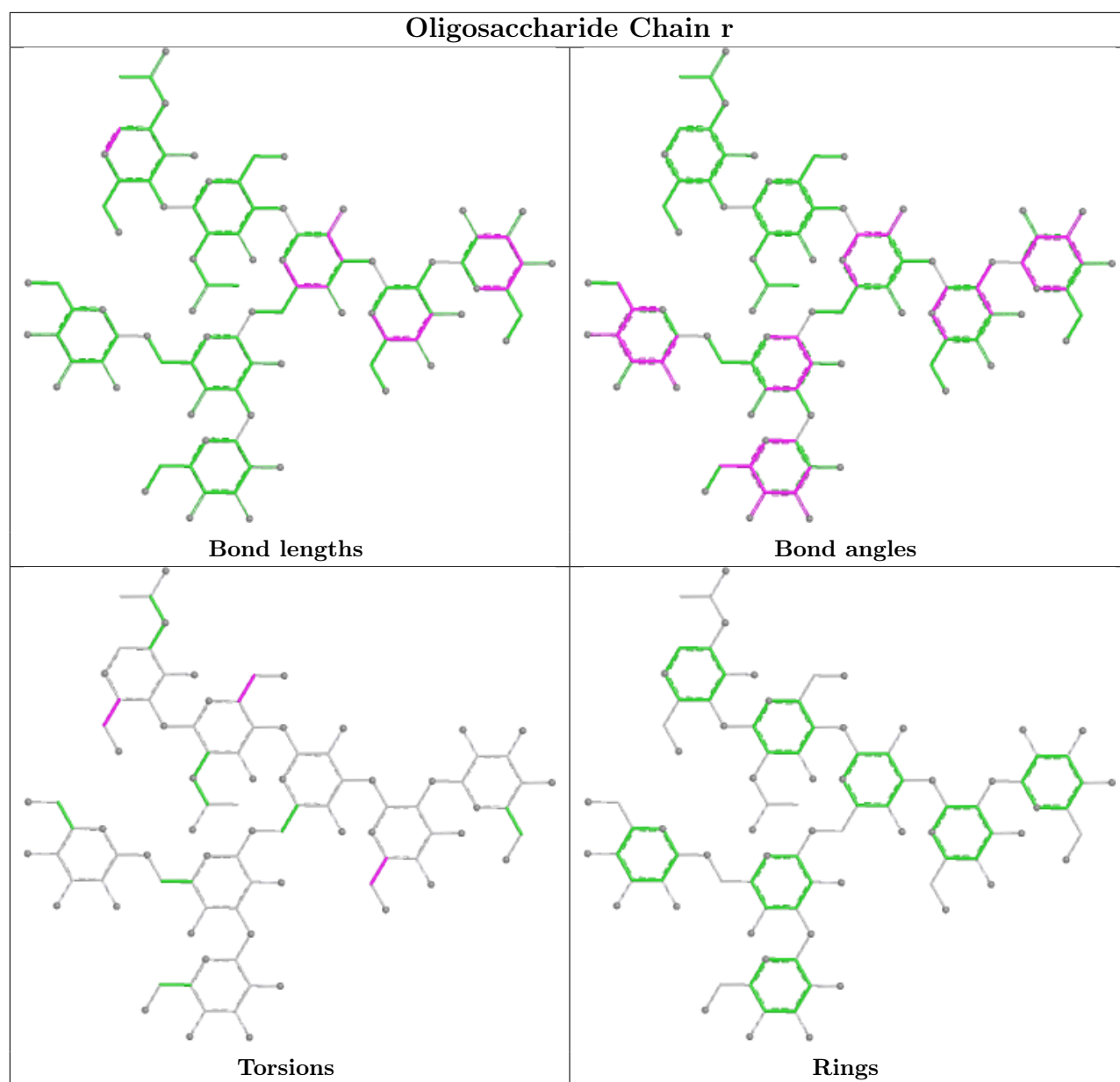


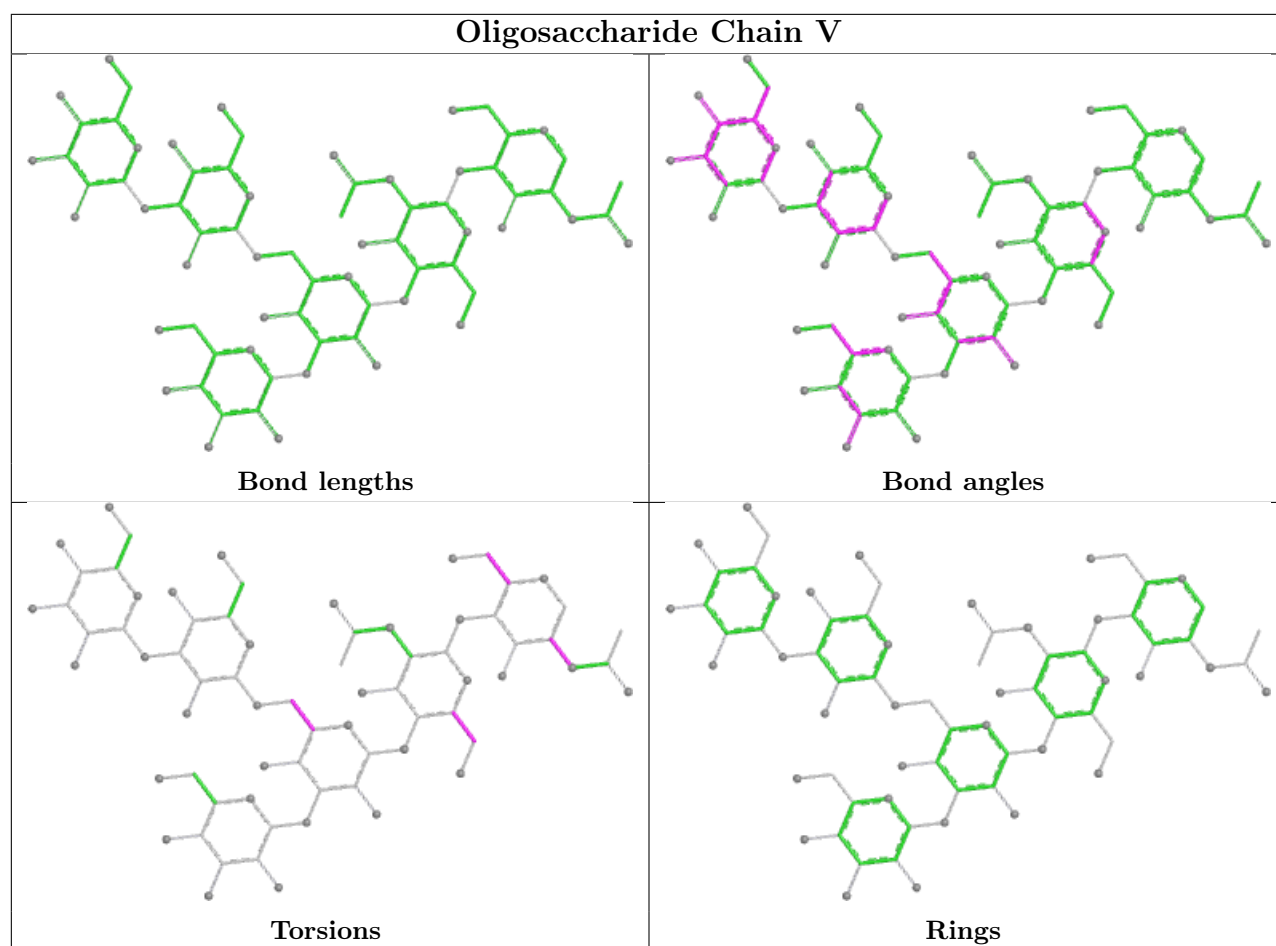


