



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 12:23 PM UTC

PDB ID : 5V8L / pdb_00005v8l
EMDB ID : EMD-8643
Title : BG505 SOSIP.664 trimer in complex with broadly neutralizing HIV antibodies
3BNC117 and PGT145
Authors : Lee, J.H.; Ward, A.B.
Deposited on : 2017-03-22
Resolution : 4.30 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.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

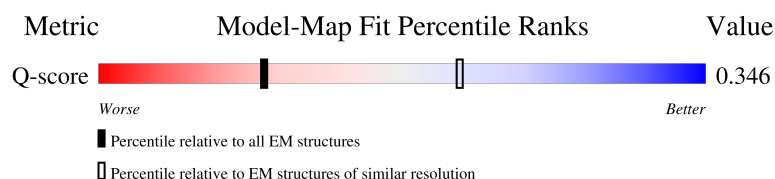
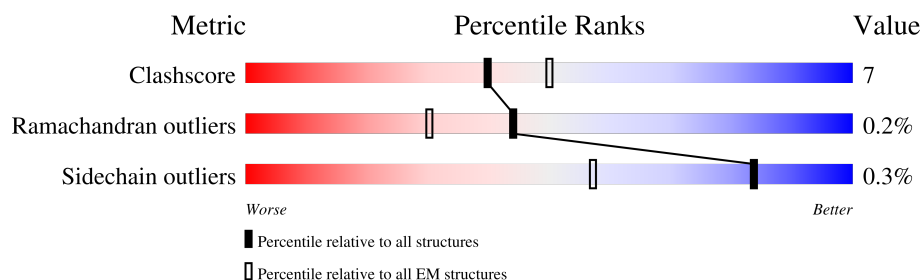
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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.



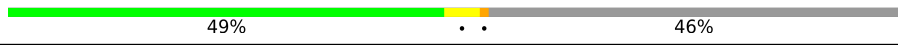
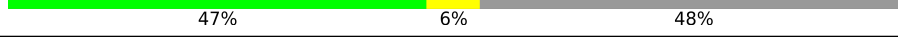
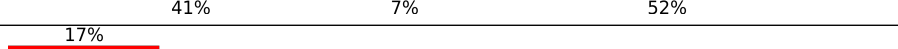
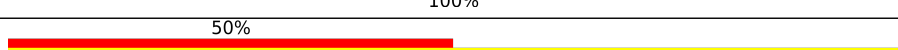
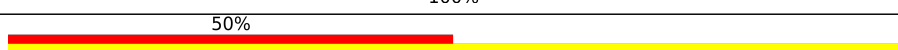
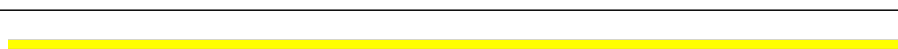
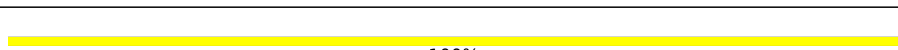
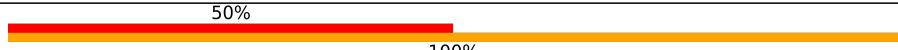
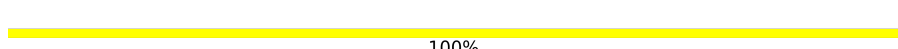
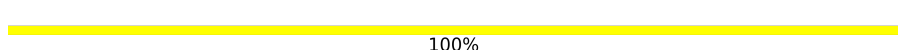
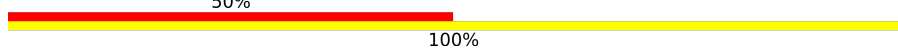
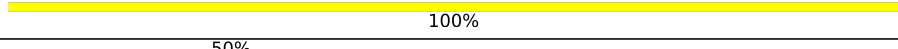
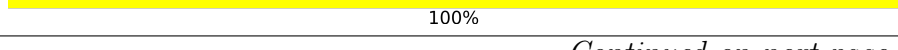
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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

Mol	Chain	Length	Quality of chain
1	A	481	
1	C	481	
1	D	481	
2	B	153	

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Mol	Chain	Length	Quality of chain
2	E	153	
2	F	153	
3	G	226	
3	H	226	
3	I	226	
4	J	267	
5	K	206	
5	L	206	
5	M	206	
6	N	219	
7	0	2	
7	1	2	
7	2	2	
7	3	2	
7	4	2	
7	O	2	
7	P	2	
7	Q	2	
7	R	2	
7	V	2	
7	W	2	
7	Z	2	
7	a	2	
7	b	2	
7	c	2	

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Mol	Chain	Length	Quality of chain
7	e	2	100%
7	h	2	50%
7	i	2	100%
7	j	2	50%
7	m	2	100%
7	n	2	100%
7	o	2	50%
7	p	2	100%
7	r	2	100%
7	u	2	50%
7	v	2	100%
7	w	2	50%
7	z	2	100%
8	S	3	33%
8	X	3	33%
8	d	3	67%
8	l	3	33%
8	y	3	67%
9	T	6	100%
10	U	7	86%
11	Y	5	20%
11	k	5	20%
11	x	5	20%
11	x	5	80%
12	f	7	14%
12	s	7	29%

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Mol	Chain	Length	Quality of chain
13	g	8	
13	q	8	
13	t	8	

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
13	NAG	q	1	-	-	X	-
13	NAG	q	2	-	-	X	-
13	MAN	q	4	-	-	X	-
14	NAG	D	639	X	-	-	-
7	NAG	Q	1	-	-	X	-
7	NAG	h	1	-	-	X	-
7	NAG	j	1	-	-	X	-
7	NAG	u	1	-	-	X	-
7	NAG	w	1	-	-	X	-
8	NAG	l	1	X	-	-	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 22934 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	450	Total	C	N	O	S	0	0
			3545	2227	625	665	28		
1	C	451	Total	C	N	O	S	0	0
			3553	2231	627	667	28		
1	D	452	Total	C	N	O	S	0	0
			3562	2236	628	670	28		

There are 21 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	126	Total	C	N	O	S	0	0
			1004	635	173	190	6		
2	E	124	Total	C	N	O	S	0	0
			987	623	170	188	6		
2	F	123	Total	C	N	O	S	0	0
			981	620	169	186	6		

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 4 is a protein called PGT145 antibody, heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	140	Total	C	N	O	S	0	0
			1094	685	191	213	5		

- Molecule 5 is a protein called 3BNC117 antibody, light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	98	Total	C	N	O	S	0	0
			783	493	137	150	3		
5	L	98	Total	C	N	O	S	0	0
			783	493	137	150	3		
5	M	98	Total	C	N	O	S	0	0
			783	493	137	150	3		

- Molecule 6 is a protein called PGT145 antibody, light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	112	Total	C	N	O	S	0	0
			859	542	153	160	4		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



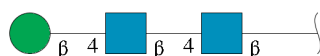
Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	2	Total	C	N	O		0	0
			28	16	2	10			
7	P	2	Total	C	N	O		0	0
			28	16	2	10			
7	Q	2	Total	C	N	O		0	0
			28	16	2	10			
7	R	2	Total	C	N	O		0	0
			28	16	2	10			
7	V	2	Total	C	N	O		0	0
			28	16	2	10			
7	W	2	Total	C	N	O		0	0
			28	16	2	10			
7	Z	2	Total	C	N	O		0	0
			28	16	2	10			
7	a	2	Total	C	N	O		0	0
			28	16	2	10			
7	b	2	Total	C	N	O		0	0
			28	16	2	10			
7	c	2	Total	C	N	O		0	0
			28	16	2	10			
7	e	2	Total	C	N	O		0	0
			28	16	2	10			
7	h	2	Total	C	N	O		0	0
			28	16	2	10			
7	i	2	Total	C	N	O		0	0
			28	16	2	10			
7	j	2	Total	C	N	O		0	0
			28	16	2	10			
7	m	2	Total	C	N	O		0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	n	2	Total	C	N	O	0	0
			28	16	2	10		
7	o	2	Total	C	N	O	0	0
			28	16	2	10		
7	p	2	Total	C	N	O	0	0
			28	16	2	10		
7	r	2	Total	C	N	O	0	0
			28	16	2	10		
7	u	2	Total	C	N	O	0	0
			28	16	2	10		
7	v	2	Total	C	N	O	0	0
			28	16	2	10		
7	w	2	Total	C	N	O	0	0
			28	16	2	10		
7	z	2	Total	C	N	O	0	0
			28	16	2	10		
7	0	2	Total	C	N	O	0	0
			28	16	2	10		
7	1	2	Total	C	N	O	0	0
			28	16	2	10		
7	2	2	Total	C	N	O	0	0
			28	16	2	10		
7	3	2	Total	C	N	O	0	0
			28	16	2	10		
7	4	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 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.



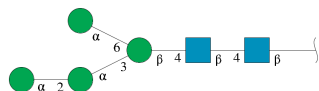
Mol	Chain	Residues	Atoms				AltConf	Trace
8	S	3	Total	C	N	O	0	0
			39	22	2	15		
8	X	3	Total	C	N	O	0	0
			39	22	2	15		
8	d	3	Total	C	N	O	0	0
			39	22	2	15		
8	l	3	Total	C	N	O	0	0
			39	22	2	15		

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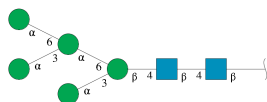
Mol	Chain	Residues	Atoms				AltConf	Trace
8	y	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 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.



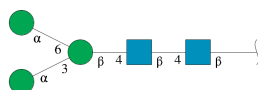
Mol	Chain	Residues	Atoms				AltConf	Trace
9	T	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
10	U	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



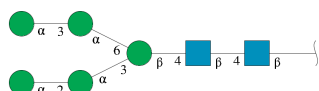
Mol	Chain	Residues	Atoms				AltConf	Trace
11	Y	5	Total	C	N	O	0	0
			61	34	2	25		
11	k	5	Total	C	N	O	0	0
			61	34	2	25		

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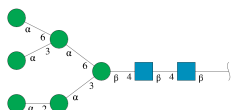
Mol	Chain	Residues	Atoms				AltConf	Trace
11	x	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
12	f	7	Total	C	N	O	0	0
			83	46	2	35		
12	s	7	Total	C	N	O	0	0
			83	46	2	35		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
13	g	8	Total	C	N	O	0	0
			94	52	2	40		
13	q	8	Total	C	N	O	0	0
			94	52	2	40		
13	t	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

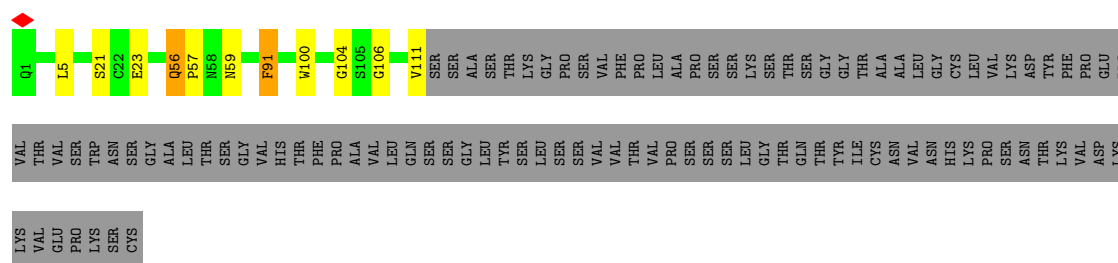


Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	N	O	0
			14	8	1	5	
14	A	1	Total	C	N	O	0
			14	8	1	5	
14	A	1	Total	C	N	O	0
			14	8	1	5	
14	A	1	Total	C	N	O	0
			14	8	1	5	
14	B	1	Total	C	N	O	0
			14	8	1	5	
14	B	1	Total	C	N	O	0
			14	8	1	5	
14	B	1	Total	C	N	O	0
			14	8	1	5	
14	C	1	Total	C	N	O	0
			14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

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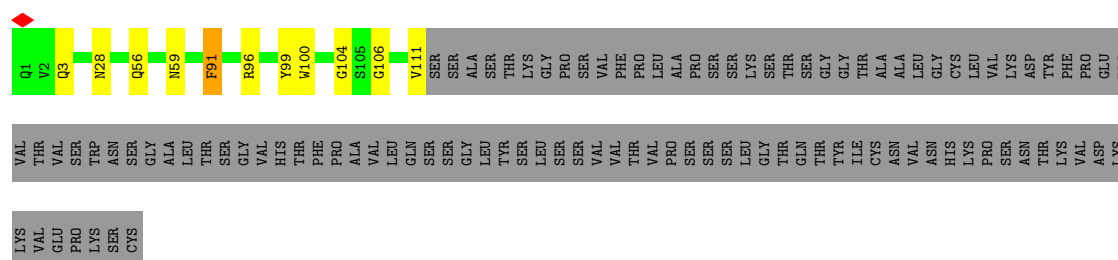
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Mol	Chain	Residues	Atoms				AltConf
14	D	1	Total 14	C 8	N 1	O 5	0
14	D	1	Total 14	C 8	N 1	O 5	0
14	E	1	Total 14	C 8	N 1	O 5	0
14	E	1	Total 14	C 8	N 1	O 5	0
14	F	1	Total 14	C 8	N 1	O 5	0
14	F	1	Total 14	C 8	N 1	O 5	0



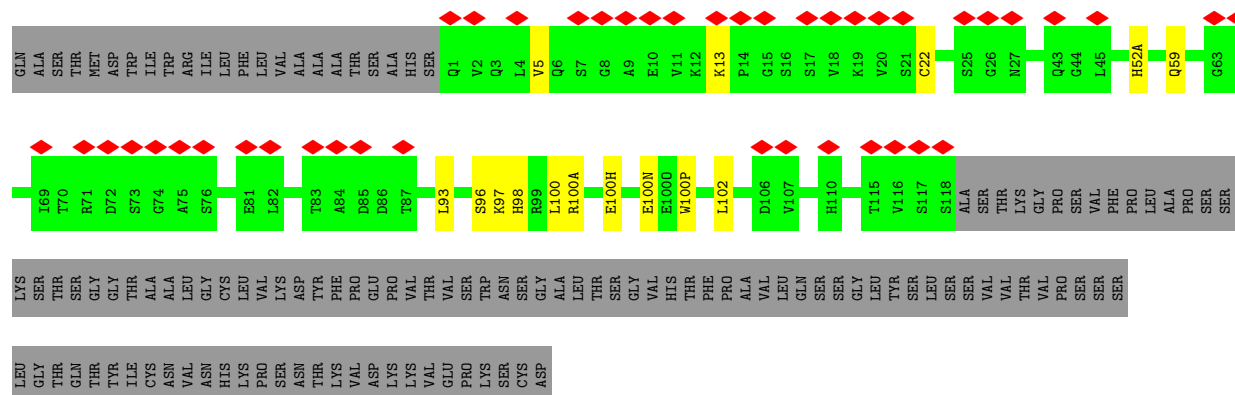
• Molecule 3: 3BNC117 antibody, heavy chain

Chain I: 49% . 46%



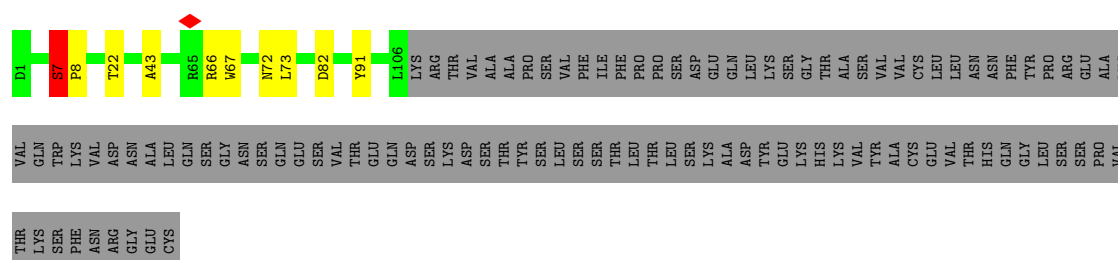
• Molecule 4: PGT145 antibody, heavy chain

Chain J: 16% 47% 6% 48%

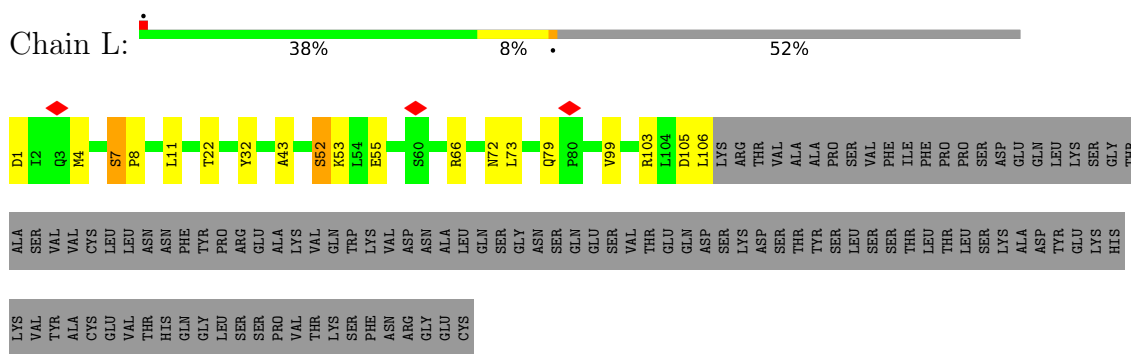


• Molecule 5: 3BNC117 antibody, light chain

Chain K: 43% . 52%



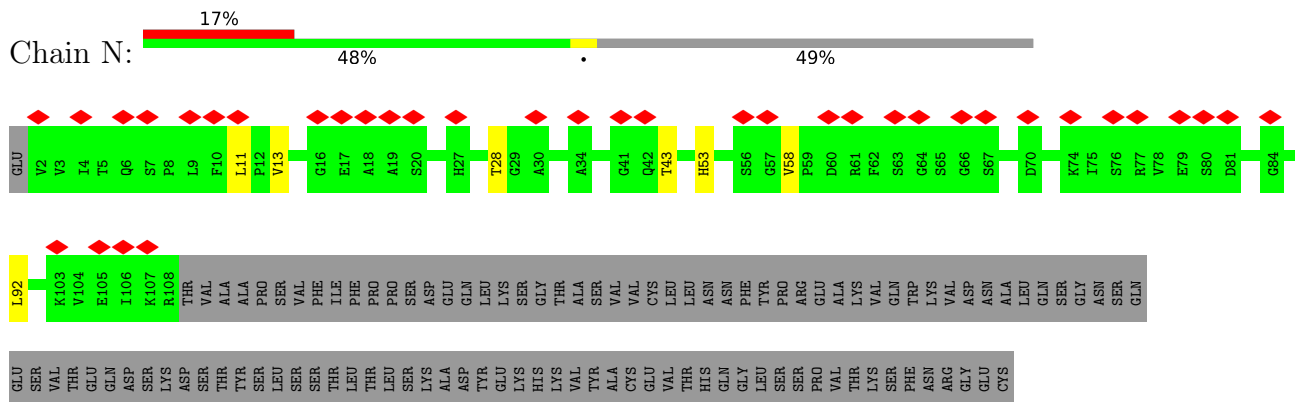
- Molecule 5: 3BNC117 antibody, light chain



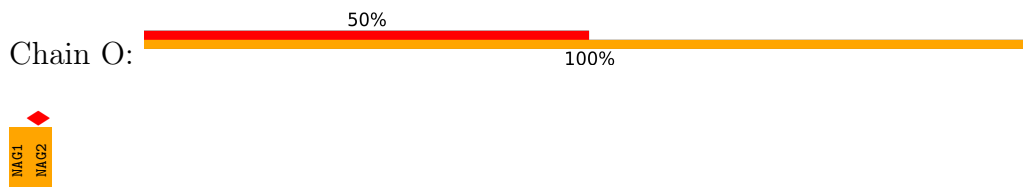
- Molecule 5: 3BNC117 antibody, light chain



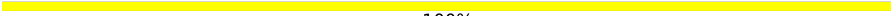
- Molecule 6: PGT145 antibody, light chain



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

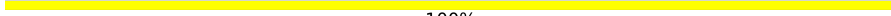


- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%

NAG1
NAG2

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

Chain Q:  100%

NAG1
NAG2

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

Chain R:  100%

NAG1
NAG2

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

Chain V:  50%

NAG1
NAG2

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

Chain W:  100%

NAG1
NAG2

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

Chain Z:  50%

NAG1
NAG2

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

Chain a:  50%



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

Chain b: 100%



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

Chain c: 50%
100%



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

Chain e: 100%



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

Chain h: 50%
50%



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

Chain i: 100%



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

Chain j: 50%
50%



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

Chain m:  100%

NAG1
NAG2

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

Chain n:  100%

NAG1
NAG2

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

Chain o:  50% 100%

♦
NAG1
NAG2

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

Chain p:  100%

NAG1
NAG2

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

Chain r:  100%

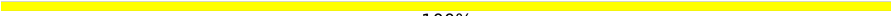
NAG1
NAG2

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

Chain u:  50% 50%

NAG1
NAG2

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

Chain v:  100%

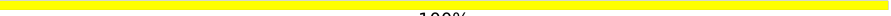
NAG1
NAG2

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

Chain w:  50%  50%

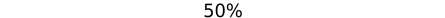
NAG1
NAG2

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

Chain z:  100%

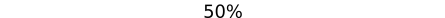
NAG1
NAG2

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

Chain 0:  50%  100%

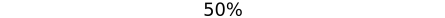
♦
NAG1
NAG2

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

Chain 1:  50%  100%

♦
NAG1
NAG2

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

Chain 2:  50%  100%

♦
NAG1
NAG2

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

Chain 3:  100%

MAG1
MAG2

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

Chain 4:  100%

MAG1
MAG2

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

Chain S:  33% 100%

MAG1
MAG2
BMA3

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

Chain X:  33% 100%

MAG1
MAG2
BMA3

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

Chain d:  67% 100%

MAG1
MAG2
BMA3

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

Chain l:  33% 33% 33%

MAG1
MAG2
BMA3

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

Chain y:  67% 33%



- Molecule 9: 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

Chain T:



- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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

Chain U:



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

Chain Y:



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

Chain k:

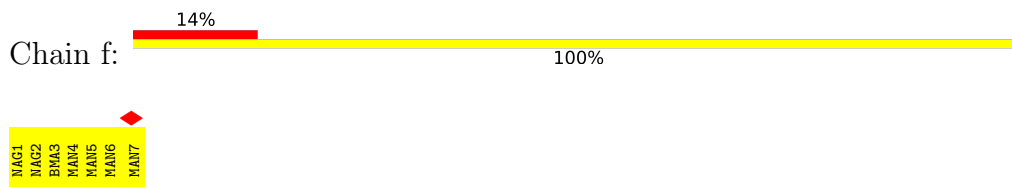


- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

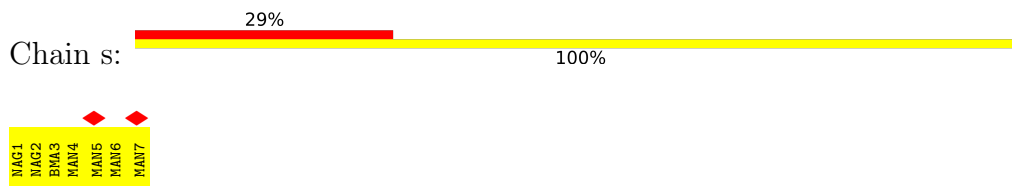
Chain x:



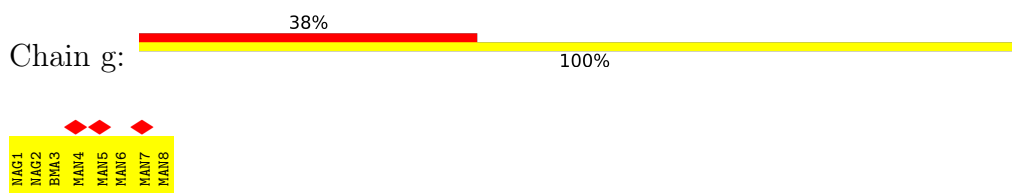
- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



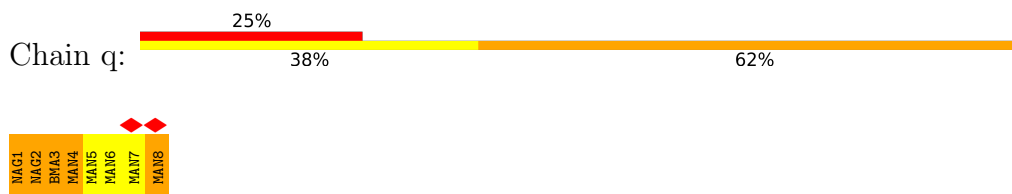
- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



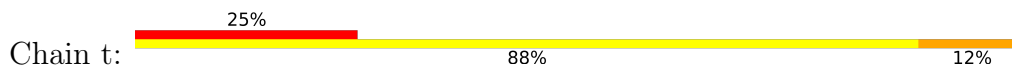
- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	65060	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	377.27997, 377.27997, 377.27997	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.90	0/3619	1.29	35/4914 (0.7%)
1	C	0.92	0/3627	1.32	40/4925 (0.8%)
1	D	0.93	0/3636	1.31	46/4937 (0.9%)
2	B	0.98	0/1021	1.11	3/1384 (0.2%)
2	E	0.98	0/1004	1.11	5/1362 (0.4%)
2	F	1.01	0/998	1.09	8/1354 (0.6%)
3	G	0.98	0/1017	1.26	6/1386 (0.4%)
3	H	0.97	0/1017	1.28	7/1386 (0.5%)
3	I	1.01	0/1017	1.31	8/1386 (0.6%)
4	J	0.82	0/1121	1.15	2/1519 (0.1%)
5	K	0.82	0/800	1.28	7/1086 (0.6%)
5	L	0.82	0/800	1.31	5/1086 (0.5%)
5	M	0.81	0/800	1.29	7/1086 (0.6%)
6	N	0.75	0/882	1.23	8/1199 (0.7%)
All	All	0.92	0/21359	1.26	187/29010 (0.6%)

There are no bond length outliers.

The worst 5 of 187 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	252	LYS	CA-C-N	10.06	131.29	120.12
1	C	252	LYS	C-N-CA	10.06	131.29	120.12
1	A	436	ALA	CA-C-N	9.49	126.49	119.66
1	A	436	ALA	C-N-CA	9.49	126.49	119.66
1	C	298	ARG	CA-C-N	9.26	129.01	119.56

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	3545	0	3481	66	0
1	C	3553	0	3488	56	0
1	D	3562	0	3494	53	0
2	B	1004	0	989	6	0
2	E	987	0	965	2	0
2	F	981	0	960	19	0
3	G	985	0	919	4	0
3	H	985	0	919	7	0
3	I	985	0	919	6	0
4	J	1094	0	1033	31	0
5	K	783	0	763	7	0
5	L	783	0	763	16	0
5	M	783	0	763	11	0
6	N	859	0	841	8	0
7	O	28	0	25	0	0
7	1	28	0	25	0	0
7	2	28	0	25	0	0
7	3	28	0	25	0	0
7	4	28	0	25	0	0
7	O	28	0	25	3	0
7	P	28	0	25	0	0
7	Q	28	0	25	15	0
7	R	28	0	25	0	0
7	V	28	0	25	6	0
7	W	28	0	25	3	0
7	Z	28	0	25	0	0
7	a	28	0	25	4	0
7	b	28	0	25	0	0
7	c	28	0	25	4	0
7	e	28	0	25	0	0
7	h	28	0	25	13	0
7	i	28	0	25	2	0
7	j	28	0	25	12	0
7	m	28	0	25	0	0
7	n	28	0	25	2	0
7	o	28	0	25	5	0
7	p	28	0	25	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	r	28	0	25	0	0
7	u	28	0	25	9	0
7	v	28	0	25	4	0
7	w	28	0	25	9	0
7	z	28	0	25	2	0
8	S	39	0	34	0	0
8	X	39	0	34	0	0
8	d	39	0	34	0	0
8	l	39	0	34	5	0
8	y	39	0	34	4	0
9	T	72	0	61	0	0
10	U	83	0	70	6	0
11	Y	61	0	52	6	0
11	k	61	0	52	2	0
11	x	61	0	52	2	0
12	f	83	0	70	0	0
12	s	83	0	70	0	0
13	g	94	0	79	2	0
13	q	94	0	79	34	0
13	t	94	0	79	6	0
14	A	56	0	52	0	0
14	B	42	0	39	0	0
14	C	56	0	52	5	0
14	D	70	0	65	3	0
14	E	28	0	26	0	0
14	F	28	0	26	0	0
All	All	22934	0	22091	305	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 7.

