



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:58 PM UTC

PDB ID : 7LX3 / pdb_00007lx3
EMDB ID : EMD-23565
Title : Cryo-EM structure of EDC-crosslinked ConSOSL.UFO.664 (ConS-EDC) in complex with bNAbs PGT122
Authors : Martin, G.M.; Ward, A.B.; Sattentau, Q.J.
Deposited on : 2021-03-03
Resolution : 3.45 Å(reported)

This is a Full wwPDB EM Validation 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

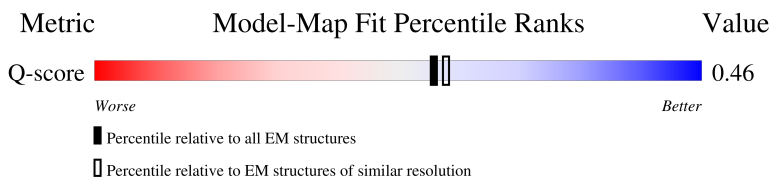
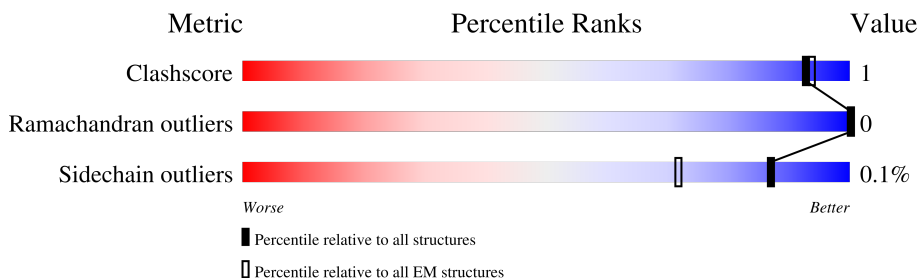
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

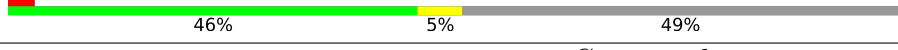
The reported resolution of this entry is 3.45 Å.

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.



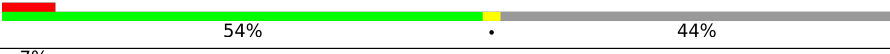
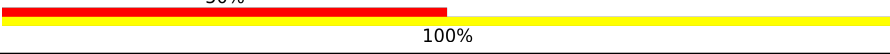
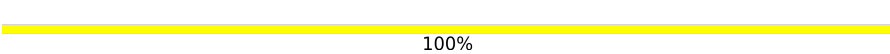
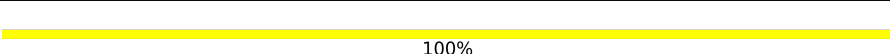
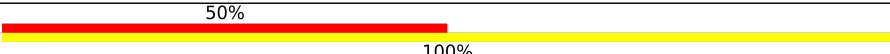
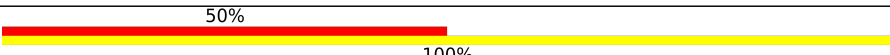
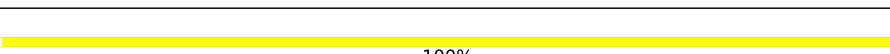
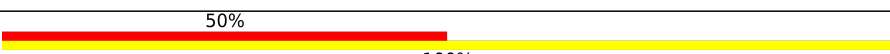
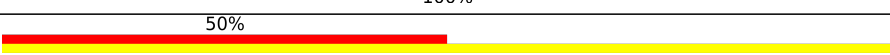
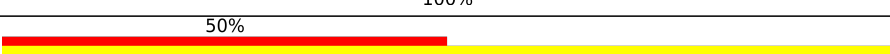
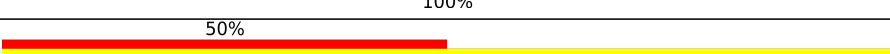
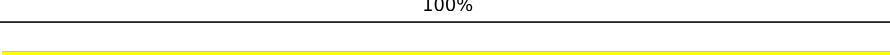
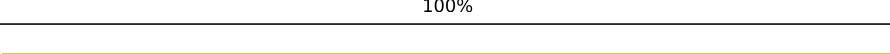
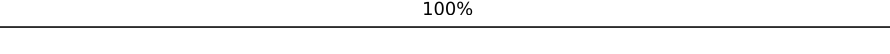
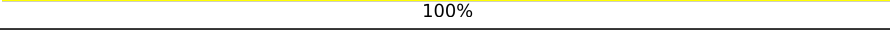
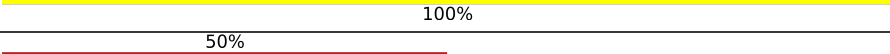
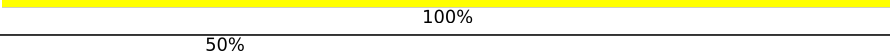
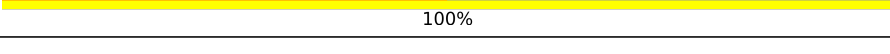
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13836 (2.95 - 3.95)

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	658	
1	B	658	
1	C	658	
2	L	213	

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Mol	Chain	Length	Quality of chain
2	M	213	
2	O	213	
3	H	235	
3	N	235	
3	P	235	
4	D	2	
4	E	2	
4	F	2	
4	G	2	
4	I	2	
4	K	2	
4	Q	2	
4	R	2	
4	S	2	
4	U	2	
4	V	2	
4	X	2	
4	Y	2	
4	Z	2	
4	a	2	
4	b	2	
4	d	2	
4	e	2	
4	f	2	
4	g	2	

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Mol	Chain	Length	Quality of chain
4	i	2	50% 100%
4	j	2	50% 100%
4	l	2	50% 100%
4	m	2	50% 100%
4	n	2	50% 100%
4	o	2	100%
4	p	2	50% 100%
4	r	2	100%
4	s	2	50% 100%
4	t	2	50% 100%
4	u	2	100%
4	w	2	50% 100%
4	x	2	50% 100%
5	J	6	33% 100%
5	c	6	33% 100%
5	q	6	33% 83% 17%
6	T	9	11% 11% 78% 11%
6	h	9	11% 11% 89%
6	v	9	11% 11% 78% 11%
7	W	6	17% 67% 17%
7	k	6	17% 83%
7	y	6	17% 83%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 20196 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 Env glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	534	Total	C	N	O	S	0	0
			4232	2675	737	788	32		
1	B	534	Total	C	N	O	S	0	0
			4232	2675	737	788	32		
1	C	534	Total	C	N	O	S	0	0
			4232	2675	737	788	32		

- Molecule 2 is a protein called PGT122 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	109	Total	C	N	O	S	0	0
			832	520	144	166	2		
2	M	109	Total	C	N	O	S	0	0
			832	520	144	166	2		
2	O	109	Total	C	N	O	S	0	0
			832	520	144	166	2		

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

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

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



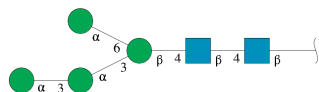
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		
4	d	2	Total	C	N	O	0	0
			28	16	2	10		
4	e	2	Total	C	N	O	0	0
			28	16	2	10		
4	f	2	Total	C	N	O	0	0
			28	16	2	10		
4	g	2	Total	C	N	O	0	0
			28	16	2	10		
4	i	2	Total	C	N	O	0	0
			28	16	2	10		
4	j	2	Total	C	N	O	0	0
			28	16	2	10		

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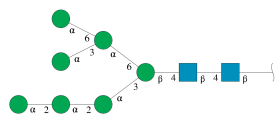
Mol	Chain	Residues	Atoms				AltConf	Trace
4	l	2	Total	C	N	O	0	0
			28	16	2	10		
4	m	2	Total	C	N	O	0	0
			28	16	2	10		
4	n	2	Total	C	N	O	0	0
			28	16	2	10		
4	o	2	Total	C	N	O	0	0
			28	16	2	10		
4	p	2	Total	C	N	O	0	0
			28	16	2	10		
4	r	2	Total	C	N	O	0	0
			28	16	2	10		
4	s	2	Total	C	N	O	0	0
			28	16	2	10		
4	t	2	Total	C	N	O	0	0
			28	16	2	10		
4	u	2	Total	C	N	O	0	0
			28	16	2	10		
4	w	2	Total	C	N	O	0	0
			28	16	2	10		
4	x	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called 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.



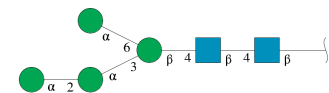
Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	6	Total	C	N	O	0	0
			72	40	2	30		
5	c	6	Total	C	N	O	0	0
			72	40	2	30		
5	q	6	Total	C	N	O	0	0
			72	40	2	30		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
6	T	9	Total	C	N	O	0	0
			105	58	2	45		
6	h	9	Total	C	N	O	0	0
			105	58	2	45		
6	v	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 7 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
7	W	6	Total	C	N	O	0	0
			72	40	2	30		
7	k	6	Total	C	N	O	0	0
			72	40	2	30		
7	y	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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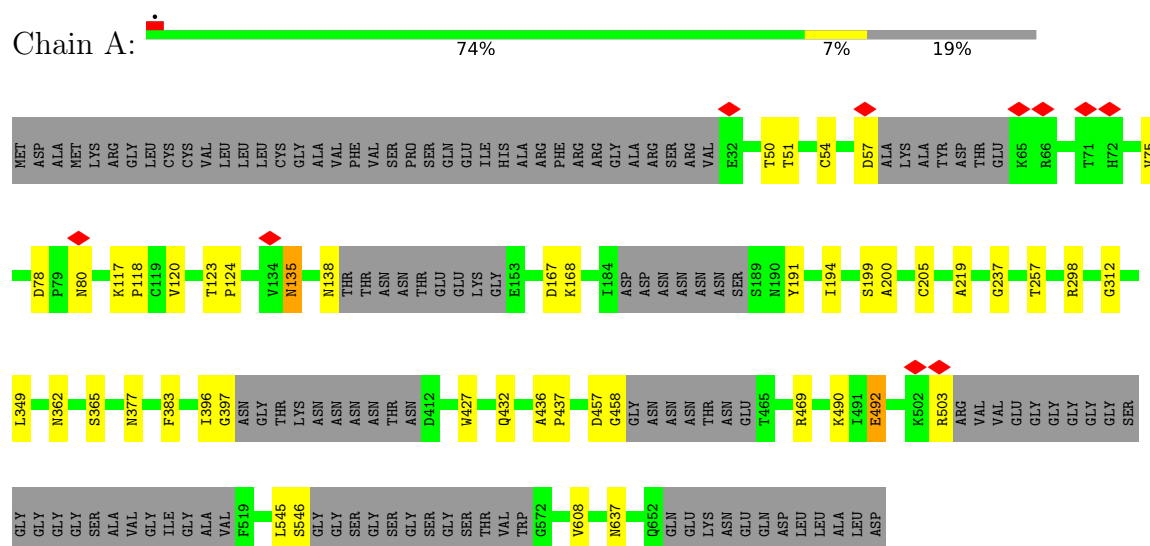
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
8	C	1	14	8	1	5	0

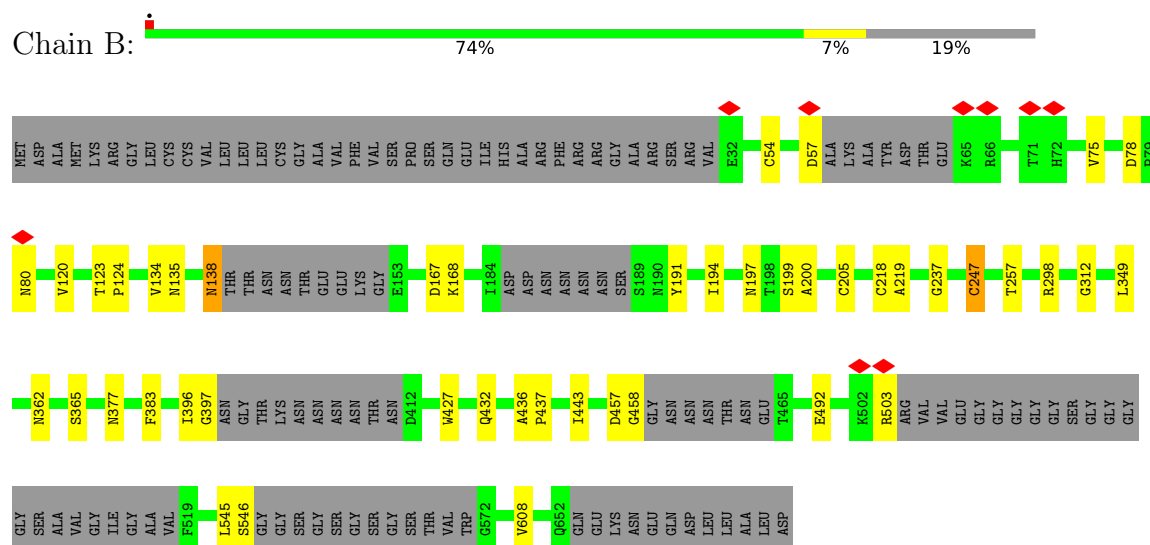
3 Residue-property plots

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.

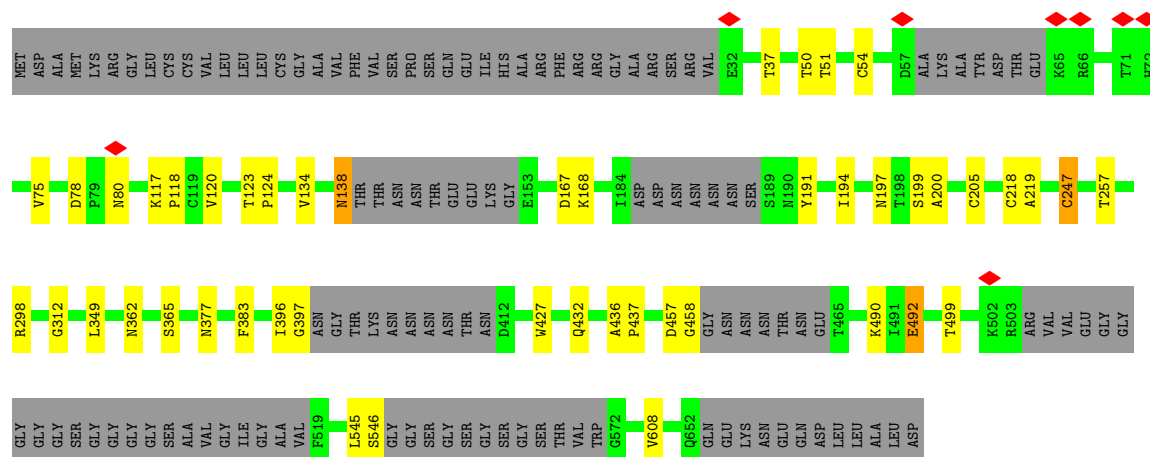
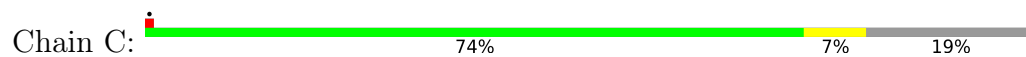
• Molecule 1: Env glycoprotein gp160



• Molecule 1: Env glycoprotein gp160



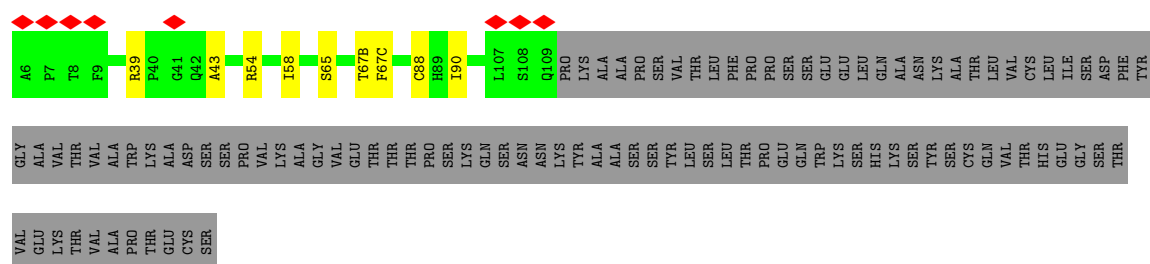
• Molecule 1: Env glycoprotein gp160



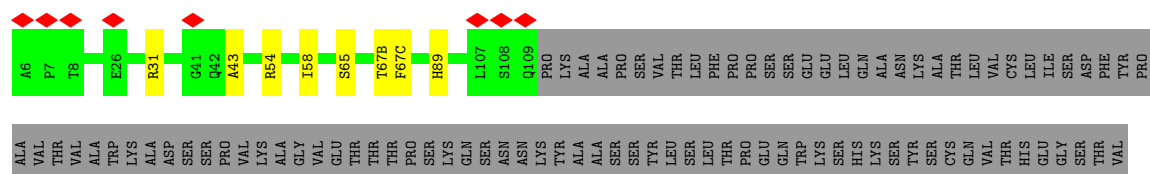
• Molecule 2: PGT122 Fab light chain



• Molecule 2: PGT122 Fab light chain



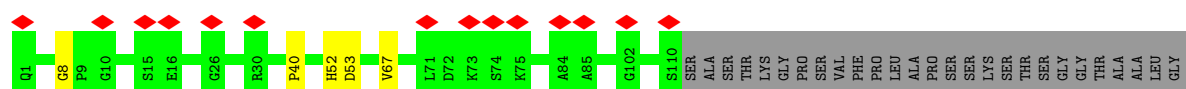
• Molecule 2: PGT122 Fab light chain



GLU
LYS
THR
VAL
ALA
PRO
THR
GLU
CYS
SER

• Molecule 3: PGT122 Fab heavy chain

Chain H:  6% 54% 44%

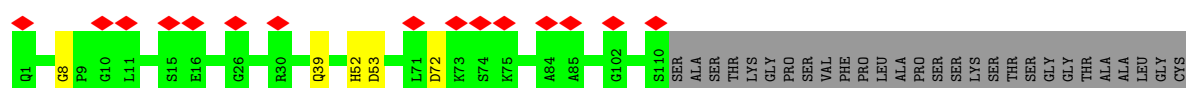


LEU VAL LYS ASP THR PHE PRO GLU PRO VAL THR VAL TRP ASN SER GLY ALA LEU THR SER GLY VAL HIS THR PHE PRO VAL LEU GLN SER SER GLY TYR SER LEU SER THR VAL LYS VAL THR VAL PRO SER PHE SER PRO LEU LEU PRO GLY THR SER GLN THR LYS THR ILE SER ASN VAL THR ALA ALA LEU GLY CYS

LYS PRO SER ASN THR LYS VAL ASP ARG GLU PRO LYS CYS

• Molecule 3: PGT122 Fab heavy chain

Chain N:  6% 54% 44%

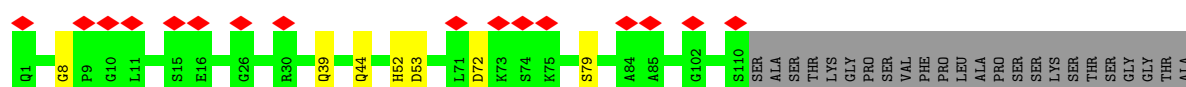


VAL LYS ASP THR PHE PRO GLU PRO VAL THR VAL TRP ASN SER GLY ALA LEU THR SER GLY VAL HIS THR PHE PRO VAL LEU GLN SER SER GLY TYR SER LEU SER THR VAL LYS VAL THR VAL PRO SER PHE SER PRO LEU LEU PRO GLY THR SER GLN THR LYS THR ILE SER ASN VAL THR ALA ALA LEU GLY CYS

PRO SER ASN THR LYS VAL ASP ARG GLU PRO LYS CYS

• Molecule 3: PGT122 Fab heavy chain

Chain P:  7% 53% 44%



LEU GLY CYS LEU VAL LYS ASP THR PHE PRO GLU PRO VAL THR VAL TRP ASN SER GLY ALA LEU THR SER GLY VAL HIS THR PHE PRO VAL LEU GLN SER SER GLY TYR SER LEU SER THR VAL LYS VAL THR VAL PRO SER PHE SER PRO LEU LEU PRO GLY THR SER GLN THR LYS THR ILE SER ASN VAL THR ALA ALA LEU GLY CYS

VAL ASN HIS LYS PRO SER ASN THR VAL LYS ASP ARG VAL GLU PRO LYS SER CYS

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

Chain D:  50% 100%



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



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



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



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



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



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



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



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



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



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



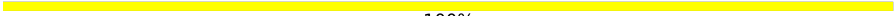
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

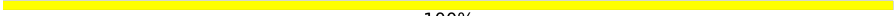


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%

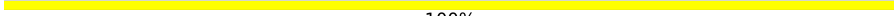
NAG1
NAG2

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

Chain a:  100%

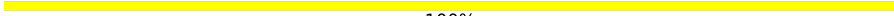
NAG1
NAG2

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

Chain b:  100%

NAG1
NAG2

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

Chain d:  100%

NAG1
NAG2

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

Chain e:  50% 100%

♦
NAG1
NAG2

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

Chain f:  50% 100%

♦
NAG1
NAG2

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

Chain g:  100%



NAG1
NAG2

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




NAG1
NAG2

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




NAG1
NAG2

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




NAG1
NAG2

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




NAG1
NAG2

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




NAG1
NAG2

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



MAG1
MAG2

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



MAG1
MAG2

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



MAG1
MAG2

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



MAG1
MAG2

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



MAG1
MAG2

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



MAG1
MAG2

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





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



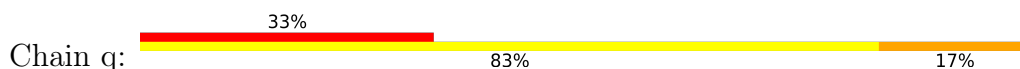
- Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 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 5: 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 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





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



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



- Molecule 7: 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 7: 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 7: 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



MAG1	MAG2	MAG3	MAG4	MAG5	MAG6
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	132156	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.061	Depositor
Minimum map value	-1.453	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.144	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	226.59999, 226.59999, 226.59999	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.12	1/4318 (0.0%)	1.21	42/5859 (0.7%)
1	B	1.14	2/4318 (0.0%)	1.22	44/5859 (0.8%)
1	C	1.14	2/4318 (0.0%)	1.21	36/5859 (0.6%)
2	L	1.12	2/854 (0.2%)	1.30	9/1169 (0.8%)
2	M	1.14	1/854 (0.1%)	1.26	10/1169 (0.9%)
2	O	1.13	1/854 (0.1%)	1.28	9/1169 (0.8%)
3	H	1.04	0/1070	1.16	4/1457 (0.3%)
3	N	1.02	0/1070	1.14	4/1457 (0.3%)
3	P	1.04	0/1070	1.16	7/1457 (0.5%)
All	All	1.12	9/18726 (0.0%)	1.21	165/25455 (0.6%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	247	CYS	CB-SG	-6.70	1.59	1.81
1	B	247	CYS	CB-SG	-6.67	1.59	1.81
2	L	89	HIS	CB-CG	-6.12	1.41	1.50
1	C	427	TRP	NE1-CE2	-5.90	1.30	1.37
2	M	88	CYS	CB-SG	-5.87	1.61	1.81
1	B	427	TRP	NE1-CE2	-5.79	1.31	1.37
2	L	91	TRP	NE1-CE2	-5.61	1.31	1.37
2	O	89	HIS	CB-CG	-5.45	1.42	1.50
1	A	427	TRP	NE1-CE2	-5.21	1.31	1.37

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	VAL	CA-C-N	8.21	128.16	120.03
1	A	75	VAL	C-N-CA	8.21	128.16	120.03
1	C	75	VAL	CA-C-N	8.09	128.04	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	75	VAL	C-N-CA	8.09	128.04	120.03
1	B	75	VAL	CA-C-N	8.05	128.00	120.03
1	B	75	VAL	C-N-CA	8.05	128.00	120.03
1	C	219	ALA	CA-C-N	7.36	127.81	120.52
1	C	219	ALA	C-N-CA	7.36	127.81	120.52
1	C	298	ARG	CA-C-N	7.36	127.52	119.87
1	C	298	ARG	C-N-CA	7.36	127.52	119.87
1	A	120	VAL	N-CA-C	7.32	119.25	109.37
1	A	298	ARG	CA-C-N	7.30	127.46	119.87
1	A	298	ARG	C-N-CA	7.30	127.46	119.87
1	B	120	VAL	N-CA-C	7.26	119.17	109.37
1	B	298	ARG	CA-C-N	7.24	127.40	119.87
1	B	298	ARG	C-N-CA	7.24	127.40	119.87
1	C	120	VAL	N-CA-C	7.24	119.14	109.37
1	B	219	ALA	CA-C-N	7.23	127.68	120.52
1	B	219	ALA	C-N-CA	7.23	127.68	120.52
2	O	58	ILE	CA-C-N	7.05	127.01	120.03
2	O	58	ILE	C-N-CA	7.05	127.01	120.03
1	A	219	ALA	CA-C-N	7.00	127.45	120.52
1	A	219	ALA	C-N-CA	7.00	127.45	120.52
2	L	58	ILE	CA-C-N	6.98	126.94	120.03
2	L	58	ILE	C-N-CA	6.98	126.94	120.03
2	M	58	ILE	CA-C-N	6.96	126.92	120.03
2	M	58	ILE	C-N-CA	6.96	126.92	120.03
1	A	205	CYS	CA-C-N	6.95	126.65	119.56
1	A	205	CYS	C-N-CA	6.95	126.65	119.56
3	N	8	GLY	CA-C-N	6.86	126.49	119.56
3	N	8	GLY	C-N-CA	6.86	126.49	119.56
1	B	205	CYS	CA-C-N	6.84	126.54	119.56
1	B	205	CYS	C-N-CA	6.84	126.54	119.56
1	B	437	PRO	N-CA-C	-6.80	103.30	110.58
3	H	8	GLY	CA-C-N	6.78	126.40	119.56
3	H	8	GLY	C-N-CA	6.78	126.40	119.56
1	C	205	CYS	CA-C-N	6.75	126.44	119.56
1	C	205	CYS	C-N-CA	6.75	126.44	119.56
3	P	8	GLY	CA-C-N	6.71	126.34	119.56
3	P	8	GLY	C-N-CA	6.71	126.34	119.56
2	M	90	ILE	N-CA-C	6.70	117.55	108.17
1	C	437	PRO	N-CA-C	-6.69	103.42	110.58
1	A	362	ASN	CA-C-N	6.59	126.97	119.92
1	A	362	ASN	C-N-CA	6.59	126.97	119.92
1	C	362	ASN	CA-C-N	6.58	126.96	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	362	ASN	C-N-CA	6.58	126.96	119.92
1	B	362	ASN	CA-C-N	6.54	126.92	119.92
1	B	362	ASN	C-N-CA	6.54	126.92	119.92
1	B	492	GLU	CA-C-N	6.41	126.53	119.87
1	B	492	GLU	C-N-CA	6.41	126.53	119.87
1	A	437	PRO	N-CA-C	-6.35	103.78	110.58
1	C	492	GLU	CA-C-N	6.31	126.43	119.87
1	C	492	GLU	C-N-CA	6.31	126.43	119.87
1	A	492	GLU	CA-C-N	6.31	126.43	119.87
1	A	492	GLU	C-N-CA	6.31	126.43	119.87
1	A	135	ASN	CA-C-N	-6.23	116.79	123.08
1	A	135	ASN	C-N-CA	-6.23	116.79	123.08
1	A	191	TYR	N-CA-C	6.23	119.17	109.52
1	C	191	TYR	N-CA-C	6.10	118.97	109.52
2	L	65	SER	CA-C-N	6.04	126.01	120.03
2	L	65	SER	C-N-CA	6.04	126.01	120.03
2	L	54	ARG	CA-C-N	6.03	126.00	120.03
2	L	54	ARG	C-N-CA	6.03	126.00	120.03
1	B	135	ASN	CA-C-N	-6.00	117.02	123.08
1	B	135	ASN	C-N-CA	-6.00	117.02	123.08
1	A	436	ALA	CA-C-N	5.96	123.95	119.66
1	A	436	ALA	C-N-CA	5.96	123.95	119.66
2	L	90	ILE	N-CA-C	5.95	116.43	107.80
2	O	65	SER	CA-C-N	5.94	125.85	119.85
2	O	65	SER	C-N-CA	5.94	125.85	119.85
3	H	67	VAL	N-CA-C	5.93	116.48	108.17
1	C	80	ASN	CA-C-N	5.92	125.86	119.76
1	C	80	ASN	C-N-CA	5.92	125.86	119.76
2	O	54	ARG	CA-C-N	5.92	125.89	120.03
2	O	54	ARG	C-N-CA	5.92	125.89	120.03
1	A	257	THR	N-CA-C	5.91	121.53	113.97
1	B	80	ASN	CA-C-N	5.91	125.84	119.76
1	B	80	ASN	C-N-CA	5.91	125.84	119.76
1	B	257	THR	N-CA-C	5.88	121.50	113.97
1	C	257	THR	N-CA-C	5.87	121.48	113.97
1	C	436	ALA	CA-C-N	5.85	123.87	119.66
1	C	436	ALA	C-N-CA	5.85	123.87	119.66
1	B	436	ALA	CA-C-N	5.82	123.85	119.66
1	B	436	ALA	C-N-CA	5.82	123.85	119.66
2	M	65	SER	CA-C-N	5.81	125.72	119.85
2	M	65	SER	C-N-CA	5.81	125.72	119.85
1	B	191	TYR	N-CA-C	5.79	118.50	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	194	ILE	N-CA-C	5.76	118.25	111.05
1	A	349	LEU	N-CA-C	-5.72	105.40	112.90
1	A	80	ASN	CA-C-N	5.72	125.63	119.85
1	A	80	ASN	C-N-CA	5.72	125.63	119.85
2	O	43	ALA	CA-C-N	5.72	125.69	120.03
2	O	43	ALA	C-N-CA	5.72	125.69	120.03
1	C	349	LEU	N-CA-C	-5.71	105.43	112.90
1	B	247	CYS	N-CA-C	5.70	116.92	108.60
1	B	194	ILE	N-CA-C	5.69	118.16	111.05
1	C	247	CYS	N-CA-C	5.69	116.91	108.60
1	A	383	PHE	CA-CB-CG	5.67	119.47	113.80
2	M	54	ARG	CA-C-N	5.65	125.85	120.31
2	M	54	ARG	C-N-CA	5.65	125.85	120.31
1	B	383	PHE	CA-CB-CG	5.64	119.44	113.80
1	B	349	LEU	N-CA-C	-5.60	105.57	112.90
1	C	383	PHE	CA-CB-CG	5.57	119.37	113.80
1	A	194	ILE	N-CA-C	5.56	118.00	111.05
2	M	43	ALA	CA-C-N	5.56	125.53	120.03
2	M	43	ALA	C-N-CA	5.56	125.53	120.03
1	C	78	ASP	CA-C-N	5.50	125.17	119.56
1	C	78	ASP	C-N-CA	5.50	125.17	119.56
1	C	432	GLN	CA-C-N	5.50	125.40	119.85
1	C	432	GLN	C-N-CA	5.50	125.40	119.85
1	B	78	ASP	CA-C-N	5.47	125.14	119.56
1	B	78	ASP	C-N-CA	5.47	125.14	119.56
1	B	432	GLN	CA-C-N	5.46	125.36	119.85
1	B	432	GLN	C-N-CA	5.46	125.36	119.85
1	B	54	CYS	CB-CA-C	-5.45	98.92	109.76
1	A	365	SER	N-CA-C	5.44	119.64	112.89
1	C	54	CYS	CB-CA-C	-5.43	98.95	109.76
1	A	432	GLN	CA-C-N	5.43	125.33	119.85
1	A	432	GLN	C-N-CA	5.43	125.33	119.85
3	H	40	PRO	N-CA-C	-5.41	102.70	111.14
1	B	608	VAL	CA-C-N	5.41	125.31	119.85
1	B	608	VAL	C-N-CA	5.41	125.31	119.85
3	P	44	GLN	CA-C-N	5.40	125.35	119.78
3	P	44	GLN	C-N-CA	5.40	125.35	119.78
2	L	43	ALA	CA-C-N	5.38	125.36	120.03
2	L	43	ALA	C-N-CA	5.38	125.36	120.03
1	A	54	CYS	CB-CA-C	-5.35	99.12	109.76
1	C	312	GLY	CA-C-N	5.34	126.51	119.84
1	C	312	GLY	C-N-CA	5.34	126.51	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	365	SER	N-CA-C	5.33	119.50	112.89
1	A	312	GLY	CA-C-N	5.29	126.46	119.84
1	A	312	GLY	C-N-CA	5.29	126.46	119.84
1	B	75	VAL	N-CA-C	5.29	120.30	108.88
1	B	237	GLY	CA-C-N	5.28	125.04	119.76
1	B	237	GLY	C-N-CA	5.28	125.04	119.76
1	C	75	VAL	N-CA-C	5.26	120.25	108.88
1	B	312	GLY	CA-C-N	5.26	126.42	119.84
1	B	312	GLY	C-N-CA	5.26	126.42	119.84
1	B	437	PRO	CA-C-N	5.24	125.14	119.85
1	B	437	PRO	C-N-CA	5.24	125.14	119.85
1	A	503	ARG	NE-CZ-NH2	-5.23	114.49	119.20
1	B	503	ARG	NE-CZ-NH2	-5.22	114.50	119.20
2	M	39	ARG	N-CA-C	-5.21	103.46	109.93
1	A	78	ASP	CA-C-N	5.20	124.81	119.56
1	A	78	ASP	C-N-CA	5.20	124.81	119.56
1	A	75	VAL	N-CA-C	5.19	120.10	108.88
1	C	608	VAL	CA-C-N	5.18	125.08	119.85
1	C	608	VAL	C-N-CA	5.18	125.08	119.85
1	A	437	PRO	CA-C-N	5.16	125.06	119.85
1	A	437	PRO	C-N-CA	5.16	125.06	119.85
3	P	39	GLN	CA-C-N	5.12	125.05	119.78
3	P	39	GLN	C-N-CA	5.12	125.05	119.78
1	B	365	SER	N-CA-C	5.11	118.78	112.54
3	N	39	GLN	CA-C-N	5.11	125.04	119.78
3	N	39	GLN	C-N-CA	5.11	125.04	119.78
3	P	79	SER	N-CA-C	5.11	117.22	108.90
2	O	31	ARG	N-CA-C	5.09	117.41	109.52
1	B	443	ILE	N-CA-C	5.09	115.23	108.11
1	A	237	GLY	CA-C-N	5.08	124.84	119.76
1	A	237	GLY	C-N-CA	5.08	124.84	119.76
1	A	608	VAL	CA-C-N	5.07	124.97	119.85
1	A	608	VAL	C-N-CA	5.07	124.97	119.85
1	B	134	VAL	N-CA-C	5.02	117.32	111.05
1	A	469	ARG	NE-CZ-NH2	-5.01	114.69	119.20
1	C	134	VAL	N-CA-C	5.00	117.31	111.05

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	4232	0	4167	14	0
1	B	4232	0	4167	11	0
1	C	4232	0	4167	14	0
2	L	832	0	786	2	0
2	M	832	0	786	1	0
2	O	832	0	786	1	0
3	H	1041	0	1021	2	0
3	N	1041	0	1021	3	0
3	P	1041	0	1021	3	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	I	28	0	25	0	0
4	K	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	U	28	0	25	0	0
4	V	28	0	25	0	0
4	X	28	0	25	0	0
4	Y	28	0	25	0	0
4	Z	28	0	25	0	0
4	a	28	0	25	0	0
4	b	28	0	25	0	0
4	d	28	0	25	0	0
4	e	28	0	25	0	0
4	f	28	0	25	0	0
4	g	28	0	25	0	0
4	i	28	0	25	0	0
4	j	28	0	25	0	0
4	l	28	0	25	0	0
4	m	28	0	25	0	0
4	n	28	0	25	0	0
4	o	28	0	25	0	0
4	p	28	0	25	0	0
4	r	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	s	28	0	25	0	0
4	t	28	0	25	0	0
4	u	28	0	25	0	0
4	w	28	0	25	0	0
4	x	28	0	25	0	0
5	J	72	0	61	0	0
5	c	72	0	61	0	0
5	q	72	0	61	1	0
6	T	105	0	88	1	0
6	h	105	0	88	0	0
6	v	105	0	88	2	0
7	W	72	0	61	1	0
7	k	72	0	61	0	0
7	y	72	0	61	0	0
8	A	70	0	65	0	0
8	B	70	0	65	0	0
8	C	70	0	65	1	0
All	All	20196	0	19572	57	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 1.