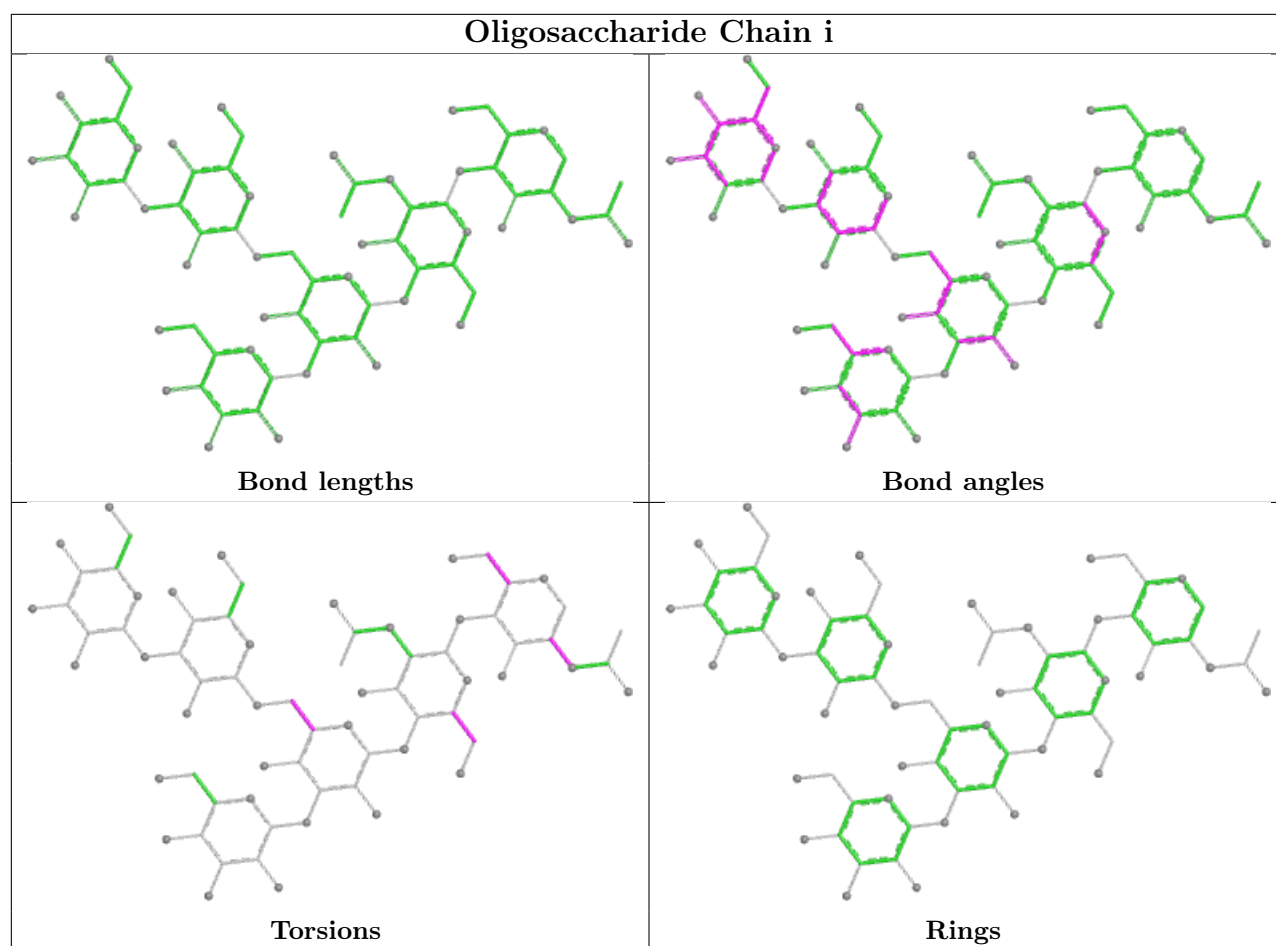


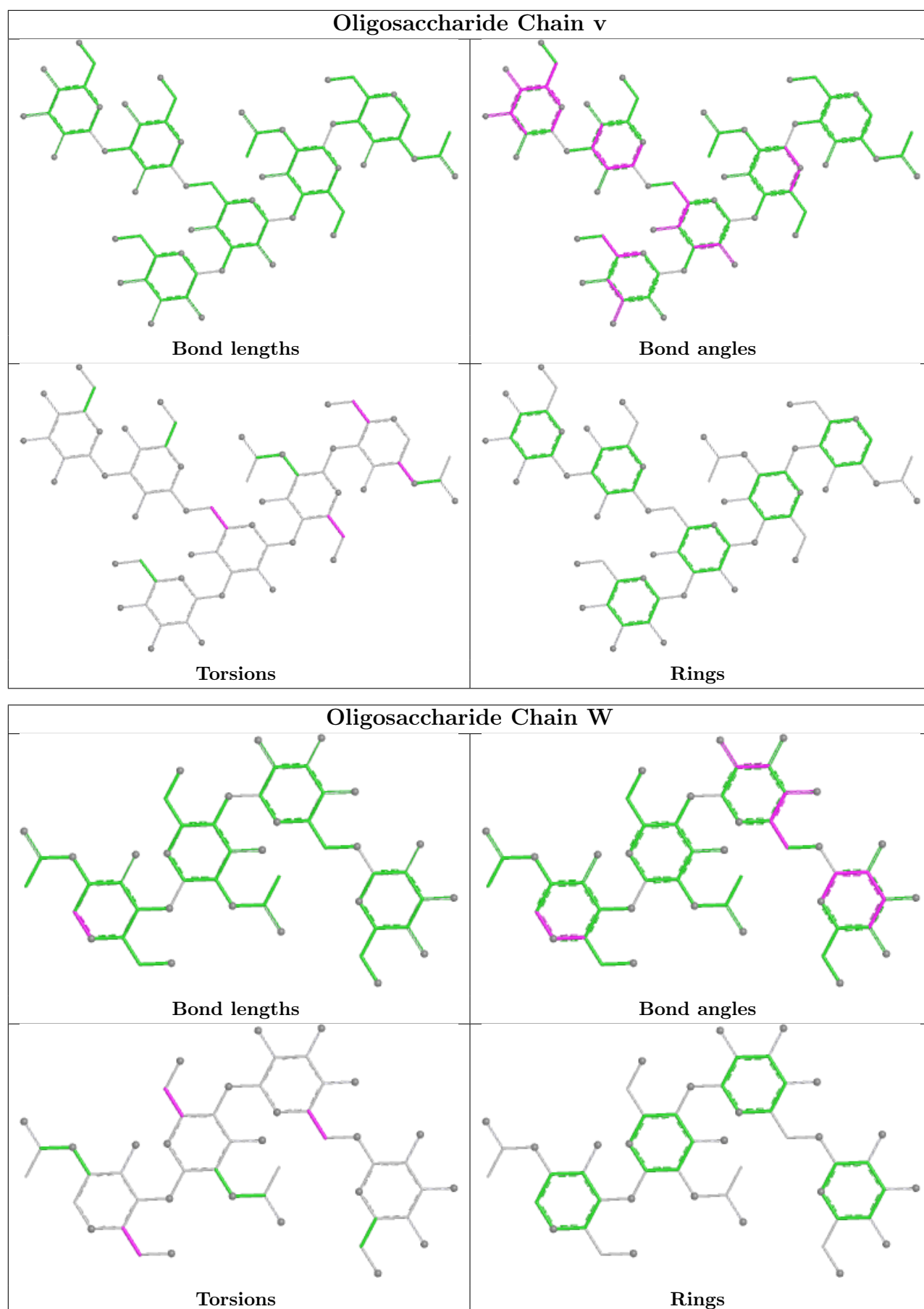