The worst 5 of 305 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)
1:A:134:VAL:HG11	7:Q:1:NAG:O7	1.16	1.28
1:C:330:HIS:HE1	7:j:1:NAG:N2	1.29	1.28
1:C:330:HIS:CE1	7:j:1:NAG:HN2	1.56	1.23
1:A:173:TYR:OH	7:Q:1:NAG:H3	1.38	1.20
1:C:87:GLU:CG	14:C:601:NAG:H82	1.72	1.19

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	444/481 (92%)	433 (98%)	11 (2%)	0	100	100
1	C	445/481 (92%)	434 (98%)	10 (2%)	1 (0%)	43	77
1	D	446/481 (93%)	439 (98%)	7 (2%)	0	100	100
2	B	122/153 (80%)	122 (100%)	0	0	100	100
2	E	120/153 (78%)	118 (98%)	2 (2%)	0	100	100
2	F	119/153 (78%)	117 (98%)	2 (2%)	0	100	100
3	G	119/226 (53%)	117 (98%)	2 (2%)	0	100	100
3	H	119/226 (53%)	117 (98%)	2 (2%)	0	100	100
3	I	119/226 (53%)	119 (100%)	0	0	100	100
4	J	138/267 (52%)	137 (99%)	1 (1%)	0	100	100
5	K	96/206 (47%)	93 (97%)	2 (2%)	1 (1%)	12	47
5	L	96/206 (47%)	92 (96%)	2 (2%)	2 (2%)	5	30
5	M	96/206 (47%)	93 (97%)	2 (2%)	1 (1%)	12	47
6	N	110/219 (50%)	108 (98%)	2 (2%)	0	100	100
All	All	2589/3684 (70%)	2539 (98%)	45 (2%)	5 (0%)	44	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	L	52	SER
1	C	80	ASN
5	M	52	SER
5	K	7	SER
5	L	7	SER

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	402/428 (94%)	399 (99%)	3 (1%)	76	79
1	C	403/428 (94%)	403 (100%)	0	100	100
1	D	404/428 (94%)	403 (100%)	1 (0%)	87	85
2	B	109/129 (84%)	107 (98%)	2 (2%)	51	67
2	E	107/129 (83%)	106 (99%)	1 (1%)	70	76
2	F	106/129 (82%)	105 (99%)	1 (1%)	70	76
3	G	102/193 (53%)	102 (100%)	0	100	100
3	H	102/193 (53%)	102 (100%)	0	100	100
3	I	102/193 (53%)	102 (100%)	0	100	100
4	J	115/223 (52%)	115 (100%)	0	100	100
5	K	86/183 (47%)	86 (100%)	0	100	100
5	L	86/183 (47%)	86 (100%)	0	100	100
5	M	86/183 (47%)	86 (100%)	0	100	100
6	N	95/191 (50%)	95 (100%)	0	100	100
All	All	2305/3213 (72%)	2297 (100%)	8 (0%)	84	84

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	618	ASN
2	E	618	ASN
2	B	637	ASN
2	B	618	ASN
1	D	65	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	56	GLN

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Mol	Chain	Res	Type
4	J	52(A)	HIS
3	I	46	GLN
4	J	98	HIS
1	C	330	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 ⓘ

137 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	$\# Z > 2$
7	NAG	0	1	7,2	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
7	NAG	0	2	7	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
7	NAG	1	1	7,2	14,14,15	0.51	0	17,19,21	2.28	3 (17%)
7	NAG	1	2	7	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
7	NAG	2	1	7,5	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
7	NAG	2	2	7	14,14,15	0.50	0	17,19,21	1.33	3 (17%)
7	NAG	3	1	7,5	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
7	NAG	3	2	7	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
7	NAG	4	1	7,5	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
7	NAG	4	2	7	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
7	NAG	O	1	1,7	14,14,15	0.78	1 (7%)	17,19,21	0.92	2 (11%)
7	NAG	O	2	7	14,14,15	0.45	0	17,19,21	1.55	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	P	1	1,7	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
7	NAG	P	2	7	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
7	NAG	Q	1	1,7	14,14,15	0.26	0	17,19,21	0.56	0
7	NAG	Q	2	7	14,14,15	0.31	0	17,19,21	0.67	1 (5%)
7	NAG	R	1	1,7	14,14,15	0.48	0	17,19,21	2.27	3 (17%)
7	NAG	R	2	7	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
8	NAG	S	1	1,8	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
8	NAG	S	2	8	14,14,15	0.51	0	17,19,21	1.34	3 (17%)
8	BMA	S	3	8	11,11,12	0.64	0	15,15,17	1.43	3 (20%)
9	NAG	T	1	1,9	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
9	NAG	T	2	9	14,14,15	0.50	0	17,19,21	1.32	3 (17%)
9	BMA	T	3	9	11,11,12	0.67	0	15,15,17	1.43	3 (20%)
9	MAN	T	4	9	11,11,12	0.55	0	15,15,17	1.49	2 (13%)
9	MAN	T	5	9	11,11,12	0.59	0	15,15,17	2.31	5 (33%)
9	MAN	T	6	9	11,11,12	0.60	0	15,15,17	2.22	3 (20%)
10	NAG	U	1	1,10	14,14,15	0.77	1 (7%)	17,19,21	0.69	0
10	NAG	U	2	10	14,14,15	0.41	0	17,19,21	0.47	0
10	BMA	U	3	10	11,11,12	1.65	4 (36%)	15,15,17	1.79	2 (13%)
10	MAN	U	4	10	11,11,12	0.61	0	15,15,17	2.21	3 (20%)
10	MAN	U	5	10	11,11,12	0.57	0	15,15,17	1.92	5 (33%)
10	MAN	U	6	10	11,11,12	0.60	0	15,15,17	2.27	6 (40%)
10	MAN	U	7	10	11,11,12	1.65	3 (27%)	15,15,17	1.28	2 (13%)
7	NAG	V	1	1,7	14,14,15	0.31	0	17,19,21	0.72	0
7	NAG	V	2	7	14,14,15	0.67	0	17,19,21	0.54	0
7	NAG	W	1	1,7	14,14,15	0.46	0	17,19,21	0.43	0
7	NAG	W	2	7	14,14,15	0.61	0	17,19,21	0.57	0
8	NAG	X	1	1,8	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
8	NAG	X	2	8	14,14,15	0.50	0	17,19,21	1.33	3 (17%)
8	BMA	X	3	8	11,11,12	0.64	0	15,15,17	1.43	3 (20%)
11	NAG	Y	1	1,11	14,14,15	0.32	0	17,19,21	0.60	0
11	NAG	Y	2	11	14,14,15	0.35	0	17,19,21	0.84	1 (5%)
11	BMA	Y	3	11	11,11,12	0.65	0	15,15,17	1.43	3 (20%)
11	MAN	Y	4	11	11,11,12	0.53	0	15,15,17	1.47	2 (13%)
11	MAN	Y	5	11	11,11,12	0.63	0	15,15,17	2.19	3 (20%)
7	NAG	Z	1	1,7	14,14,15	0.99	1 (7%)	17,19,21	1.05	1 (5%)
7	NAG	Z	2	7	14,14,15	0.50	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	a	1	1,7	14,14,15	0.49	0	17,19,21	0.56	0
7	NAG	a	2	7	14,14,15	0.41	0	17,19,21	0.45	0
7	NAG	b	1	1,7	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
7	NAG	b	2	7	14,14,15	0.50	0	17,19,21	1.32	3 (17%)
7	NAG	c	1	1,7	14,14,15	0.27	0	17,19,21	0.55	0
7	NAG	c	2	7	14,14,15	0.32	0	17,19,21	0.67	1 (5%)
8	NAG	d	1	1,8	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
8	NAG	d	2	8	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
8	BMA	d	3	8	11,11,12	0.64	0	15,15,17	1.43	3 (20%)
7	NAG	e	1	1,7	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
7	NAG	e	2	7	14,14,15	0.53	0	17,19,21	1.33	3 (17%)
12	NAG	f	1	1,12	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
12	NAG	f	2	12	14,14,15	0.50	0	17,19,21	1.33	3 (17%)
12	BMA	f	3	12	11,11,12	0.67	0	15,15,17	1.43	3 (20%)
12	MAN	f	4	12	11,11,12	0.57	0	15,15,17	1.50	2 (13%)
12	MAN	f	5	12	11,11,12	0.60	0	15,15,17	2.31	5 (33%)
12	MAN	f	6	12	11,11,12	0.59	0	15,15,17	2.21	3 (20%)
12	MAN	f	7	12	11,11,12	0.55	0	15,15,17	1.92	5 (33%)
13	NAG	g	1	1,13	14,14,15	0.76	1 (7%)	17,19,21	0.69	0
13	NAG	g	2	13	14,14,15	0.41	0	17,19,21	0.45	0
13	BMA	g	3	13	11,11,12	1.66	3 (27%)	15,15,17	1.81	2 (13%)
13	MAN	g	4	13	11,11,12	1.67	3 (27%)	15,15,17	1.27	2 (13%)
13	MAN	g	5	13	11,11,12	2.27	4 (36%)	15,15,17	1.68	3 (20%)
13	MAN	g	6	13	11,11,12	0.58	0	15,15,17	2.22	3 (20%)
13	MAN	g	7	13	11,11,12	0.58	0	15,15,17	1.93	5 (33%)
13	MAN	g	8	13	11,11,12	0.62	0	15,15,17	2.27	7 (46%)
7	NAG	h	1	1,7	14,14,15	0.32	0	17,19,21	0.73	0
7	NAG	h	2	7	14,14,15	0.67	0	17,19,21	0.54	0
7	NAG	i	1	1,7	14,14,15	0.44	0	17,19,21	0.43	0
7	NAG	i	2	7	14,14,15	0.61	0	17,19,21	0.58	0
7	NAG	j	1	1,7	14,14,15	0.40	0	17,19,21	0.76	1 (5%)
7	NAG	j	2	7	14,14,15	0.53	0	17,19,21	0.55	0
11	NAG	k	1	1,11	14,14,15	0.34	0	17,19,21	0.59	0
11	NAG	k	2	11	14,14,15	0.36	0	17,19,21	0.85	1 (5%)
11	BMA	k	3	11	11,11,12	0.66	0	15,15,17	1.45	3 (20%)
11	MAN	k	4	11	11,11,12	0.55	0	15,15,17	1.48	2 (13%)
11	MAN	k	5	11	11,11,12	0.63	0	15,15,17	2.20	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	l	1	1,8	14,14,15	0.96	1 (7%)	17,19,21	1.05	1 (5%)
8	NAG	l	2	8	14,14,15	0.52	0	17,19,21	0.56	0
8	BMA	l	3	8	11,11,12	0.62	0	15,15,17	1.42	3 (20%)
7	NAG	m	1	1,7	14,14,15	0.49	0	17,19,21	2.28	3 (17%)
7	NAG	m	2	7	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
7	NAG	n	1	1,7	14,14,15	0.49	0	17,19,21	0.57	0
7	NAG	n	2	7	14,14,15	0.40	0	17,19,21	0.44	0
7	NAG	o	1	1,7	14,14,15	0.79	1 (7%)	17,19,21	0.91	2 (11%)
7	NAG	o	2	7	14,14,15	0.45	0	17,19,21	1.55	3 (17%)
7	NAG	p	1	1,7	14,14,15	0.27	0	17,19,21	0.55	0
7	NAG	p	2	7	14,14,15	0.32	0	17,19,21	0.67	1 (5%)
13	NAG	q	1	1,13	14,14,15	1.48	4 (28%)	17,19,21	1.04	1 (5%)
13	NAG	q	2	13	14,14,15	1.35	2 (14%)	17,19,21	1.26	2 (11%)
13	BMA	q	3	13	11,11,12	1.40	2 (18%)	15,15,17	0.95	1 (6%)
13	MAN	q	4	13	11,11,12	1.50	3 (27%)	15,15,17	1.59	2 (13%)
13	MAN	q	5	13	11,11,12	1.55	3 (27%)	15,15,17	1.61	2 (13%)
13	MAN	q	6	13	11,11,12	1.64	3 (27%)	15,15,17	1.44	1 (6%)
13	MAN	q	7	13	11,11,12	1.55	3 (27%)	15,15,17	1.33	1 (6%)
13	MAN	q	8	13	11,11,12	1.45	2 (18%)	15,15,17	1.39	1 (6%)
7	NAG	r	1	1,7	14,14,15	0.49	0	17,19,21	2.27	3 (17%)
7	NAG	r	2	7	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
12	NAG	s	1	1,12	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
12	NAG	s	2	12	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
12	BMA	s	3	12	11,11,12	0.67	0	15,15,17	1.43	3 (20%)
12	MAN	s	4	12	11,11,12	0.57	0	15,15,17	1.50	3 (20%)
12	MAN	s	5	12	11,11,12	0.59	0	15,15,17	2.30	5 (33%)
12	MAN	s	6	12	11,11,12	0.59	0	15,15,17	2.22	3 (20%)
12	MAN	s	7	12	11,11,12	0.56	0	15,15,17	1.92	5 (33%)
13	NAG	t	1	1,13	14,14,15	0.77	1 (7%)	17,19,21	0.69	0
13	NAG	t	2	13	14,14,15	0.41	0	17,19,21	0.47	0
13	BMA	t	3	13	11,11,12	1.66	4 (36%)	15,15,17	1.80	2 (13%)
13	MAN	t	4	13	11,11,12	1.66	3 (27%)	15,15,17	1.27	2 (13%)
13	MAN	t	5	13	11,11,12	2.28	4 (36%)	15,15,17	1.68	3 (20%)
13	MAN	t	6	13	11,11,12	0.59	0	15,15,17	2.22	3 (20%)
13	MAN	t	7	13	11,11,12	0.58	0	15,15,17	1.93	5 (33%)
13	MAN	t	8	13	11,11,12	0.60	0	15,15,17	2.26	7 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	u	1	1,7	14,14,15	0.30	0	17,19,21	0.73	0
7	NAG	u	2	7	14,14,15	0.66	0	17,19,21	0.54	0
7	NAG	v	1	1,7	14,14,15	0.44	0	17,19,21	0.42	0
7	NAG	v	2	7	14,14,15	0.60	0	17,19,21	0.57	0
7	NAG	w	1	1,7	14,14,15	0.39	0	17,19,21	0.76	1 (5%)
7	NAG	w	2	7	14,14,15	0.54	0	17,19,21	0.55	0
11	NAG	x	1	1,11	14,14,15	0.33	0	17,19,21	0.59	0
11	NAG	x	2	11	14,14,15	0.37	0	17,19,21	0.84	1 (5%)
11	BMA	x	3	11	11,11,12	0.65	0	15,15,17	1.44	3 (20%)
11	MAN	x	4	11	11,11,12	0.53	0	15,15,17	1.47	2 (13%)
11	MAN	x	5	11	11,11,12	0.60	0	15,15,17	2.19	3 (20%)
8	NAG	y	1	1,8	14,14,15	0.97	1 (7%)	17,19,21	1.06	1 (5%)
8	NAG	y	2	8	14,14,15	0.51	0	17,19,21	0.56	0
8	BMA	y	3	8	11,11,12	0.63	0	15,15,17	1.42	3 (20%)
7	NAG	z	1	1,7	14,14,15	0.51	0	17,19,21	0.57	0
7	NAG	z	2	7	14,14,15	0.40	0	17,19,21	0.46	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
7	NAG	0	1	7,2	-	1/6/23/26	0/1/1/1
7	NAG	0	2	7	-	0/6/23/26	0/1/1/1
7	NAG	1	1	7,2	-	1/6/23/26	0/1/1/1
7	NAG	1	2	7	-	0/6/23/26	0/1/1/1
7	NAG	2	1	7,5	-	1/6/23/26	0/1/1/1
7	NAG	2	2	7	-	0/6/23/26	0/1/1/1
7	NAG	3	1	7,5	-	1/6/23/26	0/1/1/1
7	NAG	3	2	7	-	0/6/23/26	0/1/1/1
7	NAG	4	1	7,5	-	1/6/23/26	0/1/1/1
7	NAG	4	2	7	-	0/6/23/26	0/1/1/1
7	NAG	O	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	O	2	7	-	6/6/23/26	0/1/1/1
7	NAG	P	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	P	2	7	-	0/6/23/26	0/1/1/1
7	NAG	Q	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	2/6/23/26	0/1/1/1
7	NAG	R	1	1,7	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	R	2	7	-	0/6/23/26	0/1/1/1
8	NAG	S	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	S	2	8	-	0/6/23/26	0/1/1/1
8	BMA	S	3	8	-	2/2/19/22	0/1/1/1
9	NAG	T	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	T	2	9	-	0/6/23/26	0/1/1/1
9	BMA	T	3	9	-	0/2/19/22	0/1/1/1
9	MAN	T	4	9	-	0/2/19/22	0/1/1/1
9	MAN	T	5	9	-	0/2/19/22	0/1/1/1
9	MAN	T	6	9	-	0/2/19/22	0/1/1/1
10	NAG	U	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	U	2	10	-	2/6/23/26	0/1/1/1
10	BMA	U	3	10	-	0/2/19/22	0/1/1/1
10	MAN	U	4	10	-	0/2/19/22	0/1/1/1
10	MAN	U	5	10	-	0/2/19/22	0/1/1/1
10	MAN	U	6	10	-	0/2/19/22	0/1/1/1
10	MAN	U	7	10	-	2/2/19/22	0/1/1/1
7	NAG	V	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	V	2	7	-	0/6/23/26	0/1/1/1
7	NAG	W	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	W	2	7	-	2/6/23/26	0/1/1/1
8	NAG	X	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	X	2	8	-	0/6/23/26	0/1/1/1
8	BMA	X	3	8	-	2/2/19/22	0/1/1/1
11	NAG	Y	1	1,11	-	3/6/23/26	0/1/1/1
11	NAG	Y	2	11	-	2/6/23/26	0/1/1/1
11	BMA	Y	3	11	-	2/2/19/22	0/1/1/1
11	MAN	Y	4	11	-	0/2/19/22	0/1/1/1
11	MAN	Y	5	11	-	0/2/19/22	0/1/1/1
7	NAG	Z	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	2/6/23/26	0/1/1/1
7	NAG	a	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	a	2	7	-	2/6/23/26	0/1/1/1
7	NAG	b	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	b	2	7	-	0/6/23/26	0/1/1/1
7	NAG	c	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	c	2	7	-	2/6/23/26	0/1/1/1
8	NAG	d	1	1,8	-	1/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	o	2	7	-	6/6/23/26	0/1/1/1
7	NAG	p	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	p	2	7	-	2/6/23/26	0/1/1/1
13	NAG	q	1	1,13	-	0/6/23/26	0/1/1/1
13	NAG	q	2	13	-	0/6/23/26	0/1/1/1
13	BMA	q	3	13	-	0/2/19/22	0/1/1/1
13	MAN	q	4	13	-	0/2/19/22	0/1/1/1
13	MAN	q	5	13	-	0/2/19/22	0/1/1/1
13	MAN	q	6	13	-	0/2/19/22	0/1/1/1
13	MAN	q	7	13	-	0/2/19/22	0/1/1/1
13	MAN	q	8	13	-	0/2/19/22	0/1/1/1
7	NAG	r	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	r	2	7	-	0/6/23/26	0/1/1/1
12	NAG	s	1	1,12	-	1/6/23/26	0/1/1/1
12	NAG	s	2	12	-	0/6/23/26	0/1/1/1
12	BMA	s	3	12	-	0/2/19/22	0/1/1/1
12	MAN	s	4	12	-	0/2/19/22	0/1/1/1
12	MAN	s	5	12	-	0/2/19/22	0/1/1/1
12	MAN	s	6	12	-	0/2/19/22	0/1/1/1
12	MAN	s	7	12	-	0/2/19/22	0/1/1/1
13	NAG	t	1	1,13	-	2/6/23/26	0/1/1/1
13	NAG	t	2	13	-	3/6/23/26	0/1/1/1
13	BMA	t	3	13	-	0/2/19/22	0/1/1/1
13	MAN	t	4	13	-	2/2/19/22	0/1/1/1
13	MAN	t	5	13	-	0/2/19/22	0/1/1/1
13	MAN	t	6	13	-	0/2/19/22	0/1/1/1
13	MAN	t	7	13	-	0/2/19/22	0/1/1/1
13	MAN	t	8	13	-	0/2/19/22	0/1/1/1
7	NAG	u	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	u	2	7	-	0/6/23/26	0/1/1/1
7	NAG	v	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	v	2	7	-	2/6/23/26	0/1/1/1
7	NAG	w	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	w	2	7	-	2/6/23/26	0/1/1/1
11	NAG	x	1	1,11	-	3/6/23/26	0/1/1/1
11	NAG	x	2	11	-	2/6/23/26	0/1/1/1
11	BMA	x	3	11	-	2/2/19/22	0/1/1/1
11	MAN	x	4	11	-	0/2/19/22	0/1/1/1
11	MAN	x	5	11	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	y	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	y	2	8	-	2/6/23/26	0/1/1/1
8	BMA	y	3	8	-	2/2/19/22	0/1/1/1
7	NAG	z	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	z	2	7	-	2/6/23/26	0/1/1/1

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	g	5	MAN	C4-C5	4.33	1.62	1.53
13	t	5	MAN	C4-C5	4.32	1.62	1.53
13	t	5	MAN	C4-C3	3.69	1.61	1.52
13	g	5	MAN	C4-C3	3.67	1.61	1.52
7	Z	1	NAG	O5-C1	3.49	1.49	1.43

The worst 5 of 285 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	T	1	NAG	O5-C1-C2	-7.54	99.63	111.29
7	4	1	NAG	O5-C1-C2	-7.54	99.63	111.29
7	b	1	NAG	O5-C1-C2	-7.54	99.63	111.29
7	m	1	NAG	O5-C1-C2	-7.54	99.63	111.29
12	s	1	NAG	O5-C1-C2	-7.53	99.64	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	l	1	NAG	C1

5 of 140 torsion outliers are listed below:

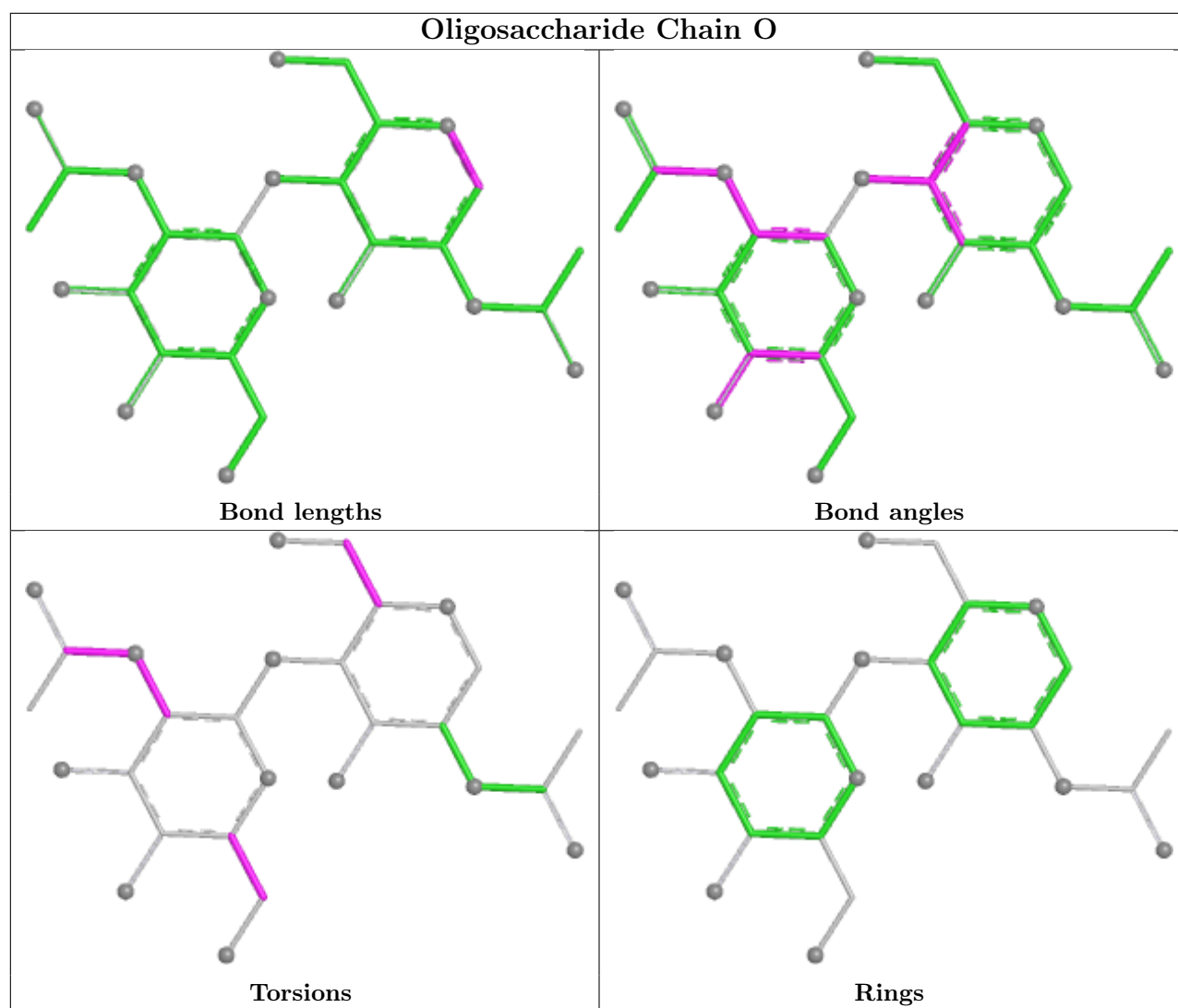
Mol	Chain	Res	Type	Atoms
7	V	1	NAG	O5-C5-C6-O6
7	h	1	NAG	O5-C5-C6-O6
7	u	1	NAG	O5-C5-C6-O6
7	v	1	NAG	O5-C5-C6-O6
7	W	1	NAG	O5-C5-C6-O6

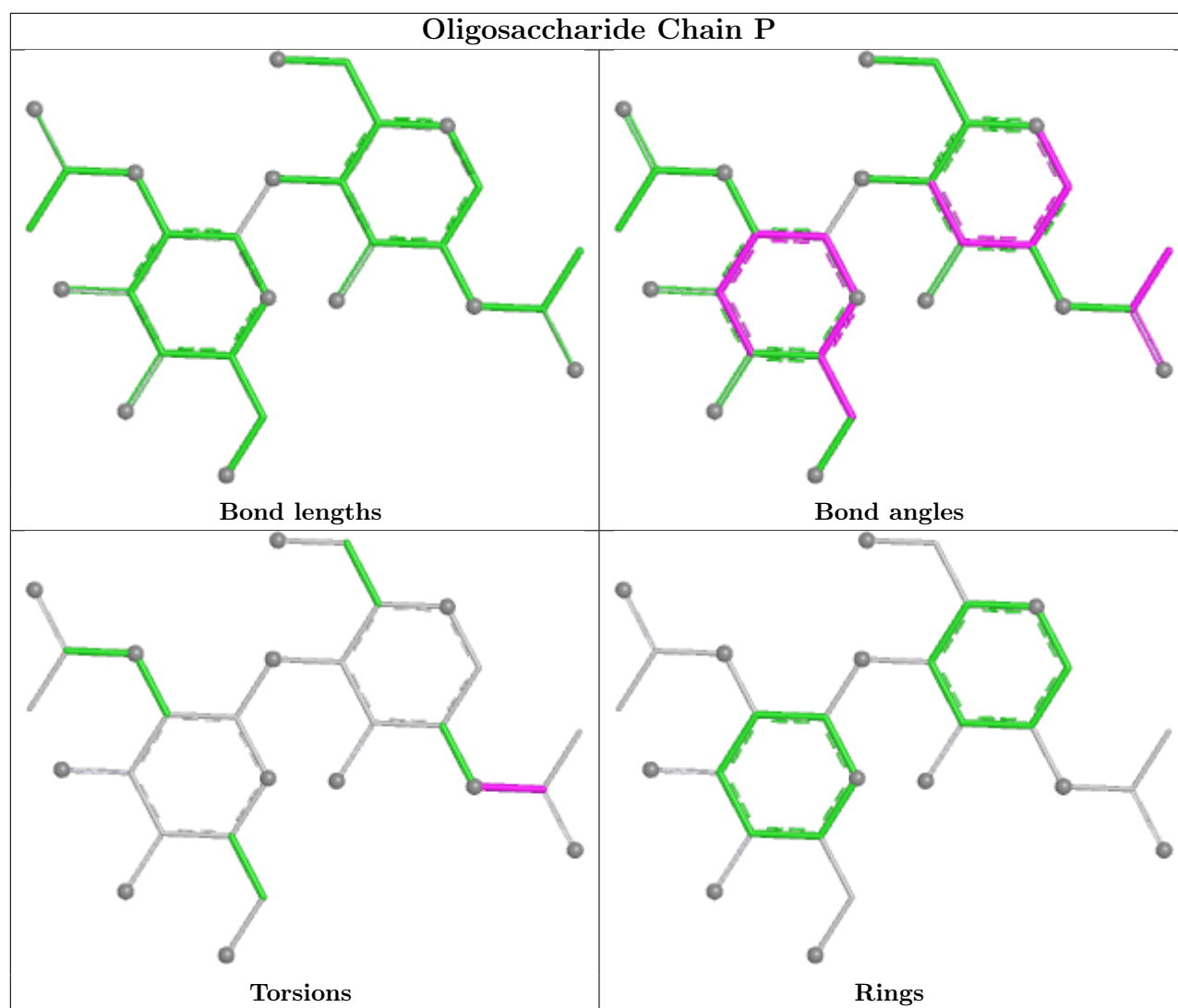
There are no ring outliers.

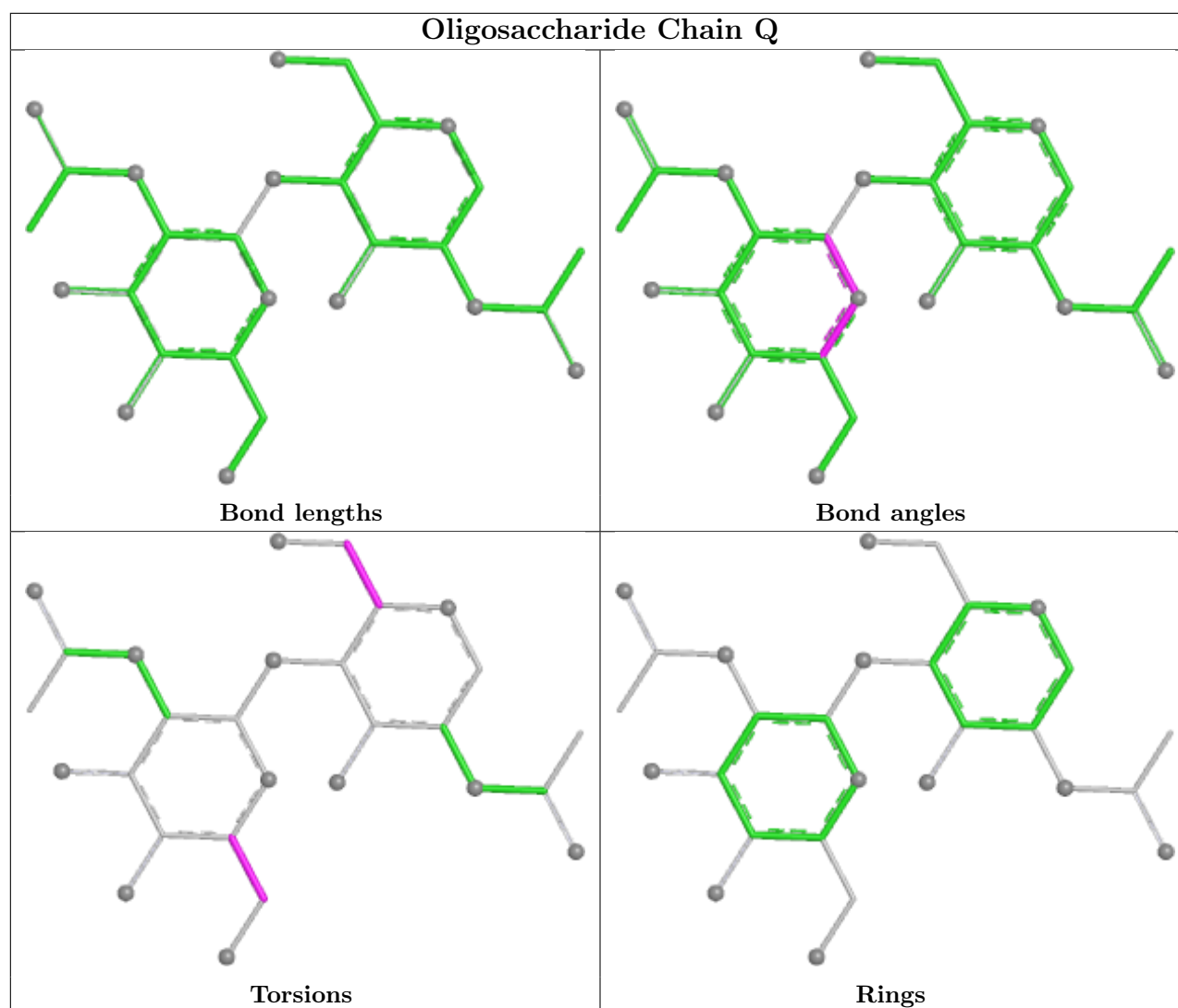
40 monomers are involved in 162 short contacts:

