



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:31 AM UTC

PDB ID : 6P65 / pdb_00006p65
EMDB ID : EMD-20260
Title : HIV Env 16055 NFL TD 2CC+ in complex with antibody 1C2 fragment anti-gen binding
Authors : Ozorowski, G.; Torres, J.L.; Ward, A.B.
Deposited on : 2019-05-31
Resolution : 3.94 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:

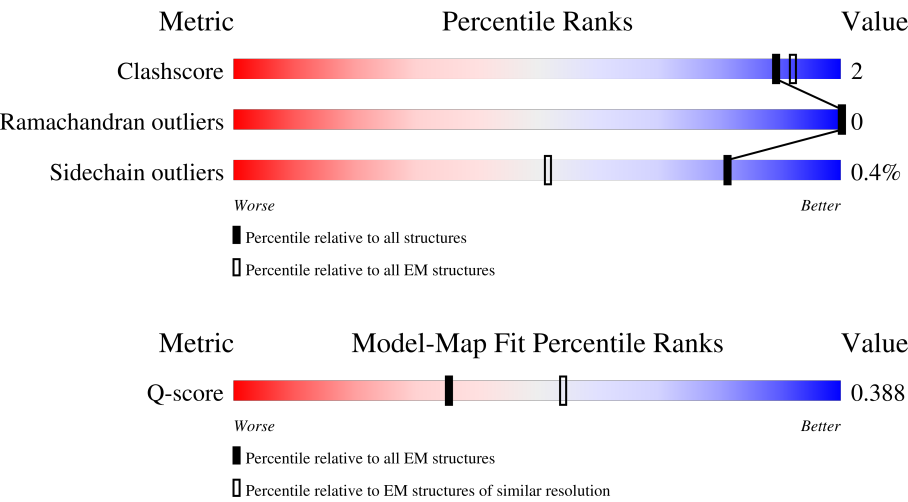
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 i

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

The reported resolution of this entry is 3.94 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	7757 (3.44 - 4.43)

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	680	5% 74% 7% 18%
1	B	680	5% 74% 7% 18%
1	E	680	5% 74% 7% 18%
2	C	259	18% 46% 51%

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Mol	Chain	Length	Quality of chain
2	F	259	
2	H	259	
3	D	235	
3	G	235	
3	L	235	
4	I	5	
4	Q	5	
4	Y	5	
4	f	5	
4	n	5	
4	u	5	
5	0	2	
5	J	2	
5	K	2	
5	M	2	
5	N	2	
5	O	2	
5	P	2	
5	R	2	
5	T	2	
5	U	2	
5	V	2	
5	W	2	
5	Z	2	
5	a	2	

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Mol	Chain	Length	Quality of chain
5	b	2	100%
5	c	2	50%
5	d	2	100%
5	e	2	100%
5	g	2	100%
5	i	2	50%
5	j	2	50%
5	k	2	50%
5	l	2	100%
5	o	2	100%
5	p	2	100%
5	q	2	100%
5	r	2	50%
5	s	2	100%
5	t	2	100%
5	v	2	100%
5	x	2	50%
5	y	2	50%
5	z	2	50%
6	S	3	33%
6	h	3	33%
6	w	3	33%
7	1	3	67%
7	X	3	67%
7	m	3	67%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20319 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 HIV Env 16055 NFL TD 2CC+.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	557	Total	C	N	O	S	0	0
			4405	2772	771	828	34		
1	B	557	Total	C	N	O	S	0	0
			4405	2772	771	828	34		
1	E	557	Total	C	N	O	S	0	0
			4405	2772	771	828	34		

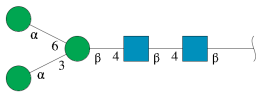
- Molecule 2 is a protein called Rabbit antibody 1C2 heavy chain fragment antigen binding.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	126	Total	C	N	O	S	0	0
			943	600	156	182	5		
2	C	126	Total	C	N	O	S	0	0
			943	600	156	182	5		
2	F	126	Total	C	N	O	S	0	0
			943	600	156	182	5		

- Molecule 3 is a protein called Rabbit antibody 1C2 kappa chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	110	Total	C	N	O	S	0	0
			820	519	133	164	4		
3	D	110	Total	C	N	O	S	0	0
			820	519	133	164	4		
3	G	110	Total	C	N	O	S	0	0
			820	519	133	164	4		

- Molecule 4 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
4	I	5	Total	C	N	O	0	0
			61	34	2	25		
4	Q	5	Total	C	N	O	0	0
			61	34	2	25		
4	Y	5	Total	C	N	O	0	0
			61	34	2	25		
4	f	5	Total	C	N	O	0	0
			61	34	2	25		
4	n	5	Total	C	N	O	0	0
			61	34	2	25		
4	u	5	Total	C	N	O	0	0
			61	34	2	25		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	2	Total	C	N	O	0	0
			28	16	2	10		
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		

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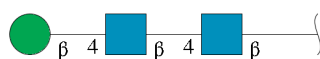
Mol	Chain	Residues	Atoms				AltConf	Trace
5	V	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	Z	2	Total	C	N	O	0	0
			28	16	2	10		
5	a	2	Total	C	N	O	0	0
			28	16	2	10		
5	b	2	Total	C	N	O	0	0
			28	16	2	10		
5	c	2	Total	C	N	O	0	0
			28	16	2	10		
5	d	2	Total	C	N	O	0	0
			28	16	2	10		
5	e	2	Total	C	N	O	0	0
			28	16	2	10		
5	g	2	Total	C	N	O	0	0
			28	16	2	10		
5	i	2	Total	C	N	O	0	0
			28	16	2	10		
5	j	2	Total	C	N	O	0	0
			28	16	2	10		
5	k	2	Total	C	N	O	0	0
			28	16	2	10		
5	l	2	Total	C	N	O	0	0
			28	16	2	10		
5	o	2	Total	C	N	O	0	0
			28	16	2	10		
5	p	2	Total	C	N	O	0	0
			28	16	2	10		
5	q	2	Total	C	N	O	0	0
			28	16	2	10		
5	r	2	Total	C	N	O	0	0
			28	16	2	10		
5	s	2	Total	C	N	O	0	0
			28	16	2	10		
5	t	2	Total	C	N	O	0	0
			28	16	2	10		
5	v	2	Total	C	N	O	0	0
			28	16	2	10		
5	x	2	Total	C	N	O	0	0
			28	16	2	10		

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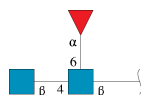
Mol	Chain	Residues	Atoms				AltConf	Trace
5	y	2	Total	C	N	O	0	0
			28	16	2	10		
5	z	2	Total	C	N	O	0	0
			28	16	2	10		
5	0	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 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
6	S	3	Total	C	N	O	0	0
			39	22	2	15		
6	h	3	Total	C	N	O	0	0
			39	22	2	15		
6	w	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
7	X	3	Total	C	N	O	0	0
			38	22	2	14		
7	m	3	Total	C	N	O	0	0
			38	22	2	14		
7	1	3	Total	C	N	O	0	0
			38	22	2	14		

- 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	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	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	

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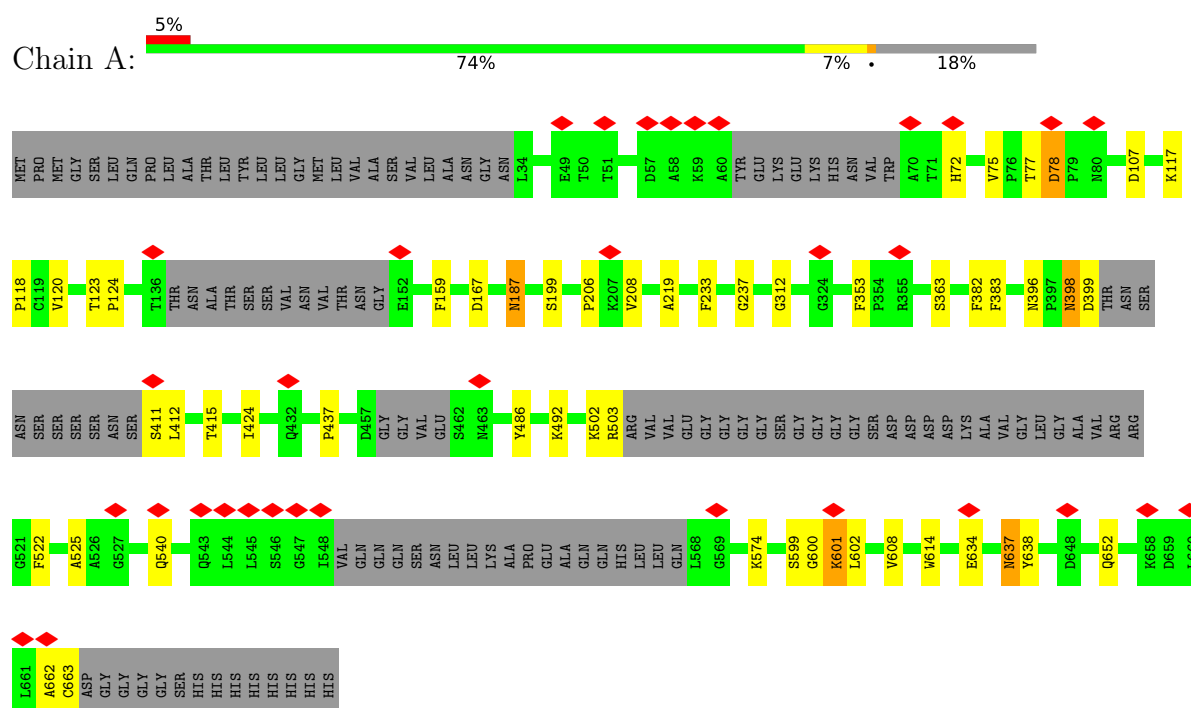
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Mol	Chain	Residues	Atoms				AltConf
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	

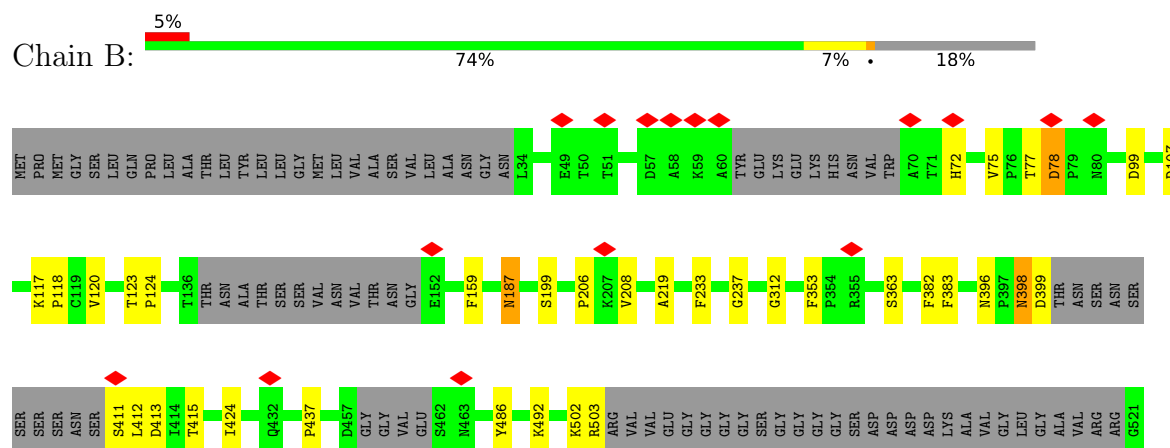
3 Residue-property plots [i](#)

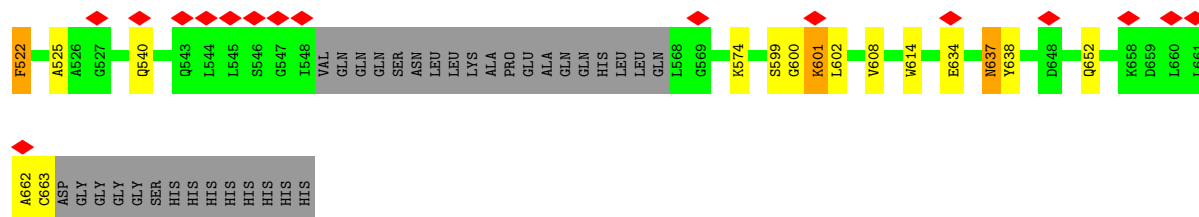
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: HIV Env 16055 NFL TD 2CC+

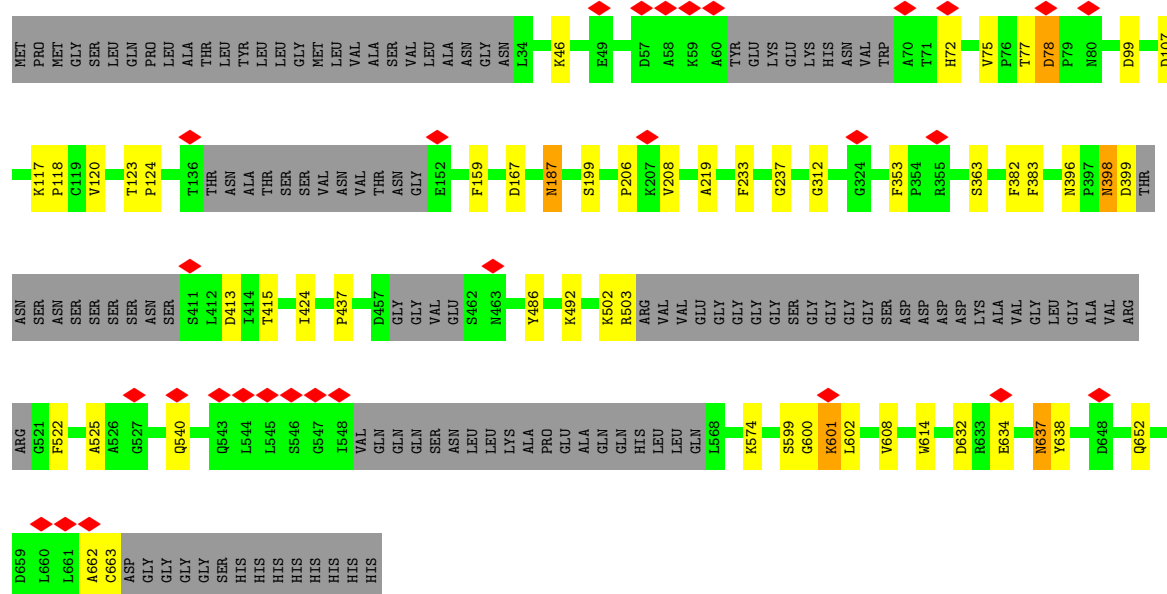
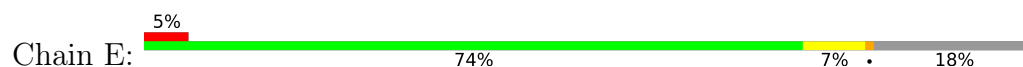


- Molecule 1: HIV Env 16055 NFL TD 2CC+

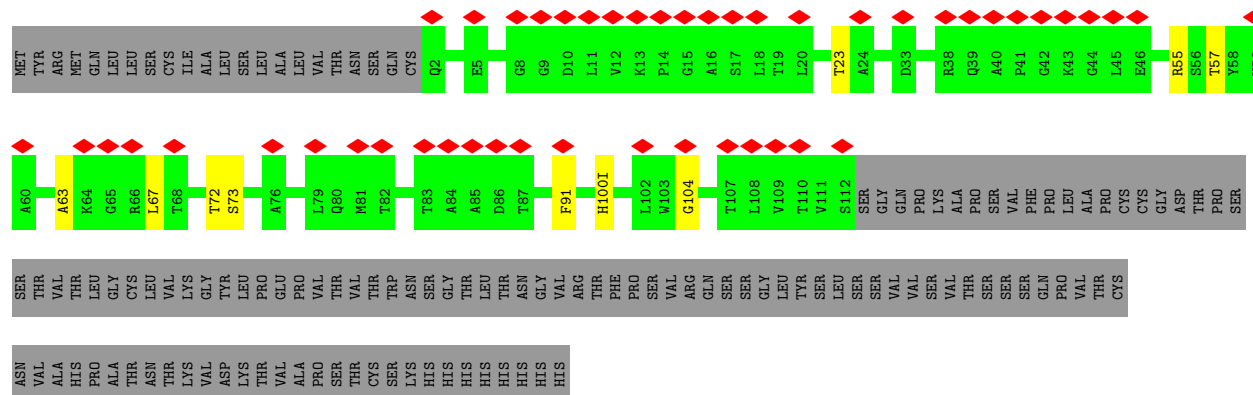




- Molecule 1: HIV Env 16055 NFL TD 2CC+

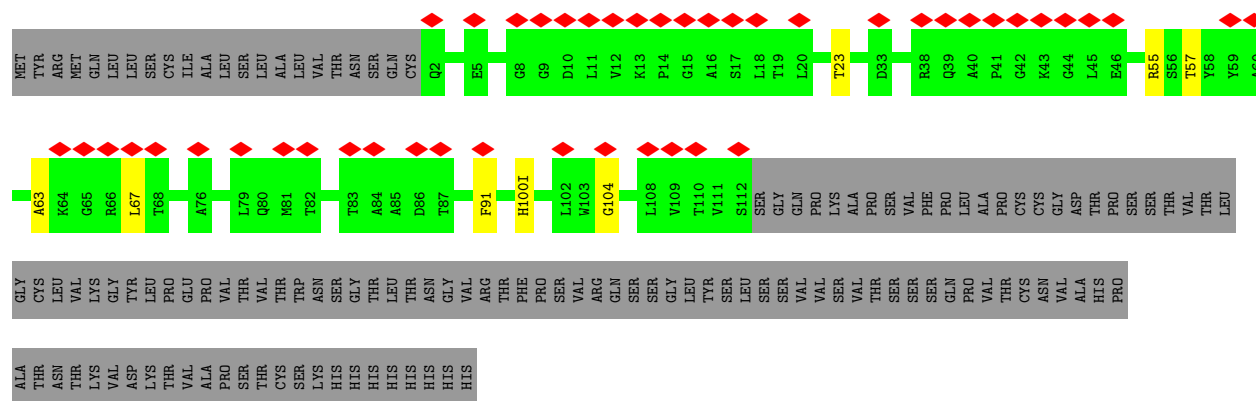


- Molecule 2: Rabbit antibody 1C2 heavy chain fragment antigen binding

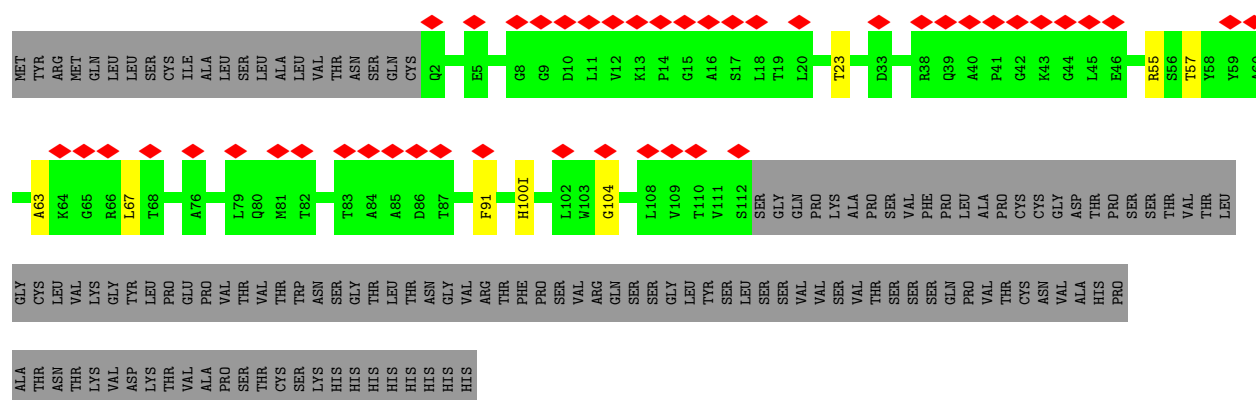


- Molecule 2: Rabbit antibody 1C2 heavy chain fragment antigen binding

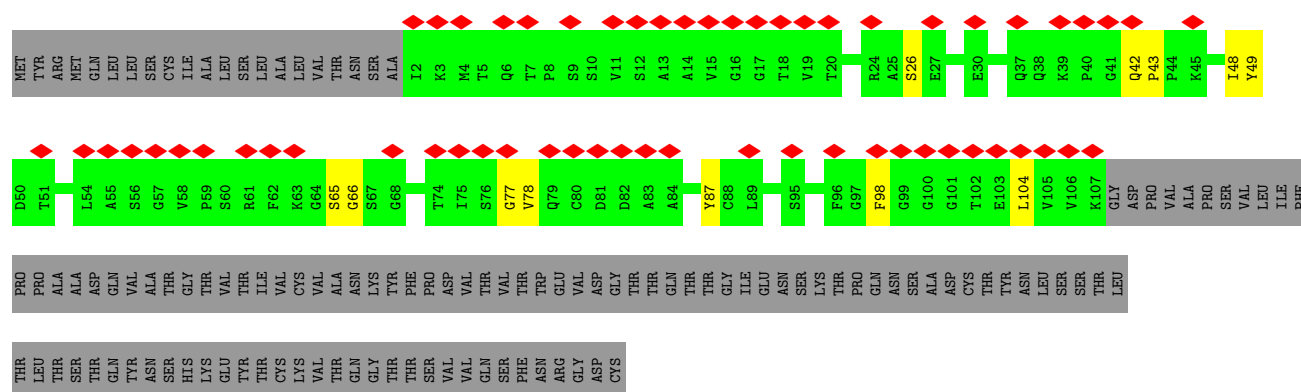
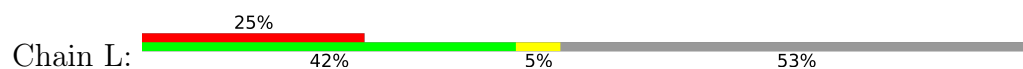




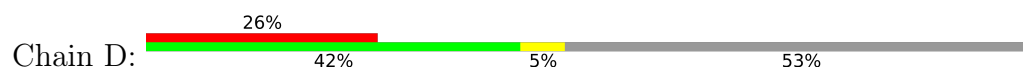
• Molecule 2: Rabbit antibody 1C2 heavy chain fragment antigen binding

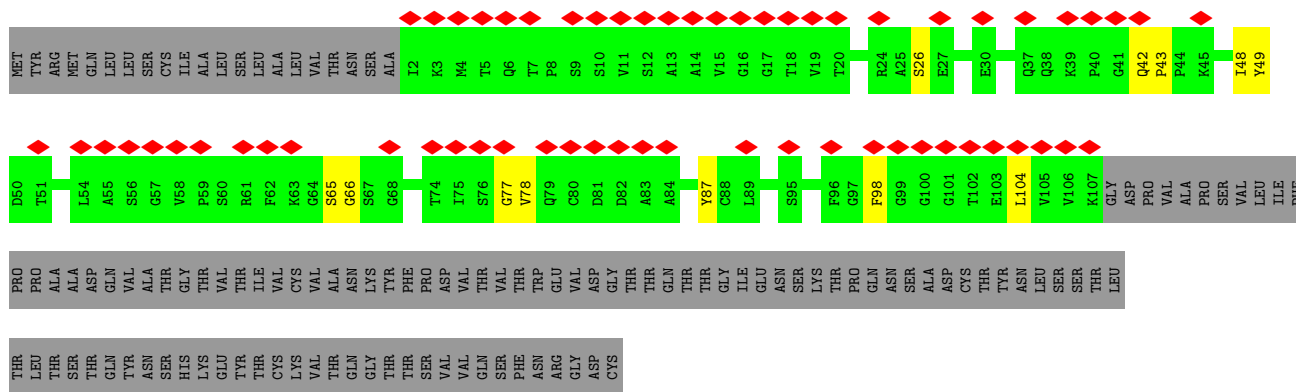


• Molecule 3: Rabbit antibody 1C2 kappa chain

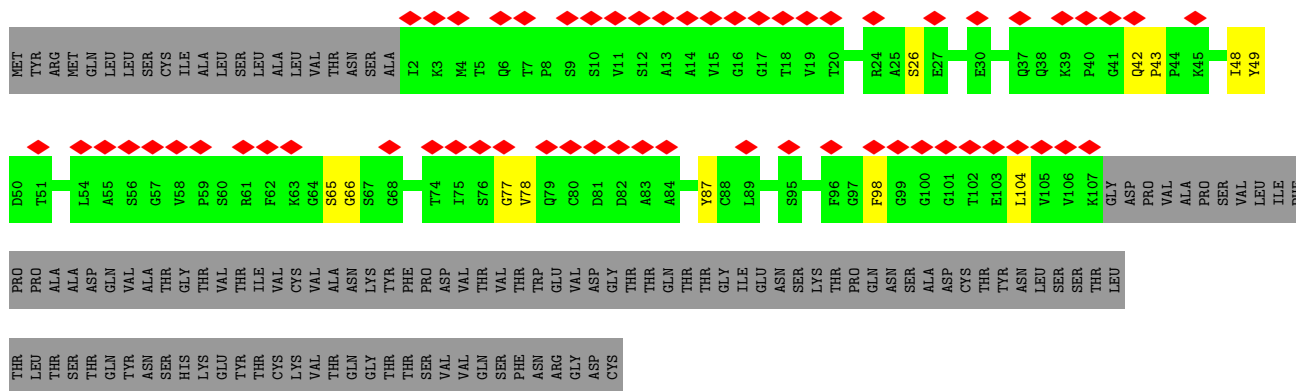
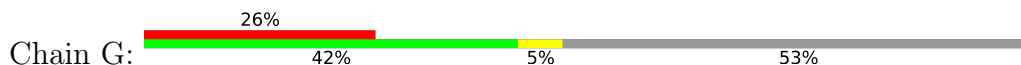


• Molecule 3: Rabbit antibody 1C2 kappa chain





• Molecule 3: Rabbit antibody 1C2 kappa chain



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



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



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



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



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



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



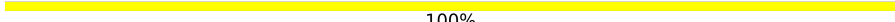
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain M:  100%

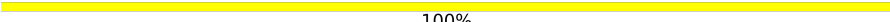
 NAG1
NAG2

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

Chain N:  50% 50%

 NAG1
NAG2

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

Chain O:  100%

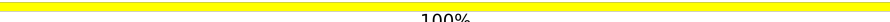
 NAG1
NAG2

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

Chain P:  50% 100%

 NAG1
NAG2

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

Chain R:  100%

 NAG1
NAG2

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

Chain T:  50% 50%

 NAG1
NAG2

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

Chain U:  50% 50%



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



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



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



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



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



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





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

Chain d:  100%



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

Chain e:  100%



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

Chain g:  100%



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

Chain i:  50% 50%



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

Chain j:  50% 50%

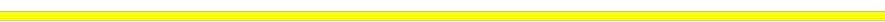


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  50% 50%



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

Chain l:  100%



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

Chain o:  100%



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

Chain p:  100%



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

Chain q:  100%

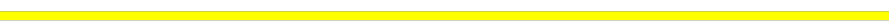


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:  50% 50%



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

Chain s:  100%



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

Chain t:  100%

MAG1
MAG2

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

Chain v:  100%

MAG1
MAG2

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

Chain x:  50% 50%

MAG1
MAG2

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

Chain y:  50% 50% 50%

MAG1
MAG2

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

Chain z:  50% 50% 50%

MAG1
MAG2

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

Chain 0:  100%

MAG1
MAG2

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



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



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	23702	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.266	Depositor
Minimum map value	-0.156	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	331.19998, 331.19998, 331.19998	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	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, FUC, NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.13	1/4492 (0.0%)	1.22	37/6094 (0.6%)
1	B	1.13	1/4492 (0.0%)	1.22	37/6094 (0.6%)
1	E	1.13	1/4492 (0.0%)	1.22	37/6094 (0.6%)
2	C	1.02	0/967	1.30	7/1317 (0.5%)
2	F	1.02	0/967	1.30	8/1317 (0.6%)
2	H	1.02	0/967	1.30	8/1317 (0.6%)
3	D	1.00	1/837 (0.1%)	1.46	10/1135 (0.9%)
3	G	0.99	1/837 (0.1%)	1.45	10/1135 (0.9%)
3	L	1.00	1/837 (0.1%)	1.45	10/1135 (0.9%)
All	All	1.10	6/18888 (0.0%)	1.27	164/25638 (0.6%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	PHE	CB-CG	-5.97	1.36	1.50
1	E	159	PHE	CB-CG	-5.94	1.36	1.50
1	A	159	PHE	CB-CG	-5.94	1.36	1.50
3	D	49	TYR	CB-CG	-5.24	1.40	1.51
3	G	49	TYR	CB-CG	-5.23	1.40	1.51
3	L	49	TYR	CB-CG	-5.22	1.40	1.51

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	492	LYS	CA-C-N	8.02	127.74	119.56
1	A	492	LYS	C-N-CA	8.02	127.74	119.56
1	E	492	LYS	CA-C-N	7.99	127.71	119.56
1	E	492	LYS	C-N-CA	7.99	127.71	119.56
1	B	492	LYS	CA-C-N	7.96	127.67	119.56
1	B	492	LYS	C-N-CA	7.96	127.67	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	98	PHE	CA-CB-CG	7.94	121.74	113.80
3	G	98	PHE	CA-CB-CG	7.93	121.73	113.80
3	D	98	PHE	CA-CB-CG	7.91	121.71	113.80
3	G	43	PRO	N-CA-C	-7.61	102.44	110.58
3	L	43	PRO	N-CA-C	-7.59	102.46	110.58
3	D	43	PRO	N-CA-C	-7.58	102.47	110.58
1	E	219	ALA	CA-C-N	7.16	127.08	119.85
1	E	219	ALA	C-N-CA	7.16	127.08	119.85
1	A	219	ALA	CA-C-N	7.16	127.08	119.85
1	A	219	ALA	C-N-CA	7.16	127.08	119.85
1	B	219	ALA	CA-C-N	7.13	127.05	119.85
1	B	219	ALA	C-N-CA	7.13	127.05	119.85
3	L	78	VAL	N-CA-C	7.09	118.94	109.37
3	D	78	VAL	N-CA-C	7.04	118.88	109.37
3	G	78	VAL	N-CA-C	7.04	118.88	109.37
3	D	42	GLN	CA-C-N	6.46	124.31	119.66
3	D	42	GLN	C-N-CA	6.46	124.31	119.66
3	L	42	GLN	CA-C-N	6.43	124.29	119.66
3	L	42	GLN	C-N-CA	6.43	124.29	119.66
3	G	42	GLN	CA-C-N	6.43	124.29	119.66
3	G	42	GLN	C-N-CA	6.43	124.29	119.66
3	D	104	LEU	N-CA-C	6.22	119.09	109.07
1	B	599	SER	N-CA-C	-6.22	101.73	110.50
3	G	104	LEU	N-CA-C	6.22	119.08	109.07
3	L	104	LEU	N-CA-C	6.21	119.07	109.07
1	A	208	VAL	N-CA-C	-6.19	101.56	109.30
1	B	208	VAL	N-CA-C	-6.18	101.57	109.30
1	A	599	SER	N-CA-C	-6.18	101.79	110.50
1	E	599	SER	N-CA-C	-6.17	101.81	110.50
1	E	522	PHE	CA-CB-CG	-6.16	107.64	113.80
1	E	208	VAL	N-CA-C	-6.15	101.61	109.30
1	E	424	ILE	N-CA-C	6.12	116.67	107.80
1	A	522	PHE	CA-CB-CG	-6.11	107.69	113.80
1	A	424	ILE	N-CA-C	6.11	116.65	107.80
1	B	522	PHE	CA-CB-CG	-6.10	107.70	113.80
1	E	120	VAL	N-CA-C	6.09	116.92	109.30
1	B	120	VAL	N-CA-C	6.09	116.91	109.30
1	A	120	VAL	N-CA-C	6.07	116.88	109.30
1	B	424	ILE	N-CA-C	6.06	116.59	107.80
2	H	100(I)	HIS	CA-CB-CG	5.96	119.76	113.80
2	C	100(I)	HIS	CA-CB-CG	5.95	119.75	113.80
2	F	100(I)	HIS	CA-CB-CG	5.93	119.73	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	67	LEU	N-CA-C	5.92	118.55	108.90
1	B	608	VAL	CA-C-N	5.91	125.81	119.85
1	B	608	VAL	C-N-CA	5.91	125.81	119.85
2	C	67	LEU	N-CA-C	5.91	118.53	108.90
1	E	608	VAL	CA-C-N	5.90	125.81	119.85
1	E	608	VAL	C-N-CA	5.90	125.81	119.85
1	A	652	GLN	N-CA-C	-5.90	105.08	112.93
1	A	608	VAL	CA-C-N	5.90	125.81	119.85
1	A	608	VAL	C-N-CA	5.90	125.81	119.85
1	B	652	GLN	N-CA-C	-5.89	105.10	112.93
1	E	652	GLN	N-CA-C	-5.89	105.10	112.93
2	H	67	LEU	N-CA-C	5.88	118.49	108.90
1	E	614	TRP	N-CA-C	-5.88	104.22	111.40
1	B	199	SER	N-CA-C	5.87	118.04	108.76
1	A	199	SER	N-CA-C	5.87	118.03	108.76
1	E	199	SER	N-CA-C	5.86	118.03	108.76
1	E	312	GLY	CA-C-N	5.86	127.16	119.84
1	E	312	GLY	C-N-CA	5.86	127.16	119.84
1	B	614	TRP	N-CA-C	-5.85	104.26	111.40
3	D	26	SER	N-CA-C	-5.85	105.23	112.90
3	G	26	SER	N-CA-C	-5.85	105.24	112.90
3	L	26	SER	N-CA-C	-5.84	105.24	112.90
1	A	614	TRP	N-CA-C	-5.84	104.28	111.40
1	A	312	GLY	CA-C-N	5.83	127.12	119.84
1	A	312	GLY	C-N-CA	5.83	127.12	119.84
1	B	312	GLY	CA-C-N	5.82	127.11	119.84
1	B	312	GLY	C-N-CA	5.82	127.11	119.84
3	G	87	TYR	N-CA-C	5.79	118.64	109.50
3	L	87	TYR	N-CA-C	5.78	118.63	109.50
3	D	87	TYR	N-CA-C	5.77	118.62	109.50
1	A	363	SER	CA-C-N	5.75	125.73	120.21
1	A	363	SER	C-N-CA	5.75	125.73	120.21
3	G	77	GLY	N-CA-C	-5.74	104.07	114.46
3	D	77	GLY	N-CA-C	-5.74	104.07	114.46
1	B	363	SER	CA-C-N	5.74	125.72	120.21
1	B	363	SER	C-N-CA	5.74	125.72	120.21
3	L	77	GLY	N-CA-C	-5.73	104.08	114.46
1	E	363	SER	CA-C-N	5.73	125.71	120.21
1	E	363	SER	C-N-CA	5.73	125.71	120.21
2	H	63	ALA	N-CA-C	5.72	117.30	110.44
2	C	91	PHE	CA-CB-CG	5.71	119.51	113.80
2	H	91	PHE	CA-CB-CG	5.70	119.50	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	63	ALA	N-CA-C	5.69	117.26	110.44
2	F	91	PHE	CA-CB-CG	5.68	119.48	113.80
2	F	63	ALA	N-CA-C	5.67	117.25	110.44
1	E	396	ASN	CA-C-N	5.65	125.33	119.56
1	E	396	ASN	C-N-CA	5.65	125.33	119.56
1	A	396	ASN	CA-C-N	5.63	125.30	119.56
1	A	396	ASN	C-N-CA	5.63	125.30	119.56
1	B	396	ASN	CA-C-N	5.61	125.28	119.56
1	B	396	ASN	C-N-CA	5.61	125.28	119.56
1	B	72	HIS	CA-CB-CG	-5.57	108.23	113.80
1	E	72	HIS	CA-CB-CG	-5.54	108.26	113.80
1	A	72	HIS	CA-CB-CG	-5.51	108.28	113.80
1	A	601	LYS	N-CA-C	5.51	119.50	112.34
1	B	601	LYS	N-CA-C	5.51	119.50	112.34
1	E	353	PHE	CA-C-N	5.50	125.47	120.03
1	E	353	PHE	C-N-CA	5.50	125.47	120.03
1	A	353	PHE	CA-C-N	5.49	125.47	120.03
1	A	353	PHE	C-N-CA	5.49	125.47	120.03
1	B	353	PHE	CA-C-N	5.49	125.46	120.03
1	B	353	PHE	C-N-CA	5.49	125.46	120.03
1	E	600	GLY	CA-C-N	5.49	129.46	120.63
1	E	600	GLY	C-N-CA	5.49	129.46	120.63
1	A	600	GLY	CA-C-N	5.48	129.45	120.63
1	A	600	GLY	C-N-CA	5.48	129.45	120.63
1	B	600	GLY	CA-C-N	5.48	129.45	120.63
1	B	600	GLY	C-N-CA	5.48	129.45	120.63
1	E	601	LYS	N-CA-C	5.46	119.44	112.34
1	B	237	GLY	CA-C-N	5.41	125.31	119.85
1	B	237	GLY	C-N-CA	5.41	125.31	119.85
1	E	237	GLY	CA-C-N	5.39	125.29	119.85
1	E	237	GLY	C-N-CA	5.39	125.29	119.85
1	A	237	GLY	CA-C-N	5.37	125.27	119.85
1	A	237	GLY	C-N-CA	5.37	125.27	119.85
1	A	206	PRO	N-CA-C	-5.33	102.83	111.14
1	E	206	PRO	N-CA-C	-5.32	102.84	111.14
1	B	206	PRO	N-CA-C	-5.32	102.85	111.14
1	A	75	VAL	N-CA-C	5.30	113.12	107.76
1	B	75	VAL	N-CA-C	5.30	113.11	107.76
1	E	75	VAL	N-CA-C	5.30	113.11	107.76
1	B	382	PHE	N-CA-C	5.26	116.99	108.41
1	A	382	PHE	N-CA-C	5.26	116.99	108.41
1	E	382	PHE	N-CA-C	5.25	116.97	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	486	TYR	N-CA-C	5.23	118.09	109.72
1	E	486	TYR	N-CA-C	5.23	118.08	109.72
1	B	486	TYR	N-CA-C	5.20	118.04	109.72
1	E	437	PRO	CA-C-N	5.14	125.04	119.85
1	E	437	PRO	C-N-CA	5.14	125.04	119.85
1	A	383	PHE	CA-CB-CG	5.13	118.93	113.80
1	B	383	PHE	CA-CB-CG	5.12	118.92	113.80
1	E	383	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	437	PRO	CA-C-N	5.12	125.02	119.85
1	A	437	PRO	C-N-CA	5.12	125.02	119.85
1	E	78	ASP	CA-C-N	5.11	124.77	119.56
1	E	78	ASP	C-N-CA	5.11	124.77	119.56
1	B	78	ASP	CA-C-N	5.10	124.76	119.56
1	B	78	ASP	C-N-CA	5.10	124.76	119.56
1	B	437	PRO	CA-C-N	5.09	125.00	119.85
1	B	437	PRO	C-N-CA	5.09	125.00	119.85
2	C	23	THR	N-CA-C	5.08	117.19	108.90
2	F	23	THR	N-CA-C	5.08	117.19	108.90
2	H	23	THR	N-CA-C	5.08	117.18	108.90
1	A	78	ASP	CA-C-N	5.06	124.72	119.56
1	A	78	ASP	C-N-CA	5.06	124.72	119.56
2	C	104	GLY	CA-C-N	5.05	124.66	119.56
2	C	104	GLY	C-N-CA	5.05	124.66	119.56
2	H	104	GLY	CA-C-N	5.03	124.64	119.56
2	H	104	GLY	C-N-CA	5.03	124.64	119.56
2	F	104	GLY	CA-C-N	5.02	124.63	119.56
2	F	104	GLY	C-N-CA	5.02	124.63	119.56
2	F	104	GLY	N-CA-C	-5.01	105.93	112.10
2	H	104	GLY	N-CA-C	-5.01	105.94	112.10
3	G	48	ILE	N-CA-C	5.01	115.92	108.46
3	L	48	ILE	N-CA-C	5.00	115.92	108.46
3	D	48	ILE	N-CA-C	5.00	115.91	108.46

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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	4405	0	4326	19	0
1	B	4405	0	4326	21	0
1	E	4405	0	4326	21	0
2	C	943	0	909	1	0
2	F	943	0	909	1	0
2	H	943	0	909	2	0
3	D	820	0	800	1	0
3	G	820	0	800	1	0
3	L	820	0	800	1	0
4	I	61	0	49	0	0
4	Q	61	0	49	0	0
4	Y	61	0	49	0	0
4	f	61	0	49	0	0
4	n	61	0	49	0	0
4	u	61	0	49	0	0
5	0	28	0	25	0	0
5	J	28	0	25	1	0
5	K	28	0	25	0	0
5	M	28	0	25	0	0
5	N	28	0	25	1	0
5	O	28	0	25	0	0
5	P	28	0	25	0	0
5	R	28	0	25	0	0
5	T	28	0	25	1	0
5	U	28	0	25	0	0
5	V	28	0	25	0	0
5	W	28	0	25	0	0
5	Z	28	0	25	1	0
5	a	28	0	25	0	0
5	b	28	0	25	0	0
5	c	28	0	25	1	0
5	d	28	0	25	0	0
5	e	28	0	25	0	0
5	g	28	0	25	0	0
5	i	28	0	25	1	0
5	j	28	0	25	0	0
5	k	28	0	25	0	0
5	l	28	0	25	0	0
5	o	28	0	25	0	0
5	p	28	0	25	0	0
5	q	28	0	25	0	0
5	r	28	0	25	1	0
5	s	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	t	28	0	25	0	0
5	v	28	0	25	0	0
5	x	28	0	25	1	0
5	y	28	0	25	0	0
5	z	28	0	25	0	0
6	S	39	0	33	0	0
6	h	39	0	33	0	0
6	w	39	0	33	0	0
7	l	38	0	34	0	0
7	X	38	0	34	0	0
7	m	38	0	34	0	0
8	A	98	0	91	2	0
8	B	98	0	91	2	0
8	E	98	0	91	2	0
All	All	20319	0	19698	70	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 2.

