



## Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 12:36 AM JST

PDB ID : 7E7D  
EMDB ID : EMD-30999  
Title : Cryo-EM structure of the SARS-CoV-2 wild-type S-Trimer from a subunit vaccine candidate  
Authors : Zheng, S.; Ma, J.  
Deposited on : 2021-02-25  
Resolution : 3.20 Å (reported)  
Based on initial model : 6VXX

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

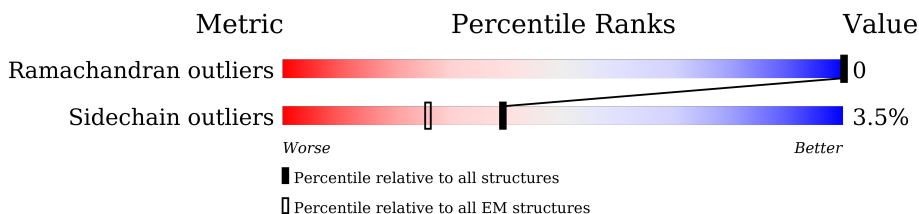
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



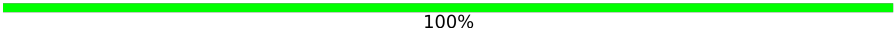




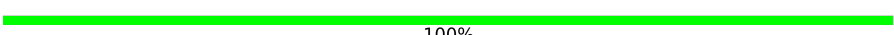









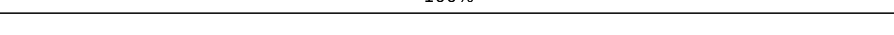
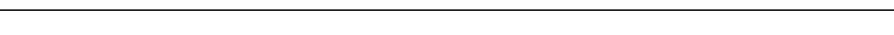
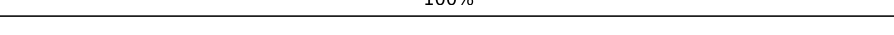
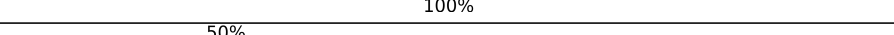
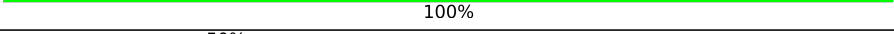
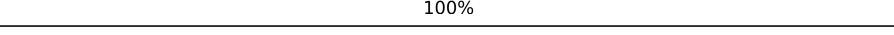
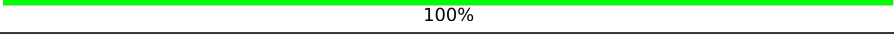
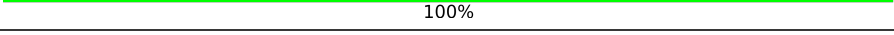
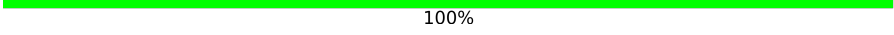

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	1520	 69% 29%
1	B	1520	 69% 29%
1	C	1520	 69% 29%
2	D	2	 100%
2	E	2	 100%
2	F	2	 100%
2	G	2	 100%
2	H	2	 50% 100%
2	I	2	 50% 100%


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Mol	Chain	Length	Quality of chain
2	J	2	 100%
2	K	2	 50% 100%
2	L	2	 100%
2	M	2	 50% 100%
2	N	2	 50% 100%
2	O	2	 100%
2	P	2	 100%
2	R	2	 100%
2	S	2	 50% 100%
2	T	2	 50% 100%
2	U	2	 100%
2	V	2	 50% 100%
2	W	2	 100%
2	X	2	 50% 100%
2	Y	2	 100%
2	Z	2	 100%
2	c	2	 100%
2	d	2	 100%
2	e	2	 50% 100%
2	f	2	 50% 100%
2	g	2	 100%
2	h	2	 50% 100%
2	i	2	 100%
2	j	2	 50% 100%
2	k	2	 50% 100%

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Mol	Chain	Length	Quality of chain
2	1	2	 100%

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 26509 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 Spike glycoprotein,Collagen alpha-1(I) chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1080	8429	5379	1406	1605	39	0	0
1	B	1080	8429	5379	1406	1605	39	0	0
1	C	1080	8429	5379	1406	1605	39	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1212	ARG	-	linker	UNP P0DTC2
A	1213	SER	-	linker	UNP P0DTC2
A	1277	ASN	ASP	variant	UNP P02452
A	1449	LYS	GLN	variant	UNP P02452
A	1492	SER	THR	variant	UNP P02452
B	1212	ARG	-	linker	UNP P0DTC2
B	1213	SER	-	linker	UNP P0DTC2
B	1277	ASN	ASP	variant	UNP P02452
B	1449	LYS	GLN	variant	UNP P02452
B	1492	SER	THR	variant	UNP P02452
C	1212	ARG	-	linker	UNP P0DTC2
C	1213	SER	-	linker	UNP P0DTC2
C	1277	ASN	ASP	variant	UNP P02452
C	1449	LYS	GLN	variant	UNP P02452
C	1492	SER	THR	variant	UNP P02452

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



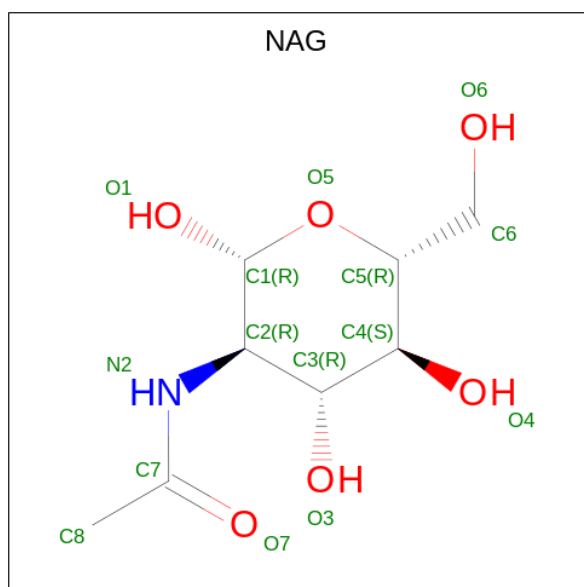
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total 28	C 16	N 2	O 10	0	0
2	E	2	Total 28	C 16	N 2	O 10	0	0
2	F	2	Total 28	C 16	N 2	O 10	0	0
2	G	2	Total 28	C 16	N 2	O 10	0	0
2	H	2	Total 28	C 16	N 2	O 10	0	0
2	I	2	Total 28	C 16	N 2	O 10	0	0
2	J	2	Total 28	C 16	N 2	O 10	0	0
2	K	2	Total 28	C 16	N 2	O 10	0	0
2	L	2	Total 28	C 16	N 2	O 10	0	0
2	M	2	Total 28	C 16	N 2	O 10	0	0
2	N	2	Total 28	C 16	N 2	O 10	0	0
2	O	2	Total 28	C 16	N 2	O 10	0	0
2	P	2	Total 28	C 16	N 2	O 10	0	0
2	R	2	Total 28	C 16	N 2	O 10	0	0
2	S	2	Total 28	C 16	N 2	O 10	0	0
2	T	2	Total 28	C 16	N 2	O 10	0	0
2	U	2	Total 28	C 16	N 2	O 10	0	0
2	V	2	Total 28	C 16	N 2	O 10	0	0
2	W	2	Total 28	C 16	N 2	O 10	0	0
2	X	2	Total 28	C 16	N 2	O 10	0	0
2	Y	2	Total 28	C 16	N 2	O 10	0	0
2	Z	2	Total 28	C 16	N 2	O 10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	c	2	Total 28	C 16	N 2	O 10	0	0
2	d	2	Total 28	C 16	N 2	O 10	0	0
2	e	2	Total 28	C 16	N 2	O 10	0	0
2	f	2	Total 28	C 16	N 2	O 10	0	0
2	g	2	Total 28	C 16	N 2	O 10	0	0
2	h	2	Total 28	C 16	N 2	O 10	0	0
2	i	2	Total 28	C 16	N 2	O 10	0	0
2	j	2	Total 28	C 16	N 2	O 10	0	0
2	k	2	Total 28	C 16	N 2	O 10	0	0
2	l	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	Total 84	C 48	N 6	O 30	0

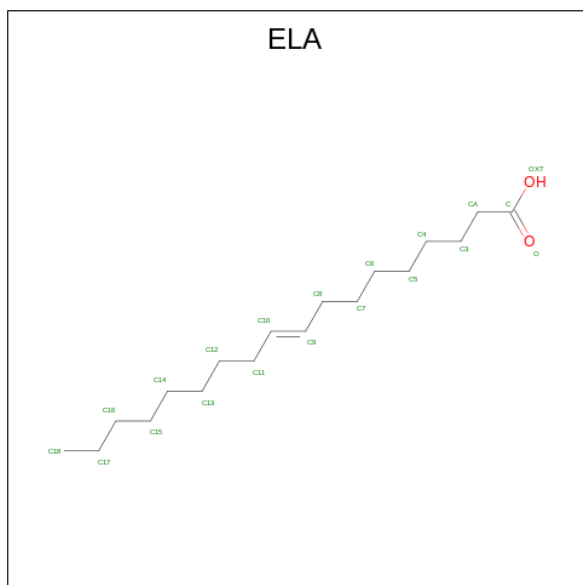
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	84	48	6	30	0
3	A	1	84	48	6	30	0
3	A	1	84	48	6	30	0
3	A	1	84	48	6	30	0
3	A	1	84	48	6	30	0
3	B	1	84	48	6	30	0
3	B	1	84	48	6	30	0
3	B	1	84	48	6	30	0
3	B	1	84	48	6	30	0
3	B	1	84	48	6	30	0
3	B	1	84	48	6	30	0
3	B	1	84	48	6	30	0
3	C	1	98	56	7	35	0
3	C	1	98	56	7	35	0
3	C	1	98	56	7	35	0
3	C	1	98	56	7	35	0
3	C	1	98	56	7	35	0
3	C	1	98	56	7	35	0
3	C	1	98	56	7	35	0

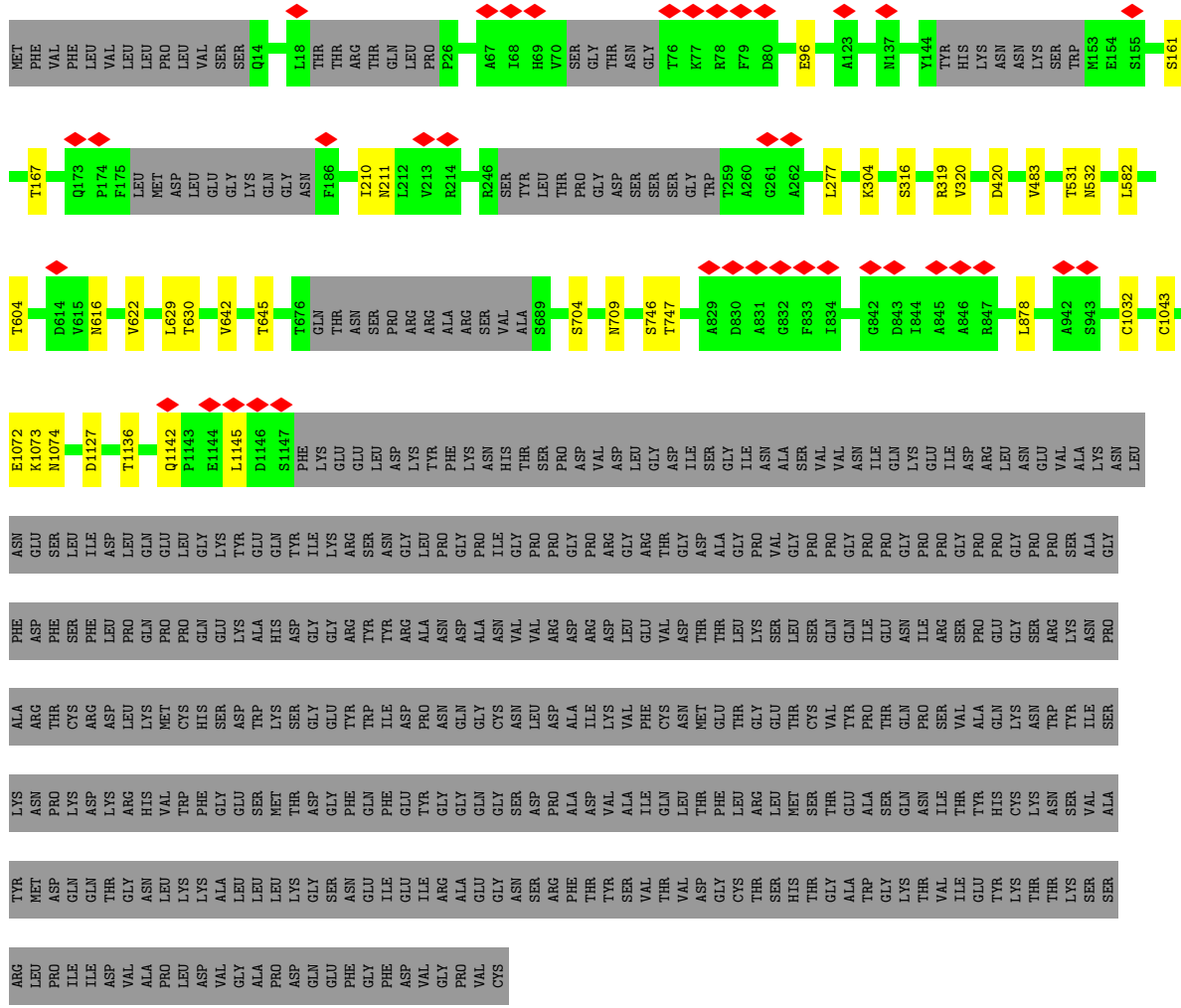
- Molecule 4 is 9-OCTADECENOIC ACID (three-letter code: ELA) (formula: C<sub>18</sub>H<sub>34</sub>O<sub>2</sub>).



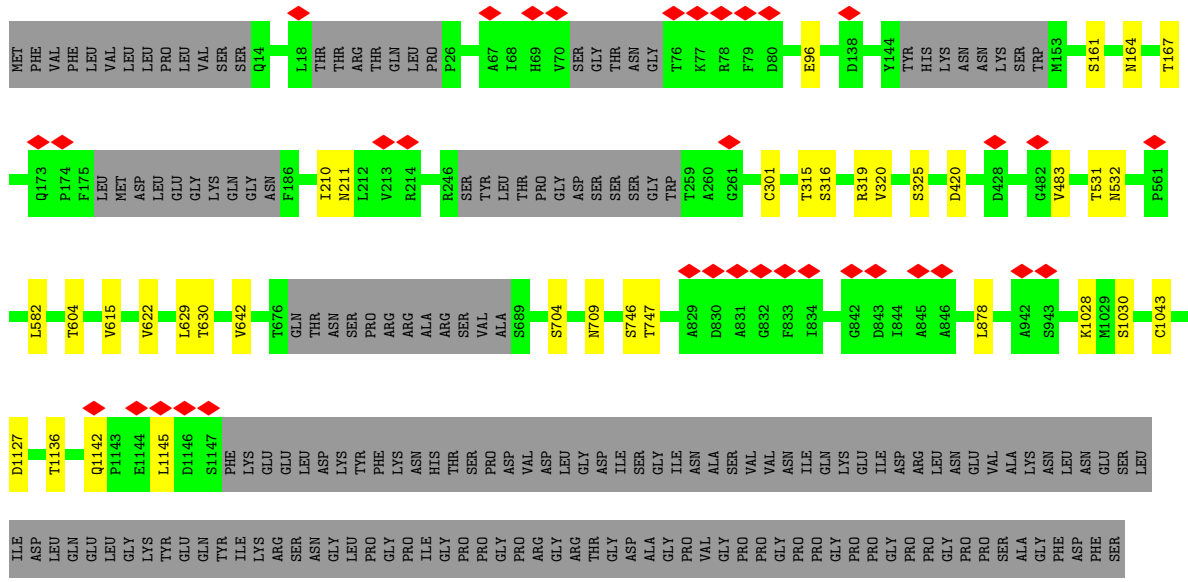


Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			40	36	4	
4	A	1	Total	C	O	0
			40	36	4	
4	B	1	Total	C	O	0
			20	18	2	





● Molecule 1: Spike glycoprotein, Collagen alpha-1(I) chain



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

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



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



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



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

Chain O:  100%



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

Chain P:  100%  
 100%



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

Chain R:  100%



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

Chain S:  50%  
 100%



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

Chain T:  50%  
 100%



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

Chain U:  100%

NAG1  
NAG2

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

Chain V:  50%  
100%NAG1  
NAG2

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

Chain W:  100%NAG1  
NAG2

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

Chain X:  50%  
100%NAG1  
NAG2

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

Chain Y:  100%NAG1  
NAG2

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

Chain Z:  100%NAG1  
NAG2

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

Chain c:  100%NAG1  
NAG2

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

Chain d:  100%



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

Chain e:  50%  
Chain e:  100%



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

Chain f:  50%  
Chain f:  100%



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

Chain g:  100%



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

Chain h:  50%  
Chain h:  100%



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

Chain i:  100%





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



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



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	173288	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.110	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	304.36002, 304.36002, 304.36002	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.46	3/8619 (0.0%)	0.56	0/11727
1	B	0.46	3/8619 (0.0%)	0.56	1/11727 (0.0%)
1	C	0.45	1/8619 (0.0%)	0.56	1/11727 (0.0%)
All	All	0.46	7/25857 (0.0%)	0.56	2/35181 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	709	ASN	CG-ND2	7.58	1.51	1.32
1	B	709	ASN	CG-ND2	7.47	1.51	1.32
1	A	709	ASN	CG-ND2	7.46	1.51	1.32
1	B	1032	CYS	CB-SG	-7.18	1.70	1.82
1	A	122	ASN	CG-ND2	5.99	1.47	1.32
1	B	1043	CYS	CB-SG	-5.42	1.73	1.81
1	A	165	ASN	CG-ND2	5.15	1.45	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	301	CYS	CA-CB-SG	5.95	124.72	114.00
1	B	616	ASN	N-CA-C	-5.28	96.75	111.00

There are no chirality outliers.

There are no planarity outliers.

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	1066/1520 (70%)	1036 (97%)	30 (3%)	0	100	100
1	B	1066/1520 (70%)	1036 (97%)	30 (3%)	0	100	100
1	C	1066/1520 (70%)	1037 (97%)	29 (3%)	0	100	100
All	All	3198/4560 (70%)	3109 (97%)	89 (3%)	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	939/1316 (71%)	905 (96%)	34 (4%)	35	69
1	B	939/1316 (71%)	907 (97%)	32 (3%)	37	70
1	C	939/1316 (71%)	906 (96%)	33 (4%)	36	69
All	All	2817/3948 (71%)	2718 (96%)	99 (4%)	39	69

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	GLU
1	A	161	SER
1	A	167	THR
1	A	210	ILE
1	A	211	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	277	LEU
1	A	315	THR
1	A	319	ARG
1	A	320	VAL
1	A	325	SER
1	A	420	ASP
1	A	483	VAL
1	A	531	THR
1	A	532	ASN
1	A	582	LEU
1	A	604	THR
1	A	629	LEU
1	A	630	THR
1	A	704	SER
1	A	746	SER
1	A	747	THR
1	A	836	GLN
1	A	839	ASP
1	A	844	ILE
1	A	848	ASP
1	A	878	LEU
1	A	1027	THR
1	A	1028	LYS
1	A	1030	SER
1	A	1031	GLU
1	A	1127	ASP
1	A	1136	THR
1	A	1142	GLN
1	A	1145	LEU
1	B	96	GLU
1	B	161	SER
1	B	167	THR
1	B	210	ILE
1	B	211	ASN
1	B	277	LEU
1	B	304	LYS
1	B	316	SER
1	B	319	ARG
1	B	320	VAL
1	B	420	ASP
1	B	483	VAL
1	B	531	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	532	ASN
1	B	582	LEU
1	B	604	THR
1	B	622	VAL
1	B	629	LEU
1	B	630	THR
1	B	642	VAL
1	B	645	THR
1	B	704	SER
1	B	746	SER
1	B	747	THR
1	B	878	LEU
1	B	1072	GLU
1	B	1073	LYS
1	B	1074	ASN
1	B	1127	ASP
1	B	1136	THR
1	B	1142	GLN
1	B	1145	LEU
1	C	96	GLU
1	C	161	SER
1	C	164	ASN
1	C	167	THR
1	C	210	ILE
1	C	211	ASN
1	C	315	THR
1	C	316	SER
1	C	319	ARG
1	C	320	VAL
1	C	325	SER
1	C	420	ASP
1	C	483	VAL
1	C	531	THR
1	C	532	ASN
1	C	582	LEU
1	C	604	THR
1	C	615	VAL
1	C	622	VAL
1	C	629	LEU
1	C	630	THR
1	C	642	VAL
1	C	704	SER

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Mol	Chain	Res	Type
1	C	746	SER
1	C	747	THR
1	C	878	LEU
1	C	1028	LYS
1	C	1030	SER
1	C	1043	CYS
1	C	1127	ASP
1	C	1136	THR
1	C	1142	GLN
1	C	1145	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	115	GLN
1	A	121	ASN
1	A	134	GLN
1	A	474	GLN
1	A	481	ASN
1	A	487	ASN
1	A	498	GLN
1	A	580	GLN
1	A	606	ASN
1	A	607	GLN
1	A	644	GLN
1	A	764	ASN
1	A	804	GLN
1	A	901	GLN
1	A	926	GLN
1	A	954	GLN
1	A	965	GLN
1	B	30	ASN
1	B	69	HIS
1	B	121	ASN
1	B	134	GLN
1	B	317	ASN
1	B	474	GLN
1	B	481	ASN
1	B	487	ASN
1	B	498	GLN
1	B	580	GLN

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Mol	Chain	Res	Type
1	B	606	ASN
1	B	607	GLN
1	B	764	ASN
1	B	804	GLN
1	B	901	GLN
1	B	926	GLN
1	B	954	GLN
1	B	965	GLN
1	C	30	ASN
1	C	69	HIS
1	C	121	ASN
1	C	134	GLN
1	C	314	GLN
1	C	474	GLN
1	C	481	ASN
1	C	487	ASN
1	C	498	GLN
1	C	580	GLN
1	C	606	ASN
1	C	607	GLN
1	C	613	GLN
1	C	764	ASN
1	C	804	GLN
1	C	901	GLN
1	C	926	GLN
1	C	954	GLN
1	C	965	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

