



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 25, 2024 – 04:05 PM EST

PDB ID : 1ZPU  
Title : Crystal Structure of Fet3p, a Multicopper Oxidase that Functions in Iron Import  
Authors : Taylor, A.B.; Stoj, C.S.; Ziegler, L.; Kosman, D.J.; Hart, P.J.  
Deposited on : 2005-05-17  
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

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:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

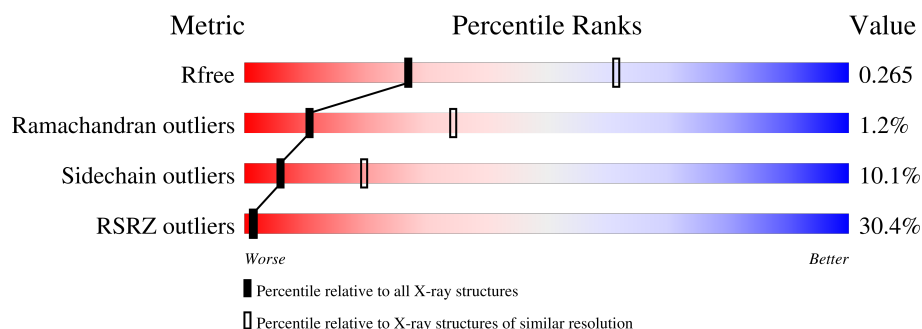
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.



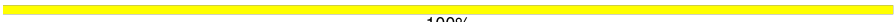
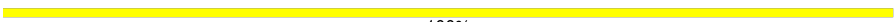
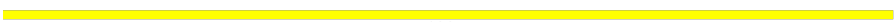











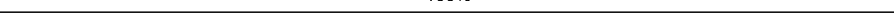
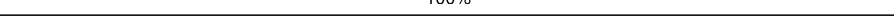
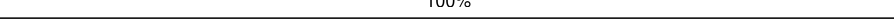

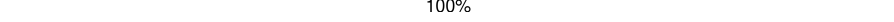
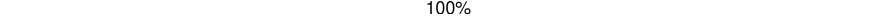

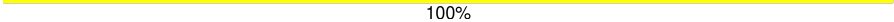

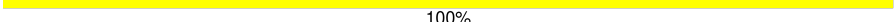
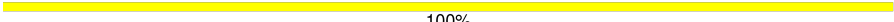
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3657 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	534	<div> <div>26%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>
1	B	534	<div> <div>10%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	C	534	<div> <div>36%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	D	534	<div> <div>21%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	E	534	<div> <div>23%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	F	534	<div> <div>64%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
2	G	5	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	J	5	 100%
2	M	5	 100%
2	O	5	 100%
2	S	5	 100%
2	U	5	 100%
2	Y	5	 100%
2	a	5	 100%
2	d	5	 40% 60%
2	f	5	 20% 80%
2	i	5	 20% 80%
2	k	5	 100%
3	H	6	 17% 83%
3	N	6	 100%
3	Z	6	 100%
3	j	6	 100%
4	I	2	 100%
4	P	2	 50% 50%
4	Q	2	 100%
4	V	2	 100%
4	b	2	 50% 50%
4	g	2	 100%
5	K	3	 33% 67%
5	L	3	 100%
5	W	3	 100%
5	X	3	 33% 67%

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Mol	Chain	Length	Quality of chain
5	c	3	<div><div style="width: 33%;"></div>33%<div style="width: 67%;"></div>67%</div>
5	h	3	<div><div style="width: 100%;"></div>100%</div>
5	l	3	<div><div style="width: 100%;"></div>100%</div>
6	R	4	<div><div style="width: 100%;"></div>100%</div>
7	T	7	<div><div style="width: 29%;"></div>29%<div style="width: 71%;"></div>71%</div>
7	e	7	<div><div style="width: 100%;"></div>100%</div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	a	1	X	-	-	-
2	NAG	f	1	X	-	-	-
3	NAG	H	1	X	-	-	-
3	NAG	N	1	X	-	-	-
3	NAG	Z	1	X	-	-	-
3	NAG	j	1	X	-	-	-
4	NAG	b	1	X	-	-	-
5	NAG	L	1	X	-	-	-
5	NAG	X	1	X	-	-	-
5	NAG	c	1	X	-	-	-
5	NAG	h	1	X	-	-	-
5	NAG	l	1	X	-	-	-
6	NAG	R	1	X	-	-	-
7	NAG	T	1	X	-	-	-
7	NAG	e	1	X	-	-	-
8	NAG	A	2006	X	-	-	-
8	NAG	A	2012	X	-	-	-
8	NAG	A	2018	X	-	-	-
8	NAG	B	2006	X	-	-	-
8	NAG	B	2012	X	-	-	-
8	NAG	B	2018	X	-	-	-
8	NAG	C	2012	X	-	-	-
8	NAG	C	2018	X	-	-	-
8	NAG	D	2006	X	-	-	-
8	NAG	E	2012	X	-	-	-
8	NAG	F	2005	X	-	-	-
8	NAG	F	2006	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	NAG	F	2009	X	-	-	-
8	NAG	F	2012	X	-	-	-

## 2 Entry composition [i](#)

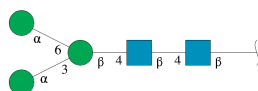
There are 9 unique types of molecules in this entry. The entry contains 27659 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Iron transport multicopper oxidase FET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	B	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	C	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	D	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	E	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	F	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			

- Molecule 2 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.



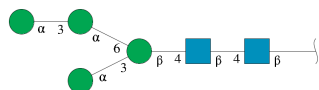
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	J	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	M	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	O	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	S	5	Total	C	N	O	0	0	0
			61	34	2	25			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	U	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	Y	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	a	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	d	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	f	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	i	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	k	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



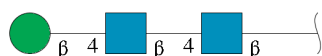
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	N	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	Z	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	j	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	b	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	g	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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				ZeroOcc	AltConf	Trace
5	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	W	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	X	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	c	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	h	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	l	3	Total	C	N	O	0	0	0
			39	22	2	15			

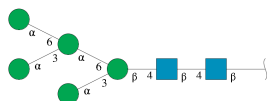
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





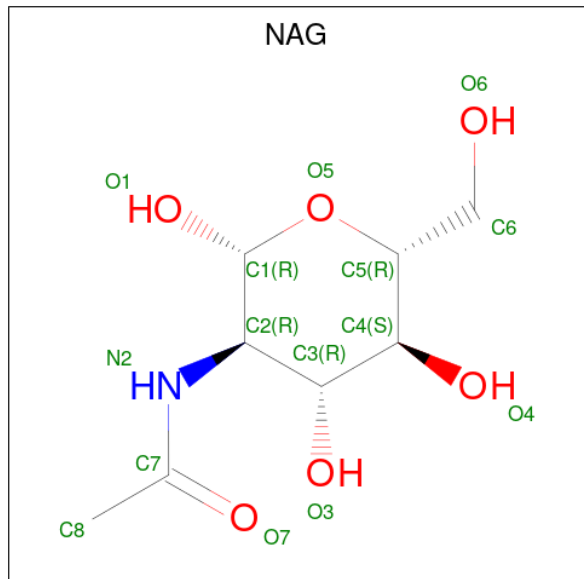
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	R	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	T	7	Total	C	N	O	0	0	0
			83	46	2	35			
7	e	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

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

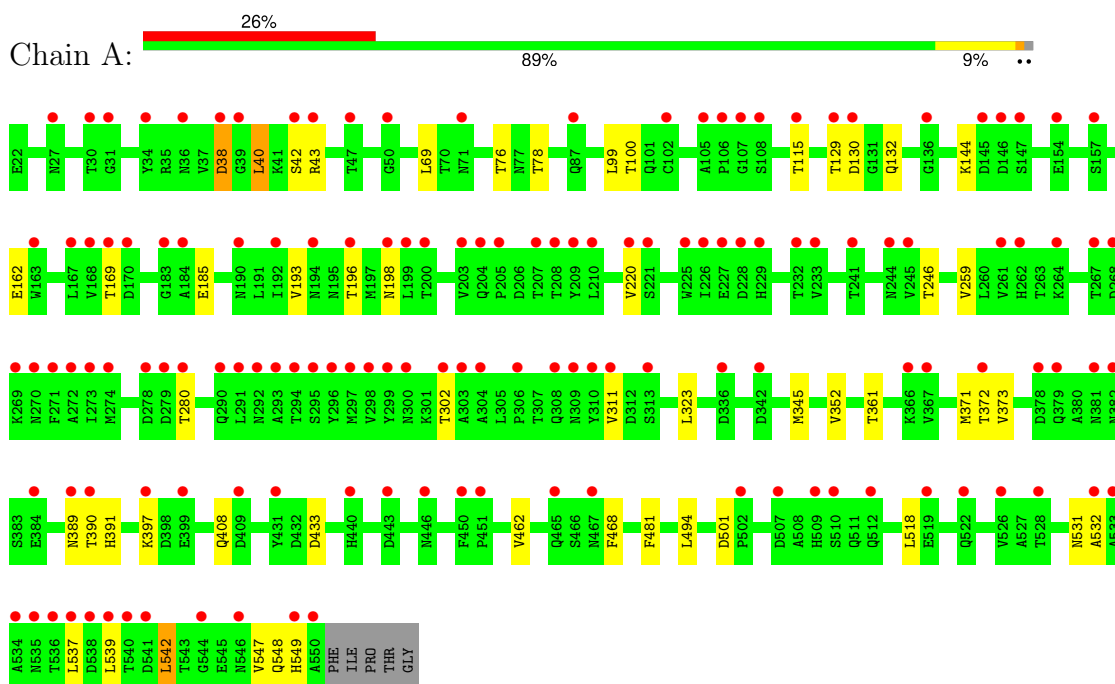
- Molecule 9 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	4	Total	Cu	0	0
			4	4		
9	B	4	Total	Cu	0	0
			4	4		
9	C	4	Total	Cu	0	0
			4	4		
9	D	4	Total	Cu	0	0
			4	4		
9	E	4	Total	Cu	0	0
			4	4		
9	F	4	Total	Cu	0	0
			4	4		

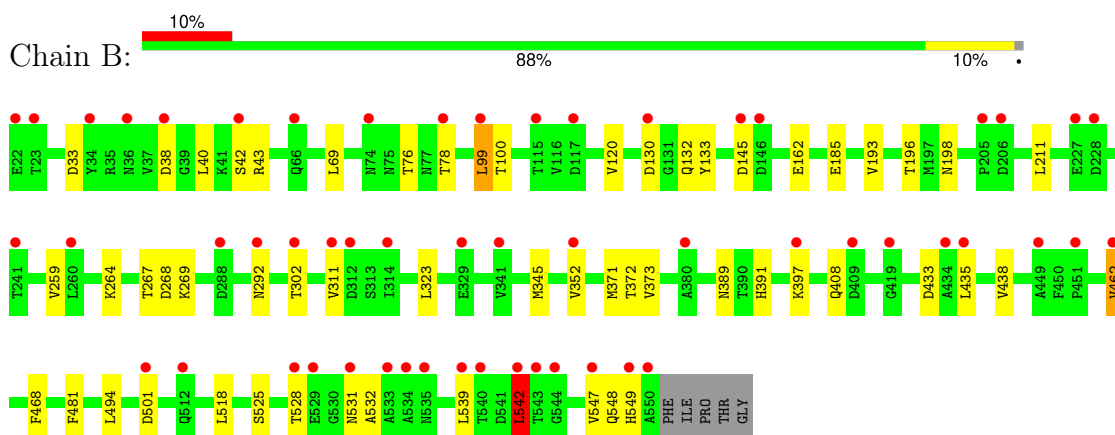
### 3 Residue-property plots

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

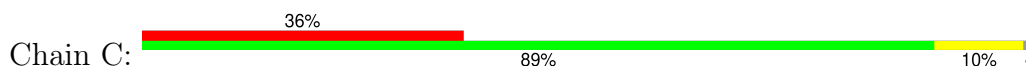
#### • Molecule 1: Iron transport multicopper oxidase FET3

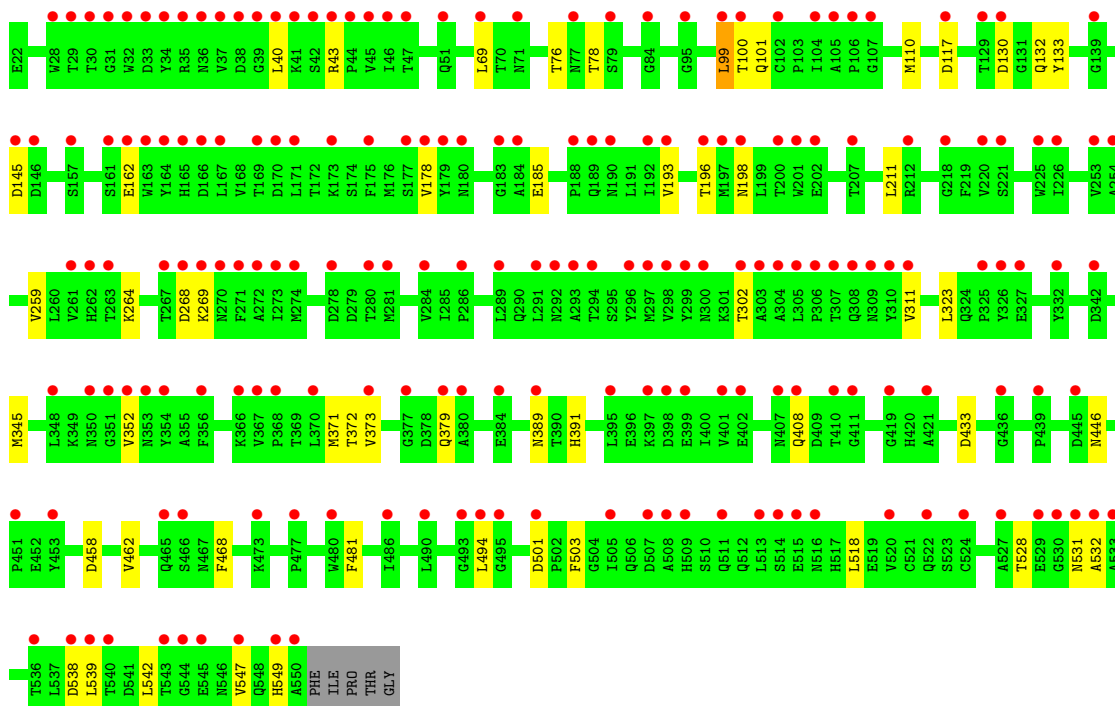


#### • Molecule 1: Iron transport multicopper oxidase FET3

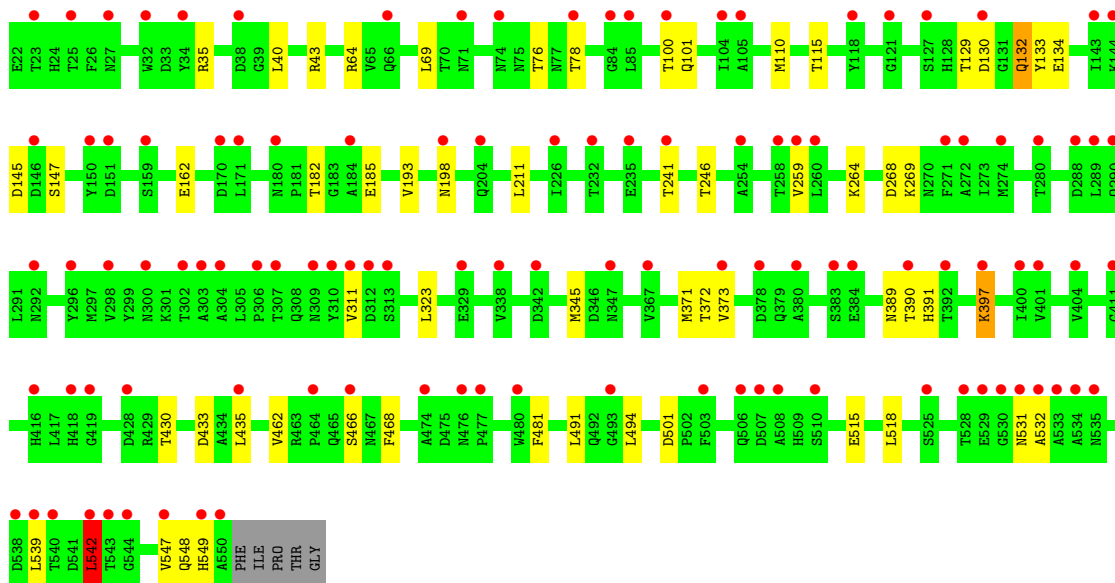
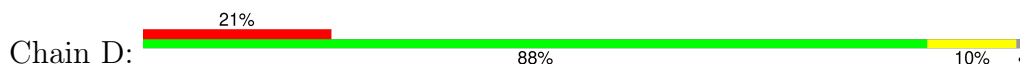


#### • Molecule 1: Iron transport multicopper oxidase FET3



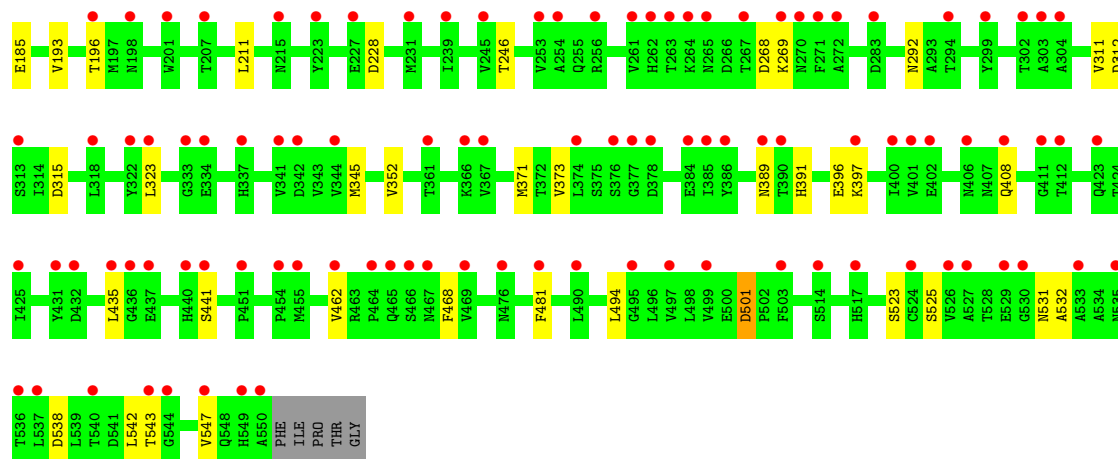


• Molecule 1: Iron transport multicopper oxidase FET3

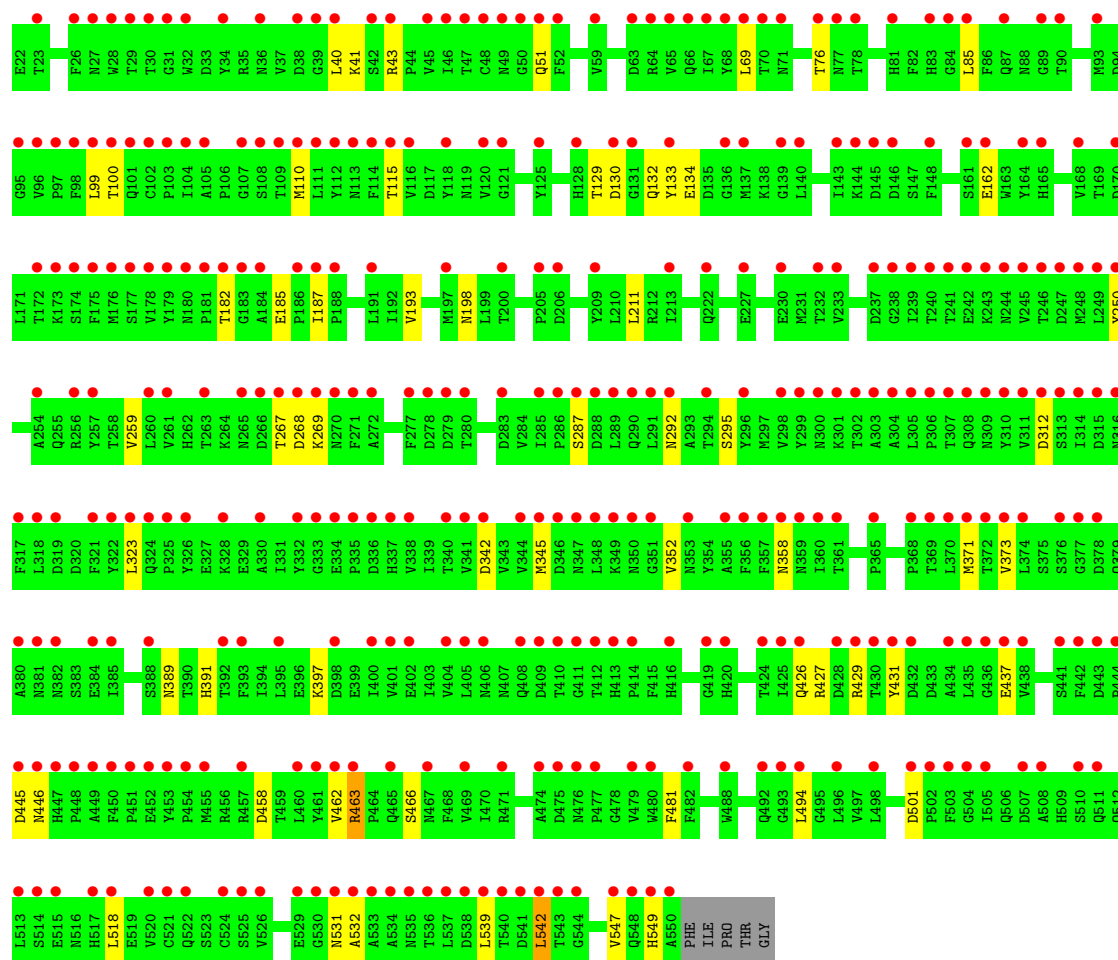
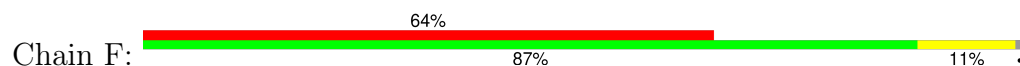


