



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 04:41 PM UTC

PDB ID : 7SKA / pdb_00007ska
EMDB ID : EMD-25178
Title : Sub-tomogram averaged structure of HIV-1 Envelope protein in native membrane
Authors : Mangala Prasad, V.; Lee, K.K.
Deposited on : 2021-10-20
Resolution : 9.10 Å(reported)
Based on initial model : 6ULC

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:

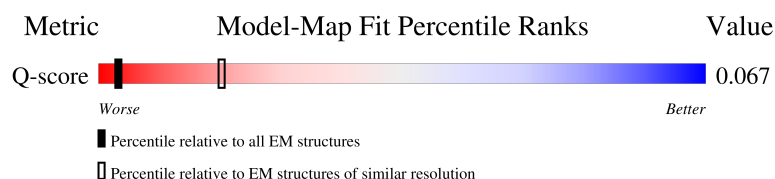
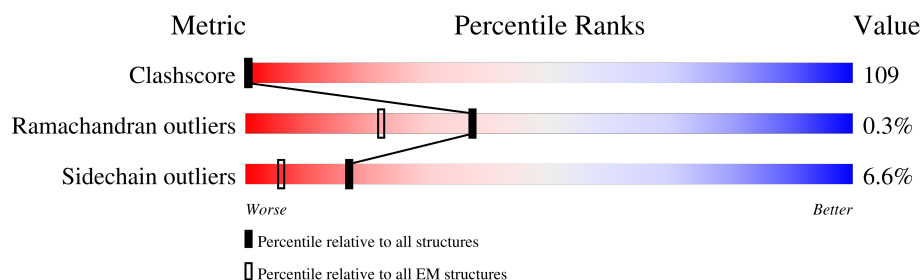
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 9.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	244 (8.60 - 9.60)

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	465	
1	N	465	
1	Y	465	
2	B	144	

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Mol	Chain	Length	Quality of chain
2	O	144	
2	Z	144	
3	F	5	
3	J	5	
3	T	5	
3	b	5	
3	j	5	
3	s	5	
4	H	6	
4	d	6	
4	k	6	
5	C	2	
5	D	2	
5	E	2	
5	G	2	
5	U	2	
5	V	2	
5	W	2	
5	X	2	
5	l	2	
5	o	2	
5	p	2	
5	q	2	
6	I	4	
6	L	4	

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Mol	Chain	Length	Quality of chain
6	a	4	
6	e	4	
6	r	4	
6	u	4	
7	K	3	
7	M	3	
7	c	3	
7	f	3	
7	t	3	
7	v	3	
8	P	6	
8	n	6	
8	w	6	
9	Q	8	
9	g	8	
9	x	8	
10	R	2	
10	h	2	
10	y	2	
11	S	6	
11	i	6	
11	m	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NAG	R	2	-	-	X	-
10	NAG	h	2	-	-	X	-
10	NAG	y	2	-	-	X	-
12	NAG	A	602	-	-	X	-
12	NAG	A	604	-	-	X	-
12	NAG	B	702	-	-	X	-
12	NAG	N	602	-	-	X	-
12	NAG	N	604	-	-	X	-
12	NAG	O	702	-	-	X	-
12	NAG	Y	602	-	-	X	-
12	NAG	Y	604	-	-	X	-
12	NAG	Z	702	-	-	X	-
5	NAG	D	1	-	-	X	-
5	NAG	V	1	-	-	X	-
5	NAG	o	1	-	-	X	-
8	FUC	P	6	-	-	X	-
8	FUC	n	6	-	-	X	-
8	FUC	w	6	-	-	X	-
9	NAG	Q	1	-	-	X	-
9	NAG	Q	2	-	-	X	-
9	NAG	Q	5	-	-	X	-
9	NAG	g	1	-	-	X	-
9	NAG	g	2	-	-	X	-
9	NAG	g	5	-	-	X	-
9	NAG	x	1	-	-	X	-
9	NAG	x	2	-	-	X	-
9	NAG	x	5	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 16743 atoms, of which 45 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	454	Total	C	N	O	S	0	0
			3575	2244	626	680	25		
1	N	454	Total	C	N	O	S	0	0
			3575	2244	626	680	25		
1	Y	454	Total	C	N	O	S	0	0
			3575	2244	626	680	25		

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	142	Total	C	N	O	S	0	0
			1136	712	204	214	6		
2	O	142	Total	C	N	O	S	0	0
			1136	712	204	214	6		
2	Z	142	Total	C	N	O	S	0	0
			1136	712	204	214	6		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	535	MET	ILE	conflict	UNP Q6TAN8
B	543	GLN	LEU	conflict	UNP Q6TAN8
B	574	ARG	LYS	conflict	UNP Q6TAN8
B	625	ASN	HIS	conflict	UNP Q6TAN8
B	626	MET	THR	conflict	UNP Q6TAN8
B	649	ALA	SER	conflict	UNP Q6TAN8
O	535	MET	ILE	conflict	UNP Q6TAN8
O	543	GLN	LEU	conflict	UNP Q6TAN8
O	574	ARG	LYS	conflict	UNP Q6TAN8
O	625	ASN	HIS	conflict	UNP Q6TAN8
O	626	MET	THR	conflict	UNP Q6TAN8
O	649	ALA	SER	conflict	UNP Q6TAN8
Z	535	MET	ILE	conflict	UNP Q6TAN8

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	543	GLN	LEU	conflict	UNP Q6TAN8
Z	574	ARG	LYS	conflict	UNP Q6TAN8
Z	625	ASN	HIS	conflict	UNP Q6TAN8
Z	626	MET	THR	conflict	UNP Q6TAN8
Z	649	ALA	SER	conflict	UNP Q6TAN8

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	5	Total	C	N	O	0	0
			61	34	2	25		
3	J	5	Total	C	N	O	0	0
			61	34	2	25		
3	T	5	Total	C	N	O	0	0
			61	34	2	25		
3	b	5	Total	C	N	O	0	0
			61	34	2	25		
3	j	5	Total	C	N	O	0	0
			61	34	2	25		
3	s	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 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
4	H	6	Total	C	N	O	0	0
			72	40	2	30		
4	d	6	Total	C	N	O	0	0
			72	40	2	30		
4	k	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 5 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
5	C	2	Total	C	N	O	0	0
			27	15	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	D	2	Total	C	N	O	0	0
			25	15	2	8		
5	E	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			27	15	2	10		
5	V	2	Total	C	N	O	0	0
			25	15	2	8		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	X	2	Total	C	N	O	0	0
			28	16	2	10		
5	l	2	Total	C	N	O	0	0
			27	15	2	10		
5	o	2	Total	C	N	O	0	0
			25	15	2	8		
5	p	2	Total	C	N	O	0	0
			28	16	2	10		
5	q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 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
6	I	4	Total	C	N	O	0	0
			50	28	2	20		
6	L	4	Total	C	N	O	0	0
			45	26	2	17		
6	a	4	Total	C	N	O	0	0
			50	28	2	20		
6	e	4	Total	C	N	O	0	0
			45	26	2	17		
6	r	4	Total	C	N	O	0	0
			50	28	2	20		
6	u	4	Total	C	N	O	0	0
			45	26	2	17		

- Molecule 7 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
7	K	3	Total	C	N	O	0	0
			37	22	2	13		
7	M	3	Total	C	N	O	0	0
			39	22	2	15		
7	c	3	Total	C	N	O	0	0
			37	22	2	13		
7	f	3	Total	C	N	O	0	0
			39	22	2	15		
7	t	3	Total	C	N	O	0	0
			37	22	2	13		
7	v	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	6	Total	C	N	O	0	0
			74	42	3	29		
8	n	6	Total	C	N	O	0	0
			74	42	3	29		
8	w	6	Total	C	N	O	0	0
			74	42	3	29		

- Molecule 9 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]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	Q	8	Total	C	N	O	0	0
			100	56	4	40		
9	g	8	Total	C	N	O	0	0
			100	56	4	40		
9	x	8	Total	C	N	O	0	0
			100	56	4	40		

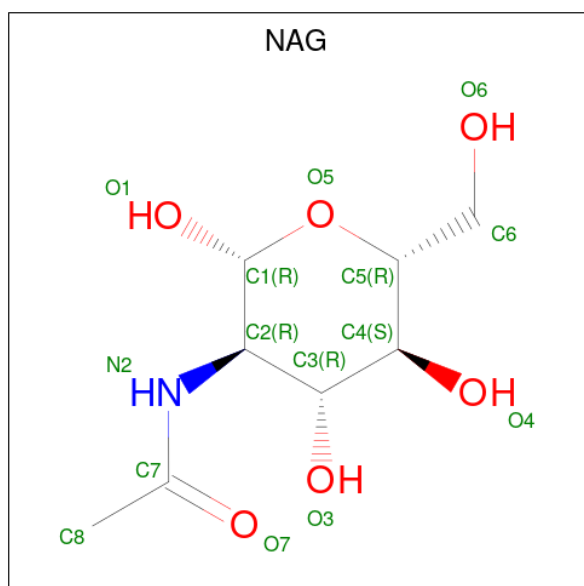
- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	R	2	Total	C	N	O	0	0
			25	14	1	10		
10	h	2	Total	C	N	O	0	0
			25	14	1	10		
10	y	2	Total	C	N	O	0	0
			25	14	1	10		

- Molecule 11 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
11	S	6	Total	C	N	O	0	0
			72	40	2	30		
11	i	6	Total	C	N	O	0	0
			72	40	2	30		
11	m	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



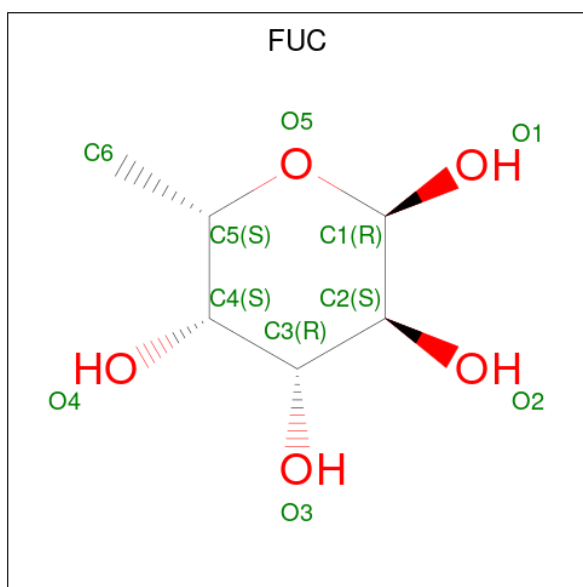
Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	H	N	O
			20	8	5	1	6
12	A	1	Total	C	H	N	O
			20	8	5	1	6

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Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total 14	C 8	N 1	O 5	0	
12	A	1	Total 14	C 8	N 1	O 5	0	
12	A	1	Total 14	C 8	N 1	O 5	0	
12	B	1	Total 20	C 8	H 5	N 1 O 6	0	
12	B	1	Total 14	C 8	N 1	O 5	0	
12	N	1	Total 20	C 8	H 5	N 1 O 6	0	
12	N	1	Total 20	C 8	H 5	N 1 O 6	0	
12	N	1	Total 14	C 8	N 1	O 5	0	
12	N	1	Total 14	C 8	N 1	O 5	0	
12	N	1	Total 14	C 8	N 1	O 5	0	
12	O	1	Total 20	C 8	H 5	N 1 O 6	0	
12	O	1	Total 14	C 8	N 1	O 5	0	
12	Y	1	Total 20	C 8	H 5	N 1 O 6	0	
12	Y	1	Total 20	C 8	H 5	N 1 O 6	0	
12	Y	1	Total 14	C 8	N 1	O 5	0	
12	Y	1	Total 14	C 8	N 1	O 5	0	
12	Y	1	Total 14	C 8	N 1	O 5	0	
12	Z	1	Total 20	C 8	H 5	N 1 O 6	0	
12	Z	1	Total 14	C 8	N 1	O 5	0	

- Molecule 13 is alpha-L-fucopyranose (CCD ID: FUC) (formula: C₆H₁₂O₅).

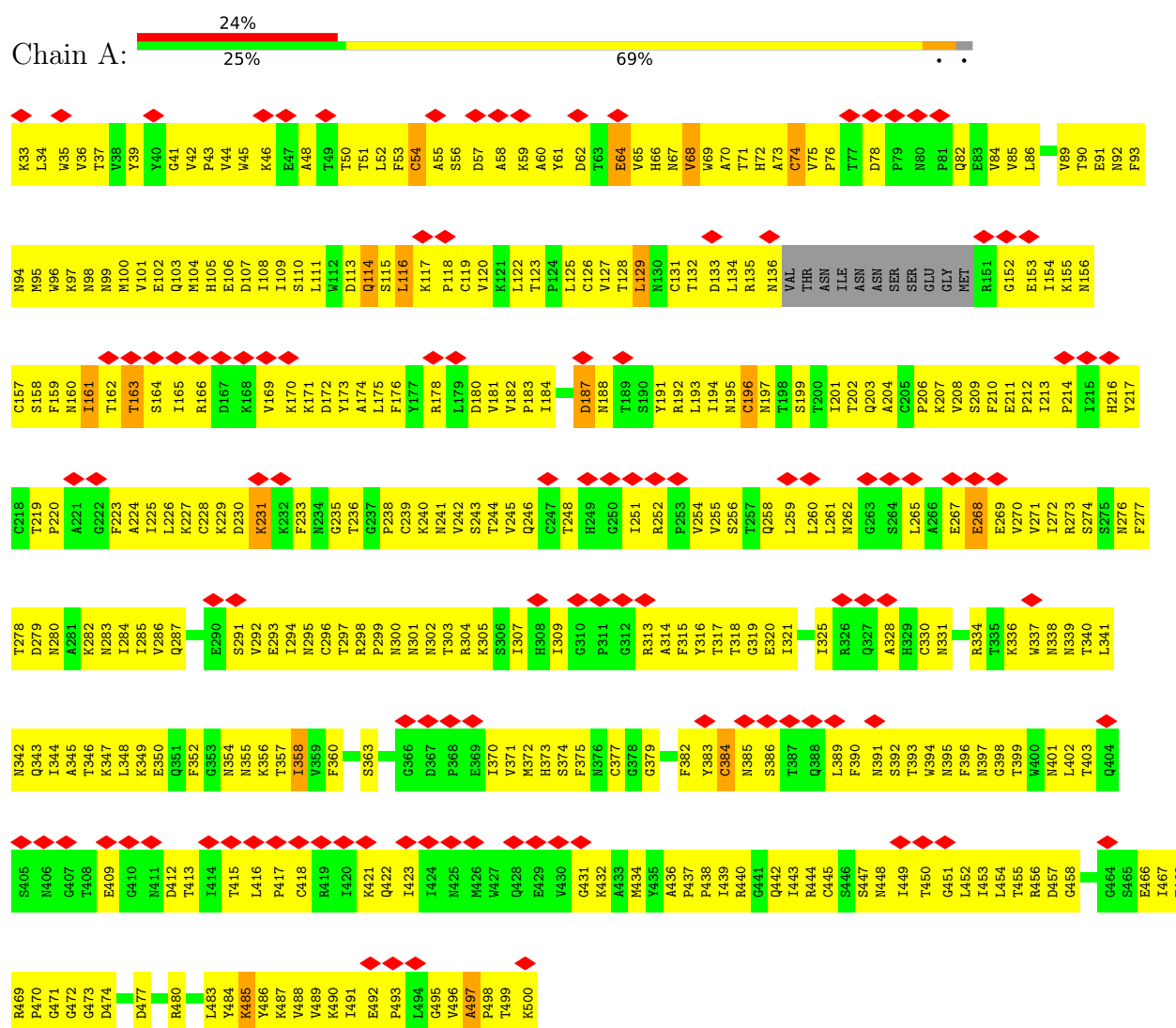


Mol	Chain	Residues	Atoms			AltConf
13	B	1	Total	C	O	0
			10	6	4	
13	O	1	Total	C	O	0
			10	6	4	
13	Z	1	Total	C	O	0
			10	6	4	

3 Residue-property plots

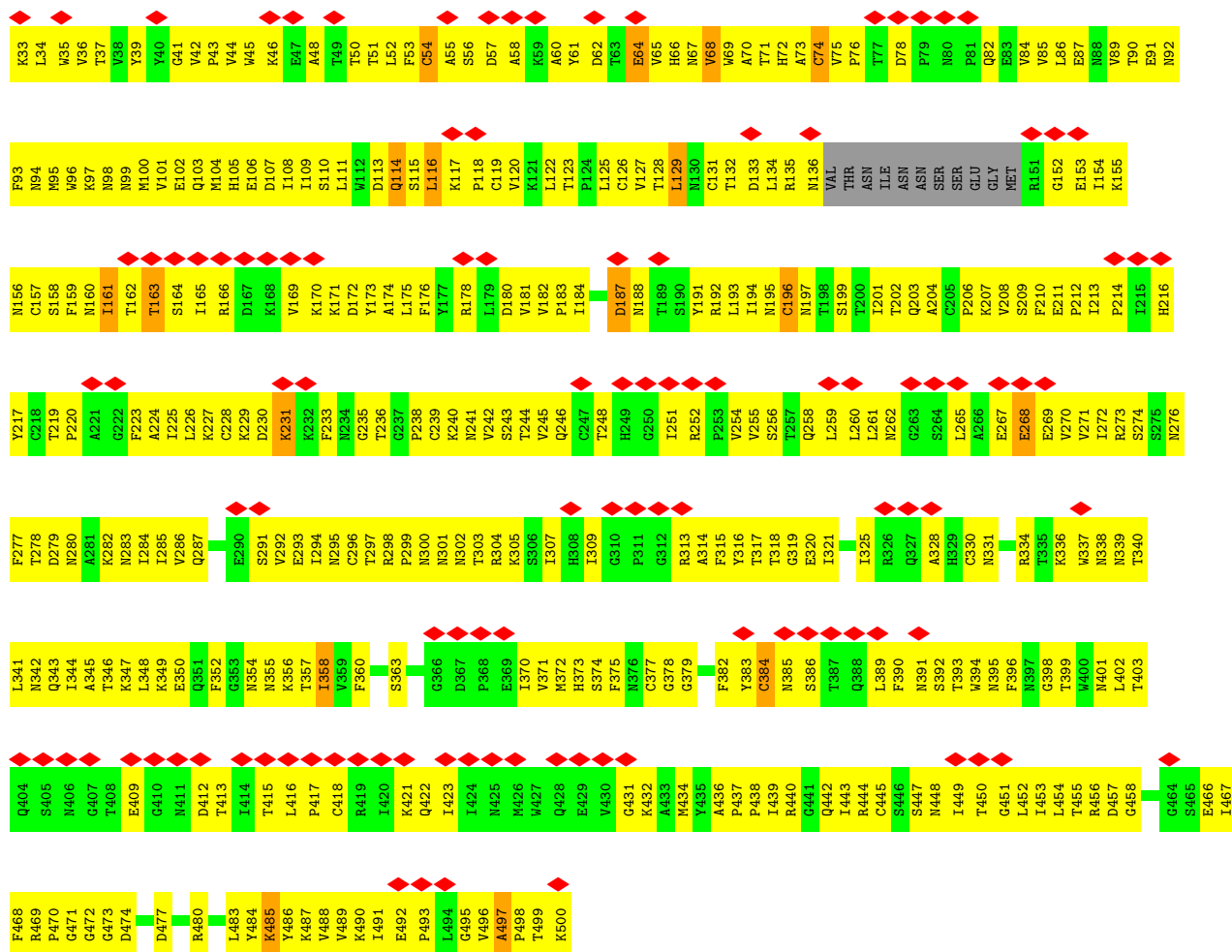
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Envelope glycoprotein gp120

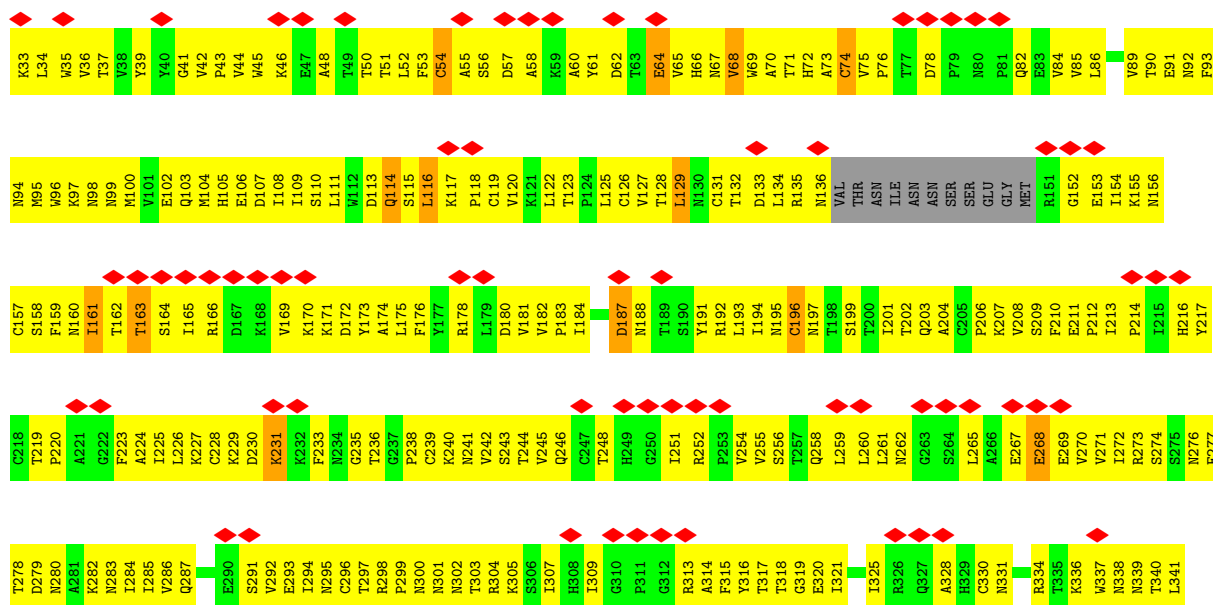


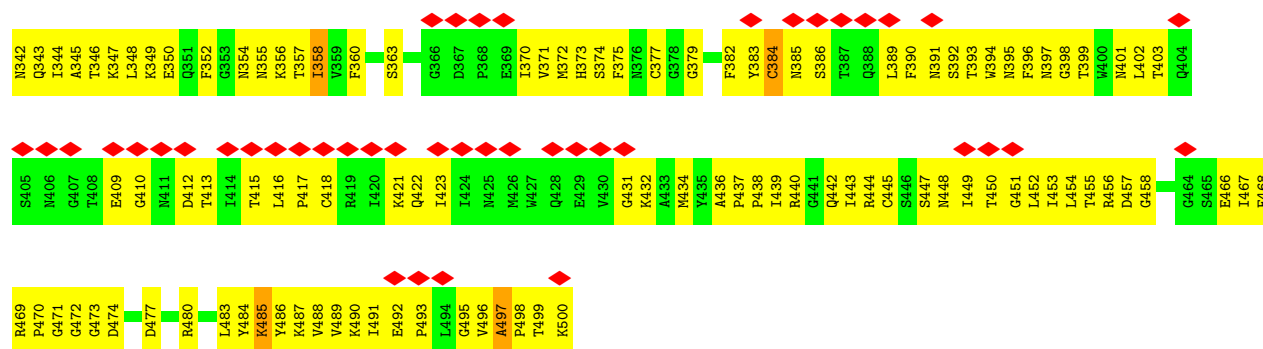
• Molecule 1: Envelope glycoprotein gp120



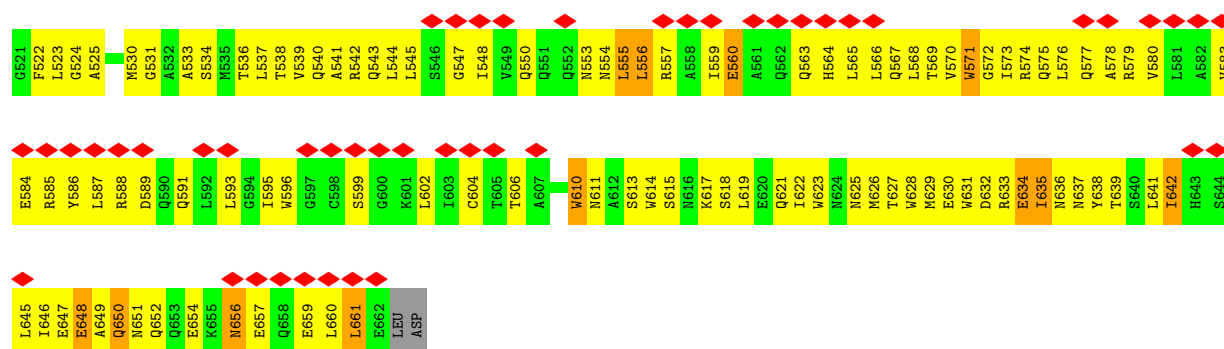


• Molecule 1: Envelope glycoprotein gp120

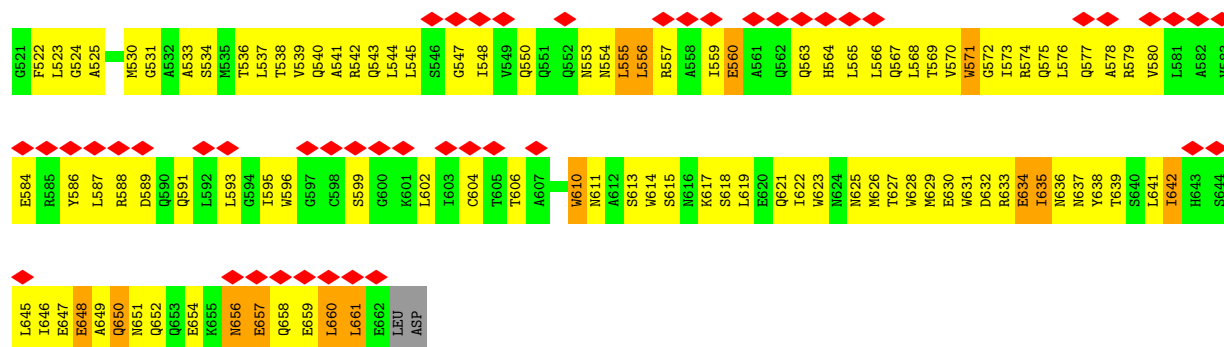




• Molecule 2: Envelope glycoprotein gp41

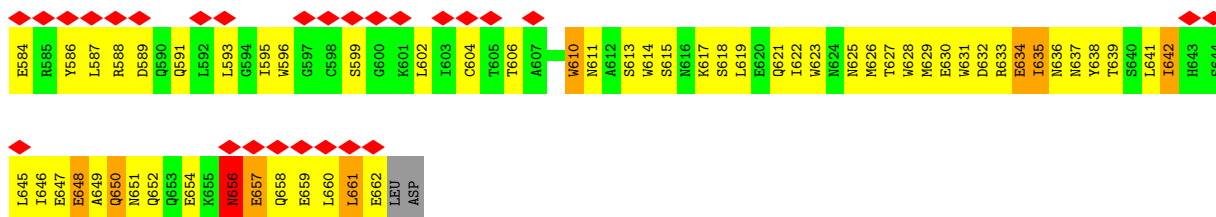


• Molecule 2: Envelope glycoprotein gp41

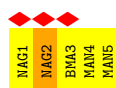


• Molecule 2: Envelope glycoprotein gp41





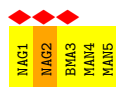
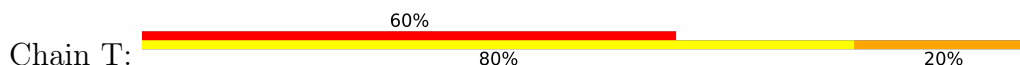
- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



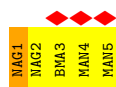
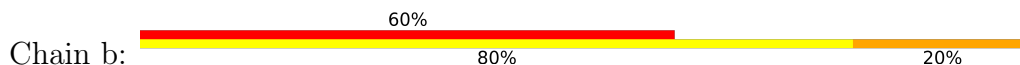
- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



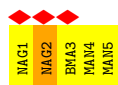
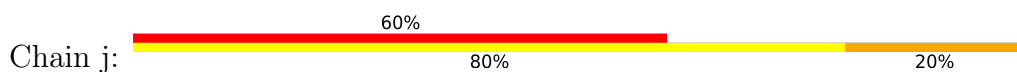
- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



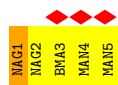
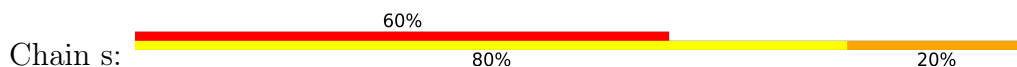
- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



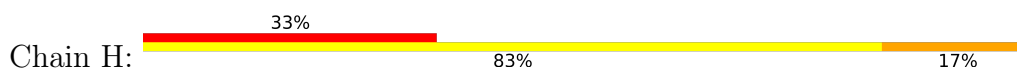
- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



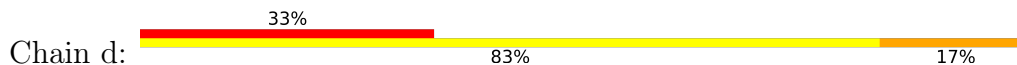
- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



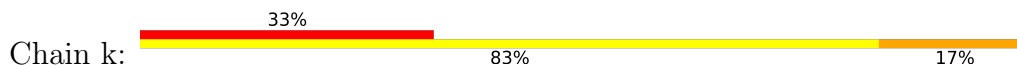
- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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





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

Chain D:  50% 50%

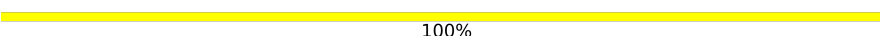


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%



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

Chain G:  100%



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

Chain U:  100% 100%



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

Chain V:  50% 50%

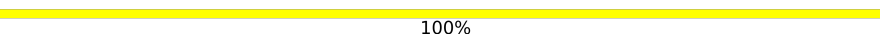


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  50% 50%

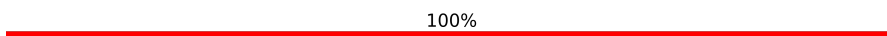


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%

NAG1
NAG2

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

Chain l:  100%
100%

NAG1
NAG2

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

Chain o:  50% 50%

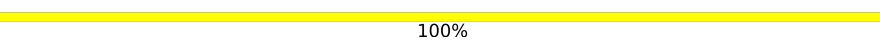
NAG1
NAG2

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

Chain p:  50% 50%

NAG1
NAG2

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

Chain q:  100%

NAG1
NAG2

- Molecule 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

Chain I:  75%
25% 50% 25%

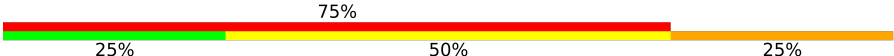
NAG1
NAG2
EMA3
MAN4

- Molecule 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

Chain L: 



- Molecule 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

Chain a: 



- Molecule 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

Chain e: 



- Molecule 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

Chain r: 



- Molecule 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

Chain u: 