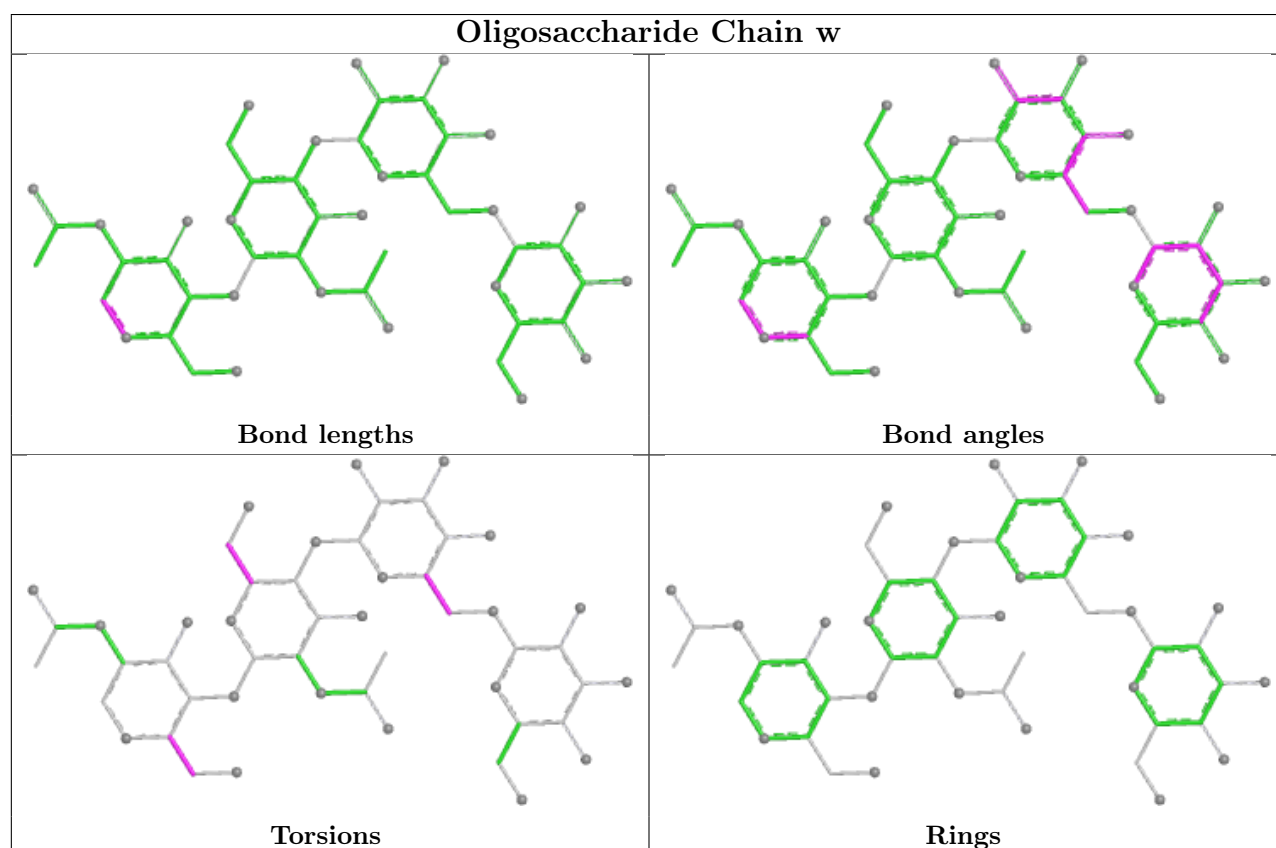
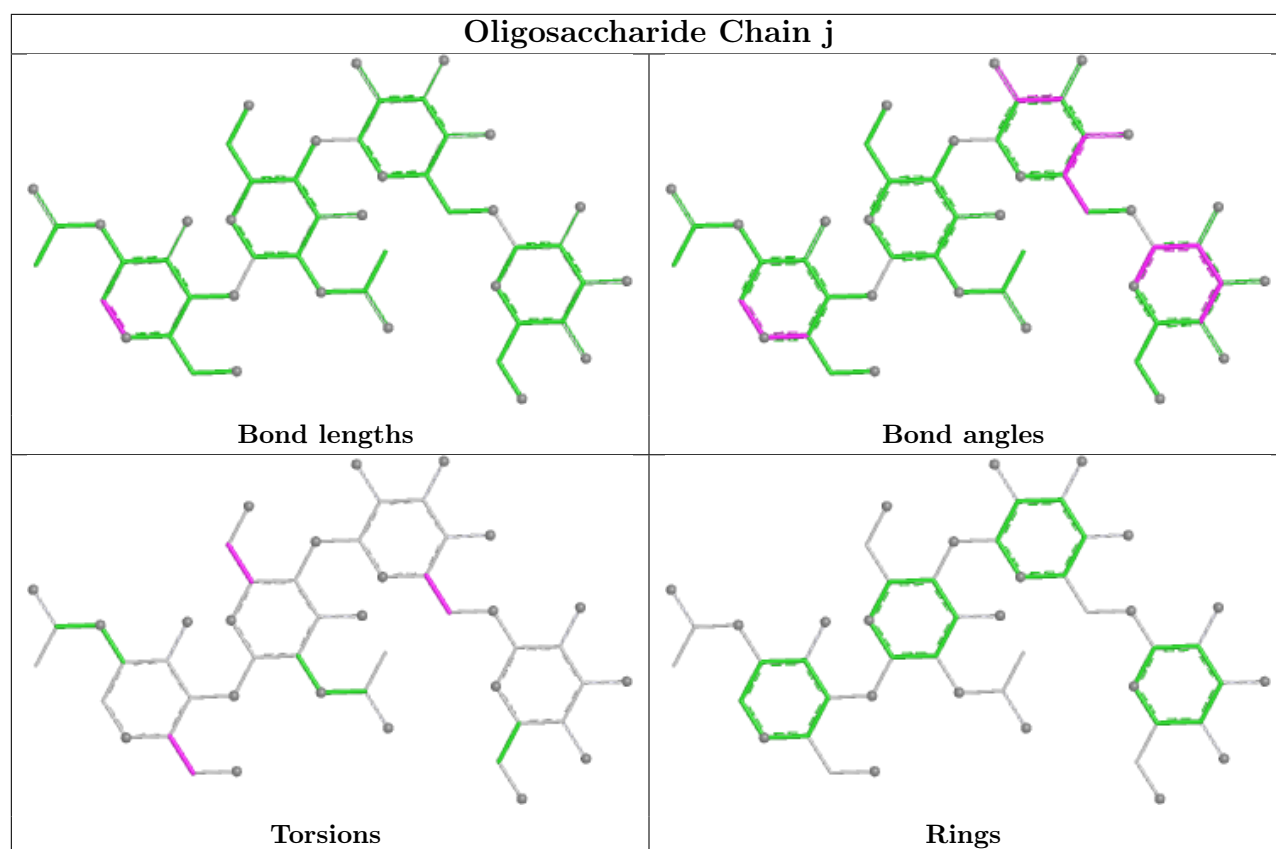












