



wwPDB EM Validation Summary Report ⓘ

Dec 16, 2024 – 10:56 PM EST

PDB ID : 6CDI
EMDB ID : EMD-7460
Title : Cryo-EM structure at 3.6 Å resolution of vaccine-elicited antibody vFP16.02 in complex with HIV-1 Env BG505 DS-SOSIP, and antibodies VRC03 and PGT122
Authors : Acharya, P.; Xu, K.; Liu, K.; Carragher, B.; Potter, C.S.; Kwong, P.D.
Deposited on : 2018-02-08
Resolution : 3.60 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:

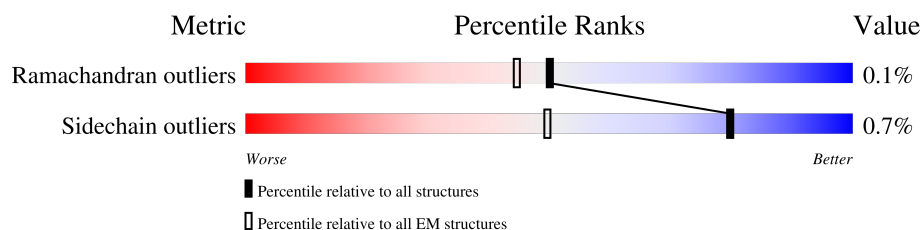
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

1 Overall quality at a glance

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




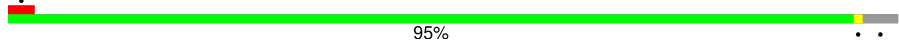
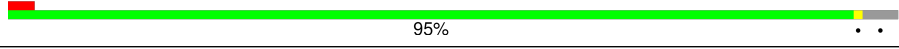
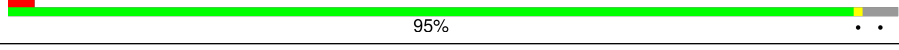
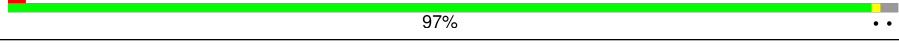
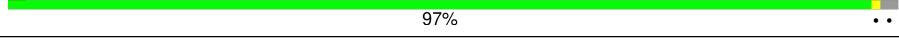
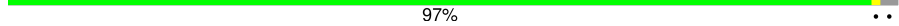
The reported resolution of this entry is 3.60 Å.

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	153	
1	D	153	
1	c	153	
2	2	473	
2	C	473	
2	d	473	
3	6	107	
3	N	107	
3	n	107	

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Mol	Chain	Length	Quality of chain
4	5	132	<div> <div>8%</div> <div>100%</div> </div>
4	M	132	<div> <div>8%</div> <div>100%</div> </div>
4	m	132	<div> <div>7%</div> <div>100%</div> </div>
5	7	102	<div> <div>99%</div> <div>.</div> </div>
5	R	102	<div> <div>99%</div> <div>.</div> </div>
5	r	102	<div> <div>99%</div> <div>.</div> </div>
6	8	227	<div> <div>56%</div> <div>44%</div> </div>
6	Q	227	<div> <div>56%</div> <div>44%</div> </div>
6	q	227	<div> <div>56%</div> <div>44%</div> </div>
7	3	211	<div> <div>8%</div> <div>55%</div> <div>45%</div> </div>
7	H	211	<div> <div>9%</div> <div>55%</div> <div>45%</div> </div>
7	h	211	<div> <div>9%</div> <div>55%</div> <div>45%</div> </div>
8	4	216	<div> <div>21%</div> <div>52%</div> <div>48%</div> </div>
8	L	216	<div> <div>19%</div> <div>52%</div> <div>48%</div> </div>
8	l	216	<div> <div>20%</div> <div>52%</div> <div>48%</div> </div>
9	B	3	<div> <div>100%</div> <div>67%</div> <div>33%</div> </div>
9	DA	3	<div> <div>67%</div> <div>33%</div> </div>
9	HA	3	<div> <div>67%</div> <div>33%</div> </div>
9	O	3	<div> <div>67%</div> <div>33%</div> </div>
9	U	3	<div> <div>67%</div> <div>33%</div> </div>
9	a	3	<div> <div>100%</div> <div>67%</div> <div>33%</div> </div>
9	k	3	<div> <div>67%</div> <div>33%</div> </div>
9	t	3	<div> <div>67%</div> <div>33%</div> </div>
9	z	3	<div> <div>100%</div> <div>67%</div> <div>33%</div> </div>
10	0	4	<div> <div>75%</div> <div>25%</div> <div>75%</div> </div>

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Mol	Chain	Length	Quality of chain
10	9	4	
10	E	4	
10	G	4	
10	MA	4	
10	Z	4	
10	b	4	
10	f	4	
10	y	4	
11	1	2	
11	F	2	
11	FA	2	
11	GA	2	
11	JA	2	
11	LA	2	
11	S	2	
11	T	2	
11	W	2	
11	Y	2	
11	e	2	
11	p	2	
11	s	2	
11	v	2	
11	x	2	
12	AA	5	
12	I	5	

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Mol	Chain	Length	Quality of chain
12	IA	5	
12	V	5	
12	g	5	
12	u	5	
13	BA	8	
13	J	8	
13	i	8	
14	CA	4	
14	K	4	
14	j	4	
15	EA	6	
15	P	6	
15	o	6	
16	KA	9	
16	X	9	
16	w	9	

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 32763 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 Glycoprotein gp41.

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

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Glycoprotein 120.

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	201	CYS	ILE	conflict	UNP Q2N0S5
d	332	ASN	THR	conflict	UNP Q2N0S5
d	433	CYS	ALA	conflict	UNP Q2N0S5
d	501	CYS	ALA	conflict	UNP Q2N0S5
2	201	CYS	ILE	conflict	UNP Q2N0S5
2	332	ASN	THR	conflict	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
2	433	CYS	ALA	conflict	UNP Q2N0S5
2	501	CYS	ALA	conflict	UNP Q2N0S5
C	201	CYS	ILE	conflict	UNP Q2N0S5
C	332	ASN	THR	conflict	UNP Q2N0S5
C	433	CYS	ALA	conflict	UNP Q2N0S5
C	501	CYS	ALA	conflict	UNP Q2N0S5

- Molecule 3 is a protein called PGT122 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	n	105	Total	C	N	O	S	0	0
			805	504	139	160	2		
3	6	105	Total	C	N	O	S	0	0
			805	504	139	160	2		
3	N	105	Total	C	N	O	S	0	0
			805	504	139	160	2		

- Molecule 4 is a protein called PGT122 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	m	132	Total	C	N	O	S	0	0
			1047	669	180	195	3		
4	5	132	Total	C	N	O	S	0	0
			1047	669	180	195	3		
4	M	132	Total	C	N	O	S	0	0
			1047	669	180	195	3		

- Molecule 5 is a protein called VRC03 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	r	102	Total	C	N	O	S	0	0
			802	510	137	152	3		
5	7	102	Total	C	N	O	S	0	0
			802	510	137	152	3		
5	R	102	Total	C	N	O	S	0	0
			802	510	137	152	3		

- Molecule 6 is a protein called VRC03 Heavy Chain.

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

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

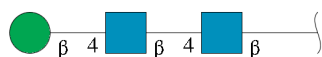
- Molecule 7 is a protein called vFP16.02 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	116	Total	C	N	O	S	0	0
			893	566	151	173	3		
7	3	116	Total	C	N	O	S	0	0
			893	566	151	173	3		
7	H	116	Total	C	N	O	S	0	0
			893	566	151	173	3		

- Molecule 8 is a protein called vFP16.02 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	l	113	Total	C	N	O	S	0	0
			875	556	146	170	3		
8	4	113	Total	C	N	O	S	0	0
			875	556	146	170	3		
8	L	113	Total	C	N	O	S	0	0
			875	556	146	170	3		

- Molecule 9 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
9	B	3	Total	C	N	O		0	0
			39	22	2	15			
9	O	3	Total	C	N	O		0	0
			39	22	2	15			
9	U	3	Total	C	N	O		0	0
			39	22	2	15			
9	a	3	Total	C	N	O		0	0
			39	22	2	15			

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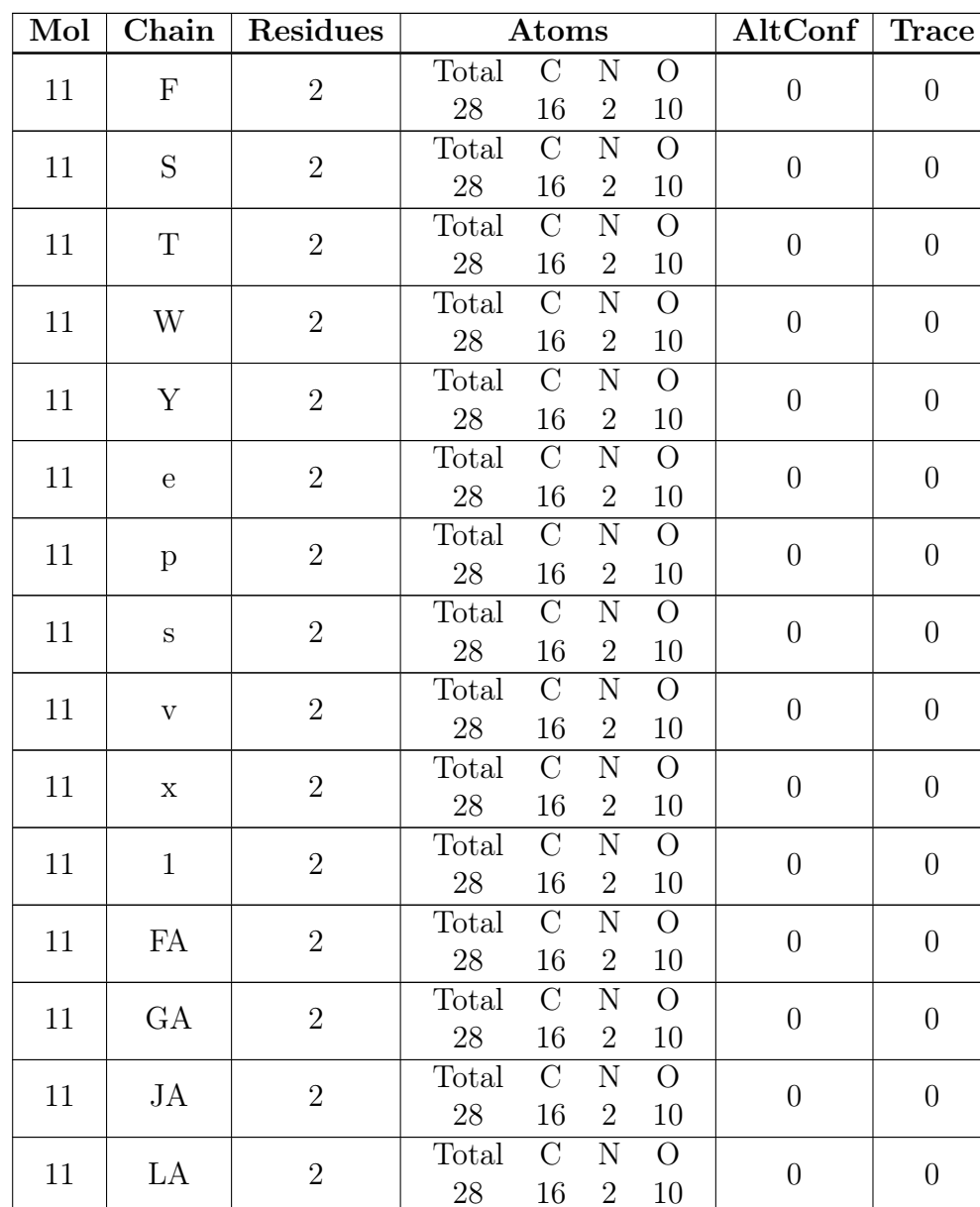
Mol	Chain	Residues	Atoms				AltConf	Trace
9	k	3	Total	C	N	O	0	0
			39	22	2	15		
9	t	3	Total	C	N	O	0	0
			39	22	2	15		
9	z	3	Total	C	N	O	0	0
			39	22	2	15		
9	DA	3	Total	C	N	O	0	0
			39	22	2	15		
9	HA	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
10	E	4	Total	C	N	O	0	0
			50	28	2	20		
10	G	4	Total	C	N	O	0	0
			50	28	2	20		
10	Z	4	Total	C	N	O	0	0
			50	28	2	20		
10	b	4	Total	C	N	O	0	0
			50	28	2	20		
10	f	4	Total	C	N	O	0	0
			50	28	2	20		
10	y	4	Total	C	N	O	0	0
			50	28	2	20		
10	0	4	Total	C	N	O	0	0
			50	28	2	20		
10	9	4	Total	C	N	O	0	0
			50	28	2	20		
10	MA	4	Total	C	N	O	0	0
			50	28	2	20		

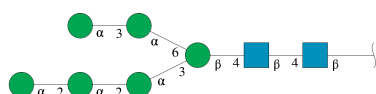
- Molecule 11 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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Mol	Chain	Residues	Atoms				AltConf	Trace
12	I	5	Total	C	N	O	0	0
			61	34	2	25		
12	V	5	Total	C	N	O	0	0
			61	34	2	25		
12	g	5	Total	C	N	O	0	0
			61	34	2	25		
12	u	5	Total	C	N	O	0	0
			61	34	2	25		
12	AA	5	Total	C	N	O	0	0
			61	34	2	25		
12	IA	5	Total	C	N	O	0	0
			61	34	2	25		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
13	J	8	Total	C	N	O	0	0
			94	52	2	40		
13	i	8	Total	C	N	O	0	0
			94	52	2	40		
13	BA	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 14 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.



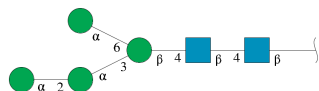
Mol	Chain	Residues	Atoms				AltConf	Trace
14	K	4	Total	C	N	O	0	0
			50	28	2	20		
14	j	4	Total	C	N	O	0	0
			50	28	2	20		

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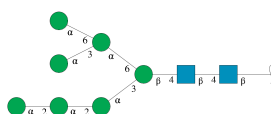
Mol	Chain	Residues	Atoms				AltConf	Trace
14	CA	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 15 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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
15	P	6	Total	C	N	O	0	0
			72	40	2	30		
15	o	6	Total	C	N	O	0	0
			72	40	2	30		
15	EA	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 16 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
16	X	9	Total	C	N	O	0	0
			105	58	2	45		
16	w	9	Total	C	N	O	0	0
			105	58	2	45		
16	KA	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 17 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

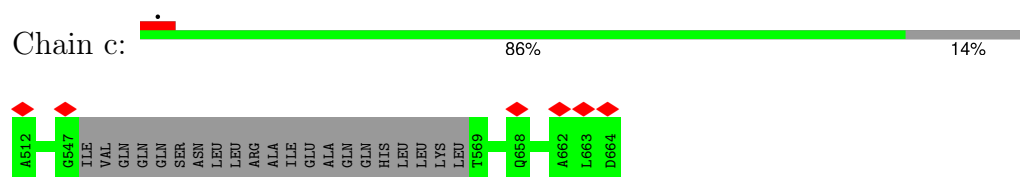


Mol	Chain	Residues	Atoms				AltConf
17	c	1	Total	C	N	O	0
			14	8	1	5	
17	d	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	2	1	Total	C	N	O	0
			14	8	1	5	
17	D	1	Total	C	N	O	0
			14	8	1	5	
17	C	1	Total	C	N	O	0
			14	8	1	5	

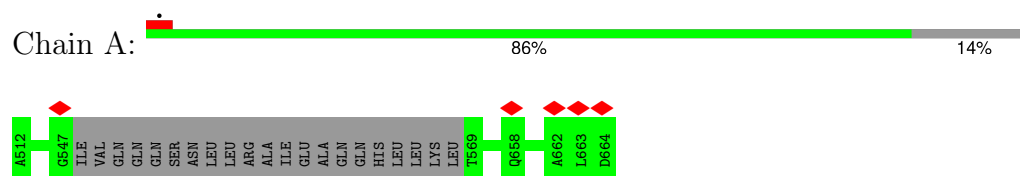
3 Residue-property plots [i](#)

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

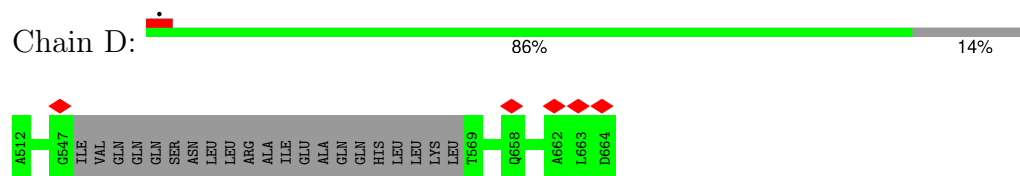
- Molecule 1: Glycoprotein gp41



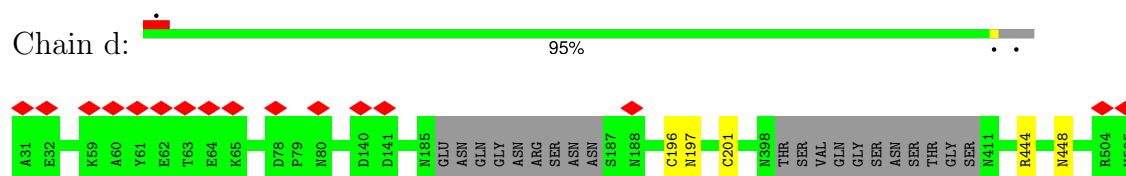
- Molecule 1: Glycoprotein gp41



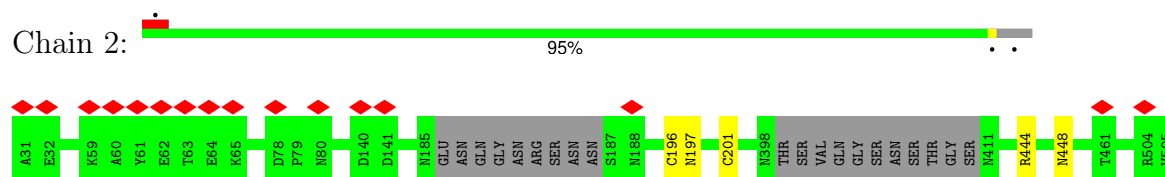
- Molecule 1: Glycoprotein gp41



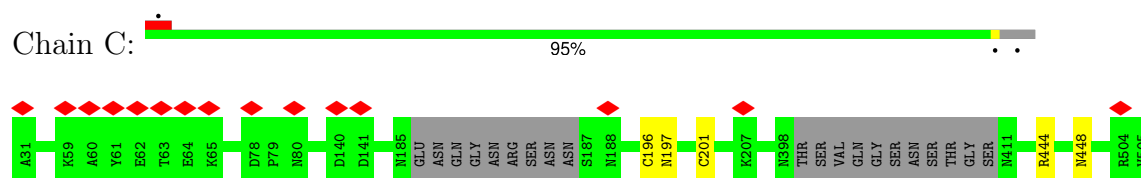
- Molecule 2: Glycoprotein 120



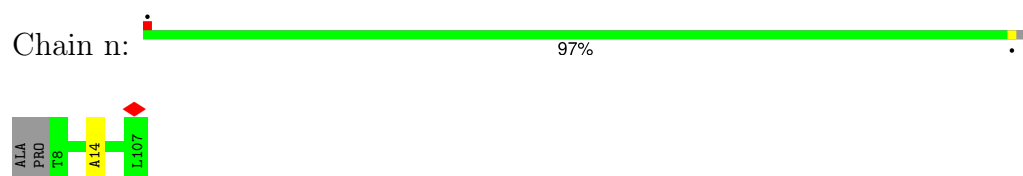
- Molecule 2: Glycoprotein 120



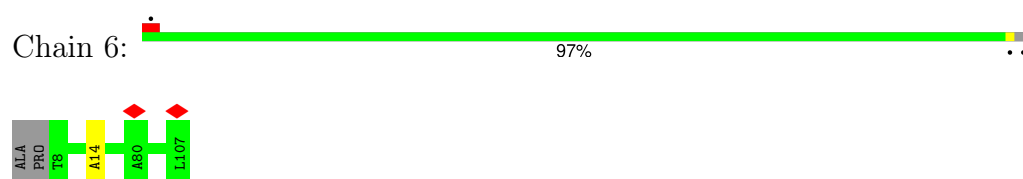
- Molecule 2: Glycoprotein 120



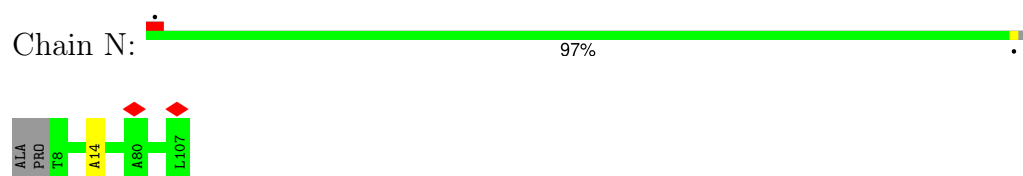
- Molecule 3: PGT122 Light Chain



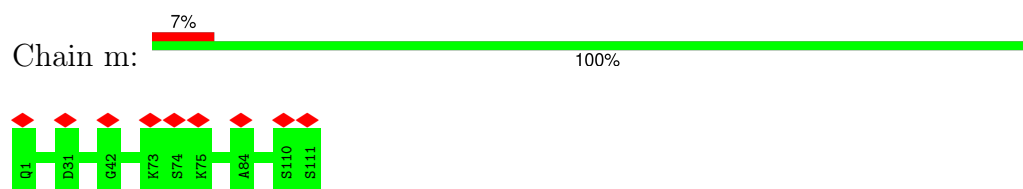
- Molecule 3: PGT122 Light Chain



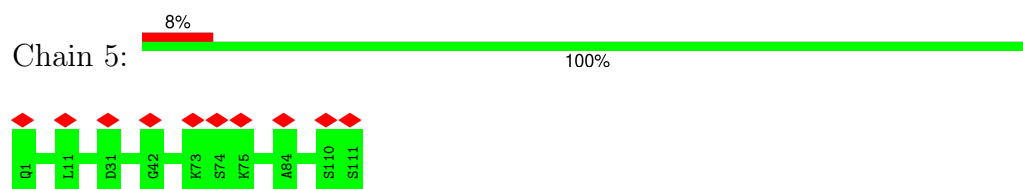
- Molecule 3: PGT122 Light Chain



- Molecule 4: PGT122 Heavy Chain

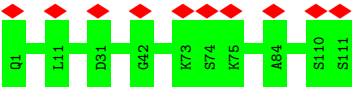


- Molecule 4: PGT122 Heavy Chain



- Molecule 4: PGT122 Heavy Chain





• Molecule 5: VRC03 light chain



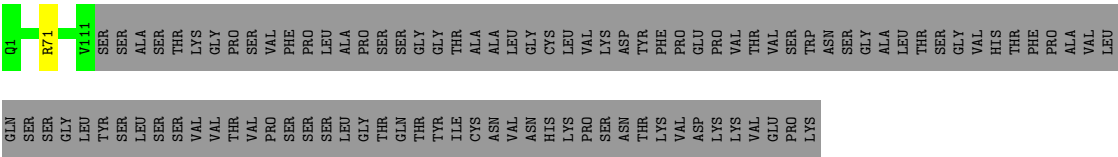
• Molecule 5: VRC03 light chain



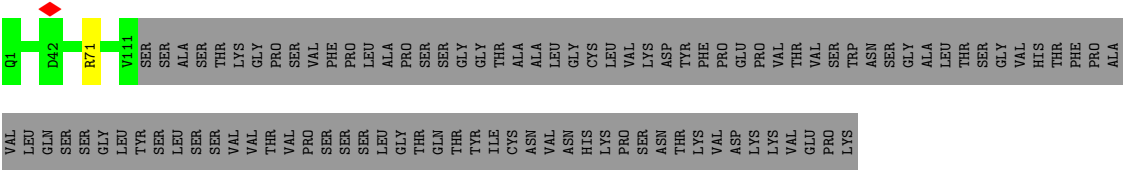
• Molecule 5: VRC03 light chain



• Molecule 6: VRC03 Heavy Chain

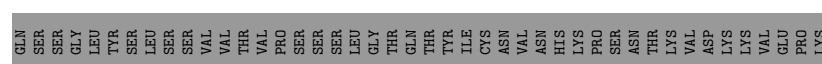
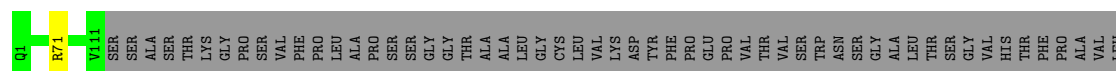


• Molecule 6: VRC03 Heavy Chain

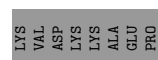
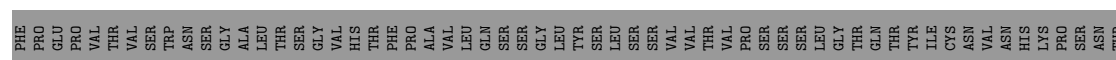
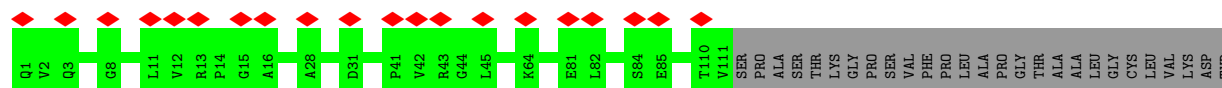


• Molecule 6: VRC03 Heavy Chain

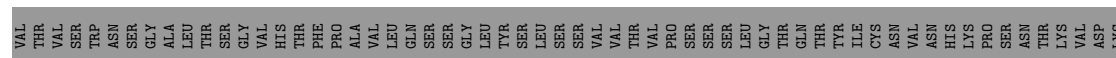
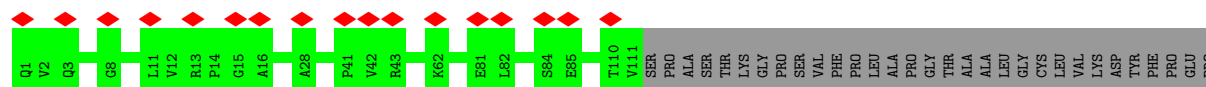




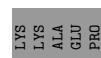
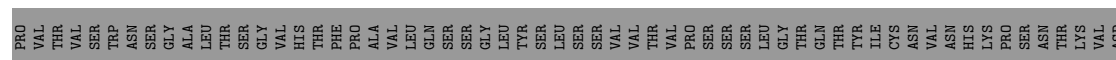
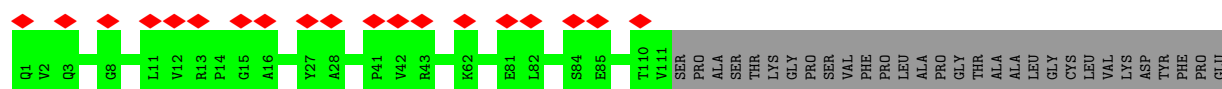
• Molecule 7: vFP16.02 Heavy Chain



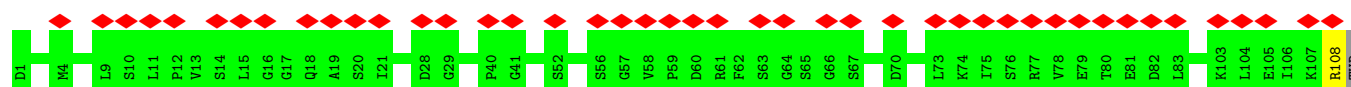
• Molecule 7: vFP16.02 Heavy Chain

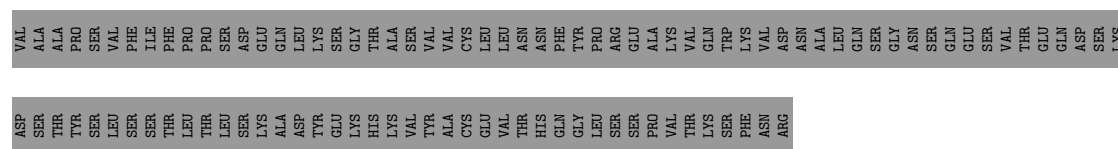


• Molecule 7: vFP16.02 Heavy Chain

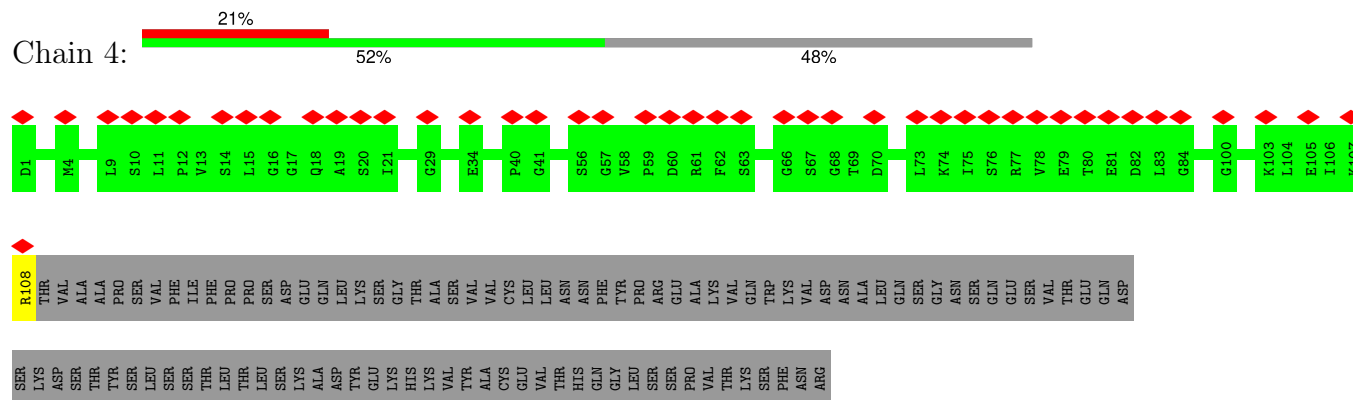


• Molecule 8: vFP16.02 Light Chain

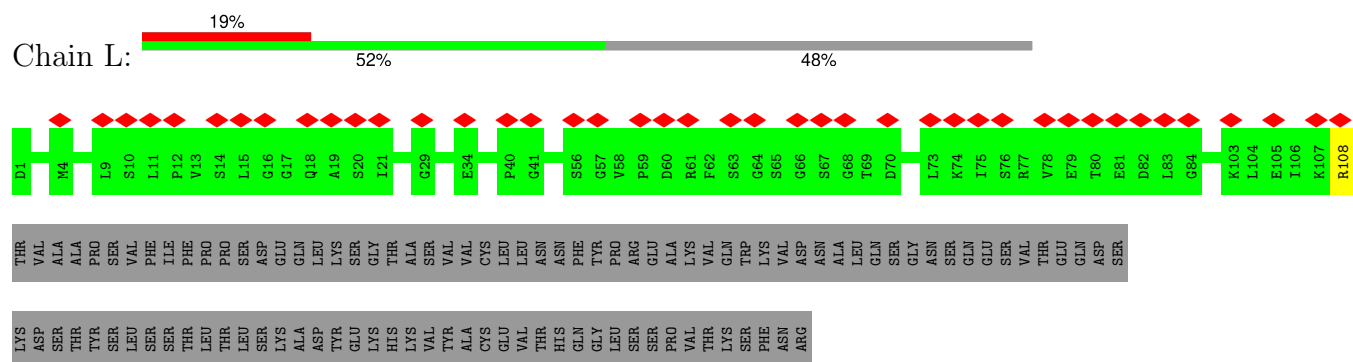




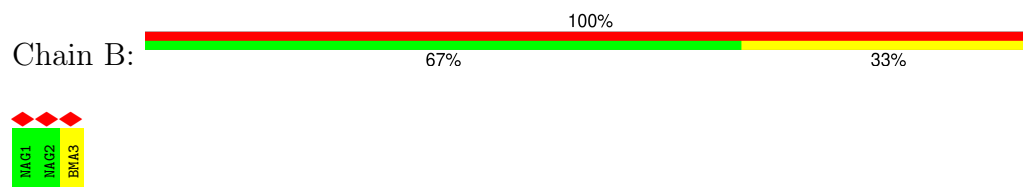
• Molecule 8: vFP16.02 Light Chain



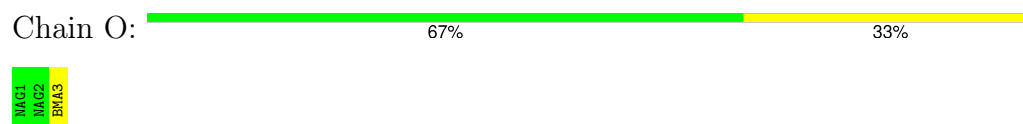
• Molecule 8: vFP16.02 Light Chain



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



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



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

Chain U:  67% 33%



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

Chain a:  100% 67% 33%



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

Chain k:  67% 33%



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

Chain t:  67% 33%



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

Chain z:  100% 67% 33%



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

Chain DA:  67% 33%

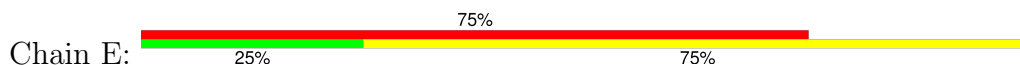


- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain HA:  67% 33%



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



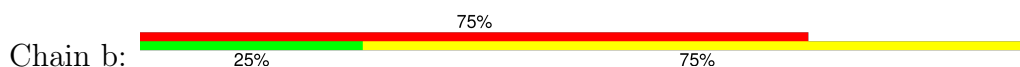
- Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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




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



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



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

Chain 0: 



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

Chain 9: 



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

Chain MA: 



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

Chain F: 



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

Chain S: 



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

Chain T: 



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



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



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



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



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



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



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





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



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



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



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

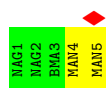


- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

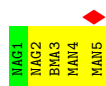


- Molecule 12: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

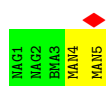




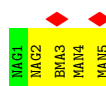
- Molecule 12: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



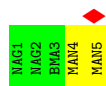
- Molecule 12: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

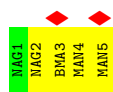


- Molecule 12: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

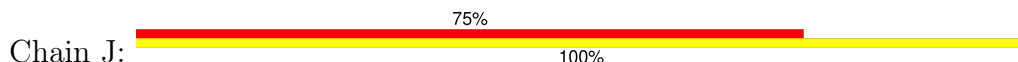


- Molecule 12: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

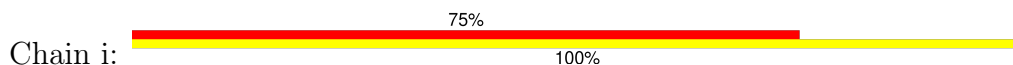




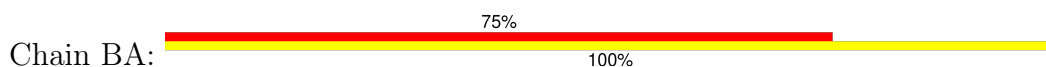
- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



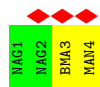
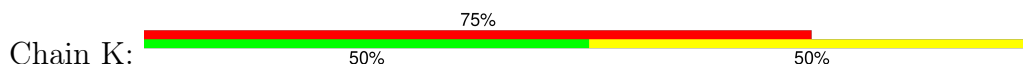
- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



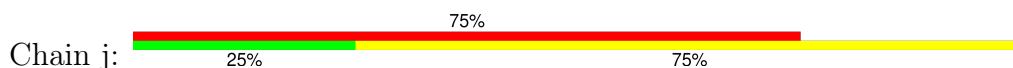
- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 14: 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

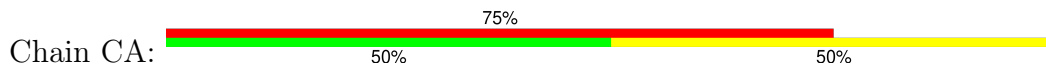


- Molecule 14: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

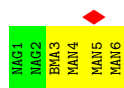




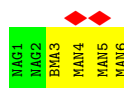
- Molecule 14: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 15: alpha-D-mannopyranose-(1-2)-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 15: alpha-D-mannopyranose-(1-2)-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 15: alpha-D-mannopyranose-(1-2)-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 16: 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



MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

● Molecule 16: 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

Chain w:  11% 89%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

● Molecule 16: 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

Chain KA:  11% 89%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	57278	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 ($e^-/\text{\AA}^2$)	67.18	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.695	Depositor
Minimum map value	-1.533	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.121	Depositor
Recommended contour level	1.01	Depositor
Map size (Å)	410.88, 410.88, 410.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.34	0/1052	0.58	0/1427
1	D	0.34	0/1052	0.58	0/1427
1	c	0.34	0/1052	0.58	0/1427
2	2	0.38	0/3638	0.58	0/4939
2	C	0.38	0/3638	0.58	0/4939
2	d	0.38	0/3638	0.58	0/4939
3	6	0.33	0/826	0.55	0/1130
3	N	0.33	0/826	0.55	0/1130
3	n	0.33	0/826	0.55	0/1130
4	5	0.30	0/1076	0.58	0/1465
4	M	0.30	0/1076	0.58	0/1465
4	m	0.30	0/1076	0.58	0/1465
5	7	0.35	0/820	0.57	0/1107
5	R	0.35	0/820	0.57	0/1107
5	r	0.35	0/820	0.57	0/1107
6	8	0.39	0/1056	0.52	0/1439
6	Q	0.39	0/1056	0.52	0/1439
6	q	0.39	0/1056	0.53	0/1439
7	3	0.33	0/913	0.53	0/1239
7	H	0.33	0/913	0.53	0/1239
7	h	0.33	0/913	0.53	0/1239
8	4	0.32	0/895	0.54	0/1210
8	L	0.32	0/895	0.54	0/1210
8	l	0.32	0/895	0.54	0/1210
All	All	0.35	0/30828	0.57	0/41868

There are no bond length outliers.