All (70) 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:398:ASN:N	1:B:398:ASN:OD1	2.32	0.62
1:E:398:ASN:N	1:E:398:ASN:OD1	2.32	0.62
1:A:398:ASN:N	1:A:398:ASN:OD1	2.32	0.61
1:B:662:ALA:O	1:B:663:CYS:C	2.45	0.59
1:A:662:ALA:O	1:A:663:CYS:C	2.45	0.59
1:A:525:ALA:H	1:A:540:GLN:HE22	1.50	0.58
1:E:662:ALA:O	1:E:663:CYS:C	2.45	0.58
1:A:637:ASN:N	1:A:637:ASN:OD1	2.36	0.57
1:E:525:ALA:H	1:E:540:GLN:HE22	1.50	0.57
1:B:525:ALA:H	1:B:540:GLN:HE22	1.50	0.56
1:E:637:ASN:N	1:E:637:ASN:OD1	2.36	0.56
1:B:637:ASN:N	1:B:637:ASN:OD1	2.36	0.55
1:B:123:THR:N	1:B:124:PRO:CD	2.70	0.55
1:E:123:THR:N	1:E:124:PRO:CD	2.70	0.54
1:A:123:THR:N	1:A:124:PRO:CD	2.70	0.54
1:E:233:PHE:CD1	5:r:1:NAG:H82	2.43	0.54
1:B:415:THR:HA	5:i:1:NAG:H81	1.90	0.53
1:A:233:PHE:CD1	5:N:1:NAG:H82	2.43	0.53
1:A:415:THR:HA	5:T:1:NAG:H81	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:PHE:CD1	5:c:1:NAG:H82	2.43	0.53
1:E:415:THR:HA	5:x:1:NAG:H81	1.90	0.52
1:A:187:ASN:OD1	1:A:187:ASN:N	2.45	0.49
1:E:187:ASN:OD1	1:E:187:ASN:N	2.45	0.49
1:B:107:ASP:OD1	1:B:574:LYS:NZ	2.46	0.49
1:A:107:ASP:OD1	1:A:574:LYS:NZ	2.46	0.49
1:B:187:ASN:OD1	1:B:187:ASN:N	2.45	0.49
1:A:399:ASP:OD1	1:A:399:ASP:C	2.55	0.48
1:E:107:ASP:OD1	1:E:574:LYS:NZ	2.46	0.48
1:B:399:ASP:C	1:B:399:ASP:OD1	2.55	0.48
3:D:65:SER:OG	3:D:66:GLY:N	2.47	0.48
1:E:399:ASP:OD1	1:E:399:ASP:C	2.55	0.47
1:A:411:SER:OG	1:A:412:LEU:N	2.47	0.47
3:G:65:SER:OG	3:G:66:GLY:N	2.47	0.47
3:L:65:SER:OG	3:L:66:GLY:N	2.47	0.47
2:C:55:ARG:NH1	2:C:57:THR:OG1	2.48	0.46
2:H:55:ARG:NH1	2:H:57:THR:OG1	2.48	0.46
1:B:411:SER:OG	1:B:412:LEU:N	2.47	0.46
2:F:55:ARG:NH1	2:F:57:THR:OG1	2.48	0.46
1:E:502:LYS:O	1:E:503:ARG:C	2.59	0.46
1:B:502:LYS:O	1:B:503:ARG:C	2.59	0.45
1:B:634:GLU:O	8:B:745:NAG:H83	2.17	0.45
1:E:638:TYR:CE1	8:E:745:NAG:H81	2.52	0.45
1:A:638:TYR:CE1	8:A:745:NAG:H81	2.52	0.45
1:A:663:CYS:O	1:A:663:CYS:SG	2.75	0.45
1:A:634:GLU:O	8:A:745:NAG:H83	2.17	0.44
1:B:413:ASP:OD1	1:B:413:ASP:N	2.47	0.44
1:B:638:TYR:CE1	8:B:745:NAG:H81	2.52	0.44
1:E:634:GLU:O	8:E:745:NAG:H83	2.17	0.44
1:E:663:CYS:O	1:E:663:CYS:SG	2.75	0.44
1:E:601:LYS:O	1:E:602:LEU:C	2.59	0.44
1:B:77:THR:OG1	1:B:78:ASP:N	2.51	0.44
1:B:663:CYS:SG	1:B:663:CYS:O	2.75	0.44
1:A:77:THR:OG1	1:A:78:ASP:N	2.51	0.44
1:A:601:LYS:O	1:A:602:LEU:C	2.59	0.44
1:B:99:ASP:OD1	1:B:99:ASP:N	2.51	0.44
1:E:46:LYS:NZ	1:E:632:ASP:OD2	2.39	0.44
1:E:77:THR:OG1	1:E:78:ASP:N	2.51	0.44
1:A:167:ASP:OD1	1:A:167:ASP:N	2.45	0.44
1:E:99:ASP:OD1	1:E:99:ASP:N	2.51	0.43
1:A:502:LYS:O	1:A:503:ARG:C	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:LYS:O	1:B:602:LEU:C	2.59	0.43
1:E:167:ASP:N	1:E:167:ASP:OD1	2.45	0.42
5:J:2:NAG:O6	5:J:2:NAG:O4	2.34	0.41
1:B:117:LYS:N	1:B:118:PRO:CD	2.83	0.41
1:E:117:LYS:N	1:E:118:PRO:CD	2.83	0.41
1:A:117:LYS:N	1:A:118:PRO:CD	2.83	0.41
1:E:413:ASP:OD1	1:E:413:ASP:N	2.47	0.41
5:Z:2:NAG:O6	5:Z:2:NAG:O4	2.34	0.41
1:B:522:PHE:O	1:B:540:GLN:NE2	2.53	0.40
2:H:72:THR:OG1	2:H:73:SER:N	2.52	0.40

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	543/680 (80%)	533 (98%)	10 (2%)	0	100	100
1	B	543/680 (80%)	533 (98%)	10 (2%)	0	100	100
1	E	543/680 (80%)	533 (98%)	10 (2%)	0	100	100
2	C	124/259 (48%)	120 (97%)	4 (3%)	0	100	100
2	F	124/259 (48%)	120 (97%)	4 (3%)	0	100	100
2	H	124/259 (48%)	120 (97%)	4 (3%)	0	100	100
3	D	108/235 (46%)	106 (98%)	2 (2%)	0	100	100
3	G	108/235 (46%)	106 (98%)	2 (2%)	0	100	100
3	L	108/235 (46%)	106 (98%)	2 (2%)	0	100	100
All	All	2325/3522 (66%)	2277 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	494/589 (84%)	491 (99%)	3 (1%)	78	81
1	B	494/589 (84%)	491 (99%)	3 (1%)	78	81
1	E	494/589 (84%)	491 (99%)	3 (1%)	78	81
2	C	97/216 (45%)	97 (100%)	0	100	100
2	F	97/216 (45%)	97 (100%)	0	100	100
2	H	97/216 (45%)	97 (100%)	0	100	100
3	D	89/199 (45%)	89 (100%)	0	100	100
3	G	89/199 (45%)	89 (100%)	0	100	100
3	L	89/199 (45%)	89 (100%)	0	100	100
All	All	2040/3012 (68%)	2031 (100%)	9 (0%)	81	84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	398	ASN
1	A	637	ASN
1	B	187	ASN
1	B	398	ASN
1	B	637	ASN
1	E	187	ASN
1	E	398	ASN
1	E	637	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	352	HIS
1	A	540	GLN
1	A	655	GLN
1	B	352	HIS

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Mol	Chain	Res	Type
1	B	540	GLN
1	B	655	GLN
1	E	352	HIS
1	E	540	GLN
1	E	655	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 ⓘ

114 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	0	1	1,5	14,14,15	0.73	0	17,19,21	1.06	2 (11%)
5	NAG	0	2	5	14,14,15	0.81	0	17,19,21	0.92	1 (5%)
7	NAG	1	1	1,7	14,14,15	0.75	0	17,19,21	0.92	0
7	NAG	1	2	7	14,14,15	0.85	0	17,19,21	0.89	1 (5%)
7	FUC	1	3	7	10,10,11	0.64	0	14,14,16	0.98	1 (7%)
4	NAG	I	1	4,1	14,14,15	0.81	0	17,19,21	1.17	2 (11%)
4	NAG	I	2	4	14,14,15	0.81	0	17,19,21	1.19	1 (5%)
4	BMA	I	3	4	11,11,12	1.86	2 (18%)	15,15,17	0.88	0
4	MAN	I	4	4	11,11,12	1.75	2 (18%)	15,15,17	1.14	2 (13%)
4	MAN	I	5	4	11,11,12	1.79	2 (18%)	15,15,17	0.99	1 (6%)
5	NAG	J	1	1,5	14,14,15	0.67	0	17,19,21	1.30	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	J	2	5	14,14,15	0.73	0	17,19,21	1.33	2 (11%)
5	NAG	K	1	1,5	14,14,15	0.85	1 (7%)	17,19,21	1.04	2 (11%)
5	NAG	K	2	5	14,14,15	0.82	0	17,19,21	0.93	1 (5%)
5	NAG	M	1	1,5	14,14,15	0.84	1 (7%)	17,19,21	1.11	0
5	NAG	M	2	5	14,14,15	0.85	0	17,19,21	0.96	1 (5%)
5	NAG	N	1	1,5	14,14,15	0.78	0	17,19,21	1.56	5 (29%)
5	NAG	N	2	5	14,14,15	0.78	0	17,19,21	0.97	1 (5%)
5	NAG	O	1	1,5	14,14,15	0.78	1 (7%)	17,19,21	1.05	1 (5%)
5	NAG	O	2	5	14,14,15	0.79	0	17,19,21	0.92	1 (5%)
5	NAG	P	1	1,5	14,14,15	0.68	0	17,19,21	1.03	1 (5%)
5	NAG	P	2	5	14,14,15	0.77	0	17,19,21	0.90	1 (5%)
4	NAG	Q	1	4,1	14,14,15	0.88	1 (7%)	17,19,21	1.07	1 (5%)
4	NAG	Q	2	4	14,14,15	0.80	1 (7%)	17,19,21	1.16	1 (5%)
4	BMA	Q	3	4	11,11,12	1.80	2 (18%)	15,15,17	1.01	1 (6%)
4	MAN	Q	4	4	11,11,12	1.73	2 (18%)	15,15,17	0.97	1 (6%)
4	MAN	Q	5	4	11,11,12	1.83	2 (18%)	15,15,17	0.99	1 (6%)
5	NAG	R	1	1,5	14,14,15	0.87	0	17,19,21	1.29	3 (17%)
5	NAG	R	2	5	14,14,15	0.78	0	17,19,21	1.05	1 (5%)
6	NAG	S	1	1,6	14,14,15	0.88	1 (7%)	17,19,21	1.15	0
6	NAG	S	2	6	14,14,15	0.87	1 (7%)	17,19,21	0.97	0
6	BMA	S	3	6	11,11,12	1.79	2 (18%)	15,15,17	0.90	0
5	NAG	T	1	1,5	14,14,15	1.16	2 (14%)	17,19,21	1.43	3 (17%)
5	NAG	T	2	5	14,14,15	0.82	0	17,19,21	1.24	2 (11%)
5	NAG	U	1	1,5	14,14,15	0.75	0	17,19,21	0.77	0
5	NAG	U	2	5	14,14,15	0.75	0	17,19,21	0.91	1 (5%)
5	NAG	V	1	1,5	14,14,15	0.64	0	17,19,21	0.89	0
5	NAG	V	2	5	14,14,15	0.80	0	17,19,21	0.85	1 (5%)
5	NAG	W	1	1,5	14,14,15	0.72	0	17,19,21	1.07	2 (11%)
5	NAG	W	2	5	14,14,15	0.80	0	17,19,21	0.93	1 (5%)
7	NAG	X	1	1,7	14,14,15	0.77	0	17,19,21	0.92	0
7	NAG	X	2	7	14,14,15	0.85	0	17,19,21	0.89	1 (5%)
7	FUC	X	3	7	10,10,11	0.65	0	14,14,16	0.98	1 (7%)
4	NAG	Y	1	4,1	14,14,15	0.80	0	17,19,21	1.16	2 (11%)
4	NAG	Y	2	4	14,14,15	0.81	0	17,19,21	1.19	1 (5%)
4	BMA	Y	3	4	11,11,12	1.85	2 (18%)	15,15,17	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	Y	4	4	11,11,12	1.75	2 (18%)	15,15,17	1.14	2 (13%)
4	MAN	Y	5	4	11,11,12	1.79	2 (18%)	15,15,17	0.99	1 (6%)
5	NAG	Z	1	1,5	14,14,15	0.67	0	17,19,21	1.30	3 (17%)
5	NAG	Z	2	5	14,14,15	0.74	0	17,19,21	1.32	2 (11%)
5	NAG	a	1	1,5	14,14,15	0.85	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	a	2	5	14,14,15	0.82	0	17,19,21	0.92	1 (5%)
5	NAG	b	1	1,5	14,14,15	0.83	1 (7%)	17,19,21	1.10	0
5	NAG	b	2	5	14,14,15	0.84	0	17,19,21	0.95	1 (5%)
5	NAG	c	1	1,5	14,14,15	0.78	0	17,19,21	1.56	5 (29%)
5	NAG	c	2	5	14,14,15	0.77	0	17,19,21	0.98	1 (5%)
5	NAG	d	1	1,5	14,14,15	0.79	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	d	2	5	14,14,15	0.79	0	17,19,21	0.92	1 (5%)
5	NAG	e	1	1,5	14,14,15	0.68	0	17,19,21	1.03	1 (5%)
5	NAG	e	2	5	14,14,15	0.76	0	17,19,21	0.90	1 (5%)
4	NAG	f	1	4,1	14,14,15	0.88	1 (7%)	17,19,21	1.06	1 (5%)
4	NAG	f	2	4	14,14,15	0.80	1 (7%)	17,19,21	1.16	1 (5%)
4	BMA	f	3	4	11,11,12	1.81	2 (18%)	15,15,17	1.00	1 (6%)
4	MAN	f	4	4	11,11,12	1.74	2 (18%)	15,15,17	0.97	1 (6%)
4	MAN	f	5	4	11,11,12	1.83	2 (18%)	15,15,17	1.00	1 (6%)
5	NAG	g	1	1,5	14,14,15	0.88	1 (7%)	17,19,21	1.29	3 (17%)
5	NAG	g	2	5	14,14,15	0.79	0	17,19,21	1.05	1 (5%)
6	NAG	h	1	1,6	14,14,15	0.89	1 (7%)	17,19,21	1.15	0
6	NAG	h	2	6	14,14,15	0.86	1 (7%)	17,19,21	0.98	0
6	BMA	h	3	6	11,11,12	1.79	2 (18%)	15,15,17	0.89	0
5	NAG	i	1	1,5	14,14,15	1.16	2 (14%)	17,19,21	1.43	3 (17%)
5	NAG	i	2	5	14,14,15	0.82	0	17,19,21	1.25	2 (11%)
5	NAG	j	1	1,5	14,14,15	0.75	0	17,19,21	0.77	0
5	NAG	j	2	5	14,14,15	0.76	0	17,19,21	0.92	1 (5%)
5	NAG	k	1	1,5	14,14,15	0.63	0	17,19,21	0.89	0
5	NAG	k	2	5	14,14,15	0.80	0	17,19,21	0.85	1 (5%)
5	NAG	l	1	1,5	14,14,15	0.73	0	17,19,21	1.06	2 (11%)
5	NAG	l	2	5	14,14,15	0.81	0	17,19,21	0.92	1 (5%)
7	NAG	m	1	1,7	14,14,15	0.75	0	17,19,21	0.93	0
7	NAG	m	2	7	14,14,15	0.84	0	17,19,21	0.89	1 (5%)
7	FUC	m	3	7	10,10,11	0.64	0	14,14,16	0.98	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	n	1	4,1	14,14,15	0.80	0	17,19,21	1.17	2 (11%)
4	NAG	n	2	4	14,14,15	0.80	0	17,19,21	1.19	1 (5%)
4	BMA	n	3	4	11,11,12	1.86	2 (18%)	15,15,17	0.88	0
4	MAN	n	4	4	11,11,12	1.75	2 (18%)	15,15,17	1.14	2 (13%)
4	MAN	n	5	4	11,11,12	1.80	2 (18%)	15,15,17	0.98	1 (6%)
5	NAG	o	1	1,5	14,14,15	0.67	0	17,19,21	1.30	3 (17%)
5	NAG	o	2	5	14,14,15	0.74	0	17,19,21	1.32	2 (11%)
5	NAG	p	1	1,5	14,14,15	0.85	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	p	2	5	14,14,15	0.83	0	17,19,21	0.93	1 (5%)
5	NAG	q	1	1,5	14,14,15	0.84	1 (7%)	17,19,21	1.11	0
5	NAG	q	2	5	14,14,15	0.84	0	17,19,21	0.96	1 (5%)
5	NAG	r	1	1,5	14,14,15	0.80	0	17,19,21	1.56	5 (29%)
5	NAG	r	2	5	14,14,15	0.78	0	17,19,21	0.98	1 (5%)
5	NAG	s	1	1,5	14,14,15	0.79	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	s	2	5	14,14,15	0.79	0	17,19,21	0.92	1 (5%)
5	NAG	t	1	1,5	14,14,15	0.68	0	17,19,21	1.03	1 (5%)
5	NAG	t	2	5	14,14,15	0.77	0	17,19,21	0.89	1 (5%)
4	NAG	u	1	4,1	14,14,15	0.87	1 (7%)	17,19,21	1.07	1 (5%)
4	NAG	u	2	4	14,14,15	0.80	1 (7%)	17,19,21	1.16	1 (5%)
4	BMA	u	3	4	11,11,12	1.80	2 (18%)	15,15,17	1.01	1 (6%)
4	MAN	u	4	4	11,11,12	1.73	2 (18%)	15,15,17	0.98	1 (6%)
4	MAN	u	5	4	11,11,12	1.82	2 (18%)	15,15,17	1.00	1 (6%)
5	NAG	v	1	1,5	14,14,15	0.87	0	17,19,21	1.29	3 (17%)
5	NAG	v	2	5	14,14,15	0.77	0	17,19,21	1.05	1 (5%)
6	NAG	w	1	1,6	14,14,15	0.88	1 (7%)	17,19,21	1.15	0
6	NAG	w	2	6	14,14,15	0.87	1 (7%)	17,19,21	0.97	0
6	BMA	w	3	6	11,11,12	1.79	2 (18%)	15,15,17	0.89	0
5	NAG	x	1	1,5	14,14,15	1.16	2 (14%)	17,19,21	1.43	3 (17%)
5	NAG	x	2	5	14,14,15	0.82	0	17,19,21	1.24	2 (11%)
5	NAG	y	1	1,5	14,14,15	0.75	0	17,19,21	0.77	0
5	NAG	y	2	5	14,14,15	0.74	0	17,19,21	0.91	1 (5%)
5	NAG	z	1	1,5	14,14,15	0.63	0	17,19,21	0.89	0
5	NAG	z	2	5	14,14,15	0.79	0	17,19,21	0.85	1 (5%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	0	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	0	2	5	-	1/6/23/26	0/1/1/1
7	NAG	1	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	1	2	7	-	1/6/23/26	0/1/1/1
7	FUC	1	3	7	-	-	0/1/1/1
4	NAG	I	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1
4	MAN	I	4	4	-	1/2/19/22	0/1/1/1
4	MAN	I	5	4	-	1/2/19/22	0/1/1/1
5	NAG	J	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	4/6/23/26	0/1/1/1
5	NAG	K	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	1/6/23/26	0/1/1/1
5	NAG	M	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	NAG	N	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	2/6/23/26	0/1/1/1
5	NAG	O	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1
5	NAG	P	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	BMA	Q	3	4	-	0/2/19/22	0/1/1/1
4	MAN	Q	4	4	-	1/2/19/22	0/1/1/1
4	MAN	Q	5	4	-	1/2/19/22	0/1/1/1
5	NAG	R	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
6	NAG	S	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	0/6/23/26	0/1/1/1
6	BMA	S	3	6	-	1/2/19/22	0/1/1/1
5	NAG	T	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	NAG	U	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	U	2	5	-	2/6/23/26	0/1/1/1
5	NAG	V	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	V	2	5	-	1/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	l	2	5	-	1/6/23/26	0/1/1/1
7	NAG	m	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	m	2	7	-	1/6/23/26	0/1/1/1
7	FUC	m	3	7	-	-	0/1/1/1
4	NAG	n	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	n	2	4	-	0/6/23/26	0/1/1/1
4	BMA	n	3	4	-	0/2/19/22	0/1/1/1
4	MAN	n	4	4	-	1/2/19/22	0/1/1/1
4	MAN	n	5	4	-	1/2/19/22	0/1/1/1
5	NAG	o	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	o	2	5	-	4/6/23/26	0/1/1/1
5	NAG	p	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	p	2	5	-	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	-	2/6/23/26	0/1/1/1
5	NAG	r	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	r	2	5	-	2/6/23/26	0/1/1/1
5	NAG	s	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	s	2	5	-	2/6/23/26	0/1/1/1
5	NAG	t	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	t	2	5	-	2/6/23/26	0/1/1/1
4	NAG	u	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	u	2	4	-	0/6/23/26	0/1/1/1
4	BMA	u	3	4	-	0/2/19/22	0/1/1/1
4	MAN	u	4	4	-	1/2/19/22	0/1/1/1
4	MAN	u	5	4	-	1/2/19/22	0/1/1/1
5	NAG	v	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	v	2	5	-	2/6/23/26	0/1/1/1
6	NAG	w	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	w	2	6	-	0/6/23/26	0/1/1/1
6	BMA	w	3	6	-	1/2/19/22	0/1/1/1
5	NAG	x	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	x	2	5	-	2/6/23/26	0/1/1/1
5	NAG	y	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	y	2	5	-	2/6/23/26	0/1/1/1
5	NAG	z	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	z	2	5	-	1/6/23/26	0/1/1/1

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	5	MAN	O2-C2	-4.25	1.34	1.43
4	I	3	BMA	O2-C2	-4.25	1.34	1.43
4	u	5	MAN	O2-C2	-4.24	1.34	1.43
4	f	5	MAN	O2-C2	-4.24	1.34	1.43
4	n	3	BMA	O2-C2	-4.20	1.34	1.43
4	Y	3	BMA	O2-C2	-4.20	1.34	1.43
4	Y	5	MAN	O2-C2	-4.20	1.34	1.43
4	n	5	MAN	O2-C2	-4.19	1.34	1.43
4	Q	3	BMA	O2-C2	-4.16	1.34	1.43
4	I	5	MAN	O2-C2	-4.16	1.34	1.43
4	f	3	BMA	O2-C2	-4.16	1.34	1.43
4	u	3	BMA	O2-C2	-4.15	1.34	1.43
4	n	4	MAN	O2-C2	-4.14	1.34	1.43
4	I	4	MAN	O2-C2	-4.14	1.34	1.43
4	Y	4	MAN	O2-C2	-4.14	1.34	1.43
6	h	3	BMA	O2-C2	-4.09	1.34	1.43
4	f	4	MAN	O2-C2	-4.09	1.34	1.43
4	Q	4	MAN	O2-C2	-4.09	1.34	1.43
4	u	4	MAN	O2-C2	-4.09	1.34	1.43
6	S	3	BMA	O2-C2	-4.08	1.34	1.43
6	w	3	BMA	O2-C2	-4.08	1.34	1.43
4	n	3	BMA	C2-C3	-2.42	1.48	1.52
5	s	1	NAG	C3-C2	-2.39	1.47	1.52
6	h	1	NAG	C3-C2	-2.38	1.47	1.52
5	d	1	NAG	C3-C2	-2.38	1.47	1.52
4	I	3	BMA	C2-C3	-2.37	1.48	1.52
4	Y	3	BMA	C2-C3	-2.35	1.48	1.52
5	O	1	NAG	C3-C2	-2.35	1.47	1.52
6	w	1	NAG	C3-C2	-2.35	1.47	1.52
6	S	1	NAG	C3-C2	-2.34	1.47	1.52
4	I	4	MAN	C2-C3	-2.33	1.48	1.52
4	Y	4	MAN	C2-C3	-2.30	1.49	1.52
5	i	1	NAG	C3-C2	-2.30	1.47	1.52
4	f	3	BMA	C2-C3	-2.30	1.49	1.52
4	n	4	MAN	C2-C3	-2.30	1.49	1.52
4	Q	3	BMA	C2-C3	-2.29	1.49	1.52
4	u	3	BMA	C2-C3	-2.28	1.49	1.52
5	T	1	NAG	C3-C2	-2.27	1.47	1.52
4	Y	5	MAN	C2-C3	-2.27	1.49	1.52
4	I	5	MAN	C2-C3	-2.26	1.49	1.52
5	x	1	NAG	C3-C2	-2.26	1.47	1.52
4	n	5	MAN	C2-C3	-2.25	1.49	1.52
5	x	1	NAG	C2-N2	-2.24	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	f	4	MAN	C2-C3	-2.24	1.49	1.52
4	u	2	NAG	C3-C2	-2.22	1.47	1.52
4	f	2	NAG	C3-C2	-2.21	1.47	1.52
4	Q	2	NAG	C3-C2	-2.20	1.47	1.52
5	T	1	NAG	C2-N2	-2.20	1.42	1.46
5	i	1	NAG	C2-N2	-2.19	1.42	1.46
4	Q	4	MAN	C2-C3	-2.18	1.49	1.52
6	w	3	BMA	C2-C3	-2.17	1.49	1.52
4	u	4	MAN	C2-C3	-2.16	1.49	1.52
6	S	3	BMA	C2-C3	-2.15	1.49	1.52
5	a	1	NAG	C3-C2	-2.15	1.48	1.52
5	K	1	NAG	C3-C2	-2.15	1.48	1.52
5	p	1	NAG	C3-C2	-2.14	1.48	1.52
6	S	2	NAG	C3-C2	-2.13	1.48	1.52
6	h	3	BMA	C2-C3	-2.13	1.49	1.52
4	Q	1	NAG	C3-C2	-2.11	1.48	1.52
5	q	1	NAG	C3-C2	-2.11	1.48	1.52
4	f	1	NAG	C3-C2	-2.11	1.48	1.52
5	M	1	NAG	C3-C2	-2.10	1.48	1.52
6	w	2	NAG	C3-C2	-2.09	1.48	1.52
6	h	2	NAG	C3-C2	-2.09	1.48	1.52
4	u	1	NAG	C3-C2	-2.08	1.48	1.52
4	Q	5	MAN	C2-C3	-2.07	1.49	1.52
4	f	5	MAN	C2-C3	-2.07	1.49	1.52
4	u	5	MAN	C2-C3	-2.06	1.49	1.52
5	b	1	NAG	C3-C2	-2.05	1.48	1.52
5	g	1	NAG	C3-C2	-2.02	1.48	1.52

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	2	NAG	C4-C3-C2	-4.22	104.84	111.02
5	o	2	NAG	C4-C3-C2	-4.20	104.86	111.02
5	Z	2	NAG	C4-C3-C2	-4.20	104.86	111.02
5	r	1	NAG	O5-C5-C6	-3.57	100.71	107.66
5	N	1	NAG	O5-C5-C6	-3.56	100.73	107.66
5	c	1	NAG	O5-C5-C6	-3.55	100.75	107.66
5	T	2	NAG	C4-C3-C2	-3.37	106.08	111.02
5	i	2	NAG	C4-C3-C2	-3.37	106.08	111.02
5	x	2	NAG	C4-C3-C2	-3.36	106.09	111.02
5	v	2	NAG	C4-C3-C2	-3.13	106.44	111.02
5	R	2	NAG	C4-C3-C2	-3.10	106.47	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	g	2	NAG	C4-C3-C2	-3.09	106.49	111.02
5	g	1	NAG	O4-C4-C3	-3.05	103.18	110.38
5	R	1	NAG	O4-C4-C3	-3.05	103.19	110.38
5	v	1	NAG	O4-C4-C3	-3.04	103.21	110.38
4	n	2	NAG	C4-C3-C2	-3.04	106.57	111.02
5	Z	1	NAG	O5-C5-C6	-3.03	101.76	107.66
5	o	1	NAG	O5-C5-C6	-3.03	101.76	107.66
5	J	1	NAG	O5-C5-C6	-3.03	101.77	107.66
4	I	2	NAG	C4-C3-C2	-3.02	106.59	111.02
4	Y	2	NAG	C4-C3-C2	-3.02	106.60	111.02
5	O	2	NAG	C4-C3-C2	-2.79	106.93	111.02
5	s	2	NAG	C4-C3-C2	-2.78	106.94	111.02
5	d	2	NAG	C4-C3-C2	-2.78	106.94	111.02
5	q	2	NAG	C4-C3-C2	-2.77	106.96	111.02
5	M	2	NAG	C4-C3-C2	-2.77	106.96	111.02
5	b	2	NAG	C4-C3-C2	-2.76	106.97	111.02
5	c	2	NAG	C4-C3-C2	-2.70	107.06	111.02
5	O	1	NAG	O4-C4-C3	-2.68	104.05	110.38
5	d	1	NAG	O4-C4-C3	-2.68	104.07	110.38
5	r	2	NAG	C4-C3-C2	-2.66	107.12	111.02
5	s	1	NAG	O4-C4-C3	-2.66	104.11	110.38
5	N	2	NAG	C4-C3-C2	-2.65	107.13	111.02
4	u	3	BMA	C2-C3-C4	-2.64	106.22	110.86
5	p	2	NAG	C4-C3-C2	-2.63	107.17	111.02
4	Q	3	BMA	C2-C3-C4	-2.63	106.24	110.86
5	K	2	NAG	C4-C3-C2	-2.62	107.17	111.02
5	i	2	NAG	O5-C1-C2	-2.62	107.24	111.29
5	W	2	NAG	C4-C3-C2	-2.61	107.19	111.02
5	T	1	NAG	O5-C1-C2	-2.61	107.25	111.29
4	f	3	BMA	C2-C3-C4	-2.61	106.27	110.86
5	x	2	NAG	O5-C1-C2	-2.61	107.26	111.29
5	i	1	NAG	O5-C1-C2	-2.60	107.27	111.29
5	x	1	NAG	O5-C1-C2	-2.59	107.28	111.29
5	T	2	NAG	O5-C1-C2	-2.59	107.28	111.29
5	a	2	NAG	C4-C3-C2	-2.58	107.24	111.02
5	l	2	NAG	C4-C3-C2	-2.58	107.24	111.02
5	0	2	NAG	C4-C3-C2	-2.58	107.24	111.02
5	j	2	NAG	C4-C3-C2	-2.55	107.28	111.02
4	I	4	MAN	C2-C3-C4	-2.55	106.37	110.86
4	Y	4	MAN	C2-C3-C4	-2.55	106.37	110.86
4	n	4	MAN	C2-C3-C4	-2.55	106.38	110.86
5	o	1	NAG	C3-C4-C5	-2.54	105.62	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	y	2	NAG	C4-C3-C2	-2.54	107.29	111.02
5	J	1	NAG	C3-C4-C5	-2.54	105.62	110.23
5	Z	1	NAG	C3-C4-C5	-2.54	105.62	110.23
5	U	2	NAG	C4-C3-C2	-2.54	107.29	111.02
4	n	1	NAG	C4-C3-C2	-2.51	107.34	111.02
4	I	1	NAG	C4-C3-C2	-2.51	107.34	111.02
4	Y	1	NAG	C4-C3-C2	-2.50	107.36	111.02
5	e	2	NAG	C4-C3-C2	-2.47	107.40	111.02
5	v	1	NAG	O5-C5-C6	-2.46	102.87	107.66
4	Q	2	NAG	C4-C3-C2	-2.46	107.41	111.02
5	g	1	NAG	O5-C5-C6	-2.46	102.88	107.66
4	f	2	NAG	C4-C3-C2	-2.45	107.43	111.02
5	R	1	NAG	O5-C5-C6	-2.45	102.90	107.66
4	u	2	NAG	C4-C3-C2	-2.43	107.45	111.02
5	t	2	NAG	C4-C3-C2	-2.43	107.45	111.02
5	P	2	NAG	C4-C3-C2	-2.43	107.45	111.02
4	I	1	NAG	O5-C1-C2	-2.40	107.58	111.29
5	r	1	NAG	C3-C4-C5	-2.38	105.91	110.23
4	n	1	NAG	O5-C1-C2	-2.38	107.61	111.29
4	u	4	MAN	C2-C3-C4	-2.38	106.68	110.86
4	Y	1	NAG	O5-C1-C2	-2.38	107.61	111.29
4	Q	4	MAN	C2-C3-C4	-2.38	106.68	110.86
5	c	1	NAG	C3-C4-C5	-2.37	105.93	110.23
5	r	1	NAG	C2-N2-C7	-2.37	119.73	122.90
4	f	4	MAN	C2-C3-C4	-2.36	106.70	110.86
5	N	1	NAG	C2-N2-C7	-2.36	119.74	122.90
5	N	1	NAG	C3-C4-C5	-2.36	105.95	110.23
5	c	1	NAG	C2-N2-C7	-2.35	119.75	122.90
5	t	1	NAG	C4-C3-C2	-2.32	107.62	111.02
5	c	1	NAG	C8-C7-N2	2.32	119.96	116.12
5	e	1	NAG	C4-C3-C2	-2.32	107.62	111.02
5	V	2	NAG	C4-C3-C2	-2.32	107.62	111.02
5	z	2	NAG	C4-C3-C2	-2.31	107.63	111.02
5	P	1	NAG	C4-C3-C2	-2.31	107.63	111.02
5	k	2	NAG	C4-C3-C2	-2.31	107.63	111.02
5	r	1	NAG	C8-C7-N2	2.30	119.94	116.12
5	c	1	NAG	C1-C2-N2	2.30	114.06	110.43
4	n	5	MAN	C2-C3-C4	-2.30	106.82	110.86
4	Y	5	MAN	C2-C3-C4	-2.30	106.82	110.86
4	I	5	MAN	C2-C3-C4	-2.30	106.82	110.86
5	N	1	NAG	C8-C7-N2	2.30	119.93	116.12
5	N	1	NAG	C1-C2-N2	2.29	114.04	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	r	1	NAG	C1-C2-N2	2.28	114.02	110.43
5	g	1	NAG	C3-C4-C5	-2.26	106.13	110.23
5	v	1	NAG	C3-C4-C5	-2.26	106.14	110.23
4	f	1	NAG	C3-C4-C5	-2.26	106.14	110.23
5	W	1	NAG	C3-C4-C5	-2.25	106.14	110.23
4	u	1	NAG	C3-C4-C5	-2.25	106.15	110.23
7	l	3	FUC	C6-C5-C4	-2.24	108.98	113.08
5	R	1	NAG	C3-C4-C5	-2.24	106.17	110.23
5	0	1	NAG	C3-C4-C5	-2.24	106.17	110.23
7	X	3	FUC	C6-C5-C4	-2.24	108.98	113.08
5	l	1	NAG	C3-C4-C5	-2.24	106.17	110.23
4	Q	1	NAG	C3-C4-C5	-2.23	106.20	110.23
7	m	3	FUC	C6-C5-C4	-2.22	109.02	113.08
7	m	2	NAG	C4-C3-C2	-2.22	107.77	111.02
7	X	2	NAG	C4-C3-C2	-2.21	107.78	111.02
7	l	2	NAG	C4-C3-C2	-2.20	107.80	111.02
5	x	1	NAG	C3-C4-C5	-2.18	106.28	110.23
5	T	1	NAG	C3-C4-C5	-2.17	106.30	110.23
5	i	1	NAG	C3-C4-C5	-2.17	106.30	110.23
5	J	2	NAG	O5-C1-C2	-2.15	107.96	111.29
5	Z	2	NAG	O5-C1-C2	-2.15	107.96	111.29
5	o	2	NAG	O5-C1-C2	-2.14	107.98	111.29
4	f	5	MAN	C2-C3-C4	-2.14	107.11	110.86
4	u	5	MAN	C2-C3-C4	-2.13	107.11	110.86
4	Q	5	MAN	C2-C3-C4	-2.12	107.13	110.86
4	I	4	MAN	C1-C2-C3	2.08	112.67	109.64
5	Z	1	NAG	O4-C4-C3	-2.07	105.50	110.38
5	J	1	NAG	O4-C4-C3	-2.06	105.52	110.38
5	o	1	NAG	O4-C4-C3	-2.06	105.53	110.38
4	Y	4	MAN	C1-C2-C3	2.05	112.63	109.64
5	a	1	NAG	O5-C5-C6	-2.05	103.67	107.66
4	n	4	MAN	C1-C2-C3	2.05	112.62	109.64
5	T	1	NAG	C1-C2-N2	-2.05	107.21	110.43
5	p	1	NAG	O5-C5-C6	-2.03	103.71	107.66
5	i	1	NAG	C1-C2-N2	-2.03	107.23	110.43
5	x	1	NAG	C1-C2-N2	-2.03	107.23	110.43
5	0	1	NAG	C1-C2-N2	-2.03	107.23	110.43
5	W	1	NAG	C1-C2-N2	-2.03	107.24	110.43
5	K	1	NAG	O5-C5-C6	-2.02	103.73	107.66
5	l	1	NAG	C1-C2-N2	-2.02	107.25	110.43
5	K	1	NAG	O4-C4-C3	-2.00	105.65	110.38

