



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 05:04 PM UTC

PDB ID : 9IKM / pdb_00009ikm
EMDB ID : EMD-60659
Title : Cryo-EM structure of TLP-4
Authors : Yan, N.; Yan, C.; Li, Z.; Wang, T.
Deposited on : 2024-06-27
Resolution : 3.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

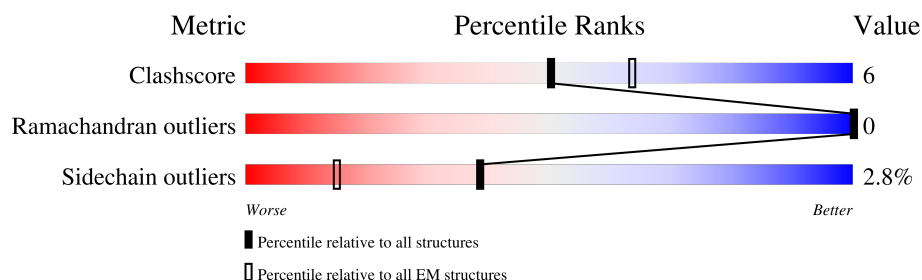
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	72	82% 18%
2	O	7	100%
2	B	7	100%
2	E	7	86% 14%
2	H	7	86% 14%
2	K	7	86% 14%
2	N	7	86% 14%
2	Q	7	86% 14%
2	T	7	71% 29%

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Mol	Chain	Length	Quality of chain
2	W	7	
2	Z	7	
2	c	7	
2	f	7	
2	i	7	
2	l	7	
2	o	7	
2	r	7	
2	u	7	
2	x	7	
3	1	29	
3	C	29	
3	F	29	
3	I	29	
3	L	29	
3	O	29	
3	R	29	
3	U	29	
3	X	29	
3	a	29	
3	d	29	
3	g	29	
3	j	29	
3	m	29	
3	p	29	

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Mol	Chain	Length	Quality of chain
3	s	29	
3	v	29	
3	y	29	
4	2	16	
4	D	16	
4	G	16	
4	J	16	
4	M	16	
4	P	16	
4	S	16	
4	V	16	
4	Y	16	
4	b	16	
4	e	16	
4	h	16	
4	k	16	
4	n	16	
4	q	16	
4	t	16	
4	w	16	
4	z	16	

2 Entry composition i

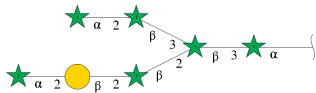
There are 4 unique types of molecules in this entry. The entry contains 9720 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TLP-4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	72	486	270	72	144	0	0

- Molecule 2 is an oligosaccharide called alpha-L-arabinofuranose-(1-2)-beta-D-galactopyranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
2	B	7	Total	C	O	0	0
			65	36	29		
2	E	7	Total	C	O	0	0
			65	36	29		
2	H	7	Total	C	O	0	0
			65	36	29		
2	K	7	Total	C	O	0	0
			65	36	29		
2	N	7	Total	C	O	0	0
			65	36	29		
2	Q	7	Total	C	O	0	0
			65	36	29		
2	T	7	Total	C	O	0	0
			65	36	29		
2	W	7	Total	C	O	0	0
			65	36	29		
2	Z	7	Total	C	O	0	0
			65	36	29		
2	c	7	Total	C	O	0	0
			65	36	29		
2	f	7	Total	C	O	0	0
			65	36	29		

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Mol	Chain	Residues	Atoms			AltConf	Trace
2	i	7	Total	C	O	0	0
			65	36	29		
2	l	7	Total	C	O	0	0
			65	36	29		
2	o	7	Total	C	O	0	0
			65	36	29		
2	r	7	Total	C	O	0	0
			65	36	29		
2	u	7	Total	C	O	0	0
			65	36	29		
2	x	7	Total	C	O	0	0
			65	36	29		
2	0	7	Total	C	O	0	0
			65	36	29		

- Molecule 3 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)-alpha-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-4)][alpha-L-arabinofuranose-(1-6)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-4)-alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)][alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)][beta-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-L-arabinofuranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose.