There are no bond angle outliers.

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	128/153 (84%)	120 (94%)	8 (6%)	0	100	100
1	D	128/153 (84%)	120 (94%)	8 (6%)	0	100	100
1	c	128/153 (84%)	120 (94%)	8 (6%)	0	100	100
2	2	447/473 (94%)	419 (94%)	28 (6%)	0	100	100
2	C	447/473 (94%)	419 (94%)	28 (6%)	0	100	100
2	d	447/473 (94%)	419 (94%)	28 (6%)	0	100	100
3	6	103/107 (96%)	95 (92%)	7 (7%)	1 (1%)	13	46
3	N	103/107 (96%)	95 (92%)	7 (7%)	1 (1%)	13	46
3	n	103/107 (96%)	95 (92%)	7 (7%)	1 (1%)	13	46
4	5	130/132 (98%)	119 (92%)	11 (8%)	0	100	100
4	M	130/132 (98%)	119 (92%)	11 (8%)	0	100	100
4	m	130/132 (98%)	119 (92%)	11 (8%)	0	100	100
5	7	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
5	R	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
5	r	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
6	8	126/227 (56%)	122 (97%)	4 (3%)	0	100	100
6	Q	126/227 (56%)	121 (96%)	5 (4%)	0	100	100
6	q	126/227 (56%)	121 (96%)	5 (4%)	0	100	100
7	3	114/211 (54%)	109 (96%)	5 (4%)	0	100	100
7	H	114/211 (54%)	109 (96%)	5 (4%)	0	100	100
7	h	114/211 (54%)	109 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	4	111/216 (51%)	105 (95%)	6 (5%)	0	100	100
8	L	111/216 (51%)	105 (95%)	6 (5%)	0	100	100
8	l	111/216 (51%)	105 (95%)	6 (5%)	0	100	100
All	All	3777/4863 (78%)	3550 (94%)	224 (6%)	3 (0%)	50	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	n	14	ALA
3	6	14	ALA
3	N	14	ALA

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	110/129 (85%)	110 (100%)	0	100	100
1	D	110/129 (85%)	110 (100%)	0	100	100
1	c	110/129 (85%)	110 (100%)	0	100	100
2	2	405/422 (96%)	400 (99%)	5 (1%)	67	82
2	C	405/422 (96%)	400 (99%)	5 (1%)	67	82
2	d	405/422 (96%)	400 (99%)	5 (1%)	67	82
3	6	88/89 (99%)	88 (100%)	0	100	100
3	N	88/89 (99%)	88 (100%)	0	100	100
3	n	88/89 (99%)	88 (100%)	0	100	100
4	5	116/116 (100%)	116 (100%)	0	100	100
4	M	116/116 (100%)	116 (100%)	0	100	100
4	m	116/116 (100%)	116 (100%)	0	100	100
5	7	86/86 (100%)	85 (99%)	1 (1%)	67	82
5	R	86/86 (100%)	85 (99%)	1 (1%)	67	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	r	86/86 (100%)	85 (99%)	1 (1%)	67	82
6	8	108/193 (56%)	107 (99%)	1 (1%)	75	87
6	Q	108/193 (56%)	107 (99%)	1 (1%)	75	87
6	q	108/193 (56%)	107 (99%)	1 (1%)	75	87
7	3	95/176 (54%)	95 (100%)	0	100	100
7	H	95/176 (54%)	95 (100%)	0	100	100
7	h	95/176 (54%)	95 (100%)	0	100	100
8	4	99/192 (52%)	98 (99%)	1 (1%)	73	85
8	L	99/192 (52%)	98 (99%)	1 (1%)	73	85
8	l	99/192 (52%)	98 (99%)	1 (1%)	73	85
All	All	3321/4209 (79%)	3297 (99%)	24 (1%)	80	90

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	8	71	ARG
2	C	197	ASN
2	C	196	CYS
2	C	201	CYS
6	q	71	ARG

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

Mol	Chain	Res	Type
2	2	315	GLN
2	C	203	GLN
2	C	315	GLN
2	d	315	GLN
2	d	203	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 ⓘ

204 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	$\# Z > 2$
10	NAG	0	1	2,10	14,14,15	0.30	0	17,19,21	0.43	0
10	NAG	0	2	10	14,14,15	0.31	0	17,19,21	0.74	1 (5%)
10	BMA	0	3	10	11,11,12	0.76	0	15,15,17	1.00	1 (6%)
10	MAN	0	4	10	11,11,12	0.87	1 (9%)	15,15,17	1.17	2 (13%)
11	NAG	1	1	11,2	14,14,15	0.48	0	17,19,21	1.04	1 (5%)
11	NAG	1	2	11	14,14,15	0.45	0	17,19,21	0.53	0
10	NAG	9	1	10	14,14,15	0.25	0	17,19,21	0.46	0
10	NAG	9	2	10	14,14,15	0.43	0	17,19,21	0.98	1 (5%)
10	BMA	9	3	10	11,11,12	0.72	0	15,15,17	1.29	1 (6%)
10	MAN	9	4	10	11,11,12	0.78	1 (9%)	15,15,17	1.23	2 (13%)
12	NAG	AA	1	12,2	14,14,15	0.25	0	17,19,21	0.53	0
12	NAG	AA	2	12	14,14,15	0.22	0	17,19,21	0.42	0
12	BMA	AA	3	12	11,11,12	0.72	0	15,15,17	0.76	0
12	MAN	AA	4	12	11,11,12	0.80	0	15,15,17	0.98	2 (13%)
12	MAN	AA	5	12	11,11,12	0.68	0	15,15,17	1.05	2 (13%)
9	NAG	B	1	9,1	14,14,15	0.23	0	17,19,21	0.54	0
9	NAG	B	2	9	14,14,15	0.39	0	17,19,21	0.51	0
9	BMA	B	3	9	11,11,12	0.77	0	15,15,17	0.85	1 (6%)
13	NAG	BA	1	2,13	14,14,15	0.60	0	17,19,21	0.99	1 (5%)
13	NAG	BA	2	13	14,14,15	0.46	0	17,19,21	0.77	1 (5%)
13	BMA	BA	3	13	11,11,12	0.78	0	15,15,17	0.91	1 (6%)
13	MAN	BA	4	13	11,11,12	2.09	3 (27%)	15,15,17	2.26	3 (20%)
13	MAN	BA	5	13	11,11,12	0.73	0	15,15,17	1.03	1 (6%)
13	MAN	BA	6	13	11,11,12	0.78	0	15,15,17	1.09	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	MAN	BA	7	13	11,11,12	0.95	1 (9%)	15,15,17	1.13	2 (13%)
13	MAN	BA	8	13	11,11,12	0.84	1 (9%)	15,15,17	1.26	2 (13%)
14	NAG	CA	1	14,2	14,14,15	0.24	0	17,19,21	0.56	0
14	NAG	CA	2	14	14,14,15	0.29	0	17,19,21	0.70	0
14	BMA	CA	3	14	11,11,12	0.79	0	15,15,17	1.28	1 (6%)
14	MAN	CA	4	14	11,11,12	0.84	0	15,15,17	1.16	2 (13%)
9	NAG	DA	1	9,2	14,14,15	0.23	0	17,19,21	0.56	0
9	NAG	DA	2	9	14,14,15	0.23	0	17,19,21	0.54	0
9	BMA	DA	3	9	11,11,12	0.78	0	15,15,17	1.05	1 (6%)
10	NAG	E	1	2,10	14,14,15	0.29	0	17,19,21	0.43	0
10	NAG	E	2	10	14,14,15	0.32	0	17,19,21	0.74	1 (5%)
10	BMA	E	3	10	11,11,12	0.77	0	15,15,17	1.00	1 (6%)
10	MAN	E	4	10	11,11,12	0.87	1 (9%)	15,15,17	1.17	2 (13%)
15	NAG	EA	1	15,2	14,14,15	0.27	0	17,19,21	0.57	0
15	NAG	EA	2	15	14,14,15	0.21	0	17,19,21	0.48	0
15	BMA	EA	3	15	11,11,12	0.99	1 (9%)	15,15,17	1.32	2 (13%)
15	MAN	EA	4	15	11,11,12	0.85	1 (9%)	15,15,17	1.32	2 (13%)
15	MAN	EA	5	15	11,11,12	0.87	1 (9%)	15,15,17	1.52	2 (13%)
15	MAN	EA	6	15	11,11,12	0.75	0	15,15,17	1.25	2 (13%)
11	NAG	F	1	11,2	14,14,15	0.49	0	17,19,21	1.03	1 (5%)
11	NAG	F	2	11	14,14,15	0.45	0	17,19,21	0.53	0
11	NAG	FA	1	11,2	14,14,15	0.27	0	17,19,21	0.50	0
11	NAG	FA	2	11	14,14,15	0.40	0	17,19,21	0.46	0
10	NAG	G	1	10	14,14,15	0.26	0	17,19,21	0.46	0
10	NAG	G	2	10	14,14,15	0.42	0	17,19,21	0.98	1 (5%)
10	BMA	G	3	10	11,11,12	0.72	0	15,15,17	1.29	1 (6%)
10	MAN	G	4	10	11,11,12	0.78	1 (9%)	15,15,17	1.23	2 (13%)
11	NAG	GA	1	11,2	14,14,15	0.19	0	17,19,21	0.55	0
11	NAG	GA	2	11	14,14,15	0.30	0	17,19,21	0.51	0
9	NAG	HA	1	9,2	14,14,15	0.30	0	17,19,21	0.50	0
9	NAG	HA	2	9	14,14,15	0.24	0	17,19,21	0.59	0
9	BMA	HA	3	9	11,11,12	1.16	1 (9%)	15,15,17	1.25	2 (13%)
12	NAG	I	1	12,2	14,14,15	0.25	0	17,19,21	0.54	0
12	NAG	I	2	12	14,14,15	0.21	0	17,19,21	0.43	0
12	BMA	I	3	12	11,11,12	0.72	0	15,15,17	0.75	0
12	MAN	I	4	12	11,11,12	0.79	0	15,15,17	0.98	2 (13%)
12	MAN	I	5	12	11,11,12	0.68	0	15,15,17	1.05	2 (13%)
12	NAG	IA	1	12,2	14,14,15	0.28	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	IA	2	12	14,14,15	0.40	0	17,19,21	0.89	1 (5%)
12	BMA	IA	3	12	11,11,12	0.71	0	15,15,17	1.21	1 (6%)
12	MAN	IA	4	12	11,11,12	0.80	0	15,15,17	0.96	2 (13%)
12	MAN	IA	5	12	11,11,12	0.88	1 (9%)	15,15,17	1.19	2 (13%)
13	NAG	J	1	2,13	14,14,15	0.60	0	17,19,21	0.99	1 (5%)
13	NAG	J	2	13	14,14,15	0.48	0	17,19,21	0.77	1 (5%)
13	BMA	J	3	13	11,11,12	0.78	0	15,15,17	0.91	1 (6%)
13	MAN	J	4	13	11,11,12	2.10	3 (27%)	15,15,17	2.25	3 (20%)
13	MAN	J	5	13	11,11,12	0.73	0	15,15,17	1.03	1 (6%)
13	MAN	J	6	13	11,11,12	0.78	0	15,15,17	1.09	2 (13%)
13	MAN	J	7	13	11,11,12	0.96	1 (9%)	15,15,17	1.14	2 (13%)
13	MAN	J	8	13	11,11,12	0.84	1 (9%)	15,15,17	1.26	2 (13%)
11	NAG	JA	1	11,2	14,14,15	0.49	0	17,19,21	0.62	0
11	NAG	JA	2	11	14,14,15	0.41	0	17,19,21	0.56	0
14	NAG	K	1	14,2	14,14,15	0.25	0	17,19,21	0.56	0
14	NAG	K	2	14	14,14,15	0.29	0	17,19,21	0.69	0
14	BMA	K	3	14	11,11,12	0.78	0	15,15,17	1.28	1 (6%)
14	MAN	K	4	14	11,11,12	0.83	0	15,15,17	1.15	2 (13%)
16	NAG	KA	1	16,2	14,14,15	0.28	0	17,19,21	0.50	0
16	NAG	KA	2	16	14,14,15	0.24	0	17,19,21	1.26	3 (17%)
16	BMA	KA	3	16	11,11,12	0.63	0	15,15,17	1.41	2 (13%)
16	MAN	KA	4	16	11,11,12	0.74	0	15,15,17	1.55	2 (13%)
16	MAN	KA	5	16	11,11,12	0.69	0	15,15,17	1.35	2 (13%)
16	MAN	KA	6	16	11,11,12	0.89	0	15,15,17	1.21	2 (13%)
16	MAN	KA	7	16	11,11,12	0.64	0	15,15,17	1.10	2 (13%)
16	MAN	KA	8	16	11,11,12	0.86	0	15,15,17	0.92	2 (13%)
16	MAN	KA	9	16	11,11,12	0.86	0	15,15,17	0.94	2 (13%)
11	NAG	LA	1	11	14,14,15	0.52	0	17,19,21	1.04	1 (5%)
11	NAG	LA	2	11	14,14,15	0.44	0	17,19,21	0.59	1 (5%)
10	NAG	MA	1	2,10	14,14,15	0.28	0	17,19,21	0.61	0
10	NAG	MA	2	10	14,14,15	0.33	0	17,19,21	0.83	1 (5%)
10	BMA	MA	3	10	11,11,12	1.08	0	15,15,17	0.89	0
10	MAN	MA	4	10	11,11,12	0.98	1 (9%)	15,15,17	1.38	2 (13%)
9	NAG	O	1	9,2	14,14,15	0.23	0	17,19,21	0.56	0
9	NAG	O	2	9	14,14,15	0.22	0	17,19,21	0.54	0
9	BMA	O	3	9	11,11,12	0.78	0	15,15,17	1.05	1 (6%)
15	NAG	P	1	15,2	14,14,15	0.27	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	NAG	P	2	15	14,14,15	0.20	0	17,19,21	0.47	0
15	BMA	P	3	15	11,11,12	0.99	1 (9%)	15,15,17	1.32	2 (13%)
15	MAN	P	4	15	11,11,12	0.86	1 (9%)	15,15,17	1.32	2 (13%)
15	MAN	P	5	15	11,11,12	0.87	1 (9%)	15,15,17	1.52	2 (13%)
15	MAN	P	6	15	11,11,12	0.76	0	15,15,17	1.25	2 (13%)
11	NAG	S	1	11,2	14,14,15	0.27	0	17,19,21	0.50	0
11	NAG	S	2	11	14,14,15	0.41	0	17,19,21	0.46	0
11	NAG	T	1	11,2	14,14,15	0.19	0	17,19,21	0.55	0
11	NAG	T	2	11	14,14,15	0.30	0	17,19,21	0.52	0
9	NAG	U	1	9,2	14,14,15	0.30	0	17,19,21	0.50	0
9	NAG	U	2	9	14,14,15	0.24	0	17,19,21	0.59	0
9	BMA	U	3	9	11,11,12	1.15	1 (9%)	15,15,17	1.25	2 (13%)
12	NAG	V	1	12,2	14,14,15	0.27	0	17,19,21	0.53	0
12	NAG	V	2	12	14,14,15	0.41	0	17,19,21	0.89	1 (5%)
12	BMA	V	3	12	11,11,12	0.70	0	15,15,17	1.22	2 (13%)
12	MAN	V	4	12	11,11,12	0.81	0	15,15,17	0.96	2 (13%)
12	MAN	V	5	12	11,11,12	0.88	1 (9%)	15,15,17	1.19	2 (13%)
11	NAG	W	1	11,2	14,14,15	0.50	0	17,19,21	0.62	0
11	NAG	W	2	11	14,14,15	0.41	0	17,19,21	0.57	0
16	NAG	X	1	16,2	14,14,15	0.28	0	17,19,21	0.49	0
16	NAG	X	2	16	14,14,15	0.24	0	17,19,21	1.26	3 (17%)
16	BMA	X	3	16	11,11,12	0.62	0	15,15,17	1.41	2 (13%)
16	MAN	X	4	16	11,11,12	0.74	0	15,15,17	1.55	2 (13%)
16	MAN	X	5	16	11,11,12	0.68	0	15,15,17	1.34	2 (13%)
16	MAN	X	6	16	11,11,12	0.88	0	15,15,17	1.21	2 (13%)
16	MAN	X	7	16	11,11,12	0.64	0	15,15,17	1.10	2 (13%)
16	MAN	X	8	16	11,11,12	0.85	0	15,15,17	0.93	2 (13%)
16	MAN	X	9	16	11,11,12	0.86	0	15,15,17	0.94	2 (13%)
11	NAG	Y	1	11	14,14,15	0.52	0	17,19,21	1.04	1 (5%)
11	NAG	Y	2	11	14,14,15	0.45	0	17,19,21	0.59	0
10	NAG	Z	1	2,10	14,14,15	0.27	0	17,19,21	0.61	0
10	NAG	Z	2	10	14,14,15	0.32	0	17,19,21	0.84	1 (5%)
10	BMA	Z	3	10	11,11,12	1.08	0	15,15,17	0.89	0
10	MAN	Z	4	10	11,11,12	0.98	1 (9%)	15,15,17	1.38	2 (13%)
9	NAG	a	1	9,1	14,14,15	0.24	0	17,19,21	0.55	0
9	NAG	a	2	9	14,14,15	0.38	0	17,19,21	0.50	0
9	BMA	a	3	9	11,11,12	0.77	0	15,15,17	0.85	1 (6%)
10	NAG	b	1	2,10	14,14,15	0.30	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	b	2	10	14,14,15	0.32	0	17,19,21	0.74	1 (5%)
10	BMA	b	3	10	11,11,12	0.76	0	15,15,17	1.00	1 (6%)
10	MAN	b	4	10	11,11,12	0.86	1 (9%)	15,15,17	1.17	2 (13%)
11	NAG	e	1	11,2	14,14,15	0.48	0	17,19,21	1.04	1 (5%)
11	NAG	e	2	11	14,14,15	0.45	0	17,19,21	0.53	0
10	NAG	f	1	10	14,14,15	0.26	0	17,19,21	0.47	0
10	NAG	f	2	10	14,14,15	0.42	0	17,19,21	0.97	1 (5%)
10	BMA	f	3	10	11,11,12	0.71	0	15,15,17	1.29	1 (6%)
10	MAN	f	4	10	11,11,12	0.78	0	15,15,17	1.22	2 (13%)
12	NAG	g	1	12,2	14,14,15	0.26	0	17,19,21	0.54	0
12	NAG	g	2	12	14,14,15	0.22	0	17,19,21	0.42	0
12	BMA	g	3	12	11,11,12	0.72	0	15,15,17	0.76	0
12	MAN	g	4	12	11,11,12	0.81	0	15,15,17	0.98	2 (13%)
12	MAN	g	5	12	11,11,12	0.67	0	15,15,17	1.06	2 (13%)
13	NAG	i	1	2,13	14,14,15	0.60	0	17,19,21	0.99	1 (5%)
13	NAG	i	2	13	14,14,15	0.47	0	17,19,21	0.77	1 (5%)
13	BMA	i	3	13	11,11,12	0.79	0	15,15,17	0.90	1 (6%)
13	MAN	i	4	13	11,11,12	2.09	3 (27%)	15,15,17	2.26	3 (20%)
13	MAN	i	5	13	11,11,12	0.73	0	15,15,17	1.03	2 (13%)
13	MAN	i	6	13	11,11,12	0.79	0	15,15,17	1.08	2 (13%)
13	MAN	i	7	13	11,11,12	0.95	1 (9%)	15,15,17	1.14	2 (13%)
13	MAN	i	8	13	11,11,12	0.84	0	15,15,17	1.25	2 (13%)
14	NAG	j	1	14,2	14,14,15	0.24	0	17,19,21	0.56	0
14	NAG	j	2	14	14,14,15	0.29	0	17,19,21	0.70	1 (5%)
14	BMA	j	3	14	11,11,12	0.79	0	15,15,17	1.28	1 (6%)
14	MAN	j	4	14	11,11,12	0.84	0	15,15,17	1.16	2 (13%)
9	NAG	k	1	9,2	14,14,15	0.23	0	17,19,21	0.56	0
9	NAG	k	2	9	14,14,15	0.23	0	17,19,21	0.54	0
9	BMA	k	3	9	11,11,12	0.79	0	15,15,17	1.05	1 (6%)
15	NAG	o	1	15,2	14,14,15	0.27	0	17,19,21	0.57	0
15	NAG	o	2	15	14,14,15	0.20	0	17,19,21	0.48	0
15	BMA	o	3	15	11,11,12	1.00	1 (9%)	15,15,17	1.32	2 (13%)
15	MAN	o	4	15	11,11,12	0.84	1 (9%)	15,15,17	1.32	2 (13%)
15	MAN	o	5	15	11,11,12	0.87	1 (9%)	15,15,17	1.52	2 (13%)
15	MAN	o	6	15	11,11,12	0.74	0	15,15,17	1.26	2 (13%)
11	NAG	p	1	11,2	14,14,15	0.27	0	17,19,21	0.49	0
11	NAG	p	2	11	14,14,15	0.40	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	s	1	11,2	14,14,15	0.18	0	17,19,21	0.55	0
11	NAG	s	2	11	14,14,15	0.31	0	17,19,21	0.51	0
9	NAG	t	1	9,2	14,14,15	0.31	0	17,19,21	0.50	0
9	NAG	t	2	9	14,14,15	0.24	0	17,19,21	0.60	0
9	BMA	t	3	9	11,11,12	1.17	1 (9%)	15,15,17	1.25	2 (13%)
12	NAG	u	1	12,2	14,14,15	0.29	0	17,19,21	0.53	0
12	NAG	u	2	12	14,14,15	0.41	0	17,19,21	0.89	1 (5%)
12	BMA	u	3	12	11,11,12	0.71	0	15,15,17	1.22	2 (13%)
12	MAN	u	4	12	11,11,12	0.81	0	15,15,17	0.96	2 (13%)
12	MAN	u	5	12	11,11,12	0.88	1 (9%)	15,15,17	1.20	2 (13%)
11	NAG	v	1	11,2	14,14,15	0.49	0	17,19,21	0.62	0
11	NAG	v	2	11	14,14,15	0.40	0	17,19,21	0.56	0
16	NAG	w	1	16,2	14,14,15	0.28	0	17,19,21	0.50	0
16	NAG	w	2	16	14,14,15	0.25	0	17,19,21	1.26	3 (17%)
16	BMA	w	3	16	11,11,12	0.61	0	15,15,17	1.42	2 (13%)
16	MAN	w	4	16	11,11,12	0.74	0	15,15,17	1.55	2 (13%)
16	MAN	w	5	16	11,11,12	0.69	0	15,15,17	1.35	2 (13%)
16	MAN	w	6	16	11,11,12	0.88	0	15,15,17	1.21	2 (13%)
16	MAN	w	7	16	11,11,12	0.64	0	15,15,17	1.10	2 (13%)
16	MAN	w	8	16	11,11,12	0.85	0	15,15,17	0.92	2 (13%)
16	MAN	w	9	16	11,11,12	0.85	0	15,15,17	0.94	2 (13%)
11	NAG	x	1	11	14,14,15	0.51	0	17,19,21	1.04	1 (5%)
11	NAG	x	2	11	14,14,15	0.44	0	17,19,21	0.59	1 (5%)
10	NAG	y	1	2,10	14,14,15	0.29	0	17,19,21	0.60	0
10	NAG	y	2	10	14,14,15	0.34	0	17,19,21	0.83	1 (5%)
10	BMA	y	3	10	11,11,12	1.07	0	15,15,17	0.89	0
10	MAN	y	4	10	11,11,12	0.99	1 (9%)	15,15,17	1.38	2 (13%)
9	NAG	z	1	9,1	14,14,15	0.23	0	17,19,21	0.54	0
9	NAG	z	2	9	14,14,15	0.38	0	17,19,21	0.50	0
9	BMA	z	3	9	11,11,12	0.77	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
10	NAG	0	1	2,10	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	0	2	10	-	1/6/23/26	0/1/1/1
10	BMA	0	3	10	-	1/2/19/22	0/1/1/1
10	MAN	0	4	10	-	2/2/19/22	0/1/1/1
11	NAG	1	1	11,2	-	4/6/23/26	0/1/1/1
11	NAG	1	2	11	-	2/6/23/26	0/1/1/1
10	NAG	9	1	10	-	0/6/23/26	0/1/1/1
10	NAG	9	2	10	-	2/6/23/26	0/1/1/1
10	BMA	9	3	10	-	2/2/19/22	0/1/1/1
10	MAN	9	4	10	-	2/2/19/22	0/1/1/1
12	NAG	AA	1	12,2	-	3/6/23/26	0/1/1/1
12	NAG	AA	2	12	-	2/6/23/26	0/1/1/1
12	BMA	AA	3	12	-	0/2/19/22	0/1/1/1
12	MAN	AA	4	12	-	1/2/19/22	0/1/1/1
12	MAN	AA	5	12	-	2/2/19/22	0/1/1/1
9	NAG	B	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	B	2	9	-	2/6/23/26	0/1/1/1
9	BMA	B	3	9	-	1/2/19/22	0/1/1/1
13	NAG	BA	1	2,13	-	4/6/23/26	0/1/1/1
13	NAG	BA	2	13	-	2/6/23/26	0/1/1/1
13	BMA	BA	3	13	-	2/2/19/22	0/1/1/1
13	MAN	BA	4	13	-	0/2/19/22	0/1/1/1
13	MAN	BA	5	13	-	0/2/19/22	0/1/1/1
13	MAN	BA	6	13	-	0/2/19/22	0/1/1/1
13	MAN	BA	7	13	-	1/2/19/22	0/1/1/1
13	MAN	BA	8	13	-	1/2/19/22	0/1/1/1
14	NAG	CA	1	14,2	-	0/6/23/26	0/1/1/1
14	NAG	CA	2	14	-	1/6/23/26	0/1/1/1
14	BMA	CA	3	14	-	2/2/19/22	0/1/1/1
14	MAN	CA	4	14	-	1/2/19/22	0/1/1/1
9	NAG	DA	1	9,2	-	1/6/23/26	0/1/1/1
9	NAG	DA	2	9	-	0/6/23/26	0/1/1/1
9	BMA	DA	3	9	-	2/2/19/22	0/1/1/1
10	NAG	E	1	2,10	-	1/6/23/26	0/1/1/1
10	NAG	E	2	10	-	1/6/23/26	0/1/1/1
10	BMA	E	3	10	-	1/2/19/22	0/1/1/1
10	MAN	E	4	10	-	2/2/19/22	0/1/1/1
15	NAG	EA	1	15,2	-	1/6/23/26	0/1/1/1
15	NAG	EA	2	15	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BMA	EA	3	15	-	2/2/19/22	0/1/1/1
15	MAN	EA	4	15	-	1/2/19/22	0/1/1/1
15	MAN	EA	5	15	-	0/2/19/22	0/1/1/1
15	MAN	EA	6	15	-	2/2/19/22	0/1/1/1
11	NAG	F	1	11,2	-	4/6/23/26	0/1/1/1
11	NAG	F	2	11	-	2/6/23/26	0/1/1/1
11	NAG	FA	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	FA	2	11	-	2/6/23/26	0/1/1/1
10	NAG	G	1	10	-	0/6/23/26	0/1/1/1
10	NAG	G	2	10	-	2/6/23/26	0/1/1/1
10	BMA	G	3	10	-	2/2/19/22	0/1/1/1
10	MAN	G	4	10	-	2/2/19/22	0/1/1/1
11	NAG	GA	1	11,2	-	1/6/23/26	0/1/1/1
11	NAG	GA	2	11	-	0/6/23/26	0/1/1/1
9	NAG	HA	1	9,2	-	2/6/23/26	0/1/1/1
9	NAG	HA	2	9	-	2/6/23/26	0/1/1/1
9	BMA	HA	3	9	-	1/2/19/22	0/1/1/1
12	NAG	I	1	12,2	-	3/6/23/26	0/1/1/1
12	NAG	I	2	12	-	2/6/23/26	0/1/1/1
12	BMA	I	3	12	-	0/2/19/22	0/1/1/1
12	MAN	I	4	12	-	1/2/19/22	0/1/1/1
12	MAN	I	5	12	-	2/2/19/22	0/1/1/1
12	NAG	IA	1	12,2	-	2/6/23/26	0/1/1/1
12	NAG	IA	2	12	-	1/6/23/26	0/1/1/1
12	BMA	IA	3	12	-	0/2/19/22	0/1/1/1
12	MAN	IA	4	12	-	0/2/19/22	0/1/1/1
12	MAN	IA	5	12	-	1/2/19/22	0/1/1/1
13	NAG	J	1	2,13	-	4/6/23/26	0/1/1/1
13	NAG	J	2	13	-	2/6/23/26	0/1/1/1
13	BMA	J	3	13	-	2/2/19/22	0/1/1/1
13	MAN	J	4	13	-	0/2/19/22	0/1/1/1
13	MAN	J	5	13	-	0/2/19/22	0/1/1/1
13	MAN	J	6	13	-	0/2/19/22	0/1/1/1
13	MAN	J	7	13	-	1/2/19/22	0/1/1/1
13	MAN	J	8	13	-	1/2/19/22	0/1/1/1
11	NAG	JA	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	JA	2	11	-	2/6/23/26	0/1/1/1
14	NAG	K	1	14,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	K	2	14	-	1/6/23/26	0/1/1/1
14	BMA	K	3	14	-	2/2/19/22	0/1/1/1
14	MAN	K	4	14	-	1/2/19/22	0/1/1/1
16	NAG	KA	1	16,2	-	2/6/23/26	0/1/1/1
16	NAG	KA	2	16	-	4/6/23/26	0/1/1/1
16	BMA	KA	3	16	-	0/2/19/22	0/1/1/1
16	MAN	KA	4	16	-	2/2/19/22	0/1/1/1
16	MAN	KA	5	16	-	2/2/19/22	0/1/1/1
16	MAN	KA	6	16	-	0/2/19/22	0/1/1/1
16	MAN	KA	7	16	-	2/2/19/22	0/1/1/1
16	MAN	KA	8	16	-	2/2/19/22	0/1/1/1
16	MAN	KA	9	16	-	0/2/19/22	0/1/1/1
11	NAG	LA	1	11	-	3/6/23/26	0/1/1/1
11	NAG	LA	2	11	-	0/6/23/26	0/1/1/1
10	NAG	MA	1	2,10	-	2/6/23/26	0/1/1/1
10	NAG	MA	2	10	-	0/6/23/26	0/1/1/1
10	BMA	MA	3	10	-	2/2/19/22	0/1/1/1
10	MAN	MA	4	10	-	2/2/19/22	0/1/1/1
9	NAG	O	1	9,2	-	1/6/23/26	0/1/1/1
9	NAG	O	2	9	-	0/6/23/26	0/1/1/1
9	BMA	O	3	9	-	2/2/19/22	0/1/1/1
15	NAG	P	1	15,2	-	1/6/23/26	0/1/1/1
15	NAG	P	2	15	-	0/6/23/26	0/1/1/1
15	BMA	P	3	15	-	2/2/19/22	0/1/1/1
15	MAN	P	4	15	-	1/2/19/22	0/1/1/1
15	MAN	P	5	15	-	0/2/19/22	0/1/1/1
15	MAN	P	6	15	-	2/2/19/22	0/1/1/1
11	NAG	S	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	S	2	11	-	2/6/23/26	0/1/1/1
11	NAG	T	1	11,2	-	1/6/23/26	0/1/1/1
11	NAG	T	2	11	-	0/6/23/26	0/1/1/1
9	NAG	U	1	9,2	-	2/6/23/26	0/1/1/1
9	NAG	U	2	9	-	2/6/23/26	0/1/1/1
9	BMA	U	3	9	-	1/2/19/22	0/1/1/1
12	NAG	V	1	12,2	-	2/6/23/26	0/1/1/1
12	NAG	V	2	12	-	1/6/23/26	0/1/1/1
12	BMA	V	3	12	-	0/2/19/22	0/1/1/1
12	MAN	V	4	12	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	V	5	12	-	1/2/19/22	0/1/1/1
11	NAG	W	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	W	2	11	-	2/6/23/26	0/1/1/1
16	NAG	X	1	16,2	-	2/6/23/26	0/1/1/1
16	NAG	X	2	16	-	4/6/23/26	0/1/1/1
16	BMA	X	3	16	-	0/2/19/22	0/1/1/1
16	MAN	X	4	16	-	2/2/19/22	0/1/1/1
16	MAN	X	5	16	-	2/2/19/22	0/1/1/1
16	MAN	X	6	16	-	0/2/19/22	0/1/1/1
16	MAN	X	7	16	-	2/2/19/22	0/1/1/1
16	MAN	X	8	16	-	2/2/19/22	0/1/1/1
16	MAN	X	9	16	-	0/2/19/22	0/1/1/1
11	NAG	Y	1	11	-	3/6/23/26	0/1/1/1
11	NAG	Y	2	11	-	0/6/23/26	0/1/1/1
10	NAG	Z	1	2,10	-	2/6/23/26	0/1/1/1
10	NAG	Z	2	10	-	0/6/23/26	0/1/1/1
10	BMA	Z	3	10	-	2/2/19/22	0/1/1/1
10	MAN	Z	4	10	-	2/2/19/22	0/1/1/1
9	NAG	a	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	a	2	9	-	2/6/23/26	0/1/1/1
9	BMA	a	3	9	-	1/2/19/22	0/1/1/1
10	NAG	b	1	2,10	-	1/6/23/26	0/1/1/1
10	NAG	b	2	10	-	1/6/23/26	0/1/1/1
10	BMA	b	3	10	-	1/2/19/22	0/1/1/1
10	MAN	b	4	10	-	2/2/19/22	0/1/1/1
11	NAG	e	1	11,2	-	4/6/23/26	0/1/1/1
11	NAG	e	2	11	-	2/6/23/26	0/1/1/1
10	NAG	f	1	10	-	0/6/23/26	0/1/1/1
10	NAG	f	2	10	-	2/6/23/26	0/1/1/1
10	BMA	f	3	10	-	2/2/19/22	0/1/1/1
10	MAN	f	4	10	-	2/2/19/22	0/1/1/1
12	NAG	g	1	12,2	-	3/6/23/26	0/1/1/1
12	NAG	g	2	12	-	2/6/23/26	0/1/1/1
12	BMA	g	3	12	-	0/2/19/22	0/1/1/1
12	MAN	g	4	12	-	1/2/19/22	0/1/1/1
12	MAN	g	5	12	-	2/2/19/22	0/1/1/1
13	NAG	i	1	2,13	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	i	2	13	-	2/6/23/26	0/1/1/1
13	BMA	i	3	13	-	2/2/19/22	0/1/1/1
13	MAN	i	4	13	-	0/2/19/22	0/1/1/1
13	MAN	i	5	13	-	0/2/19/22	0/1/1/1
13	MAN	i	6	13	-	0/2/19/22	0/1/1/1
13	MAN	i	7	13	-	1/2/19/22	0/1/1/1
13	MAN	i	8	13	-	1/2/19/22	0/1/1/1
14	NAG	j	1	14,2	-	0/6/23/26	0/1/1/1
14	NAG	j	2	14	-	1/6/23/26	0/1/1/1
14	BMA	j	3	14	-	2/2/19/22	0/1/1/1
14	MAN	j	4	14	-	1/2/19/22	0/1/1/1
9	NAG	k	1	9,2	-	1/6/23/26	0/1/1/1
9	NAG	k	2	9	-	0/6/23/26	0/1/1/1
9	BMA	k	3	9	-	2/2/19/22	0/1/1/1
15	NAG	o	1	15,2	-	1/6/23/26	0/1/1/1
15	NAG	o	2	15	-	0/6/23/26	0/1/1/1
15	BMA	o	3	15	-	2/2/19/22	0/1/1/1
15	MAN	o	4	15	-	1/2/19/22	0/1/1/1
15	MAN	o	5	15	-	0/2/19/22	0/1/1/1
15	MAN	o	6	15	-	2/2/19/22	0/1/1/1
11	NAG	p	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	p	2	11	-	2/6/23/26	0/1/1/1
11	NAG	s	1	11,2	-	1/6/23/26	0/1/1/1
11	NAG	s	2	11	-	0/6/23/26	0/1/1/1
9	NAG	t	1	9,2	-	2/6/23/26	0/1/1/1
9	NAG	t	2	9	-	2/6/23/26	0/1/1/1
9	BMA	t	3	9	-	1/2/19/22	0/1/1/1
12	NAG	u	1	12,2	-	2/6/23/26	0/1/1/1
12	NAG	u	2	12	-	1/6/23/26	0/1/1/1
12	BMA	u	3	12	-	0/2/19/22	0/1/1/1
12	MAN	u	4	12	-	0/2/19/22	0/1/1/1
12	MAN	u	5	12	-	1/2/19/22	0/1/1/1
11	NAG	v	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	v	2	11	-	2/6/23/26	0/1/1/1
16	NAG	w	1	16,2	-	2/6/23/26	0/1/1/1
16	NAG	w	2	16	-	4/6/23/26	0/1/1/1
16	BMA	w	3	16	-	0/2/19/22	0/1/1/1
16	MAN	w	4	16	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	MAN	w	5	16	-	2/2/19/22	0/1/1/1
16	MAN	w	6	16	-	0/2/19/22	0/1/1/1
16	MAN	w	7	16	-	2/2/19/22	0/1/1/1
16	MAN	w	8	16	-	2/2/19/22	0/1/1/1
16	MAN	w	9	16	-	0/2/19/22	0/1/1/1
11	NAG	x	1	11	-	3/6/23/26	0/1/1/1
11	NAG	x	2	11	-	0/6/23/26	0/1/1/1
10	NAG	y	1	2,10	-	2/6/23/26	0/1/1/1
10	NAG	y	2	10	-	0/6/23/26	0/1/1/1
10	BMA	y	3	10	-	2/2/19/22	0/1/1/1
10	MAN	y	4	10	-	2/2/19/22	0/1/1/1
9	NAG	z	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	z	2	9	-	2/6/23/26	0/1/1/1
9	BMA	z	3	9	-	1/2/19/22	0/1/1/1

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J	4	MAN	C1-C2	4.28	1.62	1.52
13	BA	4	MAN	C1-C2	4.27	1.62	1.52
13	i	4	MAN	C1-C2	4.26	1.62	1.52
13	J	4	MAN	O5-C1	4.11	1.50	1.43
13	BA	4	MAN	O5-C1	4.07	1.50	1.43

The worst 5 of 210 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	BA	4	MAN	C1-O5-C5	7.40	122.11	112.19
13	J	4	MAN	C1-O5-C5	7.38	122.08	112.19
13	i	4	MAN	C1-O5-C5	7.38	122.08	112.19
16	w	4	MAN	C1-O5-C5	5.20	119.15	112.19
16	KA	4	MAN	C1-O5-C5	5.18	119.12	112.19

There are no chirality outliers.