• Molecule 1: Iron transport multicopper oxidase FET3






• Molecule 1: Iron transport multicopper oxidase FET3



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

Chain G:  100%


MAG1  
MAG2  
BMA3  
MAN4  
MAN5

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

Chain J:  100%


MAG1  
MAG2  
BMA3  
MAN4  
MAN5

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

Chain M:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

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

Chain O:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

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

Chain S:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

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

Chain U:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

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

nose

Chain Y:  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5

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

Chain a:  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5

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

Chain d:  40% 60%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5

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

Chain f:  20% 80%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5

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

Chain i:  20% 80%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5

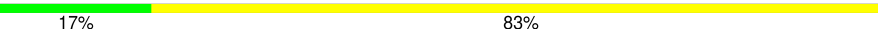
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5



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

Chain H:  17% 83%

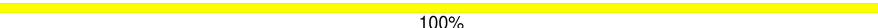
NAG1  
NAG2  
BMA3  
MAN4  
MAN5  
MAN6

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

Chain N:  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5  
MAN6

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

Chain Z:  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5  
MAN6

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

Chain j:  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5  
MAN6

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

Chain I:  100%

NAG1  
NAG2

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

Chain P:  50% 50%

NAG1  
NAG2

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

Chain Q:  100%

MAG1  
MAG2

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

Chain V:  100%

MAG1  
MAG2

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

Chain b:  50% 50%

MAG1  
MAG2

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

Chain g:  100%

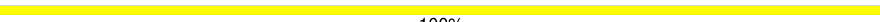
MAG1  
MAG2

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

Chain K:  33% 67%


MAG1  
MAG2  
BMA3

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

Chain L:  100%

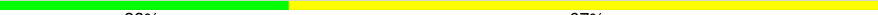
MAG1  
MAG2  
BMA3

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

Chain W:  100%

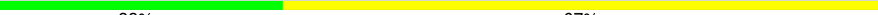
MAG1  
MAG2  
BMA3

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

Chain X:  33% 67%


MAG1  
MAG2  
BMA3

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

Chain c:  33% 67%

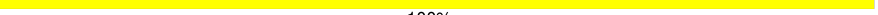
MAG1  
MAG2  
BMA3

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

Chain h:  100%

MAG1  
MAG2  
BMA3

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

Chain l:  100%

MAG1  
MAG2  
BMA3

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

Chain R:  100%

MAG1  
MAG2  
BMA3  
MAN4

- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  29% 71%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 7:  $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-6)] $\alpha$ -D-mannopyranose-(1-6)-[ $\alpha$ -D-mannopyranose-(1-3)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain e:

100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.53Å 168.53Å 174.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.80) 98.2 (50.00-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.226 , 0.257 0.235 , 0.265	Depositor DCC
$R_{free}$ test set	6726 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.6	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 70.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.010 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	27659	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3641e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, CU1, 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	0.50	0/4373	0.66	2/5981 (0.0%)
1	B	0.50	0/4373	0.66	3/5981 (0.1%)
1	C	0.55	5/4373 (0.1%)	0.64	2/5981 (0.0%)
1	D	0.51	3/4373 (0.1%)	0.60	2/5981 (0.0%)
1	E	0.44	1/4373 (0.0%)	0.58	1/5981 (0.0%)
1	F	0.99	20/4373 (0.5%)	0.77	11/5981 (0.2%)
All	All	0.61	29/26238 (0.1%)	0.65	21/35886 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	463	ARG	CZ-NH1	40.06	1.85	1.33
1	F	250	TYR	CE2-CZ	15.67	1.58	1.38
1	F	250	TYR	CG-CD2	15.35	1.59	1.39
1	D	515	GLU	CD-OE1	13.48	1.40	1.25
1	F	250	TYR	CE1-CZ	13.27	1.55	1.38

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	463	ARG	NE-CZ-NH2	-25.91	107.34	120.30
1	F	463	ARG	NE-CZ-NH1	10.71	125.66	120.30

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*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	445	ASP	CB-CG-OD2	-9.31	109.92	118.30
1	F	429	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	F	463	ARG	NH1-CZ-NH2	-8.13	110.46	119.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	463	ARG	Sidechain

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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	527/534 (99%)	497 (94%)	23 (4%)	7 (1%)	10	32
1	B	527/534 (99%)	498 (94%)	23 (4%)	6 (1%)	12	37
1	C	527/534 (99%)	495 (94%)	27 (5%)	5 (1%)	14	42
1	D	527/534 (99%)	497 (94%)	22 (4%)	8 (2%)	8	29
1	E	527/534 (99%)	497 (94%)	24 (5%)	6 (1%)	12	37
1	F	527/534 (99%)	498 (94%)	23 (4%)	6 (1%)	12	37
All	All	3162/3204 (99%)	2982 (94%)	142 (4%)	38 (1%)	11	34

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	531	ASN
1	C	130	ASP
1	D	130	ASP
1	E	130	ASP

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	477/481 (99%)	430 (90%)	47 (10%)	6	21
1	B	477/481 (99%)	425 (89%)	52 (11%)	5	17
1	C	477/481 (99%)	431 (90%)	46 (10%)	7	22
1	D	477/481 (99%)	425 (89%)	52 (11%)	5	17
1	E	477/481 (99%)	432 (91%)	45 (9%)	7	23
1	F	477/481 (99%)	429 (90%)	48 (10%)	6	20
All	All	2862/2886 (99%)	2572 (90%)	290 (10%)	6	20

5 of 290 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	441	SER
1	F	539	LEU
1	E	525	SER
1	F	193	VAL
1	B	548	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	51	GLN
1	E	549	HIS
1	C	66	GLN
1	F	309	ASN

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Mol	Chain	Res	Type
1	E	195	ASN

### 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 ⓘ

135 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	G	1	2,1	14,14,15	0.71	0	17,19,21	1.37	3 (17%)
2	NAG	G	2	2	14,14,15	0.53	0	17,19,21	1.07	2 (11%)
2	BMA	G	3	2	11,11,12	0.81	0	15,15,17	1.71	2 (13%)
2	MAN	G	4	2	11,11,12	0.58	0	15,15,17	1.33	1 (6%)
2	MAN	G	5	2	11,11,12	0.73	0	15,15,17	2.09	2 (13%)
3	NAG	H	1	3,1	14,14,15	0.78	0	17,19,21	2.11	4 (23%)
3	NAG	H	2	3	14,14,15	0.63	0	17,19,21	0.85	0
3	BMA	H	3	3	11,11,12	0.73	0	15,15,17	1.82	3 (20%)
3	MAN	H	4	3	11,11,12	0.60	0	15,15,17	1.03	1 (6%)
3	MAN	H	5	3	11,11,12	0.71	0	15,15,17	1.09	1 (6%)
3	MAN	H	6	3	11,11,12	0.67	0	15,15,17	1.54	3 (20%)
4	NAG	I	1	4,1	14,14,15	0.63	0	17,19,21	2.17	5 (29%)
4	NAG	I	2	4	14,14,15	1.09	1 (7%)	17,19,21	1.32	2 (11%)
2	NAG	J	1	2,1	14,14,15	0.72	0	17,19,21	1.73	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	J	2	2	14,14,15	0.62	0	17,19,21	2.05	3 (17%)
2	BMA	J	3	2	11,11,12	0.71	0	15,15,17	1.30	2 (13%)
2	MAN	J	4	2	11,11,12	0.72	0	15,15,17	1.59	2 (13%)
2	MAN	J	5	2	11,11,12	0.69	0	15,15,17	1.74	1 (6%)
5	NAG	K	1	1,5	14,14,15	0.51	0	17,19,21	2.04	3 (17%)
5	NAG	K	2	5	14,14,15	0.47	0	17,19,21	0.94	0
5	BMA	K	3	5	11,11,12	0.92	0	15,15,17	1.07	1 (6%)
5	NAG	L	1	1,5	14,14,15	0.49	0	17,19,21	1.88	5 (29%)
5	NAG	L	2	5	14,14,15	0.54	0	17,19,21	1.14	2 (11%)
5	BMA	L	3	5	11,11,12	0.63	0	15,15,17	1.92	2 (13%)
2	NAG	M	1	2,1	14,14,15	0.70	0	17,19,21	0.99	1 (5%)
2	NAG	M	2	2	14,14,15	0.60	0	17,19,21	1.10	1 (5%)
2	BMA	M	3	2	11,11,12	0.75	0	15,15,17	0.92	1 (6%)
2	MAN	M	4	2	11,11,12	0.70	0	15,15,17	2.65	5 (33%)
2	MAN	M	5	2	11,11,12	0.45	0	15,15,17	1.34	3 (20%)
3	NAG	N	1	3,1	14,14,15	0.69	0	17,19,21	1.53	4 (23%)
3	NAG	N	2	3	14,14,15	0.57	0	17,19,21	1.04	1 (5%)
3	BMA	N	3	3	11,11,12	0.75	0	15,15,17	1.37	2 (13%)
3	MAN	N	4	3	11,11,12	0.61	0	15,15,17	2.08	2 (13%)
3	MAN	N	5	3	11,11,12	0.54	0	15,15,17	1.22	1 (6%)
3	MAN	N	6	3	11,11,12	0.55	0	15,15,17	1.06	1 (6%)
2	NAG	O	1	2,1	14,14,15	0.56	0	17,19,21	1.68	3 (17%)
2	NAG	O	2	2	14,14,15	0.74	0	17,19,21	1.28	3 (17%)
2	BMA	O	3	2	11,11,12	0.75	0	15,15,17	1.51	4 (26%)
2	MAN	O	4	2	11,11,12	0.61	0	15,15,17	1.93	5 (33%)
2	MAN	O	5	2	11,11,12	1.67	2 (18%)	15,15,17	2.23	4 (26%)
4	NAG	P	1	4,1	14,14,15	0.56	0	17,19,21	0.96	0
4	NAG	P	2	4	14,14,15	0.50	0	17,19,21	0.98	1 (5%)
4	NAG	Q	1	4,1	14,14,15	0.47	0	17,19,21	1.87	4 (23%)
4	NAG	Q	2	4	14,14,15	0.48	0	17,19,21	1.18	1 (5%)
6	NAG	R	1	1,6	14,14,15	0.73	0	17,19,21	1.61	2 (11%)
6	NAG	R	2	6	14,14,15	0.62	0	17,19,21	1.21	2 (11%)
6	BMA	R	3	6	11,11,12	0.54	0	15,15,17	0.90	1 (6%)
6	MAN	R	4	6	11,11,12	0.53	0	15,15,17	2.04	4 (26%)
2	NAG	S	1	2,1	14,14,15	0.74	0	17,19,21	1.37	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	S	2	2	14,14,15	0.61	0	17,19,21	1.36	3 (17%)
2	BMA	S	3	2	11,11,12	0.56	0	15,15,17	1.77	3 (20%)
2	MAN	S	4	2	11,11,12	0.56	0	15,15,17	1.36	2 (13%)
2	MAN	S	5	2	11,11,12	0.62	0	15,15,17	1.18	1 (6%)
7	NAG	T	1	1,7	14,14,15	0.91	1 (7%)	17,19,21	2.10	7 (41%)
7	NAG	T	2	7	14,14,15	0.44	0	17,19,21	0.94	0
7	BMA	T	3	7	11,11,12	0.58	0	15,15,17	1.80	3 (20%)
7	MAN	T	4	7	11,11,12	0.60	0	15,15,17	1.28	1 (6%)
7	MAN	T	5	7	11,11,12	0.70	0	15,15,17	0.75	0
7	MAN	T	6	7	11,11,12	0.55	0	15,15,17	2.10	1 (6%)
7	MAN	T	7	7	11,11,12	0.75	0	15,15,17	1.72	3 (20%)
2	NAG	U	1	2,1	14,14,15	0.48	0	17,19,21	1.98	2 (11%)
2	NAG	U	2	2	14,14,15	0.74	1 (7%)	17,19,21	1.30	4 (23%)
2	BMA	U	3	2	11,11,12	0.68	0	15,15,17	1.16	2 (13%)
2	MAN	U	4	2	11,11,12	0.77	0	15,15,17	1.43	3 (20%)
2	MAN	U	5	2	11,11,12	0.59	0	15,15,17	1.61	2 (13%)
4	NAG	V	1	4,1	14,14,15	0.51	0	17,19,21	1.16	1 (5%)
4	NAG	V	2	4	14,14,15	1.20	2 (14%)	17,19,21	1.46	2 (11%)
5	NAG	W	1	1,5	14,14,15	1.99	3 (21%)	17,19,21	0.92	0
5	NAG	W	2	5	14,14,15	1.77	3 (21%)	17,19,21	2.25	4 (23%)
5	BMA	W	3	5	11,11,12	2.48	1 (9%)	15,15,17	1.70	4 (26%)
5	NAG	X	1	1,5	14,14,15	0.49	0	17,19,21	1.80	5 (29%)
5	NAG	X	2	5	14,14,15	0.42	0	17,19,21	1.21	2 (11%)
5	BMA	X	3	5	11,11,12	0.66	0	15,15,17	0.88	0
2	NAG	Y	1	2,1	14,14,15	0.54	0	17,19,21	0.95	1 (5%)
2	NAG	Y	2	2	14,14,15	0.58	0	17,19,21	1.23	3 (17%)
2	BMA	Y	3	2	11,11,12	0.57	0	15,15,17	1.29	2 (13%)
2	MAN	Y	4	2	11,11,12	0.57	0	15,15,17	1.25	1 (6%)
2	MAN	Y	5	2	11,11,12	0.62	0	15,15,17	1.08	1 (6%)
3	NAG	Z	1	3,1	14,14,15	0.62	0	17,19,21	1.77	3 (17%)
3	NAG	Z	2	3	14,14,15	0.69	0	17,19,21	0.96	1 (5%)
3	BMA	Z	3	3	11,11,12	0.70	0	15,15,17	1.75	4 (26%)
3	MAN	Z	4	3	11,11,12	0.59	0	15,15,17	1.09	1 (6%)
3	MAN	Z	5	3	11,11,12	0.62	0	15,15,17	0.91	1 (6%)
3	MAN	Z	6	3	11,11,12	1.07	1 (9%)	15,15,17	1.83	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	a	1	2,1	14,14,15	0.40	0	17,19,21	1.23	1 (5%)
2	NAG	a	2	2	14,14,15	0.57	0	17,19,21	1.01	2 (11%)
2	BMA	a	3	2	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
2	MAN	a	4	2	11,11,12	0.54	0	15,15,17	1.46	1 (6%)
2	MAN	a	5	2	11,11,12	0.60	0	15,15,17	1.53	2 (13%)
4	NAG	b	1	4,1	14,14,15	1.38	2 (14%)	17,19,21	1.66	3 (17%)
4	NAG	b	2	4	14,14,15	0.50	0	17,19,21	0.69	0
5	NAG	c	1	1,5	14,14,15	0.53	0	17,19,21	1.38	2 (11%)
5	NAG	c	2	5	14,14,15	0.54	0	17,19,21	0.82	0
5	BMA	c	3	5	11,11,12	0.54	0	15,15,17	0.88	1 (6%)
2	NAG	d	1	2,1	14,14,15	0.60	0	17,19,21	1.11	1 (5%)
2	NAG	d	2	2	14,14,15	0.54	0	17,19,21	0.82	0
2	BMA	d	3	2	11,11,12	0.76	0	15,15,17	1.91	4 (26%)
2	MAN	d	4	2	11,11,12	0.59	0	15,15,17	0.61	0
2	MAN	d	5	2	11,11,12	0.54	0	15,15,17	1.38	1 (6%)
7	NAG	e	1	1,7	14,14,15	0.56	0	17,19,21	1.08	1 (5%)
7	NAG	e	2	7	14,14,15	0.49	0	17,19,21	1.26	2 (11%)
7	BMA	e	3	7	11,11,12	0.61	0	15,15,17	1.41	4 (26%)
7	MAN	e	4	7	11,11,12	0.62	0	15,15,17	1.42	3 (20%)
7	MAN	e	5	7	11,11,12	0.55	0	15,15,17	0.98	1 (6%)
7	MAN	e	6	7	11,11,12	0.70	0	15,15,17	1.54	2 (13%)
7	MAN	e	7	7	11,11,12	0.52	0	15,15,17	1.52	1 (6%)
2	NAG	f	1	2,1	14,14,15	0.53	0	17,19,21	1.45	3 (17%)
2	NAG	f	2	2	14,14,15	0.50	0	17,19,21	0.95	0
2	BMA	f	3	2	11,11,12	0.62	0	15,15,17	0.97	1 (6%)
2	MAN	f	4	2	11,11,12	0.56	0	15,15,17	1.34	1 (6%)
2	MAN	f	5	2	11,11,12	0.56	0	15,15,17	1.37	1 (6%)
4	NAG	g	1	4,1	14,14,15	0.55	0	17,19,21	1.22	2 (11%)
4	NAG	g	2	4	14,14,15	0.59	0	17,19,21	1.05	1 (5%)
5	NAG	h	1	1,5	14,14,15	0.60	0	17,19,21	1.68	4 (23%)
5	NAG	h	2	5	14,14,15	0.61	0	17,19,21	1.11	1 (5%)
5	BMA	h	3	5	11,11,12	0.86	0	15,15,17	1.78	3 (20%)
2	NAG	i	1	2,1	14,14,15	0.60	0	17,19,21	0.96	0
2	NAG	i	2	2	14,14,15	0.59	0	17,19,21	1.19	1 (5%)
2	BMA	i	3	2	11,11,12	0.64	0	15,15,17	1.31	3 (20%)
2	MAN	i	4	2	11,11,12	0.64	0	15,15,17	1.79	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MAN	i	5	2	11,11,12	0.49	0	15,15,17	1.57	1 (6%)
3	NAG	j	1	3,1	14,14,15	0.63	0	17,19,21	1.49	3 (17%)
3	NAG	j	2	3	14,14,15	0.75	0	17,19,21	1.50	2 (11%)
3	BMA	j	3	3	11,11,12	0.78	0	15,15,17	0.90	2 (13%)
3	MAN	j	4	3	11,11,12	1.19	1 (9%)	15,15,17	1.42	2 (13%)
3	MAN	j	5	3	11,11,12	0.94	1 (9%)	15,15,17	0.92	1 (6%)
3	MAN	j	6	3	11,11,12	0.58	0	15,15,17	1.55	2 (13%)
2	NAG	k	1	2,1	14,14,15	0.52	0	17,19,21	1.24	1 (5%)
2	NAG	k	2	2	14,14,15	0.55	0	17,19,21	1.07	2 (11%)
2	BMA	k	3	2	11,11,12	0.69	0	15,15,17	1.22	1 (6%)
2	MAN	k	4	2	11,11,12	0.66	0	15,15,17	0.87	1 (6%)
2	MAN	k	5	2	11,11,12	1.57	1 (9%)	15,15,17	1.70	2 (13%)
5	NAG	l	1	1,5	14,14,15	0.51	0	17,19,21	1.11	1 (5%)
5	NAG	l	2	5	14,14,15	0.57	0	17,19,21	1.52	4 (23%)
5	BMA	l	3	5	11,11,12	1.84	2 (18%)	15,15,17	0.98	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	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	2/2/19/22	0/1/1/1
2	MAN	G	4	2	-	2/2/19/22	0/1/1/1
2	MAN	G	5	2	-	2/2/19/22	1/1/1/1
3	NAG	H	1	3,1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
3	MAN	H	4	3	-	2/2/19/22	0/1/1/1
3	MAN	H	5	3	-	0/2/19/22	0/1/1/1
3	MAN	H	6	3	-	2/2/19/22	0/1/1/1
4	NAG	I	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	J	2	2	-	5/6/23/26	0/1/1/1

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

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

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

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

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	3	BMA	O6-C6	7.78	1.75	1.42
2	k	5	MAN	O6-C6	4.89	1.63	1.42
5	l	3	BMA	O6-C6	4.81	1.62	1.42
5	W	1	NAG	C8-C7	4.59	1.60	1.50
5	W	2	NAG	C8-C7	4.54	1.60	1.50

The worst 5 of 274 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	5	MAN	C1-O5-C5	7.27	121.93	112.19
2	M	4	MAN	C1-O5-C5	7.15	121.77	112.19
2	O	5	MAN	C1-O5-C5	6.84	121.35	112.19
2	U	1	NAG	C1-O5-C5	6.74	121.22	112.19
7	T	6	MAN	C1-O5-C5	6.61	121.04	112.19

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	a	1	NAG	C1
2	f	1	NAG	C1
3	H	1	NAG	C1
3	N	1	NAG	C1
3	Z	1	NAG	C1

5 of 250 torsion outliers are listed below:

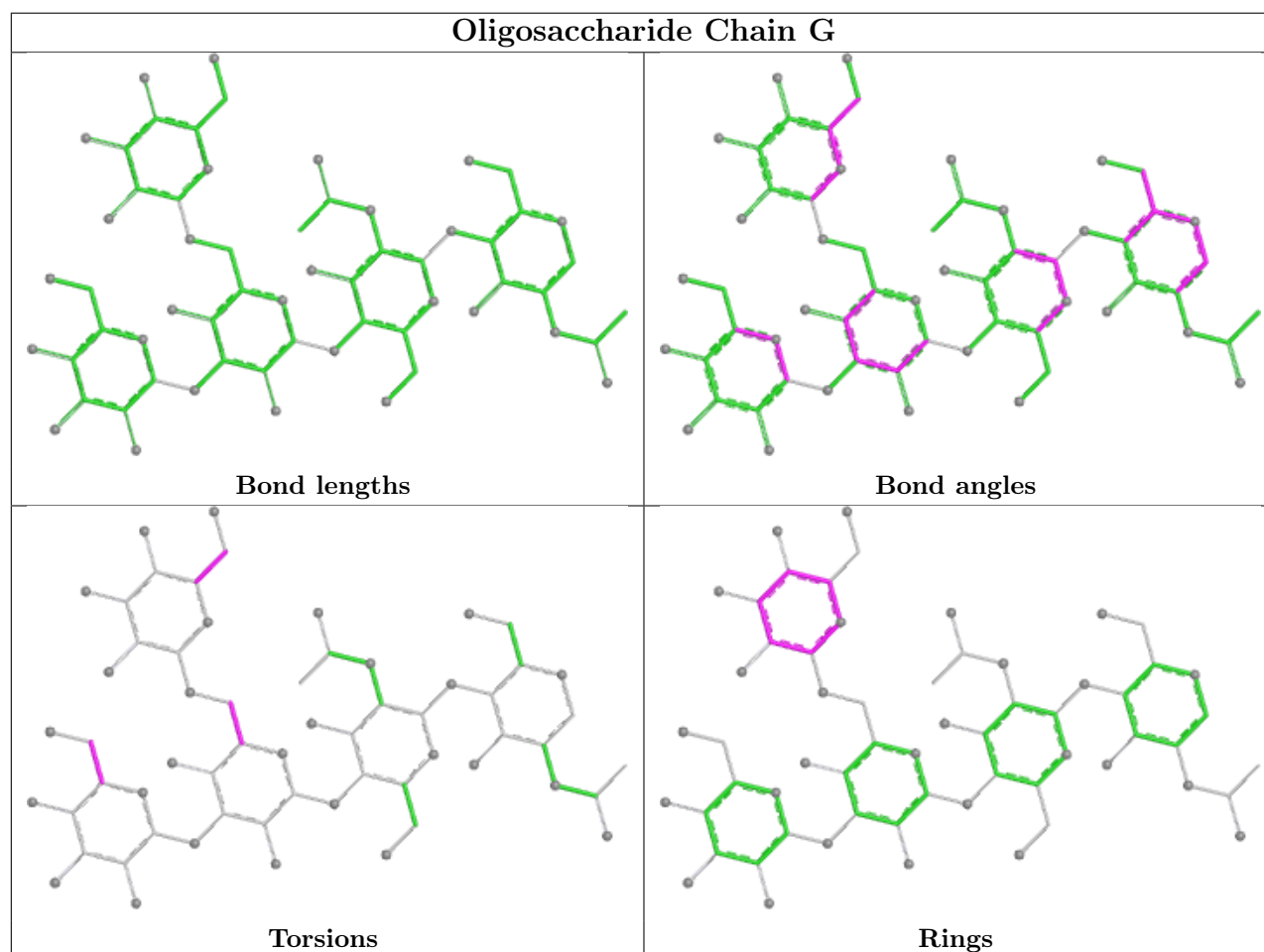
Mol	Chain	Res	Type	Atoms
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	O	1	NAG	C8-C7-N2-C2
2	O	1	NAG	O7-C7-N2-C2
2	U	1	NAG	C8-C7-N2-C2

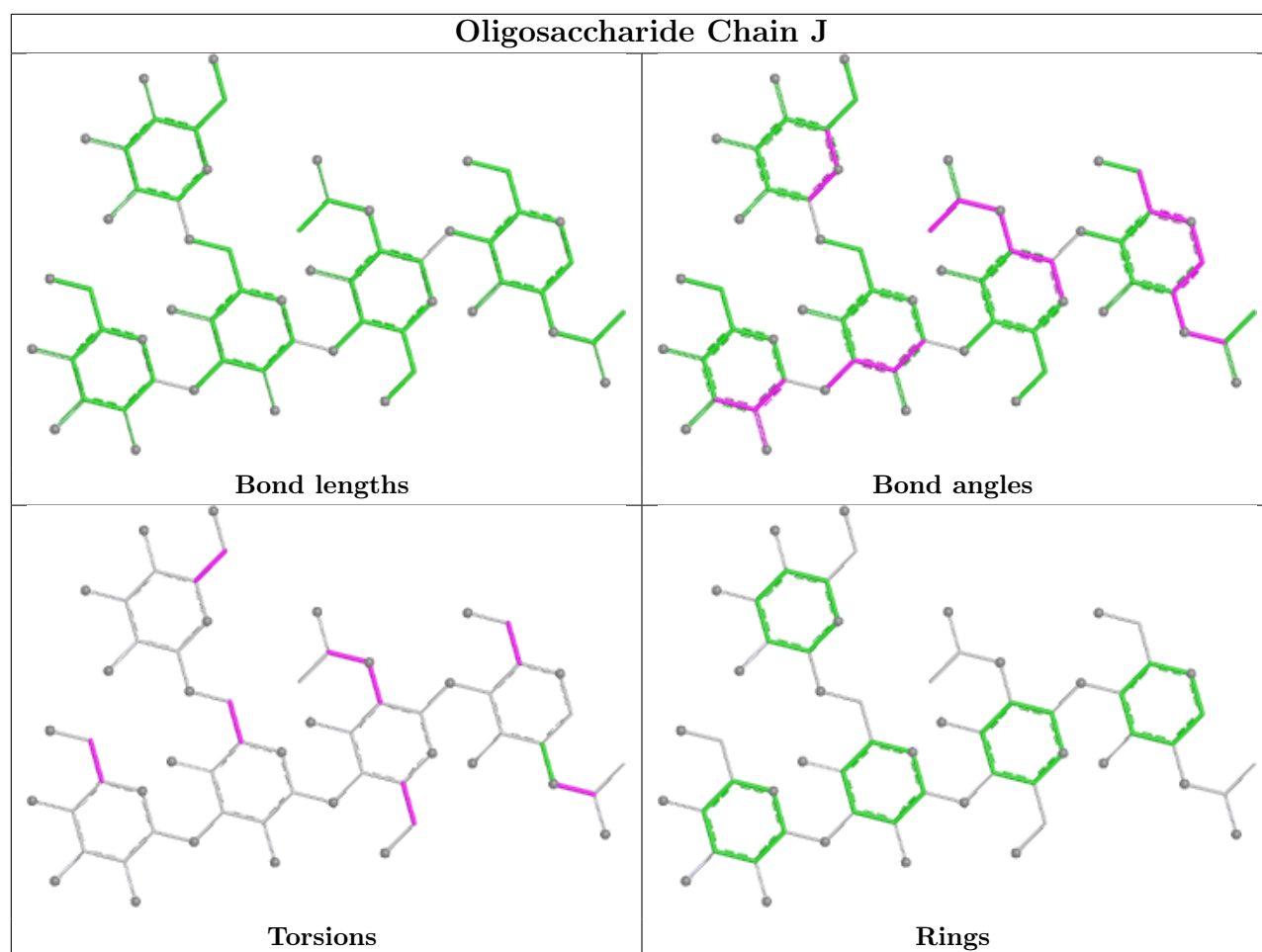
All (5) ring outliers are listed below:

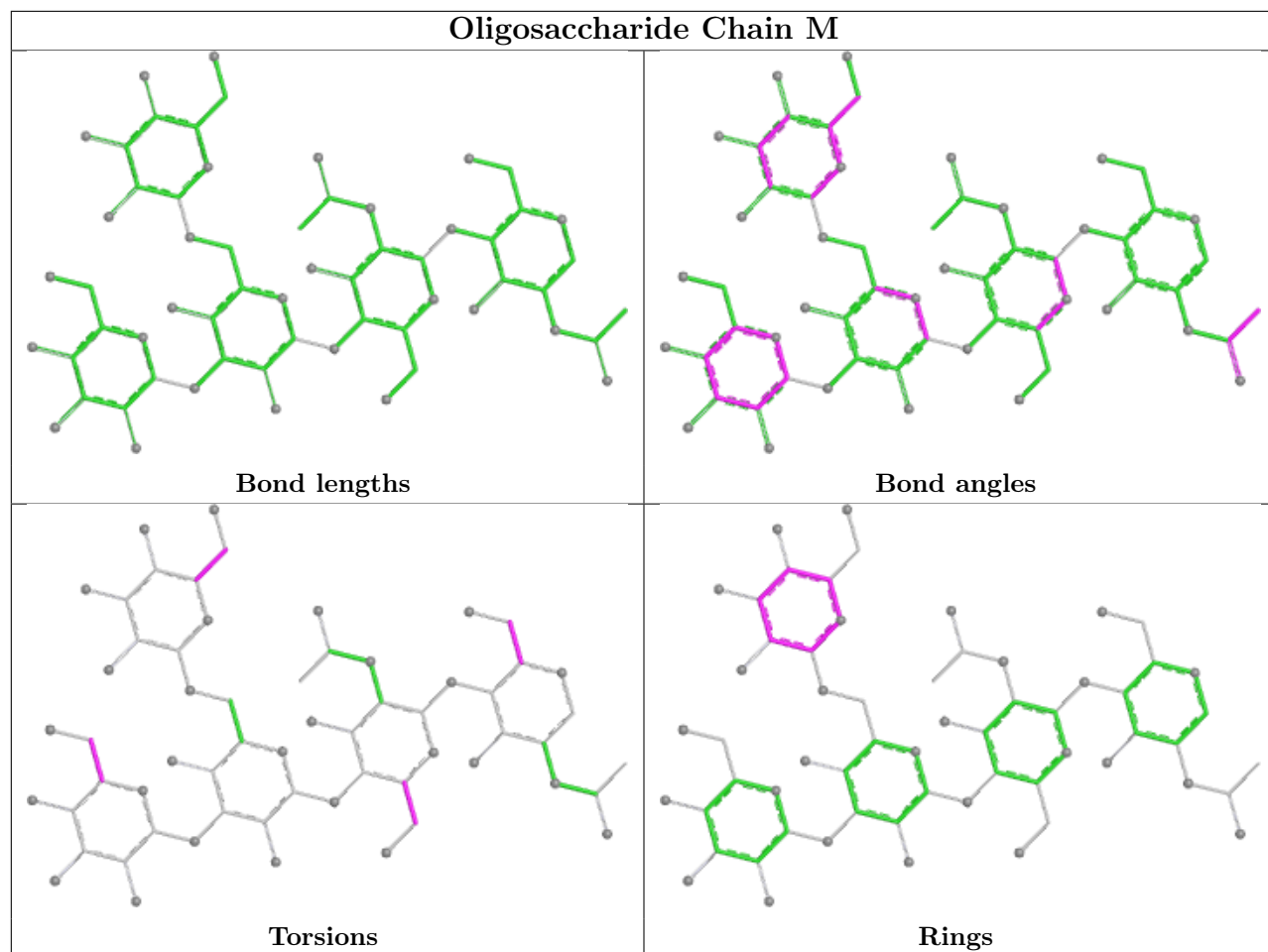
Mol	Chain	Res	Type	Atoms
2	G	5	MAN	C1-C2-C3-C4-C5-O5
2	k	5	MAN	C1-C2-C3-C4-C5-O5
2	f	4	MAN	C1-C2-C3-C4-C5-O5
2	i	5	MAN	C1-C2-C3-C4-C5-O5
2	M	5	MAN	C1-C2-C3-C4-C5-O5

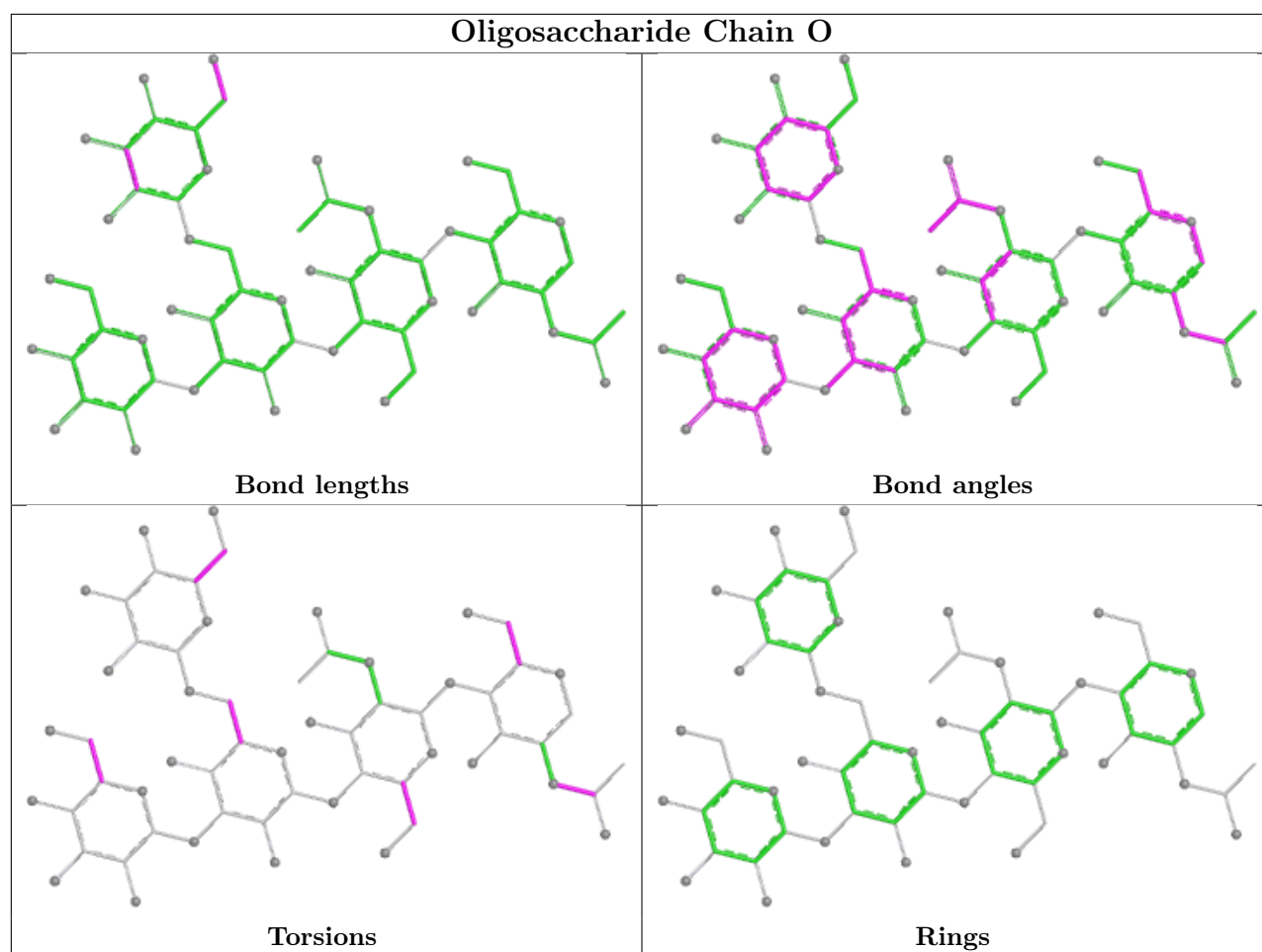
No monomer is involved in short contacts.

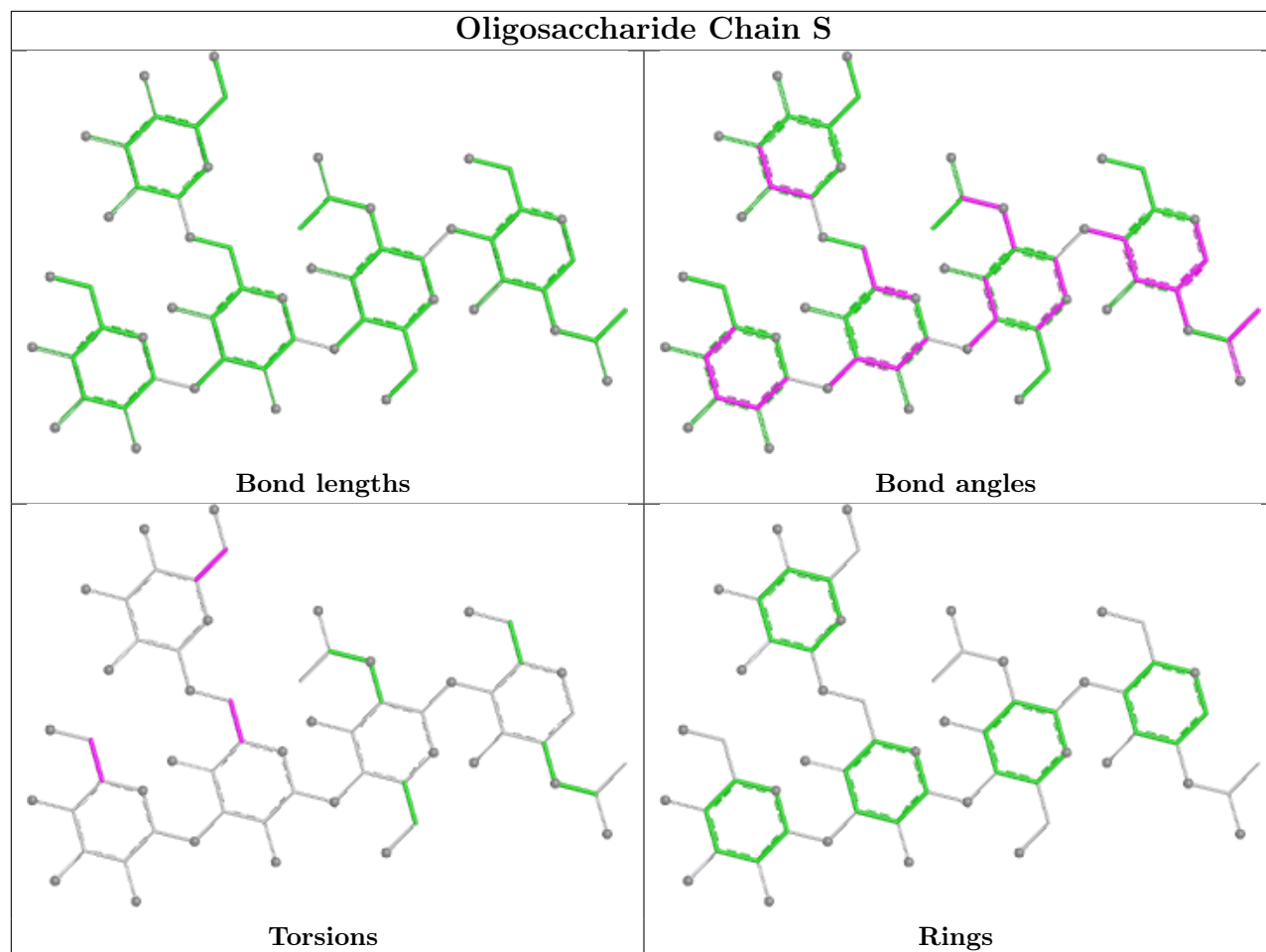
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