All (57) 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:B:545:LEU:O	1:B:546:SER:C	2.48	0.57
1:C:545:LEU:O	1:C:546:SER:C	2.46	0.56
1:A:545:LEU:O	1:A:546:SER:C	2.51	0.54
8:C:704:NAG:O6	8:C:704:NAG:O4	2.25	0.54
1:C:138:ASN:C	1:C:138:ASN:OD1	2.51	0.52
1:C:167:ASP:OD2	1:C:168:LYS:NZ	2.42	0.52
1:A:167:ASP:OD2	1:A:168:LYS:NZ	2.42	0.52
1:B:138:ASN:OD1	1:B:138:ASN:C	2.53	0.51
3:P:52:HIS:CG	3:P:53:ASP:H	2.29	0.51
3:N:52:HIS:CG	3:N:53:ASP:H	2.29	0.50
3:P:52:HIS:CG	3:P:53:ASP:N	2.80	0.50
3:H:52:HIS:CG	3:H:53:ASP:H	2.29	0.50
1:B:167:ASP:OD2	1:B:168:LYS:NZ	2.44	0.50
1:C:490:LYS:NZ	1:C:492:GLU:OE2	2.44	0.49
3:N:52:HIS:CG	3:N:53:ASP:N	2.80	0.49
1:A:490:LYS:NZ	1:A:492:GLU:OE2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:52:HIS:CG	3:H:53:ASP:N	2.81	0.48
1:C:123:THR:N	1:C:124:PRO:CD	2.76	0.48
1:A:123:THR:N	1:A:124:PRO:CD	2.76	0.48
1:B:123:THR:N	1:B:124:PRO:CD	2.76	0.48
5:q:4:MAN:O6	5:q:4:MAN:O4	2.31	0.47
1:B:377:ASN:OD1	1:B:377:ASN:C	2.58	0.47
6:T:9:MAN:O6	6:T:9:MAN:O4	2.27	0.46
1:A:138:ASN:OD1	1:A:138:ASN:C	2.58	0.46
1:B:197:ASN:OD1	1:B:197:ASN:N	2.49	0.46
1:C:457:ASP:O	1:C:458:GLY:C	2.59	0.46
1:B:457:ASP:O	1:B:458:GLY:C	2.59	0.46
1:A:396:ILE:O	1:A:397:GLY:C	2.60	0.45
1:A:457:ASP:O	1:A:458:GLY:C	2.59	0.45
1:C:218:CYS:HA	1:C:247:CYS:HB3	1.99	0.45
1:A:377:ASN:OD1	1:A:377:ASN:C	2.59	0.45
1:B:218:CYS:HA	1:B:247:CYS:HB3	1.99	0.45
1:C:37:THR:OG1	1:C:499:THR:OG1	2.20	0.45
7:W:6:MAN:O6	7:W:6:MAN:O4	2.31	0.44
3:P:72:ASP:C	3:P:72:ASP:OD1	2.62	0.43
1:C:377:ASN:OD1	1:C:377:ASN:C	2.62	0.43
1:C:396:ILE:O	1:C:397:GLY:C	2.61	0.42
1:A:637:ASN:OD1	1:A:637:ASN:N	2.47	0.42
2:L:25:GLU:OE1	2:L:25:GLU:N	2.51	0.42
1:A:50:THR:OG1	1:A:51:THR:N	2.51	0.42
1:C:50:THR:OG1	1:C:51:THR:N	2.50	0.42
1:B:396:ILE:O	1:B:397:GLY:C	2.60	0.42
3:N:72:ASP:OD1	3:N:72:ASP:C	2.62	0.42
1:A:57:ASP:OD1	1:A:57:ASP:C	2.62	0.42
1:A:199:SER:OG	1:A:200:ALA:N	2.52	0.42
1:C:199:SER:OG	1:C:200:ALA:N	2.52	0.42
1:B:57:ASP:OD1	1:B:57:ASP:C	2.62	0.41
1:A:135:ASN:OD1	1:A:135:ASN:N	2.52	0.41
2:L:67(B):THR:OG1	2:L:67(C):PHE:N	2.53	0.41
6:v:8:MAN:O6	6:v:8:MAN:O4	2.34	0.41
6:v:9:MAN:O6	6:v:9:MAN:O4	2.30	0.41
1:C:197:ASN:OD1	1:C:197:ASN:N	2.50	0.41
1:A:117:LYS:N	1:A:118:PRO:CD	2.84	0.40
2:O:67(B):THR:OG1	2:O:67(C):PHE:N	2.53	0.40
1:C:117:LYS:N	1:C:118:PRO:CD	2.84	0.40
1:B:199:SER:OG	1:B:200:ALA:N	2.54	0.40
2:M:67(B):THR:OG1	2:M:67(C):PHE:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/658 (79%)	512 (99%)	6 (1%)	0	100	100
1	B	518/658 (79%)	512 (99%)	6 (1%)	0	100	100
1	C	518/658 (79%)	513 (99%)	5 (1%)	0	100	100
2	L	107/213 (50%)	106 (99%)	1 (1%)	0	100	100
2	M	107/213 (50%)	106 (99%)	1 (1%)	0	100	100
2	O	107/213 (50%)	106 (99%)	1 (1%)	0	100	100
3	H	129/235 (55%)	129 (100%)	0	0	100	100
3	N	129/235 (55%)	129 (100%)	0	0	100	100
3	P	129/235 (55%)	129 (100%)	0	0	100	100
All	All	2262/3318 (68%)	2242 (99%)	20 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	478/571 (84%)	478 (100%)	0	100	100
1	B	478/571 (84%)	477 (100%)	1 (0%)	87	84
1	C	478/571 (84%)	477 (100%)	1 (0%)	87	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	91/181 (50%)	91 (100%)	0	100	100
2	M	91/181 (50%)	91 (100%)	0	100	100
2	O	91/181 (50%)	91 (100%)	0	100	100
3	H	115/205 (56%)	115 (100%)	0	100	100
3	N	115/205 (56%)	115 (100%)	0	100	100
3	P	115/205 (56%)	115 (100%)	0	100	100
All	All	2052/2871 (72%)	2050 (100%)	2 (0%)	87	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	138	ASN
1	C	138	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	ASN
1	A	432	GLN
1	B	92	ASN
1	B	422	GLN
1	B	425	ASN
1	B	432	GLN
1	C	92	ASN
1	C	422	GLN
1	C	425	ASN
1	C	432	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

129 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
4	NAG	D	1	4,1	14,14,15	1.03	1 (7%)	17,19,21	0.87	0
4	NAG	D	2	4	14,14,15	0.72	1 (7%)	17,19,21	0.85	1 (5%)
4	NAG	E	1	4,1	14,14,15	0.93	1 (7%)	17,19,21	1.50	4 (23%)
4	NAG	E	2	4	14,14,15	0.93	1 (7%)	17,19,21	0.71	0
4	NAG	F	1	4,1	14,14,15	0.98	1 (7%)	17,19,21	1.02	1 (5%)
4	NAG	F	2	4	14,14,15	0.72	1 (7%)	17,19,21	0.83	1 (5%)
4	NAG	G	1	4,1	14,14,15	0.98	1 (7%)	17,19,21	0.78	0
4	NAG	G	2	4	14,14,15	0.68	0	17,19,21	0.92	1 (5%)
4	NAG	I	1	4,1	14,14,15	1.11	1 (7%)	17,19,21	1.83	5 (29%)
4	NAG	I	2	4	14,14,15	0.92	1 (7%)	17,19,21	0.74	0
5	NAG	J	1	1,5	14,14,15	1.00	1 (7%)	17,19,21	0.76	0
5	NAG	J	2	5	14,14,15	0.66	0	17,19,21	1.10	1 (5%)
5	BMA	J	3	5	11,11,12	0.51	0	15,15,17	0.79	1 (6%)
5	MAN	J	4	5	11,11,12	0.57	0	15,15,17	0.93	1 (6%)
5	MAN	J	5	5	11,11,12	0.59	0	15,15,17	0.79	1 (6%)
5	MAN	J	6	5	11,11,12	0.69	0	15,15,17	0.76	1 (6%)
4	NAG	K	1	4,1	14,14,15	0.88	1 (7%)	17,19,21	0.86	0
4	NAG	K	2	4	14,14,15	0.61	0	17,19,21	0.90	1 (5%)
4	NAG	Q	1	4,1	14,14,15	1.15	1 (7%)	17,19,21	0.91	0
4	NAG	Q	2	4	14,14,15	0.77	1 (7%)	17,19,21	0.68	0
4	NAG	R	1	4,1	14,14,15	1.03	1 (7%)	17,19,21	1.11	2 (11%)
4	NAG	R	2	4	14,14,15	0.72	1 (7%)	17,19,21	0.93	1 (5%)
4	NAG	S	1	4,1	14,14,15	0.82	1 (7%)	17,19,21	0.91	0
4	NAG	S	2	4	14,14,15	0.72	1 (7%)	17,19,21	0.87	1 (5%)
6	NAG	T	1	1,6	14,14,15	0.77	1 (7%)	17,19,21	1.11	3 (17%)
6	NAG	T	2	6	14,14,15	0.69	0	17,19,21	1.35	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	T	3	6	11,11,12	0.44	0	15,15,17	1.04	1 (6%)
6	MAN	T	4	6	11,11,12	0.47	0	15,15,17	0.75	0
6	MAN	T	5	6	11,11,12	0.57	0	15,15,17	1.15	1 (6%)
6	MAN	T	6	6	11,11,12	0.60	0	15,15,17	0.74	1 (6%)
6	MAN	T	7	6	11,11,12	0.59	0	15,15,17	0.75	1 (6%)
6	MAN	T	8	6	11,11,12	0.61	0	15,15,17	0.81	1 (6%)
6	MAN	T	9	6	11,11,12	0.63	0	15,15,17	0.83	1 (6%)
4	NAG	U	1	4,1	14,14,15	0.98	1 (7%)	17,19,21	1.16	1 (5%)
4	NAG	U	2	4	14,14,15	0.71	1 (7%)	17,19,21	0.93	1 (5%)
4	NAG	V	1	4,1	14,14,15	1.01	1 (7%)	17,19,21	0.93	0
4	NAG	V	2	4	14,14,15	0.78	1 (7%)	17,19,21	0.72	1 (5%)
7	NAG	W	1	1,7	14,14,15	0.97	1 (7%)	17,19,21	0.76	1 (5%)
7	NAG	W	2	7	14,14,15	0.72	1 (7%)	17,19,21	1.01	2 (11%)
7	BMA	W	3	7	11,11,12	0.51	0	15,15,17	0.78	1 (6%)
7	MAN	W	4	7	11,11,12	0.64	0	15,15,17	0.82	0
7	MAN	W	5	7	11,11,12	0.53	0	15,15,17	0.91	1 (6%)
7	MAN	W	6	7	11,11,12	0.57	0	15,15,17	0.90	1 (6%)
4	NAG	X	1	4,1	14,14,15	1.02	1 (7%)	17,19,21	0.90	0
4	NAG	X	2	4	14,14,15	0.70	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	Y	1	4,1	14,14,15	0.97	1 (7%)	17,19,21	1.56	5 (29%)
4	NAG	Y	2	4	14,14,15	1.00	1 (7%)	17,19,21	0.71	0
4	NAG	Z	1	4,1	14,14,15	0.97	1 (7%)	17,19,21	0.97	0
4	NAG	Z	2	4	14,14,15	0.71	1 (7%)	17,19,21	0.85	1 (5%)
4	NAG	a	1	4,1	14,14,15	0.98	1 (7%)	17,19,21	0.78	0
4	NAG	a	2	4	14,14,15	0.68	0	17,19,21	0.92	1 (5%)
4	NAG	b	1	4,1	14,14,15	0.95	1 (7%)	17,19,21	1.56	3 (17%)
4	NAG	b	2	4	14,14,15	0.93	1 (7%)	17,19,21	0.80	1 (5%)
5	NAG	c	1	1,5	14,14,15	1.00	1 (7%)	17,19,21	0.73	0
5	NAG	c	2	5	14,14,15	0.66	0	17,19,21	1.10	1 (5%)
5	BMA	c	3	5	11,11,12	0.52	0	15,15,17	0.79	1 (6%)
5	MAN	c	4	5	11,11,12	0.56	0	15,15,17	0.93	1 (6%)
5	MAN	c	5	5	11,11,12	0.58	0	15,15,17	0.79	1 (6%)
5	MAN	c	6	5	11,11,12	0.70	0	15,15,17	0.75	1 (6%)
4	NAG	d	1	4,1	14,14,15	0.88	1 (7%)	17,19,21	0.85	0
4	NAG	d	2	4	14,14,15	0.62	0	17,19,21	0.90	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	e	1	4,1	14,14,15	1.14	1 (7%)	17,19,21	0.90	0
4	NAG	e	2	4	14,14,15	0.77	1 (7%)	17,19,21	0.68	0
4	NAG	f	1	4,1	14,14,15	1.04	1 (7%)	17,19,21	1.13	2 (11%)
4	NAG	f	2	4	14,14,15	0.71	1 (7%)	17,19,21	0.94	1 (5%)
4	NAG	g	1	4,1	14,14,15	0.82	1 (7%)	17,19,21	0.91	0
4	NAG	g	2	4	14,14,15	0.71	1 (7%)	17,19,21	0.86	1 (5%)
6	NAG	h	1	1,6	14,14,15	0.76	1 (7%)	17,19,21	1.10	3 (17%)
6	NAG	h	2	6	14,14,15	0.71	0	17,19,21	1.33	3 (17%)
6	BMA	h	3	6	11,11,12	0.40	0	15,15,17	1.00	1 (6%)
6	MAN	h	4	6	11,11,12	0.46	0	15,15,17	0.76	0
6	MAN	h	5	6	11,11,12	0.58	0	15,15,17	1.05	1 (6%)
6	MAN	h	6	6	11,11,12	0.61	0	15,15,17	0.85	1 (6%)
6	MAN	h	7	6	11,11,12	0.57	0	15,15,17	0.84	1 (6%)
6	MAN	h	8	6	11,11,12	0.59	0	15,15,17	0.78	1 (6%)
6	MAN	h	9	6	11,11,12	0.64	0	15,15,17	0.95	1 (6%)
4	NAG	i	1	4,1	14,14,15	0.95	1 (7%)	17,19,21	1.20	1 (5%)
4	NAG	i	2	4	14,14,15	0.70	1 (7%)	17,19,21	0.92	1 (5%)
4	NAG	j	1	4,1	14,14,15	1.03	1 (7%)	17,19,21	0.94	0
4	NAG	j	2	4	14,14,15	0.77	1 (7%)	17,19,21	0.73	1 (5%)
7	NAG	k	1	1,7	14,14,15	1.00	1 (7%)	17,19,21	0.70	0
7	NAG	k	2	7	14,14,15	0.67	0	17,19,21	0.99	2 (11%)
7	BMA	k	3	7	11,11,12	0.49	0	15,15,17	0.81	1 (6%)
7	MAN	k	4	7	11,11,12	0.64	0	15,15,17	1.00	0
7	MAN	k	5	7	11,11,12	0.57	0	15,15,17	0.84	1 (6%)
7	MAN	k	6	7	11,11,12	0.56	0	15,15,17	0.89	1 (6%)
4	NAG	l	1	4,1	14,14,15	1.01	1 (7%)	17,19,21	0.90	0
4	NAG	l	2	4	14,14,15	0.72	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	m	1	4,1	14,14,15	0.94	1 (7%)	17,19,21	1.59	4 (23%)
4	NAG	m	2	4	14,14,15	0.97	1 (7%)	17,19,21	0.70	0
4	NAG	n	1	4,1	14,14,15	0.95	1 (7%)	17,19,21	0.99	1 (5%)
4	NAG	n	2	4	14,14,15	0.70	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	o	1	4,1	14,14,15	0.96	1 (7%)	17,19,21	0.77	0
4	NAG	o	2	4	14,14,15	0.67	0	17,19,21	0.92	1 (5%)
4	NAG	p	1	4,1	14,14,15	1.08	1 (7%)	17,19,21	1.83	5 (29%)
4	NAG	p	2	4	14,14,15	0.93	1 (7%)	17,19,21	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	q	1	1,5	14,14,15	1.00	1 (7%)	17,19,21	0.72	0
5	NAG	q	2	5	14,14,15	0.66	0	17,19,21	1.09	1 (5%)
5	BMA	q	3	5	11,11,12	0.50	0	15,15,17	0.79	1 (6%)
5	MAN	q	4	5	11,11,12	0.56	0	15,15,17	0.93	1 (6%)
5	MAN	q	5	5	11,11,12	0.58	0	15,15,17	0.79	1 (6%)
5	MAN	q	6	5	11,11,12	0.70	0	15,15,17	0.76	1 (6%)
4	NAG	r	1	4,1	14,14,15	0.88	1 (7%)	17,19,21	0.84	0
4	NAG	r	2	4	14,14,15	0.62	0	17,19,21	0.90	1 (5%)
4	NAG	s	1	4,1	14,14,15	1.14	1 (7%)	17,19,21	0.90	0
4	NAG	s	2	4	14,14,15	0.79	1 (7%)	17,19,21	0.67	0
4	NAG	t	1	4,1	14,14,15	1.03	1 (7%)	17,19,21	1.12	2 (11%)
4	NAG	t	2	4	14,14,15	0.70	0	17,19,21	0.94	1 (5%)
4	NAG	u	1	4,1	14,14,15	0.83	1 (7%)	17,19,21	0.90	0
4	NAG	u	2	4	14,14,15	0.72	1 (7%)	17,19,21	0.86	1 (5%)
6	NAG	v	1	1,6	14,14,15	0.76	1 (7%)	17,19,21	1.10	2 (11%)
6	NAG	v	2	6	14,14,15	0.64	0	17,19,21	1.32	1 (5%)
6	BMA	v	3	6	11,11,12	0.42	0	15,15,17	1.09	1 (6%)
6	MAN	v	4	6	11,11,12	0.49	0	15,15,17	0.70	0
6	MAN	v	5	6	11,11,12	0.57	0	15,15,17	1.08	1 (6%)
6	MAN	v	6	6	11,11,12	0.61	0	15,15,17	0.72	1 (6%)
6	MAN	v	7	6	11,11,12	0.58	0	15,15,17	0.78	1 (6%)
6	MAN	v	8	6	11,11,12	0.61	0	15,15,17	0.79	1 (6%)
6	MAN	v	9	6	11,11,12	0.74	0	15,15,17	0.78	0
4	NAG	w	1	4,1	14,14,15	0.99	1 (7%)	17,19,21	1.16	1 (5%)
4	NAG	w	2	4	14,14,15	0.70	1 (7%)	17,19,21	0.96	1 (5%)
4	NAG	x	1	4,1	14,14,15	1.03	1 (7%)	17,19,21	0.93	0
4	NAG	x	2	4	14,14,15	0.78	1 (7%)	17,19,21	0.72	1 (5%)
7	NAG	y	1	1,7	14,14,15	1.04	1 (7%)	17,19,21	0.63	0
7	NAG	y	2	7	14,14,15	0.63	0	17,19,21	0.97	1 (5%)
7	BMA	y	3	7	11,11,12	0.51	0	15,15,17	0.81	1 (6%)
7	MAN	y	4	7	11,11,12	0.60	0	15,15,17	0.93	0
7	MAN	y	5	7	11,11,12	0.56	0	15,15,17	0.85	1 (6%)
7	MAN	y	6	7	11,11,12	0.58	0	15,15,17	0.90	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

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

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

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

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

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	1	NAG	C1-C2	3.98	1.57	1.52
4	s	1	NAG	C1-C2	3.93	1.57	1.52
4	e	1	NAG	C1-C2	3.90	1.57	1.52
4	D	1	NAG	C1-C2	3.68	1.57	1.52
4	X	1	NAG	C1-C2	3.65	1.57	1.52
4	l	1	NAG	C1-C2	3.61	1.57	1.52
7	y	1	NAG	C1-C2	3.55	1.57	1.52
4	w	1	NAG	C1-C2	3.47	1.57	1.52
4	x	1	NAG	C1-C2	3.46	1.57	1.52
4	U	1	NAG	C1-C2	3.45	1.57	1.52
4	j	1	NAG	C1-C2	3.44	1.57	1.52
4	V	1	NAG	C1-C2	3.37	1.56	1.52
4	i	1	NAG	C1-C2	3.34	1.56	1.52
4	Y	2	NAG	C1-C2	3.33	1.56	1.52
5	q	1	NAG	C1-C2	3.31	1.56	1.52
4	F	1	NAG	C1-C2	3.30	1.56	1.52
4	G	1	NAG	C1-C2	3.28	1.56	1.52
7	k	1	NAG	C1-C2	3.28	1.56	1.52
4	a	1	NAG	C1-C2	3.27	1.56	1.52
5	J	1	NAG	C1-C2	3.27	1.56	1.52
5	c	1	NAG	C1-C2	3.27	1.56	1.52
4	f	1	NAG	C1-C2	3.26	1.56	1.52
4	Z	1	NAG	C1-C2	3.24	1.56	1.52
4	m	2	NAG	C1-C2	3.23	1.56	1.52
4	o	1	NAG	C1-C2	3.22	1.56	1.52
4	R	1	NAG	C1-C2	3.22	1.56	1.52
4	n	1	NAG	C1-C2	3.21	1.56	1.52
4	t	1	NAG	C1-C2	3.20	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	W	1	NAG	C1-C2	3.14	1.56	1.52
4	p	2	NAG	C1-C2	3.12	1.56	1.52
4	I	2	NAG	C1-C2	3.10	1.56	1.52
4	b	2	NAG	C1-C2	3.10	1.56	1.52
4	I	1	NAG	C1-C2	3.09	1.56	1.52
4	E	2	NAG	C1-C2	3.04	1.56	1.52
4	r	1	NAG	C1-C2	3.02	1.56	1.52
4	d	1	NAG	C1-C2	3.01	1.56	1.52
4	p	1	NAG	C1-C2	3.00	1.56	1.52
4	K	1	NAG	C1-C2	2.99	1.56	1.52
4	u	1	NAG	C1-C2	2.77	1.56	1.52
4	Y	1	NAG	C1-C2	2.73	1.56	1.52
4	g	1	NAG	C1-C2	2.72	1.56	1.52
4	S	1	NAG	C1-C2	2.71	1.56	1.52
4	b	1	NAG	C1-C2	2.61	1.55	1.52
4	m	1	NAG	C1-C2	2.58	1.55	1.52
4	E	1	NAG	C1-C2	2.57	1.55	1.52
4	x	2	NAG	C1-C2	2.52	1.55	1.52
4	V	2	NAG	C1-C2	2.50	1.55	1.52
4	j	2	NAG	C1-C2	2.48	1.55	1.52
4	s	2	NAG	C1-C2	2.46	1.55	1.52
6	T	1	NAG	C1-C2	2.46	1.55	1.52
6	v	1	NAG	C1-C2	2.43	1.55	1.52
6	h	1	NAG	C1-C2	2.39	1.55	1.52
4	Q	2	NAG	C1-C2	2.39	1.55	1.52
4	e	2	NAG	C1-C2	2.37	1.55	1.52
7	W	2	NAG	C1-C2	2.24	1.55	1.52
4	F	2	NAG	C1-C2	2.16	1.55	1.52
4	Z	2	NAG	C1-C2	2.13	1.55	1.52
4	D	2	NAG	C1-C2	2.12	1.55	1.52
4	n	2	NAG	C1-C2	2.10	1.55	1.52
4	l	2	NAG	C1-C2	2.09	1.55	1.52
4	R	2	NAG	C1-C2	2.06	1.55	1.52
4	f	2	NAG	C1-C2	2.06	1.55	1.52
4	S	2	NAG	C1-C2	2.05	1.55	1.52
4	u	2	NAG	C1-C2	2.04	1.55	1.52
4	X	2	NAG	C1-C2	2.03	1.55	1.52
4	i	2	NAG	C1-C2	2.03	1.55	1.52
4	U	2	NAG	C1-C2	2.03	1.55	1.52
4	w	2	NAG	C1-C2	2.01	1.55	1.52
4	g	2	NAG	C1-C2	2.01	1.55	1.52

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	O4-C4-C3	-4.69	99.33	110.38
4	p	1	NAG	O4-C4-C3	-4.63	99.47	110.38
4	m	1	NAG	C3-C4-C5	-3.79	103.36	110.23
4	b	1	NAG	C3-C4-C5	-3.71	103.50	110.23
4	b	1	NAG	O4-C4-C3	-3.46	102.21	110.38
4	E	1	NAG	C3-C4-C5	-3.45	103.98	110.23
4	Y	1	NAG	C3-C4-C5	-3.37	104.13	110.23
4	p	1	NAG	C3-C4-C5	-3.35	104.15	110.23
4	I	1	NAG	C3-C4-C5	-3.25	104.34	110.23
6	v	3	BMA	C2-C3-C4	-3.14	105.33	110.86
6	T	3	BMA	C2-C3-C4	-3.05	105.50	110.86
4	a	2	NAG	C4-C3-C2	-3.00	106.62	111.02
4	o	2	NAG	C4-C3-C2	-3.00	106.62	111.02
6	h	3	BMA	C2-C3-C4	-2.98	105.62	110.86
4	G	2	NAG	C4-C3-C2	-2.98	106.65	111.02
6	T	5	MAN	C2-C3-C4	-2.90	105.76	110.86
4	w	2	NAG	C4-C3-C2	-2.87	106.81	111.02
4	Y	1	NAG	O4-C4-C3	-2.86	103.64	110.38
4	p	1	NAG	O5-C5-C6	-2.83	102.16	107.66
4	K	2	NAG	C4-C3-C2	-2.81	106.90	111.02
4	r	2	NAG	C4-C3-C2	-2.80	106.92	111.02
6	v	2	NAG	C3-C4-C5	-2.79	105.17	110.23
4	I	1	NAG	O5-C5-C6	-2.79	102.23	107.66
4	d	2	NAG	C4-C3-C2	-2.78	106.94	111.02
4	U	2	NAG	C4-C3-C2	-2.78	106.95	111.02
4	f	2	NAG	C4-C3-C2	-2.77	106.96	111.02
4	t	2	NAG	C4-C3-C2	-2.75	106.98	111.02
4	i	2	NAG	C4-C3-C2	-2.74	107.00	111.02
4	R	2	NAG	C4-C3-C2	-2.72	107.04	111.02
4	f	1	NAG	O4-C4-C3	-2.70	104.00	110.38
5	J	4	MAN	C2-C3-C4	-2.70	106.12	110.86
4	R	1	NAG	O4-C4-C3	-2.69	104.04	110.38
5	q	4	MAN	C2-C3-C4	-2.68	106.14	110.86
5	c	4	MAN	C2-C3-C4	-2.68	106.14	110.86
5	q	3	BMA	C2-C3-C4	-2.68	106.15	110.86
4	t	1	NAG	O4-C4-C3	-2.68	104.07	110.38
7	W	5	MAN	C2-C3-C4	-2.67	106.17	110.86
6	h	9	MAN	C2-C3-C4	-2.66	106.18	110.86
6	v	5	MAN	C2-C3-C4	-2.66	106.18	110.86
5	c	3	BMA	C2-C3-C4	-2.65	106.21	110.86
4	S	2	NAG	C4-C3-C2	-2.64	107.15	111.02
5	J	3	BMA	C2-C3-C4	-2.63	106.23	110.86
4	u	2	NAG	C4-C3-C2	-2.62	107.18	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	g	2	NAG	C4-C3-C2	-2.60	107.21	111.02
6	h	5	MAN	C2-C3-C4	-2.60	106.29	110.86
4	i	1	NAG	C1-O5-C5	-2.59	108.71	112.19
4	Z	2	NAG	C4-C3-C2	-2.59	107.22	111.02
7	y	3	BMA	C2-C3-C4	-2.56	106.36	110.86
7	y	2	NAG	C3-C4-C5	-2.55	105.60	110.23
7	k	3	BMA	C2-C3-C4	-2.55	106.37	110.86
4	n	2	NAG	C4-C3-C2	-2.53	107.31	111.02
4	m	1	NAG	O4-C4-C3	-2.51	104.46	110.38
7	W	3	BMA	C2-C3-C4	-2.50	106.46	110.86
4	t	1	NAG	C3-C4-C5	-2.49	105.71	110.23
4	f	1	NAG	C3-C4-C5	-2.47	105.75	110.23
7	y	6	MAN	C2-C3-C4	-2.47	106.52	110.86
7	y	5	MAN	C2-C3-C4	-2.46	106.53	110.86
4	F	2	NAG	C4-C3-C2	-2.46	107.41	111.02
7	k	6	MAN	C2-C3-C4	-2.44	106.57	110.86
7	W	6	MAN	C2-C3-C4	-2.44	106.58	110.86
4	R	1	NAG	C3-C4-C5	-2.44	105.82	110.23
7	k	2	NAG	C3-C4-C5	-2.43	105.83	110.23
4	l	2	NAG	C4-C3-C2	-2.42	107.47	111.02
7	k	5	MAN	C2-C3-C4	-2.41	106.61	110.86
6	h	2	NAG	C3-C4-C5	-2.41	105.86	110.23
4	U	1	NAG	C1-O5-C5	-2.41	108.95	112.19
4	w	1	NAG	C1-O5-C5	-2.41	108.95	112.19
4	X	2	NAG	C4-C3-C2	-2.41	107.48	111.02
4	D	2	NAG	C4-C3-C2	-2.41	107.49	111.02
5	J	5	MAN	C2-C3-C4	-2.41	106.63	110.86
7	W	2	NAG	C3-C4-C5	-2.39	105.89	110.23
5	q	5	MAN	C2-C3-C4	-2.39	106.66	110.86
4	m	1	NAG	O5-C5-C6	-2.38	103.02	107.66
5	c	5	MAN	C2-C3-C4	-2.37	106.70	110.86
6	h	7	MAN	C2-C3-C4	-2.36	106.71	110.86
4	I	1	NAG	O5-C1-C2	-2.33	107.68	111.29
6	h	6	MAN	C2-C3-C4	-2.32	106.78	110.86
6	v	1	NAG	C1-O5-C5	-2.32	109.08	112.19
4	p	1	NAG	C4-C3-C2	2.32	114.41	111.02
6	T	9	MAN	C2-C3-C4	-2.31	106.80	110.86
6	T	2	NAG	C4-C3-C2	-2.31	107.63	111.02
4	Y	1	NAG	O5-C5-C6	-2.31	103.17	107.66
4	E	1	NAG	C1-O5-C5	-2.29	109.11	112.19
4	b	1	NAG	O5-C5-C6	-2.29	103.21	107.66
6	h	1	NAG	C1-O5-C5	-2.28	109.13	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	1	NAG	C1-O5-C5	-2.28	109.13	112.19
6	T	2	NAG	C6-C5-C4	-2.27	107.44	113.02
6	h	8	MAN	C2-C3-C4	-2.27	106.87	110.86
4	m	1	NAG	C1-O5-C5	-2.25	109.17	112.19
4	E	1	NAG	O5-C5-C6	-2.25	103.28	107.66
4	F	1	NAG	C4-C3-C2	-2.25	107.72	111.02
6	v	8	MAN	C2-C3-C4	-2.22	106.95	110.86
5	J	2	NAG	C4-C3-C2	-2.22	107.77	111.02
6	T	8	MAN	C2-C3-C4	-2.22	106.96	110.86
4	E	1	NAG	O4-C4-C3	-2.21	105.17	110.38
7	W	2	NAG	O4-C4-C3	-2.17	105.25	110.38
5	c	6	MAN	C2-C3-C4	-2.17	107.04	110.86
5	c	2	NAG	C4-C3-C2	-2.16	107.85	111.02
7	W	1	NAG	C3-C4-C5	-2.16	106.31	110.23
4	b	2	NAG	C4-C3-C2	-2.16	107.85	111.02
4	j	2	NAG	C4-C3-C2	-2.16	107.85	111.02
6	T	6	MAN	C2-C3-C4	-2.16	107.06	110.86
5	q	6	MAN	C2-C3-C4	-2.16	107.07	110.86
6	T	2	NAG	C3-C4-C5	-2.15	106.33	110.23
4	I	1	NAG	C4-C3-C2	2.15	114.17	111.02
5	J	6	MAN	C2-C3-C4	-2.15	107.08	110.86
6	T	7	MAN	C2-C3-C4	-2.15	107.09	110.86
6	v	7	MAN	C2-C3-C4	-2.14	107.09	110.86
6	h	2	NAG	O4-C4-C5	-2.14	104.05	109.32
4	Y	1	NAG	C2-N2-C7	-2.14	120.03	122.90
4	V	2	NAG	C4-C3-C2	-2.14	107.89	111.02
6	h	2	NAG	C4-C3-C2	-2.13	107.89	111.02
5	q	2	NAG	C4-C3-C2	-2.13	107.90	111.02
4	x	2	NAG	C4-C3-C2	-2.12	107.91	111.02
6	T	1	NAG	C1-C2-N2	-2.11	107.10	110.43
6	h	1	NAG	C1-C2-N2	-2.09	107.14	110.43
6	T	1	NAG	C3-C4-C5	-2.09	106.45	110.23
4	p	1	NAG	O5-C1-C2	-2.08	108.07	111.29
4	Y	1	NAG	C1-O5-C5	-2.05	109.44	112.19
4	n	1	NAG	C4-C3-C2	-2.04	108.03	111.02
6	h	1	NAG	C3-C4-C5	-2.03	106.55	110.23
7	k	2	NAG	O4-C4-C3	-2.02	105.60	110.38
6	v	1	NAG	C1-C2-N2	-2.02	107.25	110.43
6	v	6	MAN	C2-C3-C4	-2.02	107.31	110.86