5 of 282 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	X	8	MAN	C4-C5-C6-O6
16	w	8	MAN	C4-C5-C6-O6

Continued on next page...

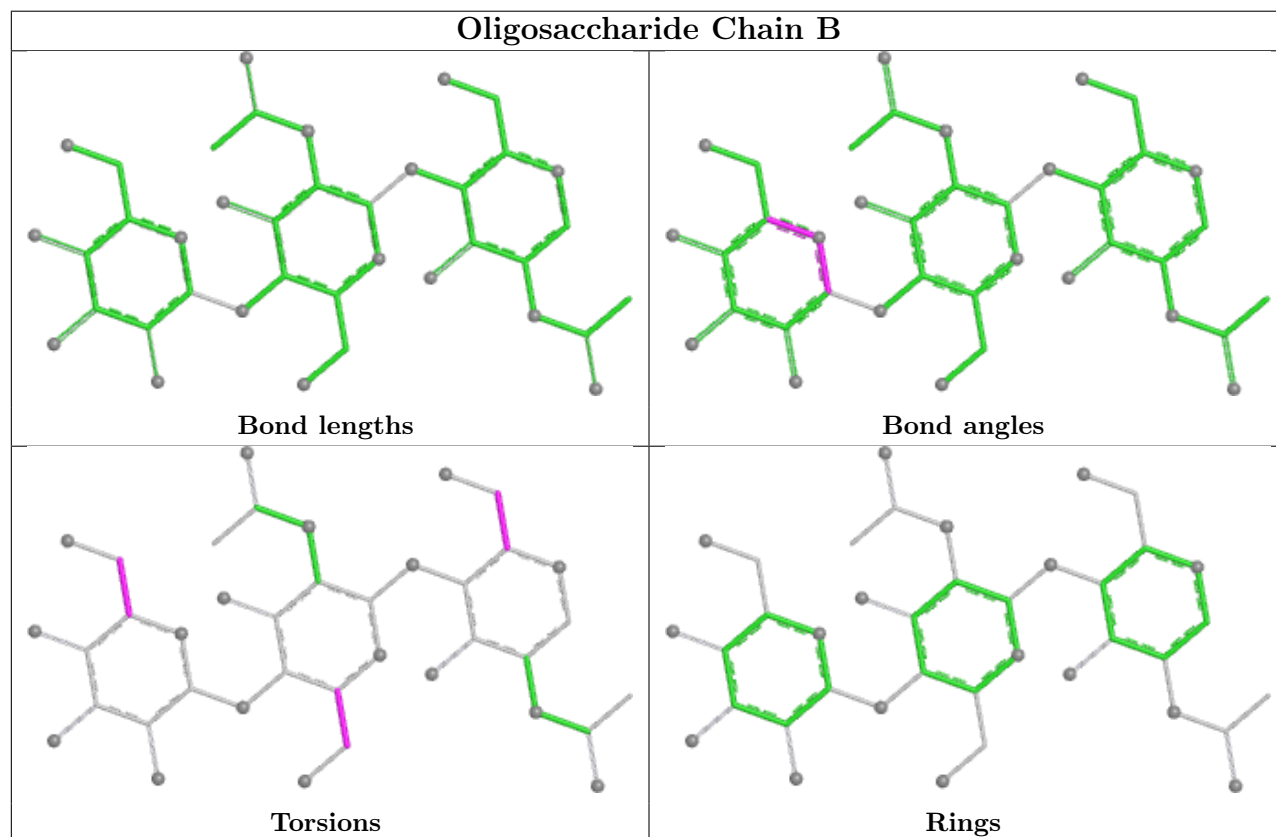
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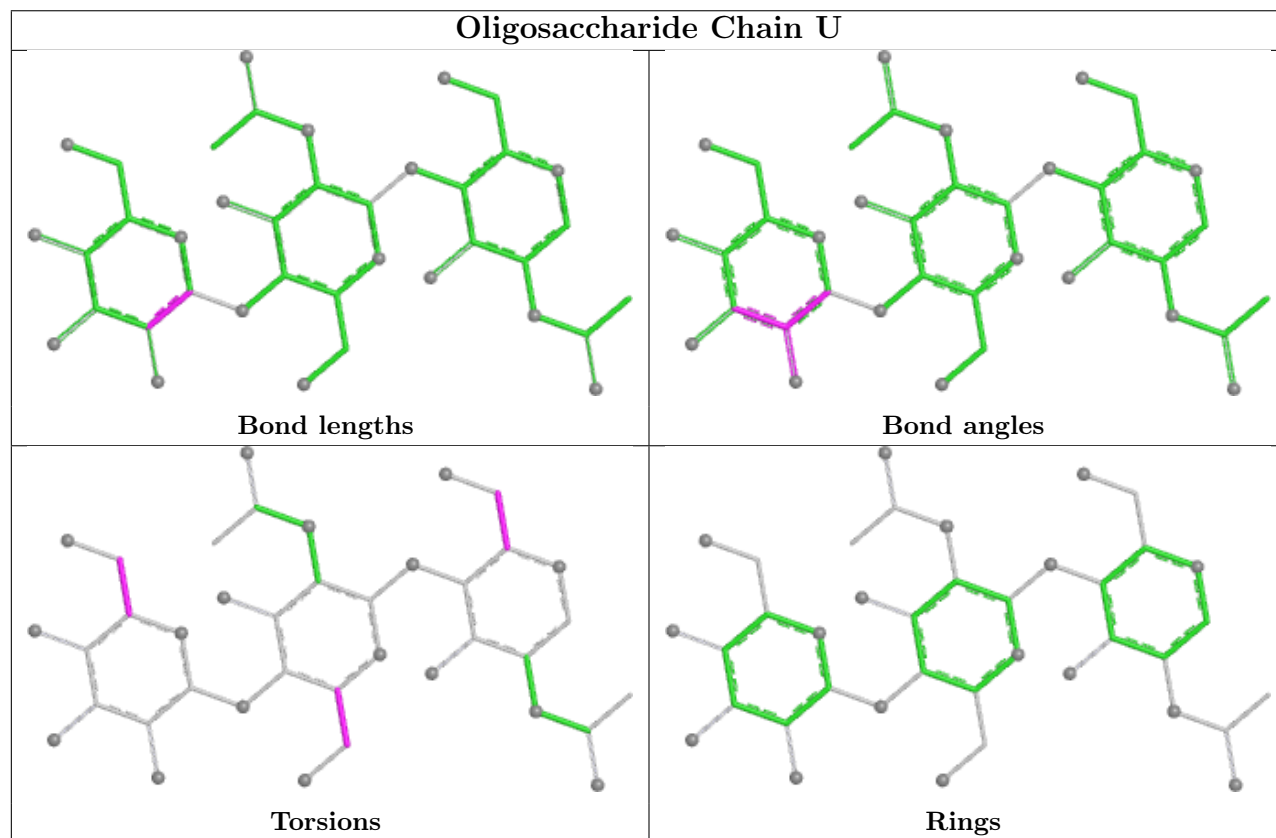
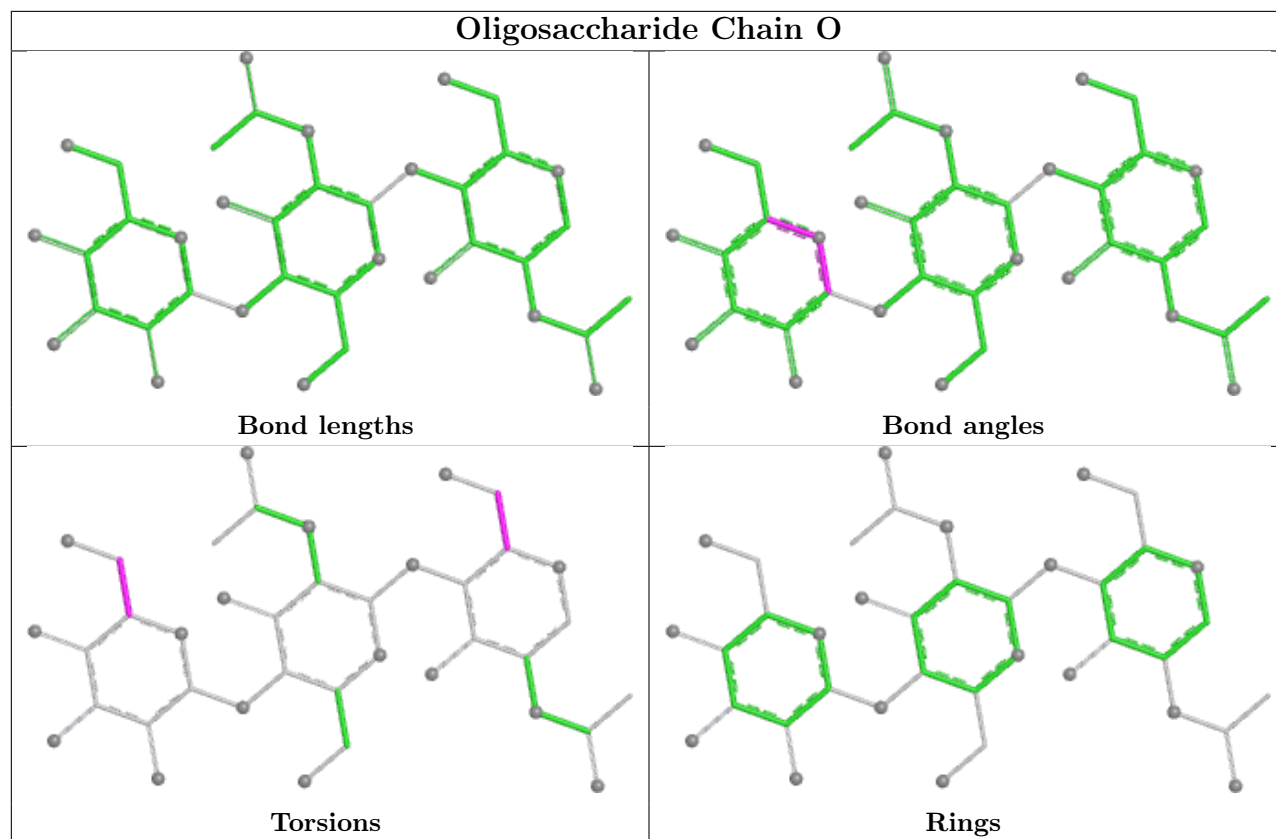
Mol	Chain	Res	Type	Atoms
16	KA	8	MAN	C4-C5-C6-O6
12	V	1	NAG	O5-C5-C6-O6
12	u	1	NAG	O5-C5-C6-O6

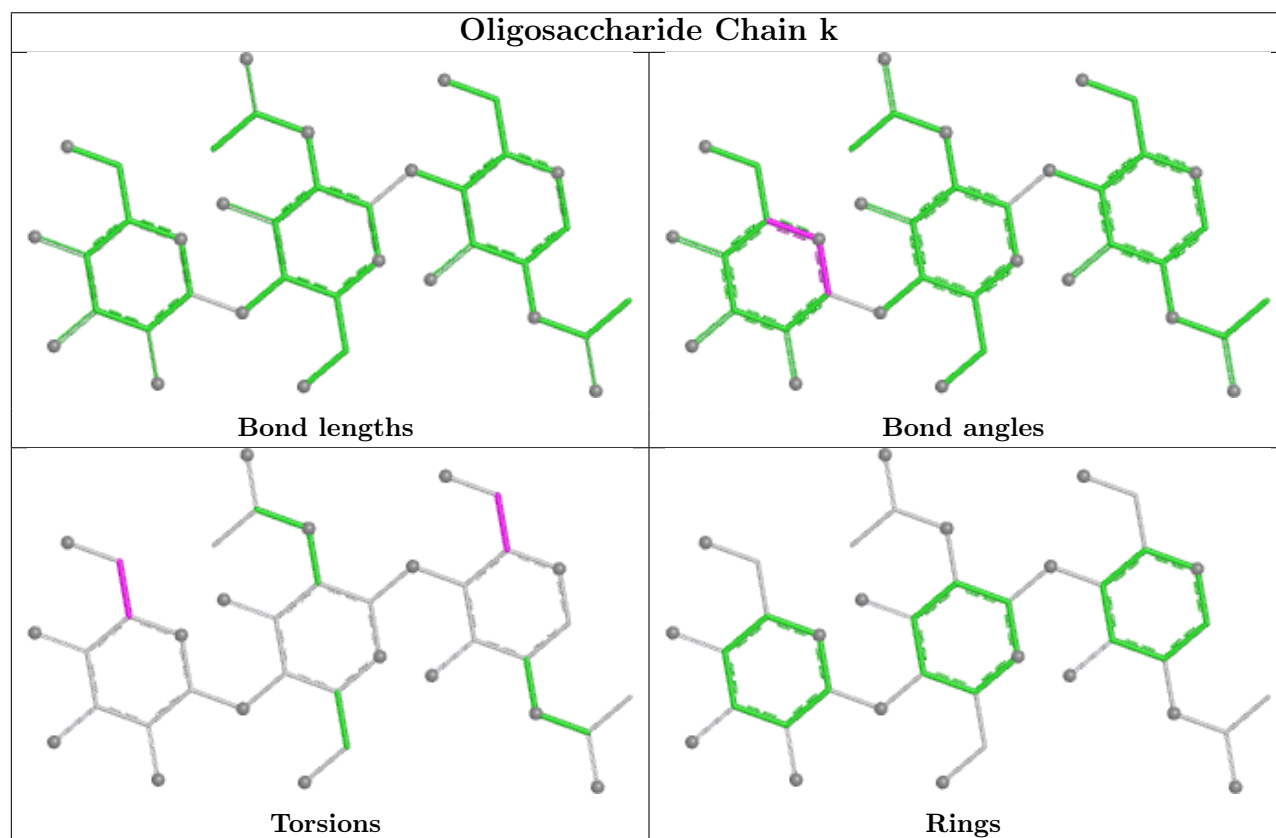
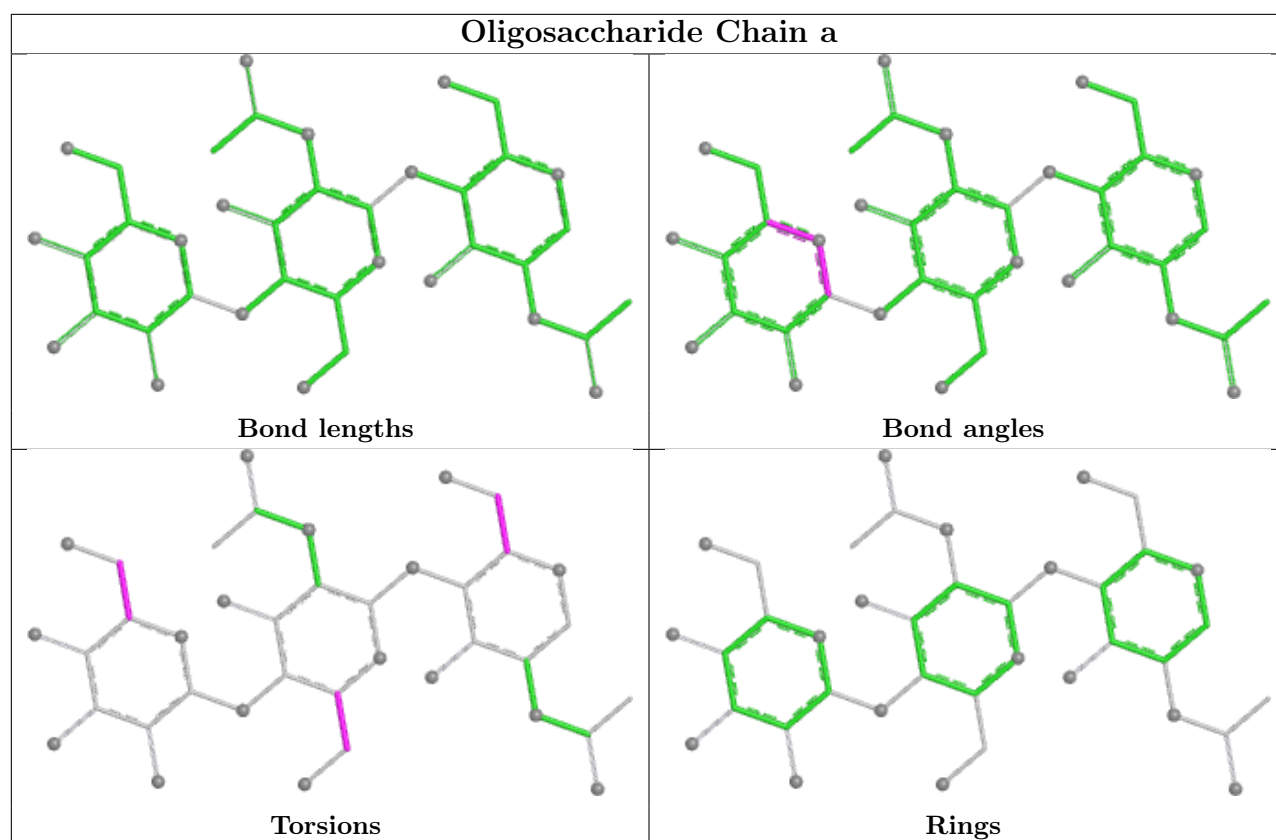
There are no ring outliers.

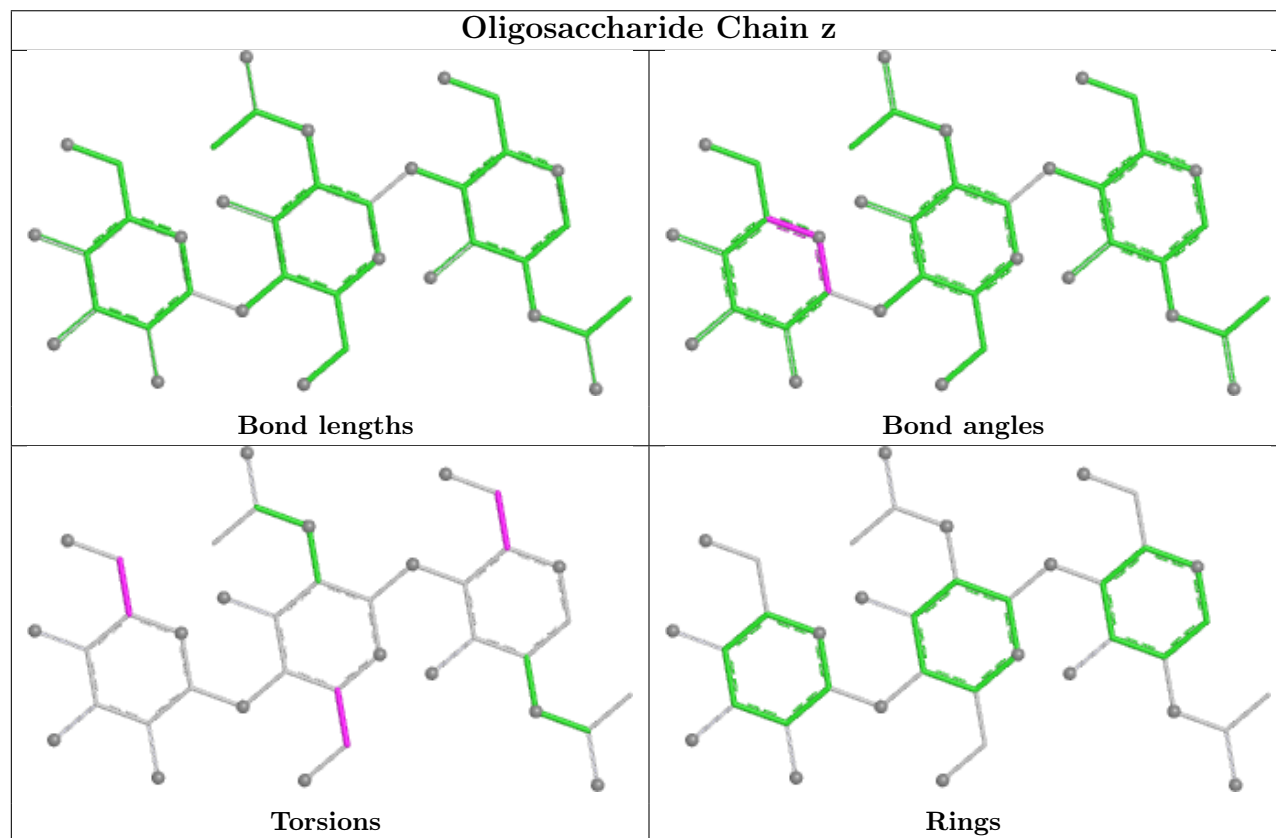
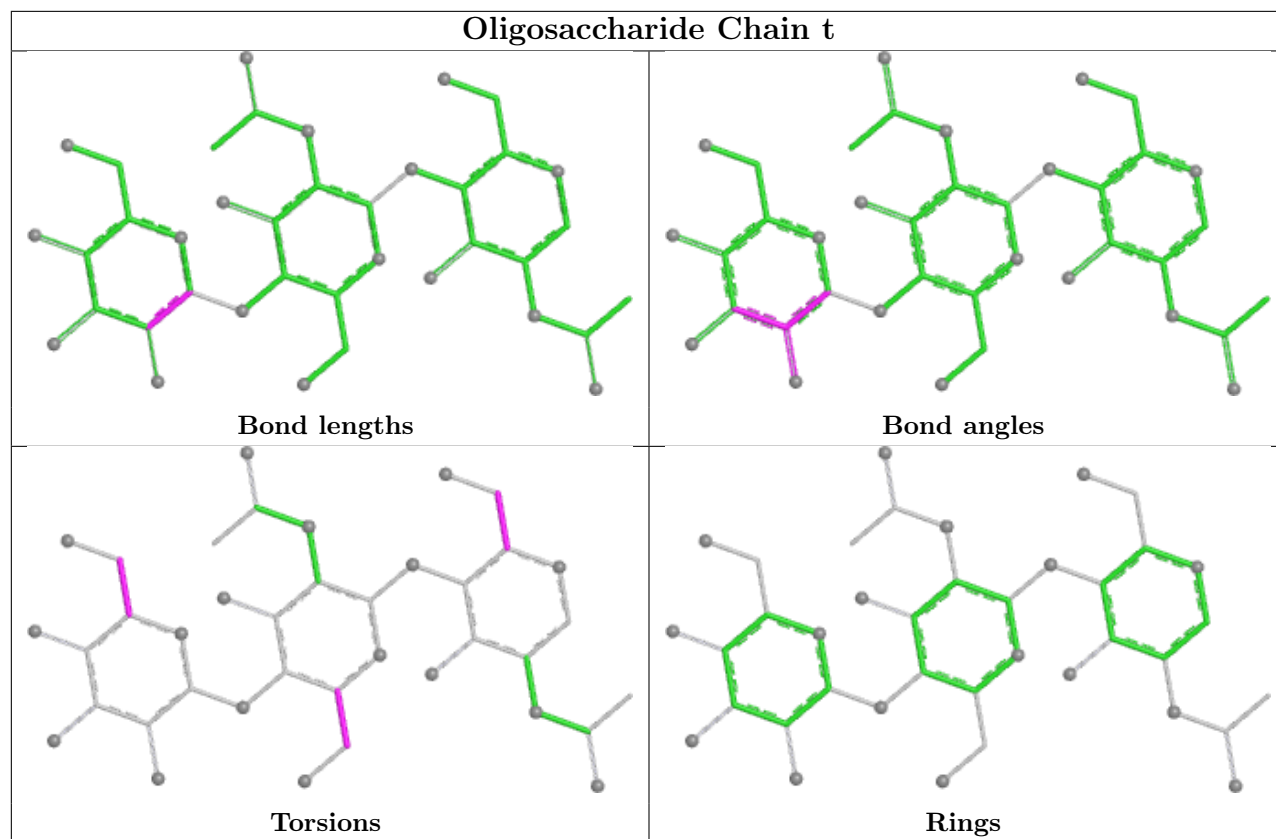
No monomer is involved in short contacts.

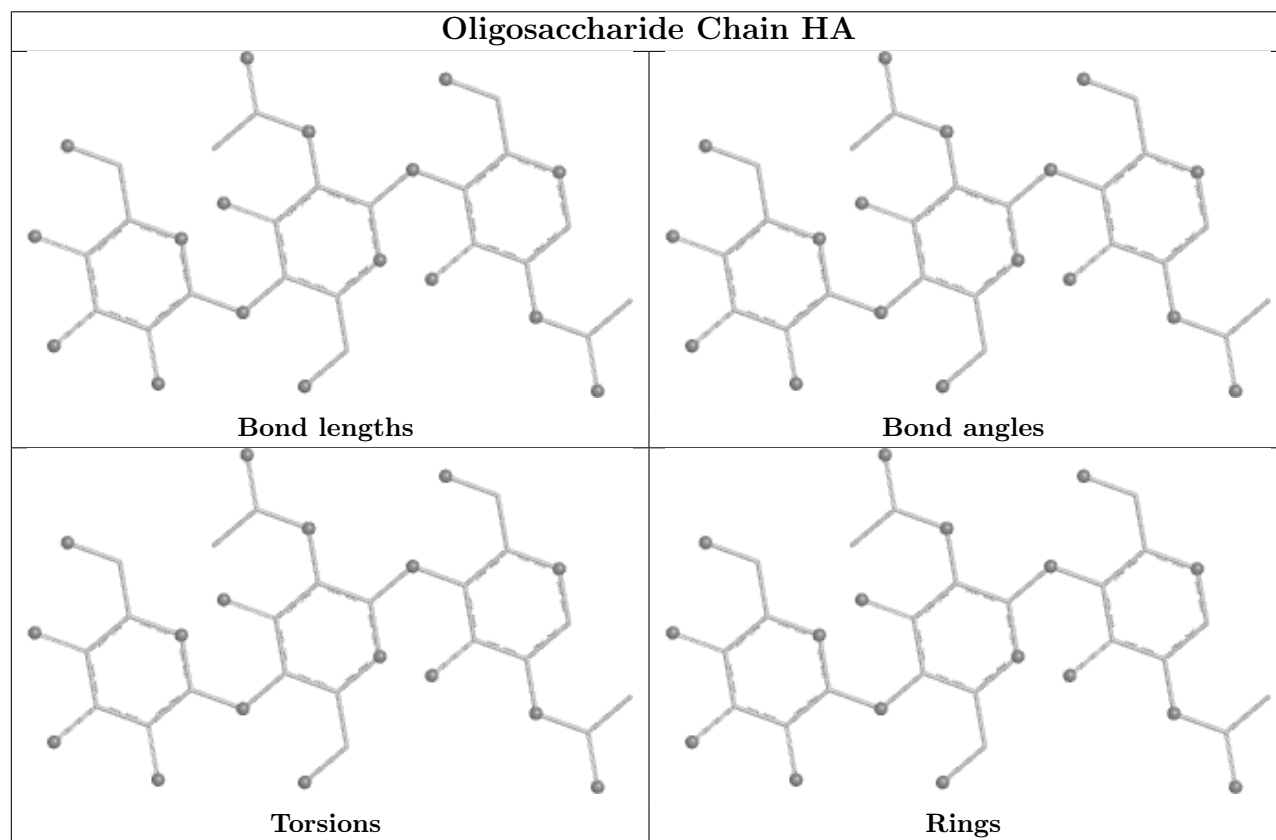
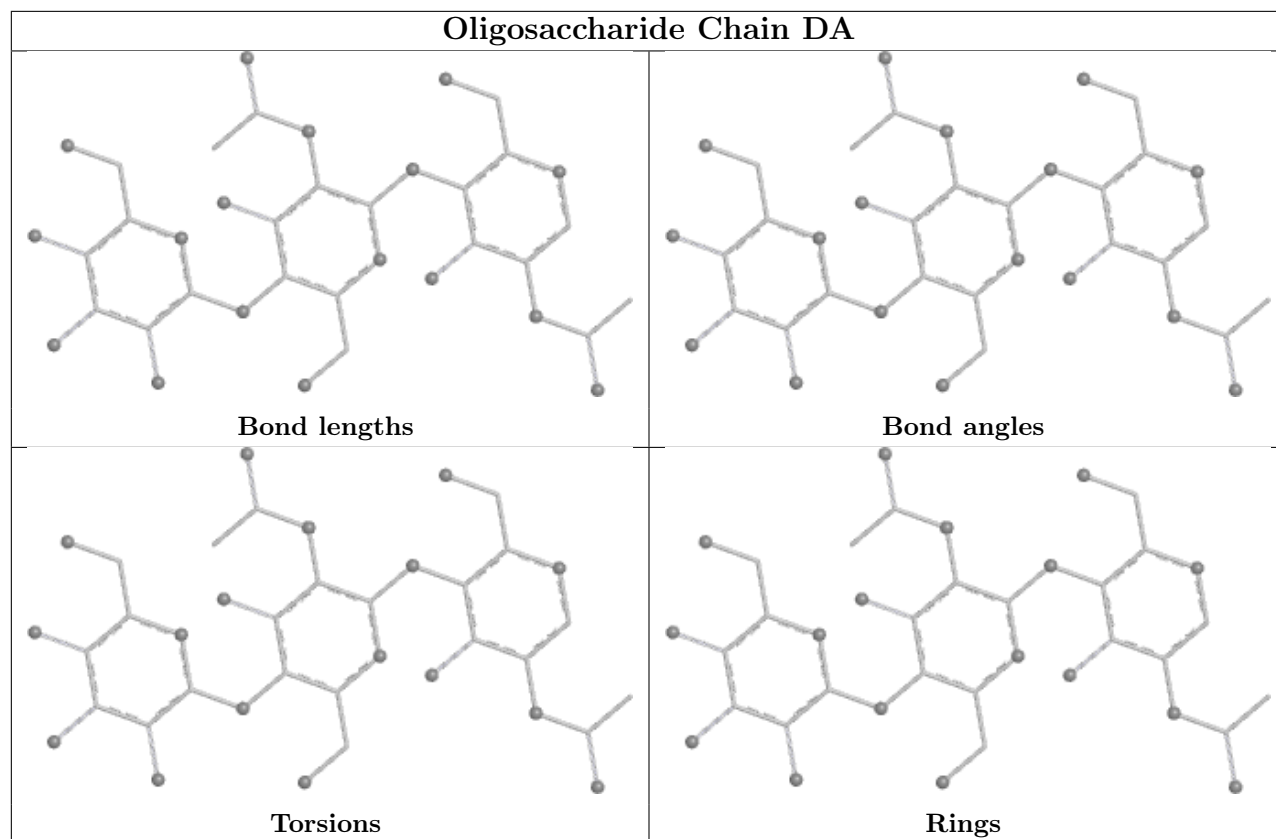
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

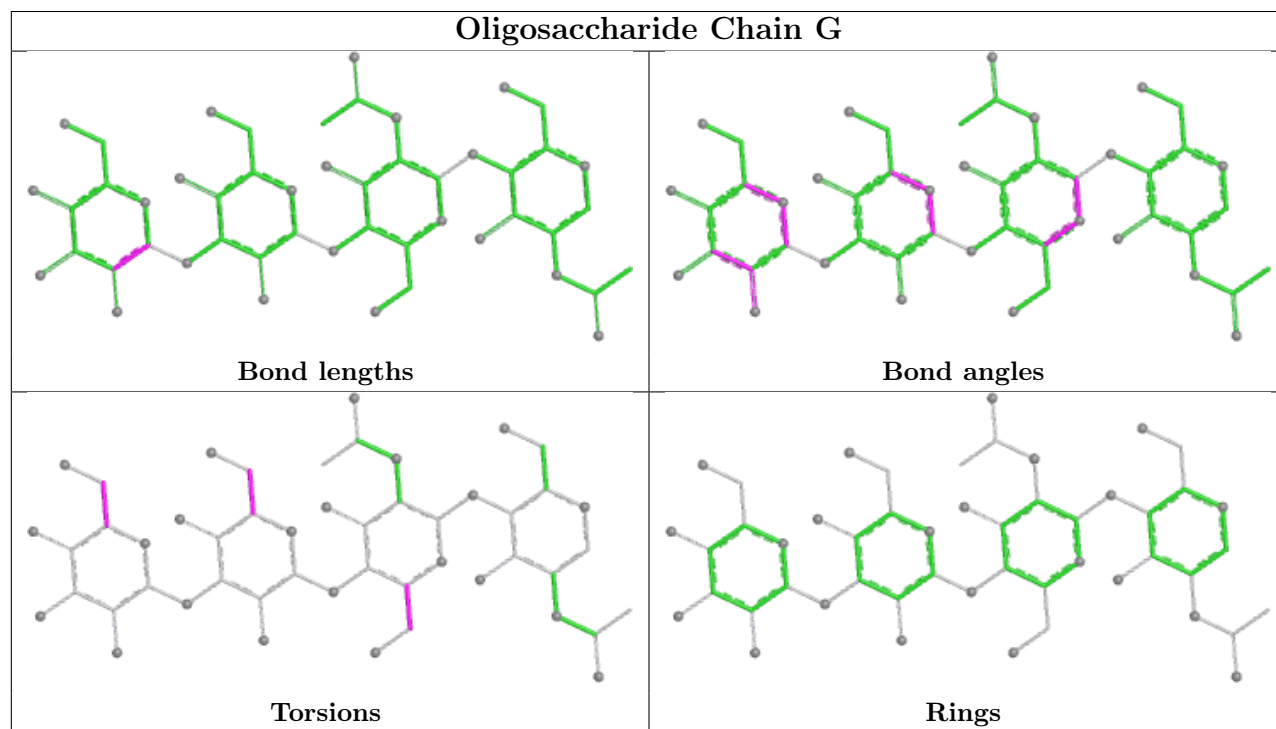
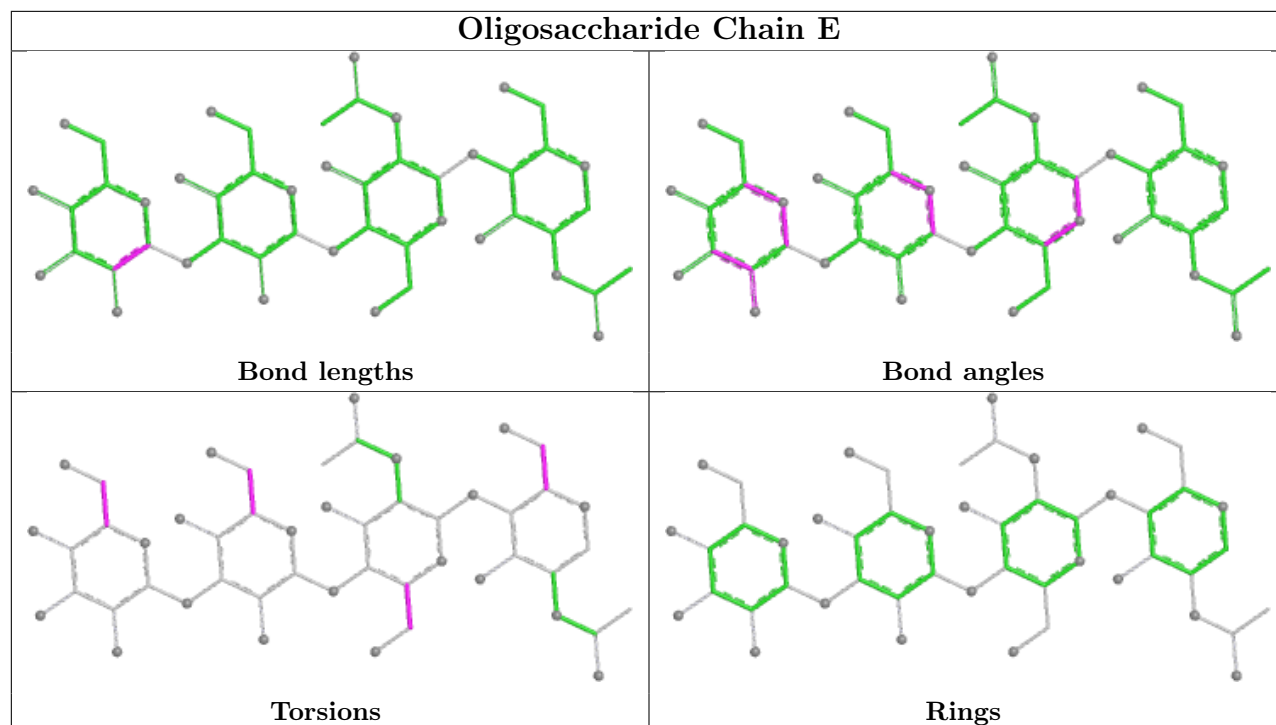