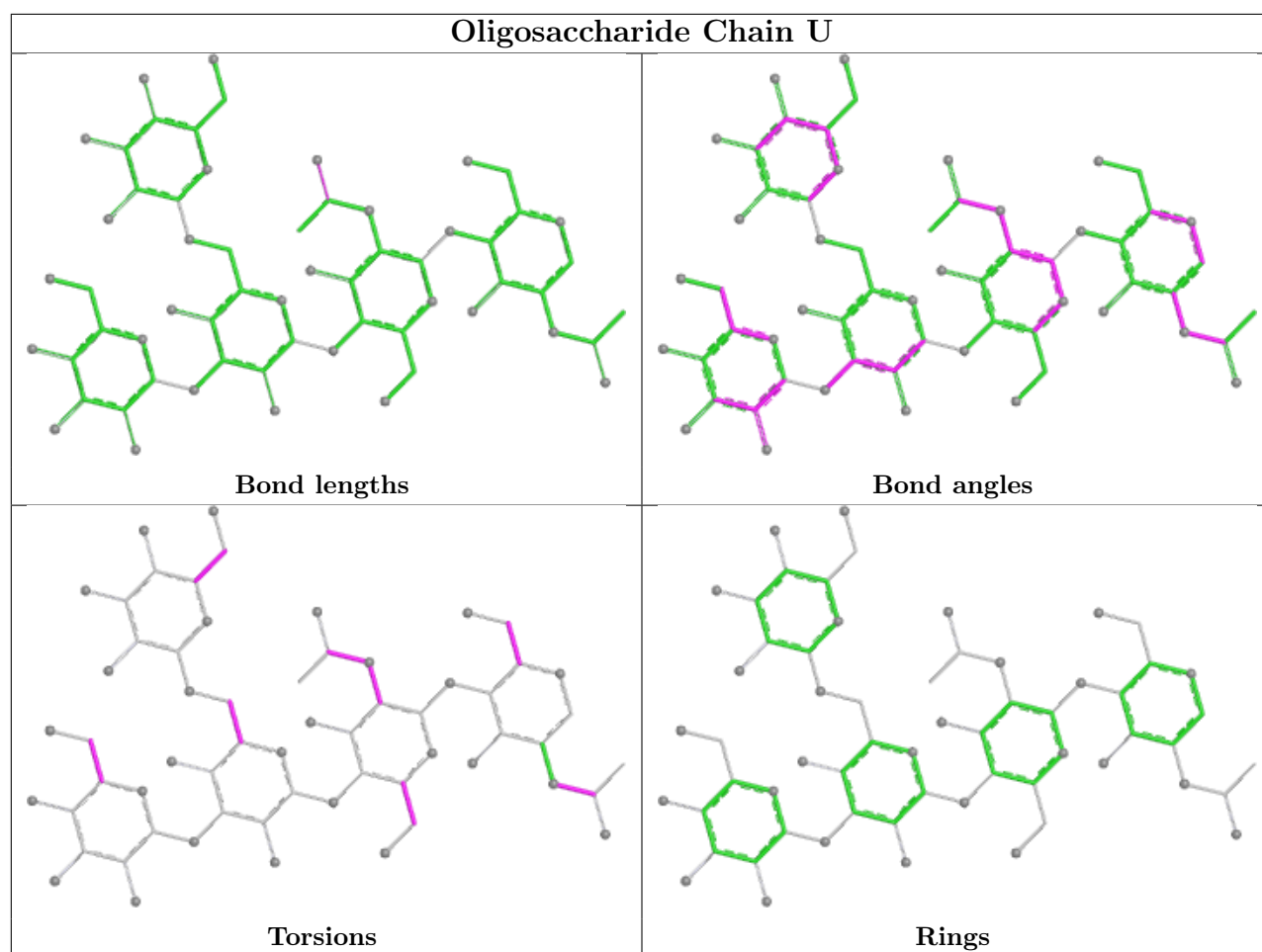


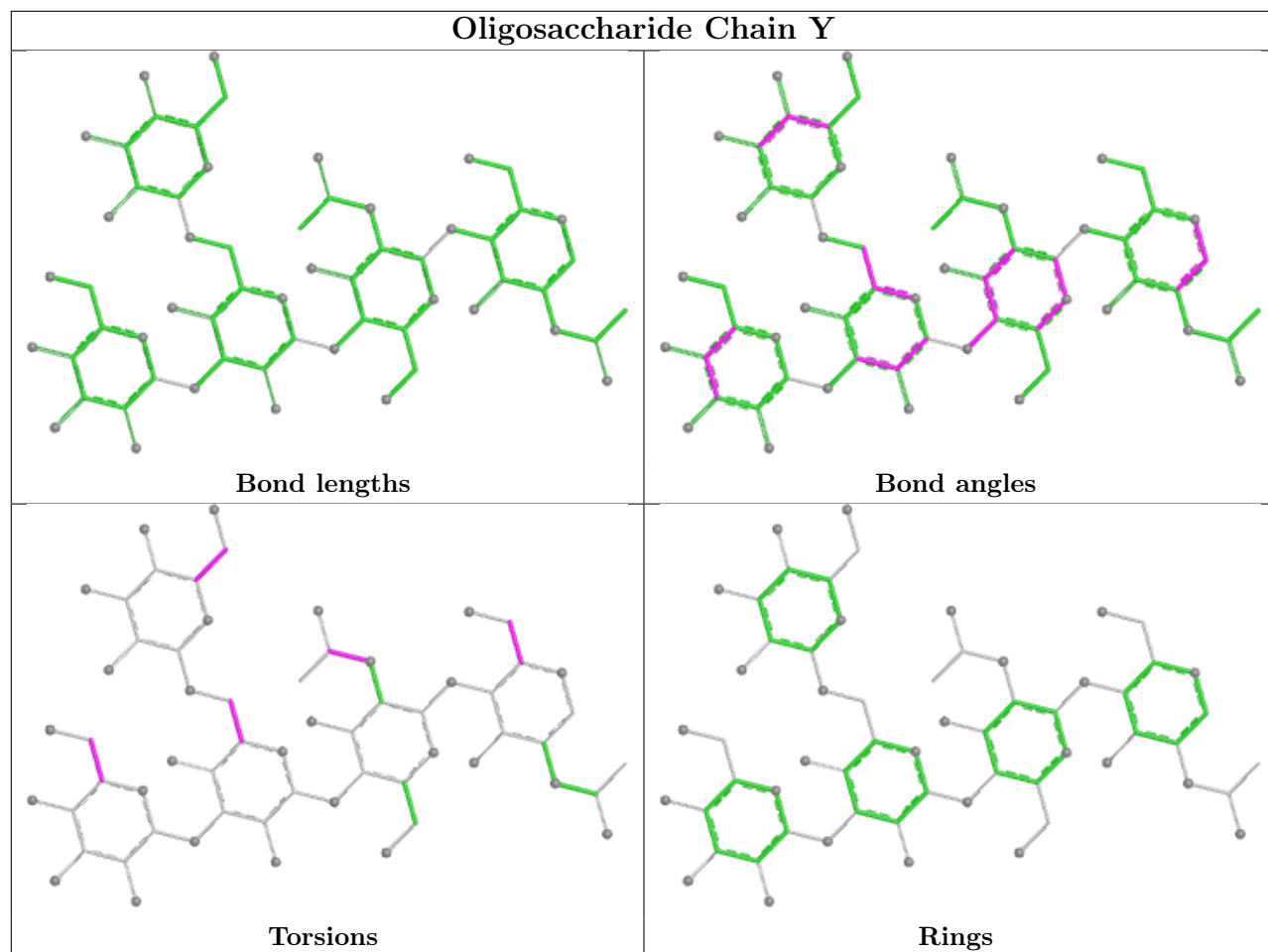




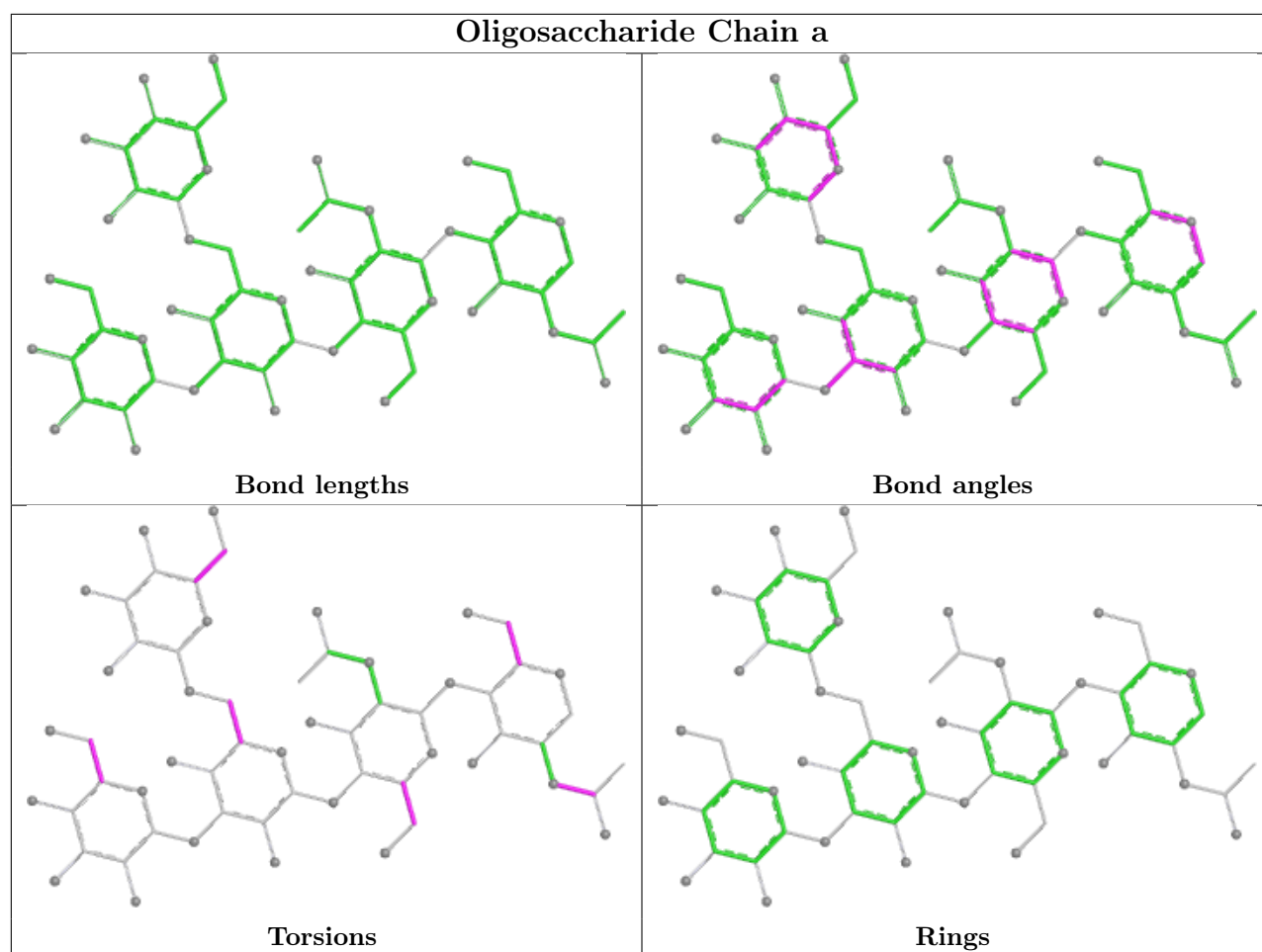


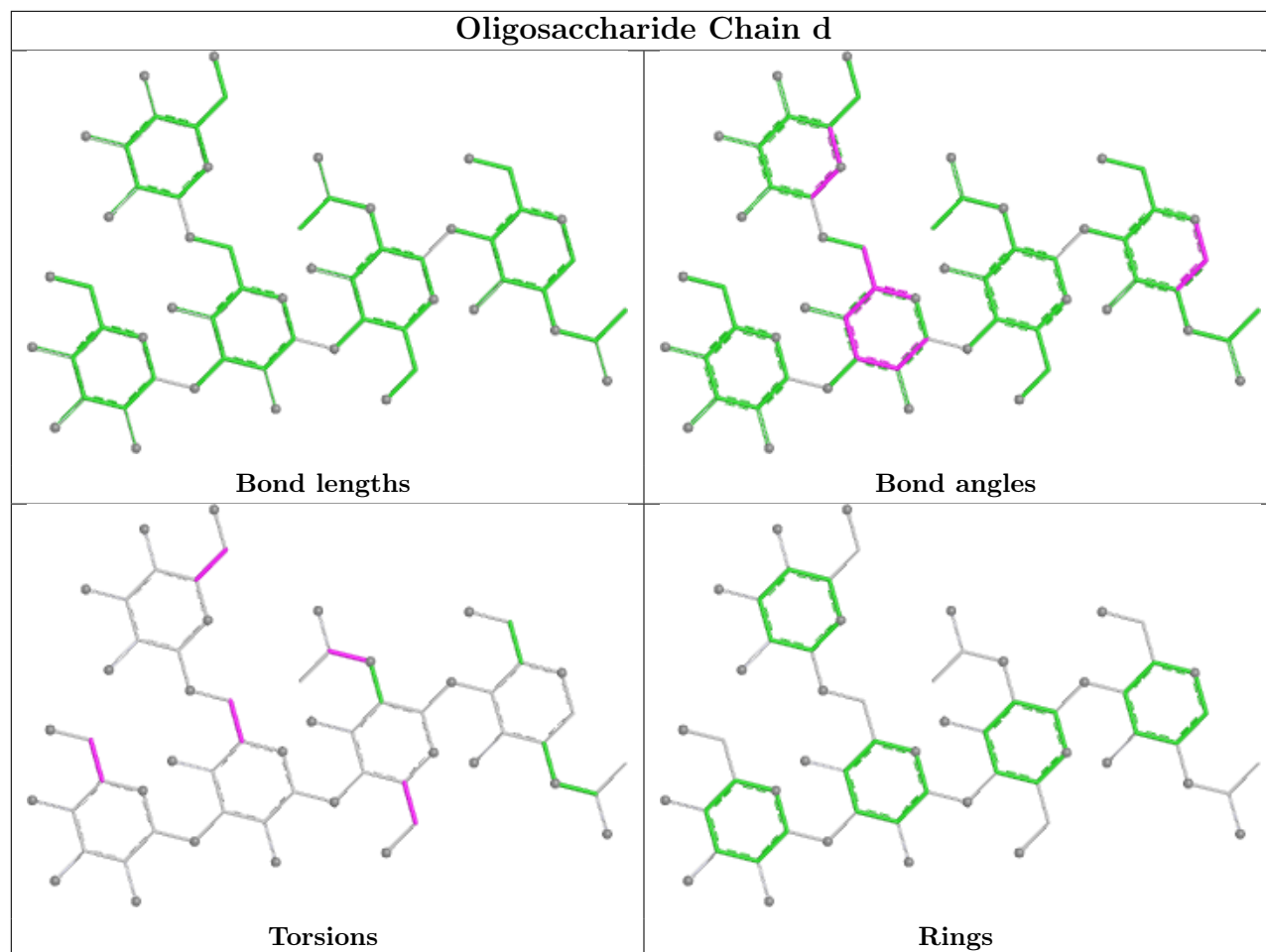


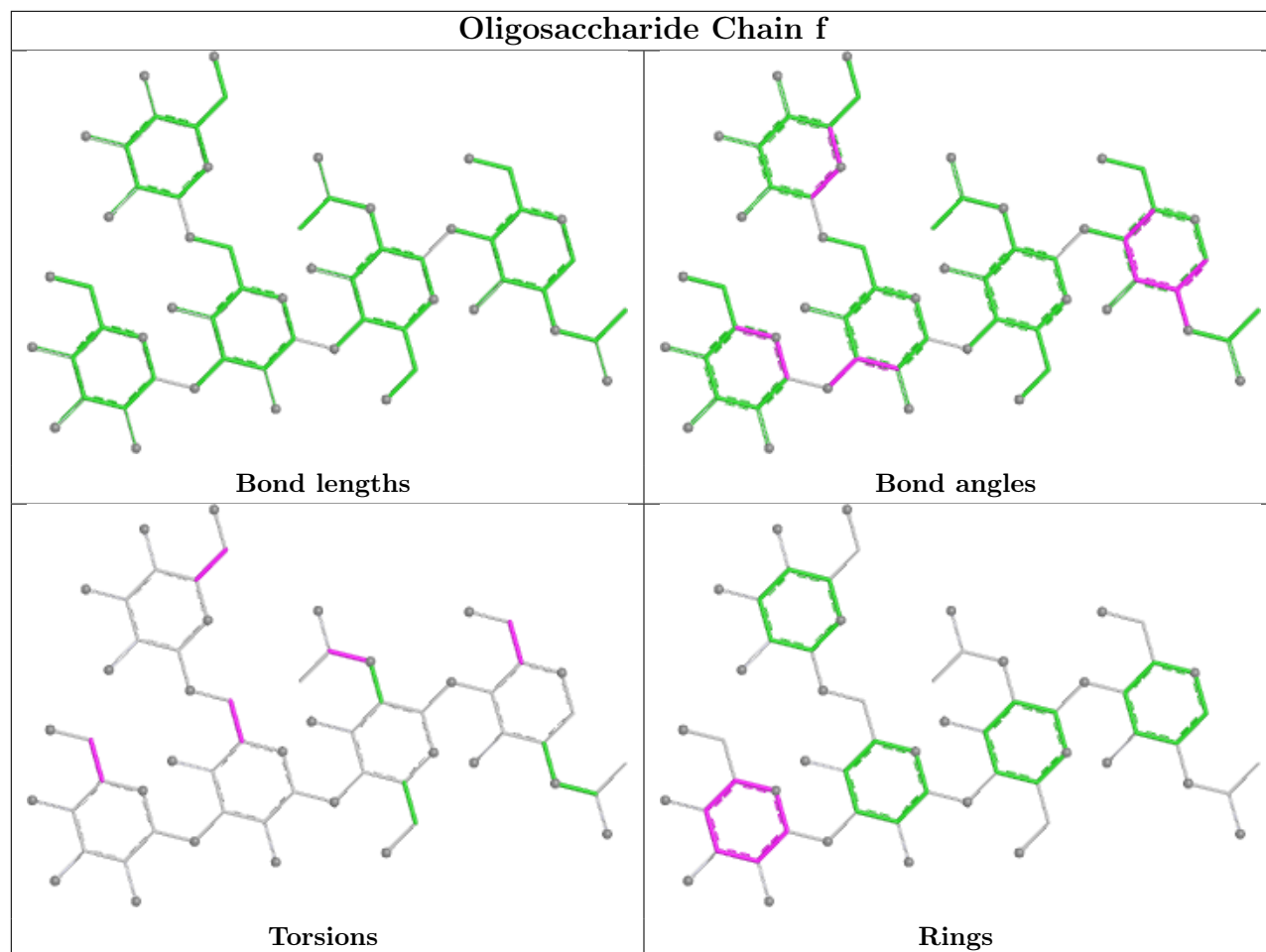


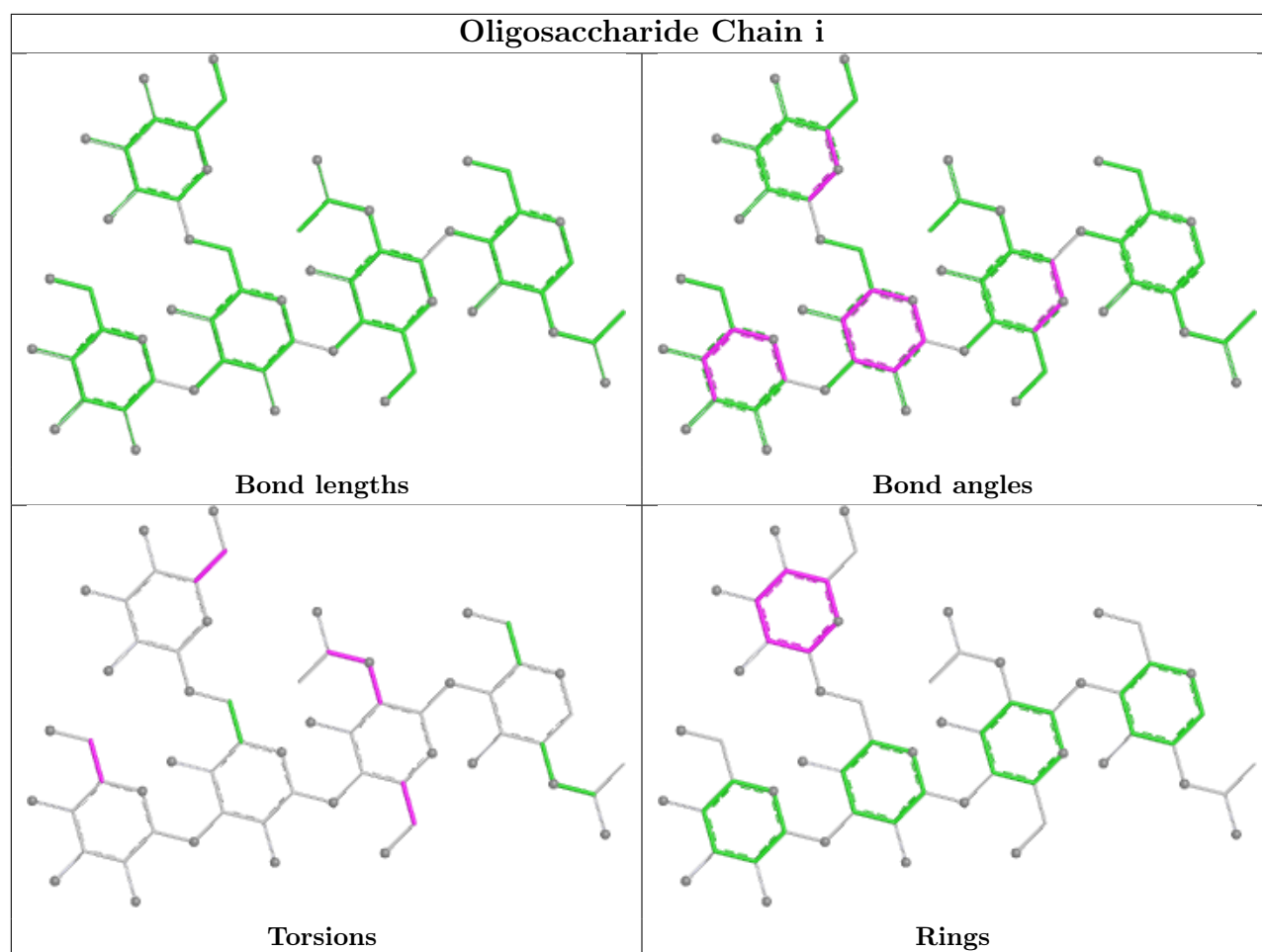


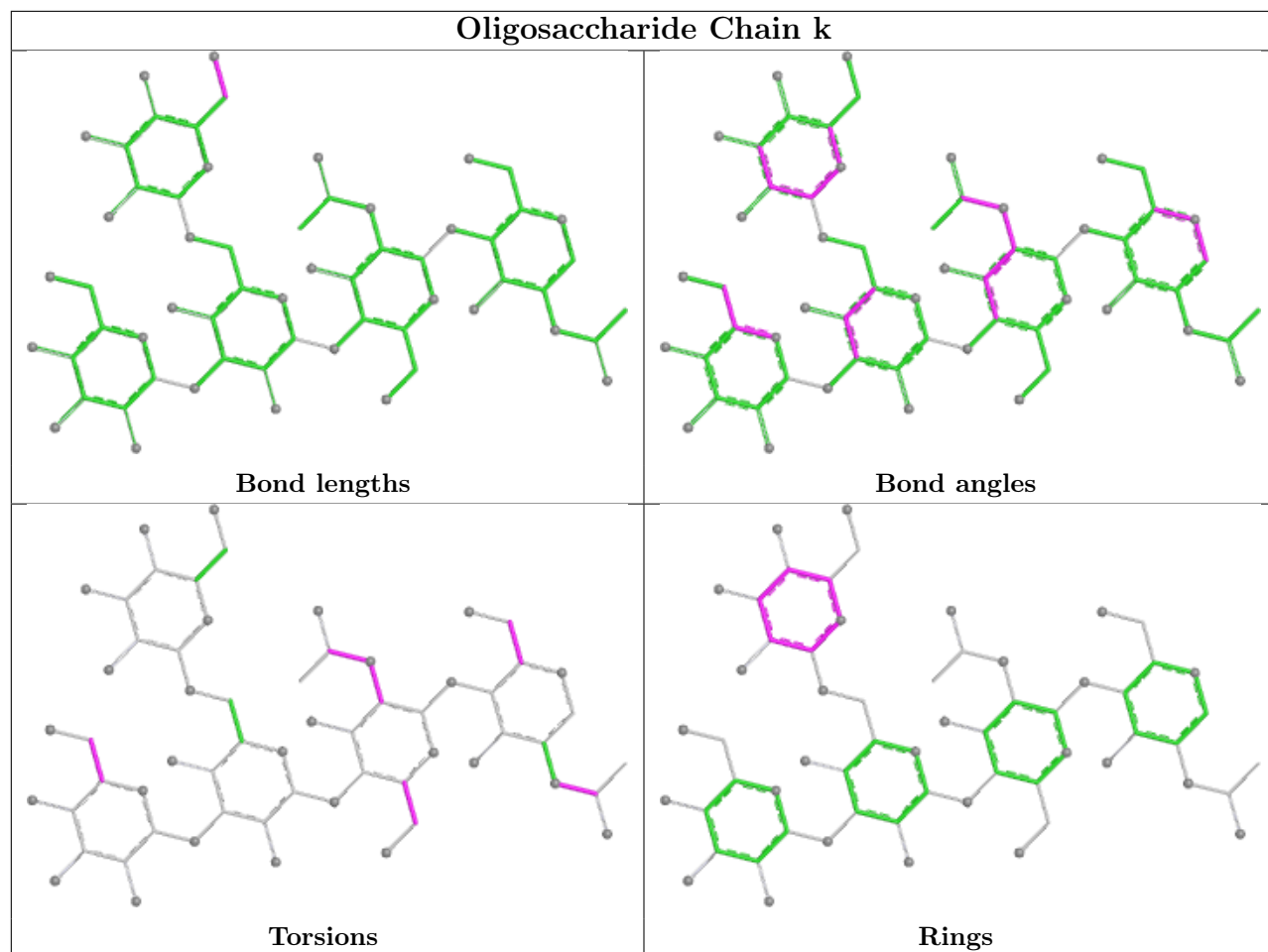