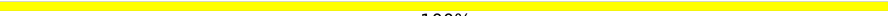


- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

NAG1
NAG2
BMA3

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  33% 33% 67%

NAG1
NAG2
BMA3

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  100%

NAG1
NAG2
BMA3

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:  33% 33% 67%

NAG1
NAG2
BMA3

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:  100%

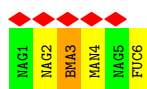
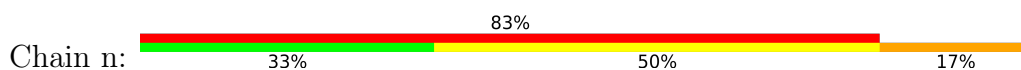
NAG1
NAG2
BMA3

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

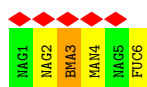
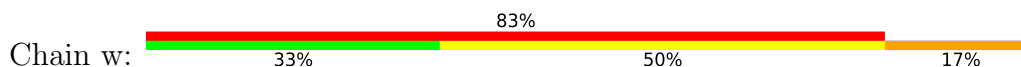
Chain P:  33% 83% 67%

NAG1
NAG2
BMA3
MAN4
NAG5
FUC6

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



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



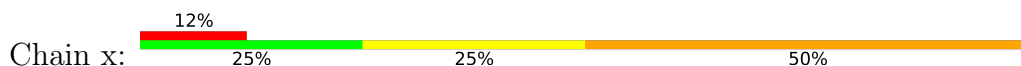
- Molecule 9: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



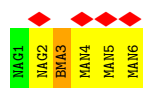
- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose



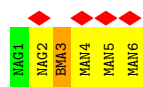
- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose



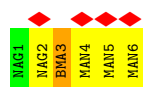
- Molecule 11: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: 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 11: 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



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of subtomograms used	32802	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 ($e^-/\text{\AA}^2$)	68	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	58000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	30.607	Depositor
Minimum map value	-12.715	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.989	Depositor
Recommended contour level	2.77	Depositor
Map size (Å)	309.59998, 309.59998, 309.59998	wwPDB
Map dimensions	120, 120, 120	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.5799997, 2.5799997, 2.5799997	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, NAG, FUC, GAL, 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	1/3652 (0.0%)	0.56	0/4963
1	N	0.34	1/3652 (0.0%)	0.56	0/4963
1	Y	0.34	1/3652 (0.0%)	0.56	0/4963
2	B	0.48	0/1155	0.73	2/1567 (0.1%)
2	O	0.49	0/1155	0.73	2/1567 (0.1%)
2	Z	0.48	0/1155	0.74	2/1567 (0.1%)
All	All	0.38	3/14421 (0.0%)	0.61	6/19590 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	497	ALA	C-N	-5.87	1.27	1.33
1	Y	497	ALA	C-N	-5.86	1.27	1.33
1	A	497	ALA	C-N	-5.83	1.27	1.33

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	635	ILE	N-CA-C	-10.34	103.28	113.20
2	B	635	ILE	N-CA-C	-10.30	103.31	113.20
2	Z	635	ILE	N-CA-C	-10.29	103.32	113.20
2	O	560	GLU	O-C-N	-5.03	116.27	122.11
2	B	560	GLU	O-C-N	-5.02	116.29	122.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3575	0	3506	845	0
1	N	3575	0	3506	846	0
1	Y	3575	0	3506	846	0
2	B	1136	0	1122	507	0
2	O	1136	0	1122	509	0
2	Z	1136	0	1122	507	0
3	F	61	0	52	1	0
3	J	61	0	52	1	0
3	T	61	0	52	1	0
3	b	61	0	52	1	0
3	j	61	0	52	1	0
3	s	61	0	52	1	0
4	H	72	0	61	5	0
4	d	72	0	61	5	0
4	k	72	0	61	5	0
5	C	27	0	22	2	0
5	D	25	0	18	9	0
5	E	28	0	25	1	0
5	G	28	0	25	3	0
5	U	27	0	22	2	0
5	V	25	0	18	9	0
5	W	28	0	25	1	0
5	X	28	0	25	3	0
5	l	27	0	22	2	0
5	o	25	0	18	8	0
5	p	28	0	25	1	0
5	q	28	0	25	3	0
6	I	50	0	43	7	0
6	L	45	0	31	5	0
6	a	50	0	43	6	0
6	e	45	0	31	5	0
6	r	50	0	43	7	0
6	u	45	0	31	5	0
7	K	37	0	30	5	0
7	M	39	0	34	5	0
7	c	37	0	30	5	0
7	f	39	0	34	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	t	37	0	30	6	0
7	v	39	0	34	6	0
8	P	74	0	61	15	0
8	n	74	0	61	16	0
8	w	74	0	61	16	0
9	Q	100	0	85	34	0
9	g	100	0	85	32	0
9	x	100	0	85	32	0
10	R	25	0	22	13	0
10	h	25	0	22	13	0
10	y	25	0	22	13	0
11	S	72	0	61	1	0
11	i	72	0	61	1	0
11	m	72	0	61	1	0
12	A	72	10	69	26	0
12	B	29	5	28	11	0
12	N	72	10	69	27	0
12	O	29	5	28	11	0
12	Y	72	10	69	27	0
12	Z	29	5	28	11	0
13	B	10	0	10	5	0
13	O	10	0	10	4	0
13	Z	10	0	10	4	0
All	All	16698	45	16071	3558	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 109.

The worst 5 of 3558 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:652:GLN:NE2	2:Z:538:THR:HB	1.42	1.33
2:B:637:ASN:O	2:B:641:LEU:HG	1.21	1.32
1:Y:331:ASN:HD21	7:t:1:NAG:C1	1.43	1.32
2:O:637:ASN:O	2:O:641:LEU:HG	1.22	1.31
1:A:331:ASN:HD21	7:K:1:NAG:C1	1.43	1.31

There are no symmetry-related clashes.

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	450/465 (97%)	410 (91%)	40 (9%)	0	100	100
1	N	450/465 (97%)	410 (91%)	40 (9%)	0	100	100
1	Y	450/465 (97%)	410 (91%)	40 (9%)	0	100	100
2	B	140/144 (97%)	117 (84%)	21 (15%)	2 (1%)	9	40
2	O	140/144 (97%)	118 (84%)	20 (14%)	2 (1%)	9	40
2	Z	140/144 (97%)	118 (84%)	20 (14%)	2 (1%)	9	40
All	All	1770/1827 (97%)	1583 (89%)	181 (10%)	6 (0%)	37	72

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	656	ASN
2	O	656	ASN
2	Z	656	ASN
2	B	555	LEU
2	O	555	LEU

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	407/417 (98%)	388 (95%)	19 (5%)	23	45
1	N	407/417 (98%)	388 (95%)	19 (5%)	23	45
1	Y	407/417 (98%)	388 (95%)	19 (5%)	23	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	121/123 (98%)	105 (87%)	16 (13%)	4	15
2	O	121/123 (98%)	105 (87%)	16 (13%)	4	15
2	Z	121/123 (98%)	105 (87%)	16 (13%)	4	15
All	All	1584/1620 (98%)	1479 (93%)	105 (7%)	17	37

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	587	LEU
1	Y	64	GLU
2	Z	654	GLU
2	O	610	TRP
2	O	656	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	567	GLN
1	Y	331	ASN
2	O	616	ASN
1	Y	66	HIS
1	Y	373	HIS

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 ⓘ

180 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	13,13,15	0.36	0	14,17,21	0.76	0
5	NAG	C	2	5	14,14,15	0.39	0	17,19,21	0.41	0
5	NAG	D	1	5	14,14,15	0.94	1 (7%)	17,19,21	1.22	2 (11%)
5	NAG	D	2	5	11,11,15	1.39	1 (9%)	7,13,21	0.98	0
5	NAG	E	1	5	14,14,15	0.37	0	17,19,21	0.36	0
5	NAG	E	2	5	14,14,15	0.41	0	17,19,21	0.48	0
3	NAG	F	1	3	14,14,15	1.15	2 (14%)	17,19,21	1.17	1 (5%)
3	NAG	F	2	3	14,14,15	1.18	2 (14%)	17,19,21	0.62	0
3	BMA	F	3	3	11,11,12	1.89	3 (27%)	15,15,17	1.14	2 (13%)
3	MAN	F	4	3	11,11,12	1.01	0	15,15,17	1.39	2 (13%)
3	MAN	F	5	3	11,11,12	1.56	1 (9%)	15,15,17	1.61	3 (20%)
5	NAG	G	1	5	14,14,15	0.26	0	17,19,21	0.41	0
5	NAG	G	2	5	14,14,15	0.32	0	17,19,21	0.40	0
4	NAG	H	1	4	14,14,15	0.30	0	17,19,21	0.75	1 (5%)
4	NAG	H	2	4	14,14,15	0.26	0	17,19,21	0.38	0
4	BMA	H	3	4	11,11,12	0.61	0	15,15,17	0.82	0
4	MAN	H	4	4	11,11,12	0.81	1 (9%)	15,15,17	0.85	1 (6%)
4	MAN	H	5	4	11,11,12	0.53	0	15,15,17	0.96	1 (6%)
4	MAN	H	6	4	11,11,12	0.56	0	15,15,17	0.95	1 (6%)
6	NAG	I	1	6	14,14,15	0.54	0	17,19,21	0.70	0
6	NAG	I	2	6	14,14,15	0.35	0	17,19,21	0.43	0
6	BMA	I	3	6	11,11,12	0.70	0	15,15,17	0.73	0
6	MAN	I	4	6	11,11,12	0.69	0	15,15,17	0.81	1 (6%)
3	NAG	J	1	3	14,14,15	1.17	2 (14%)	17,19,21	1.17	1 (5%)
3	NAG	J	2	3	14,14,15	1.20	2 (14%)	17,19,21	0.63	0
3	BMA	J	3	3	11,11,12	1.89	3 (27%)	15,15,17	1.13	1 (6%)
3	MAN	J	4	3	11,11,12	1.00	0	15,15,17	1.40	1 (6%)
3	MAN	J	5	3	11,11,12	1.56	1 (9%)	15,15,17	1.60	3 (20%)
7	NAG	K	1	7	14,14,15	1.24	1 (7%)	17,19,21	0.86	0
7	NAG	K	2	7	14,14,15	0.43	0	17,19,21	0.76	0
7	BMA	K	3	7	9,9,12	1.28	1 (11%)	11,11,17	1.53	2 (18%)
6	NAG	L	1	6	13,13,15	0.35	0	16,18,21	0.47	0
6	NAG	L	2	6	13,13,15	0.52	0	14,17,21	0.93	1 (7%)
6	BMA	L	3	6	8,8,12	0.97	1 (12%)	8,10,17	1.83	3 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	L	4	6	11,11,12	0.55	0	15,15,17	0.87	1 (6%)
7	NAG	M	1	7	14,14,15	0.65	0	17,19,21	0.55	0
7	NAG	M	2	7	14,14,15	0.53	0	17,19,21	0.51	0
7	BMA	M	3	7	11,11,12	0.50	0	15,15,17	0.84	0
8	NAG	P	1	8	14,14,15	0.20	0	17,19,21	0.51	0
8	NAG	P	2	8	14,14,15	0.21	0	17,19,21	0.61	0
8	BMA	P	3	8	11,11,12	1.01	1 (9%)	15,15,17	0.86	0
8	MAN	P	4	8	11,11,12	0.75	1 (9%)	15,15,17	1.11	1 (6%)
8	NAG	P	5	8	14,14,15	0.43	0	17,19,21	0.47	0
8	FUC	P	6	8	10,10,11	0.86	0	14,14,16	0.91	0
9	NAG	Q	1	9	14,14,15	0.94	1 (7%)	17,19,21	1.58	5 (29%)
9	NAG	Q	2	9	14,14,15	1.13	1 (7%)	17,19,21	1.29	2 (11%)
9	BMA	Q	3	9	11,11,12	0.72	0	15,15,17	1.03	1 (6%)
9	MAN	Q	4	9	11,11,12	1.14	2 (18%)	15,15,17	1.24	2 (13%)
9	NAG	Q	5	9	14,14,15	0.19	0	17,19,21	0.49	0
9	GAL	Q	6	9	11,11,12	0.49	0	15,15,17	0.81	0
9	NAG	Q	7	9	14,14,15	0.68	0	17,19,21	0.47	0
9	GAL	Q	8	9	11,11,12	0.48	0	15,15,17	0.64	0
10	MAN	R	1	10	11,11,12	0.91	1 (9%)	15,15,17	1.46	4 (26%)
10	NAG	R	2	10	14,14,15	0.97	1 (7%)	17,19,21	1.31	1 (5%)
11	NAG	S	1	11	14,14,15	0.27	0	17,19,21	0.37	0
11	NAG	S	2	11	14,14,15	0.50	0	17,19,21	0.63	0
11	BMA	S	3	11	11,11,12	0.64	0	15,15,17	1.01	1 (6%)
11	MAN	S	4	11	11,11,12	0.93	1 (9%)	15,15,17	1.24	3 (20%)
11	MAN	S	5	11	11,11,12	0.65	0	15,15,17	0.94	1 (6%)
11	MAN	S	6	11	11,11,12	0.60	0	15,15,17	1.04	2 (13%)
3	NAG	T	1	3	14,14,15	1.13	2 (14%)	17,19,21	1.17	1 (5%)
3	NAG	T	2	3	14,14,15	1.18	2 (14%)	17,19,21	0.62	0
3	BMA	T	3	3	11,11,12	1.88	3 (27%)	15,15,17	1.15	2 (13%)
3	MAN	T	4	3	11,11,12	1.02	0	15,15,17	1.39	2 (13%)
3	MAN	T	5	3	11,11,12	1.56	1 (9%)	15,15,17	1.61	3 (20%)
5	NAG	U	1	5	13,13,15	0.37	0	14,17,21	0.75	0
5	NAG	U	2	5	14,14,15	0.39	0	17,19,21	0.40	0
5	NAG	V	1	5	14,14,15	0.94	1 (7%)	17,19,21	1.22	3 (17%)
5	NAG	V	2	5	11,11,15	1.39	1 (9%)	7,13,21	0.98	0
5	NAG	W	1	5	14,14,15	0.35	0	17,19,21	0.36	0
5	NAG	W	2	5	14,14,15	0.41	0	17,19,21	0.48	0
5	NAG	X	1	5	14,14,15	0.26	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	X	2	5	14,14,15	0.31	0	17,19,21	0.40	0
6	NAG	a	1	6	14,14,15	0.55	0	17,19,21	0.69	0
6	NAG	a	2	6	14,14,15	0.34	0	17,19,21	0.43	0
6	BMA	a	3	6	11,11,12	0.71	0	15,15,17	0.73	0
6	MAN	a	4	6	11,11,12	0.69	0	15,15,17	0.81	1 (6%)
3	NAG	b	1	3	14,14,15	1.18	2 (14%)	17,19,21	1.17	1 (5%)
3	NAG	b	2	3	14,14,15	1.20	2 (14%)	17,19,21	0.63	0
3	BMA	b	3	3	11,11,12	1.88	3 (27%)	15,15,17	1.14	1 (6%)
3	MAN	b	4	3	11,11,12	1.00	0	15,15,17	1.40	1 (6%)
3	MAN	b	5	3	11,11,12	1.56	1 (9%)	15,15,17	1.60	3 (20%)
7	NAG	c	1	7	14,14,15	1.24	1 (7%)	17,19,21	0.86	0
7	NAG	c	2	7	14,14,15	0.42	0	17,19,21	0.77	0
7	BMA	c	3	7	9,9,12	1.29	1 (11%)	11,11,17	1.53	3 (27%)
4	NAG	d	1	4	14,14,15	0.30	0	17,19,21	0.75	1 (5%)
4	NAG	d	2	4	14,14,15	0.28	0	17,19,21	0.38	0
4	BMA	d	3	4	11,11,12	0.60	0	15,15,17	0.82	0
4	MAN	d	4	4	11,11,12	0.81	1 (9%)	15,15,17	0.85	1 (6%)
4	MAN	d	5	4	11,11,12	0.53	0	15,15,17	0.96	1 (6%)
4	MAN	d	6	4	11,11,12	0.56	0	15,15,17	0.96	2 (13%)
6	NAG	e	1	6	13,13,15	0.36	0	16,18,21	0.48	0
6	NAG	e	2	6	13,13,15	0.52	0	14,17,21	0.93	1 (7%)
6	BMA	e	3	6	8,8,12	0.98	1 (12%)	8,10,17	1.82	3 (37%)
6	MAN	e	4	6	11,11,12	0.54	0	15,15,17	0.87	1 (6%)
7	NAG	f	1	7	14,14,15	0.65	0	17,19,21	0.55	0
7	NAG	f	2	7	14,14,15	0.53	0	17,19,21	0.51	0
7	BMA	f	3	7	11,11,12	0.50	0	15,15,17	0.84	0
9	NAG	g	1	9	14,14,15	0.94	1 (7%)	17,19,21	1.59	5 (29%)
9	NAG	g	2	9	14,14,15	1.13	1 (7%)	17,19,21	1.29	2 (11%)
9	BMA	g	3	9	11,11,12	0.71	0	15,15,17	1.03	1 (6%)
9	MAN	g	4	9	11,11,12	1.13	2 (18%)	15,15,17	1.25	2 (13%)
9	NAG	g	5	9	14,14,15	0.19	0	17,19,21	0.48	0
9	GAL	g	6	9	11,11,12	0.48	0	15,15,17	0.80	0
9	NAG	g	7	9	14,14,15	0.69	1 (7%)	17,19,21	0.47	0
9	GAL	g	8	9	11,11,12	0.47	0	15,15,17	0.64	0
10	MAN	h	1	10	11,11,12	0.90	1 (9%)	15,15,17	1.46	4 (26%)
10	NAG	h	2	10	14,14,15	0.97	1 (7%)	17,19,21	1.32	1 (5%)
11	NAG	i	1	11	14,14,15	0.26	0	17,19,21	0.37	0
11	NAG	i	2	11	14,14,15	0.49	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BMA	i	3	11	11,11,12	0.65	0	15,15,17	1.01	1 (6%)
11	MAN	i	4	11	11,11,12	0.93	1 (9%)	15,15,17	1.25	3 (20%)
11	MAN	i	5	11	11,11,12	0.64	0	15,15,17	0.94	1 (6%)
11	MAN	i	6	11	11,11,12	0.61	0	15,15,17	1.03	2 (13%)
3	NAG	j	1	3	14,14,15	1.15	2 (14%)	17,19,21	1.17	1 (5%)
3	NAG	j	2	3	14,14,15	1.19	2 (14%)	17,19,21	0.63	0
3	BMA	j	3	3	11,11,12	1.89	3 (27%)	15,15,17	1.14	2 (13%)
3	MAN	j	4	3	11,11,12	1.01	0	15,15,17	1.39	2 (13%)
3	MAN	j	5	3	11,11,12	1.55	1 (9%)	15,15,17	1.61	3 (20%)
4	NAG	k	1	4	14,14,15	0.30	0	17,19,21	0.76	1 (5%)
4	NAG	k	2	4	14,14,15	0.28	0	17,19,21	0.38	0
4	BMA	k	3	4	11,11,12	0.61	0	15,15,17	0.82	0
4	MAN	k	4	4	11,11,12	0.80	1 (9%)	15,15,17	0.85	1 (6%)
4	MAN	k	5	4	11,11,12	0.54	0	15,15,17	0.96	1 (6%)
4	MAN	k	6	4	11,11,12	0.56	0	15,15,17	0.95	1 (6%)
5	NAG	l	1	5	13,13,15	0.36	0	14,17,21	0.76	0
5	NAG	l	2	5	14,14,15	0.39	0	17,19,21	0.41	0
11	NAG	m	1	11	14,14,15	0.26	0	17,19,21	0.36	0
11	NAG	m	2	11	14,14,15	0.50	0	17,19,21	0.63	0
11	BMA	m	3	11	11,11,12	0.63	0	15,15,17	1.01	1 (6%)
11	MAN	m	4	11	11,11,12	0.94	1 (9%)	15,15,17	1.25	3 (20%)
11	MAN	m	5	11	11,11,12	0.65	0	15,15,17	0.94	1 (6%)
11	MAN	m	6	11	11,11,12	0.61	0	15,15,17	1.03	2 (13%)
8	NAG	n	1	8	14,14,15	0.20	0	17,19,21	0.51	0
8	NAG	n	2	8	14,14,15	0.21	0	17,19,21	0.61	0
8	BMA	n	3	8	11,11,12	1.01	1 (9%)	15,15,17	0.86	0
8	MAN	n	4	8	11,11,12	0.76	1 (9%)	15,15,17	1.12	1 (6%)
8	NAG	n	5	8	14,14,15	0.42	0	17,19,21	0.47	0
8	FUC	n	6	8	10,10,11	0.85	0	14,14,16	0.91	0
5	NAG	o	1	5	14,14,15	0.94	1 (7%)	17,19,21	1.22	2 (11%)
5	NAG	o	2	5	11,11,15	1.38	1 (9%)	7,13,21	0.99	0
5	NAG	p	1	5	14,14,15	0.38	0	17,19,21	0.36	0
5	NAG	p	2	5	14,14,15	0.42	0	17,19,21	0.48	0
5	NAG	q	1	5	14,14,15	0.25	0	17,19,21	0.42	0
5	NAG	q	2	5	14,14,15	0.31	0	17,19,21	0.40	0
6	NAG	r	1	6	14,14,15	0.54	0	17,19,21	0.70	0
6	NAG	r	2	6	14,14,15	0.34	0	17,19,21	0.43	0
6	BMA	r	3	6	11,11,12	0.69	0	15,15,17	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	r	4	6	11,11,12	0.69	0	15,15,17	0.81	1 (6%)
3	NAG	s	1	3	14,14,15	1.17	2 (14%)	17,19,21	1.17	1 (5%)
3	NAG	s	2	3	14,14,15	1.19	2 (14%)	17,19,21	0.63	0
3	BMA	s	3	3	11,11,12	1.90	3 (27%)	15,15,17	1.13	1 (6%)
3	MAN	s	4	3	11,11,12	1.00	0	15,15,17	1.40	2 (13%)
3	MAN	s	5	3	11,11,12	1.57	1 (9%)	15,15,17	1.61	3 (20%)
7	NAG	t	1	7	14,14,15	1.23	1 (7%)	17,19,21	0.86	0
7	NAG	t	2	7	14,14,15	0.41	0	17,19,21	0.76	0
7	BMA	t	3	7	9,9,12	1.28	1 (11%)	11,11,17	1.52	2 (18%)
6	NAG	u	1	6	13,13,15	0.36	0	16,18,21	0.47	0
6	NAG	u	2	6	13,13,15	0.52	0	14,17,21	0.93	1 (7%)
6	BMA	u	3	6	8,8,12	0.98	1 (12%)	8,10,17	1.82	3 (37%)
6	MAN	u	4	6	11,11,12	0.56	0	15,15,17	0.87	1 (6%)
7	NAG	v	1	7	14,14,15	0.64	0	17,19,21	0.55	0
7	NAG	v	2	7	14,14,15	0.53	0	17,19,21	0.50	0
7	BMA	v	3	7	11,11,12	0.50	0	15,15,17	0.84	0
8	NAG	w	1	8	14,14,15	0.20	0	17,19,21	0.51	0
8	NAG	w	2	8	14,14,15	0.21	0	17,19,21	0.61	0
8	BMA	w	3	8	11,11,12	1.00	1 (9%)	15,15,17	0.86	0
8	MAN	w	4	8	11,11,12	0.76	1 (9%)	15,15,17	1.11	1 (6%)
8	NAG	w	5	8	14,14,15	0.43	0	17,19,21	0.46	0
8	FUC	w	6	8	10,10,11	0.87	0	14,14,16	0.91	0
9	NAG	x	1	9	14,14,15	0.94	1 (7%)	17,19,21	1.57	5 (29%)
9	NAG	x	2	9	14,14,15	1.14	1 (7%)	17,19,21	1.29	2 (11%)
9	BMA	x	3	9	11,11,12	0.71	0	15,15,17	1.03	1 (6%)
9	MAN	x	4	9	11,11,12	1.13	2 (18%)	15,15,17	1.24	2 (13%)
9	NAG	x	5	9	14,14,15	0.19	0	17,19,21	0.48	0
9	GAL	x	6	9	11,11,12	0.49	0	15,15,17	0.81	0
9	NAG	x	7	9	14,14,15	0.67	0	17,19,21	0.48	0
9	GAL	x	8	9	11,11,12	0.48	0	15,15,17	0.64	0
10	MAN	y	1	10	11,11,12	0.90	1 (9%)	15,15,17	1.46	4 (26%)
10	NAG	y	2	10	14,14,15	0.98	1 (7%)	17,19,21	1.31	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1	5	-	2/5/22/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1
5	NAG	D	1	5	-	2/6/23/26	0/1/1/1
5	NAG	D	2	5	-	0/5/15/26	0/1/1/1
5	NAG	E	1	5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3	-	3/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
3	MAN	F	4	3	-	1/2/19/22	0/1/1/1
3	MAN	F	5	3	-	2/2/19/22	0/1/1/1
5	NAG	G	1	5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4	-	3/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1
4	MAN	H	4	4	-	1/2/19/22	0/1/1/1
4	MAN	H	5	4	-	0/2/19/22	0/1/1/1
4	MAN	H	6	4	-	1/2/19/22	0/1/1/1
6	NAG	I	1	6	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1
6	BMA	I	3	6	-	1/2/19/22	0/1/1/1
6	MAN	I	4	6	-	2/2/19/22	0/1/1/1
3	NAG	J	1	3	-	3/6/23/26	0/1/1/1
3	NAG	J	2	3	-	1/6/23/26	0/1/1/1
3	BMA	J	3	3	-	2/2/19/22	0/1/1/1
3	MAN	J	4	3	-	1/2/19/22	0/1/1/1
3	MAN	J	5	3	-	2/2/19/22	0/1/1/1
7	NAG	K	1	7	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	0/6/23/26	0/1/1/1
7	BMA	K	3	7	-	0/2/13/22	0/1/1/1
6	NAG	L	1	6	-	1/4/21/26	0/1/1/1
6	NAG	L	2	6	-	2/5/22/26	0/1/1/1
6	BMA	L	3	6	-	-	0/1/1/1
6	MAN	L	4	6	-	0/2/19/22	0/1/1/1
7	NAG	M	1	7	-	0/6/23/26	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
8	NAG	P	1	8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	P	2	8	-	2/6/23/26	0/1/1/1
8	BMA	P	3	8	-	2/2/19/22	0/1/1/1
8	MAN	P	4	8	-	2/2/19/22	0/1/1/1
8	NAG	P	5	8	-	2/6/23/26	0/1/1/1
8	FUC	P	6	8	-	-	0/1/1/1
9	NAG	Q	1	9	-	2/6/23/26	0/1/1/1
9	NAG	Q	2	9	-	4/6/23/26	0/1/1/1
9	BMA	Q	3	9	-	2/2/19/22	1/1/1/1
9	MAN	Q	4	9	-	0/2/19/22	0/1/1/1
9	NAG	Q	5	9	-	4/6/23/26	0/1/1/1
9	GAL	Q	6	9	-	0/2/19/22	0/1/1/1
9	NAG	Q	7	9	-	0/6/23/26	0/1/1/1
9	GAL	Q	8	9	-	1/2/19/22	0/1/1/1
10	MAN	R	1	10	-	2/2/19/22	0/1/1/1
10	NAG	R	2	10	-	3/6/23/26	0/1/1/1
11	NAG	S	1	11	-	0/6/23/26	0/1/1/1
11	NAG	S	2	11	-	0/6/23/26	0/1/1/1
11	BMA	S	3	11	-	2/2/19/22	0/1/1/1
11	MAN	S	4	11	-	0/2/19/22	0/1/1/1
11	MAN	S	5	11	-	0/2/19/22	0/1/1/1
11	MAN	S	6	11	-	2/2/19/22	0/1/1/1
3	NAG	T	1	3	-	3/6/23/26	0/1/1/1
3	NAG	T	2	3	-	1/6/23/26	0/1/1/1
3	BMA	T	3	3	-	2/2/19/22	0/1/1/1
3	MAN	T	4	3	-	1/2/19/22	0/1/1/1
3	MAN	T	5	3	-	2/2/19/22	0/1/1/1
5	NAG	U	1	5	-	2/5/22/26	0/1/1/1
5	NAG	U	2	5	-	2/6/23/26	0/1/1/1
5	NAG	V	1	5	-	2/6/23/26	0/1/1/1
5	NAG	V	2	5	-	0/5/15/26	0/1/1/1
5	NAG	W	1	5	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	0/6/23/26	0/1/1/1
5	NAG	X	1	5	-	0/6/23/26	0/1/1/1
5	NAG	X	2	5	-	2/6/23/26	0/1/1/1
6	NAG	a	1	6	-	2/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
6	BMA	a	3	6	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	a	4	6	-	2/2/19/22	0/1/1/1
3	NAG	b	1	3	-	3/6/23/26	0/1/1/1
3	NAG	b	2	3	-	1/6/23/26	0/1/1/1
3	BMA	b	3	3	-	2/2/19/22	0/1/1/1
3	MAN	b	4	3	-	1/2/19/22	0/1/1/1
3	MAN	b	5	3	-	2/2/19/22	0/1/1/1
7	NAG	c	1	7	-	2/6/23/26	0/1/1/1
7	NAG	c	2	7	-	0/6/23/26	0/1/1/1
7	BMA	c	3	7	-	0/2/13/22	0/1/1/1
4	NAG	d	1	4	-	3/6/23/26	0/1/1/1
4	NAG	d	2	4	-	2/6/23/26	0/1/1/1
4	BMA	d	3	4	-	2/2/19/22	0/1/1/1
4	MAN	d	4	4	-	1/2/19/22	0/1/1/1
4	MAN	d	5	4	-	0/2/19/22	0/1/1/1
4	MAN	d	6	4	-	1/2/19/22	0/1/1/1
6	NAG	e	1	6	-	1/4/21/26	0/1/1/1
6	NAG	e	2	6	-	2/5/22/26	0/1/1/1
6	BMA	e	3	6	-	-	0/1/1/1
6	MAN	e	4	6	-	0/2/19/22	0/1/1/1
7	NAG	f	1	7	-	0/6/23/26	0/1/1/1
7	NAG	f	2	7	-	0/6/23/26	0/1/1/1
7	BMA	f	3	7	-	0/2/19/22	0/1/1/1
9	NAG	g	1	9	-	2/6/23/26	0/1/1/1
9	NAG	g	2	9	-	4/6/23/26	0/1/1/1
9	BMA	g	3	9	-	2/2/19/22	1/1/1/1
9	MAN	g	4	9	-	0/2/19/22	0/1/1/1
9	NAG	g	5	9	-	4/6/23/26	0/1/1/1
9	GAL	g	6	9	-	0/2/19/22	0/1/1/1
9	NAG	g	7	9	-	0/6/23/26	0/1/1/1
9	GAL	g	8	9	-	1/2/19/22	0/1/1/1
10	MAN	h	1	10	-	2/2/19/22	0/1/1/1
10	NAG	h	2	10	-	3/6/23/26	0/1/1/1
11	NAG	i	1	11	-	0/6/23/26	0/1/1/1
11	NAG	i	2	11	-	0/6/23/26	0/1/1/1
11	BMA	i	3	11	-	2/2/19/22	0/1/1/1
11	MAN	i	4	11	-	0/2/19/22	0/1/1/1
11	MAN	i	5	11	-	0/2/19/22	0/1/1/1
11	MAN	i	6	11	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	j	1	3	-	3/6/23/26	0/1/1/1
3	NAG	j	2	3	-	1/6/23/26	0/1/1/1
3	BMA	j	3	3	-	2/2/19/22	0/1/1/1
3	MAN	j	4	3	-	1/2/19/22	0/1/1/1
3	MAN	j	5	3	-	2/2/19/22	0/1/1/1
4	NAG	k	1	4	-	3/6/23/26	0/1/1/1
4	NAG	k	2	4	-	1/6/23/26	0/1/1/1
4	BMA	k	3	4	-	2/2/19/22	0/1/1/1
4	MAN	k	4	4	-	1/2/19/22	0/1/1/1
4	MAN	k	5	4	-	0/2/19/22	0/1/1/1
4	MAN	k	6	4	-	1/2/19/22	0/1/1/1
5	NAG	l	1	5	-	2/5/22/26	0/1/1/1
5	NAG	l	2	5	-	2/6/23/26	0/1/1/1
11	NAG	m	1	11	-	0/6/23/26	0/1/1/1
11	NAG	m	2	11	-	0/6/23/26	0/1/1/1
11	BMA	m	3	11	-	2/2/19/22	0/1/1/1
11	MAN	m	4	11	-	0/2/19/22	0/1/1/1
11	MAN	m	5	11	-	0/2/19/22	0/1/1/1
11	MAN	m	6	11	-	2/2/19/22	0/1/1/1
8	NAG	n	1	8	-	0/6/23/26	0/1/1/1
8	NAG	n	2	8	-	2/6/23/26	0/1/1/1
8	BMA	n	3	8	-	2/2/19/22	0/1/1/1
8	MAN	n	4	8	-	2/2/19/22	0/1/1/1
8	NAG	n	5	8	-	2/6/23/26	0/1/1/1
8	FUC	n	6	8	-	-	0/1/1/1
5	NAG	o	1	5	-	2/6/23/26	0/1/1/1
5	NAG	o	2	5	-	0/5/15/26	0/1/1/1
5	NAG	p	1	5	-	2/6/23/26	0/1/1/1
5	NAG	p	2	5	-	0/6/23/26	0/1/1/1
5	NAG	q	1	5	-	0/6/23/26	0/1/1/1
5	NAG	q	2	5	-	2/6/23/26	0/1/1/1
6	NAG	r	1	6	-	2/6/23/26	0/1/1/1
6	NAG	r	2	6	-	2/6/23/26	0/1/1/1
6	BMA	r	3	6	-	1/2/19/22	0/1/1/1
6	MAN	r	4	6	-	2/2/19/22	0/1/1/1
3	NAG	s	1	3	-	3/6/23/26	0/1/1/1
3	NAG	s	2	3	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	s	3	3	-	2/2/19/22	0/1/1/1
3	MAN	s	4	3	-	1/2/19/22	0/1/1/1
3	MAN	s	5	3	-	2/2/19/22	0/1/1/1
7	NAG	t	1	7	-	2/6/23/26	0/1/1/1
7	NAG	t	2	7	-	0/6/23/26	0/1/1/1
7	BMA	t	3	7	-	0/2/13/22	0/1/1/1
6	NAG	u	1	6	-	1/4/21/26	0/1/1/1
6	NAG	u	2	6	-	2/5/22/26	0/1/1/1
6	BMA	u	3	6	-	-	0/1/1/1
6	MAN	u	4	6	-	0/2/19/22	0/1/1/1
7	NAG	v	1	7	-	0/6/23/26	0/1/1/1
7	NAG	v	2	7	-	0/6/23/26	0/1/1/1
7	BMA	v	3	7	-	0/2/19/22	0/1/1/1
8	NAG	w	1	8	-	0/6/23/26	0/1/1/1
8	NAG	w	2	8	-	2/6/23/26	0/1/1/1
8	BMA	w	3	8	-	2/2/19/22	0/1/1/1
8	MAN	w	4	8	-	2/2/19/22	0/1/1/1
8	NAG	w	5	8	-	2/6/23/26	0/1/1/1
8	FUC	w	6	8	-	-	0/1/1/1
9	NAG	x	1	9	-	2/6/23/26	0/1/1/1
9	NAG	x	2	9	-	4/6/23/26	0/1/1/1
9	BMA	x	3	9	-	2/2/19/22	1/1/1/1
9	MAN	x	4	9	-	0/2/19/22	0/1/1/1
9	NAG	x	5	9	-	4/6/23/26	0/1/1/1
9	GAL	x	6	9	-	0/2/19/22	0/1/1/1
9	NAG	x	7	9	-	0/6/23/26	0/1/1/1
9	GAL	x	8	9	-	1/2/19/22	0/1/1/1
10	MAN	y	1	10	-	2/2/19/22	0/1/1/1
10	NAG	y	2	10	-	3/6/23/26	0/1/1/1