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	1	NAG	O5-C5-C6-O6
5	Z	1	NAG	O5-C5-C6-O6
5	o	1	NAG	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6
5	i	2	NAG	O5-C5-C6-O6
5	q	2	NAG	O5-C5-C6-O6
5	x	2	NAG	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
5	a	1	NAG	O5-C5-C6-O6
5	j	2	NAG	O5-C5-C6-O6
5	p	1	NAG	O5-C5-C6-O6
5	y	2	NAG	O5-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
5	R	2	NAG	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
5	r	2	NAG	O5-C5-C6-O6
5	v	2	NAG	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
5	d	2	NAG	O5-C5-C6-O6
5	e	2	NAG	O5-C5-C6-O6
5	g	2	NAG	O5-C5-C6-O6
5	s	2	NAG	O5-C5-C6-O6
5	t	2	NAG	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	Z	1	NAG	C4-C5-C6-O6
5	o	1	NAG	C4-C5-C6-O6
5	R	1	NAG	O5-C5-C6-O6
5	g	1	NAG	O5-C5-C6-O6
5	v	1	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	o	2	NAG	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
5	k	2	NAG	O5-C5-C6-O6
5	z	2	NAG	O5-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
5	e	2	NAG	C4-C5-C6-O6
5	t	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	X	1	NAG	C4-C5-C6-O6
7	m	1	NAG	C4-C5-C6-O6
7	l	1	NAG	C4-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
5	i	1	NAG	O5-C5-C6-O6
5	x	1	NAG	O5-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	b	2	NAG	C4-C5-C6-O6
5	q	2	NAG	C4-C5-C6-O6
4	Q	4	MAN	O5-C5-C6-O6
4	f	4	MAN	O5-C5-C6-O6
4	u	4	MAN	O5-C5-C6-O6
5	R	1	NAG	C4-C5-C6-O6
5	g	1	NAG	C4-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
5	r	1	NAG	O5-C5-C6-O6
5	v	1	NAG	C4-C5-C6-O6
4	I	5	MAN	O5-C5-C6-O6
4	Y	5	MAN	O5-C5-C6-O6
4	n	5	MAN	O5-C5-C6-O6
7	X	2	NAG	O5-C5-C6-O6
7	m	2	NAG	O5-C5-C6-O6
7	l	2	NAG	O5-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
5	p	2	NAG	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
5	a	1	NAG	C4-C5-C6-O6
5	p	1	NAG	C4-C5-C6-O6
5	W	2	NAG	O5-C5-C6-O6
5	l	2	NAG	O5-C5-C6-O6
5	0	2	NAG	O5-C5-C6-O6
6	S	3	BMA	O5-C5-C6-O6
6	h	3	BMA	O5-C5-C6-O6
6	w	3	BMA	O5-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
5	i	2	NAG	C4-C5-C6-O6
5	x	2	NAG	C4-C5-C6-O6
4	Q	5	MAN	O5-C5-C6-O6
4	f	5	MAN	O5-C5-C6-O6
4	u	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	j	2	NAG	C4-C5-C6-O6
5	U	2	NAG	C4-C5-C6-O6
5	y	2	NAG	C4-C5-C6-O6
7	l	1	NAG	O5-C5-C6-O6
7	m	1	NAG	O5-C5-C6-O6
7	X	1	NAG	O5-C5-C6-O6
4	I	4	MAN	O5-C5-C6-O6
4	Y	4	MAN	O5-C5-C6-O6
4	n	4	MAN	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
4	n	1	NAG	O5-C5-C6-O6
5	N	1	NAG	C4-C5-C6-O6
5	c	1	NAG	C4-C5-C6-O6
5	r	1	NAG	C4-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
5	i	1	NAG	C4-C5-C6-O6
5	x	1	NAG	C4-C5-C6-O6
5	r	2	NAG	C4-C5-C6-O6
5	N	2	NAG	C4-C5-C6-O6
5	c	2	NAG	C4-C5-C6-O6
5	R	2	NAG	C4-C5-C6-O6
5	g	2	NAG	C4-C5-C6-O6
5	v	2	NAG	C4-C5-C6-O6
5	J	2	NAG	C3-C2-N2-C7
5	Z	2	NAG	C3-C2-N2-C7
5	o	2	NAG	C3-C2-N2-C7
5	O	2	NAG	C4-C5-C6-O6
5	d	2	NAG	C4-C5-C6-O6
5	s	2	NAG	C4-C5-C6-O6
5	J	2	NAG	C1-C2-N2-C7
5	Z	2	NAG	C1-C2-N2-C7
5	o	2	NAG	C1-C2-N2-C7
5	o	2	NAG	C4-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
5	Z	2	NAG	C4-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 8 short contacts:

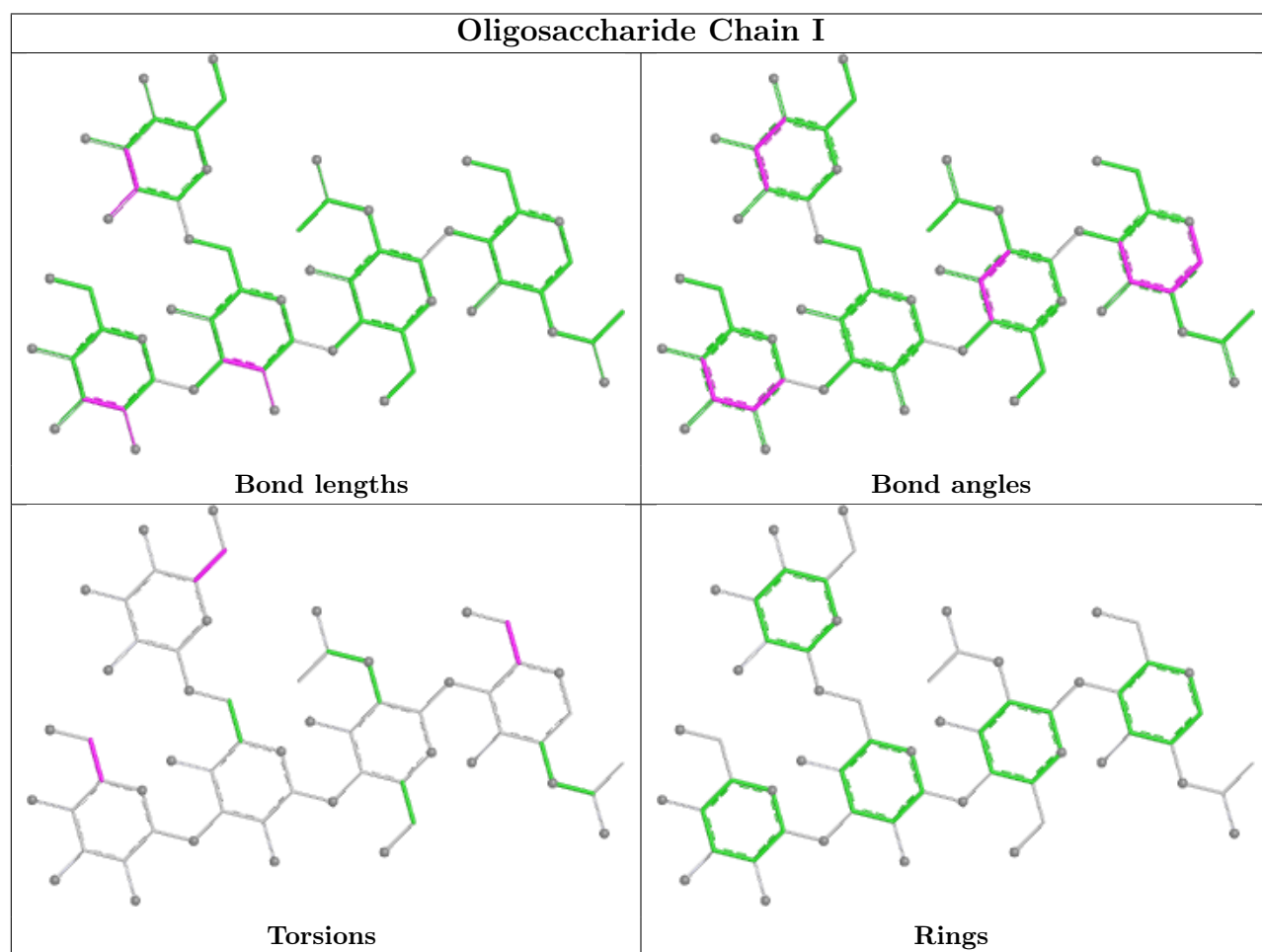
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	1	NAG	1	0

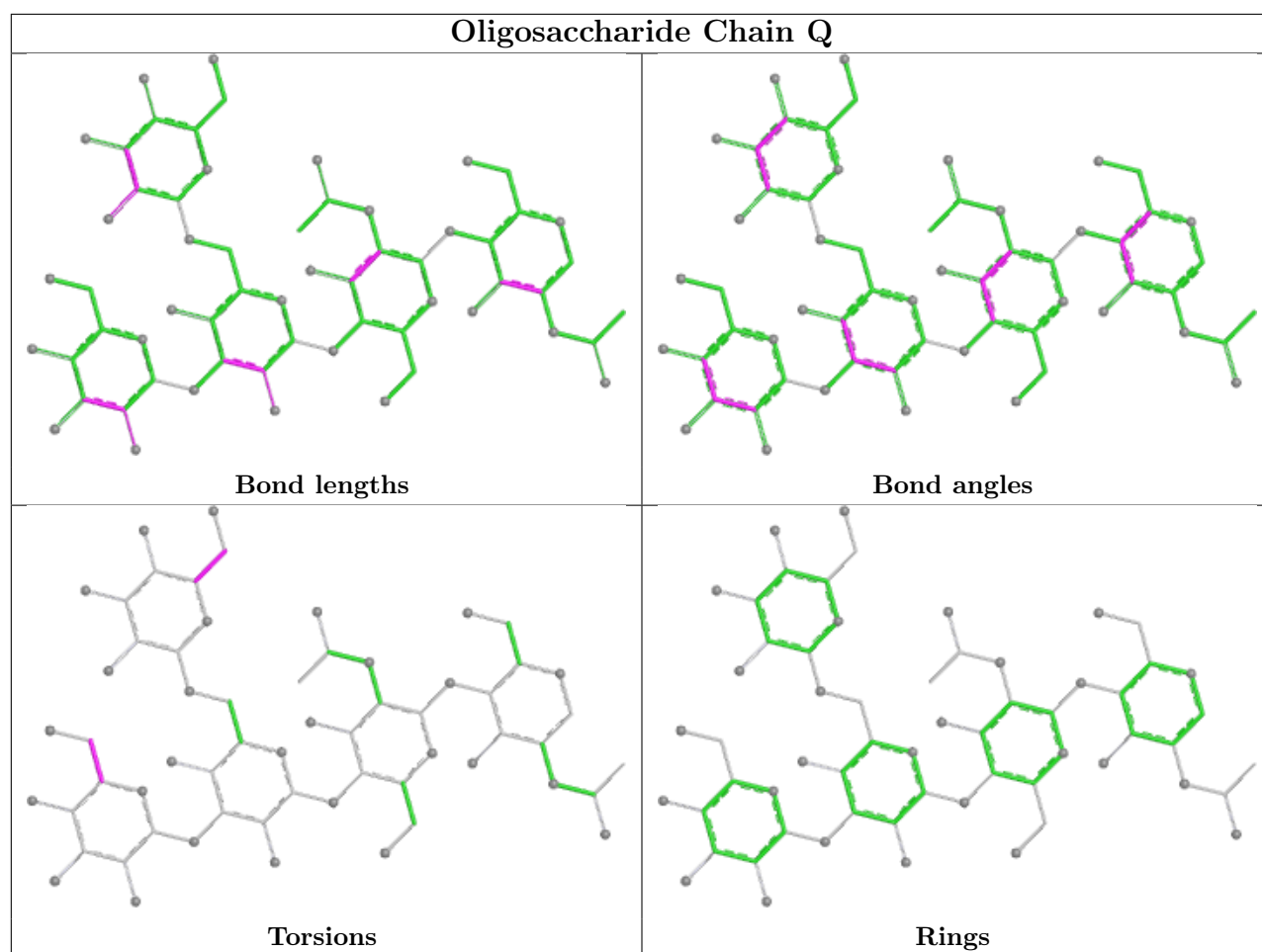
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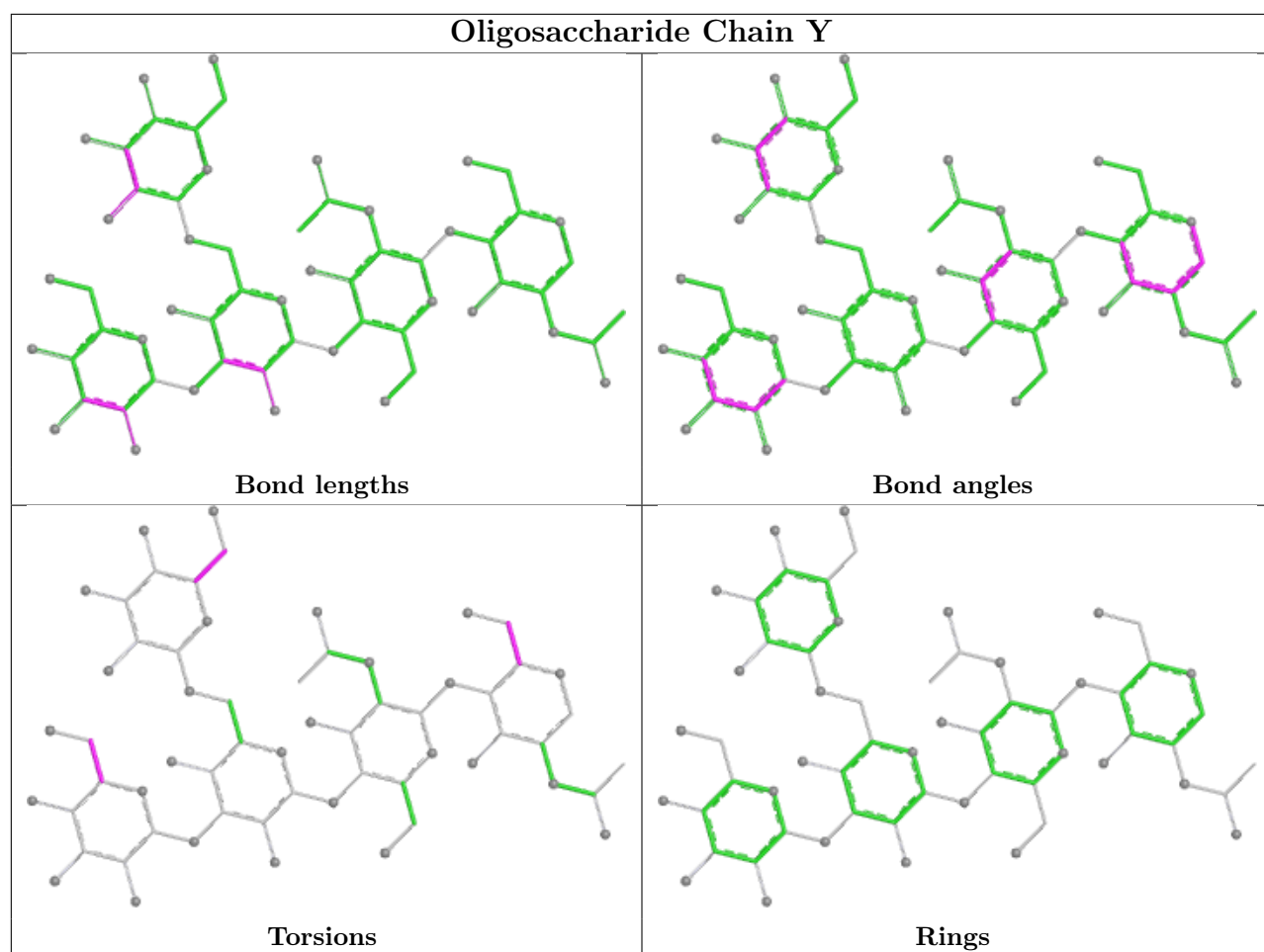
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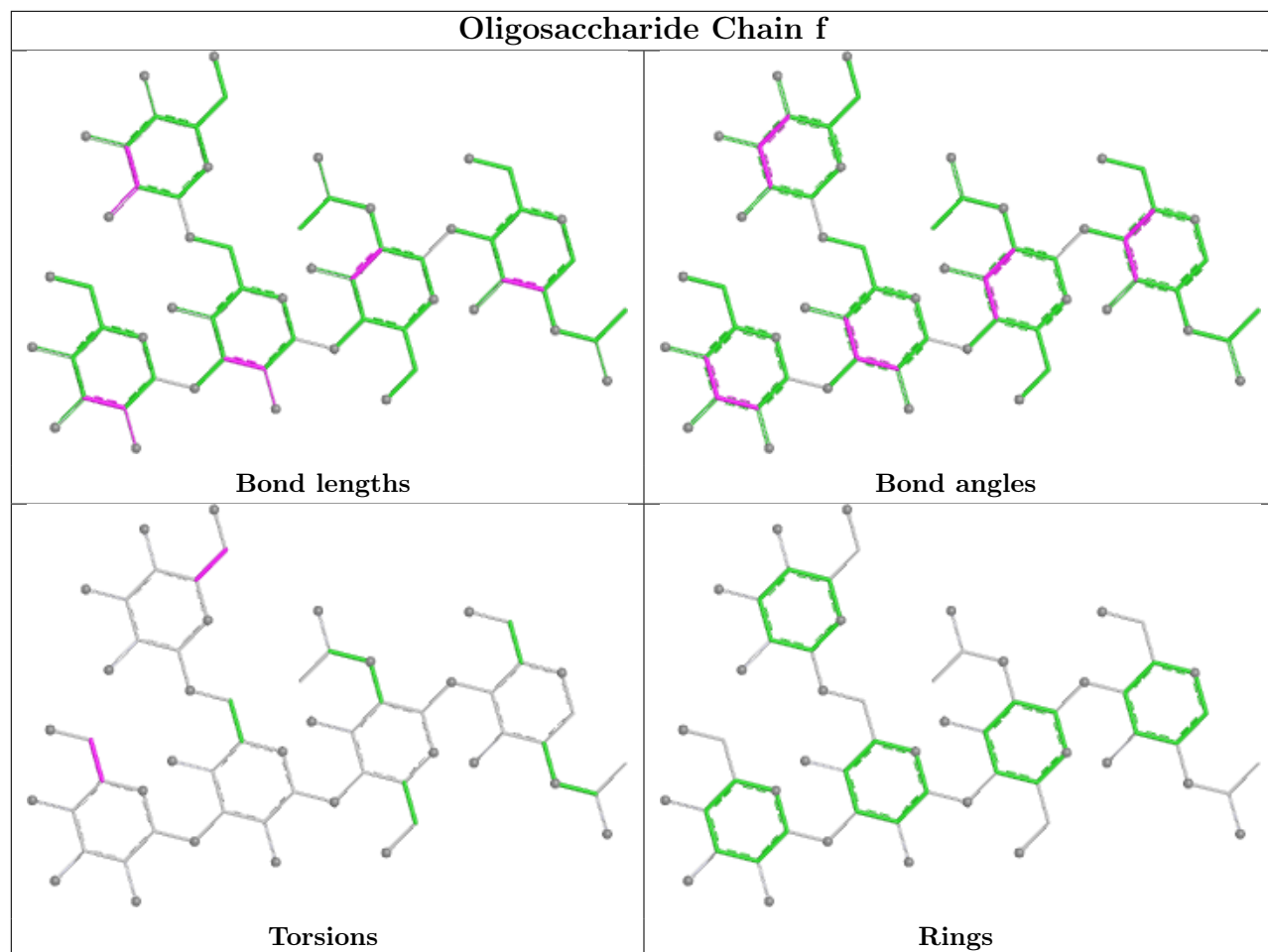
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	i	1	NAG	1	0
5	x	1	NAG	1	0
5	J	2	NAG	1	0
5	Z	2	NAG	1	0
5	r	1	NAG	1	0
5	N	1	NAG	1	0
5	c	1	NAG	1	0

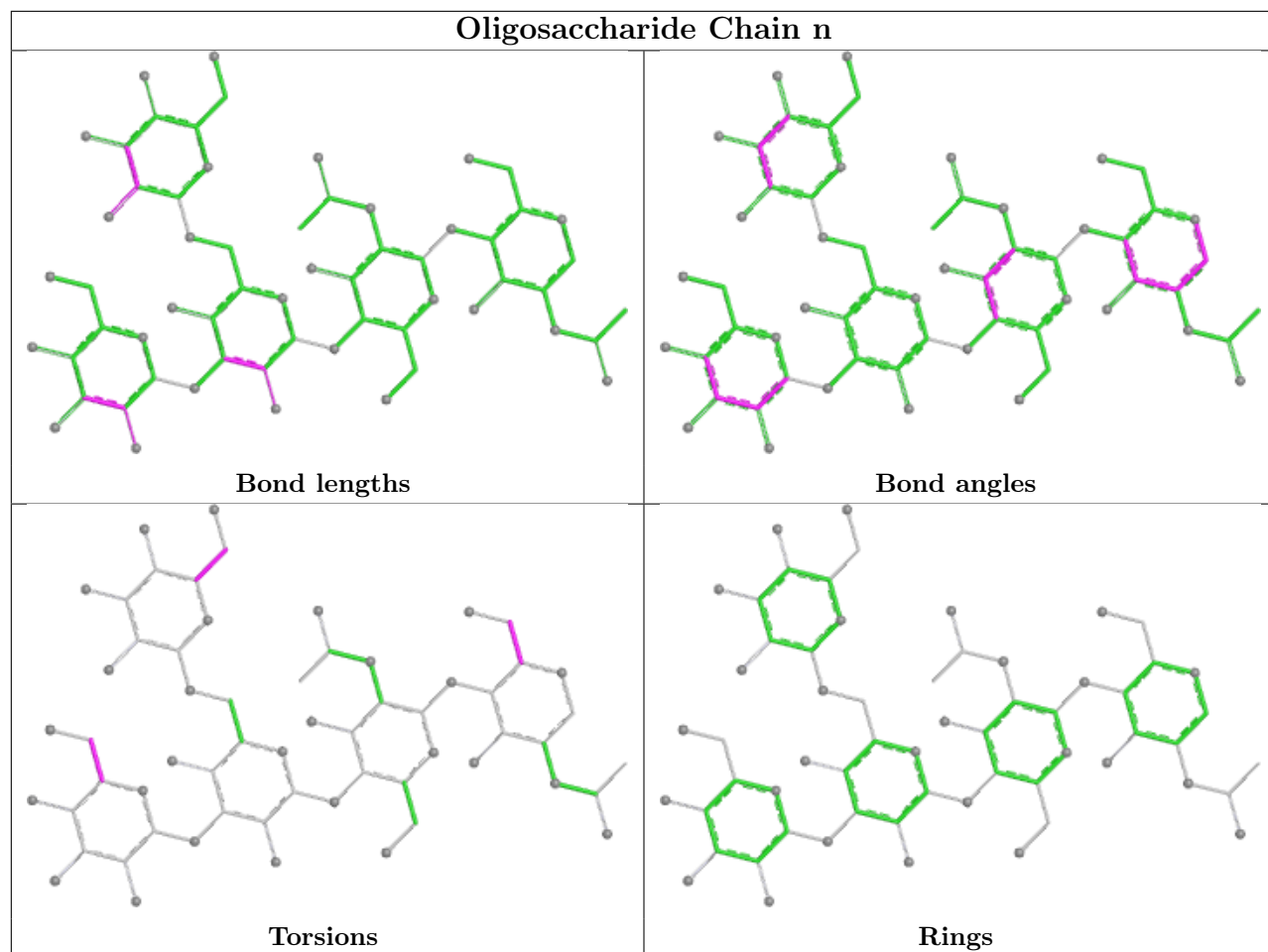
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