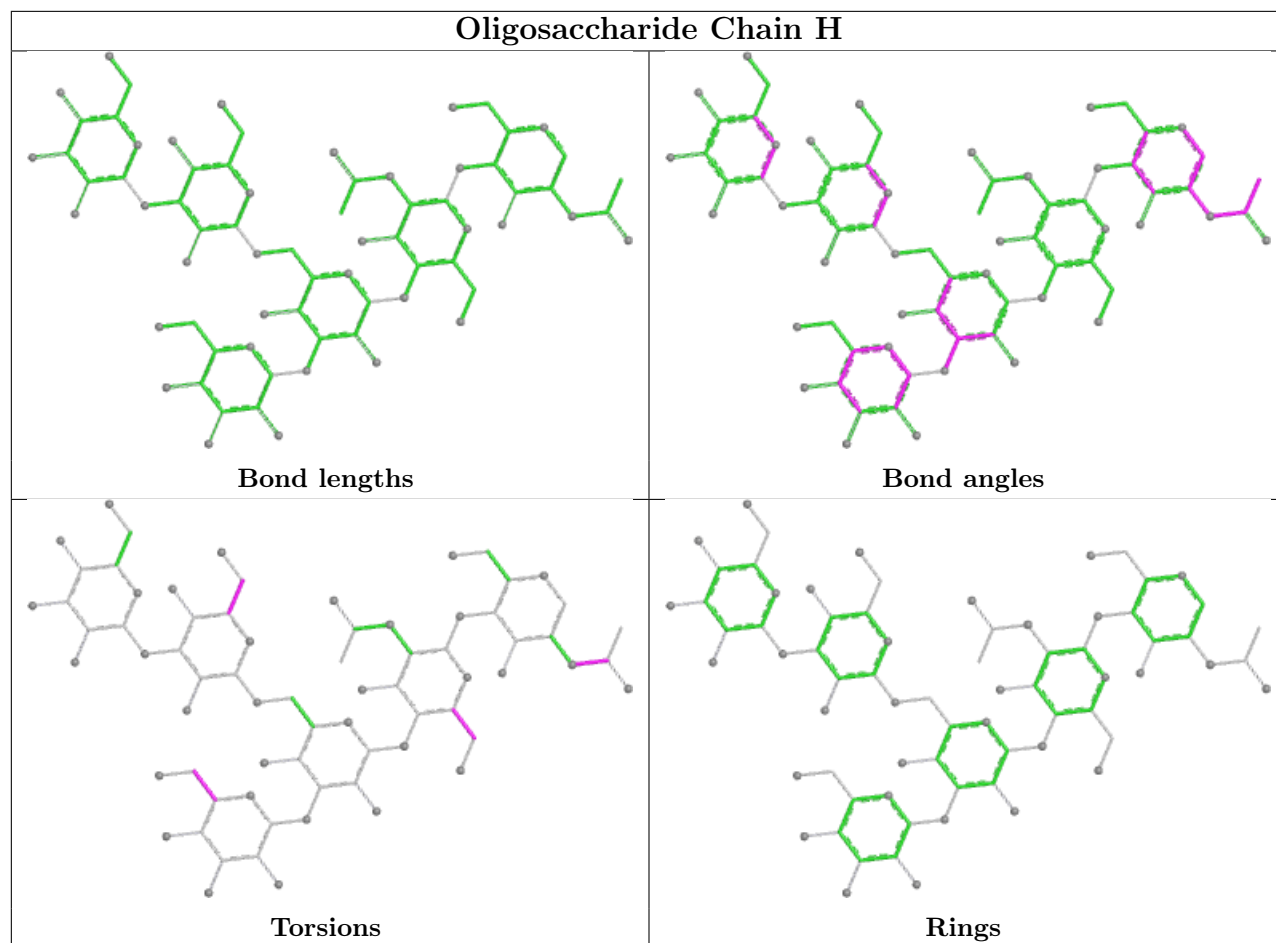


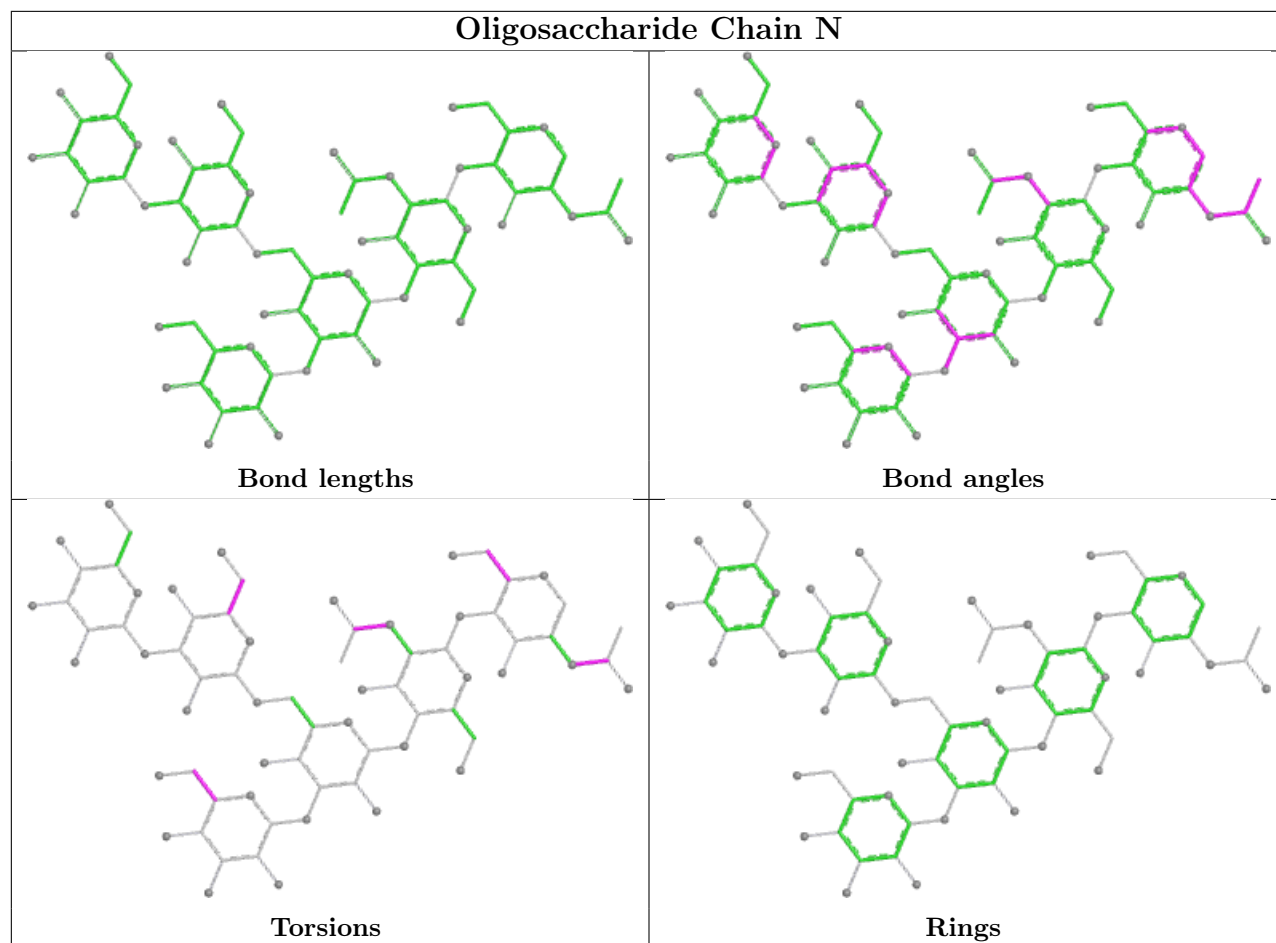


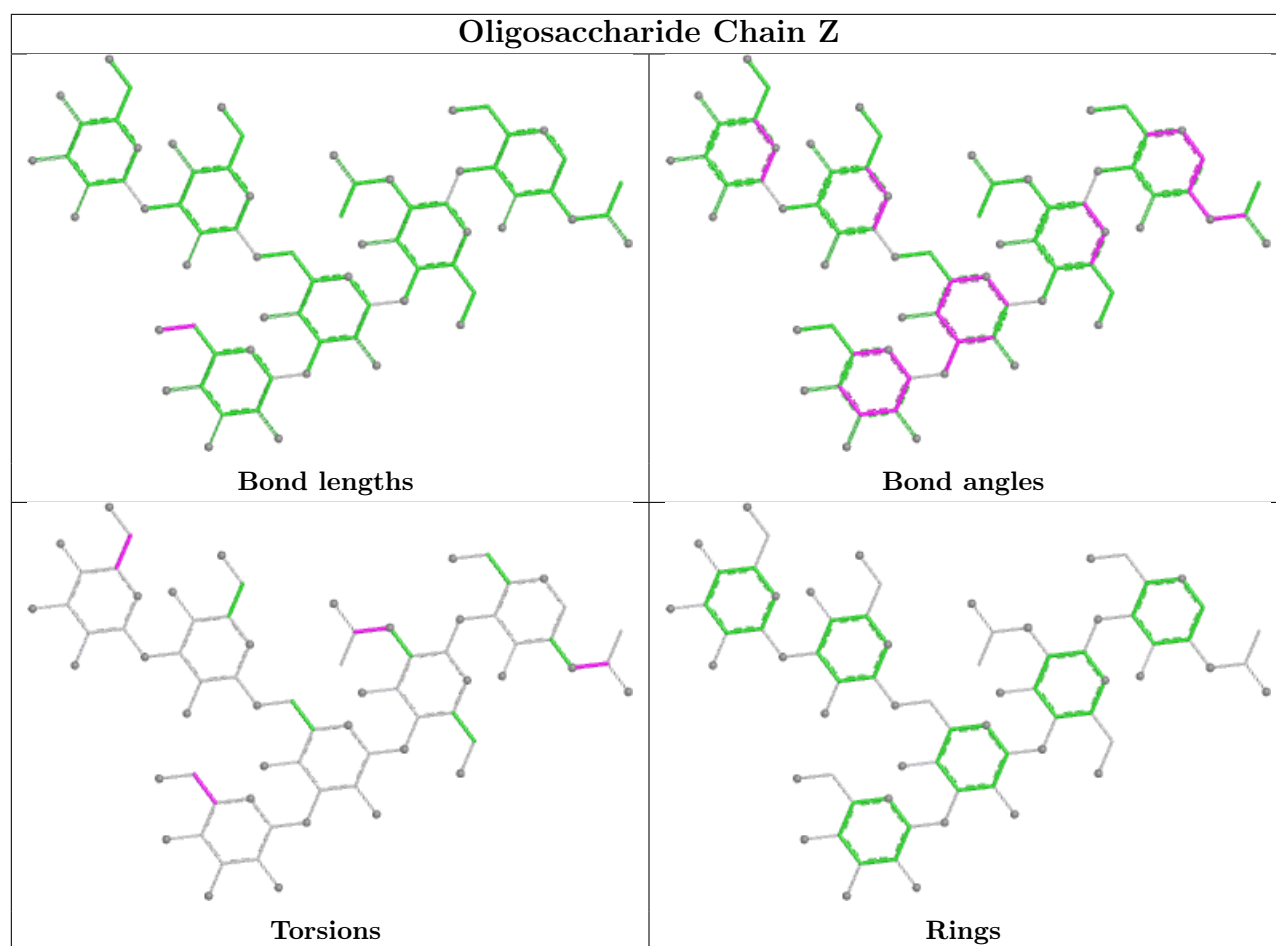




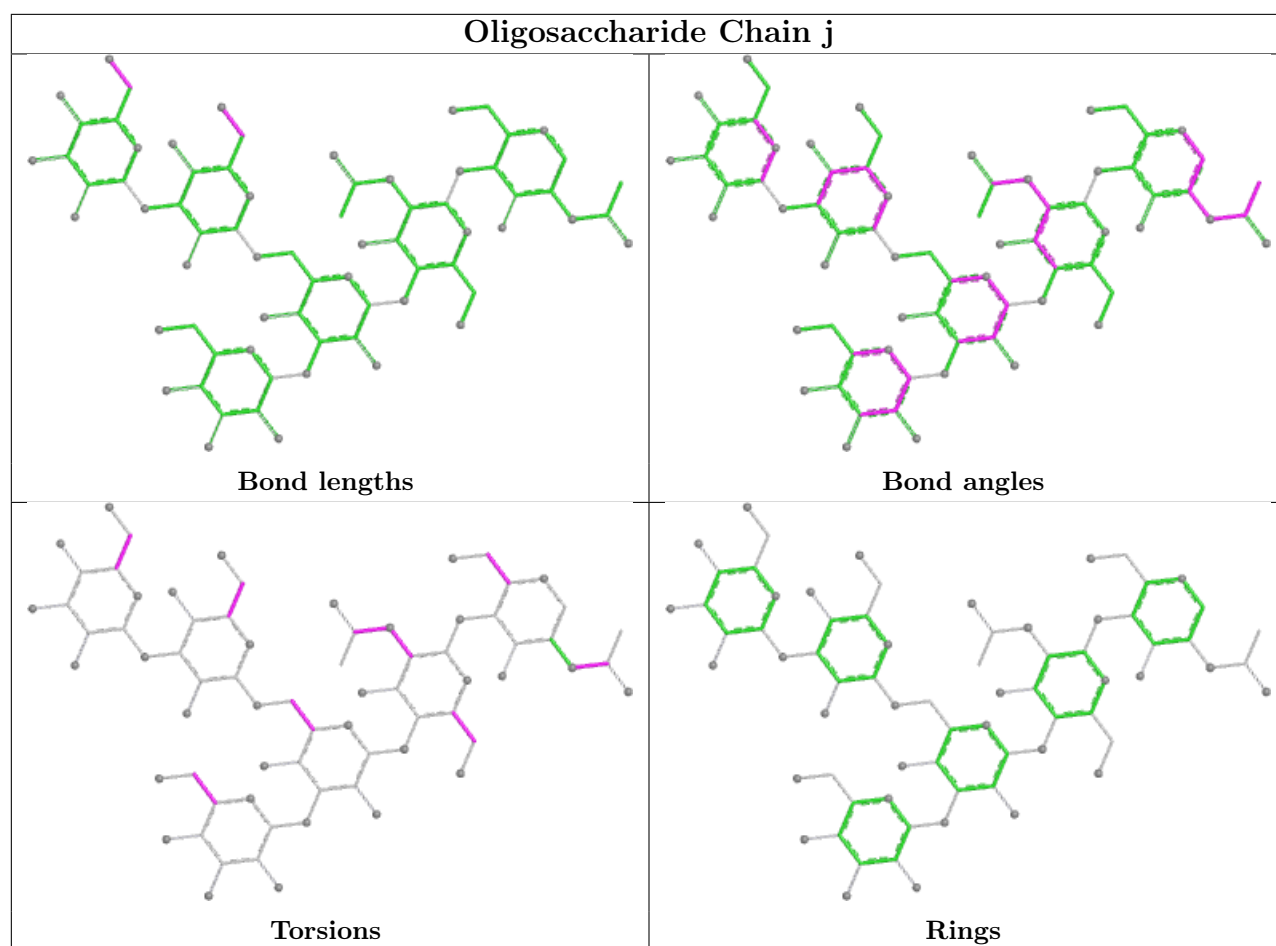


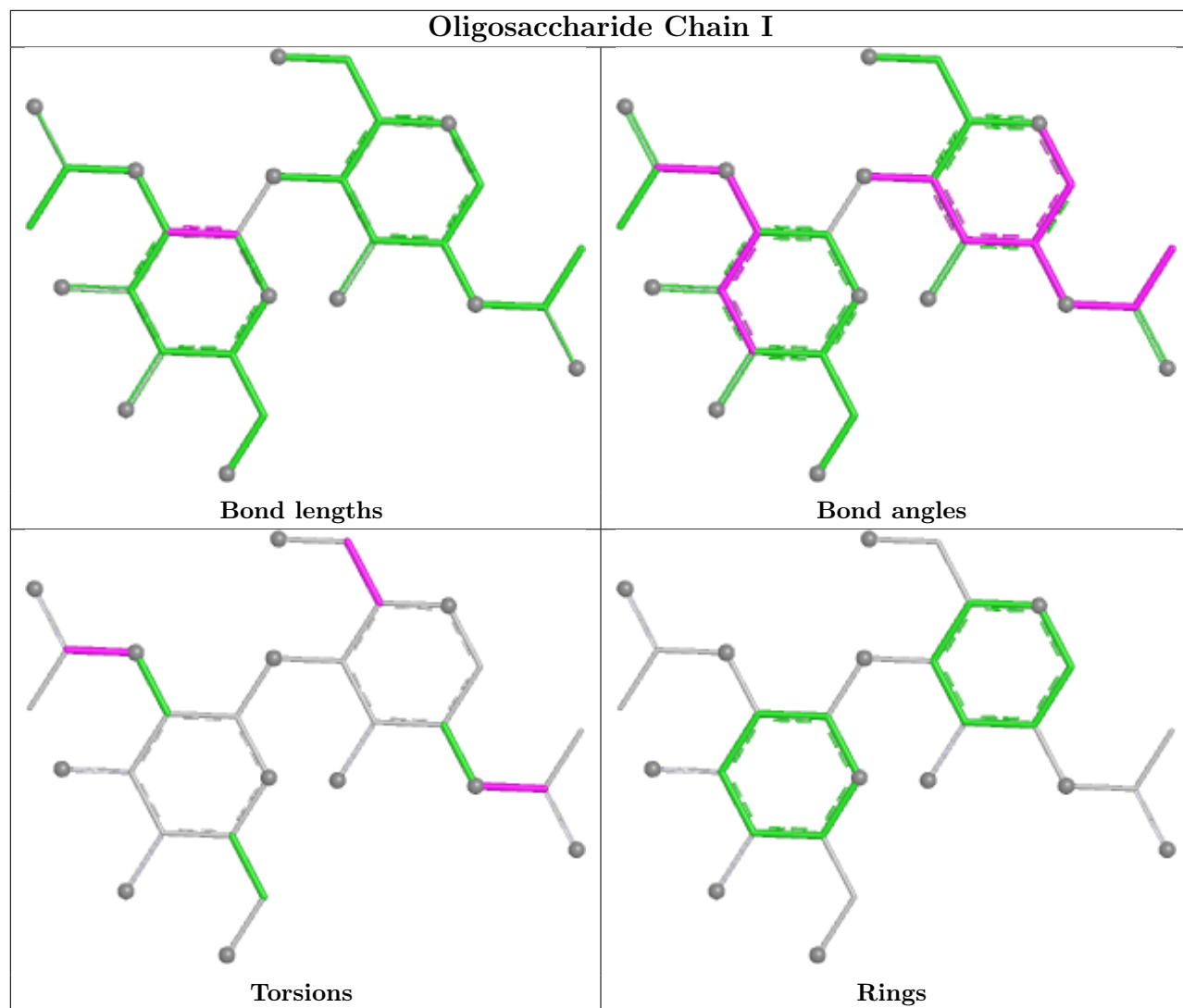


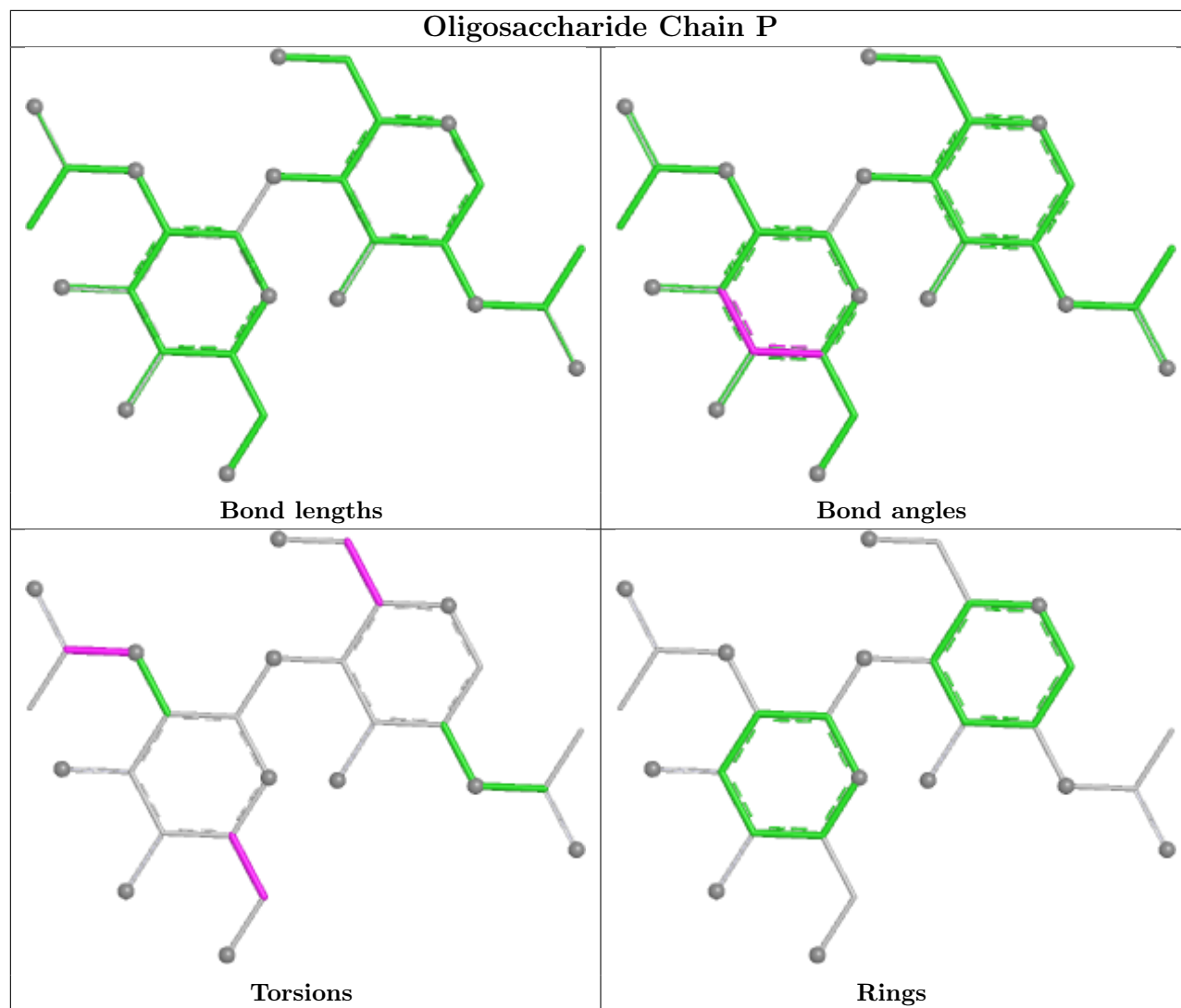