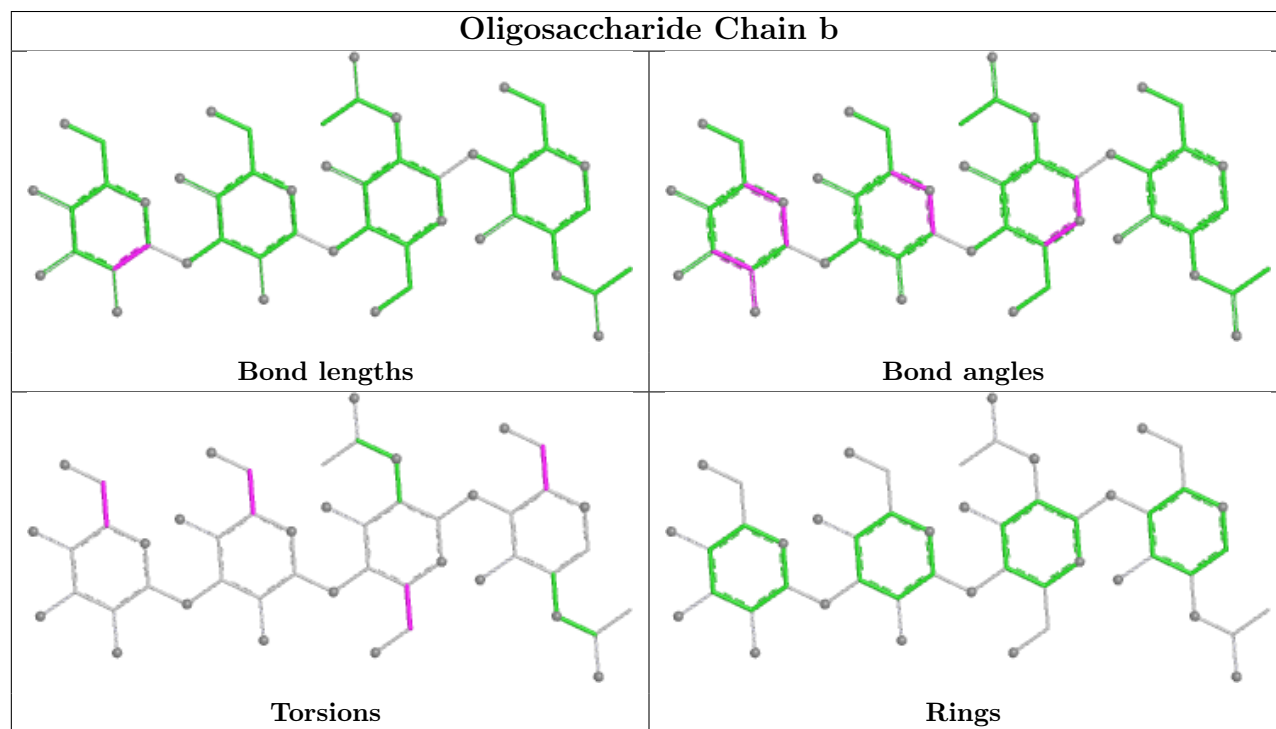
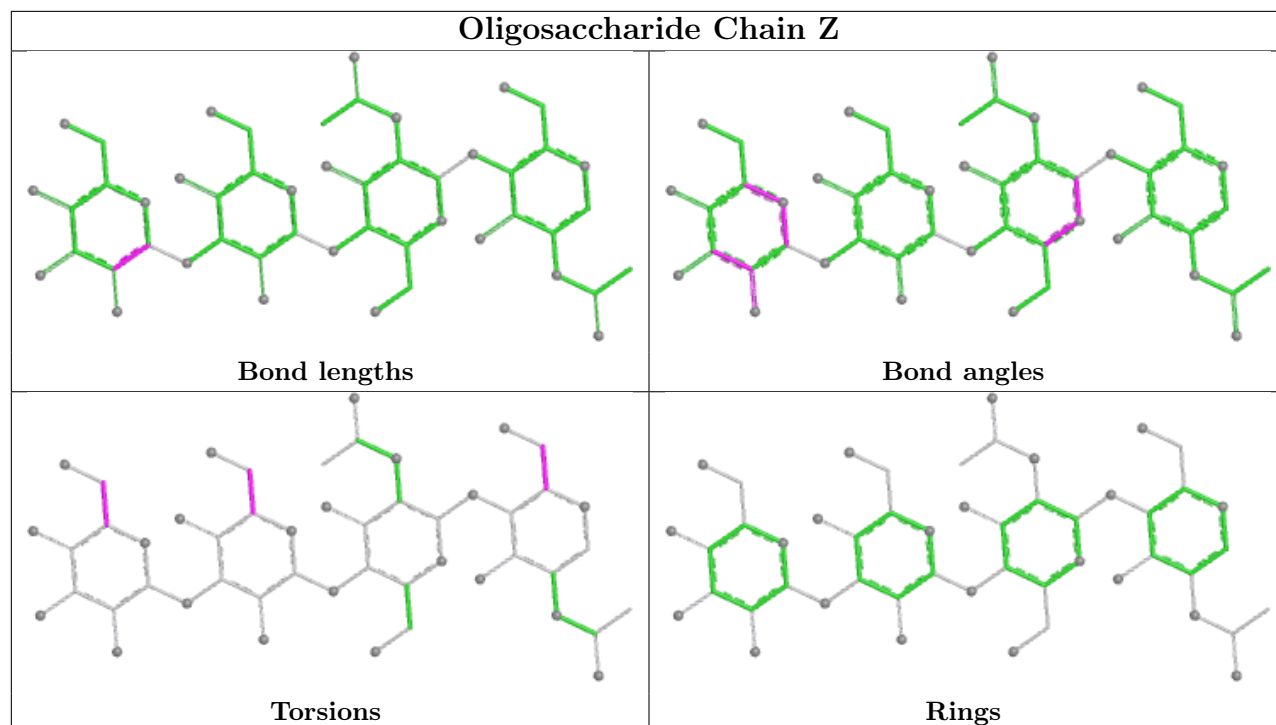


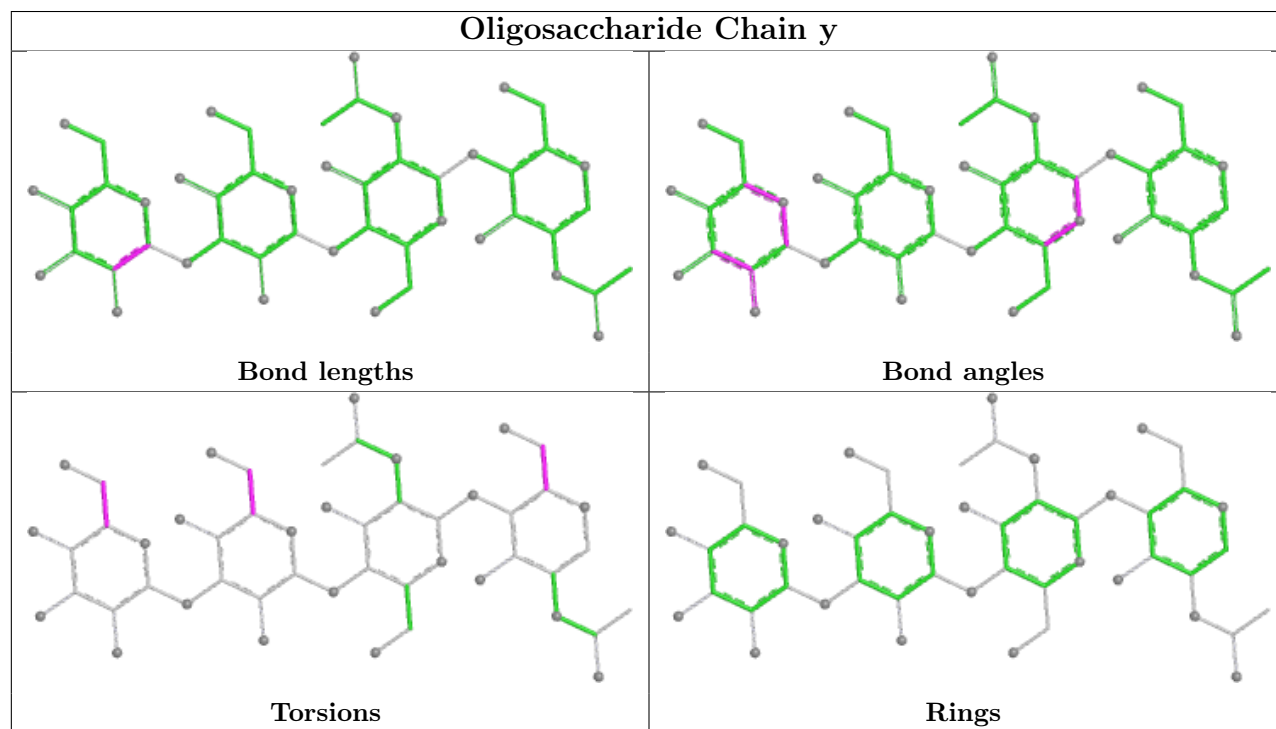
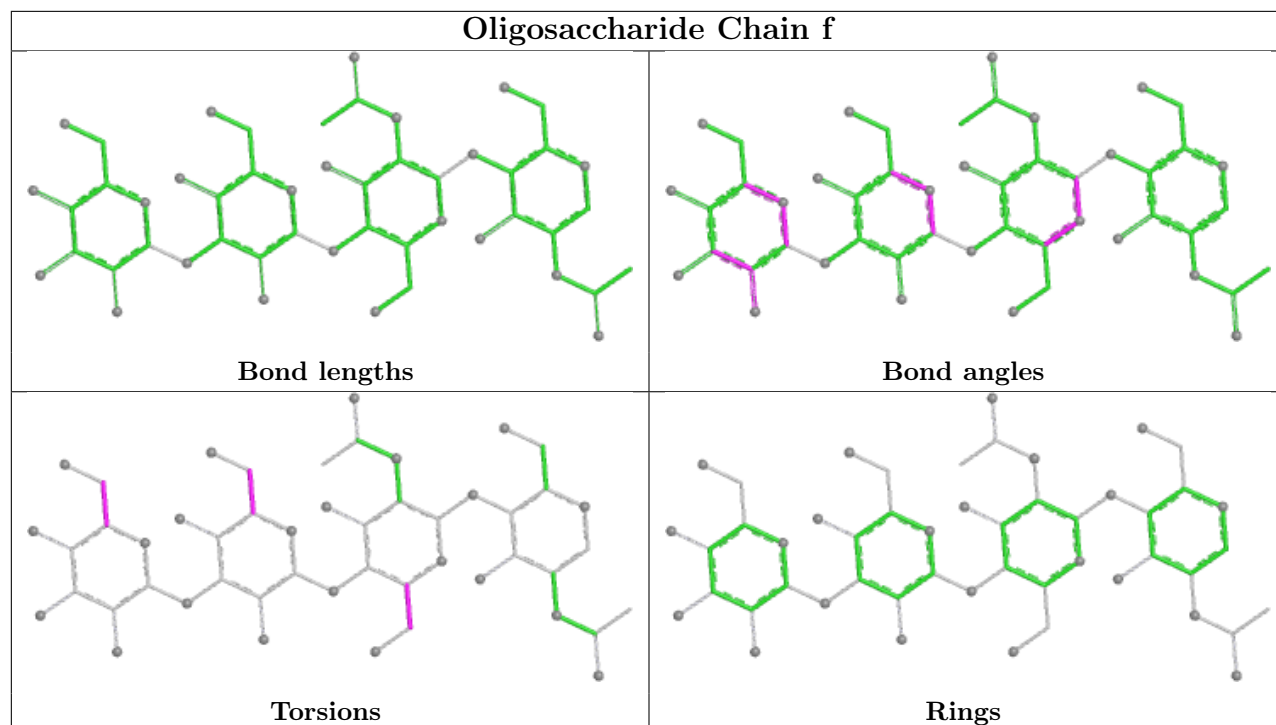


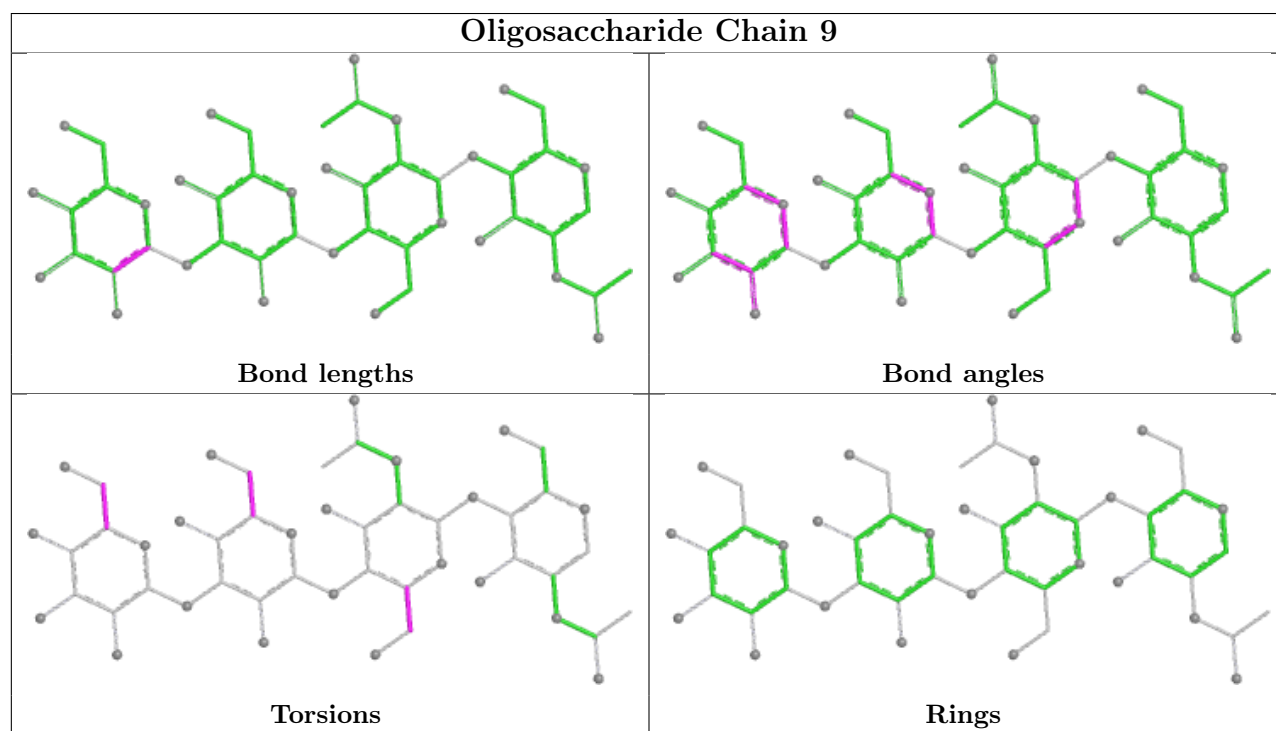
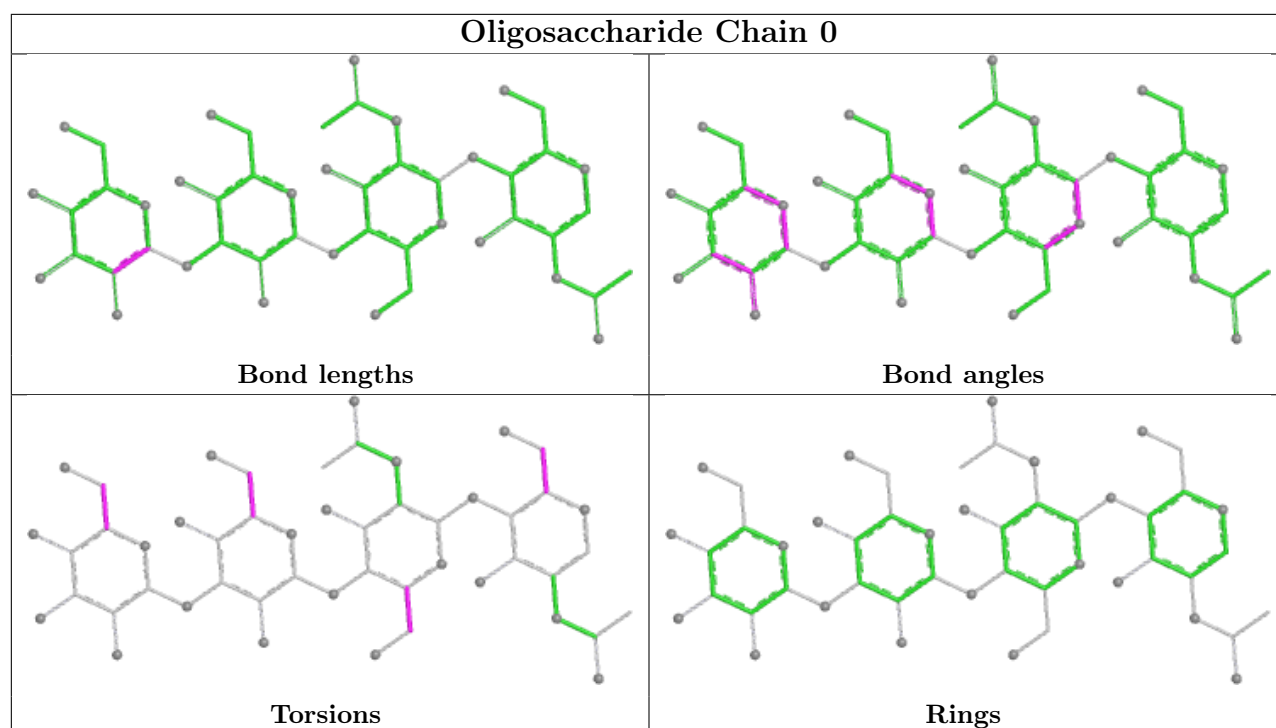