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	W	5	MAN	C4-C5-C6-O6
5	c	3	BMA	C4-C5-C6-O6
5	q	3	BMA	C4-C5-C6-O6
5	J	3	BMA	C4-C5-C6-O6
6	h	2	NAG	O5-C5-C6-O6
7	W	5	MAN	O5-C5-C6-O6
7	k	3	BMA	O5-C5-C6-O6
7	y	3	BMA	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
4	o	2	NAG	C4-C5-C6-O6
5	c	3	BMA	O5-C5-C6-O6
6	h	7	MAN	O5-C5-C6-O6
7	W	3	BMA	O5-C5-C6-O6
5	J	3	BMA	O5-C5-C6-O6
5	q	3	BMA	O5-C5-C6-O6
6	v	7	MAN	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
6	T	7	MAN	O5-C5-C6-O6
7	y	3	BMA	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
4	o	2	NAG	O5-C5-C6-O6
7	k	3	BMA	C4-C5-C6-O6
6	T	7	MAN	C4-C5-C6-O6
6	T	9	MAN	O5-C5-C6-O6
6	h	9	MAN	O5-C5-C6-O6
6	h	7	MAN	C4-C5-C6-O6
7	W	3	BMA	C4-C5-C6-O6
4	p	1	NAG	O5-C5-C6-O6
6	h	2	NAG	C4-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
6	v	7	MAN	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	l	1	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	p	1	NAG	C4-C5-C6-O6
4	m	1	NAG	O5-C5-C6-O6
6	h	5	MAN	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	l	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	v	5	MAN	O5-C5-C6-O6
6	T	5	MAN	O5-C5-C6-O6
4	w	2	NAG	O5-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
4	n	2	NAG	O5-C5-C6-O6
5	J	5	MAN	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
5	c	5	MAN	O5-C5-C6-O6
5	q	5	MAN	O5-C5-C6-O6
6	v	9	MAN	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
7	y	5	MAN	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	g	2	NAG	O5-C5-C6-O6
4	u	2	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
6	T	6	MAN	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	b	2	NAG	O5-C5-C6-O6
4	i	2	NAG	O5-C5-C6-O6
6	h	8	MAN	O5-C5-C6-O6
6	v	2	NAG	O5-C5-C6-O6
7	W	6	MAN	O5-C5-C6-O6
6	v	6	MAN	O5-C5-C6-O6
7	k	6	MAN	O5-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
5	J	4	MAN	O5-C5-C6-O6
7	y	6	MAN	O5-C5-C6-O6
5	c	4	MAN	O5-C5-C6-O6
6	v	8	MAN	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	m	2	NAG	O5-C5-C6-O6
5	q	4	MAN	O5-C5-C6-O6
7	y	5	MAN	O5-C5-C6-O6
4	l	1	NAG	C4-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	f	2	NAG	O5-C5-C6-O6
4	t	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	e	2	NAG	O5-C5-C6-O6
4	s	2	NAG	O5-C5-C6-O6

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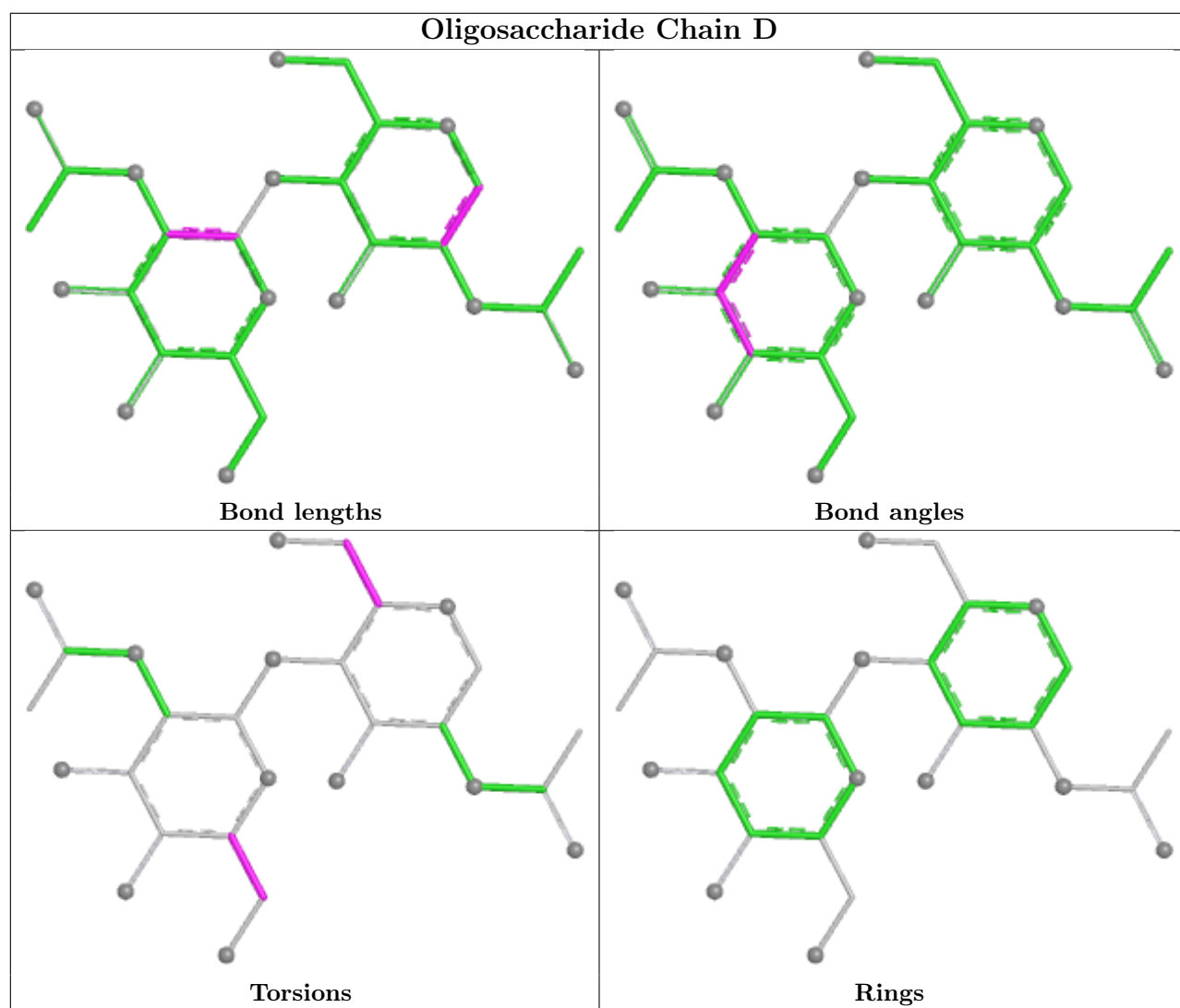
Mol	Chain	Res	Type	Atoms
5	c	6	MAN	O5-C5-C6-O6
5	q	6	MAN	O5-C5-C6-O6
6	T	8	MAN	O5-C5-C6-O6
6	v	4	MAN	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	d	2	NAG	O5-C5-C6-O6
4	r	2	NAG	O5-C5-C6-O6
4	p	2	NAG	O5-C5-C6-O6
5	J	6	MAN	O5-C5-C6-O6
6	h	6	MAN	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	j	2	NAG	O5-C5-C6-O6
4	x	2	NAG	O5-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
6	h	5	MAN	C4-C5-C6-O6
6	T	9	MAN	C4-C5-C6-O6
6	h	4	MAN	C4-C5-C6-O6
6	h	9	MAN	C4-C5-C6-O6
4	r	1	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	d	1	NAG	O5-C5-C6-O6
6	T	4	MAN	C4-C5-C6-O6
4	m	1	NAG	C4-C5-C6-O6
6	v	5	MAN	C4-C5-C6-O6
6	T	5	MAN	C4-C5-C6-O6
4	g	1	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	u	1	NAG	O5-C5-C6-O6

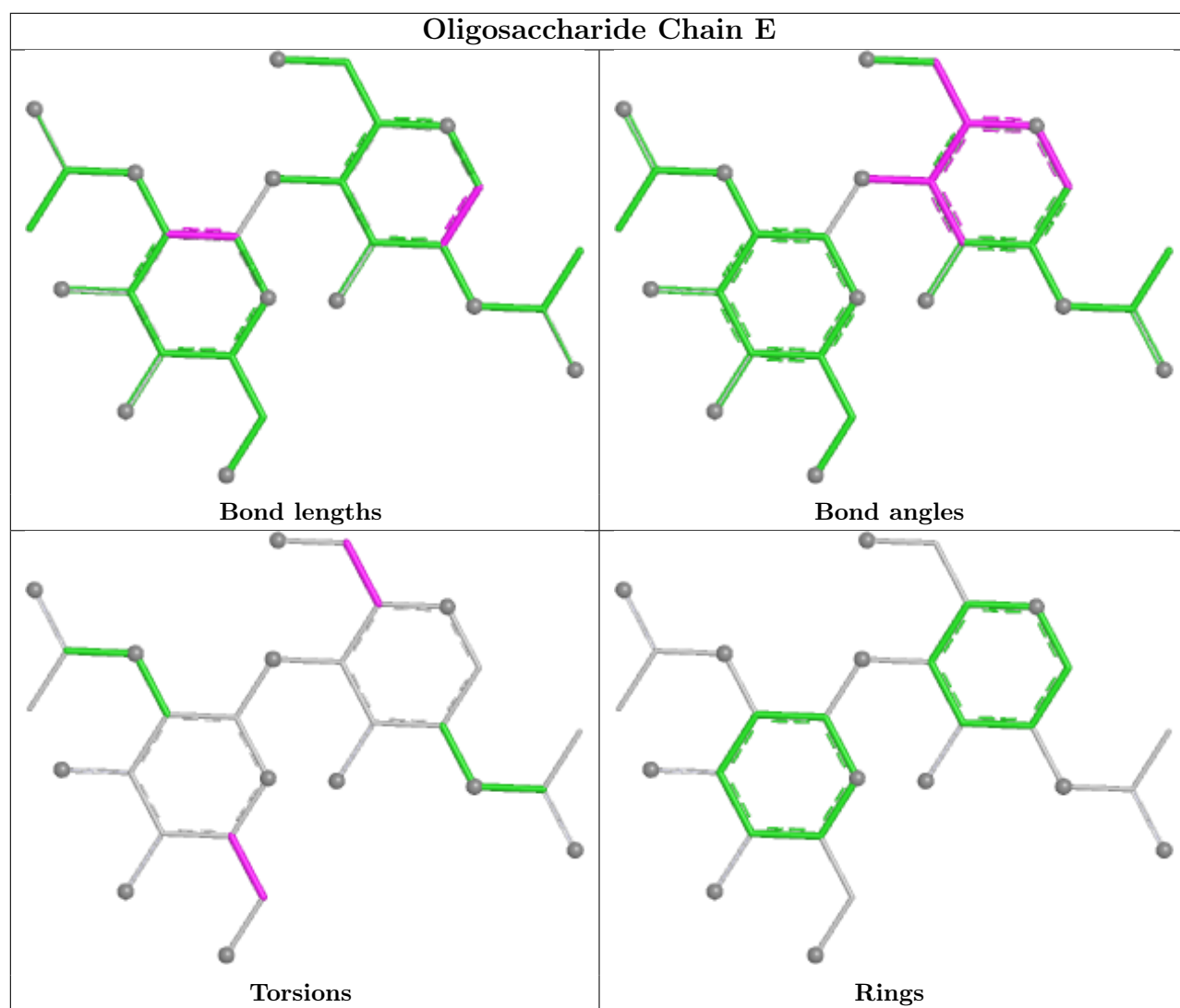
There are no ring outliers.

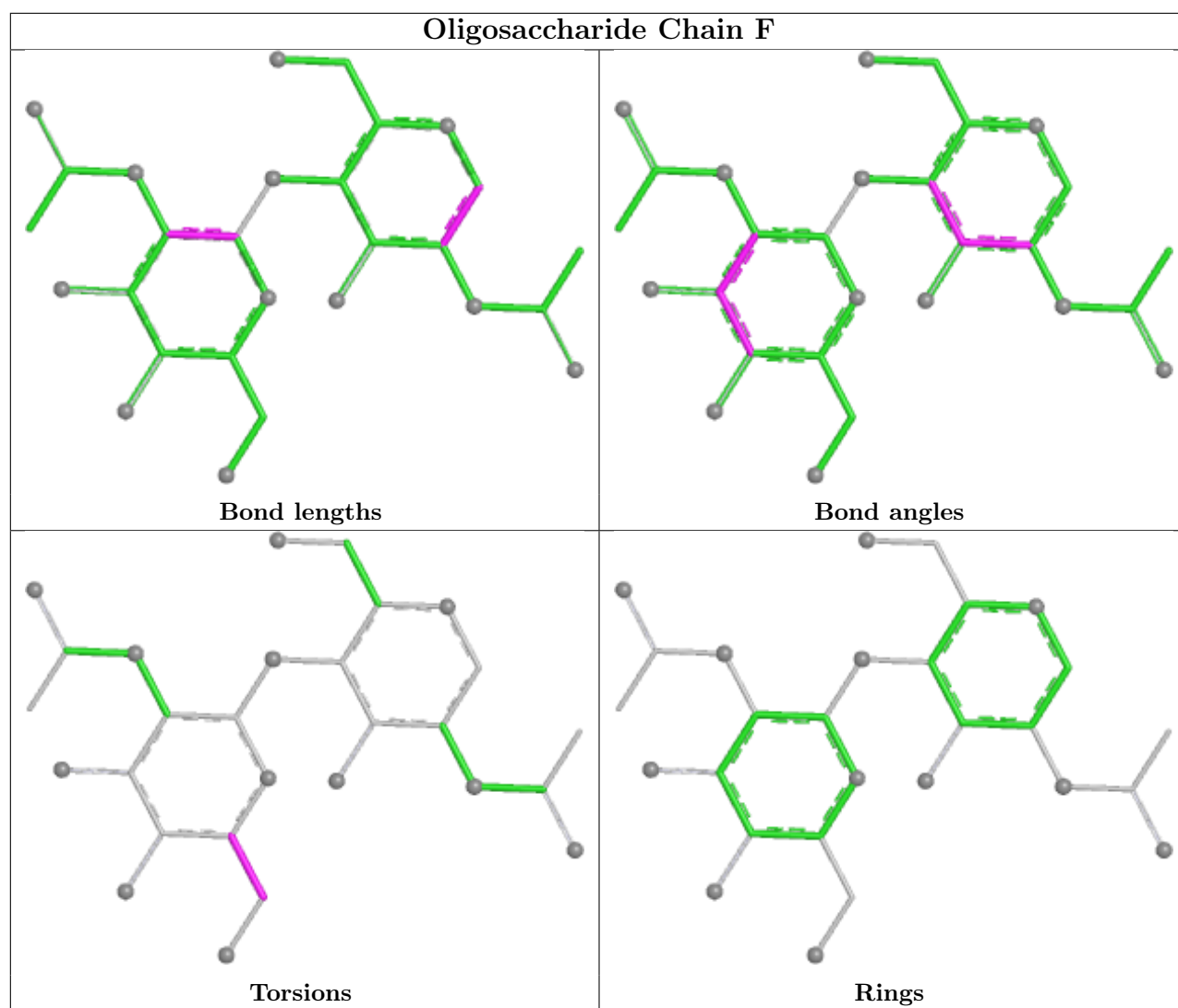
5 monomers are involved in 5 short contacts:

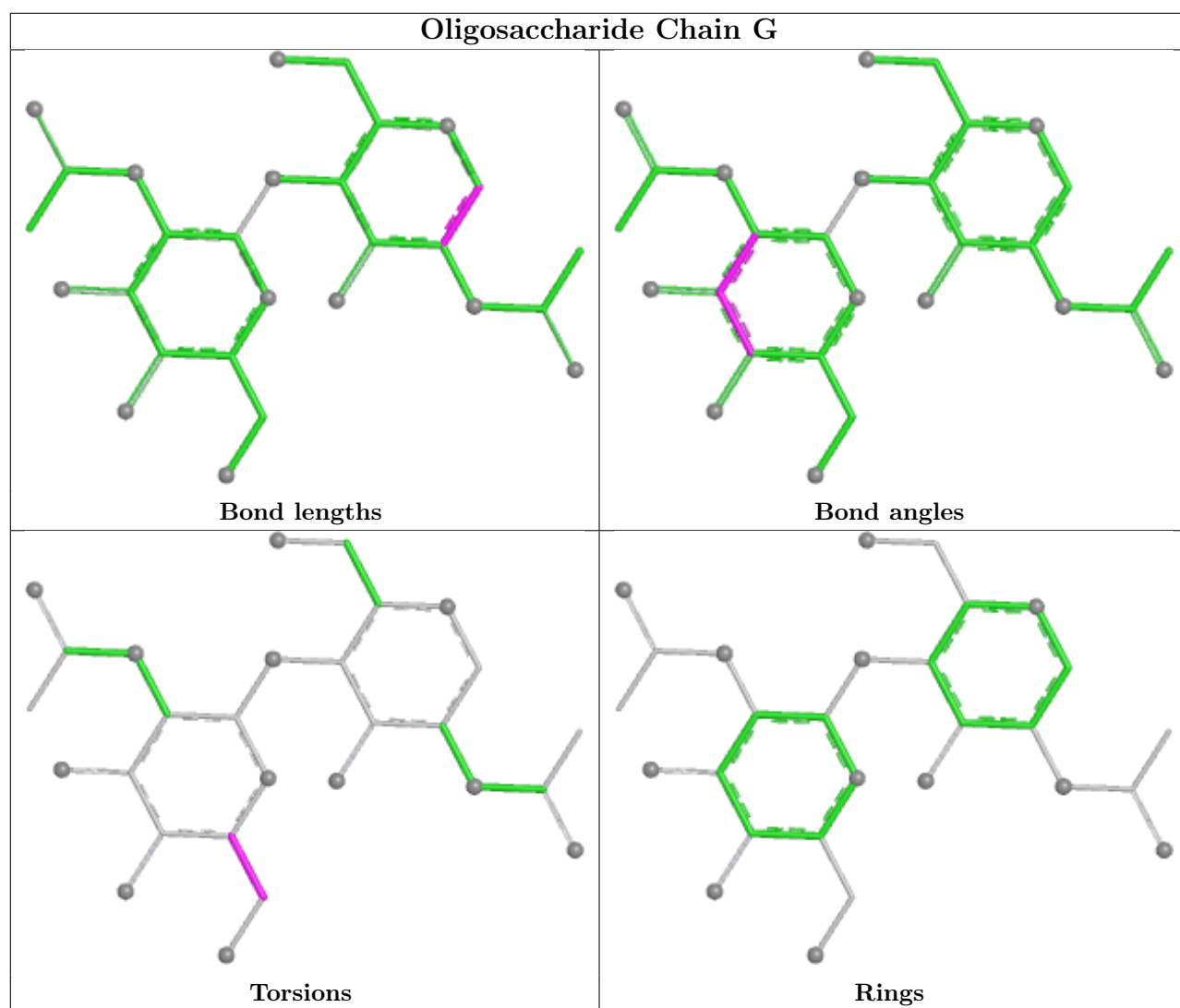
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	q	4	MAN	1	0
6	v	9	MAN	1	0
7	W	6	MAN	1	0
6	v	8	MAN	1	0
6	T	9	MAN	1	0

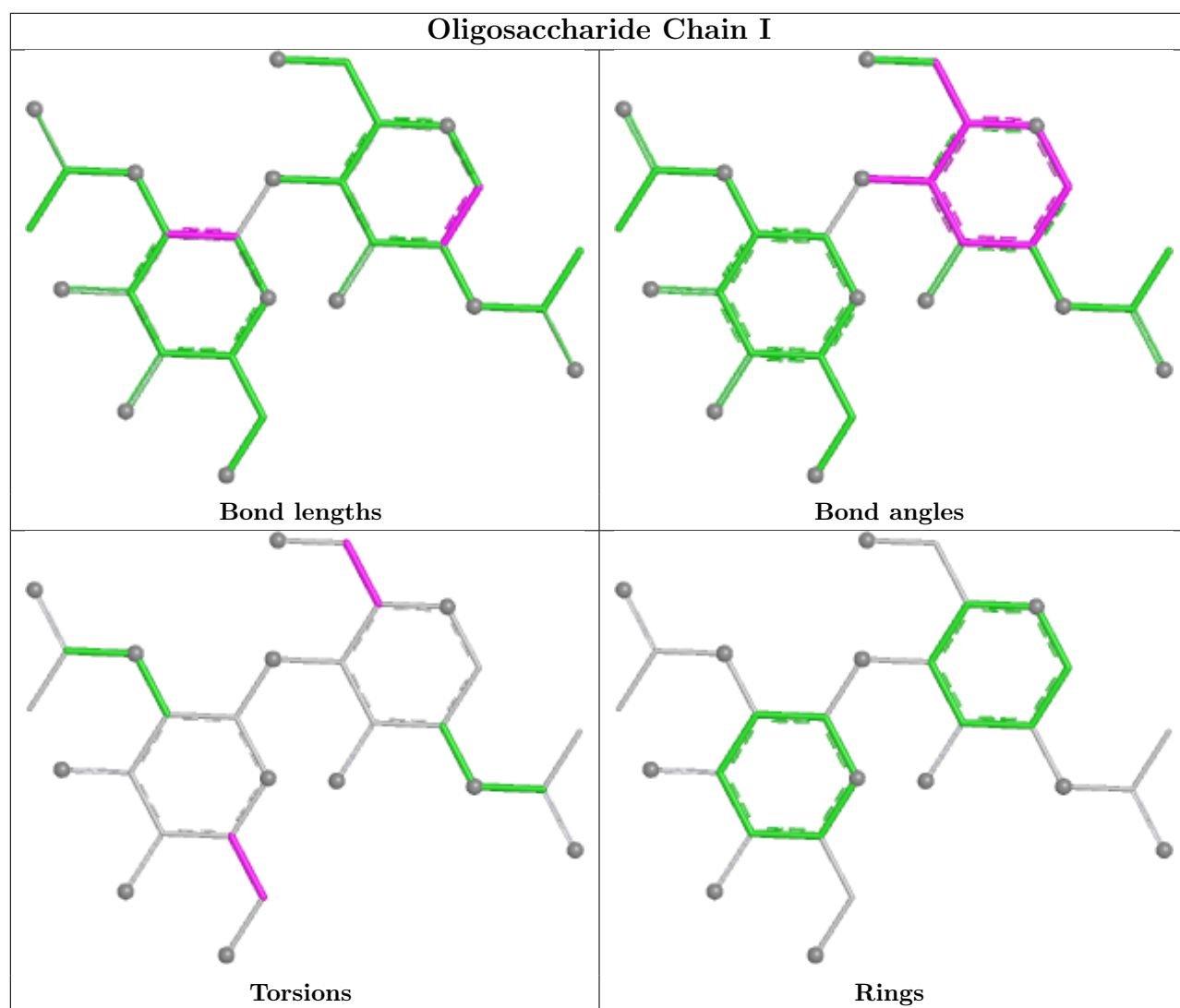
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