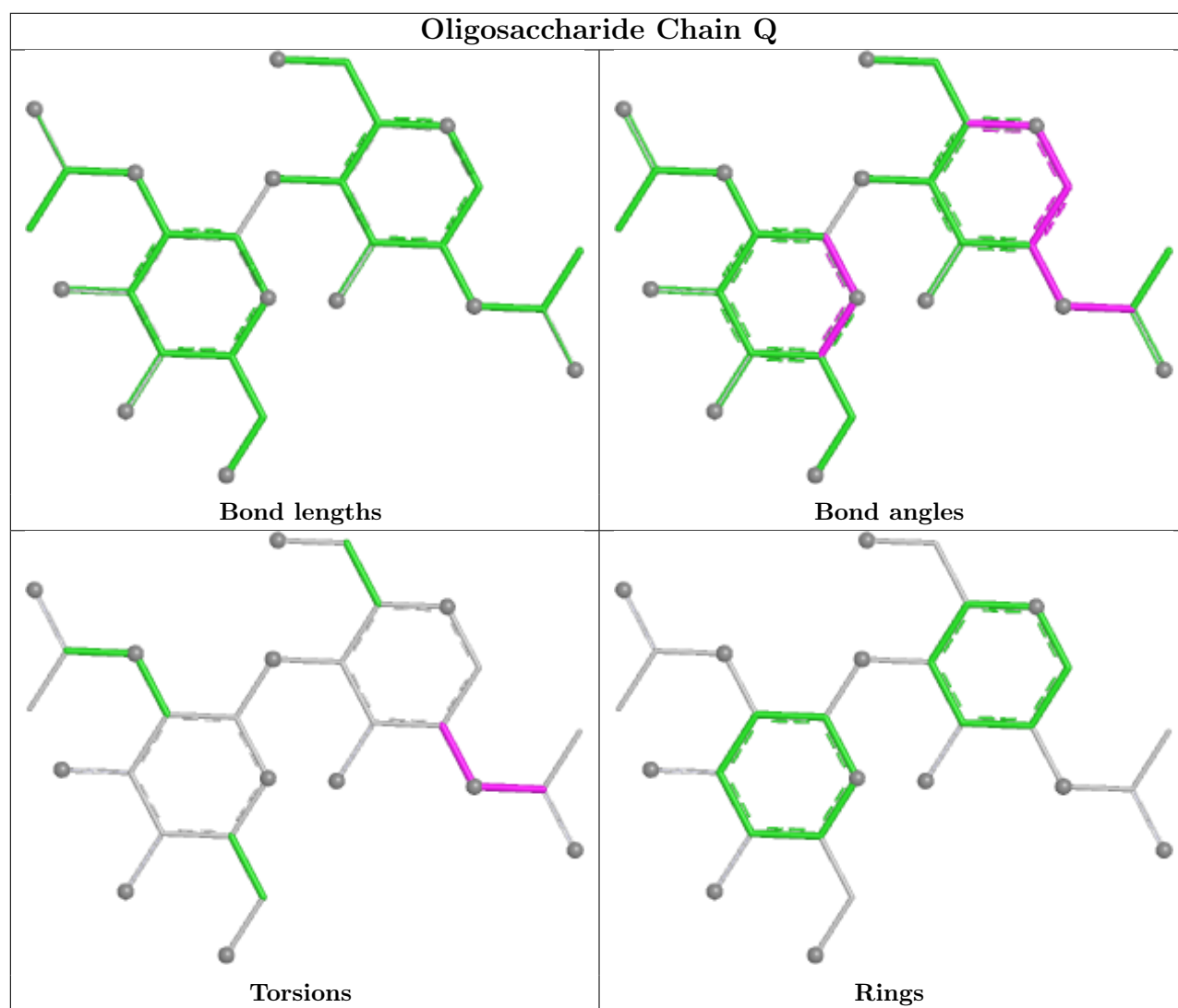


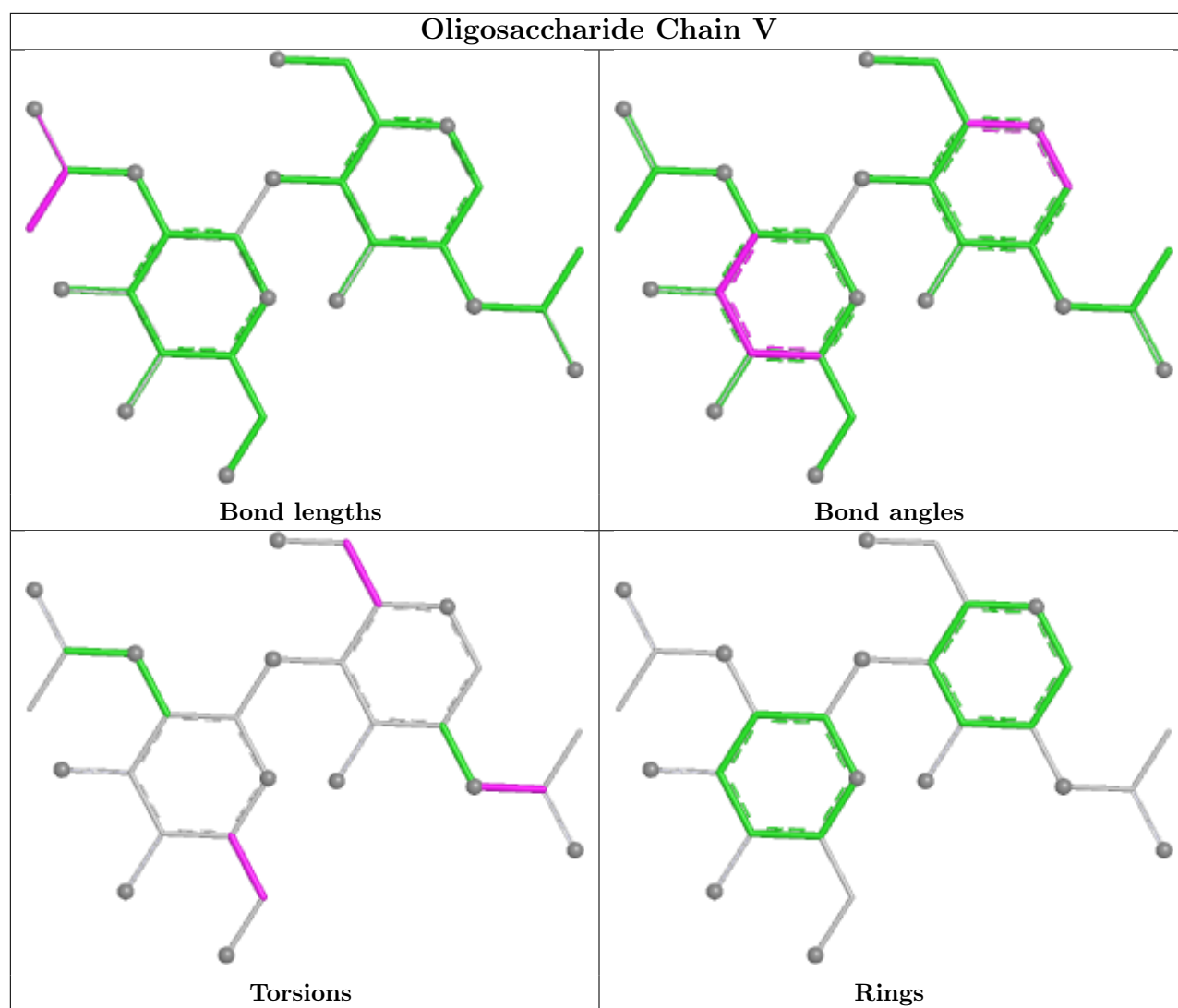


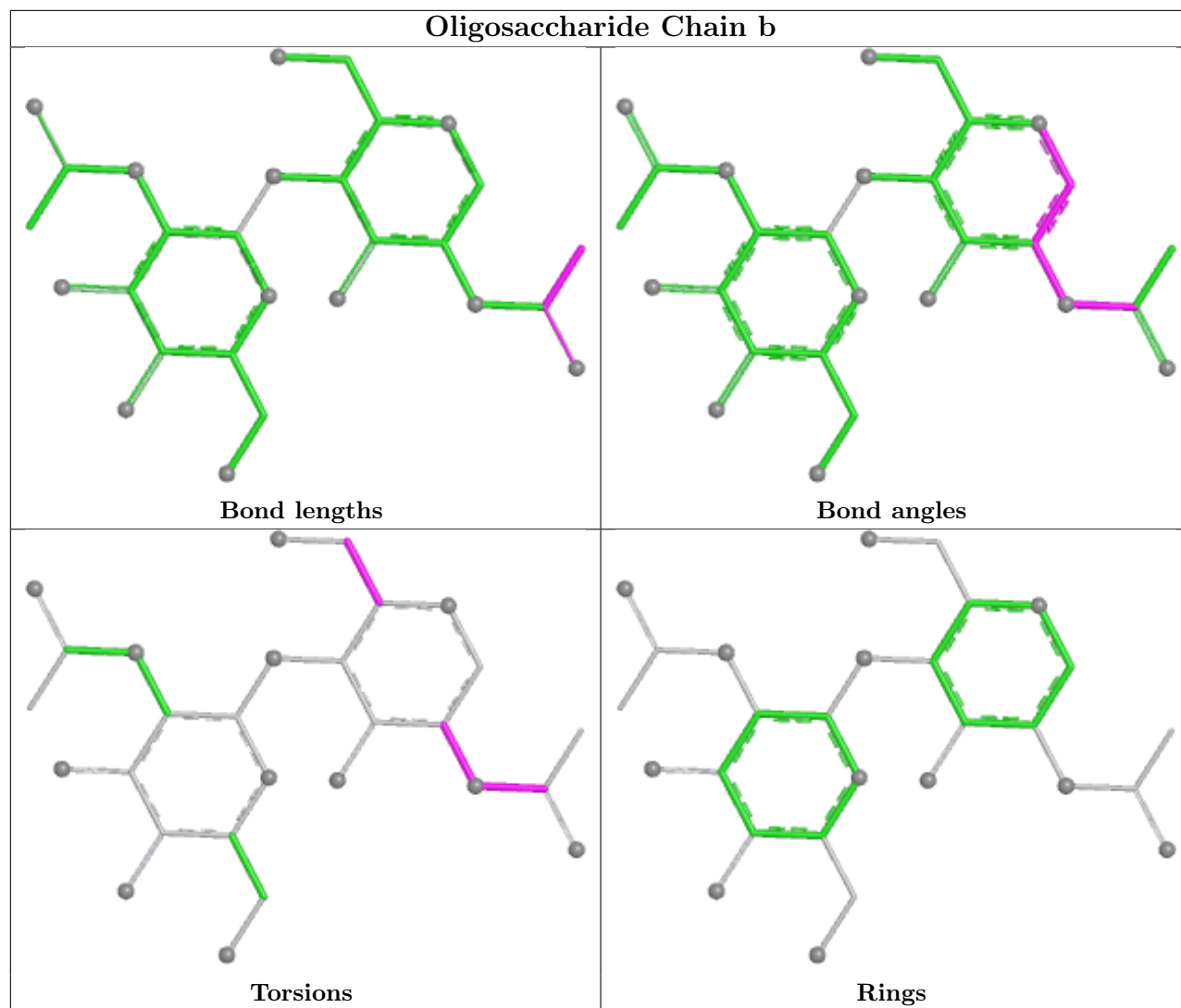


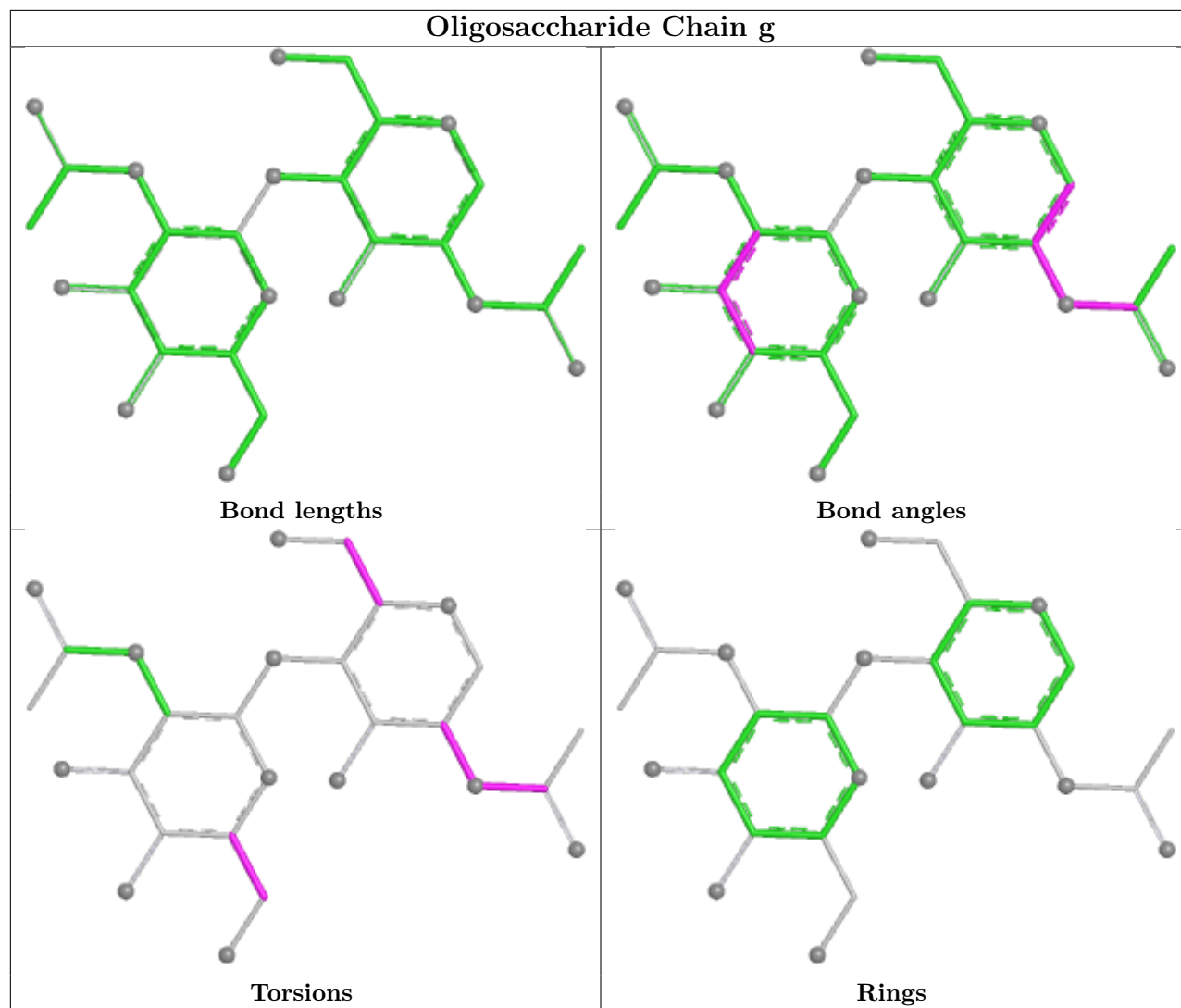




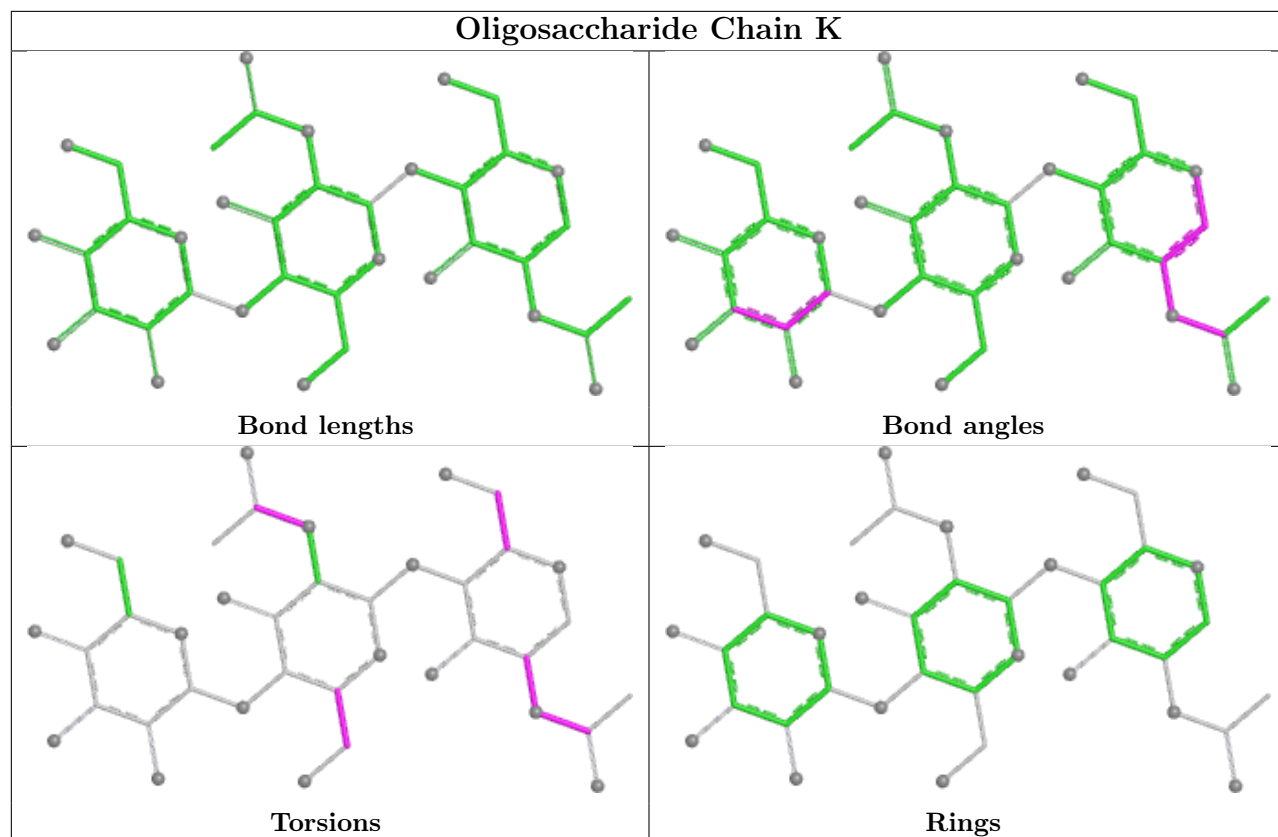




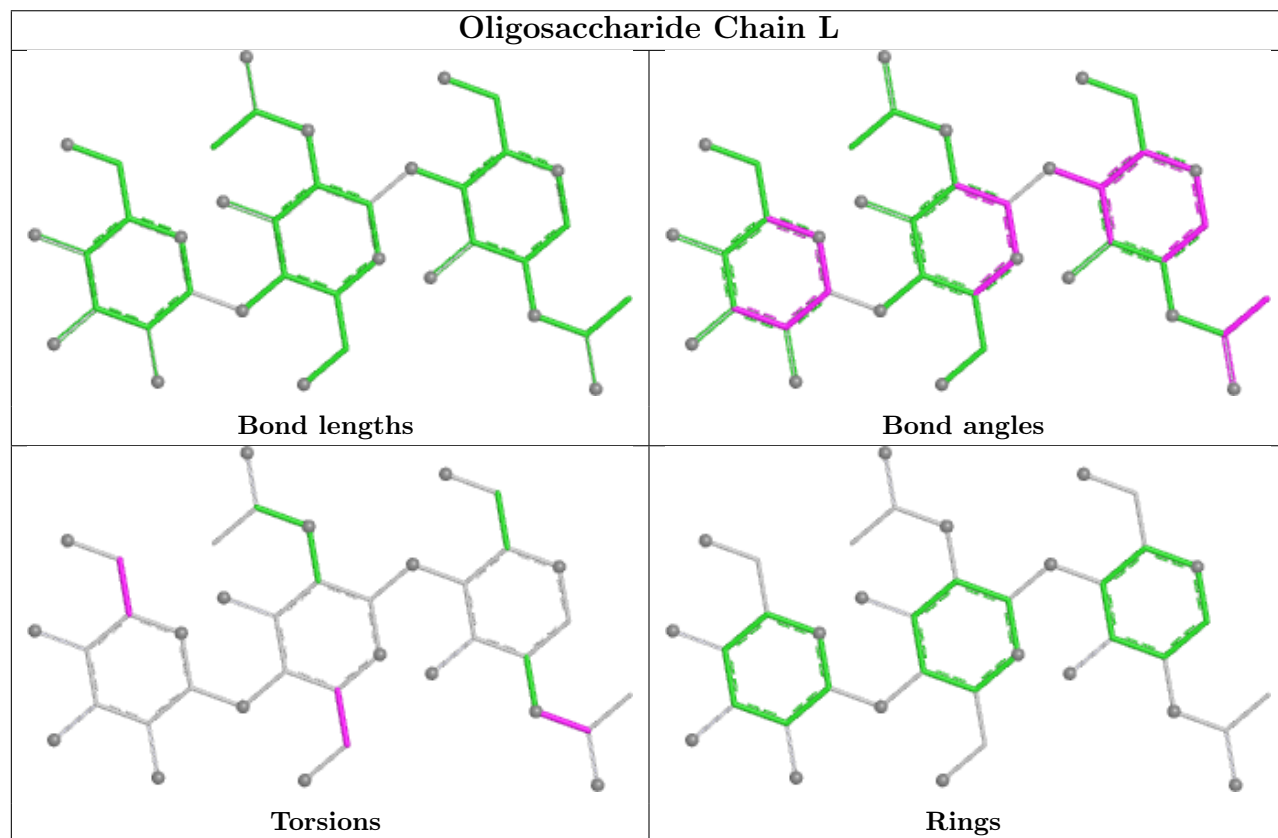




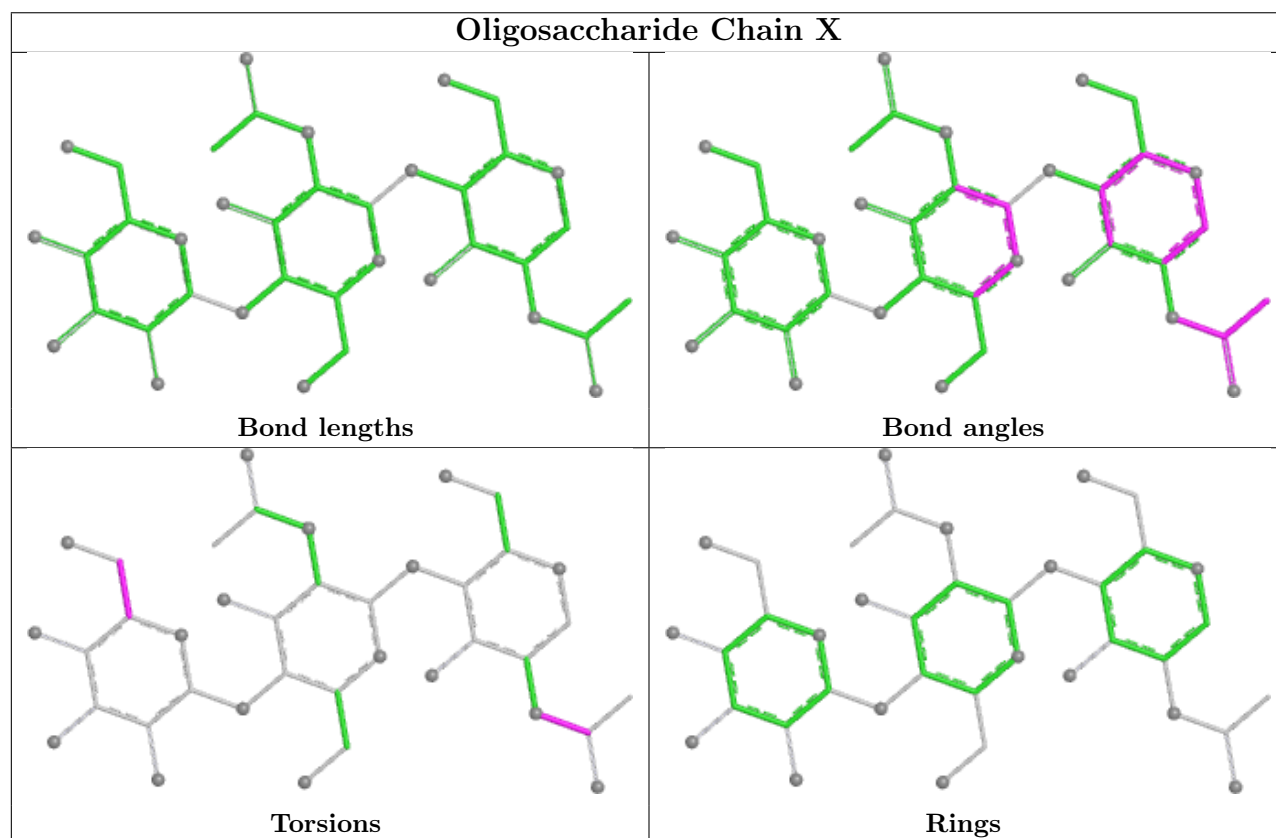