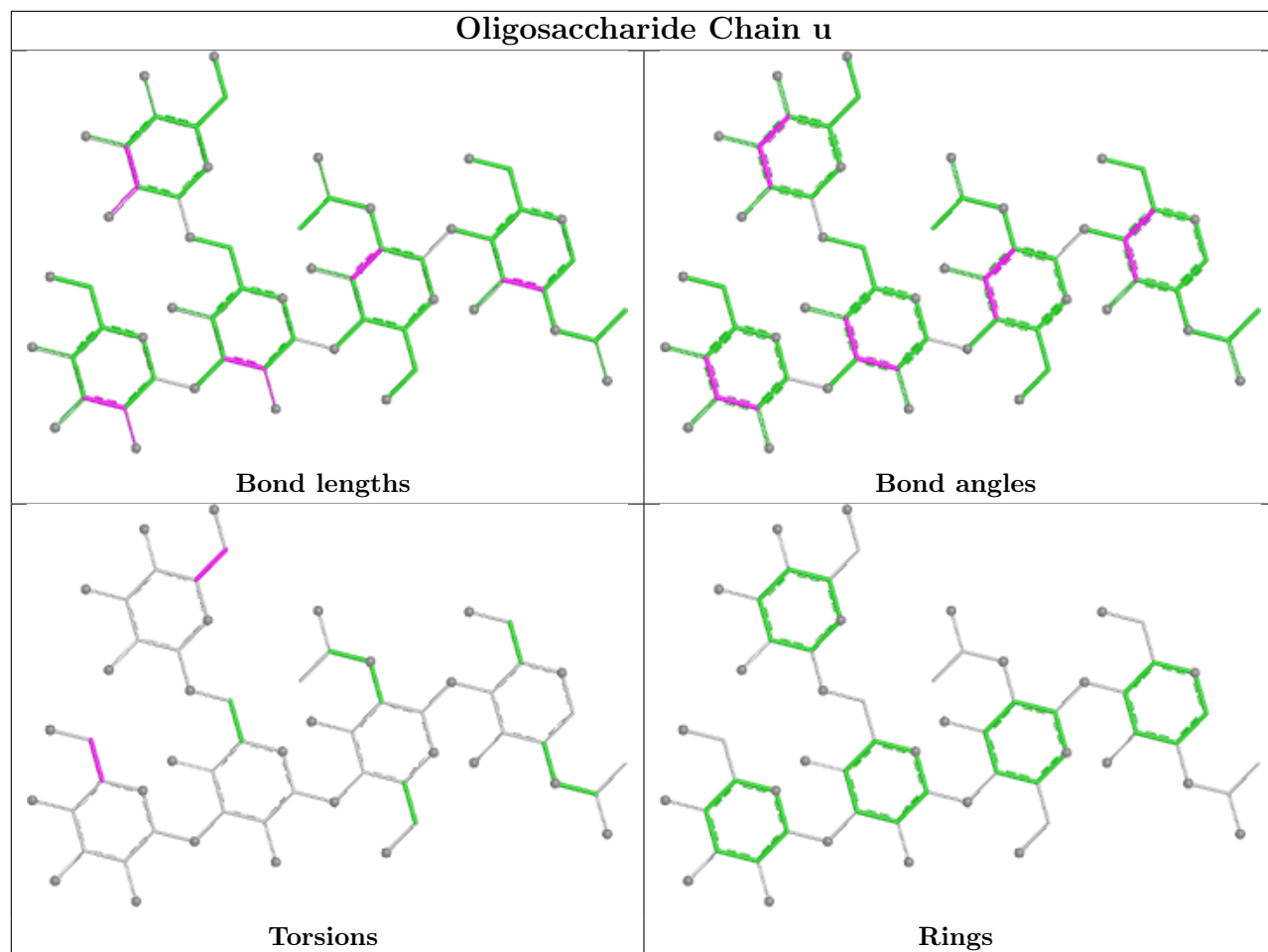


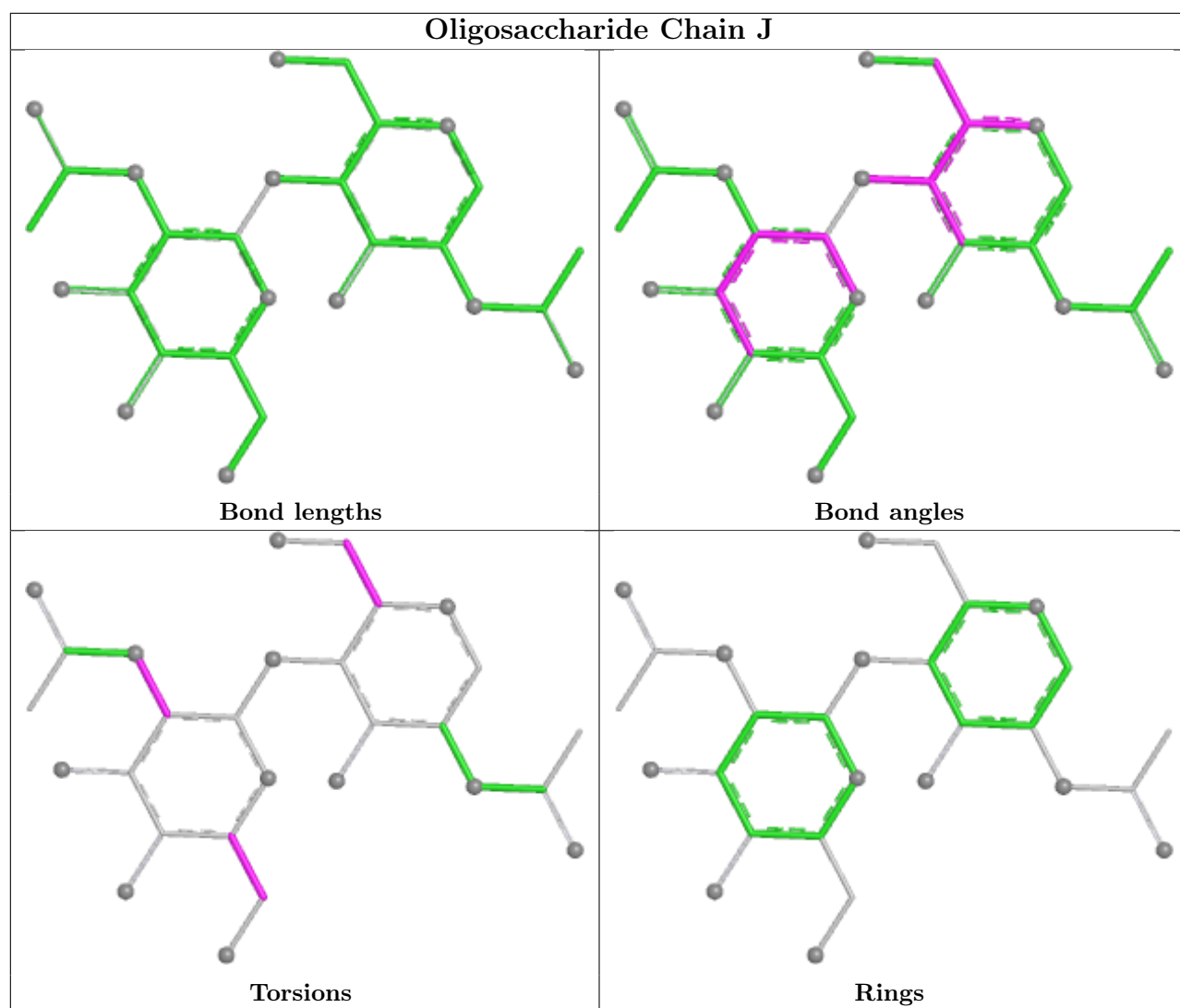


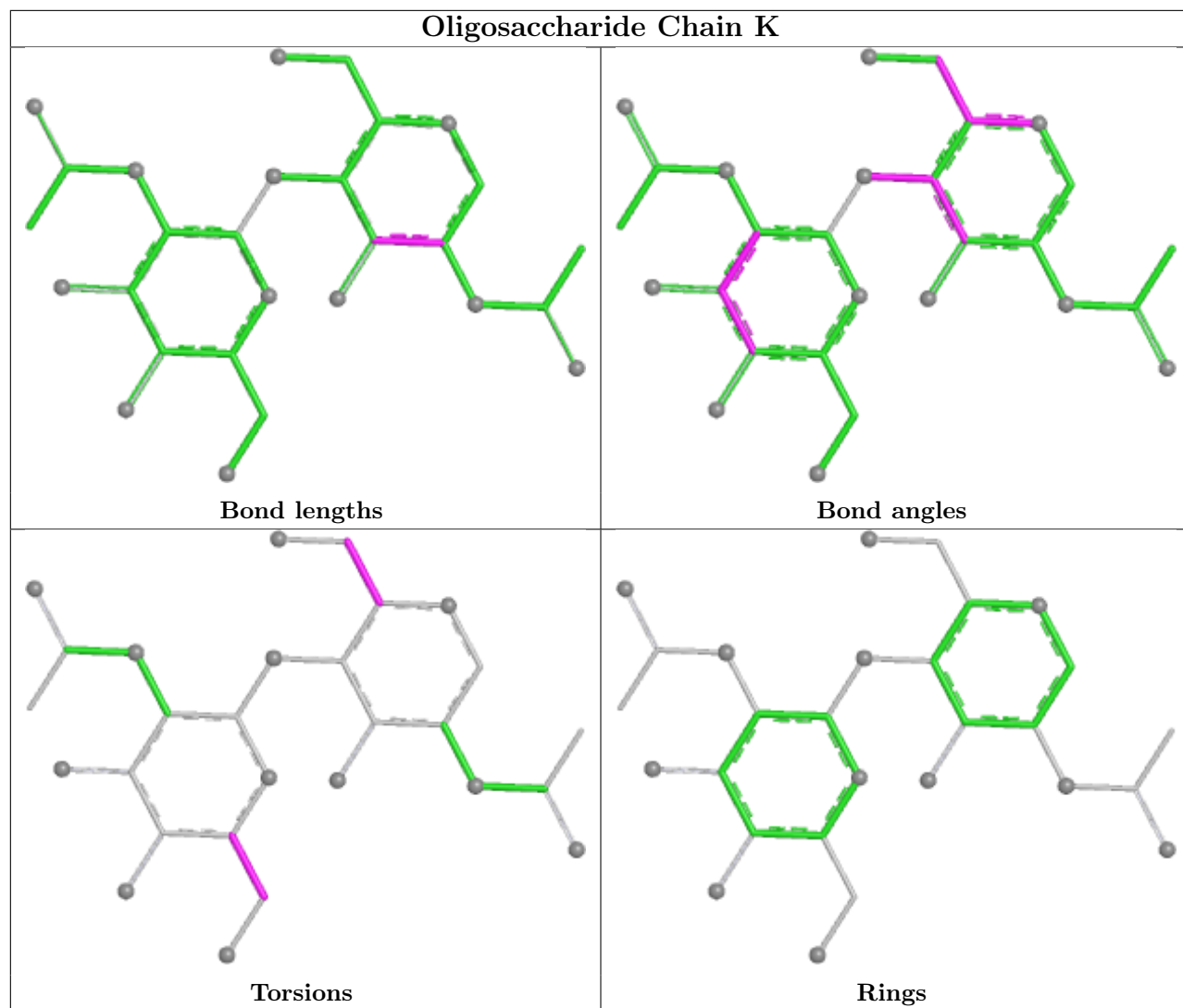


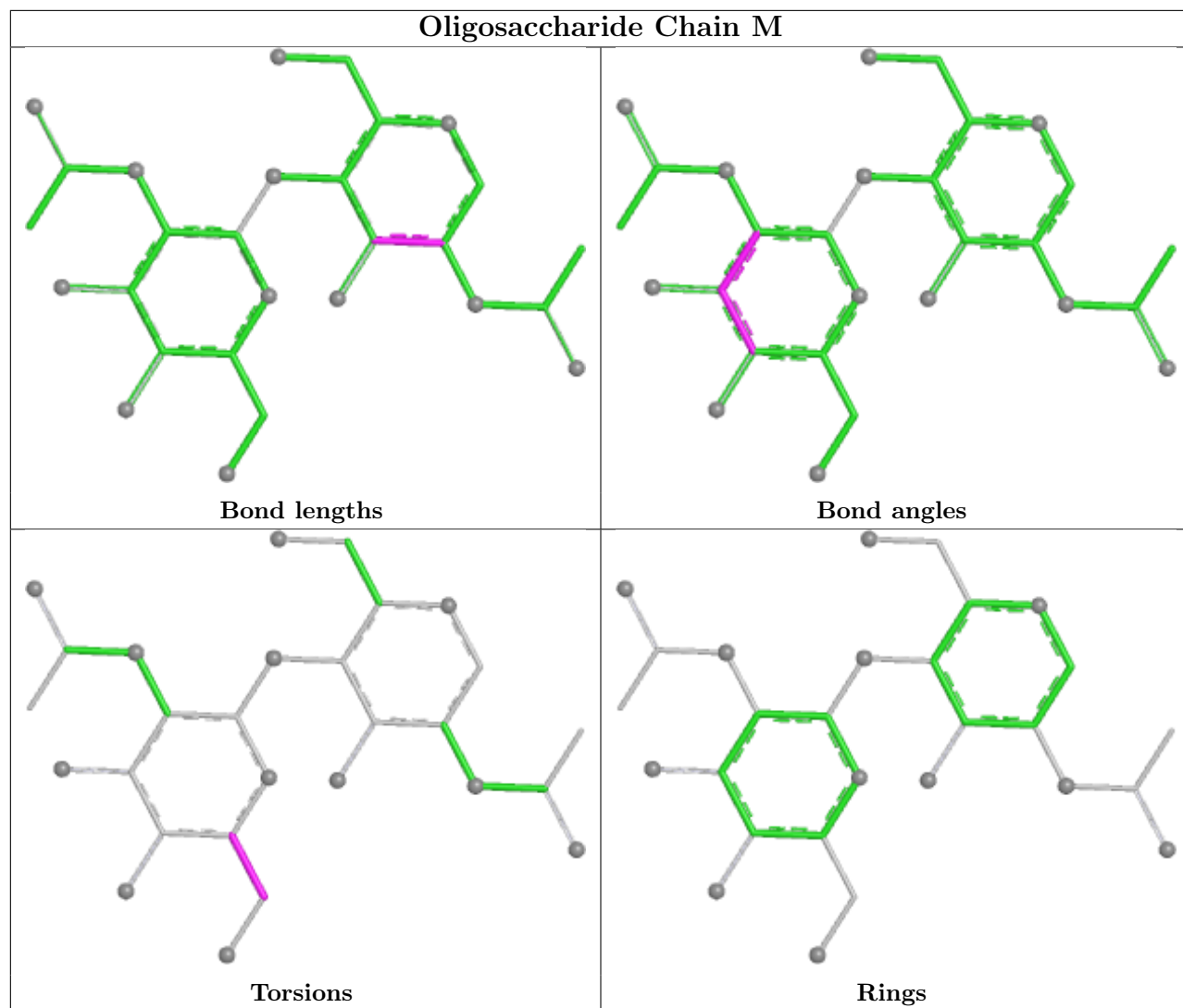


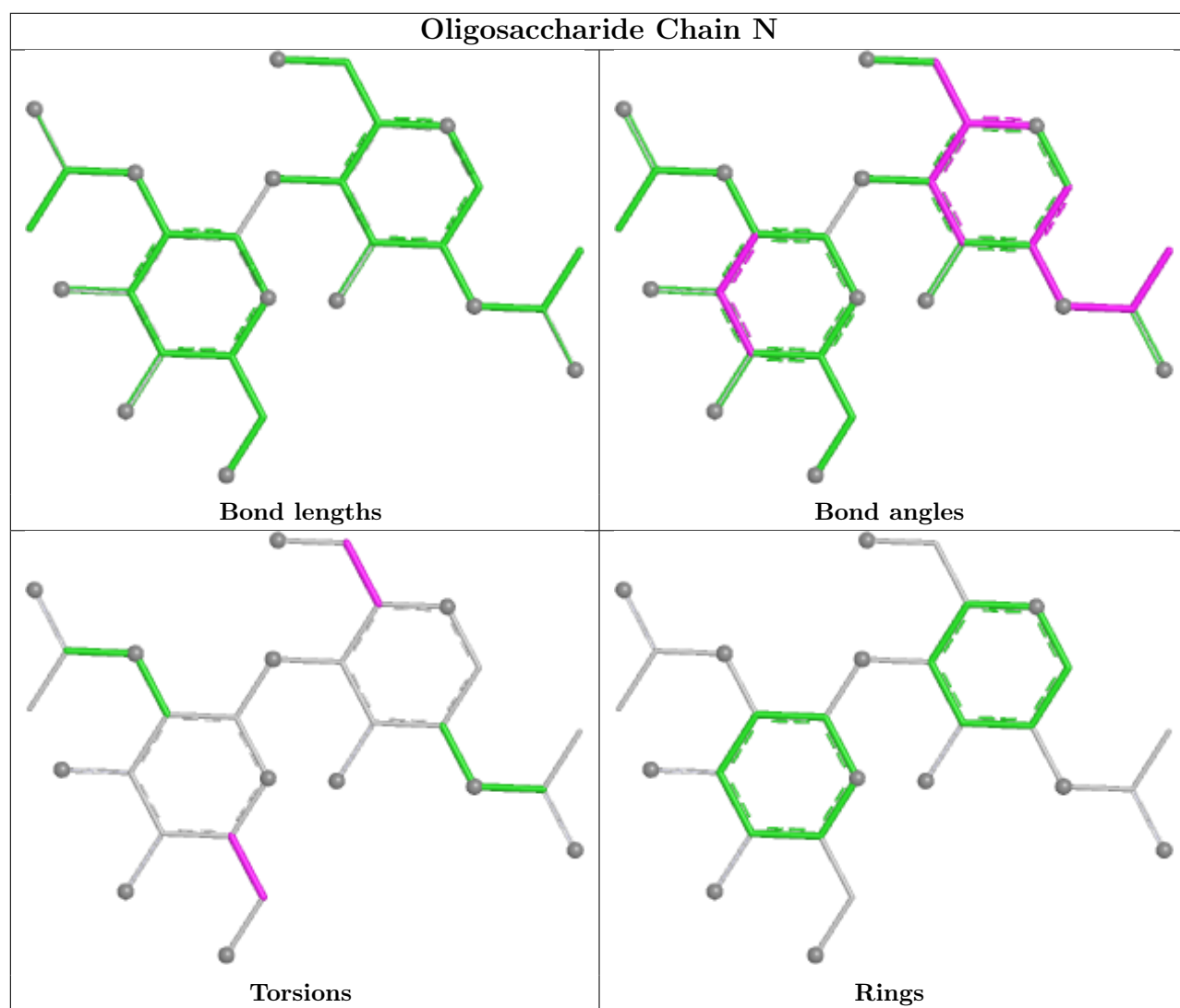


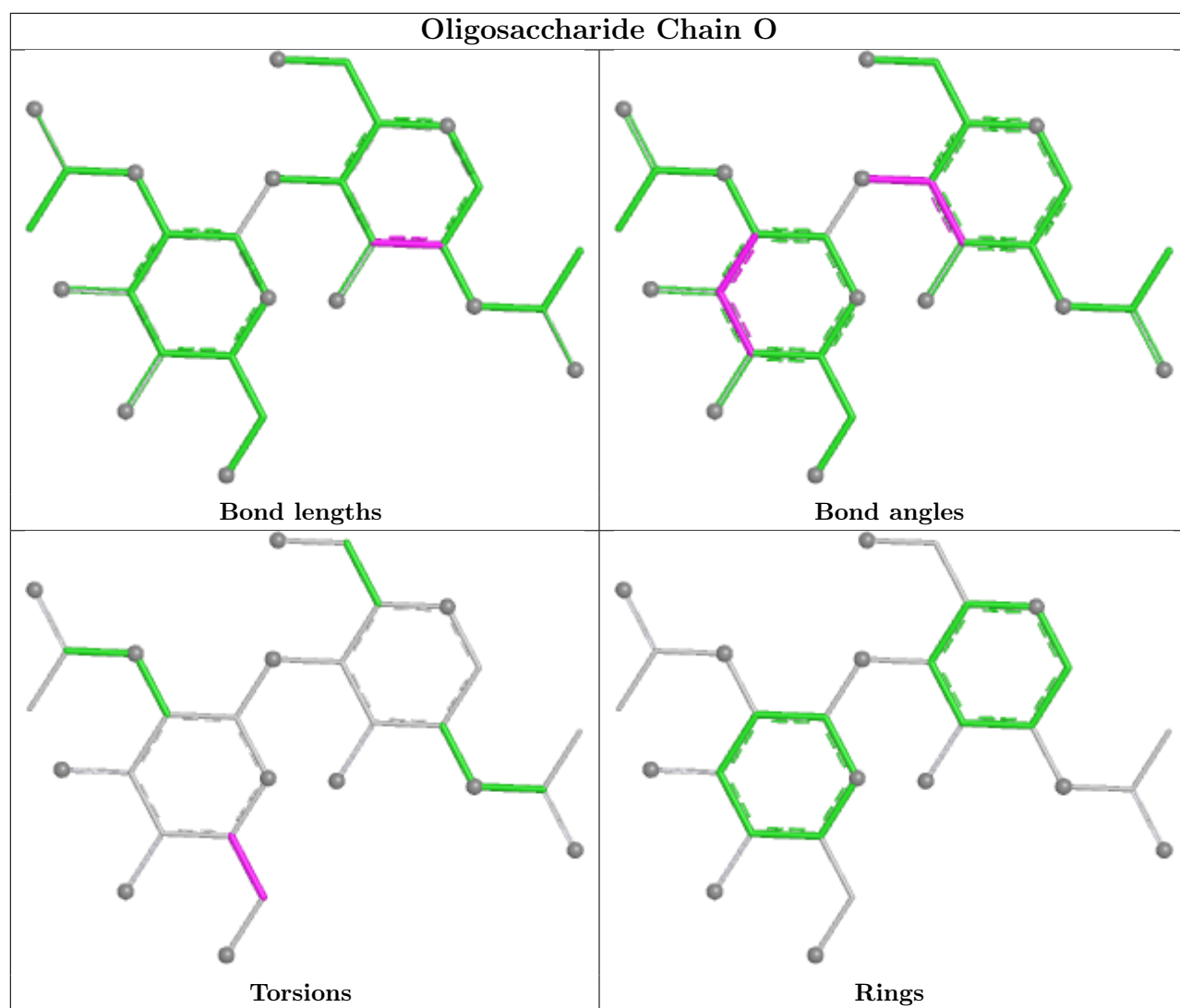


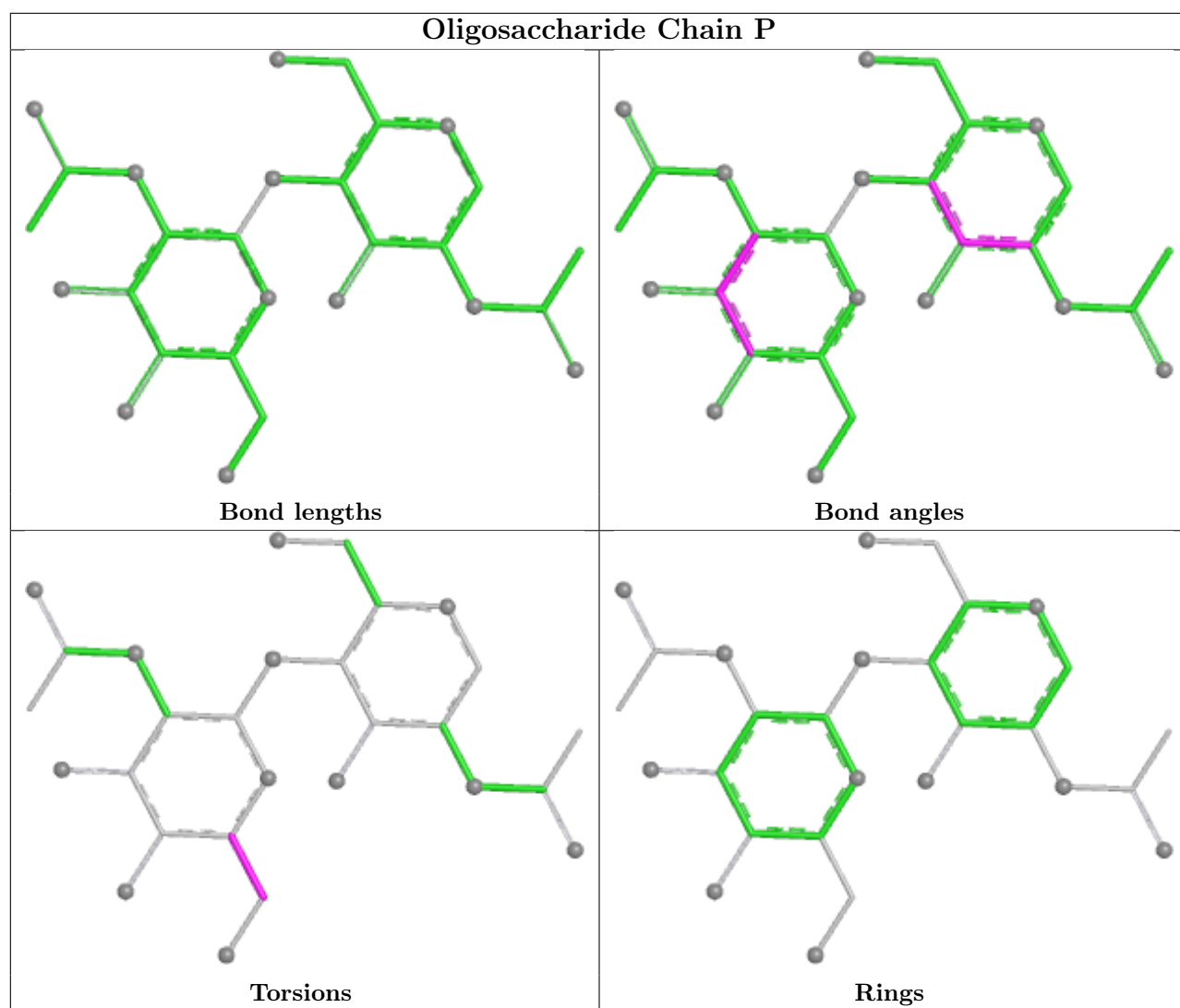


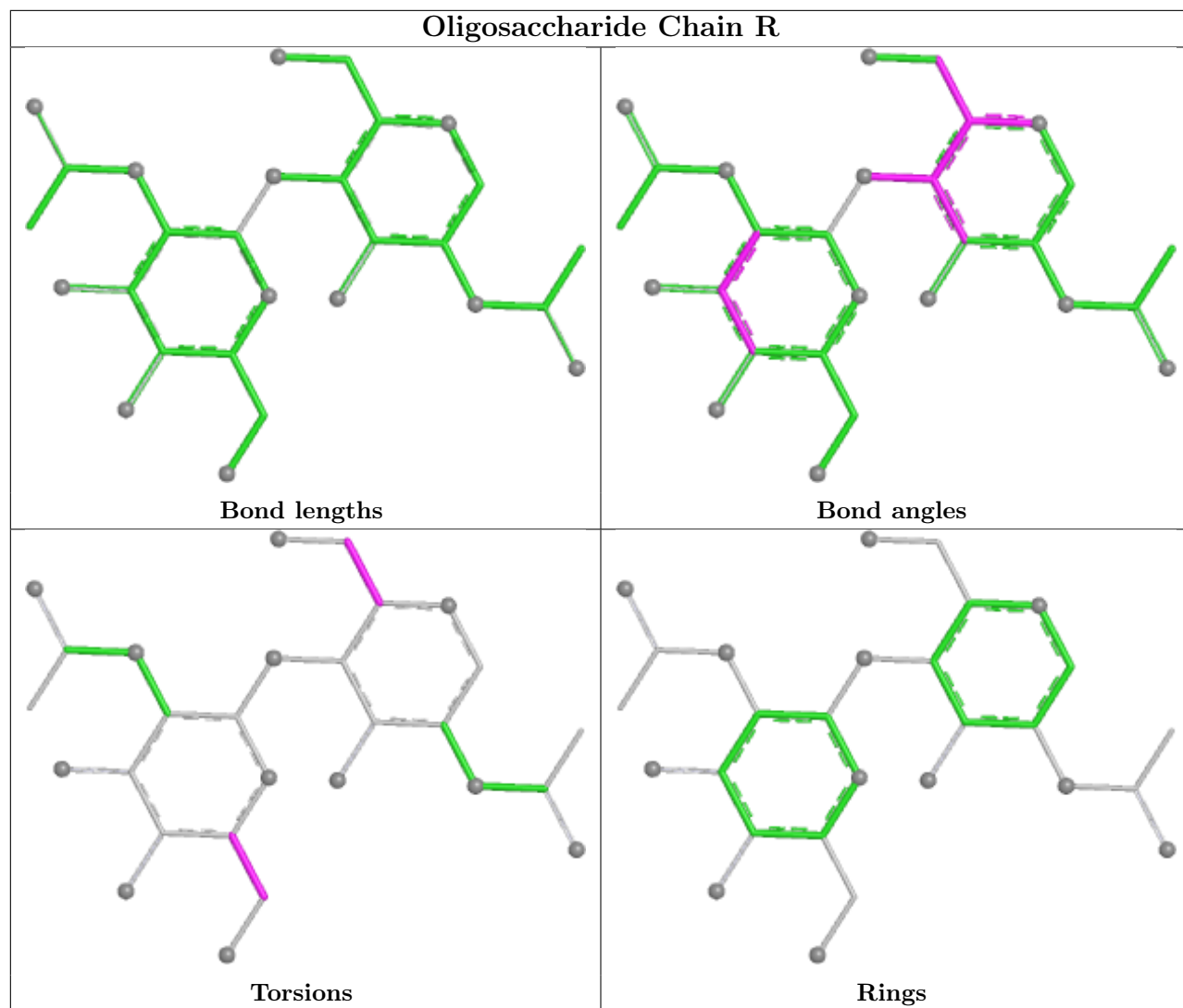


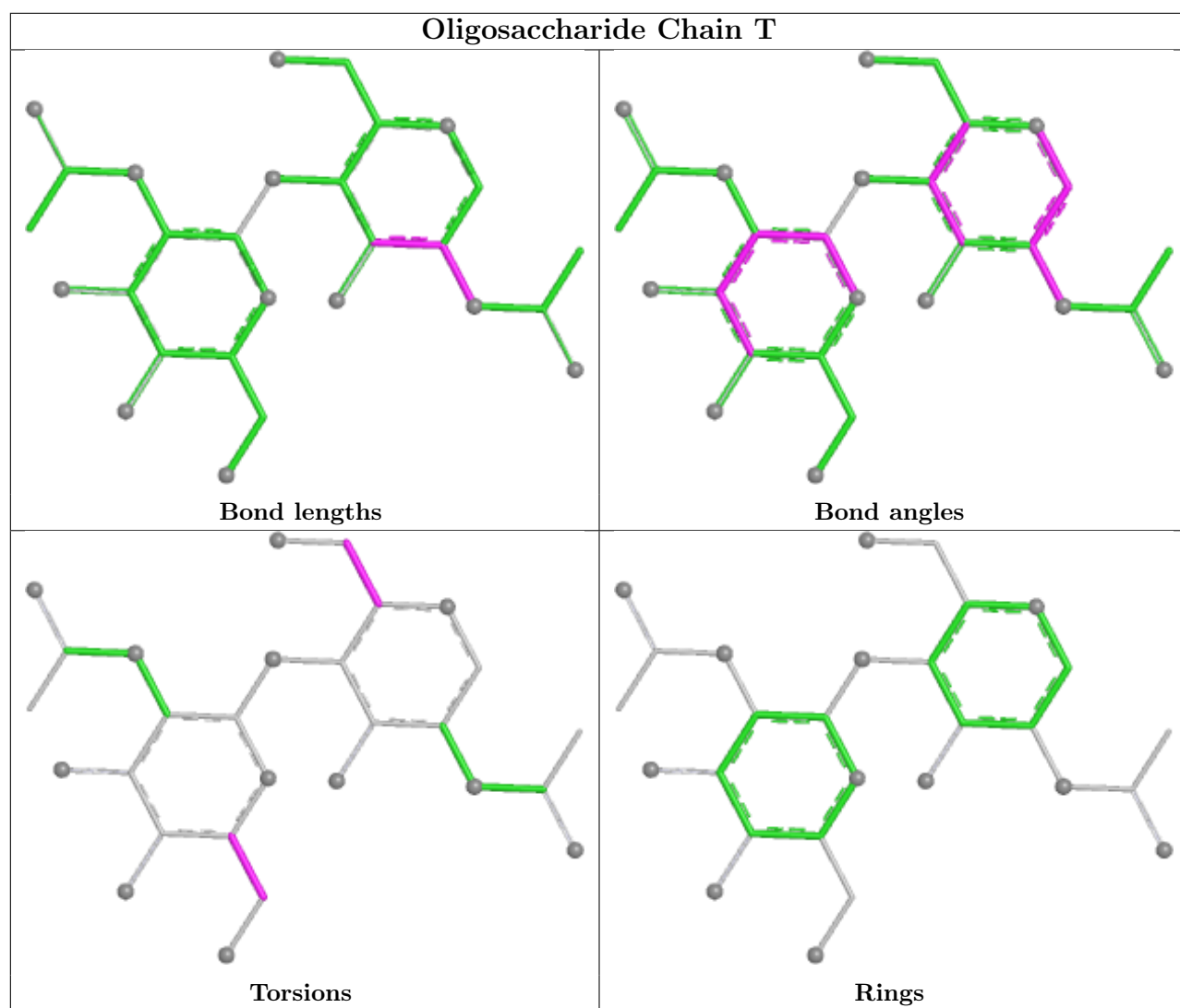


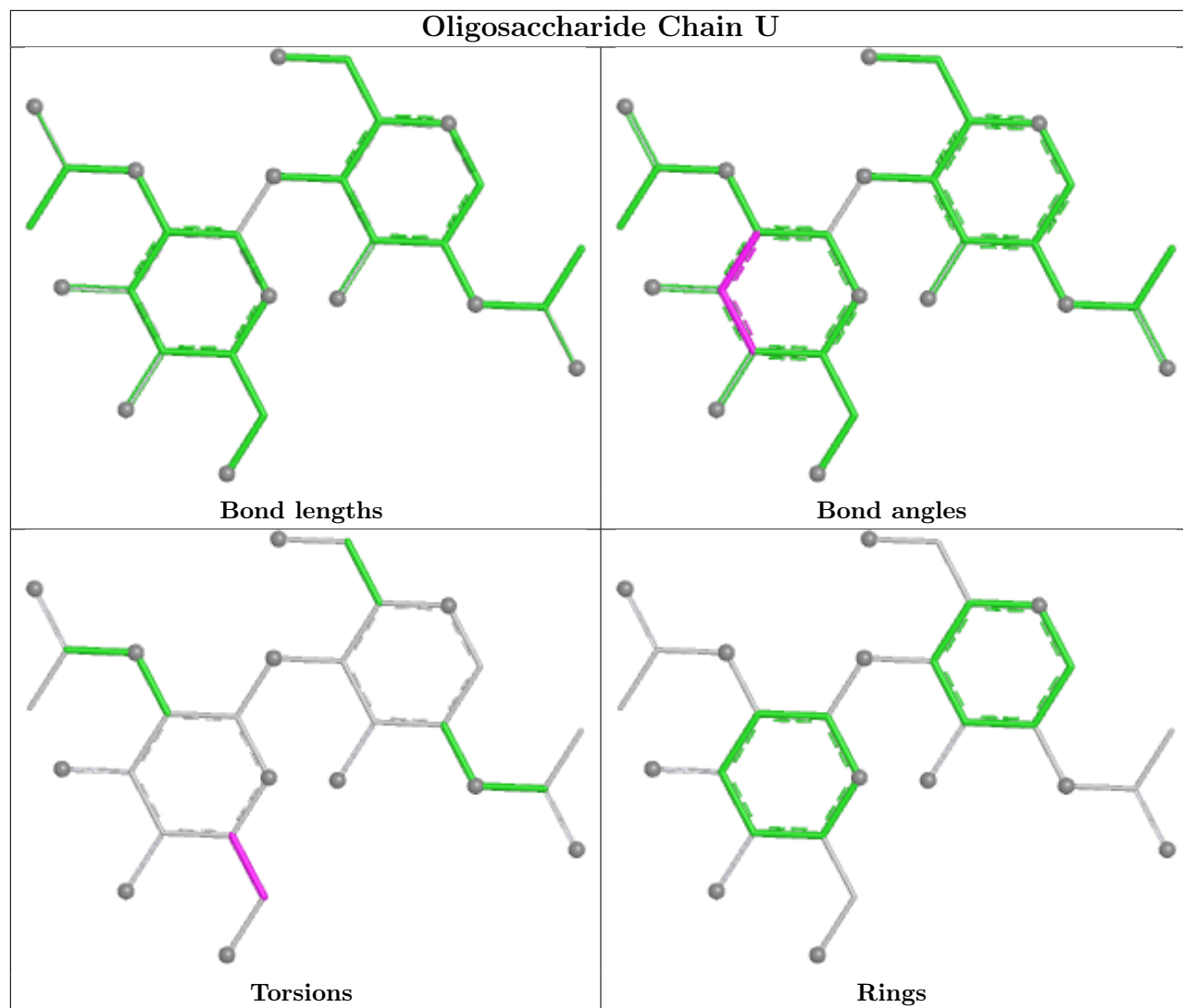


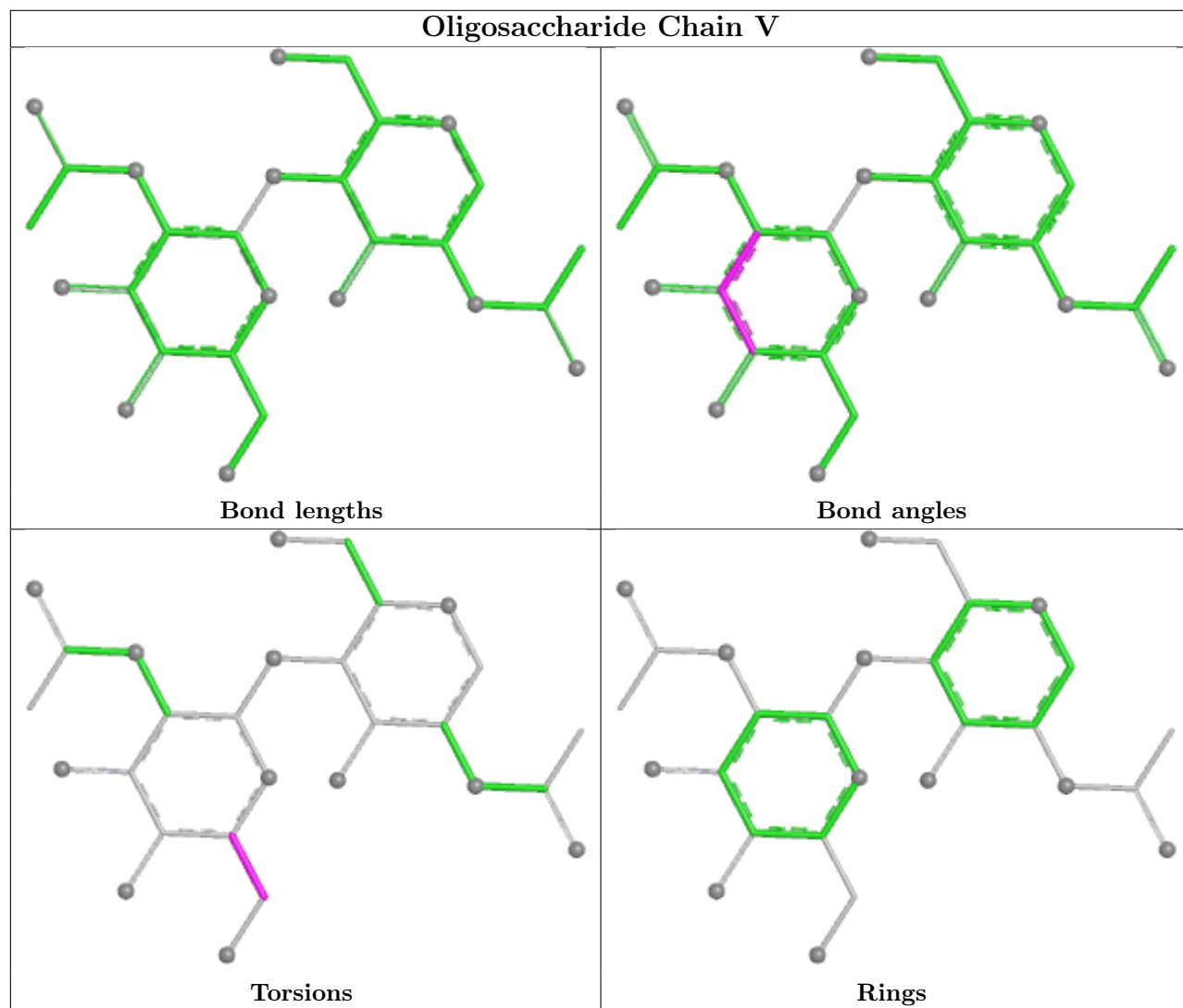


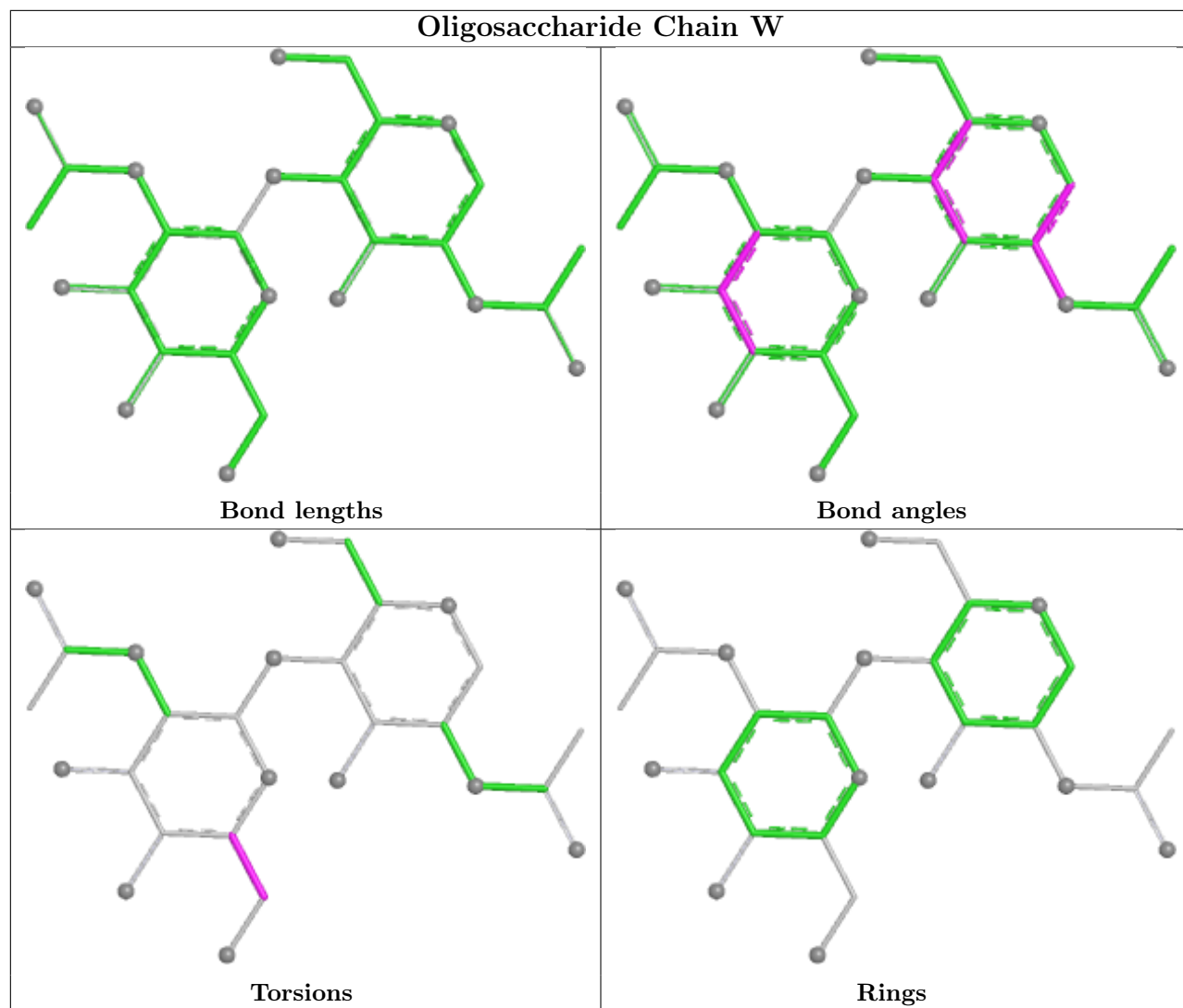


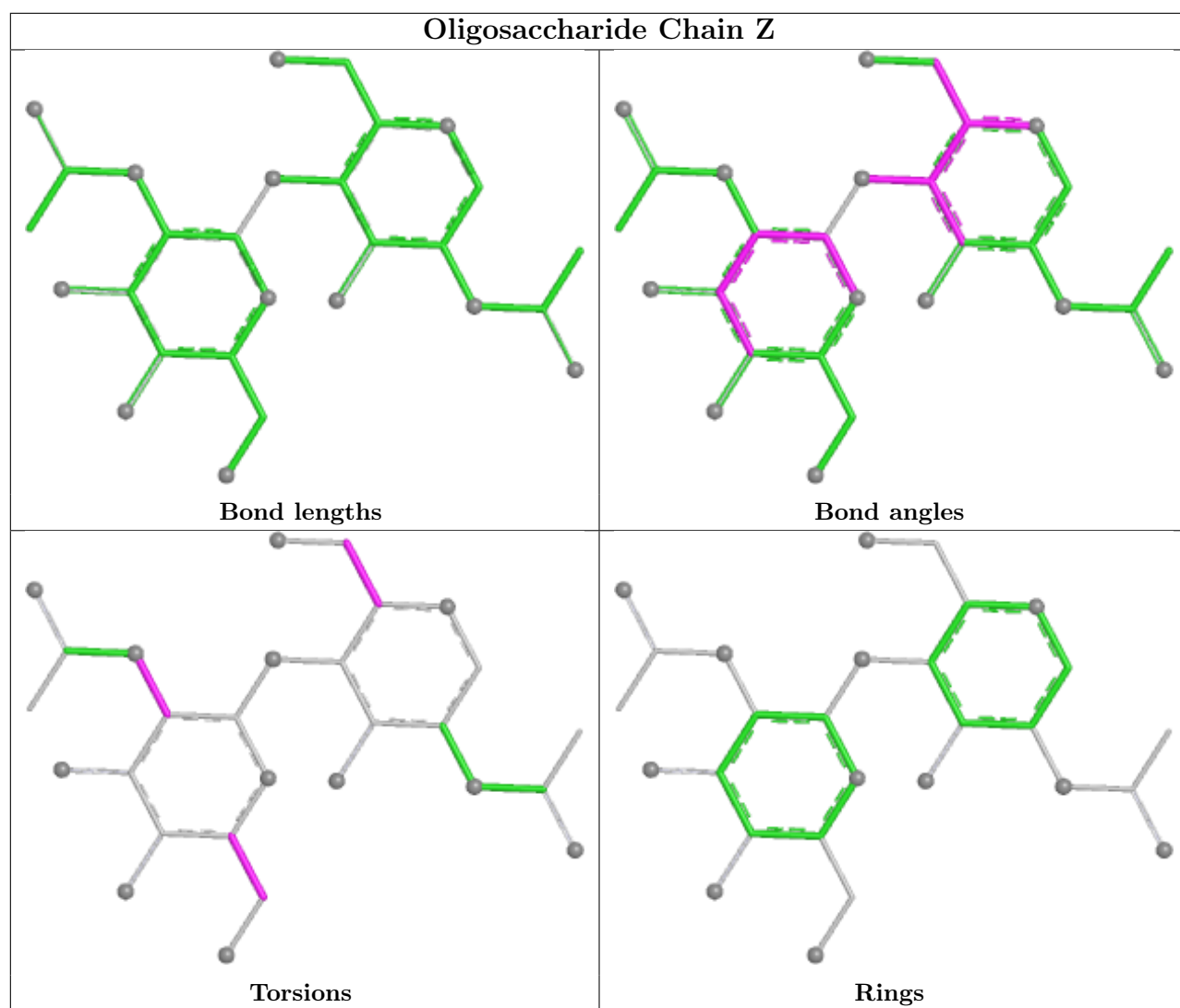


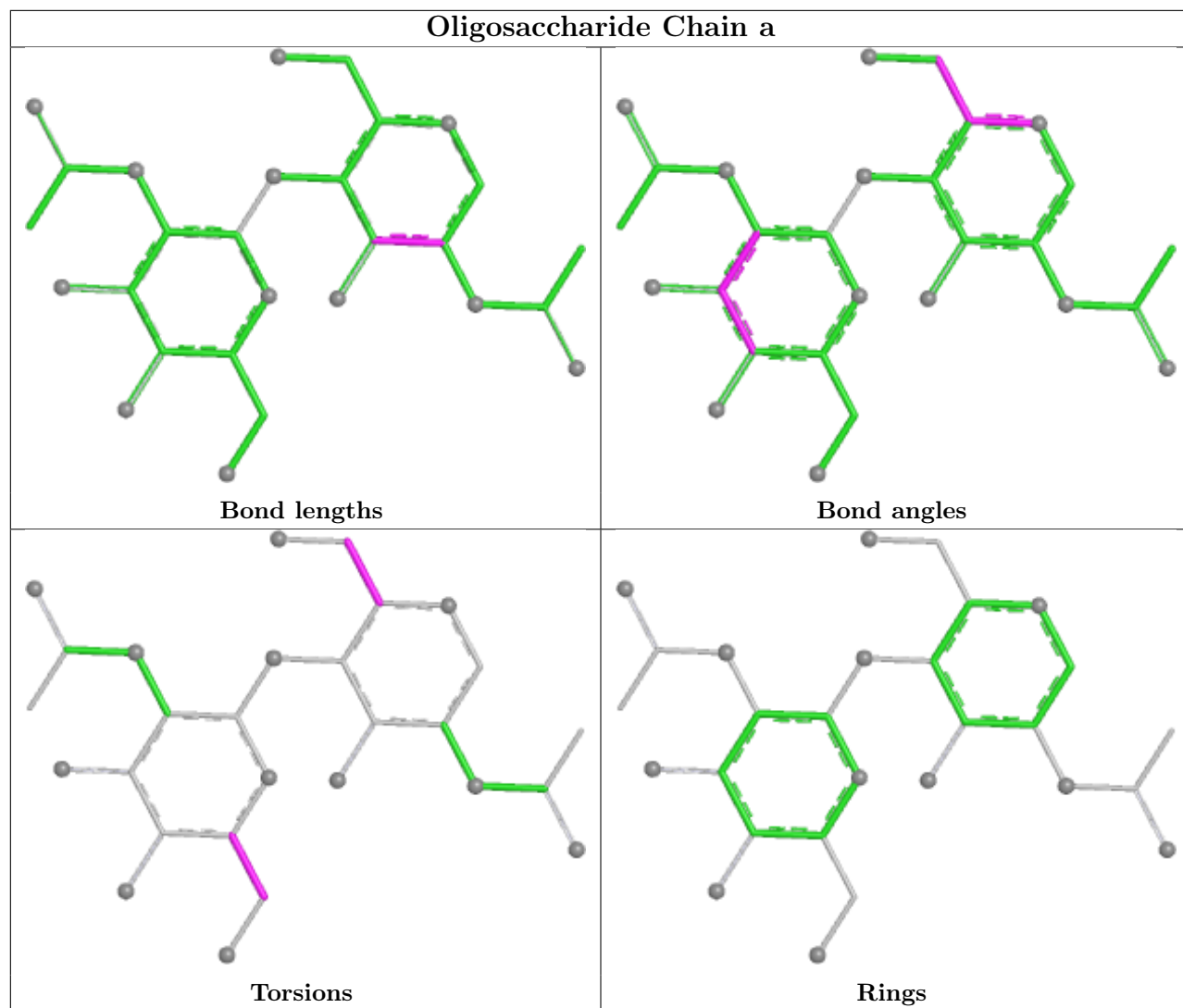


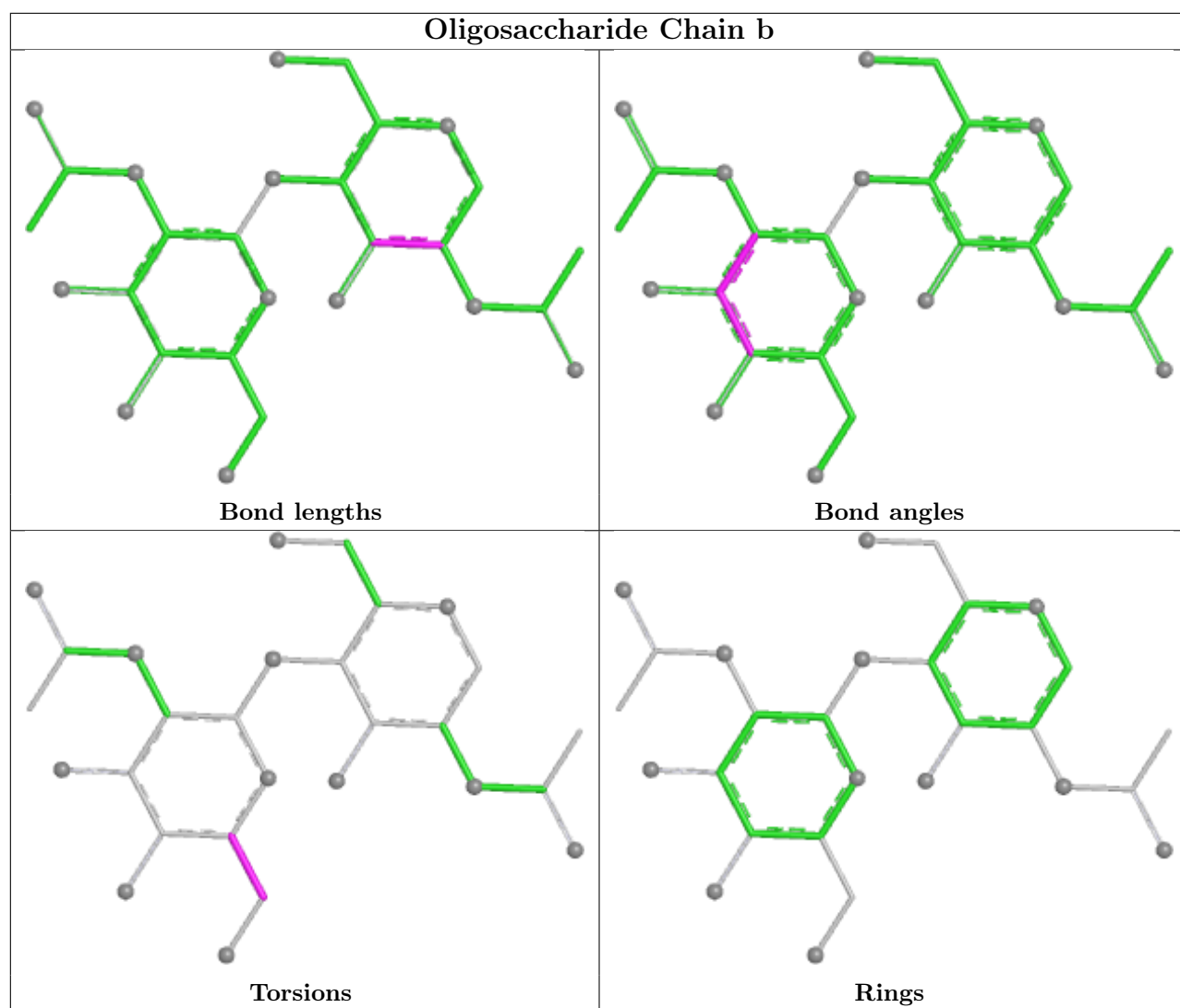


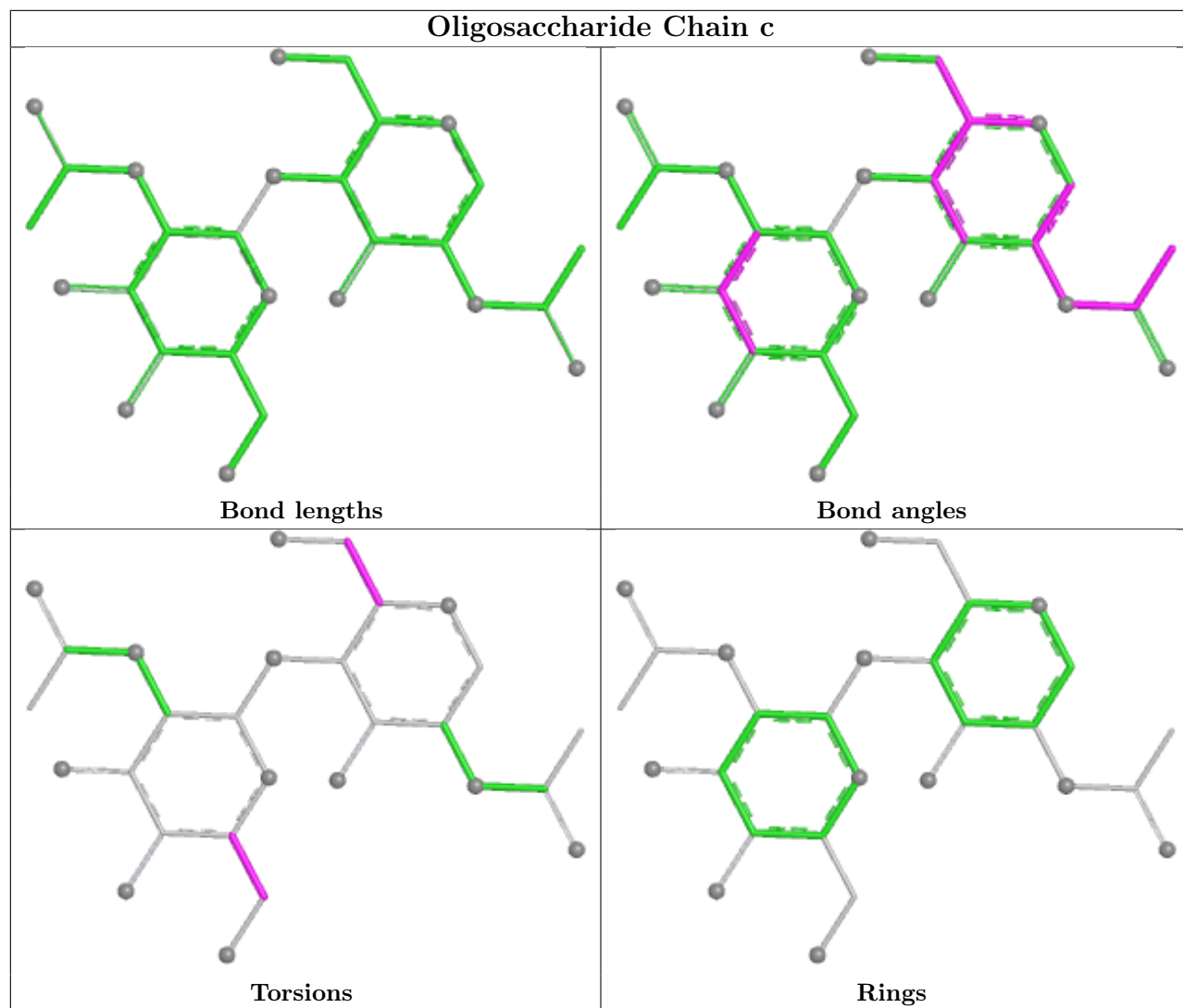


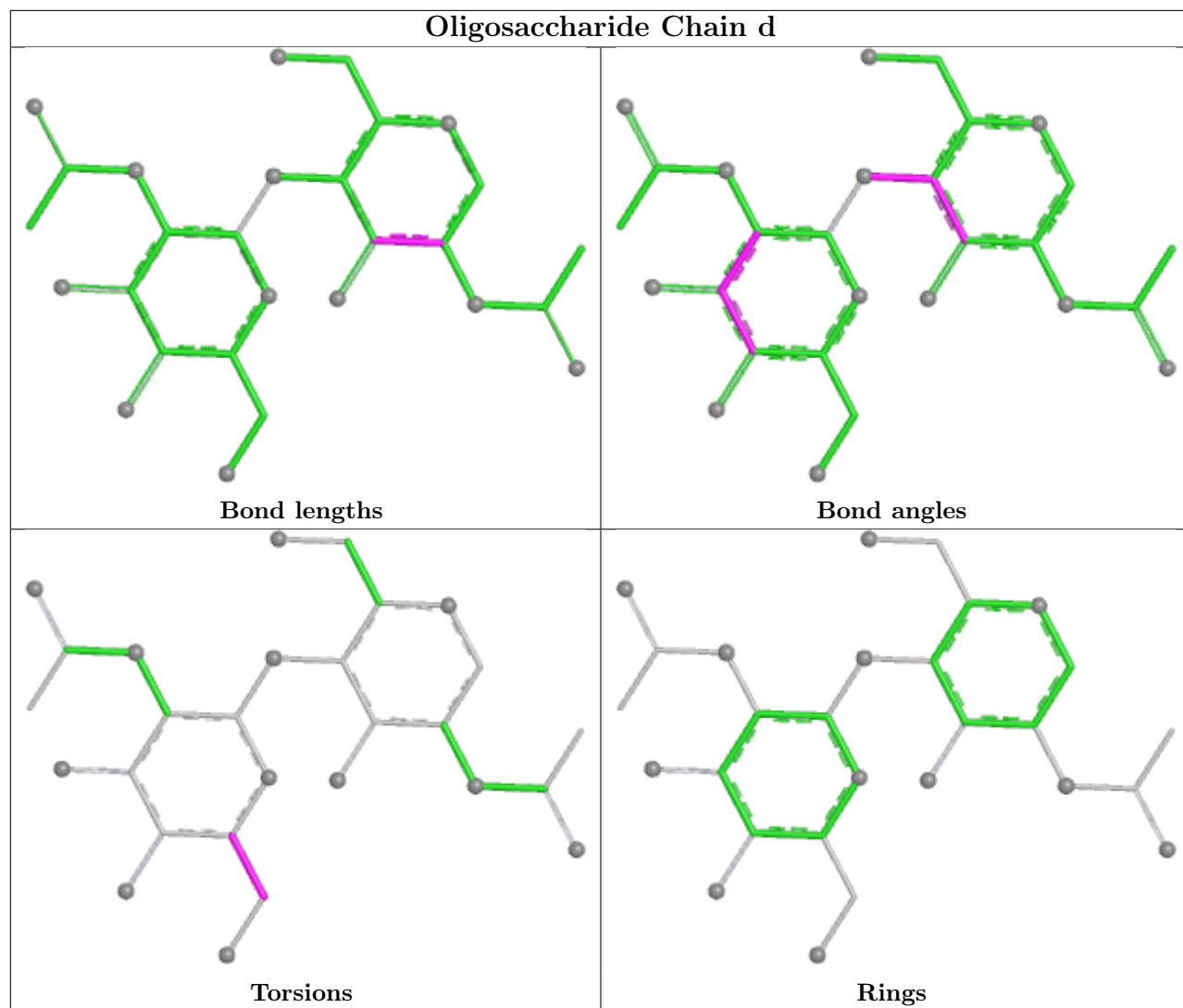


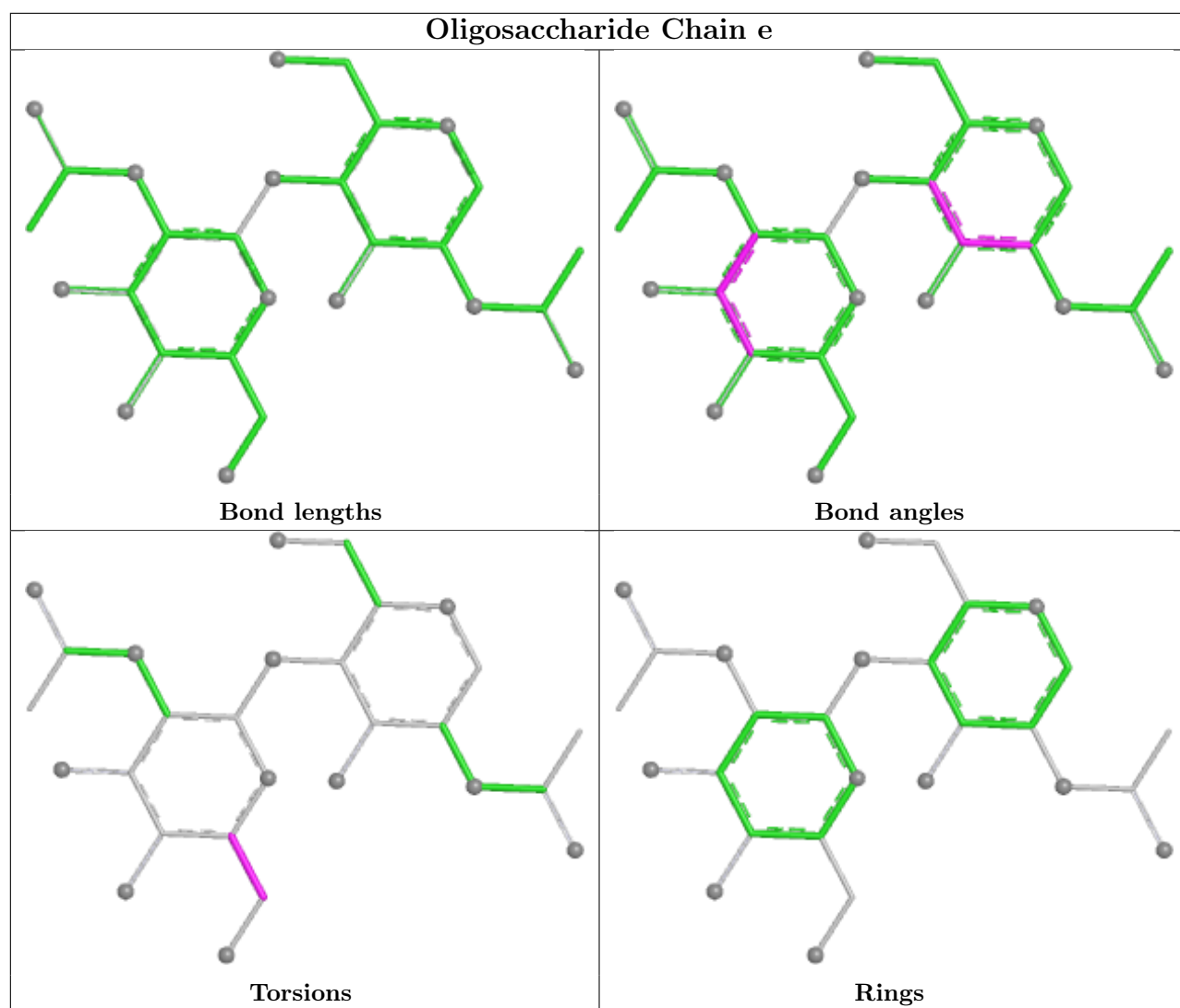


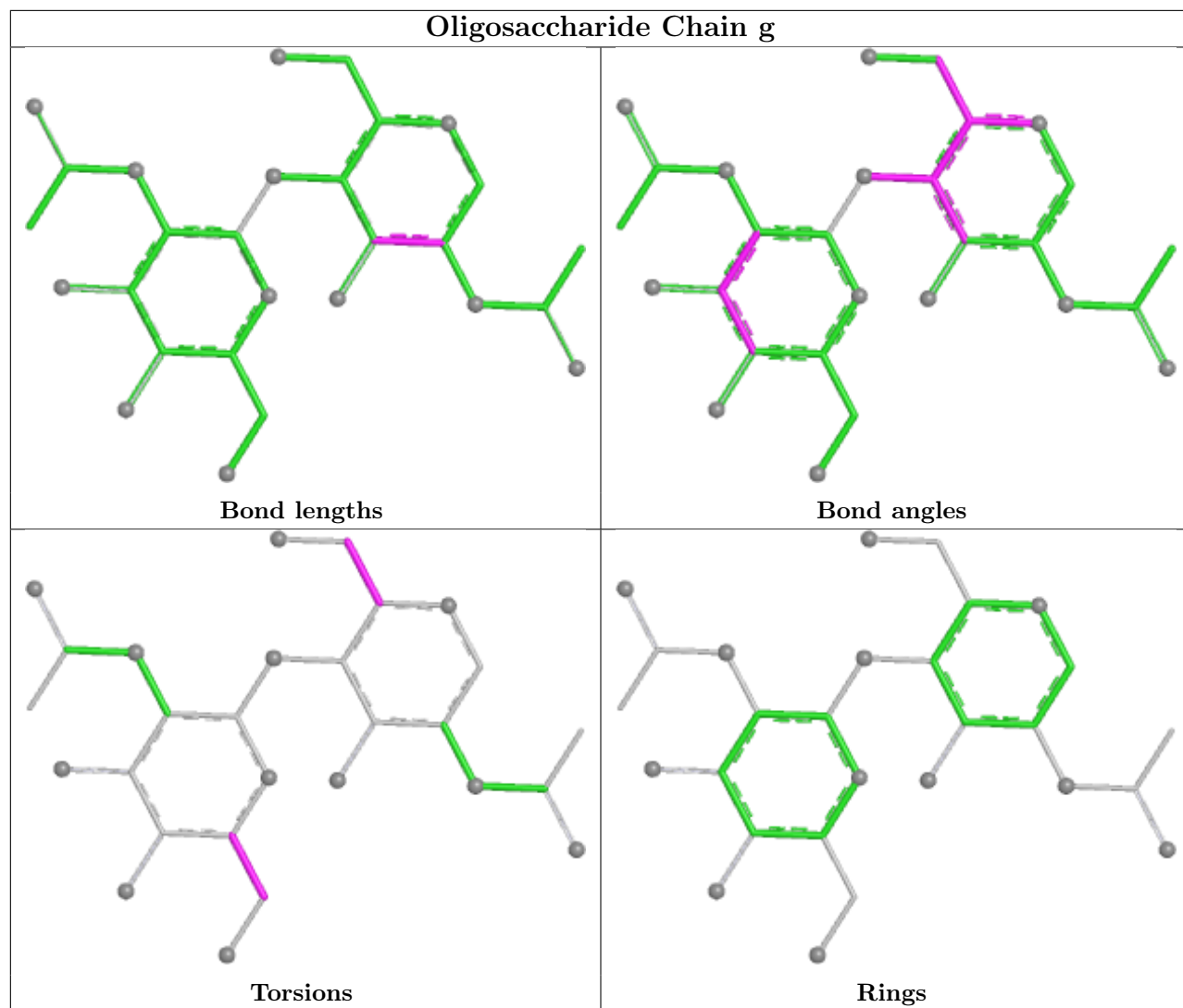


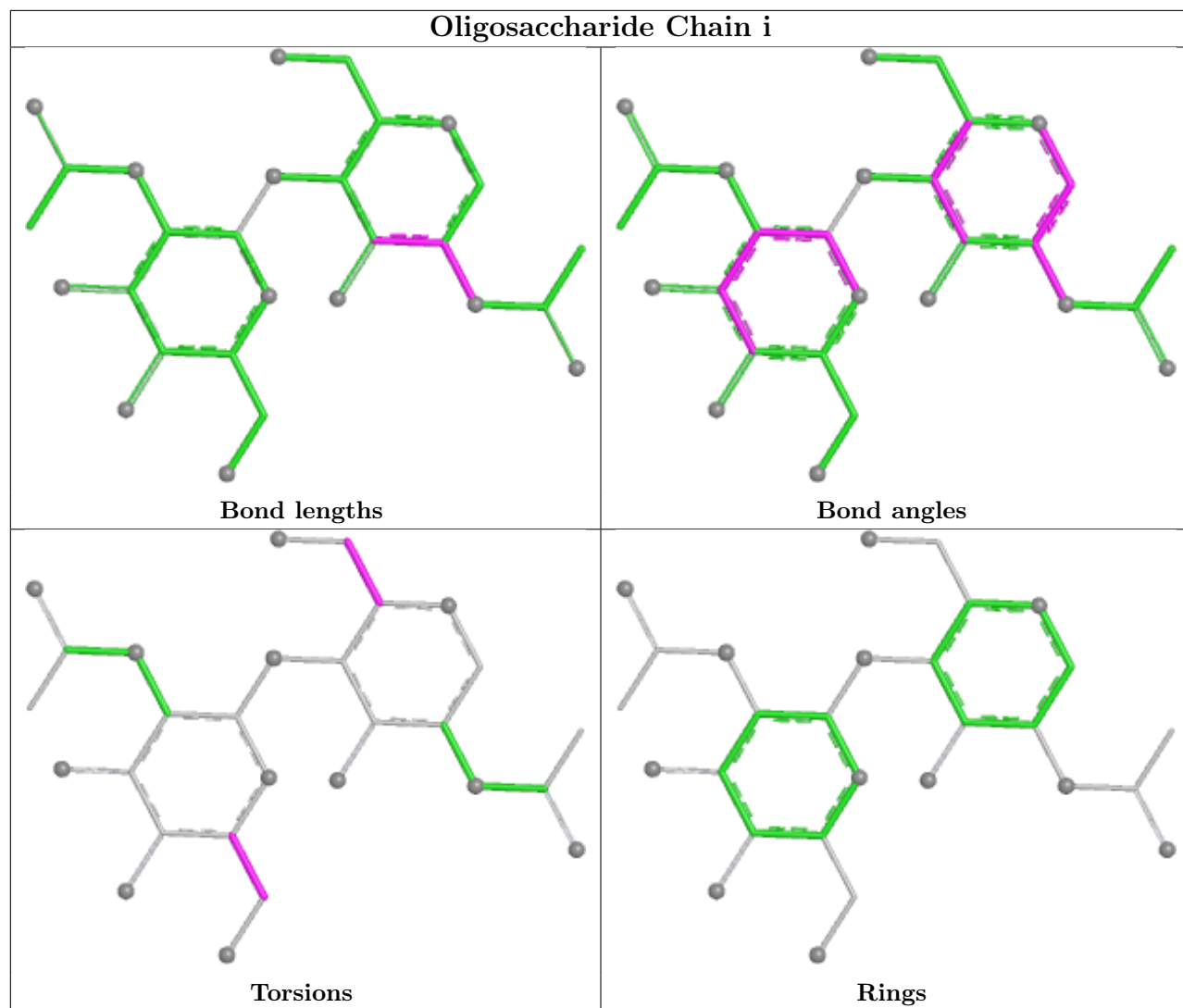


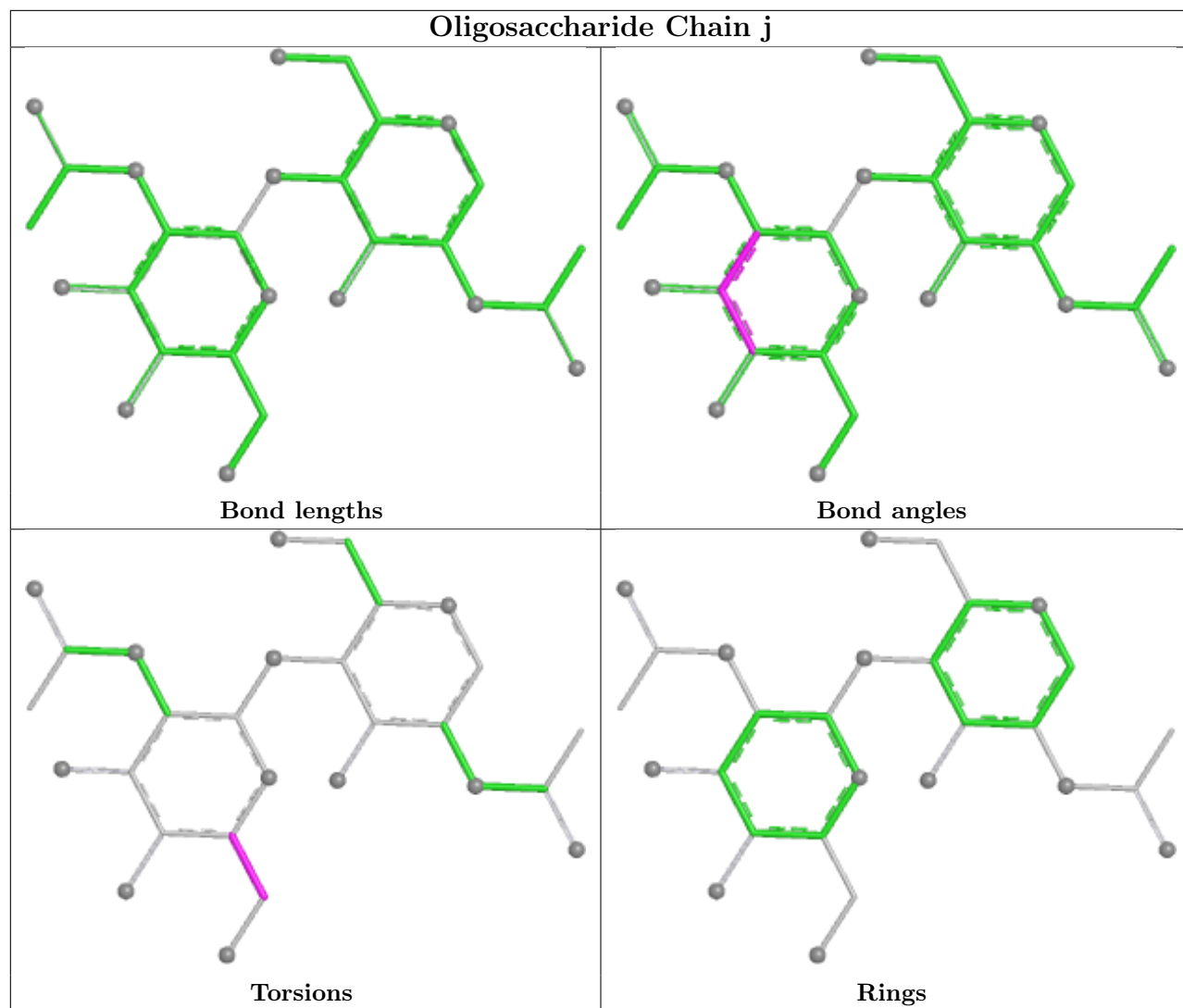


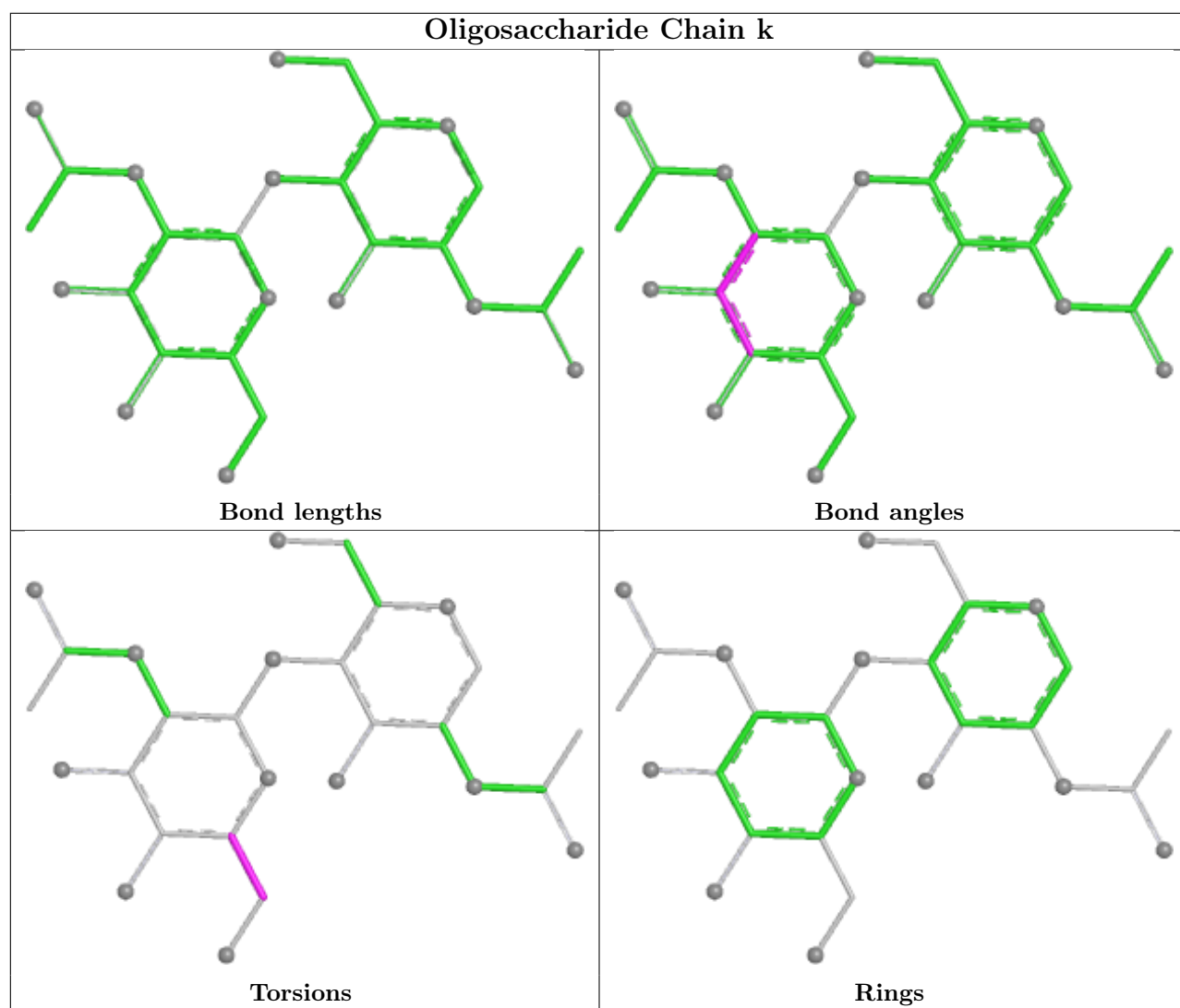


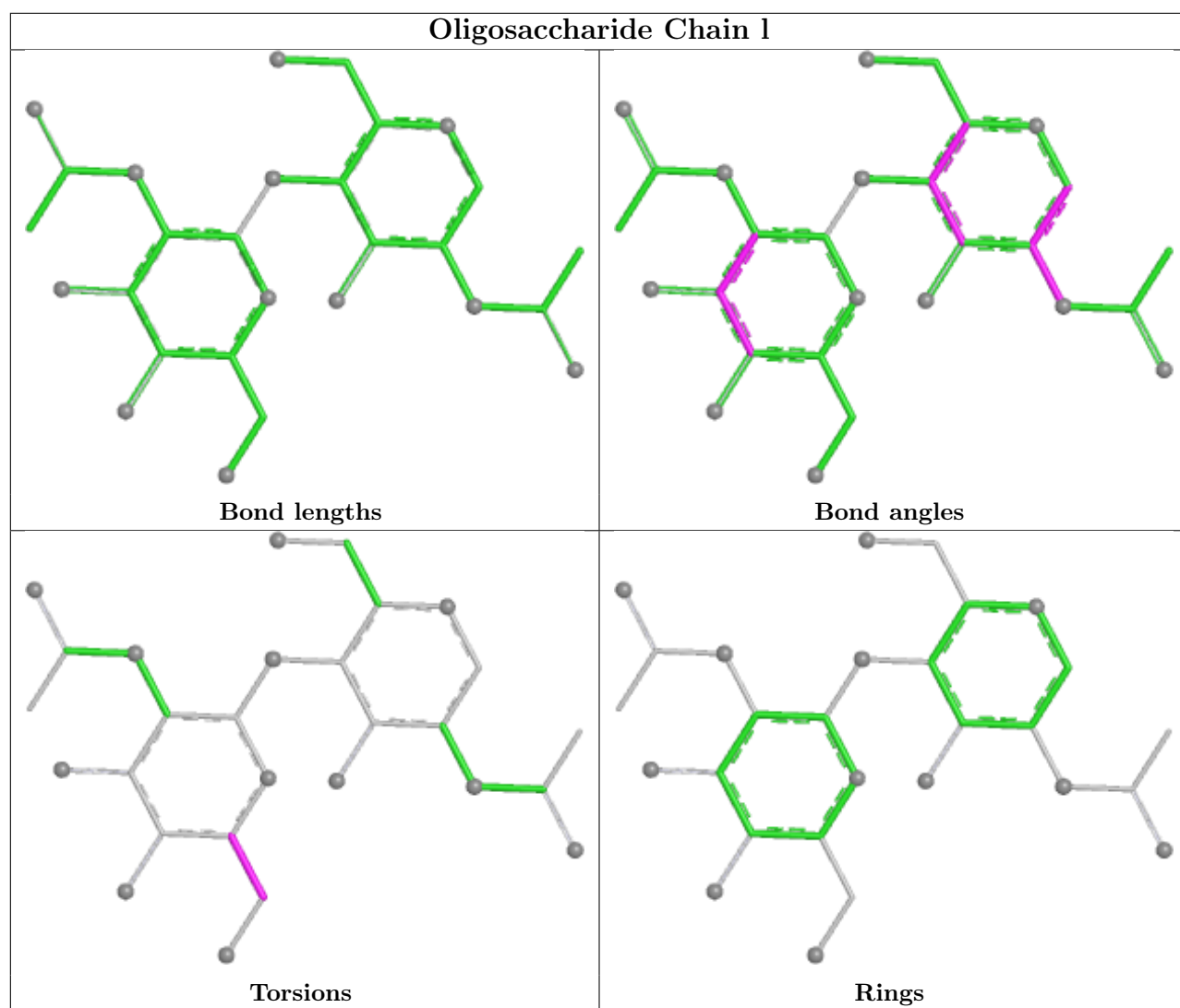


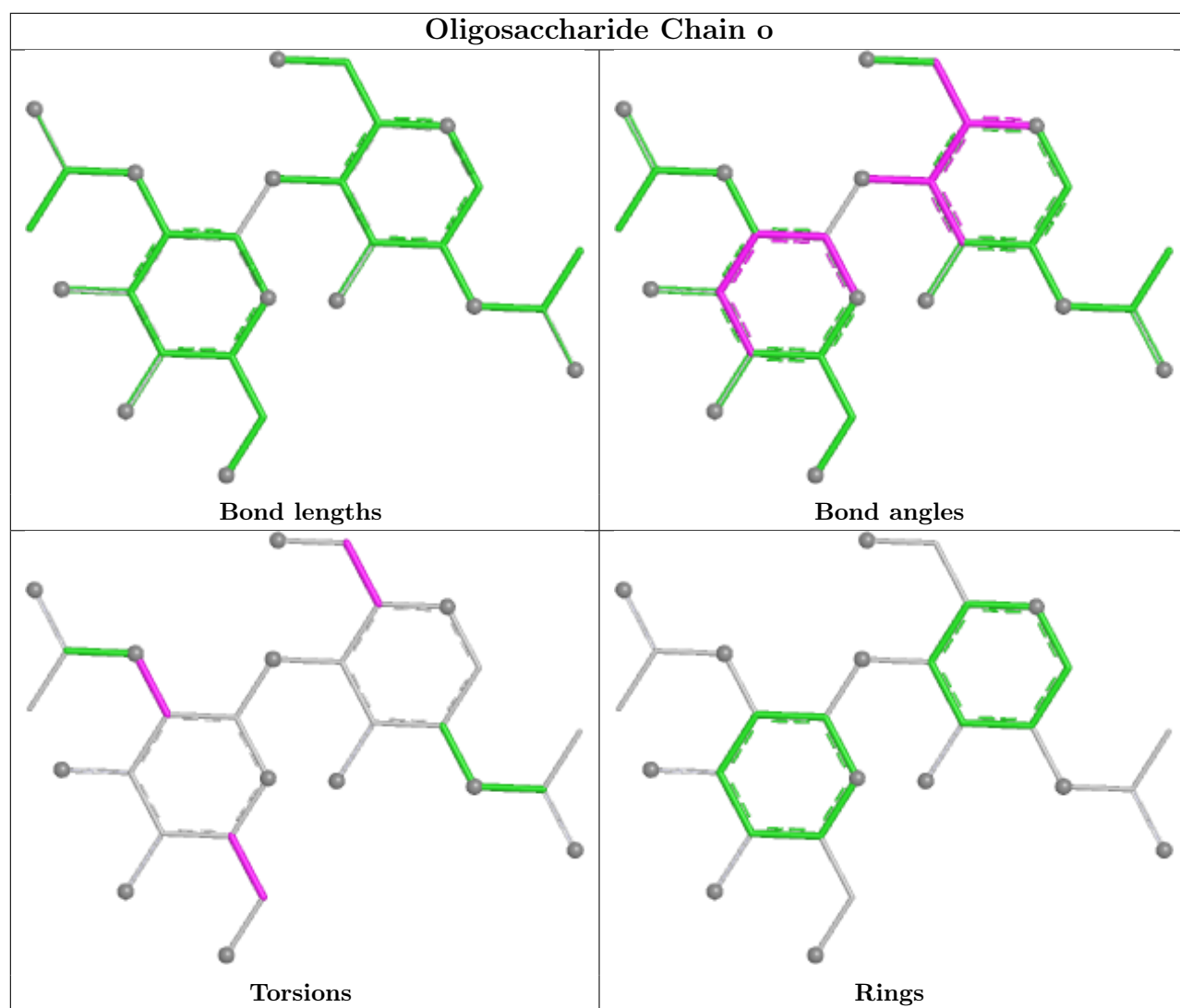


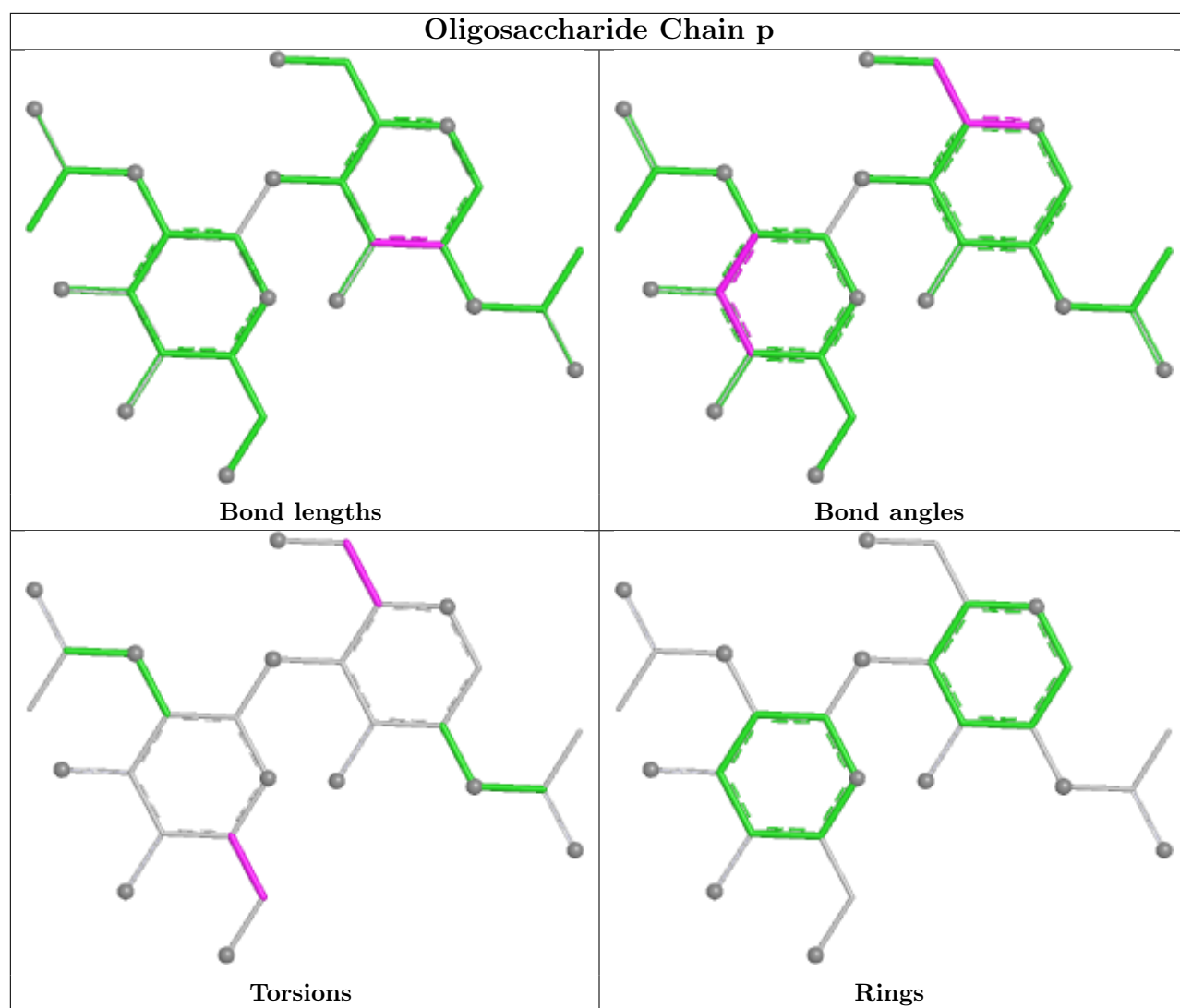


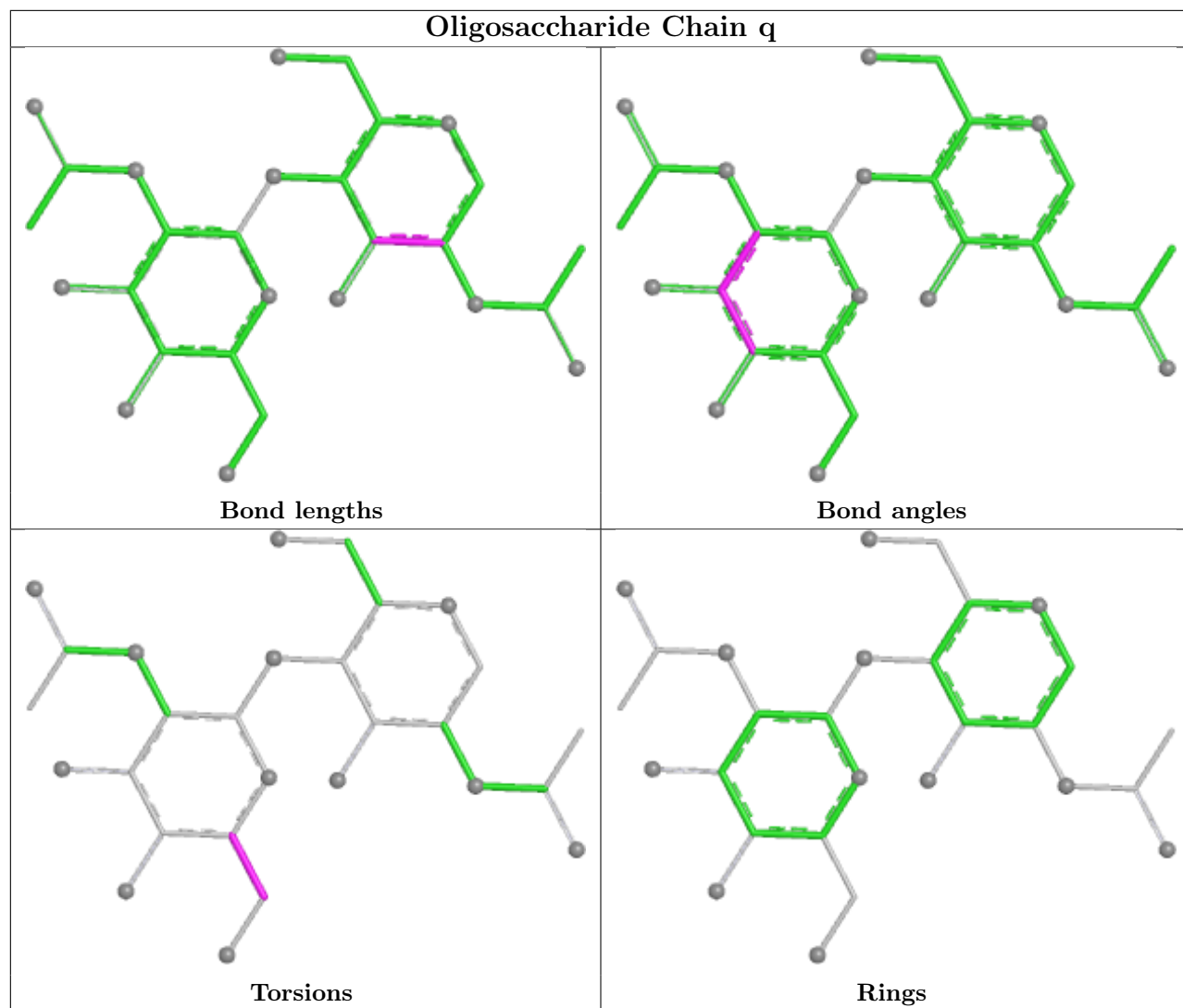


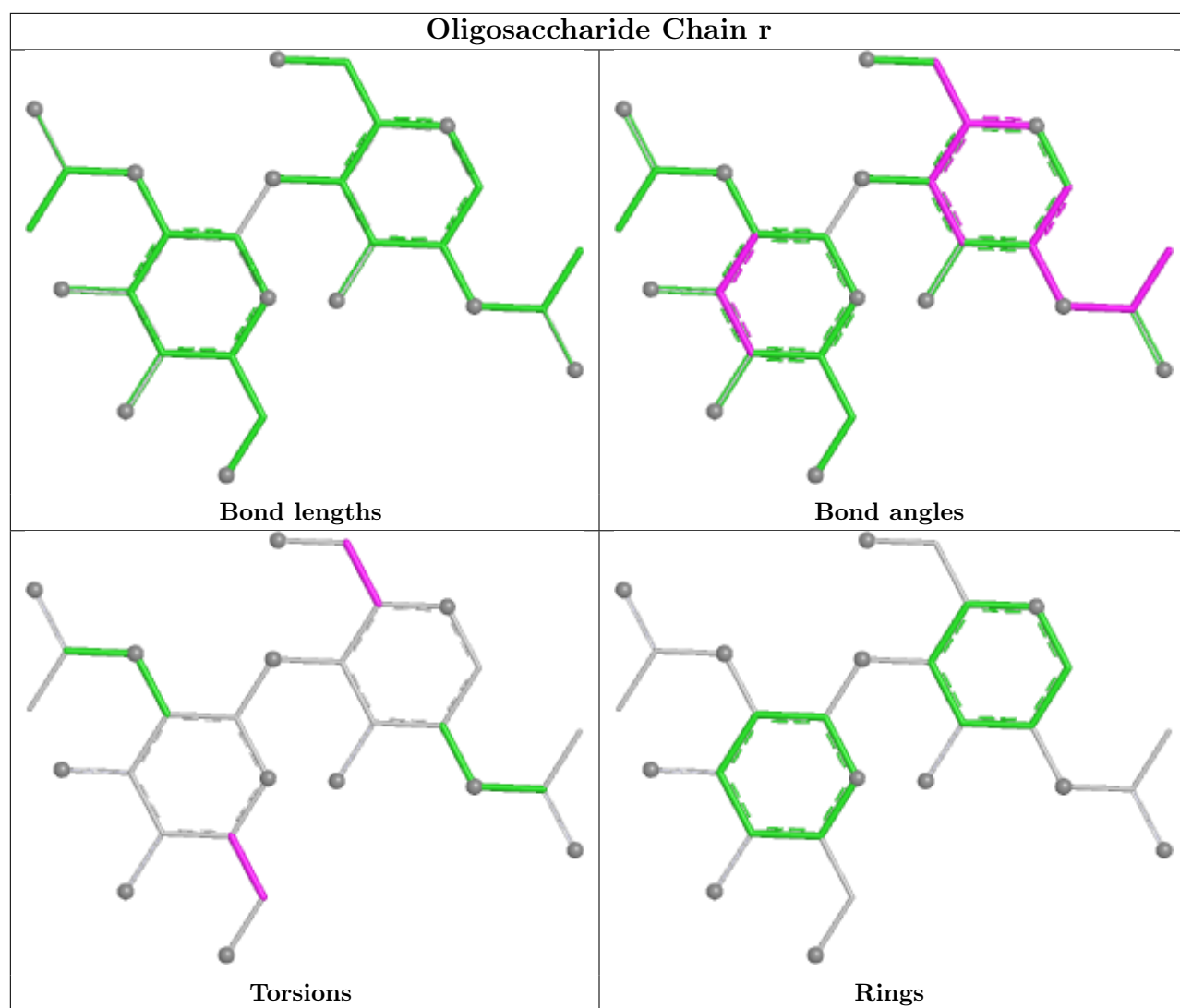


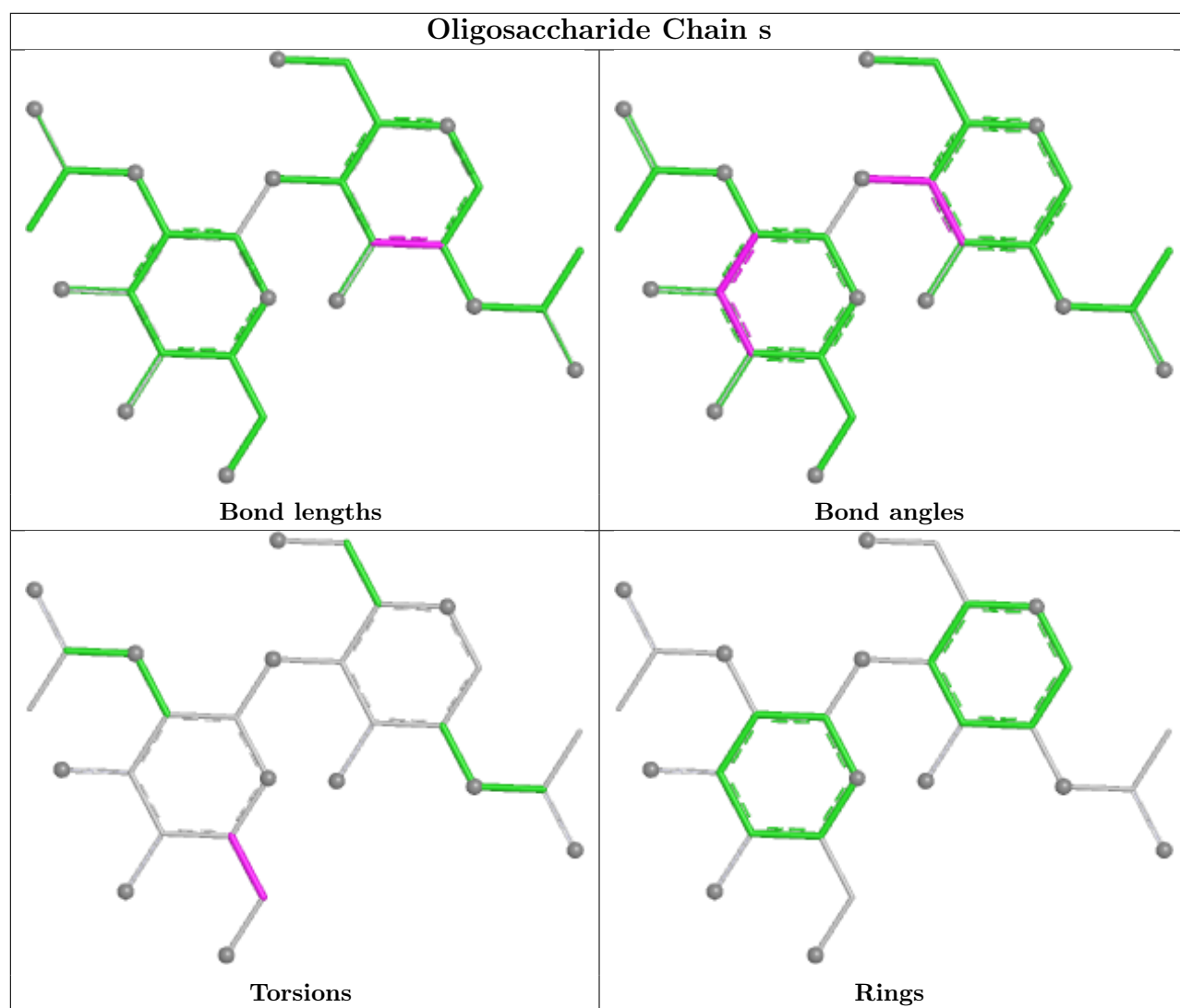


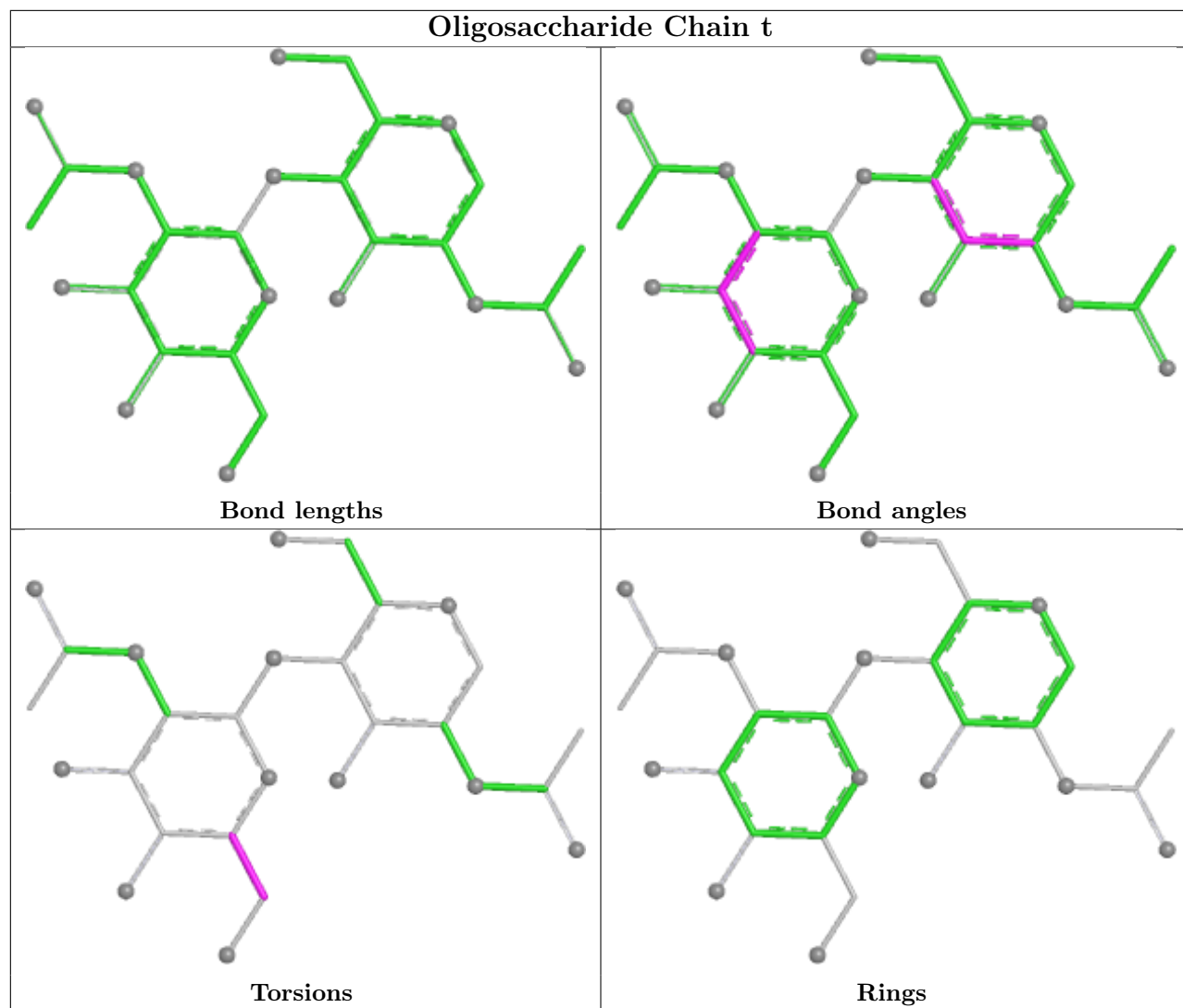


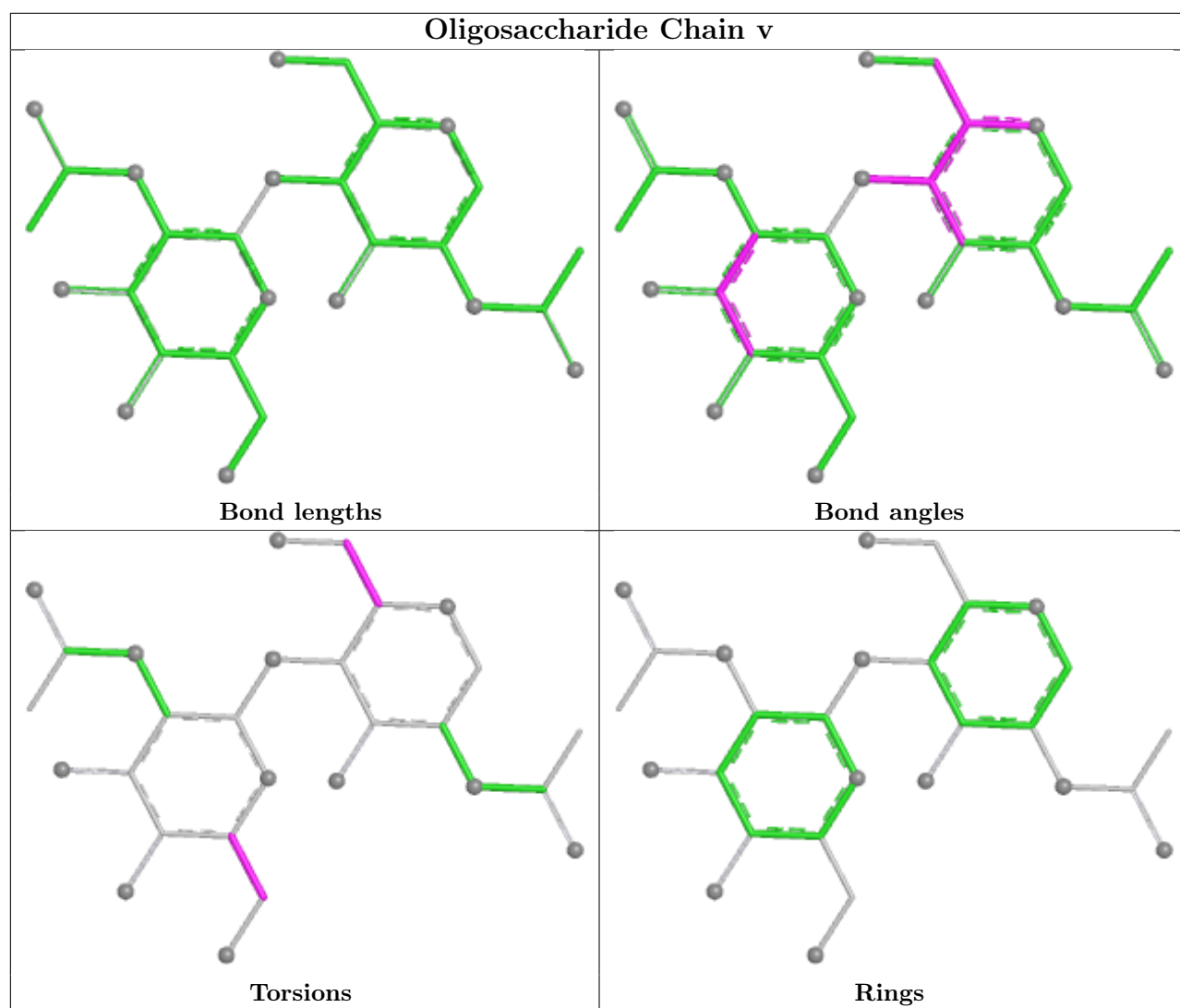


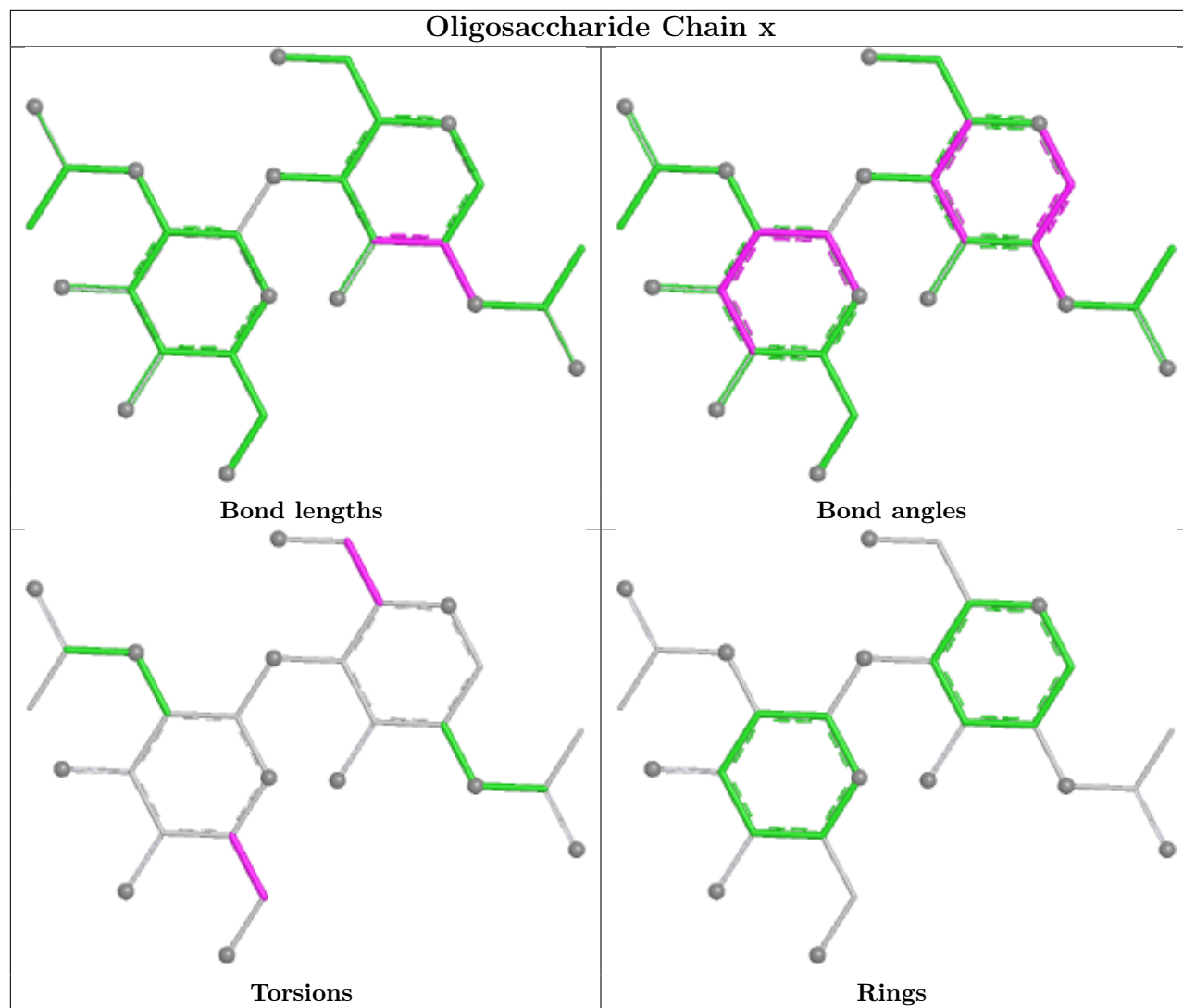


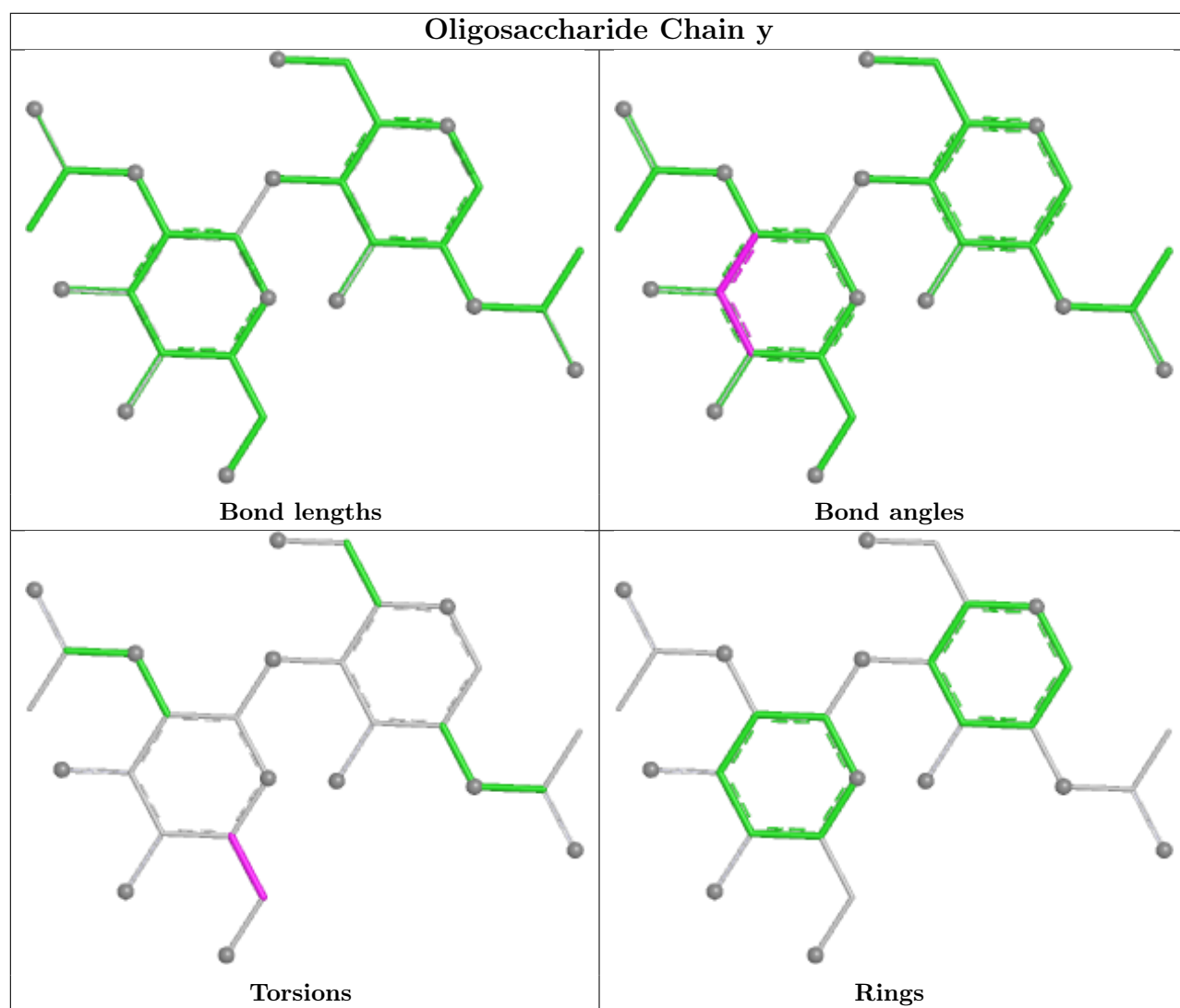


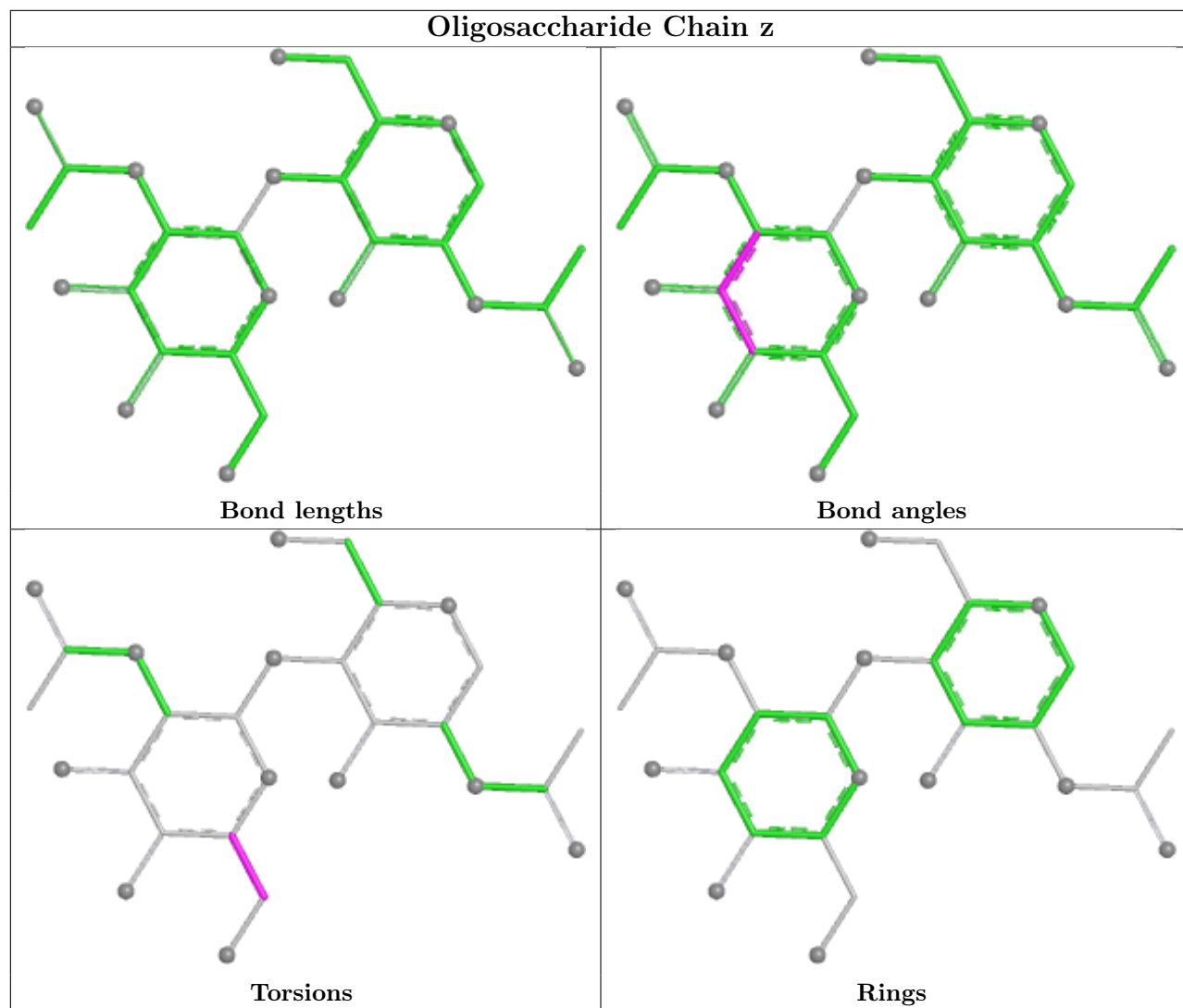


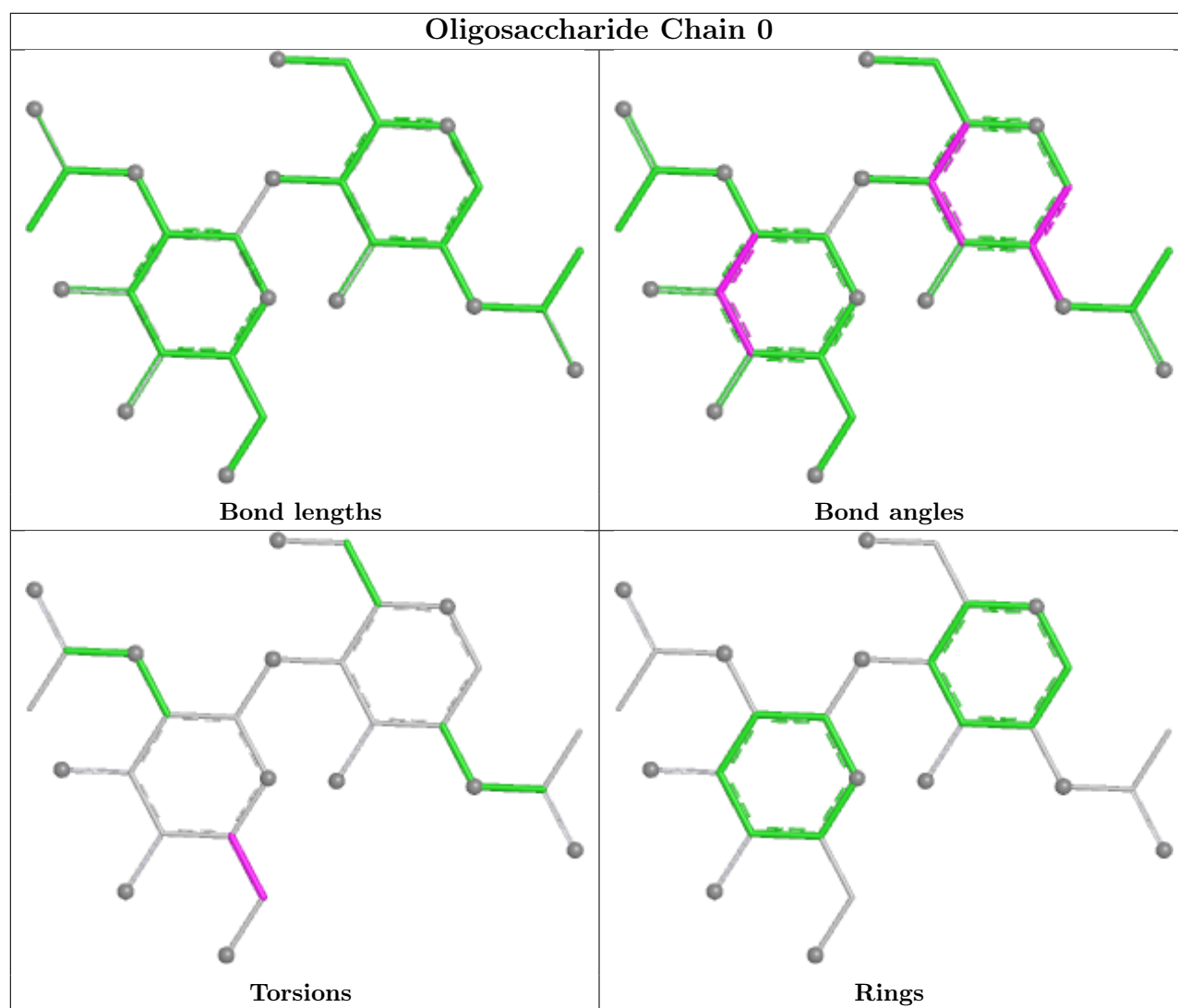


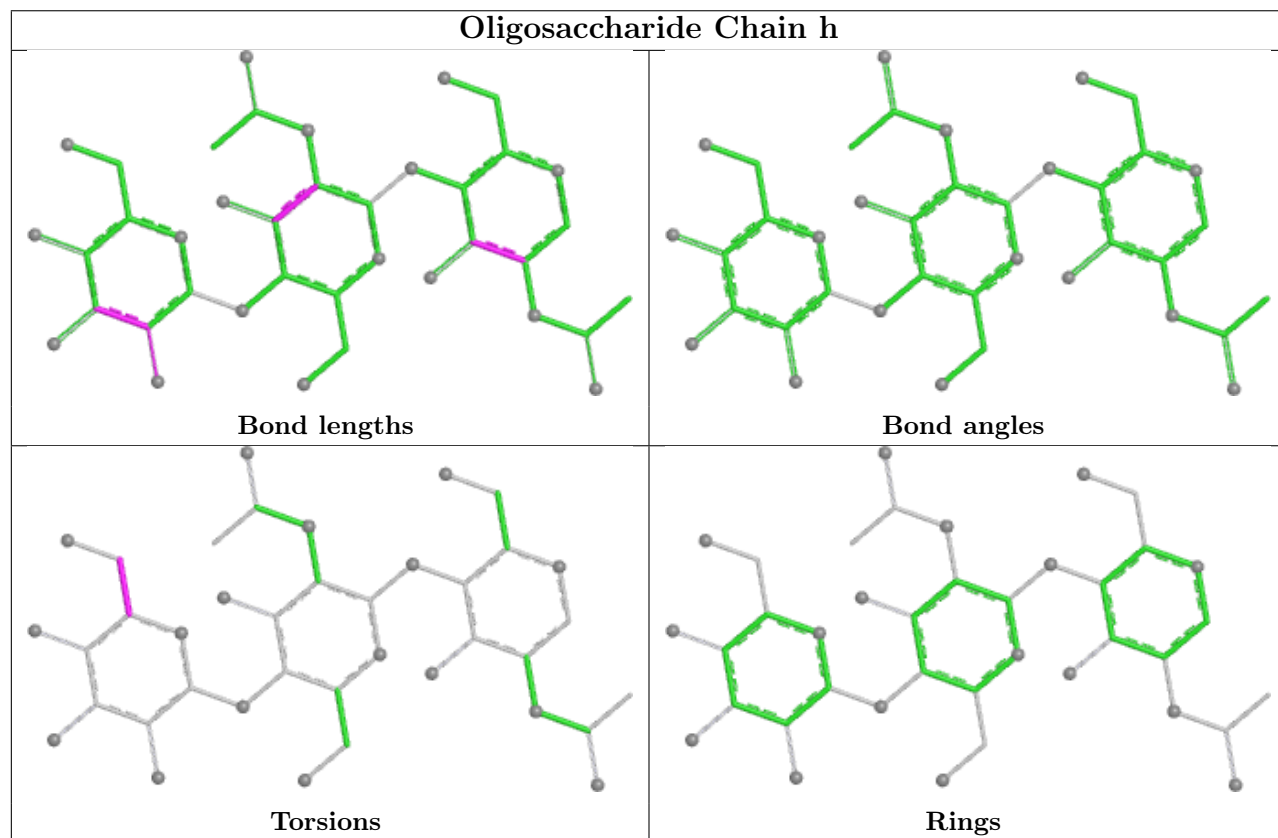