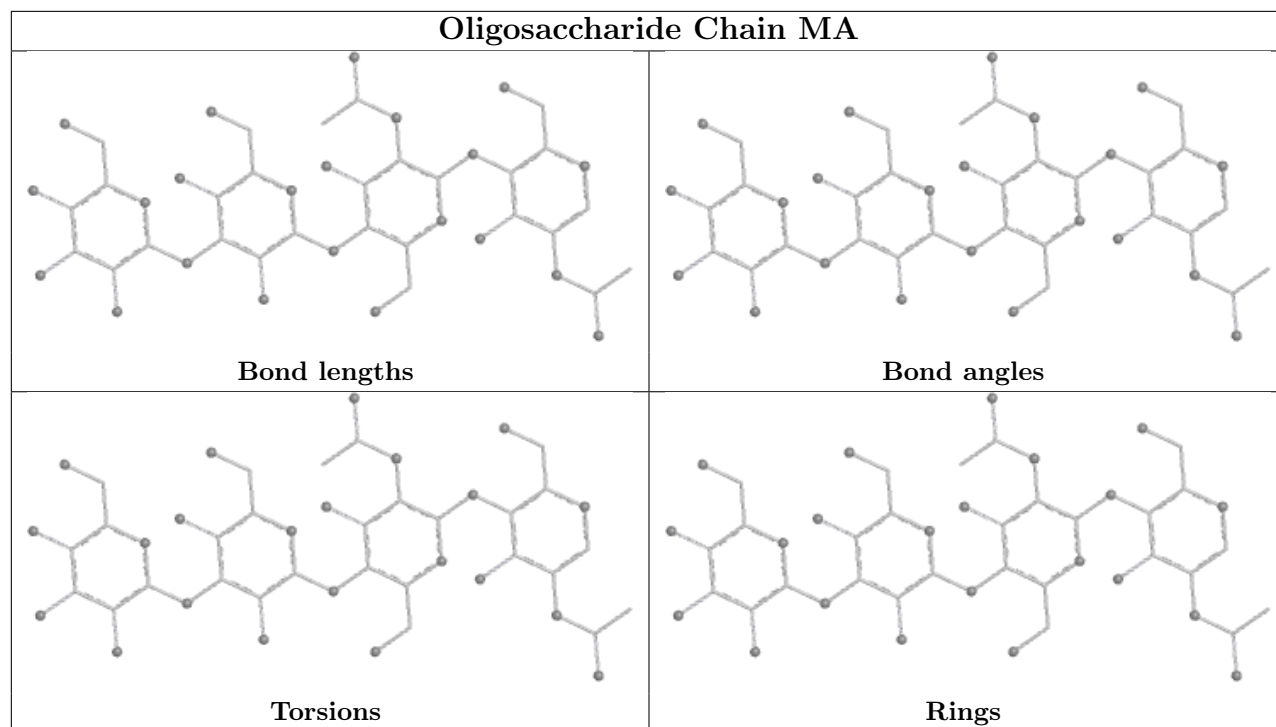


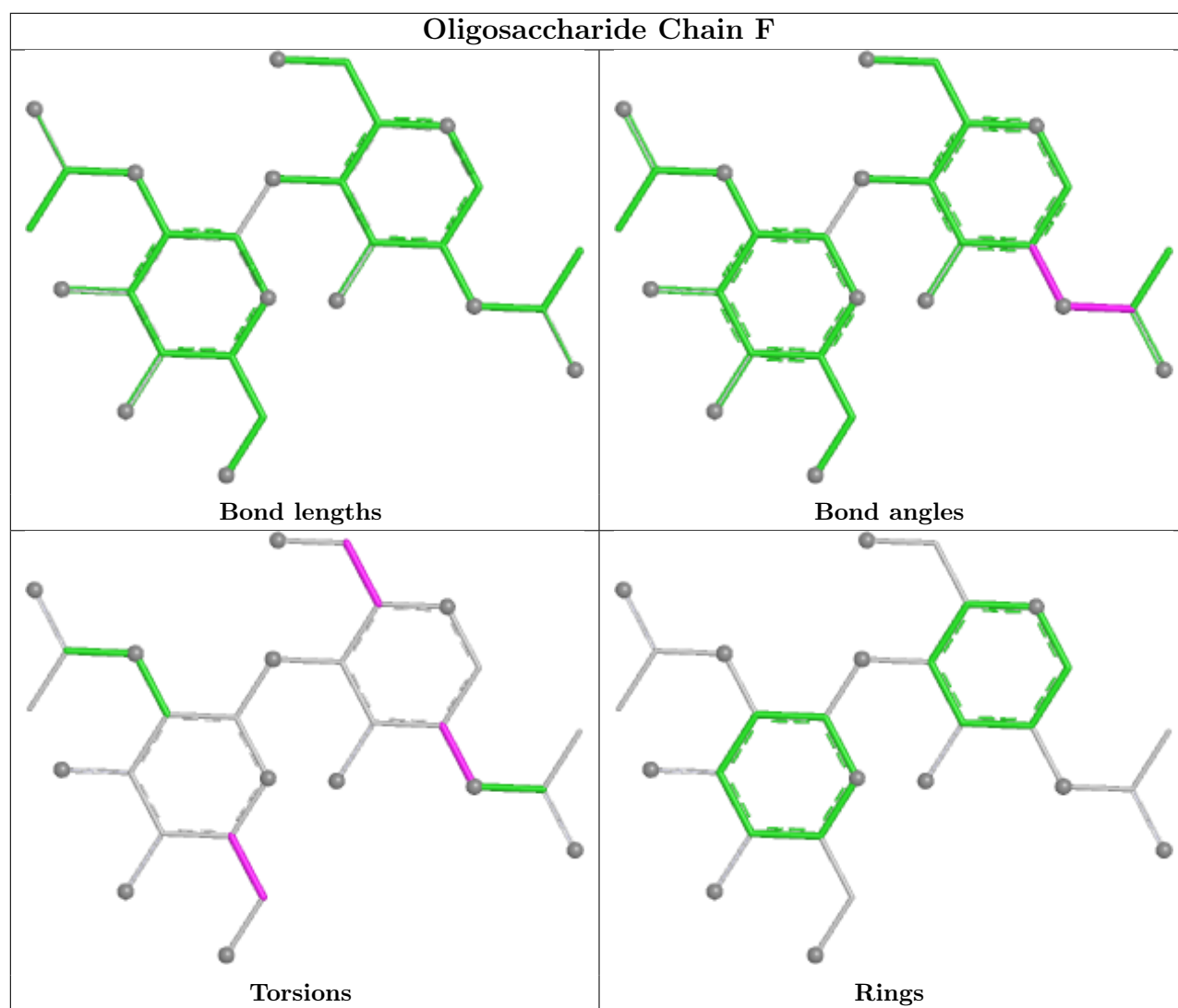


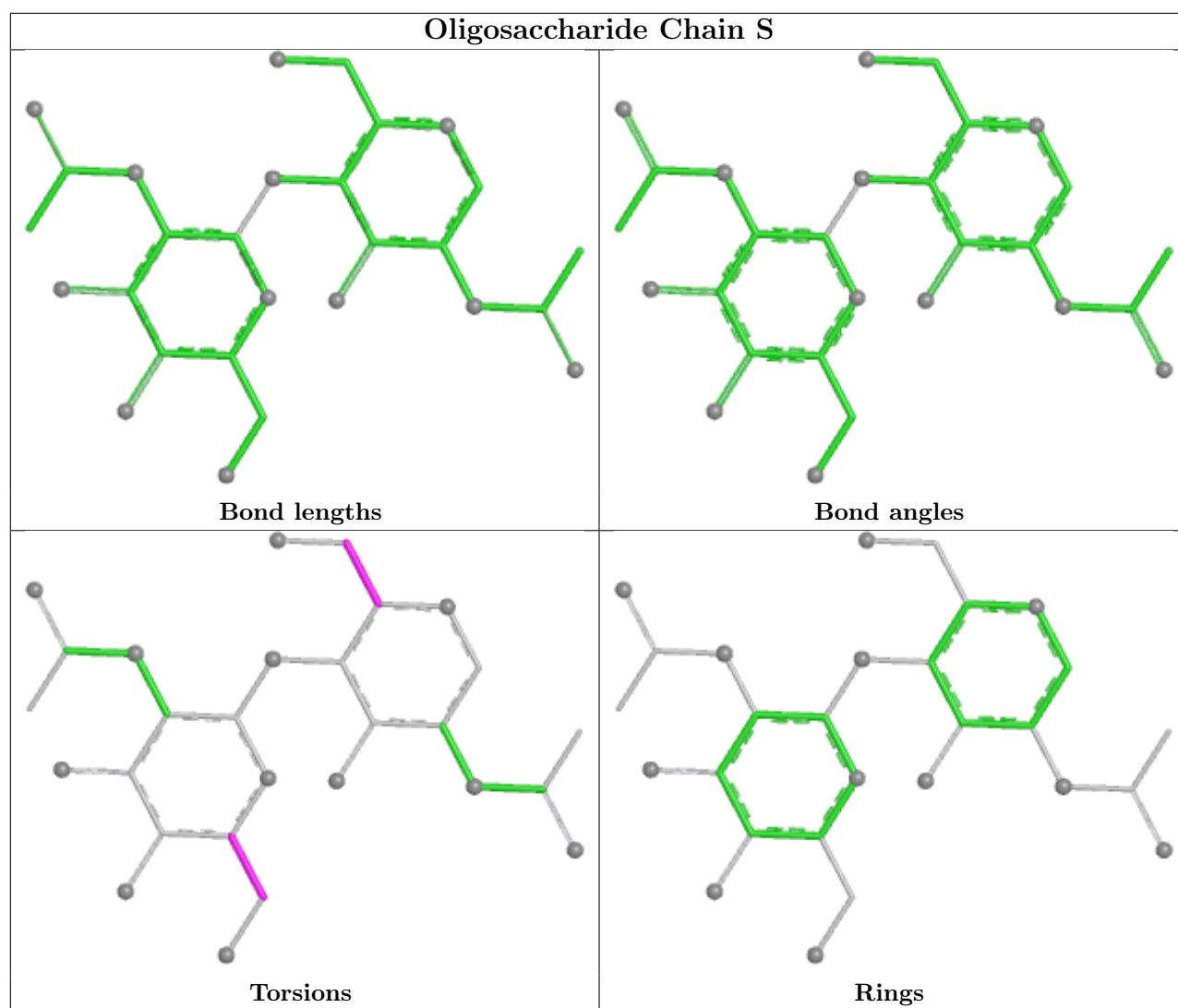


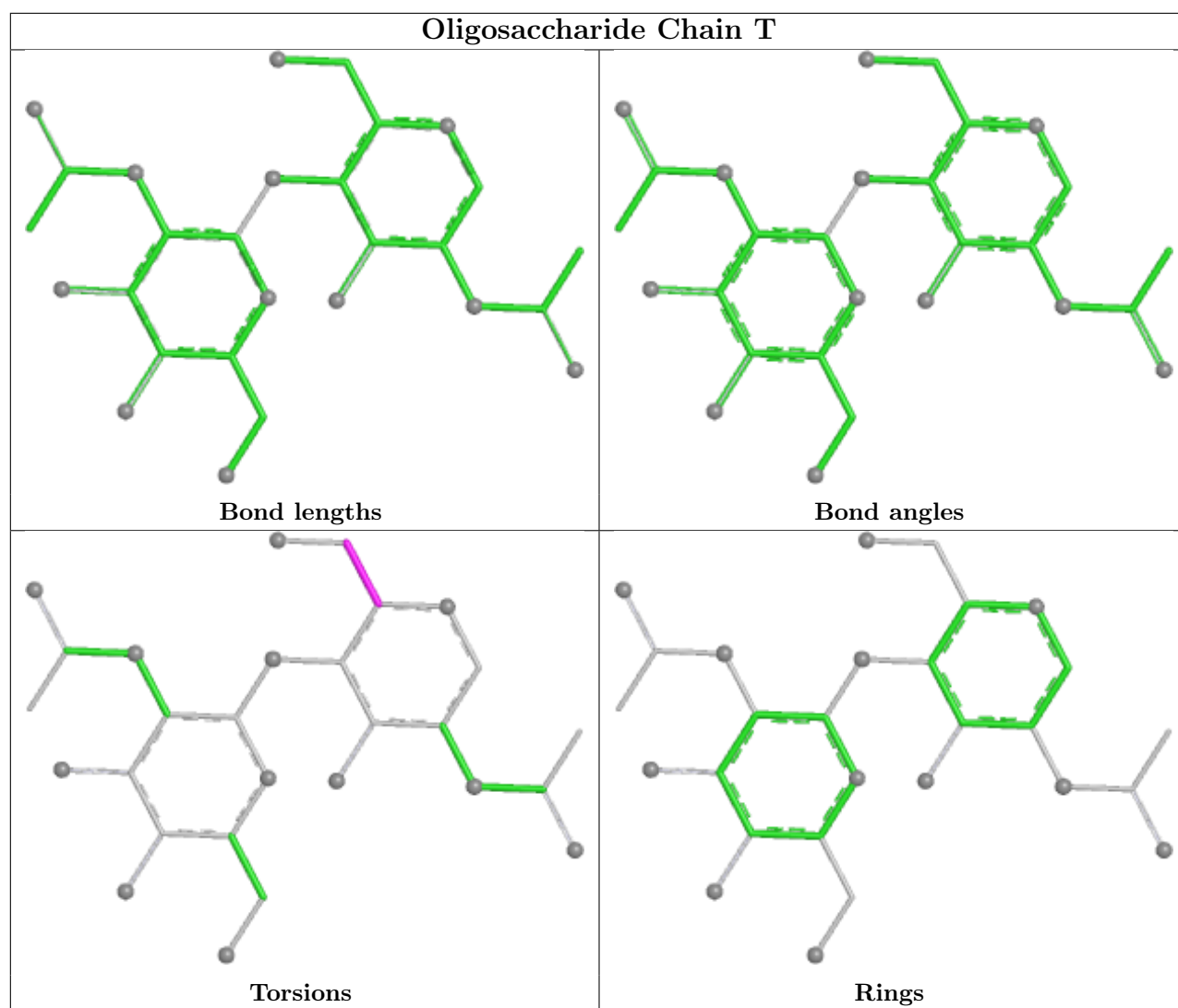


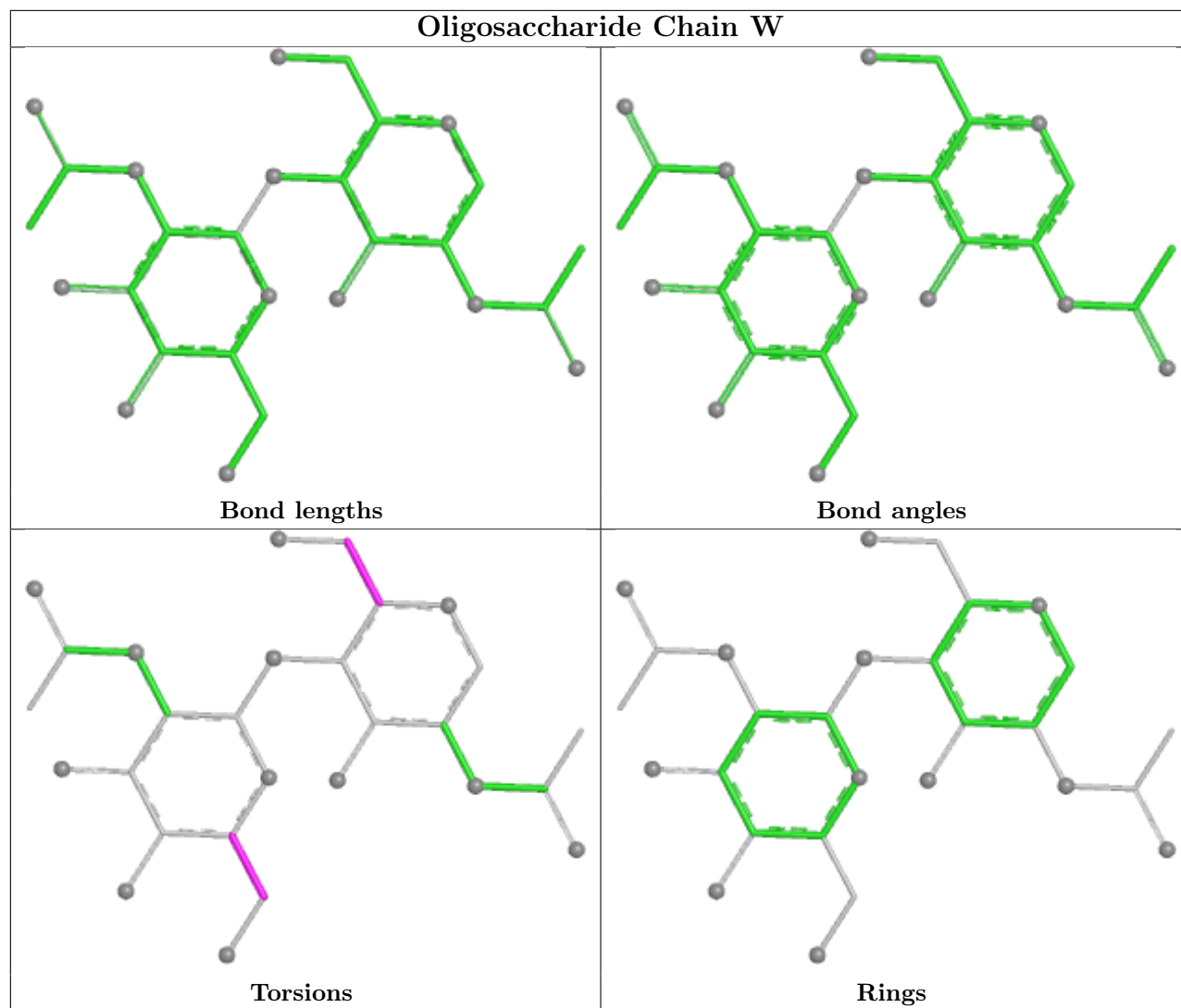


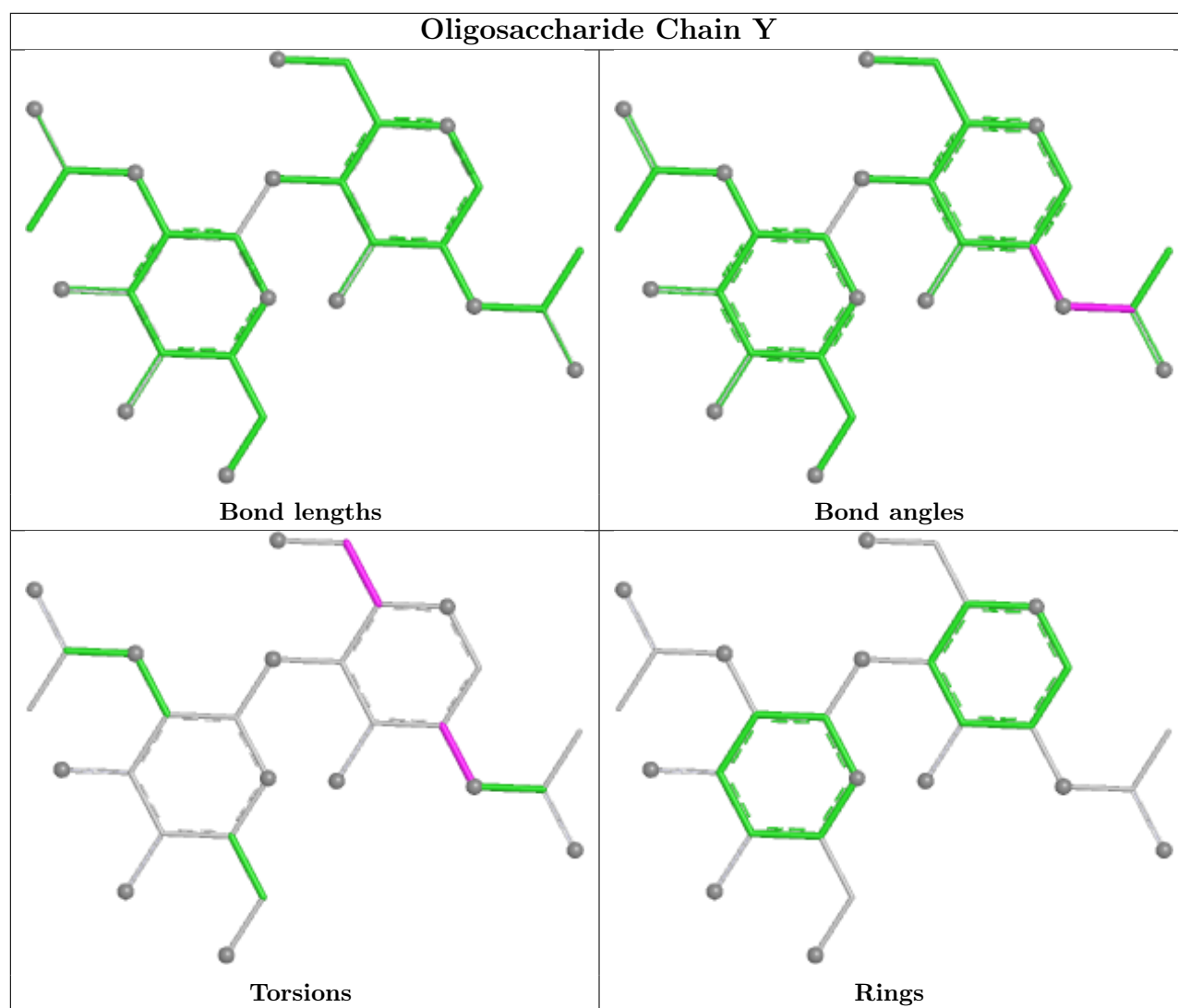


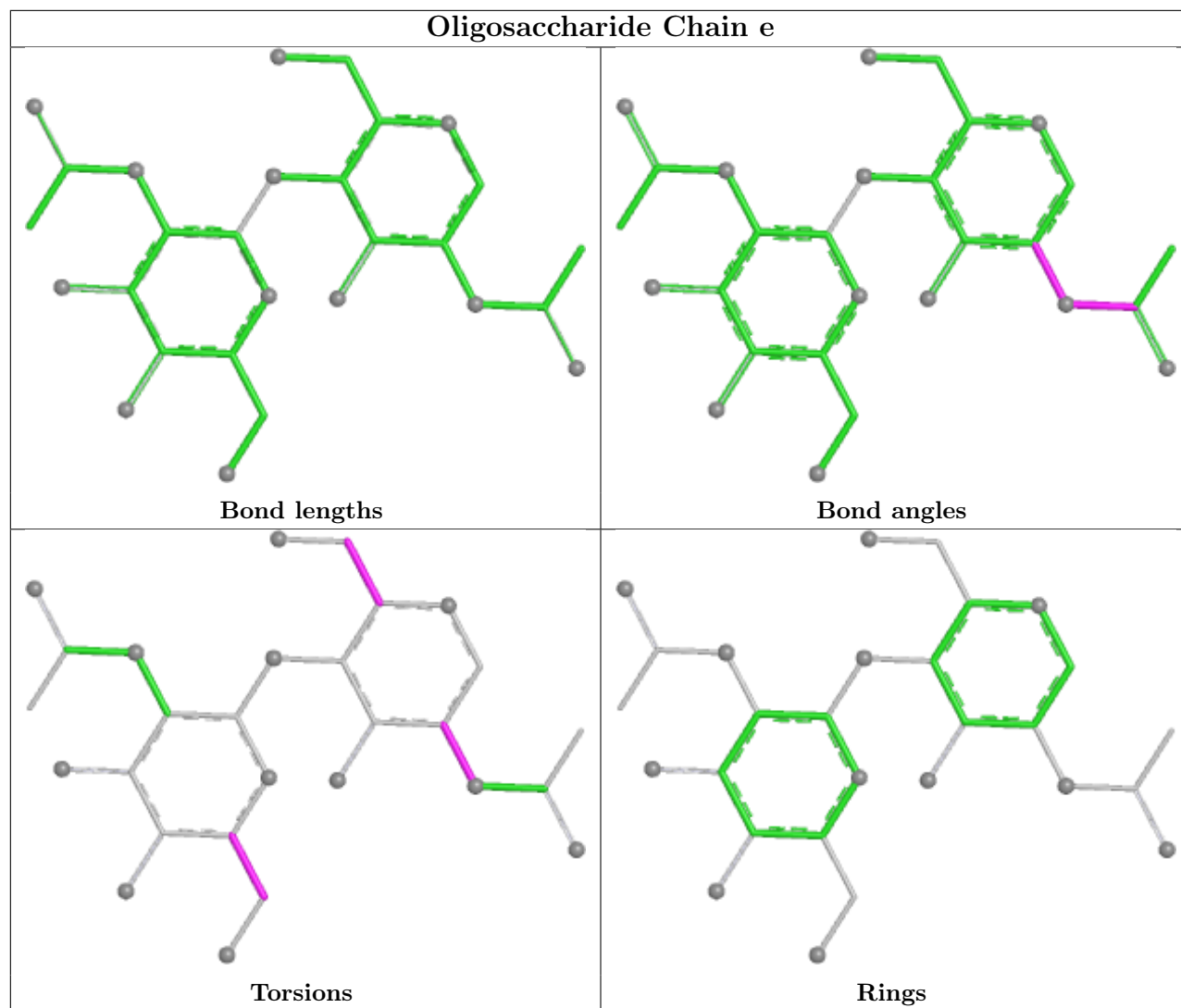


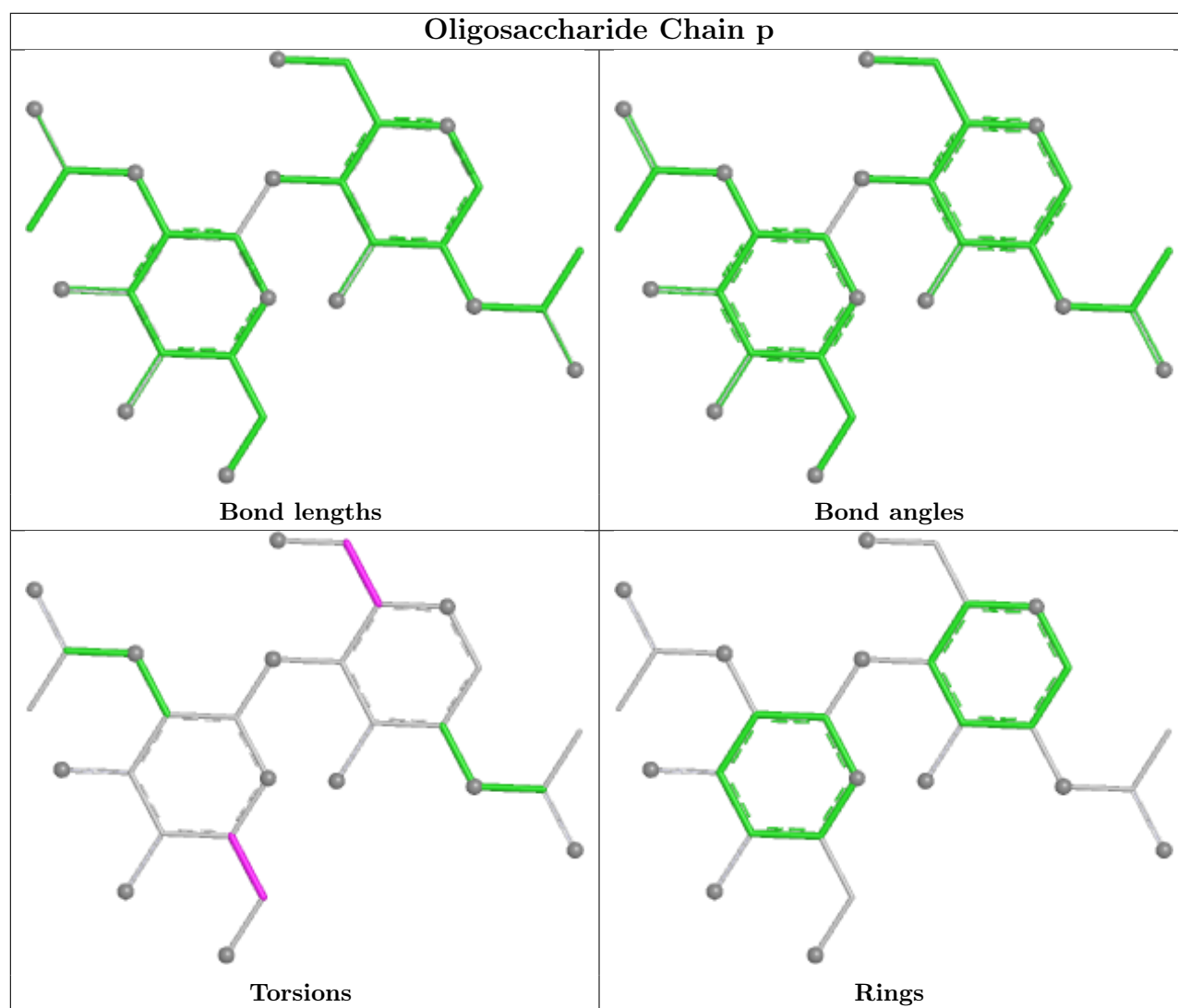


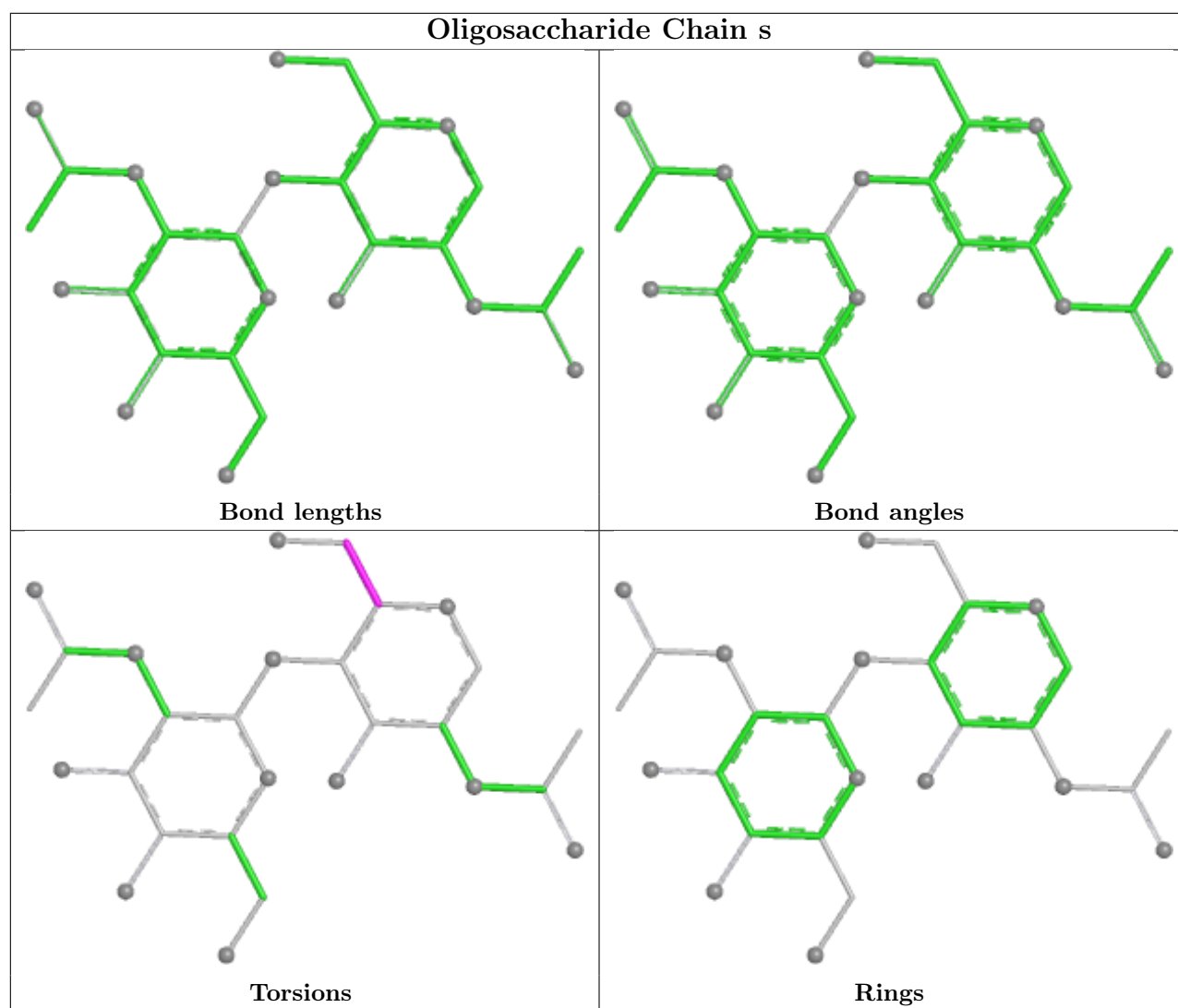


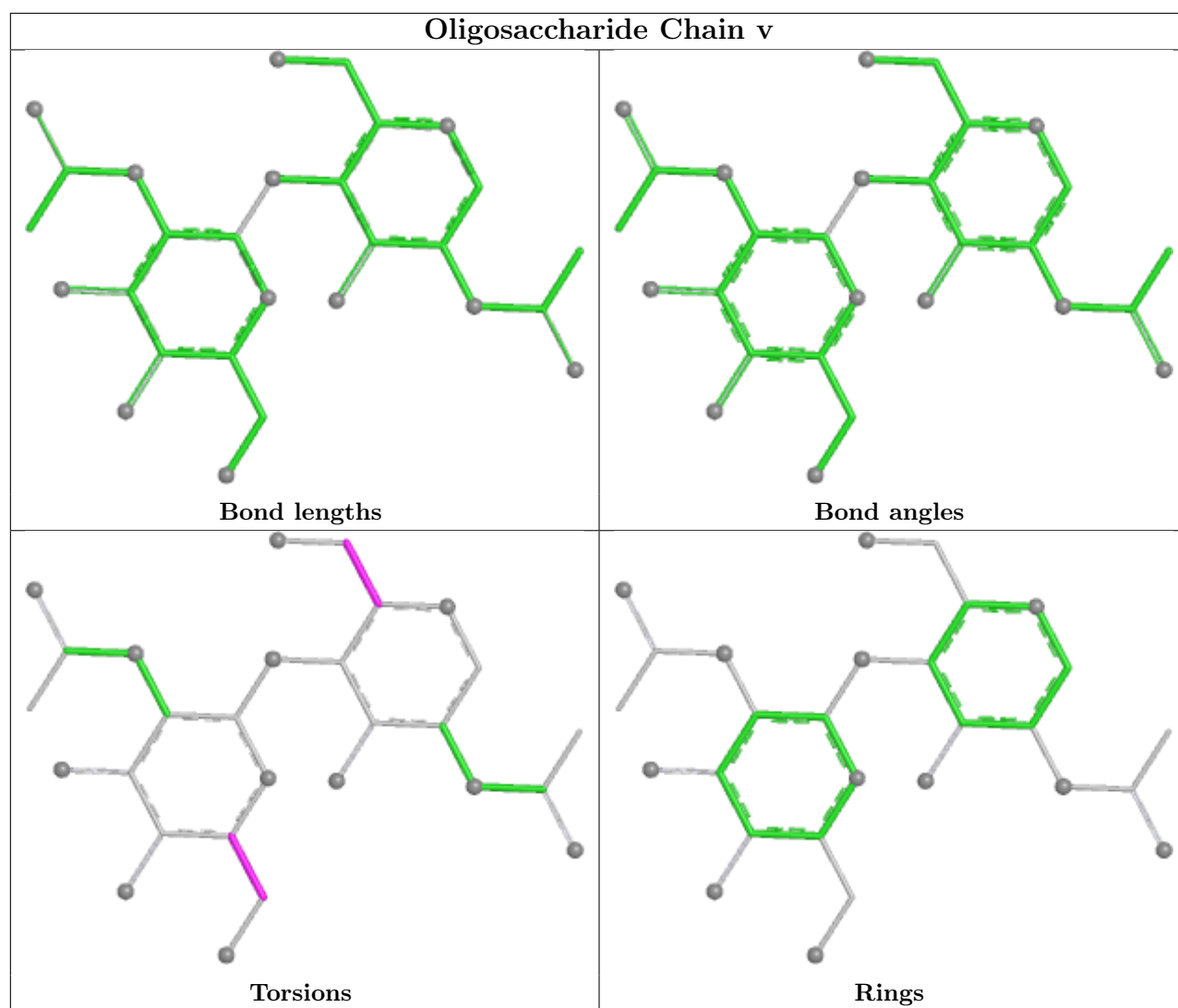


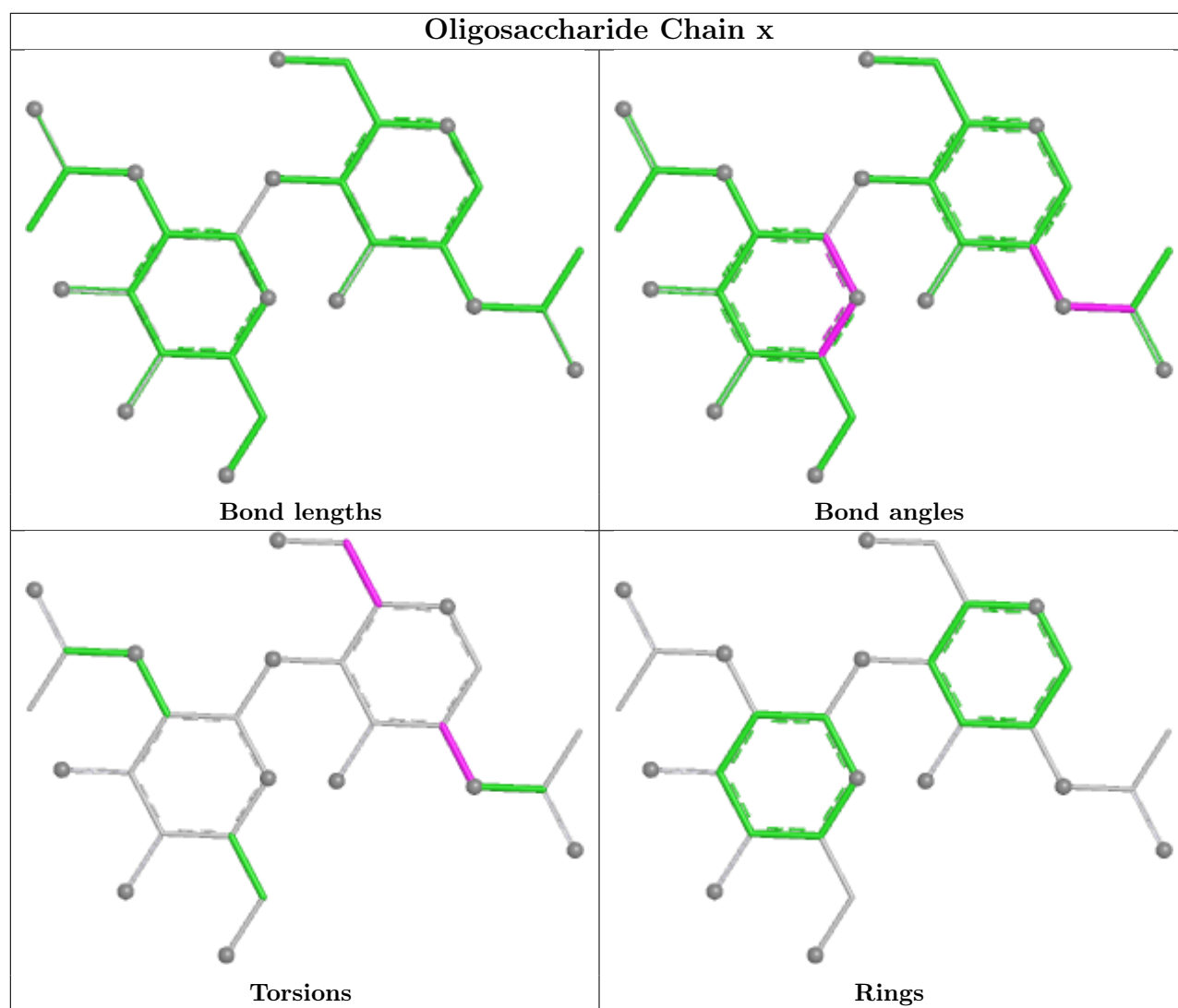


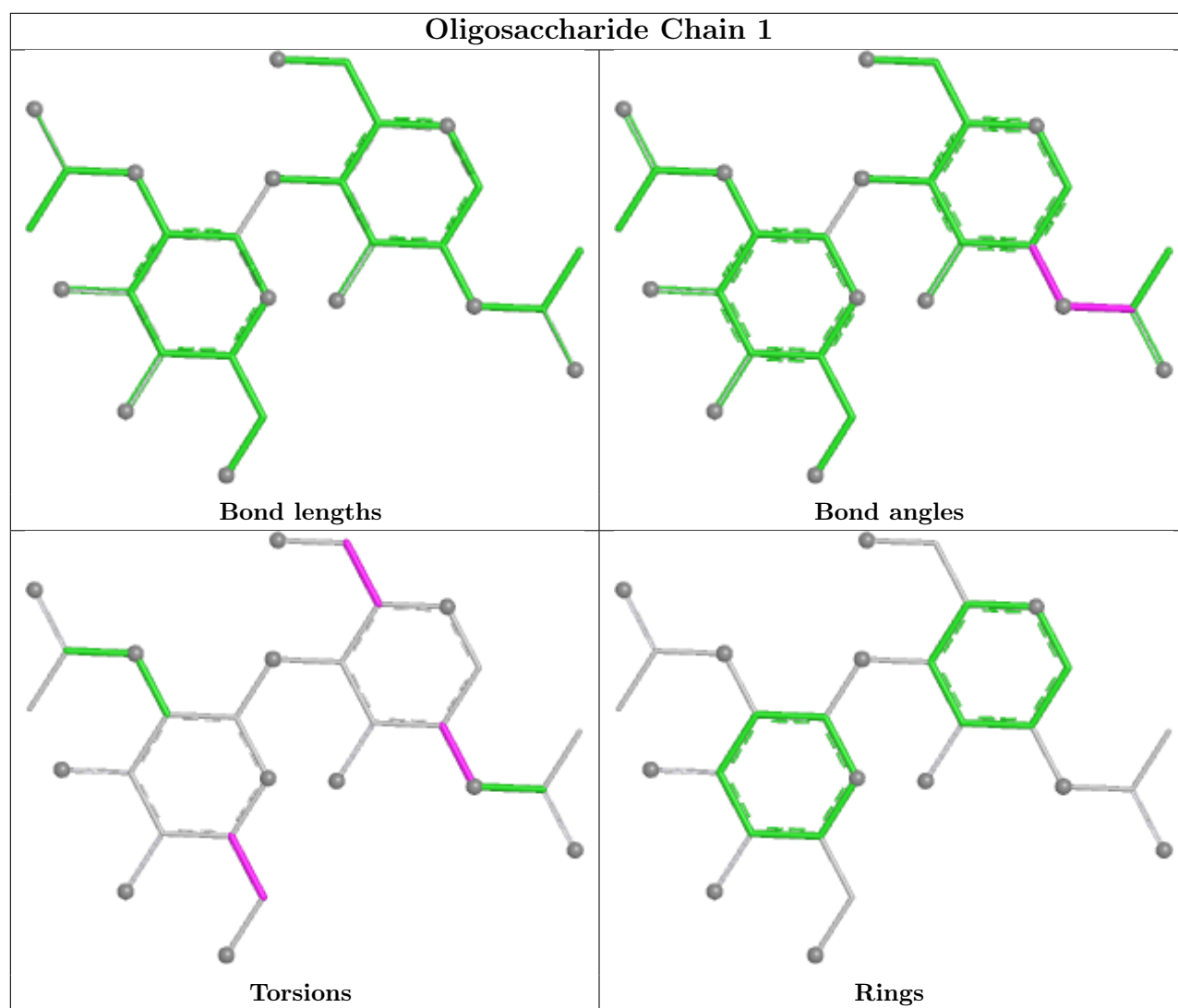


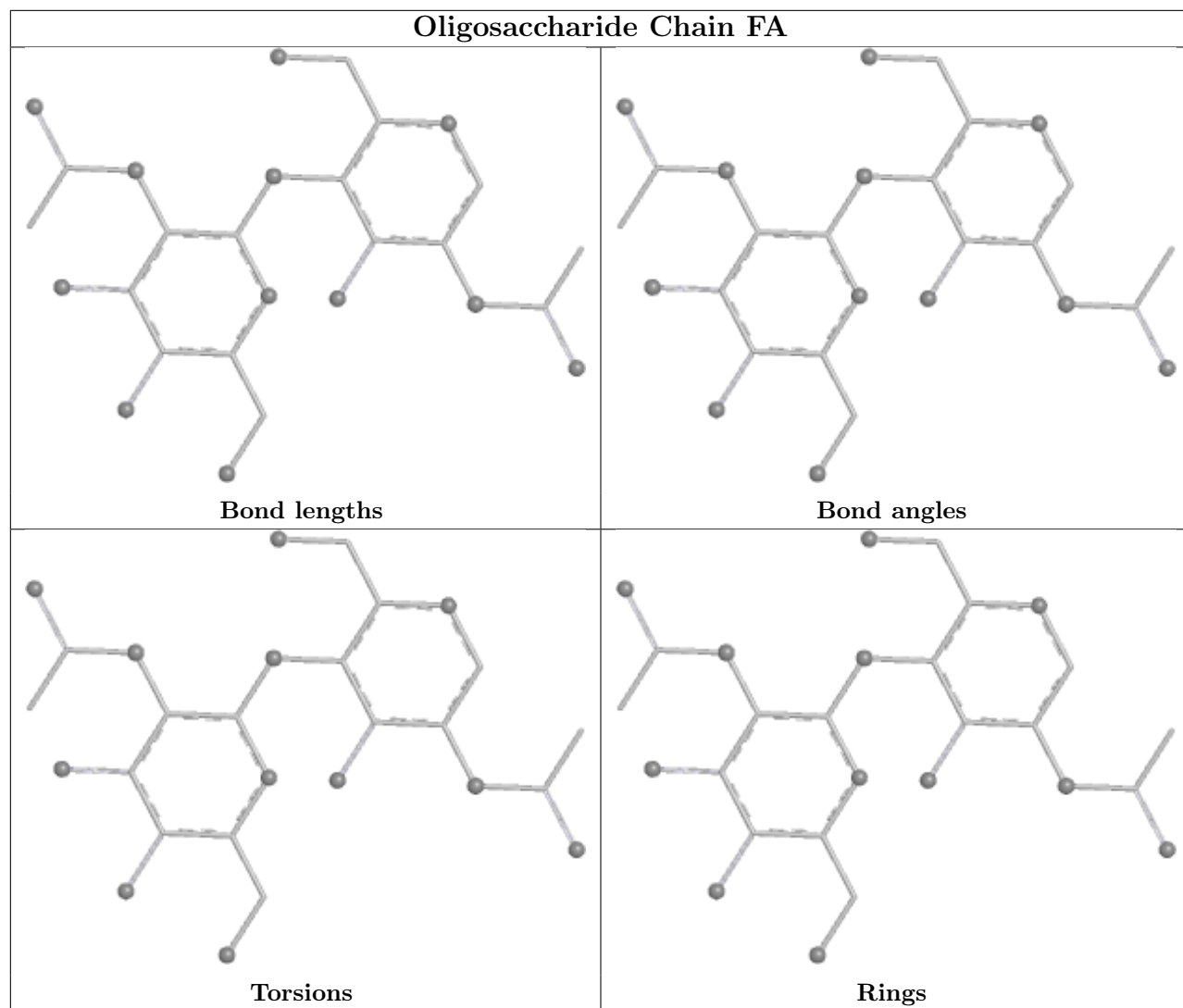


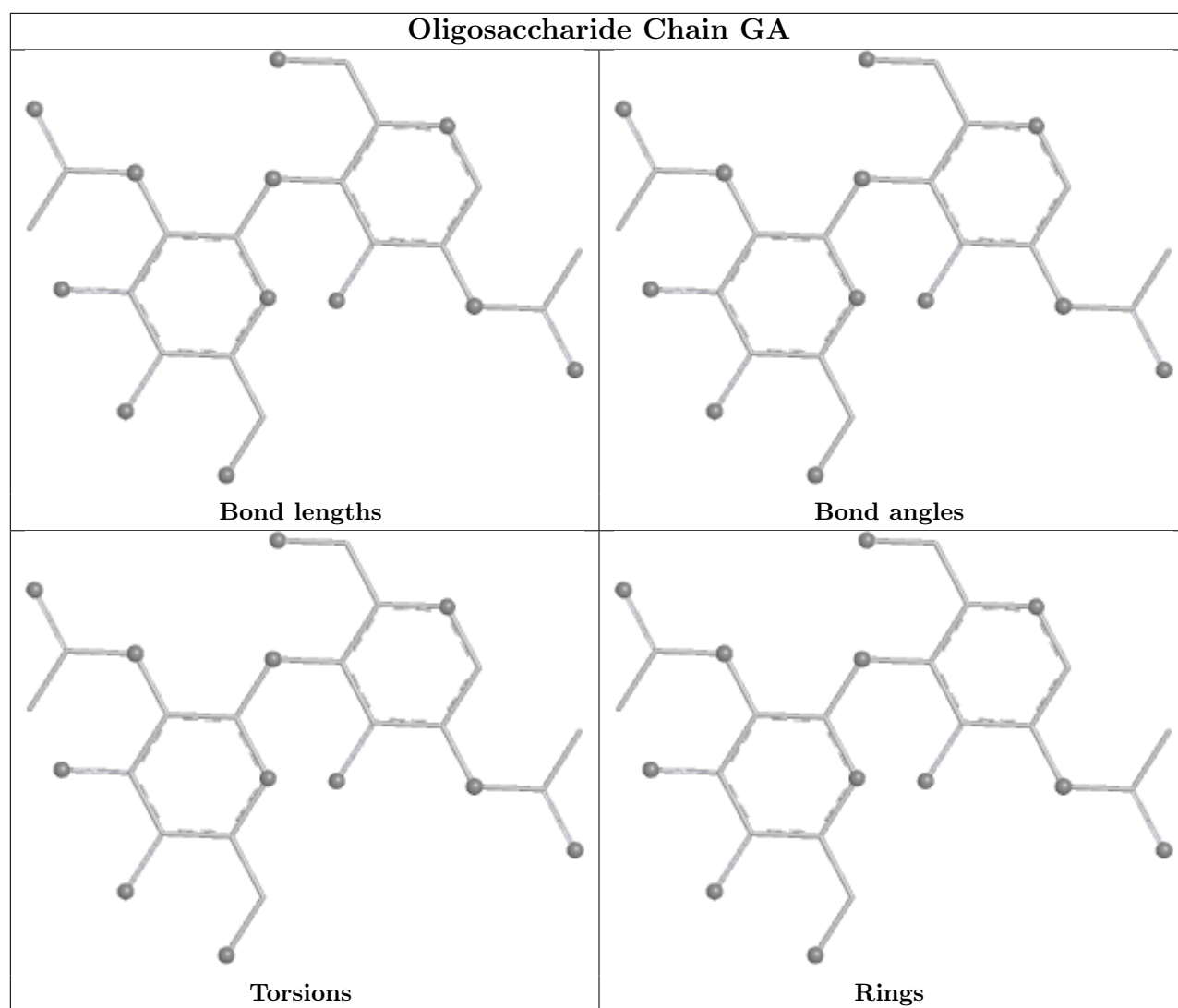