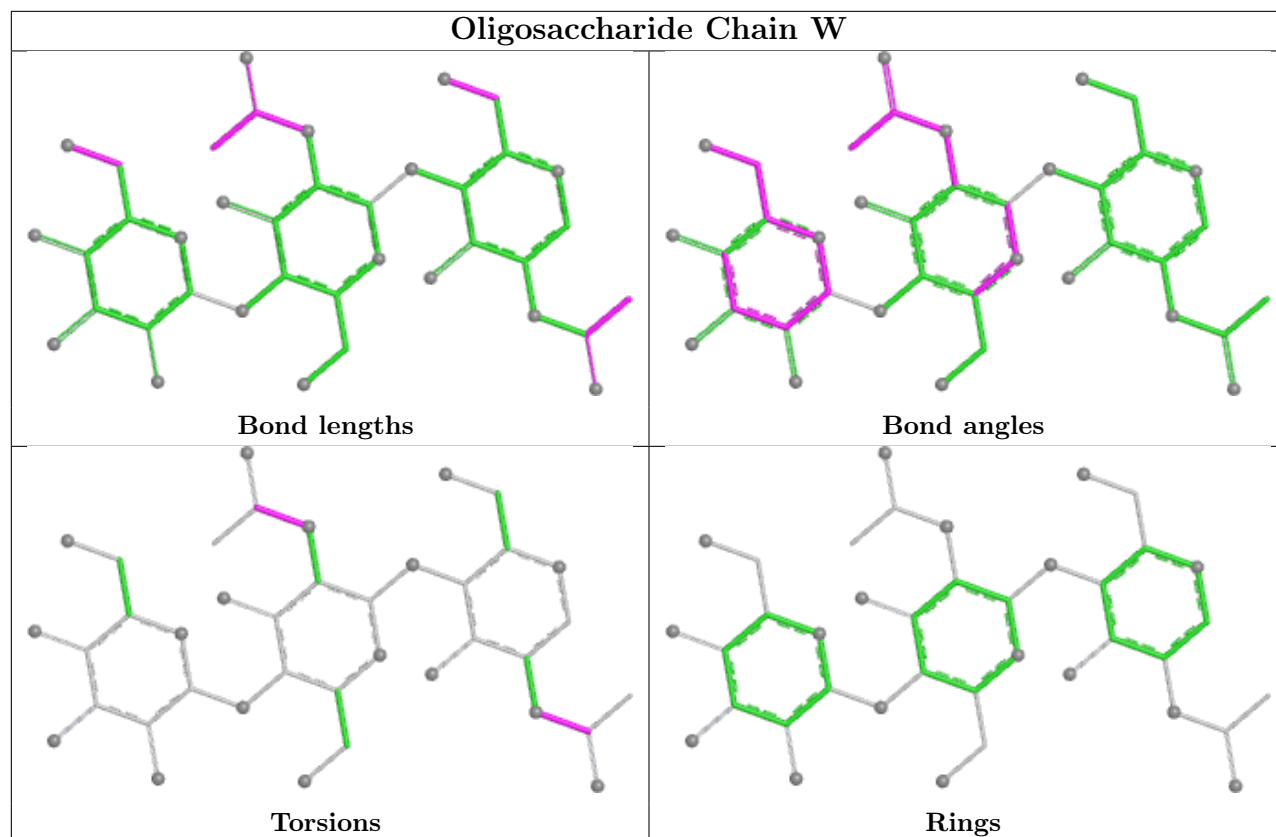
## Oligosaccharide Chain K

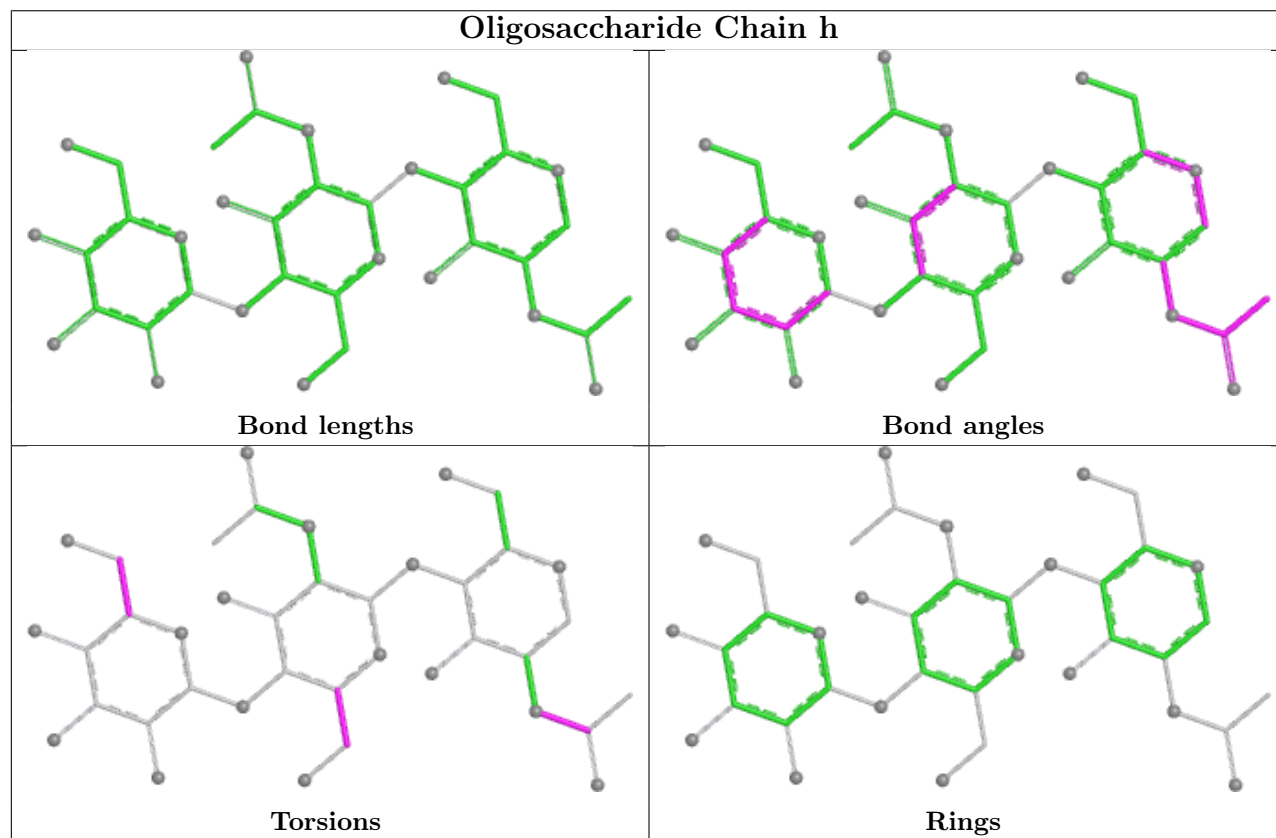
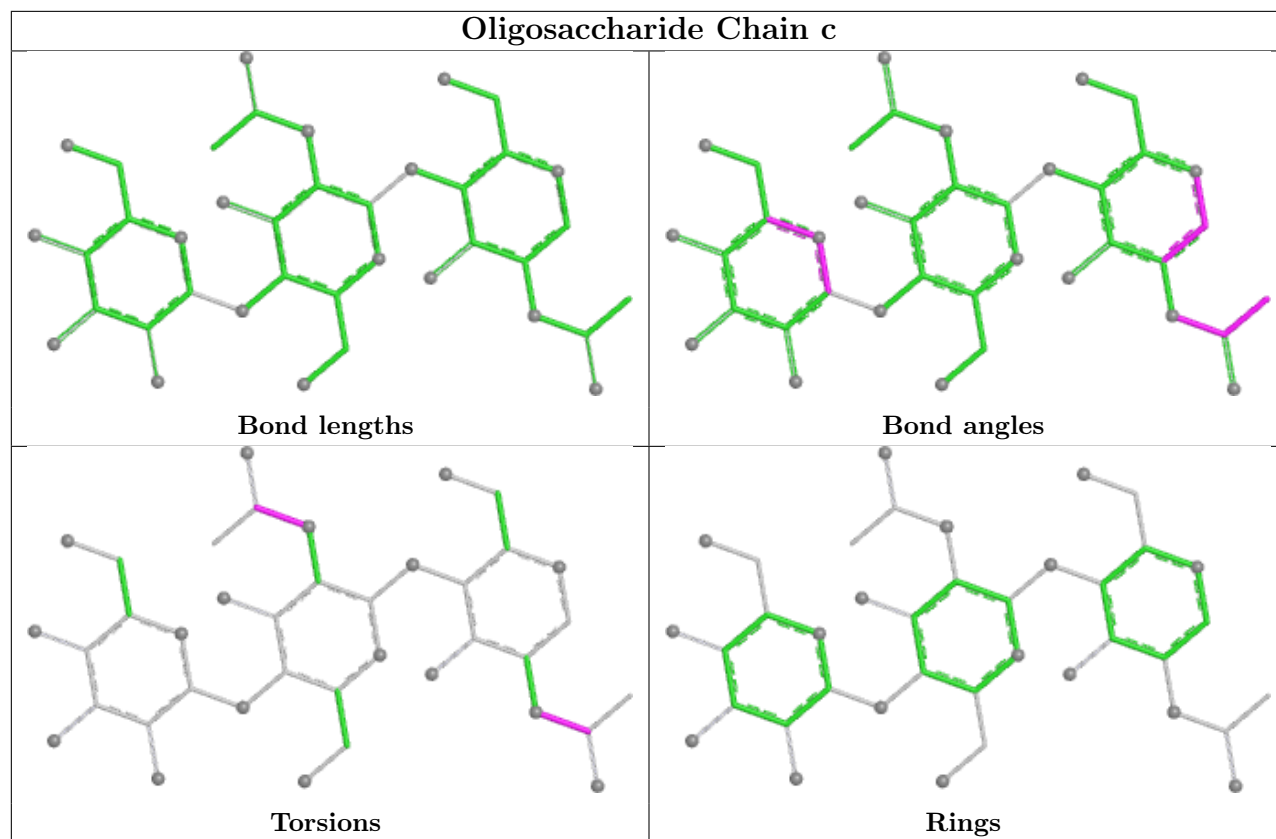


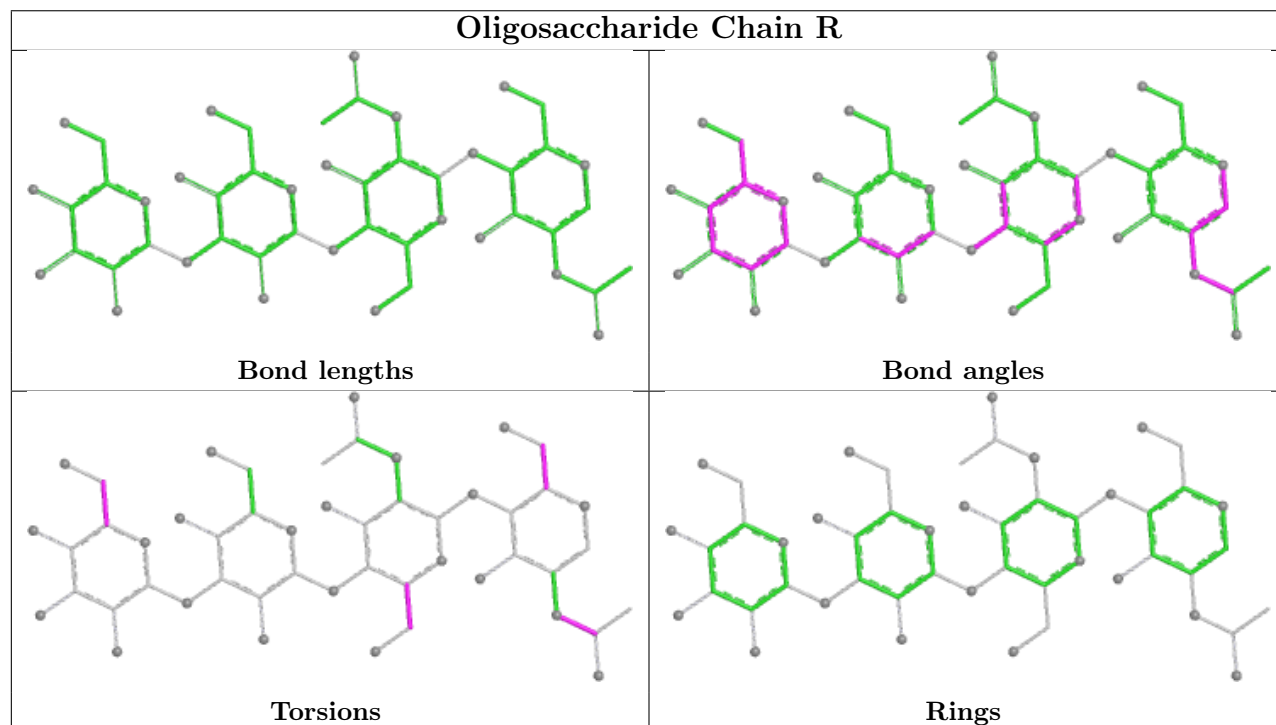
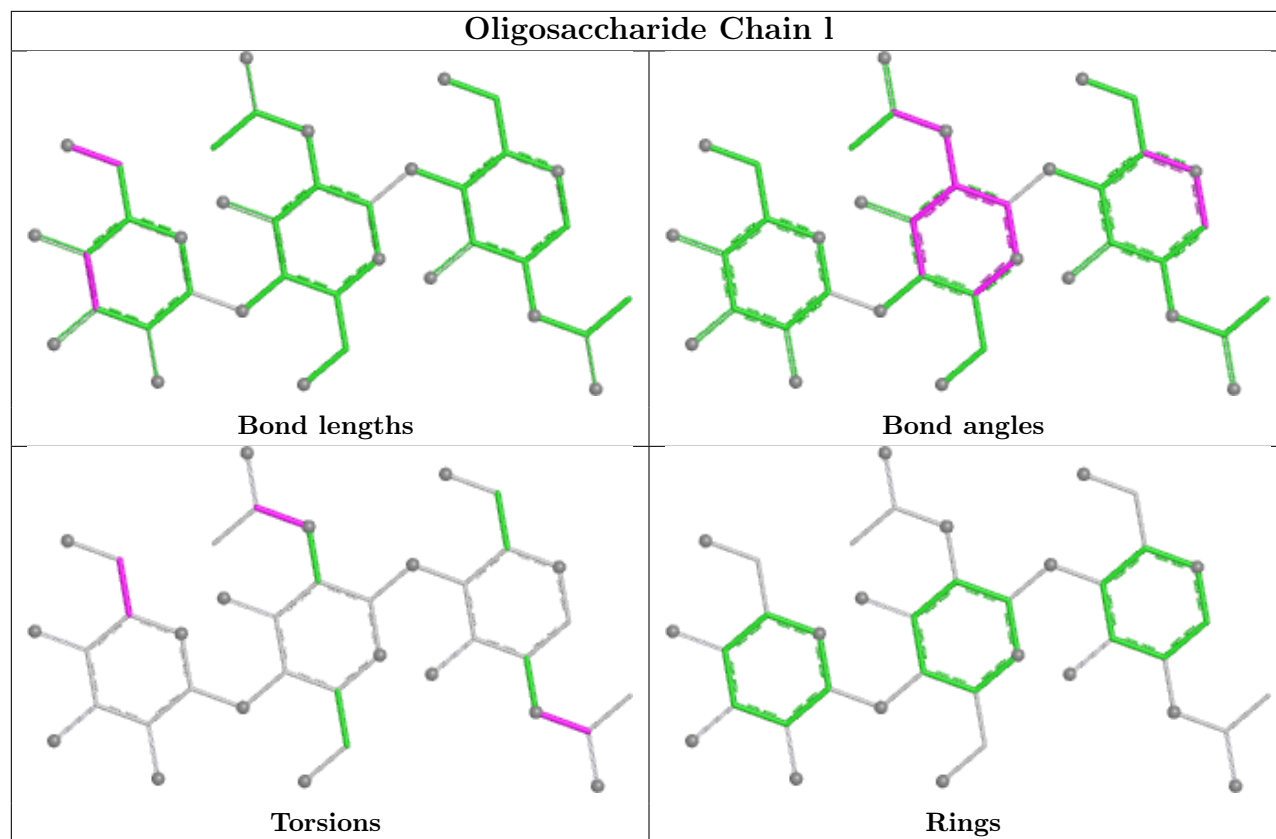
## Oligosaccharide Chain L