64 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
2	NAG	D	1	1,2	14,14,15	0.46	0	17,19,21	0.99	1 (5%)
2	NAG	D	2	2	14,14,15	0.24	0	17,19,21	1.05	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.45	0	17,19,21	0.58	0
2	NAG	E	2	2	14,14,15	0.18	0	17,19,21	0.41	0
2	NAG	F	1	1,2	14,14,15	0.35	0	17,19,21	0.69	0
2	NAG	F	2	2	14,14,15	0.32	0	17,19,21	0.62	0
2	NAG	G	1	1,2	14,14,15	0.24	0	17,19,21	0.38	0
2	NAG	G	2	2	14,14,15	0.19	0	17,19,21	0.43	0
2	NAG	H	1	1,2	14,14,15	0.28	0	17,19,21	0.42	0
2	NAG	H	2	2	14,14,15	0.25	0	17,19,21	0.37	0
2	NAG	I	1	1,2	14,14,15	0.35	0	17,19,21	0.53	0
2	NAG	I	2	2	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	J	1	1,2	14,14,15	0.32	0	17,19,21	0.47	0
2	NAG	J	2	2	14,14,15	0.23	0	17,19,21	0.42	0
2	NAG	K	1	1,2	14,14,15	0.31	0	17,19,21	1.05	1 (5%)
2	NAG	K	2	2	14,14,15	0.30	0	17,19,21	0.55	0
2	NAG	L	1	1,2	14,14,15	0.31	0	17,19,21	0.44	0
2	NAG	L	2	2	14,14,15	0.19	0	17,19,21	0.50	0
2	NAG	M	1	1,2	14,14,15	0.32	0	17,19,21	0.61	0
2	NAG	M	2	2	14,14,15	0.30	0	17,19,21	0.70	0
2	NAG	N	1	1,2	14,14,15	0.30	0	17,19,21	0.67	0
2	NAG	N	2	2	14,14,15	0.24	0	17,19,21	0.96	1 (5%)
2	NAG	O	1	1,2	14,14,15	0.35	0	17,19,21	0.47	0
2	NAG	O	2	2	14,14,15	0.23	0	17,19,21	0.53	0
2	NAG	P	1	1,2	14,14,15	0.47	0	17,19,21	0.58	0
2	NAG	P	2	2	14,14,15	0.19	0	17,19,21	0.41	0
2	NAG	R	1	1,2	14,14,15	0.24	0	17,19,21	0.37	0
2	NAG	R	2	2	14,14,15	0.20	0	17,19,21	0.44	0
2	NAG	S	1	1,2	14,14,15	0.28	0	17,19,21	0.43	0
2	NAG	S	2	2	14,14,15	0.25	0	17,19,21	0.37	0
2	NAG	T	1	1,2	14,14,15	0.35	0	17,19,21	0.52	0
2	NAG	T	2	2	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	U	1	1,2	14,14,15	0.33	0	17,19,21	0.47	0
2	NAG	U	2	2	14,14,15	0.24	0	17,19,21	0.42	0
2	NAG	V	1	1,2	14,14,15	0.34	0	17,19,21	0.50	0
2	NAG	V	2	2	14,14,15	0.19	0	17,19,21	0.44	0
2	NAG	W	1	1,2	14,14,15	0.31	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	W	2	2	14,14,15	0.18	0	17,19,21	0.50	0
2	NAG	X	1	1,2	14,14,15	0.32	0	17,19,21	0.61	0
2	NAG	X	2	2	14,14,15	0.29	0	17,19,21	0.73	0
2	NAG	Y	1	1,2	14,14,15	0.29	0	17,19,21	0.63	0
2	NAG	Y	2	2	14,14,15	0.31	0	17,19,21	0.52	0
2	NAG	Z	1	1,2	14,14,15	0.35	0	17,19,21	0.47	0
2	NAG	Z	2	2	14,14,15	0.25	0	17,19,21	0.53	0
2	NAG	c	1	1,2	14,14,15	0.38	0	17,19,21	0.62	0
2	NAG	c	2	2	14,14,15	0.31	0	17,19,21	0.73	0
2	NAG	d	1	1,2	14,14,15	0.25	0	17,19,21	0.38	0
2	NAG	d	2	2	14,14,15	0.21	0	17,19,21	0.44	0
2	NAG	e	1	1,2	14,14,15	0.27	0	17,19,21	0.43	0
2	NAG	e	2	2	14,14,15	0.26	0	17,19,21	0.37	0
2	NAG	f	1	1,2	14,14,15	0.35	0	17,19,21	0.52	0
2	NAG	f	2	2	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	g	1	1,2	14,14,15	0.33	0	17,19,21	0.47	0
2	NAG	g	2	2	14,14,15	0.24	0	17,19,21	0.42	0
2	NAG	h	1	1,2	14,14,15	0.34	0	17,19,21	0.49	0
2	NAG	h	2	2	14,14,15	0.19	0	17,19,21	0.44	0
2	NAG	i	1	1,2	14,14,15	0.31	0	17,19,21	0.45	0
2	NAG	i	2	2	14,14,15	0.18	0	17,19,21	0.50	0
2	NAG	j	1	1,2	14,14,15	0.31	0	17,19,21	0.65	0
2	NAG	j	2	2	14,14,15	0.26	0	17,19,21	0.68	0
2	NAG	k	1	1,2	14,14,15	0.29	0	17,19,21	0.62	0
2	NAG	k	2	2	14,14,15	0.32	0	17,19,21	0.52	0
2	NAG	l	1	1,2	14,14,15	0.34	0	17,19,21	0.47	0
2	NAG	l	2	2	14,14,15	0.24	0	17,19,21	0.53	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
2	NAG	D	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	K	2	2	-	4/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	4/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	N	2	2	-	5/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	1/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	P	2	2	-	1/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
2	NAG	S	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	2/6/23/26	0/1/1/1
2	NAG	T	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	T	2	2	-	0/6/23/26	0/1/1/1
2	NAG	U	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	U	2	2	-	0/6/23/26	0/1/1/1
2	NAG	V	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	V	2	2	-	2/6/23/26	0/1/1/1
2	NAG	W	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	W	2	2	-	2/6/23/26	0/1/1/1
2	NAG	X	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	X	2	2	-	4/6/23/26	0/1/1/1
2	NAG	Y	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	3/6/23/26	0/1/1/1
2	NAG	Z	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	1/6/23/26	0/1/1/1
2	NAG	c	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	c	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	d	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	d	2	2	-	0/6/23/26	0/1/1/1
2	NAG	e	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	e	2	2	-	2/6/23/26	0/1/1/1
2	NAG	f	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	f	2	2	-	0/6/23/26	0/1/1/1
2	NAG	g	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	g	2	2	-	0/6/23/26	0/1/1/1
2	NAG	h	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	h	2	2	-	2/6/23/26	0/1/1/1
2	NAG	i	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	i	2	2	-	2/6/23/26	0/1/1/1
2	NAG	j	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	j	2	2	-	4/6/23/26	0/1/1/1
2	NAG	k	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	k	2	2	-	3/6/23/26	0/1/1/1
2	NAG	l	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	l	2	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C1-O5-C5	3.22	116.56	112.19
2	D	1	NAG	O5-C1-C2	2.12	114.63	111.29
2	K	1	NAG	C1-O5-C5	2.08	115.00	112.19
2	N	2	NAG	C2-N2-C7	2.07	125.84	122.90

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	N	1	NAG	C1-C2-N2-C7
2	N	2	NAG	O7-C7-N2-C2
2	N	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	W	2	NAG	O5-C5-C6-O6
2	i	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	j	2	NAG	O5-C5-C6-O6
2	X	2	NAG	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O7-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
2	X	2	NAG	C8-C7-N2-C2
2	c	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C1-C2-N2-C7
2	P	1	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	W	2	NAG	C4-C5-C6-O6
2	i	2	NAG	C4-C5-C6-O6
2	M	2	NAG	C8-C7-N2-C2
2	X	2	NAG	O7-C7-N2-C2
2	j	2	NAG	C8-C7-N2-C2
2	j	2	NAG	O7-C7-N2-C2
2	O	1	NAG	O5-C5-C6-O6
2	l	1	NAG	O5-C5-C6-O6
2	X	2	NAG	C4-C5-C6-O6
2	c	1	NAG	C4-C5-C6-O6
2	Z	1	NAG	O5-C5-C6-O6
2	N	2	NAG	C1-C2-N2-C7
2	M	2	NAG	O5-C5-C6-O6
2	Y	2	NAG	O5-C5-C6-O6
2	k	2	NAG	O5-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	j	2	NAG	C4-C5-C6-O6
2	Z	1	NAG	C4-C5-C6-O6
2	l	1	NAG	C4-C5-C6-O6
2	h	2	NAG	O5-C5-C6-O6
2	V	1	NAG	C4-C5-C6-O6
2	h	1	NAG	C4-C5-C6-O6
2	V	2	NAG	O5-C5-C6-O6
2	Y	2	NAG	C4-C5-C6-O6
2	k	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	V	2	NAG	C4-C5-C6-O6
2	h	2	NAG	C4-C5-C6-O6
2	M	2	NAG	O7-C7-N2-C2
2	N	1	NAG	C8-C7-N2-C2
2	H	2	NAG	O5-C5-C6-O6
2	S	2	NAG	O5-C5-C6-O6
2	e	2	NAG	O5-C5-C6-O6
2	k	1	NAG	O5-C5-C6-O6
2	Y	1	NAG	O5-C5-C6-O6
2	Y	1	NAG	C1-C2-N2-C7
2	k	1	NAG	C1-C2-N2-C7
2	H	2	NAG	C4-C5-C6-O6
2	S	2	NAG	C4-C5-C6-O6
2	e	2	NAG	C4-C5-C6-O6
2	Y	1	NAG	C4-C5-C6-O6
2	k	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
2	N	1	NAG	O7-C7-N2-C2
2	V	1	NAG	O5-C5-C6-O6
2	h	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	P	1	NAG	C1-C2-N2-C7
2	D	1	NAG	C4-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C1-C2-N2-C7
2	N	2	NAG	C4-C5-C6-O6
2	X	1	NAG	C4-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	I	1	NAG	C3-C2-N2-C7
2	T	1	NAG	C3-C2-N2-C7
2	Y	2	NAG	C3-C2-N2-C7
2	f	1	NAG	C3-C2-N2-C7
2	k	2	NAG	C3-C2-N2-C7
2	D	1	NAG	O5-C5-C6-O6
2	c	1	NAG	C8-C7-N2-C2
2	L	1	NAG	C1-C2-N2-C7
2	W	1	NAG	C1-C2-N2-C7
2	i	1	NAG	C1-C2-N2-C7
2	E	1	NAG	C3-C2-N2-C7

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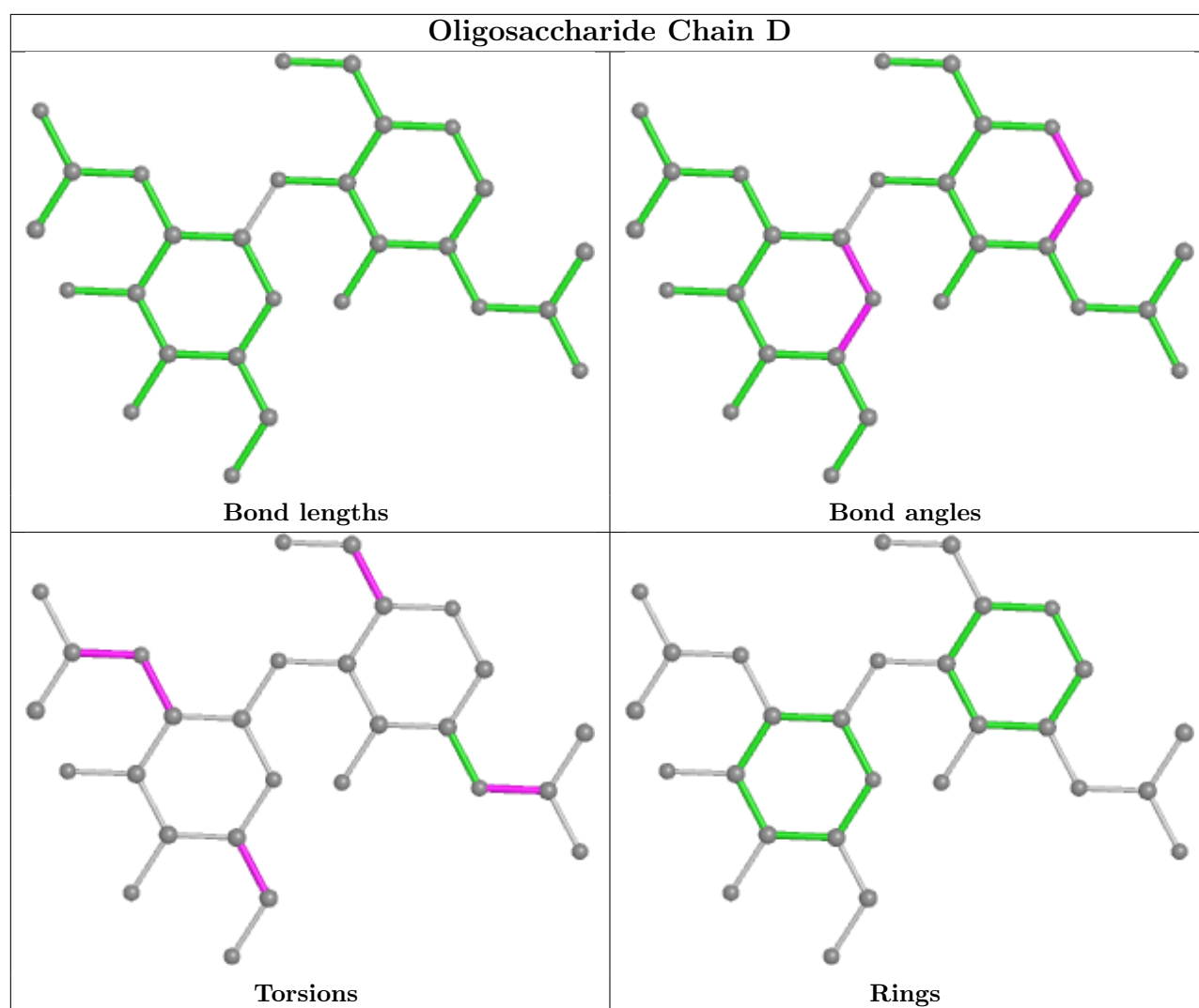
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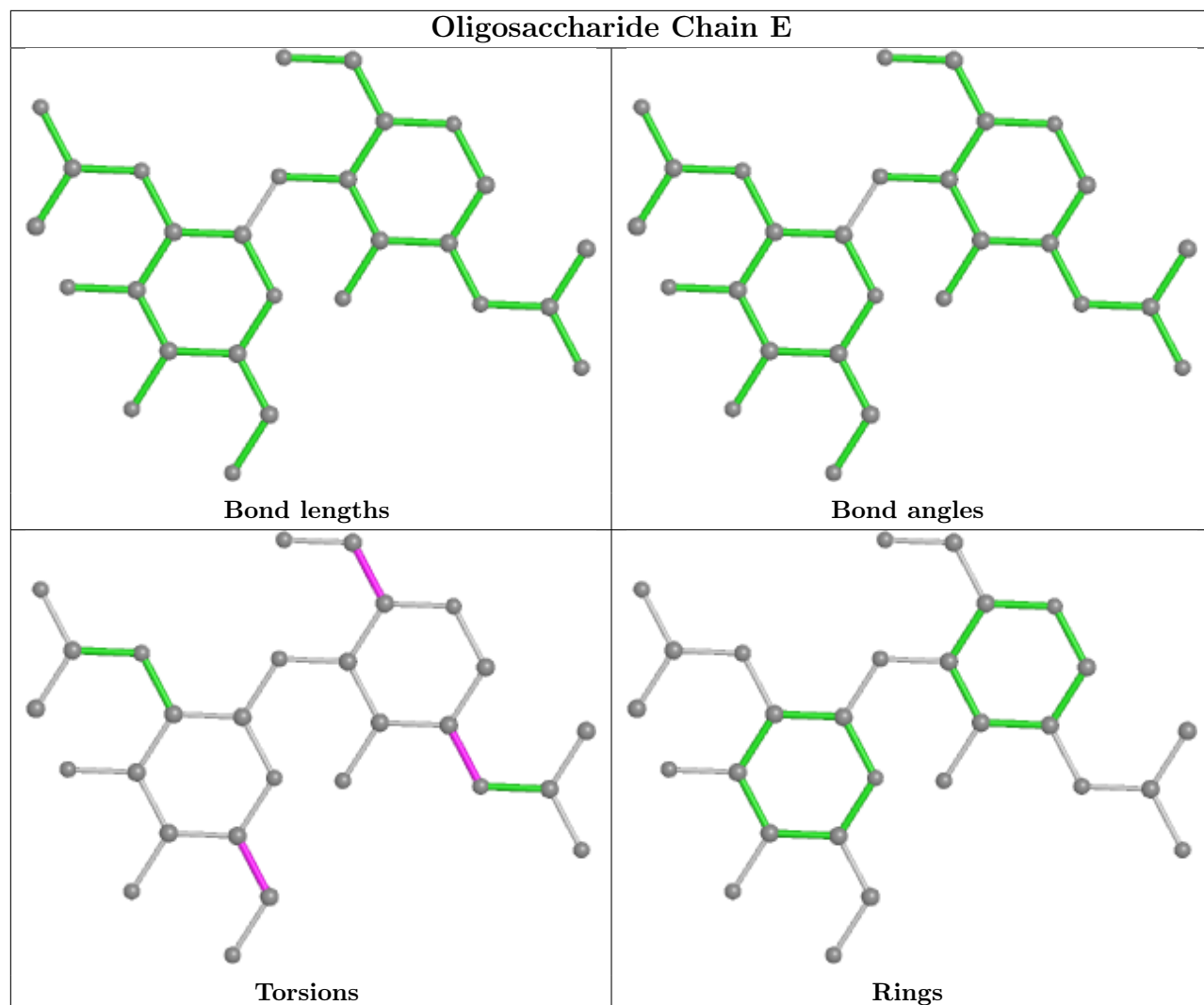
Mol	Chain	Res	Type	Atoms
2	K	1	NAG	C3-C2-N2-C7
2	O	2	NAG	C3-C2-N2-C7
2	P	1	NAG	C3-C2-N2-C7
2	Z	2	NAG	C3-C2-N2-C7
2	1	2	NAG	C3-C2-N2-C7

There are no ring outliers.

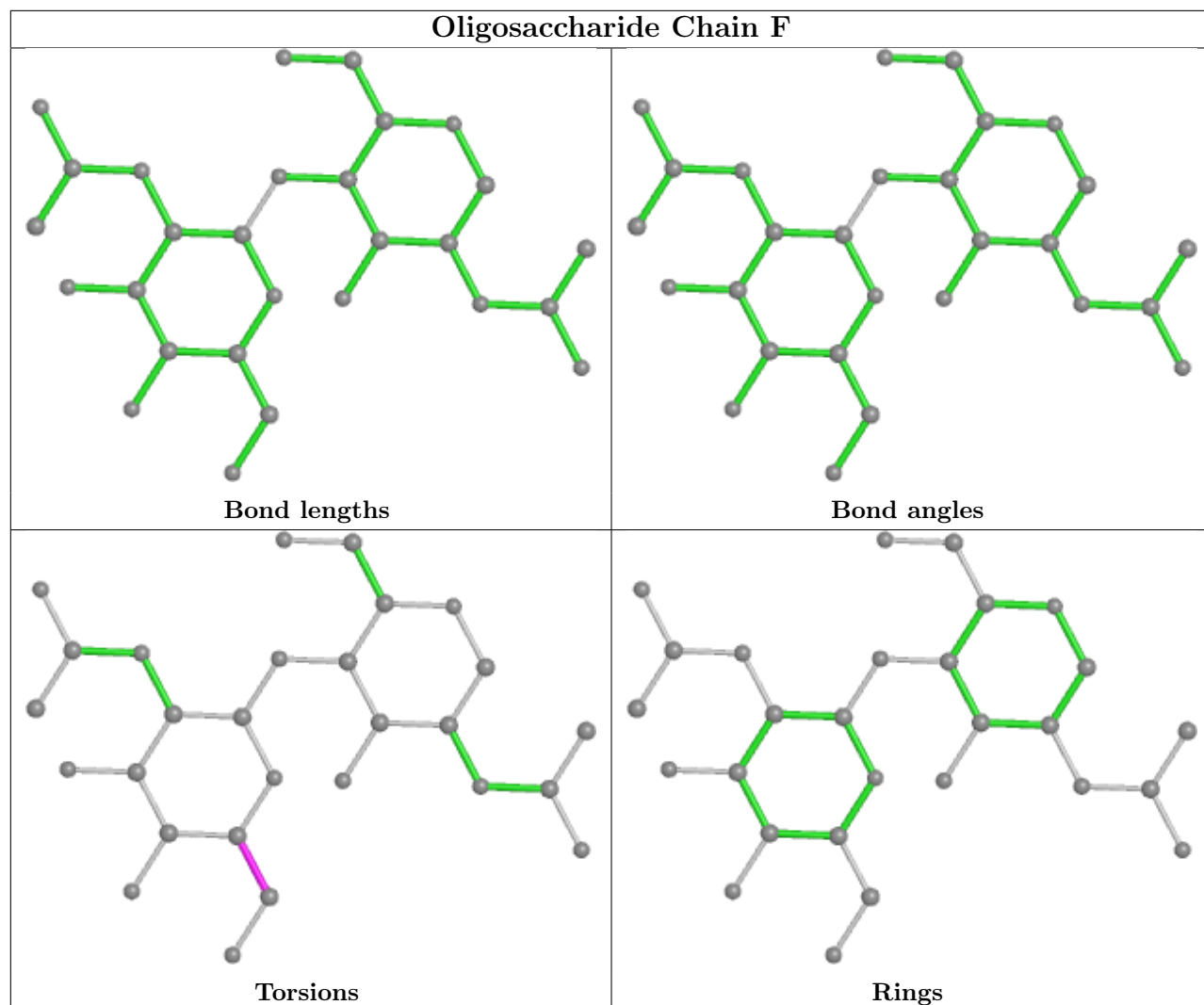
No monomer is involved in short contacts.

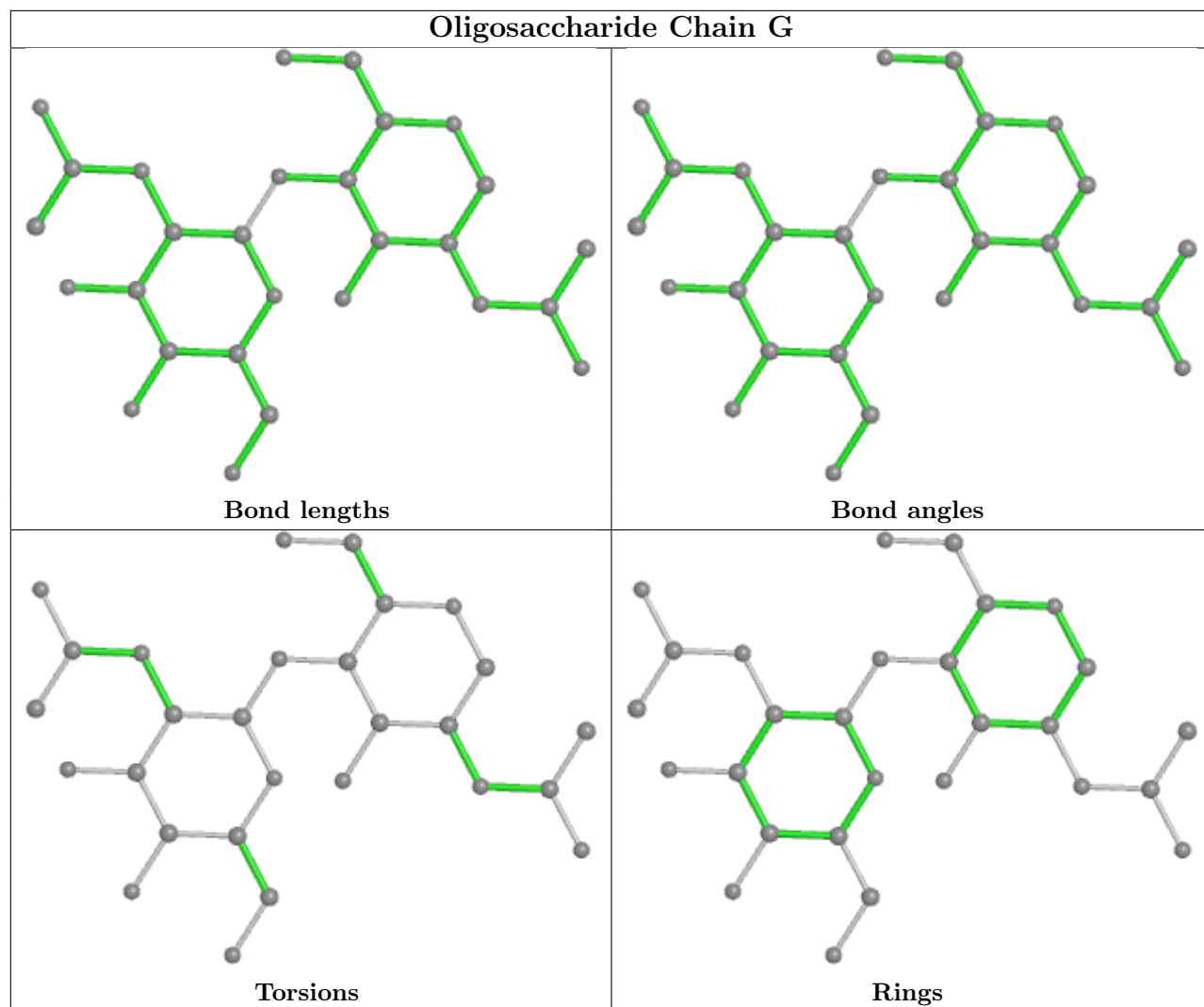
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