5.6 Ligand geometry

21 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	F	631	1	14,14,15	0.51	0	17,19,21	0.41	0
11	NAG	G	604	1	14,14,15	0.42	0	17,19,21	0.65	1 (5%)
11	NAG	G	645	1	14,14,15	0.47	0	17,19,21	0.56	0
11	NAG	F	645	1	14,14,15	0.47	0	17,19,21	0.56	0
11	NAG	A	604	1	14,14,15	0.41	0	17,19,21	0.65	1 (5%)
11	NAG	F	604	1	14,14,15	0.41	0	17,19,21	0.65	1 (5%)
11	NAG	A	645	1	14,14,15	0.47	0	17,19,21	0.56	0
11	NAG	G	634	1	14,14,15	0.50	0	17,19,21	0.42	0
11	NAG	J	702	2	14,14,15	0.53	0	17,19,21	0.53	0
11	NAG	A	634	1	14,14,15	0.50	0	17,19,21	0.42	0
11	NAG	F	611	1	14,14,15	0.52	0	17,19,21	0.51	0
11	NAG	I	702	2	14,14,15	0.53	0	17,19,21	0.54	0
11	NAG	B	701	2	14,14,15	0.35	0	17,19,21	0.62	0
11	NAG	I	701	2	14,14,15	0.35	0	17,19,21	0.61	0
11	NAG	F	634	1	14,14,15	0.32	0	17,19,21	0.40	0
11	NAG	G	611	1	14,14,15	0.53	0	17,19,21	0.51	0
11	NAG	A	633	1	14,14,15	0.32	0	17,19,21	0.40	0
11	NAG	A	611	1	14,14,15	0.52	0	17,19,21	0.51	0
11	NAG	B	702	2	14,14,15	0.53	0	17,19,21	0.54	0
11	NAG	G	633	1	14,14,15	0.33	0	17,19,21	0.41	0
11	NAG	J	701	2	14,14,15	0.35	0	17,19,21	0.61	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
11	NAG	F	631	1	-	2/6/23/26	0/1/1/1
11	NAG	G	604	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	G	645	1	-	0/6/23/26	0/1/1/1
11	NAG	F	645	1	-	0/6/23/26	0/1/1/1
11	NAG	A	604	1	-	2/6/23/26	0/1/1/1
11	NAG	F	604	1	-	2/6/23/26	0/1/1/1
11	NAG	A	645	1	-	0/6/23/26	0/1/1/1
11	NAG	G	634	1	-	2/6/23/26	0/1/1/1
11	NAG	J	702	2	-	2/6/23/26	0/1/1/1
11	NAG	A	634	1	-	2/6/23/26	0/1/1/1
11	NAG	F	611	1	-	2/6/23/26	0/1/1/1
11	NAG	I	702	2	-	2/6/23/26	0/1/1/1
11	NAG	B	701	2	-	3/6/23/26	0/1/1/1
11	NAG	I	701	2	-	3/6/23/26	0/1/1/1
11	NAG	F	634	1	-	2/6/23/26	0/1/1/1
11	NAG	G	611	1	-	2/6/23/26	0/1/1/1
11	NAG	A	633	1	-	2/6/23/26	0/1/1/1
11	NAG	A	611	1	-	2/6/23/26	0/1/1/1
11	NAG	B	702	2	-	2/6/23/26	0/1/1/1
11	NAG	G	633	1	-	2/6/23/26	0/1/1/1
11	NAG	J	701	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	604	NAG	C1-O5-C5	2.07	114.97	112.19
11	F	604	NAG	C1-O5-C5	2.07	114.96	112.19
11	G	604	NAG	C1-O5-C5	2.07	114.96	112.19

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	633	NAG	O5-C5-C6-O6
11	A	634	NAG	O5-C5-C6-O6
11	F	631	NAG	O5-C5-C6-O6
11	F	634	NAG	O5-C5-C6-O6
11	G	633	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

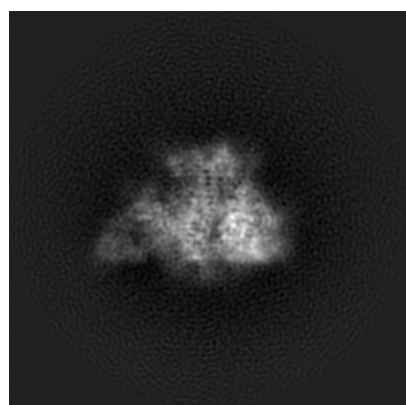
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8644. These allow visual inspection of the internal detail of the map and identification of artifacts.

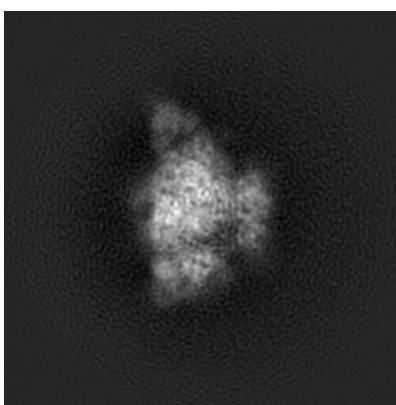
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

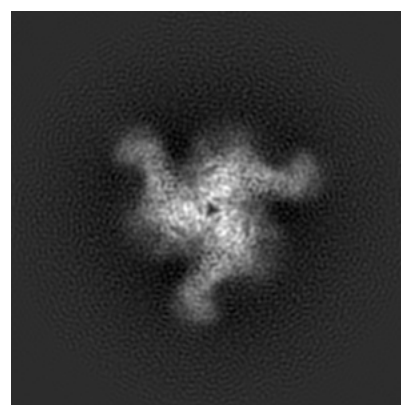
6.1.1 Primary map



X



Y

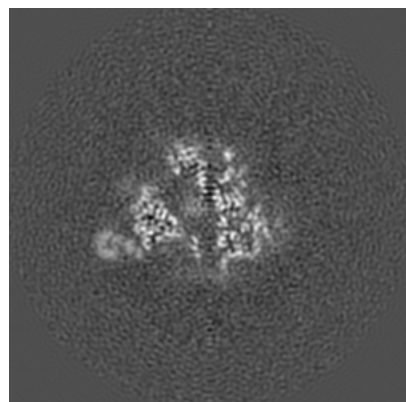


Z

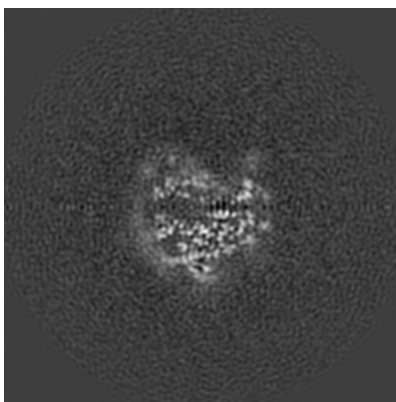
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