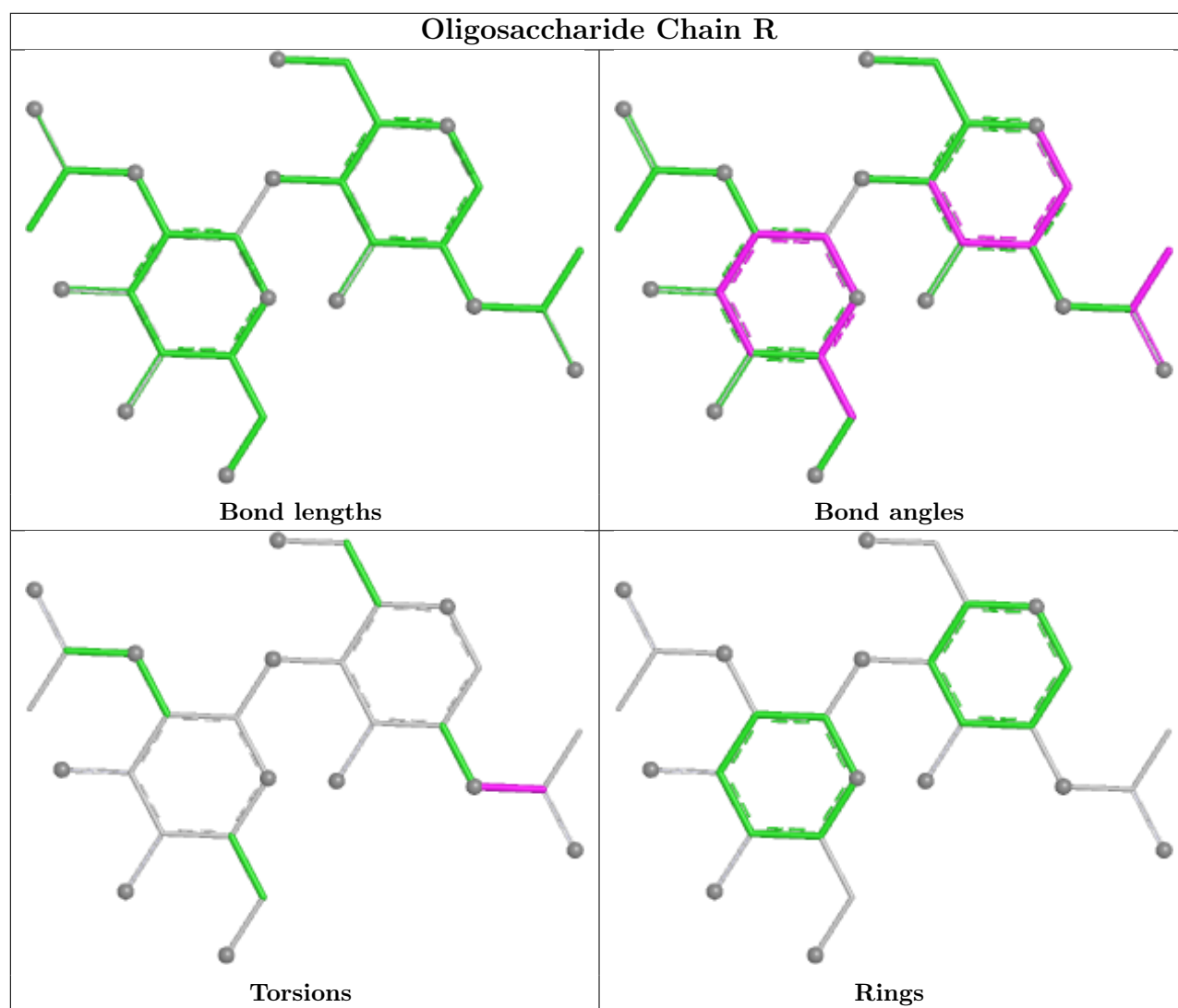
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	u	1	NAG	9	0
7	o	1	NAG	4	0
7	v	2	NAG	1	0
7	z	1	NAG	2	0
11	Y	1	NAG	6	0
7	n	2	NAG	2	0
11	x	2	NAG	1	0
11	k	1	NAG	2	0
7	w	1	NAG	9	0
10	U	1	NAG	5	0
7	O	2	NAG	1	0
7	v	1	NAG	4	0
7	W	2	NAG	1	0
13	q	1	NAG	7	0
7	i	2	NAG	1	0
7	p	1	NAG	5	0
13	q	3	BMA	5	0
7	n	1	NAG	2	0
13	q	4	MAN	9	0
7	o	2	NAG	1	0
8	l	1	NAG	5	0
7	z	2	NAG	2	0
10	U	2	NAG	1	0
13	g	2	NAG	2	0
7	c	1	NAG	4	0
7	a	1	NAG	4	0
7	O	1	NAG	2	0
8	y	2	NAG	3	0
7	W	1	NAG	3	0
8	y	1	NAG	1	0
7	h	1	NAG	13	0
13	q	2	NAG	11	0
11	x	1	NAG	2	0
7	j	1	NAG	12	0
13	q	8	MAN	2	0
13	t	1	NAG	4	0
7	Q	1	NAG	15	0
7	V	1	NAG	6	0
13	t	2	NAG	2	0
7	i	1	NAG	2	0

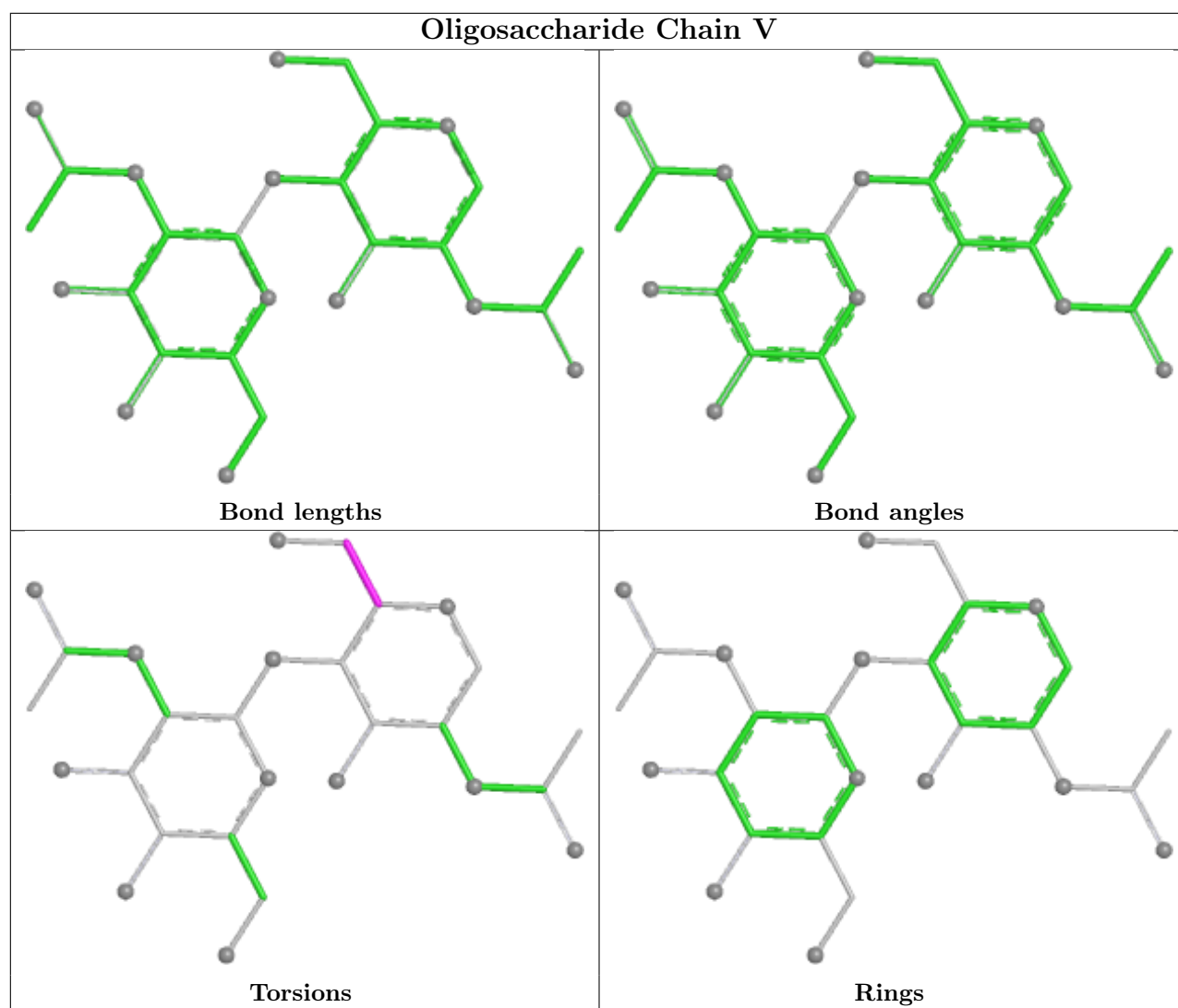
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