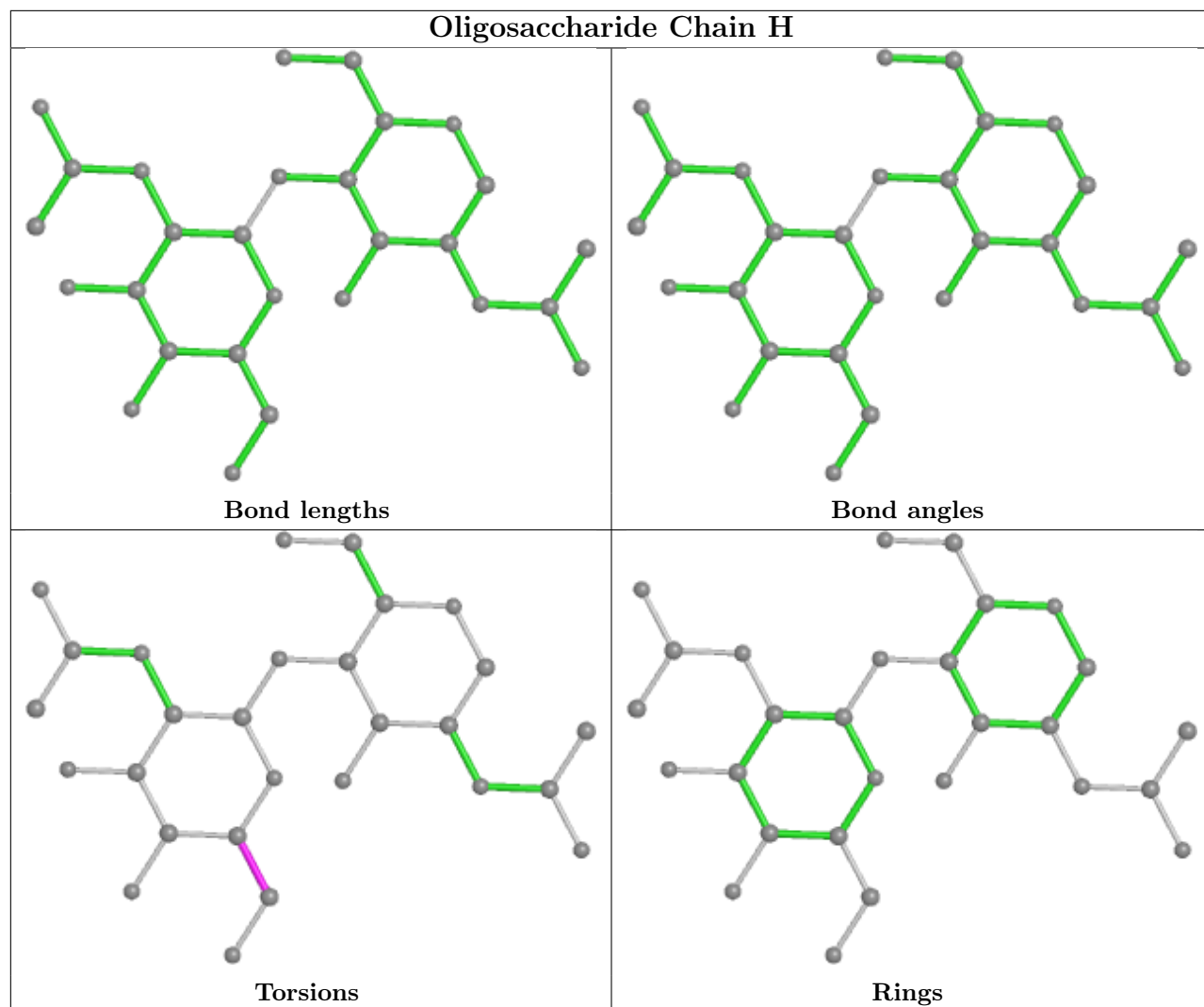


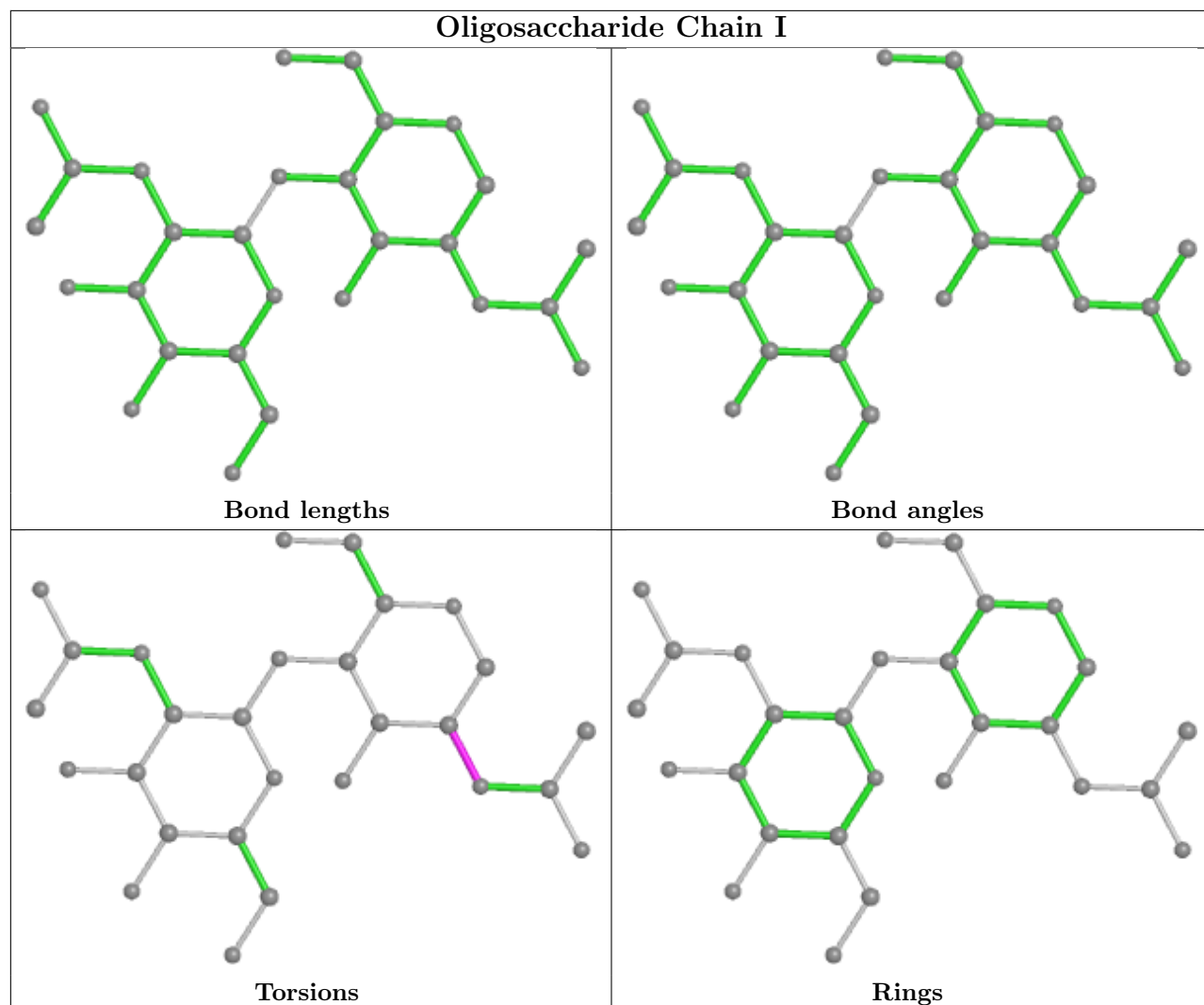


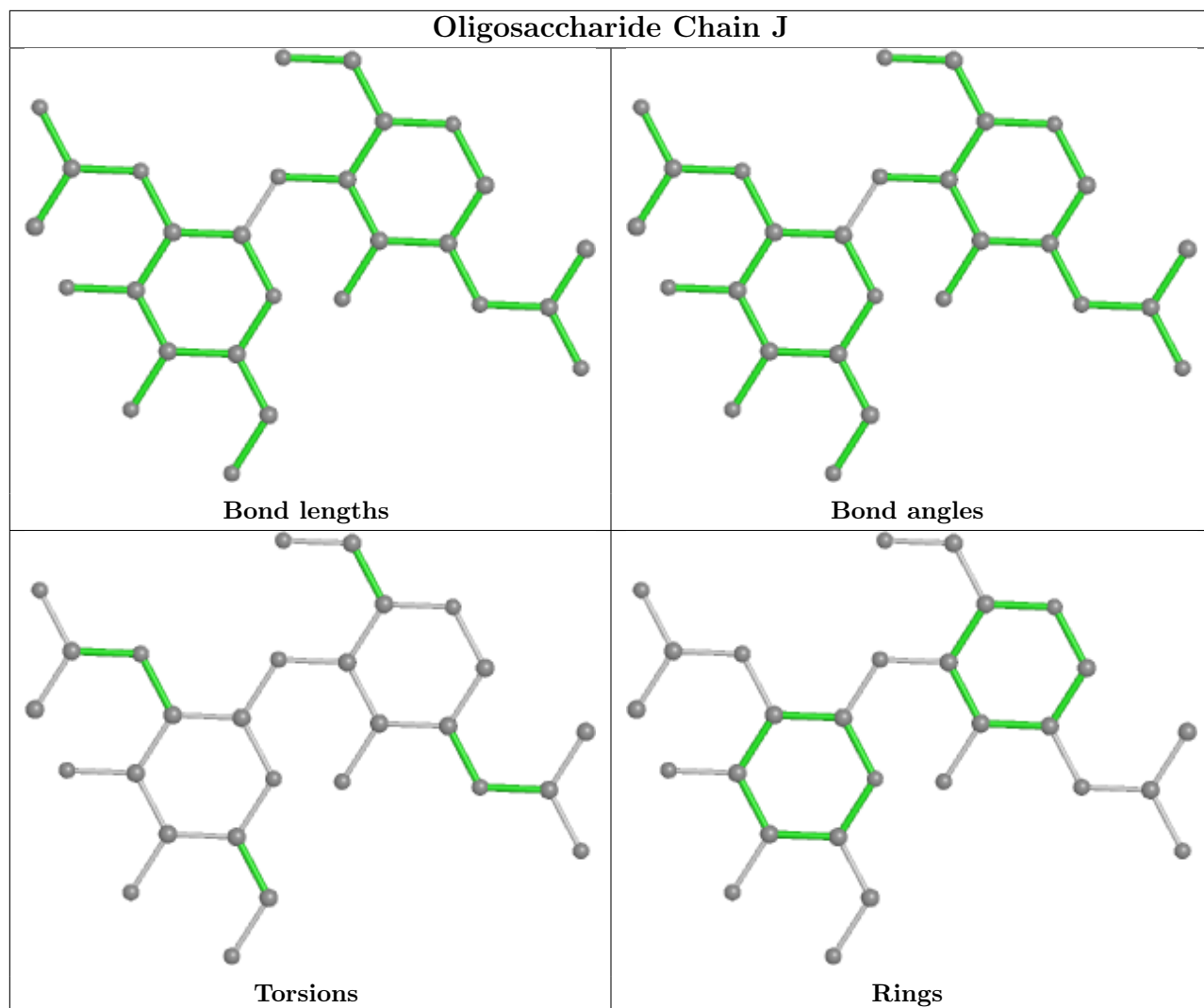


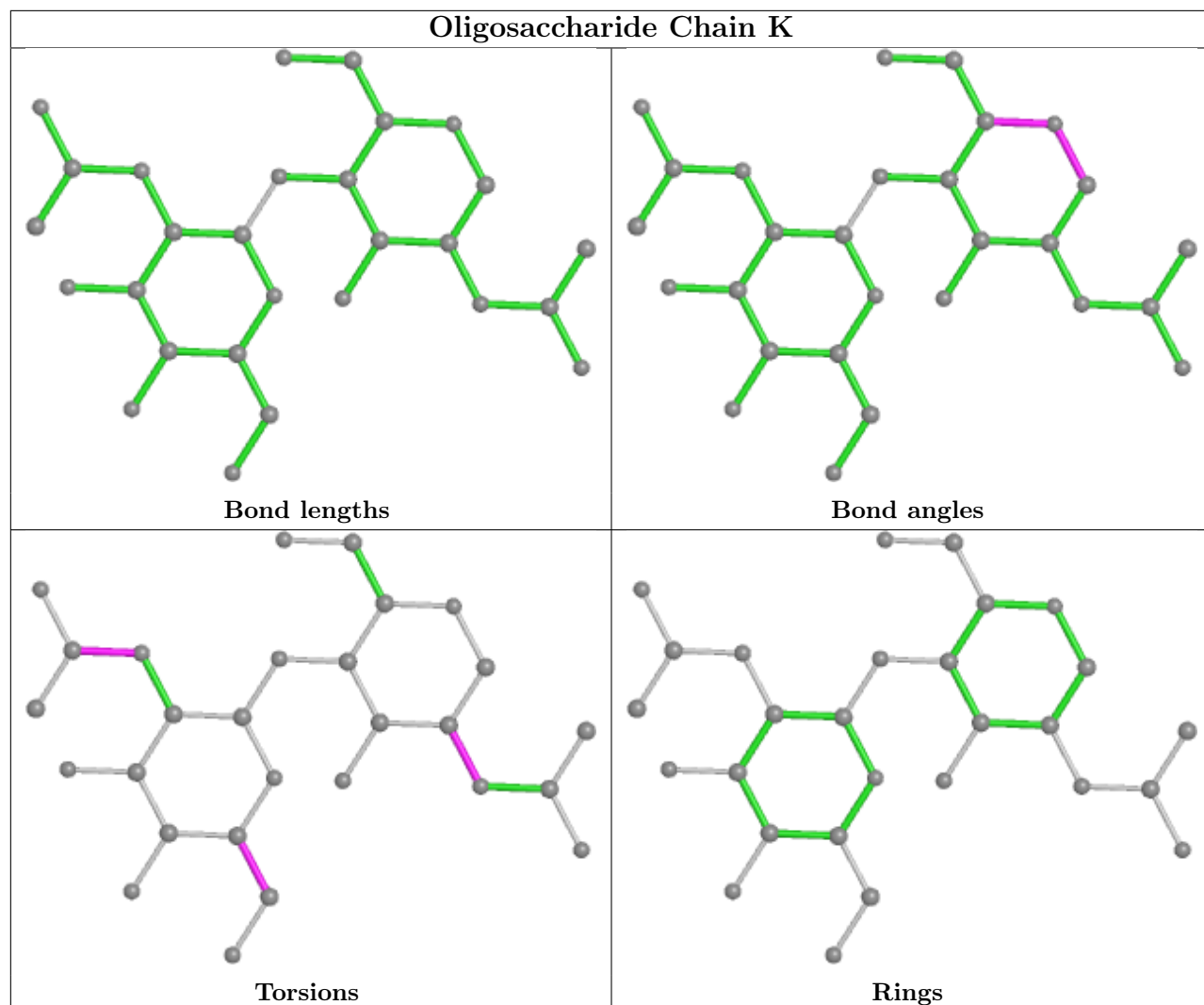


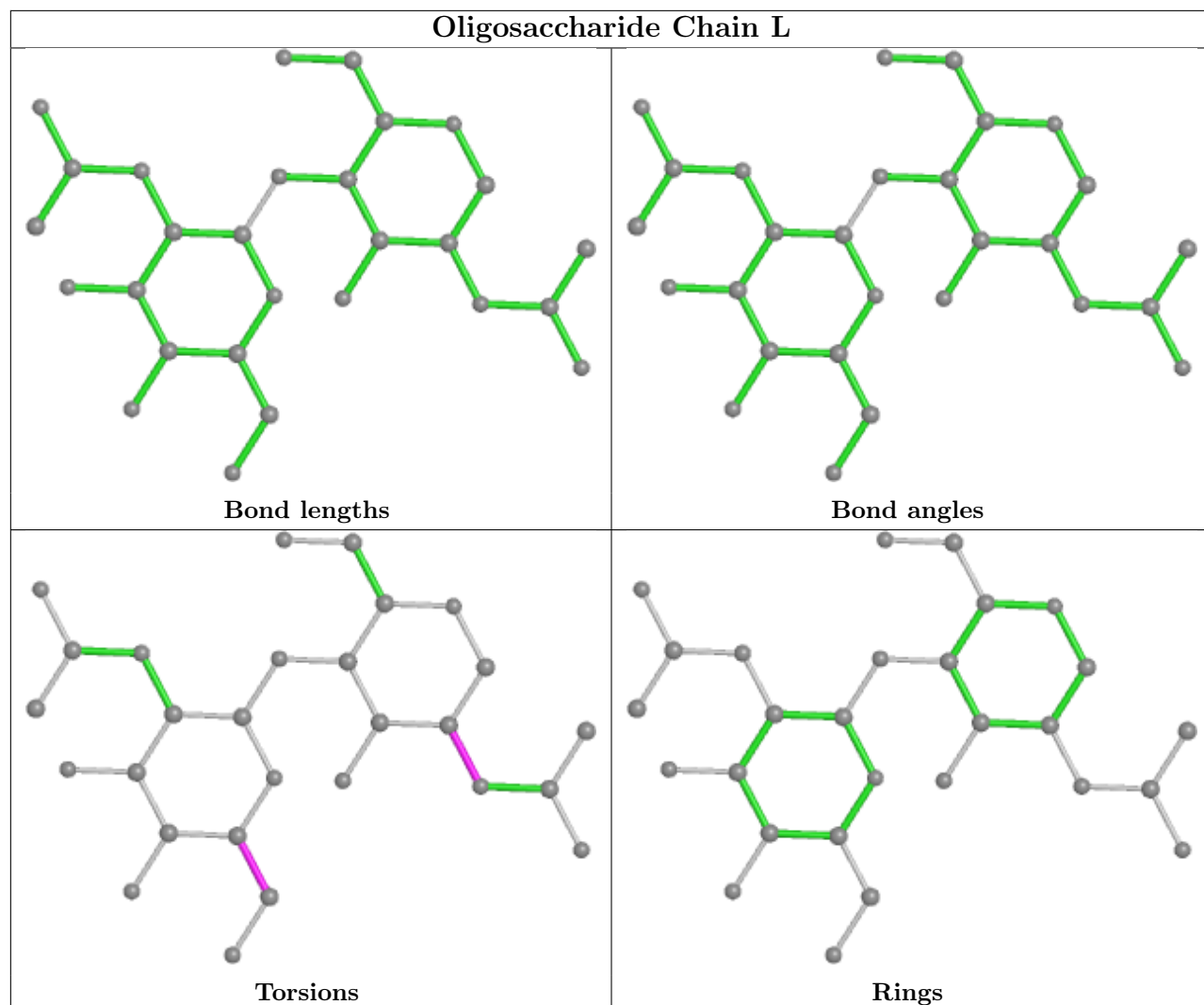


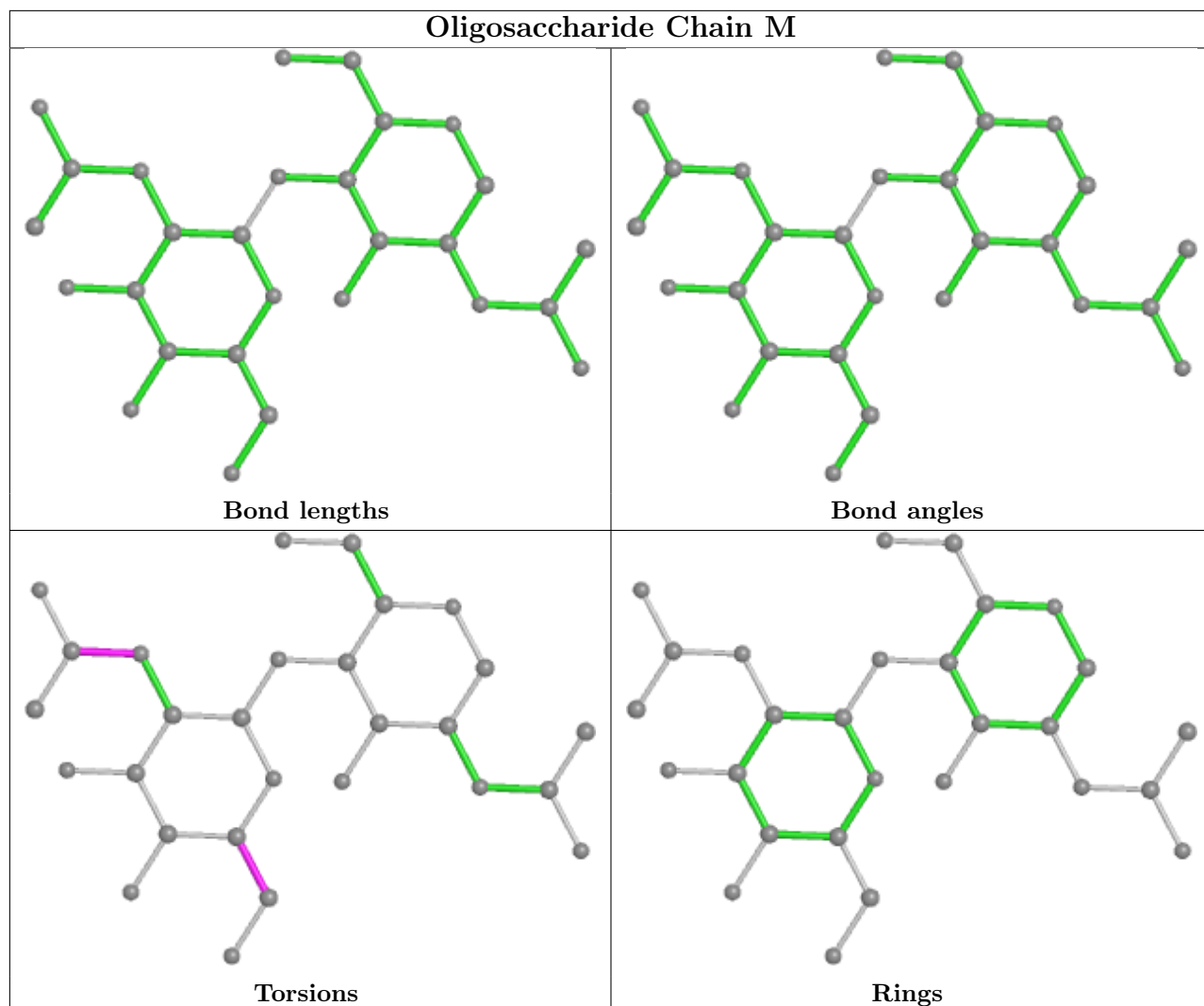




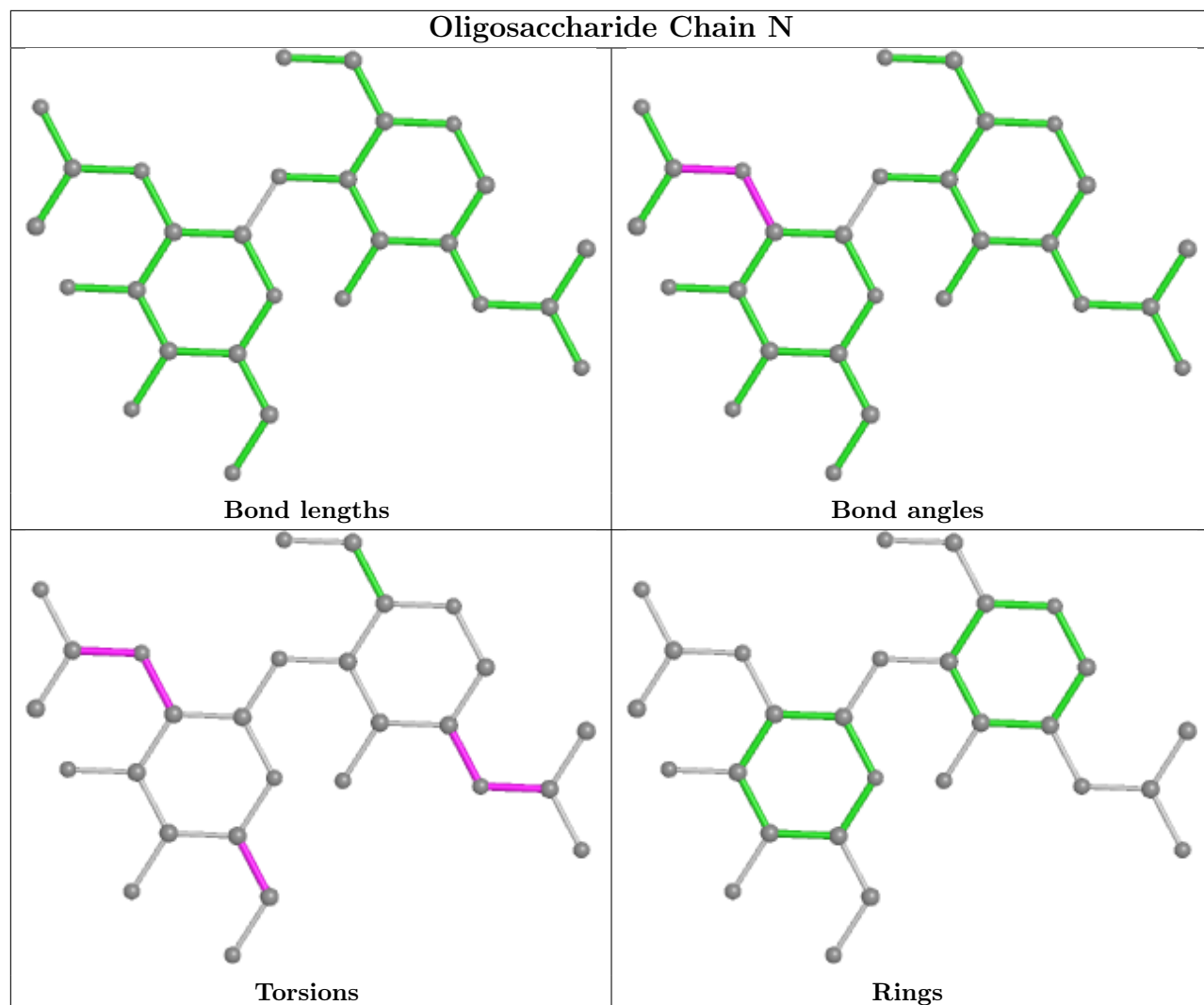


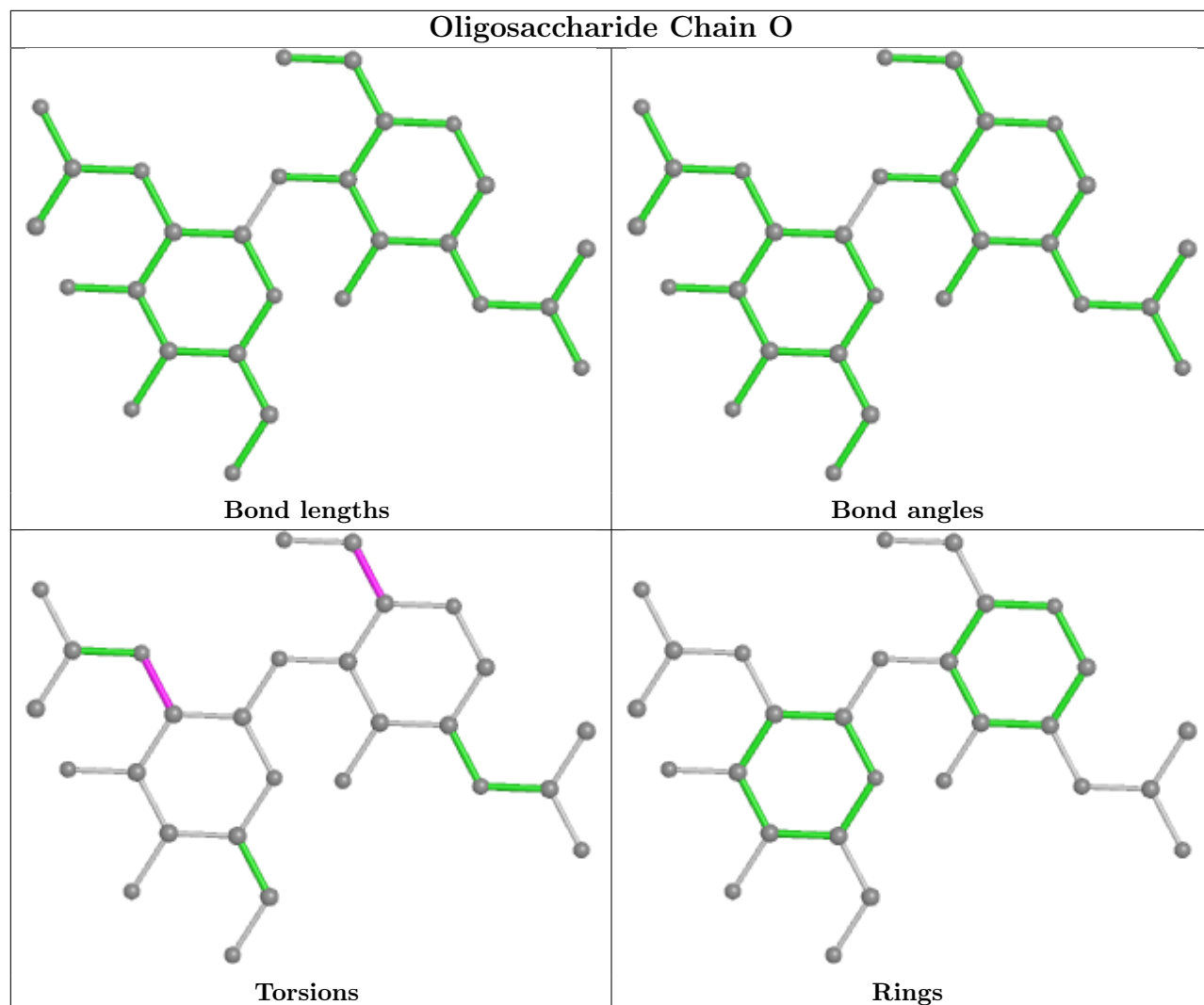


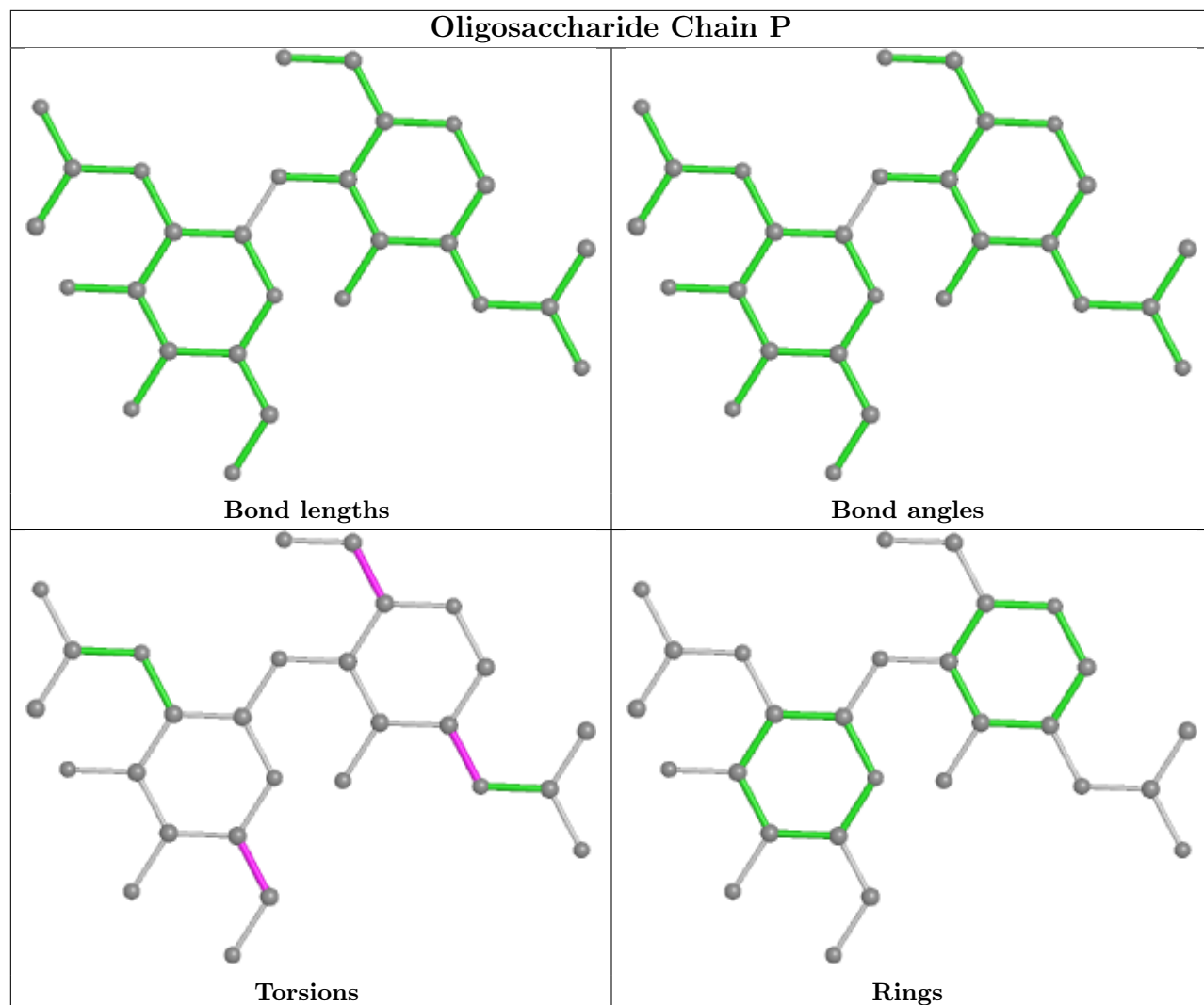


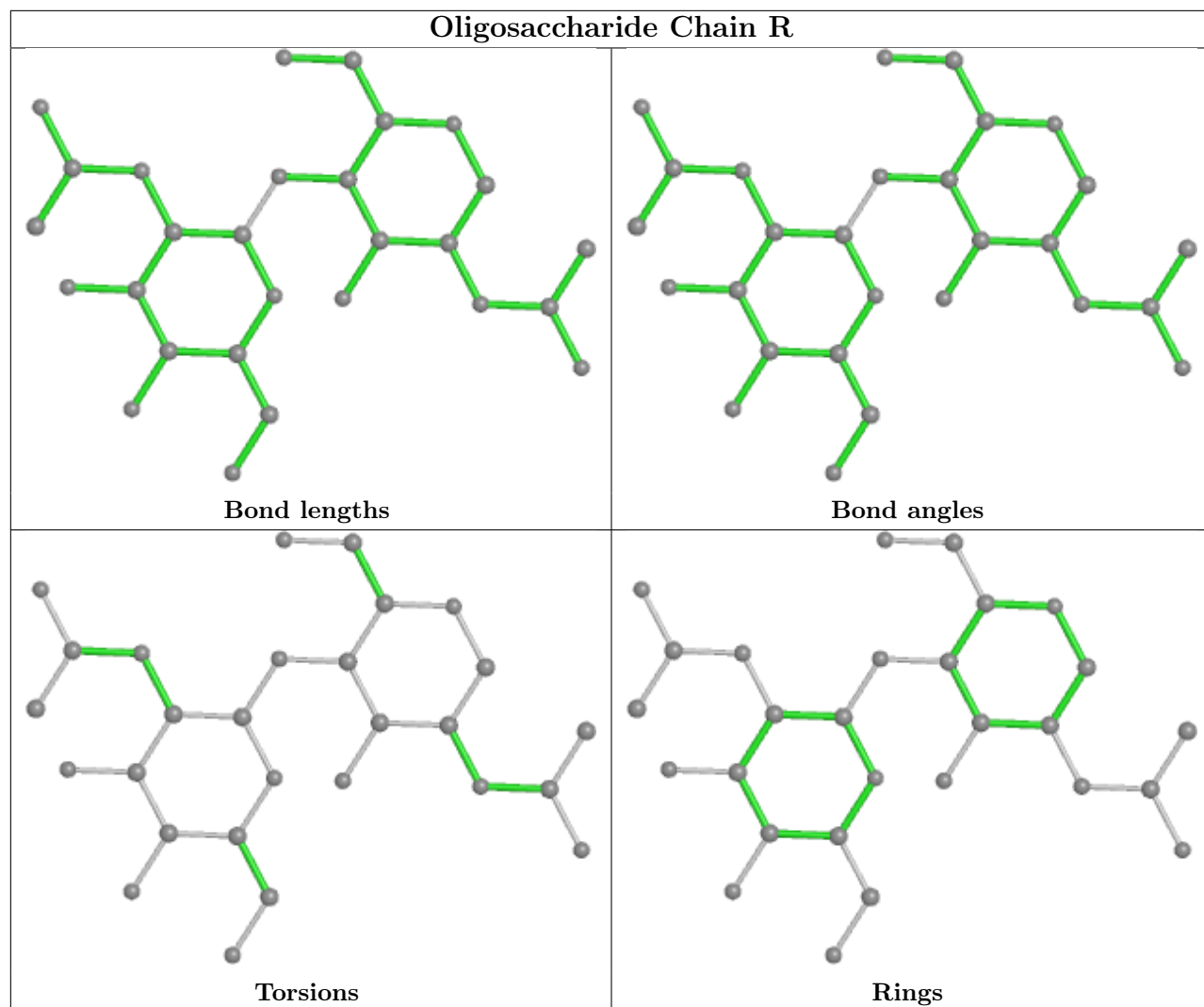


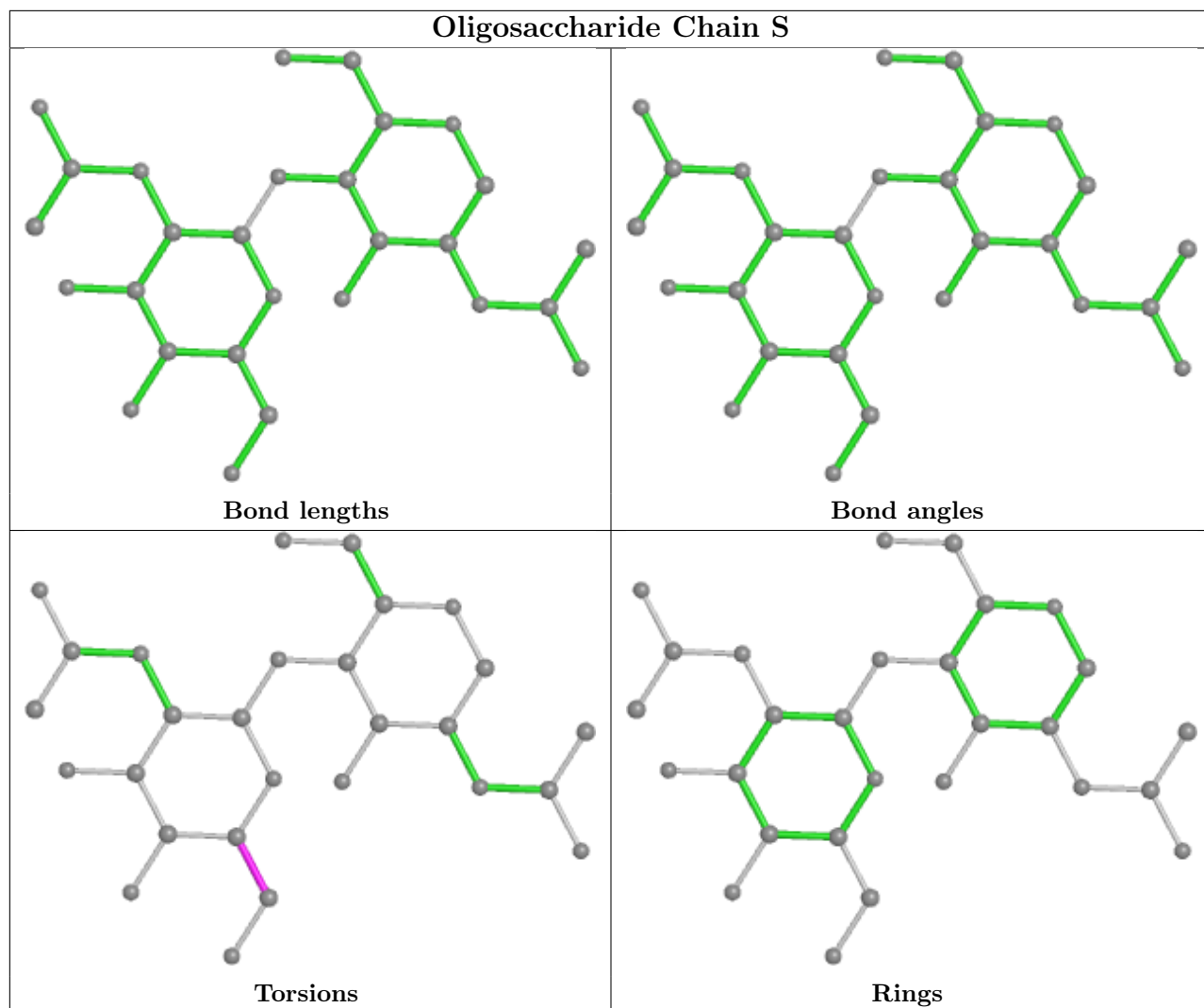


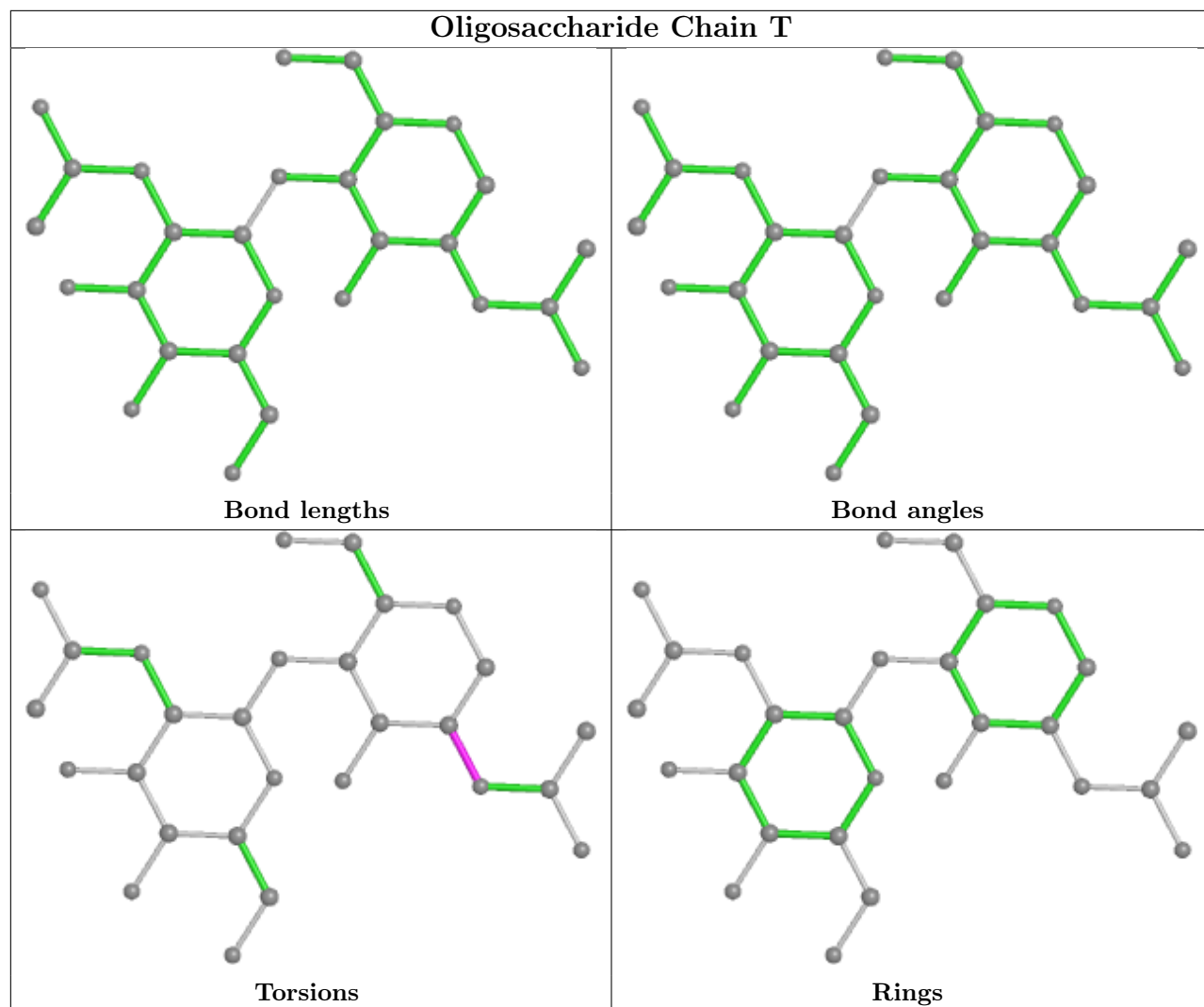


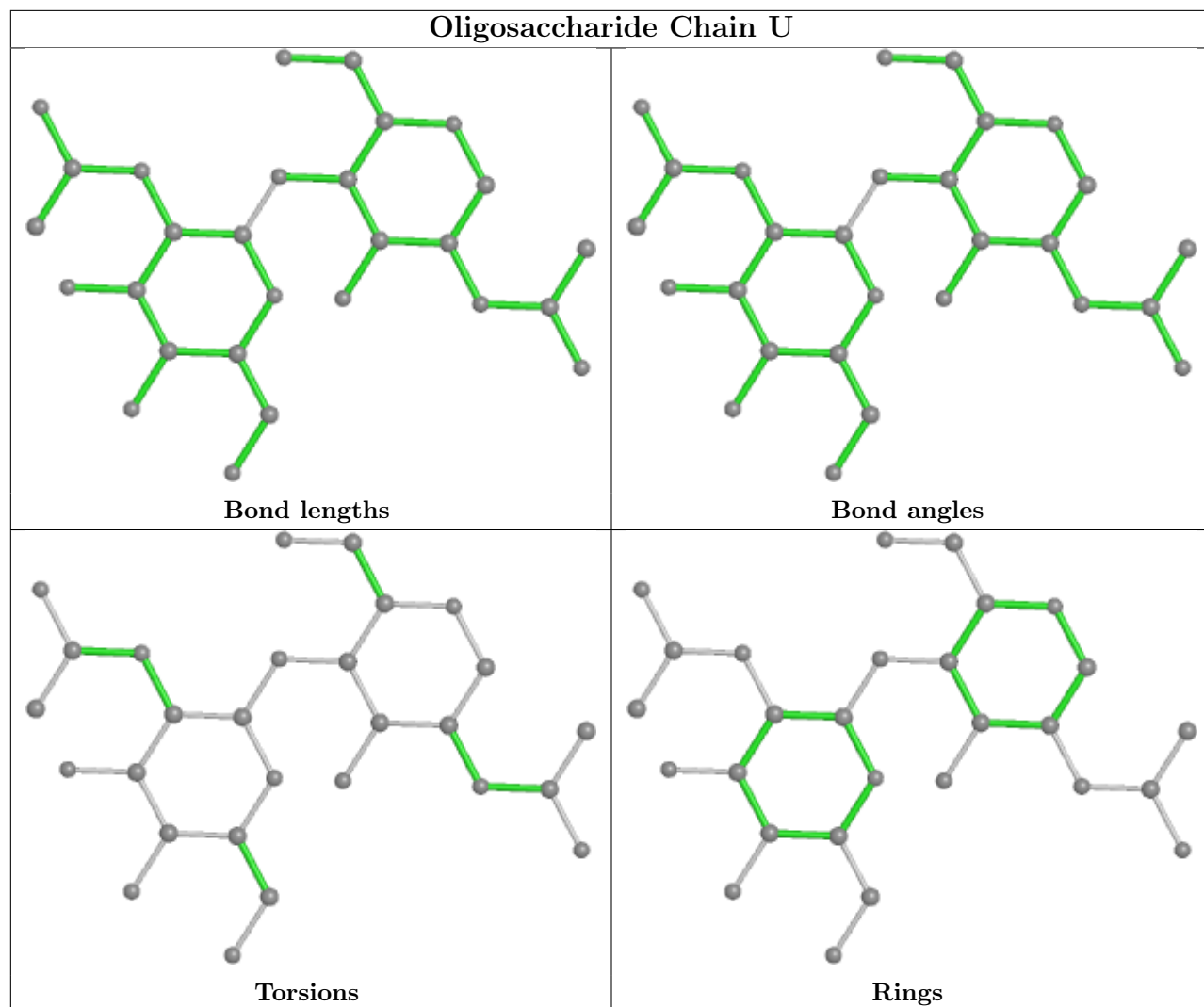


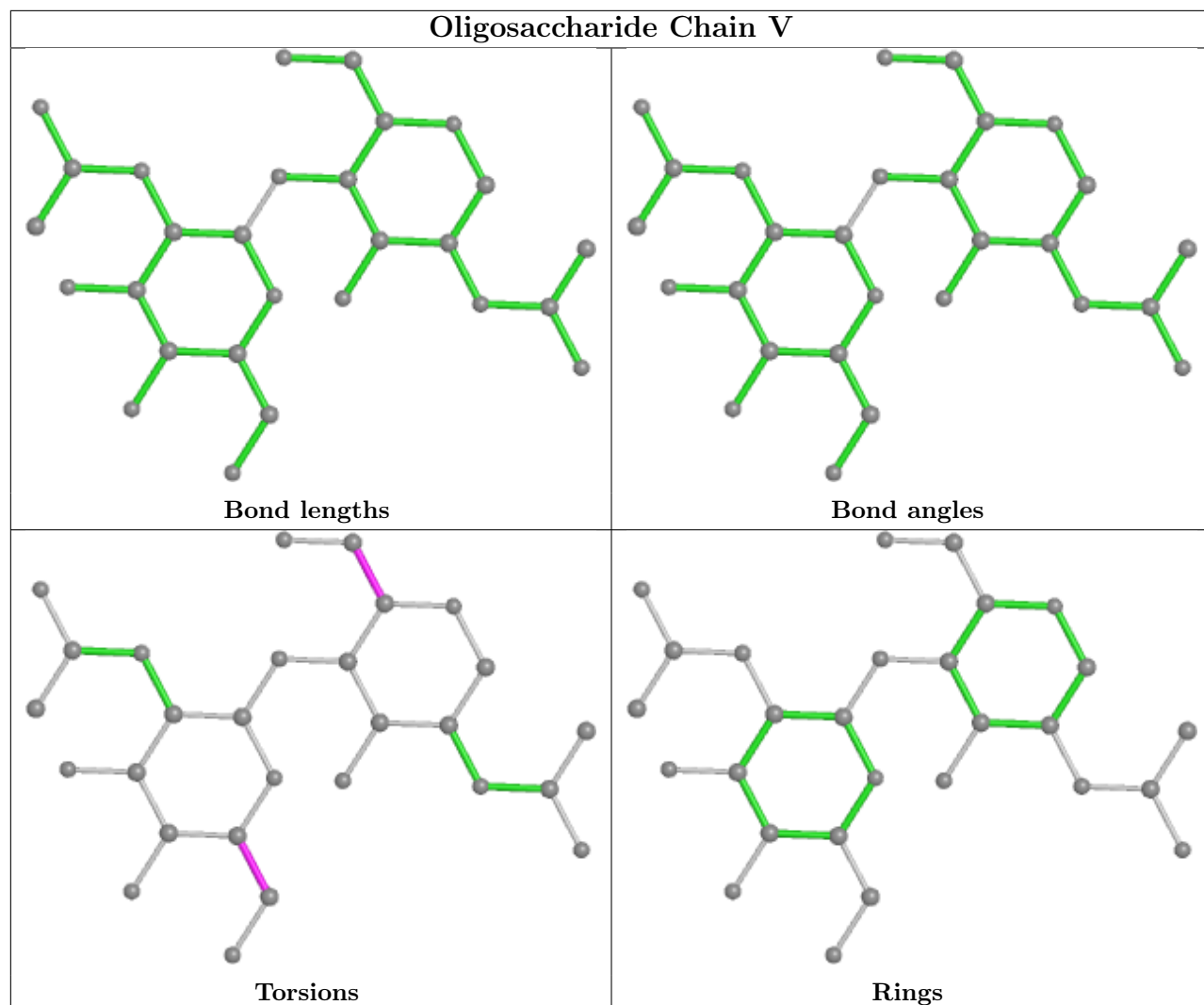




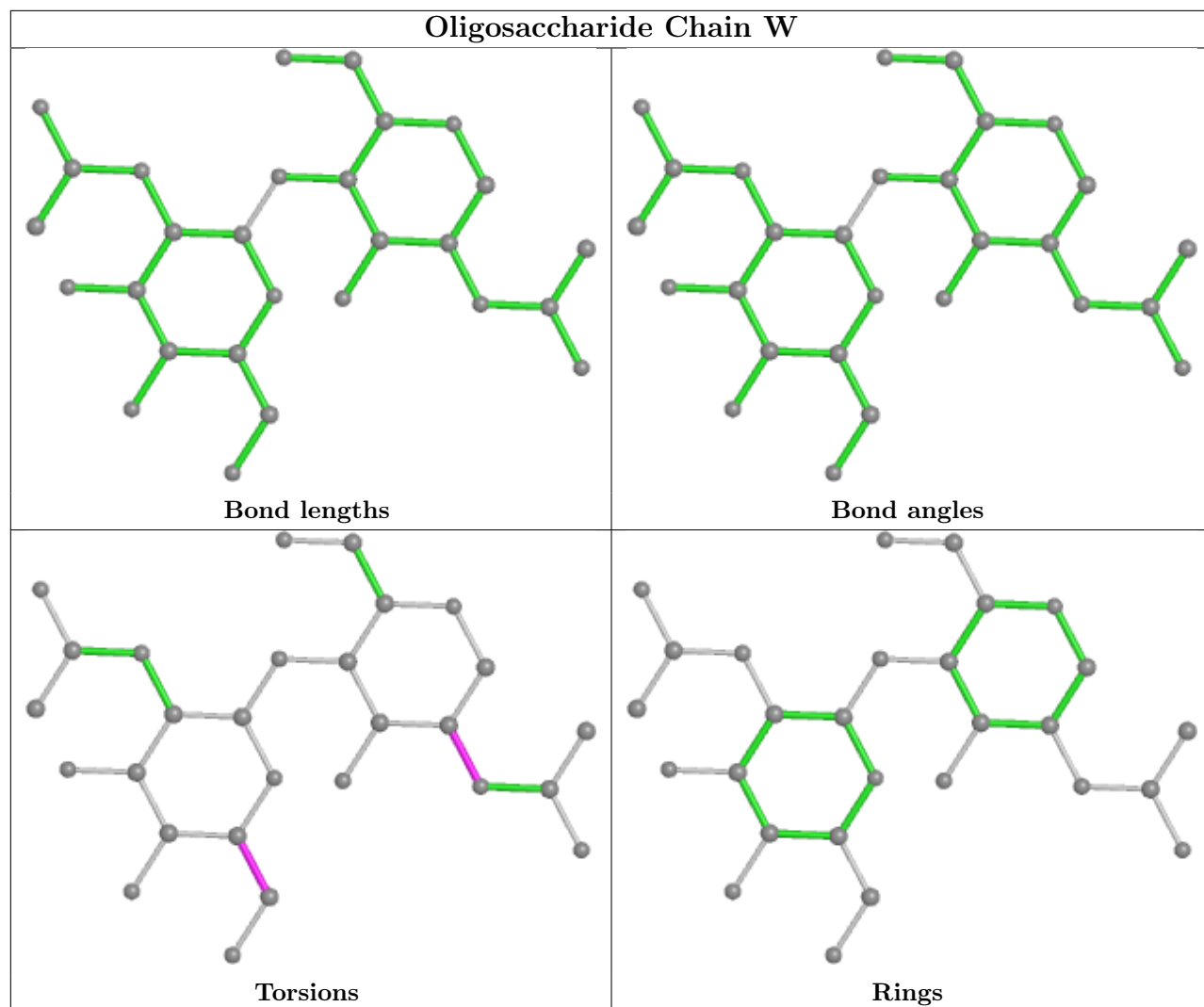


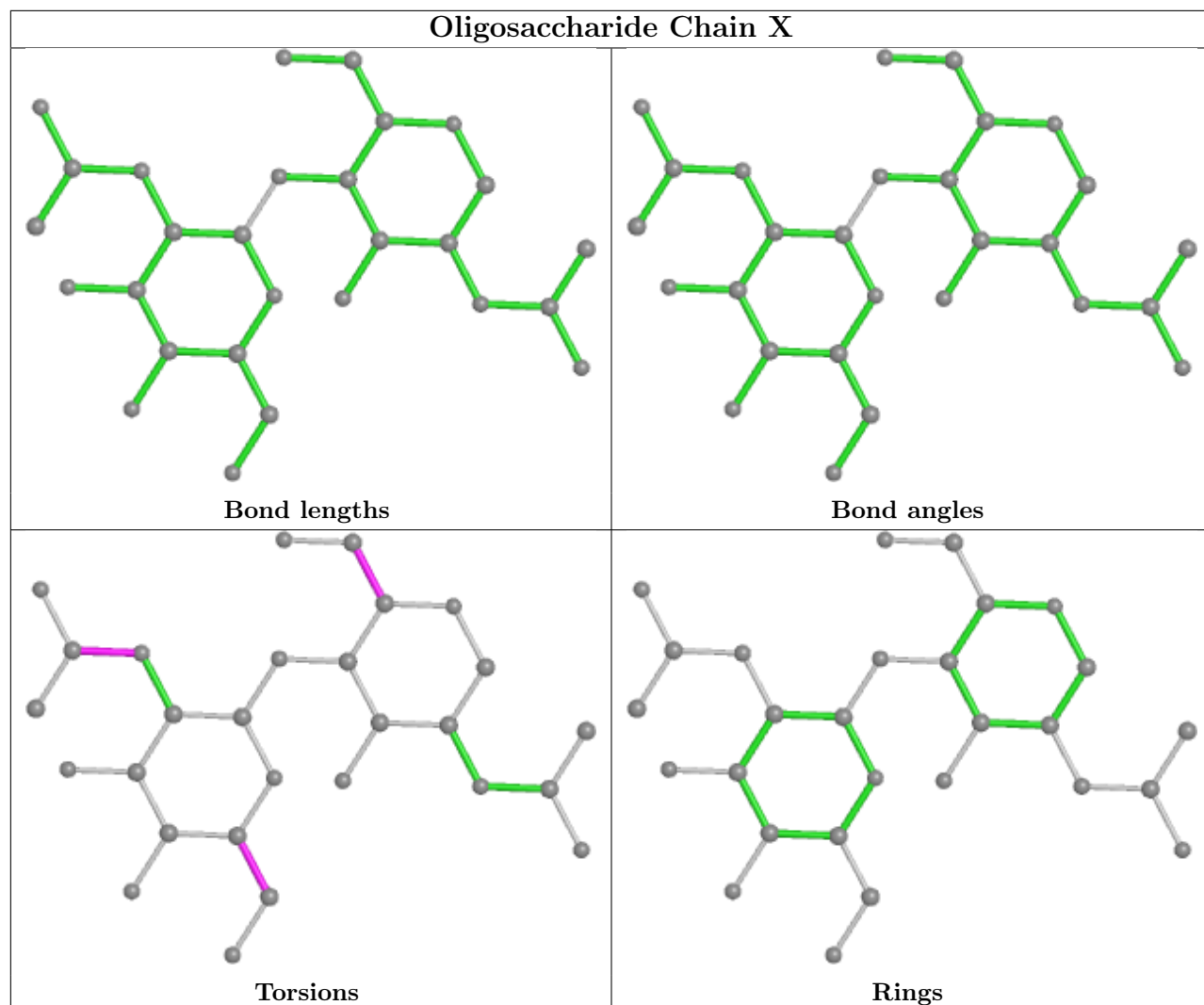


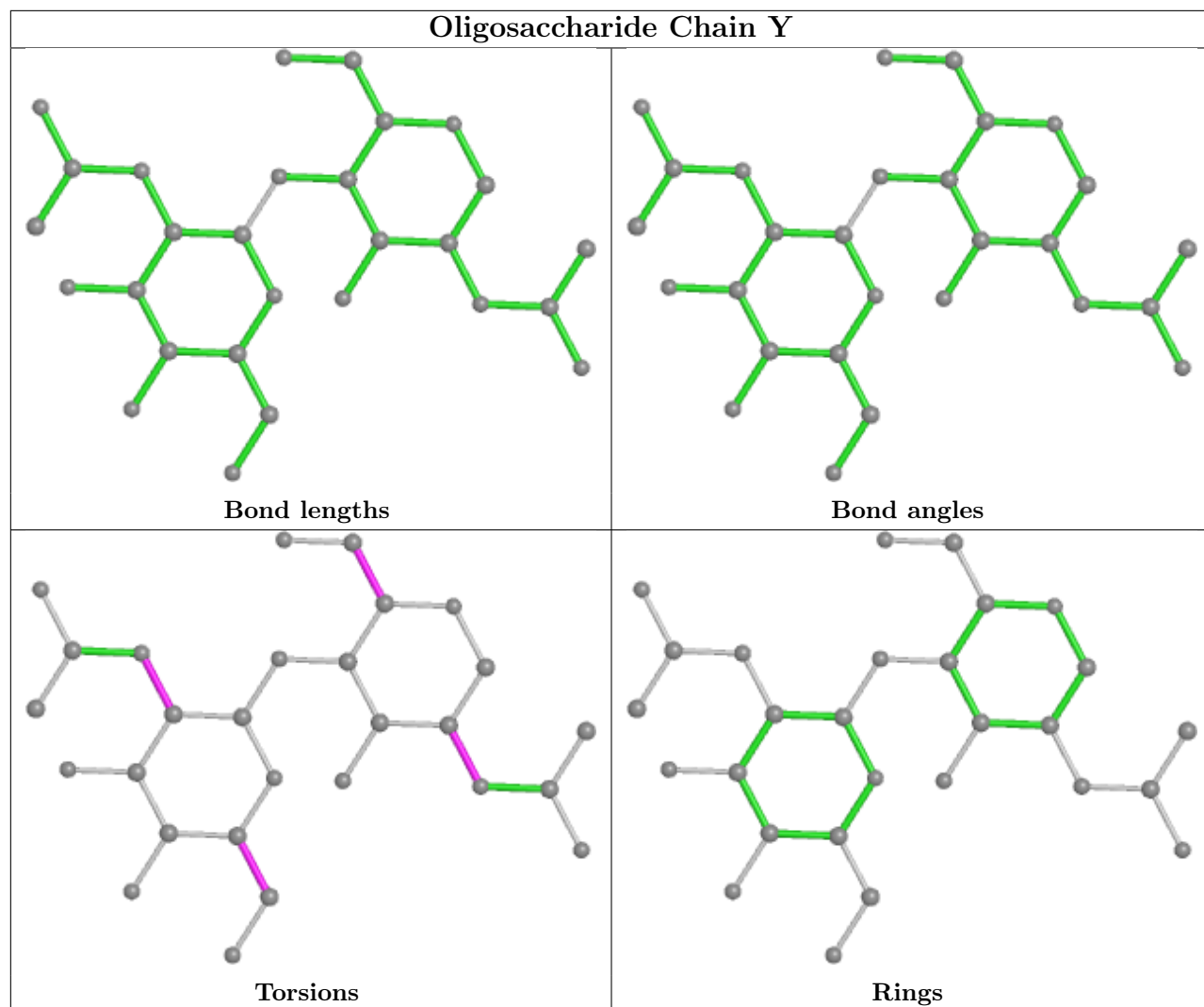


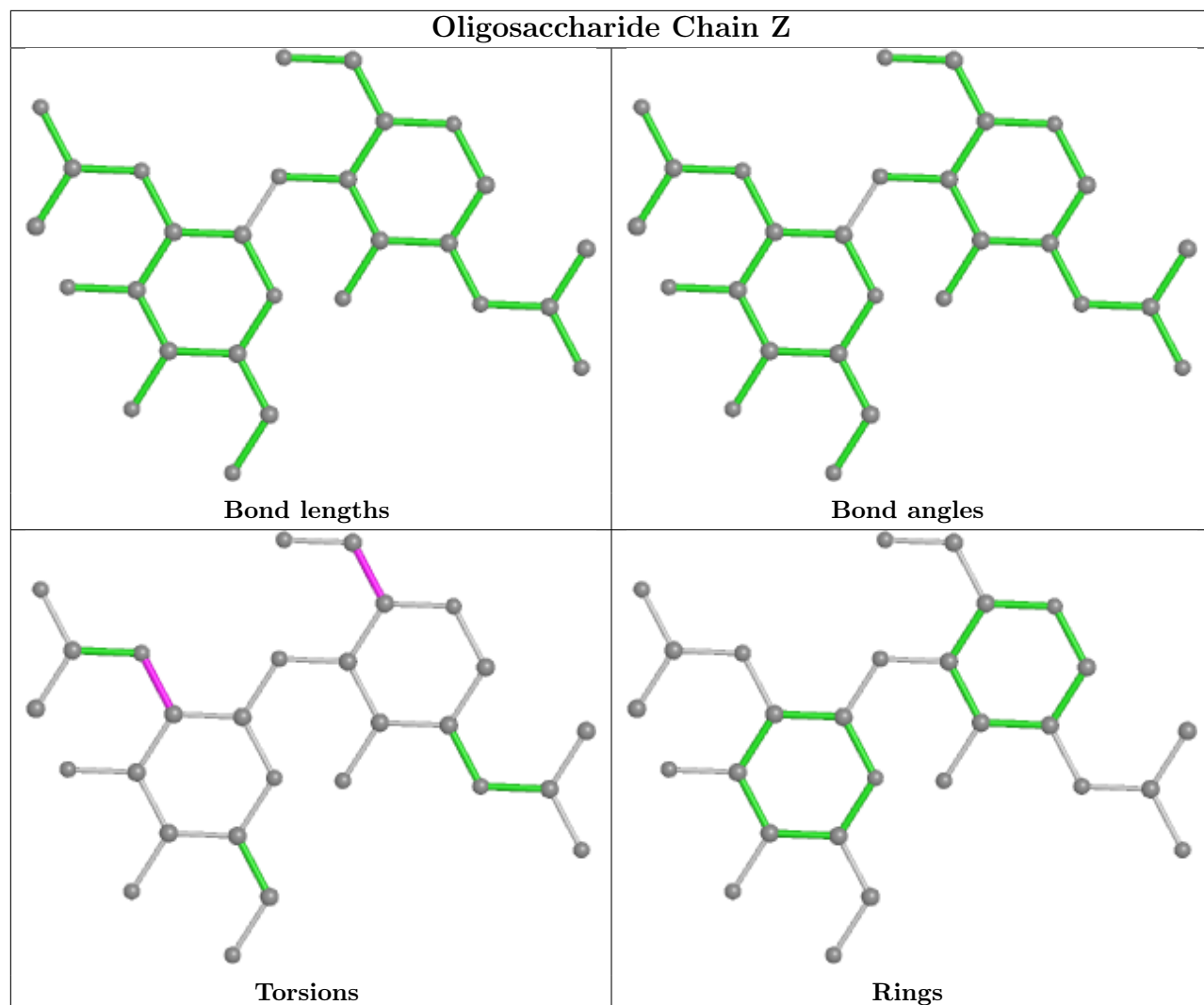


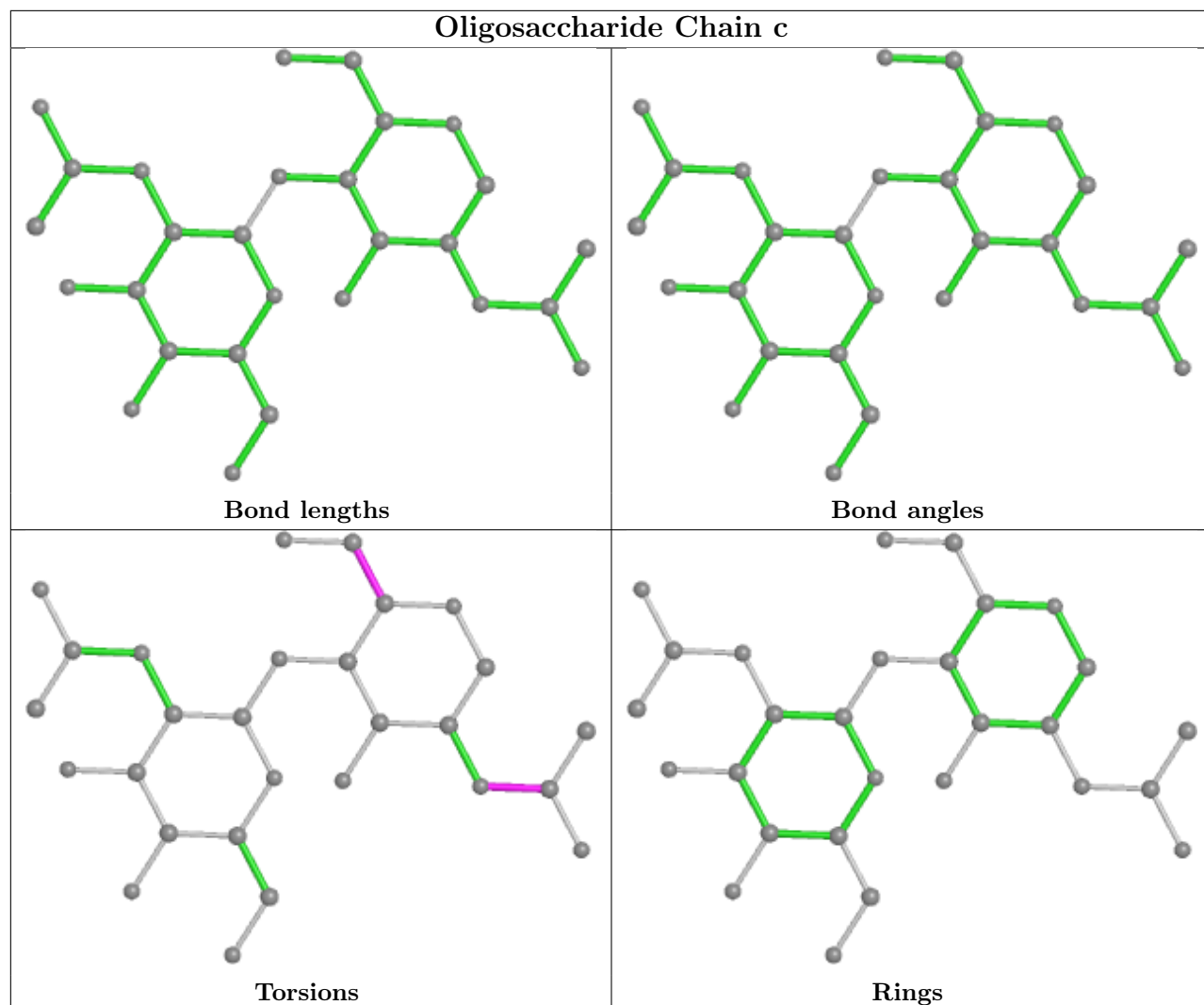


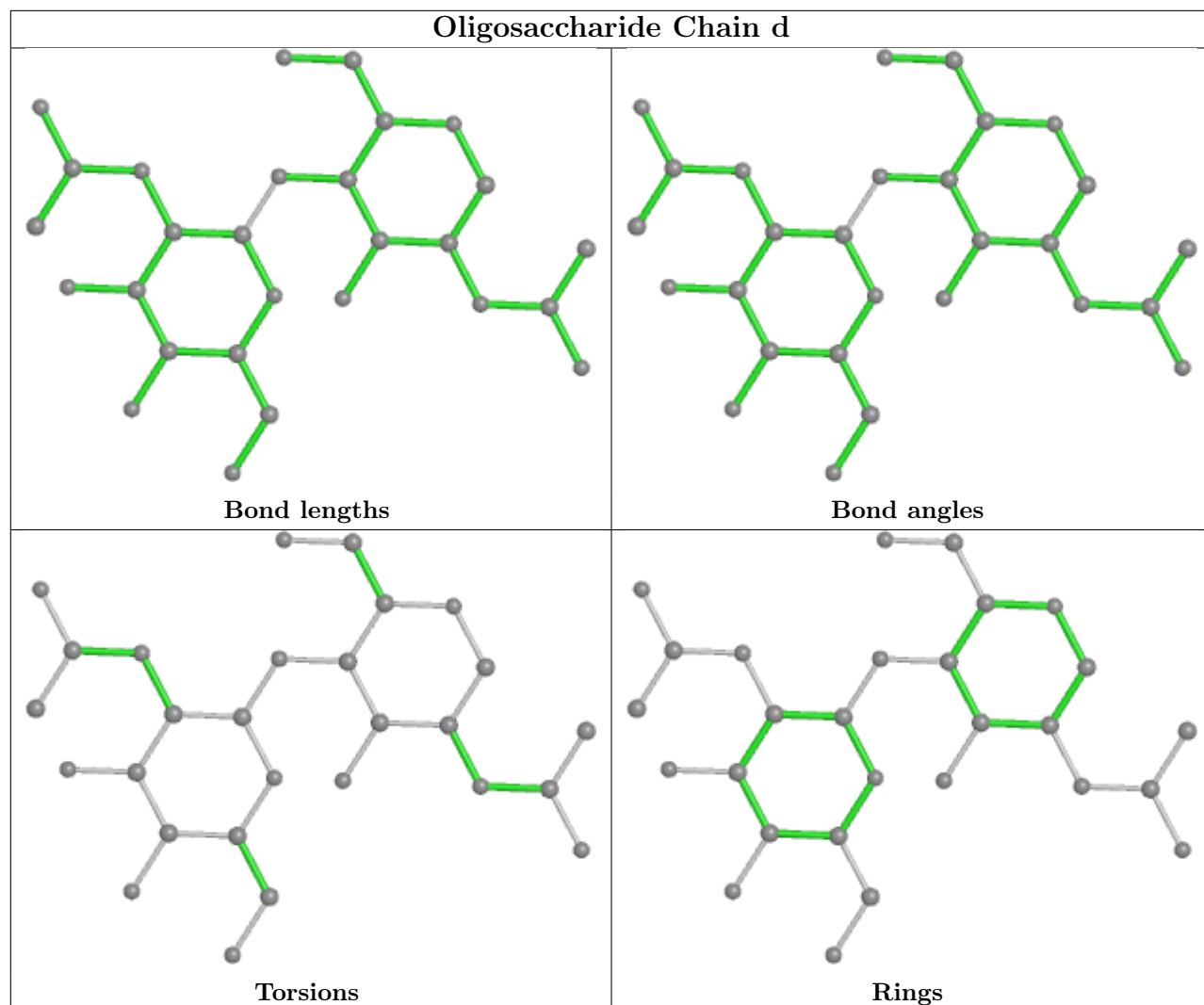


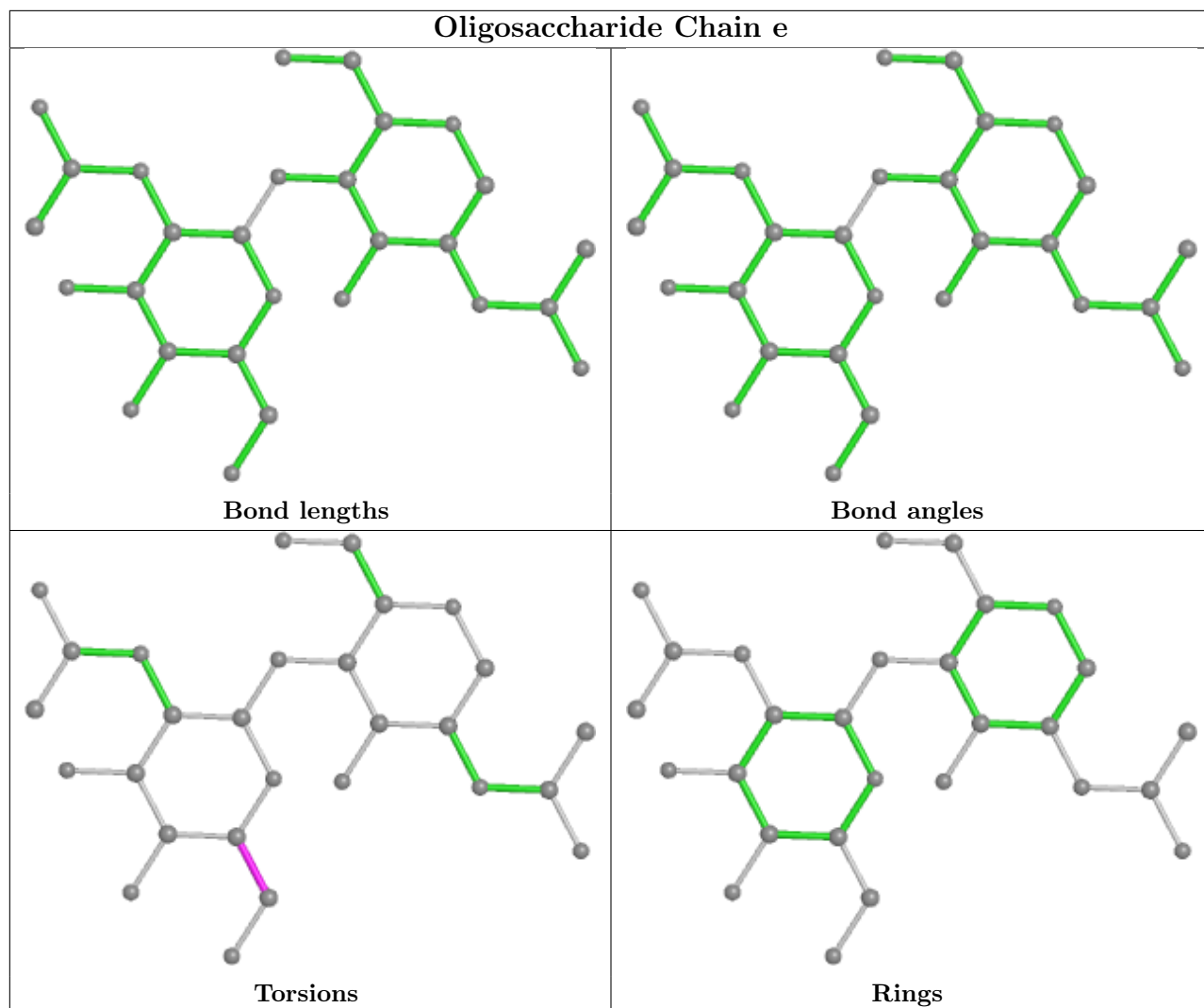


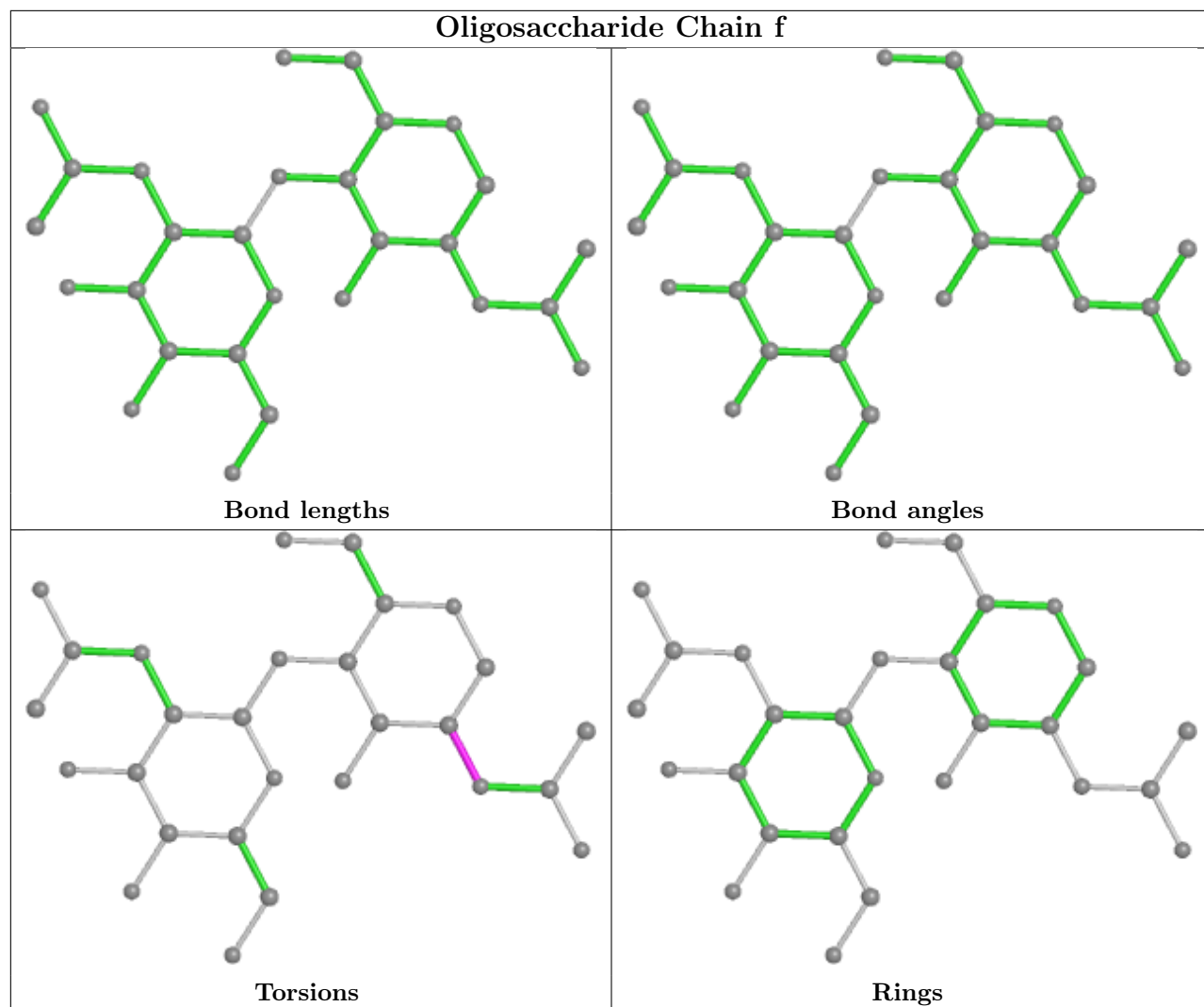




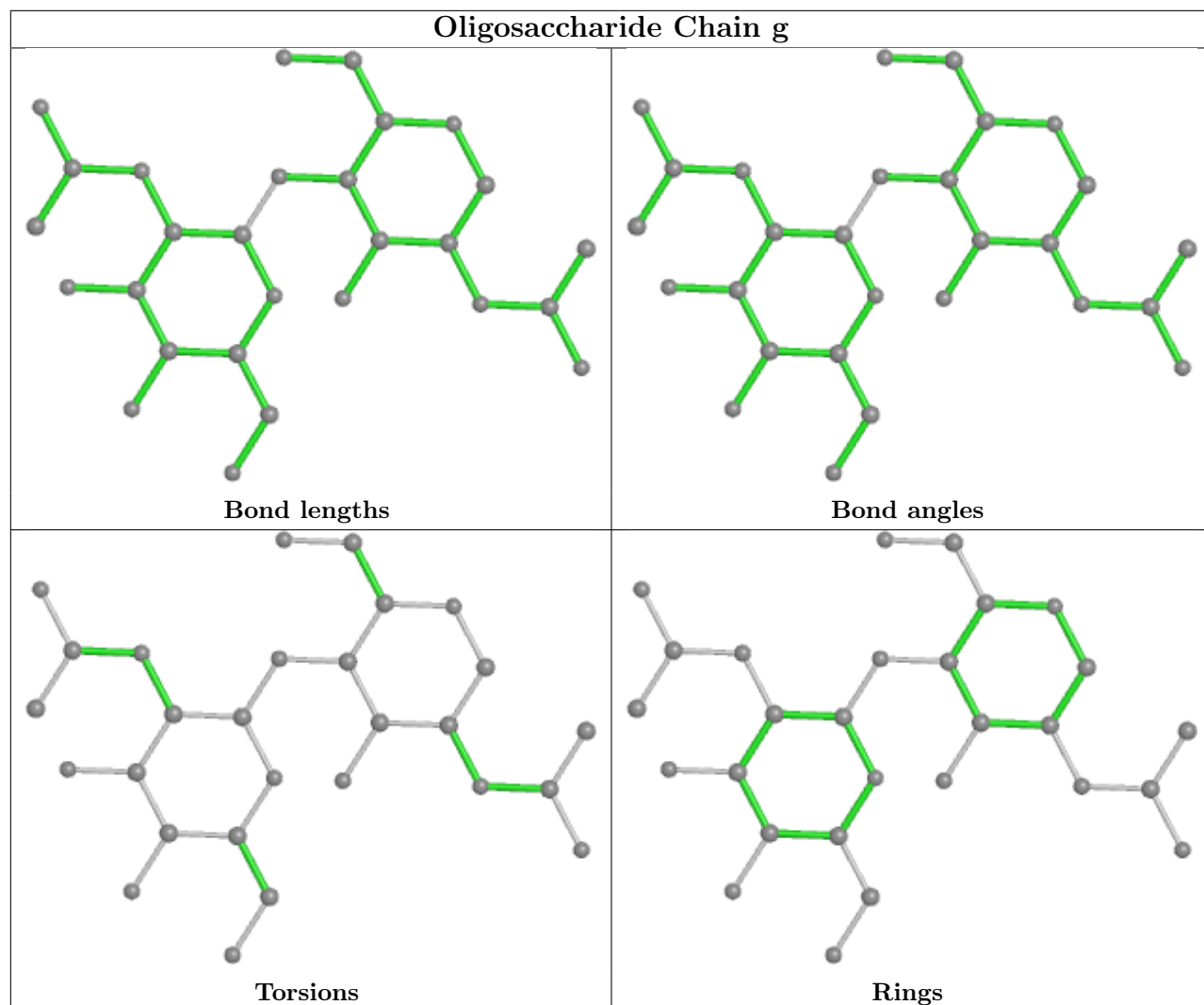


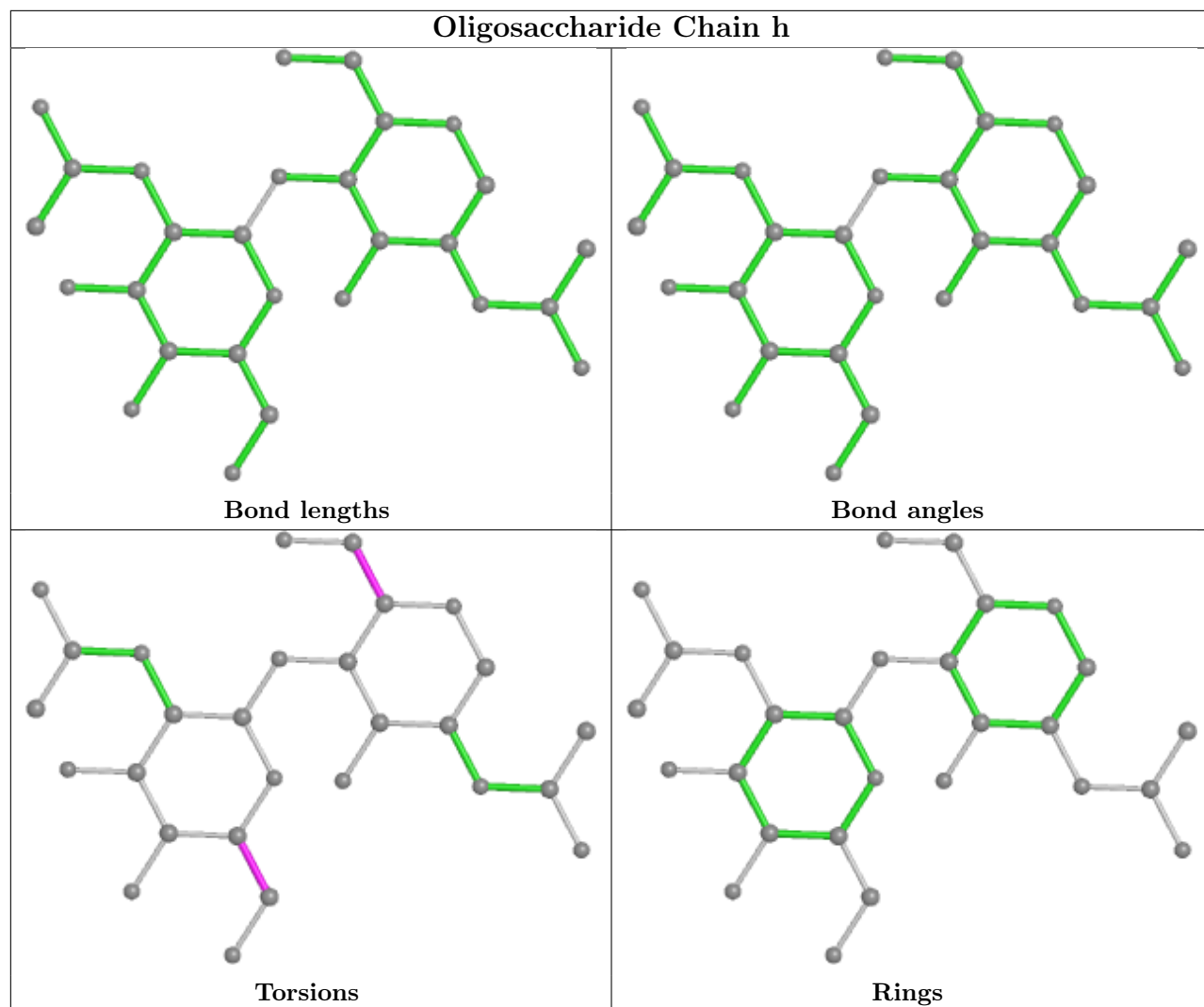


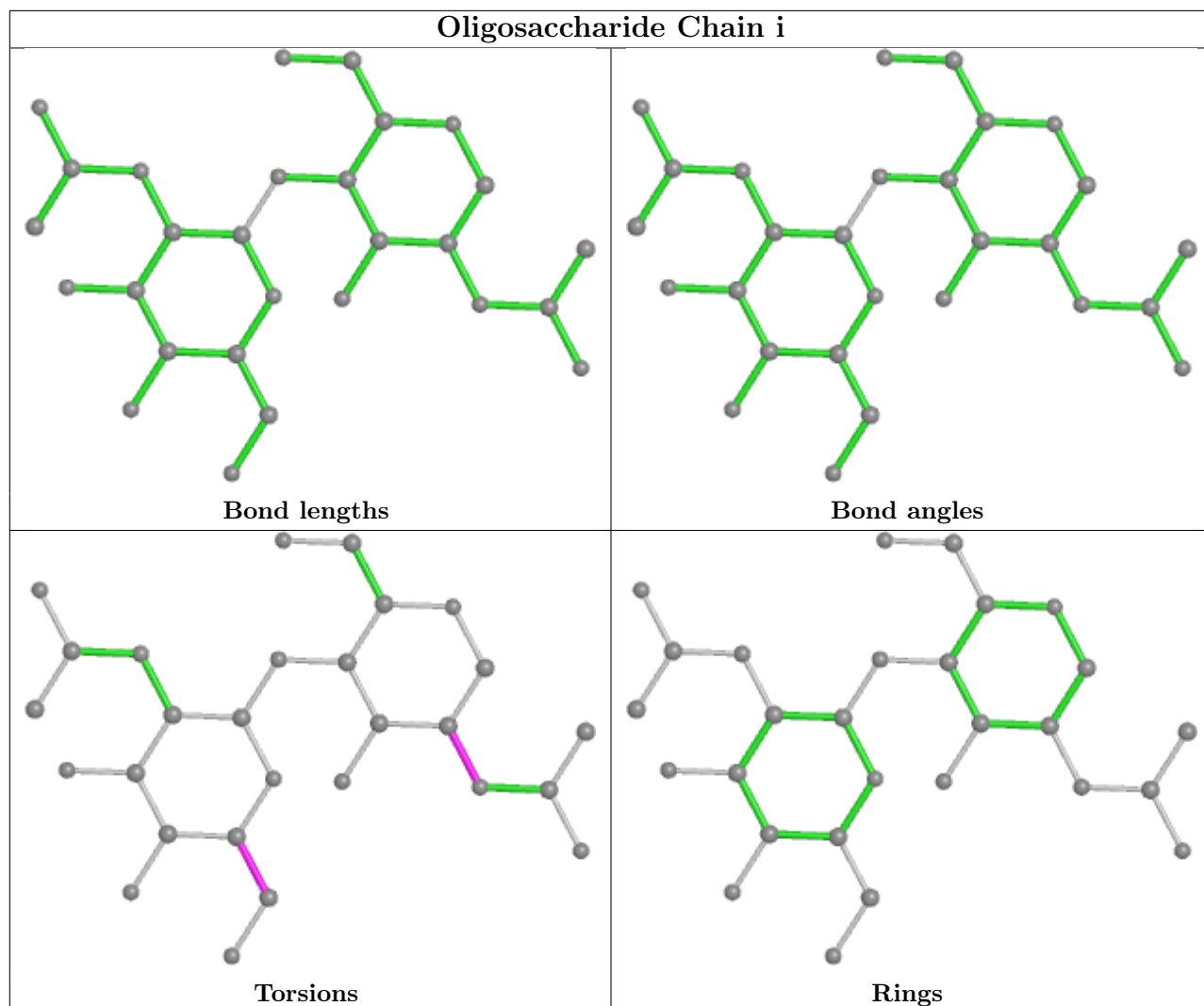


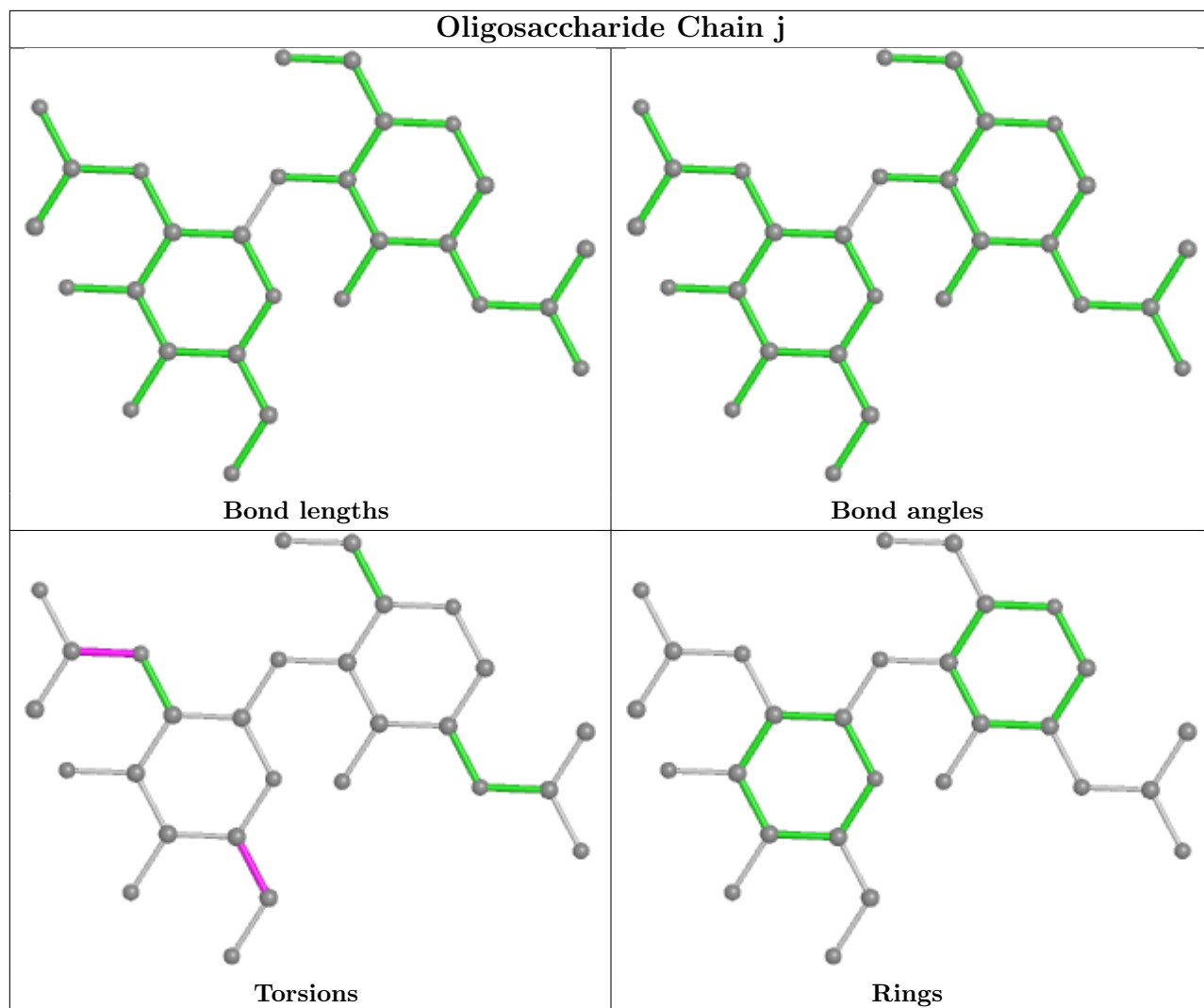


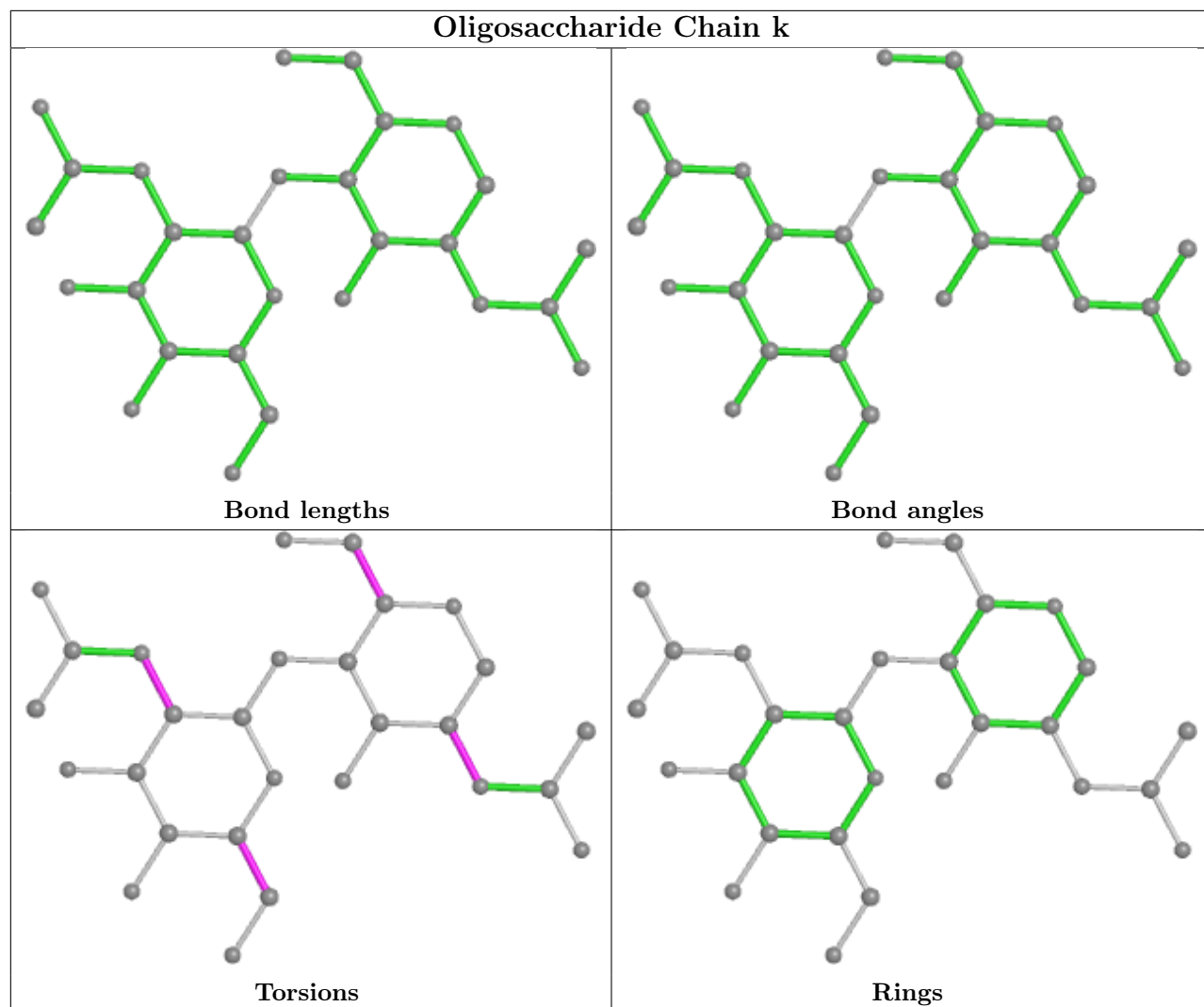


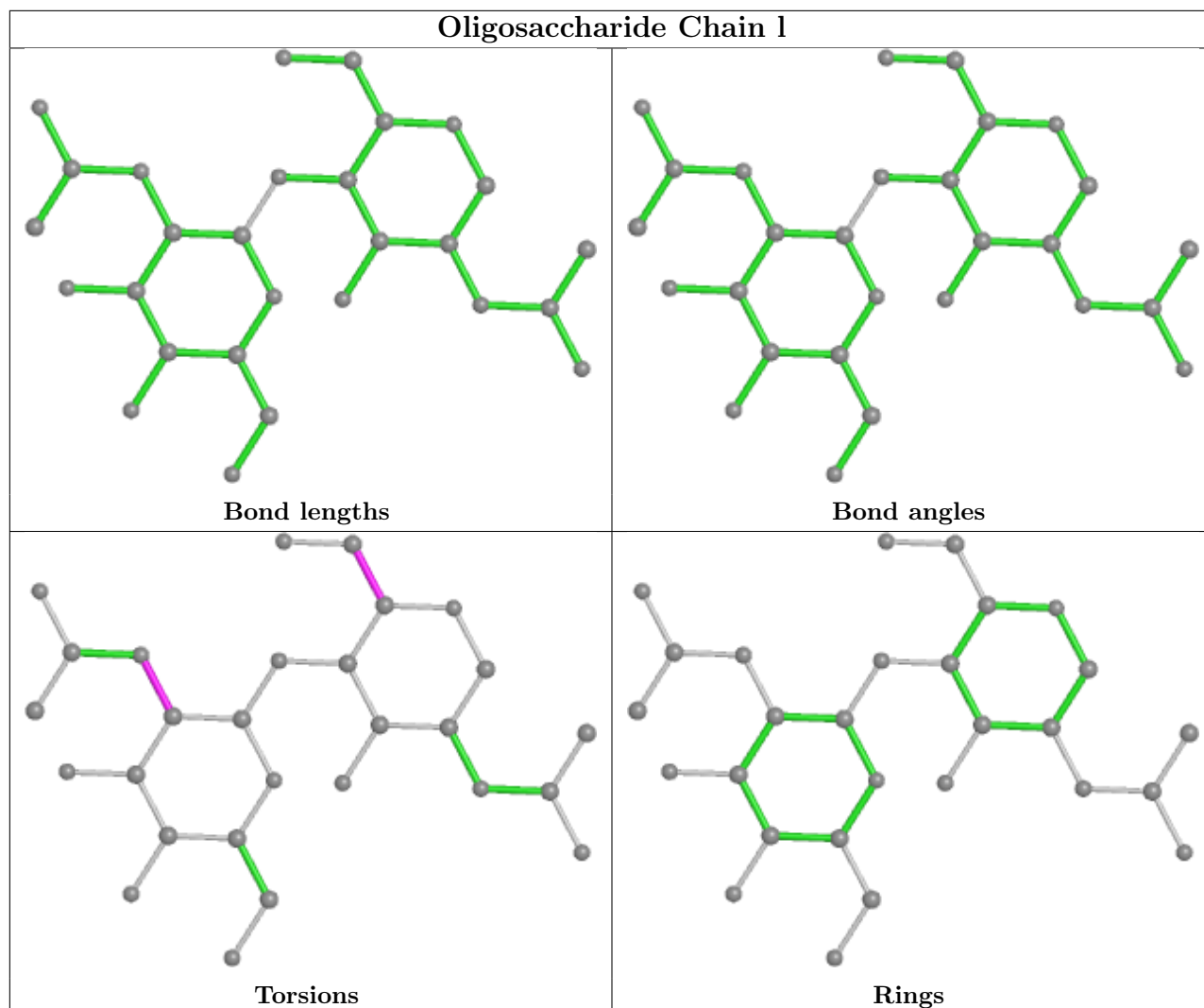