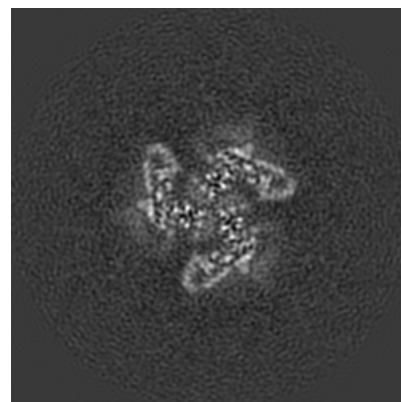
6.2.1 Primary map



X Index: 128



Y Index: 128

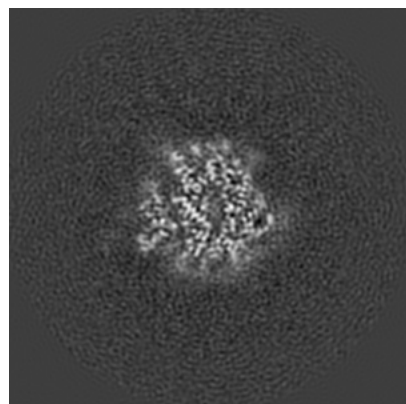


Z Index: 128

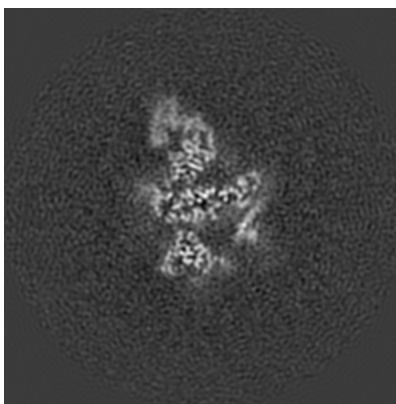
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

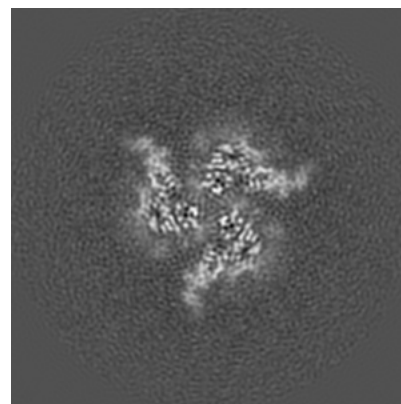
6.3.1 Primary map



X Index: 135



Y Index: 142

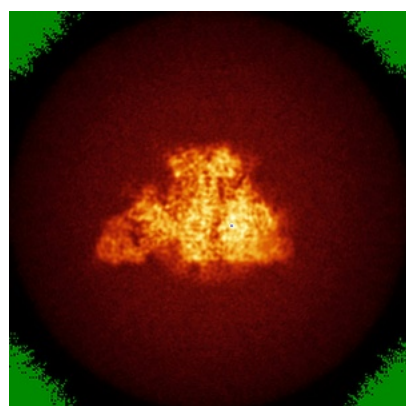


Z Index: 123

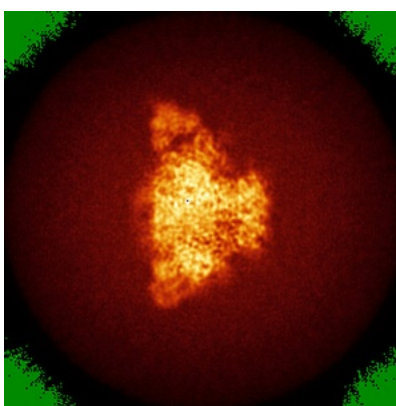
The images above show the largest variance slices of the map in three orthogonal directions.