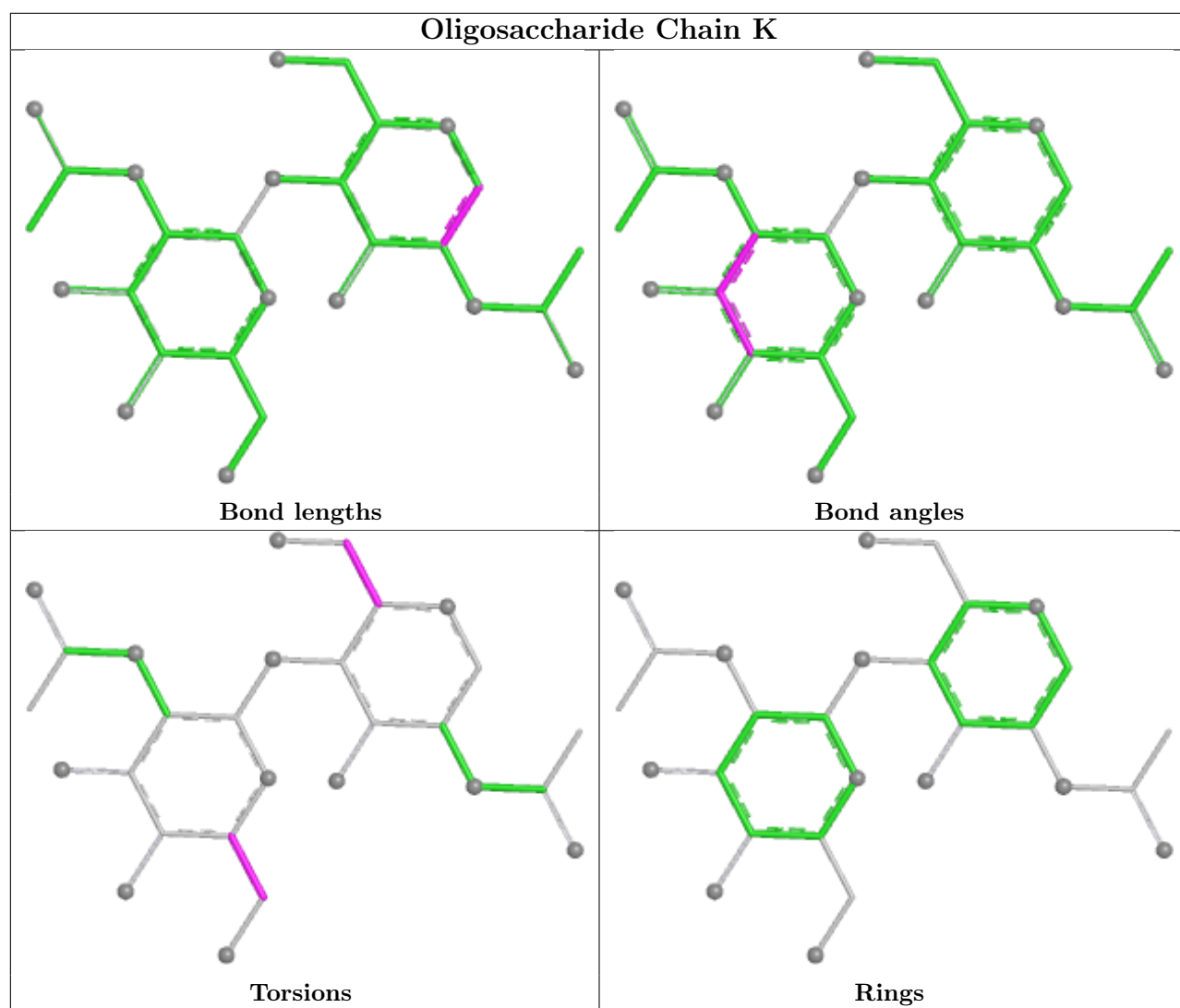


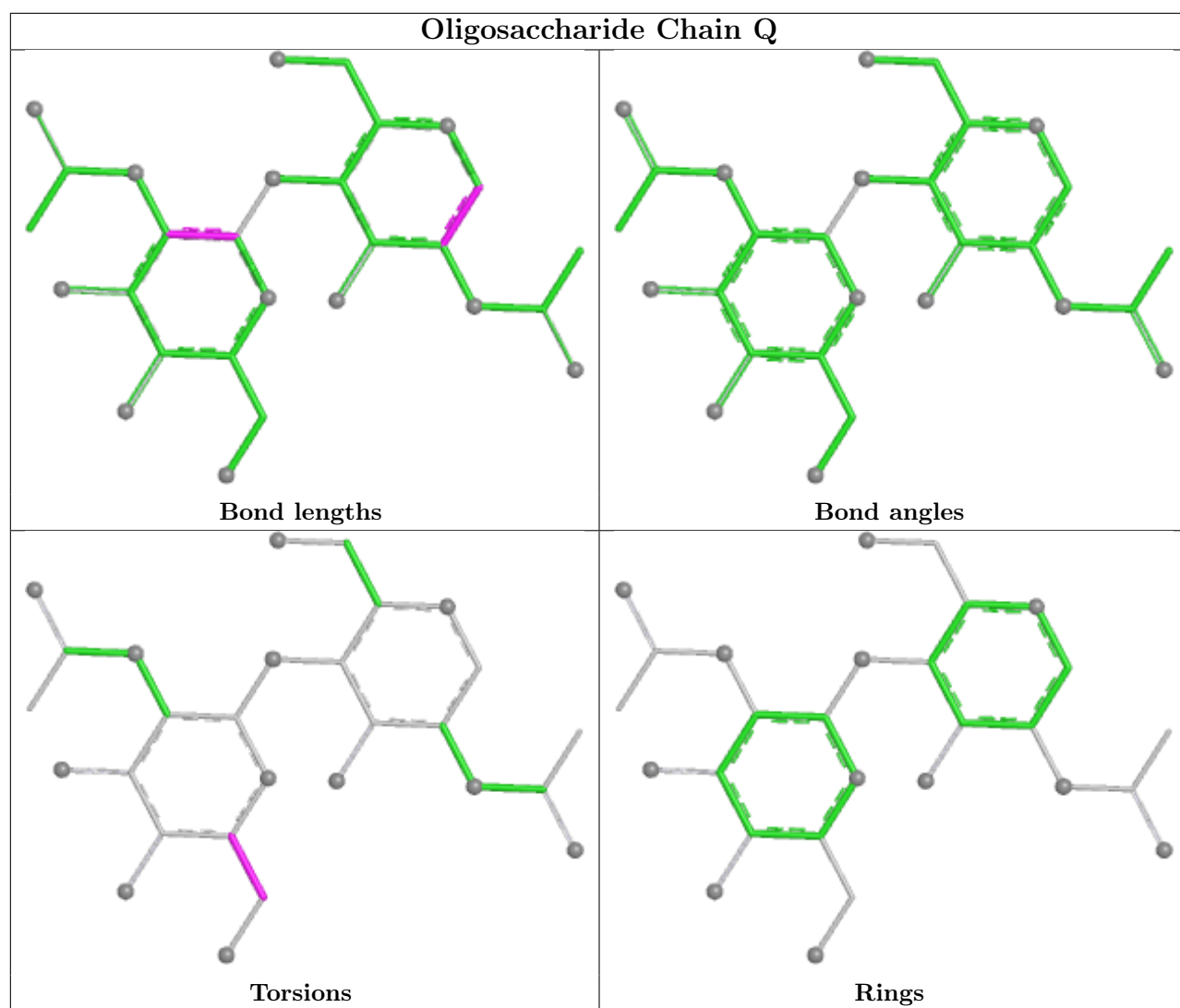


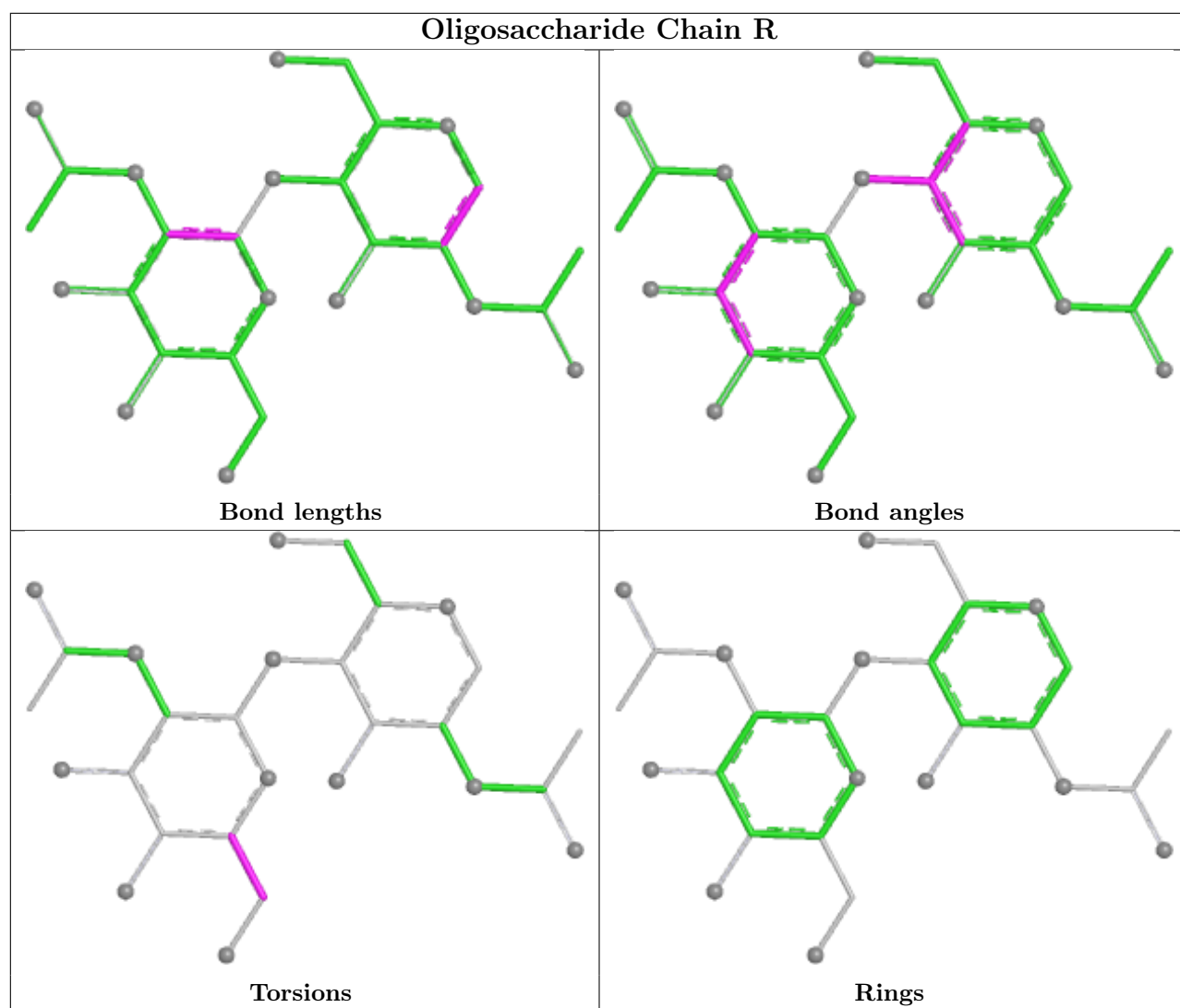


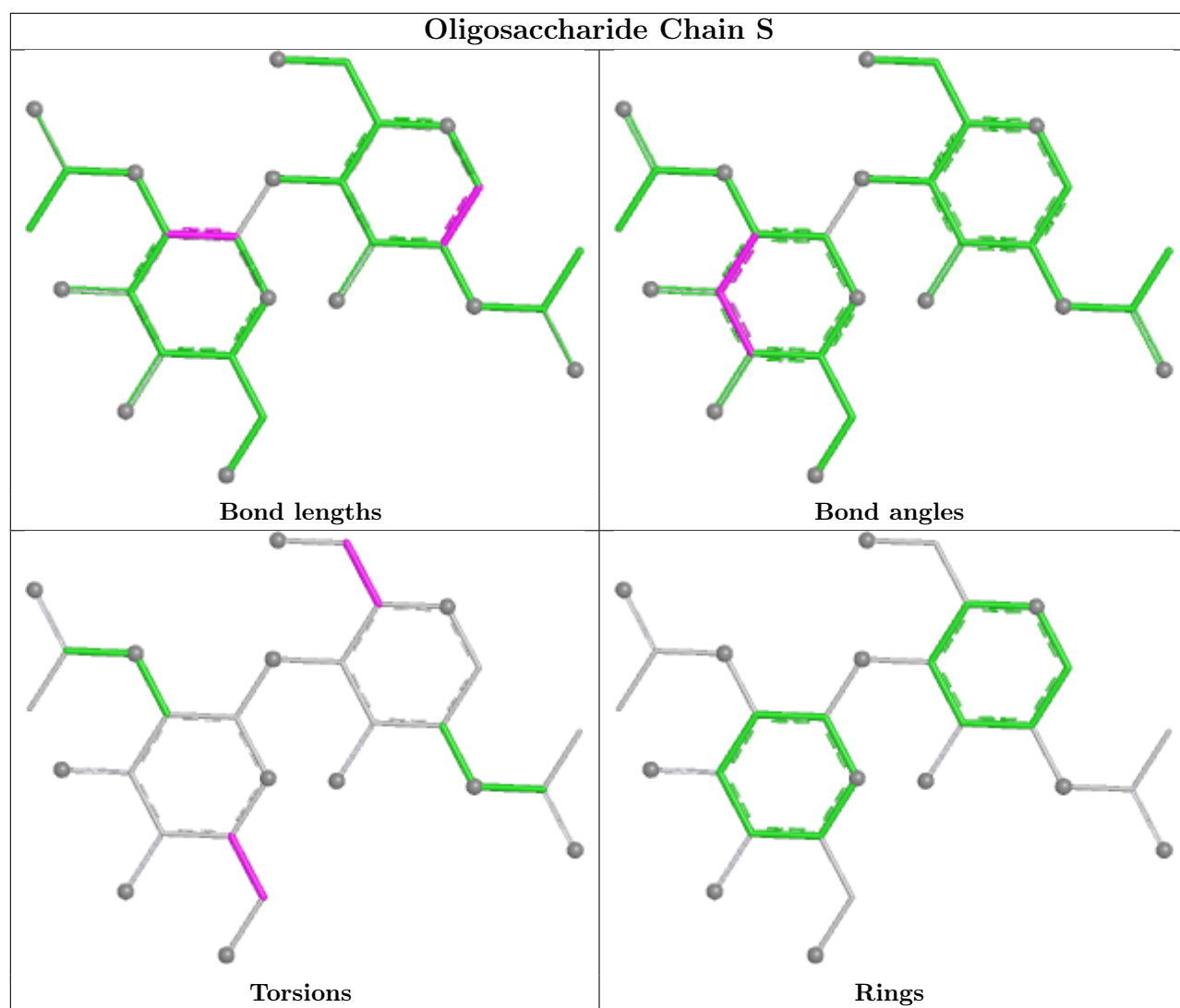


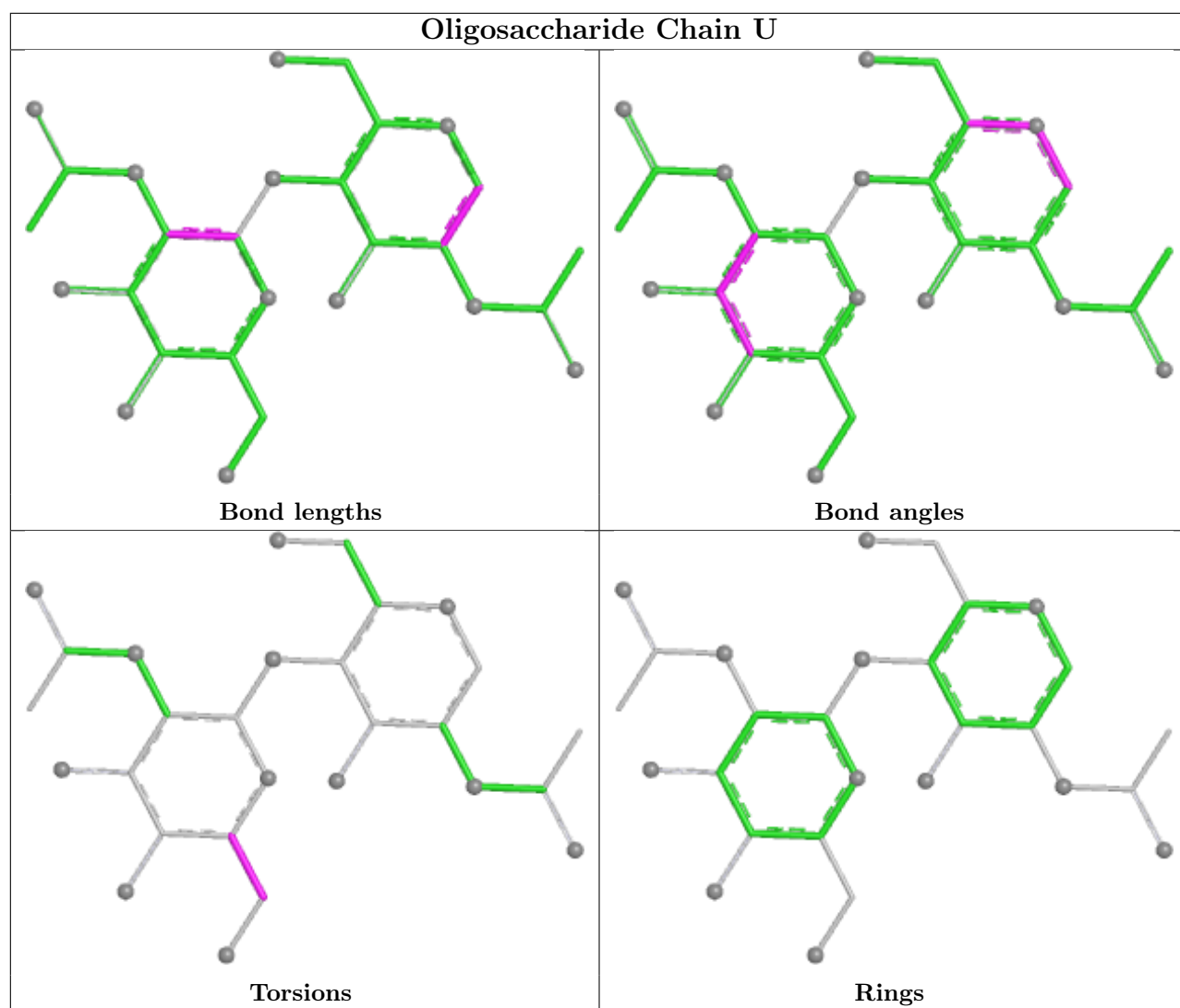


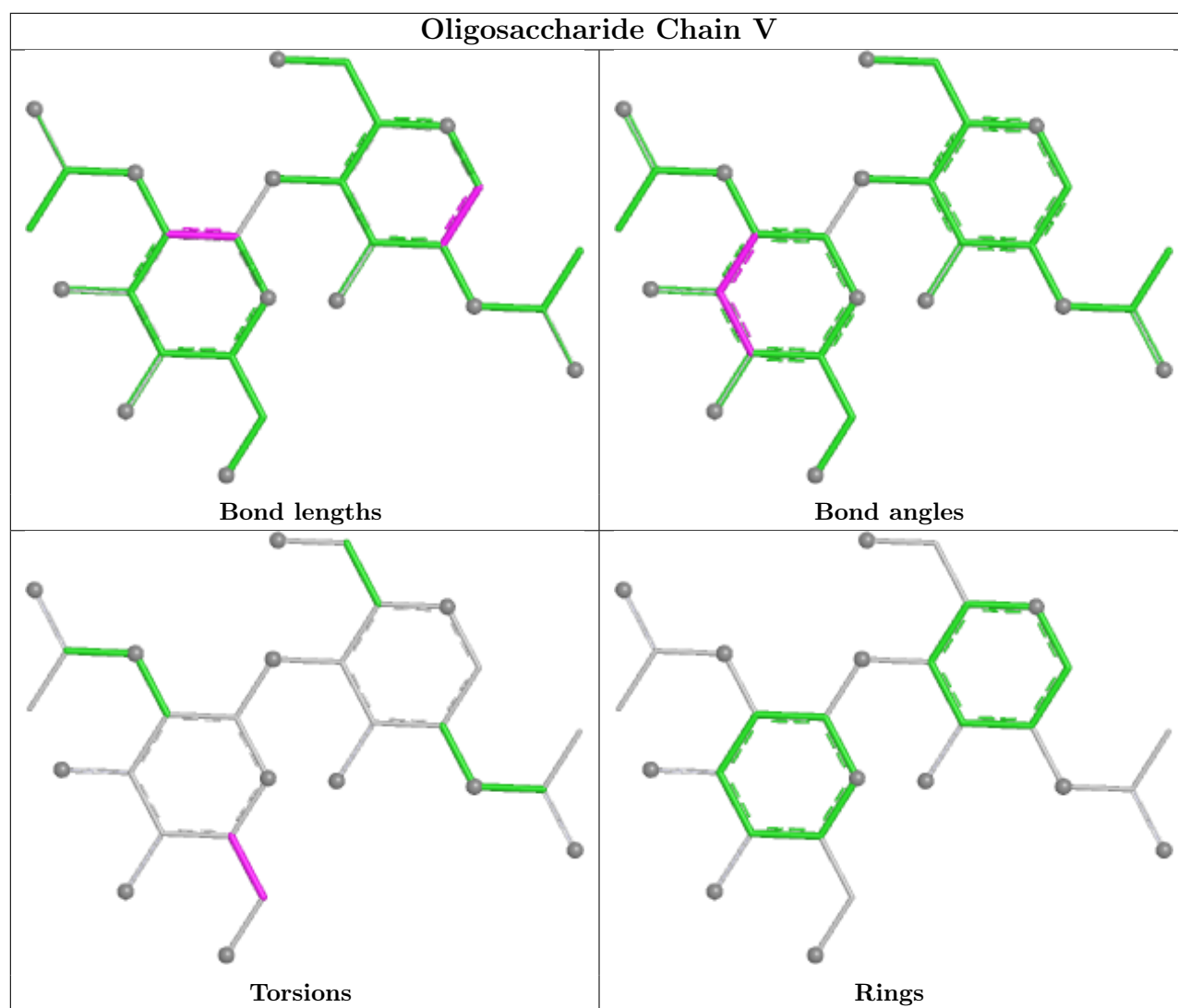


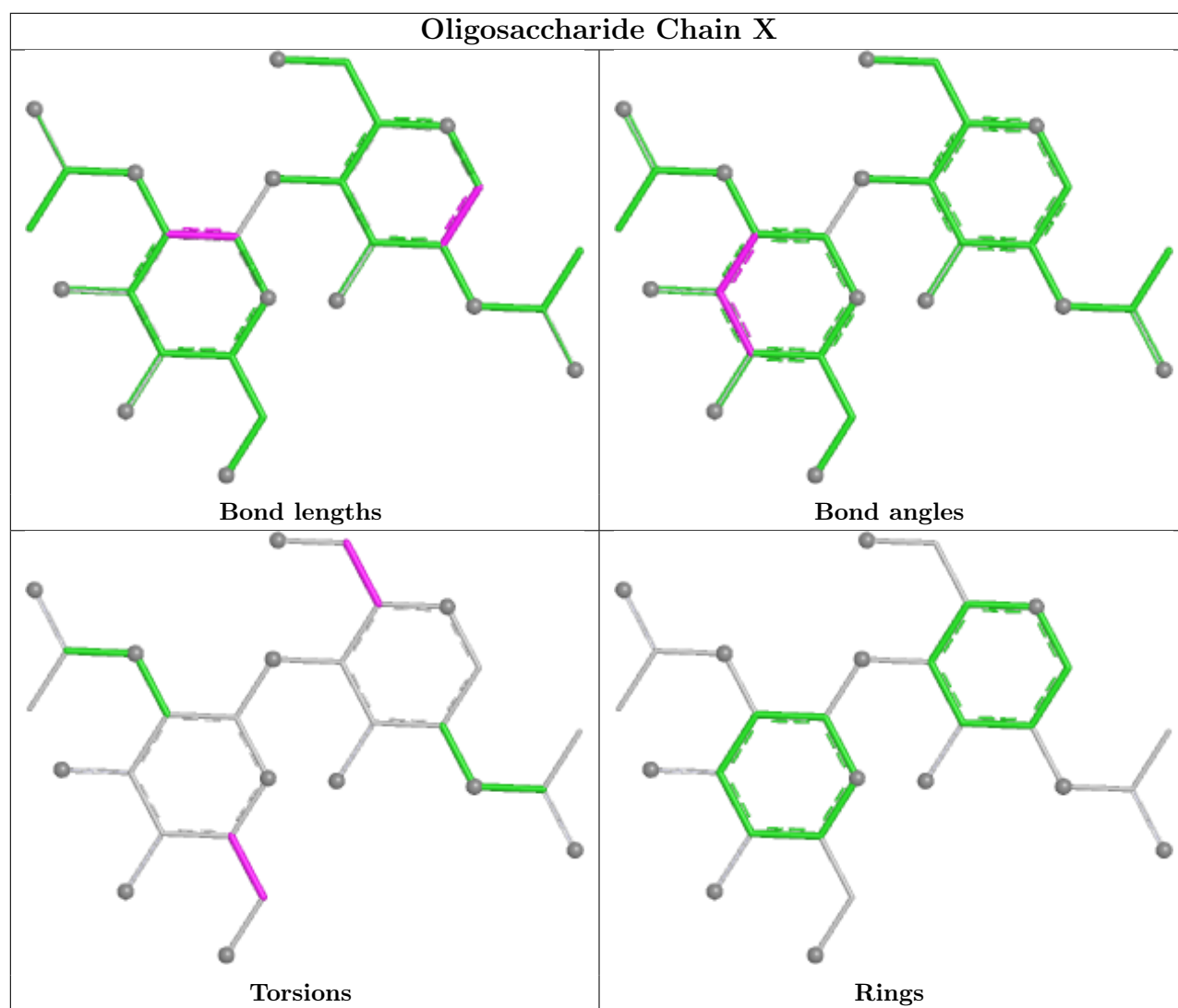


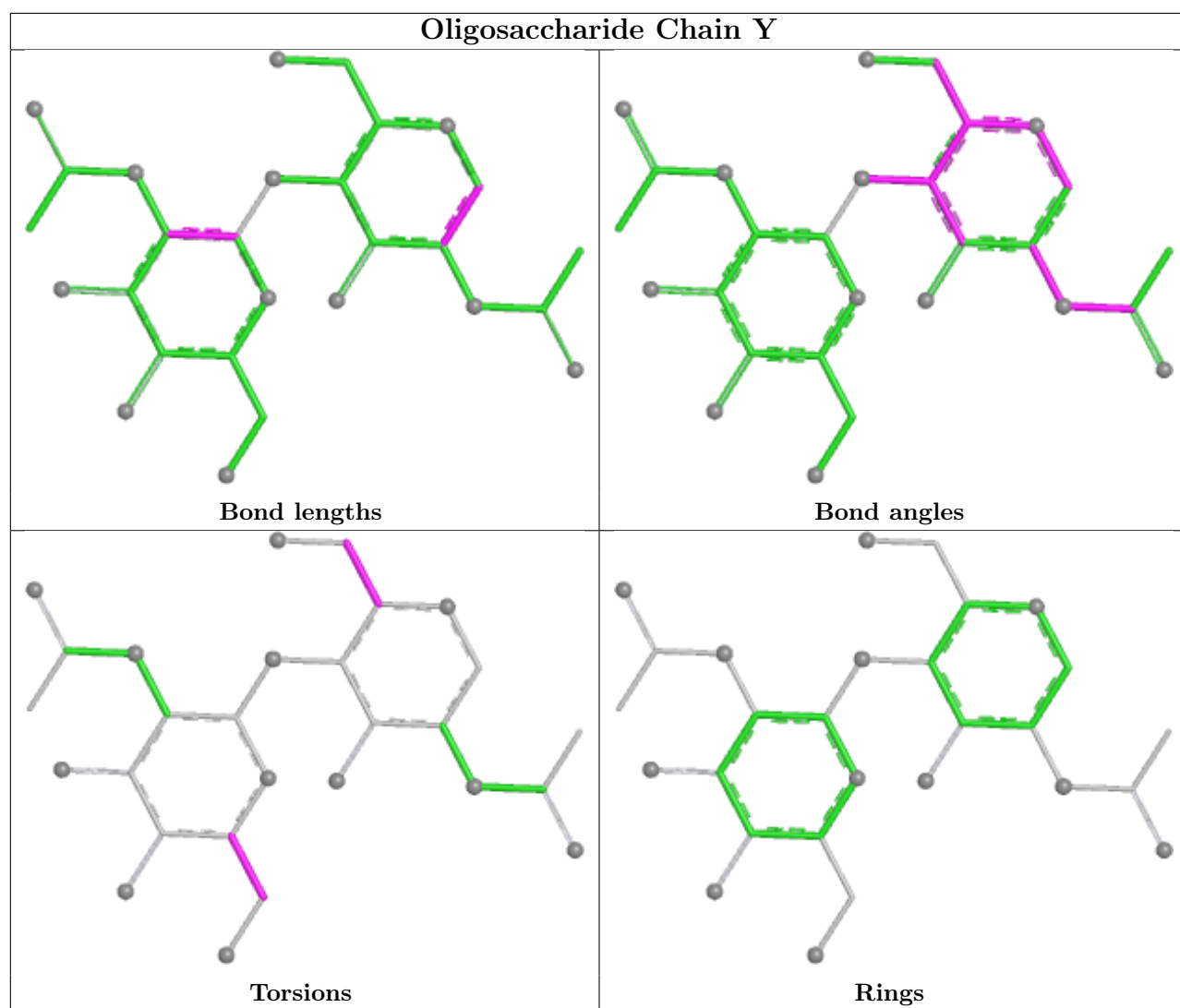


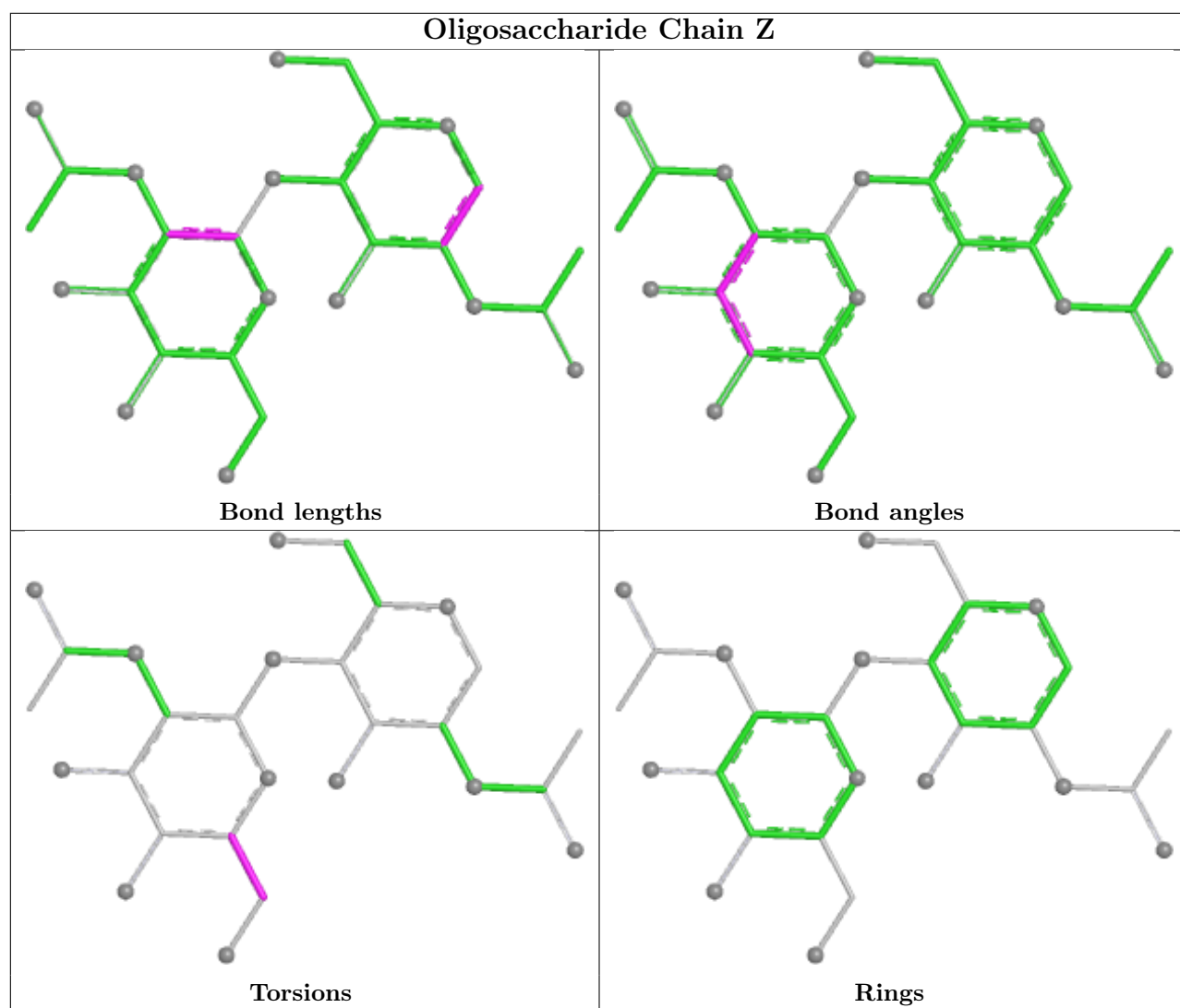


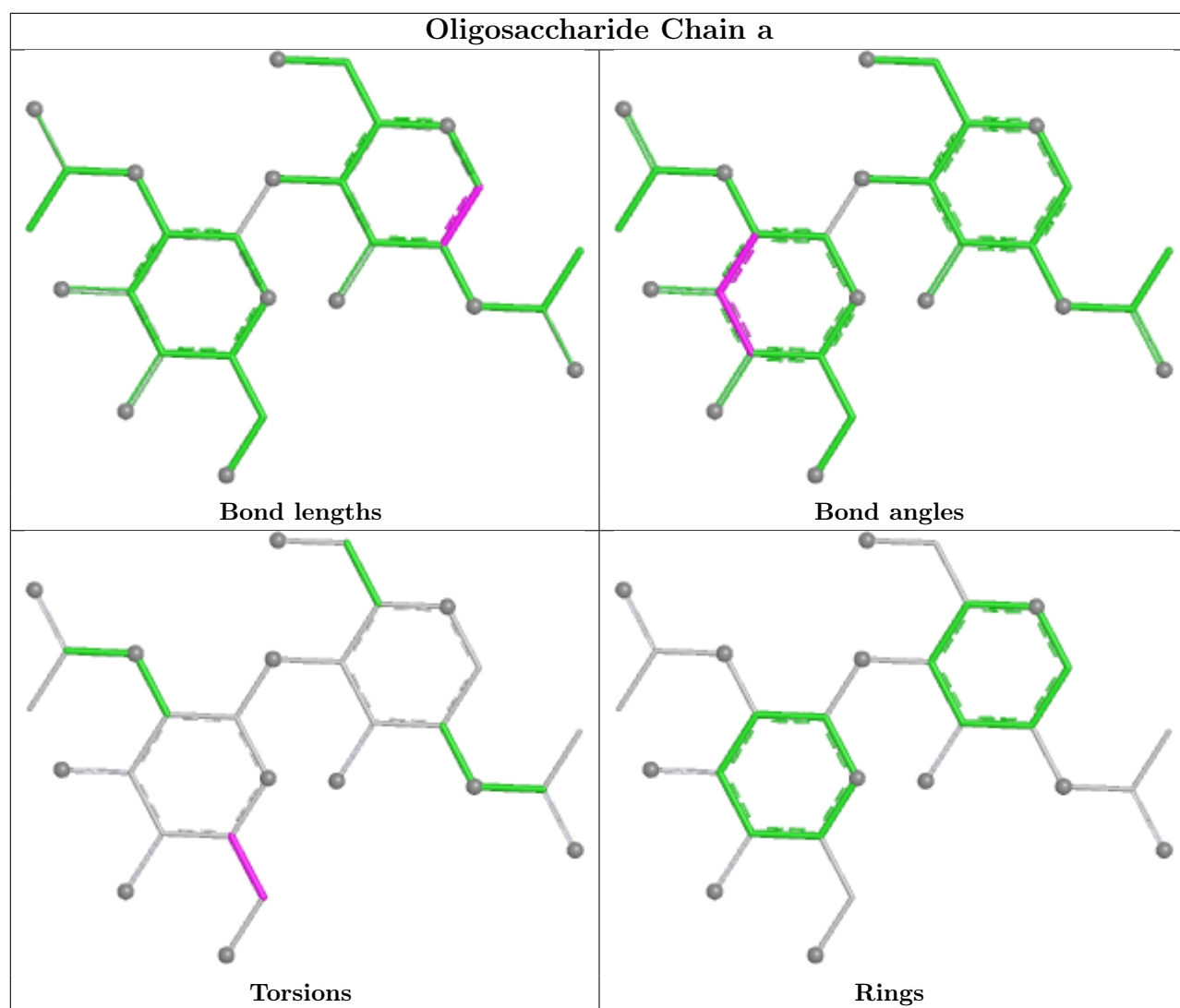