## 5.6 Ligand geometry [i](#)

22 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	$\# Z  > 2$
3	NAG	B	1603	1	14,14,15	0.32	0	17,19,21	0.51	0
3	NAG	A	1603	1	14,14,15	0.25	0	17,19,21	0.50	0
3	NAG	B	1606	1	14,14,15	0.42	0	17,19,21	1.12	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	B	1605	1	14,14,15	0.33	0	17,19,21	0.46	0
3	NAG	A	1601	1	14,14,15	0.15	0	17,19,21	0.60	0
3	NAG	C	1605	1	14,14,15	0.59	0	17,19,21	0.50	0
3	NAG	C	1607	1	14,14,15	0.27	0	17,19,21	0.70	0
3	NAG	C	1602	1	14,14,15	0.31	0	17,19,21	0.52	0
4	ELA	A	1607	-	19,19,19	0.80	1 (5%)	19,19,19	0.72	0
3	NAG	B	1604	1	14,14,15	0.24	0	17,19,21	0.49	0
3	NAG	A	1608	1	14,14,15	0.23	0	17,19,21	0.97	2 (11%)
3	NAG	C	1601	1	14,14,15	0.14	0	17,19,21	0.61	0
3	NAG	A	1604	1	14,14,15	0.33	0	17,19,21	0.47	0
3	NAG	C	1603	1	14,14,15	0.24	0	17,19,21	0.49	0
3	NAG	A	1602	1	14,14,15	0.32	0	17,19,21	0.52	0
4	ELA	B	1601	-	19,19,19	0.80	1 (5%)	19,19,19	0.74	0
3	NAG	C	1604	1	14,14,15	0.33	0	17,19,21	0.47	0
3	NAG	B	1607	1	14,14,15	0.26	0	17,19,21	0.97	1 (5%)
3	NAG	A	1605	1	14,14,15	0.58	0	17,19,21	0.50	0
3	NAG	B	1602	1	14,14,15	0.14	0	17,19,21	0.61	0
4	ELA	A	1606	-	19,19,19	0.81	1 (5%)	19,19,19	0.72	0
3	NAG	C	1606	1	14,14,15	0.25	0	17,19,21	0.94	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