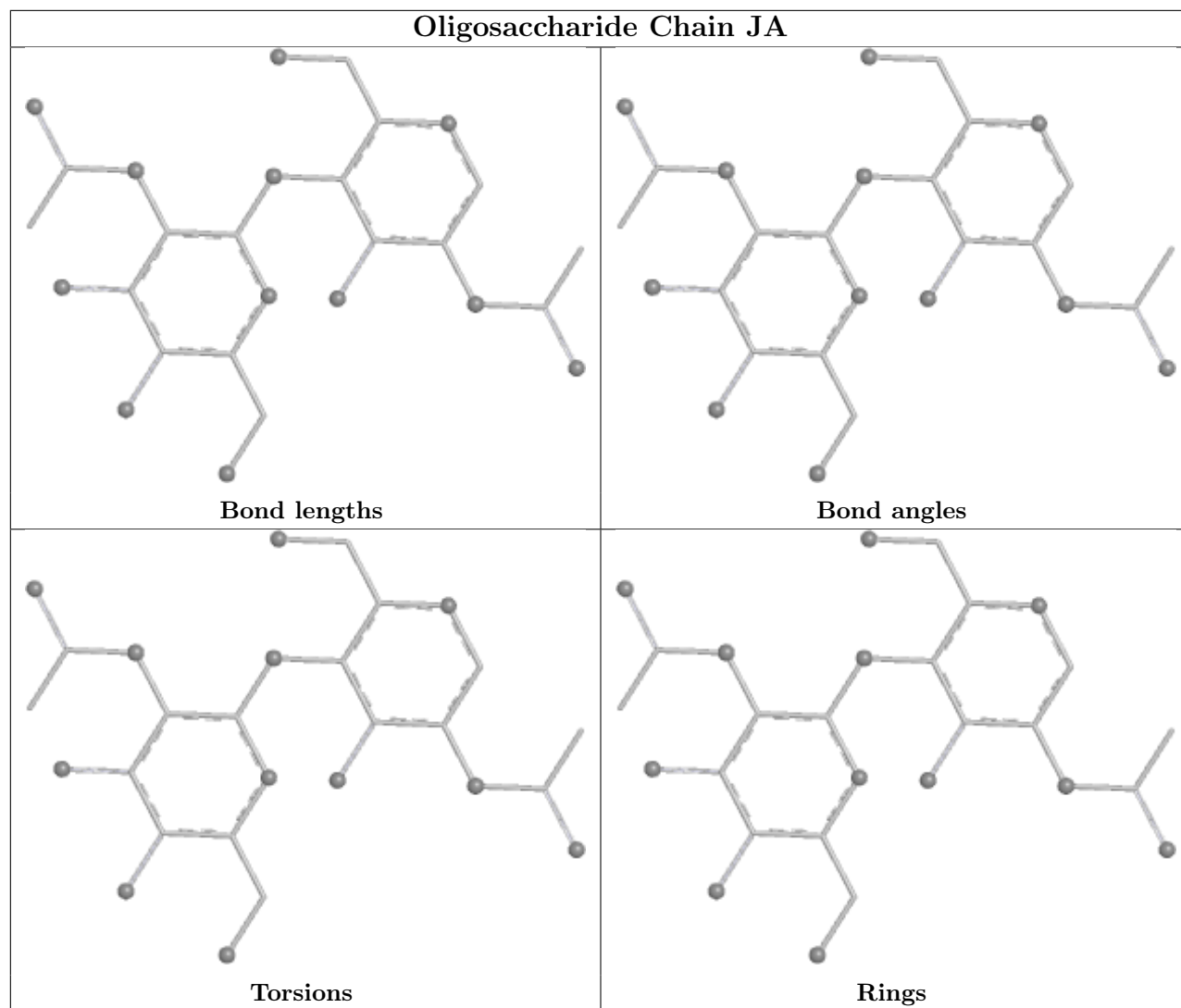


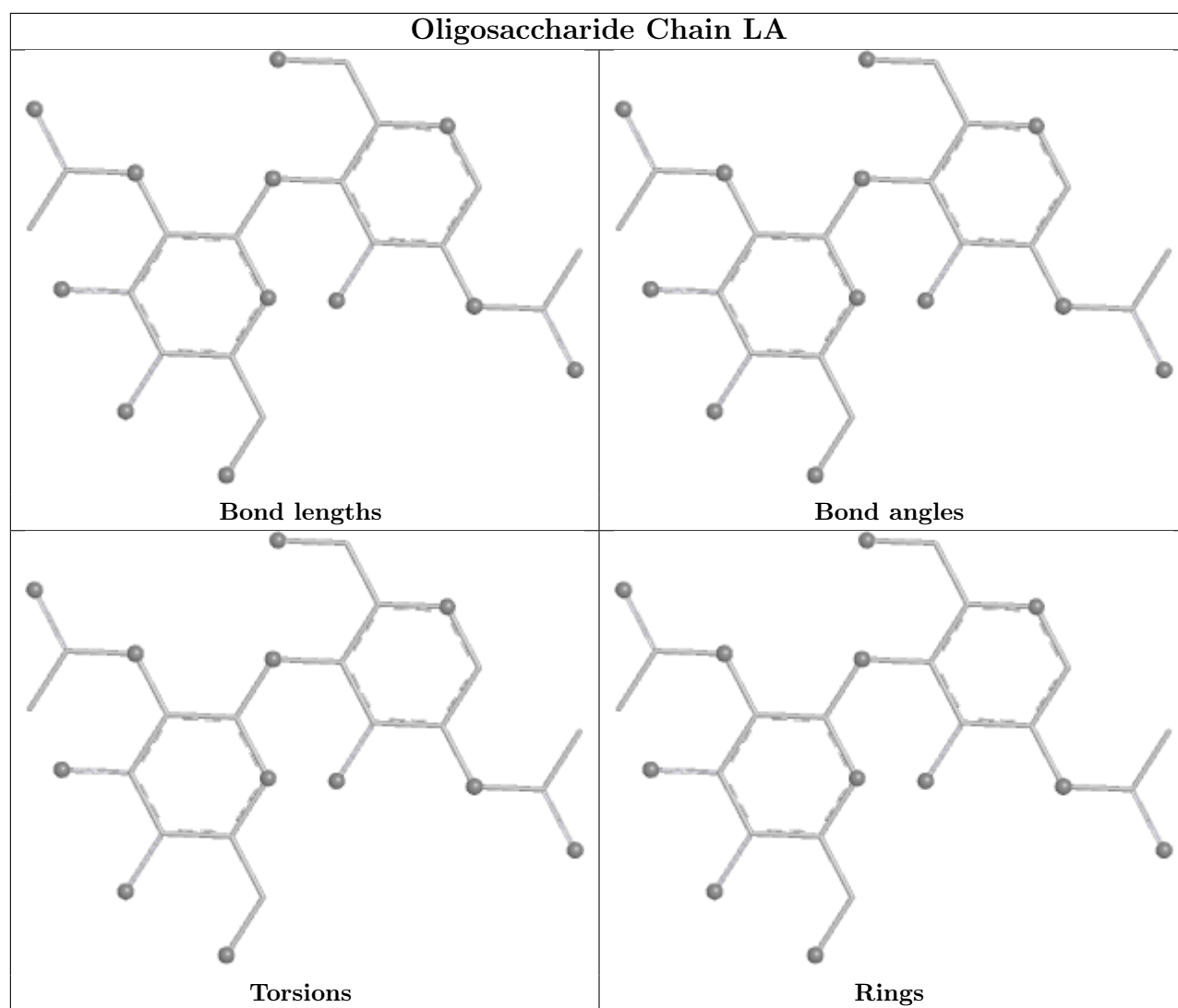


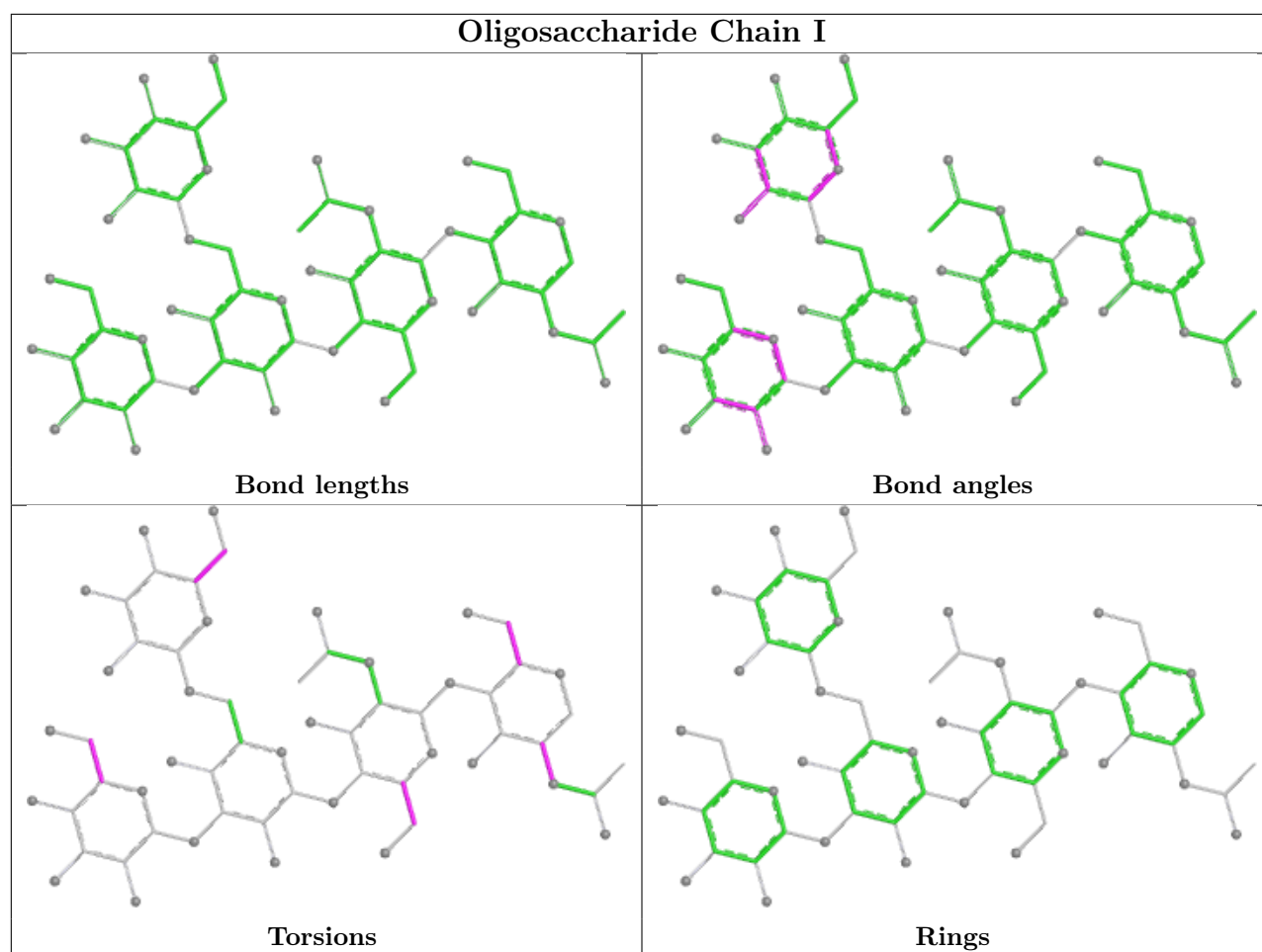


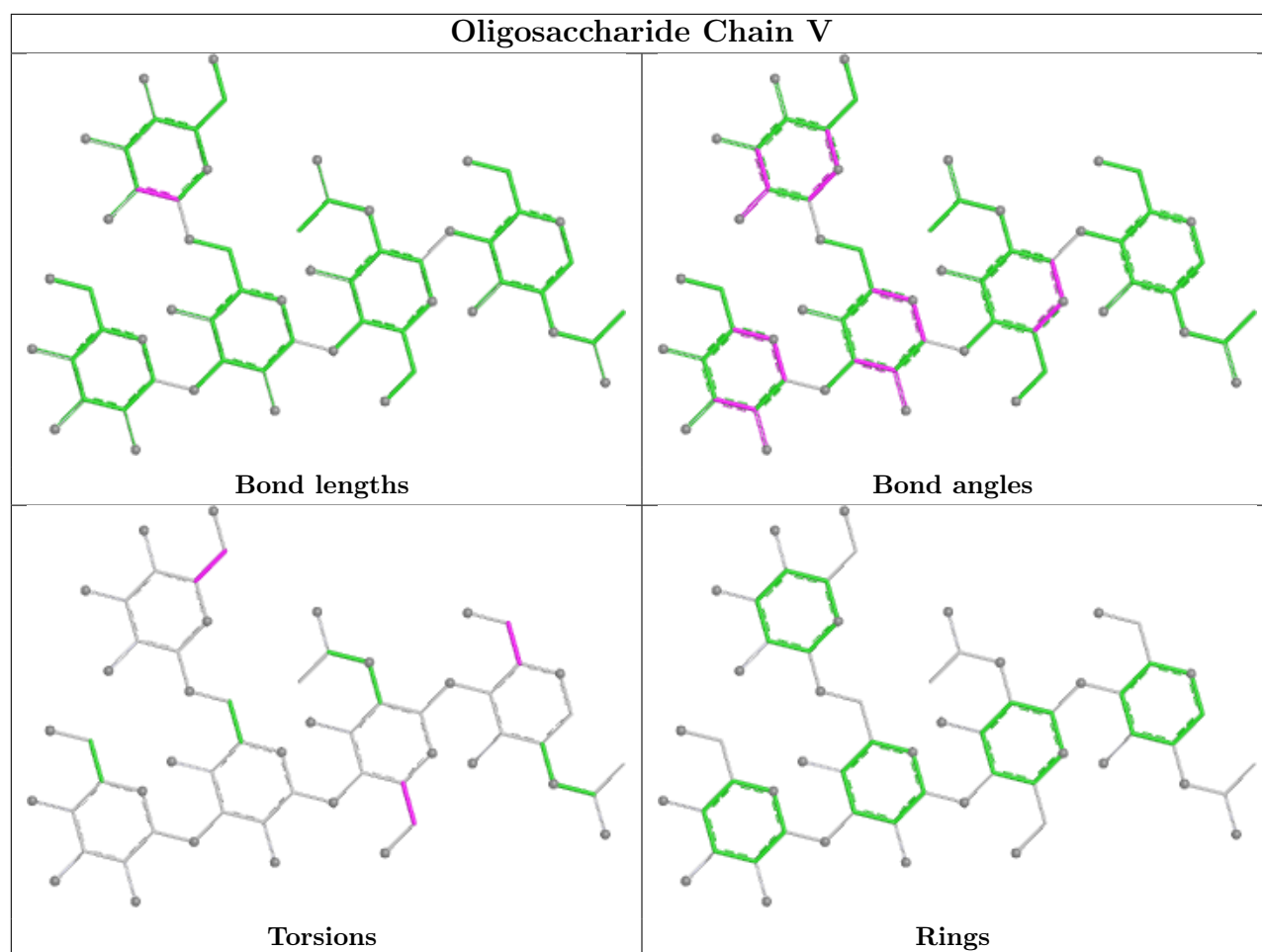


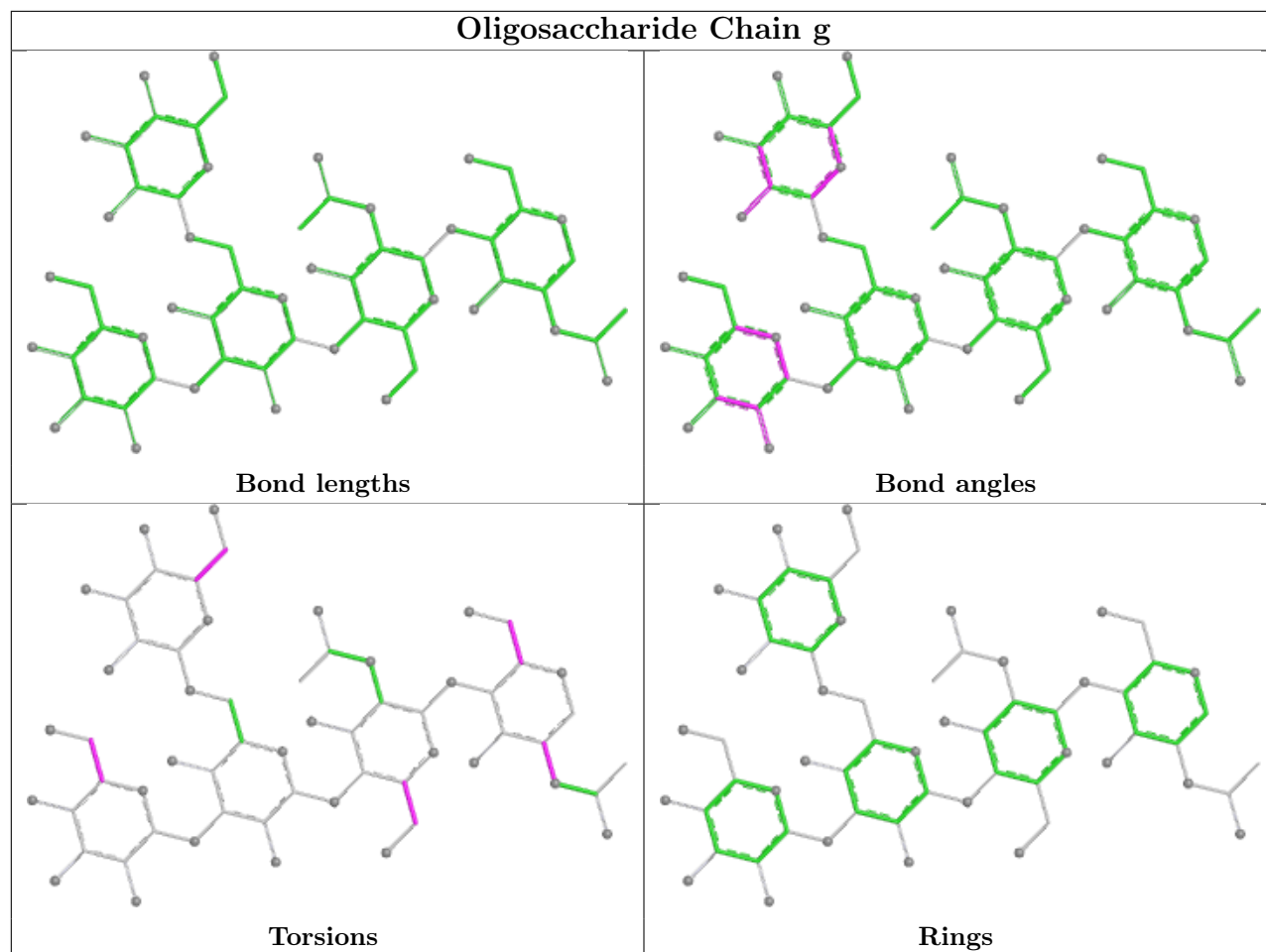


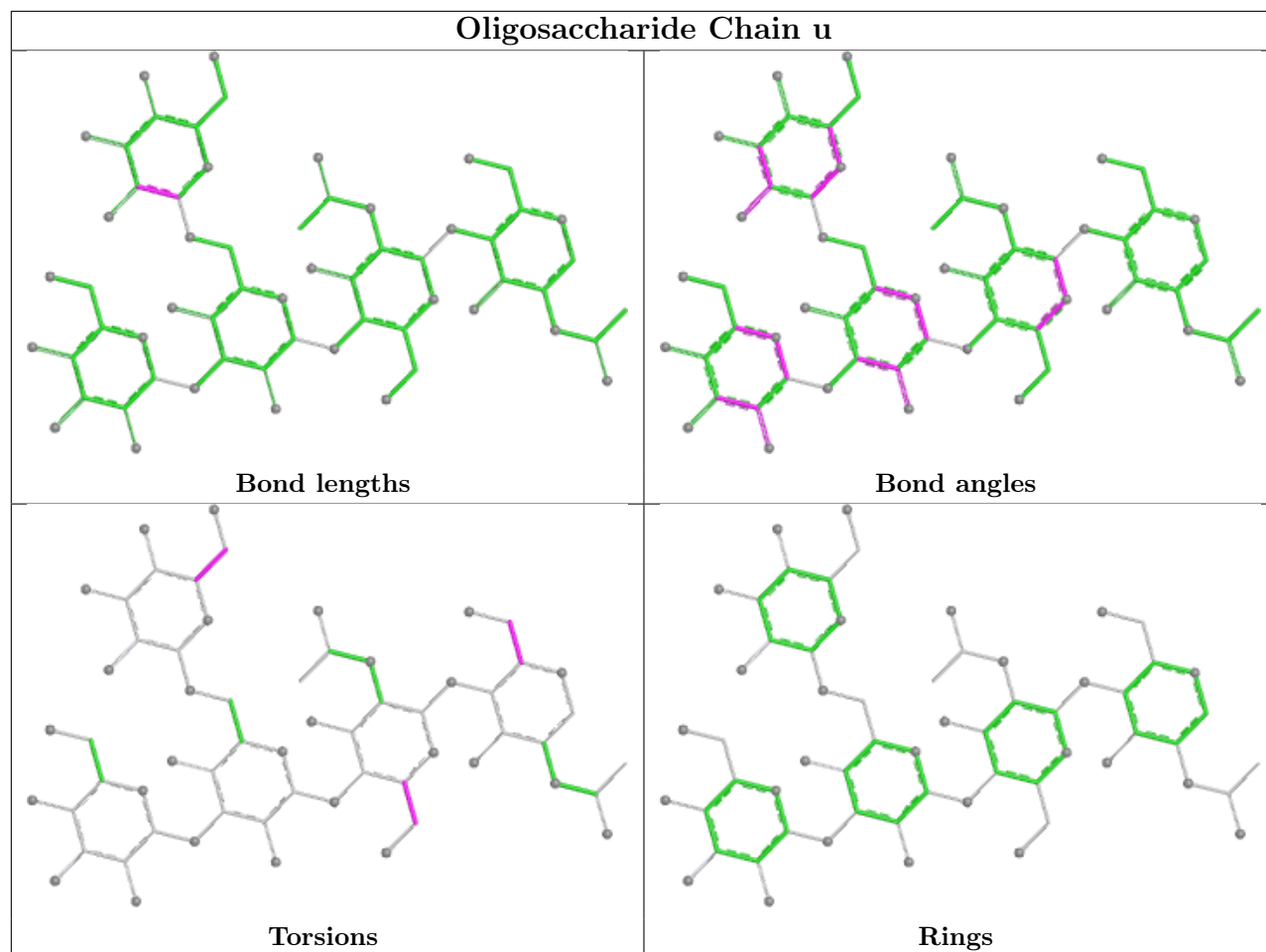


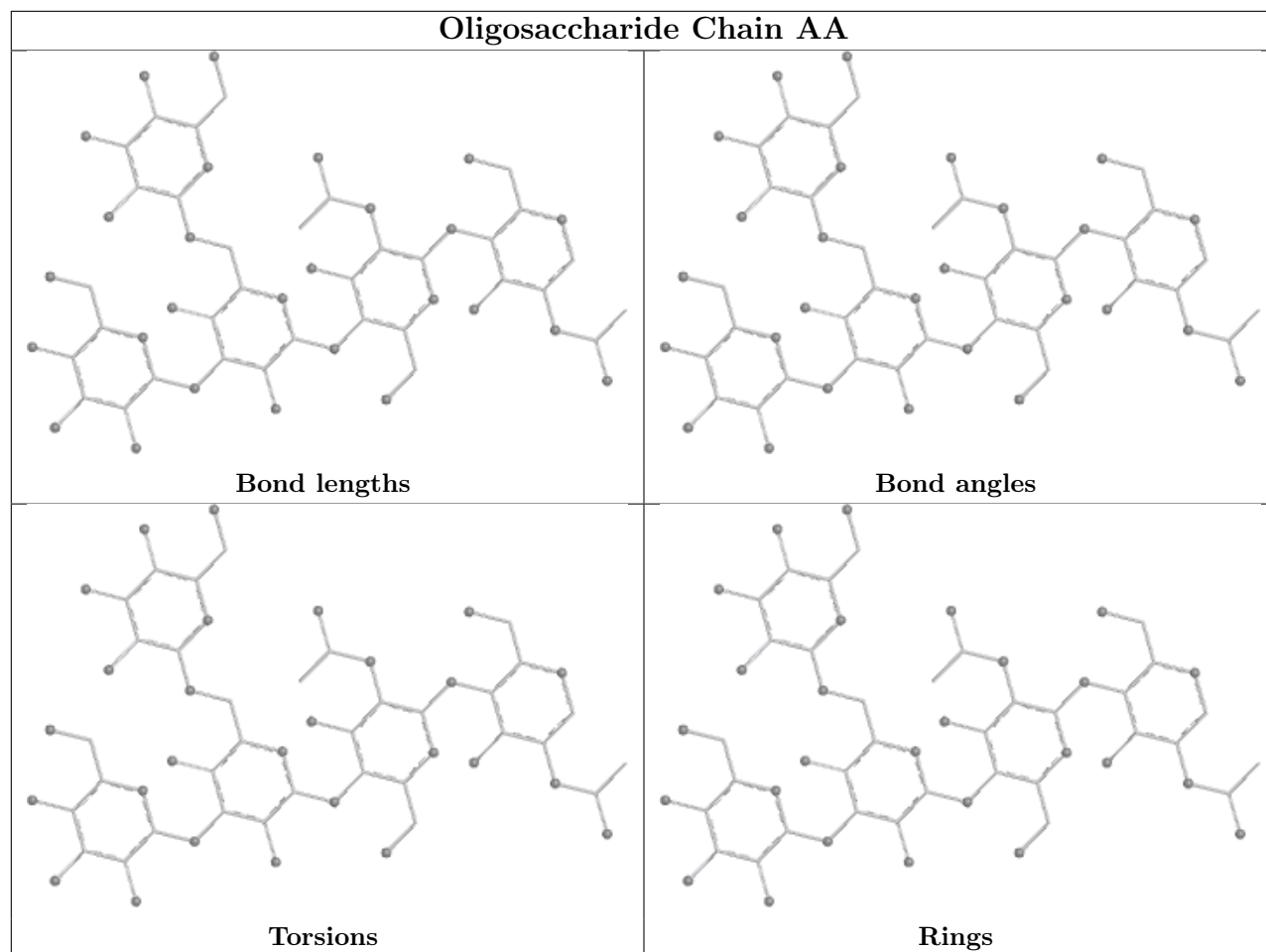


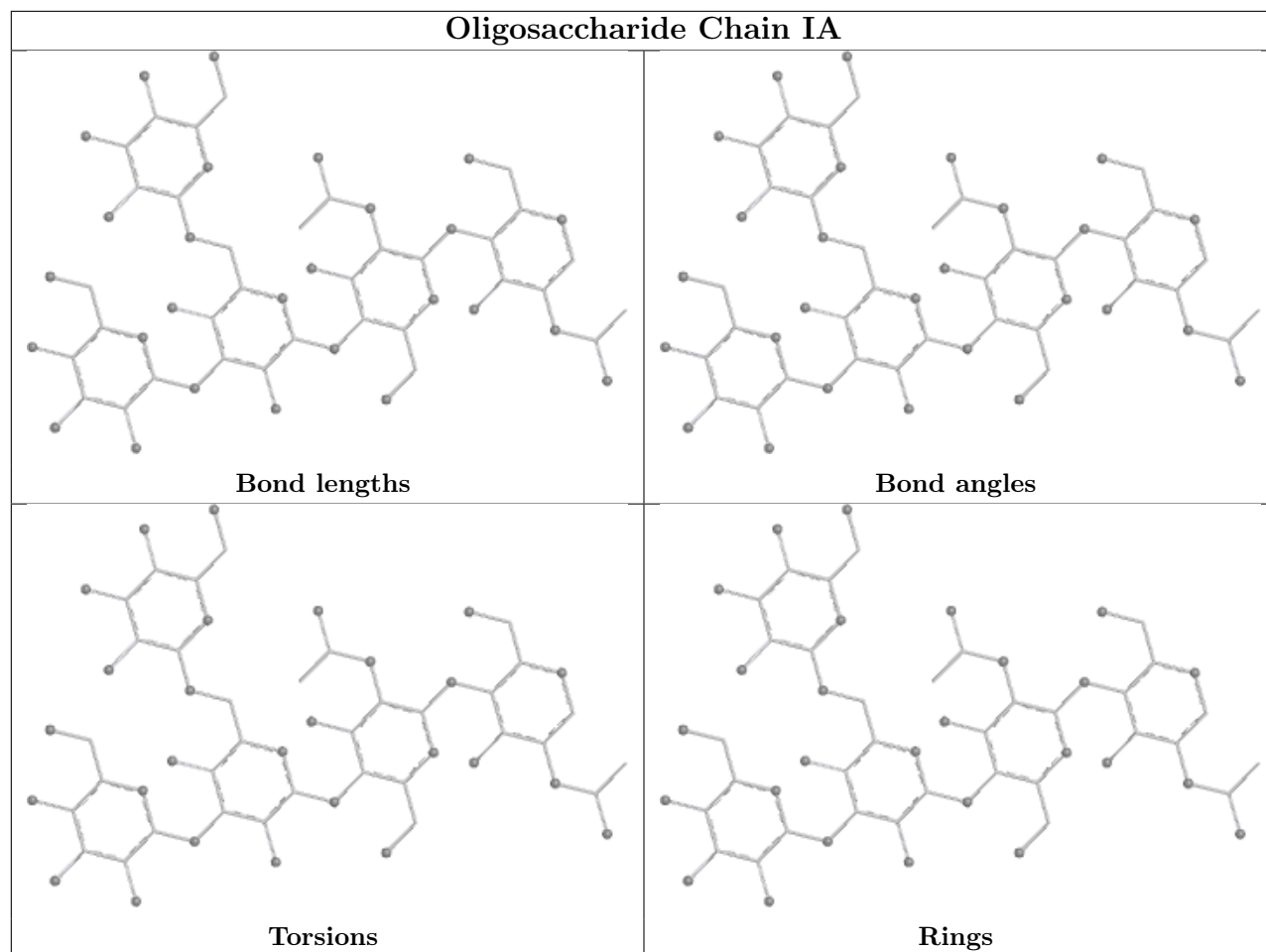




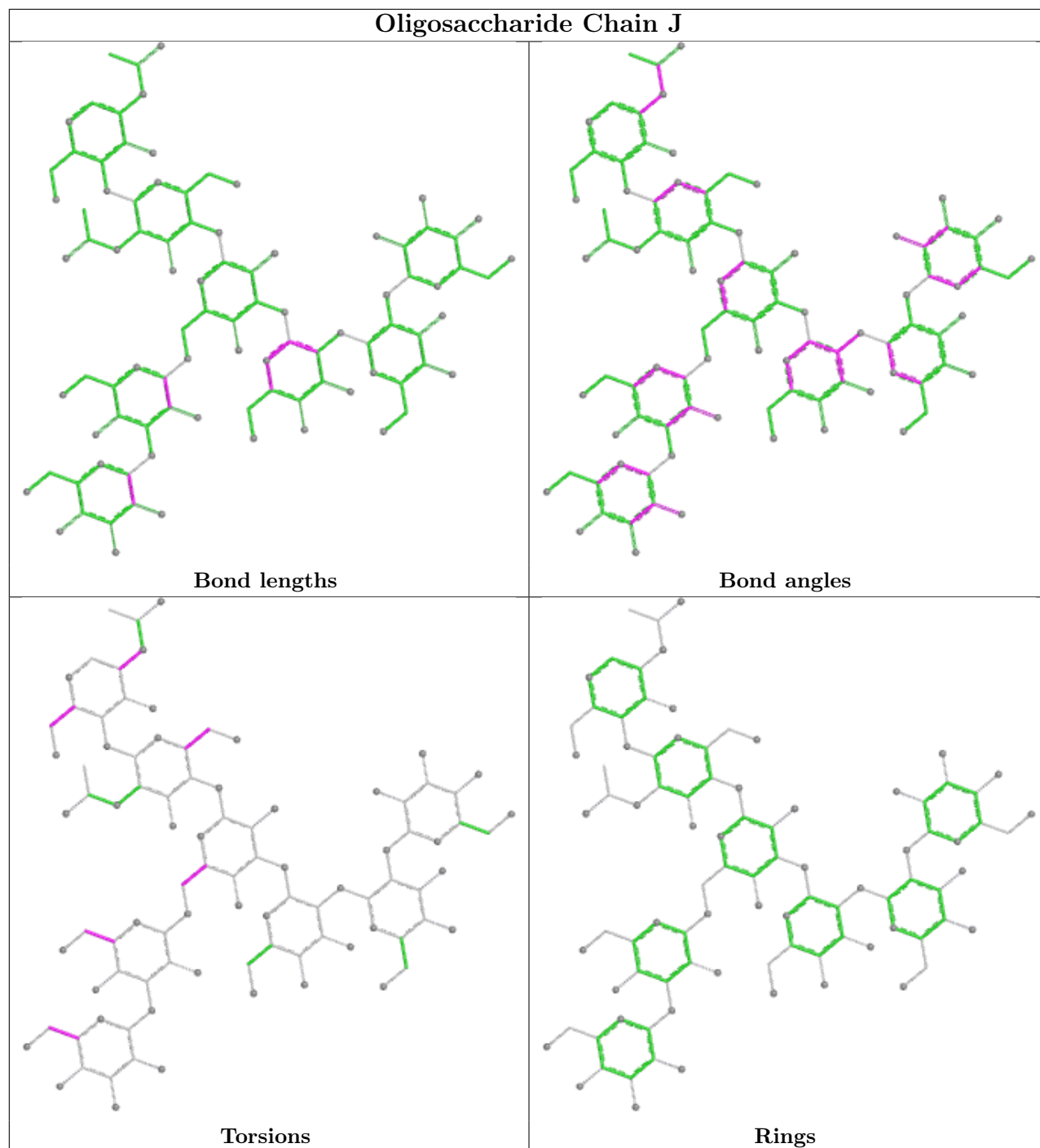


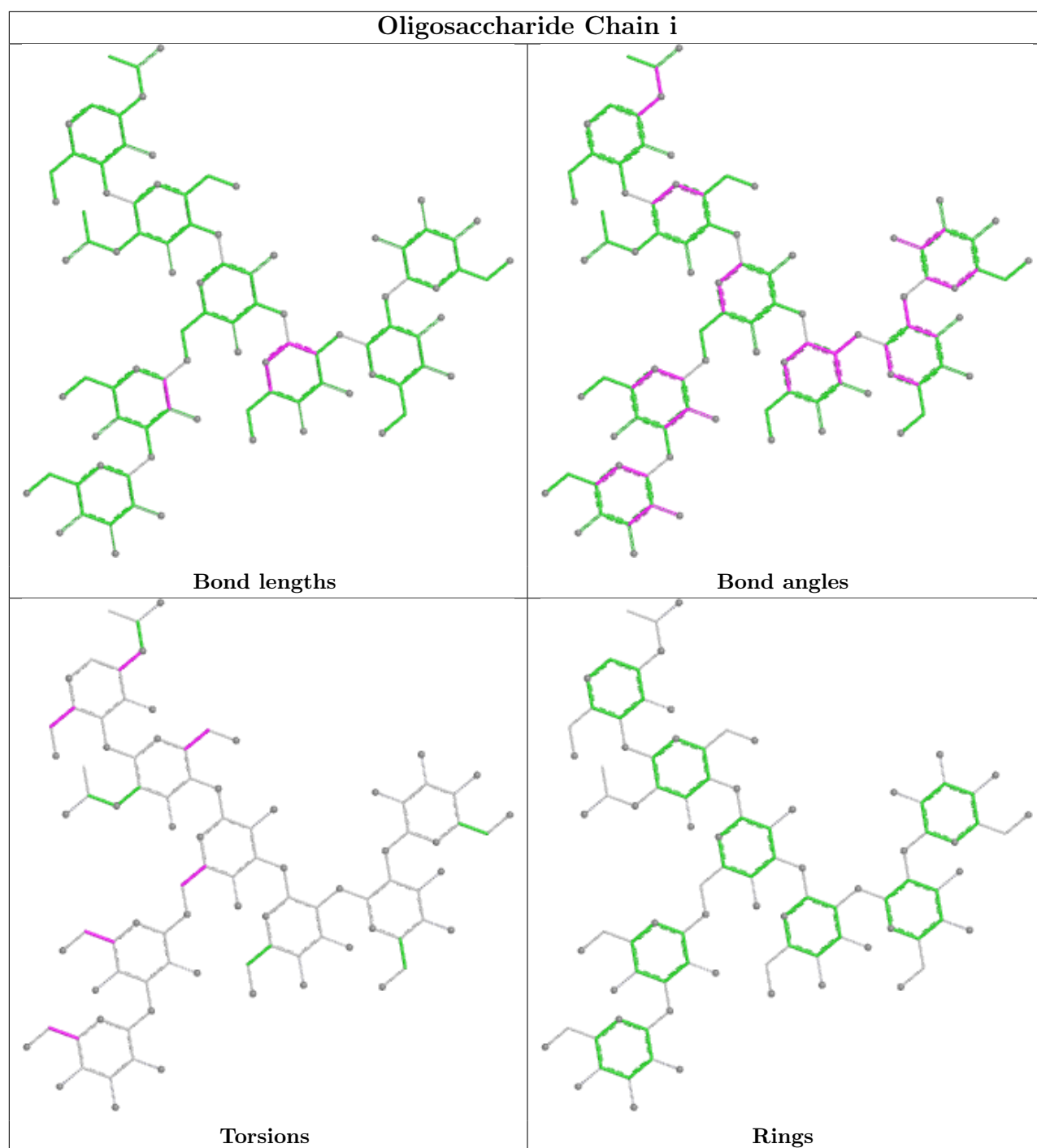


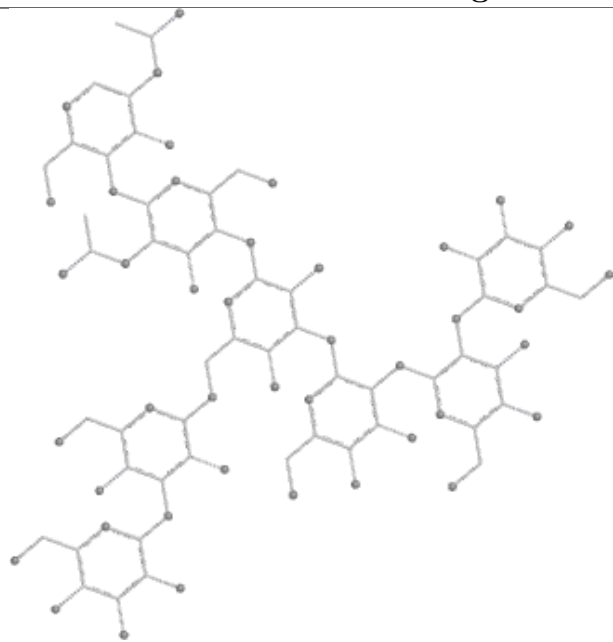
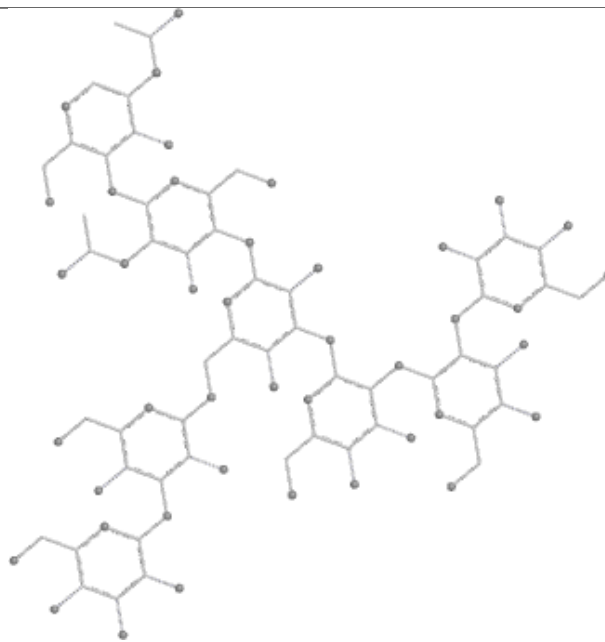
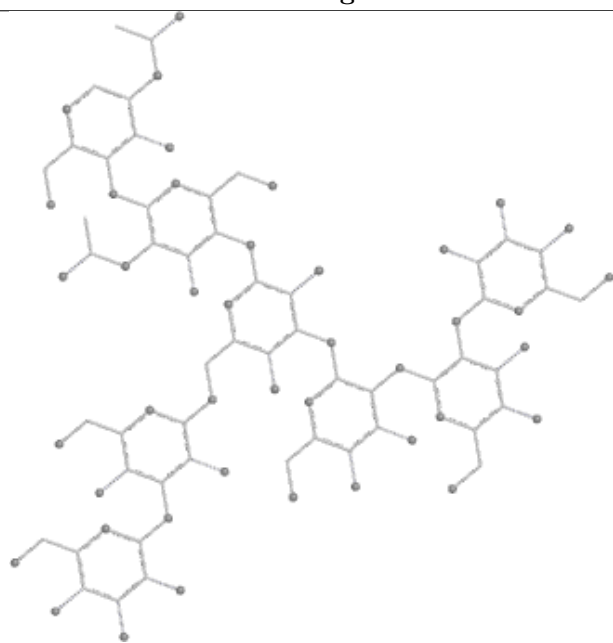
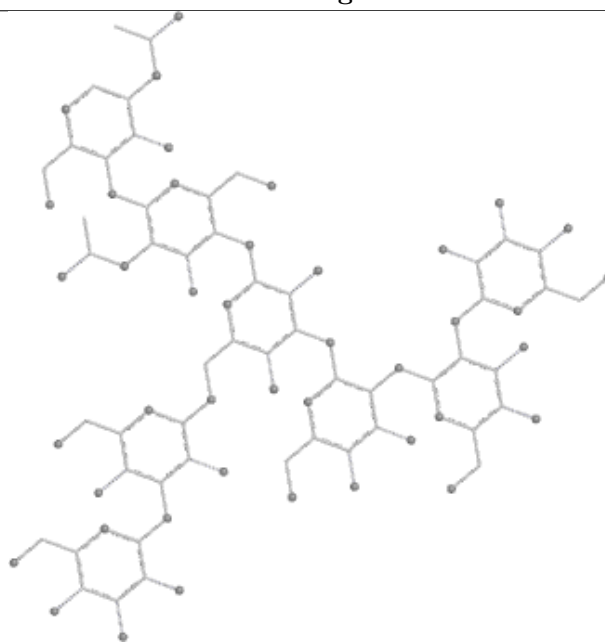