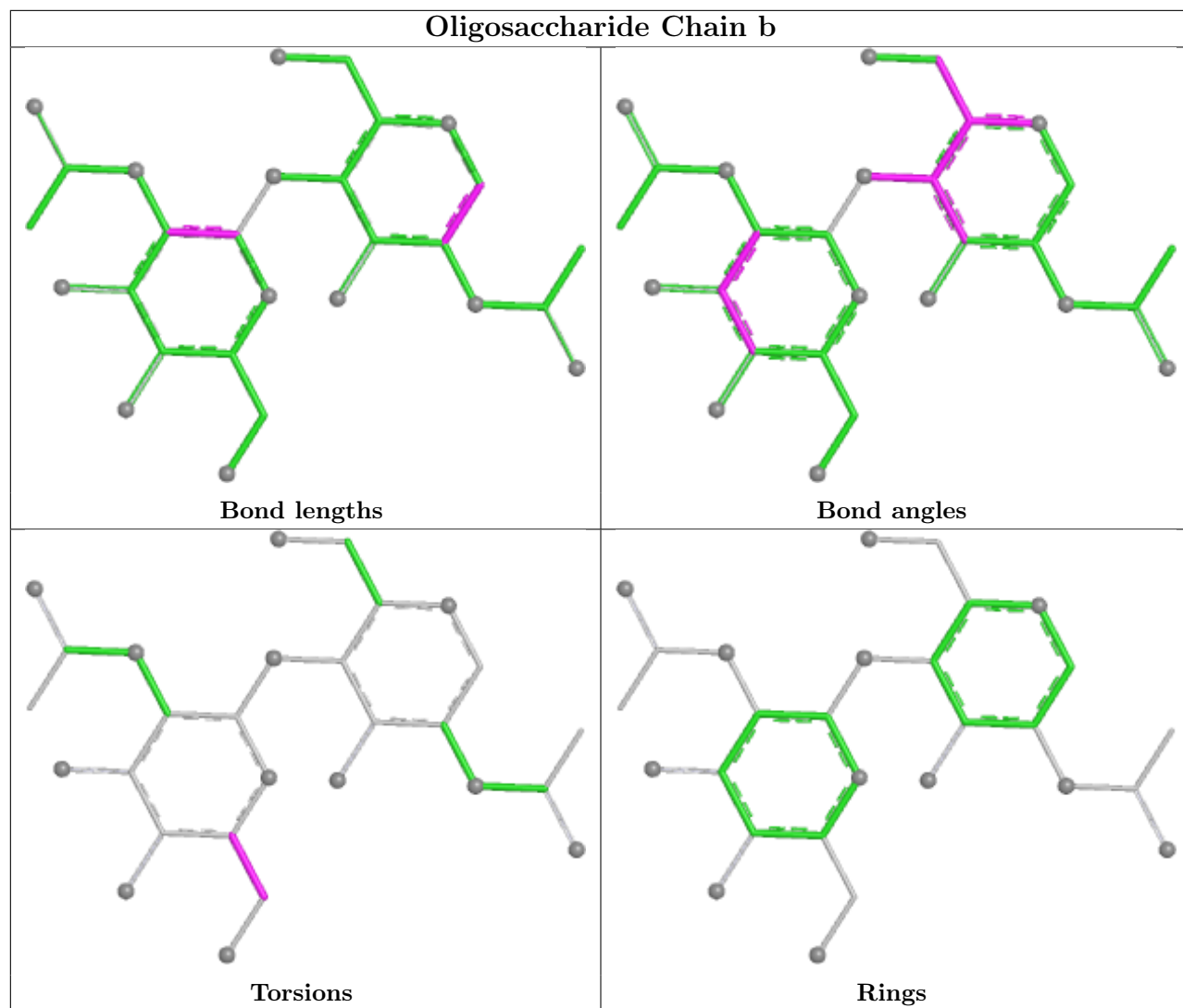


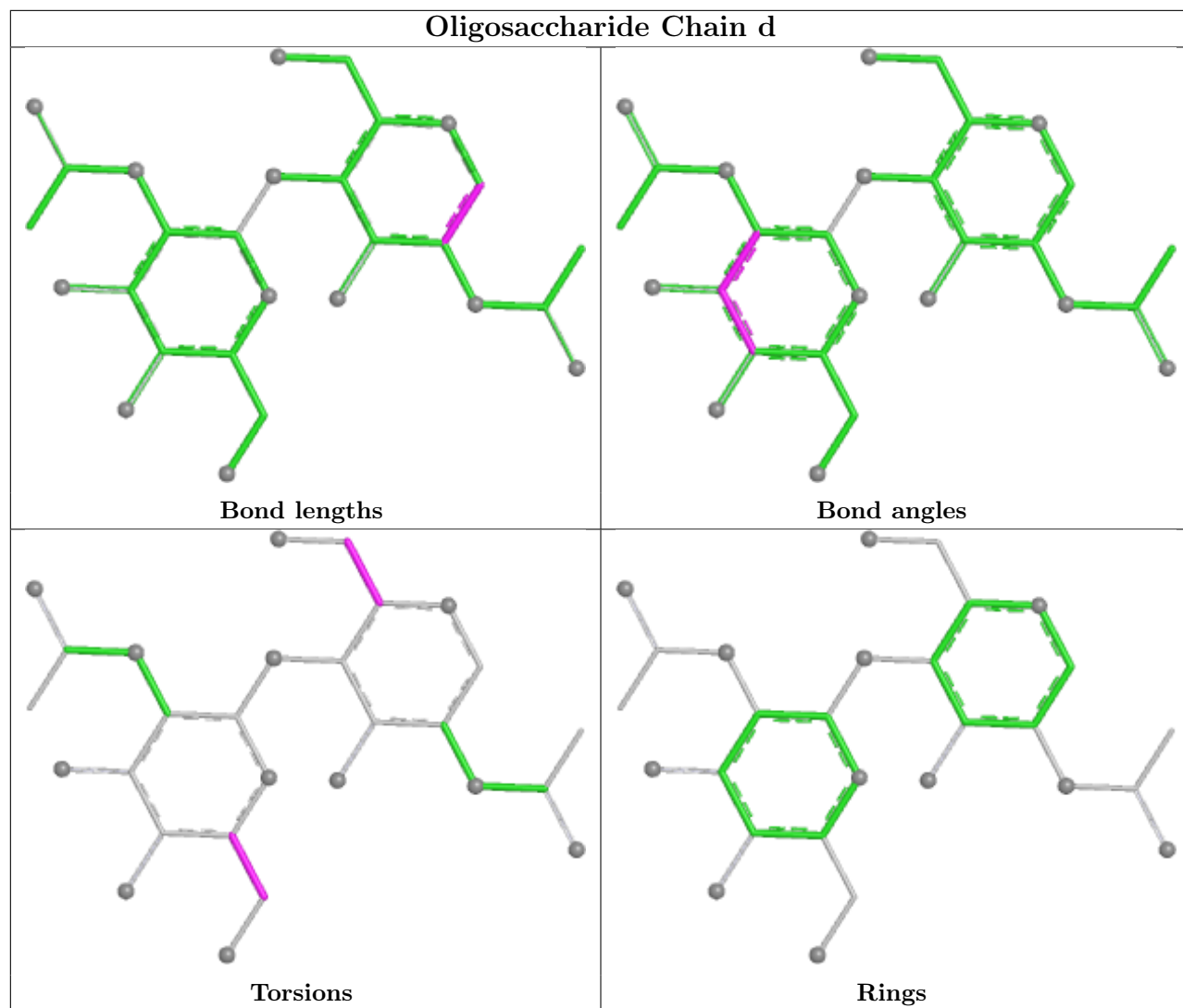


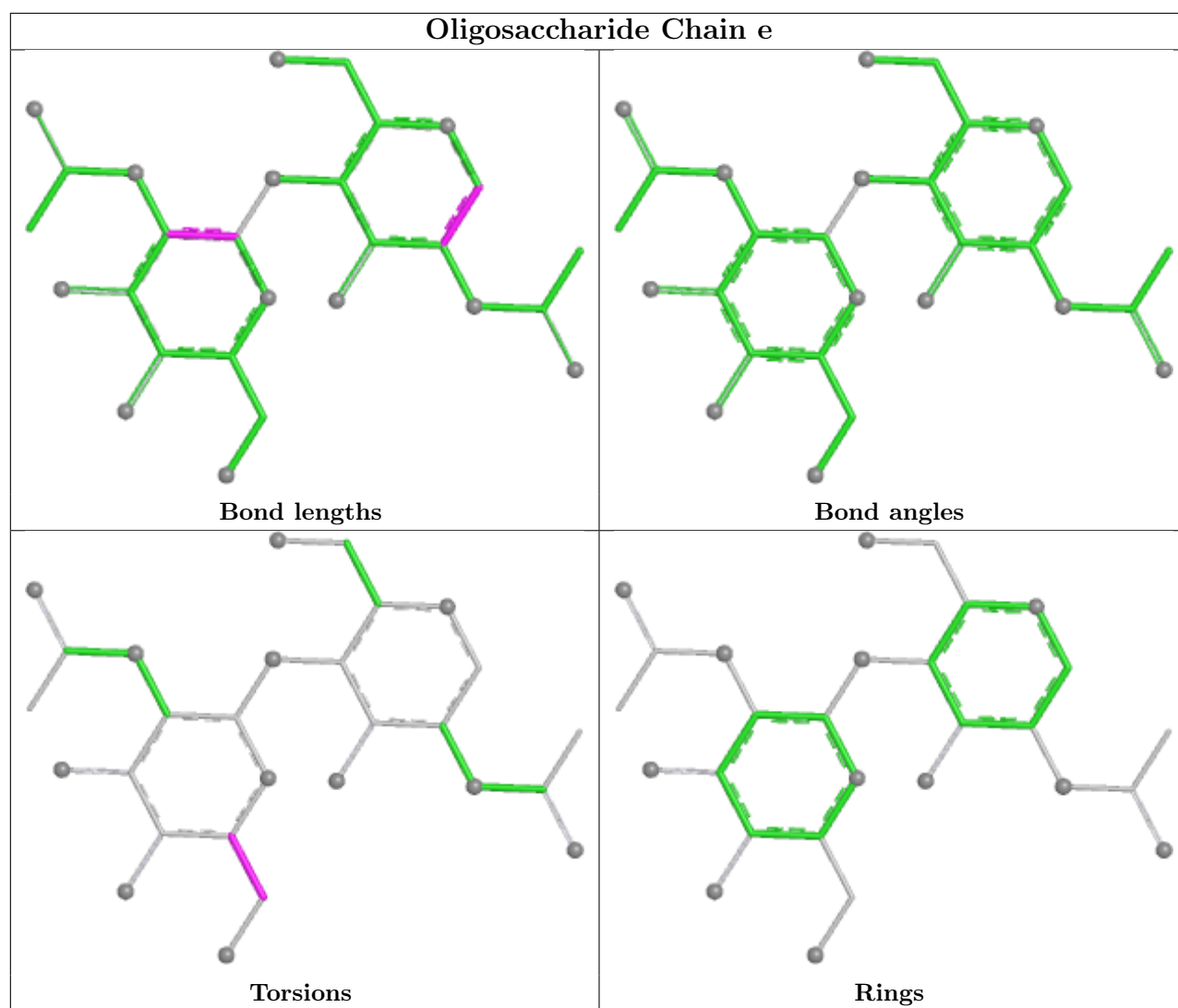


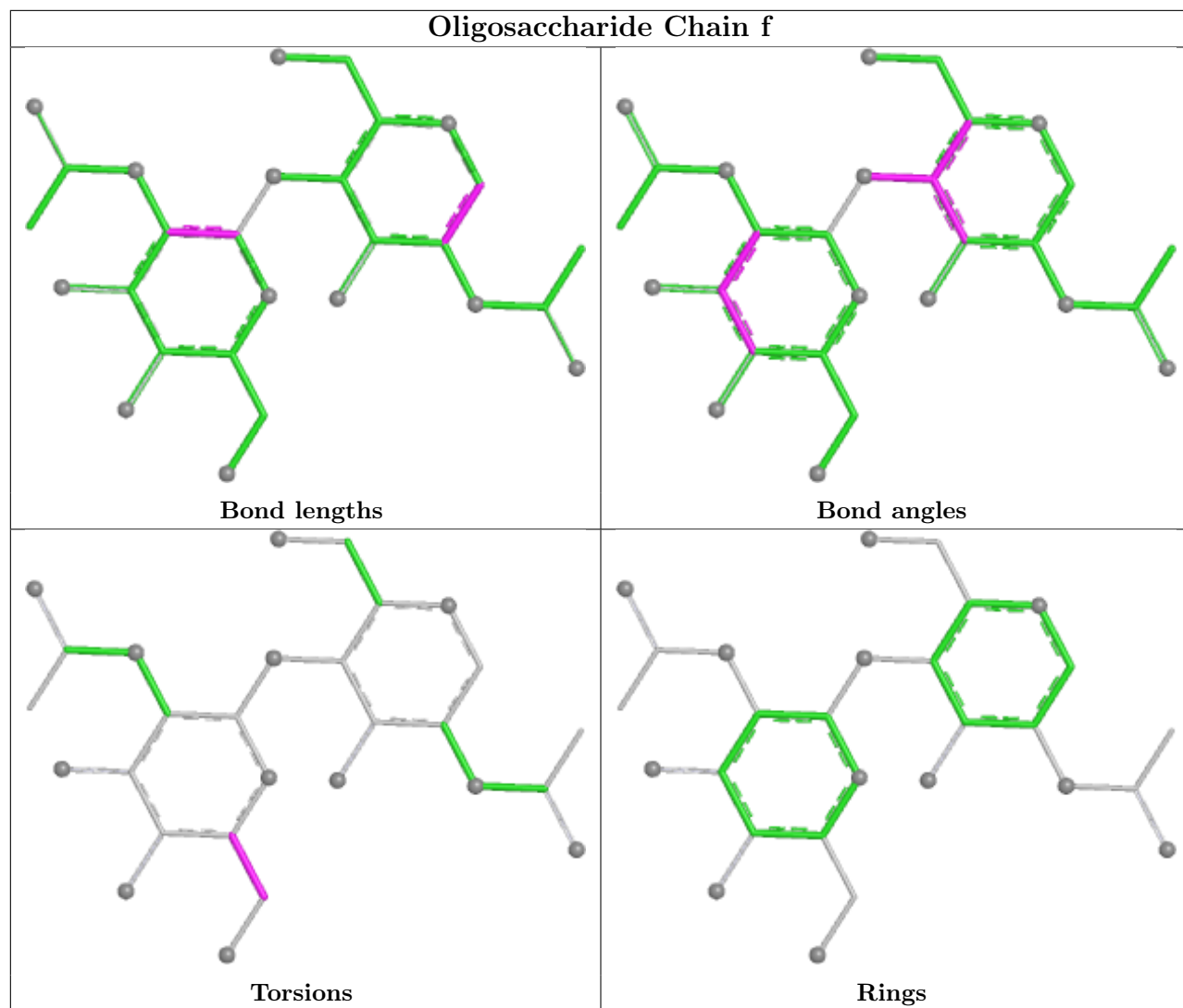


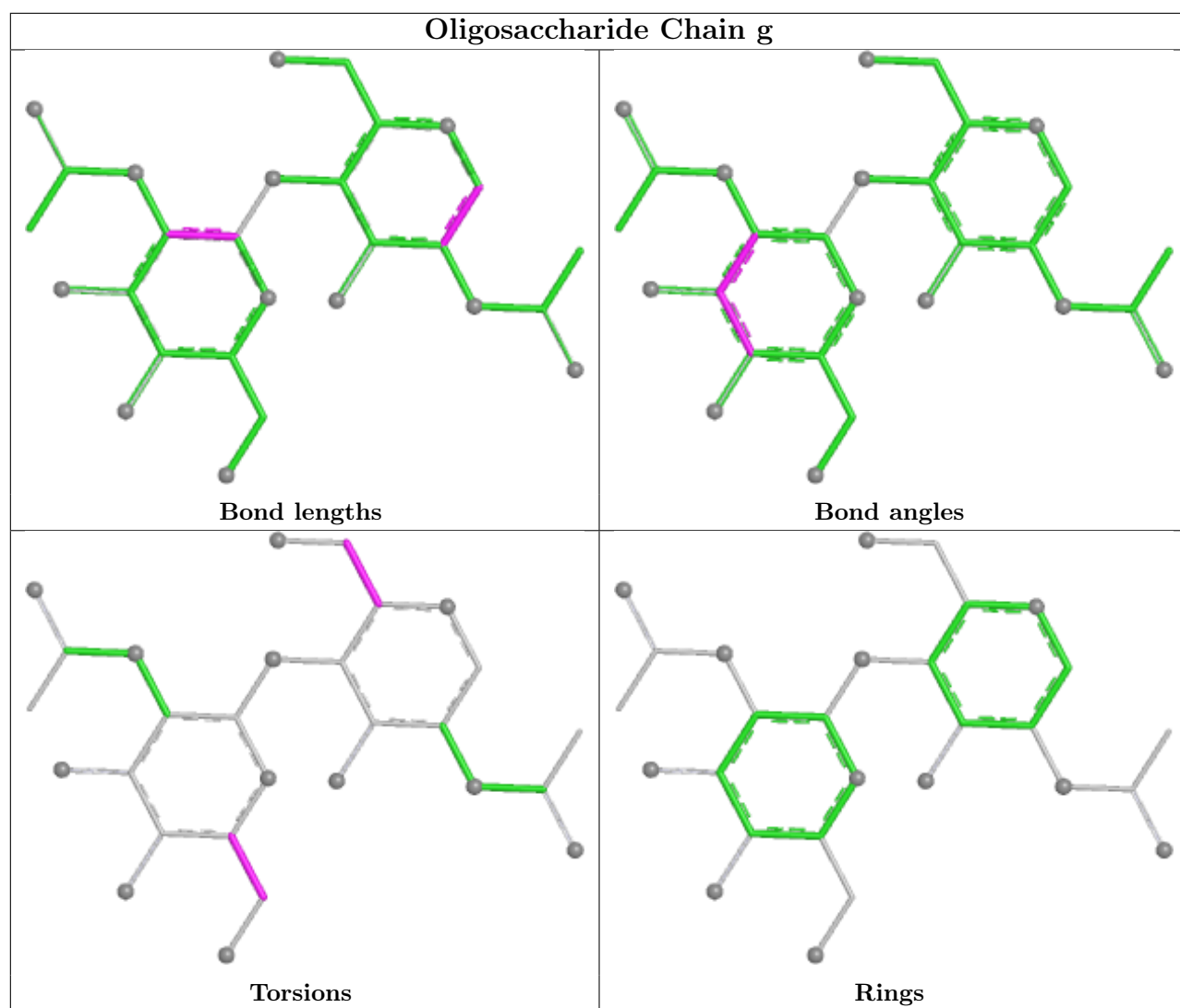


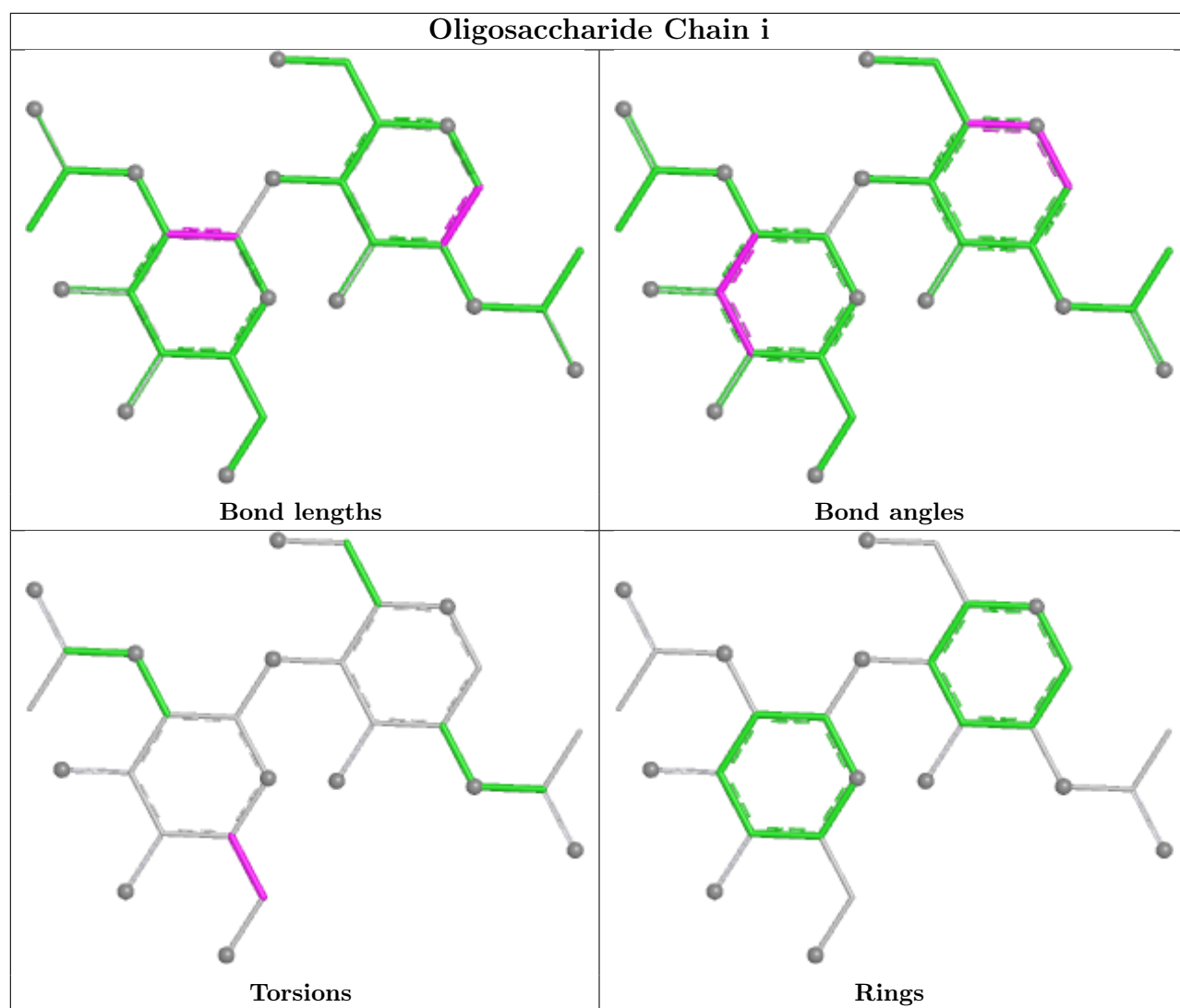


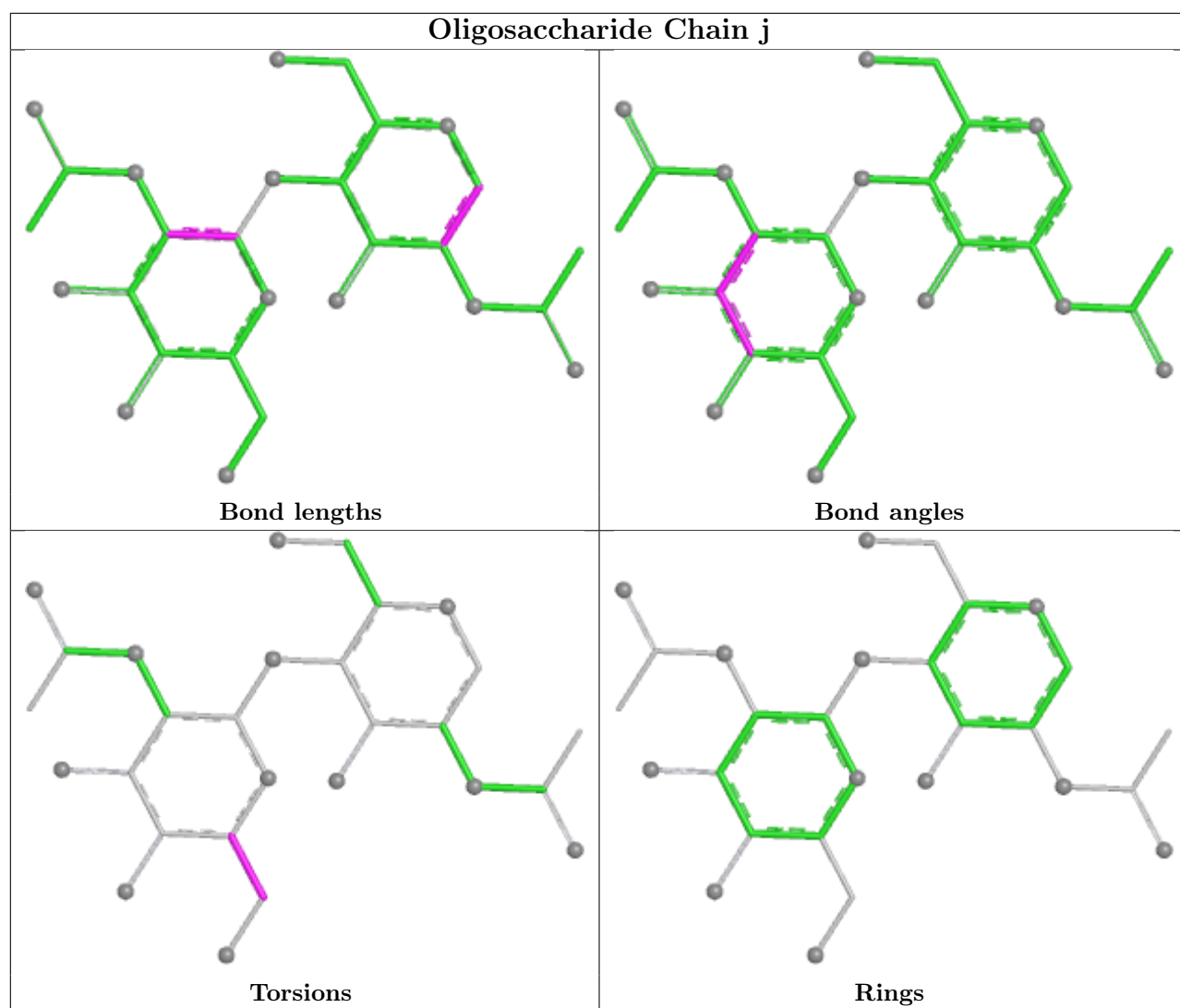


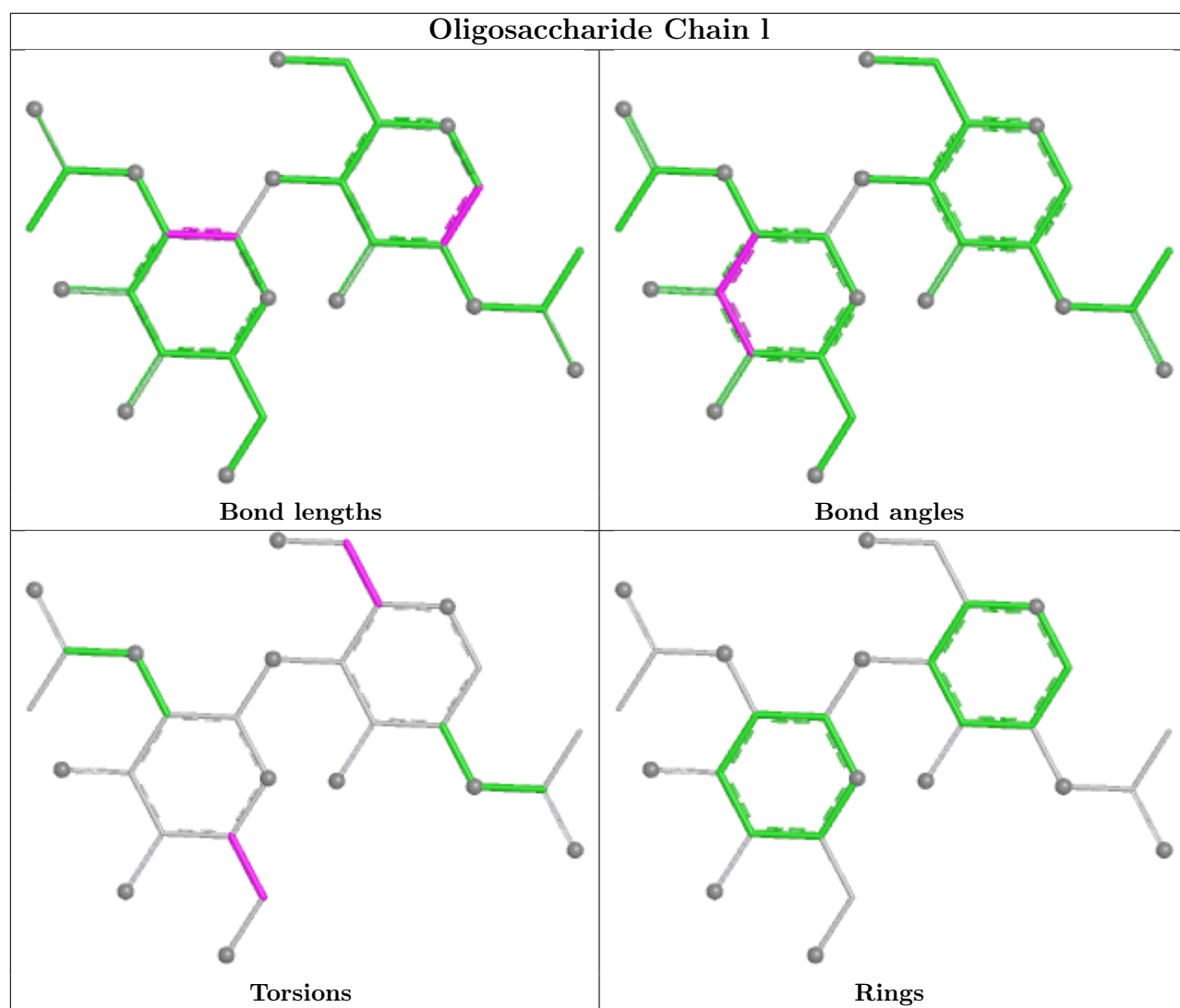


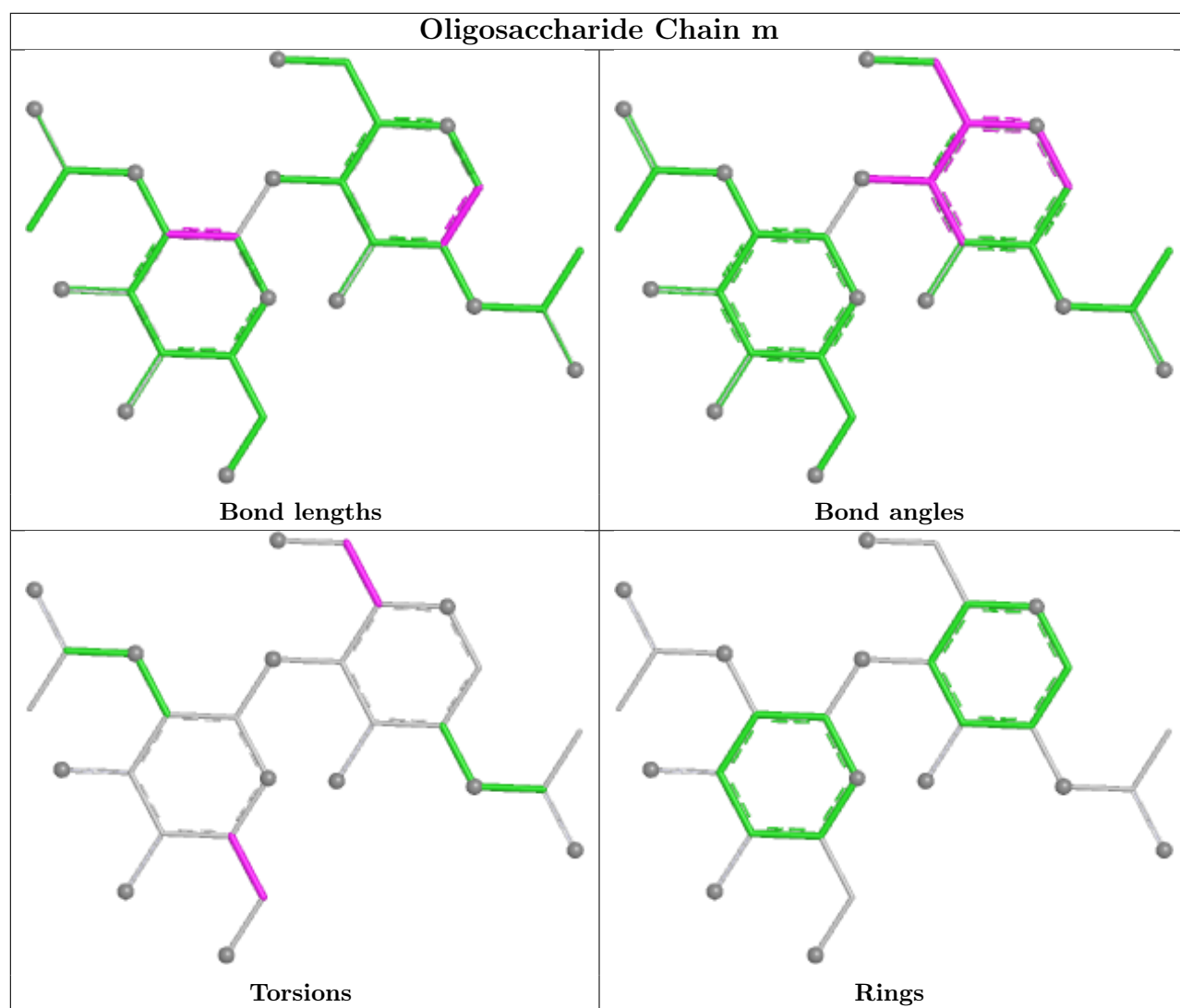


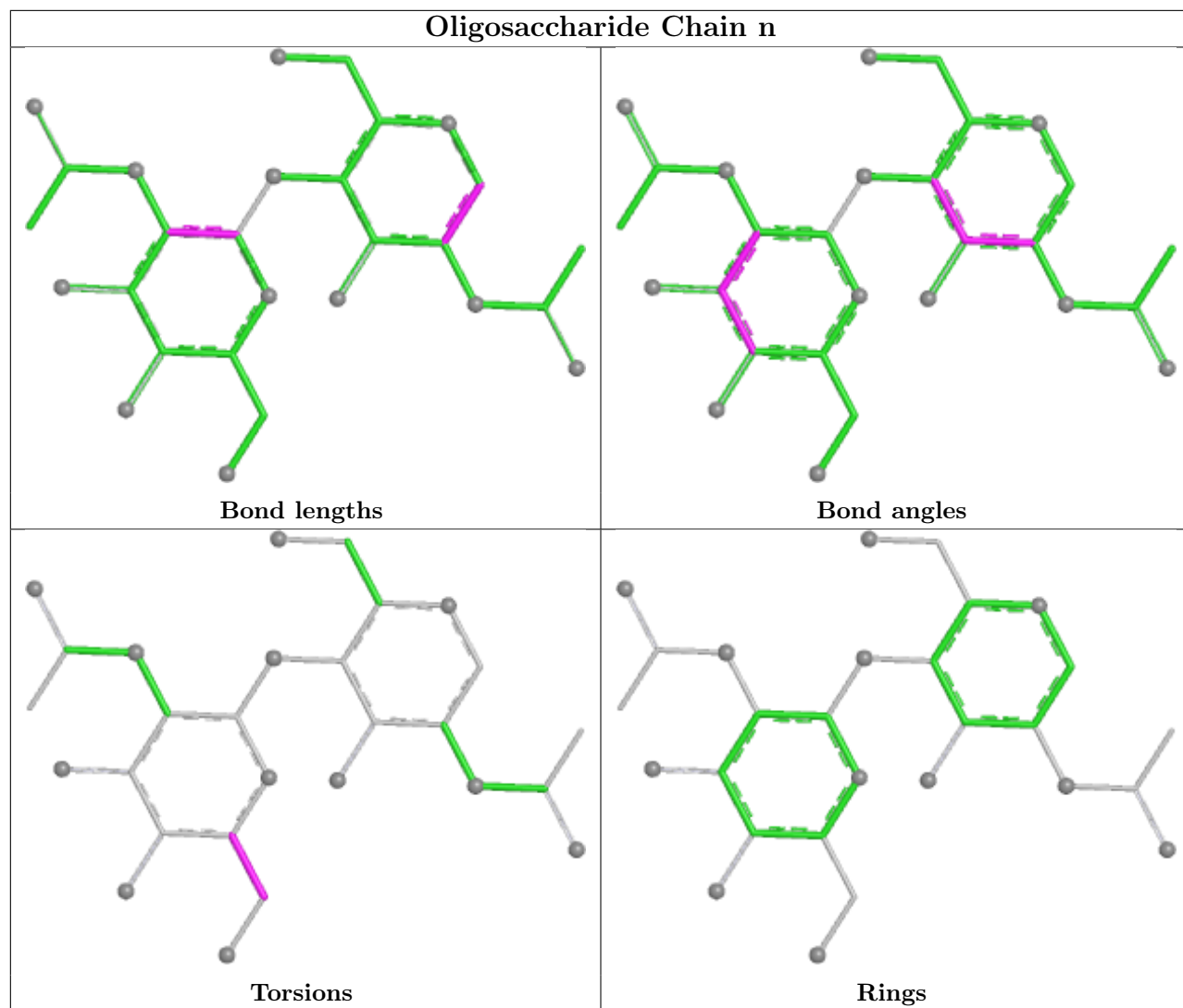