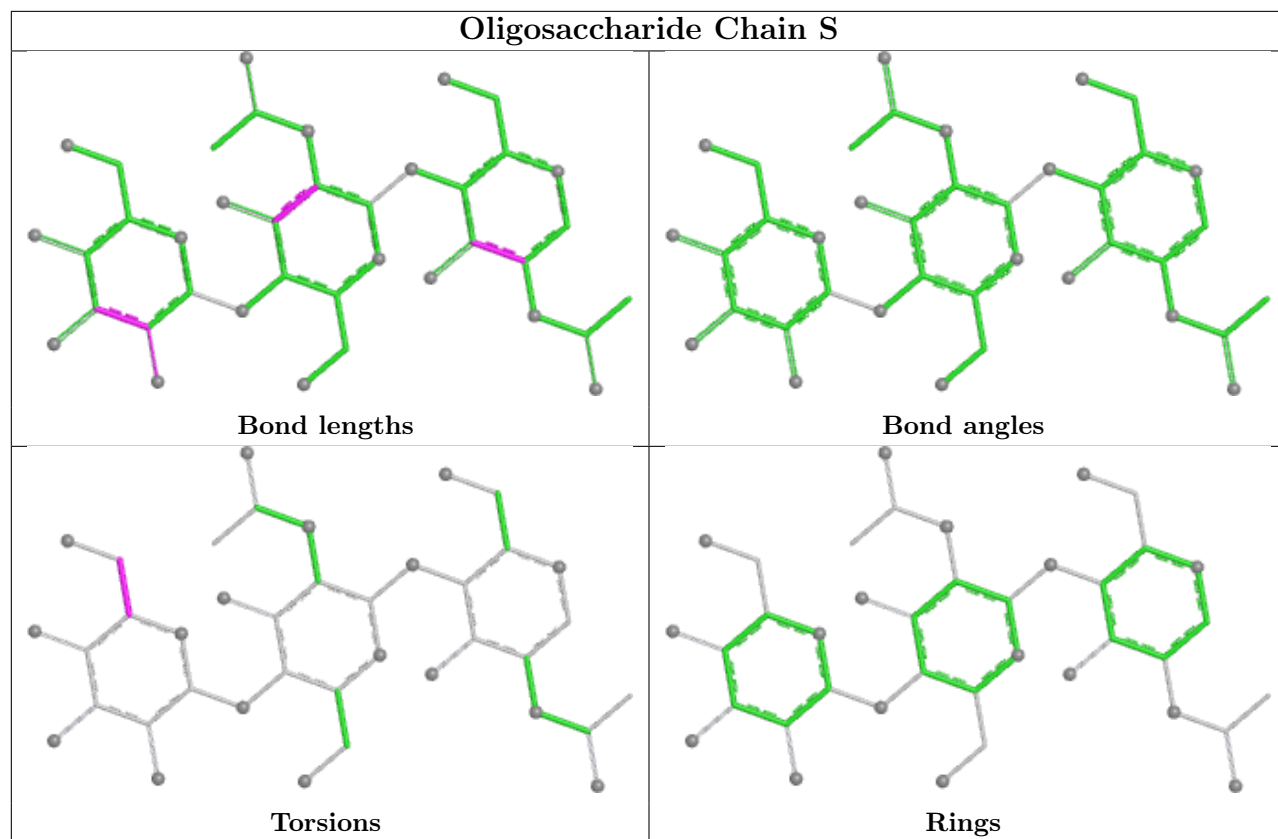


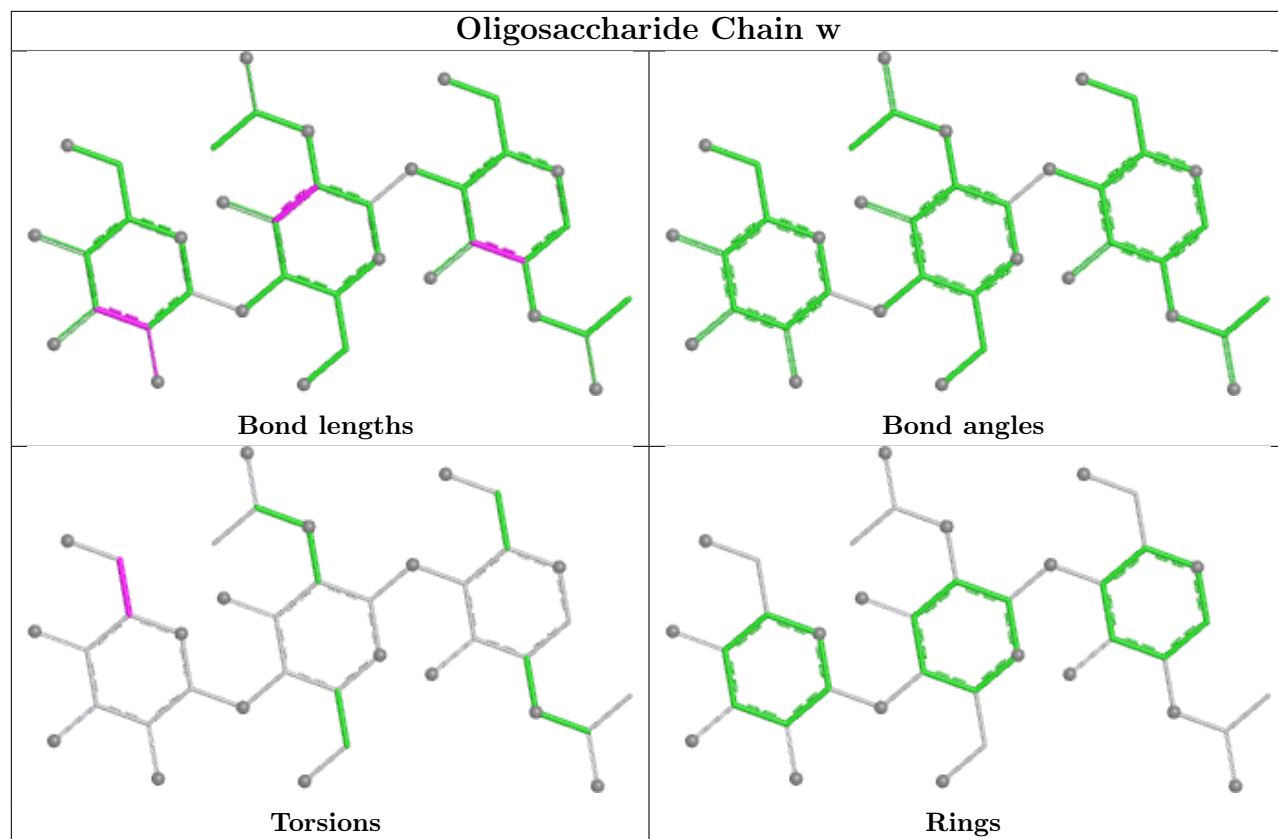


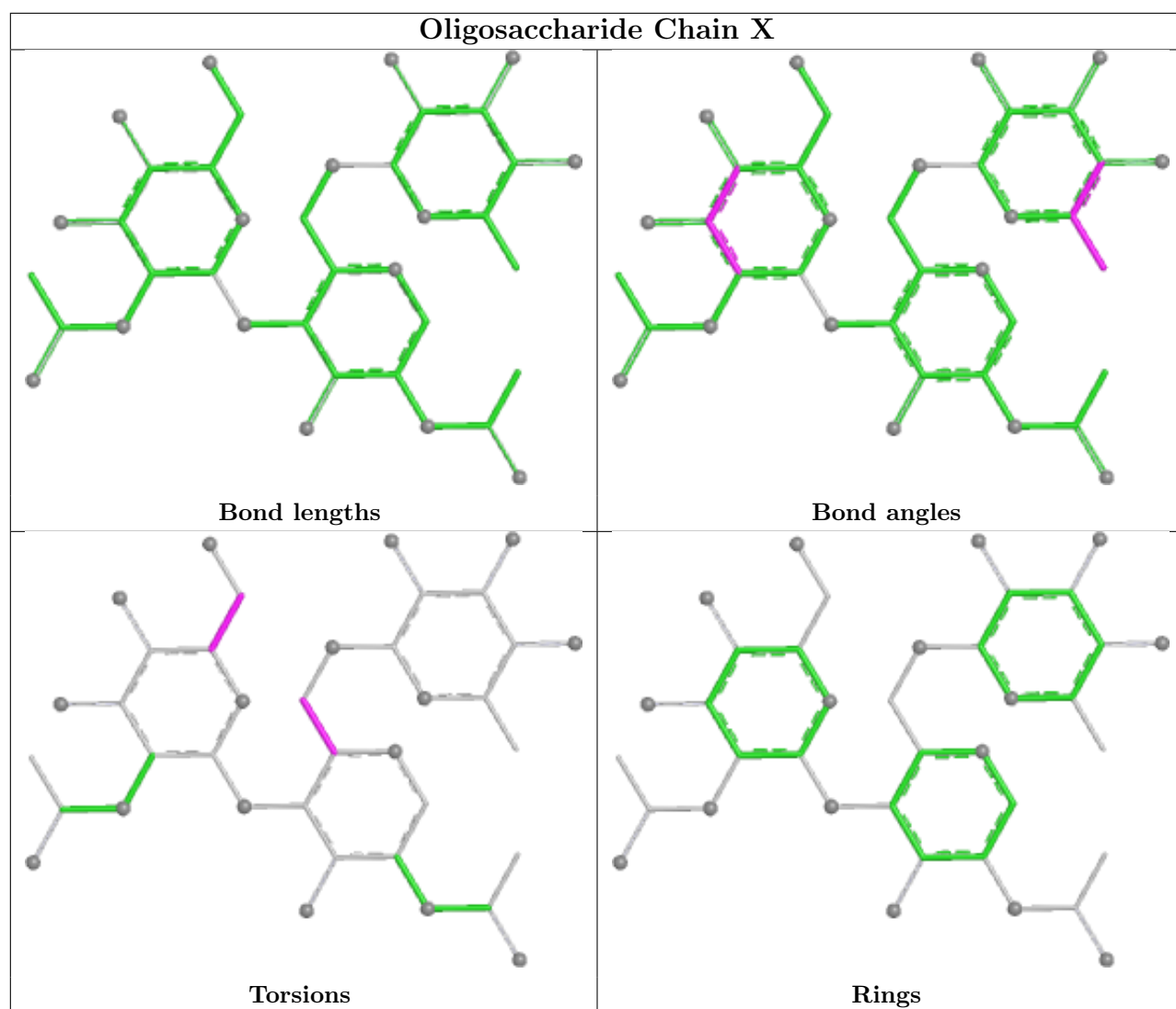


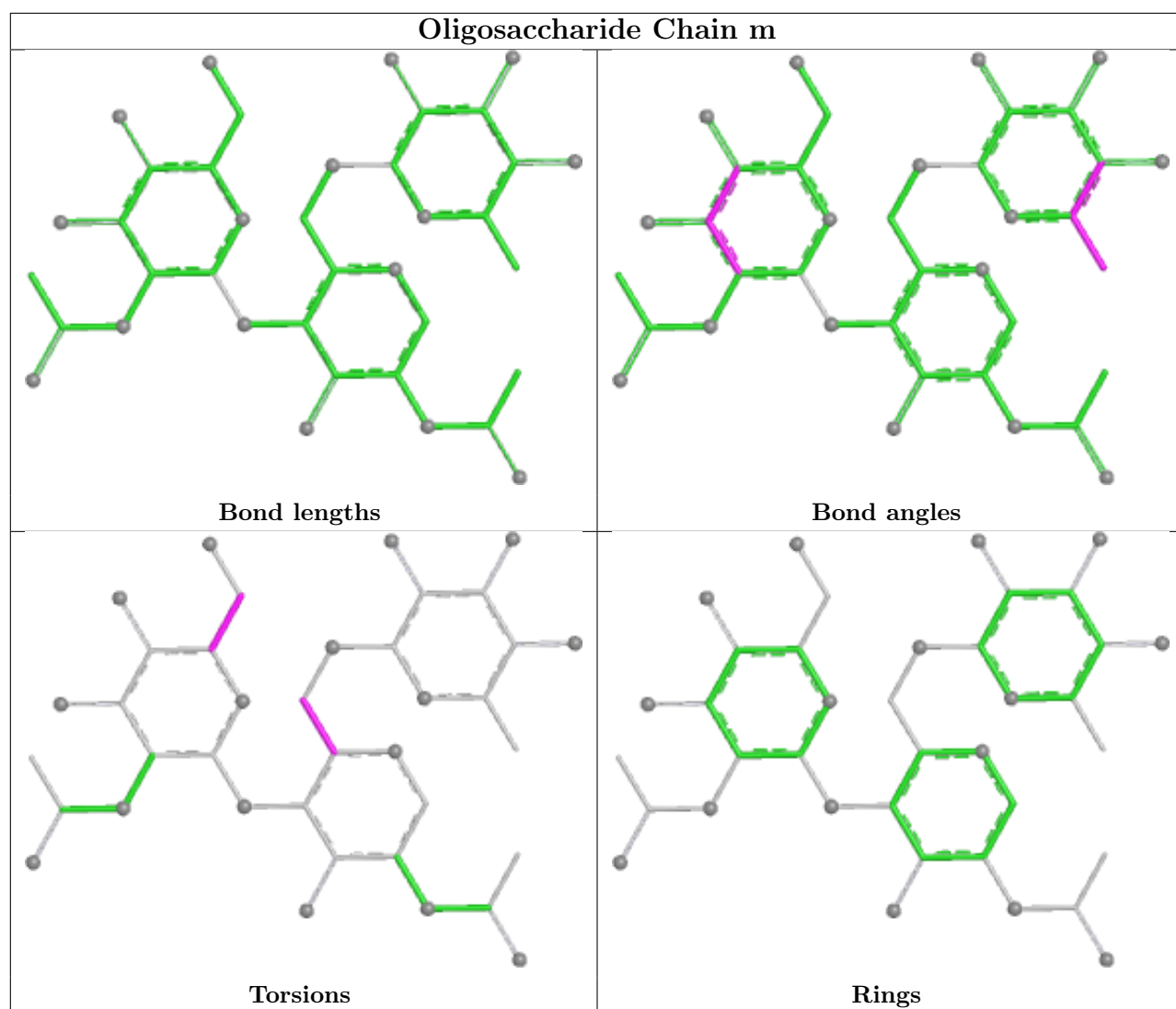


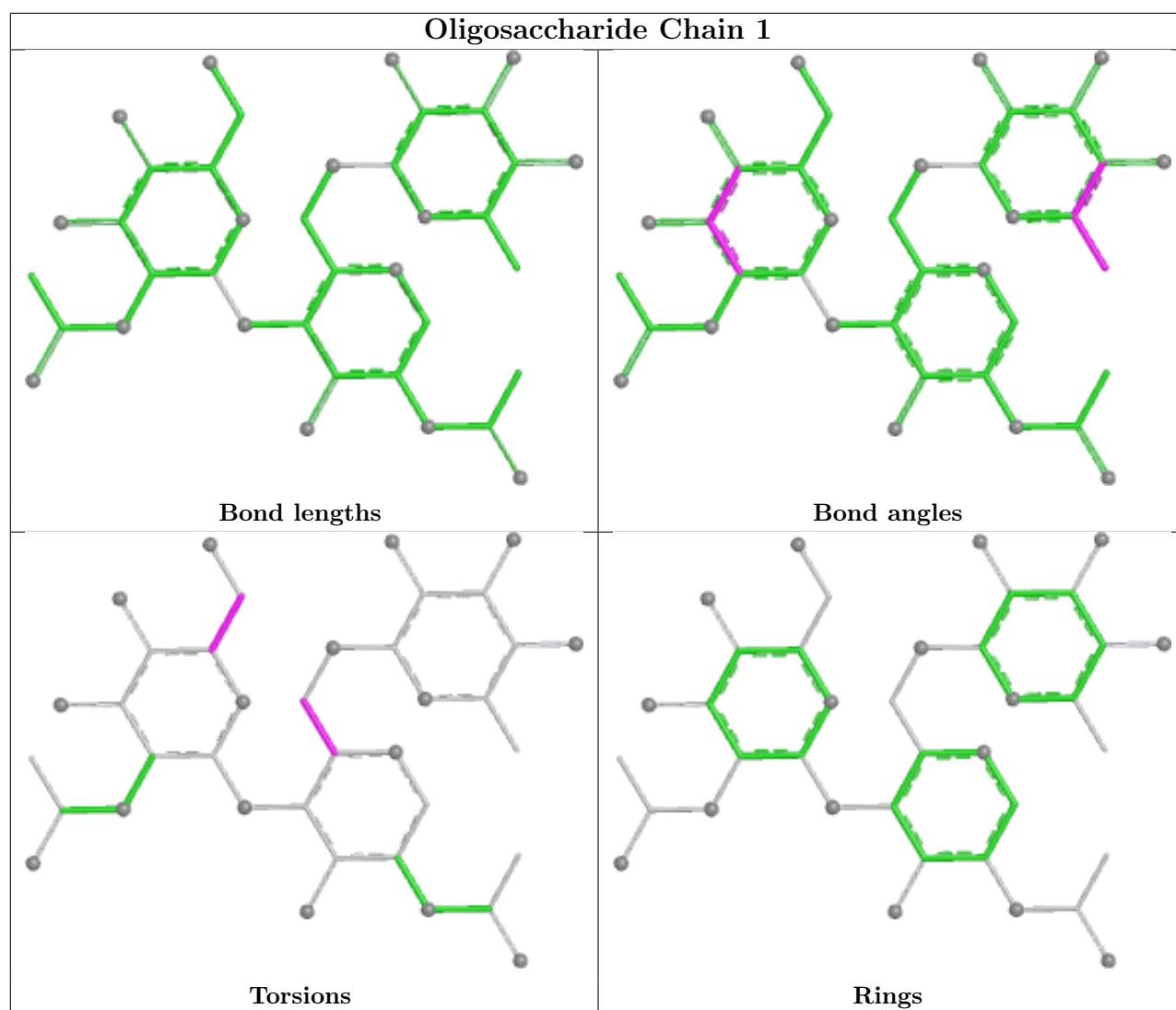












5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	NAG	E	745	1	14,14,15	0.94	0	17,19,21	1.04	1 (5%)
8	NAG	E	729	1	14,14,15	0.81	0	17,19,21	0.77	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	A	745	1	14,14,15	0.94	1 (7%)	17,19,21	1.04	1 (5%)
8	NAG	A	739	1	14,14,15	0.83	0	17,19,21	1.00	1 (5%)
8	NAG	E	738	1	14,14,15	0.86	0	17,19,21	0.90	1 (5%)
8	NAG	E	739	1	14,14,15	0.83	0	17,19,21	1.00	1 (5%)
8	NAG	A	741	1	14,14,15	0.80	0	17,19,21	1.11	1 (5%)
8	NAG	A	740	1	14,14,15	0.79	1 (7%)	17,19,21	0.98	1 (5%)
8	NAG	E	741	1	14,14,15	0.81	0	17,19,21	1.10	1 (5%)
8	NAG	B	740	1	14,14,15	0.78	0	17,19,21	0.98	1 (5%)
8	NAG	B	710	1	14,14,15	0.93	1 (7%)	17,19,21	0.88	1 (5%)
8	NAG	A	710	1	14,14,15	0.93	1 (7%)	17,19,21	0.88	1 (5%)
8	NAG	B	729	1	14,14,15	0.81	1 (7%)	17,19,21	0.77	1 (5%)
8	NAG	B	745	1	14,14,15	0.94	0	17,19,21	1.04	1 (5%)
8	NAG	E	710	1	14,14,15	0.93	1 (7%)	17,19,21	0.88	1 (5%)
8	NAG	E	740	1	14,14,15	0.78	1 (7%)	17,19,21	0.98	1 (5%)
8	NAG	B	738	1	14,14,15	0.86	0	17,19,21	0.90	1 (5%)
8	NAG	A	738	1	14,14,15	0.87	0	17,19,21	0.90	1 (5%)
8	NAG	A	729	1	14,14,15	0.81	1 (7%)	17,19,21	0.77	1 (5%)
8	NAG	B	739	1	14,14,15	0.83	0	17,19,21	1.00	1 (5%)
8	NAG	B	741	1	14,14,15	0.80	0	17,19,21	1.11	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	E	745	1	-	1/6/23/26	0/1/1/1