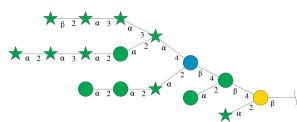
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	29	Total	C	N	O	0	0
			290	160	1	129		
3	F	29	Total	C	N	O	0	0
			290	160	1	129		
3	I	29	Total	C	N	O	0	0
			290	160	1	129		
3	L	29	Total	C	N	O	0	0
			290	160	1	129		
3	O	29	Total	C	N	O	0	0
			290	160	1	129		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	R	29	Total	C	N	O	0	0
			290	160	1	129		
3	U	29	Total	C	N	O	0	0
			290	160	1	129		
3	X	29	Total	C	N	O	0	0
			290	160	1	129		
3	a	29	Total	C	N	O	0	0
			290	160	1	129		
3	d	29	Total	C	N	O	0	0
			290	160	1	129		
3	g	29	Total	C	N	O	0	0
			290	160	1	129		
3	j	29	Total	C	N	O	0	0
			290	160	1	129		
3	m	29	Total	C	N	O	0	0
			290	160	1	129		
3	p	29	Total	C	N	O	0	0
			290	160	1	129		
3	s	29	Total	C	N	O	0	0
			290	160	1	129		
3	v	29	Total	C	N	O	0	0
			290	160	1	129		
3	y	29	Total	C	N	O	0	0
			290	160	1	129		
3	1	29	Total	C	N	O	0	0
			290	160	1	129		

- Molecule 4 is an oligosaccharide called alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
4	D	16	Total	C	O	0	0
			158	87	71		
4	G	16	Total	C	O	0	0
			158	87	71		

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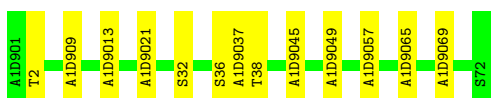
Mol	Chain	Residues	Atoms			AltConf	Trace
4	J	16	Total 158	C 87	O 71	0	0
4	M	16	Total 158	C 87	O 71	0	0
4	P	16	Total 158	C 87	O 71	0	0
4	S	16	Total 158	C 87	O 71	0	0
4	V	16	Total 158	C 87	O 71	0	0
4	Y	16	Total 158	C 87	O 71	0	0
4	b	16	Total 158	C 87	O 71	0	0
4	e	16	Total 158	C 87	O 71	0	0
4	h	16	Total 158	C 87	O 71	0	0
4	k	16	Total 158	C 87	O 71	0	0
4	n	16	Total 158	C 87	O 71	0	0
4	q	16	Total 158	C 87	O 71	0	0
4	t	16	Total 158	C 87	O 71	0	0
4	w	16	Total 158	C 87	O 71	0	0
4	z	16	Total 158	C 87	O 71	0	0
4	2	16	Total 158	C 87	O 71	0	0

3 Residue-property plots [i](#)

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

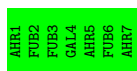
- Molecule 1: TLP-4

Chain A:  82% 18%



- Molecule 2: alpha-L-arabinofuranose-(1-2)-beta-D-galactopyranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain B:  100%



- Molecule 2: alpha-L-arabinofuranose-(1-2)-beta-D-galactopyranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain E:  86% 14%



- Molecule 2: alpha-L-arabinofuranose-(1-2)-beta-D-galactopyranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain H:  86% 14%



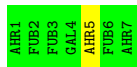
- Molecule 2: alpha-L-arabinofuranose-(1-2)-beta-D-galactopyranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain K:  86% 14%



- Molecule 2: alpha-L-arabinofuranose-(1-2)-beta-D-galactopyranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain N:  86% 14%



- Molecule 2: alpha-L-arabinofuranose-(1-2)-beta-D-galactopyranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain Q:  86% 14%



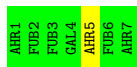
- Molecule 2: alpha-L-arabinofuranose-(1-2)-beta-D-galactopyranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain T:  71% 29%