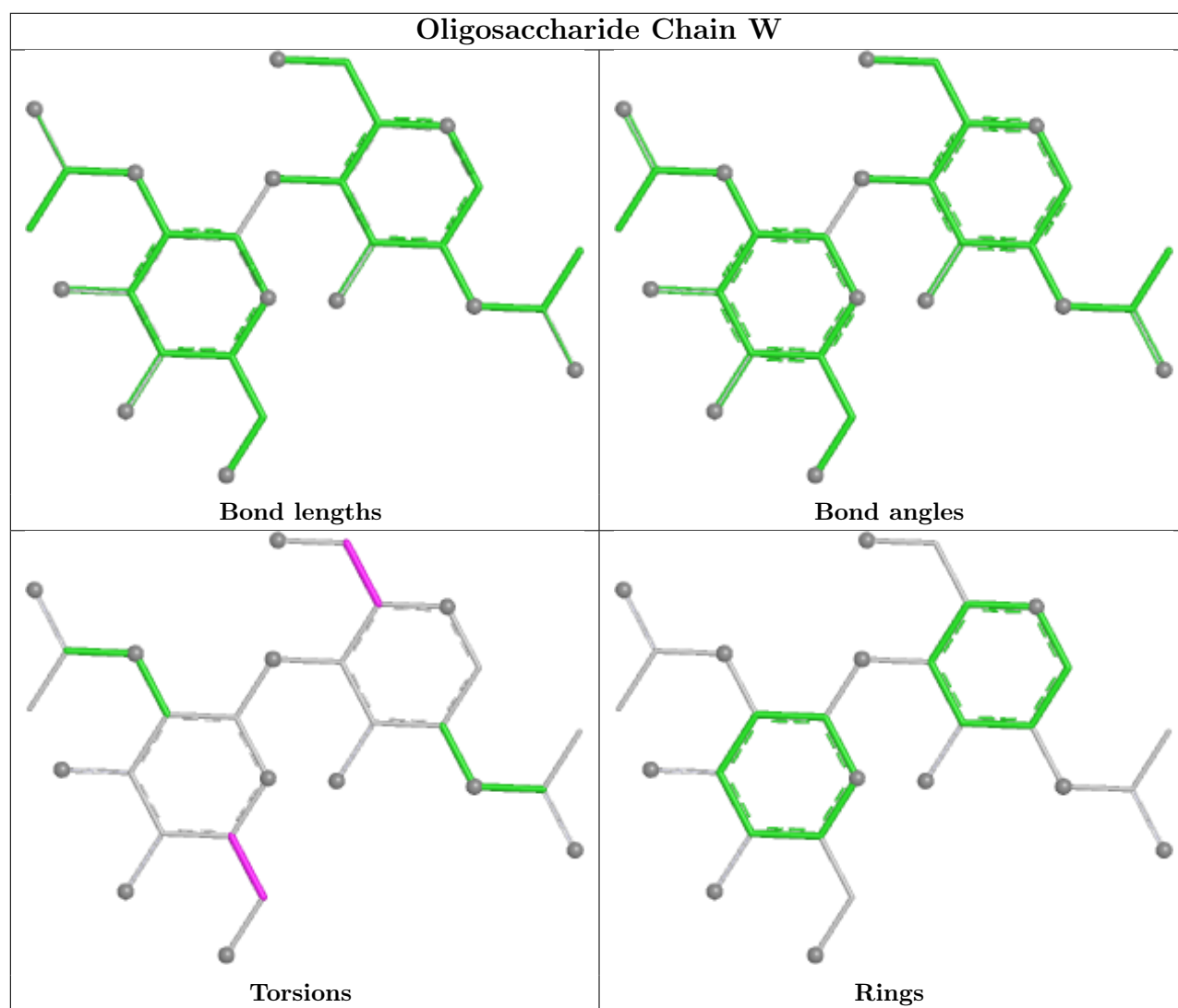


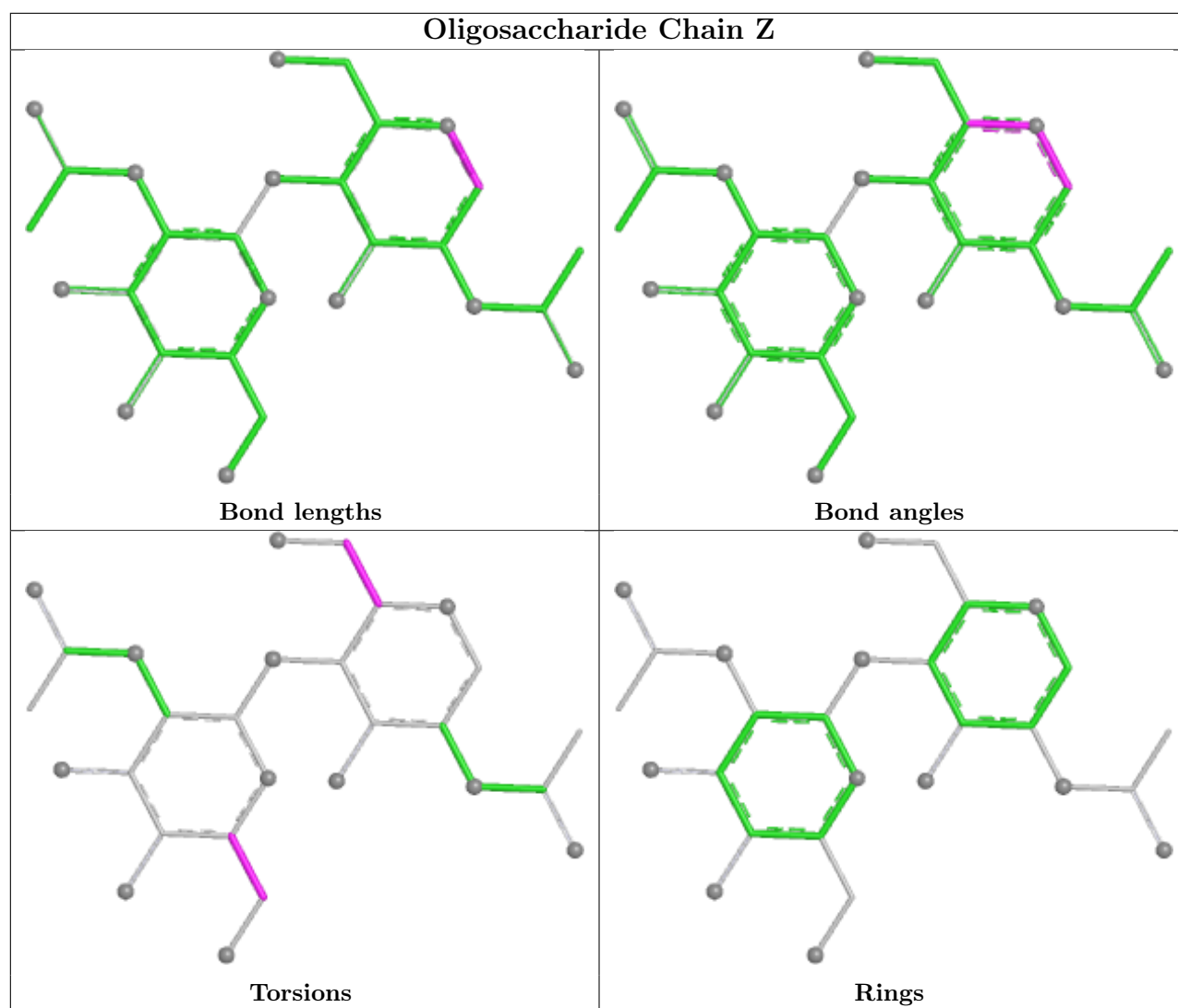


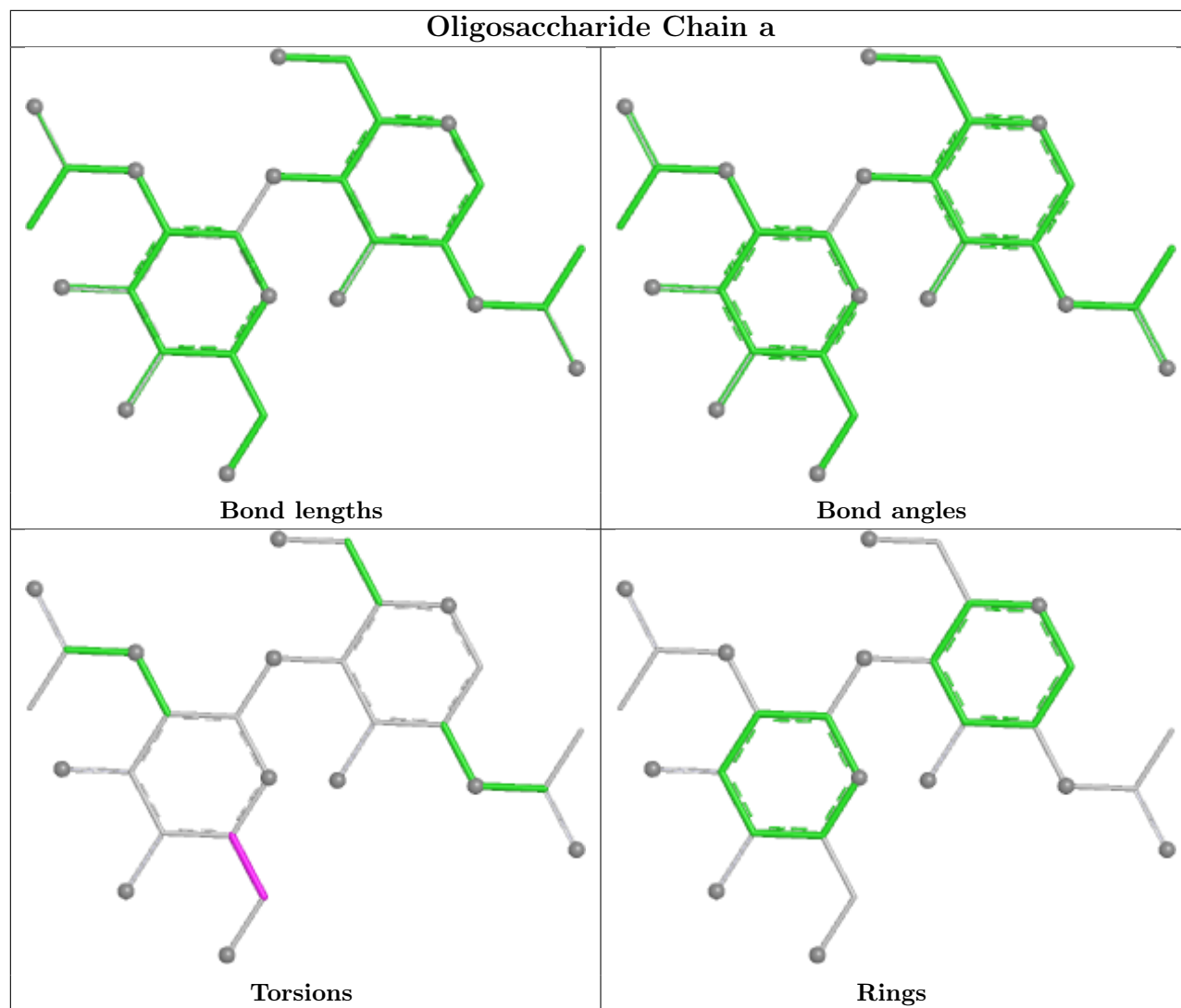


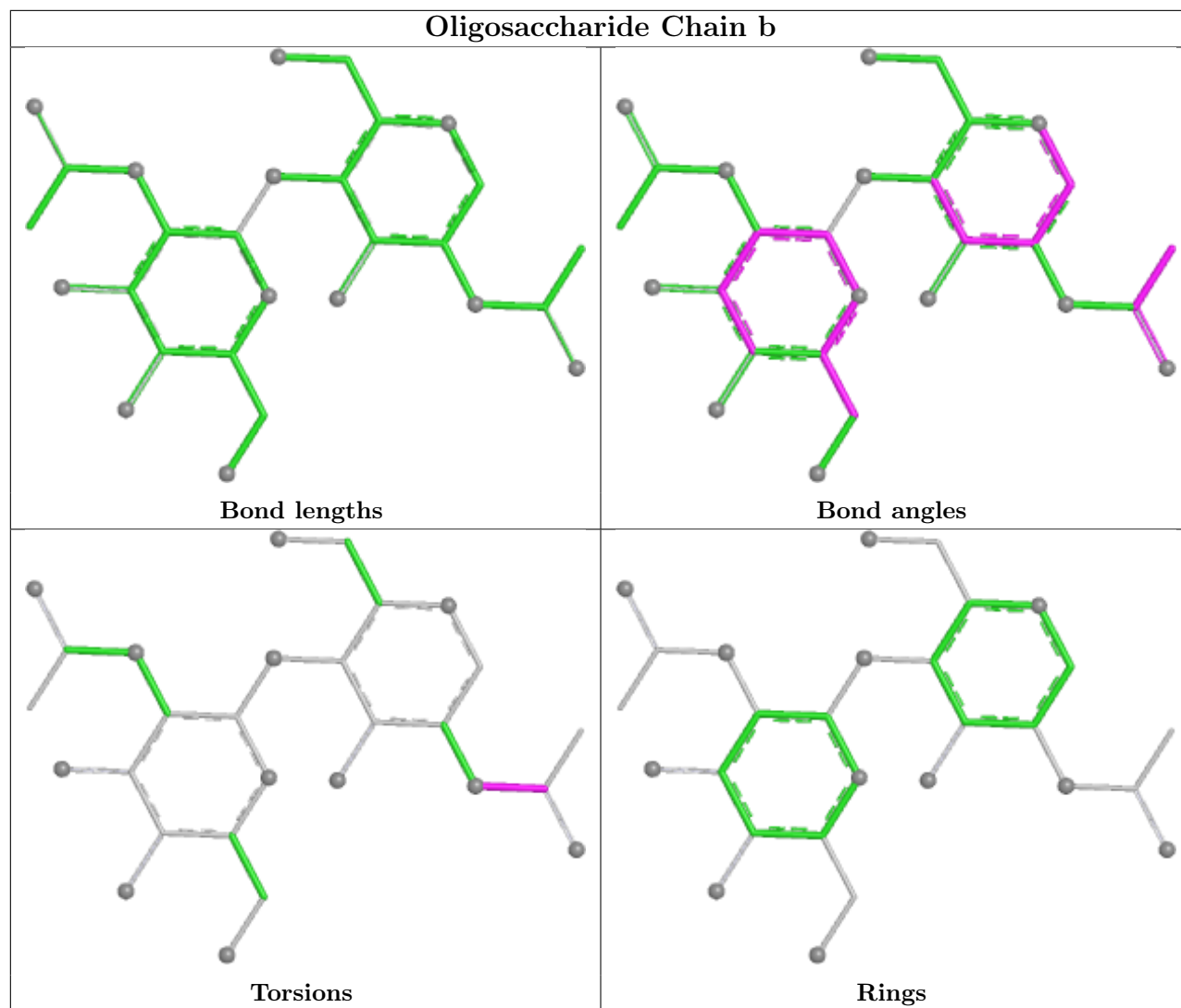


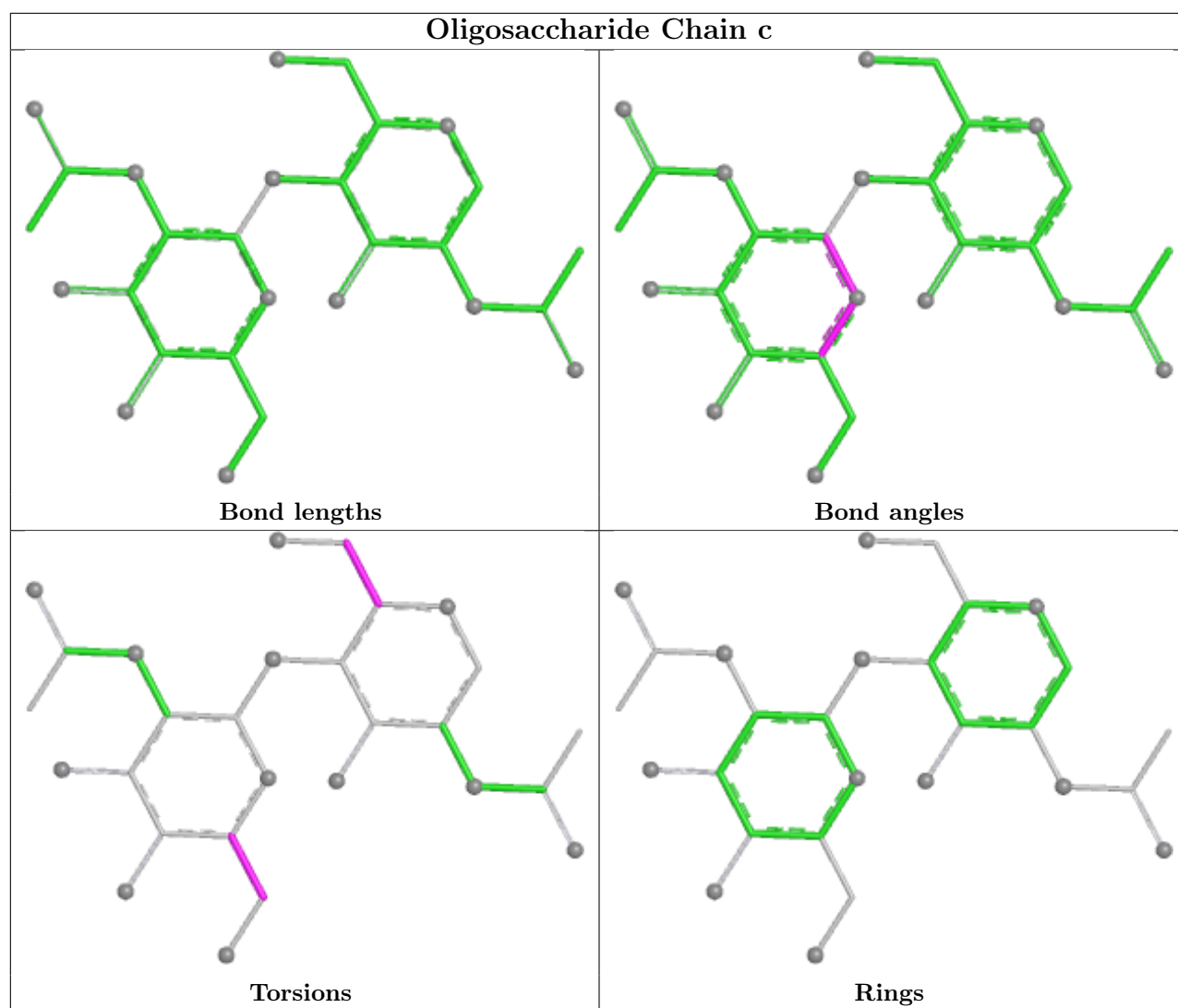


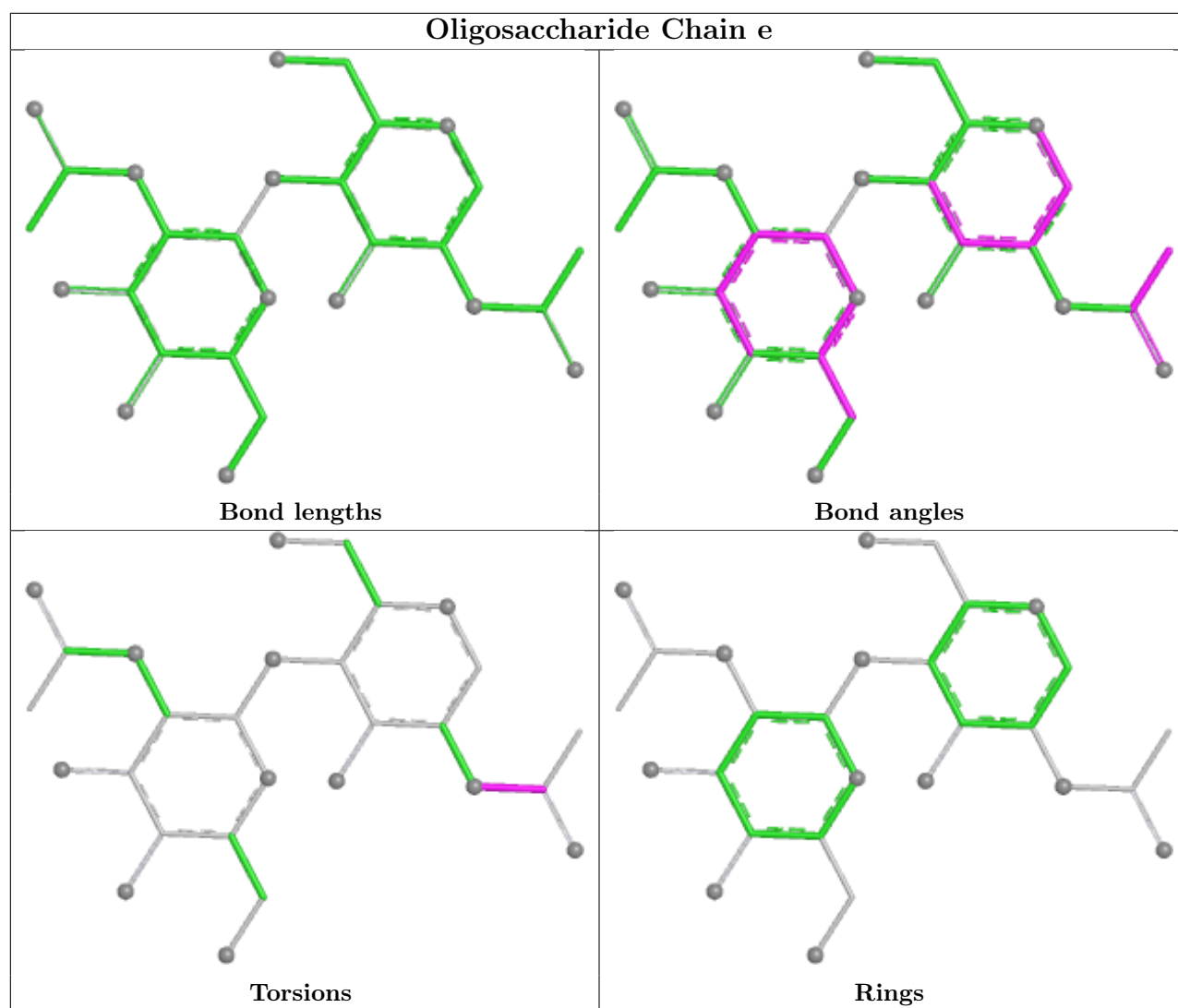


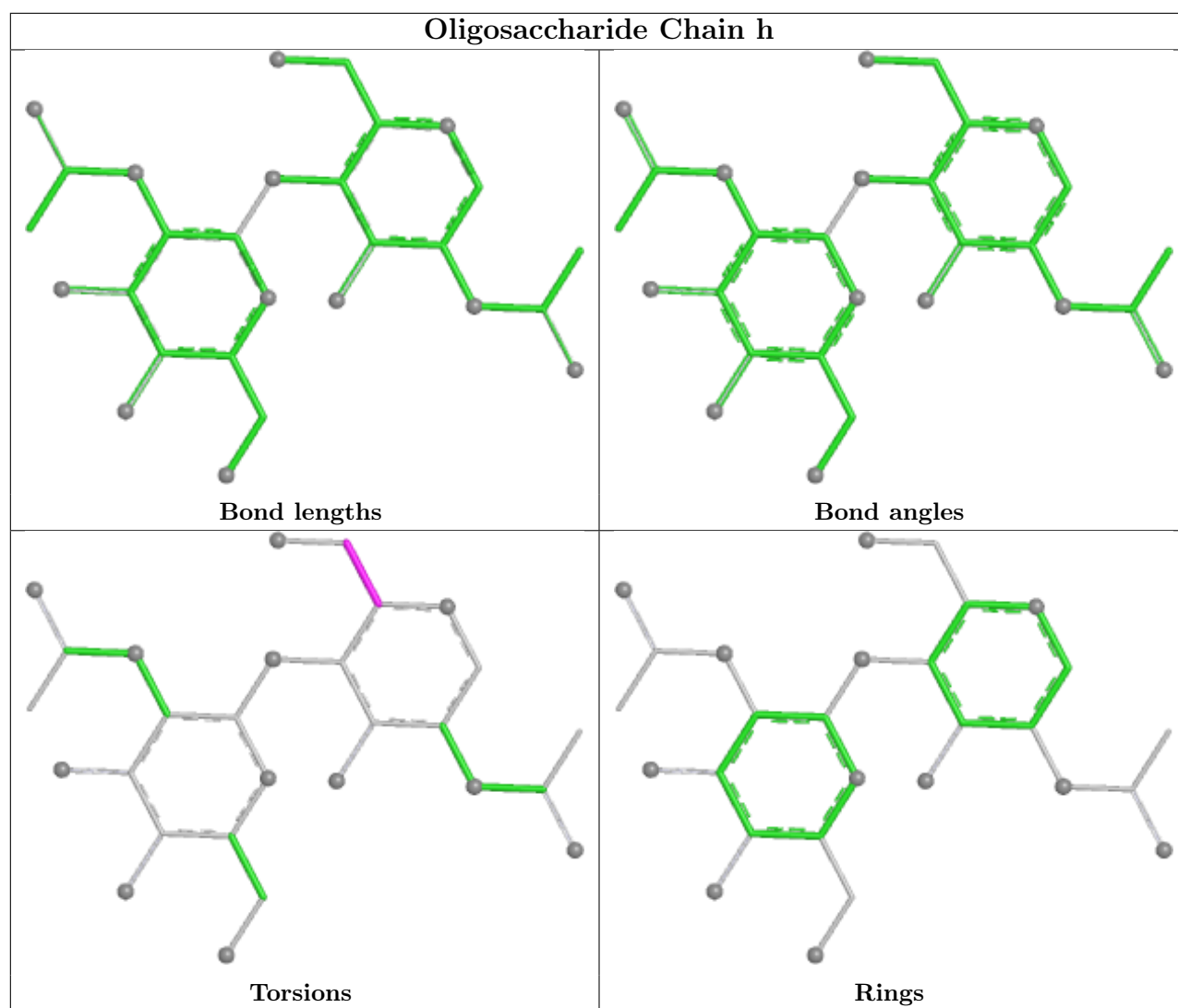


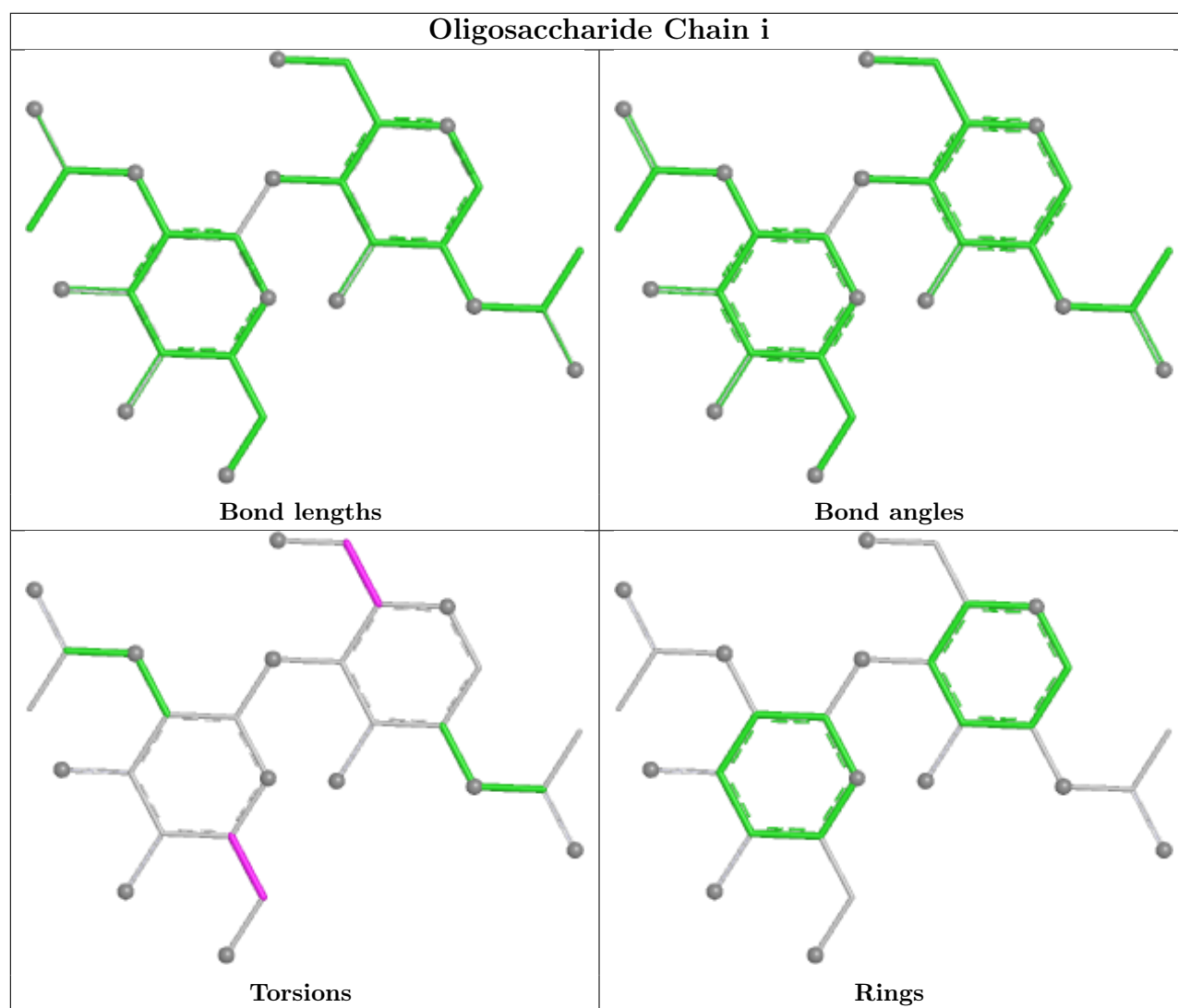


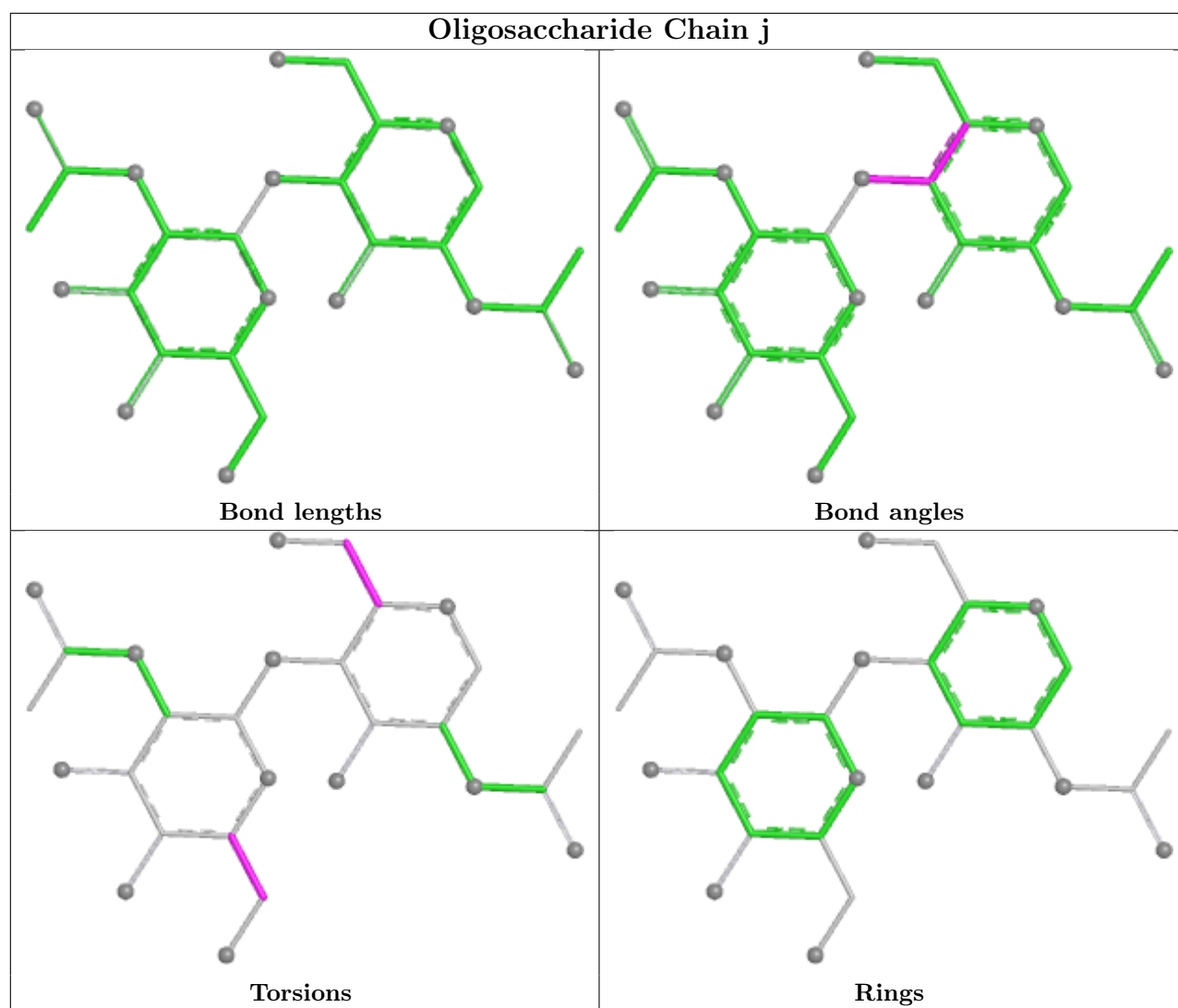


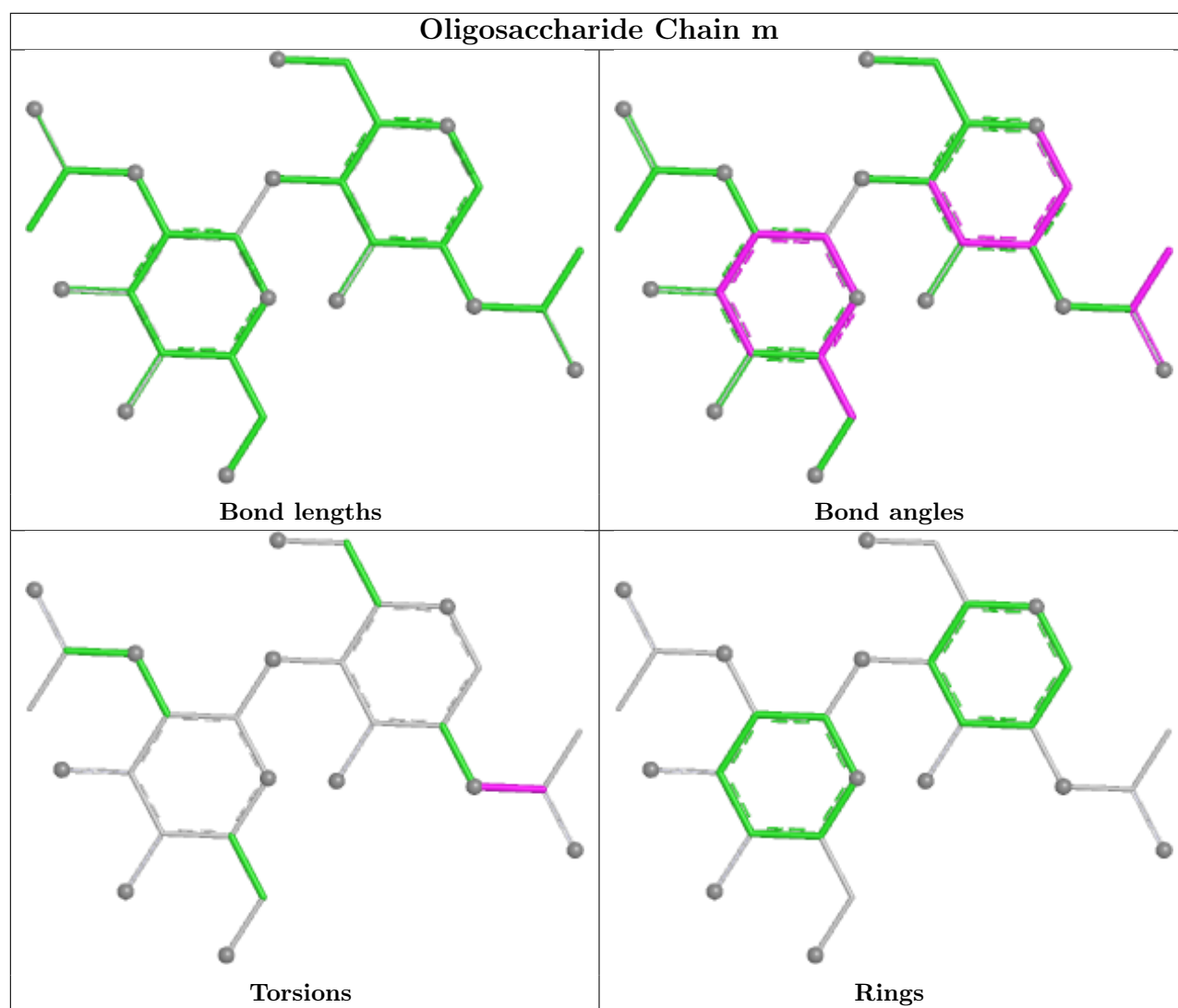


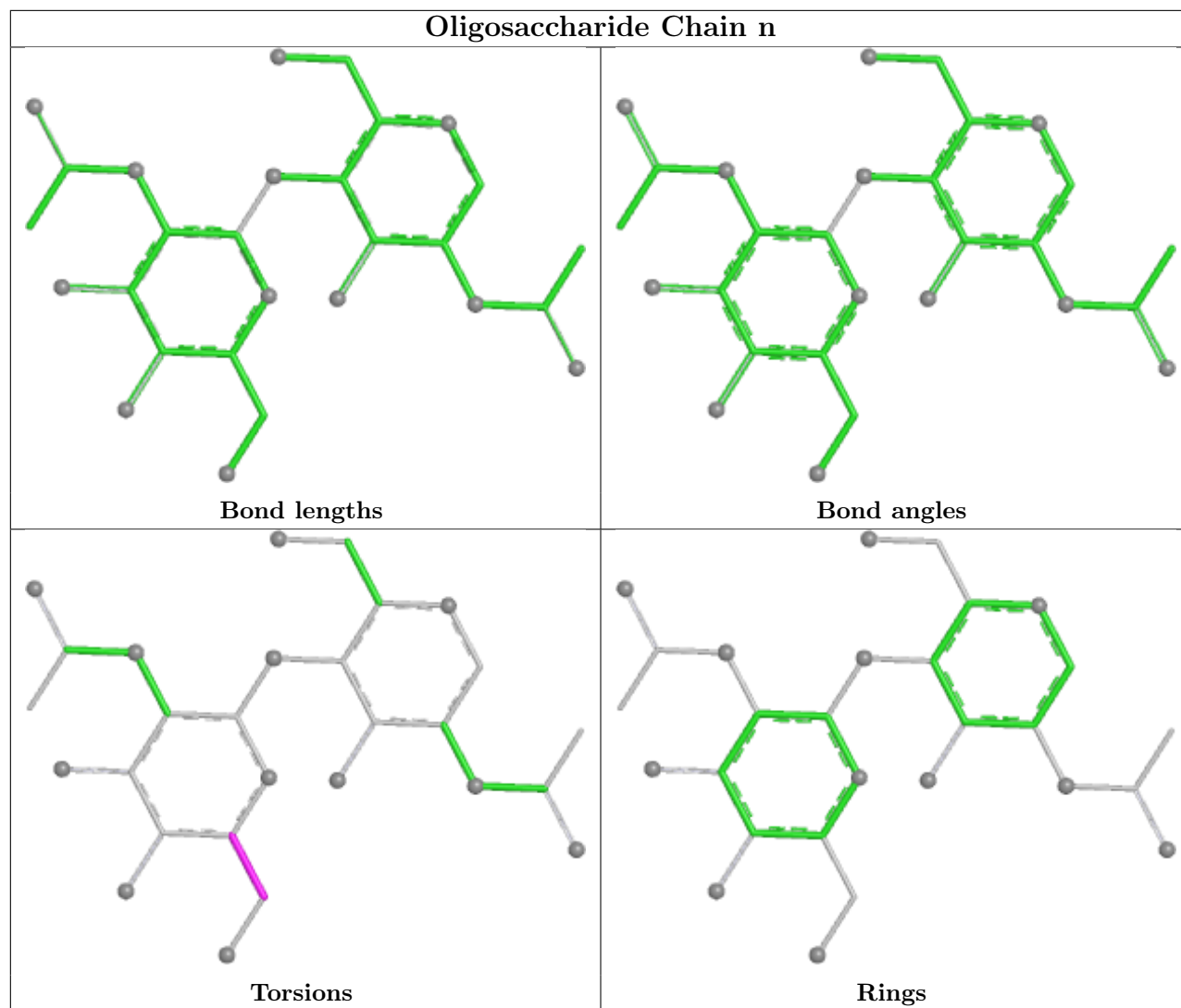


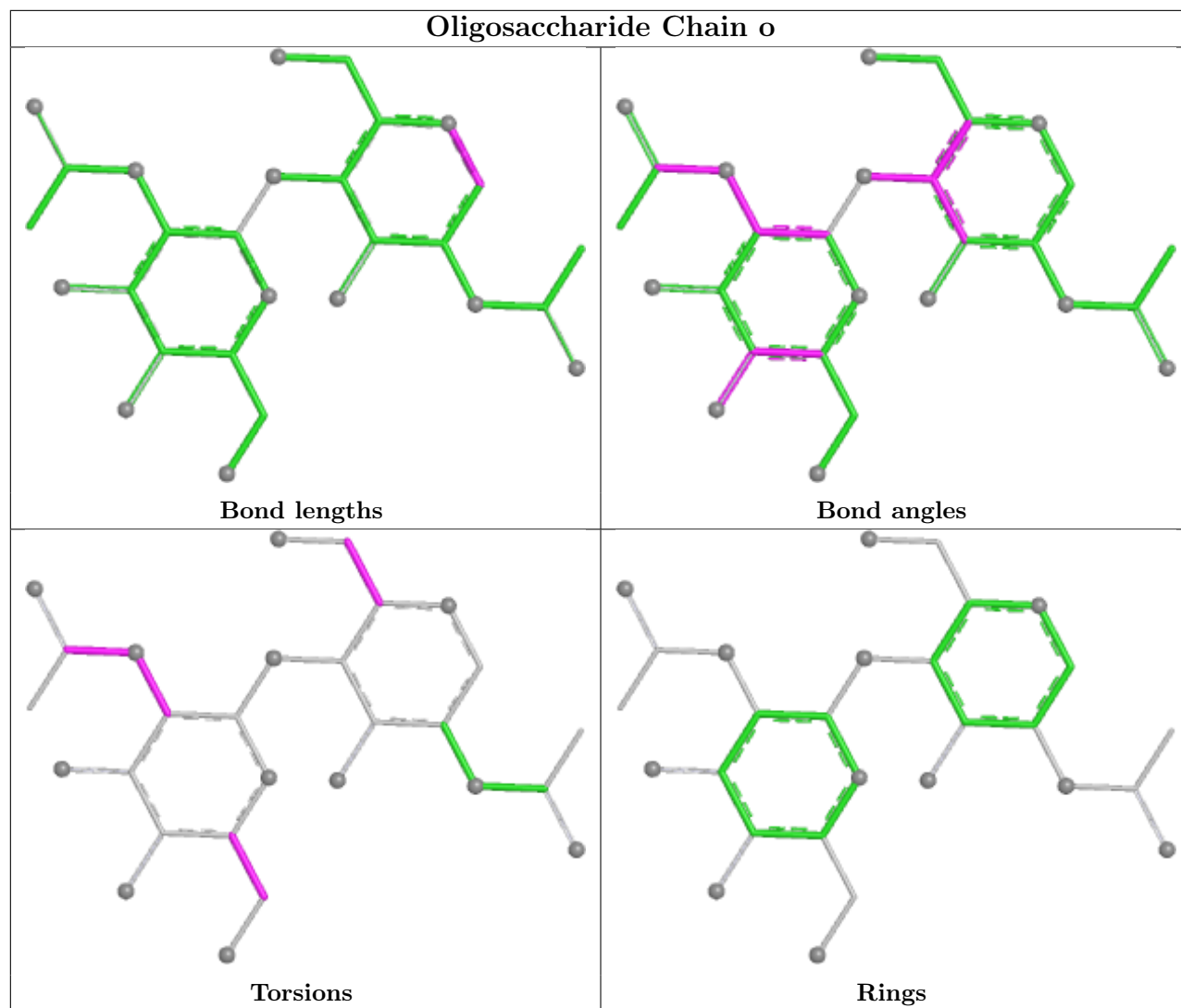