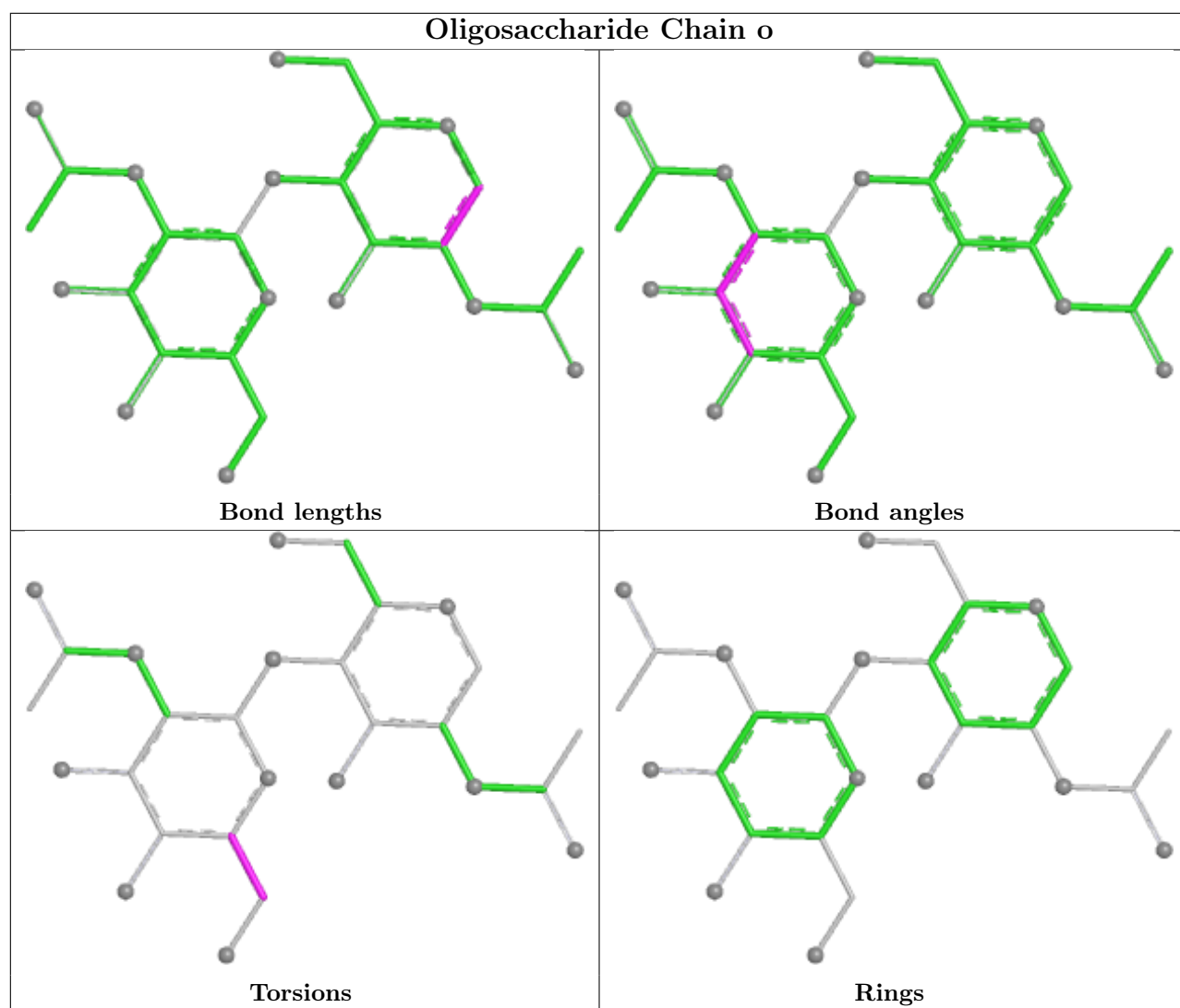


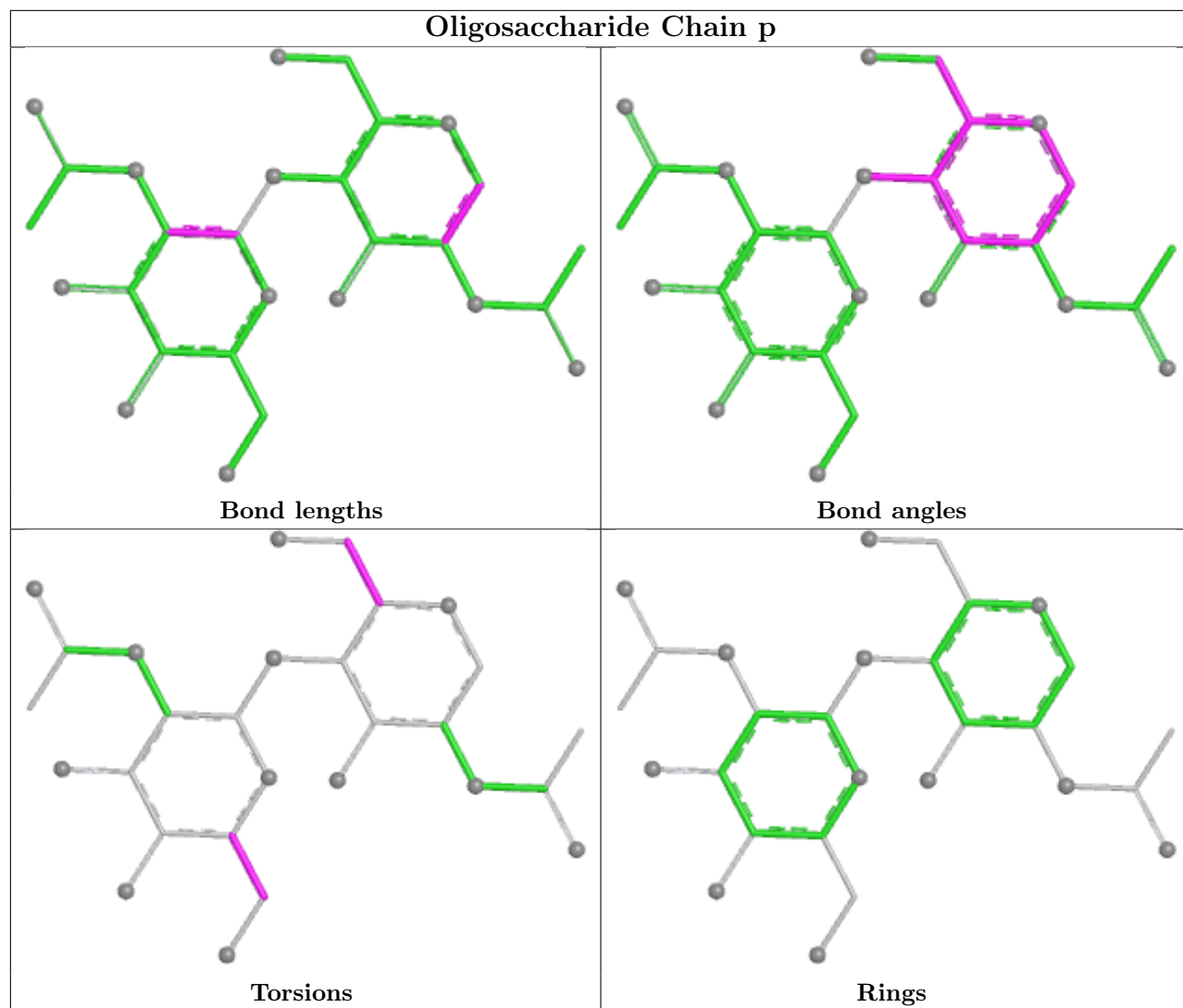


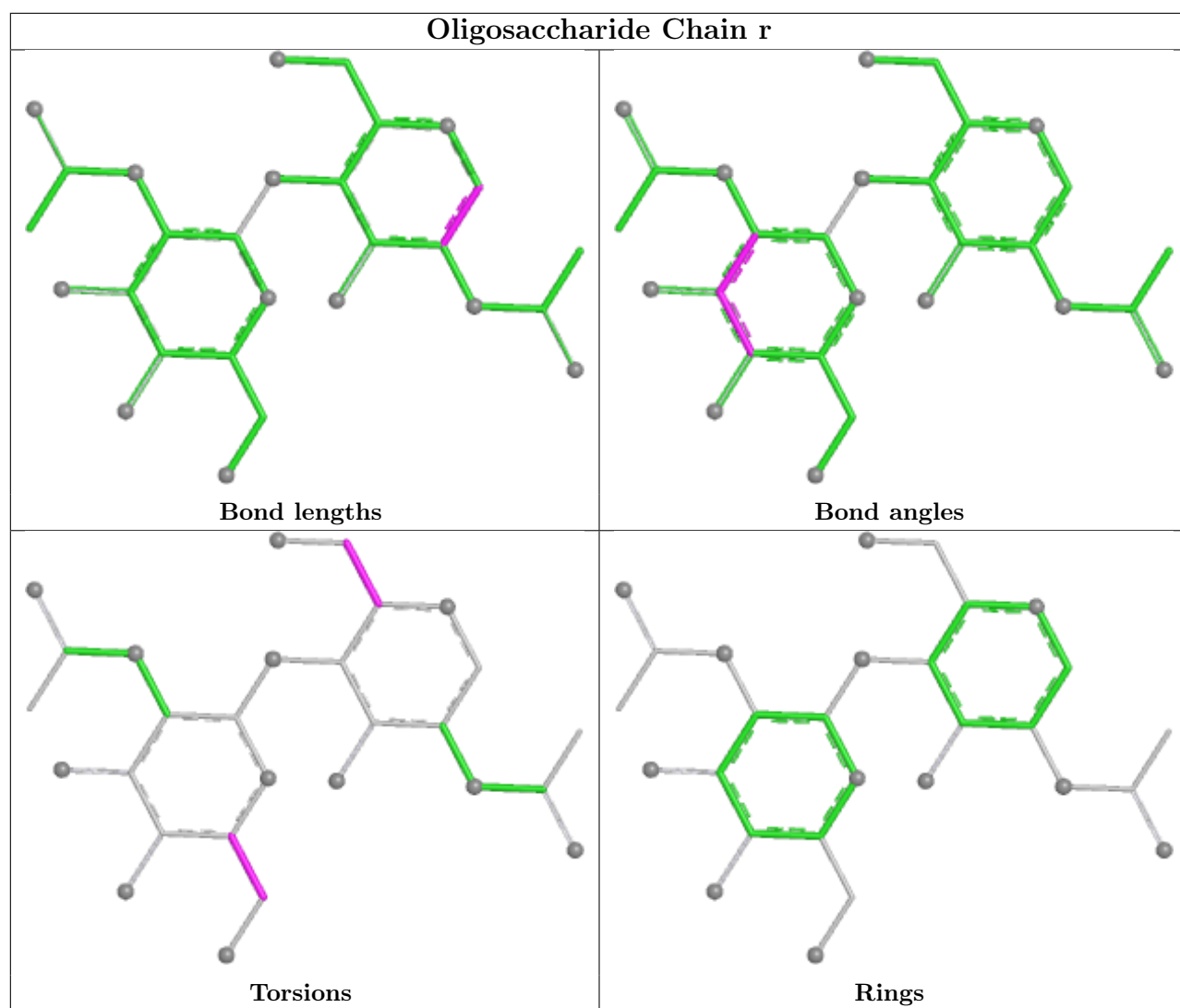


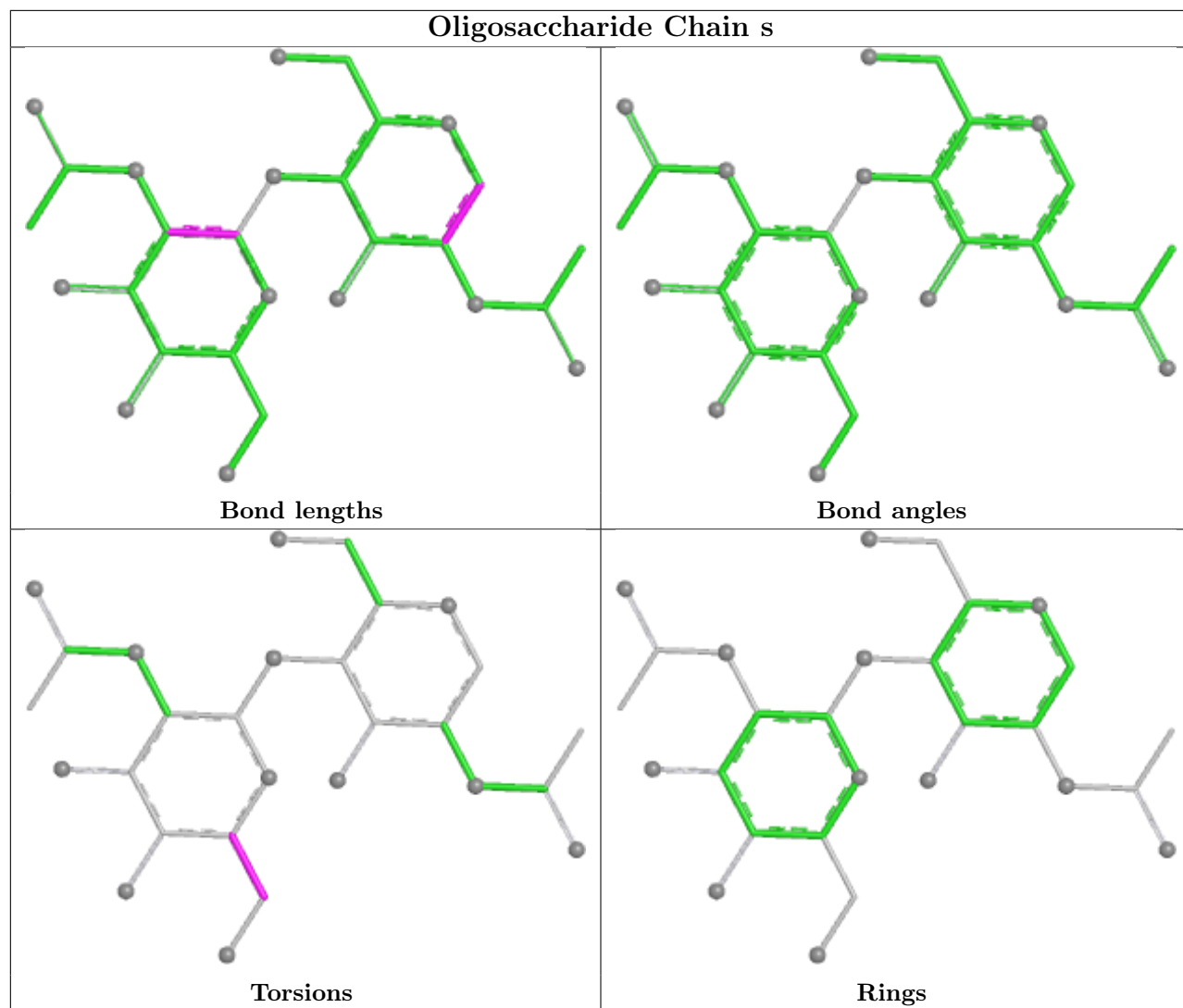


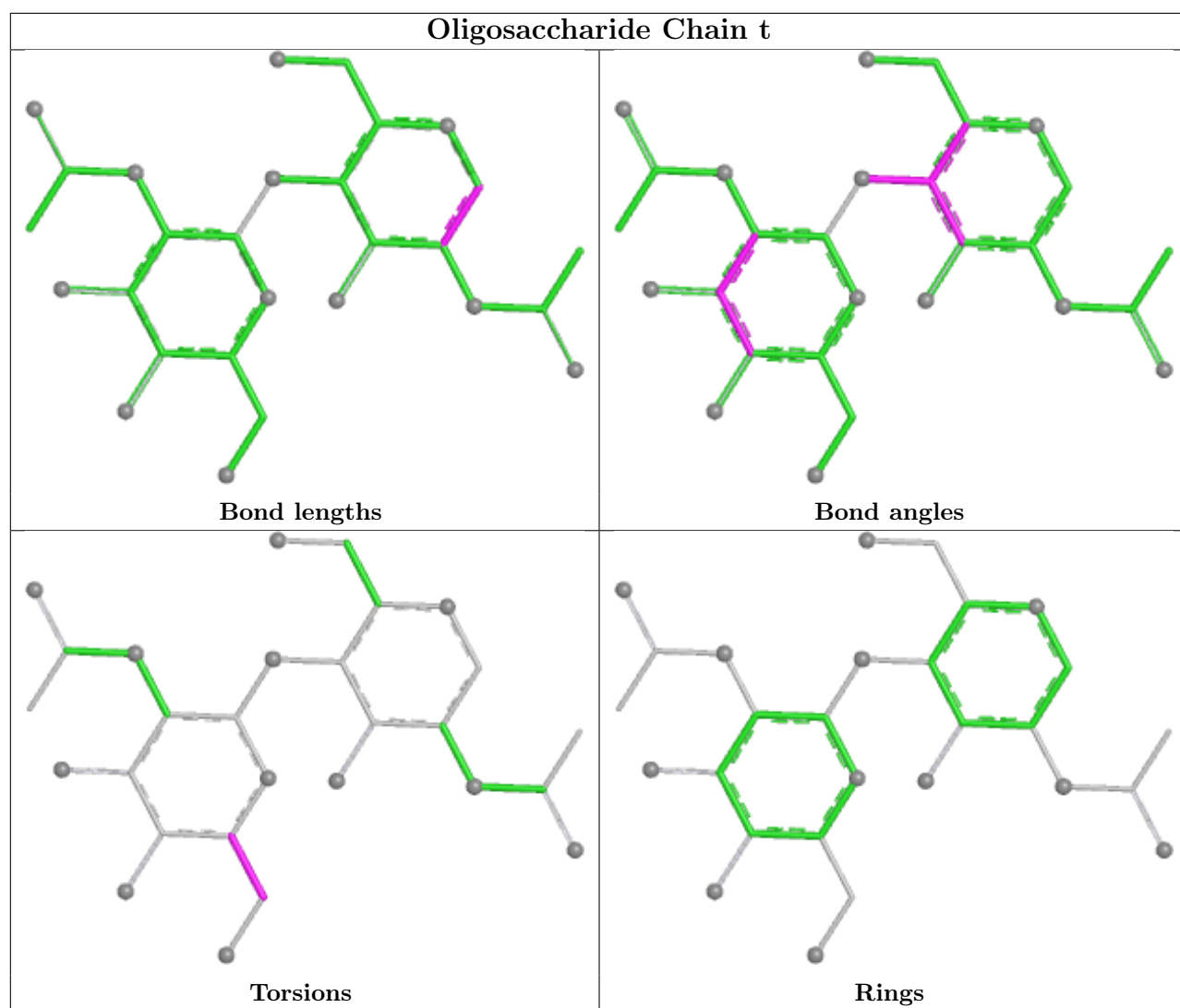


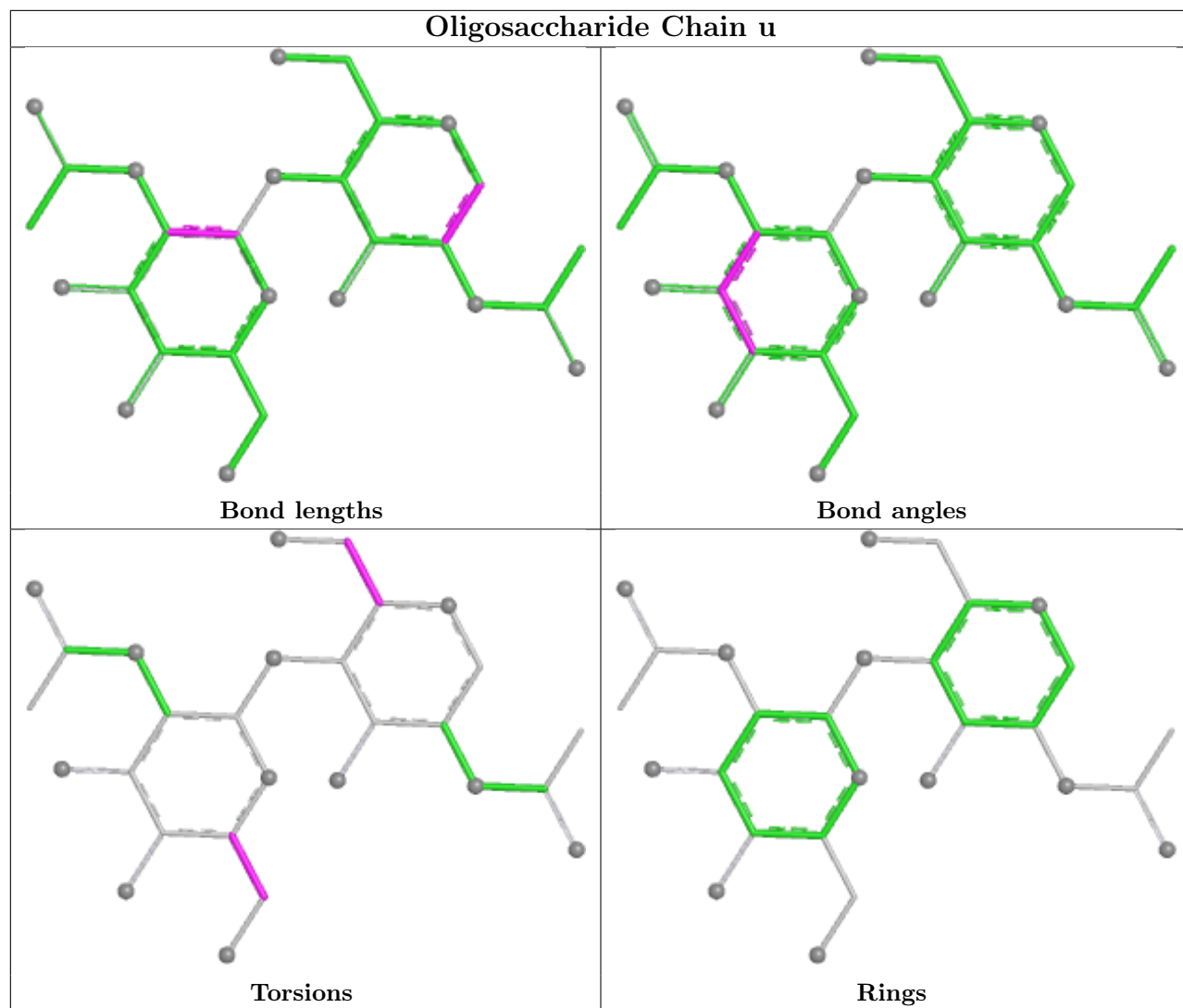


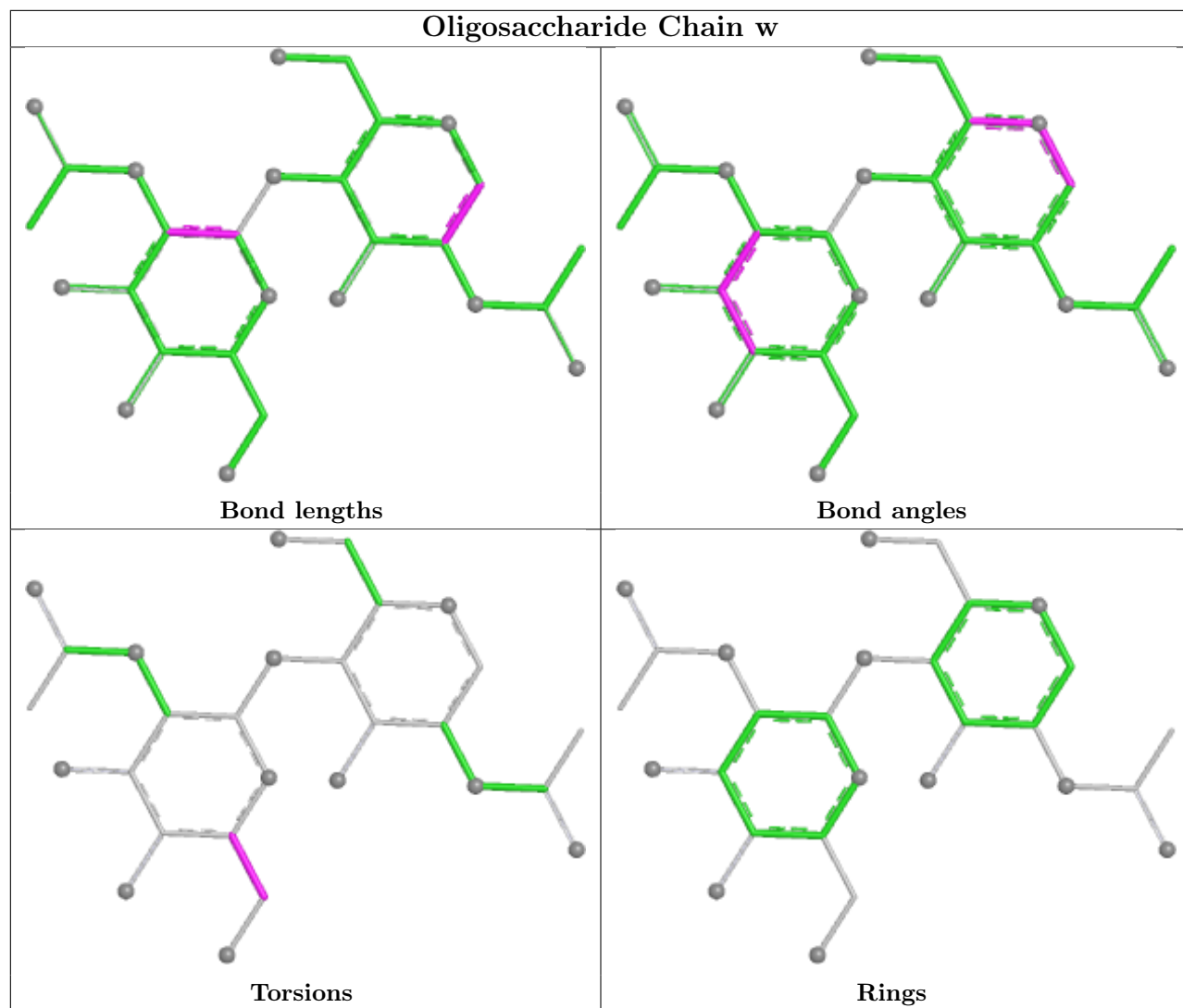


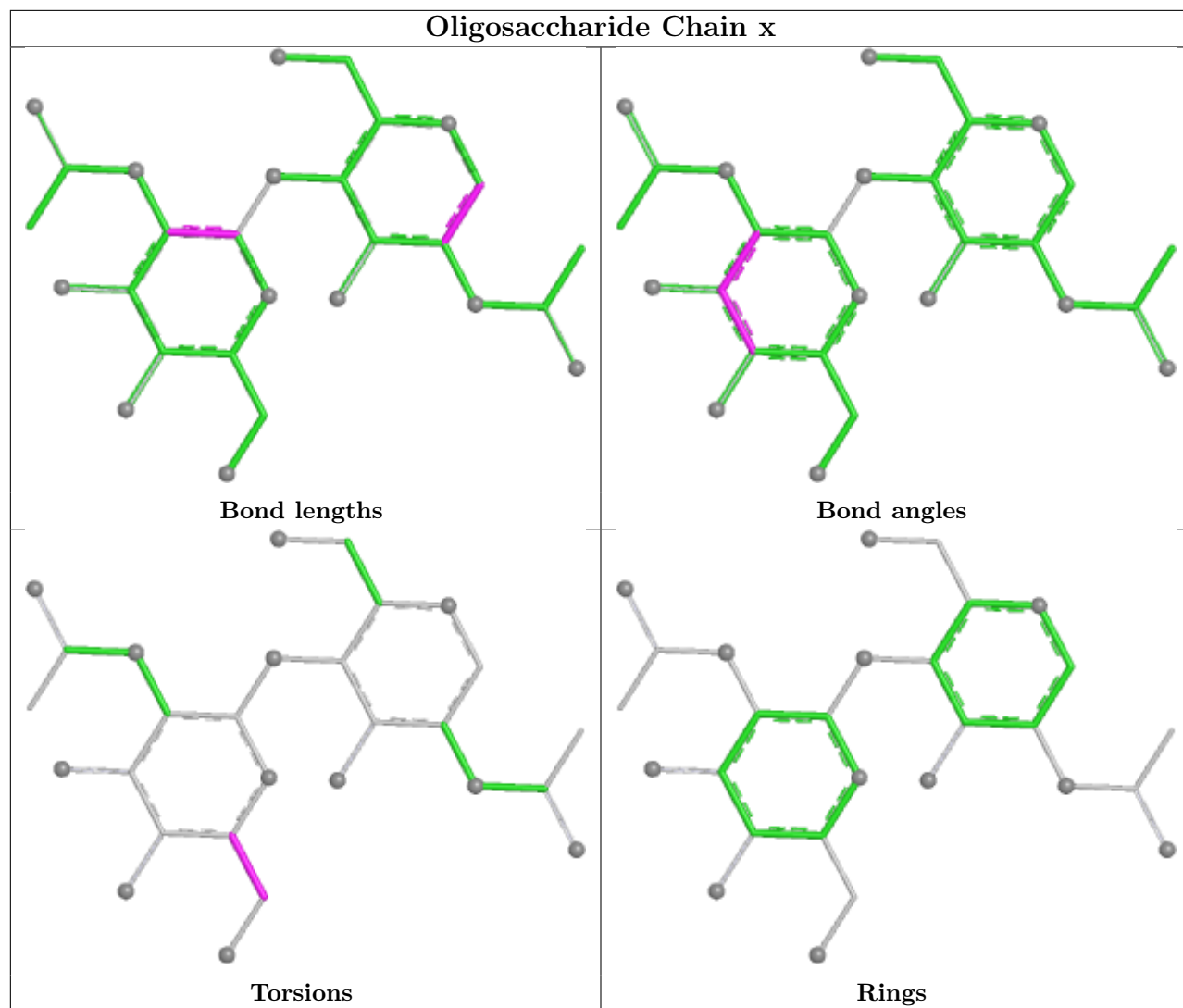


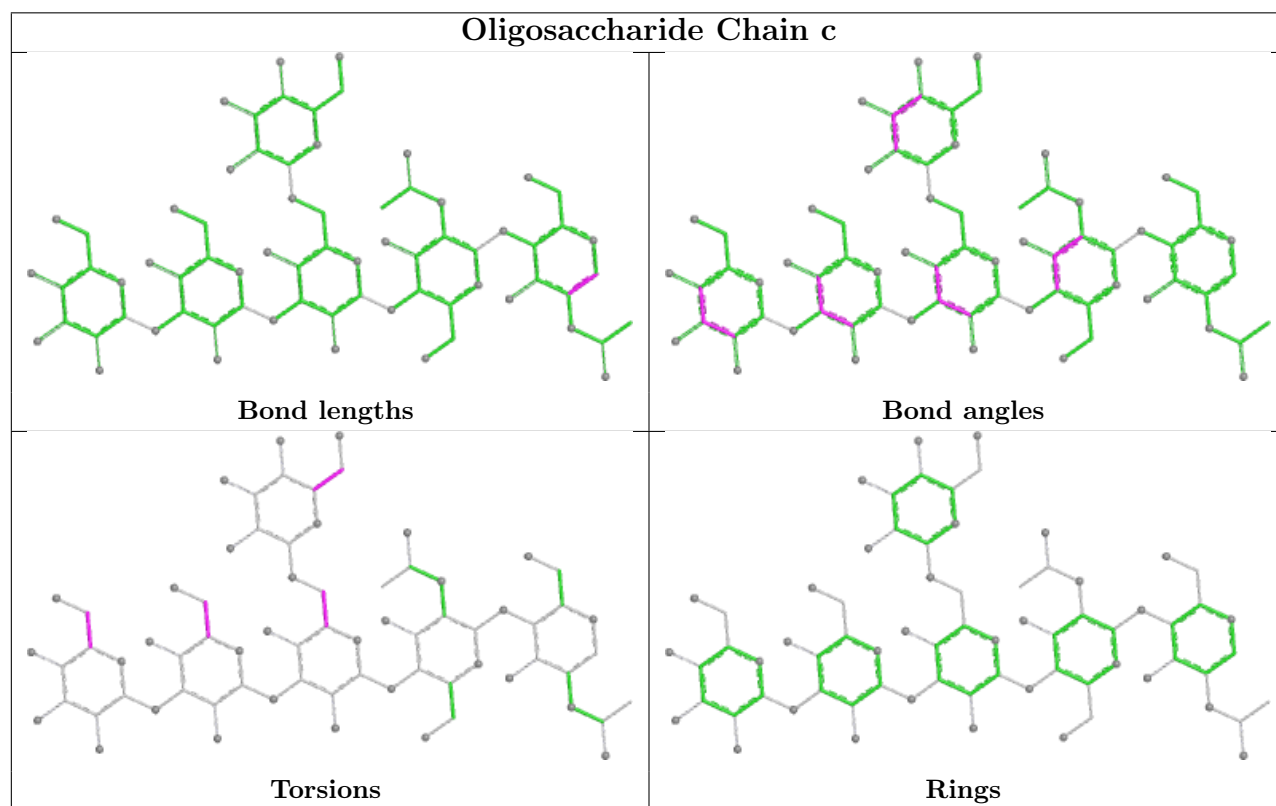
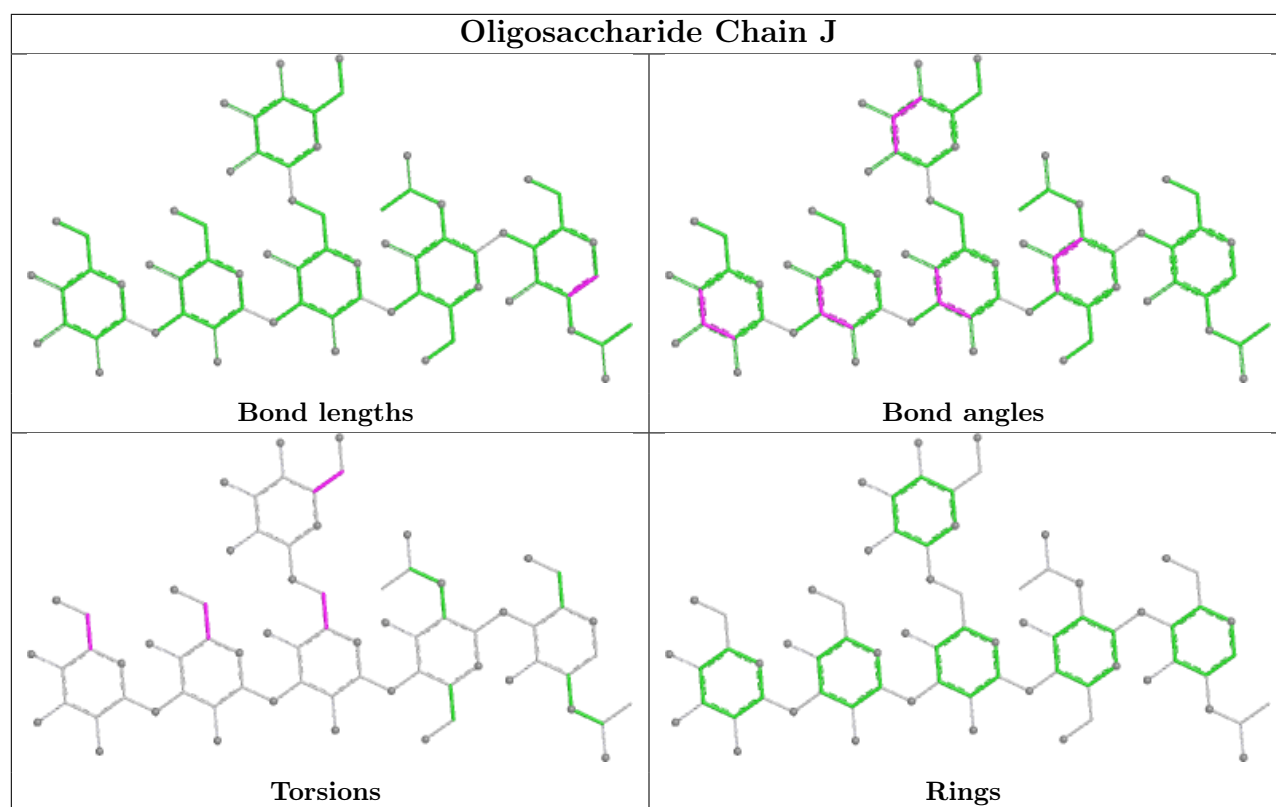