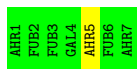
- Molecule 2: alpha-L-arabinofuranose-(1-2)-beta-D-galactopyranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain W:  86% 14%



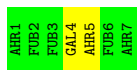
- Molecule 2: alpha-L-arabinofuranose-(1-2)-beta-D-galactopyranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain Z:  86% 14%



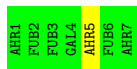
- Molecule 2: alpha-L-arabinofuranose-(1-2)-beta-D-galactopyranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain c:  71% 29%



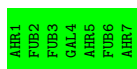
- Molecule 2: alpha-L-arabinofuranose-(1-2)-beta-D-galactopyranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain f:  86% 14%



- Molecule 2: alpha-L-arabinofuranose-(1-2)-beta-D-galactopyranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain i:  100%



- Molecule 2: alpha-L-arabinofuranose-(1-2)-beta-D-galactopyranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain l:  100%



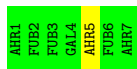
- Molecule 2: alpha-L-arabinofuranose-(1-2)-beta-D-galactopyranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain o:  57% 43%



- Molecule 2: alpha-L-arabinofuranose-(1-2)-beta-D-galactopyranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain r:  86% 14%



- Molecule 2: alpha-L-arabinofuranose-(1-2)-beta-D-galactopyranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain u:  71% 29%



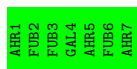
- Molecule 2: alpha-L-arabinofuranose-(1-2)-beta-D-galactopyranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain x:  71% 29%



- Molecule 2: alpha-L-arabinofuranose-(1-2)-beta-D-galactopyranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain 0:  100%



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

Chain C:  48% 38% 14%



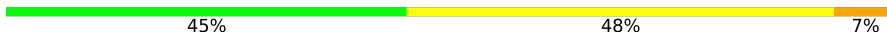
- Molecule 3: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)-alpha-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-4)][alpha-L-arabinofuranose-(1-6)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-4)-alpha-D-mannopyranose-(1-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

nose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain F:  41% 55%

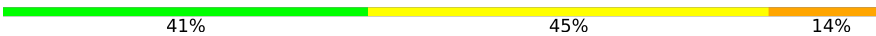


• Molecule 3: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)-alpha-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-4)]alpha-L-arabinofuranose-(1-6)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-4)-alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-L-arabinofuranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain I:  45% 48% 7%



• Molecule 3: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)-alpha-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-4)]alpha-L-arabinofuranose-(1-6)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-4)-alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-L-arabinofuranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

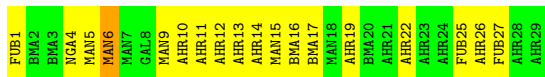
Chain L:  41% 45% 14%



• Molecule 3: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)-alpha-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-4)]alpha-L-arabinofuranose-(1-6)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-4)-alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-L-arabinofuranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

nose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain O:  38% 59%



● Molecule 3: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)-alpha-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-4)]alpha-L-arabinofuranose-(1-6)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-4)-alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-L-arabinofuranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain R:  48% 45% 7%



● Molecule 3: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)-alpha-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-4)]alpha-L-arabinofuranose-(1-6)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-4)-alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-L-arabinofuranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain U:  48% 45% 7%



● Molecule 3: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)-alpha-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-4)]alpha-L-arabinofuranose-(1-6)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-4)-alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-L-arabinofuranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

nose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain X:  45% 48% 7%

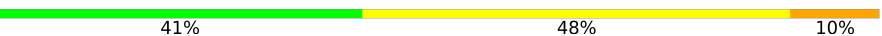


• Molecule 3: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)-alpha-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-4)]alpha-L-arabinofuranose-(1-6)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-4)-alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-L-arabinofuranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain a:  38% 48% 14%



• Molecule 3: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)-alpha-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-4)]alpha-L-arabinofuranose-(1-6)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-4)-alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-L-arabinofuranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain d:  41% 48% 10%