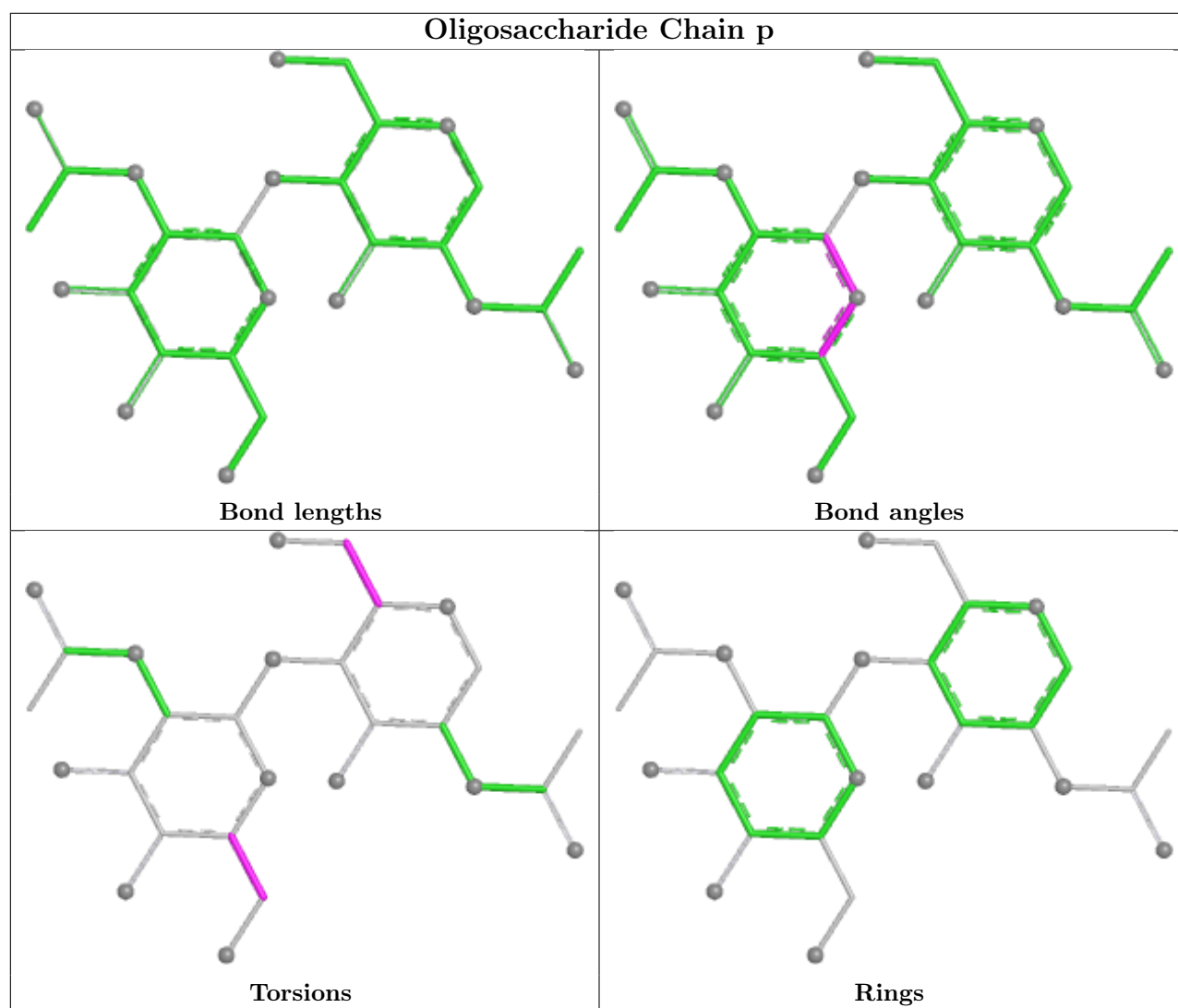


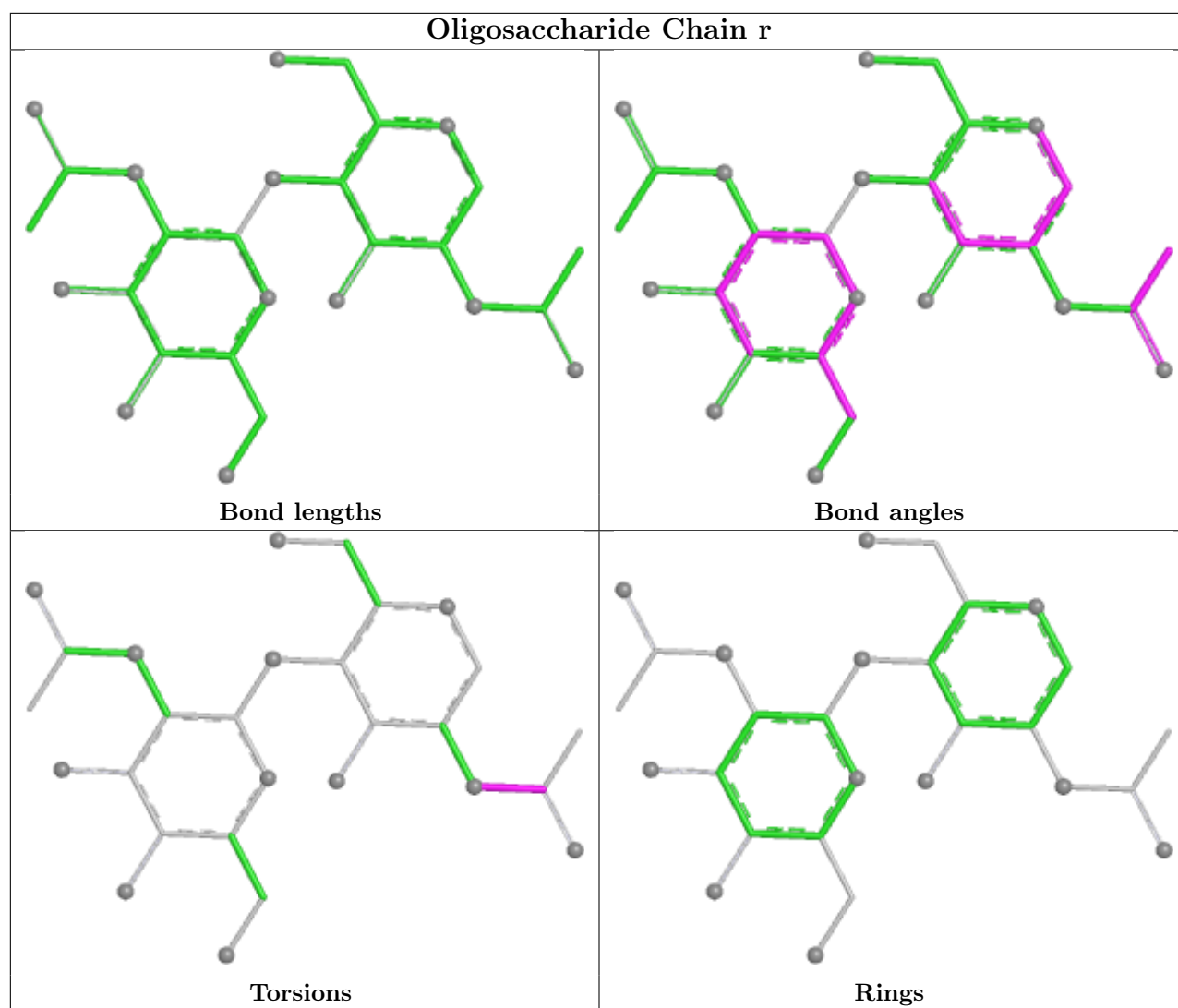


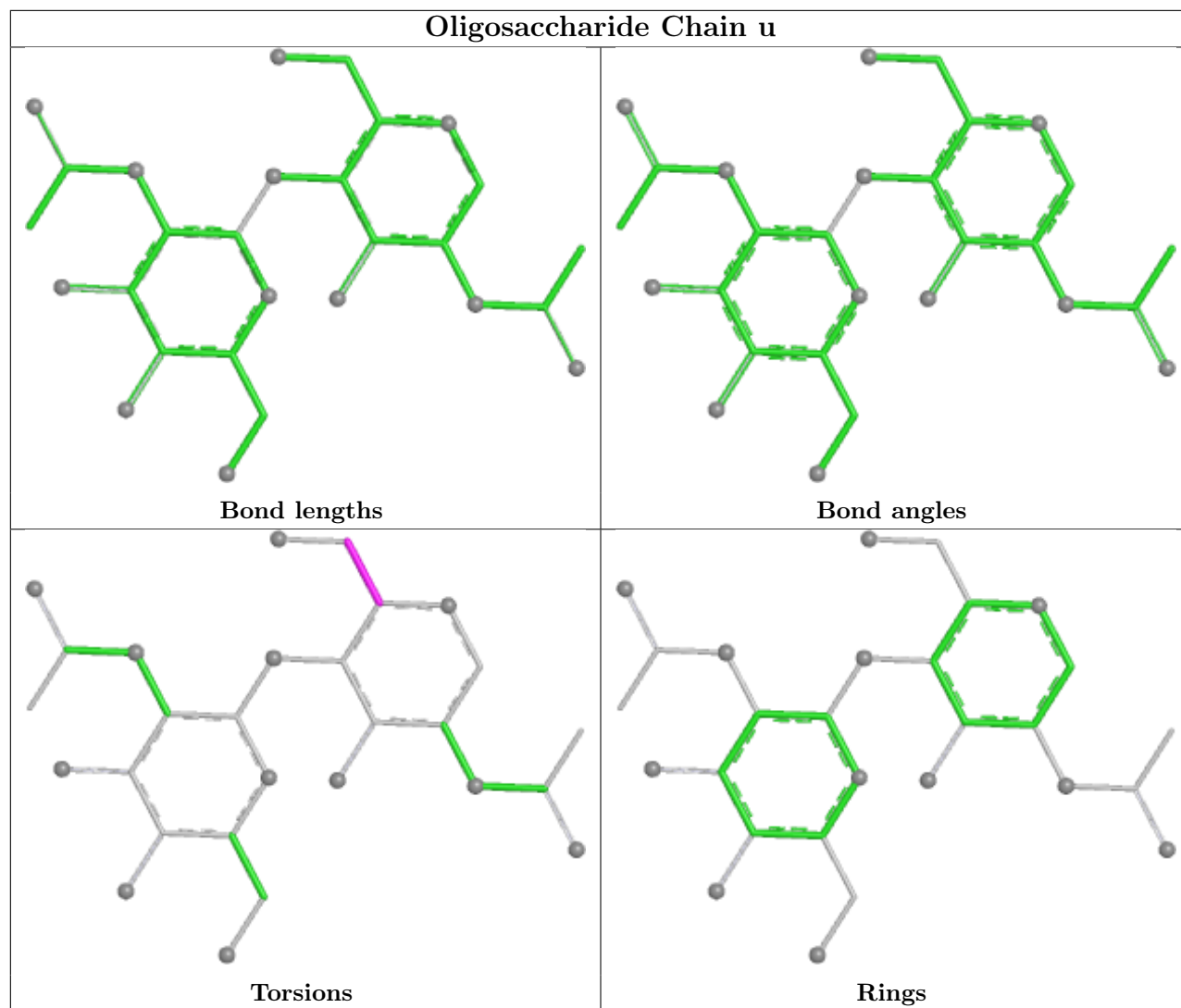


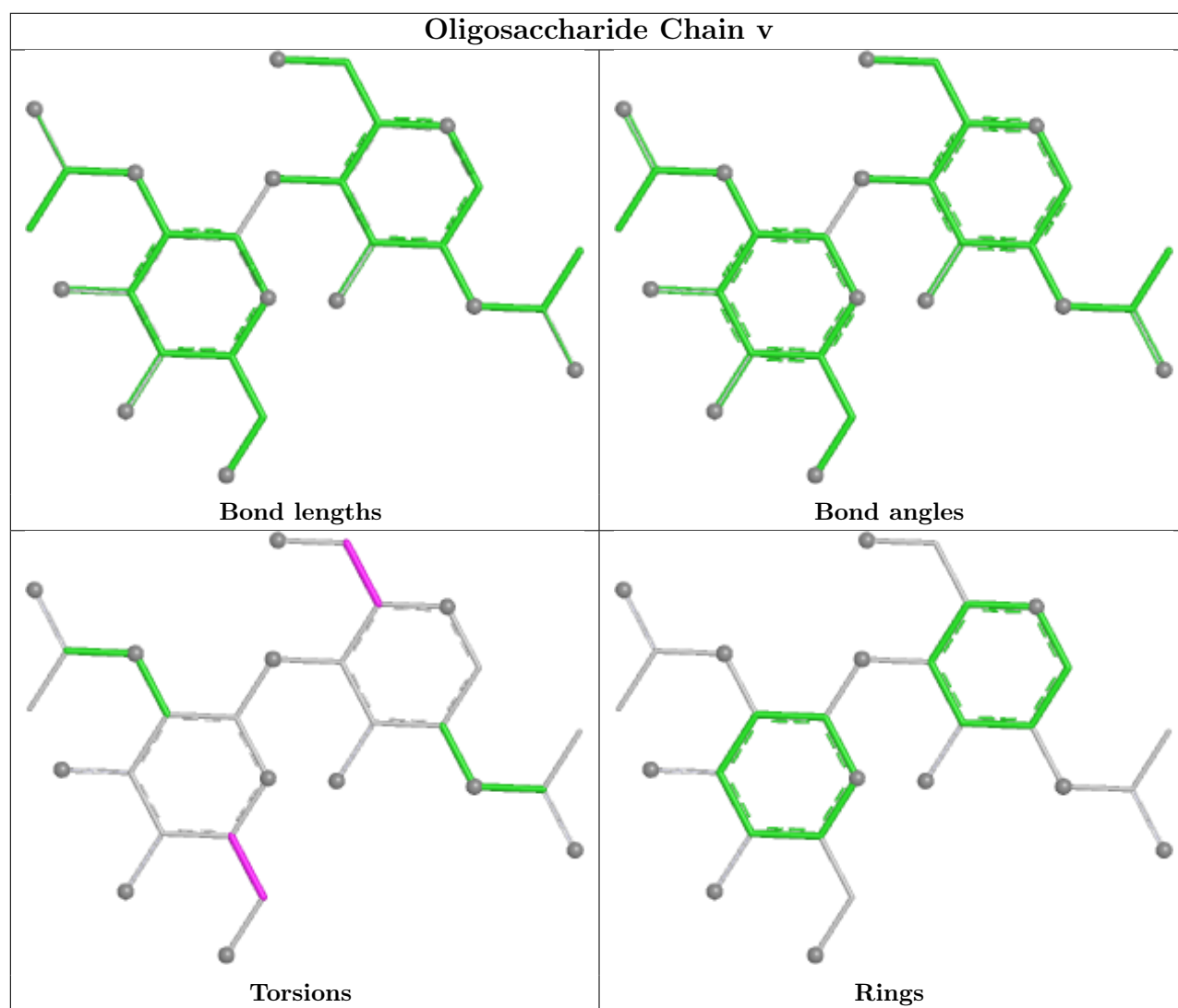


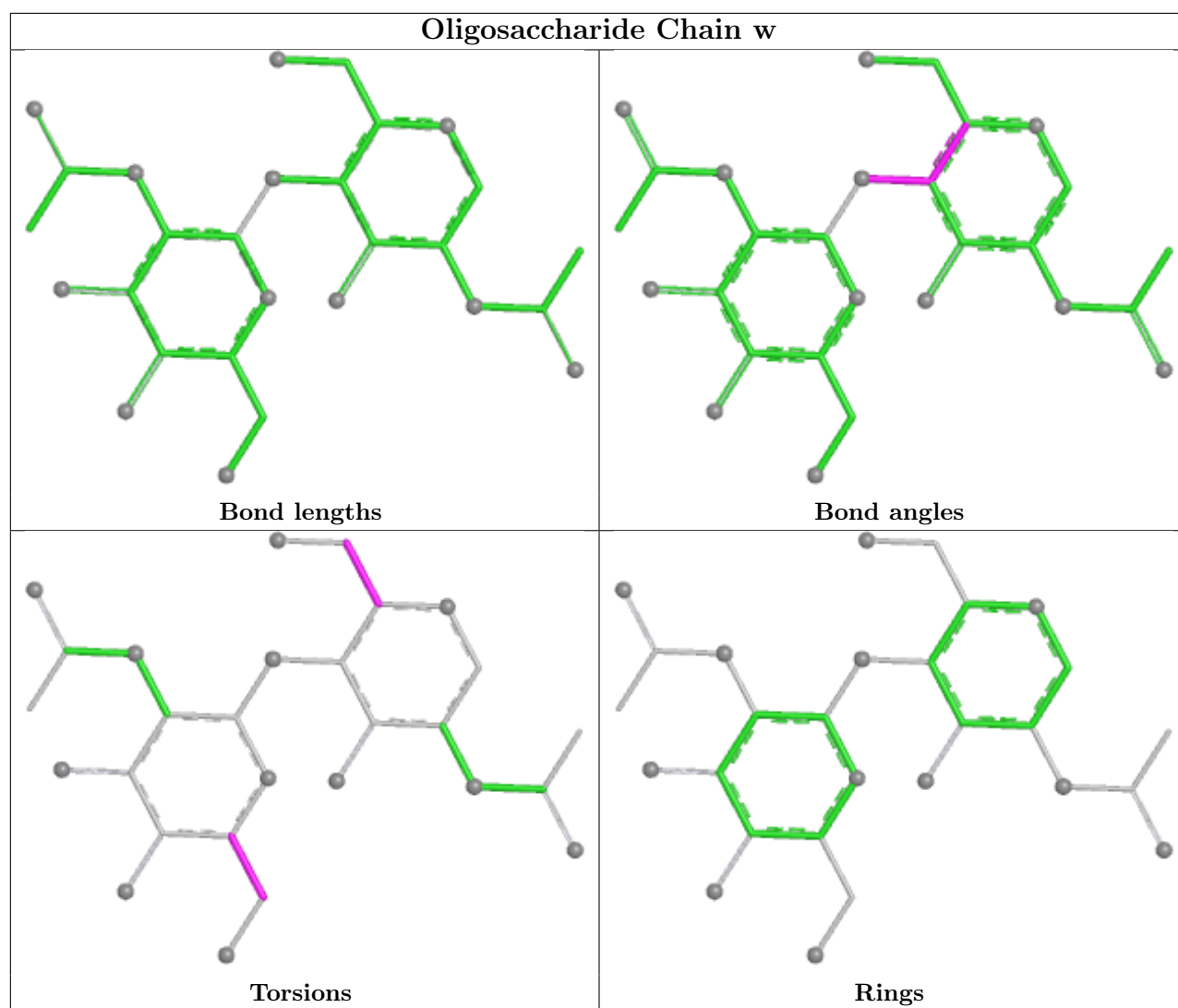


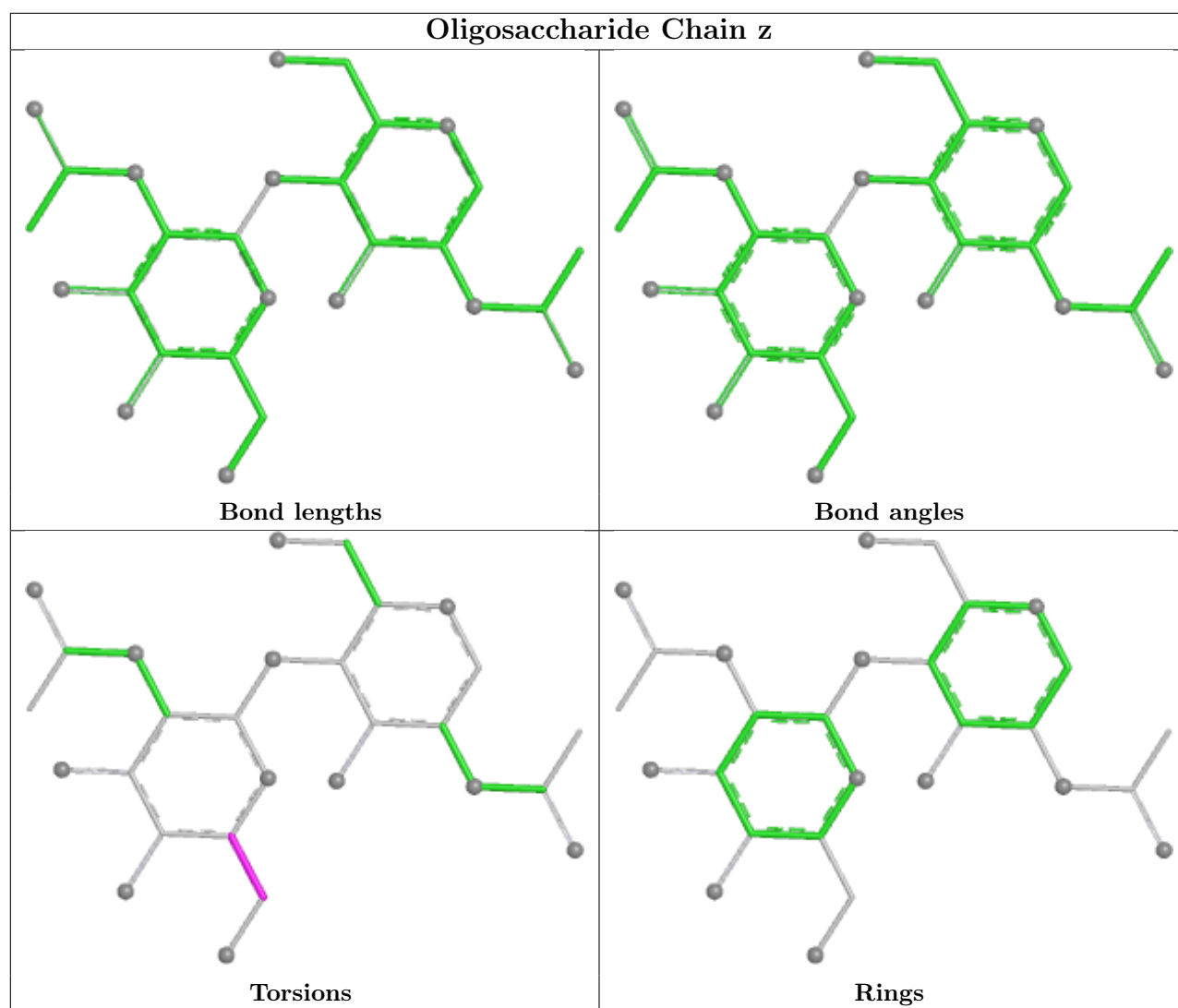


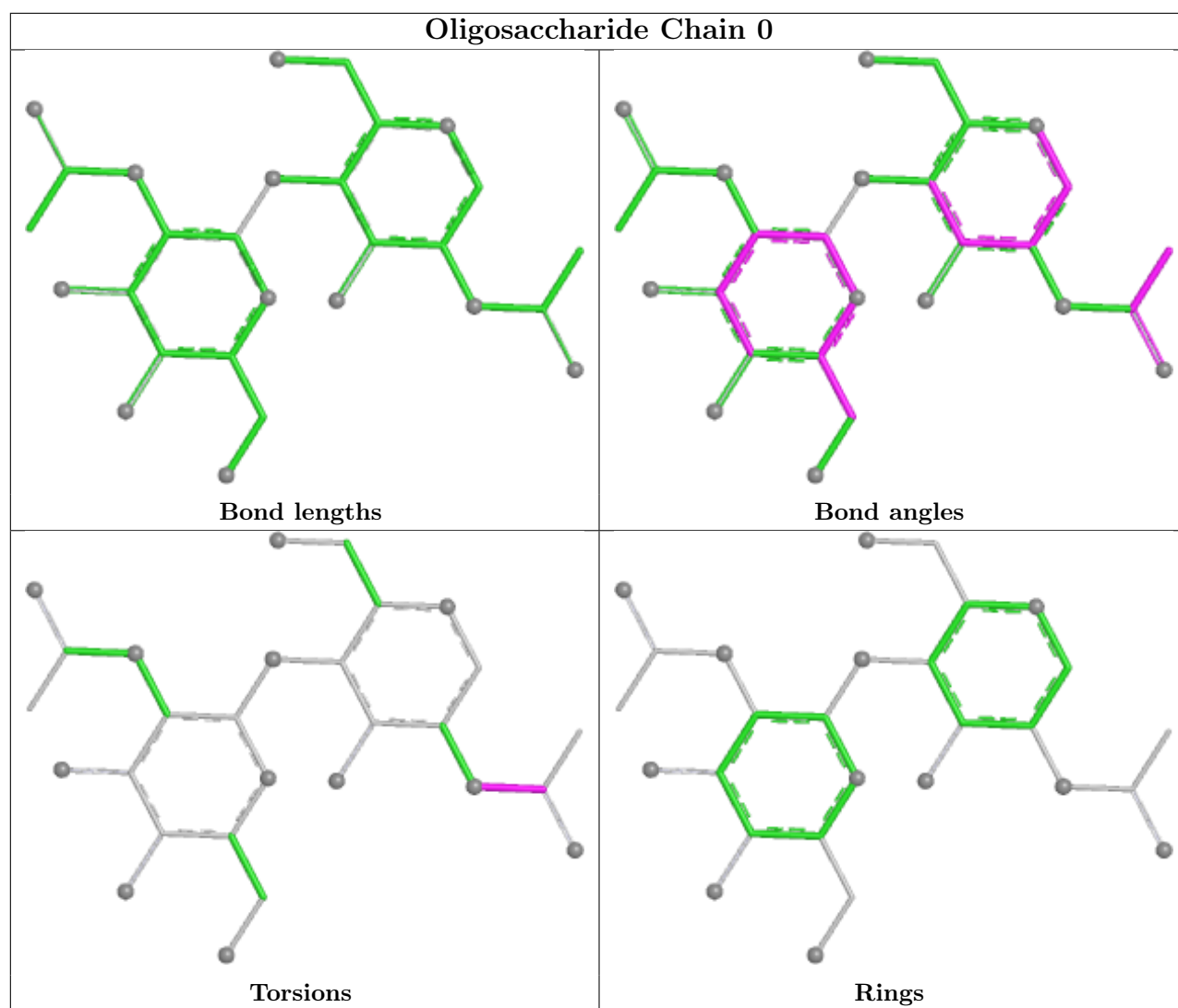


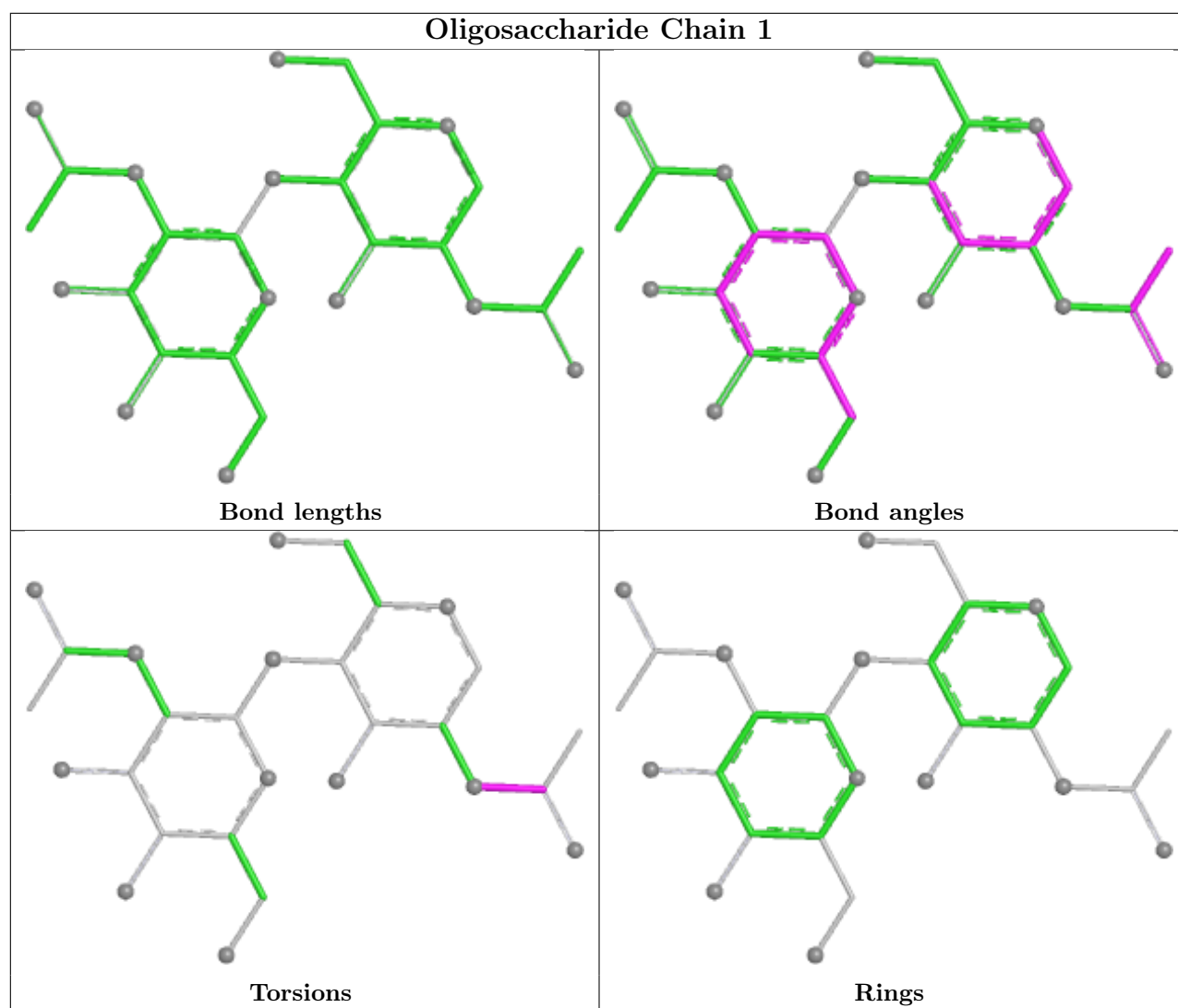


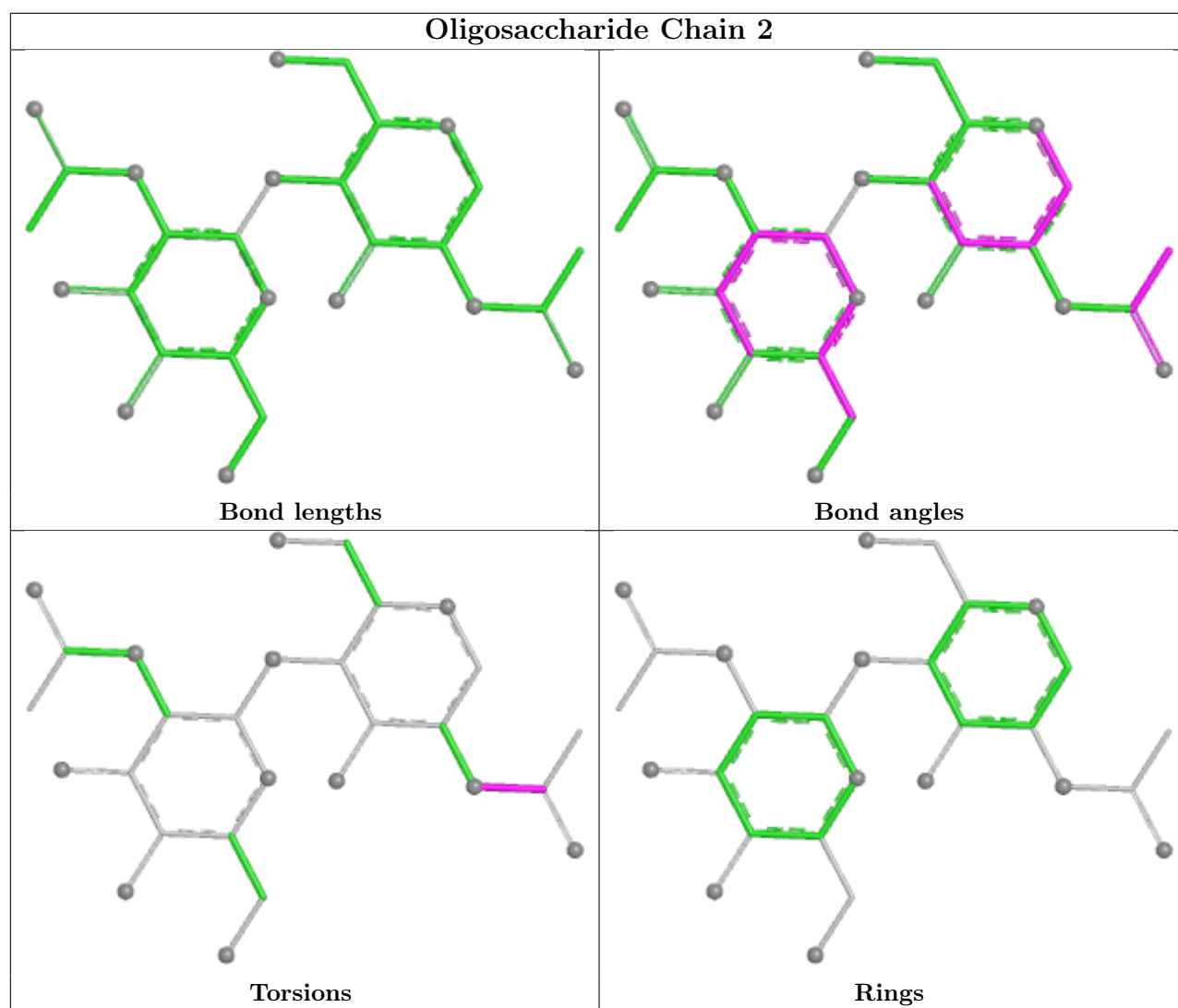


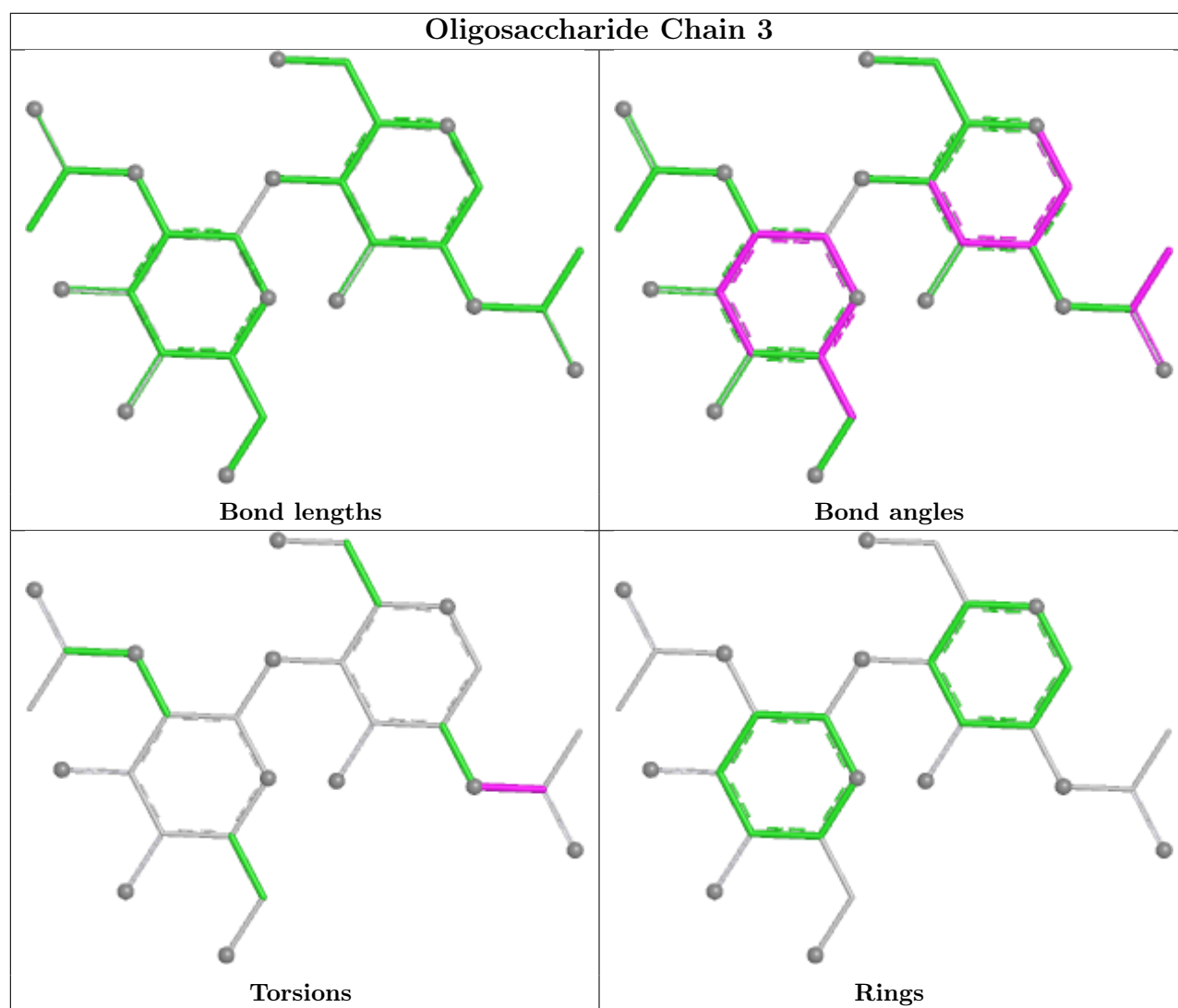


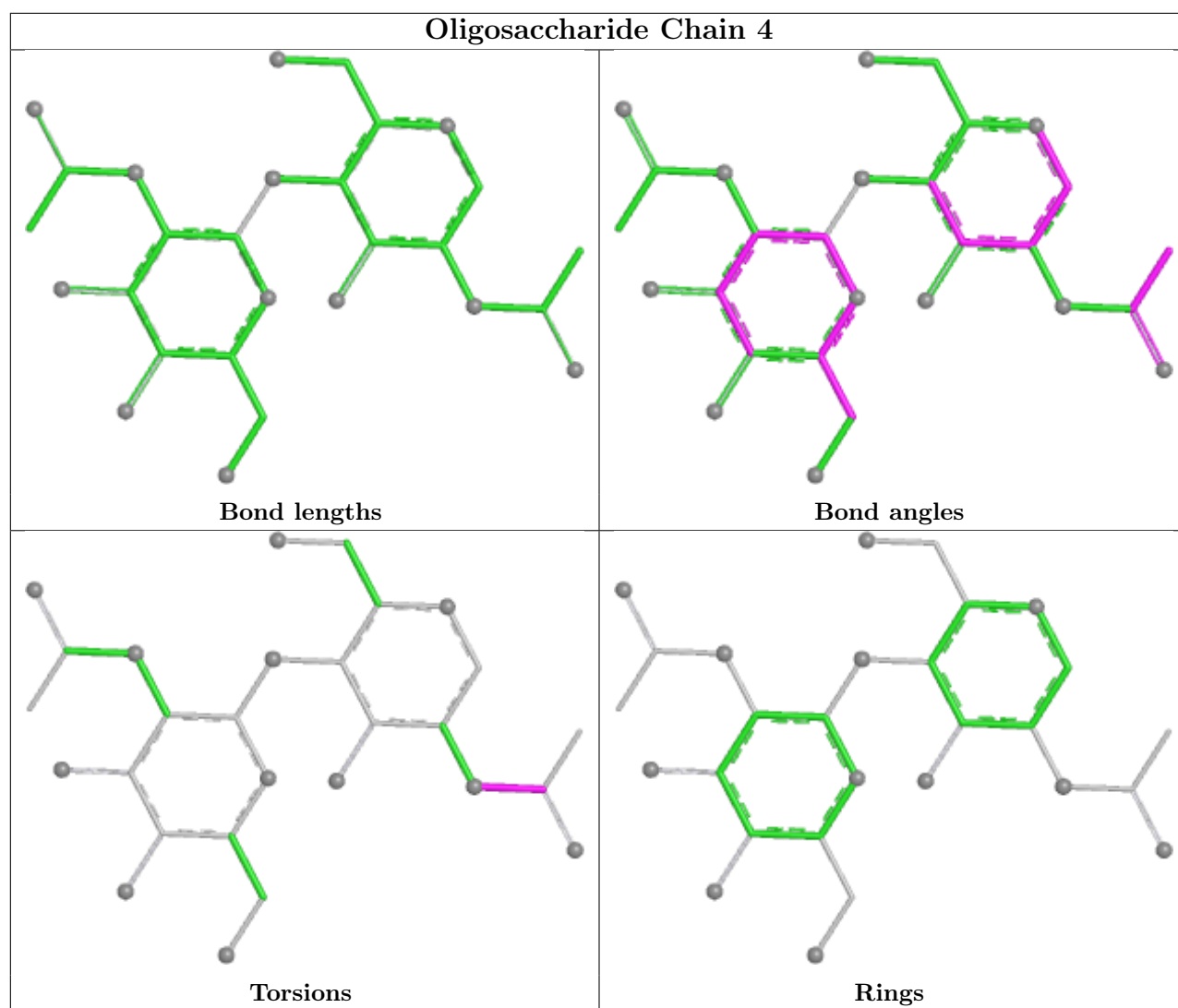


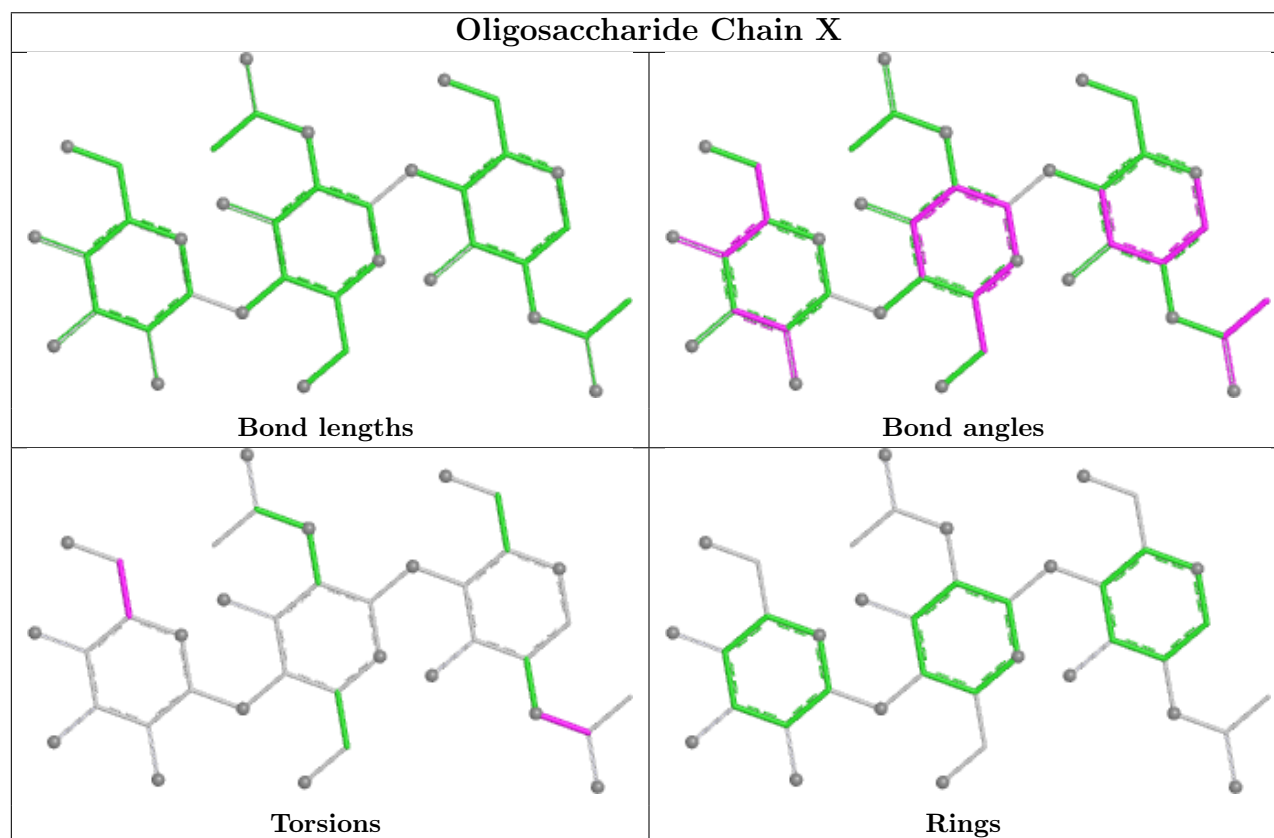
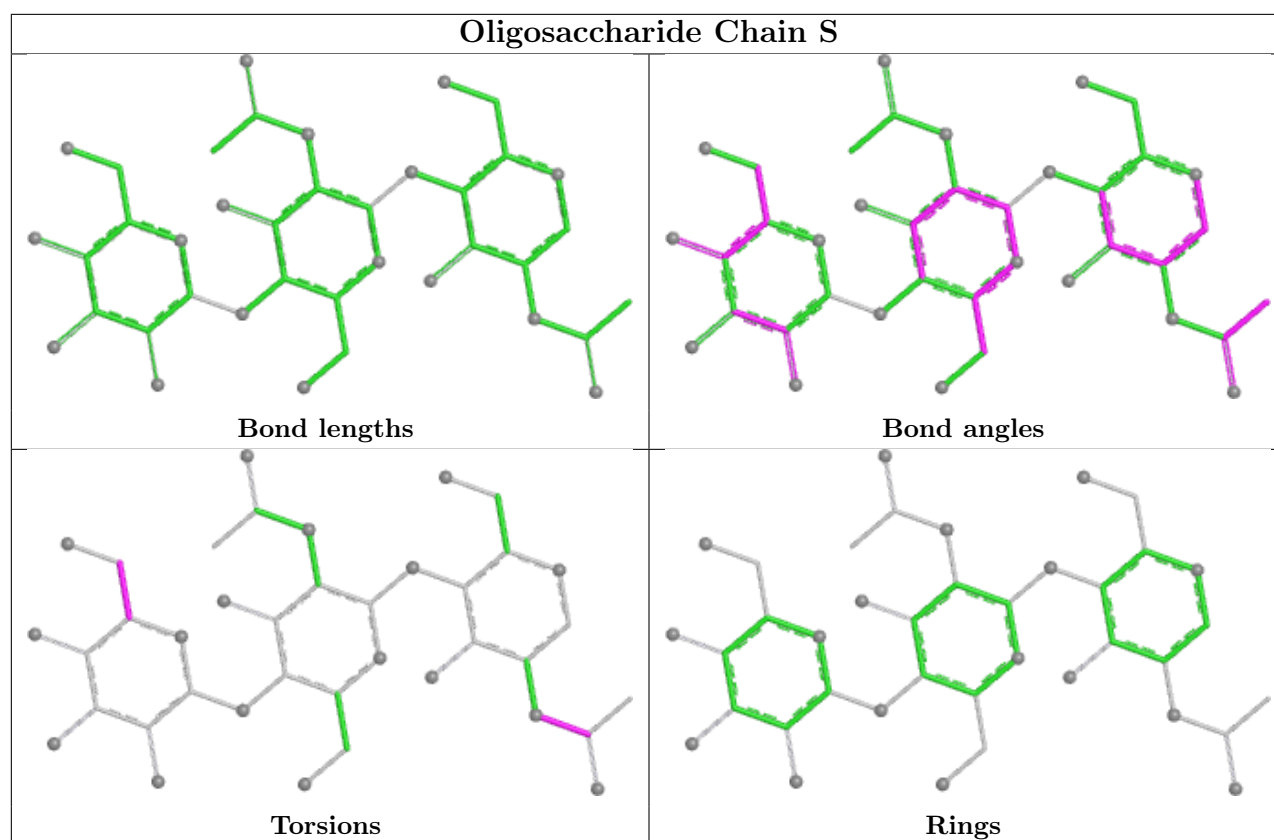