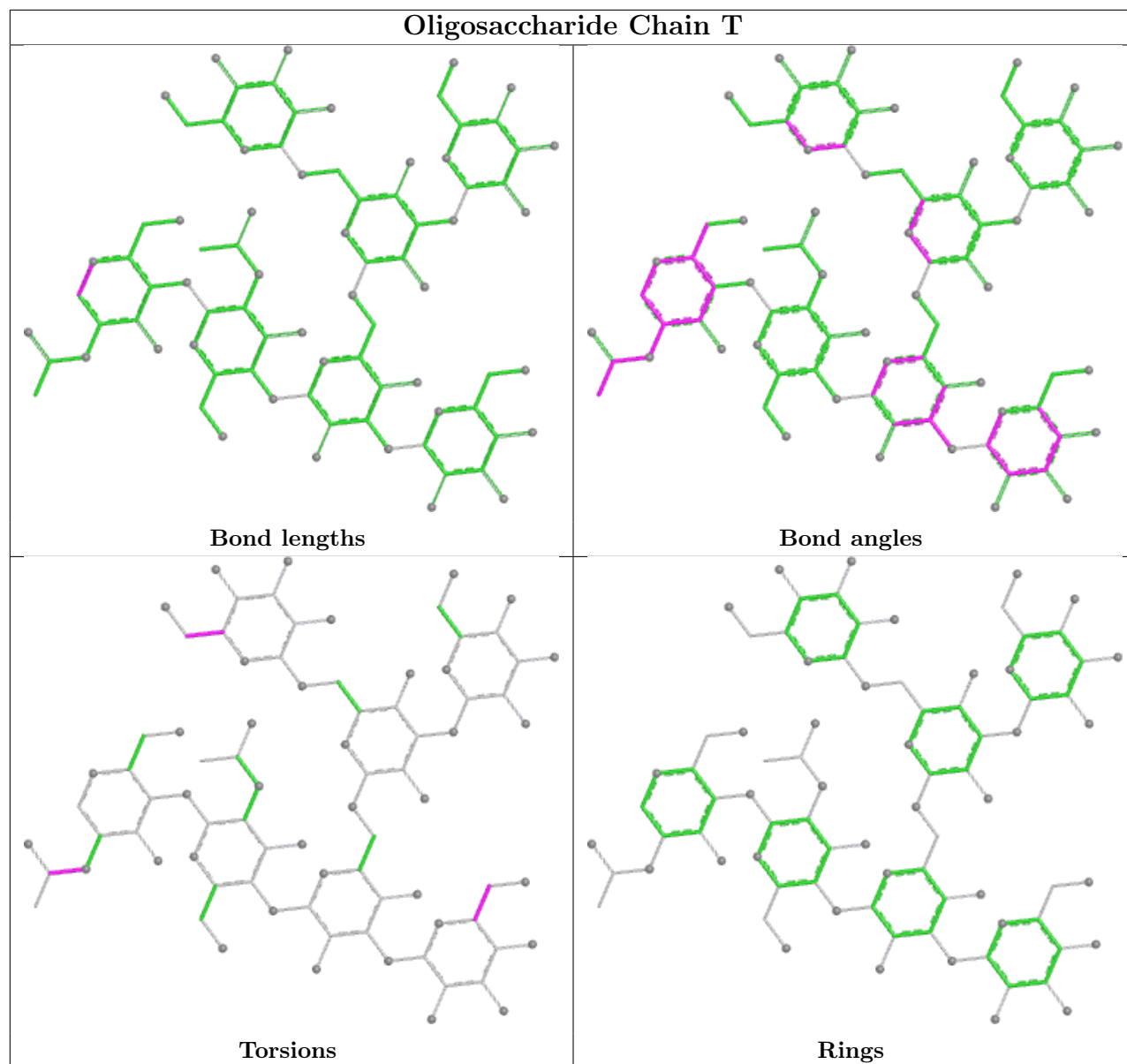


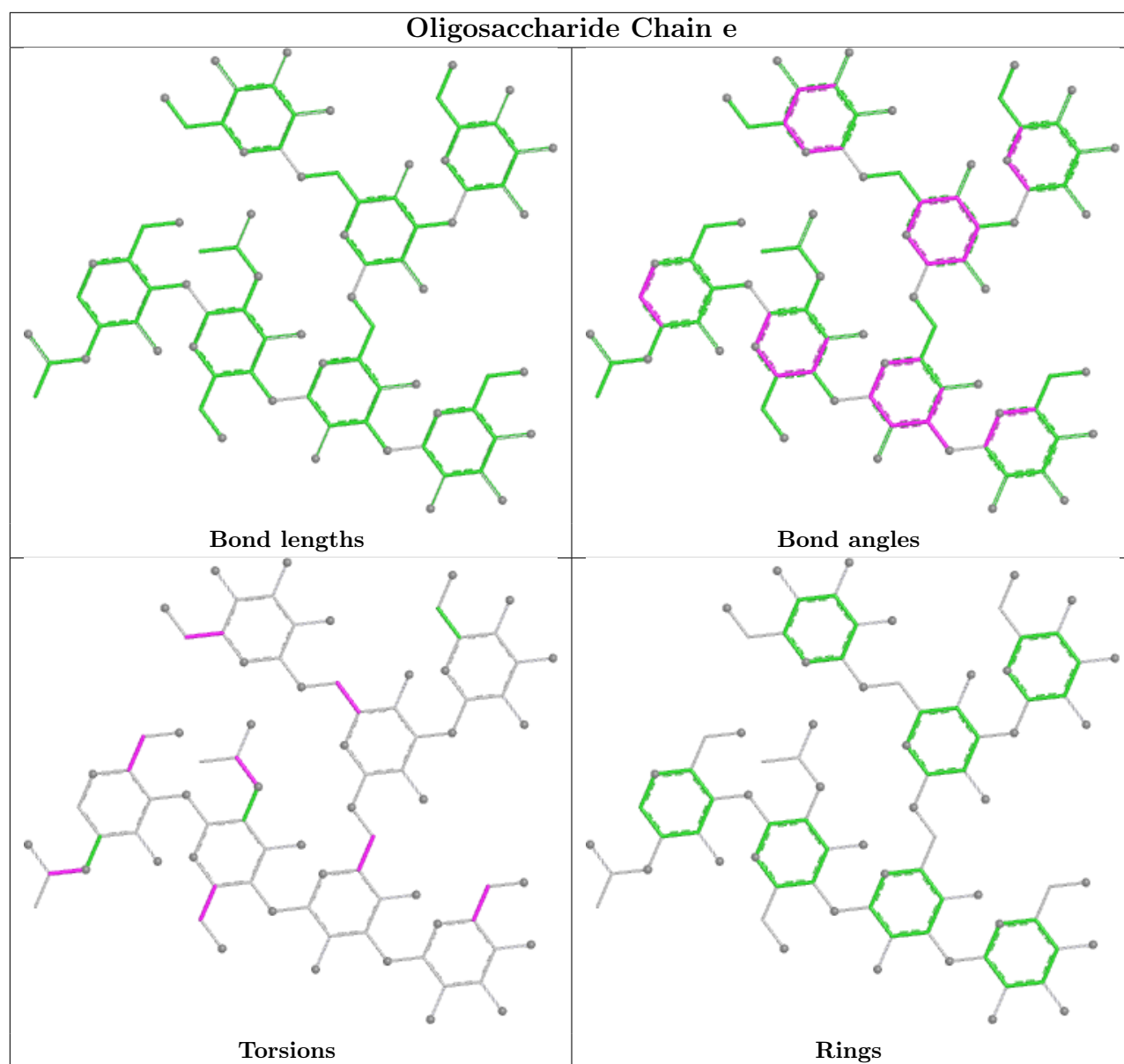












## 5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 24 are monoatomic - leaving 31 for Mogul analysis.

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	D	2008	1	14,14,15	0.48	0	17,19,21	1.09	1 (5%)
8	NAG	A	2018	1	14,14,15	0.70	0	17,19,21	1.55	2 (11%)
8	NAG	F	2012	1	14,14,15	0.48	0	17,19,21	1.39	2 (11%)
8	NAG	B	2005	1	14,14,15	0.58	0	17,19,21	1.00	2 (11%)
8	NAG	A	2006	1	14,14,15	0.88	0	17,19,21	1.17	3 (17%)
8	NAG	F	2014	1	14,14,15	0.46	0	17,19,21	1.28	2 (11%)
8	NAG	B	2006	1	14,14,15	0.67	0	17,19,21	1.01	1 (5%)
8	NAG	F	2008	1	14,14,15	0.55	0	17,19,21	1.13	1 (5%)
8	NAG	F	2005	1	14,14,15	4.26	4 (28%)	17,19,21	1.96	4 (23%)
8	NAG	E	2012	1	14,14,15	3.43	2 (14%)	17,19,21	1.50	3 (17%)
8	NAG	F	2009	1	14,14,15	0.88	0	17,19,21	1.59	4 (23%)
8	NAG	C	2018	1	14,14,15	5.07	3 (21%)	17,19,21	2.19	4 (23%)
8	NAG	F	2006	1	14,14,15	4.11	4 (28%)	17,19,21	1.98	4 (23%)
8	NAG	C	2005	1	14,14,15	0.54	0	17,19,21	1.70	4 (23%)
8	NAG	B	2014	1	14,14,15	0.46	0	17,19,21	2.00	3 (17%)
8	NAG	C	2014	1	14,14,15	0.54	0	17,19,21	1.82	3 (17%)
8	NAG	D	2006	1	14,14,15	3.86	3 (21%)	17,19,21	2.07	4 (23%)
8	NAG	D	2014	1	14,14,15	0.52	0	17,19,21	0.91	0
8	NAG	C	2006	1	14,14,15	0.47	0	17,19,21	1.45	1 (5%)
8	NAG	E	2005	1	14,14,15	0.55	0	17,19,21	0.88	1 (5%)
8	NAG	A	2014	1	14,14,15	0.64	0	17,19,21	1.08	0
8	NAG	E	2006	1	14,14,15	0.68	0	17,19,21	1.88	4 (23%)
8	NAG	E	2014	1	14,14,15	0.47	0	17,19,21	1.86	2 (11%)
8	NAG	B	2012	1	14,14,15	0.53	0	17,19,21	1.21	1 (5%)
8	NAG	A	2008	1	14,14,15	0.48	0	17,19,21	0.92	1 (5%)
8	NAG	B	2018	1	14,14,15	0.80	1 (7%)	17,19,21	1.26	1 (5%)
8	NAG	D	2012	1	14,14,15	0.67	0	17,19,21	1.02	1 (5%)
8	NAG	C	2012	1	14,14,15	0.54	0	17,19,21	1.60	2 (11%)
8	NAG	D	2005	1	14,14,15	0.52	0	17,19,21	1.17	2 (11%)
8	NAG	E	2008	1	14,14,15	0.52	0	17,19,21	0.94	0
8	NAG	A	2012	1	14,14,15	0.54	0	17,19,21	1.21	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	D	2008	1	-	0/6/23/26	0/1/1/1
8	NAG	A	2018	1	1/1/5/7	3/6/23/26	0/1/1/1
8	NAG	F	2012	1	1/1/5/7	5/6/23/26	0/1/1/1
8	NAG	B	2005	1	-	4/6/23/26	0/1/1/1
8	NAG	A	2006	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	F	2014	1	-	2/6/23/26	0/1/1/1
8	NAG	B	2006	1	1/1/5/7	2/6/23/26	0/1/1/1
8	NAG	F	2008	1	-	0/6/23/26	0/1/1/1
8	NAG	F	2005	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	E	2012	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	F	2009	1	1/1/5/7	5/6/23/26	0/1/1/1
8	NAG	C	2018	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	F	2006	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	C	2005	1	-	4/6/23/26	0/1/1/1
8	NAG	D	2006	1	1/1/5/7	2/6/23/26	0/1/1/1
8	NAG	B	2014	1	-	4/6/23/26	0/1/1/1
8	NAG	C	2014	1	-	4/6/23/26	0/1/1/1
8	NAG	D	2014	1	-	4/6/23/26	0/1/1/1
8	NAG	C	2006	1	-	2/6/23/26	0/1/1/1
8	NAG	E	2005	1	-	2/6/23/26	0/1/1/1
8	NAG	A	2014	1	-	2/6/23/26	0/1/1/1
8	NAG	E	2006	1	-	3/6/23/26	0/1/1/1
8	NAG	E	2014	1	-	2/6/23/26	0/1/1/1
8	NAG	B	2012	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	A	2008	1	-	0/6/23/26	0/1/1/1
8	NAG	B	2018	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	D	2012	1	-	5/6/23/26	0/1/1/1
8	NAG	C	2012	1	1/1/5/7	2/6/23/26	0/1/1/1
8	NAG	D	2005	1	-	4/6/23/26	0/1/1/1
8	NAG	E	2008	1	-	2/6/23/26	0/1/1/1
8	NAG	A	2012	1	1/1/5/7	3/6/23/26	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	2018	NAG	O7-C7	14.52	1.55	1.23
8	F	2006	NAG	C8-C7	14.37	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	2006	NAG	O7-C7	11.91	1.49	1.23
8	C	2018	NAG	C8-C7	11.45	1.74	1.50
8	E	2012	NAG	C8-C7	10.37	1.72	1.50

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	2014	NAG	C1-O5-C5	6.36	120.71	112.19
8	C	2014	NAG	C1-O5-C5	5.97	120.19	112.19
8	F	2005	NAG	C1-O5-C5	5.46	119.51	112.19
8	D	2006	NAG	C8-C7-N2	-5.31	107.31	116.12
8	B	2014	NAG	C1-O5-C5	5.25	119.22	112.19

5 of 14 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	2006	NAG	C1
8	A	2012	NAG	C1
8	A	2018	NAG	C1
8	B	2006	NAG	C1
8	B	2012	NAG	C1

5 of 94 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	2012	NAG	C8-C7-N2-C2
8	A	2012	NAG	O7-C7-N2-C2
8	A	2014	NAG	O7-C7-N2-C2
8	B	2005	NAG	C8-C7-N2-C2
8	B	2005	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

**Warning:** The R factor obtained from EDS is 0.3081, which does not match the depositor's R factor of 0.22563. Please interpret the results in this section carefully.

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	529/534 (99%)	1.54	140 (26%)	2 2	67, 69, 71, 74	0
1	B	529/534 (99%)	1.08	55 (10%)	13 10	67, 69, 71, 74	0
1	C	529/534 (99%)	1.72	193 (36%)	1 1	67, 69, 71, 74	0
1	D	529/534 (99%)	1.45	112 (21%)	3 3	67, 69, 71, 73	0
1	E	529/534 (99%)	1.51	122 (23%)	2 3	68, 69, 71, 73	0
1	F	529/534 (99%)	2.56	342 (64%)	0 0	68, 69, 71, 73	0
All	All	3174/3204 (99%)	1.64	964 (30%)	1 1	67, 69, 71, 74	0

The worst 5 of 964 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	550	ALA	7.6
1	F	436	GLY	7.2
1	D	533	ALA	6.5
1	F	533	ALA	6.4
1	F	454	PRO	6.3

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

SUGAR-RSR INFOmissingINFO

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	NAG	E	2005	14/15	0.29	0.23	70,71,71,71	0
8	NAG	E	2012	14/15	0.35	0.23	73,74,77,77	0
8	NAG	F	2012	14/15	0.35	0.22	72,73,75,75	0
8	NAG	F	2006	14/15	0.37	0.23	67,68,70,70	0
8	NAG	C	2018	14/15	0.52	0.19	74,76,77,78	0
8	NAG	E	2008	14/15	0.53	0.22	72,72,73,73	0
8	NAG	A	2018	14/15	0.53	0.20	78,80,82,82	0
8	NAG	D	2014	14/15	0.54	0.21	65,66,67,67	0
8	NAG	E	2006	14/15	0.55	0.22	73,74,75,76	0
8	NAG	F	2008	14/15	0.56	0.23	71,71,72,72	0
8	NAG	B	2014	14/15	0.56	0.22	67,70,71,71	0
8	NAG	B	2018	14/15	0.60	0.18	80,83,83,83	0
8	NAG	F	2005	14/15	0.61	0.18	67,70,71,72	0
8	NAG	F	2009	14/15	0.61	0.19	66,69,69,69	0
8	NAG	C	2006	14/15	0.61	0.19	74,76,77,78	0
8	NAG	D	2006	14/15	0.63	0.18	65,68,70,71	0
8	NAG	A	2006	14/15	0.64	0.19	71,73,74,74	0
8	NAG	C	2012	14/15	0.69	0.18	75,77,79,80	0
8	NAG	A	2012	14/15	0.71	0.18	76,79,80,81	0
8	NAG	D	2012	14/15	0.72	0.16	73,74,76,77	0
8	NAG	D	2008	14/15	0.73	0.19	70,71,73,73	0
8	NAG	D	2005	14/15	0.73	0.18	71,72,74,75	0
8	NAG	F	2014	14/15	0.74	0.16	59,62,63,64	0
8	NAG	B	2006	14/15	0.76	0.14	74,76,78,79	0
8	NAG	A	2014	14/15	0.79	0.16	67,67,71,72	0
8	NAG	B	2012	14/15	0.79	0.15	74,75,79,79	0
8	NAG	B	2005	14/15	0.83	0.14	64,67,69,70	0
8	NAG	C	2005	14/15	0.83	0.16	64,68,70,70	0
8	NAG	E	2014	14/15	0.84	0.13	52,56,57,58	0
8	NAG	A	2008	14/15	0.86	0.15	68,69,70,70	0
8	NAG	C	2014	14/15	0.88	0.12	53,55,57,58	0
9	CU1	F	1001	1/1	0.89	0.19	90,90,90,90	0
9	CU1	D	1004	1/1	0.92	0.18	100,100,100,100	0
9	CU1	F	1004	1/1	0.94	0.17	100,100,100,100	0
9	CU1	C	1004	1/1	0.95	0.16	100,100,100,100	0
9	CU1	F	1003	1/1	0.95	0.14	91,91,91,91	0
9	CU1	A	1004	1/1	0.95	0.12	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	CU1	E	1004	1/1	0.96	0.15	100,100,100,100	0
9	CU1	C	1001	1/1	0.96	0.08	85,85,85,85	0
9	CU1	F	1002	1/1	0.96	0.11	96,96,96,96	0
9	CU1	E	1001	1/1	0.96	0.14	88,88,88,88	0
9	CU1	E	1003	1/1	0.96	0.14	99,99,99,99	0
9	CU1	D	1002	1/1	0.97	0.07	87,87,87,87	0
9	CU1	E	1002	1/1	0.97	0.16	93,93,93,93	0
9	CU1	D	1003	1/1	0.97	0.07	89,89,89,89	0
9	CU1	B	1004	1/1	0.97	0.08	100,100,100,100	0
9	CU1	D	1001	1/1	0.98	0.05	86,86,86,86	0
9	CU1	C	1003	1/1	0.98	0.05	83,83,83,83	0
9	CU1	B	1002	1/1	0.98	0.09	88,88,88,88	0
9	CU1	B	1003	1/1	0.99	0.09	87,87,87,87	0
9	CU1	A	1003	1/1	0.99	0.10	89,89,89,89	0
9	CU1	A	1001	1/1	0.99	0.03	82,82,82,82	0
9	CU1	C	1002	1/1	0.99	0.04	85,85,85,85	0
9	CU1	B	1001	1/1	0.99	0.05	87,87,87,87	0
9	CU1	A	1002	1/1	0.99	0.09	87,87,87,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.