• Molecule 3: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)-alpha-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-4)]alpha-L-arabinofuranose-(1-6)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-4)-alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-L-arabinofuranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

nose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain g:  48% 45% 7%

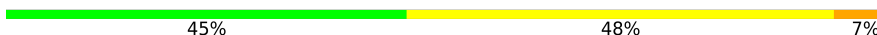


● Molecule 3: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)-alpha-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-4)]alpha-L-arabinofuranose-(1-6)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-4)-alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-L-arabinofuranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain j:  52% 38% 10%



● Molecule 3: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)-alpha-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-4)]alpha-L-arabinofuranose-(1-6)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-4)-alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-L-arabinofuranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain m:  45% 48% 7%



● Molecule 3: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)-alpha-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-4)]alpha-L-arabinofuranose-(1-6)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-4)-alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-L-arabinofuranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

nose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain p:  52% 41% 7%

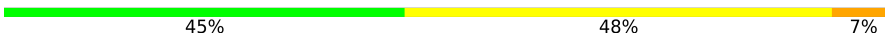


• Molecule 3: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)-alpha-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-4)]alpha-L-arabinofuranose-(1-6)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-4)-alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-L-arabinofuranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain s:  41% 45% 14%



• Molecule 3: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)-alpha-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-4)]alpha-L-arabinofuranose-(1-6)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-4)-alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-L-arabinofuranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain v:  45% 48% 7%



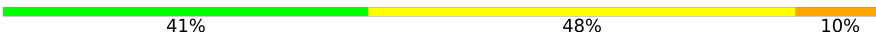
• Molecule 3: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)-alpha-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-4)]alpha-L-arabinofuranose-(1-6)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-4)-alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-L-arabinofuranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

nose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain y:  48% 45% 7%



• Molecule 3: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)-alpha-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-4)]alpha-L-arabinofuranose-(1-6)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-4)-alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-6)]beta-D-mannopyranose-(1-6)]beta-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-L-arabinofuranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-beta-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]beta-L-arabinofuranose

Chain 1:  41% 48% 10%



• Molecule 4: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose

Chain D:  69% 31%



• Molecule 4: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose

Chain G:  62% 38%



• Molecule 4: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose

Chain J:  56% 44%



• Molecule 4: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose

Chain M:  62% 38%



• Molecule 4: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose

Chain P:  69% 31%



• Molecule 4: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose

Chain S:  62% 38%



• Molecule 4: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose

ose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose

Chain V:  56% 44%

GAL1	BNA2	BCC3	AHR4	MAN5	AHR6	AHR7	AHR8	AHR9	AHR10	FUB11	AHR12	MAN13	MAN14	MAN15	AHR16
------	------	------	------	------	------	------	------	------	-------	-------	-------	-------	-------	-------	-------

● Molecule 4: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose

Chain Y:  50% 50%

GAL1	BNA2	BCC3	AHR4	MAN5	AHR6	AHR7	AHR8	AHR9	AHR10	FUB11	AHR12	MAN13	MAN14	MAN15	AHR16
------	------	------	------	------	------	------	------	------	-------	-------	-------	-------	-------	-------	-------

● Molecule 4: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose

Chain b:  62% 25% 12%

GAL1	BNA2	BCC3	AHR4	MAN5	AHR6	AHR7	AHR8	AHR9	AHR10	FUB11	AHR12	MAN13	MAN14	MAN15	AHR16
------	------	------	------	------	------	------	------	------	-------	-------	-------	-------	-------	-------	-------

● Molecule 4: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose

Chain e:  62% 38%

GAL1	BNA2	BCC3	AHR4	MAN5	AHR6	AHR7	AHR8	AHR9	AHR10	FUB11	AHR12	MAN13	MAN14	MAN15	AHR16
------	------	------	------	------	------	------	------	------	-------	-------	-------	-------	-------	-------	-------

● Molecule 4: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1

-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose

Chain h:  62% 38%



• Molecule 4: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose

Chain k:  50% 44% 6%



• Molecule 4: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose

Chain n:  62% 25% 12%



• Molecule 4: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose

Chain q:  75% 25%



• Molecule 4: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-a

lpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose

Chain t:  62% 31% 6%



• Molecule 4: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose

Chain w:  62% 38%



• Molecule 4: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose

Chain z:  62% 31% 6%



• Molecule 4: alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-2)-alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)]beta-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-galactopyranose