8	NAG	E	729	1	-	1/6/23/26	0/1/1/1
8	NAG	A	745	1	-	1/6/23/26	0/1/1/1
8	NAG	A	739	1	-	2/6/23/26	0/1/1/1
8	NAG	E	738	1	-	1/6/23/26	0/1/1/1
8	NAG	E	739	1	-	2/6/23/26	0/1/1/1
8	NAG	A	741	1	-	1/6/23/26	0/1/1/1
8	NAG	A	740	1	-	1/6/23/26	0/1/1/1
8	NAG	E	741	1	-	1/6/23/26	0/1/1/1
8	NAG	B	740	1	-	1/6/23/26	0/1/1/1
8	NAG	B	710	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	710	1	-	2/6/23/26	0/1/1/1
8	NAG	B	729	1	-	1/6/23/26	0/1/1/1
8	NAG	B	745	1	-	1/6/23/26	0/1/1/1
8	NAG	E	710	1	-	2/6/23/26	0/1/1/1
8	NAG	E	740	1	-	1/6/23/26	0/1/1/1
8	NAG	B	738	1	-	1/6/23/26	0/1/1/1
8	NAG	A	738	1	-	1/6/23/26	0/1/1/1
8	NAG	A	729	1	-	1/6/23/26	0/1/1/1
8	NAG	B	739	1	-	2/6/23/26	0/1/1/1
8	NAG	B	741	1	-	1/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	710	NAG	C3-C2	-2.02	1.48	1.52
8	A	710	NAG	C3-C2	-2.02	1.48	1.52
8	B	710	NAG	C3-C2	-2.01	1.48	1.52
8	E	740	NAG	C3-C2	-2.01	1.48	1.52
8	B	729	NAG	C3-C2	-2.01	1.48	1.52
8	A	729	NAG	C3-C2	-2.00	1.48	1.52
8	A	740	NAG	C3-C2	-2.00	1.48	1.52
8	A	745	NAG	C1-C2	2.00	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	741	NAG	C4-C3-C2	-3.36	106.09	111.02
8	A	741	NAG	C4-C3-C2	-3.36	106.10	111.02
8	E	741	NAG	C4-C3-C2	-3.34	106.12	111.02
8	A	739	NAG	C4-C3-C2	-3.09	106.49	111.02
8	E	739	NAG	C4-C3-C2	-3.08	106.50	111.02
8	B	739	NAG	C4-C3-C2	-3.07	106.52	111.02
8	E	745	NAG	C4-C3-C2	-2.96	106.67	111.02
8	B	745	NAG	C4-C3-C2	-2.94	106.70	111.02
8	A	745	NAG	C4-C3-C2	-2.93	106.72	111.02
8	E	740	NAG	C4-C3-C2	-2.59	107.22	111.02
8	A	740	NAG	C4-C3-C2	-2.59	107.23	111.02