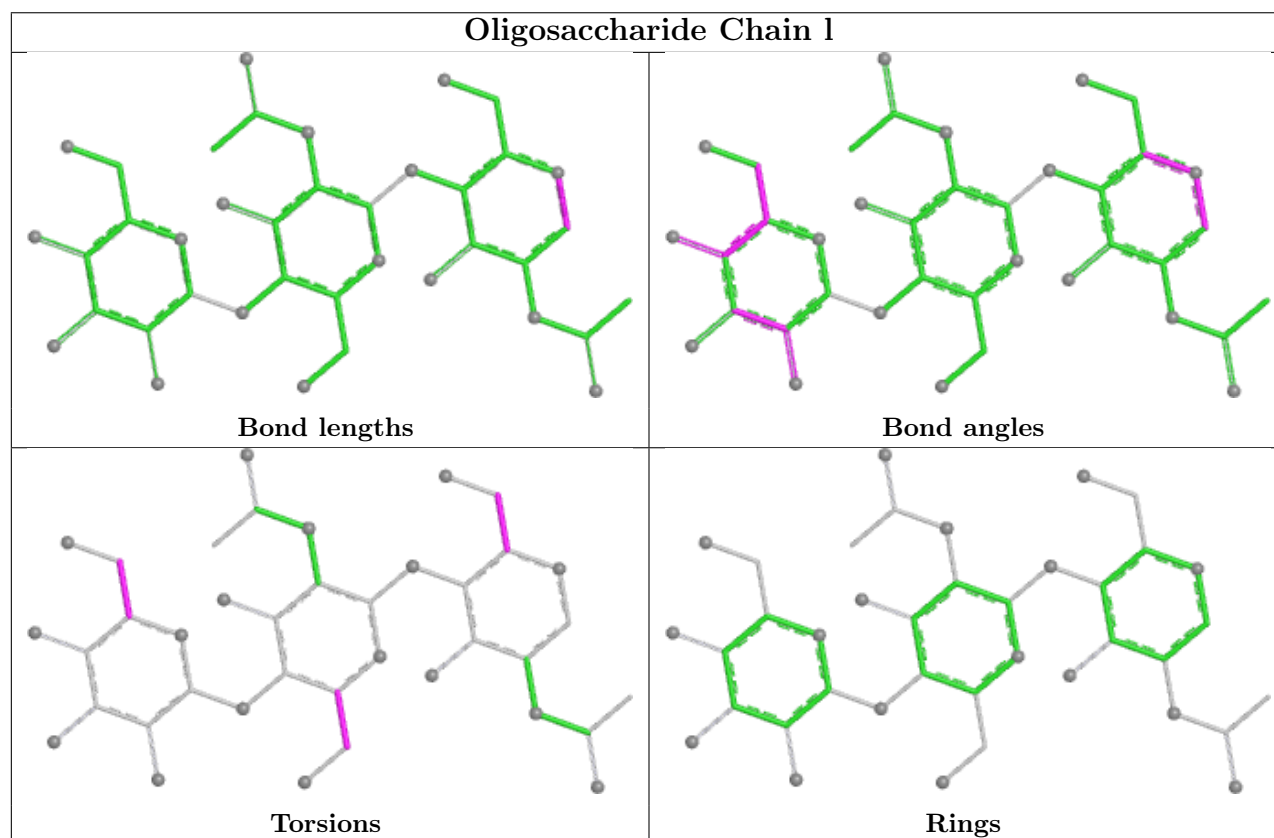
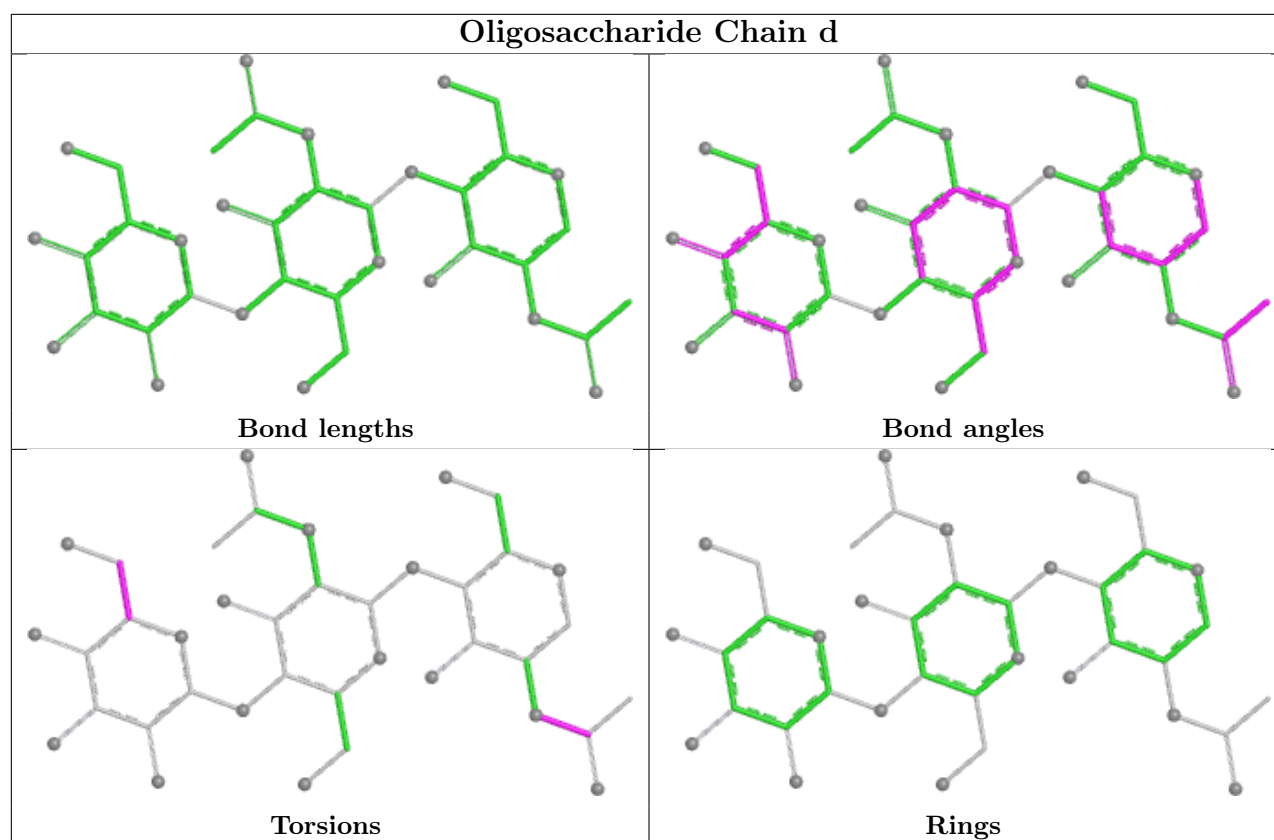