Chain 2:  69% 31%



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-134.79°, rise=12.41 Å, axial sym=C1	Depositor
Number of segments used	27189	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	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: A1D9O, AHR, MAN, BMA, FUB, NGA, BGC, GAL

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	0.23	0/306	0.35	0/396

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	486	0	288	5	0
2	0	65	0	9	0	0
2	B	65	0	9	0	0
2	E	65	0	9	0	0
2	H	65	0	9	0	0
2	K	65	0	9	0	0
2	N	65	0	9	0	0
2	Q	65	0	9	0	0
2	T	65	0	9	1	0
2	W	65	0	9	0	0
2	Z	65	0	9	0	0
2	c	65	0	9	1	0
2	f	65	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	i	65	0	9	0	0
2	l	65	0	9	0	0
2	o	65	0	9	2	0
2	r	65	0	9	0	0
2	u	65	0	9	1	0
2	x	65	0	9	1	0
3	1	290	0	110	4	0
3	C	290	0	110	7	0
3	F	290	0	110	2	0
3	I	290	0	110	4	0
3	L	290	0	110	5	0
3	O	290	0	110	2	0
3	R	290	0	110	3	0
3	U	290	0	110	3	0
3	X	290	0	110	3	0
3	a	290	0	110	5	0
3	d	290	0	110	4	0
3	g	290	0	110	2	0
3	j	290	0	110	4	0
3	m	290	0	110	3	0
3	p	290	0	110	3	0
3	s	290	0	110	5	0
3	v	290	0	110	3	0
3	y	290	0	110	3	0
4	2	158	0	62	1	0
4	D	158	0	62	0	0
4	G	158	0	62	1	0
4	J	158	0	62	2	0
4	M	158	0	62	2	0
4	P	158	0	62	0	0
4	S	158	0	62	1	0
4	V	158	0	62	1	0
4	Y	158	0	62	2	0
4	b	158	0	62	4	0
4	e	158	0	62	2	0
4	h	158	0	62	1	0
4	k	158	0	62	3	0
4	n	158	0	62	2	0
4	q	158	0	62	0	0
4	t	158	0	62	4	0
4	w	158	0	62	1	0
4	z	158	0	62	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9720	0	3546	74	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:13:MAN:O5	4:b:14:MAN:H5	1.74	0.87
3:I:11:AHR:C5	2:c:4:GAL:O6	2.30	0.79
4:b:13:MAN:H4	4:b:14:MAN:H3	1.63	0.78
1:A:36:SER:HB2	3:C:25:FUB:O2	1.84	0.77
4:t:13:MAN:H4	4:t:14:MAN:H3	1.73	0.70
2:T:4:GAL:O6	3:a:11:AHR:C5	2.41	0.69
4:b:13:MAN:C1	4:b:14:MAN:H5	2.30	0.62
3:C:5:MAN:O3	3:C:25:FUB:C1	2.48	0.61
1:A:38:THR:CG2	3:C:25:FUB:O3	2.49	0.60
3:I:5:MAN:H62	3:I:6:MAN:H2	1.86	0.58
3:R:5:MAN:H62	3:R:6:MAN:H2	1.86	0.58
3:F:5:MAN:H62	3:F:6:MAN:H2	1.86	0.58
3:X:5:MAN:H62	3:X:6:MAN:H2	1.86	0.58