3	NAG	B	1603	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1603	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1606	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1605	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1601	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1605	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1607	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1602	1	-	2/6/23/26	0/1/1/1
4	ELA	A	1607	-	-	8/17/17/17	-
3	NAG	B	1604	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1608	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1601	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1604	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1603	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1602	1	-	2/6/23/26	0/1/1/1
4	ELA	B	1601	-	-	6/17/17/17	-
3	NAG	C	1604	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1607	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1605	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1602	1	-	0/6/23/26	0/1/1/1
4	ELA	A	1606	-	-	8/17/17/17	-
3	NAG	C	1606	1	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1606	ELA	OXT-C	3.00	1.40	1.30
4	A	1607	ELA	OXT-C	2.97	1.40	1.30
4	B	1601	ELA	OXT-C	2.97	1.40	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1606	NAG	C1-O5-C5	3.50	116.94	112.19
3	C	1606	NAG	C2-N2-C7	2.73	126.79	122.90
3	B	1607	NAG	C2-N2-C7	2.44	126.37	122.90
3	A	1608	NAG	C1-O5-C5	2.31	115.33	112.19
3	A	1608	NAG	C2-N2-C7	2.20	126.03	122.90

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1607	NAG	C8-C7-N2-C2
3	B	1607	NAG	O7-C7-N2-C2
3	C	1606	NAG	C8-C7-N2-C2
3	C	1606	NAG	O7-C7-N2-C2
3	C	1607	NAG	C8-C7-N2-C2
3	C	1607	NAG	O7-C7-N2-C2
3	C	1607	NAG	O5-C5-C6-O6
3	A	1608	NAG	C8-C7-N2-C2
3	A	1608	NAG	O7-C7-N2-C2
3	C	1607	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	1602	NAG	C8-C7-N2-C2
3	A	1602	NAG	O7-C7-N2-C2
3	B	1603	NAG	C8-C7-N2-C2
3	B	1603	NAG	O7-C7-N2-C2
3	C	1602	NAG	C8-C7-N2-C2
3	C	1602	NAG	O7-C7-N2-C2
4	B	1601	ELA	C4-C3-CA-C
3	A	1603	NAG	O5-C5-C6-O6
3	B	1604	NAG	O5-C5-C6-O6
3	C	1603	NAG	O5-C5-C6-O6
3	A	1608	NAG	C1-C2-N2-C7
4	A	1607	ELA	C6-C7-C8-C9
4	B	1601	ELA	C12-C13-C14-C15
4	A	1607	ELA	C11-C12-C13-C14
4	B	1601	ELA	C11-C12-C13-C14
4	A	1606	ELA	C14-C15-C16-C17
4	B	1601	ELA	C5-C6-C7-C8
4	B	1601	ELA	C6-C7-C8-C9
4	A	1606	ELA	CA-C3-C4-C5
4	A	1607	ELA	CA-C3-C4-C5
4	A	1606	ELA	C13-C14-C15-C16
4	A	1607	ELA	C5-C6-C7-C8
4	A	1606	ELA	C6-C7-C8-C9
4	A	1606	ELA	C11-C12-C13-C14
3	B	1607	NAG	C1-C2-N2-C7
4	A	1607	ELA	C12-C13-C14-C15
4	A	1606	ELA	C5-C6-C7-C8
4	A	1606	ELA	C4-C5-C6-C7
3	A	1605	NAG	C1-C2-N2-C7
3	C	1605	NAG	C1-C2-N2-C7