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

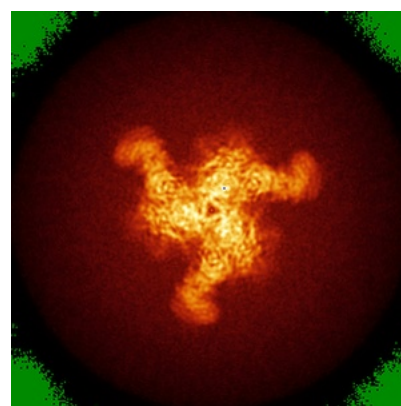
6.4.1 Primary map



X



Y

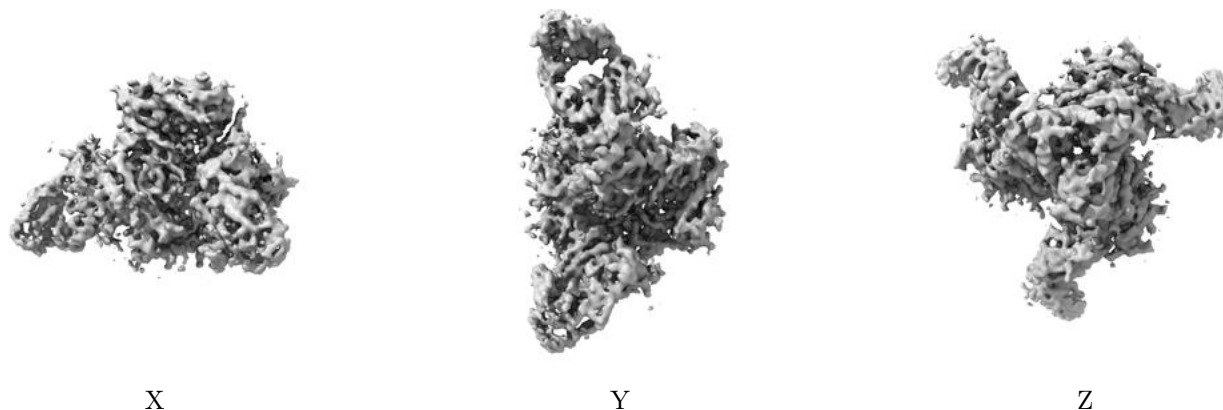


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

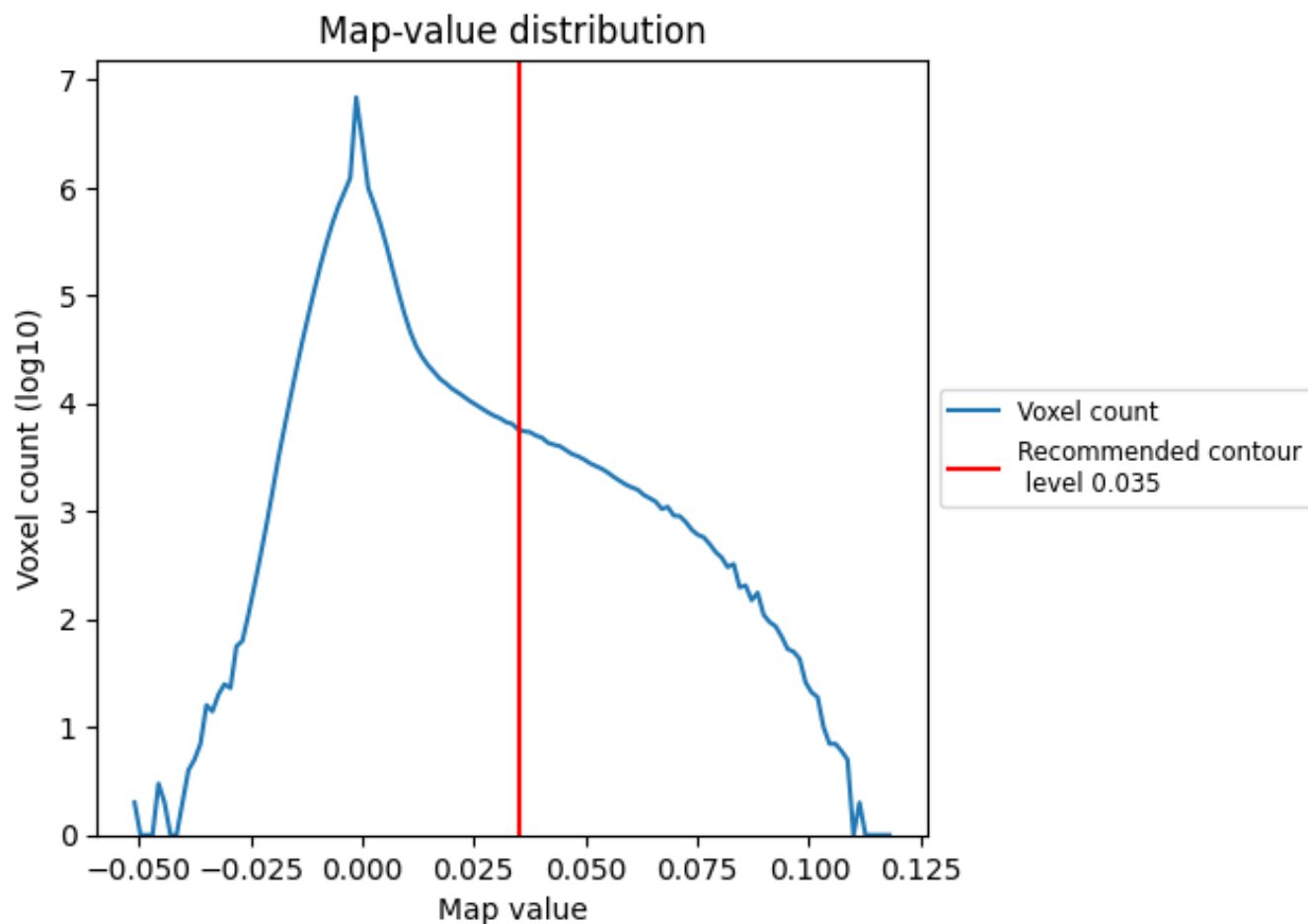
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

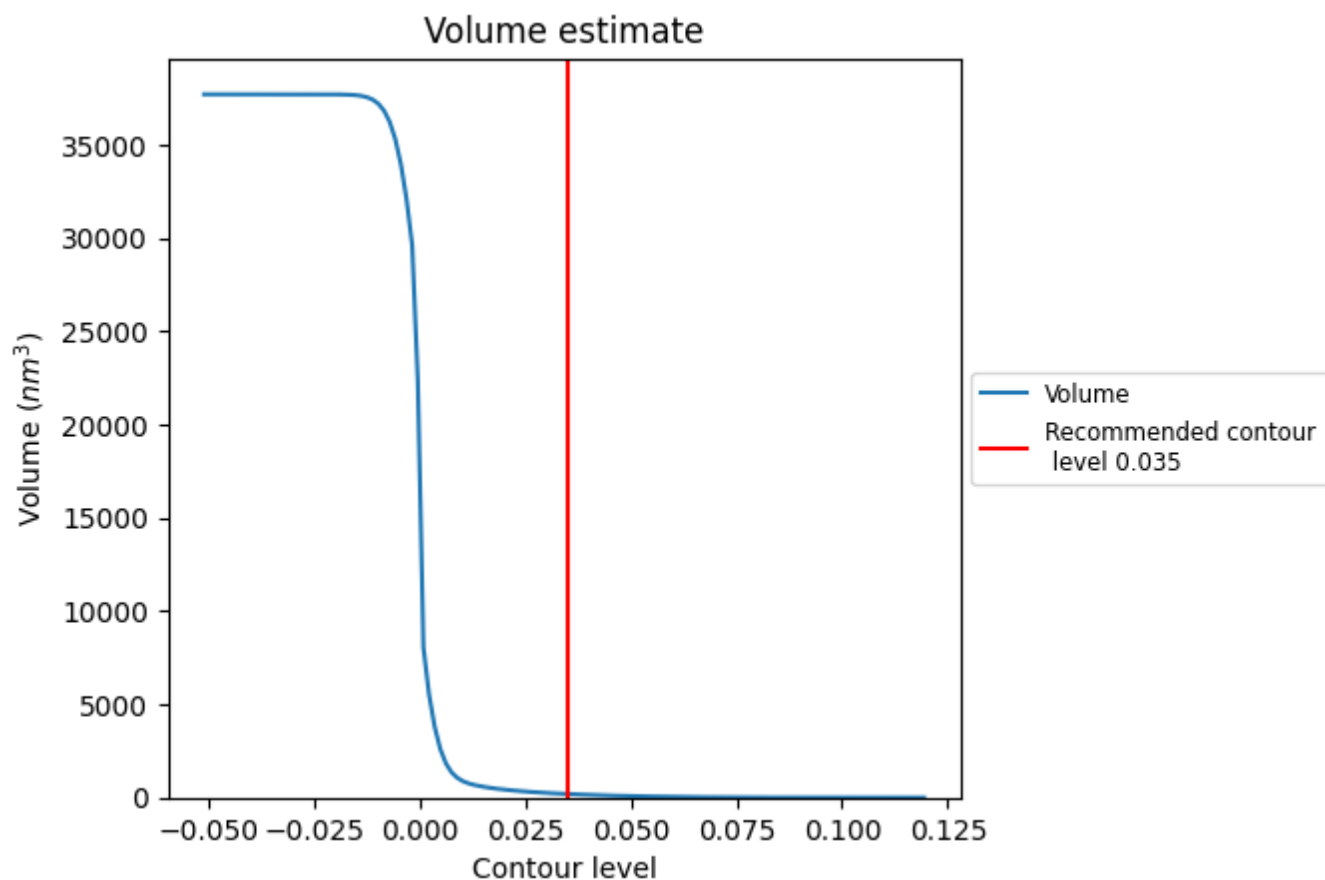
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