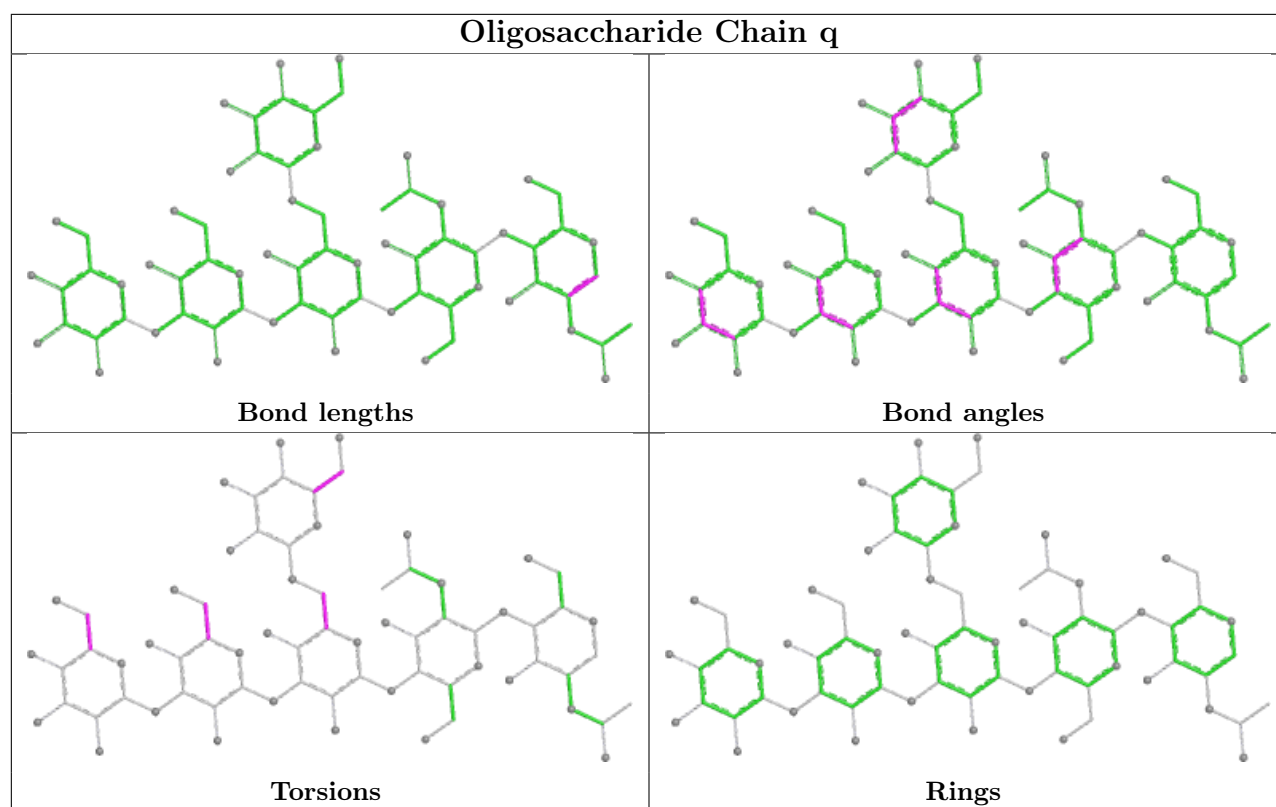


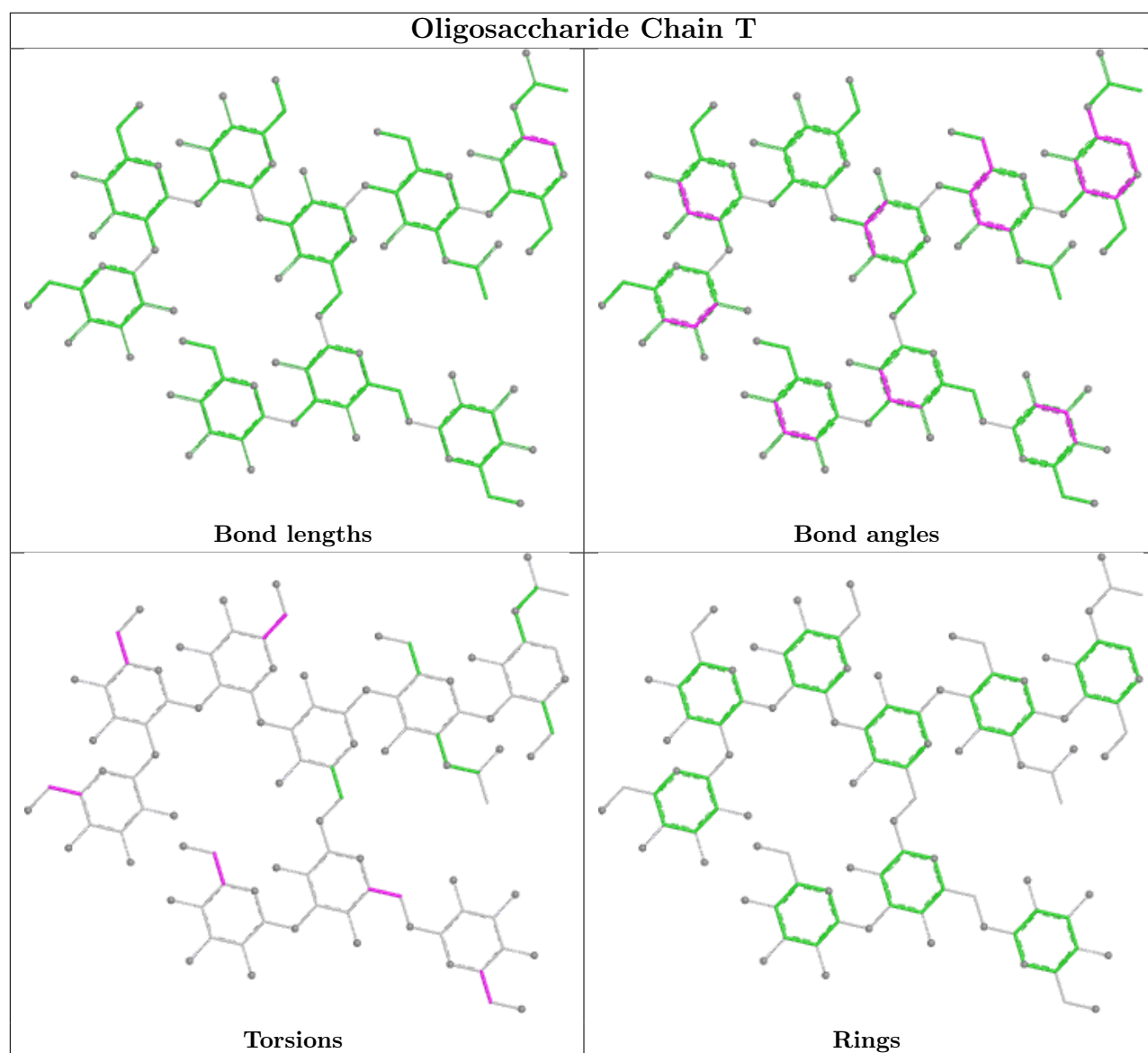


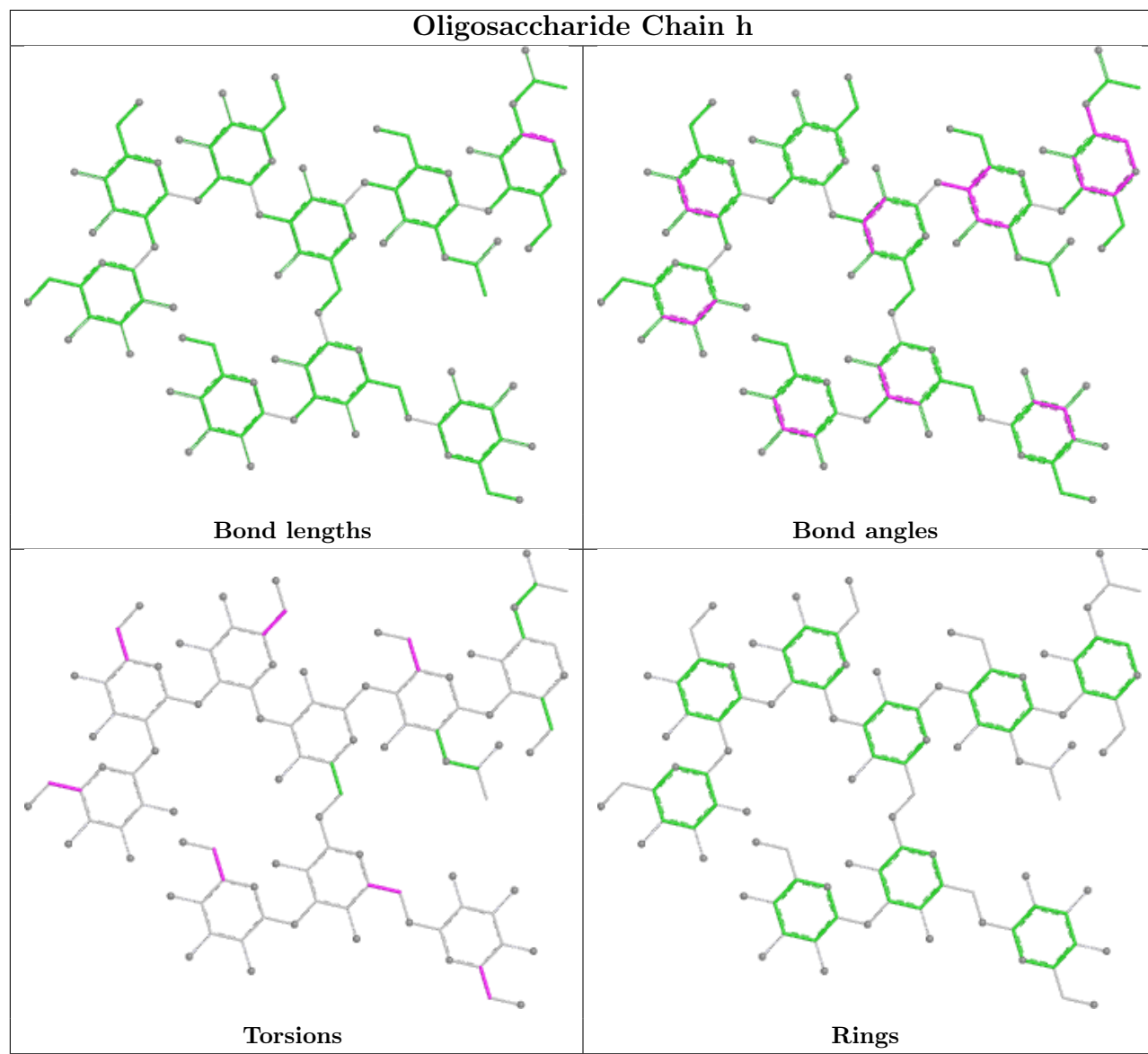


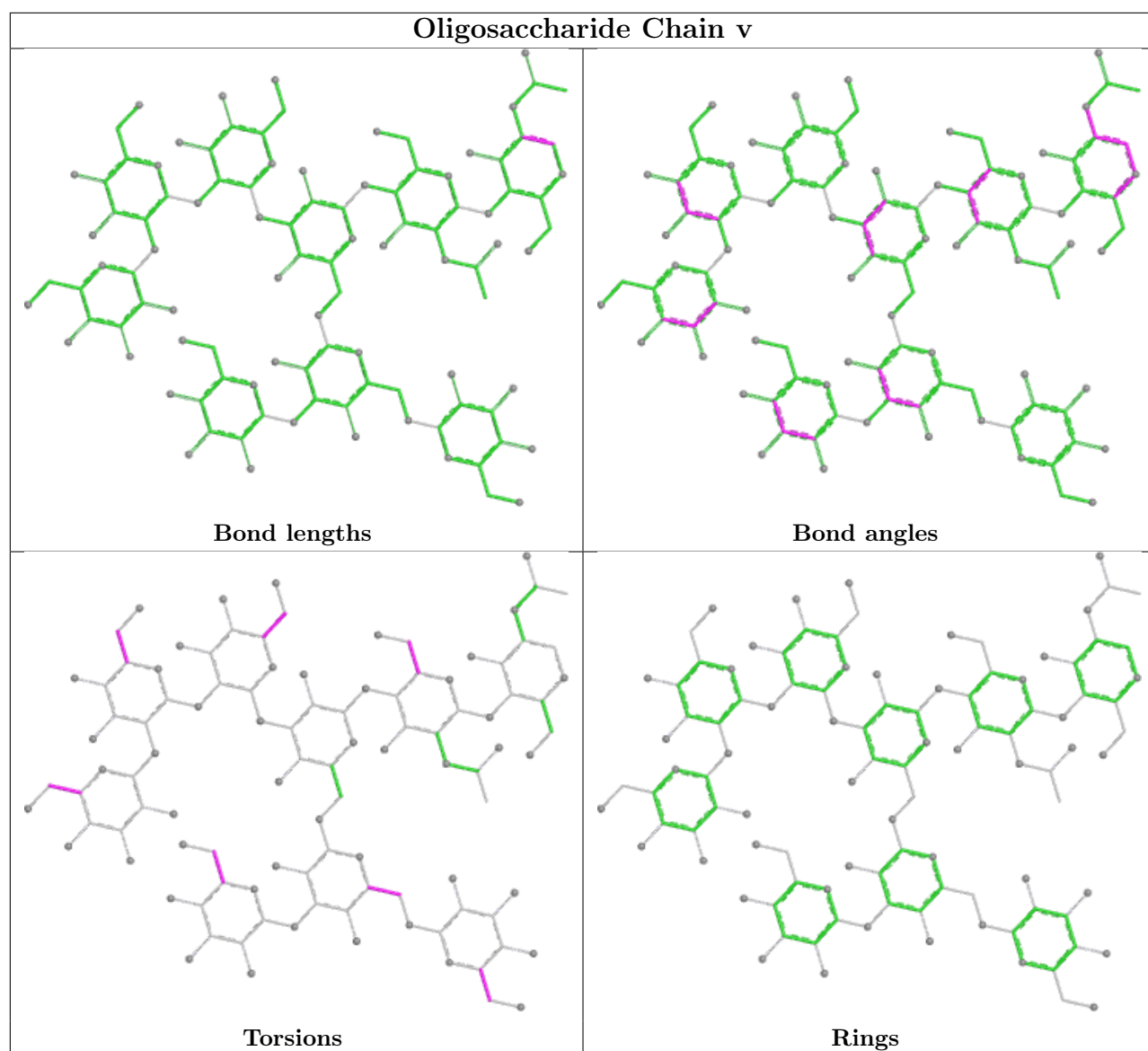


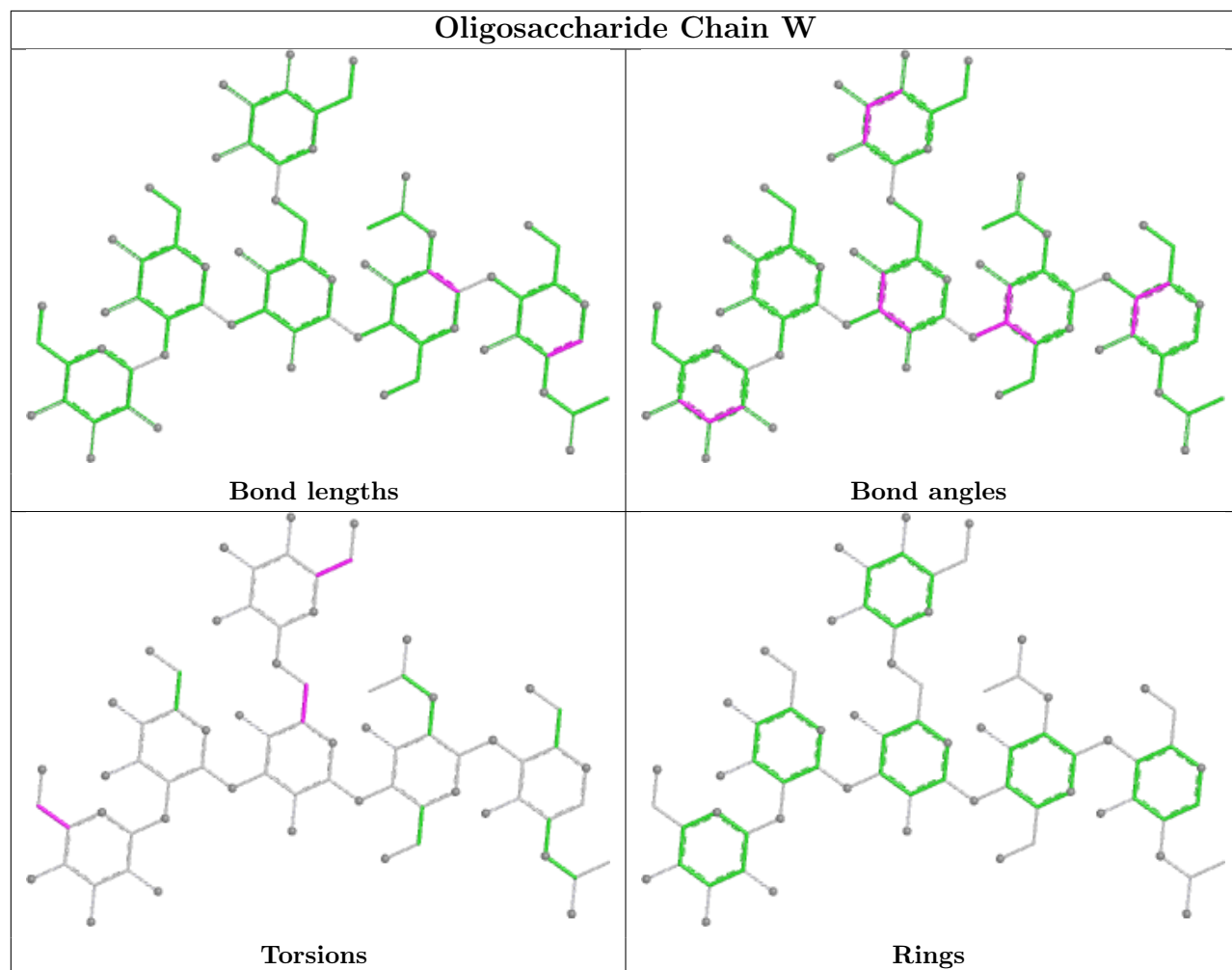


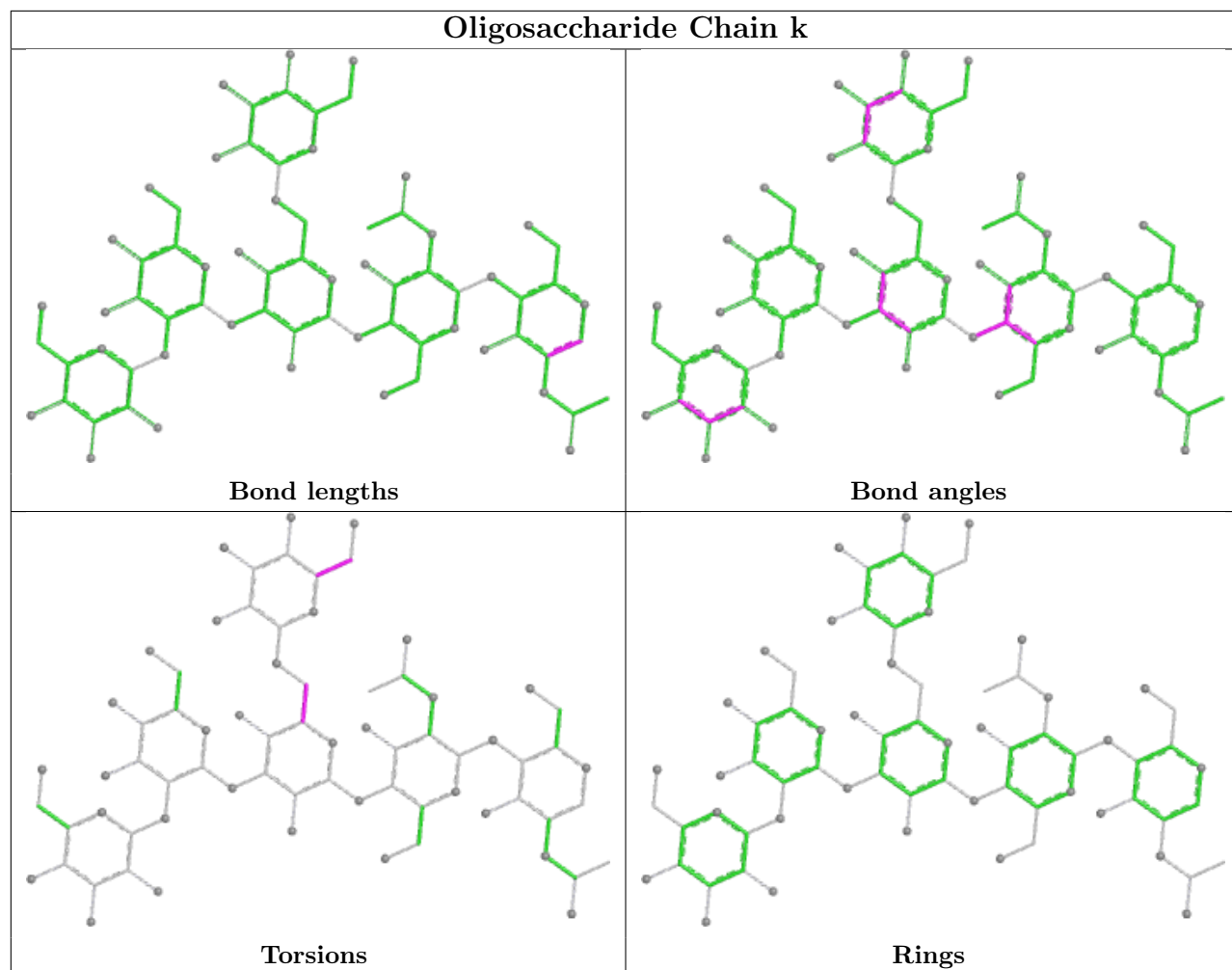


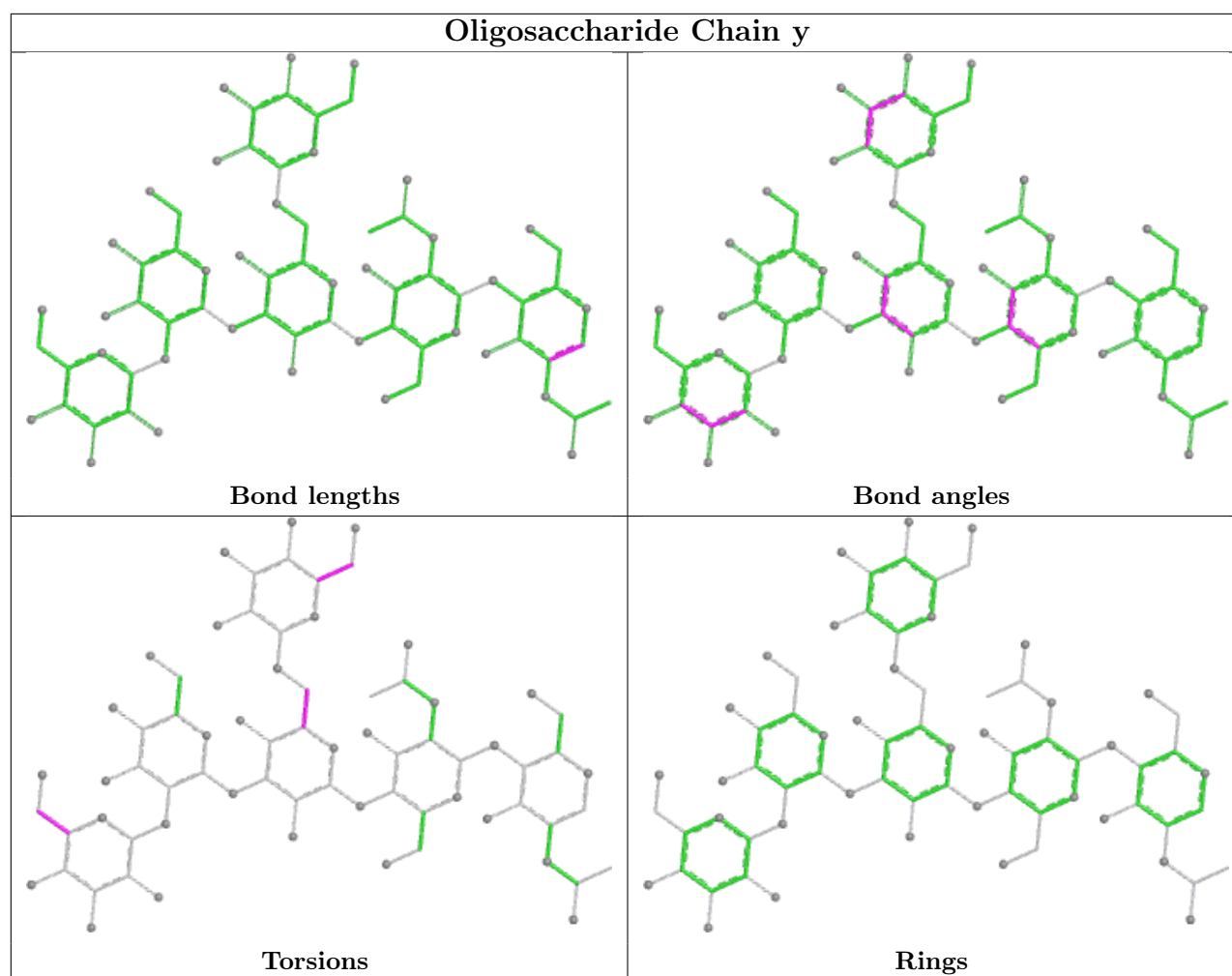












5.6 Ligand geometry [i](#)

15 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
8	NAG	A	705	1	14,14,15	1.11	1 (7%)	17,19,21	0.98	1 (5%)
8	NAG	C	704	1	14,14,15	1.06	1 (7%)	17,19,21	0.92	1 (5%)
8	NAG	A	704	1	14,14,15	1.04	1 (7%)	17,19,21	0.88	1 (5%)
8	NAG	A	701	1	14,14,15	1.04	1 (7%)	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	A	702	1	14,14,15	0.93	1 (7%)	17,19,21	1.31	3 (17%)
8	NAG	A	703	1	14,14,15	0.95	1 (7%)	17,19,21	1.17	2 (11%)
8	NAG	B	702	1	14,14,15	0.93	1 (7%)	17,19,21	1.26	2 (11%)
8	NAG	B	701	1	14,14,15	1.02	1 (7%)	17,19,21	0.59	0
8	NAG	B	704	1	14,14,15	1.06	1 (7%)	17,19,21	0.86	1 (5%)
8	NAG	B	705	1	14,14,15	1.05	1 (7%)	17,19,21	1.04	1 (5%)
8	NAG	C	702	1	14,14,15	0.89	1 (7%)	17,19,21	1.27	2 (11%)
8	NAG	C	703	1	14,14,15	0.98	1 (7%)	17,19,21	1.16	2 (11%)
8	NAG	C	705	1	14,14,15	1.09	1 (7%)	17,19,21	1.01	1 (5%)
8	NAG	B	703	1	14,14,15	0.95	1 (7%)	17,19,21	1.16	2 (11%)
8	NAG	C	701	1	14,14,15	1.05	1 (7%)	17,19,21	0.58	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
8	NAG	A	705	1	-	1/6/23/26	0/1/1/1
8	NAG	C	704	1	-	2/6/23/26	0/1/1/1
8	NAG	A	704	1	-	1/6/23/26	0/1/1/1
8	NAG	A	701	1	-	1/6/23/26	0/1/1/1
8	NAG	A	702	1	-	2/6/23/26	0/1/1/1
8	NAG	A	703	1	-	2/6/23/26	0/1/1/1
8	NAG	B	702	1	-	2/6/23/26	0/1/1/1
8	NAG	B	701	1	-	1/6/23/26	0/1/1/1
8	NAG	B	704	1	-	1/6/23/26	0/1/1/1
8	NAG	B	705	1	-	1/6/23/26	0/1/1/1
8	NAG	C	702	1	-	2/6/23/26	0/1/1/1
8	NAG	C	703	1	-	1/6/23/26	0/1/1/1
8	NAG	C	705	1	-	1/6/23/26	0/1/1/1
8	NAG	B	703	1	-	1/6/23/26	0/1/1/1
8	NAG	C	701	1	-	1/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	705	NAG	C1-C2	3.85	1.57	1.52
8	C	705	NAG	C1-C2	3.78	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	701	NAG	C1-C2	3.76	1.57	1.52
8	A	701	NAG	C1-C2	3.72	1.57	1.52
8	B	704	NAG	C1-C2	3.70	1.57	1.52
8	C	704	NAG	C1-C2	3.68	1.57	1.52
8	B	701	NAG	C1-C2	3.68	1.57	1.52
8	A	704	NAG	C1-C2	3.64	1.57	1.52
8	B	705	NAG	C1-C2	3.61	1.57	1.52
8	C	703	NAG	C1-C2	3.29	1.56	1.52
8	B	702	NAG	C1-C2	3.15	1.56	1.52
8	A	702	NAG	C1-C2	3.14	1.56	1.52
8	B	703	NAG	C1-C2	3.13	1.56	1.52
8	A	703	NAG	C1-C2	3.08	1.56	1.52
8	C	702	NAG	C1-C2	3.03	1.56	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	702	NAG	C4-C3-C2	-3.64	105.68	111.02
8	B	702	NAG	C4-C3-C2	-3.47	105.93	111.02
8	C	702	NAG	C4-C3-C2	-3.43	106.00	111.02
8	A	703	NAG	C4-C3-C2	-3.42	106.00	111.02
8	C	703	NAG	C4-C3-C2	-3.27	106.23	111.02
8	B	703	NAG	C4-C3-C2	-3.25	106.25	111.02
8	B	705	NAG	C4-C3-C2	-3.08	106.51	111.02
8	C	705	NAG	C4-C3-C2	-2.89	106.78	111.02
8	A	705	NAG	C4-C3-C2	-2.83	106.87	111.02
8	C	704	NAG	C4-C3-C2	-2.37	107.55	111.02
8	A	704	NAG	C4-C3-C2	-2.32	107.61	111.02
8	B	704	NAG	C4-C3-C2	-2.29	107.66	111.02
8	C	702	NAG	C1-O5-C5	-2.19	109.25	112.19
8	B	703	NAG	C1-C2-N2	-2.18	106.99	110.43
8	C	703	NAG	C1-C2-N2	-2.18	107.00	110.43
8	A	703	NAG	C1-C2-N2	-2.09	107.15	110.43
8	A	702	NAG	C1-O5-C5	-2.06	109.42	112.19
8	B	702	NAG	C1-O5-C5	-2.06	109.43	112.19
8	A	702	NAG	C2-N2-C7	-2.00	120.22	122.90

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	702	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	C	702	NAG	C4-C5-C6-O6
8	B	702	NAG	C4-C5-C6-O6
8	A	703	NAG	O5-C5-C6-O6
8	C	704	NAG	O5-C5-C6-O6
8	A	702	NAG	O5-C5-C6-O6
8	B	702	NAG	O5-C5-C6-O6
8	C	702	NAG	O5-C5-C6-O6
8	C	703	NAG	O5-C5-C6-O6
8	B	703	NAG	O5-C5-C6-O6
8	B	704	NAG	O5-C5-C6-O6
8	C	701	NAG	O5-C5-C6-O6
8	A	701	NAG	O5-C5-C6-O6
8	B	701	NAG	O5-C5-C6-O6
8	B	705	NAG	O5-C5-C6-O6
8	C	705	NAG	O5-C5-C6-O6
8	A	705	NAG	O5-C5-C6-O6
8	A	703	NAG	C4-C5-C6-O6
8	A	704	NAG	O5-C5-C6-O6
8	C	704	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	704	NAG	1	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.