8	B	740	NAG	C4-C3-C2	-2.58	107.24	111.02
8	A	738	NAG	C4-C3-C2	-2.47	107.40	111.02
8	E	738	NAG	C4-C3-C2	-2.47	107.40	111.02
8	B	738	NAG	C4-C3-C2	-2.45	107.43	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	710	NAG	C4-C3-C2	-2.34	107.59	111.02
8	A	710	NAG	C4-C3-C2	-2.32	107.61	111.02
8	E	710	NAG	C4-C3-C2	-2.32	107.62	111.02
8	E	729	NAG	C4-C3-C2	-2.11	107.93	111.02
8	B	729	NAG	C4-C3-C2	-2.10	107.93	111.02
8	A	729	NAG	C4-C3-C2	-2.10	107.94	111.02

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	739	NAG	O5-C5-C6-O6
8	B	739	NAG	O5-C5-C6-O6
8	E	739	NAG	O5-C5-C6-O6
8	B	710	NAG	O5-C5-C6-O6
8	A	710	NAG	O5-C5-C6-O6
8	E	710	NAG	O5-C5-C6-O6
8	A	729	NAG	O5-C5-C6-O6
8	B	729	NAG	O5-C5-C6-O6
8	E	729	NAG	O5-C5-C6-O6
8	A	741	NAG	O5-C5-C6-O6
8	B	741	NAG	O5-C5-C6-O6
8	E	741	NAG	O5-C5-C6-O6
8	A	739	NAG	C4-C5-C6-O6
8	E	739	NAG	C4-C5-C6-O6
8	B	739	NAG	C4-C5-C6-O6
8	A	745	NAG	O5-C5-C6-O6
8	E	745	NAG	O5-C5-C6-O6
8	A	740	NAG	O5-C5-C6-O6
8	B	740	NAG	O5-C5-C6-O6
8	B	745	NAG	O5-C5-C6-O6
8	E	740	NAG	O5-C5-C6-O6
8	A	738	NAG	O5-C5-C6-O6
8	B	738	NAG	O5-C5-C6-O6
8	E	738	NAG	O5-C5-C6-O6
8	E	710	NAG	C4-C5-C6-O6
8	A	710	NAG	C4-C5-C6-O6
8	B	710	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	745	NAG	2	0
8	A	745	NAG	2	0
8	B	745	NAG	2	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.

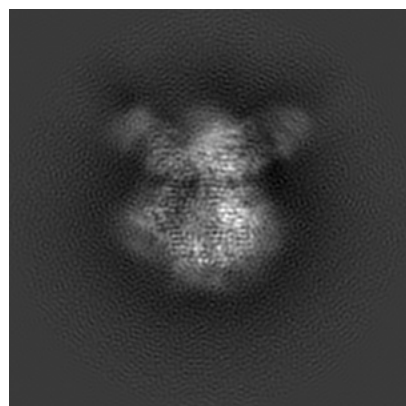
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20260. These allow visual inspection of the internal detail of the map and identification of artifacts.