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	c	1	NAG	O5-C1	-4.32	1.36	1.43
7	K	1	NAG	O5-C1	-4.31	1.36	1.43
7	t	1	NAG	O5-C1	-4.29	1.36	1.43
3	s	5	MAN	O5-C1	-4.26	1.36	1.43
3	J	5	MAN	O5-C1	-4.25	1.36	1.43

The worst 5 of 157 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	h	2	NAG	C1-O5-C5	4.83	118.66	112.19
10	R	2	NAG	C1-O5-C5	4.83	118.66	112.19
10	y	2	NAG	C1-O5-C5	4.82	118.65	112.19
3	s	5	MAN	C1-O5-C5	-3.94	106.91	112.19
3	T	5	MAN	C1-O5-C5	-3.93	106.92	112.19

There are no chirality outliers.

5 of 235 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C3-C2-N2-C7
3	J	1	NAG	C3-C2-N2-C7
3	T	1	NAG	C3-C2-N2-C7
3	b	1	NAG	C3-C2-N2-C7
3	j	1	NAG	C3-C2-N2-C7

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	Q	3	BMA	C1-C2-C3-C4-C5-O5
9	x	3	BMA	C1-C2-C3-C4-C5-O5
9	g	3	BMA	C1-C2-C3-C4-C5-O5

112 monomers are involved in 284 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	m	2	NAG	1	0
6	e	2	NAG	4	0
11	i	3	BMA	1	0
5	G	1	NAG	2	0
5	W	1	NAG	1	0
9	Q	1	NAG	9	0
7	M	1	NAG	2	0
9	g	3	BMA	3	0
6	a	1	NAG	5	0
9	g	4	MAN	1	0
4	k	2	NAG	1	0
5	U	1	NAG	2	0
6	u	3	BMA	3	0
5	X	2	NAG	3	0
9	x	4	MAN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Q	7	NAG	1	0
6	u	2	NAG	4	0
3	T	2	NAG	1	0
11	m	3	BMA	1	0
7	c	1	NAG	4	0
9	g	2	NAG	7	0
7	K	3	BMA	1	0
9	g	6	GAL	3	0
8	w	3	BMA	1	0
9	g	5	NAG	10	0
6	I	4	MAN	1	0
8	w	6	FUC	15	0
6	u	4	MAN	1	0
6	L	1	NAG	1	0
5	C	2	NAG	2	0
10	R	1	MAN	1	0
6	r	3	BMA	1	0
3	s	1	NAG	1	0
7	v	3	BMA	4	0
4	d	2	NAG	1	0
7	K	2	NAG	1	0
6	I	3	BMA	1	0
5	p	1	NAG	1	0
7	t	2	NAG	2	0
9	Q	5	NAG	11	0
5	X	1	NAG	2	0
11	S	3	BMA	1	0
5	V	1	NAG	9	0
9	x	6	GAL	3	0
10	h	1	MAN	1	0
6	e	1	NAG	1	0
7	c	2	NAG	1	0
3	J	1	NAG	1	0
11	i	2	NAG	1	0
4	d	3	BMA	1	0
10	y	2	NAG	12	0
9	Q	4	MAN	1	0
4	H	3	BMA	1	0
7	v	1	NAG	2	0
6	r	4	MAN	1	0
9	x	5	NAG	10	0
5	q	1	NAG	2	0

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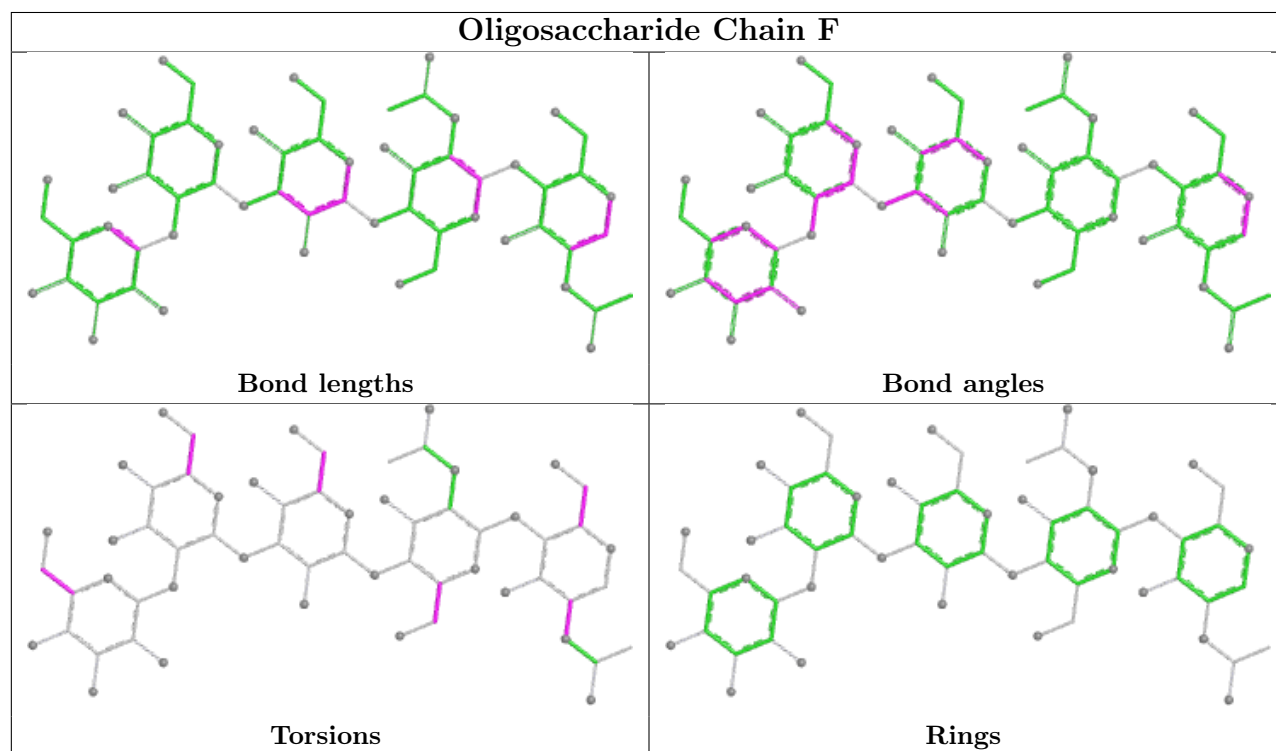
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1	NAG	2	0
8	n	3	BMA	1	0
10	R	2	NAG	12	0
5	E	1	NAG	1	0
10	y	1	MAN	1	0
3	F	2	NAG	1	0
8	P	6	FUC	15	0
7	c	3	BMA	1	0
10	h	2	NAG	12	0
9	Q	2	NAG	8	0
5	D	1	NAG	9	0
7	K	1	NAG	4	0
7	f	2	NAG	4	0
5	U	2	NAG	2	0
6	e	4	MAN	1	0
9	Q	6	GAL	3	0
4	H	2	NAG	1	0
6	L	2	NAG	4	0
8	n	2	NAG	1	0
3	b	1	NAG	1	0
5	l	2	NAG	2	0
7	M	2	NAG	3	0
4	d	1	NAG	4	0
11	S	2	NAG	1	0
6	u	1	NAG	1	0
8	w	2	NAG	1	0
6	L	4	MAN	1	0
4	k	1	NAG	4	0
7	f	1	NAG	2	0
6	r	1	NAG	6	0
9	Q	3	BMA	3	0
7	f	3	BMA	4	0
5	q	2	NAG	3	0
9	g	1	NAG	9	0
5	o	1	NAG	8	0
7	t	1	NAG	4	0
6	a	3	BMA	1	0
7	v	2	NAG	4	0
4	H	1	NAG	4	0
5	l	1	NAG	2	0
9	x	3	BMA	3	0
8	n	6	FUC	15	0

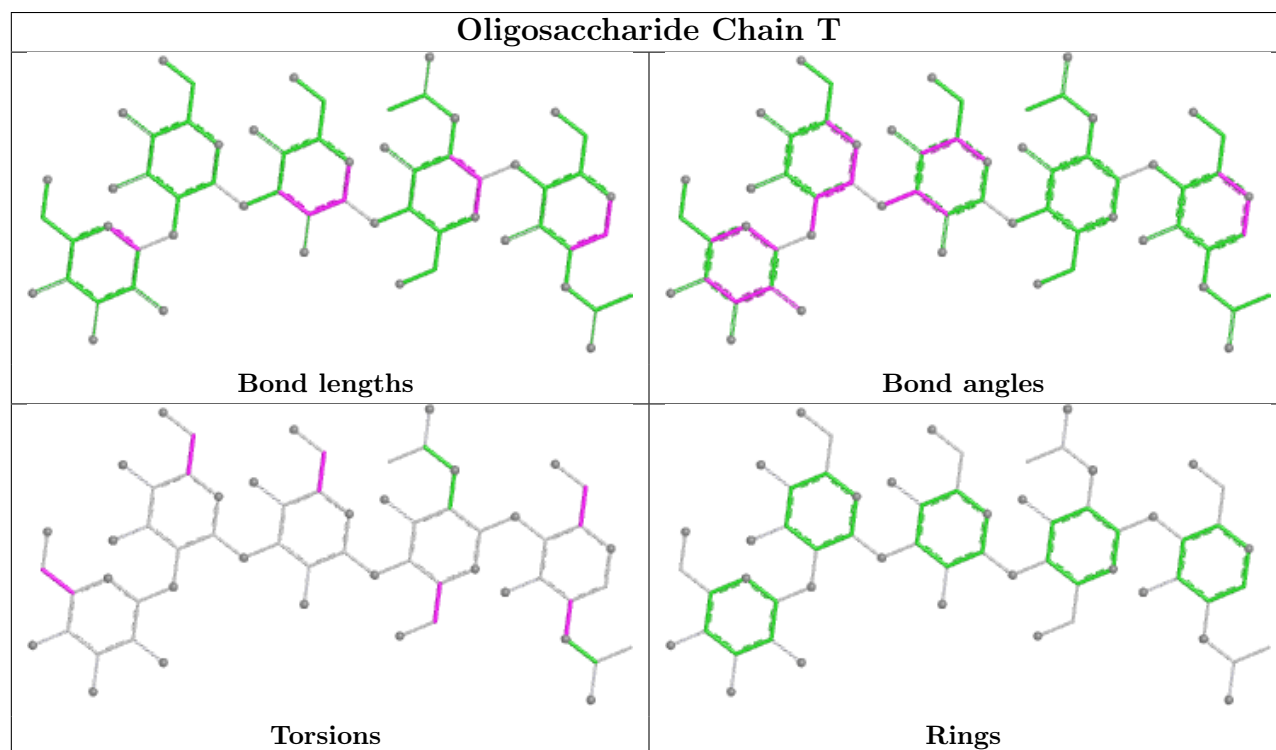
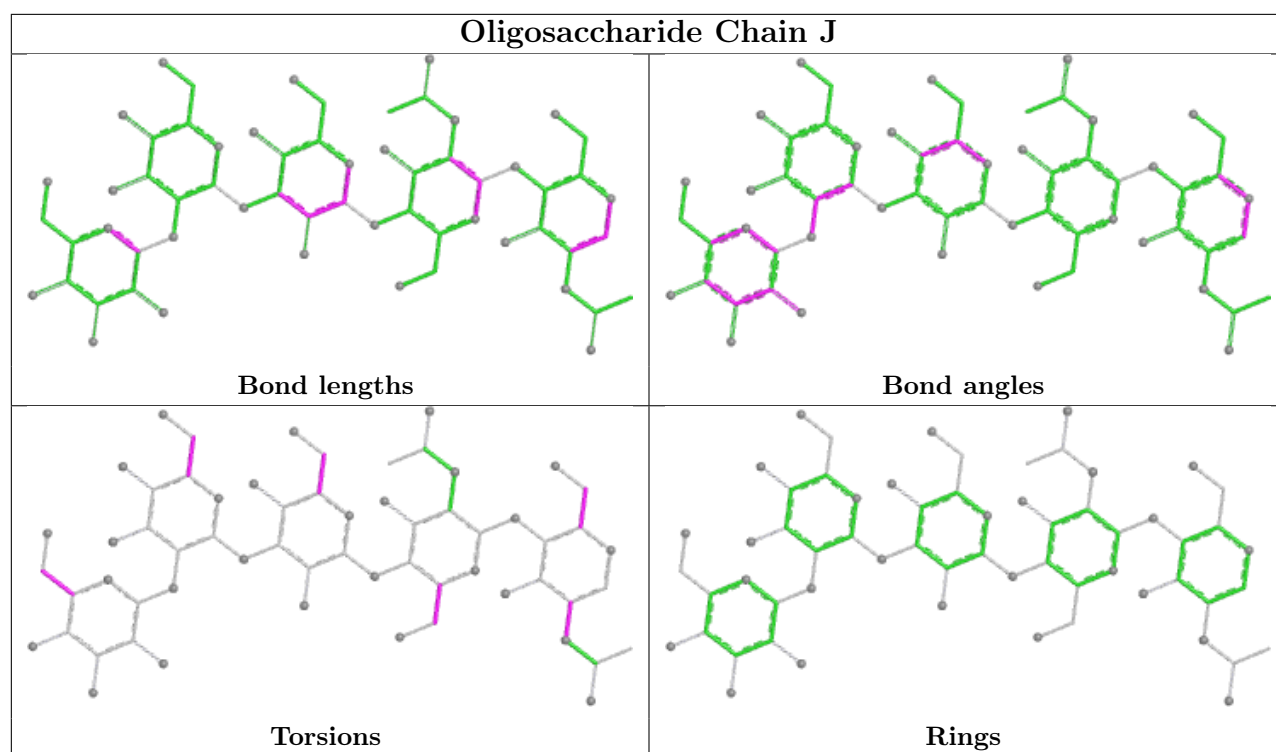
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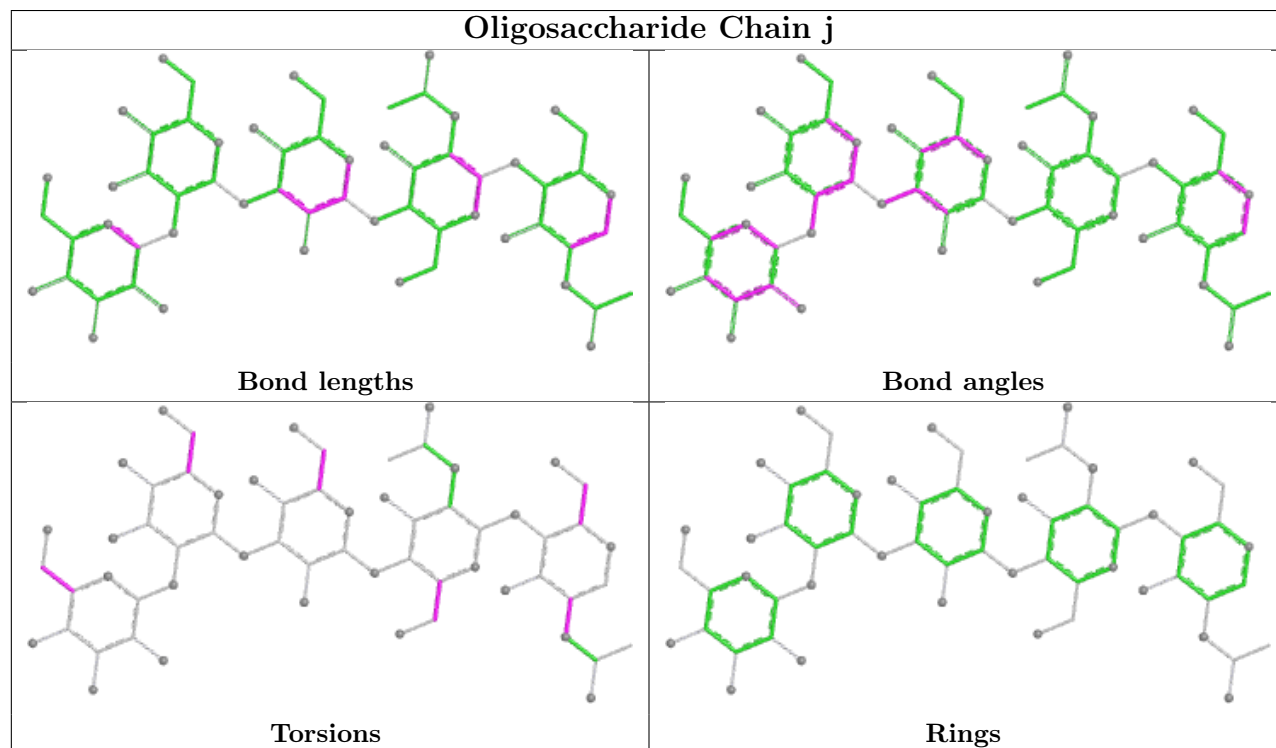
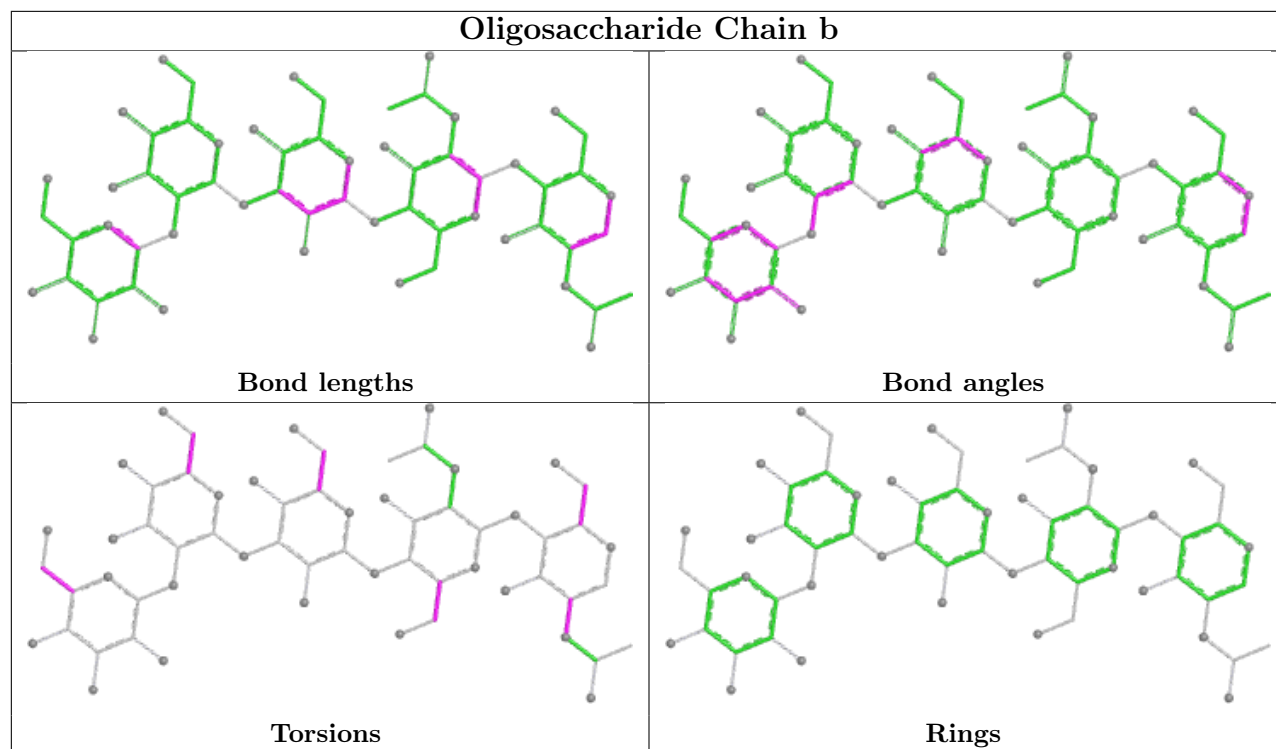
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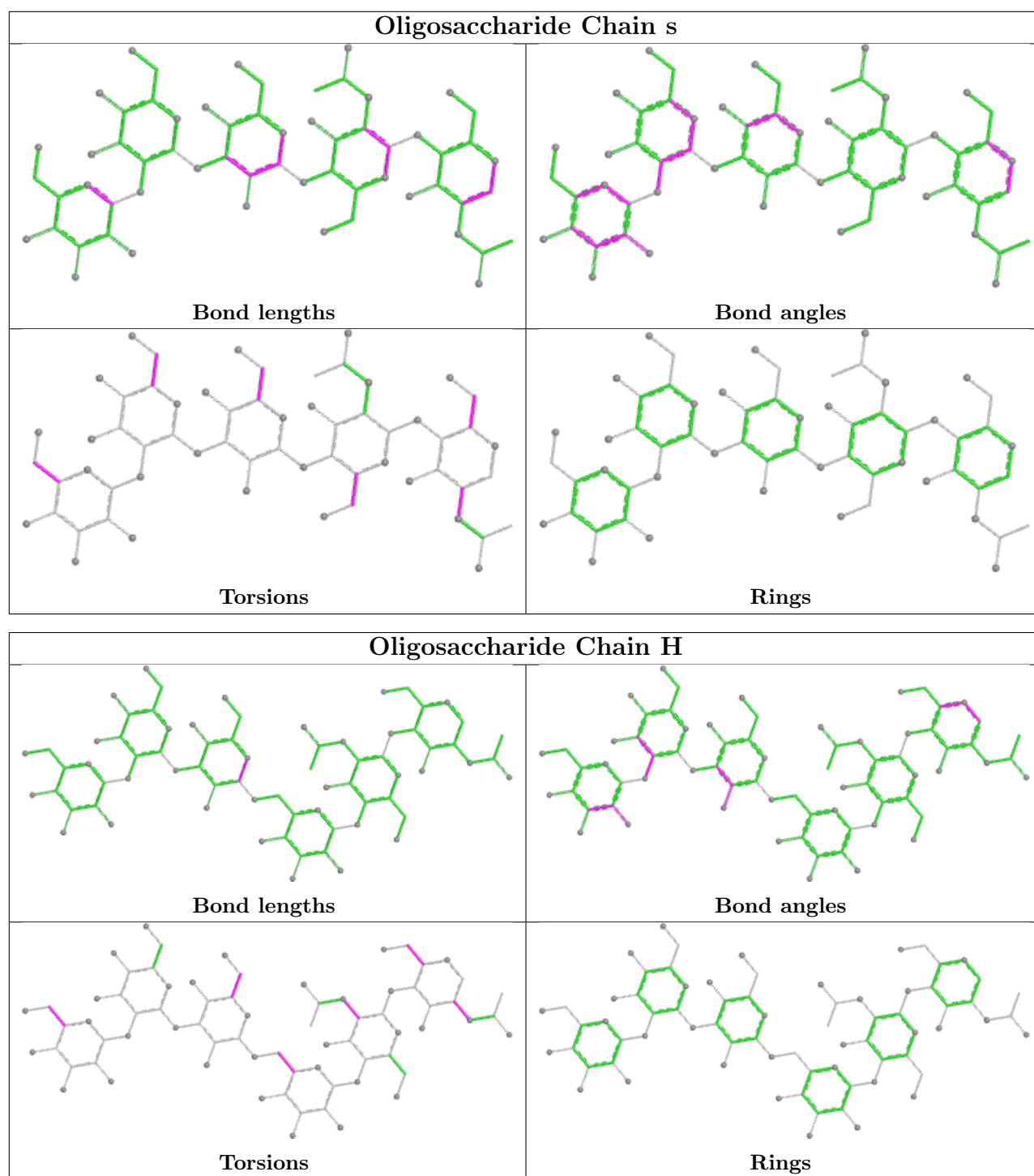
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	e	3	BMA	3	0
5	G	2	NAG	3	0
6	a	4	MAN	1	0
7	t	3	BMA	1	0
8	P	2	NAG	1	0
7	M	3	BMA	3	0
9	x	1	NAG	9	0
9	x	2	NAG	7	0
4	k	3	BMA	1	0
6	L	3	BMA	3	0
3	j	2	NAG	1	0
6	I	1	NAG	6	0
9	g	7	NAG	1	0

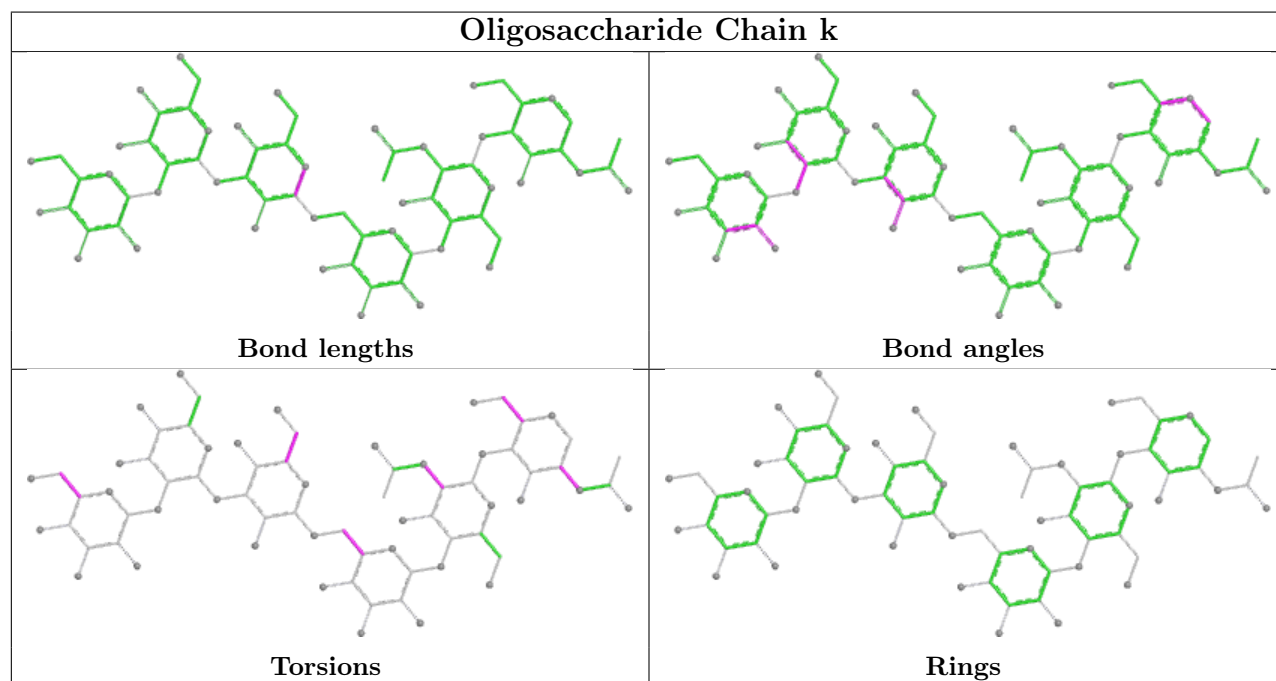
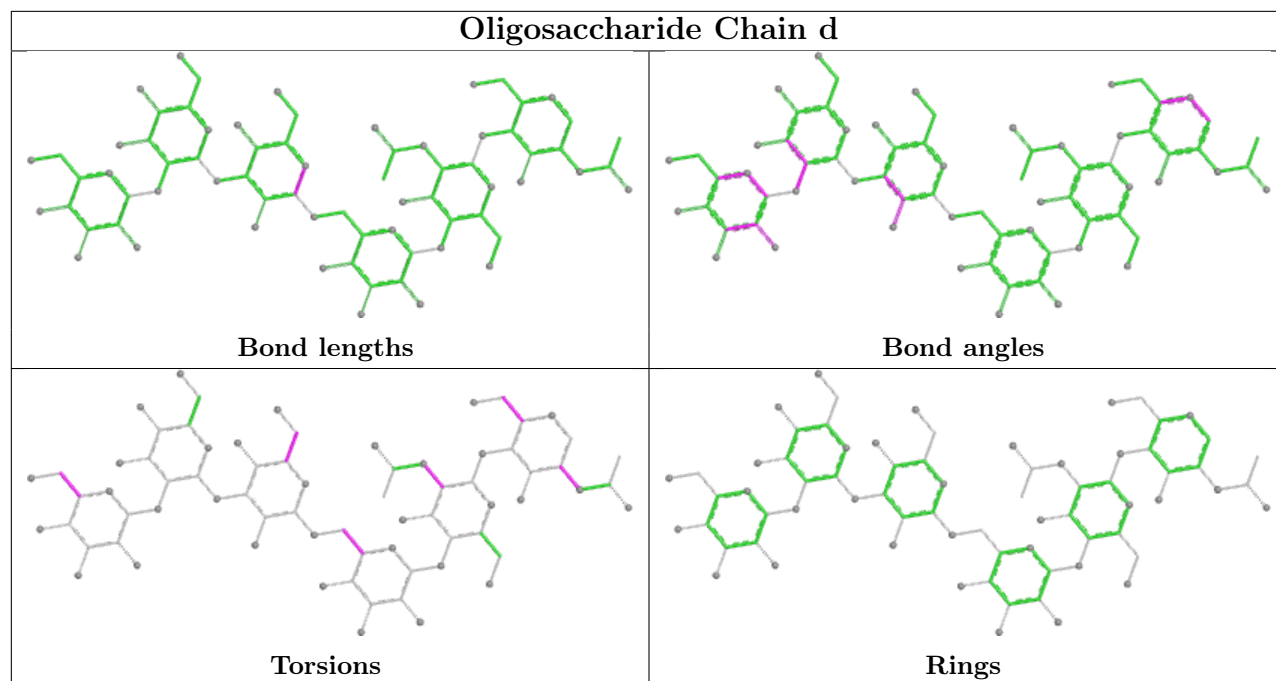
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