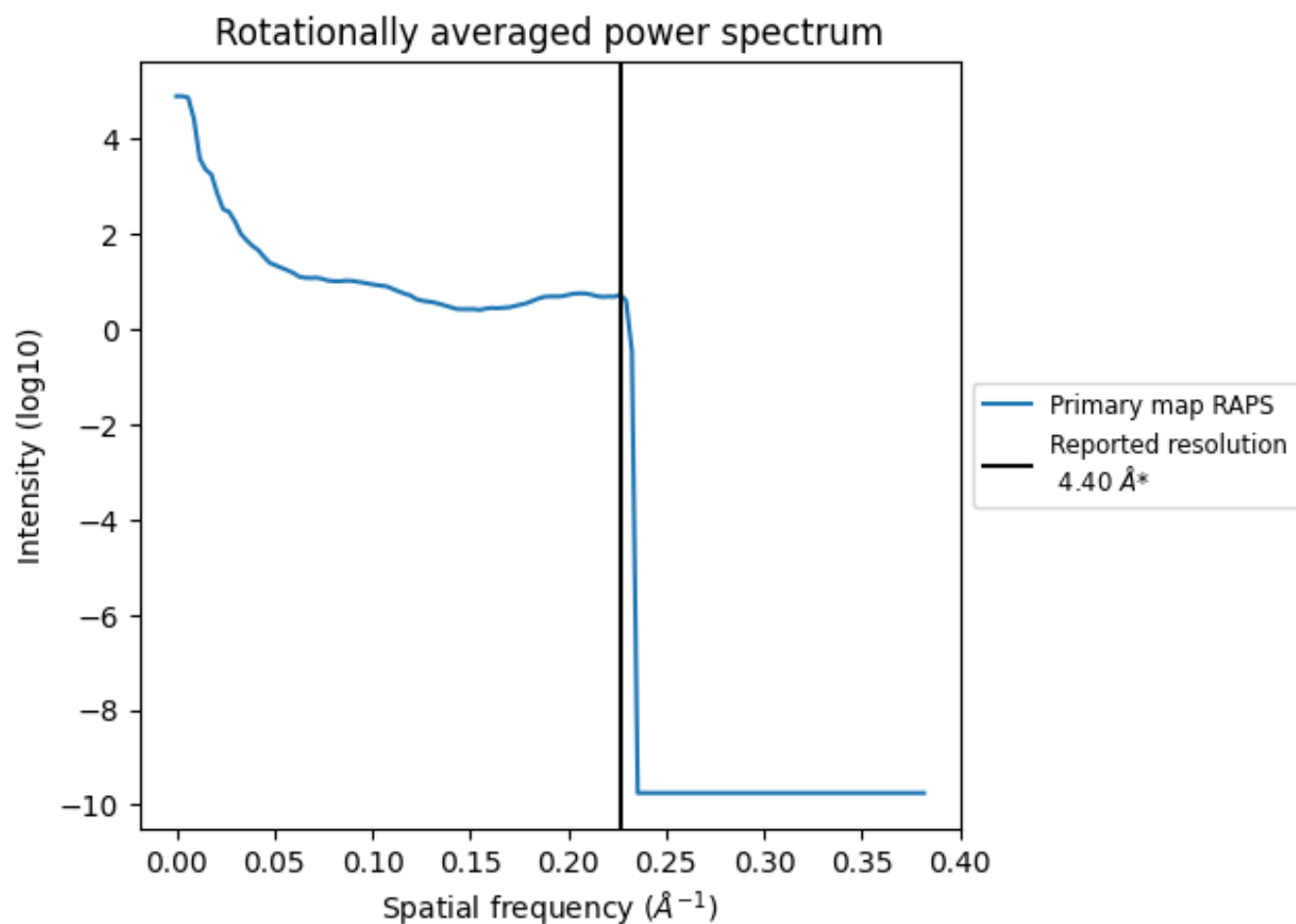
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm³; this corresponds to an approximate mass of 173 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 0.227 Å⁻¹

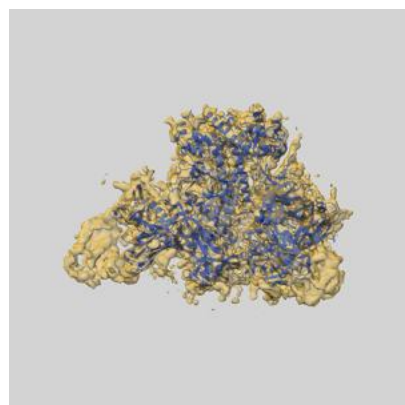
8 Fourier-Shell correlation

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

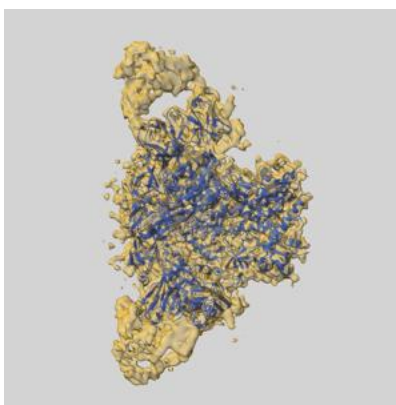
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8644 and PDB model 5V8M. Per-residue inclusion information can be found in section 3 on page 12.

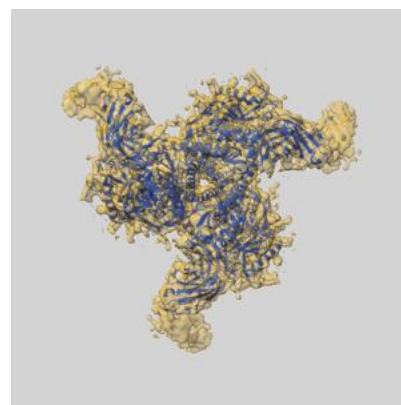
9.1 Map-model overlay [i](#)