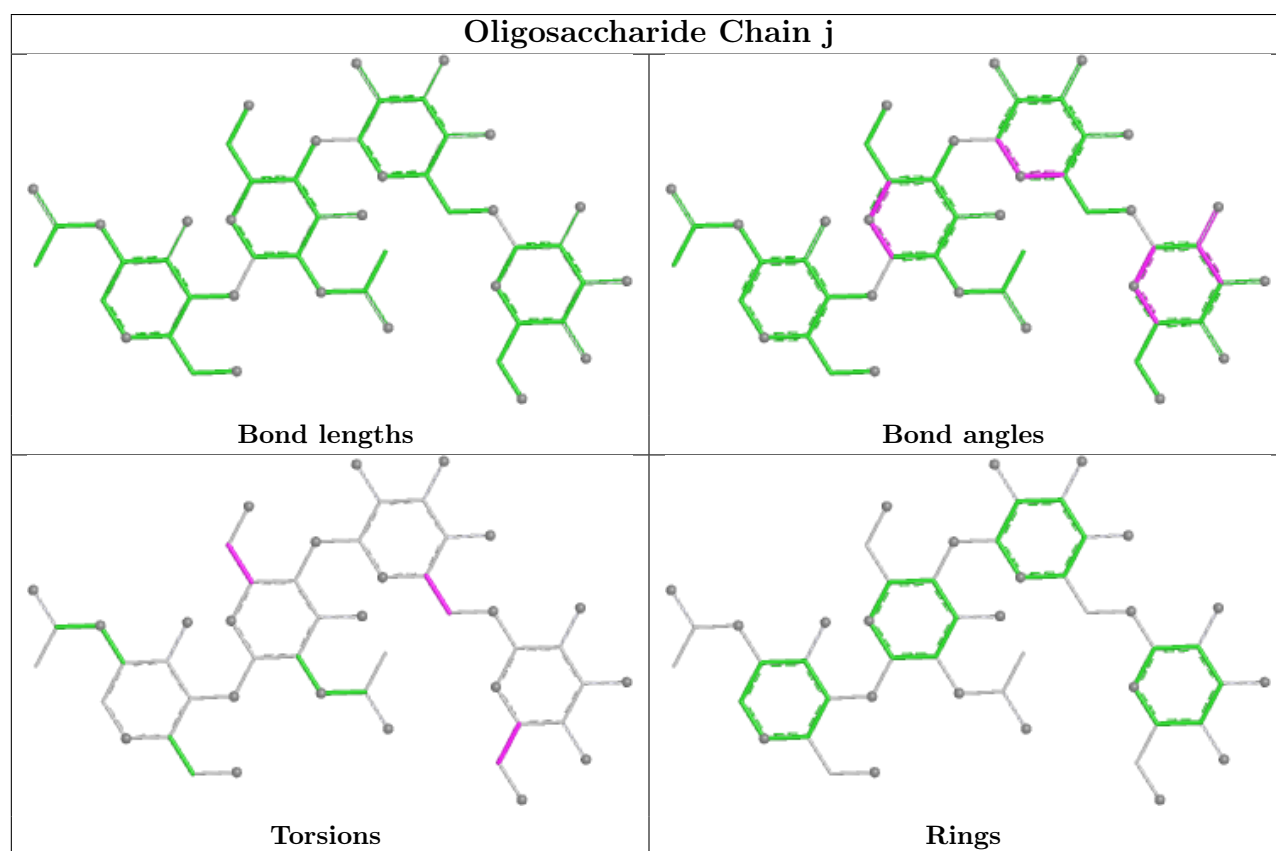
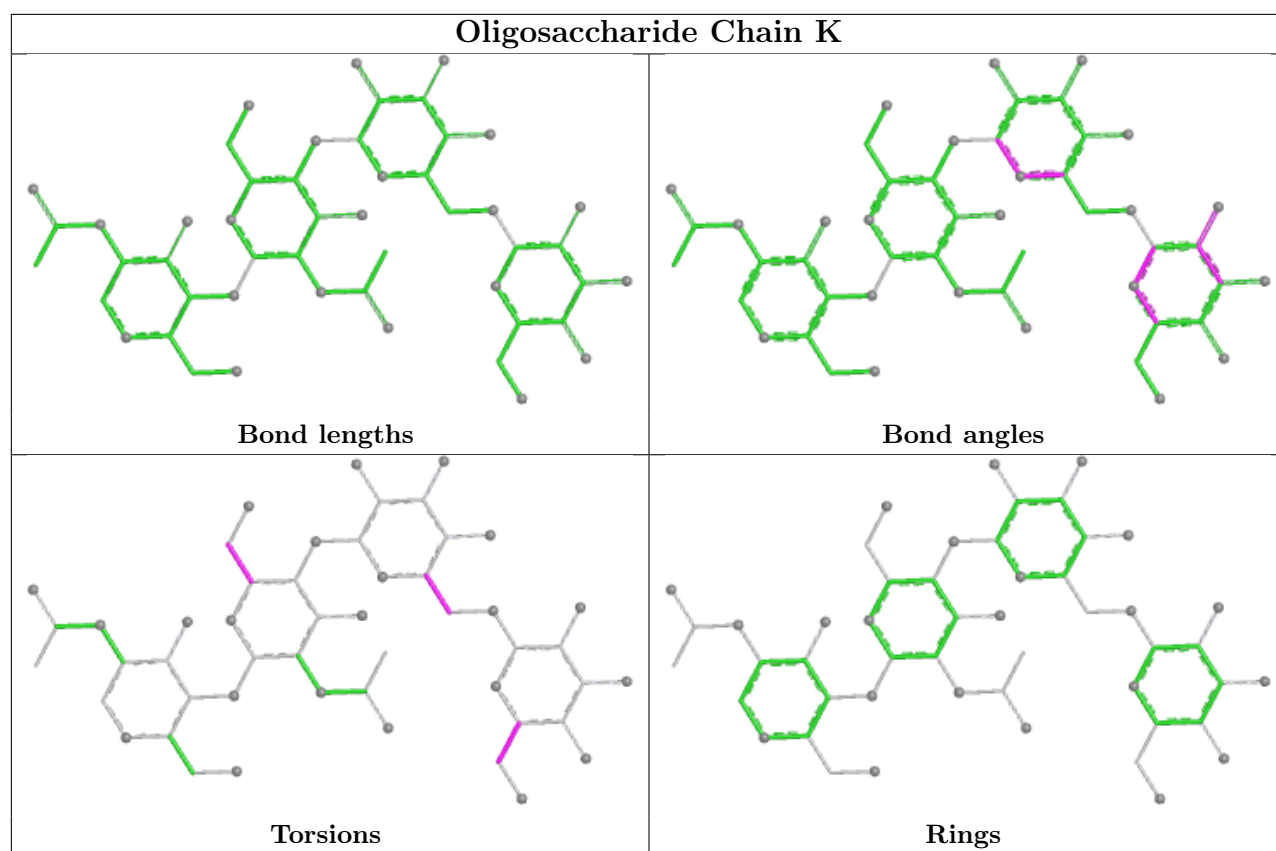


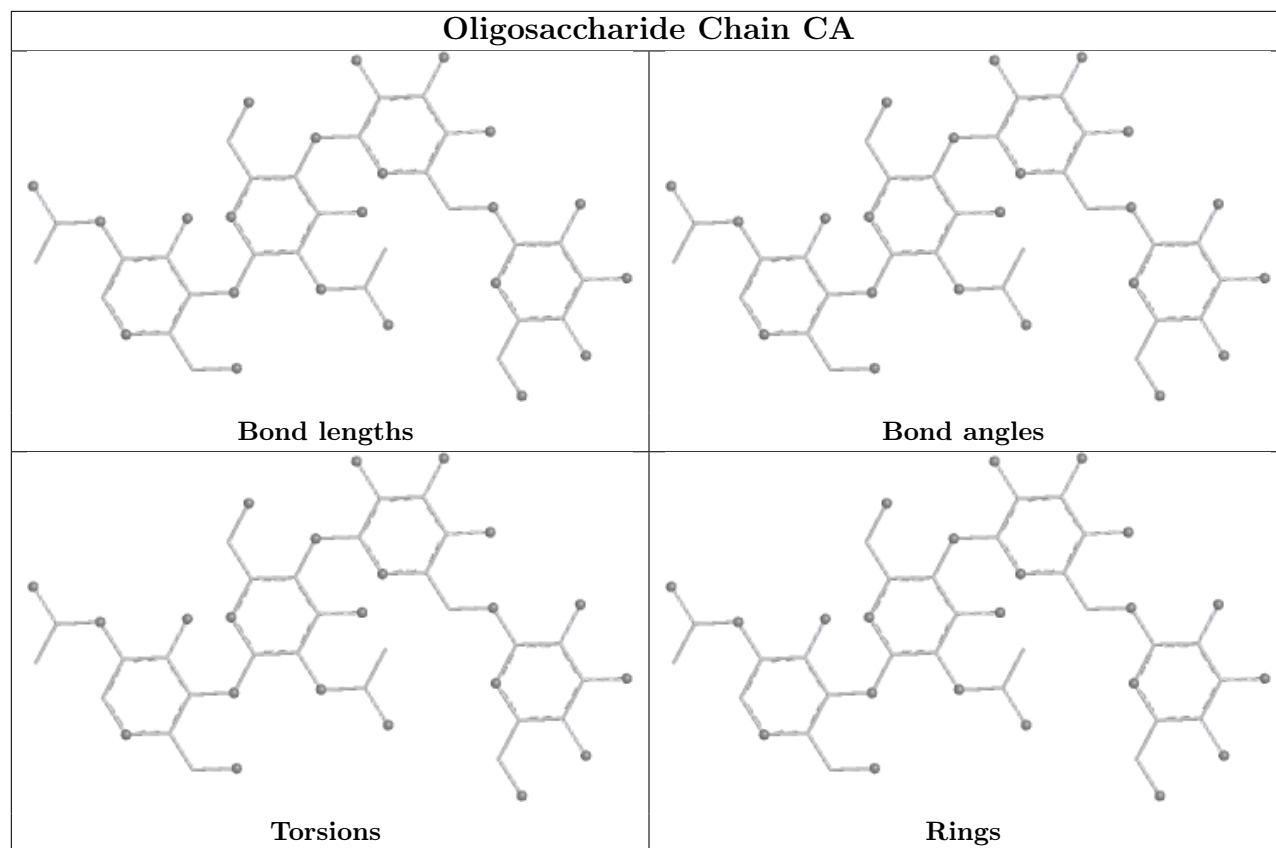
Oligosaccharide Chain J

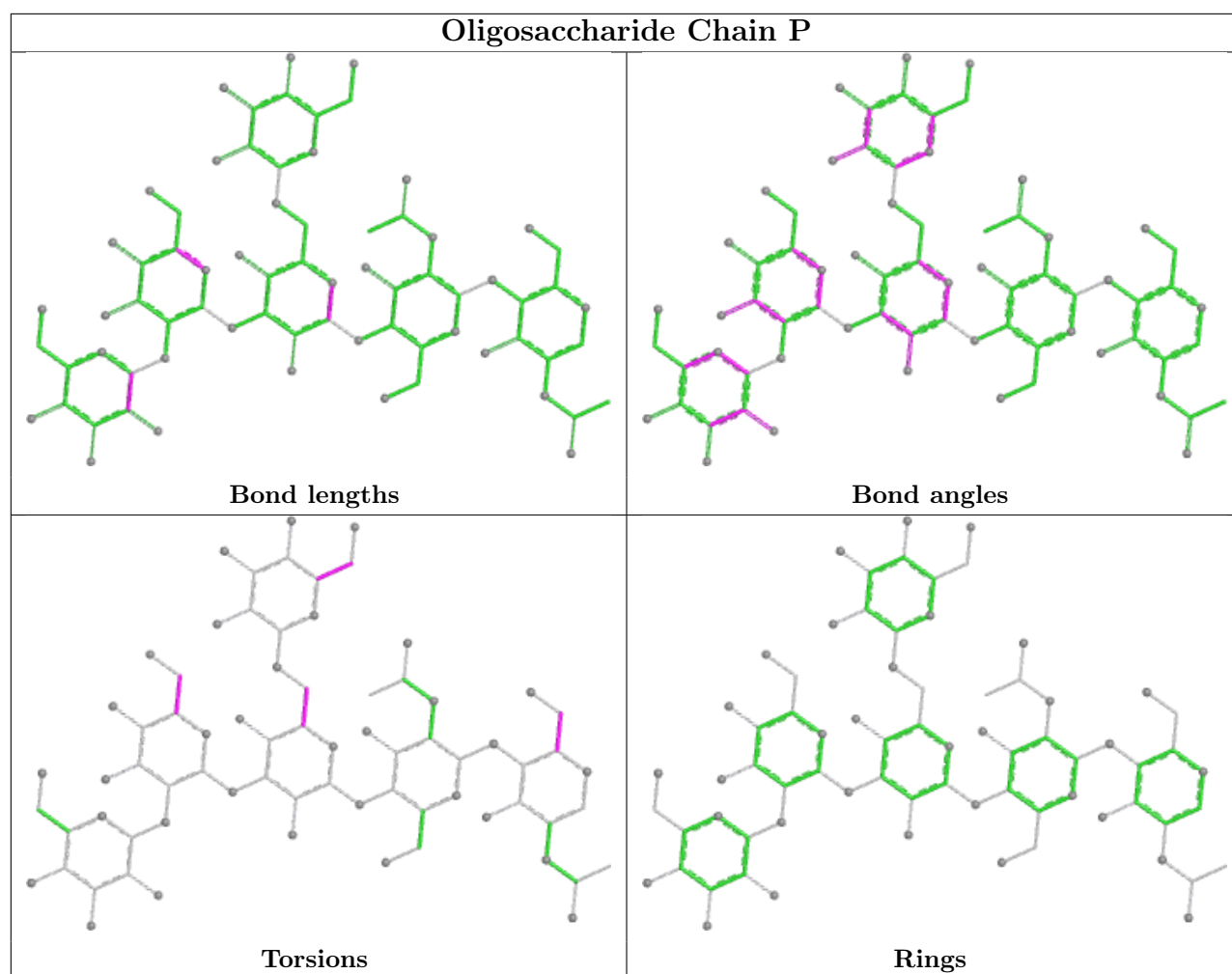


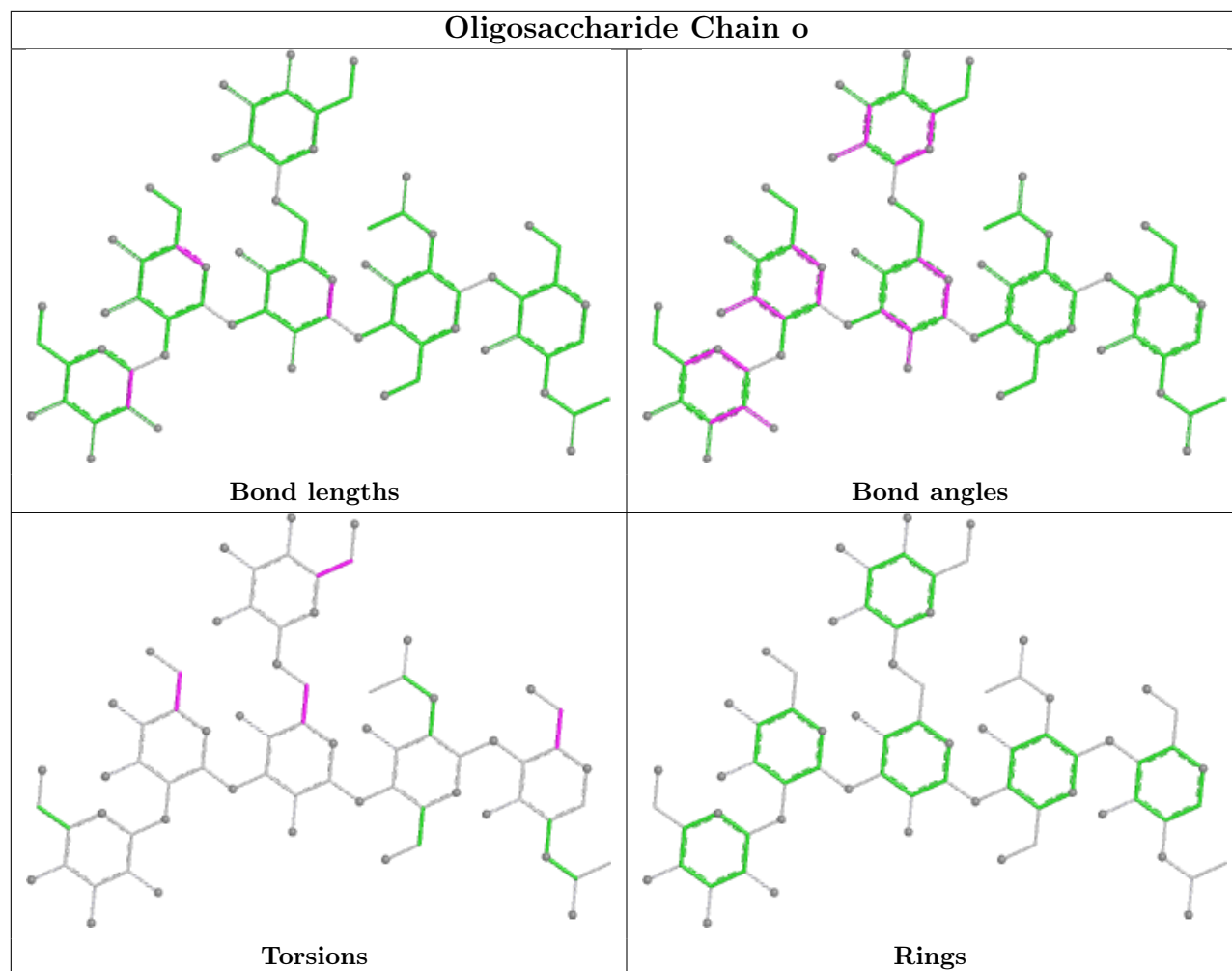


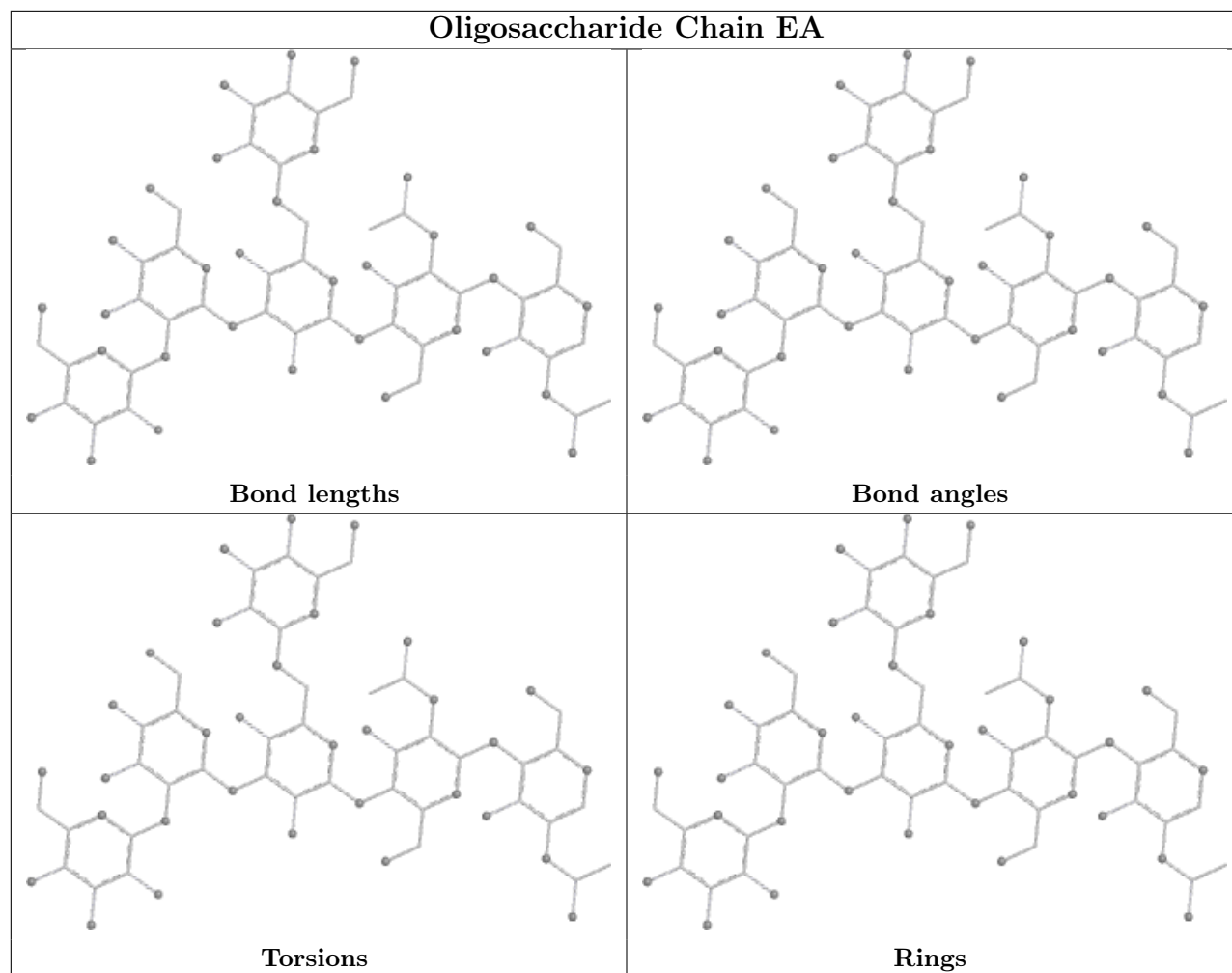
Oligosaccharide Chain BA**Bond lengths****Bond angles****Torsions****Rings**

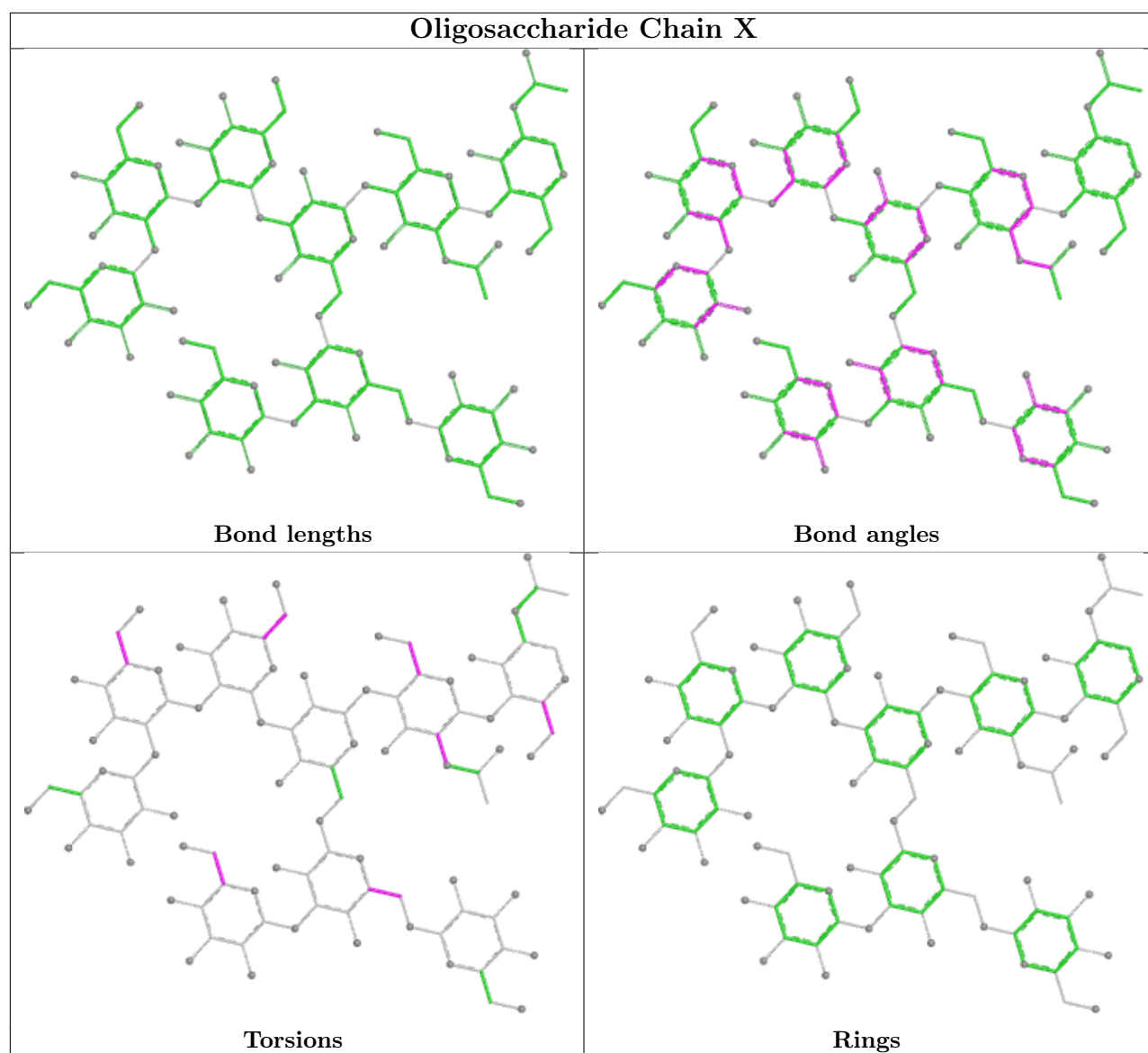


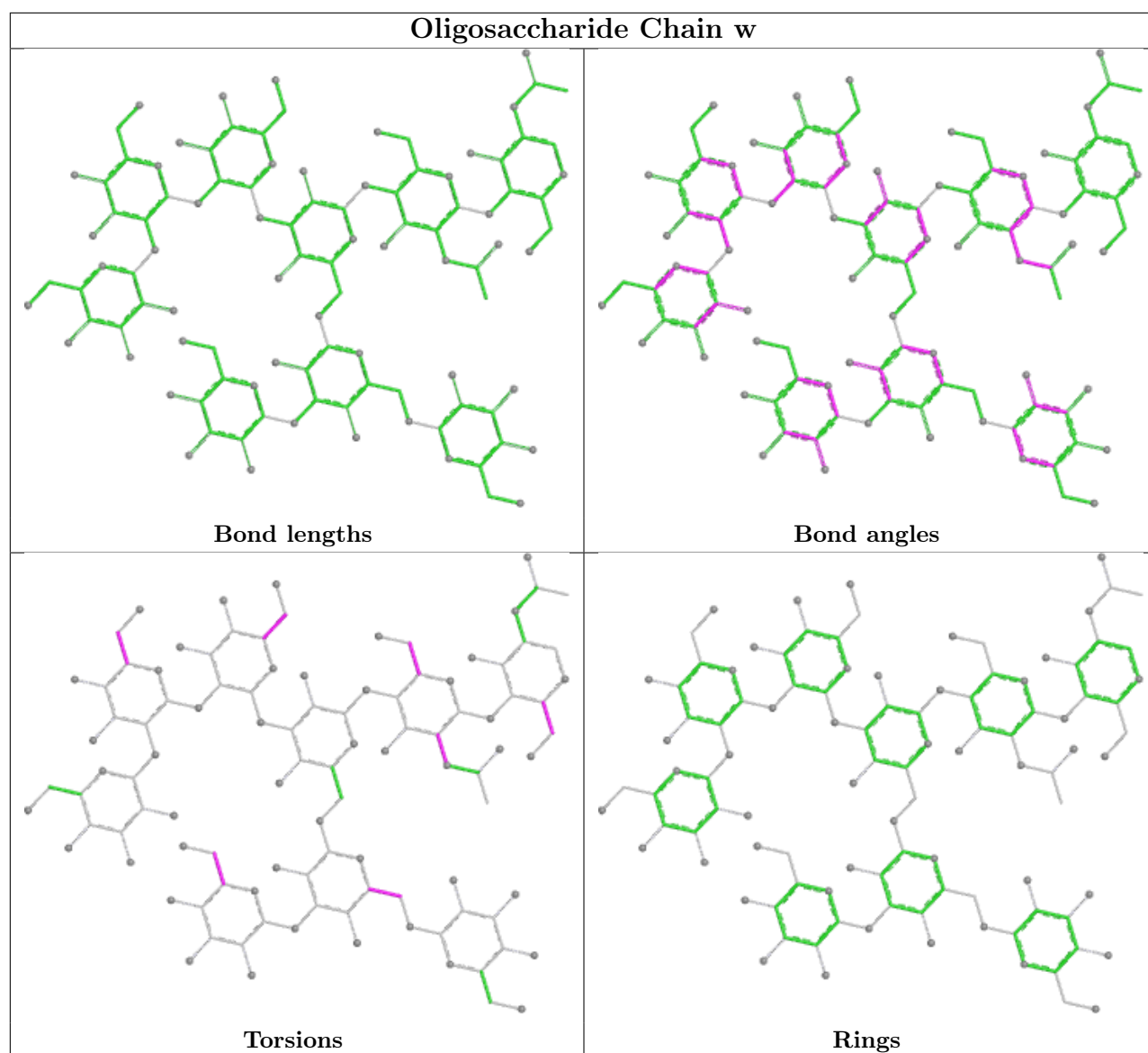


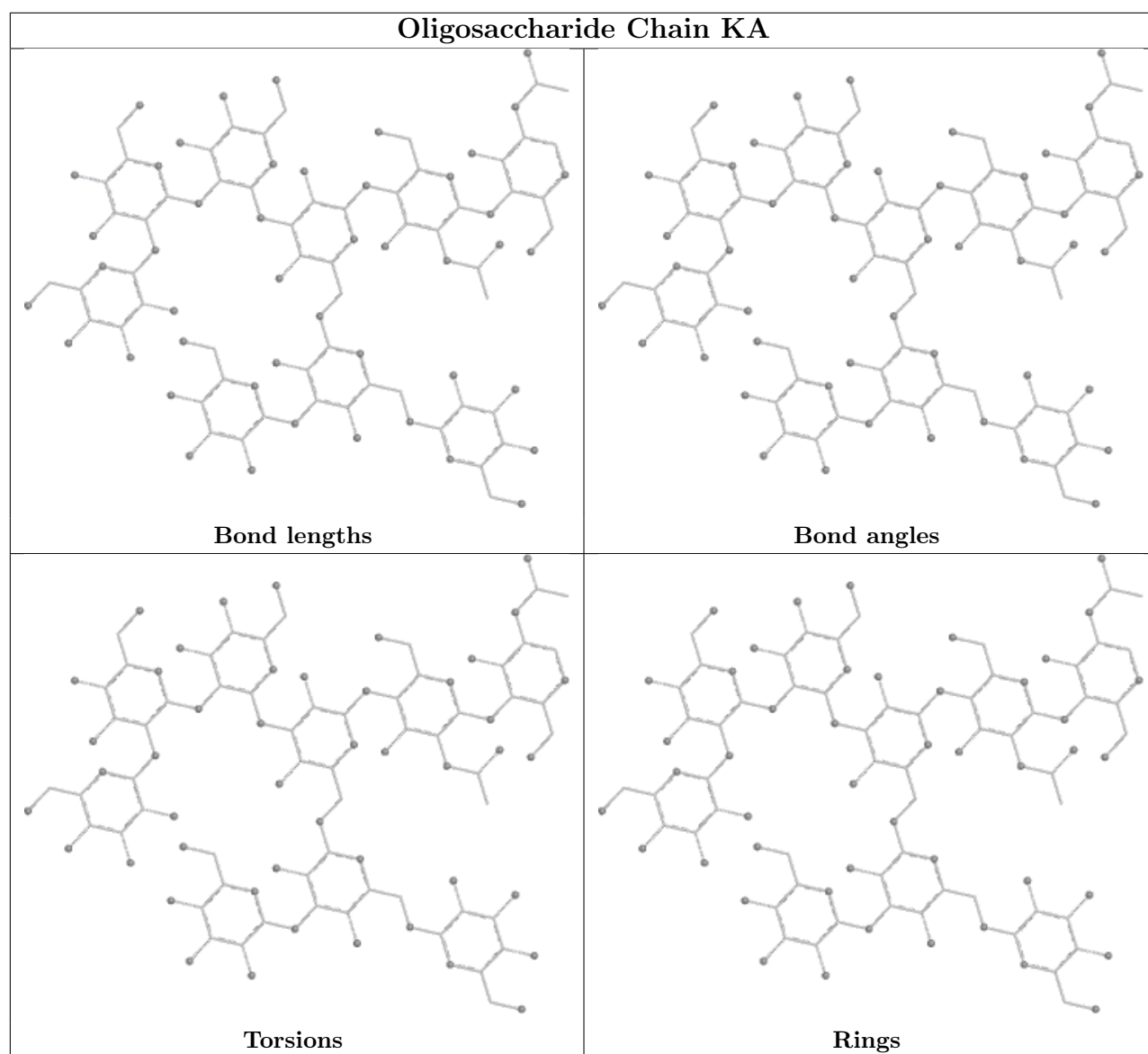




Oligosaccharide Chain EA







5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
17	NAG	A	701	1	14,14,15	0.24	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	NAG	2	601	2	14,14,15	0.29	0	17,19,21	0.53	0
17	NAG	D	701	1	14,14,15	0.24	0	17,19,21	0.48	0
17	NAG	d	601	2	14,14,15	0.28	0	17,19,21	0.51	0
17	NAG	c	701	1	14,14,15	0.24	0	17,19,21	0.48	0
17	NAG	C	601	2	14,14,15	0.28	0	17,19,21	0.52	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
17	NAG	A	701	1	-	0/6/23/26	0/1/1/1
17	NAG	2	601	2	-	3/6/23/26	0/1/1/1
17	NAG	D	701	1	-	0/6/23/26	0/1/1/1
17	NAG	d	601	2	-	3/6/23/26	0/1/1/1
17	NAG	c	701	1	-	0/6/23/26	0/1/1/1
17	NAG	C	601	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	d	601	NAG	O5-C5-C6-O6
17	2	601	NAG	O5-C5-C6-O6
17	C	601	NAG	O5-C5-C6-O6
17	d	601	NAG	C4-C5-C6-O6
17	2	601	NAG	C4-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.

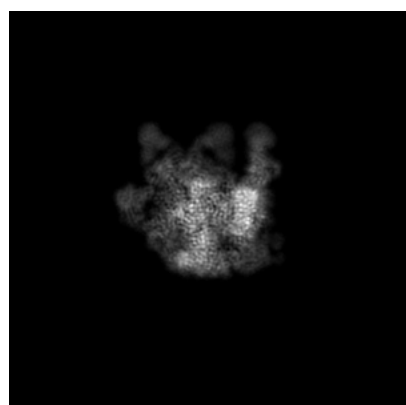
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7460. These allow visual inspection of the internal detail of the map and identification of artifacts.