4	A	1607	ELA	C4-C5-C6-C7
3	A	1603	NAG	C4-C5-C6-O6
3	B	1604	NAG	C4-C5-C6-O6
3	C	1603	NAG	C4-C5-C6-O6
3	A	1608	NAG	O5-C5-C6-O6
3	C	1605	NAG	C4-C5-C6-O6
3	A	1605	NAG	C4-C5-C6-O6
4	B	1601	ELA	C3-C4-C5-C6
4	A	1607	ELA	C4-C3-CA-C
3	C	1606	NAG	C3-C2-N2-C7
3	C	1606	NAG	C1-C2-N2-C7
3	B	1606	NAG	C8-C7-N2-C2

*Continued on next page...*

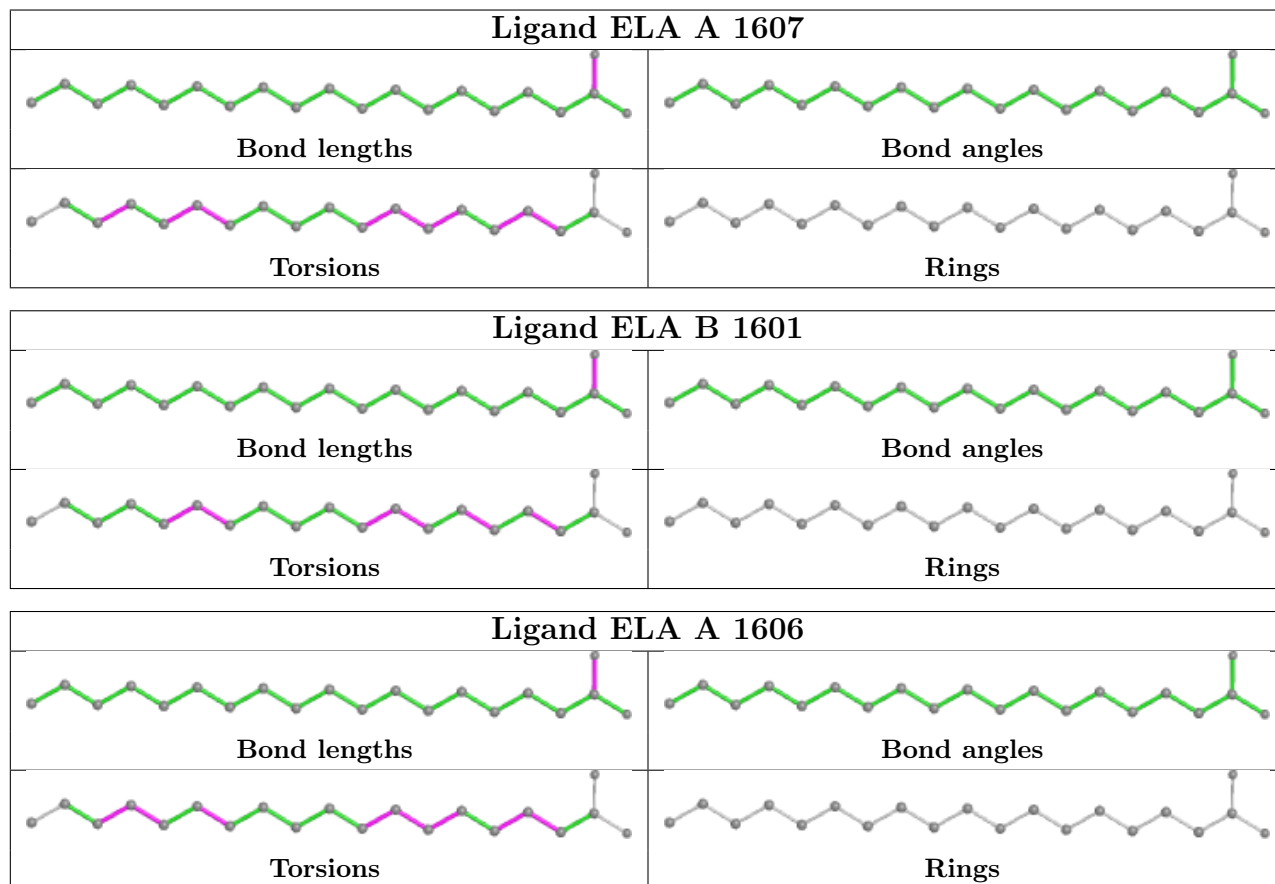
Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1607	ELA	C14-C15-C16-C17
4	A	1606	ELA	C4-C3-CA-C
3	B	1606	NAG	O7-C7-N2-C2
3	A	1605	NAG	C3-C2-N2-C7
3	C	1605	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.

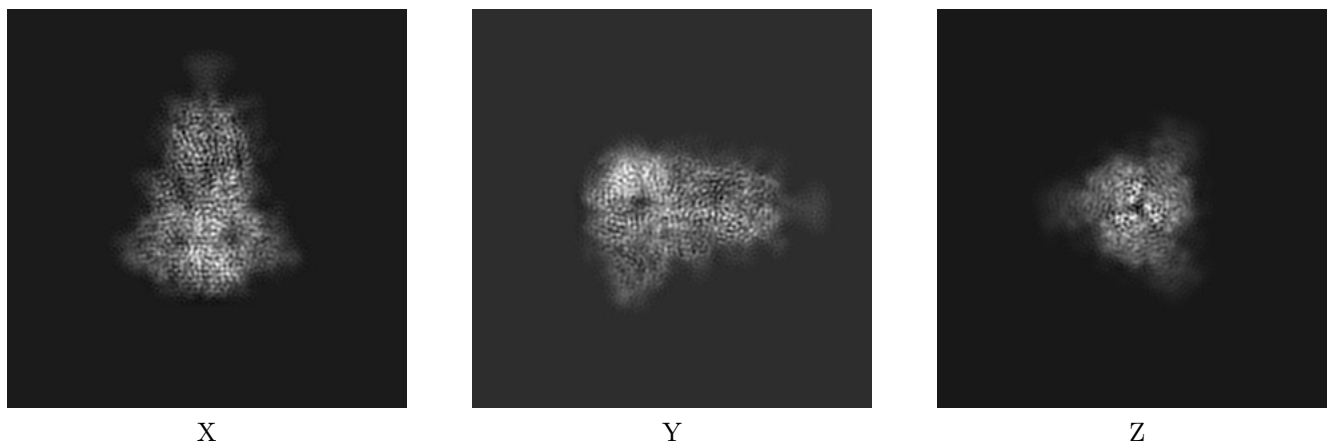
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30999. 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](#)

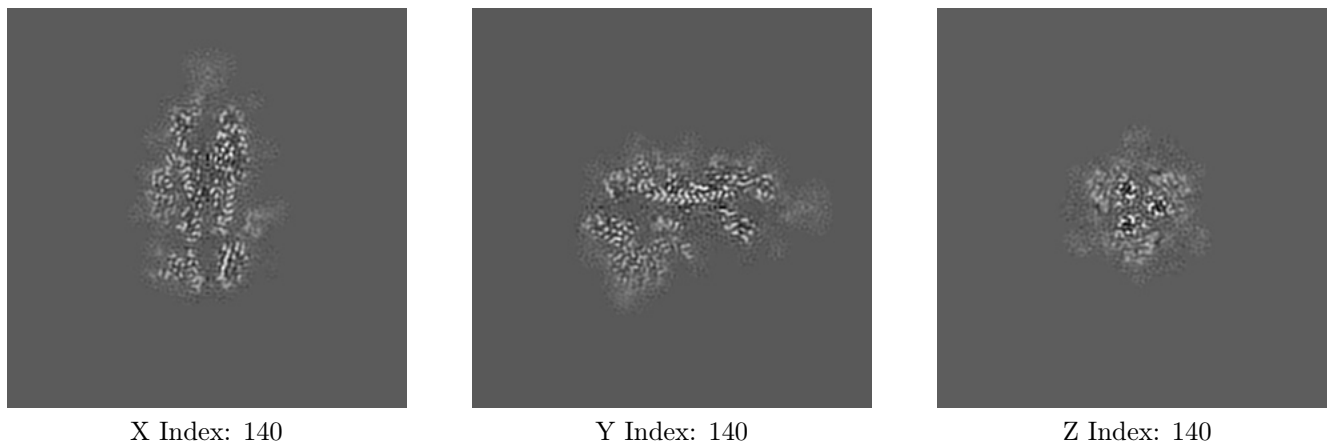
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

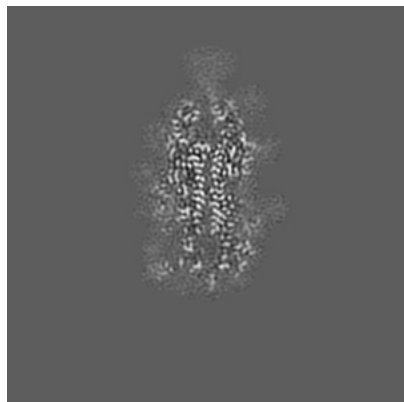
#### 6.2.1 Primary map



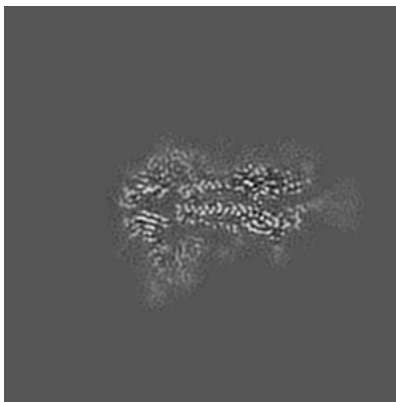
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

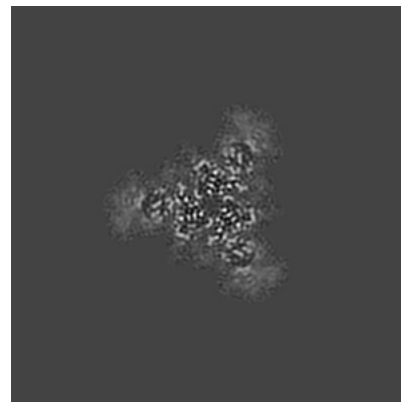
### 6.3.1 Primary map



X Index: 135



Y Index: 134

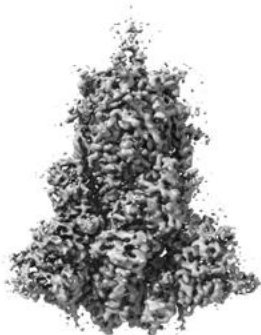


Z Index: 106

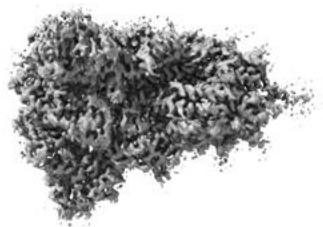
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