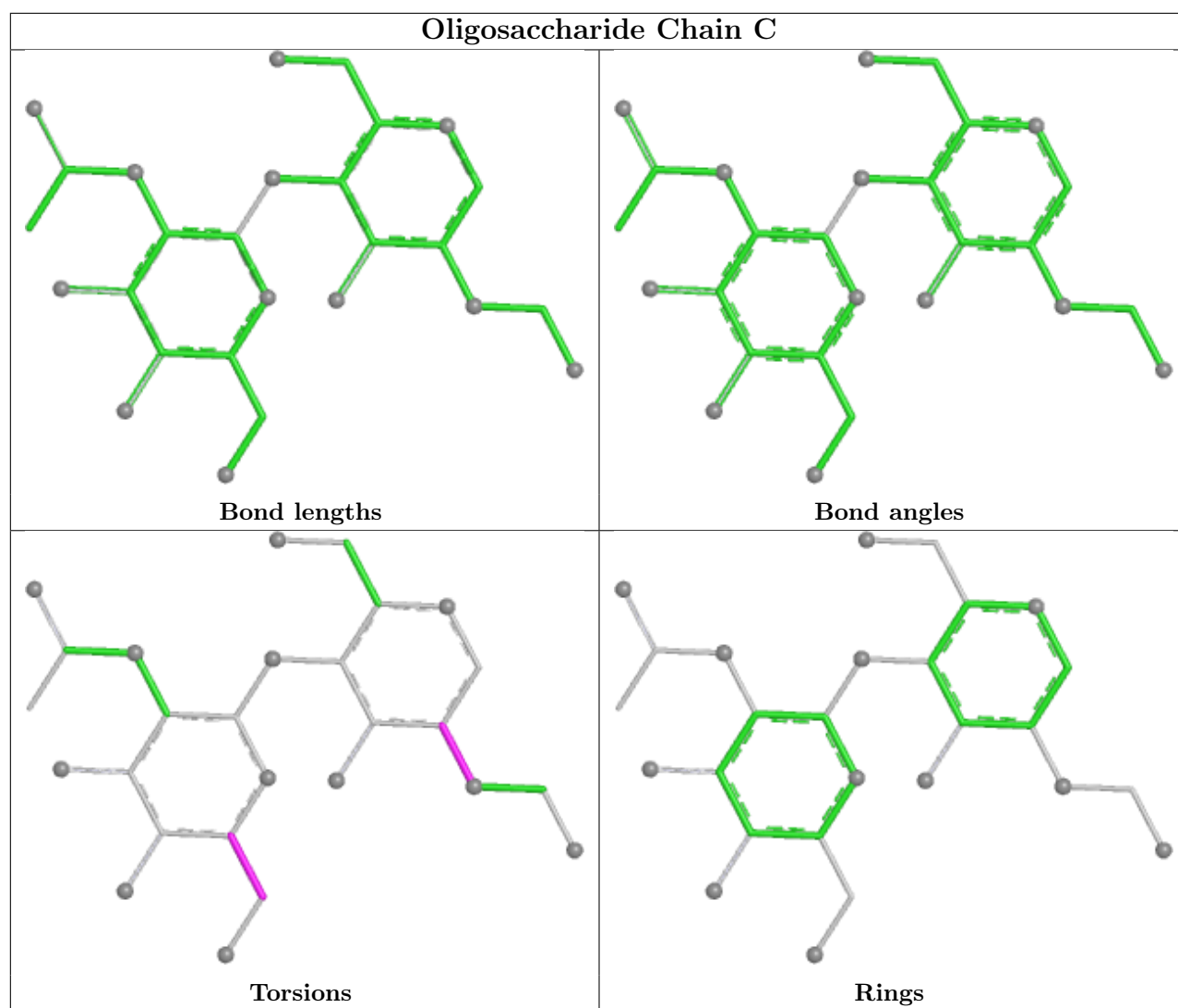


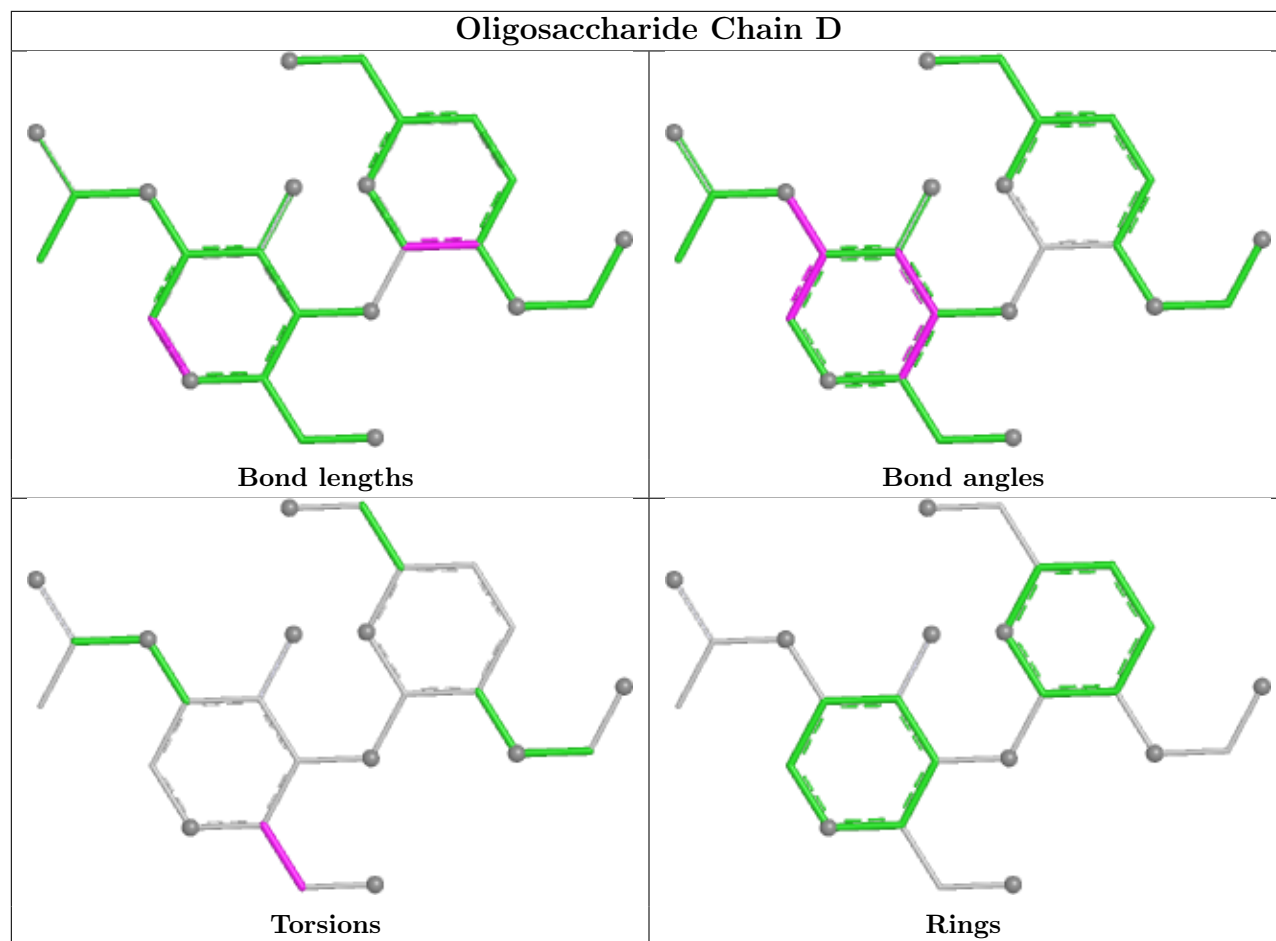


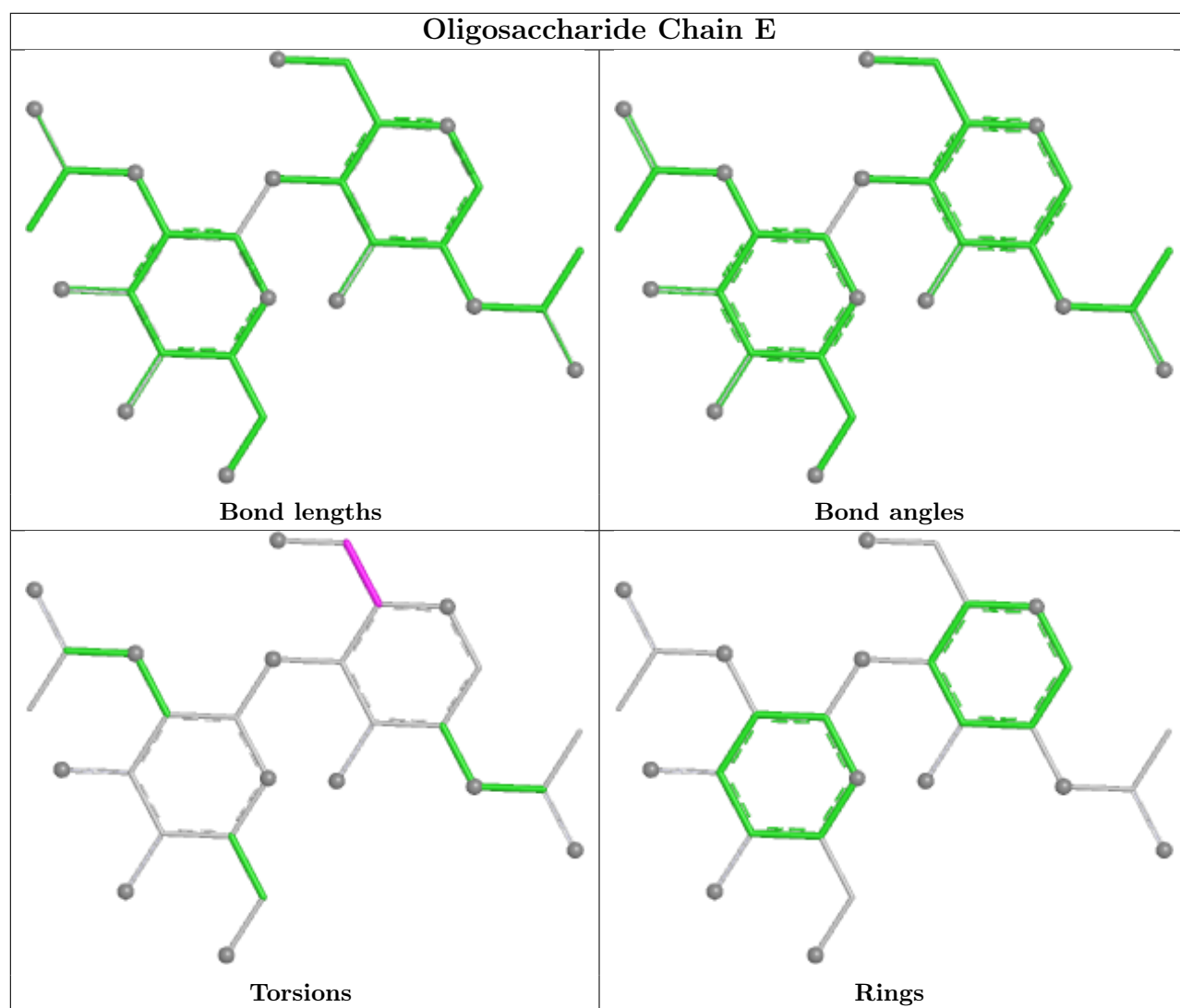


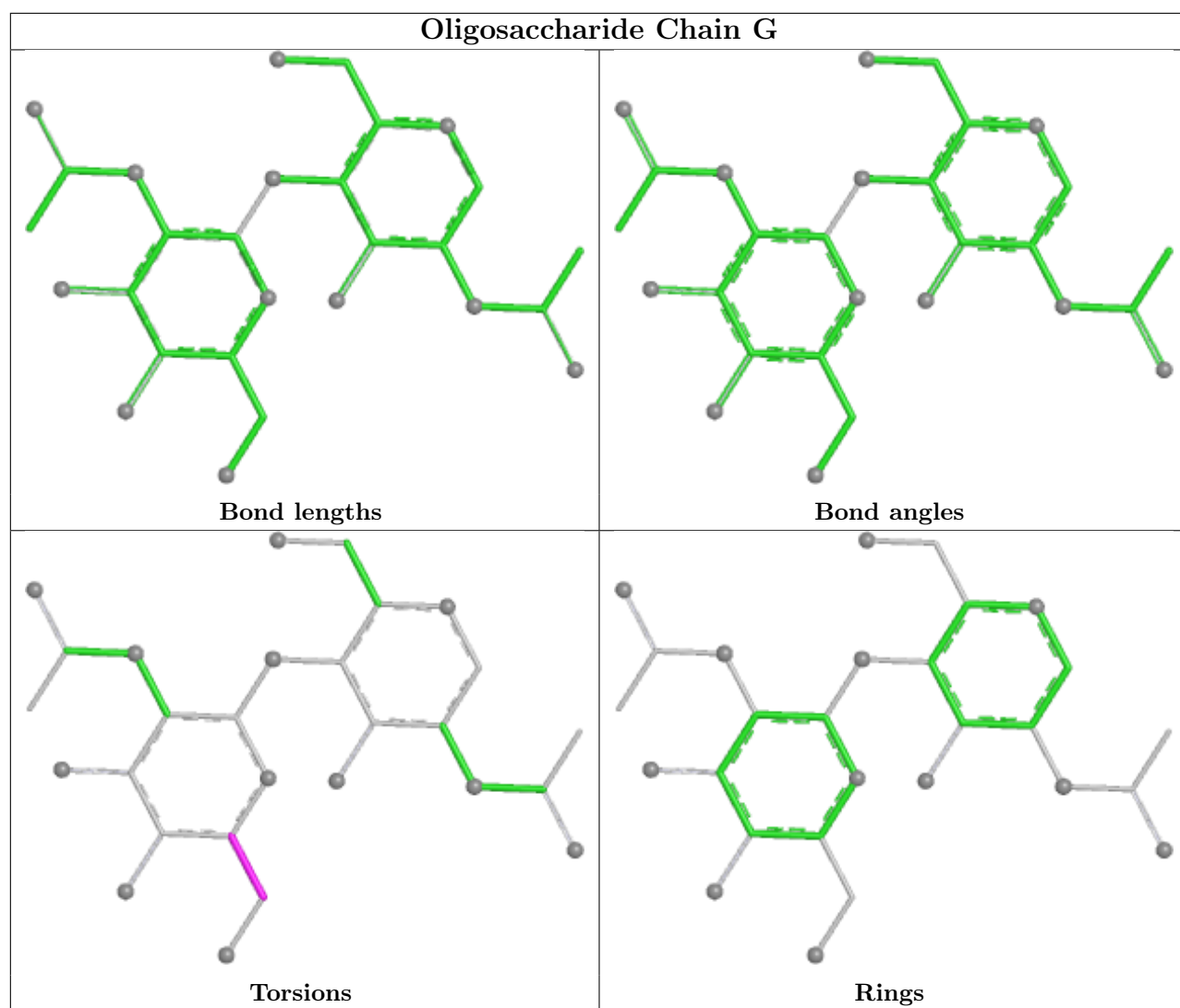


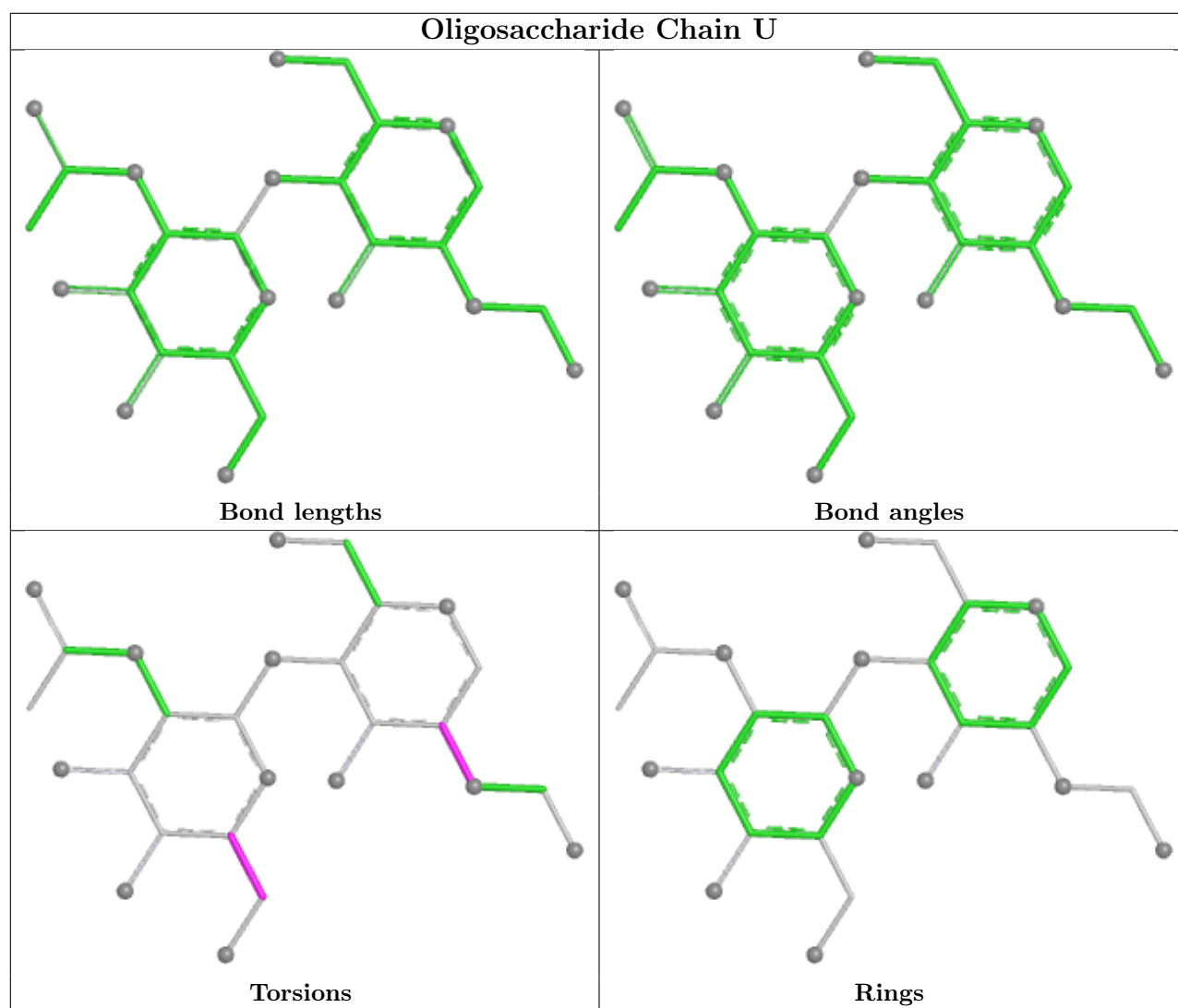


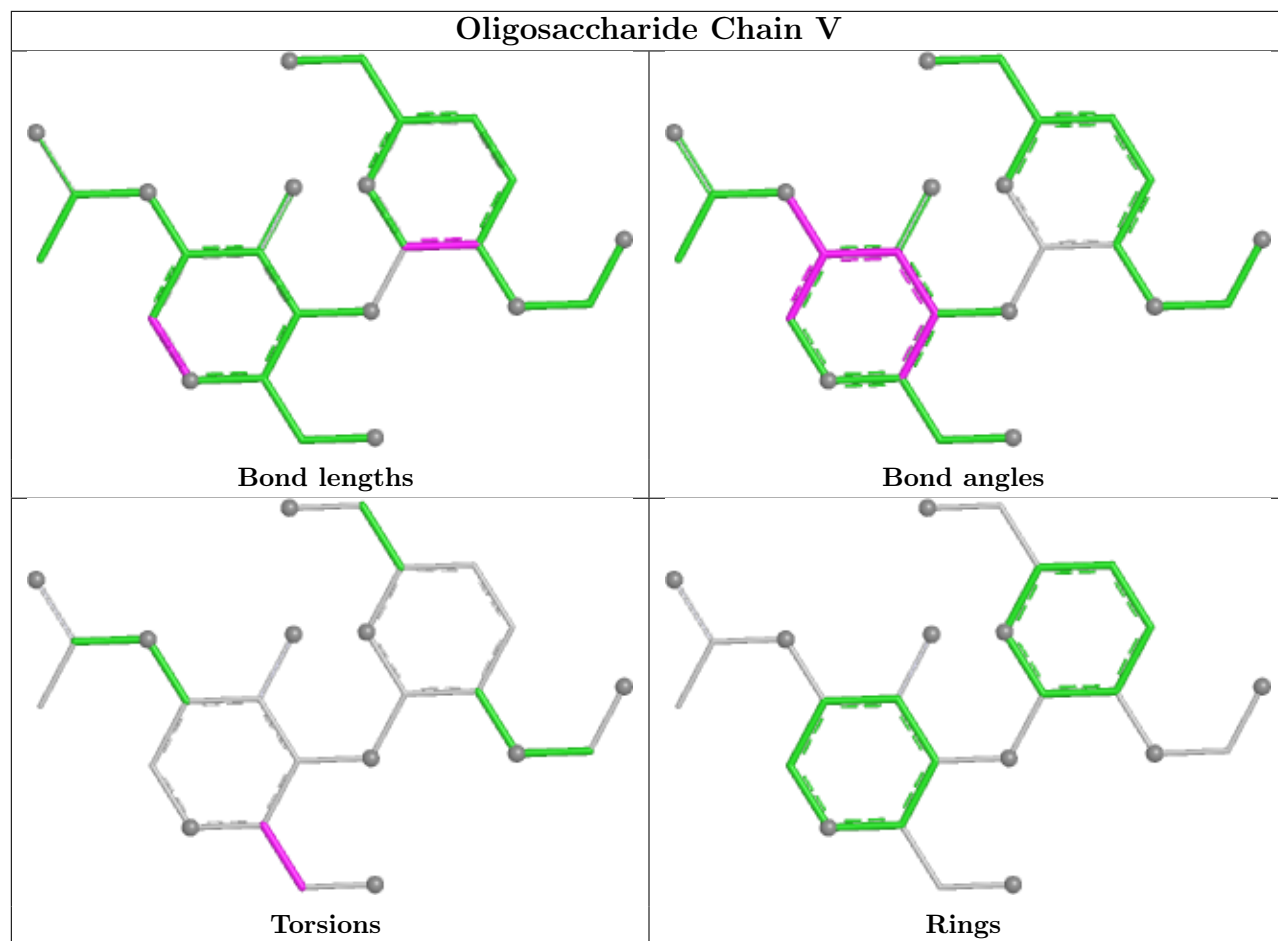


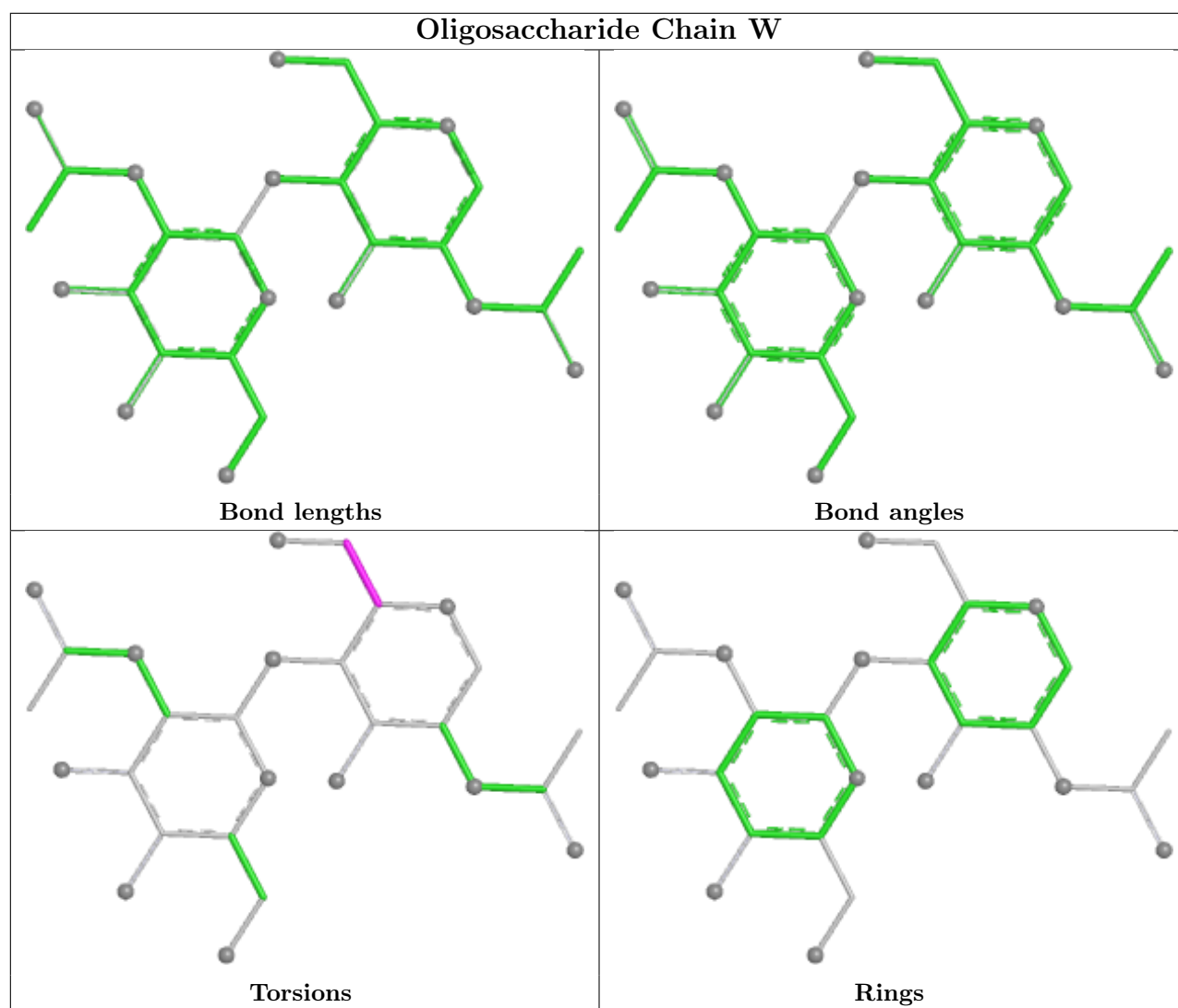


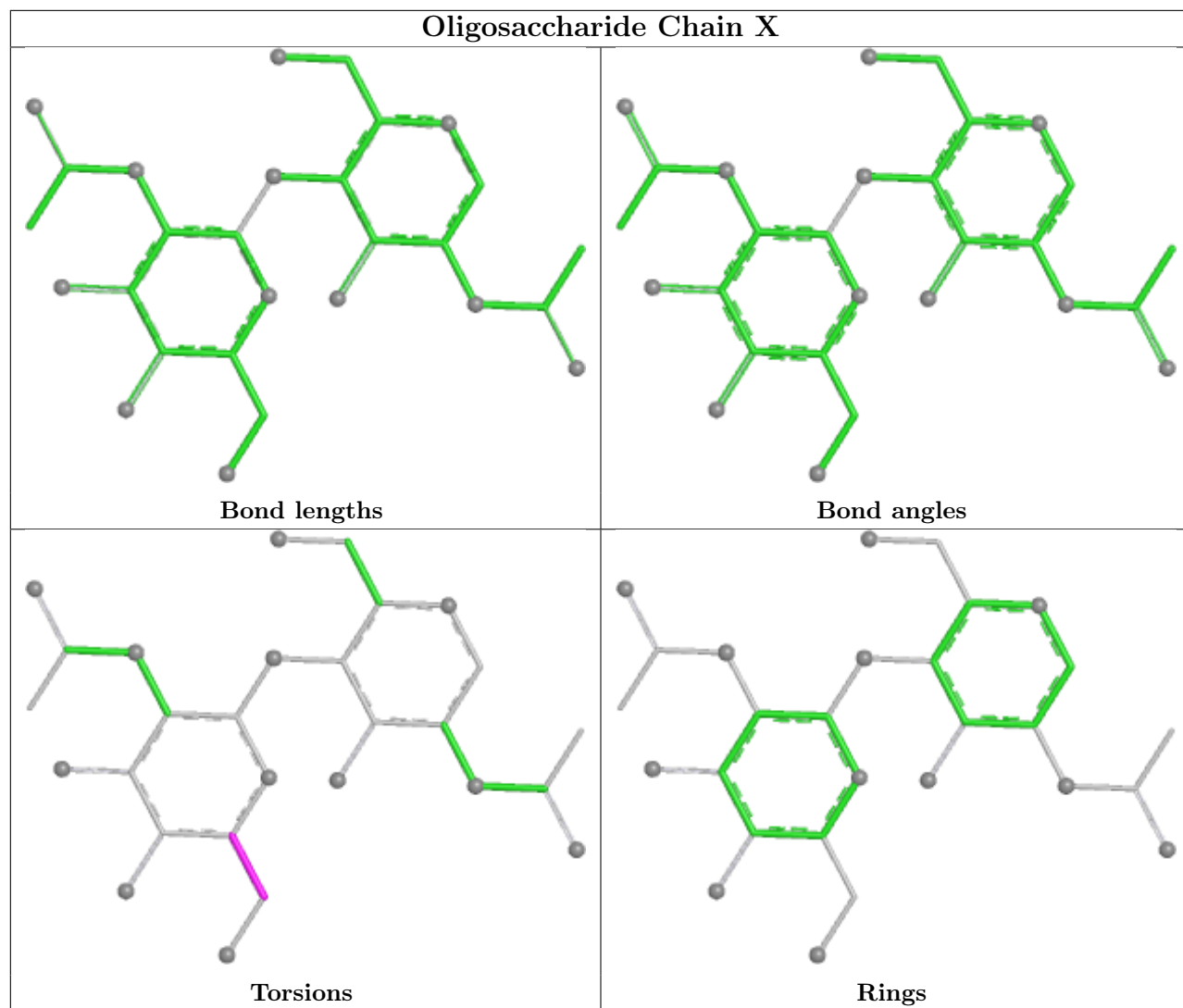