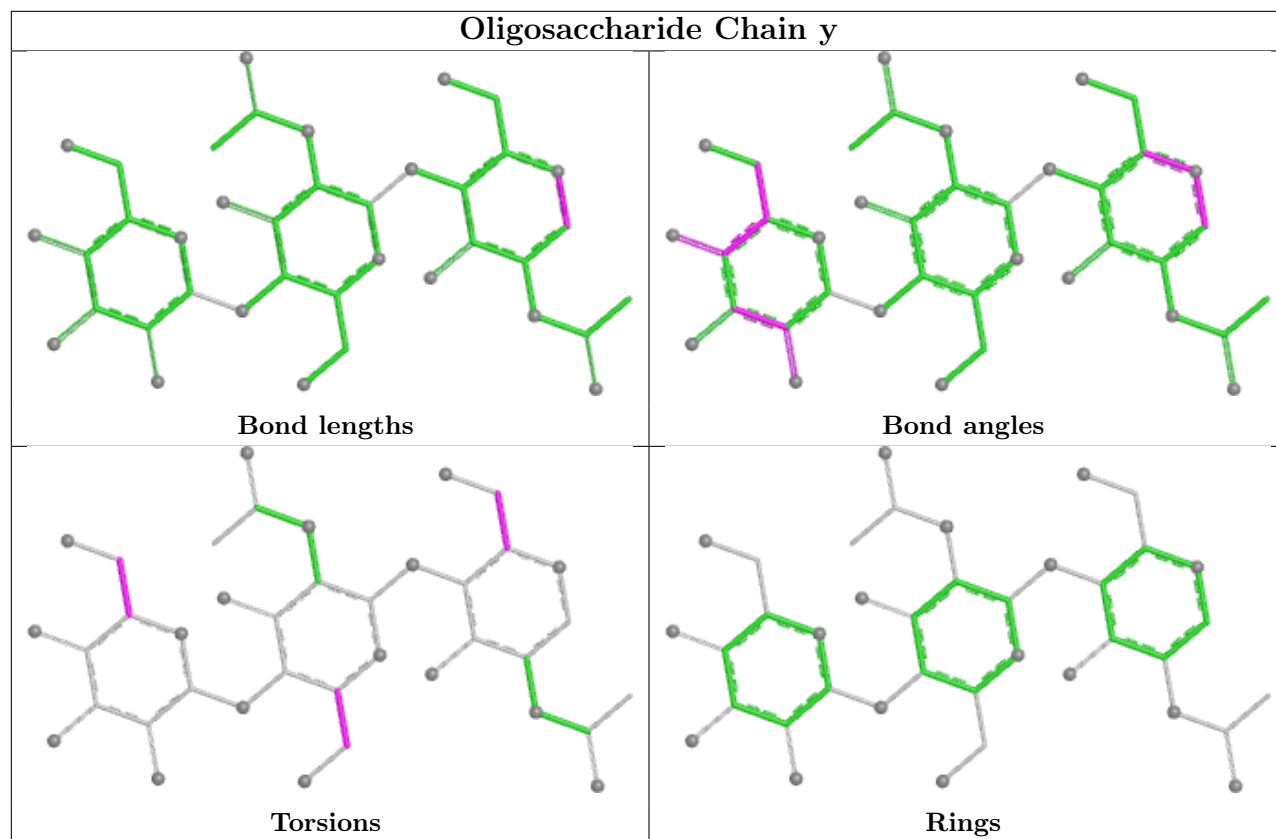


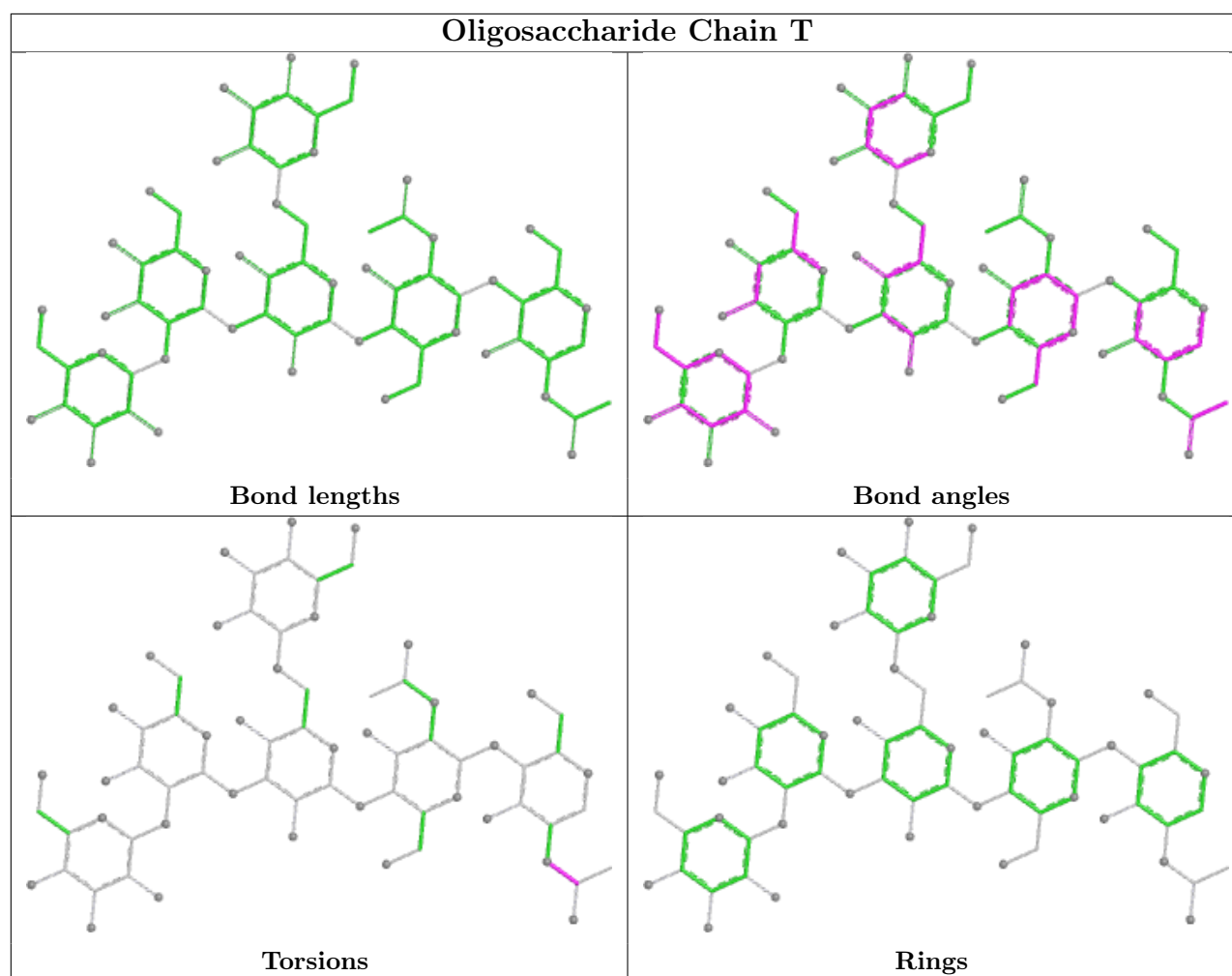


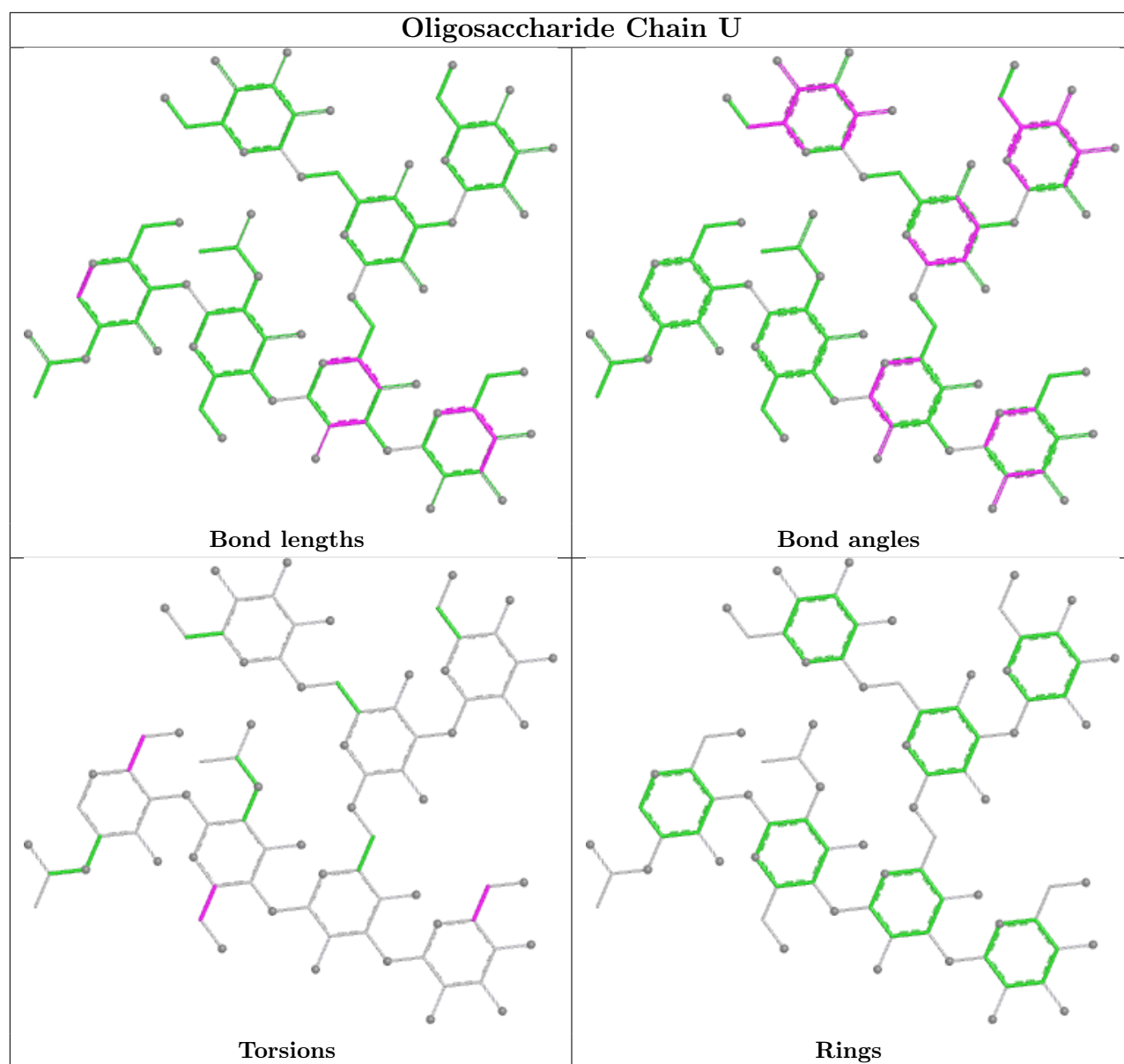


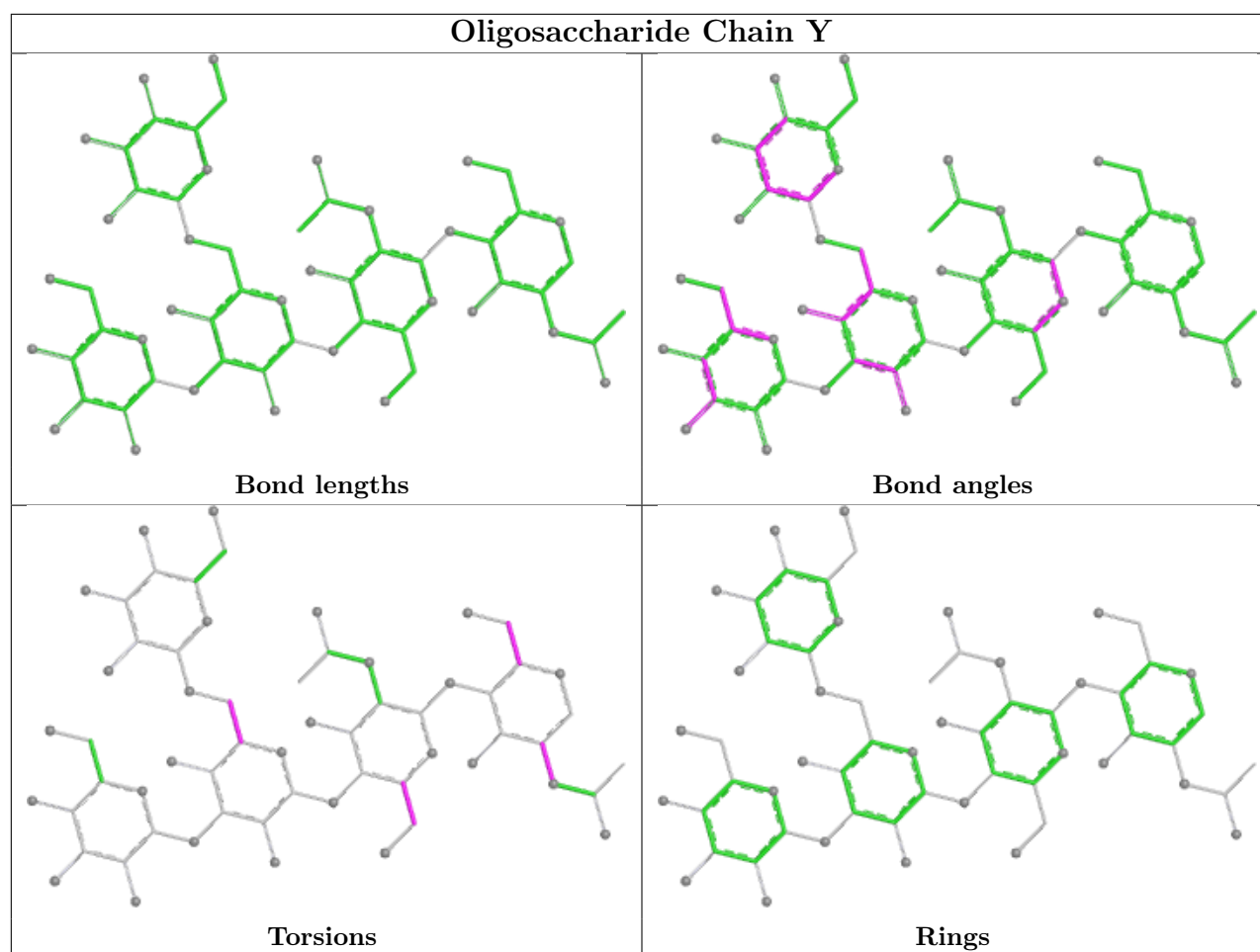


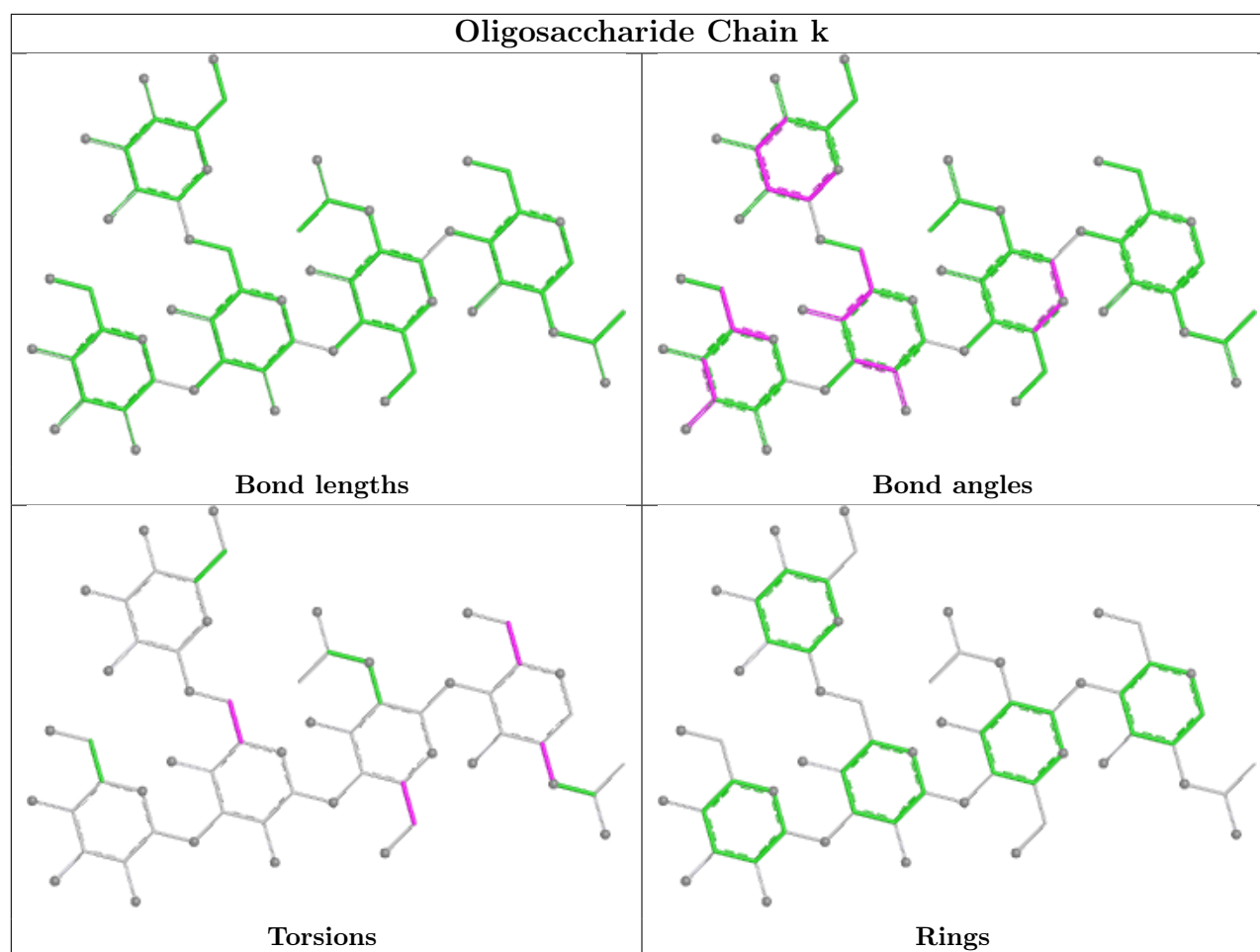


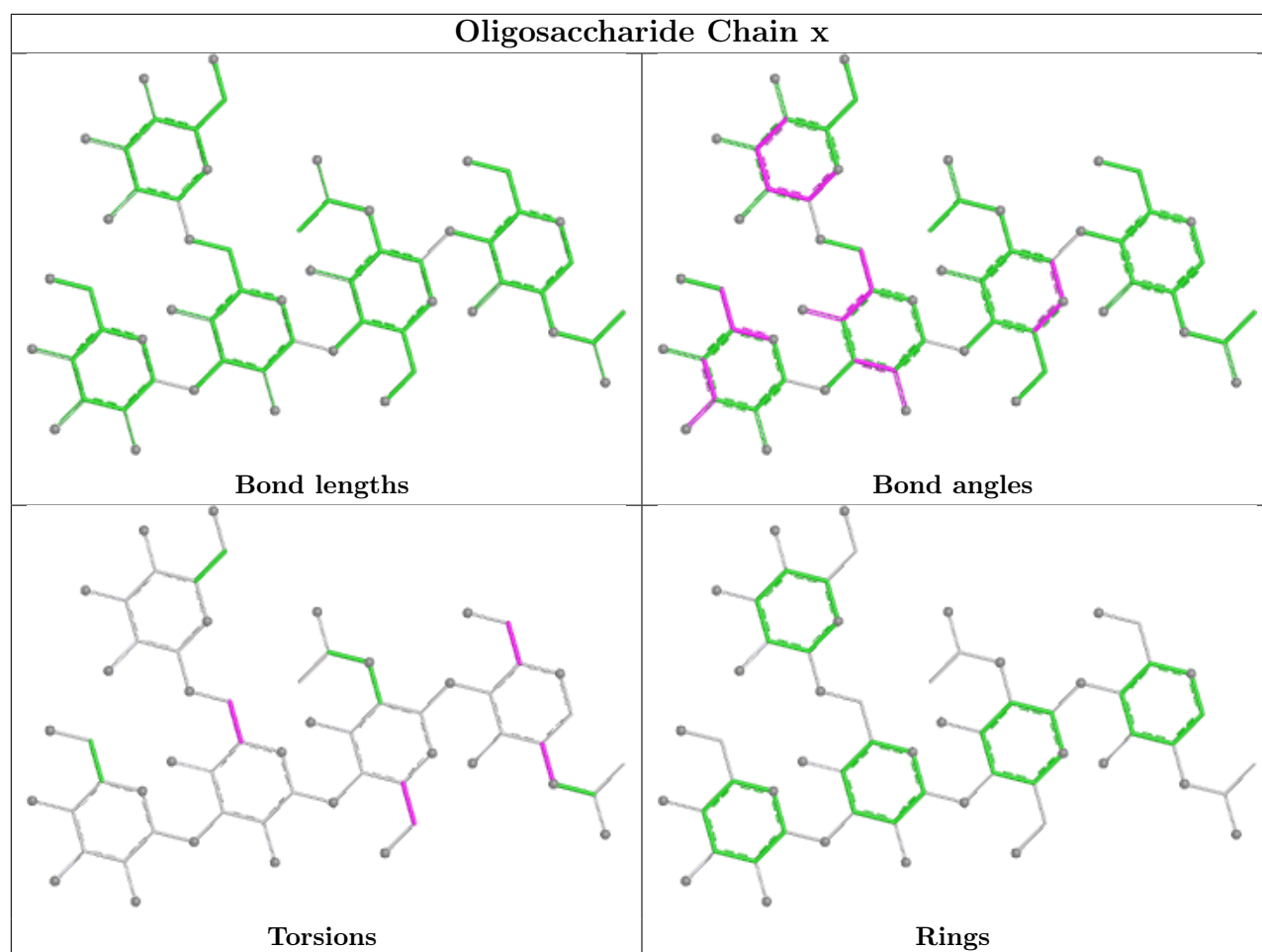


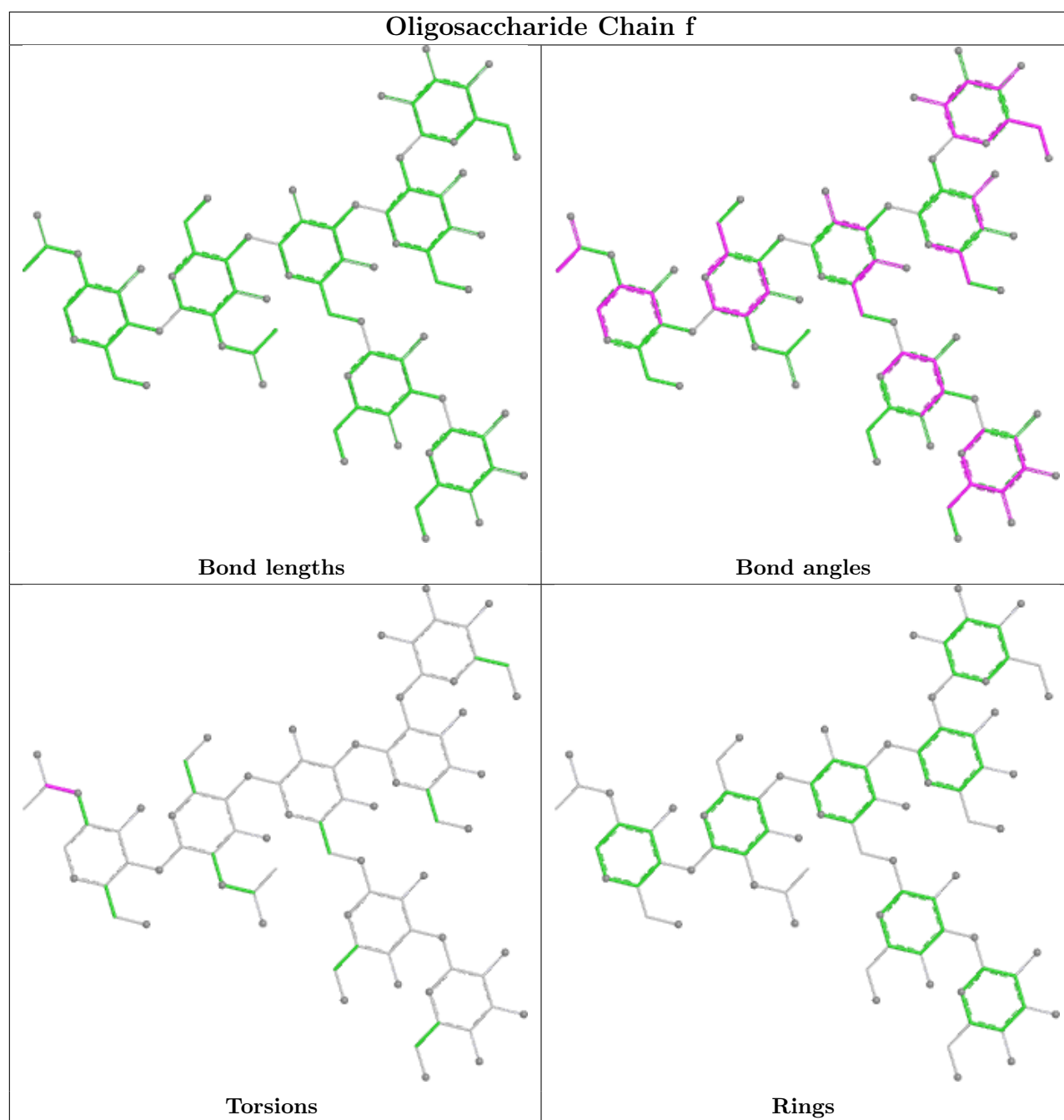


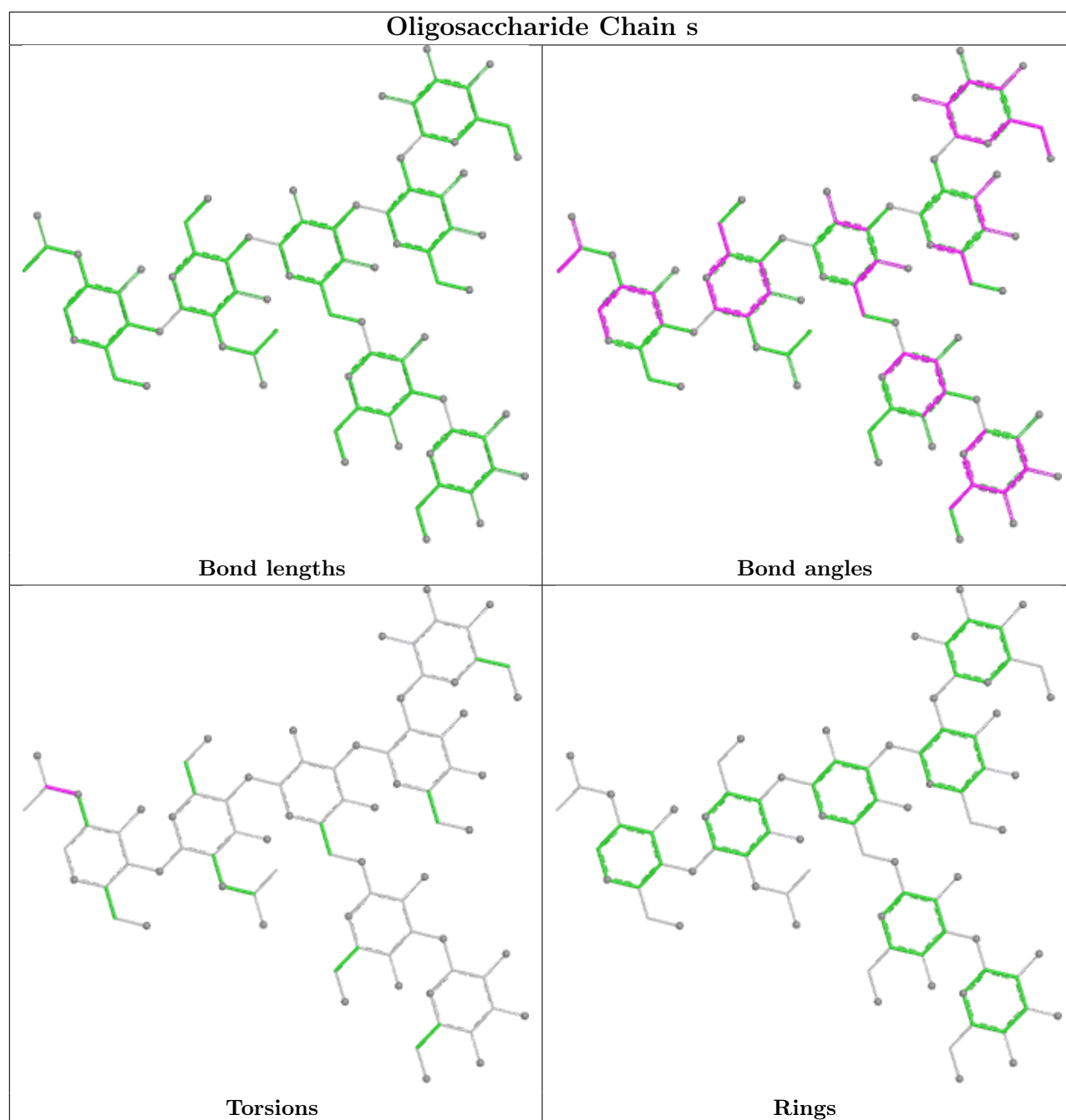


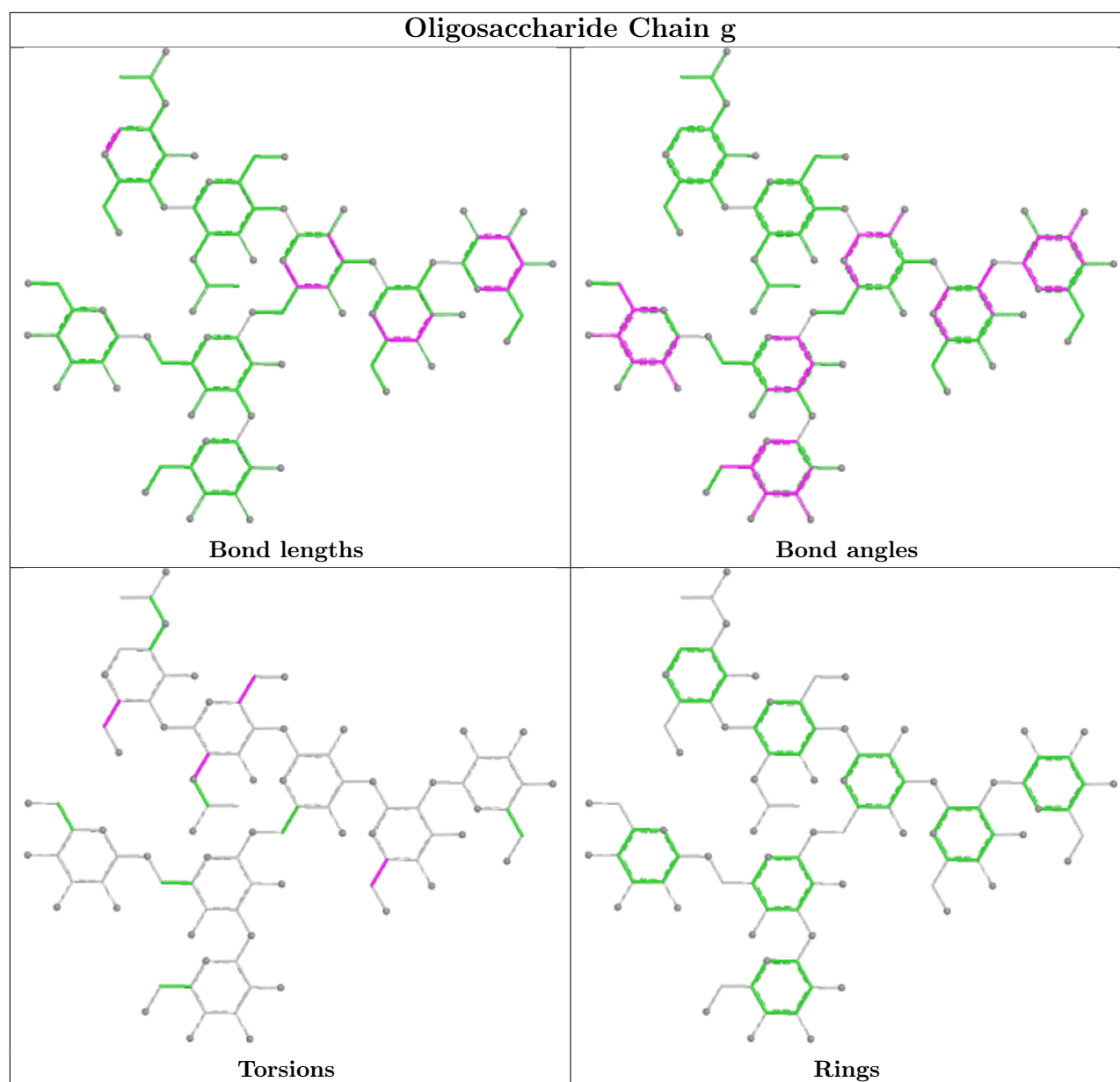


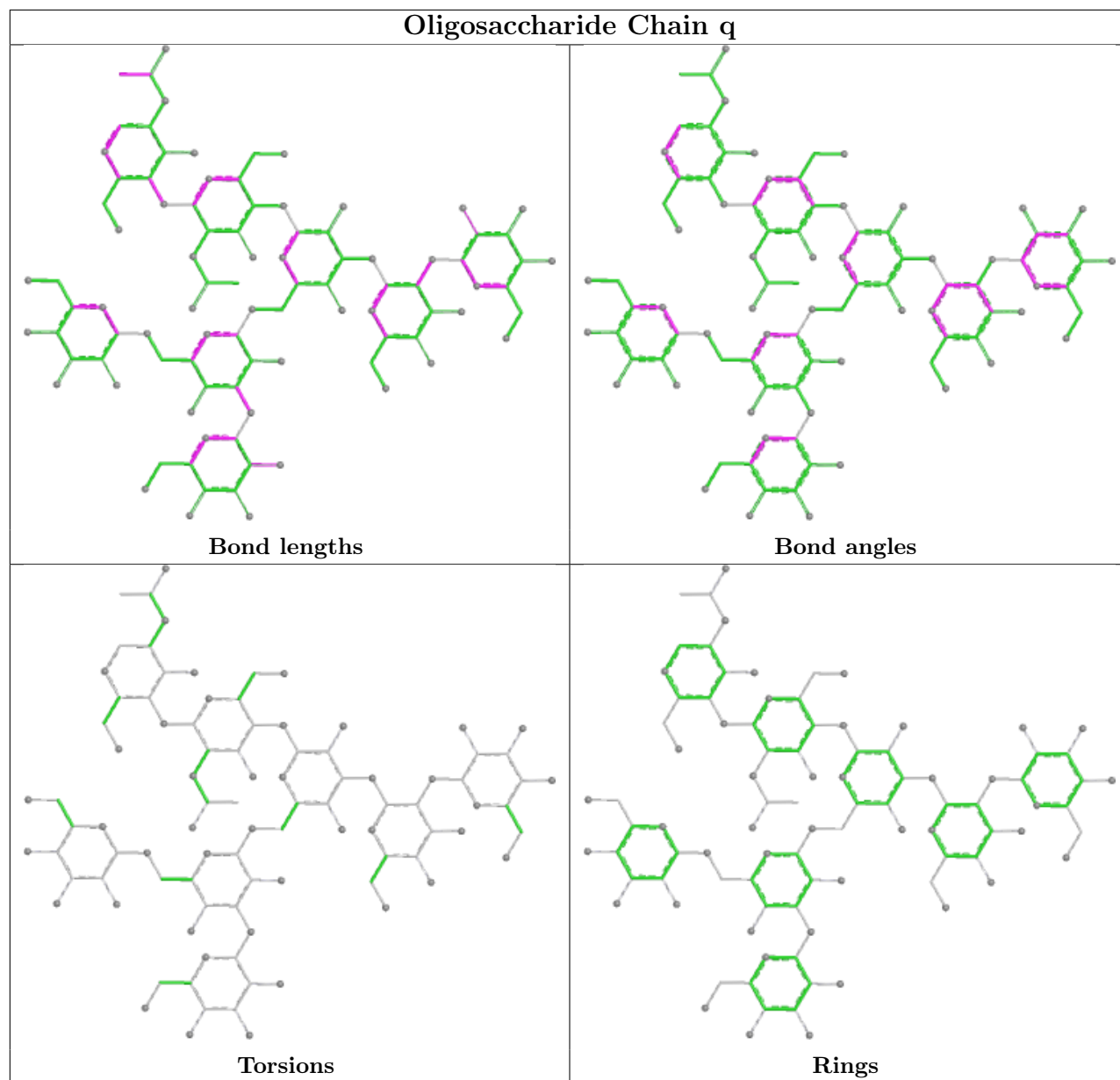


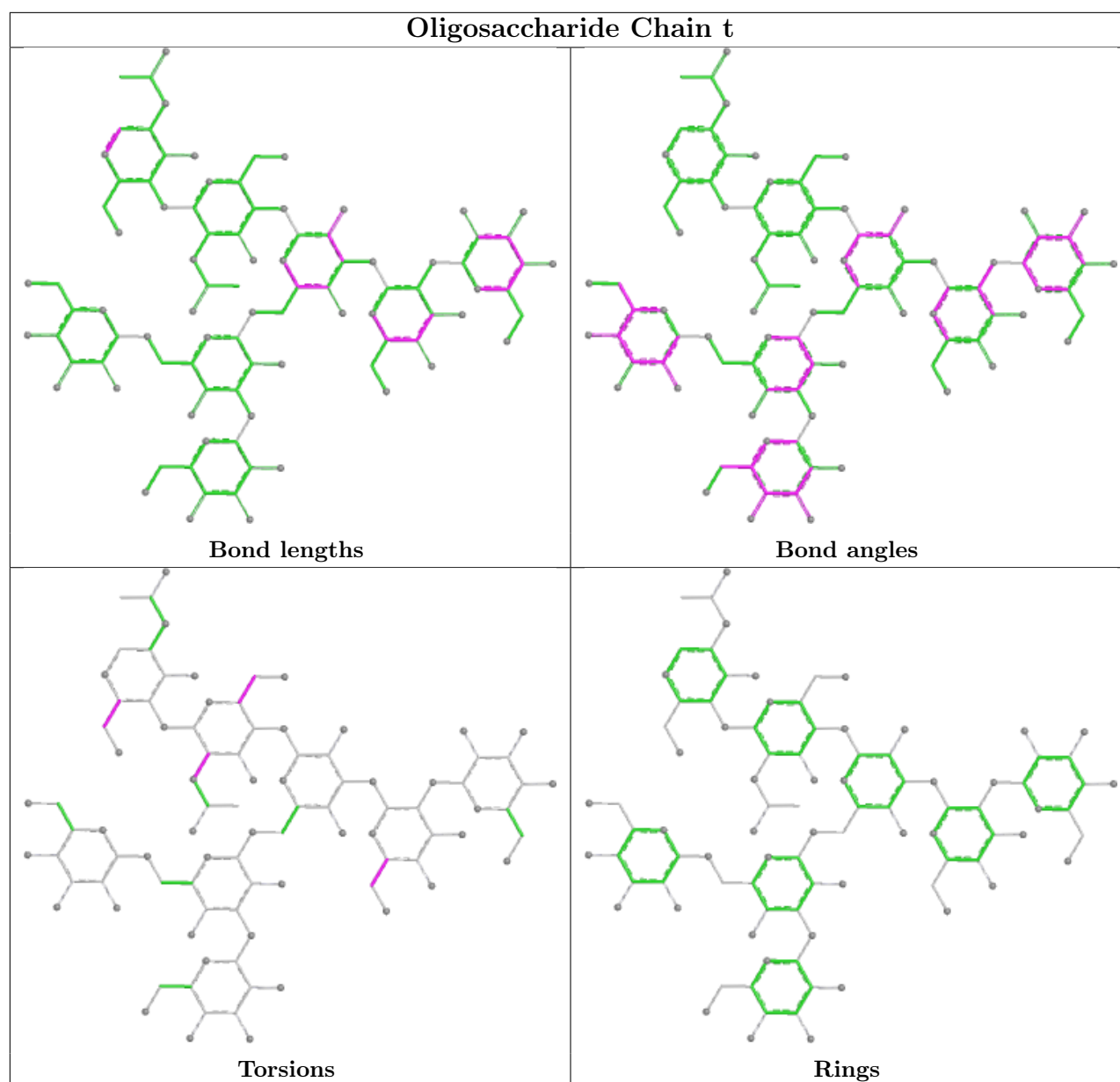












5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	NAG	D	639	1	14,14,15	0.51	0	17,19,21	0.42	0
14	NAG	F	704	2	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
14	NAG	A	633	1	14,14,15	0.30	0	17,19,21	0.41	0
14	NAG	C	611	1	14,14,15	0.51	0	17,19,21	0.52	0
14	NAG	D	603	1	14,14,15	0.41	0	17,19,21	0.66	1 (5%)
14	NAG	C	634	1	14,14,15	0.51	0	17,19,21	0.42	0
14	NAG	C	633	1	14,14,15	0.33	0	17,19,21	0.42	0
14	NAG	E	701	2	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
14	NAG	A	642	1	14,14,15	0.47	0	17,19,21	0.56	0
14	NAG	D	616	1	14,14,15	0.53	0	17,19,21	0.52	0
14	NAG	A	612	1	14,14,15	0.52	0	17,19,21	0.51	0
14	NAG	D	648	1	14,14,15	0.48	0	17,19,21	0.55	0
14	NAG	C	601	1	14,14,15	0.79	1 (7%)	17,19,21	0.92	2 (11%)
14	NAG	A	634	1	14,14,15	0.51	0	17,19,21	0.41	0
14	NAG	D	638	1	14,14,15	0.33	0	17,19,21	0.40	0
14	NAG	F	703	2	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
14	NAG	B	703	2	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
14	NAG	B	701	2	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
14	NAG	B	702	2	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
14	NAG	E	702	2	14,14,15	0.51	0	17,19,21	2.27	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	D	639	1	1/1/5/7	2/6/23/26	0/1/1/1
14	NAG	F	704	2	-	1/6/23/26	0/1/1/1
14	NAG	A	633	1	-	2/6/23/26	0/1/1/1
14	NAG	C	611	1	-	2/6/23/26	0/1/1/1
14	NAG	D	603	1	-	2/6/23/26	0/1/1/1
14	NAG	C	634	1	-	2/6/23/26	0/1/1/1
14	NAG	C	633	1	-	2/6/23/26	0/1/1/1
14	NAG	E	701	2	-	1/6/23/26	0/1/1/1
14	NAG	A	642	1	-	0/6/23/26	0/1/1/1
14	NAG	D	616	1	-	2/6/23/26	0/1/1/1
14	NAG	A	612	1	-	2/6/23/26	0/1/1/1
14	NAG	D	648	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	C	601	1	-	2/6/23/26	0/1/1/1
14	NAG	A	634	1	-	2/6/23/26	0/1/1/1
14	NAG	D	638	1	-	2/6/23/26	0/1/1/1
14	NAG	F	703	2	-	1/6/23/26	0/1/1/1
14	NAG	B	703	2	-	1/6/23/26	0/1/1/1
14	NAG	B	701	2	-	1/6/23/26	0/1/1/1
14	NAG	B	702	2	-	1/6/23/26	0/1/1/1
14	NAG	E	702	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	601	NAG	O5-C1	-2.19	1.40	1.43

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	703	NAG	O5-C1-C2	-7.52	99.65	111.29
14	B	702	NAG	O5-C1-C2	-7.52	99.66	111.29
14	F	703	NAG	O5-C1-C2	-7.51	99.67	111.29
14	E	702	NAG	O5-C1-C2	-7.51	99.67	111.29
14	F	704	NAG	O5-C1-C2	-7.51	99.68	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	D	639	NAG	C1

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	633	NAG	O5-C5-C6-O6
14	A	634	NAG	O5-C5-C6-O6
14	C	601	NAG	O5-C5-C6-O6
14	C	633	NAG	O5-C5-C6-O6
14	C	634	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	D	648	NAG	3	0
14	C	601	NAG	5	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.

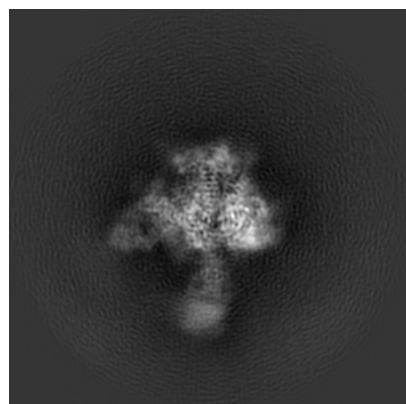
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8643. These allow visual inspection of the internal detail of the map and identification of artifacts.

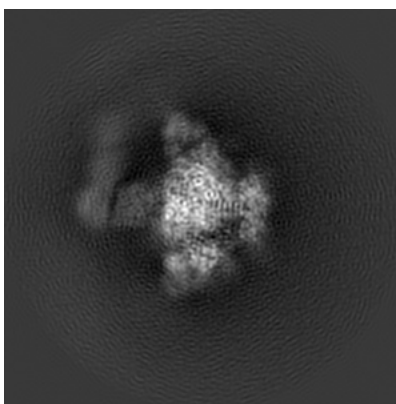
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

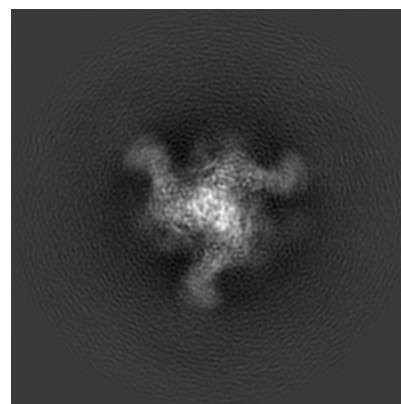
6.1.1 Primary map



X

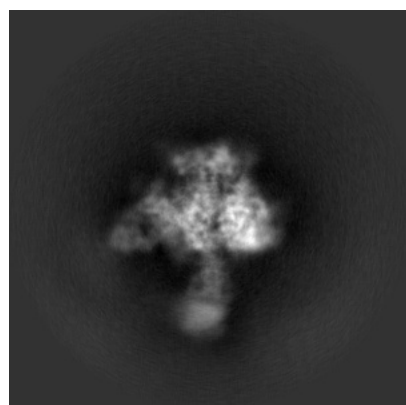


Y

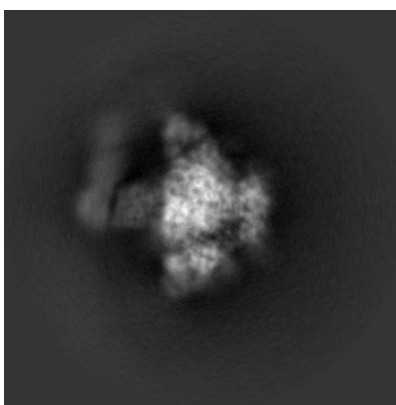


Z

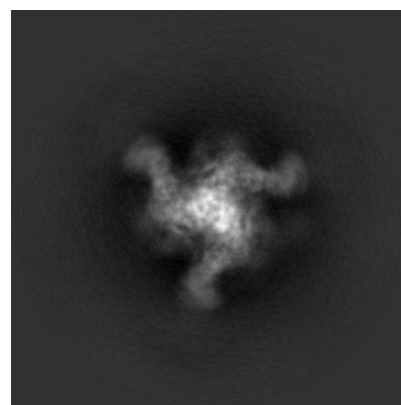
6.1.2 Raw map



X



Y

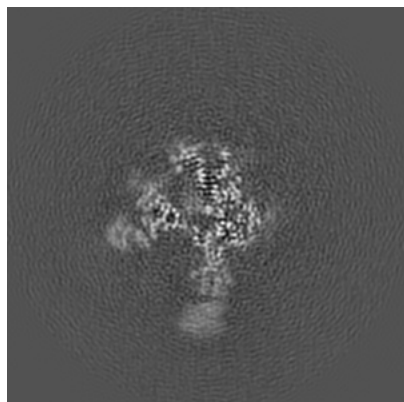


Z

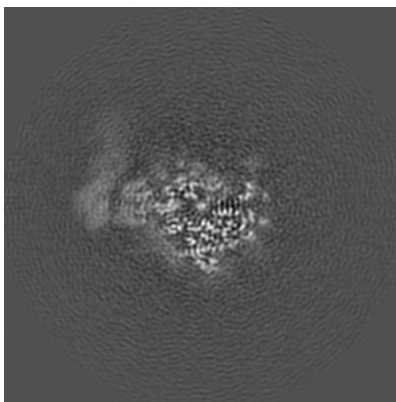
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

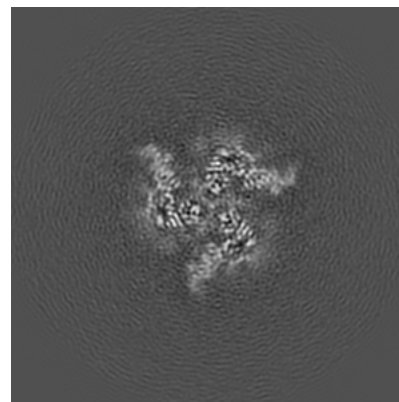
6.2.1 Primary map



X Index: 144

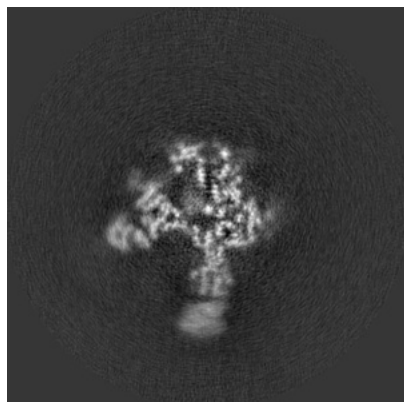


Y Index: 144

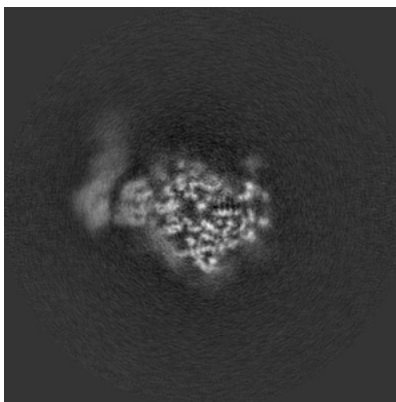


Z Index: 144

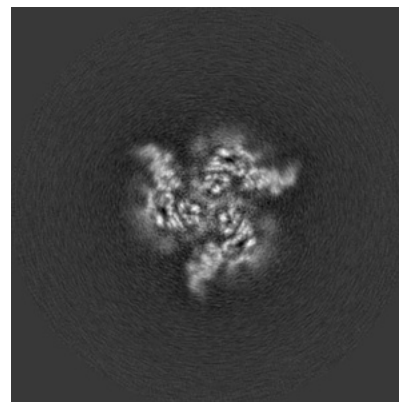
6.2.2 Raw map



X Index: 144



Y Index: 144

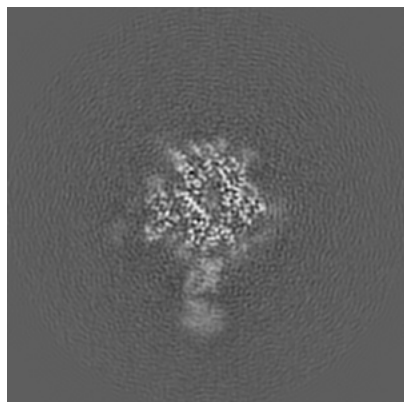


Z Index: 144

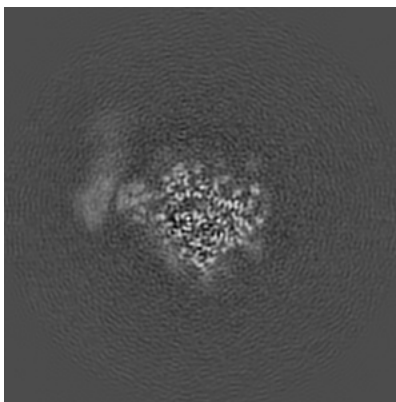
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

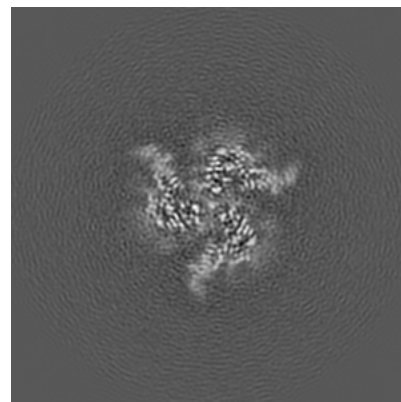
6.3.1 Primary map



X Index: 152

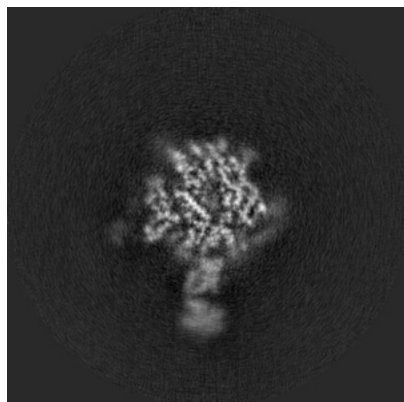


Y Index: 140

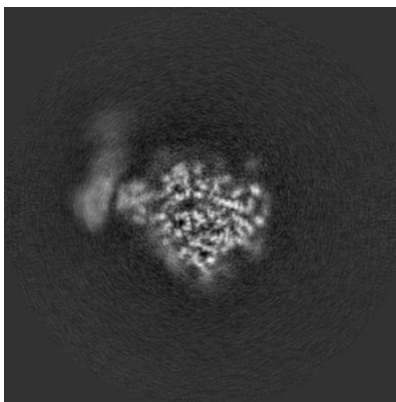


Z Index: 143

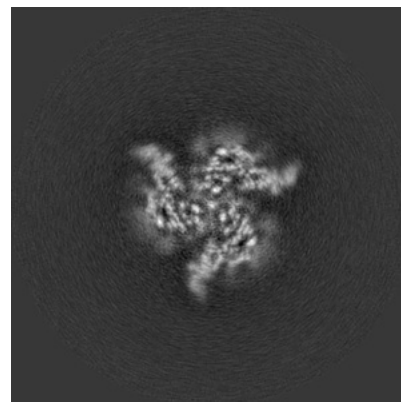
6.3.2 Raw map



X Index: 152



Y Index: 140

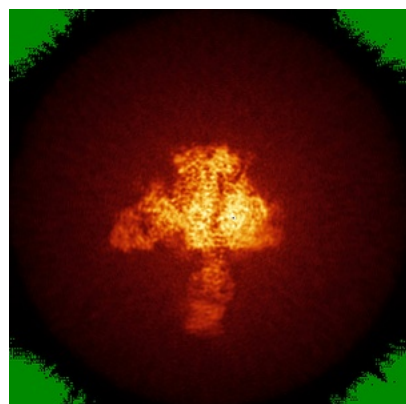


Z Index: 143

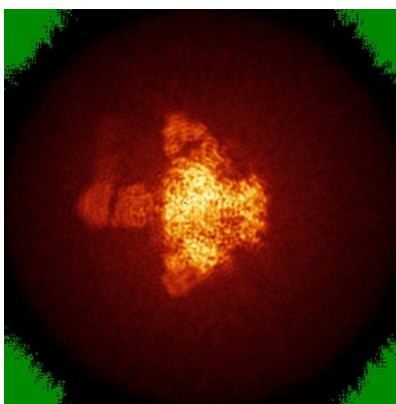
The images above show the largest variance slices of the map in three orthogonal directions.