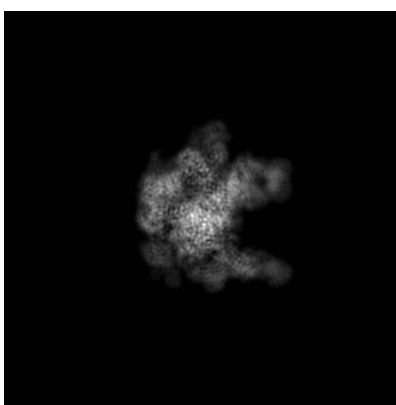
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

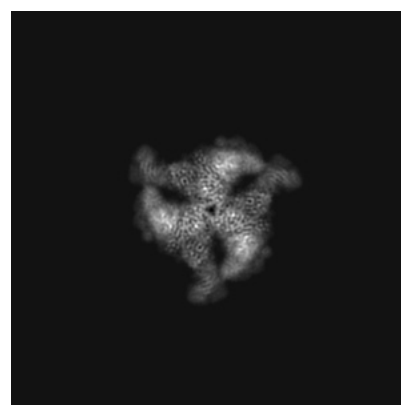
6.1.1 Primary map



X



Y

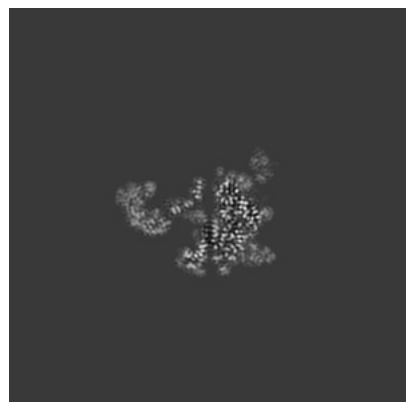


Z

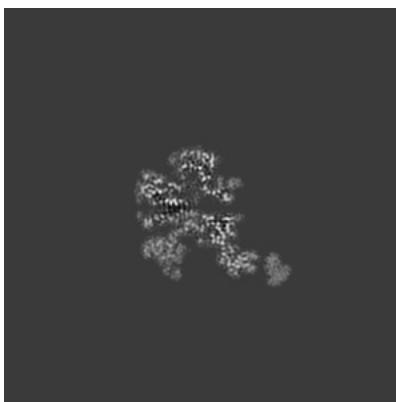
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

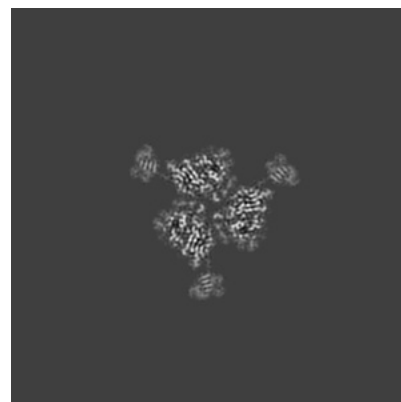
6.2.1 Primary map



X Index: 192



Y Index: 192

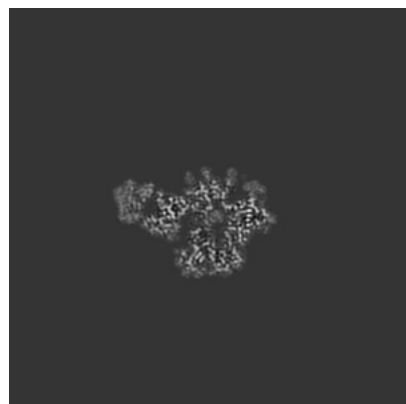


Z Index: 192

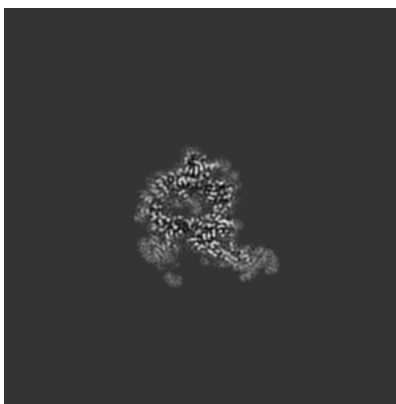
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

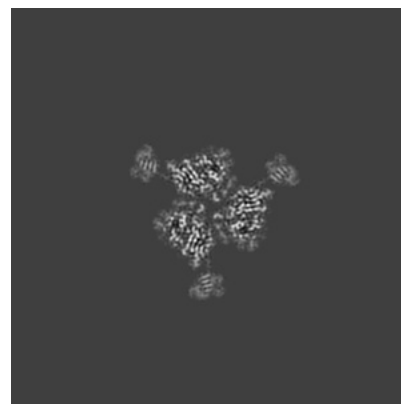
6.3.1 Primary map



X Index: 183



Y Index: 180

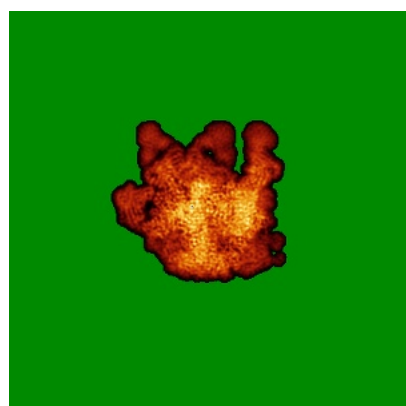


Z Index: 192

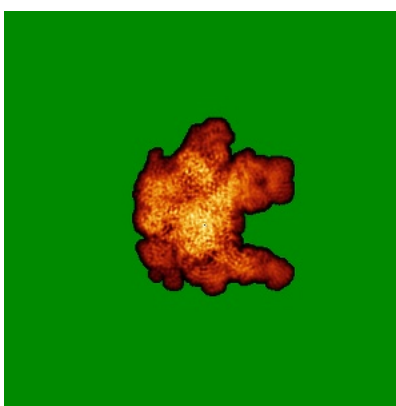
The images above show the largest variance slices of the map in three orthogonal directions.

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

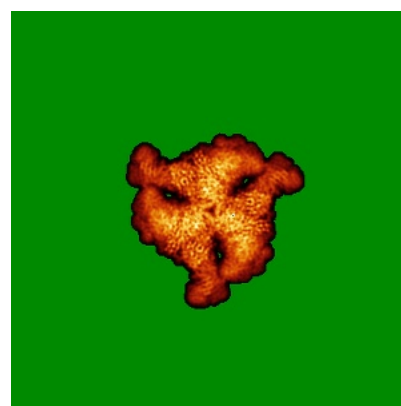
6.4.1 Primary map



X



Y



Z

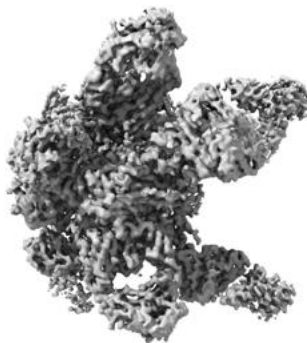
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

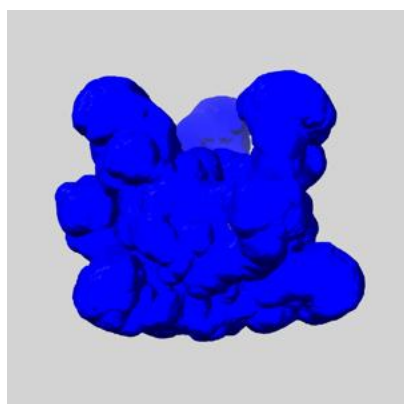
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

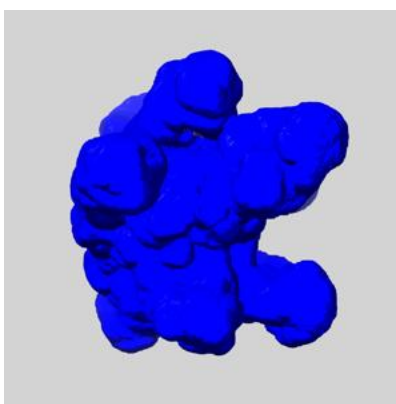
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

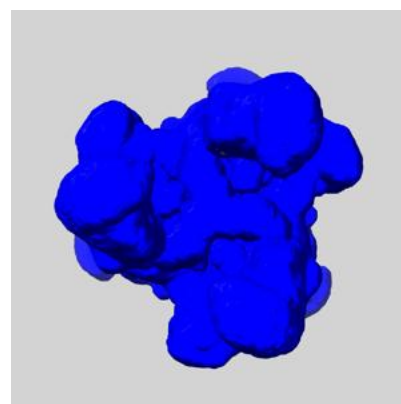
6.6.1 emd_7460_msk_1.map [i](#)



X

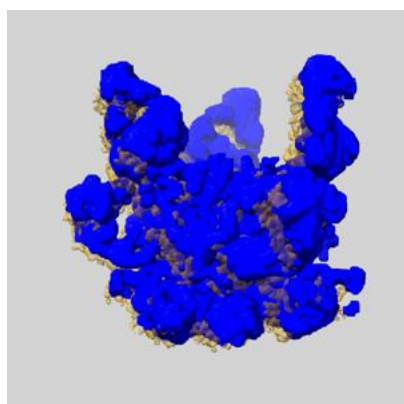


Y

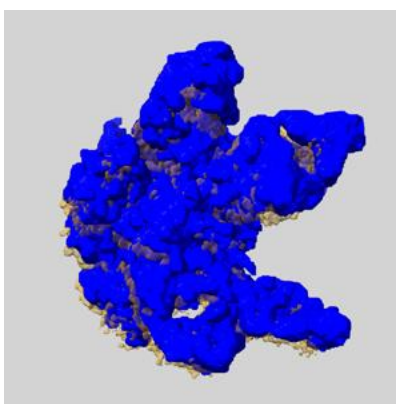


Z

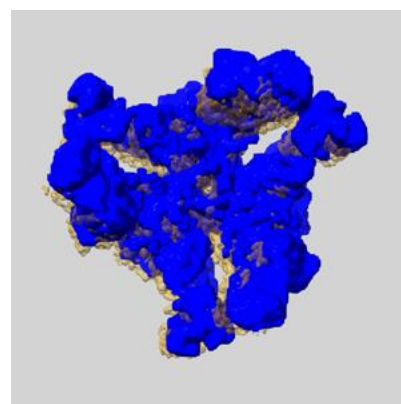
6.6.2 emd_7460_msk_2.map [i](#)



X



Y

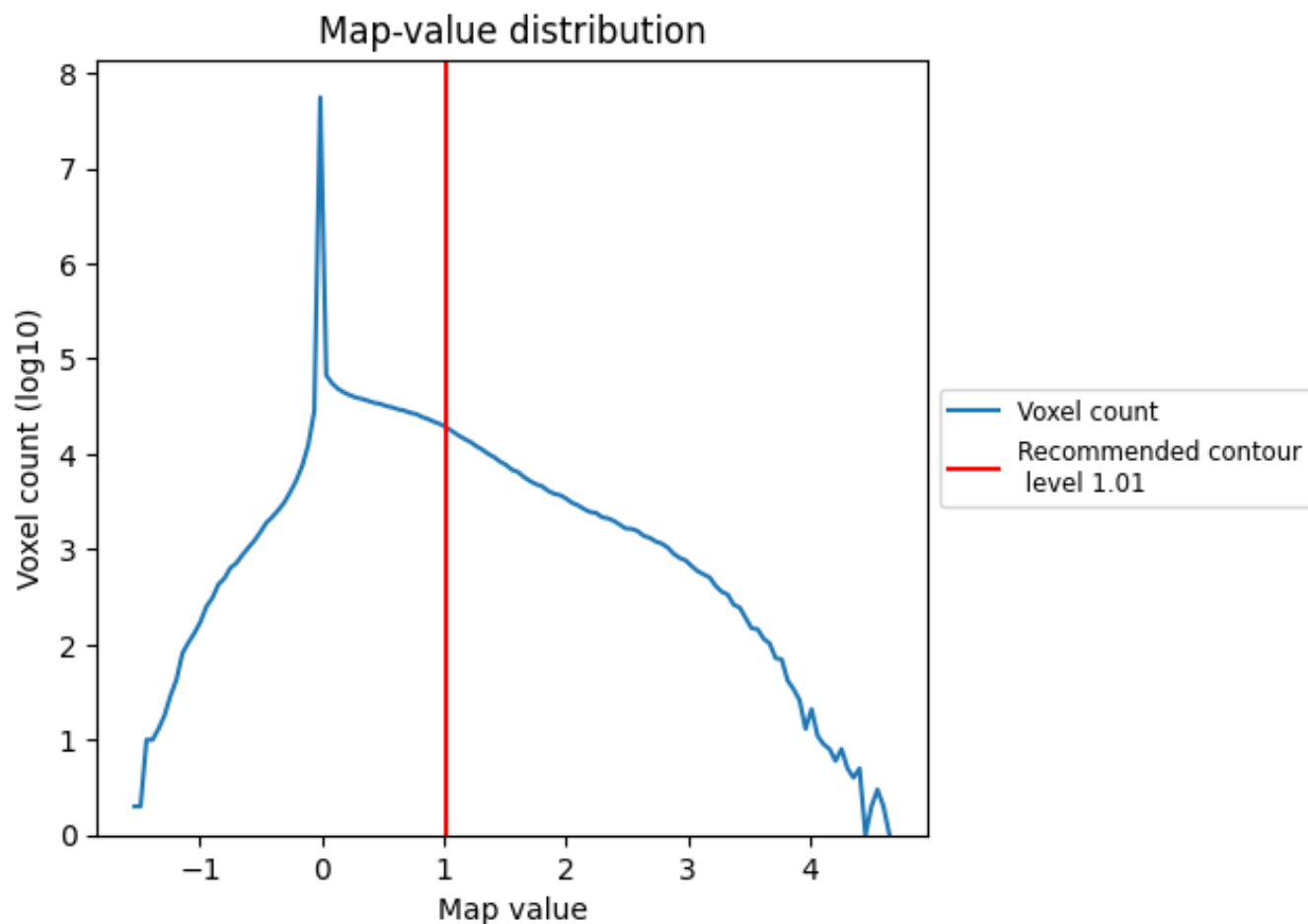


Z

7 Map analysis [i](#)

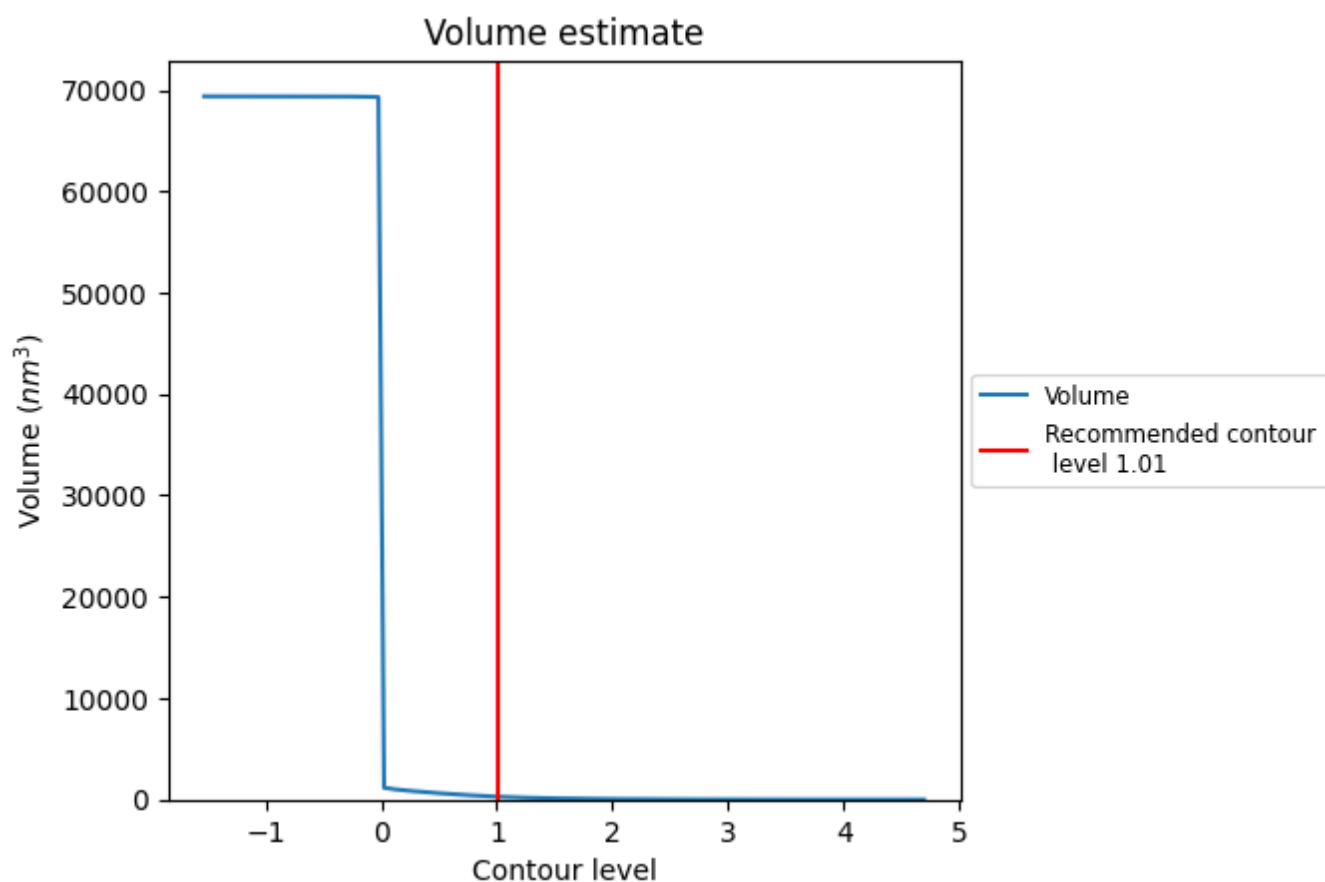
This section contains the results of statistical analysis of the map.

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.

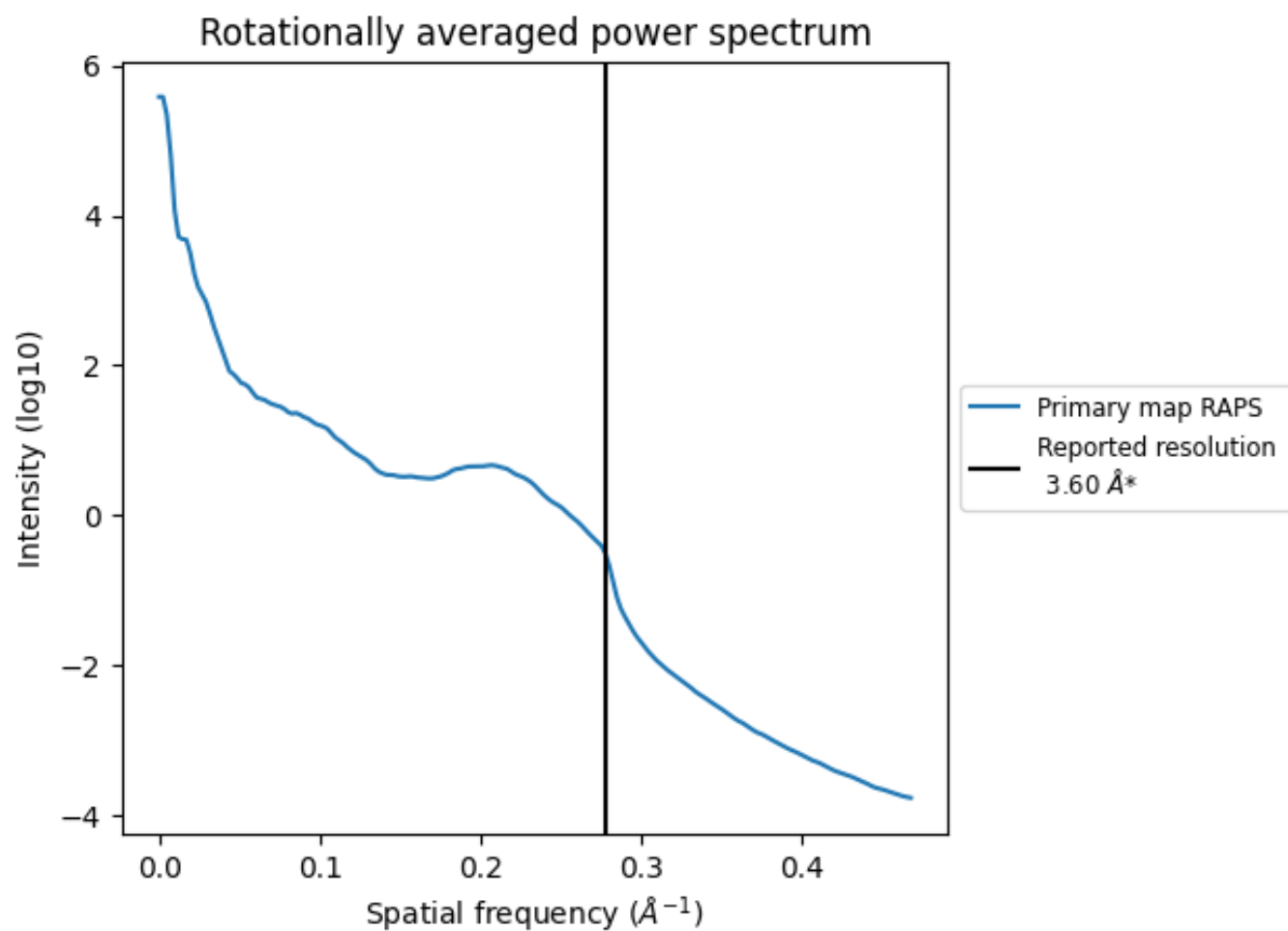
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 283 nm³; this corresponds to an approximate mass of 255 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 ⓘ

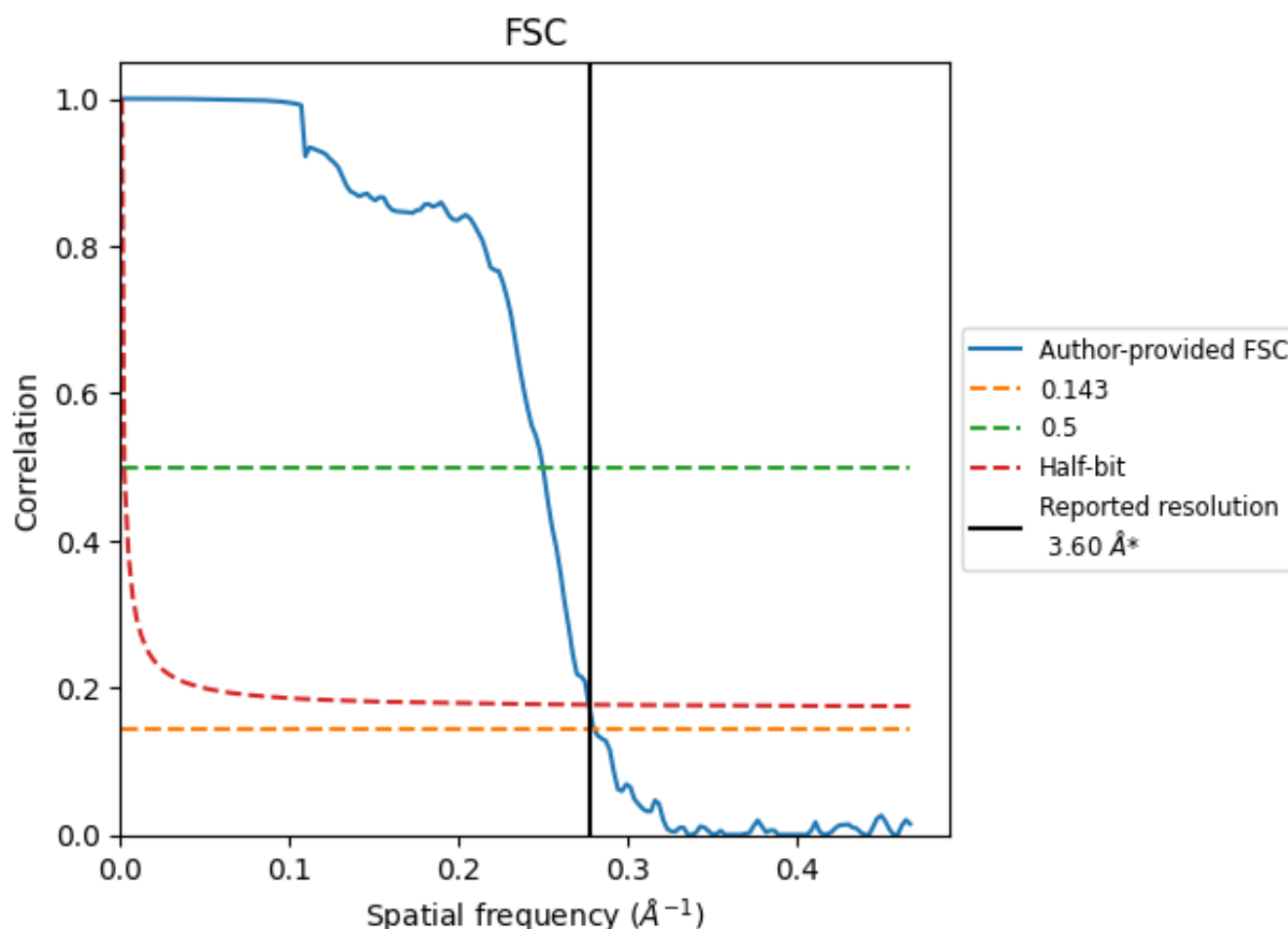


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

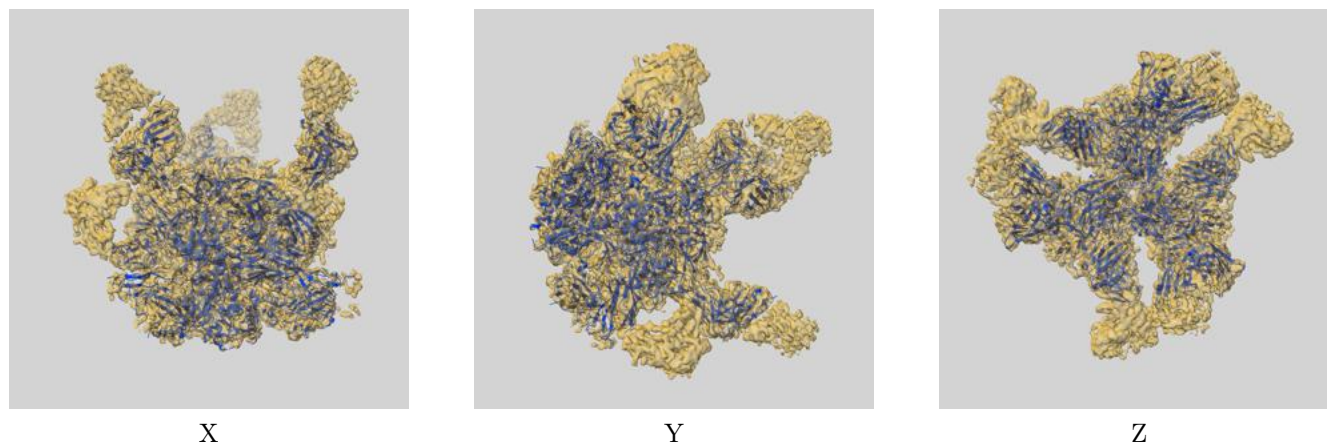
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.57	4.00	3.61
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

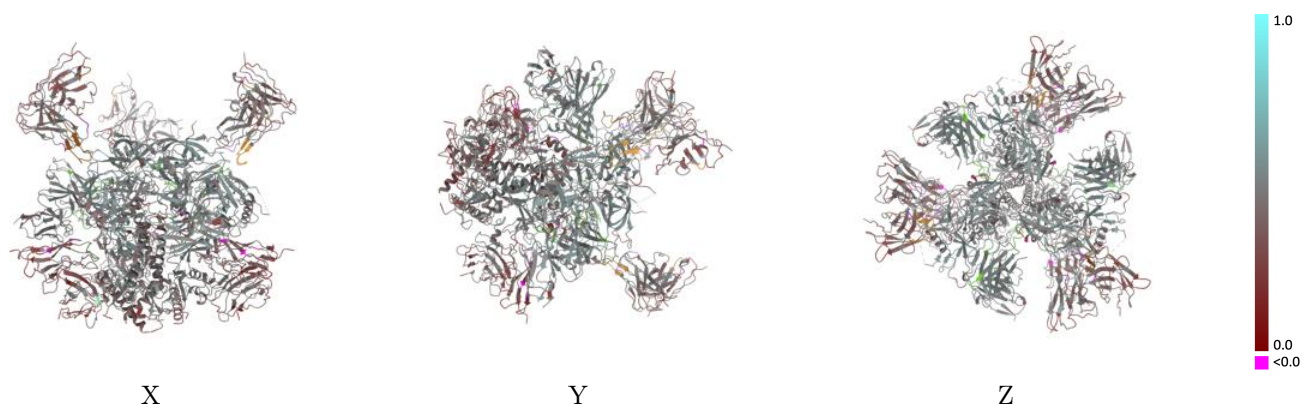
This section contains information regarding the fit between EMDB map EMD-7460 and PDB model 6CDI. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



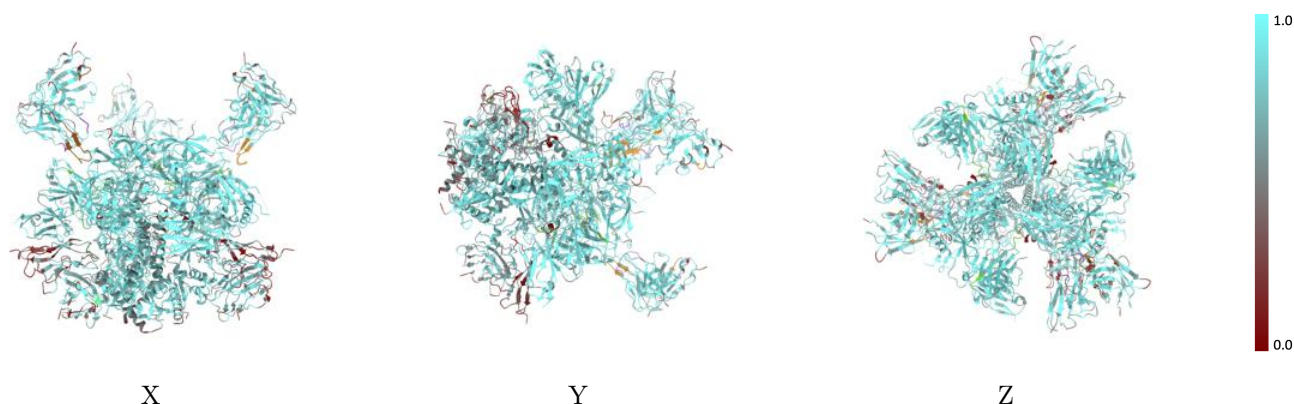
The images above show the 3D surface view of the map at the recommended contour level 1.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



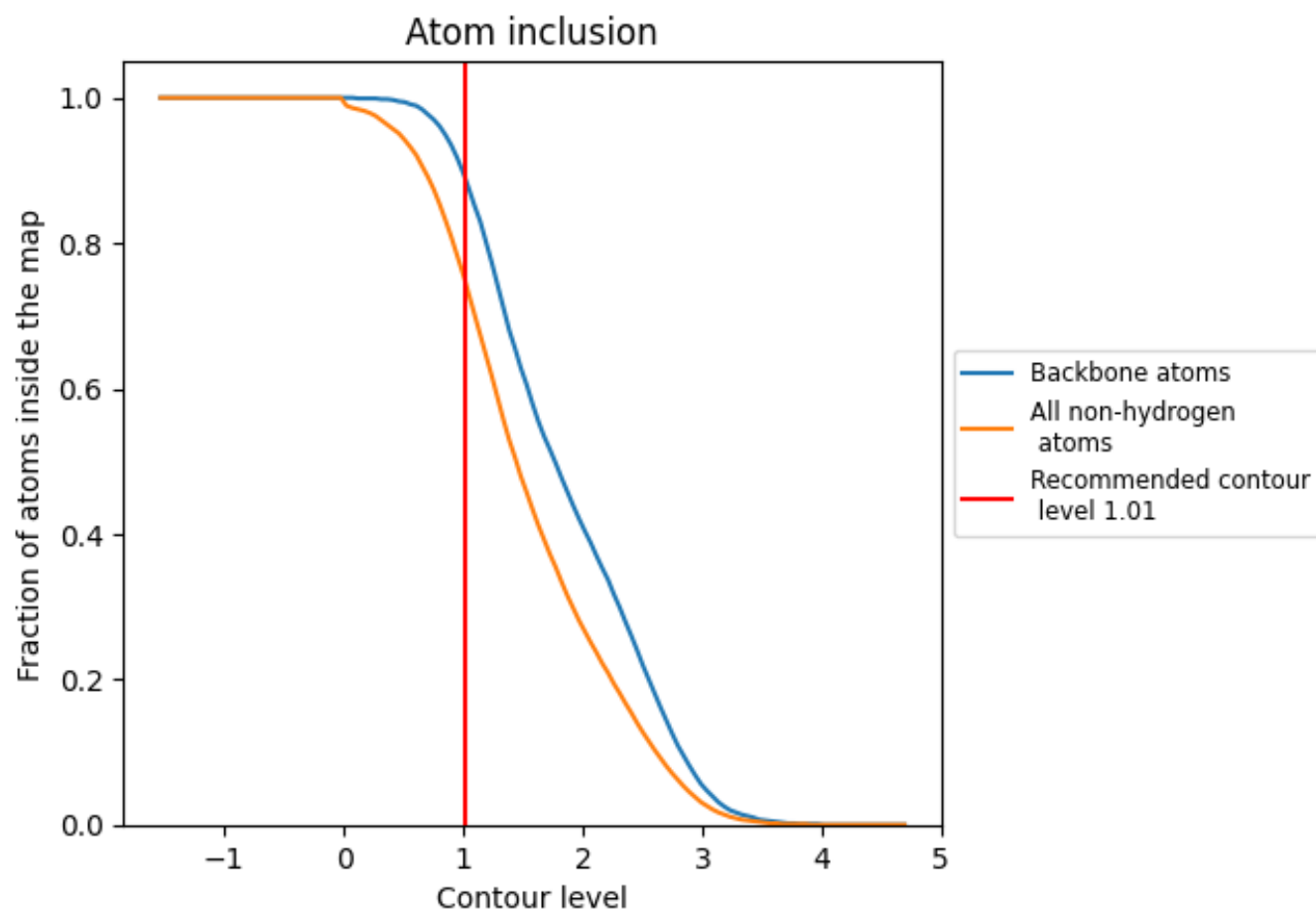
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.01).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ



















































































The table lists the average atom inclusion at the recommended contour level (1.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7520	 0.4320
0	 0.2400	 0.1720
1	 0.5710	 0.3310
2	 0.8220	 0.4750
3	 0.6190	 0.3580
4	 0.4790	 0.3300
5	 0.7770	 0.3880
6	 0.8070	 0.4250
7	 0.8510	 0.4780
8	 0.8520	 0.4960
9	 0.7200	 0.4380
A	 0.7650	 0.4400
AA	 0.5570	 0.4660
B	 0.0260	 -0.0370
BA	 0.1920	 0.0600
C	 0.8310	 0.4840
CA	 0.2800	 0.1690
D	 0.7720	 0.4450
DA	 0.6920	 0.4250
E	 0.2400	 0.1850
EA	 0.6530	 0.4470
F	 0.5710	 0.3140
FA	 0.7140	 0.4800
G	 0.7200	 0.4350
GA	 0.6070	 0.4360
H	 0.6280	 0.3580
HA	 0.8720	 0.5030
I	 0.5900	 0.4630
IA	 0.5570	 0.4270
J	 0.1920	 0.0740
JA	 0.4640	 0.3750
K	 0.2800	 0.1850
KA	 0.8000	 0.4610
L	 0.4900	 0.3280
LA	 0.4640	 0.3940



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Chain	Atom inclusion	Q-score
M	 0.7890	 0.3900
MA	 0.7000	 0.4830
N	 0.8070	 0.4280
O	 0.6920	 0.4260
P	 0.6110	 0.4470
Q	 0.8530	 0.5080
R	 0.8600	 0.4840
S	 0.6430	 0.4810
T	 0.6430	 0.4140
U	 0.8210	 0.5160
V	 0.6070	 0.4200
W	 0.4640	 0.3610
X	 0.7620	 0.4490
Y	 0.5000	 0.3900
Z	 0.7000	 0.4710
a	 0.0260	 -0.0120
b	 0.2400	 0.1780
c	 0.7780	 0.4400
d	 0.8190	 0.4730
e	 0.6070	 0.3370
f	 0.7200	 0.4350
g	 0.5740	 0.4630
h	 0.6090	 0.3600
i	 0.1920	 0.0740
j	 0.2800	 0.1720
k	 0.6410	 0.4180
l	 0.4840	 0.3290
m	 0.7800	 0.3870
n	 0.8060	 0.4220
o	 0.6250	 0.4540
p	 0.6790	 0.4680
q	 0.8500	 0.4980
r	 0.8540	 0.4760
s	 0.6430	 0.4470
t	 0.8970	 0.4940
u	 0.5570	 0.4070
v	 0.4640	 0.3780
w	 0.8190	 0.4710
x	 0.4640	 0.3820
y	 0.7400	 0.4750
z	 0.0260	 -0.0090