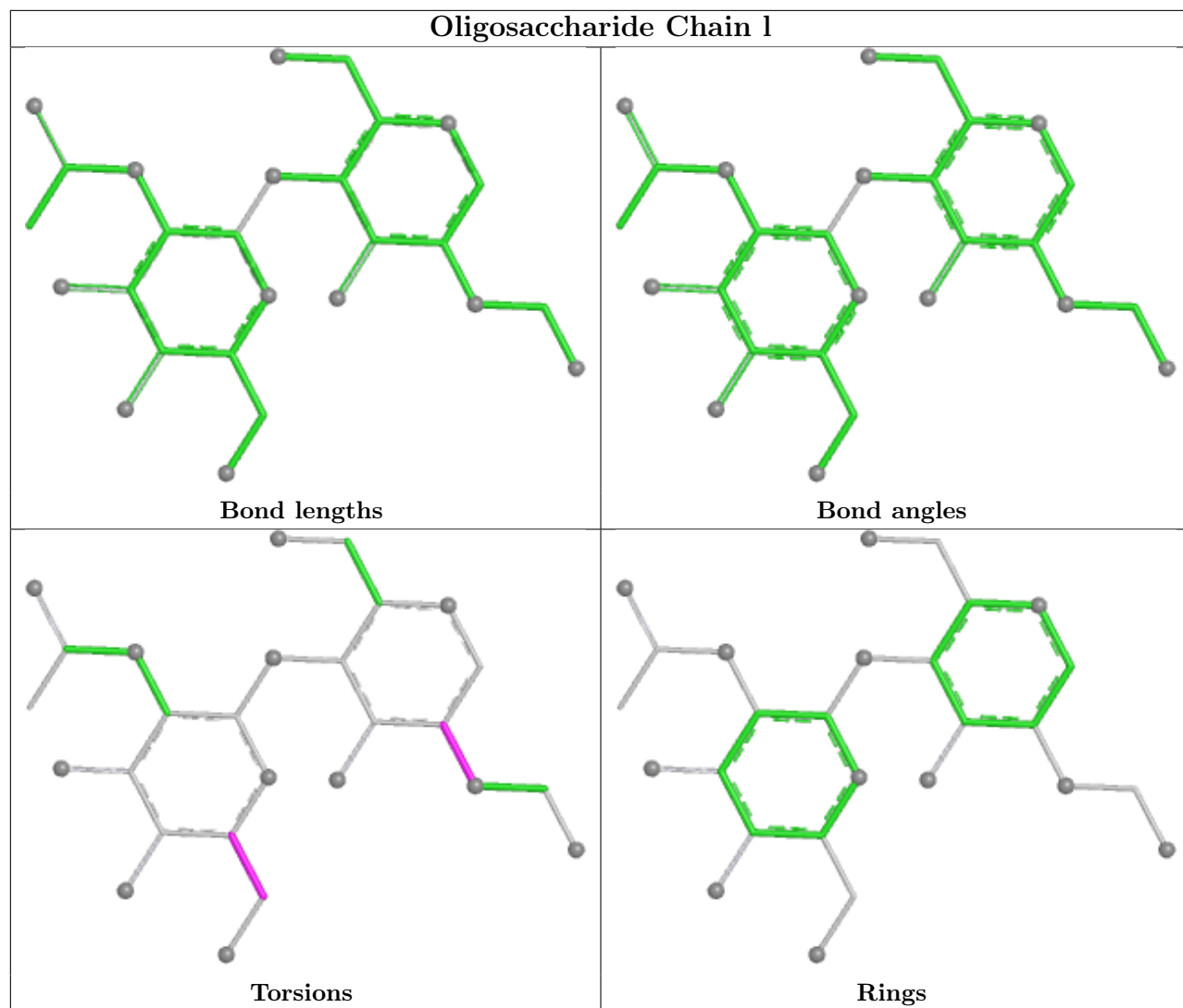


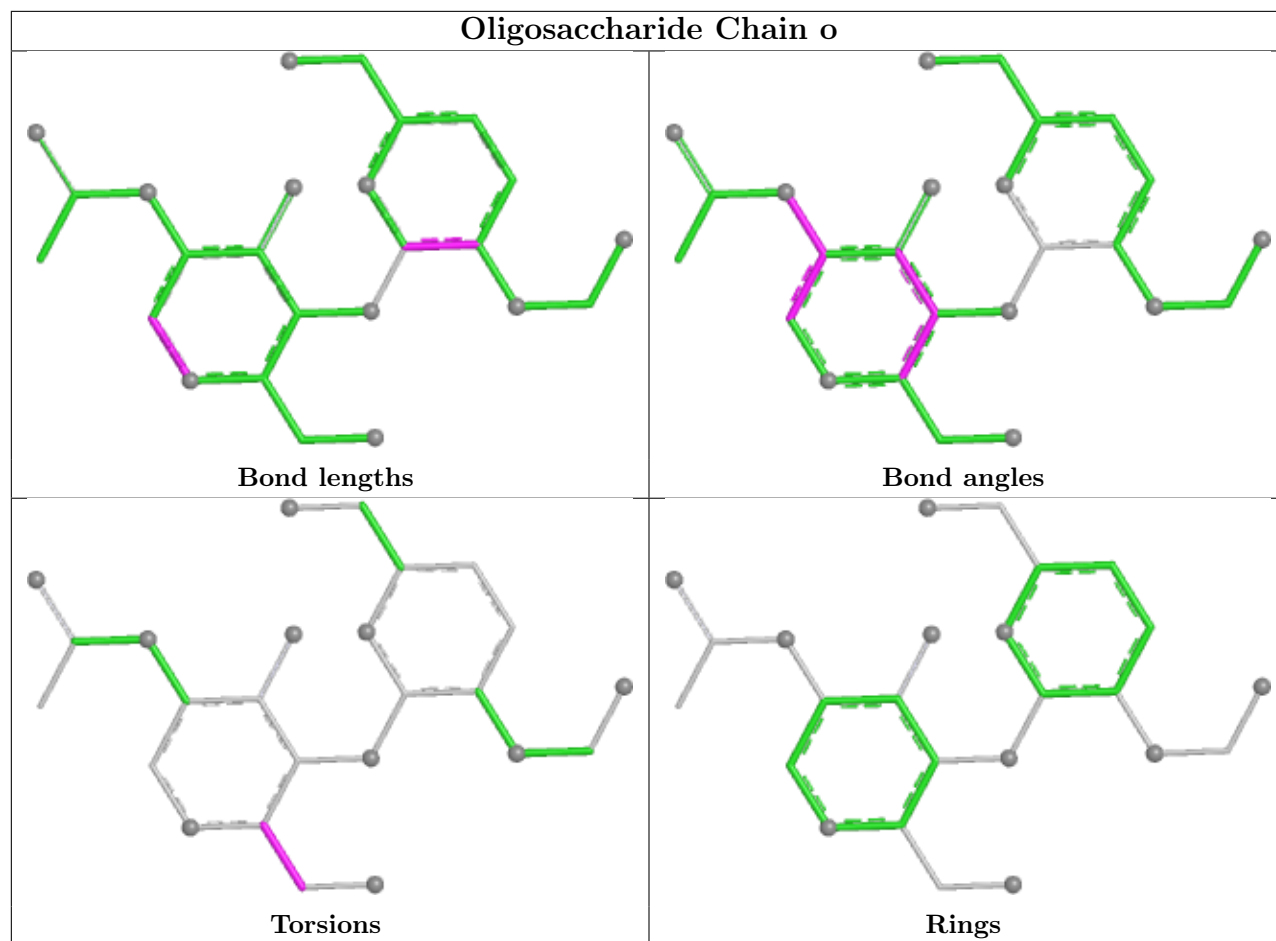


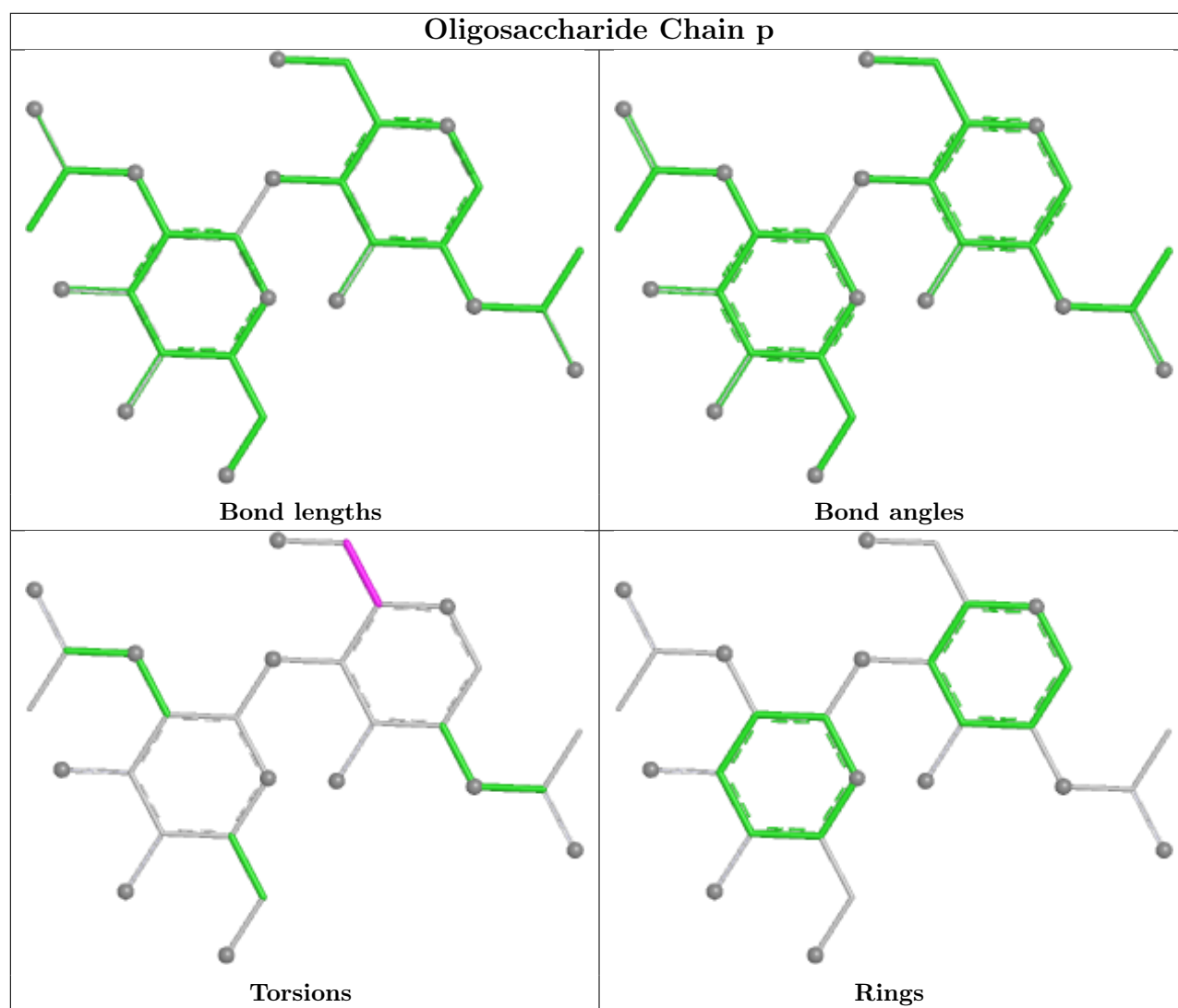


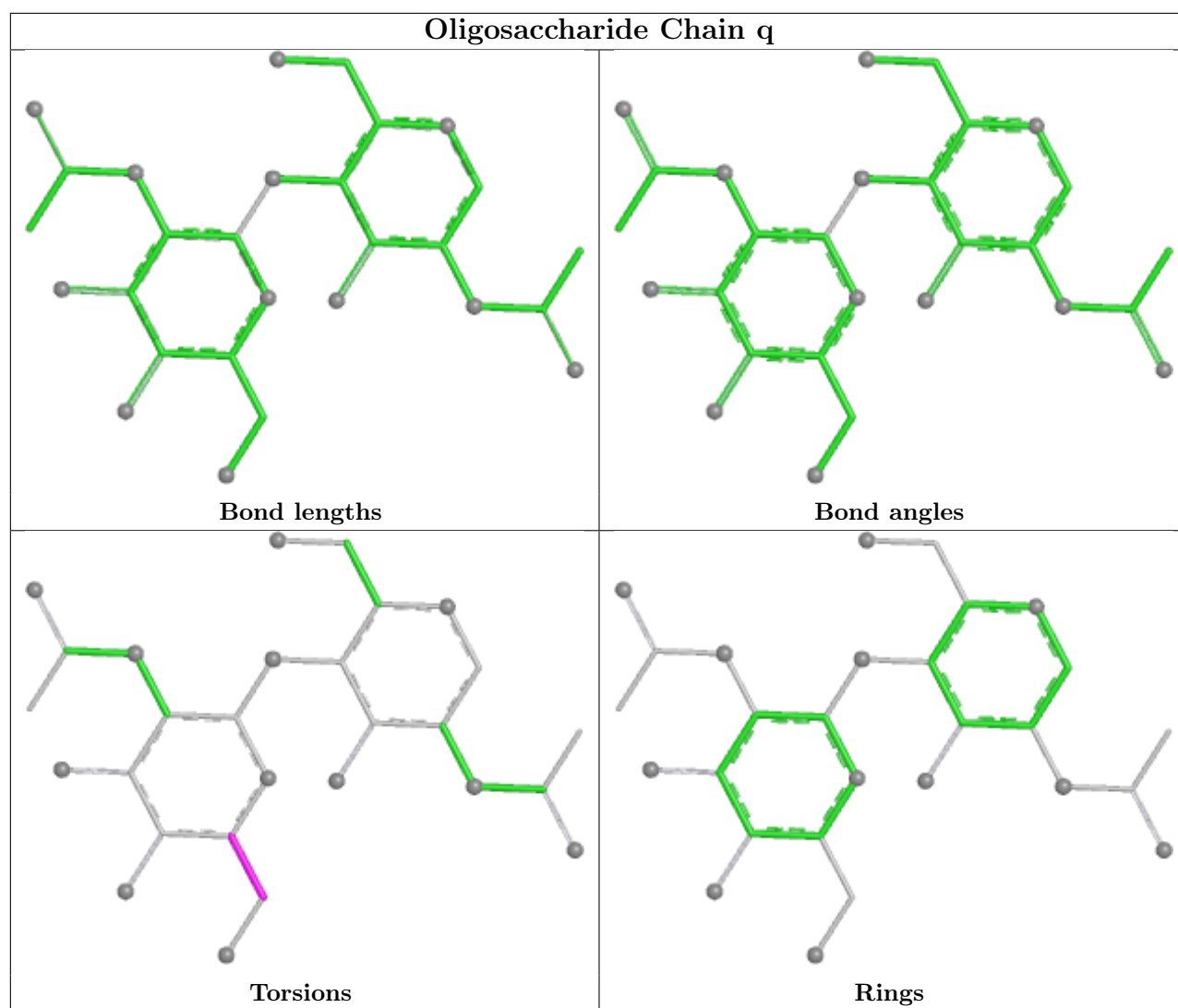


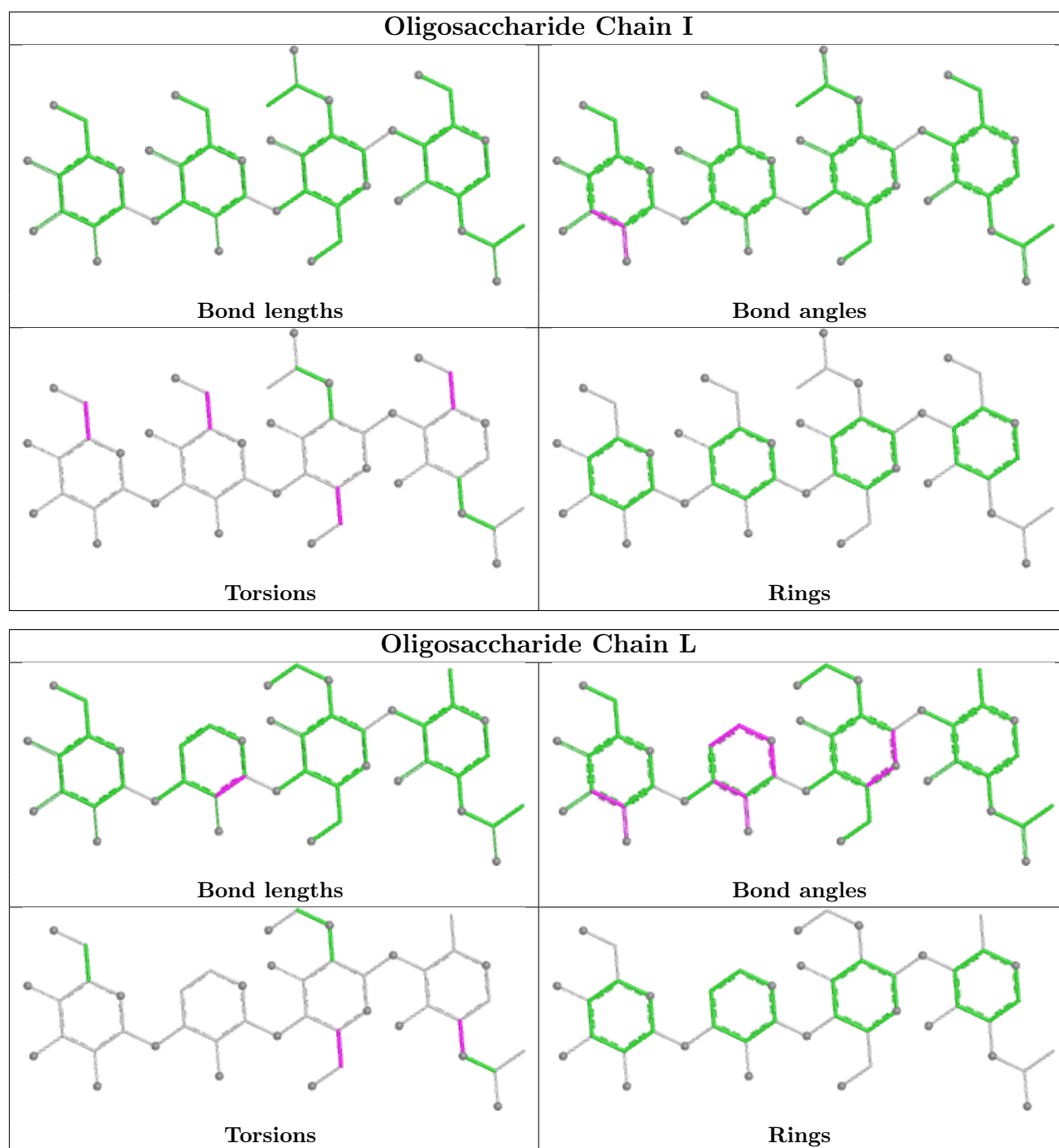


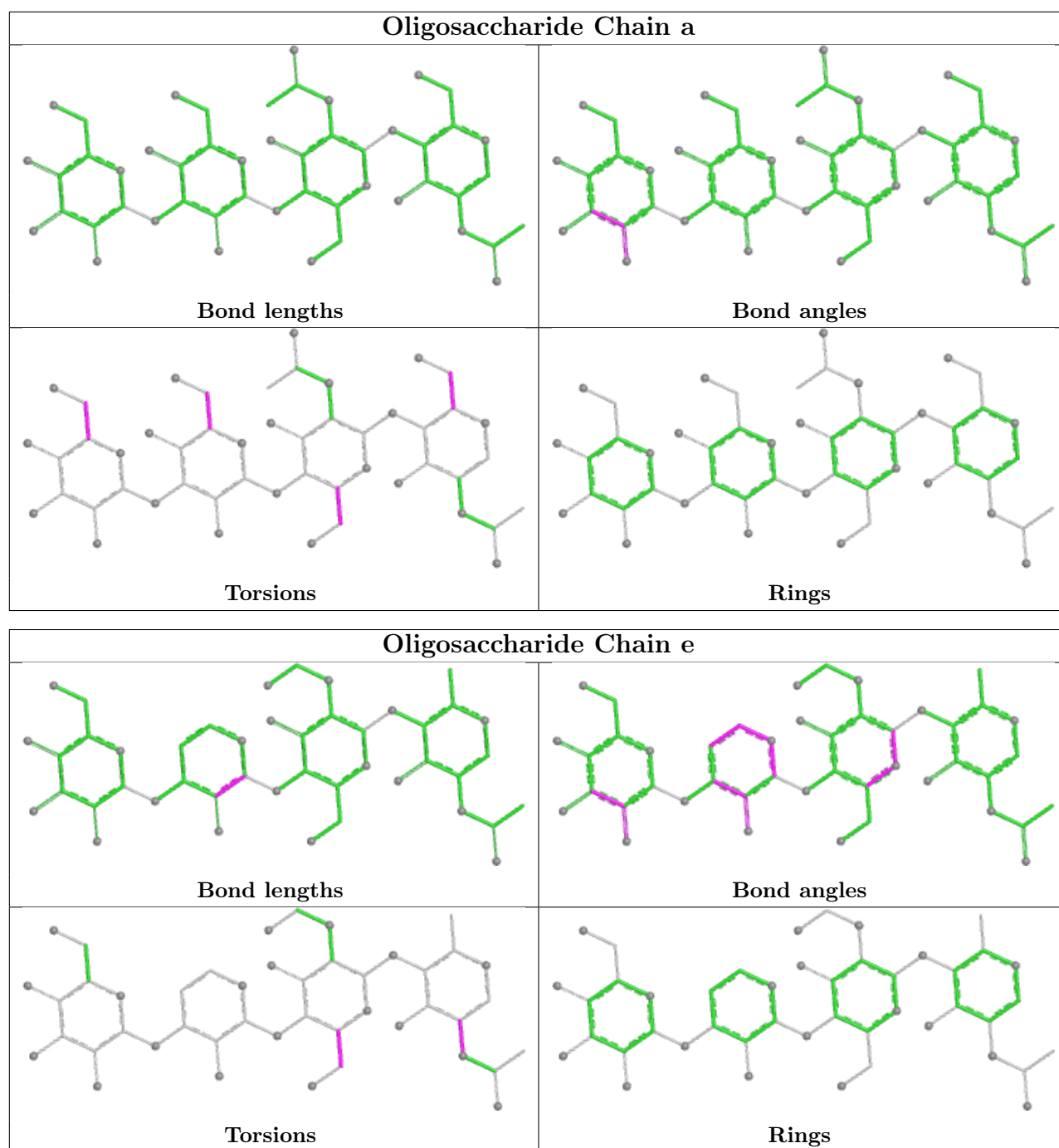


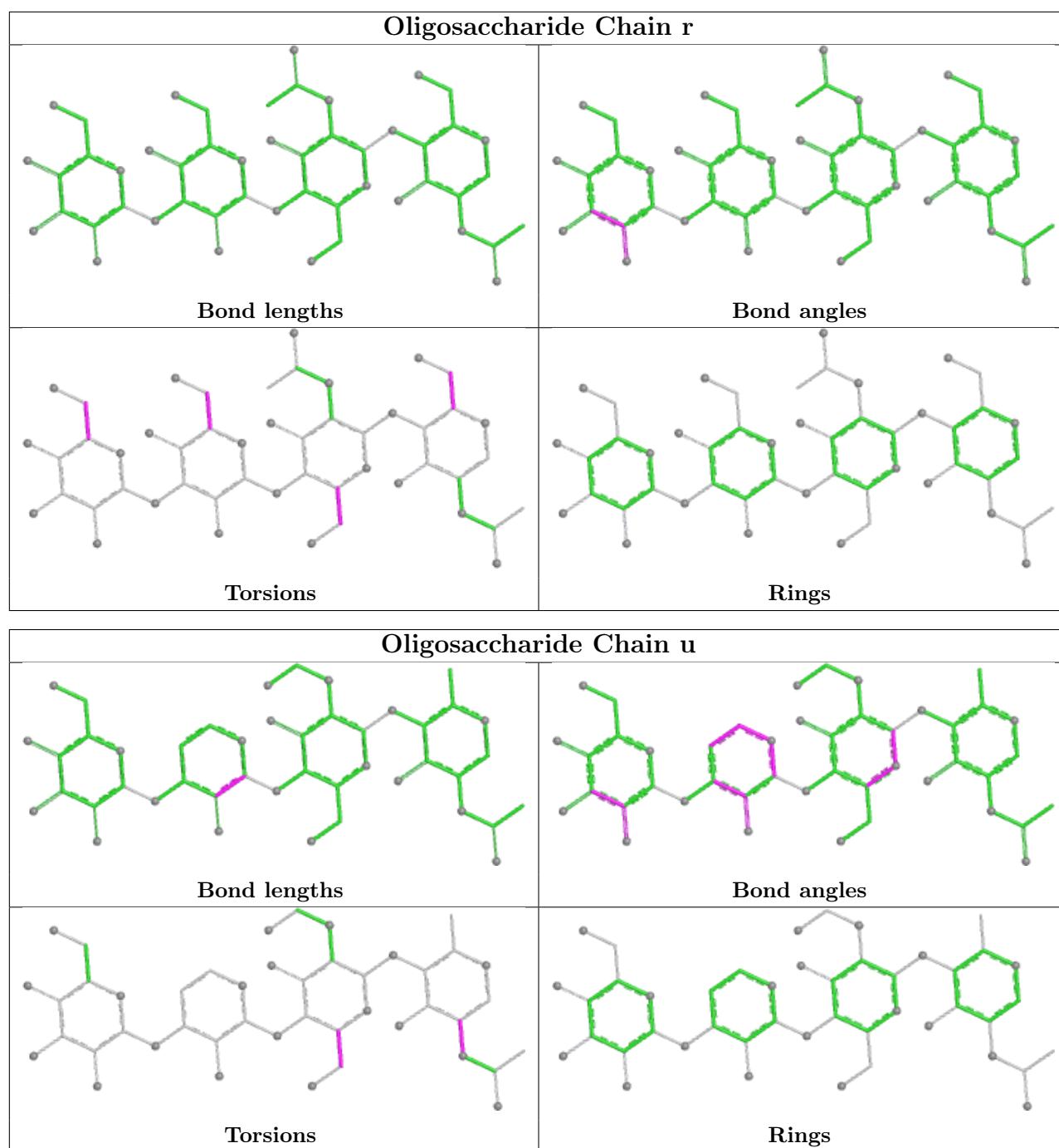


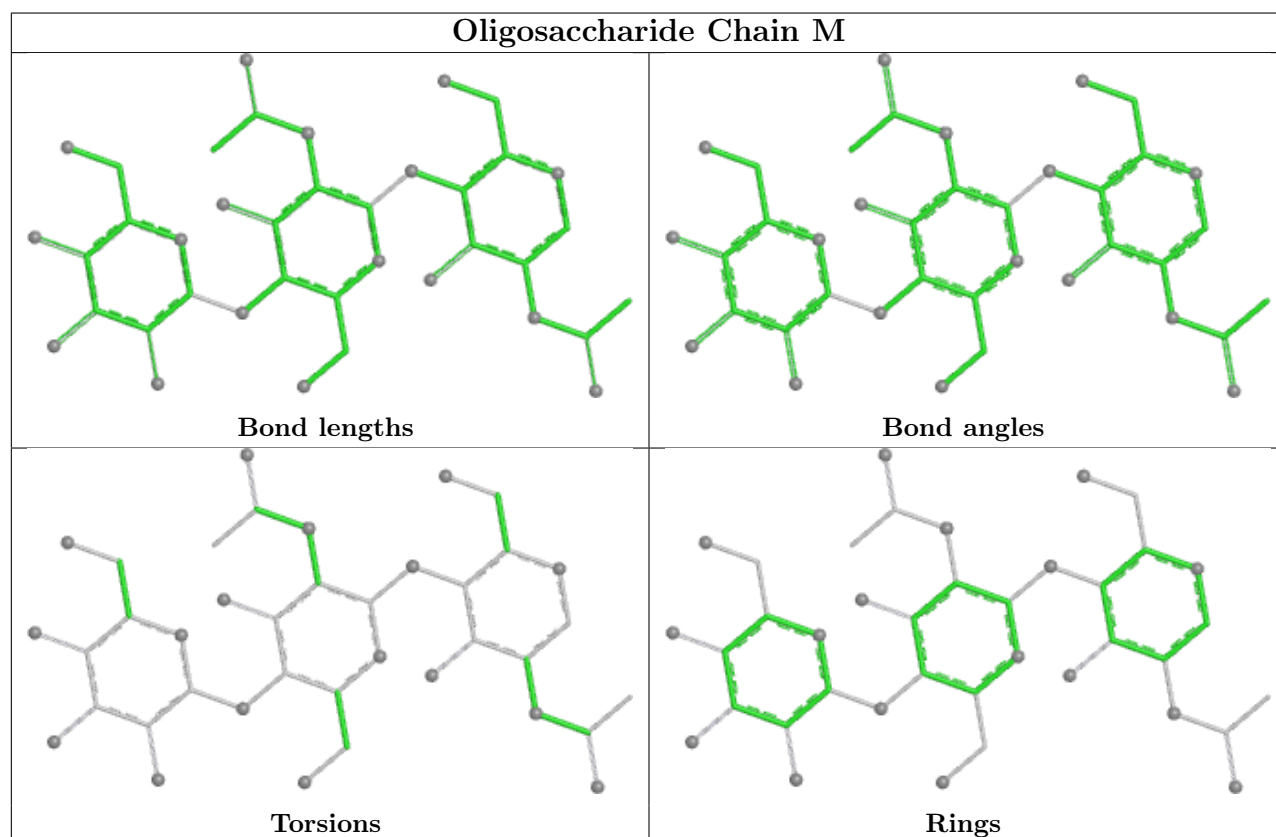
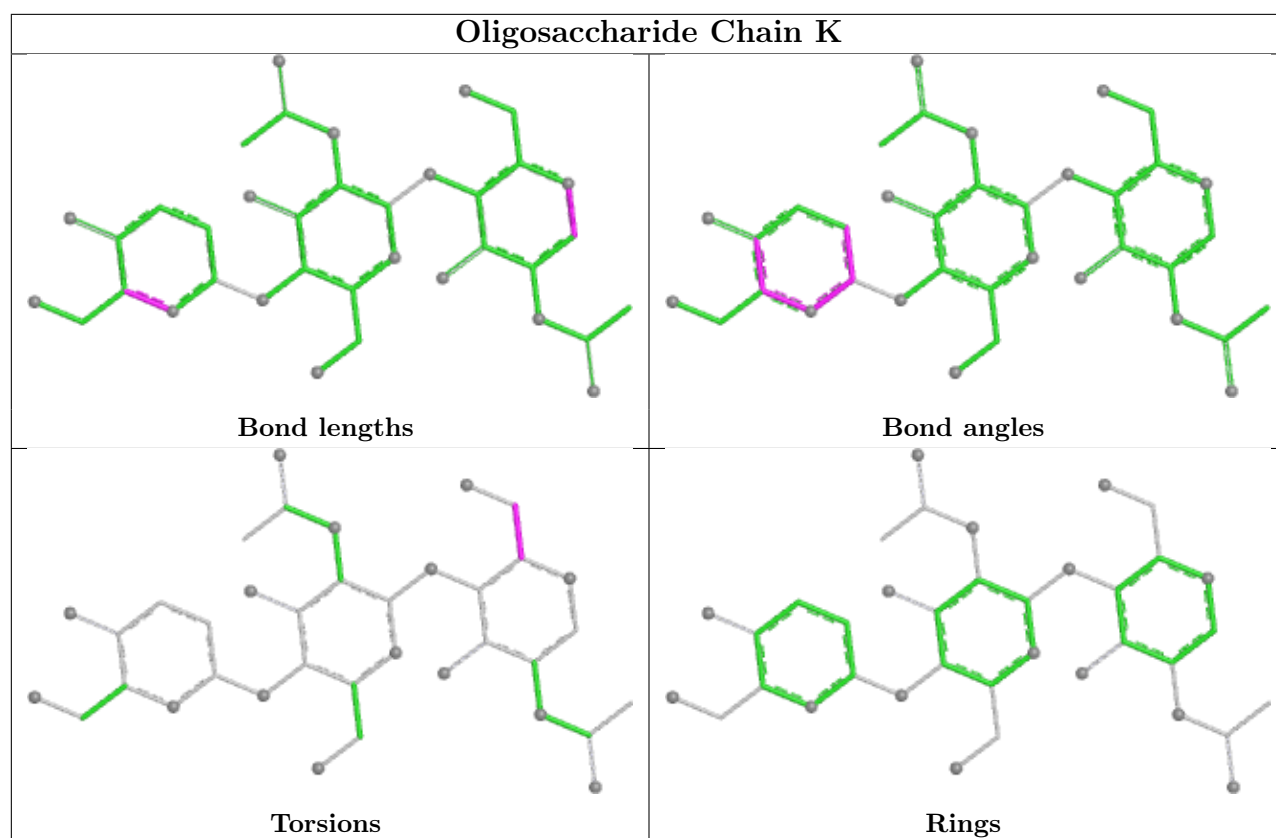