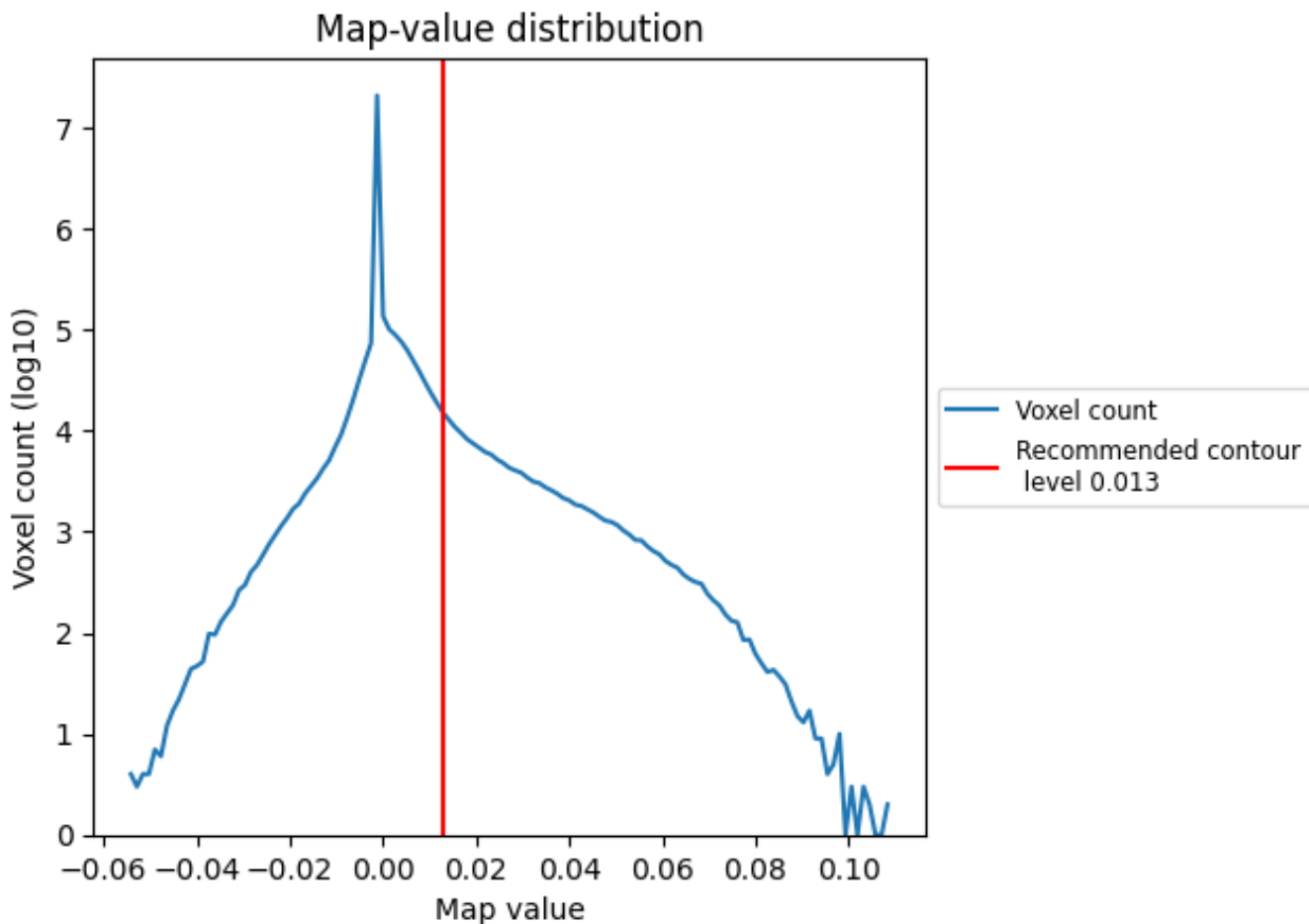
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

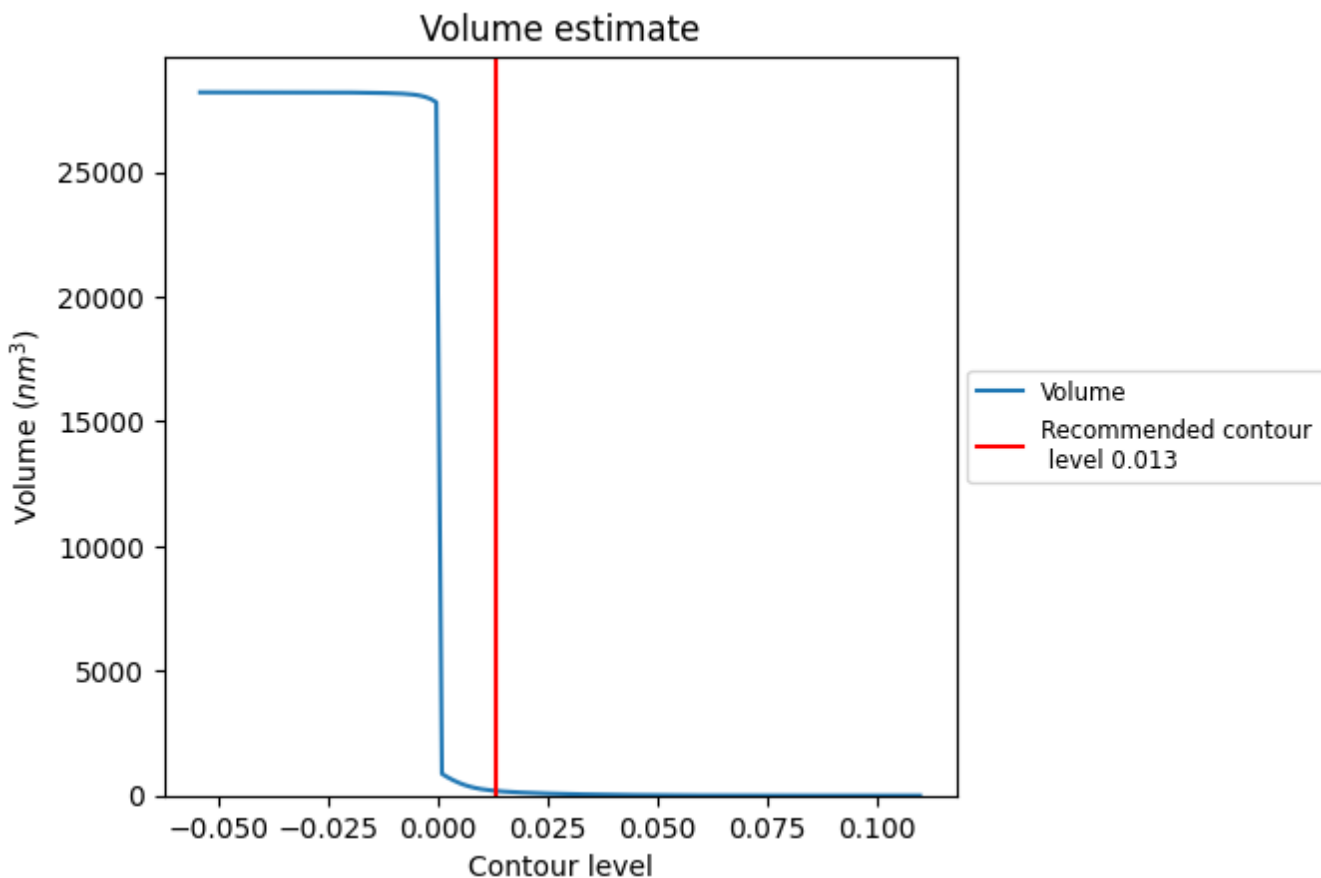
This section contains the results of statistical analysis of the map.

### 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 [\(i\)](#)

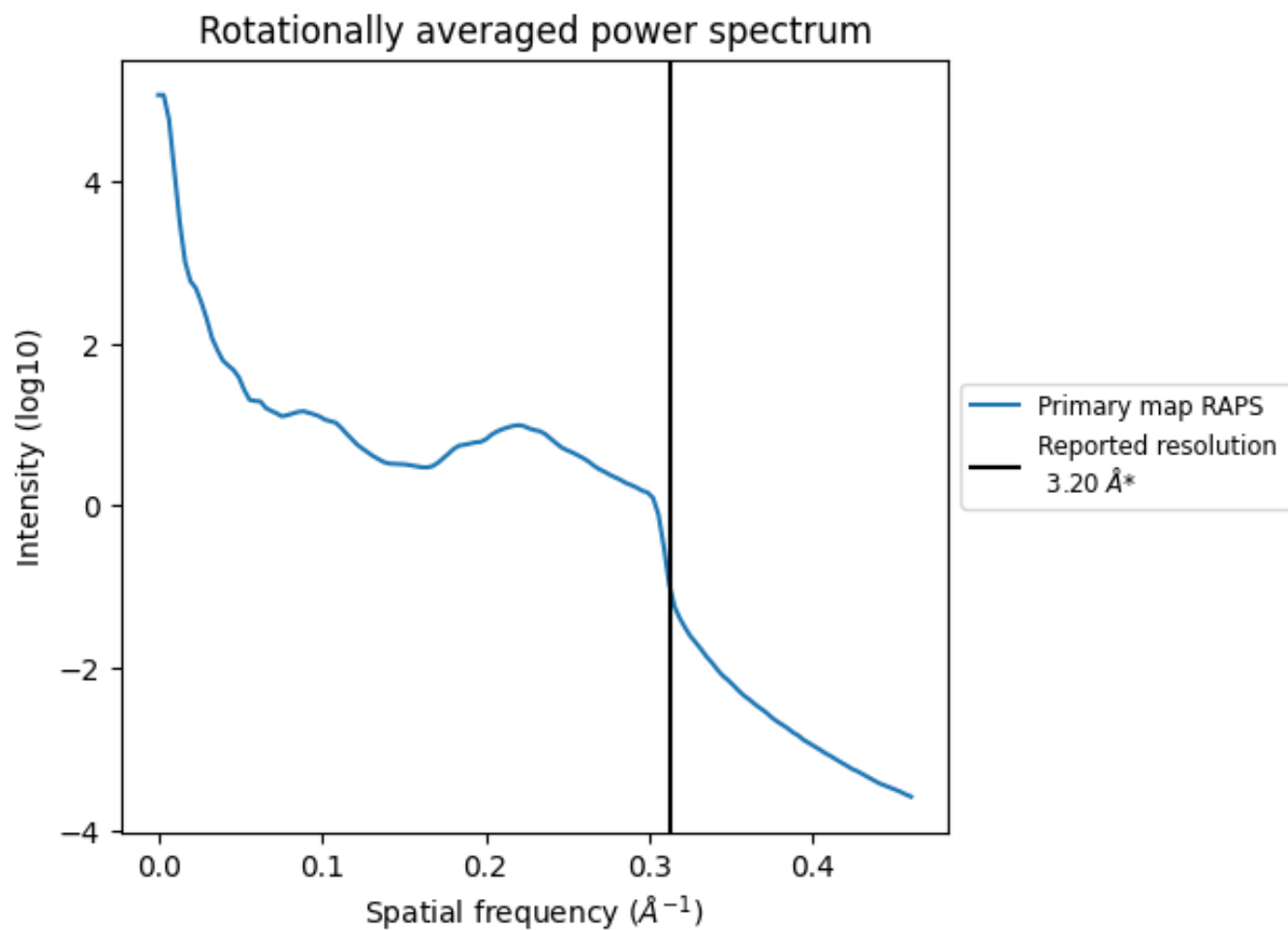


The volume at the recommended contour level is 191 nm<sup>3</sup>; this corresponds to an approximate mass of 172 kDa.

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 [i](#)

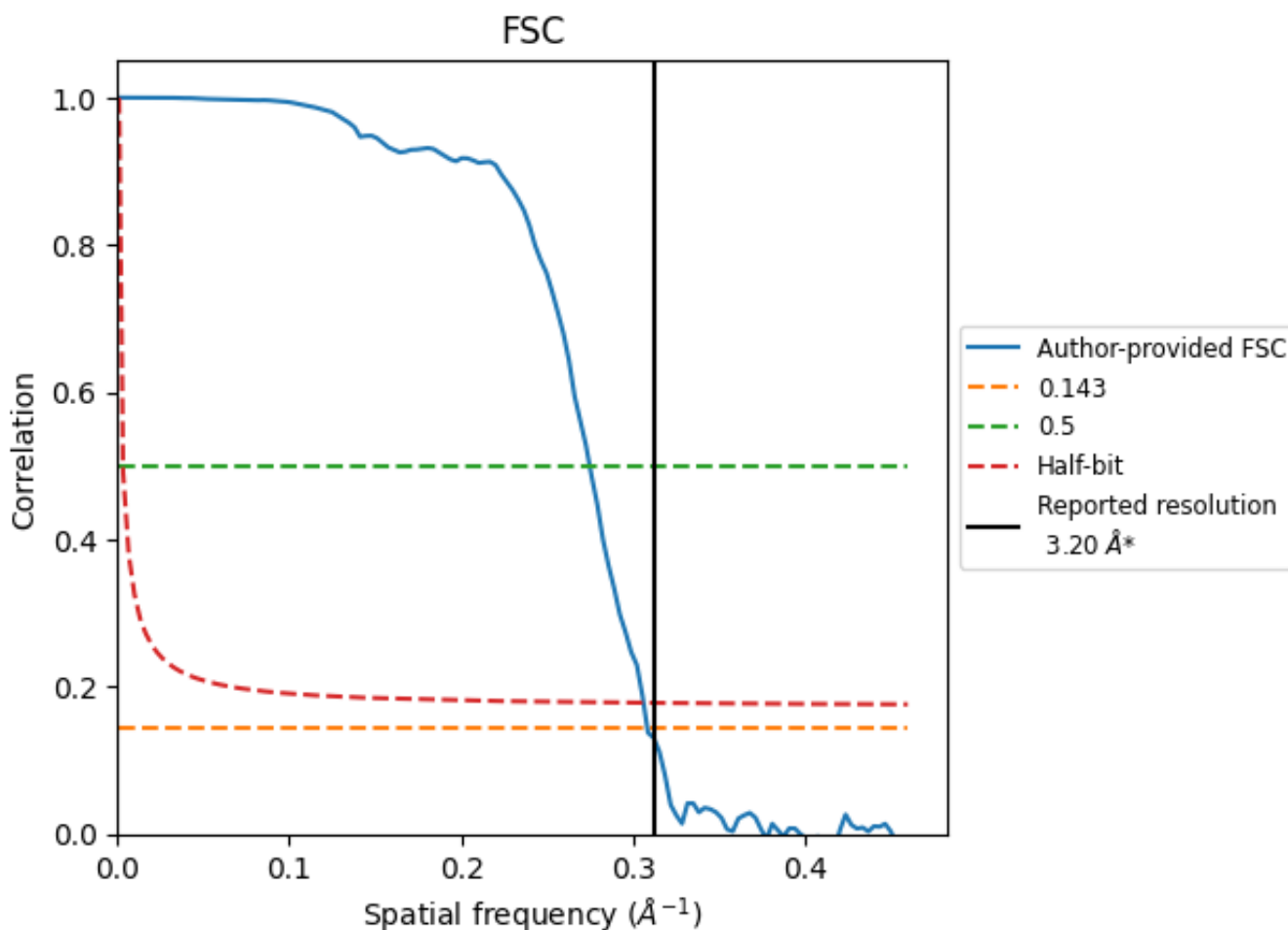


\*Reported resolution corresponds to spatial frequency of  $0.312 \text{\AA}^{-1}$

## 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 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

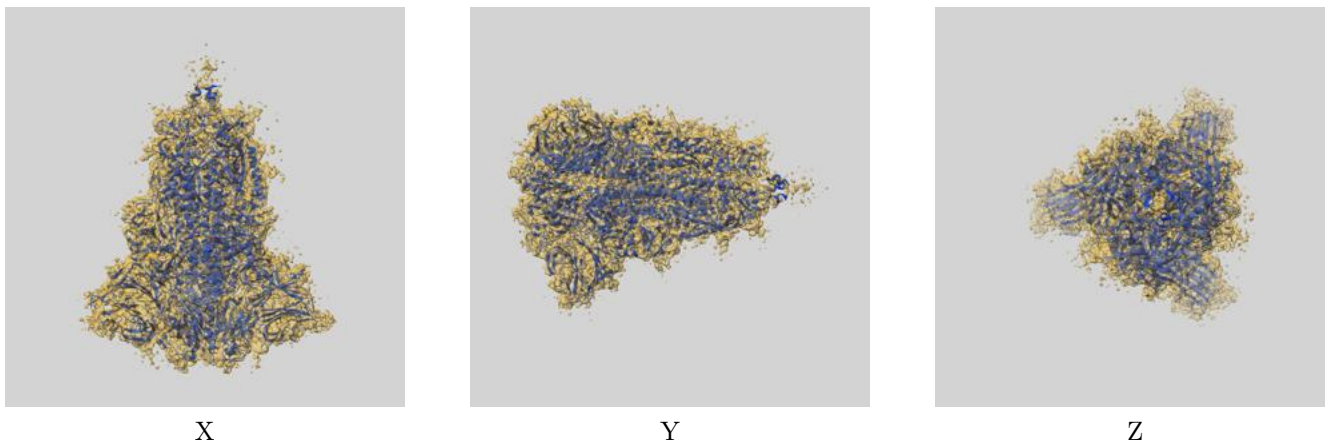
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.24	3.64	3.27
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

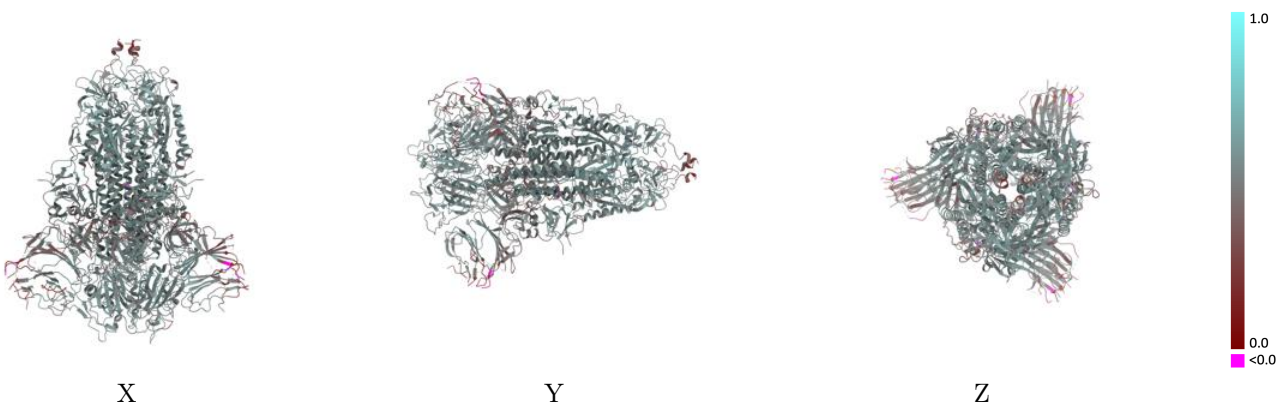
This section contains information regarding the fit between EMDB map EMD-30999 and PDB model 7E7D. Per-residue inclusion information can be found in section 3 on page 10.

### 9.1 Map-model overlay [i](#)



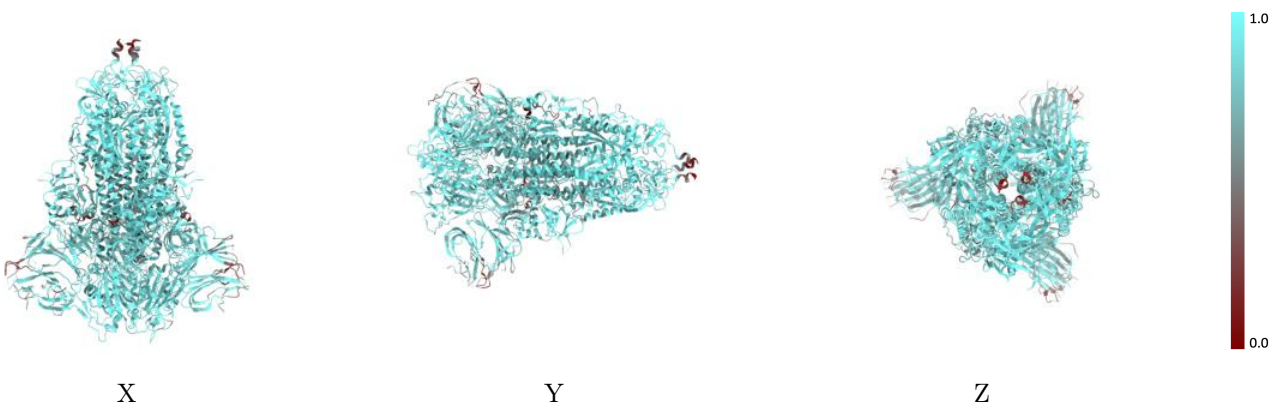
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



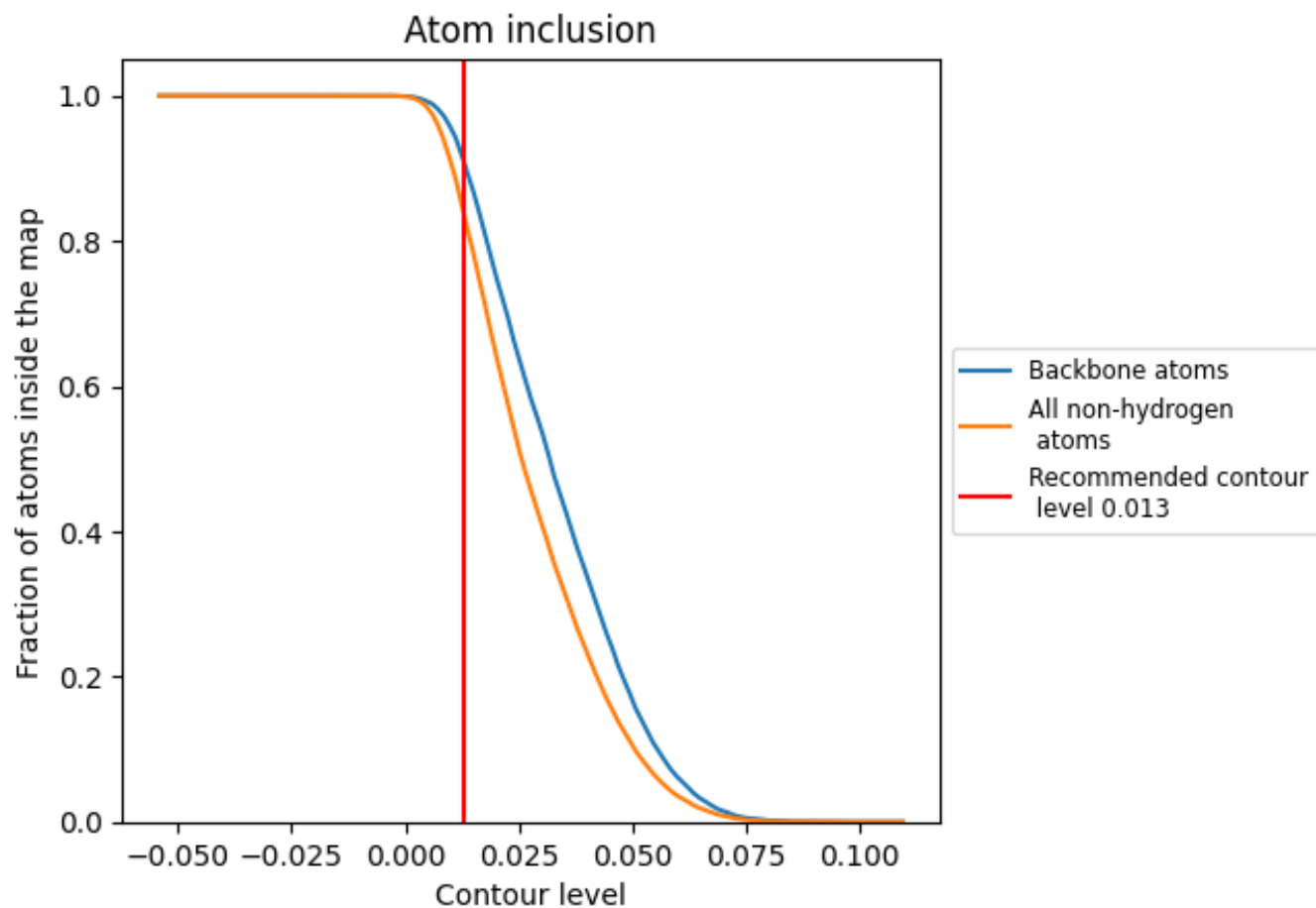
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 84% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8362	 0.5010
A	 0.8515	 0.5080
B	 0.8485	 0.5060
C	 0.8412	 0.5000
D	 0.6786	 0.3930
E	 0.1071	 0.1880
F	 0.7143	 0.4780
G	 0.6429	 0.3910
H	 0.4286	 0.3820
I	 0.2857	 0.2900
J	 0.6786	 0.4520
K	 0.2500	 0.2700
L	 0.7857	 0.4400
M	 0.3214	 0.3660
N	 0.6429	 0.4230
O	 0.7143	 0.5000
P	 0.1071	 0.1930
R	 0.6786	 0.3970
S	 0.5000	 0.3780
T	 0.3929	 0.3080
U	 0.6429	 0.4550
V	 0.2857	 0.2600
W	 0.7500	 0.4350
X	 0.3214	 0.3270
Y	 0.7143	 0.4260
Z	 0.6786	 0.4930
c	 0.7857	 0.4700
d	 0.6429	 0.4240
e	 0.4643	 0.3710
f	 0.2857	 0.3270
g	 0.7857	 0.4590
h	 0.3571	 0.2560
i	 0.7143	 0.4370
j	 0.3571	 0.3180
k	 0.6429	 0.4430
l	 0.6071	 0.4530