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

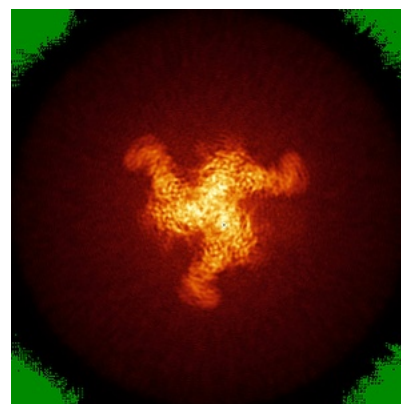
6.4.1 Primary map



X



Y

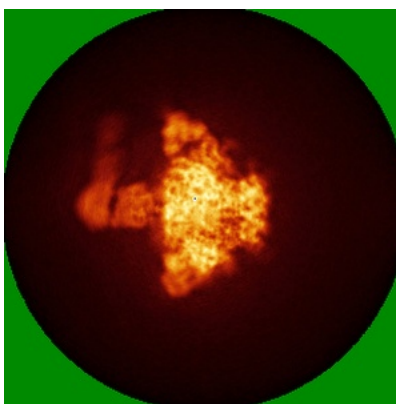


Z

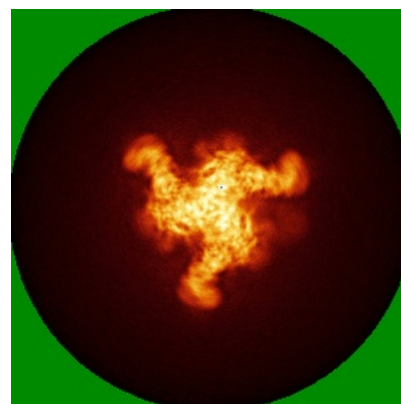
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

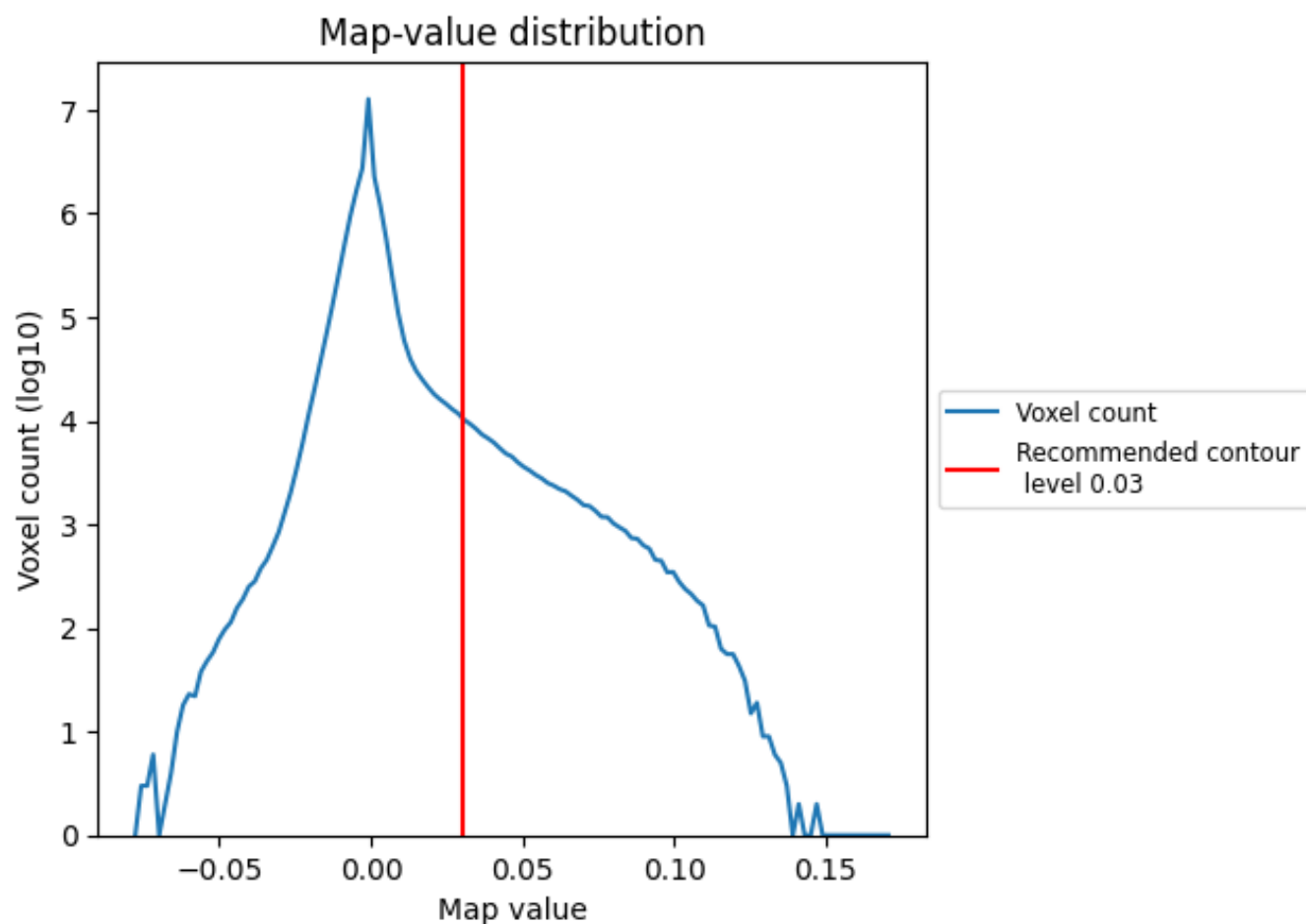
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

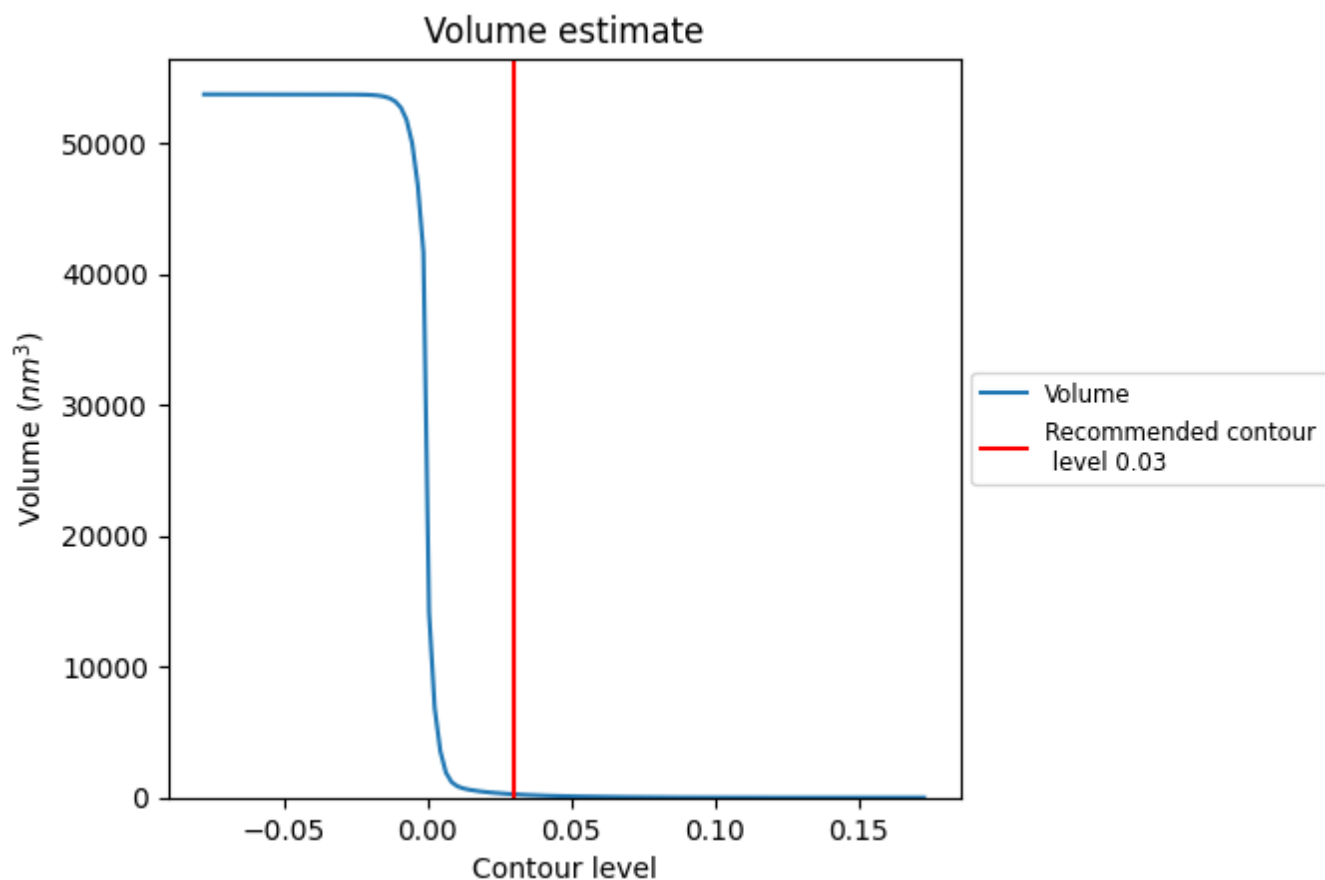
This section contains the results of statistical analysis of the map.

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.

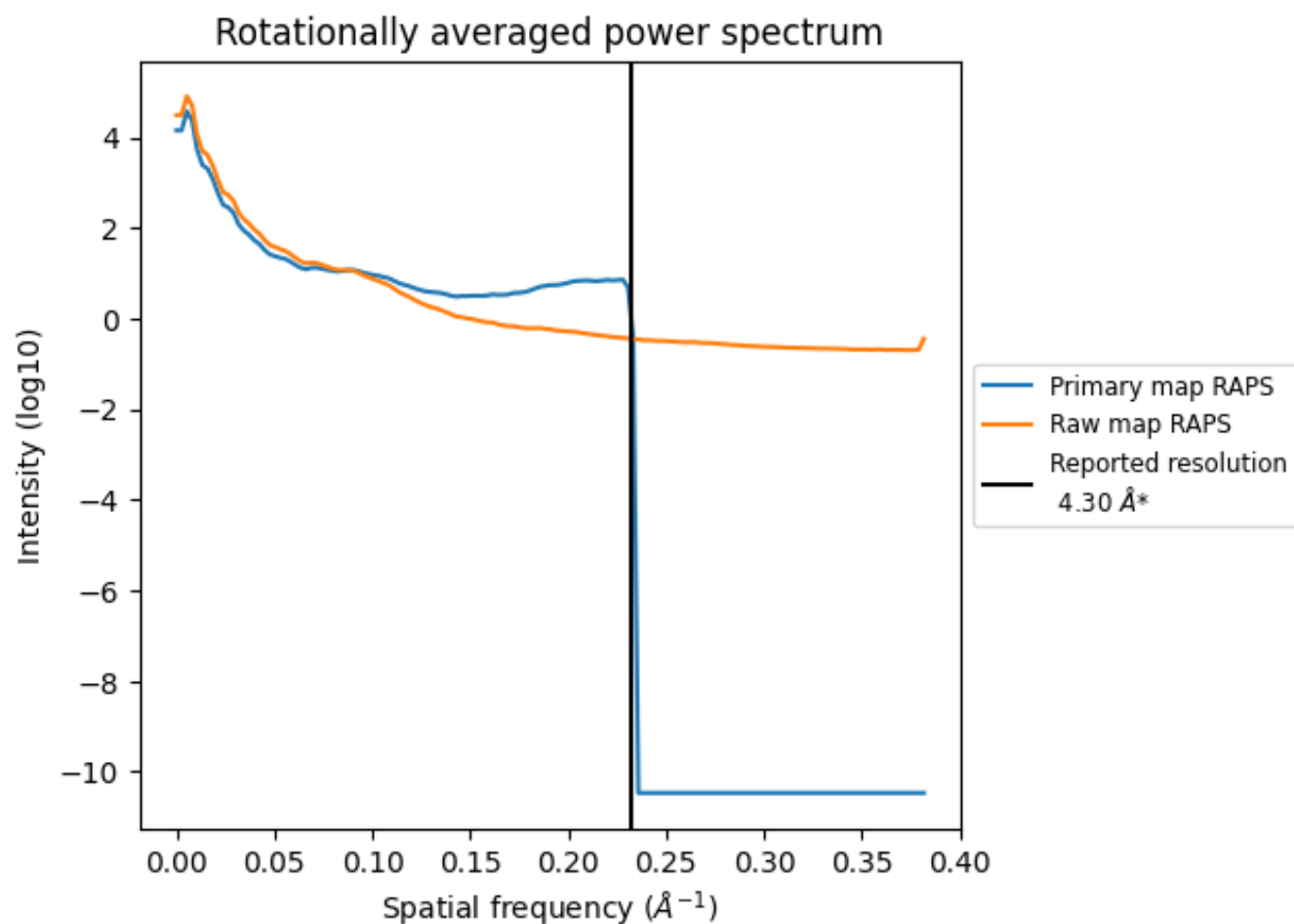
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 252 nm³; this corresponds to an approximate mass of 228 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 ⓘ

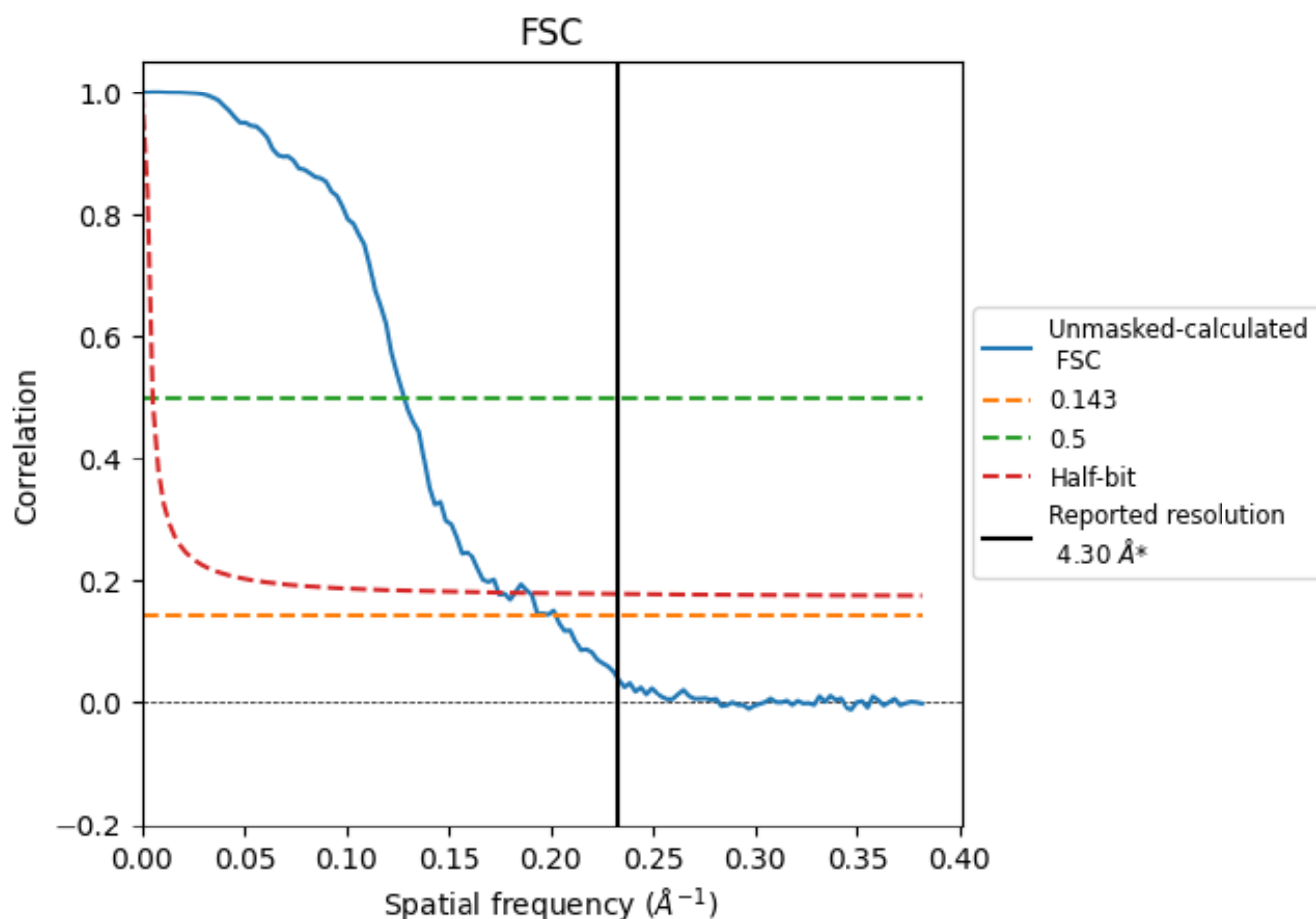


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

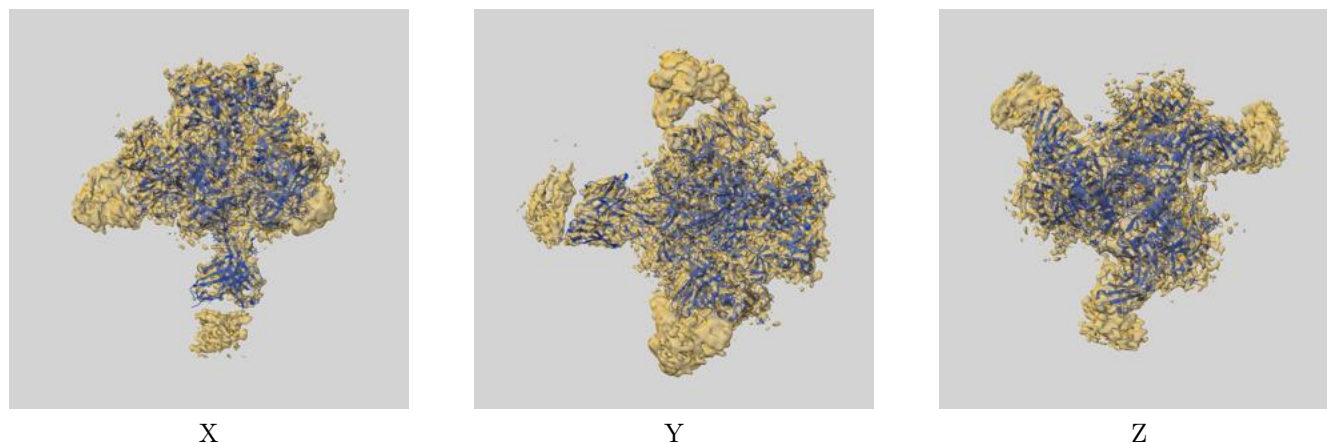
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.94	7.81	5.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.94 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

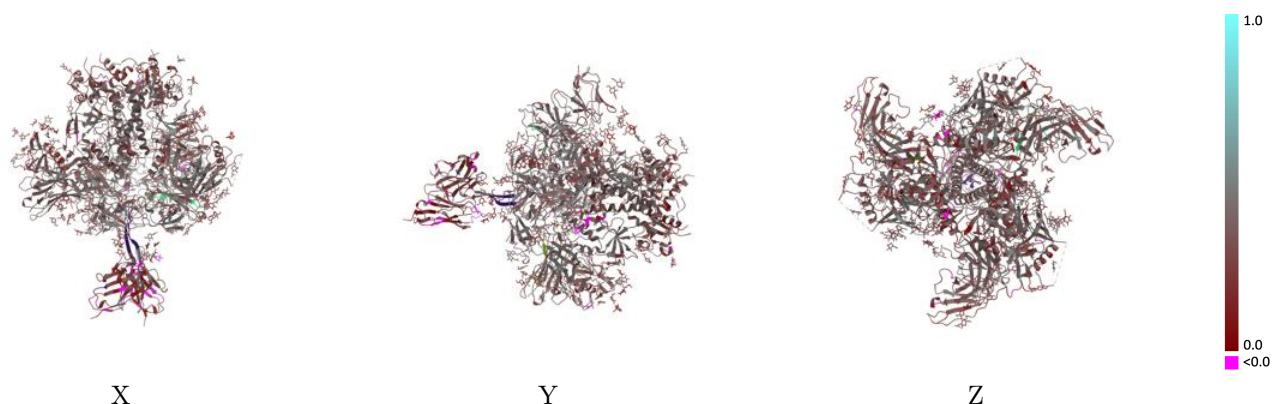
This section contains information regarding the fit between EMDB map EMD-8643 and PDB model 5V8L. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



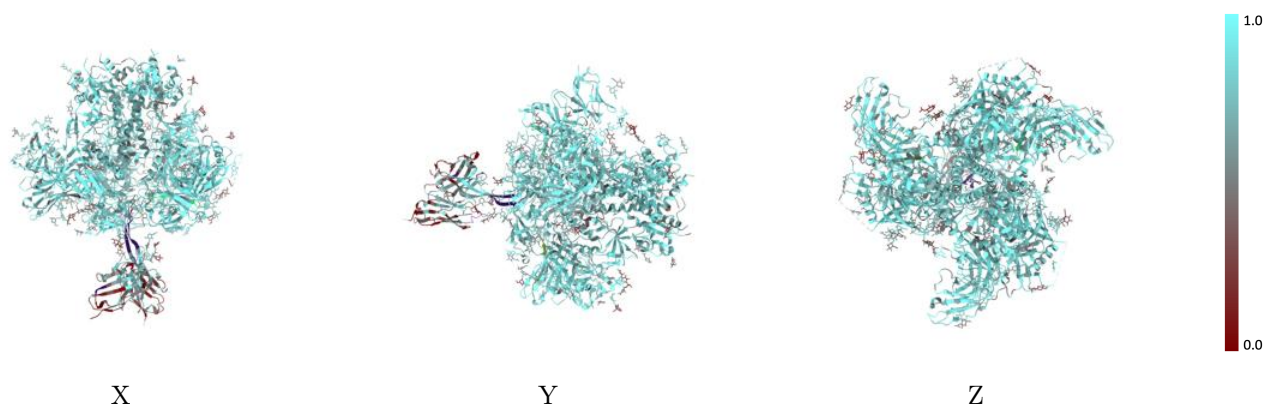
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



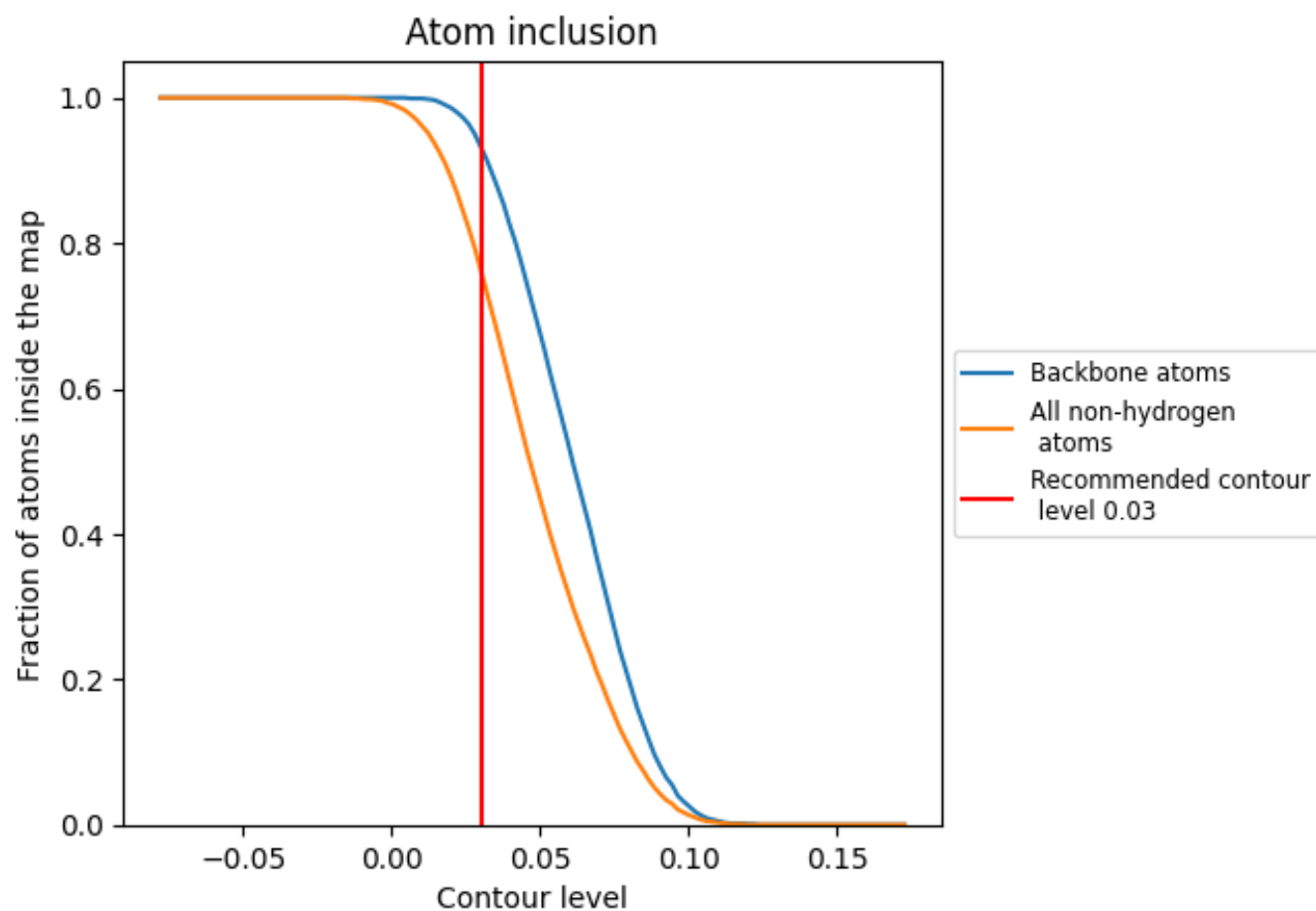
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7640	 0.3460
0	 0.2860	 0.2220
1	 0.4290	 0.3450
2	 0.5000	 0.2110
3	 0.5710	 0.2220
4	 0.6070	 0.2580
A	 0.8040	 0.3640
B	 0.7760	 0.3180
C	 0.8030	 0.3750
D	 0.8080	 0.3780
E	 0.7920	 0.3380
F	 0.7730	 0.3250
G	 0.8370	 0.3810
H	 0.8260	 0.3880
I	 0.8390	 0.3930
J	 0.5450	 0.2580
K	 0.7840	 0.3320
L	 0.7740	 0.3170
M	 0.7870	 0.3500
N	 0.5230	 0.2360
O	 0.4290	 0.2690
P	 0.7140	 0.3160
Q	 0.7140	 0.3470
R	 0.3930	 0.2490
S	 0.4620	 0.2450
T	 0.7640	 0.3690
U	 0.7350	 0.2970
V	 0.5360	 0.2690
W	 0.3930	 0.2590
X	 0.6410	 0.3410
Y	 0.6070	 0.2530
Z	 0.6790	 0.2220
a	 0.6430	 0.3340
b	 0.7860	 0.3430
c	 0.5710	 0.2820



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Chain	Atom inclusion	Q-score
d	 0.4870	 0.1400
e	 0.5360	 0.3290
f	 0.5900	 0.3040
g	 0.5960	 0.2670
h	 0.5710	 0.3390
i	 0.5710	 0.3070
j	 0.6430	 0.3270
k	 0.5410	 0.1720
l	 0.7690	 0.2240
m	 0.5360	 0.2690
n	 0.6070	 0.2970
o	 0.3930	 0.3060
p	 0.6790	 0.3370
q	 0.5320	 0.2030
r	 0.5710	 0.2350
s	 0.5900	 0.2890
t	 0.6920	 0.2980
u	 0.6070	 0.2960
v	 0.5710	 0.2530
w	 0.6070	 0.2310
x	 0.6560	 0.2690
y	 0.6670	 0.1470
z	 0.5360	 0.3120