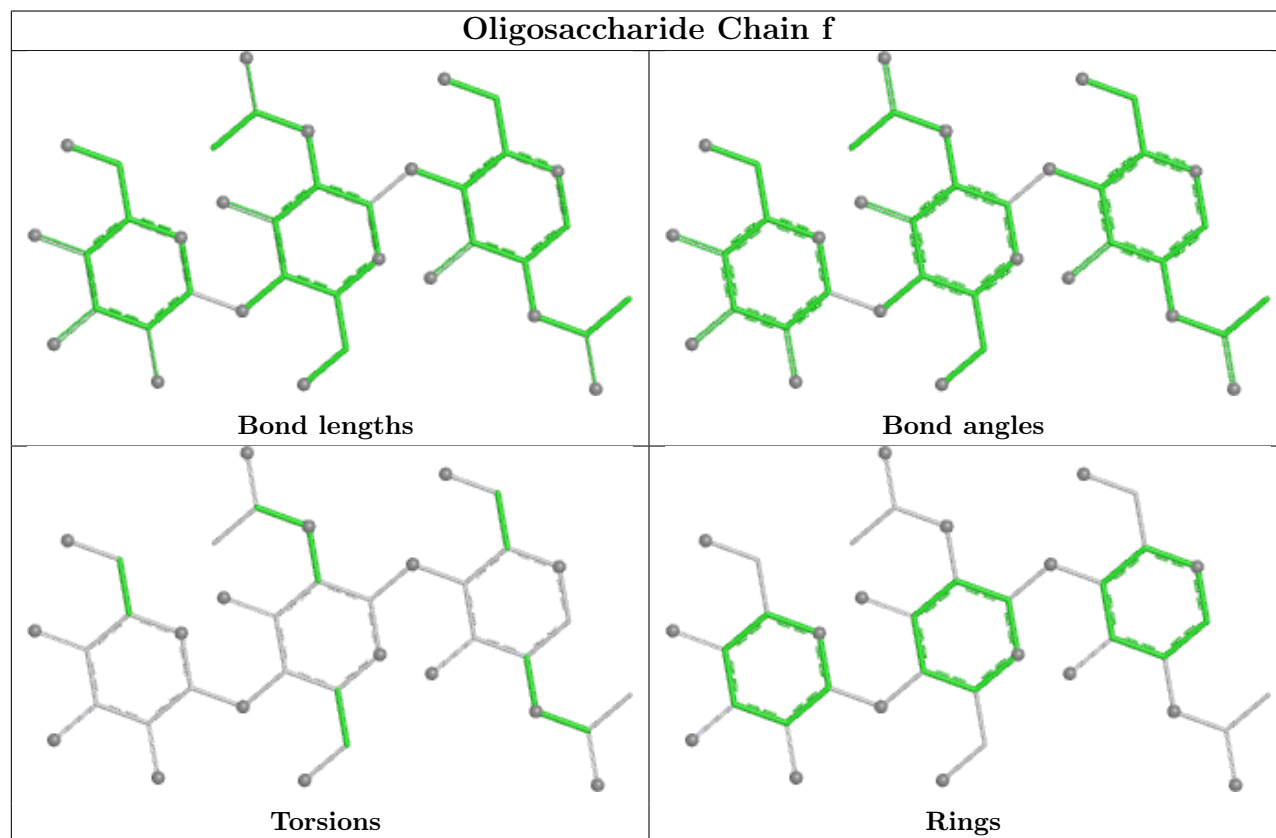
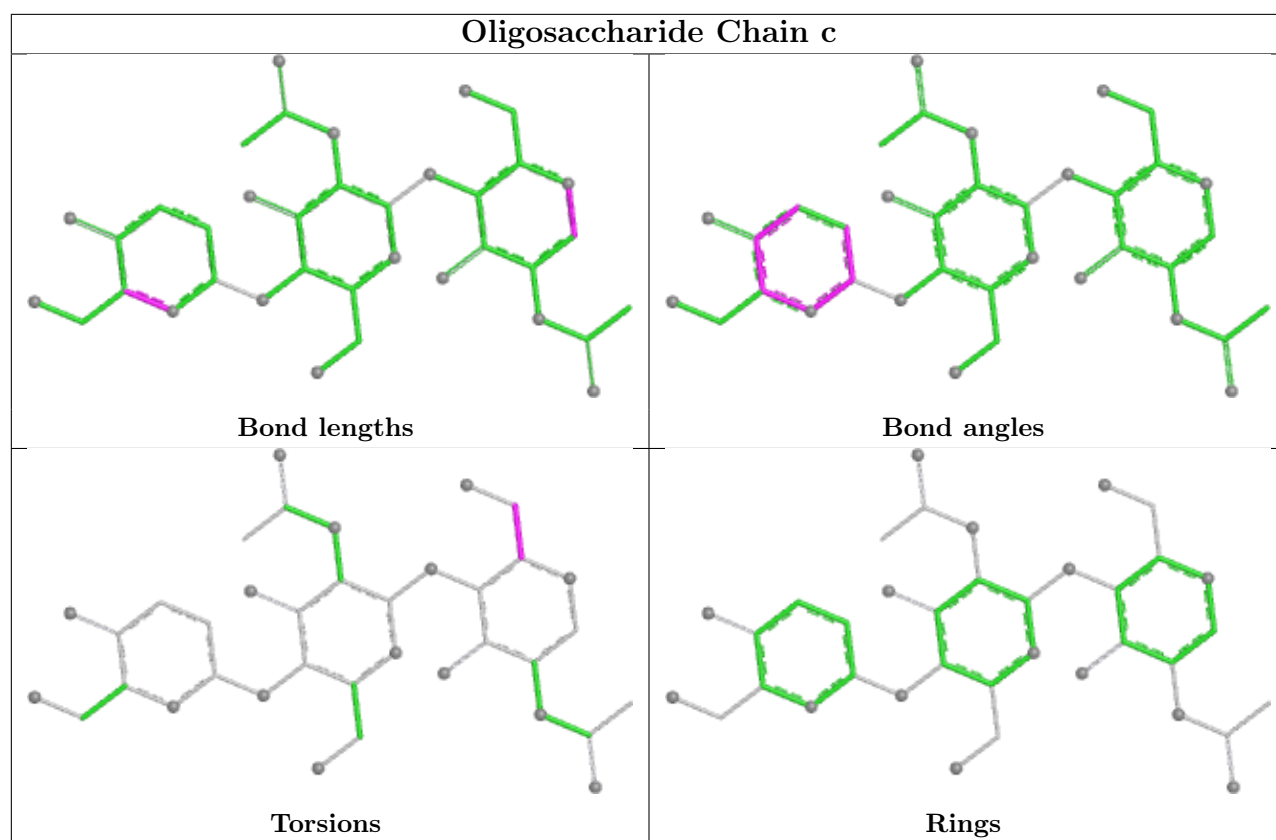


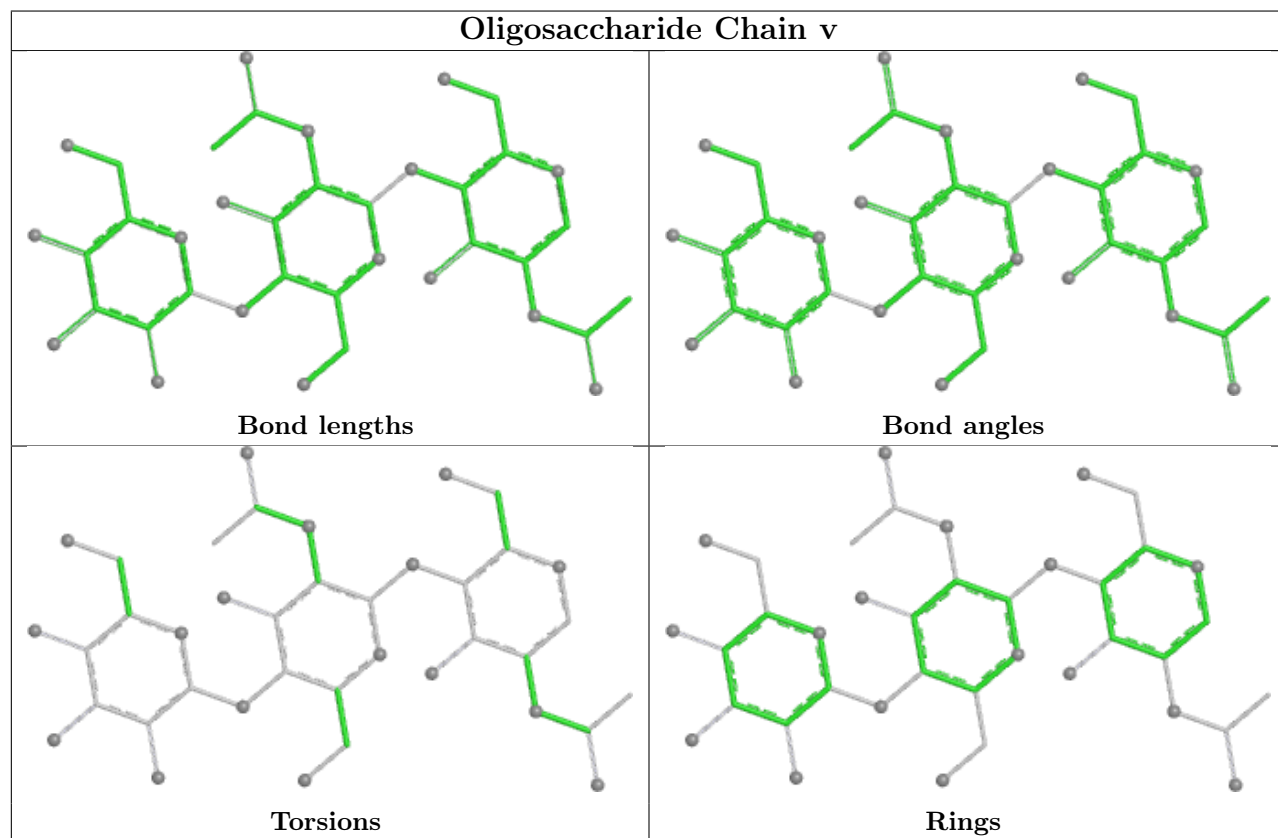
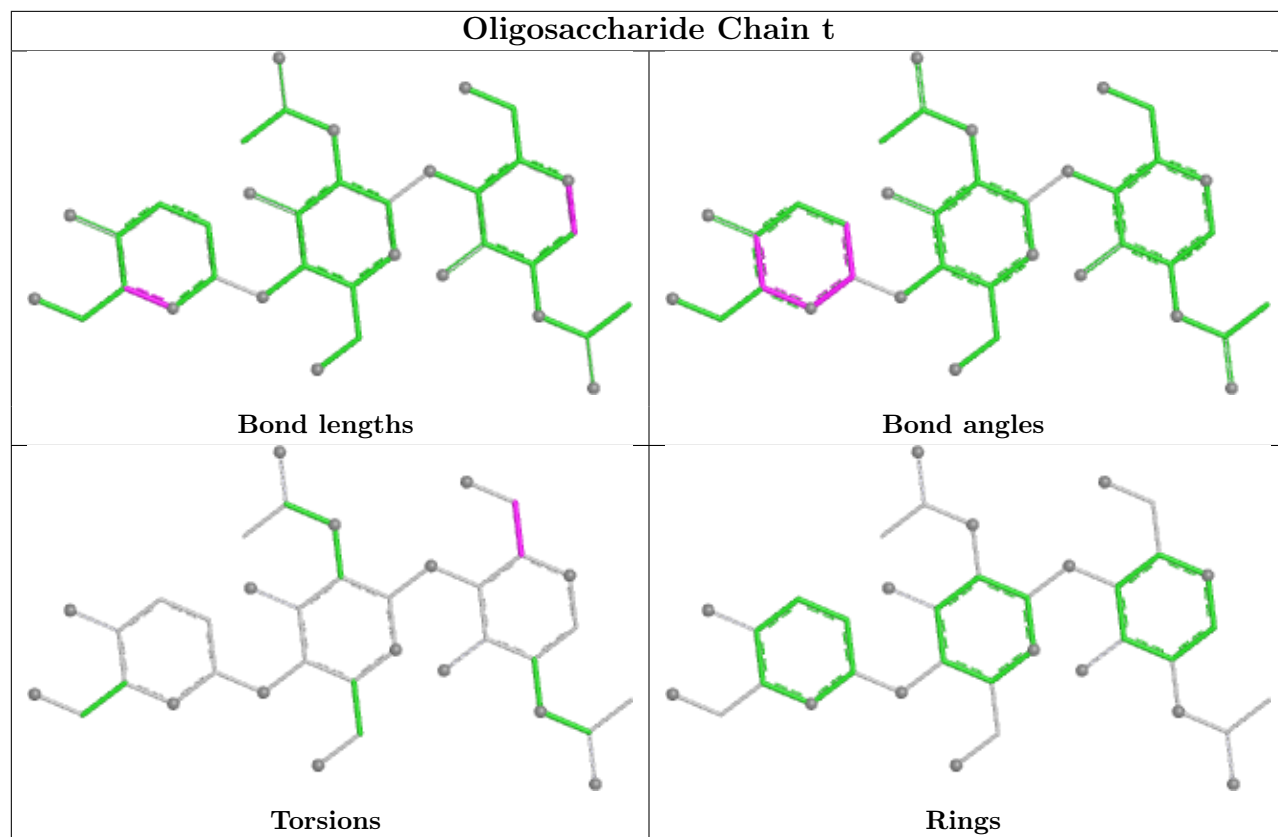


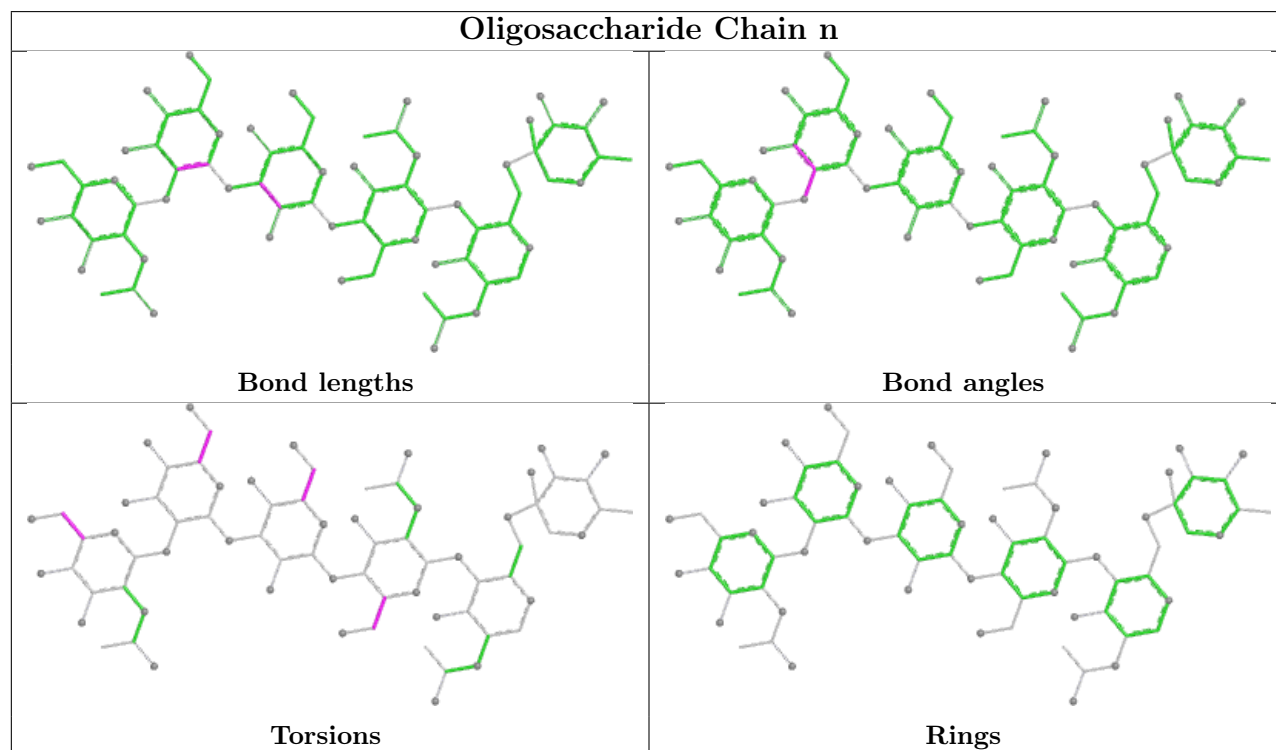
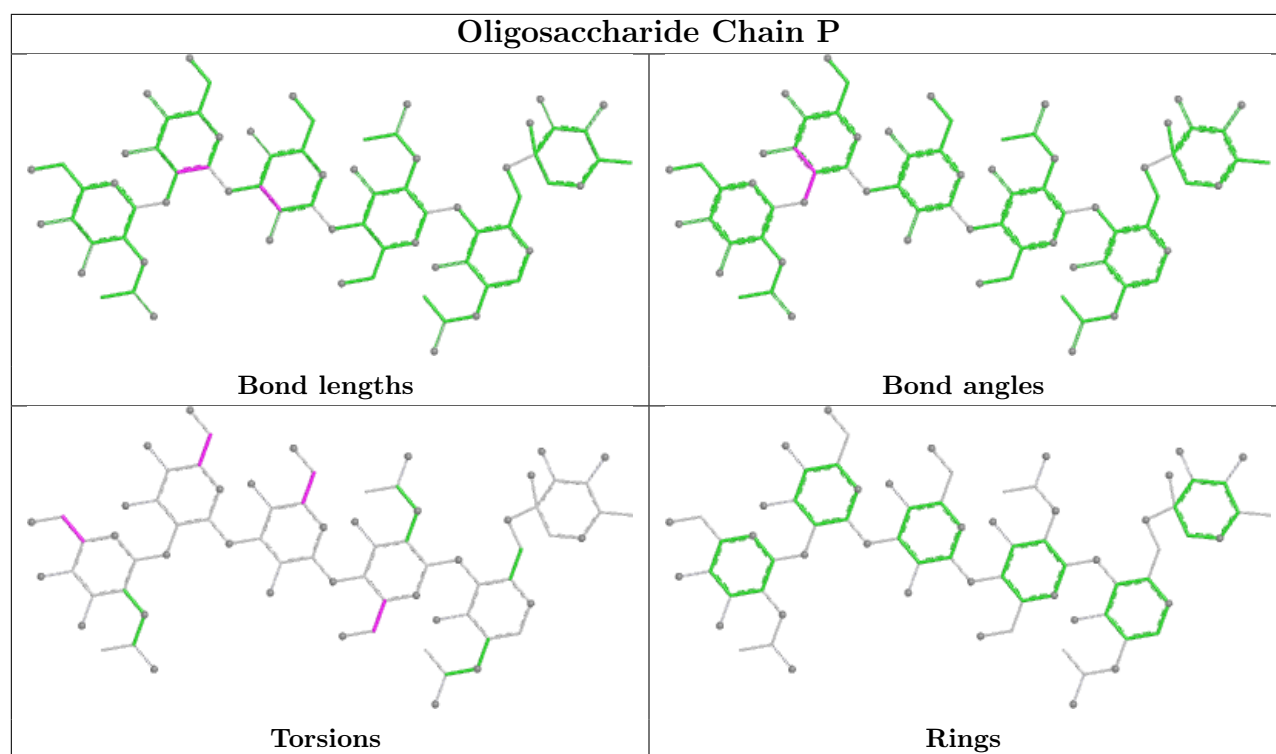


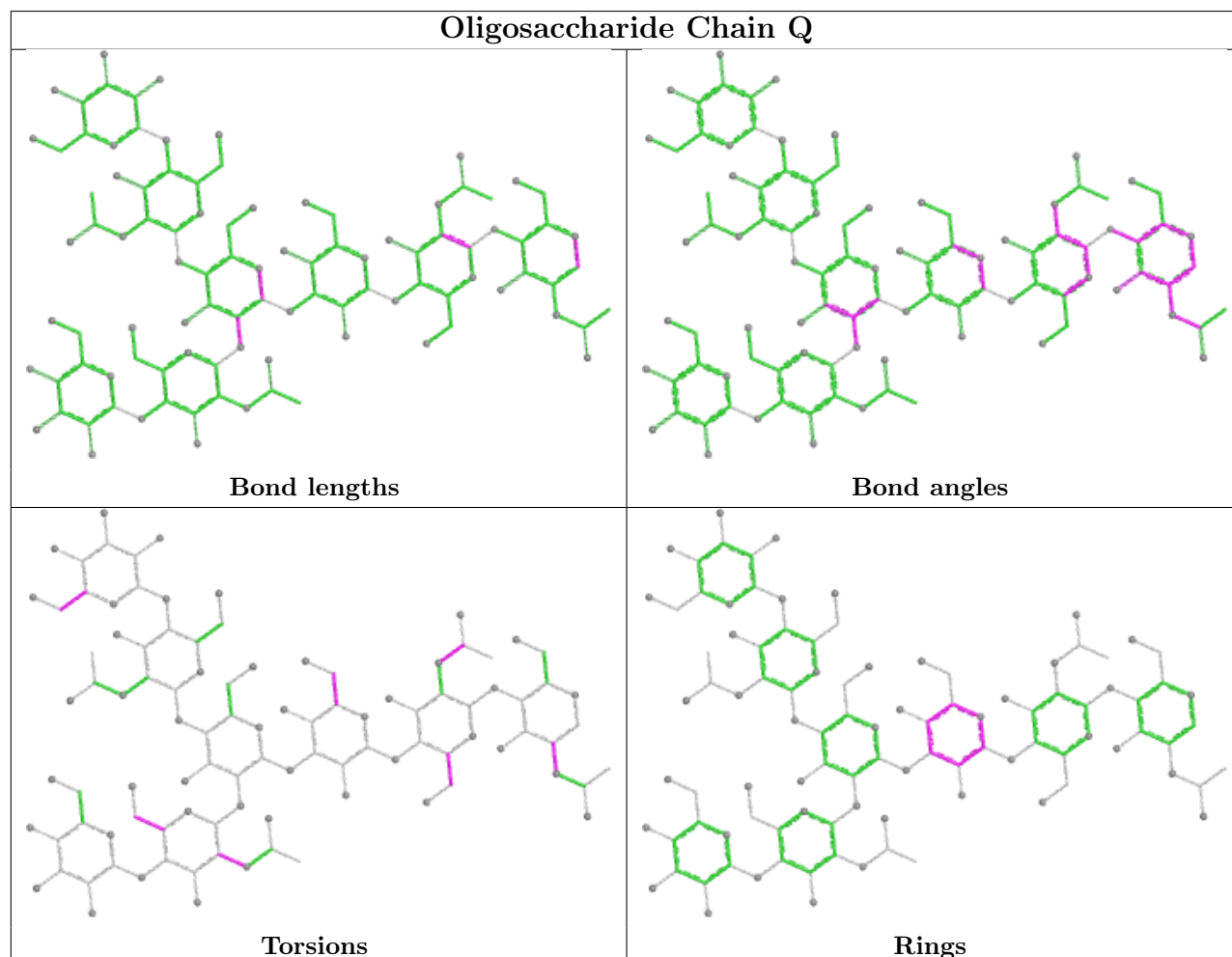
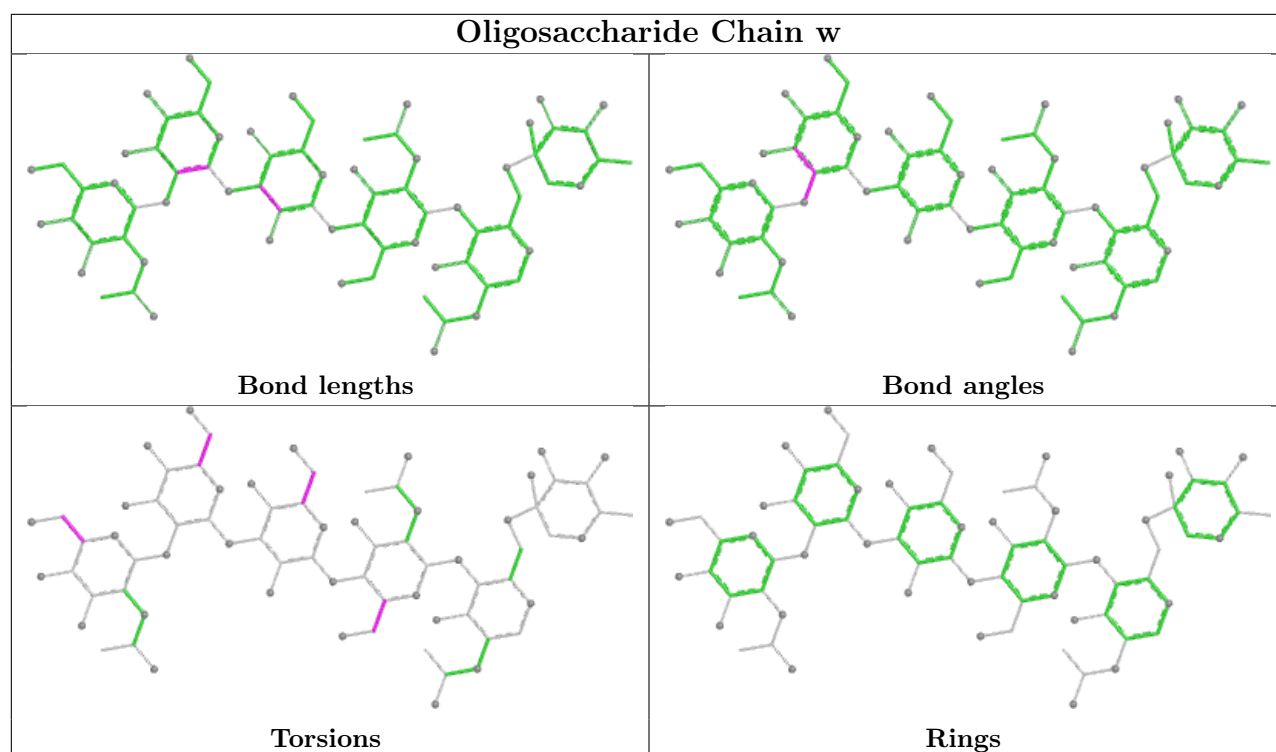