X



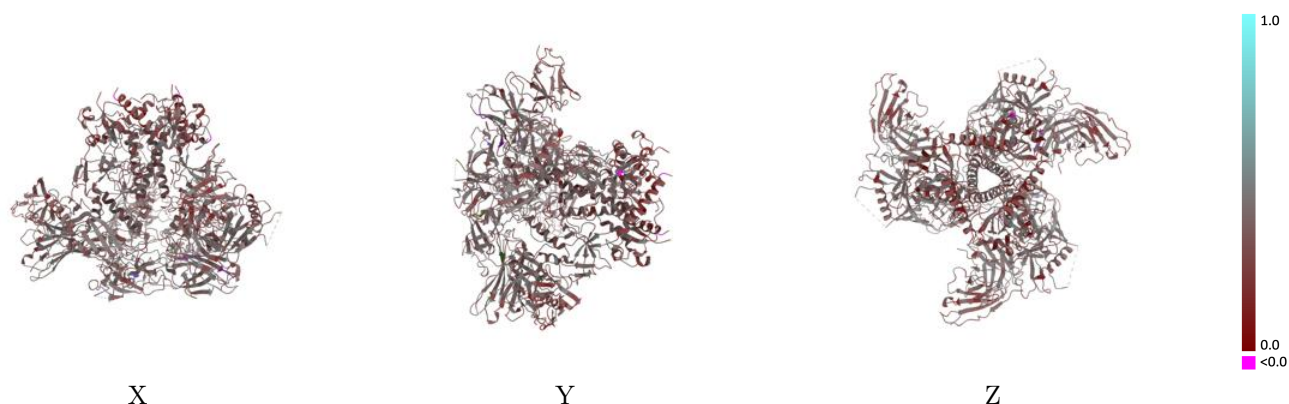
Y



Z

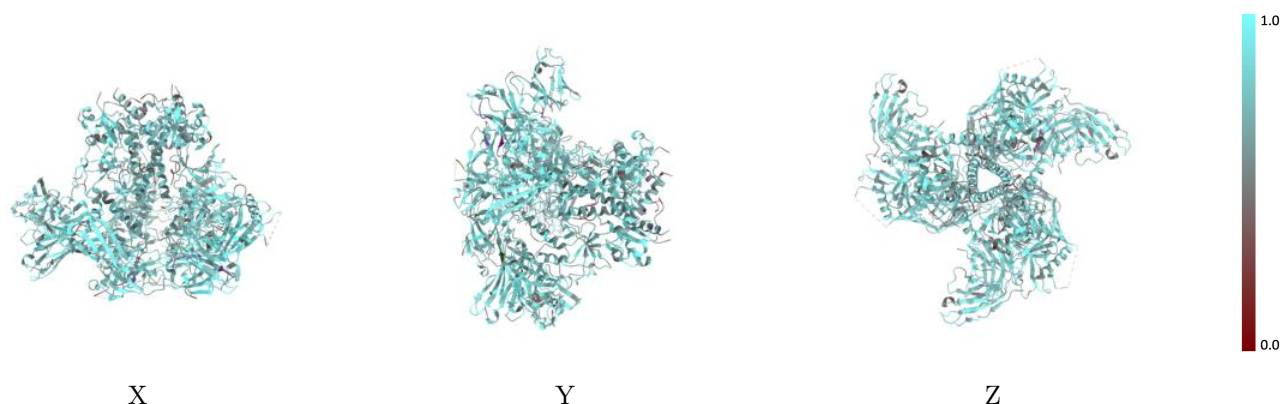
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



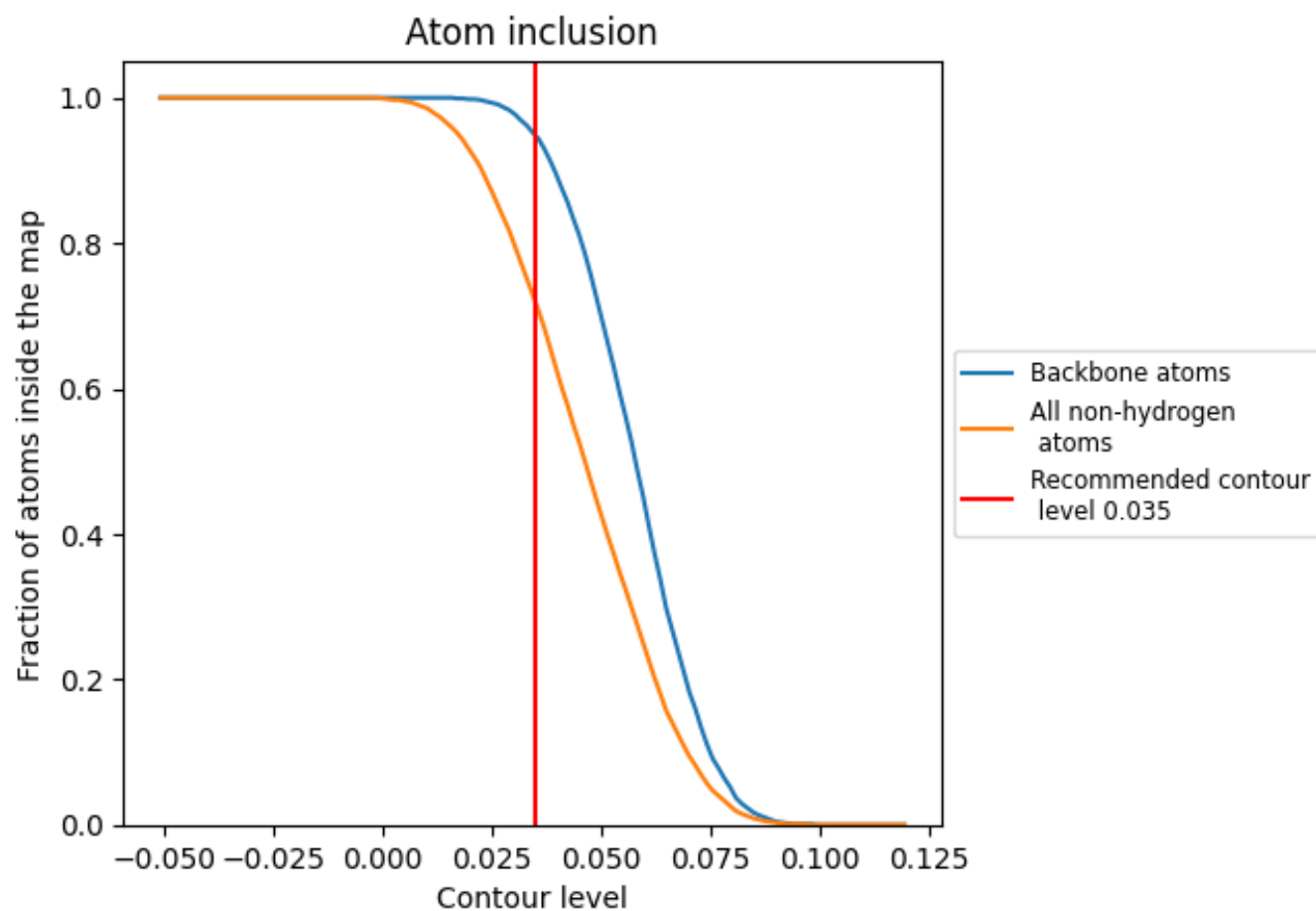
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 72% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7170	 0.3470
A	 0.7440	 0.3680
B	 0.6890	 0.2910
C	 0.2050	 0.2380
D	 0.4640	 0.2370
E	 0.3570	 0.3160
F	 0.7450	 0.3680
G	 0.7460	 0.3690
H	 0.8070	 0.3810
I	 0.6870	 0.2970
J	 0.6900	 0.2930
K	 0.6790	 0.3890
L	 0.7200	 0.3270
M	 0.3860	 0.3000
N	 0.5530	 0.3110
O	 0.3930	 0.2740
P	 0.4290	 0.2910
Q	 0.4640	 0.2180
R	 0.7990	 0.3780
S	 0.8030	 0.3790
T	 0.7180	 0.3230
U	 0.7200	 0.3230
V	 0.3890	 0.2840
W	 0.5000	 0.2210
X	 0.5000	 0.3160
Y	 0.4640	 0.2950
Z	 0.2310	 0.2520
a	 0.5000	 0.2450
b	 0.3570	 0.3210
c	 0.6430	 0.4100
d	 0.3860	 0.3040
e	 0.5430	 0.3190
f	 0.3930	 0.2740
g	 0.4640	 0.2870
h	 0.4640	 0.2360



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Chain	Atom inclusion	Q-score
i	 0.3750	 0.2850
j	 0.5000	 0.2280
k	 0.5000	 0.3170
l	 0.4640	 0.3340
m	 0.2310	 0.2500
n	 0.4640	 0.2390
o	 0.3570	 0.3280
p	 0.6430	 0.3850
q	 0.3860	 0.2910
r	 0.5530	 0.3240
s	 0.3570	 0.2740
t	 0.4640	 0.2930
u	 0.4640	 0.2080
v	 0.3750	 0.2850
w	 0.5000	 0.2290
x	 0.5000	 0.3130
y	 0.4640	 0.3070