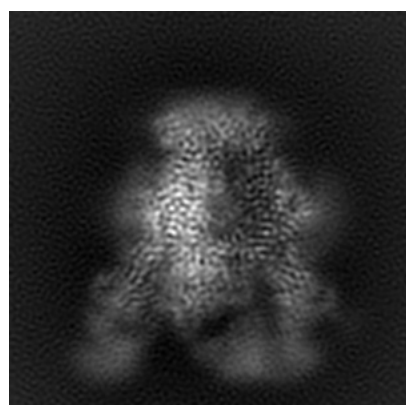
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23565. These allow visual inspection of the internal detail of the map and identification of artifacts.

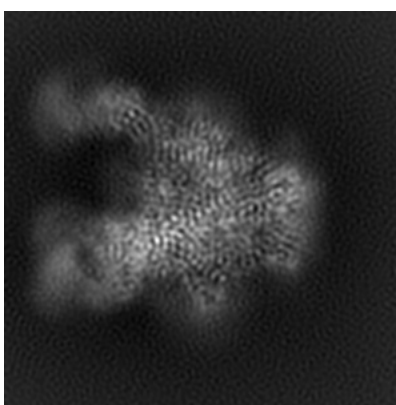
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

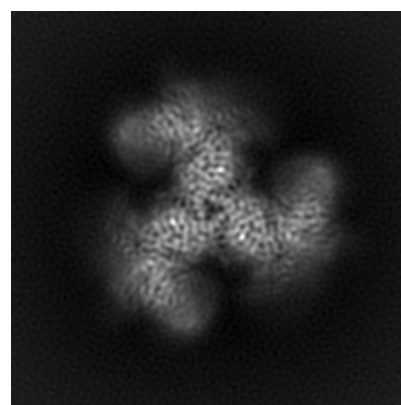
6.1.1 Primary map



X



Y

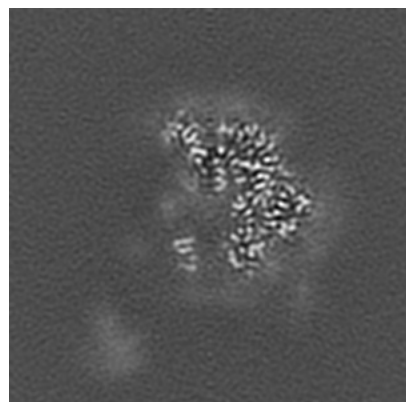


Z

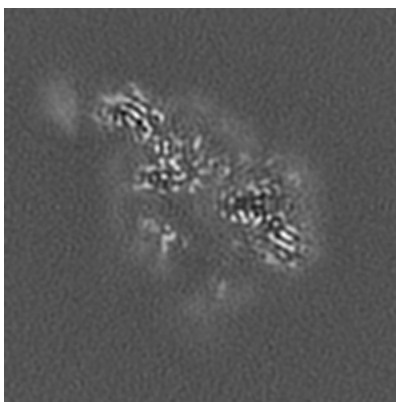
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

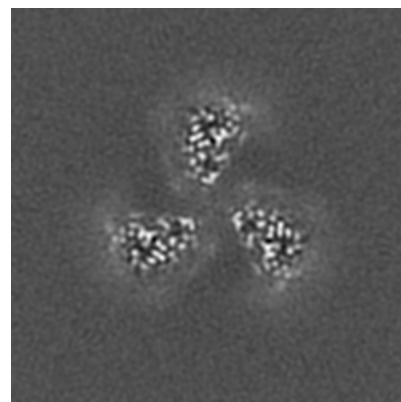
6.2.1 Primary map



X Index: 110



Y Index: 110

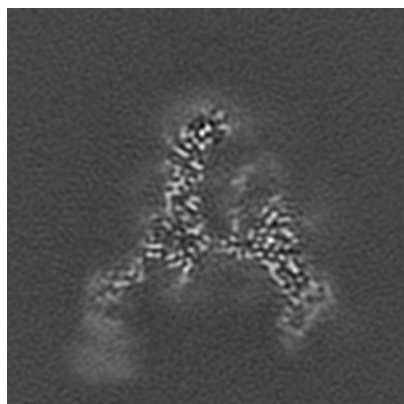


Z Index: 110

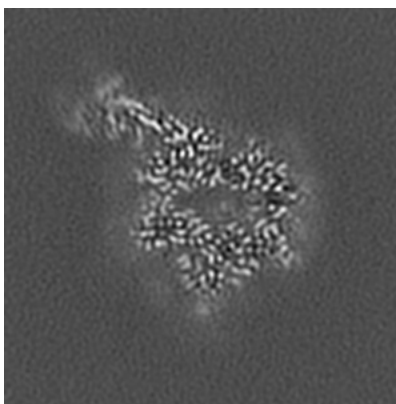
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

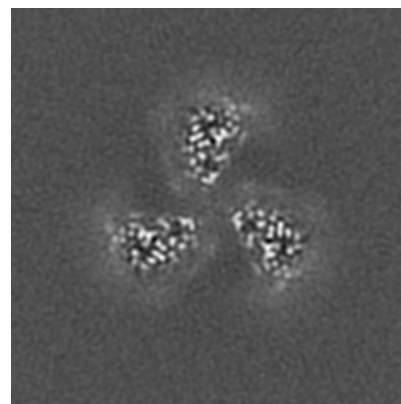
6.3.1 Primary map



X Index: 95



Y Index: 99

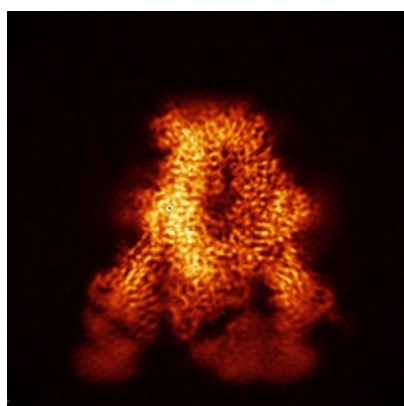


Z Index: 110

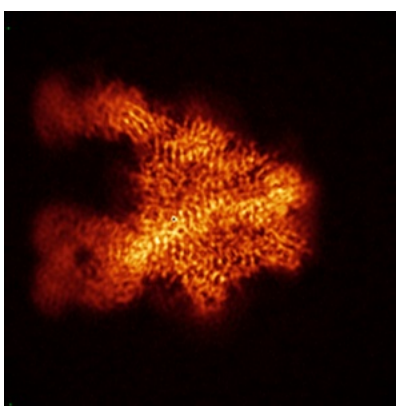
The images above show the largest variance slices of the map in three orthogonal directions.

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

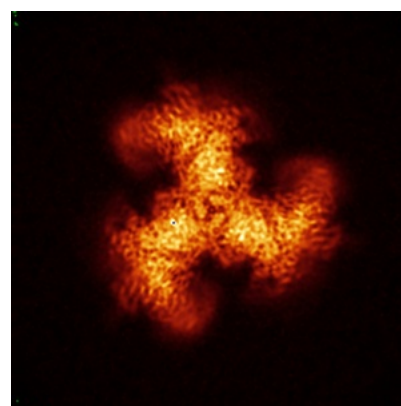
6.4.1 Primary map



X



Y

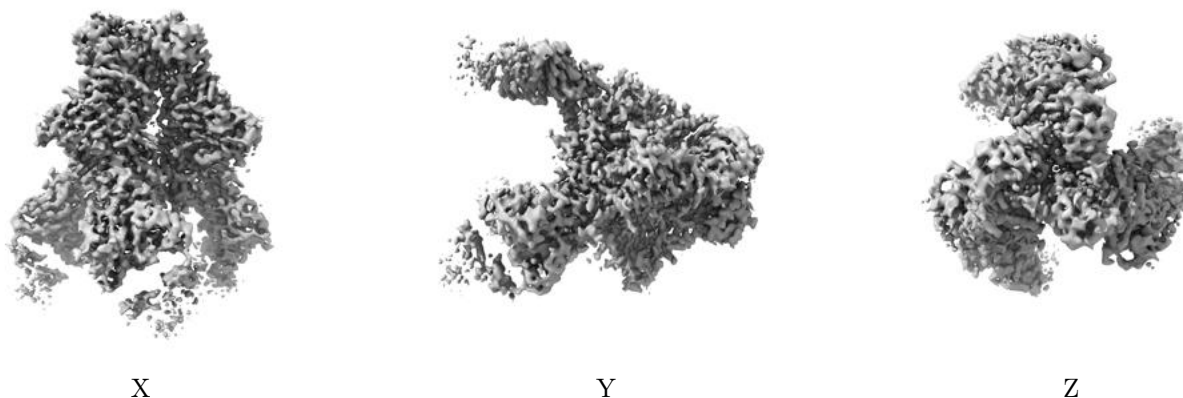


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

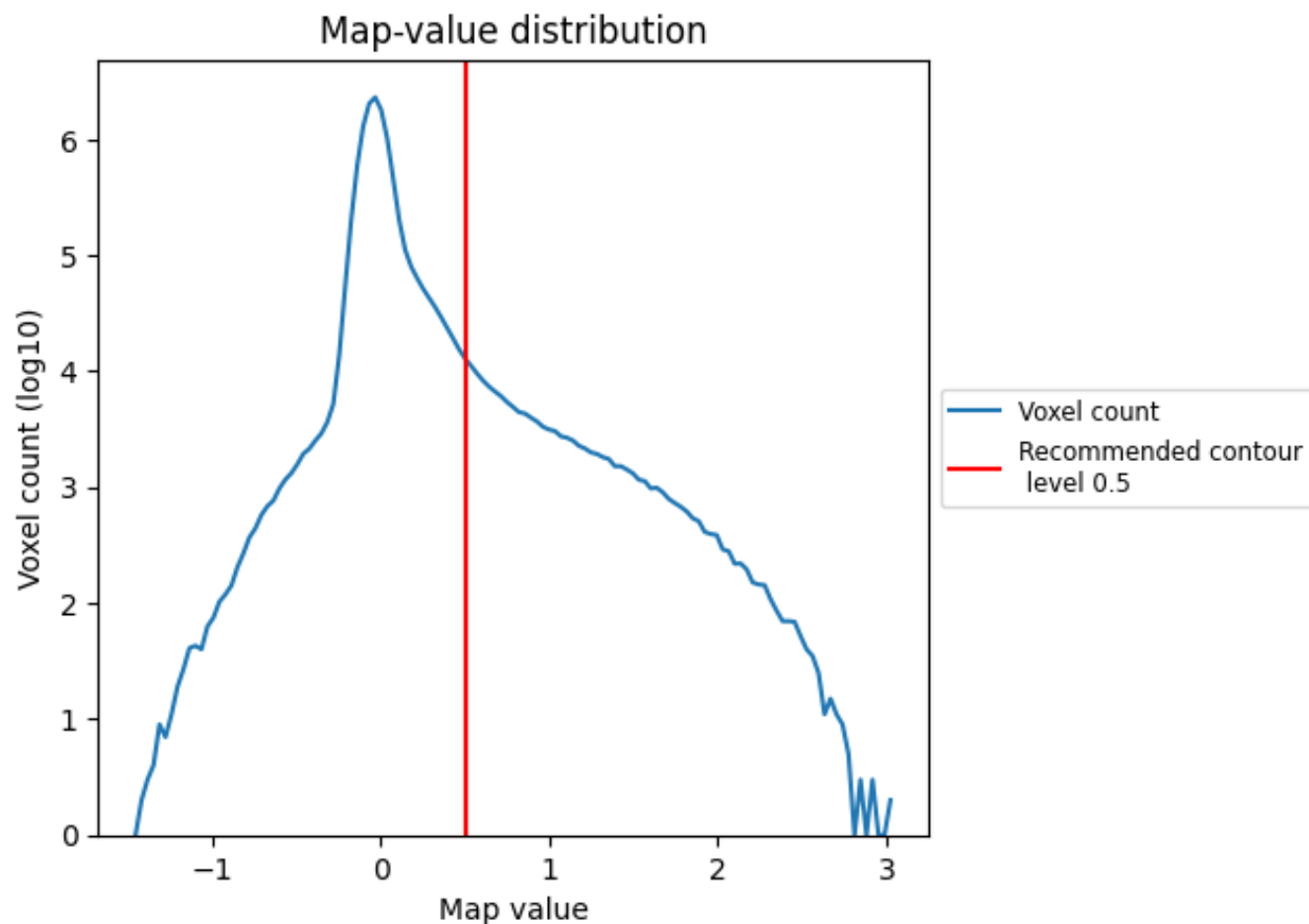
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

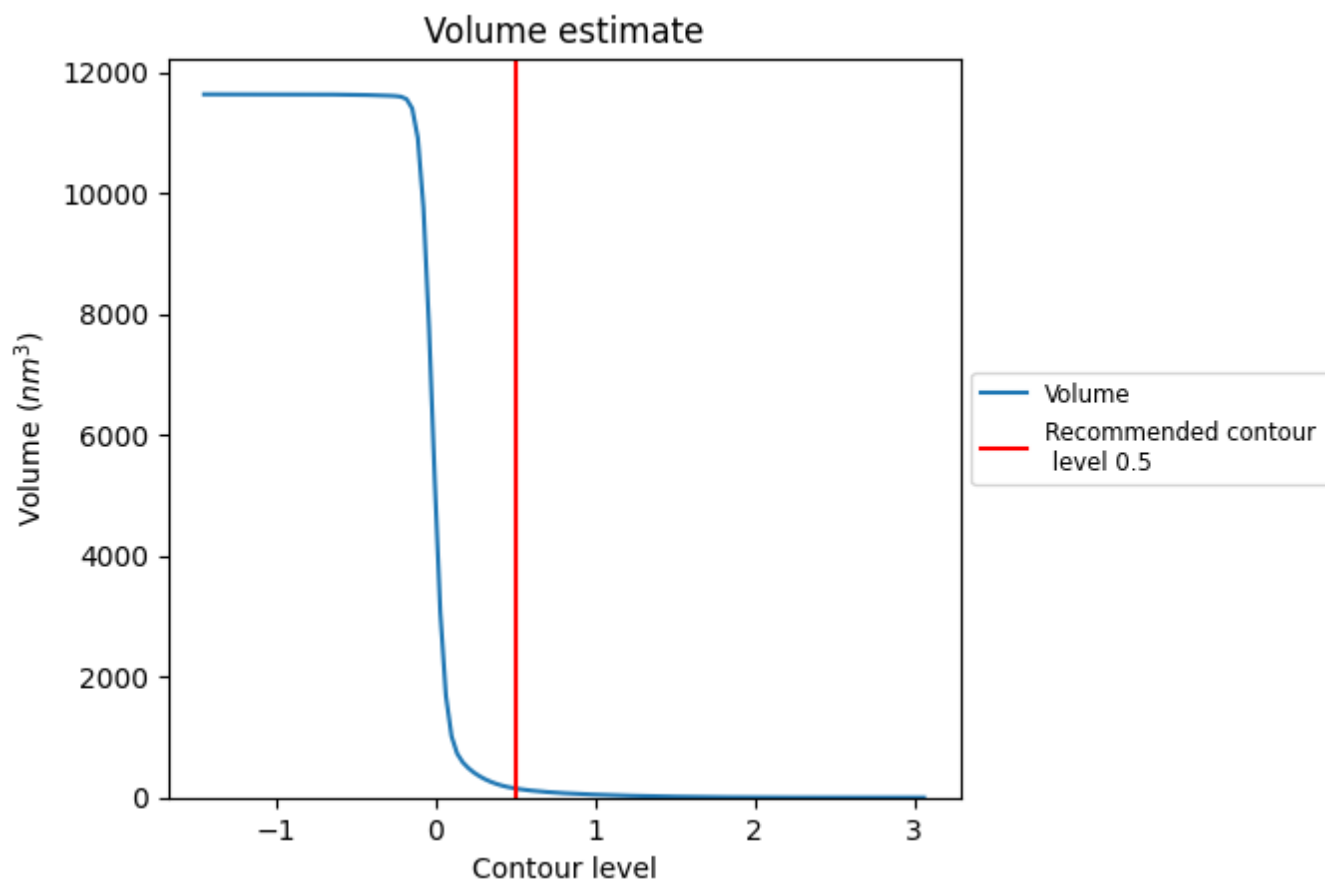
This section contains the results of statistical analysis of the map.

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.

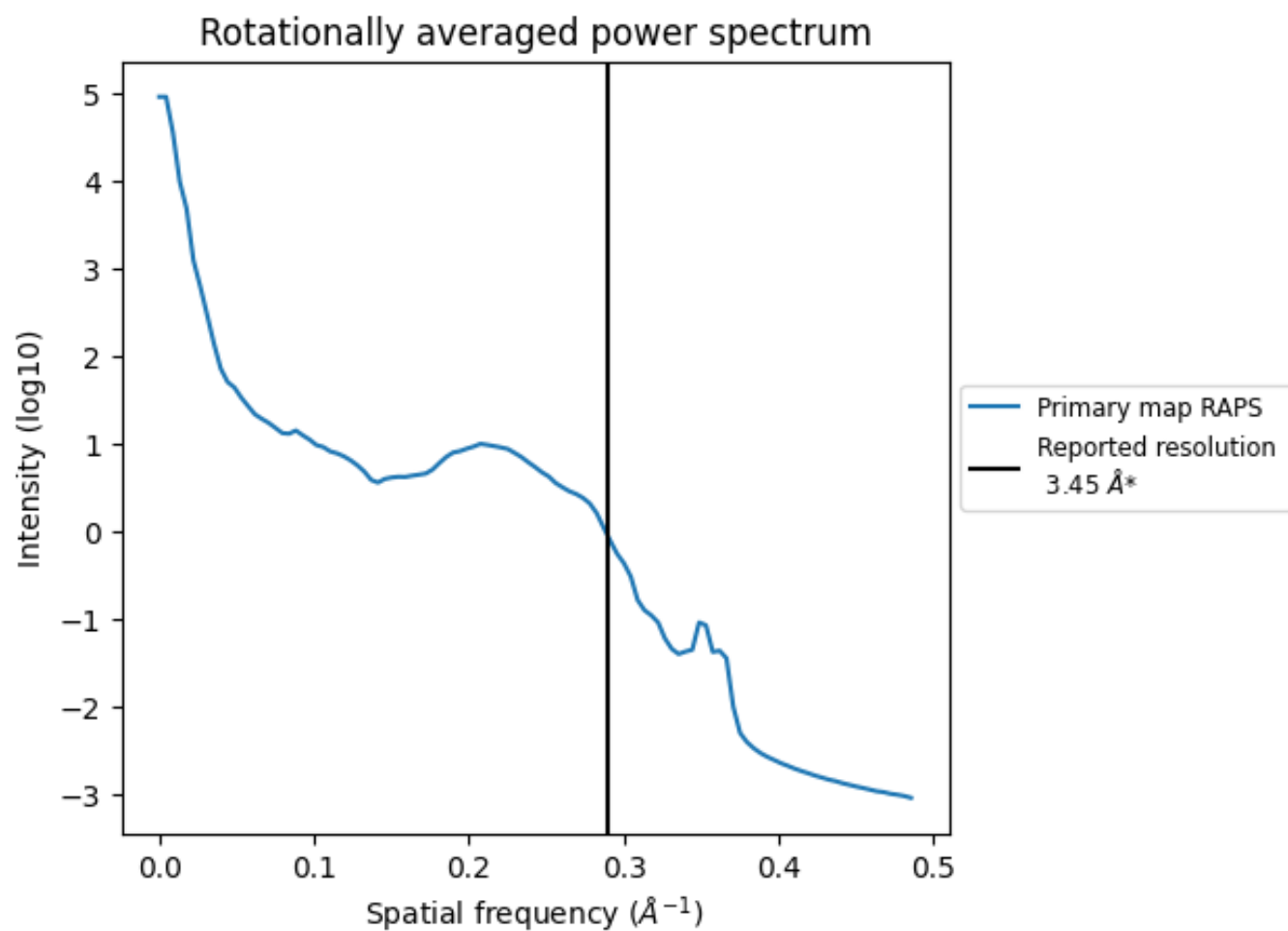
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 150 nm³; this corresponds to an approximate mass of 136 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 0.290 Å⁻¹

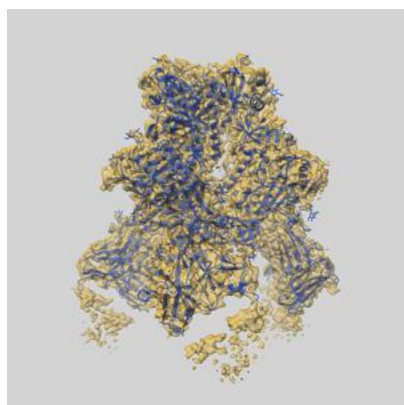
8 Fourier-Shell correlation

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

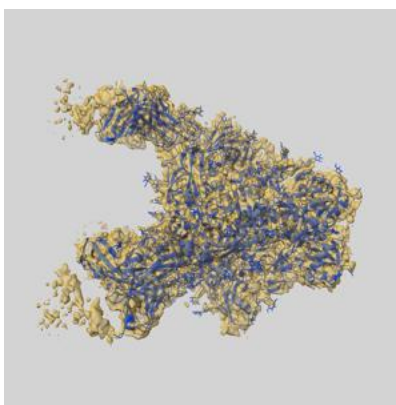
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23565 and PDB model 7LX3. Per-residue inclusion information can be found in section [3](#) on page [11](#).

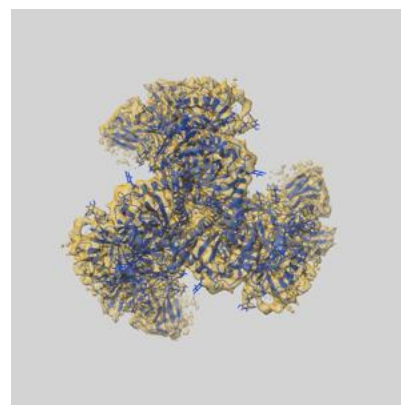
9.1 Map-model overlay [i](#)



X



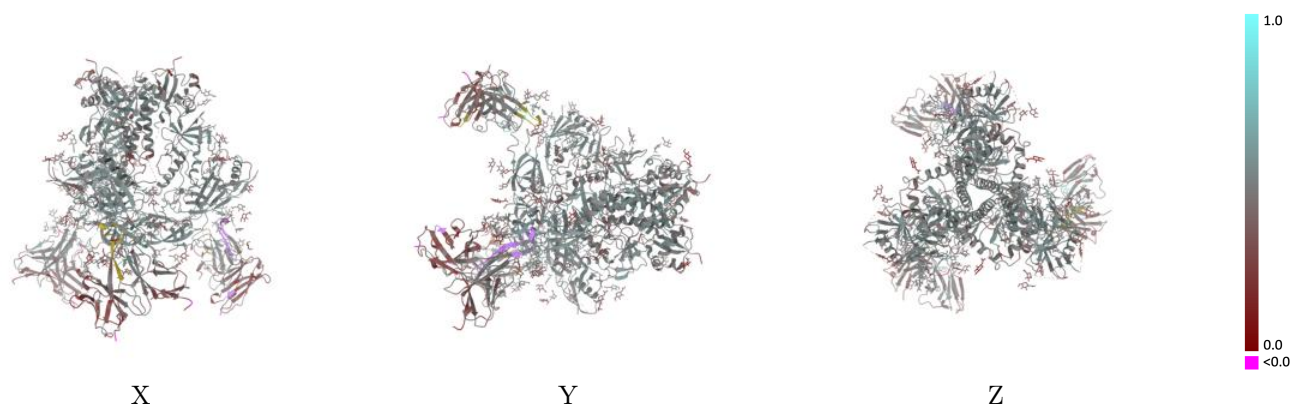
Y



Z

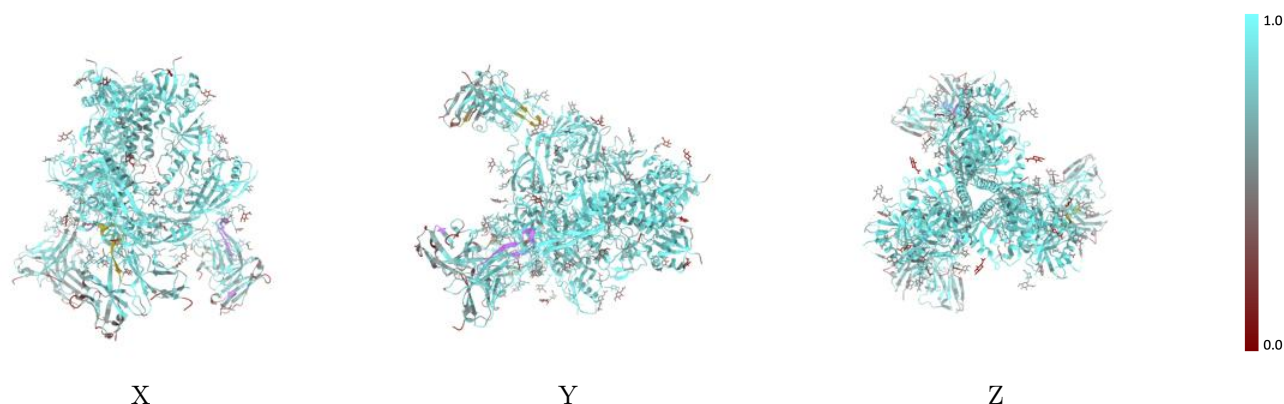
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



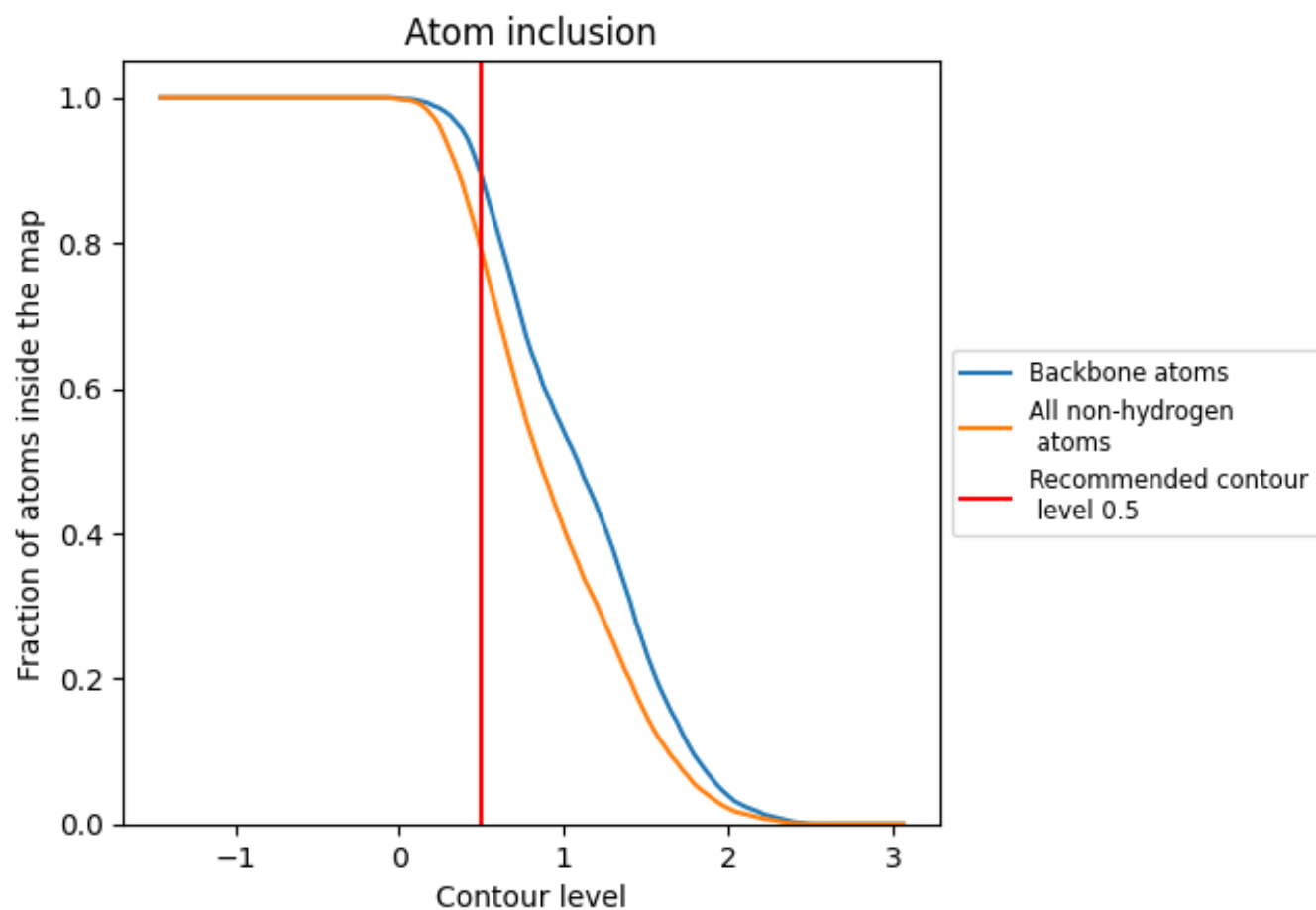
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 79% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7880	 0.4600
A	 0.8400	 0.4930
B	 0.8390	 0.4920
C	 0.8410	 0.4920
D	 0.3210	 0.4290
E	 0.5360	 0.3680
F	 0.5000	 0.4410
G	 0.4640	 0.3000
H	 0.6940	 0.3760
I	 0.5000	 0.3420
J	 0.7360	 0.4670
K	 0.6790	 0.3900
L	 0.7580	 0.4240
M	 0.7460	 0.4250
N	 0.6870	 0.3750
O	 0.7470	 0.4220
P	 0.6900	 0.3740
Q	 0.3210	 0.3420
R	 0.5000	 0.3350
S	 0.6790	 0.5160
T	 0.7900	 0.4730
U	 0.5360	 0.4060
V	 0.5710	 0.4330
W	 0.7360	 0.4430
X	 0.3210	 0.4260
Y	 0.5360	 0.3600
Z	 0.5360	 0.4350
a	 0.4640	 0.2950
b	 0.5710	 0.3630
c	 0.7220	 0.4680
d	 0.6790	 0.4080
e	 0.3210	 0.3490
f	 0.5000	 0.3210
g	 0.6790	 0.5230
h	 0.8090	 0.4620



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Chain	Atom inclusion	Q-score
i	 0.5360	 0.4010
j	 0.5710	 0.4420
k	 0.7640	 0.4470
l	 0.3210	 0.4130
m	 0.5360	 0.3620
n	 0.5000	 0.4290
o	 0.5710	 0.3010
p	 0.5360	 0.3350
q	 0.7220	 0.4660
r	 0.6790	 0.4010
s	 0.3210	 0.3240
t	 0.4290	 0.3080
u	 0.6790	 0.5140
v	 0.7620	 0.4460
w	 0.5360	 0.3900
x	 0.5710	 0.4380
y	 0.7640	 0.4480