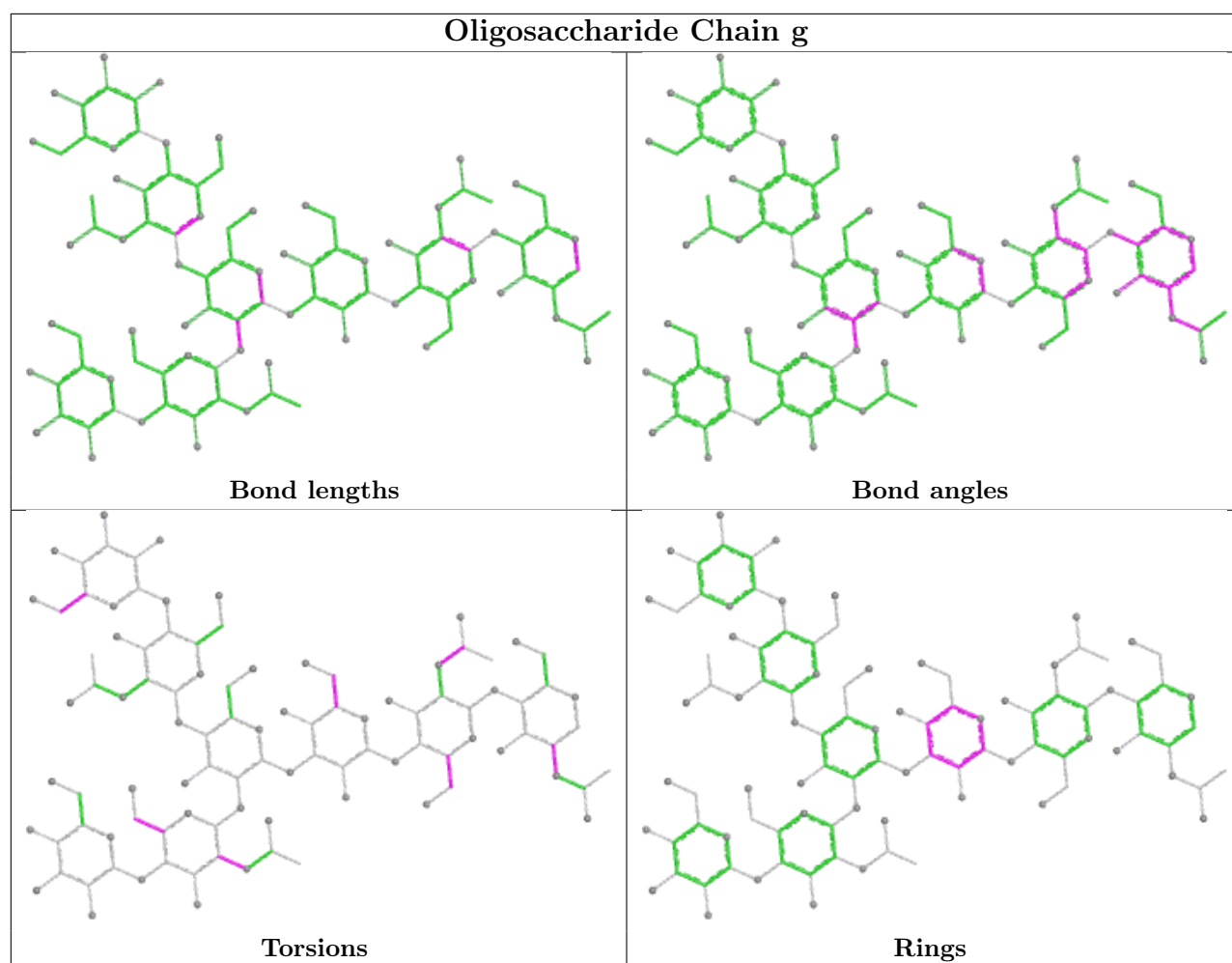


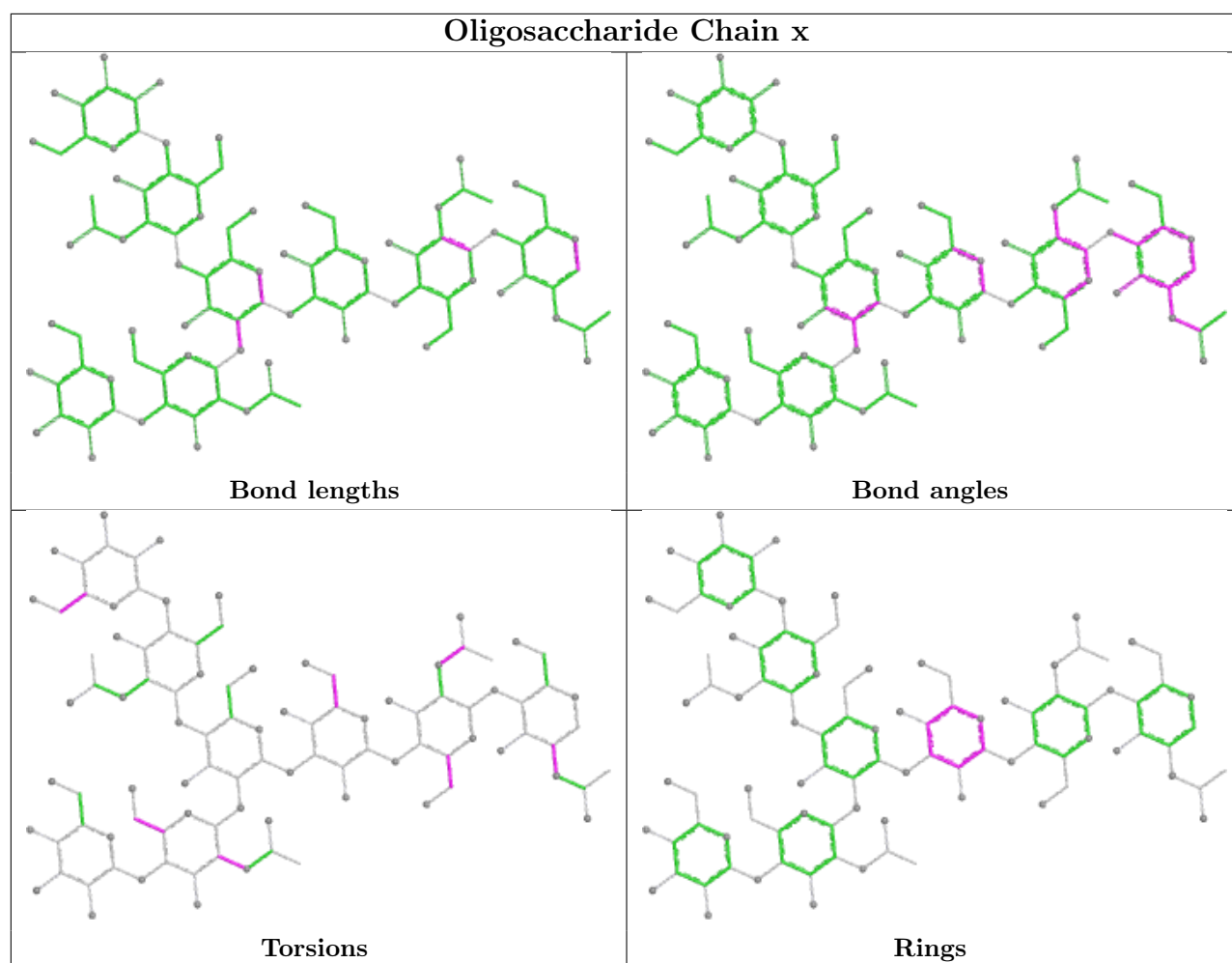


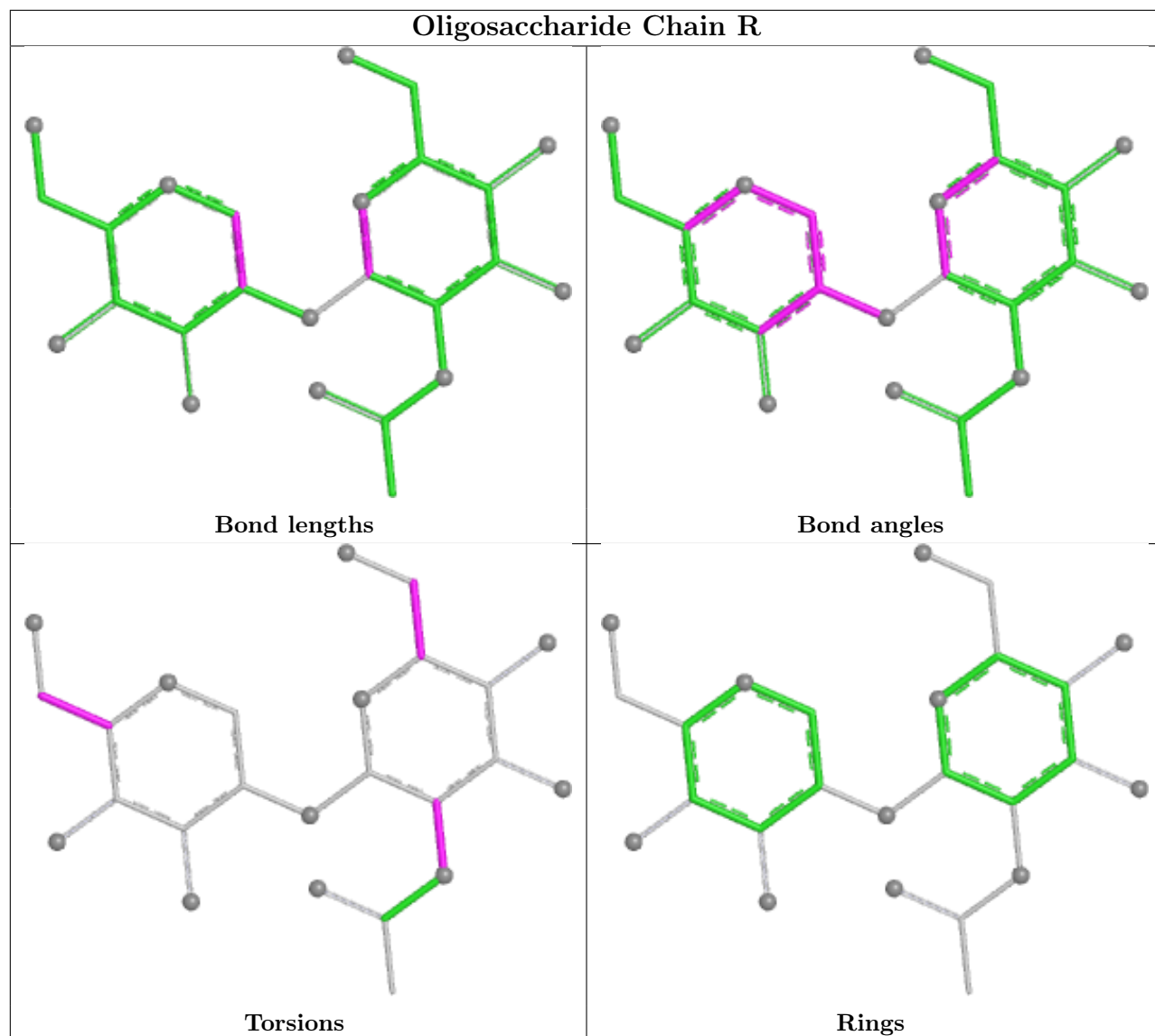


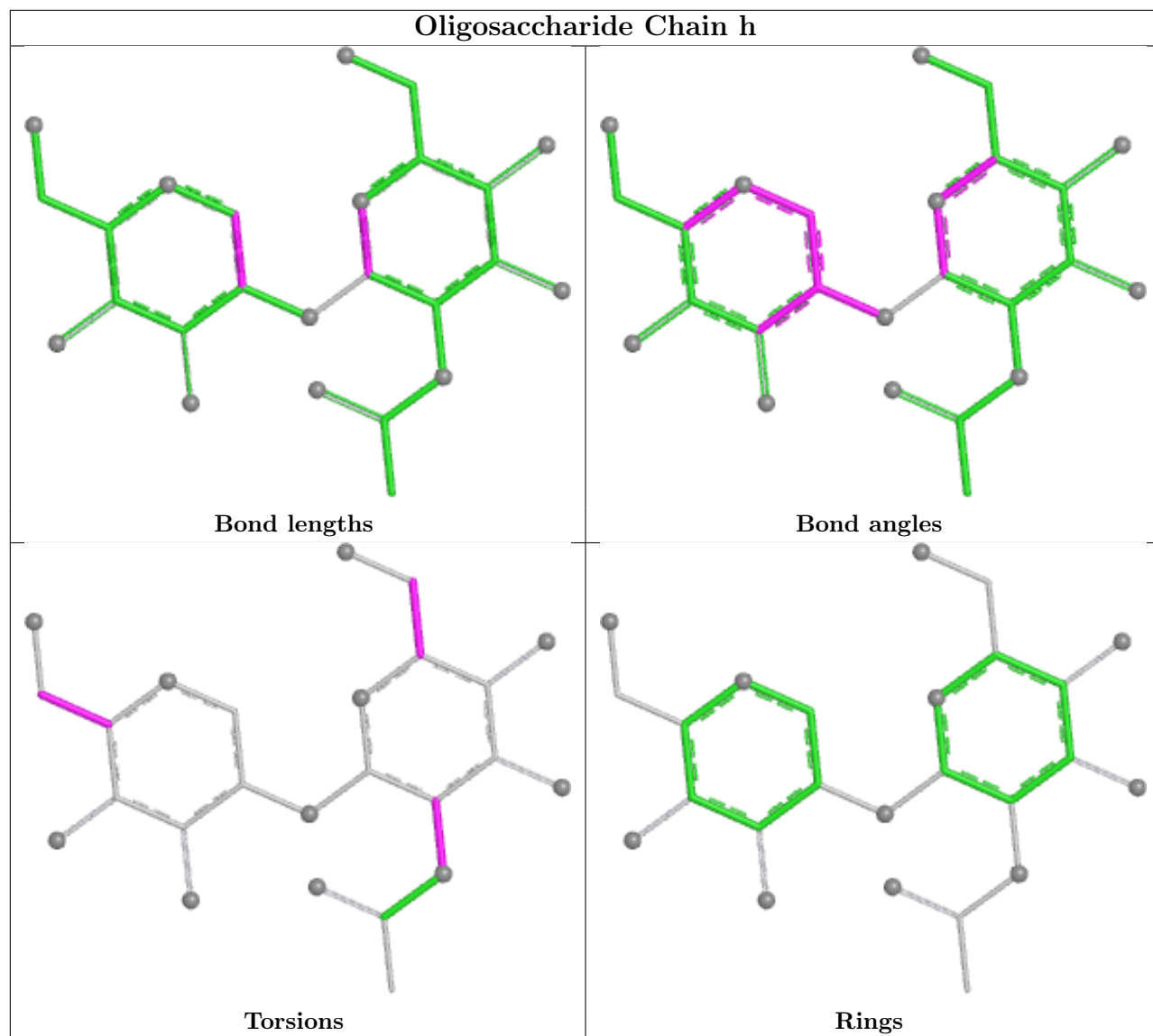


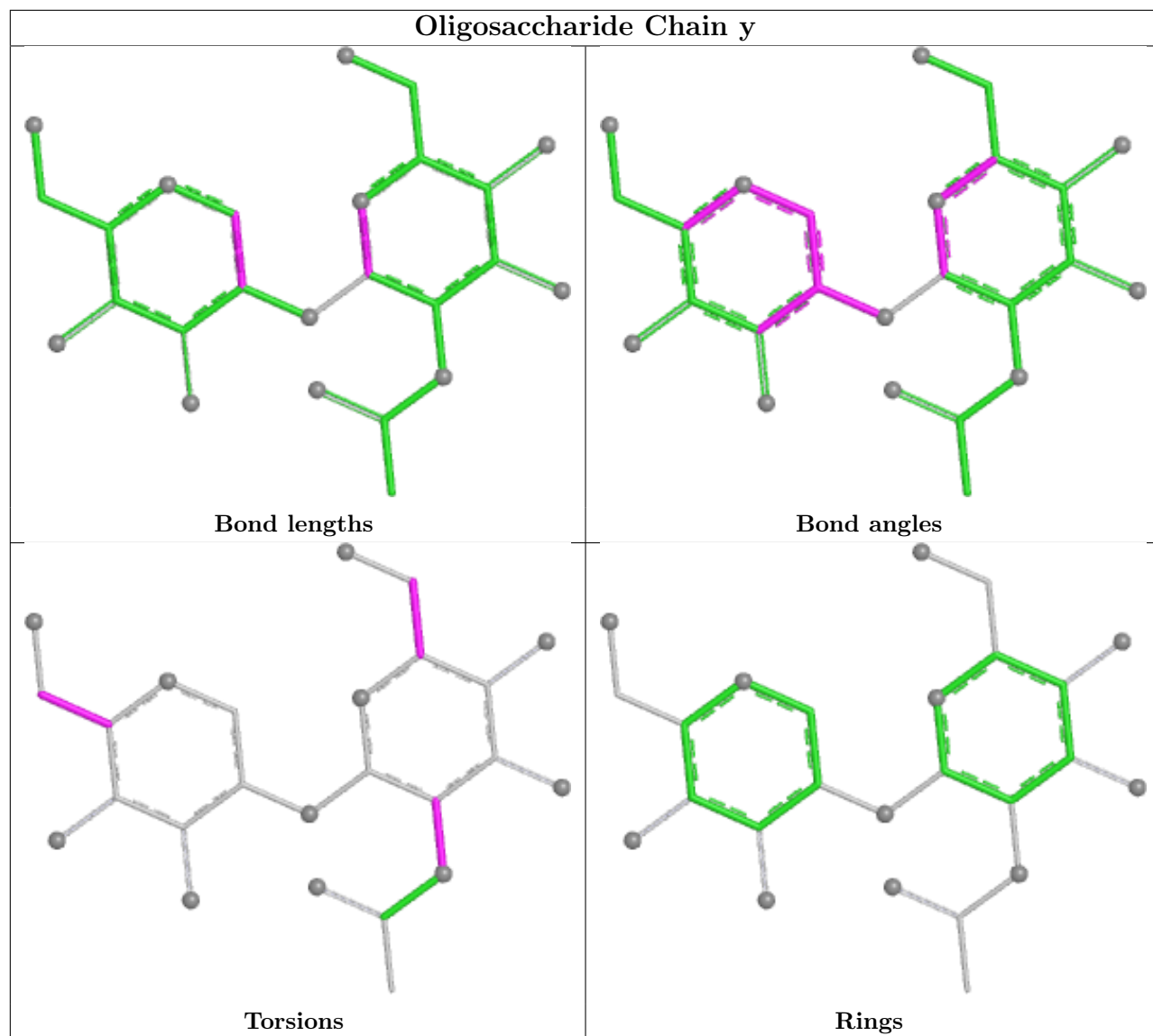


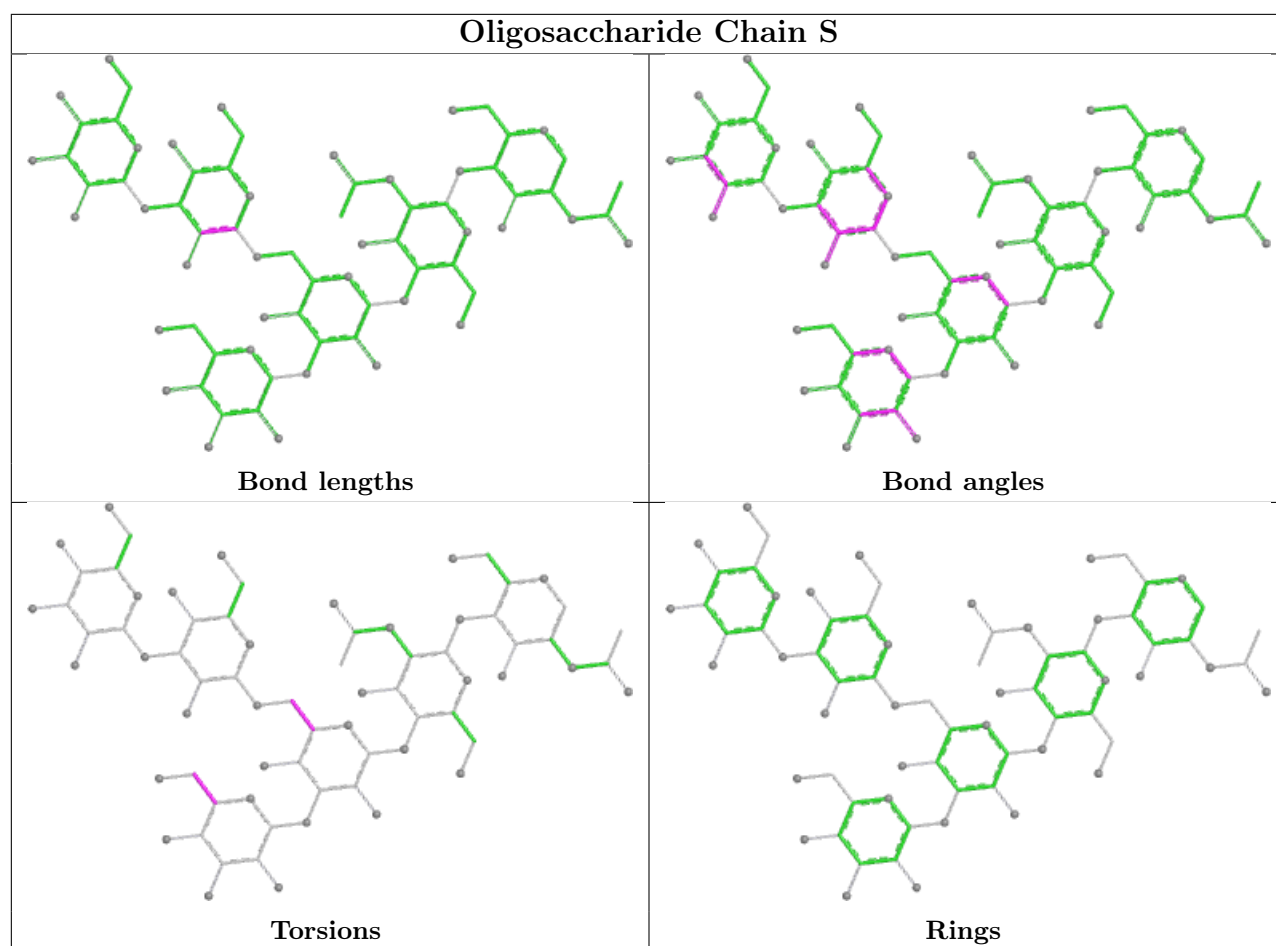


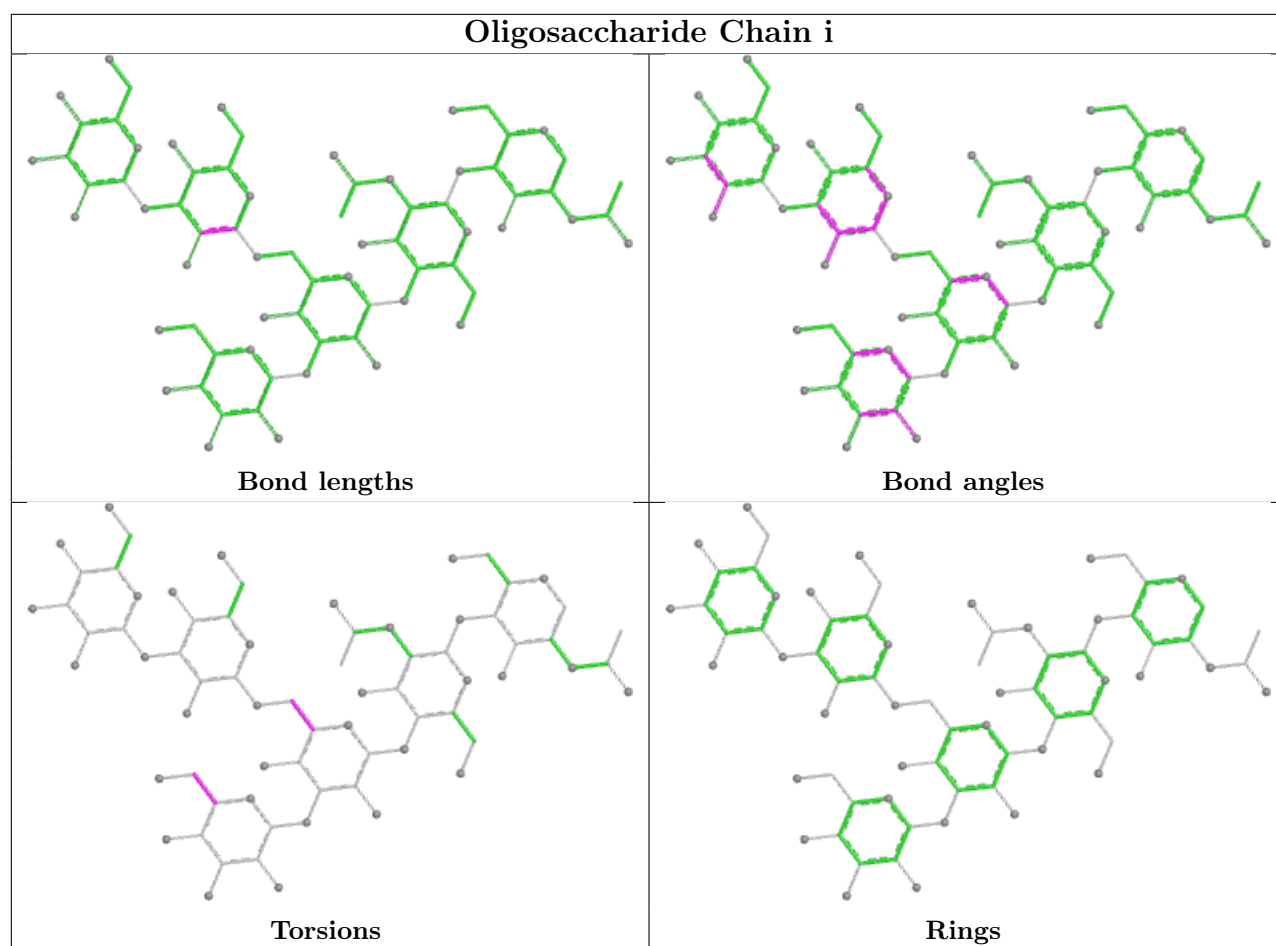


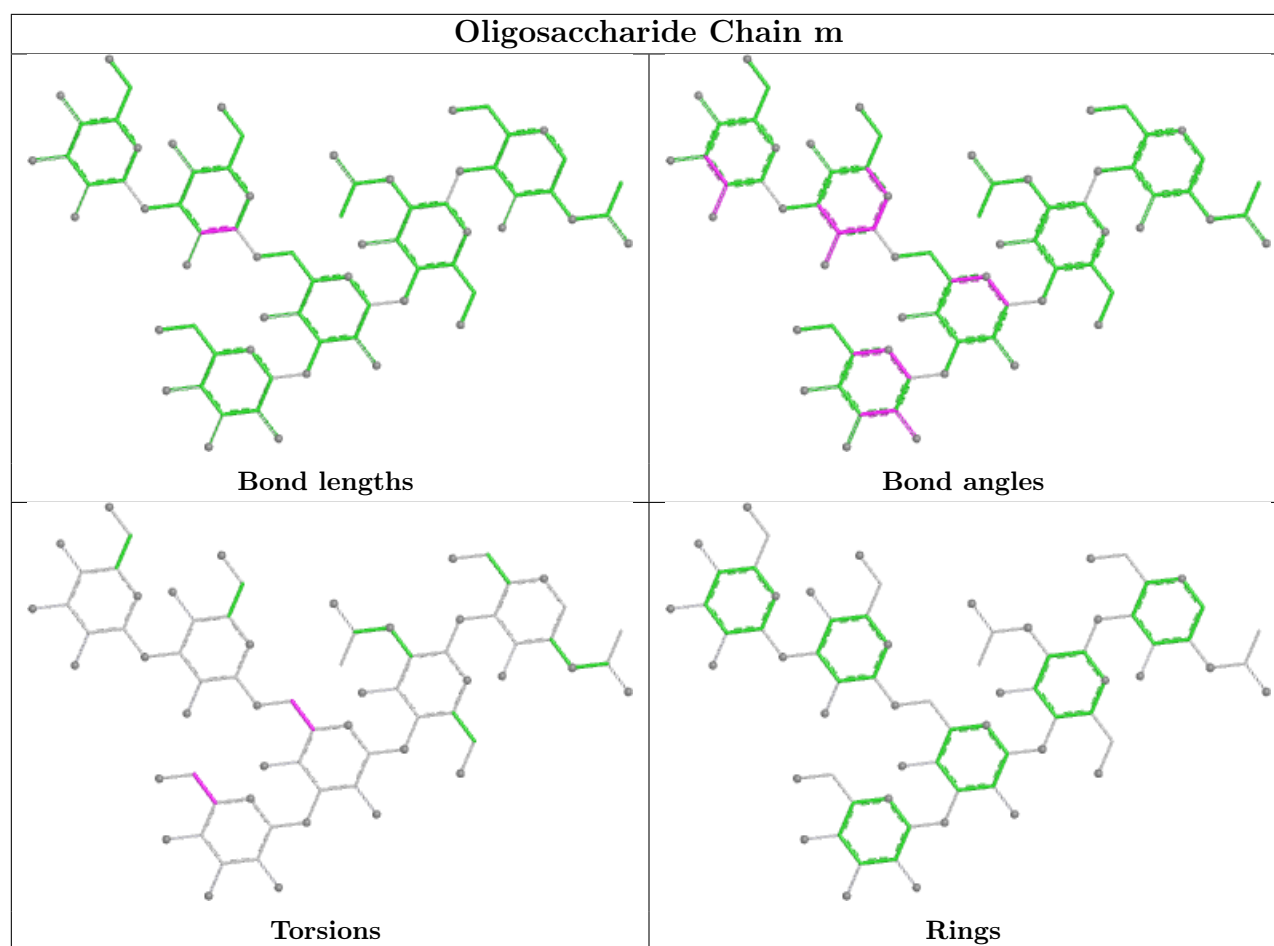












5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
12	NAG	N	603	-	14,14,15	0.54	0	17,19,21	0.62	0
12	NAG	Y	605	-	14,14,15	0.31	0	17,19,21	0.35	0
12	NAG	A	602	-	15,15,15	0.23	0	21,21,21	0.28	0
12	NAG	N	601	-	15,15,15	0.16	0	21,21,21	0.28	0
12	NAG	Y	603	-	14,14,15	0.52	0	17,19,21	0.63	0
12	NAG	A	604	-	14,14,15	0.31	0	17,19,21	0.52	0
12	NAG	N	605	-	14,14,15	0.32	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	Y	602	-	15,15,15	0.23	0	21,21,21	0.28	0
12	NAG	N	602	-	15,15,15	0.24	0	21,21,21	0.28	0
13	FUC	O	703	-	10,10,11	0.71	0	14,14,16	0.88	0
12	NAG	O	702	-	14,14,15	0.40	0	17,19,21	0.40	0
12	NAG	Y	604	-	14,14,15	0.32	0	17,19,21	0.51	0
12	NAG	Y	601	-	15,15,15	0.16	0	21,21,21	0.28	0
12	NAG	N	604	-	14,14,15	0.31	0	17,19,21	0.52	0
12	NAG	O	701	-	15,15,15	0.20	0	21,21,21	0.26	0
12	NAG	Z	701	-	15,15,15	0.22	0	21,21,21	0.26	0
12	NAG	A	603	-	14,14,15	0.54	0	17,19,21	0.62	0
12	NAG	B	701	-	15,15,15	0.22	0	21,21,21	0.26	0
12	NAG	A	605	-	14,14,15	0.31	0	17,19,21	0.36	0
13	FUC	B	703	-	10,10,11	0.71	0	14,14,16	0.88	0
13	FUC	Z	703	-	10,10,11	0.73	0	14,14,16	0.87	0
12	NAG	B	702	-	14,14,15	0.40	0	17,19,21	0.40	0
12	NAG	Z	702	-	14,14,15	0.41	0	17,19,21	0.40	0
12	NAG	A	601	-	15,15,15	0.16	0	21,21,21	0.28	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
12	NAG	N	603	-	-	2/6/23/26	0/1/1/1
12	NAG	Y	605	-	-	2/6/23/26	0/1/1/1
12	NAG	A	602	-	-	0/6/26/26	0/1/1/1
12	NAG	N	601	-	-	0/6/26/26	0/1/1/1
12	NAG	Y	603	-	-	2/6/23/26	0/1/1/1
12	NAG	A	604	-	-	2/6/23/26	0/1/1/1
12	NAG	N	605	-	-	2/6/23/26	0/1/1/1
12	NAG	Y	602	-	-	0/6/26/26	0/1/1/1
12	NAG	N	602	-	-	0/6/26/26	0/1/1/1
13	FUC	O	703	-	-	-	0/1/1/1
12	NAG	O	702	-	-	2/6/23/26	0/1/1/1
12	NAG	Y	604	-	-	2/6/23/26	0/1/1/1
12	NAG	Y	601	-	-	0/6/26/26	0/1/1/1
12	NAG	N	604	-	-	2/6/23/26	0/1/1/1
12	NAG	O	701	-	-	0/6/26/26	0/1/1/1
12	NAG	Z	701	-	-	0/6/26/26	0/1/1/1
12	NAG	A	603	-	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	B	701	-	-	0/6/26/26	0/1/1/1
12	NAG	A	605	-	-	2/6/23/26	0/1/1/1
13	FUC	B	703	-	-	-	0/1/1/1
13	FUC	Z	703	-	-	-	0/1/1/1
12	NAG	B	702	-	-	2/6/23/26	0/1/1/1
12	NAG	Z	702	-	-	2/6/23/26	0/1/1/1
12	NAG	A	601	-	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	603	NAG	C1-C2-N2-C7
12	N	603	NAG	C1-C2-N2-C7
12	Y	603	NAG	C1-C2-N2-C7
12	A	605	NAG	O5-C5-C6-O6
12	B	702	NAG	O5-C5-C6-O6

There are no ring outliers.