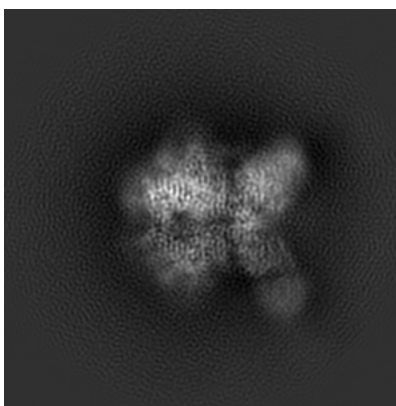
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

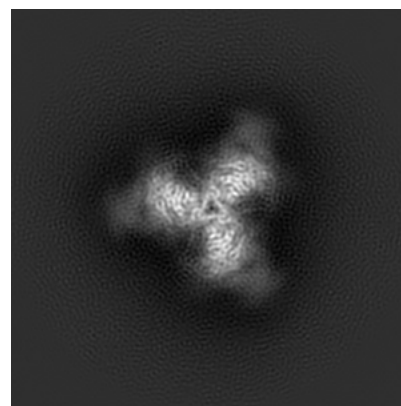
6.1.1 Primary map



X

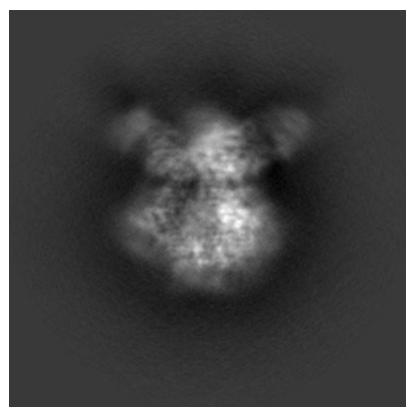


Y

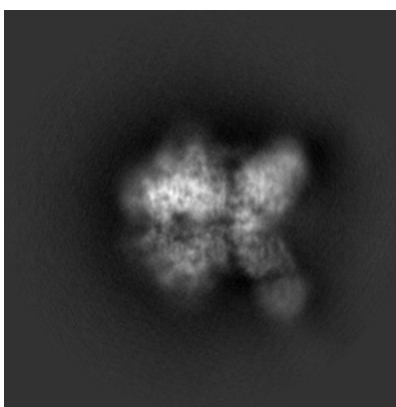


Z

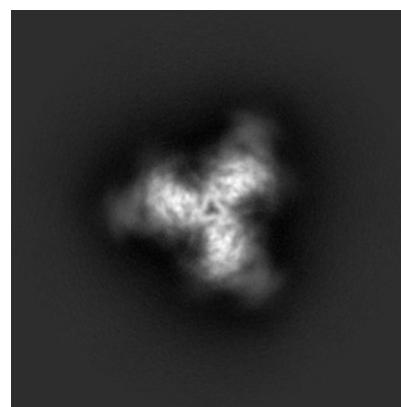
6.1.2 Raw map



X



Y

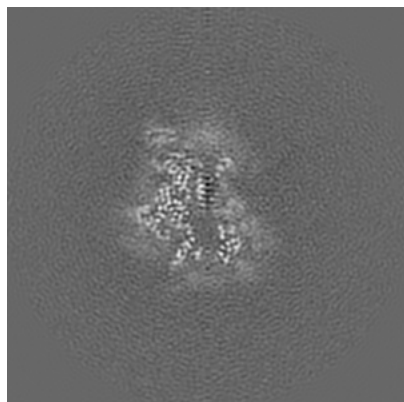


Z

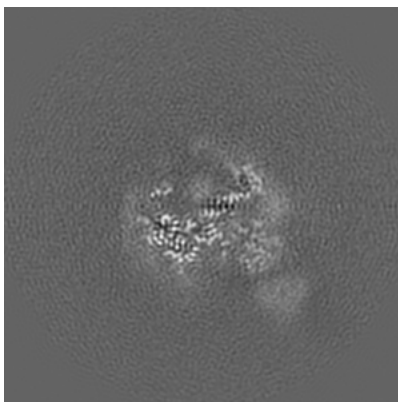
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

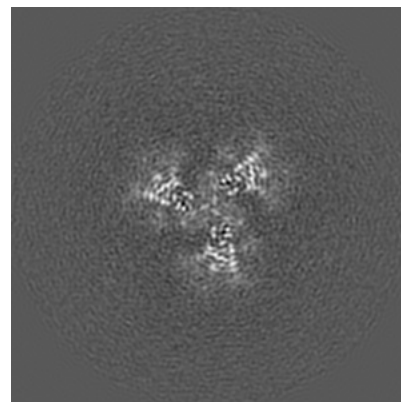
6.2.1 Primary map



X Index: 144

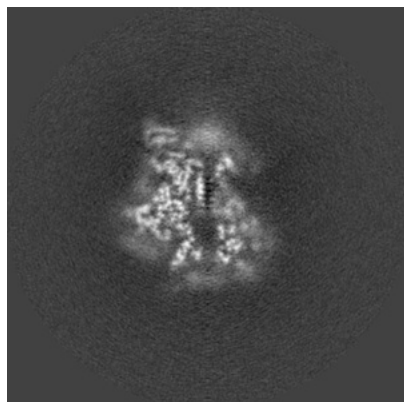


Y Index: 144

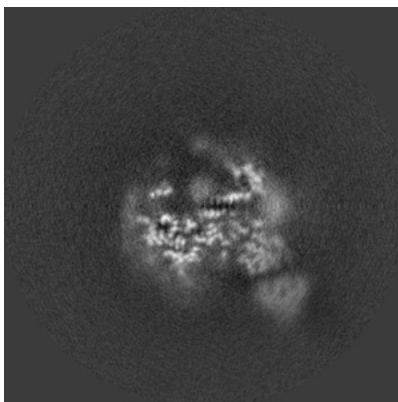


Z Index: 144

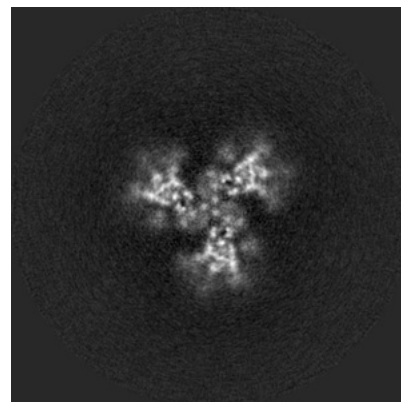
6.2.2 Raw map



X Index: 144



Y Index: 144

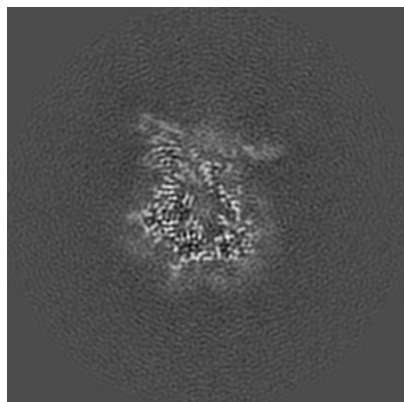


Z Index: 144

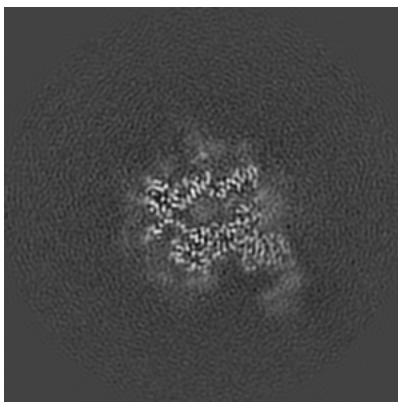
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

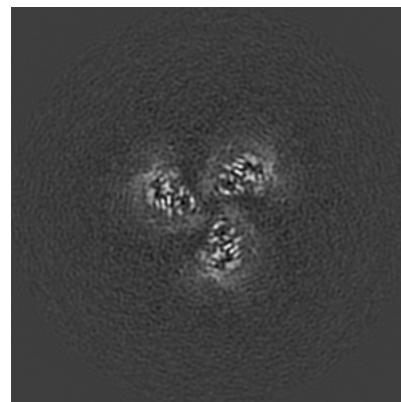
6.3.1 Primary map



X Index: 152

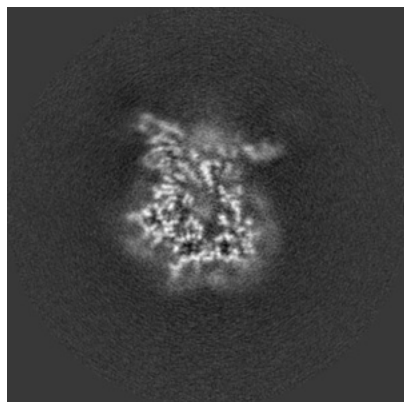


Y Index: 154

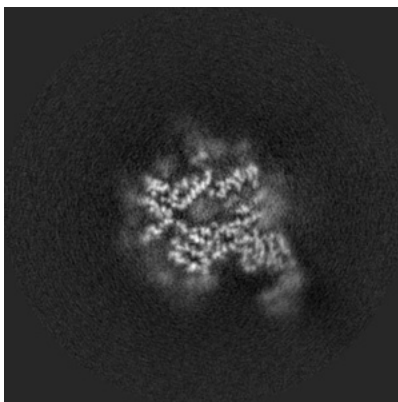


Z Index: 135

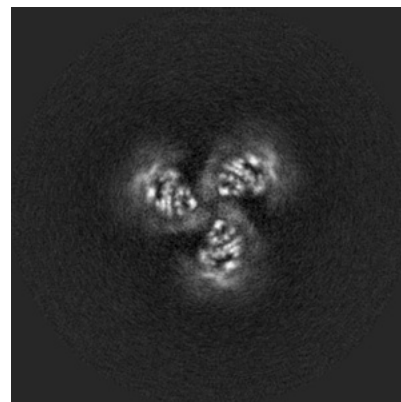
6.3.2 Raw map



X Index: 152



Y Index: 154

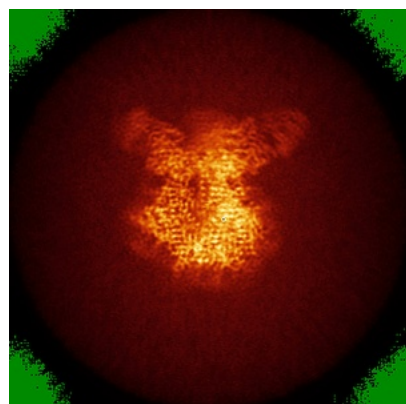


Z Index: 136

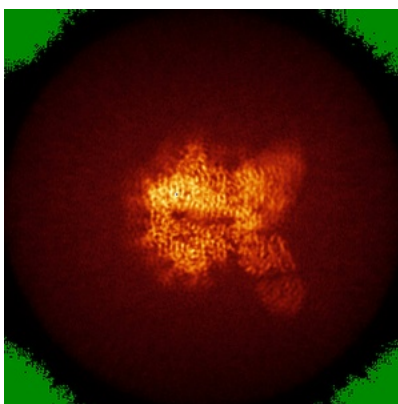
The images above show the largest variance slices of the map in three orthogonal directions.

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

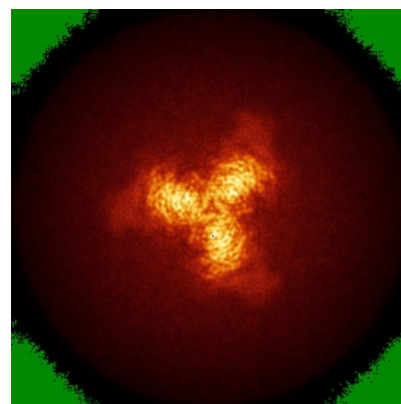
6.4.1 Primary map



X

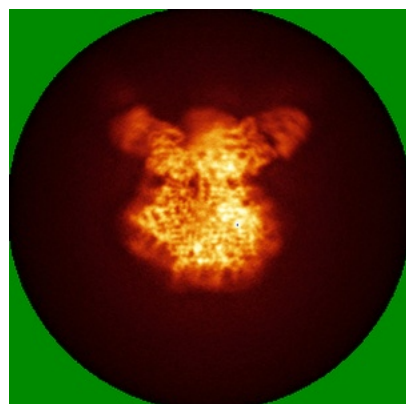


Y

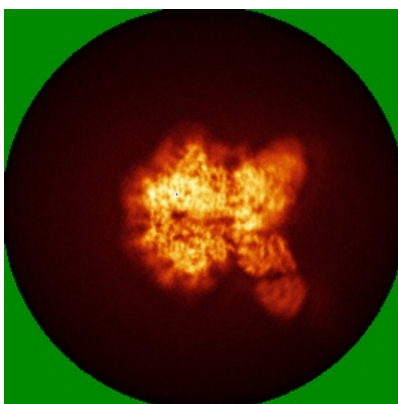


Z

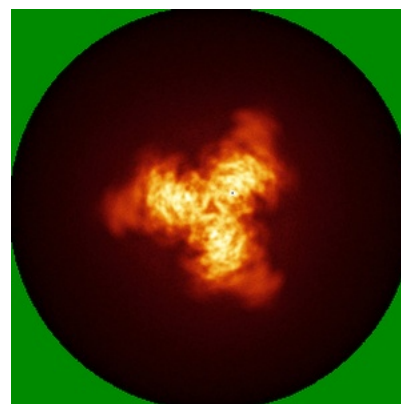
6.4.2 Raw map



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.

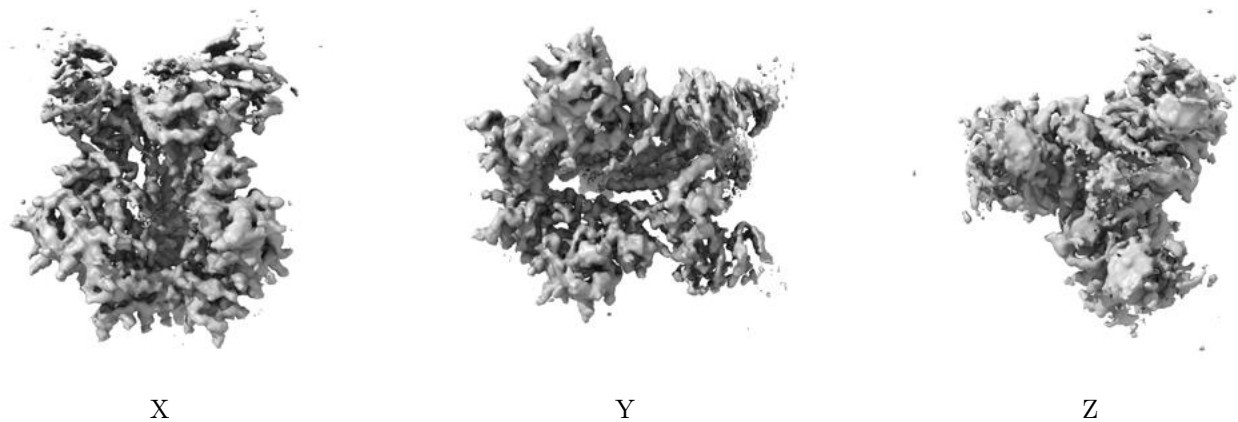
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

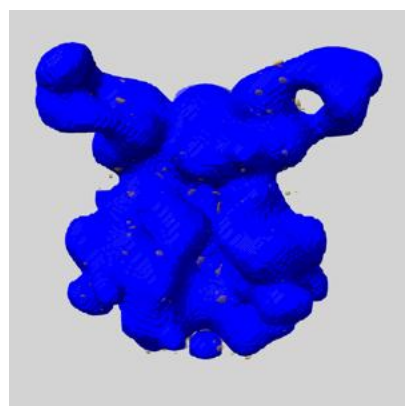
6.6 Mask visualisation [i](#)

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

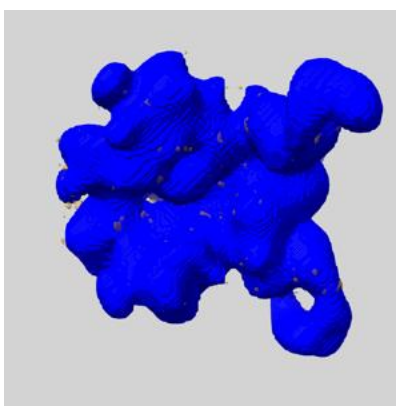
A mask typically either:

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

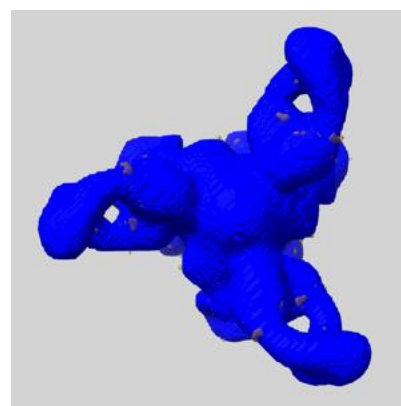
6.6.1 emd_20260_msk_1.map [i](#)



X



Y

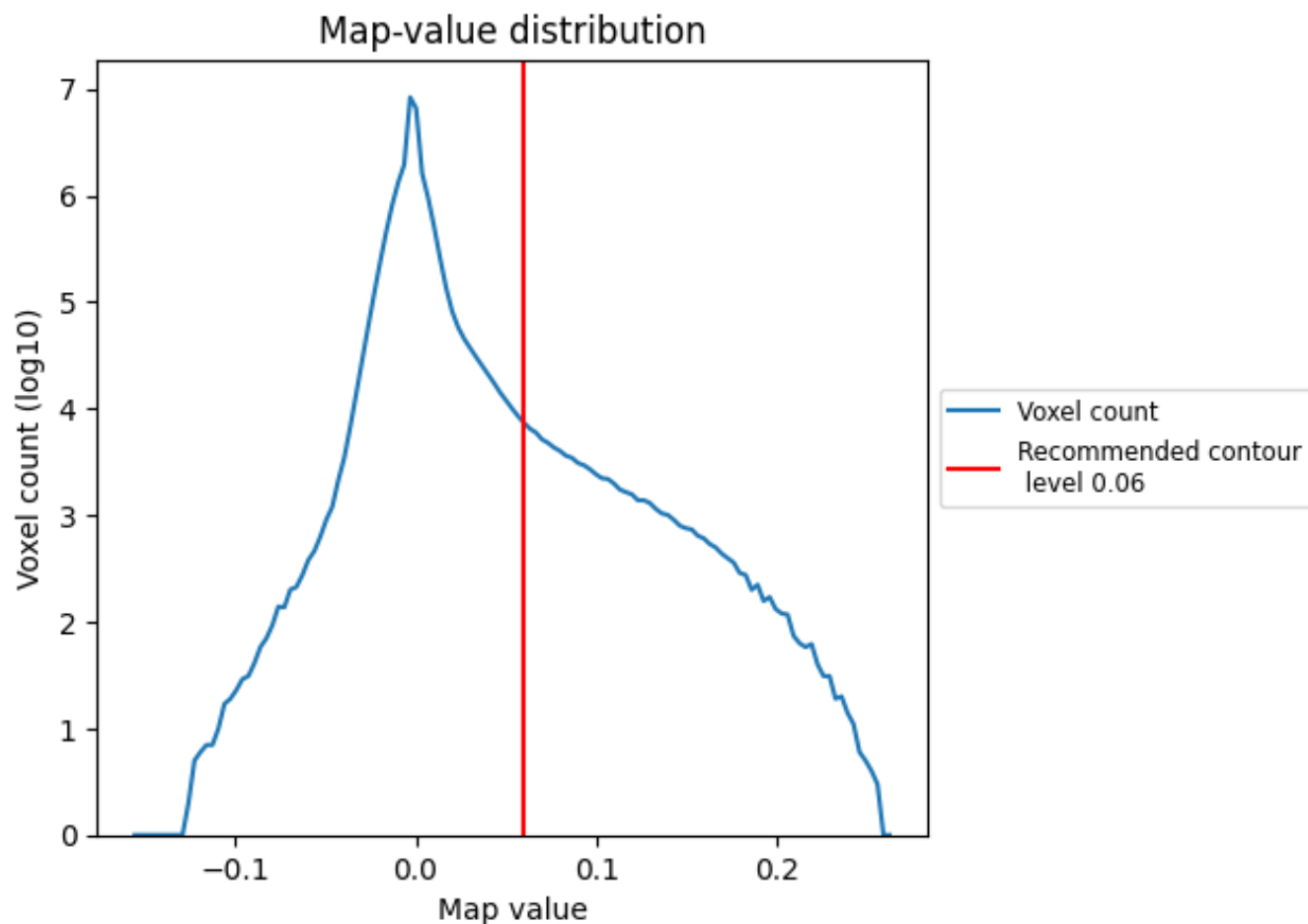


Z

7 Map analysis [i](#)

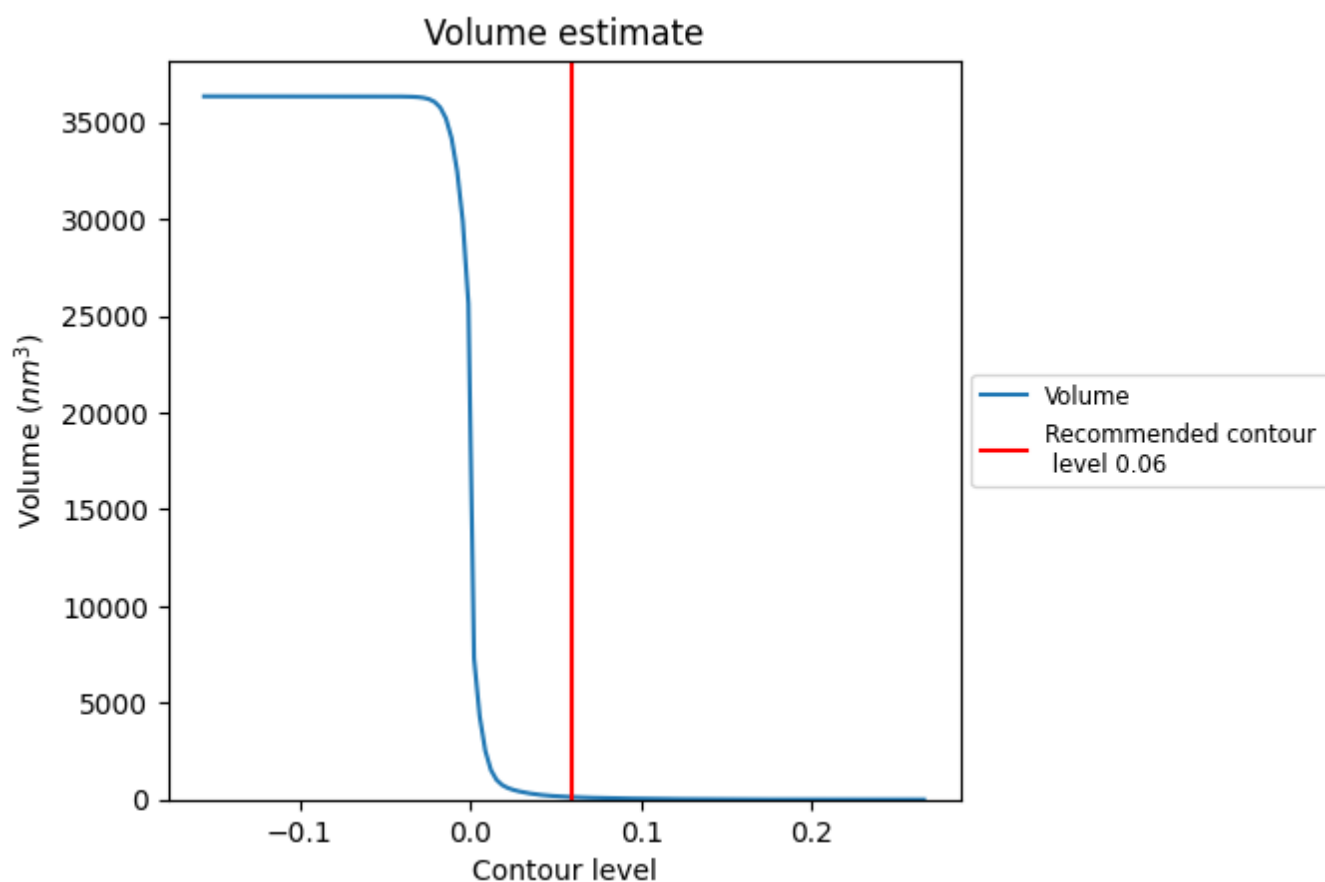
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

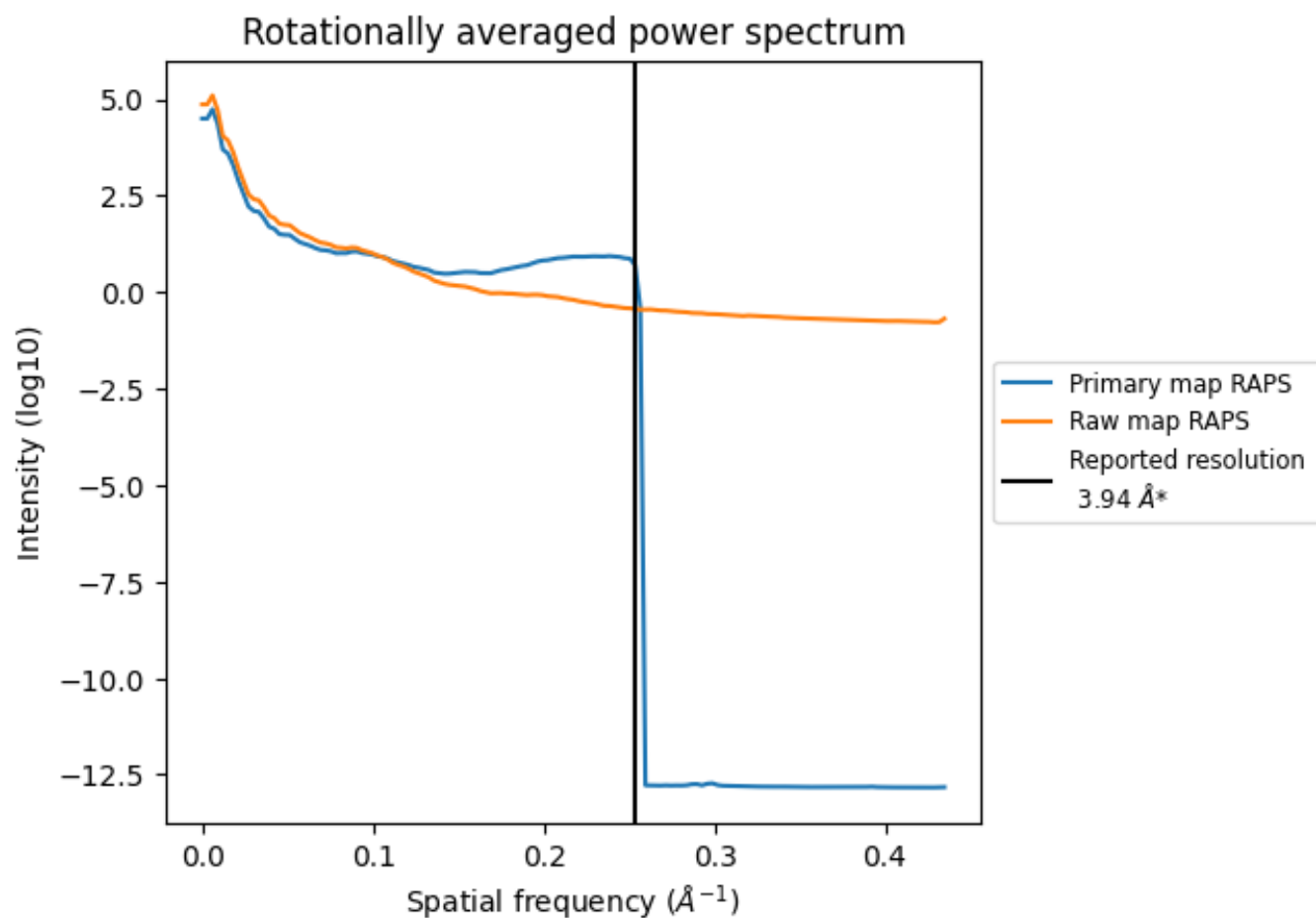
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 128 nm³; this corresponds to an approximate mass of 115 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 ⓘ

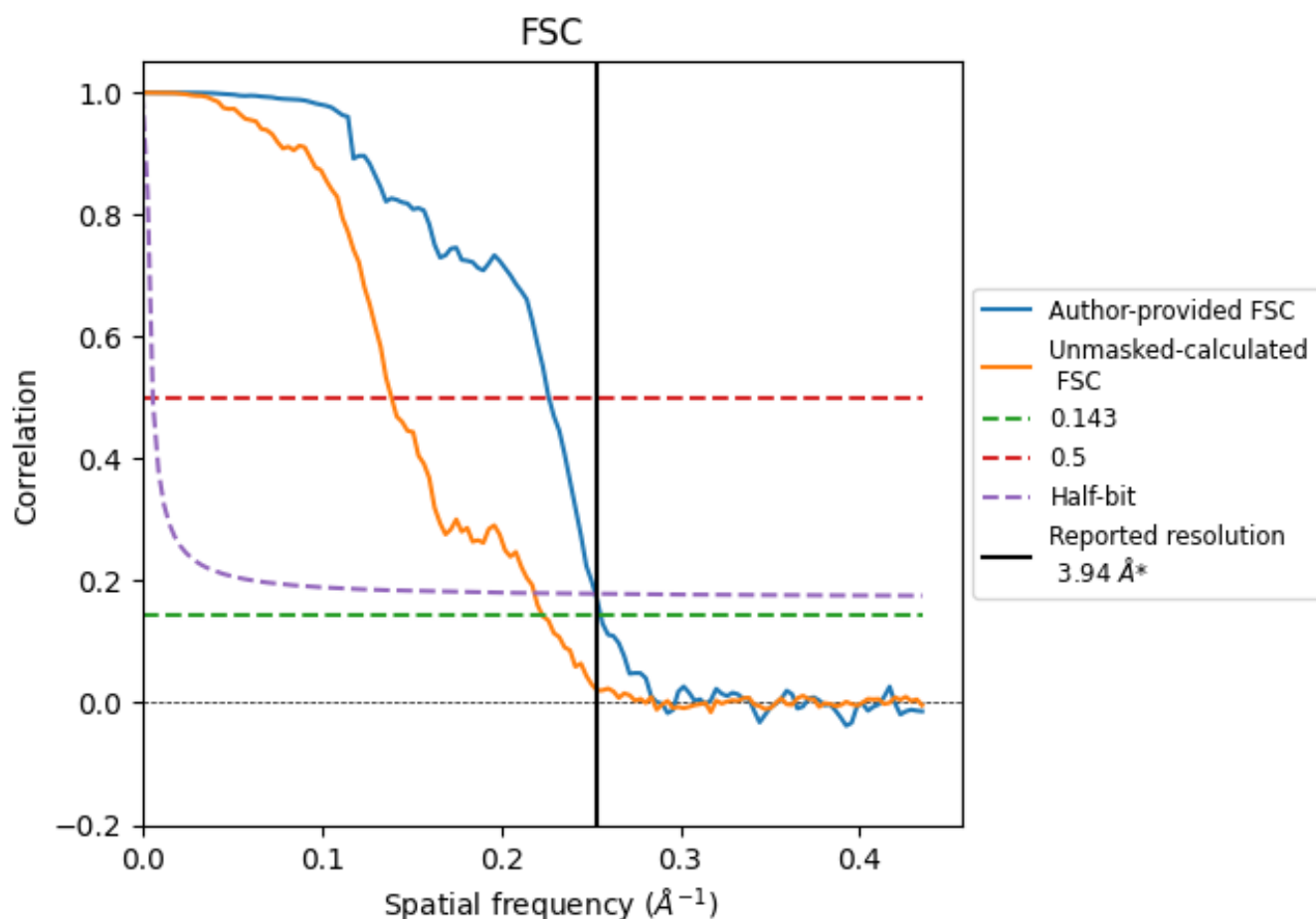


*Reported resolution corresponds to spatial frequency of 0.254 Å⁻¹

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 0.254 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

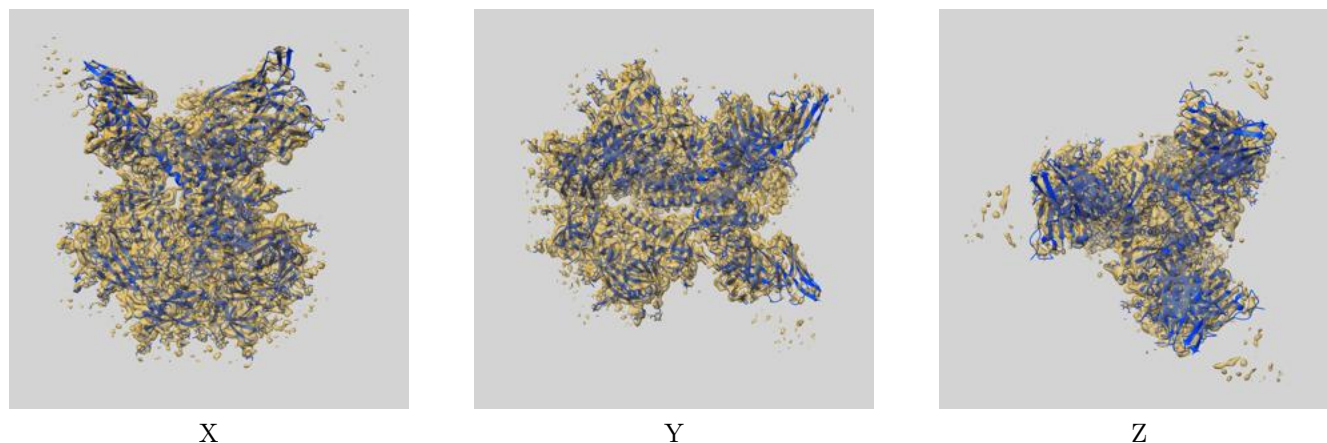
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.94	-	-
Author-provided FSC curve	3.91	4.41	3.96
Unmasked-calculated*	4.48	7.19	4.57

*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 4.48 differs from the reported value 3.94 by more than 10 %

9 Map-model fit [i](#)

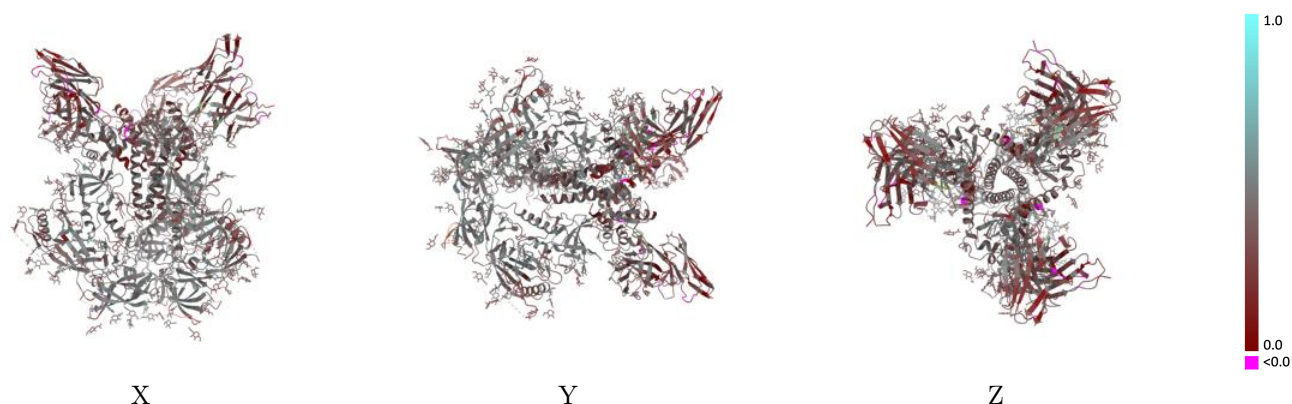
This section contains information regarding the fit between EMDB map EMD-20260 and PDB model 6P65. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



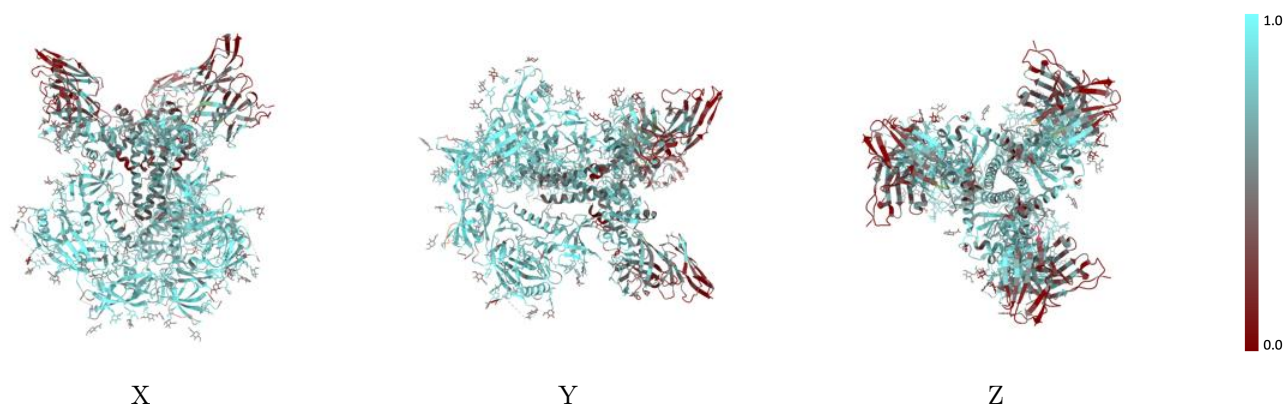
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



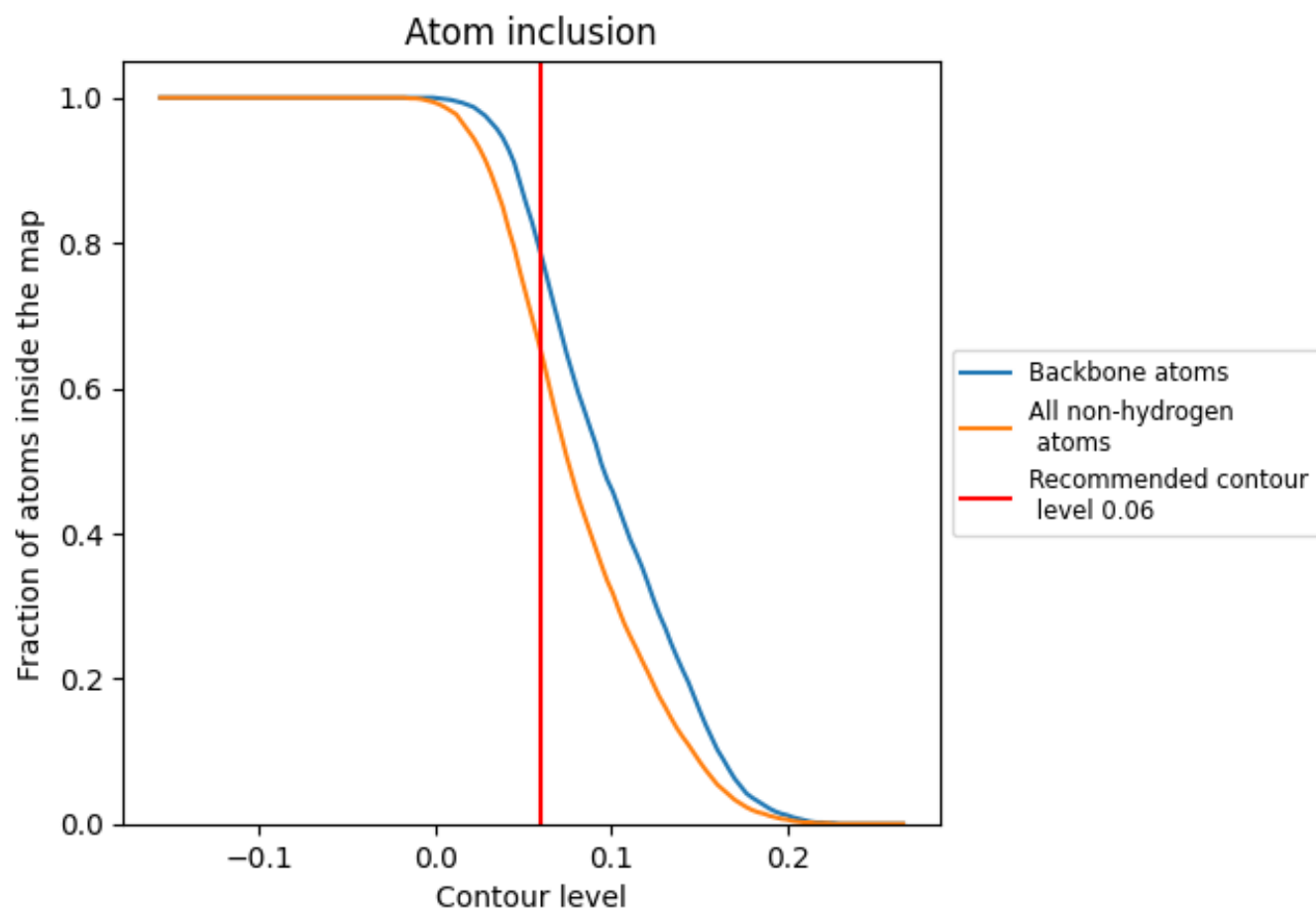
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 65% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6530	 0.3880
0	 0.6070	 0.3880
1	 0.3950	 0.3600
A	 0.7430	 0.4180
B	 0.7440	 0.4170
C	 0.4890	 0.3180
D	 0.3750	 0.2980
E	 0.7420	 0.4180
F	 0.4850	 0.3140
G	 0.3800	 0.2990
H	 0.4810	 0.3170
I	 0.5410	 0.4030
J	 0.8210	 0.4370
K	 0.6790	 0.4370
L	 0.3760	 0.2980
M	 0.5710	 0.4340
N	 0.5000	 0.3120
O	 0.6430	 0.3920
P	 0.5710	 0.4440
Q	 0.8690	 0.4660
R	 0.5000	 0.3110
S	 0.6410	 0.4120
T	 0.7140	 0.4030
U	 0.4290	 0.3720
V	 0.6070	 0.3990
W	 0.6070	 0.4000
X	 0.3950	 0.3680
Y	 0.5410	 0.4000
Z	 0.8210	 0.4150
a	 0.6790	 0.4410
b	 0.5710	 0.4330
c	 0.5000	 0.3140
d	 0.6430	 0.3970
e	 0.6070	 0.4550
f	 0.8690	 0.4590



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Chain	Atom inclusion	Q-score
g	 0.4640	 0.2870
h	 0.6670	 0.4160
i	 0.6790	 0.4050
j	 0.4640	 0.3860
k	 0.6070	 0.4160
l	 0.6070	 0.3950
m	 0.4210	 0.3570
n	 0.5410	 0.4090
o	 0.8210	 0.4160
p	 0.6790	 0.4500
q	 0.5710	 0.4300
r	 0.5000	 0.3200
s	 0.6790	 0.4020
t	 0.6070	 0.4530
u	 0.8690	 0.4700
v	 0.4640	 0.2950
w	 0.6410	 0.4280
x	 0.6790	 0.3950
y	 0.4290	 0.3620
z	 0.6070	 0.4230