18 monomers are involved in 126 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	N	603	NAG	4	0
12	A	602	NAG	8	0
12	Y	603	NAG	4	0
12	A	604	NAG	14	0
12	Y	602	NAG	8	0
12	N	602	NAG	8	0
13	O	703	FUC	4	0
12	O	702	NAG	7	0
12	Y	604	NAG	15	0
12	N	604	NAG	15	0
12	O	701	NAG	4	0
12	Z	701	NAG	4	0
12	A	603	NAG	4	0
12	B	701	NAG	4	0
13	B	703	FUC	5	0
13	Z	703	FUC	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	702	NAG	7	0
12	Z	702	NAG	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25178. 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

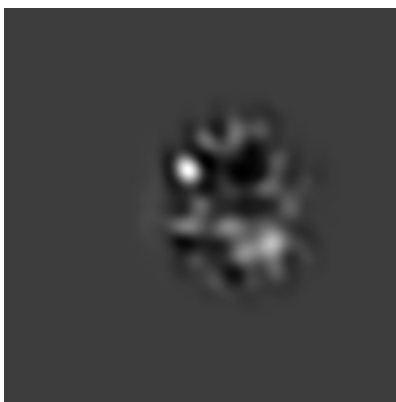
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 60



Y Index: 60



Z Index: 60

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: 57



Y Index: 49



Z Index: 69

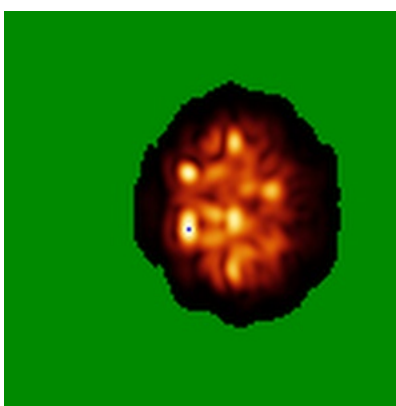
The images above show the largest variance slices of the map in three orthogonal directions.

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

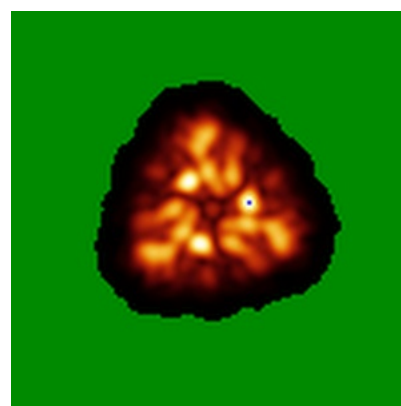
6.4.1 Primary map



X



Y

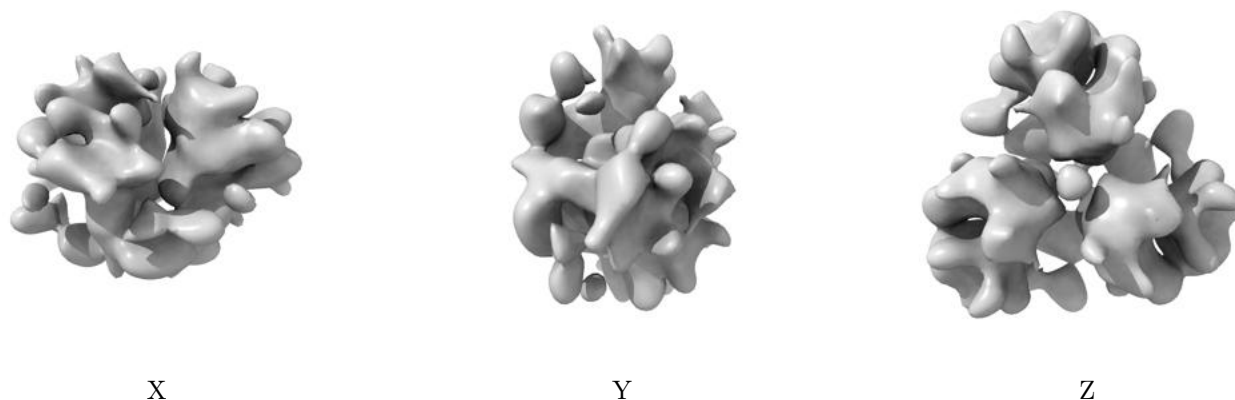


Z

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

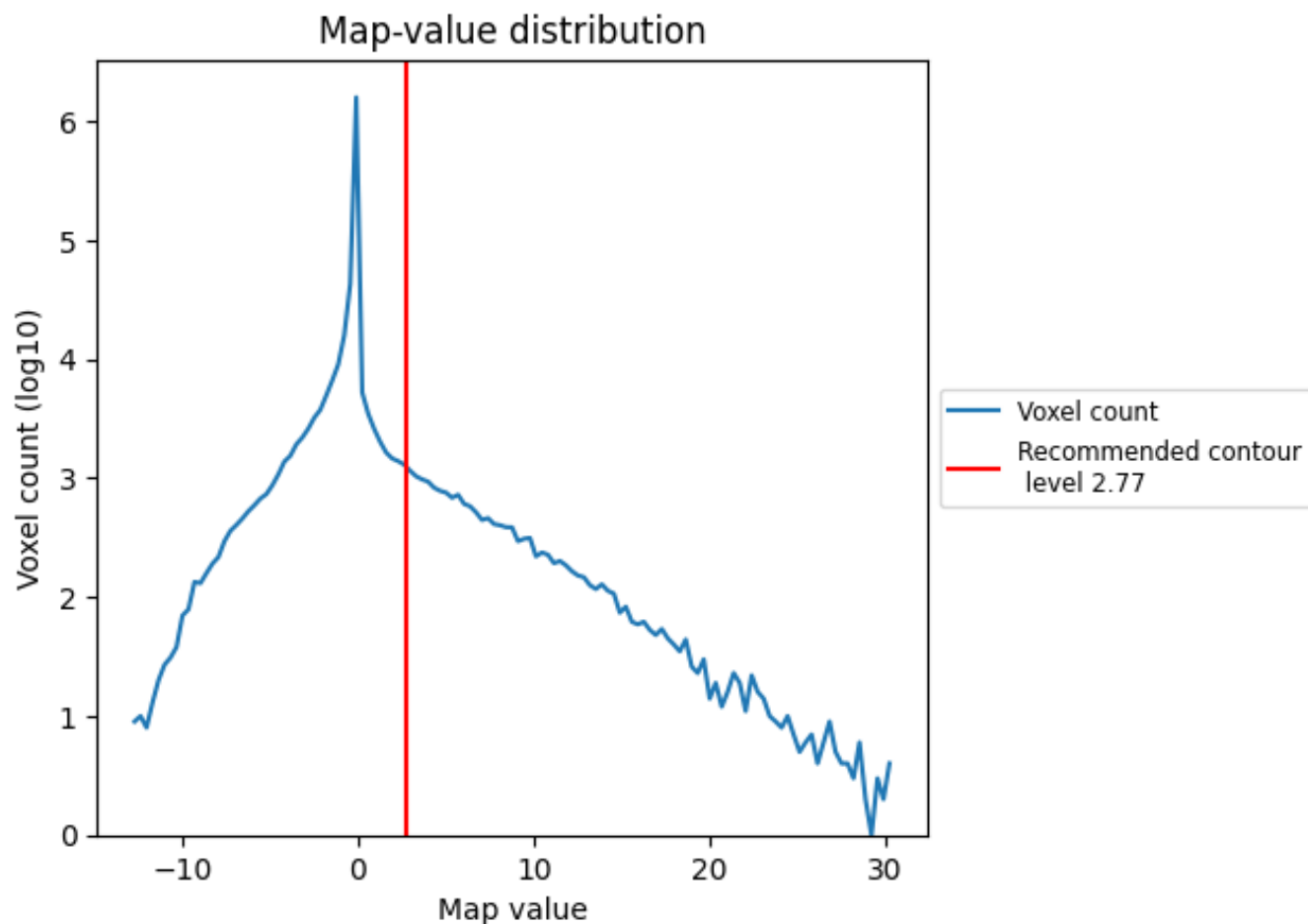
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

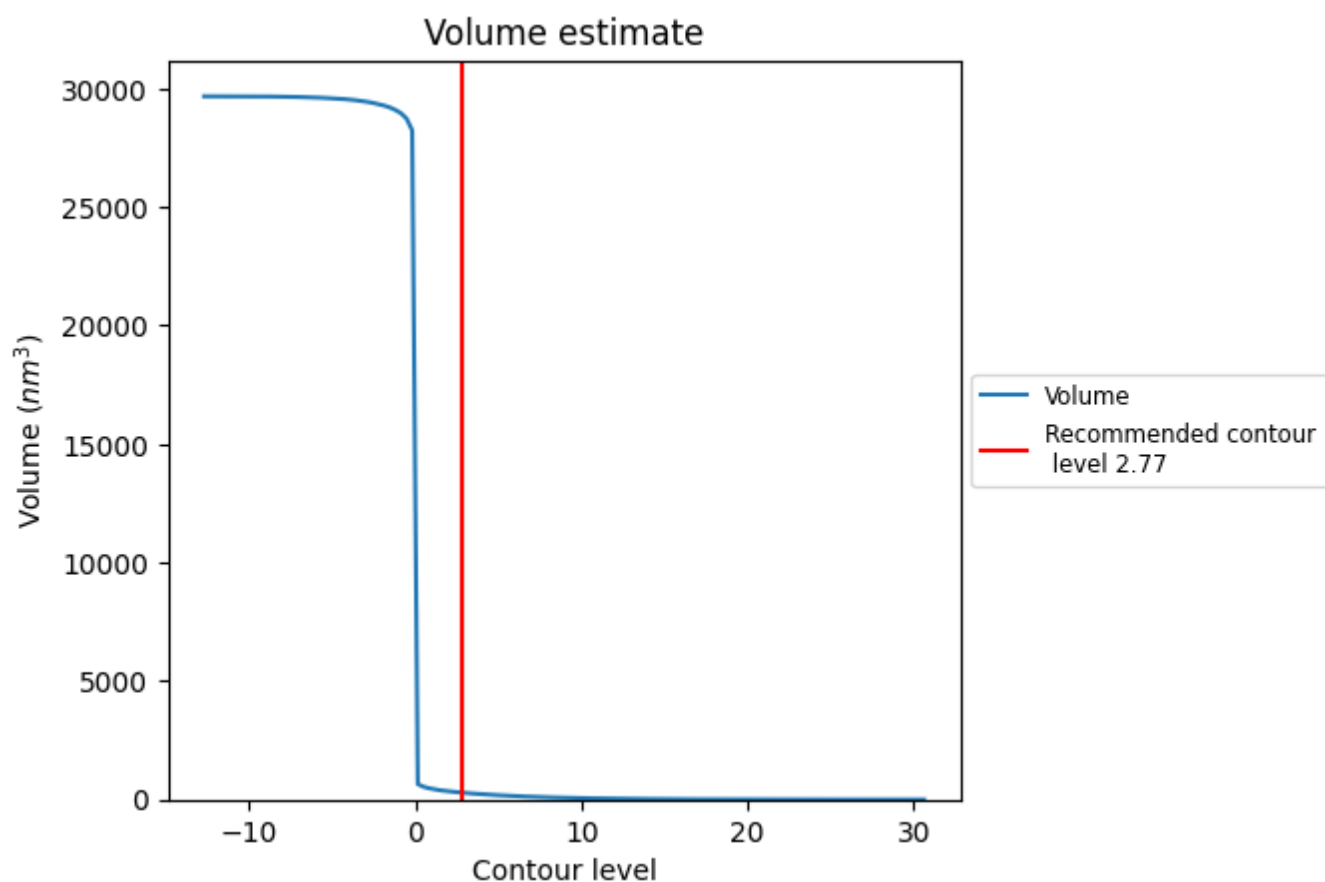
This section contains the results of statistical analysis of the map.

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.

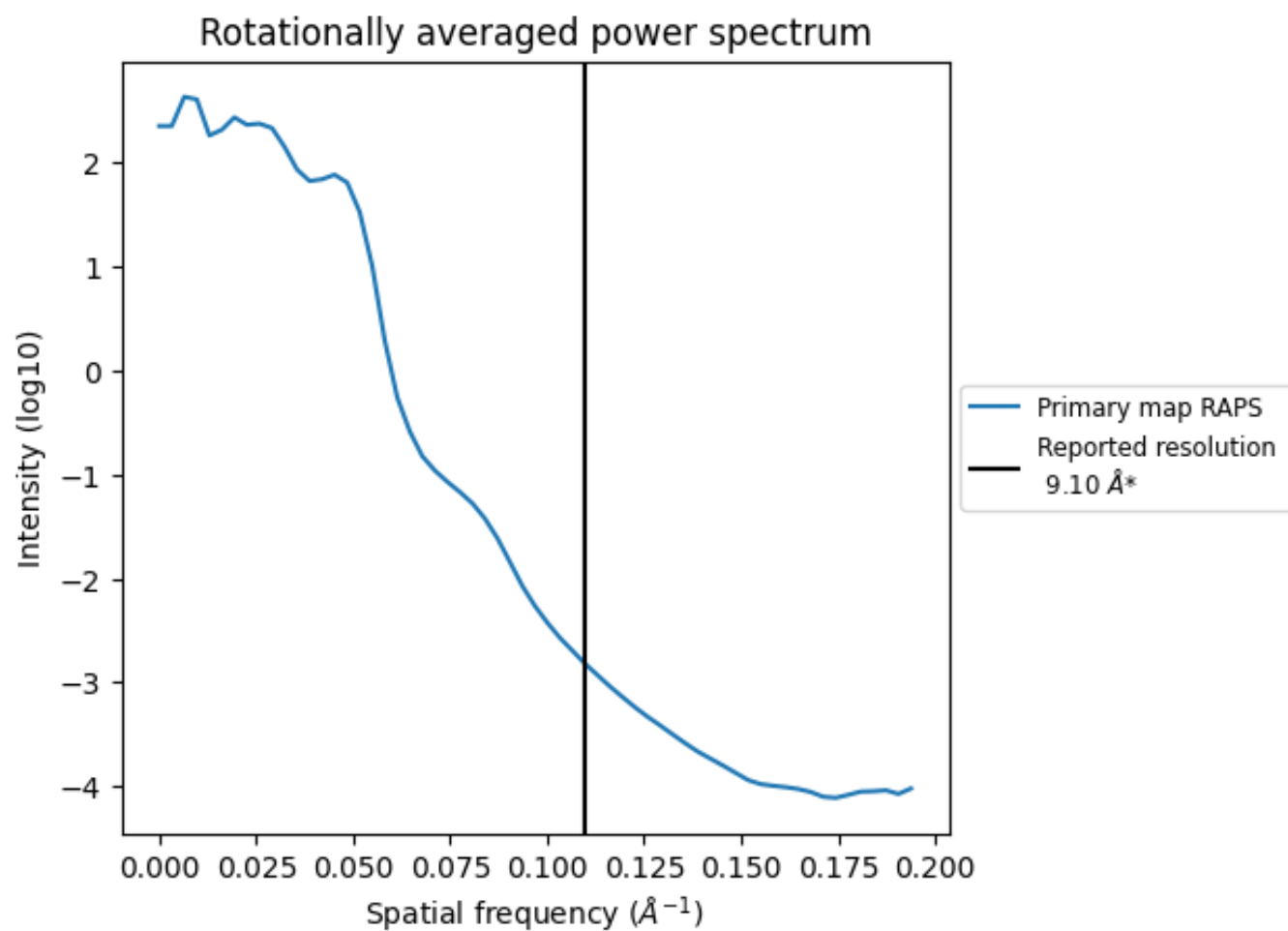
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 294 nm^3 ; this corresponds to an approximate mass of 266 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 ⓘ

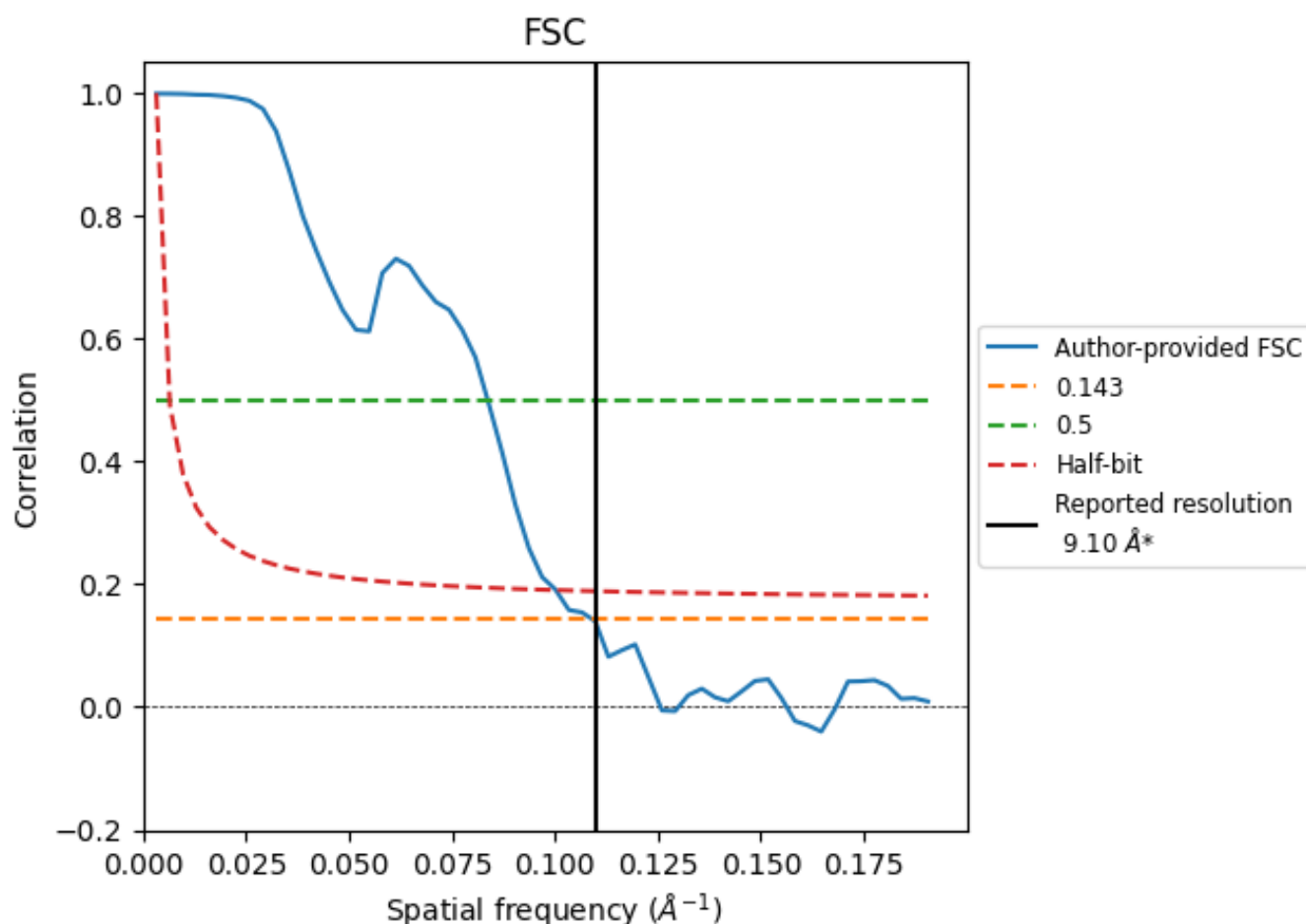


*Reported resolution corresponds to spatial frequency of 0.110 Å⁻¹

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 0.110 Å⁻¹

8.2 Resolution estimates [i](#)

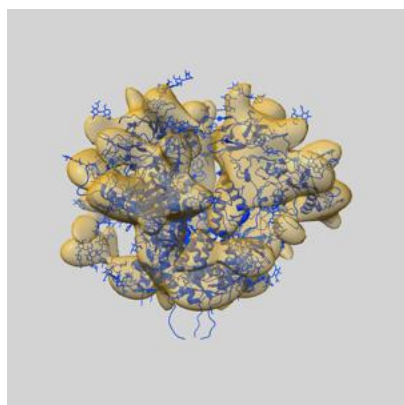
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.10	-	-
Author-provided FSC curve	9.17	11.95	9.98
Unmasked-calculated*	-	-	-

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

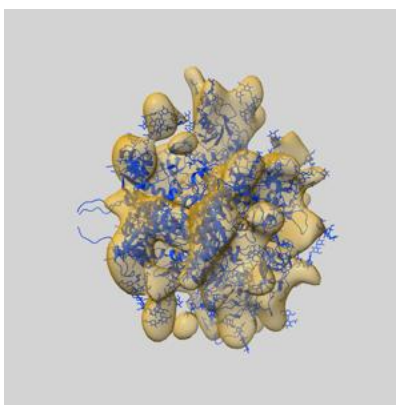
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25178 and PDB model 7SKA. Per-residue inclusion information can be found in section [3](#) on page [13](#).

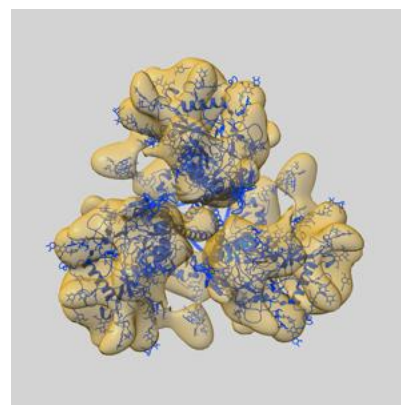
9.1 Map-model overlay [i](#)



X



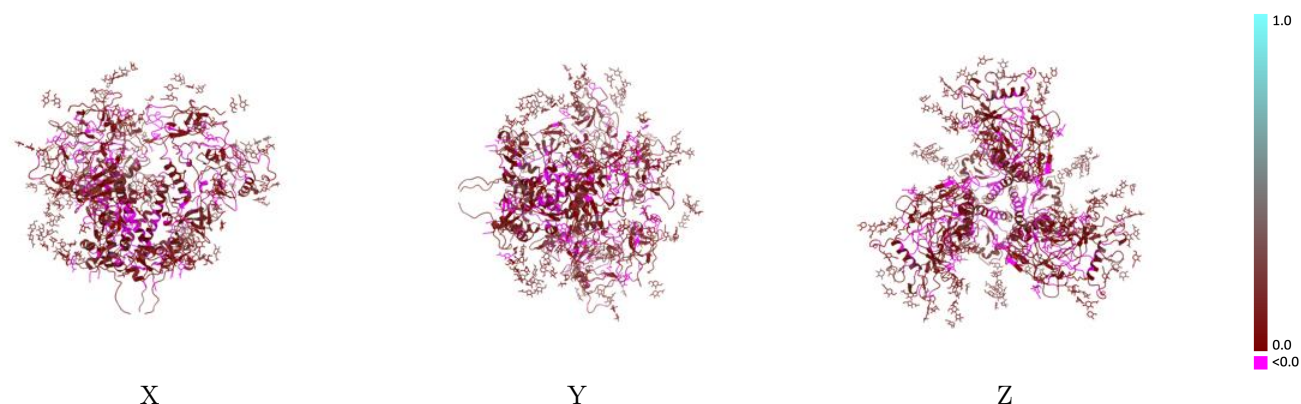
Y



Z

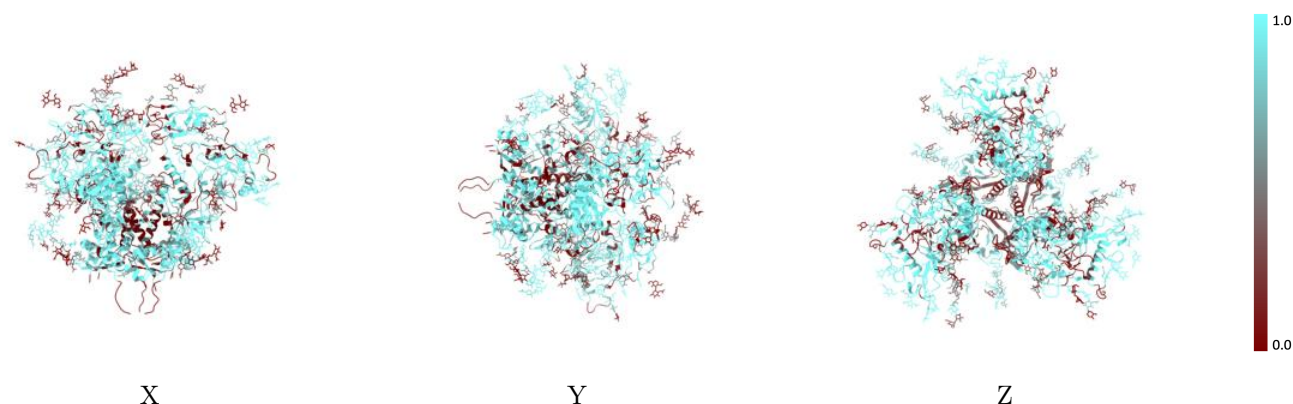
The images above show the 3D surface view of the map at the recommended contour level 2.77 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



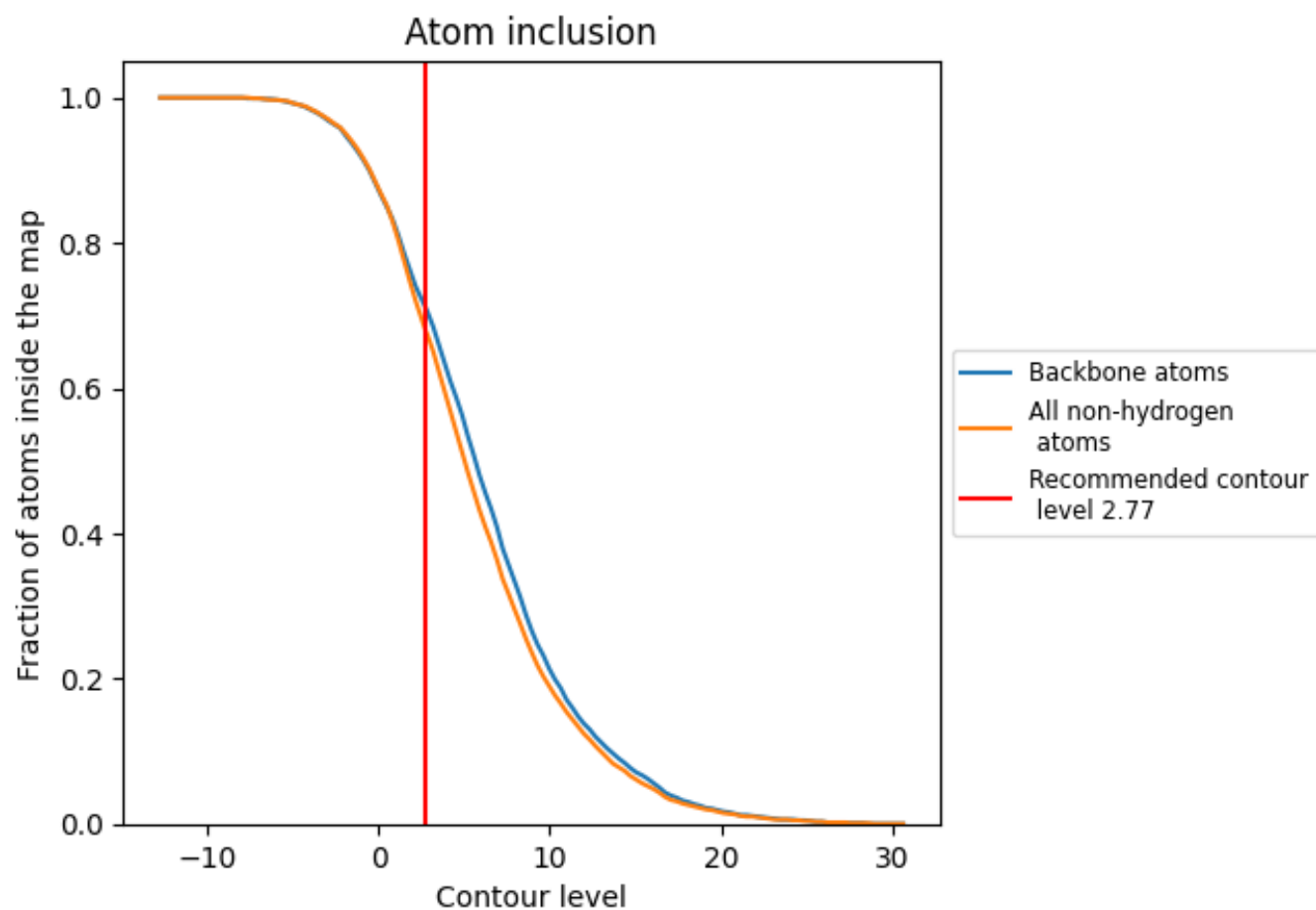
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.77).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (2.77) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6780	 0.0670
A	 0.7230	 0.0530
B	 0.6420	 0.0790
C	 0.0000	 0.1400
D	 0.4400	 0.1170
E	 1.0000	 0.1340
F	 0.4920	 0.0970
G	 0.8930	 0.1800
H	 0.5560	 0.1090
I	 0.1400	 0.1890
J	 0.2950	 0.0840
K	 0.6490	 0.1110
L	 0.9560	 0.1410
M	 0.9740	 0.3120
N	 0.7230	 0.0510
O	 0.6410	 0.0810
P	 0.1350	 0.0880
Q	 0.8300	 0.1560
R	 0.6000	 0.0680
S	 0.2080	 0.0280
T	 0.4920	 0.0740
U	 0.0000	 0.1630
V	 0.4400	 0.1250
W	 1.0000	 0.1200
X	 0.8930	 0.1960
Y	 0.7240	 0.0500
Z	 0.6410	 0.0800
a	 0.1400	 0.1840
b	 0.3110	 0.0870
c	 0.6490	 0.1080
d	 0.5420	 0.1140
e	 0.9560	 0.1370
f	 0.9740	 0.3080
g	 0.8400	 0.1660
h	 0.6000	 0.0920



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Chain	Atom inclusion	Q-score
i	 0.2080	 0.0150
j	 0.4920	 0.0860
k	 0.5420	 0.1140
l	 0.0000	 0.1370
m	 0.2220	 0.0230
n	 0.1350	 0.1010
o	 0.4400	 0.1240
p	 1.0000	 0.1490
q	 0.8930	 0.2040
r	 0.1400	 0.1830
s	 0.2790	 0.0840
t	 0.6490	 0.1080
u	 0.9560	 0.1390
v	 0.9740	 0.3090
w	 0.1350	 0.1090
x	 0.8400	 0.1710
y	 0.6000	 0.0820