3:v:5:MAN:H62	3:v:6:MAN:H2	1.86	0.58
3:m:5:MAN:H62	3:m:6:MAN:H2	1.86	0.58
3:p:5:MAN:H62	3:p:6:MAN:H2	1.86	0.57
3:j:5:MAN:H62	3:j:6:MAN:H2	1.86	0.57
3:g:5:MAN:H62	3:g:6:MAN:H2	1.86	0.57
3:a:5:MAN:H62	3:a:6:MAN:H2	1.86	0.57
3:j:11:AHR:C5	2:o:4:GAL:O6	2.53	0.57
3:L:5:MAN:H62	3:L:6:MAN:H2	1.85	0.57
3:d:5:MAN:H62	3:d:6:MAN:H2	1.86	0.57
3:y:5:MAN:H62	3:y:6:MAN:H2	1.86	0.57
3:O:5:MAN:H62	3:O:6:MAN:H2	1.86	0.57
3:U:5:MAN:H62	3:U:6:MAN:H2	1.86	0.57
3:s:5:MAN:H62	3:s:6:MAN:H2	1.86	0.57
3:1:5:MAN:H62	3:1:6:MAN:H2	1.86	0.56
4:n:13:MAN:C1	4:n:14:MAN:H5	2.35	0.56
1:A:36:SER:CB	3:C:25:FUB:O2	2.55	0.54
3:p:11:AHR:C5	2:u:4:GAL:O6	2.57	0.53
1:A:38:THR:HG22	3:C:25:FUB:O3	2.07	0.52
3:j:24:AHR:O5	2:o:6:FUB:O3	2.29	0.50
3:C:8:GAL:O3	3:C:9:MAN:O5	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:z:13:MAN:O5	4:z:14:MAN:H5	2.13	0.48
3:C:1:FUB:O3	4:e:16:HR:O3	2.32	0.48
3:d:17:BMA:HO2	4:e:5:MAN:HO3	1.61	0.47
3:y:17:BMA:O2	4:z:5:MAN:O3	2.32	0.47
3:1:17:BMA:O2	4:2:5:MAN:O3	2.32	0.47
3:a:17:BMA:O2	4:b:5:MAN:O3	2.32	0.47
3:L:17:BMA:O2	4:M:5:MAN:O3	2.32	0.46
3:I:17:BMA:O2	4:J:5:MAN:O3	2.32	0.46
3:m:17:BMA:O2	4:n:5:MAN:O3	2.32	0.46
4:t:13:MAN:H4	4:t:14:MAN:C3	2.44	0.46
3:v:17:BMA:O2	4:w:5:MAN:O3	2.32	0.46
3:L:17:BMA:HO2	4:M:5:MAN:HO3	1.64	0.45
3:R:17:BMA:O2	4:S:5:MAN:O3	2.32	0.45
3:j:17:BMA:O2	4:k:5:MAN:O3	2.32	0.44
3:s:17:BMA:O2	4:t:5:MAN:O3	2.32	0.44
4:G:16:HR:O3	3:1:1:FUB:O3	2.35	0.43
3:s:17:BMA:HO2	4:t:5:MAN:HO3	1.66	0.43
3:d:1:FUB:O3	4:h:16:HR:O3	2.36	0.43
3:U:17:BMA:O2	4:V:5:MAN:O3	2.32	0.43
4:k:13:MAN:H4	4:k:14:MAN:H3	2.01	0.42
3:s:11:HR:C5	2:x:4:GAL:O6	2.68	0.42
1:A:32:SER:HA	4:k:1:GAL:H62	2.02	0.42
3:F:4:NGA:H3	3:F:16:BMA:H2	2.02	0.42
4:J:16:HR:O3	3:L:1:FUB:O3	2.38	0.42
3:g:4:NGA:H3	3:g:16:BMA:H2	2.02	0.41
3:v:4:NGA:H3	3:v:16:BMA:H2	2.02	0.41
3:I:4:NGA:H3	3:I:16:BMA:H2	2.02	0.41
3:R:4:NGA:H3	3:R:16:BMA:H2	2.02	0.41
3:X:4:NGA:H3	3:X:16:BMA:H2	2.02	0.41
3:p:4:NGA:H3	3:p:16:BMA:H2	2.02	0.41
3:m:4:NGA:H3	3:m:16:BMA:H2	2.02	0.41
3:O:4:NGA:H3	3:O:16:BMA:H2	2.02	0.41
3:X:17:BMA:HO2	4:Y:5:MAN:HO3	1.61	0.41
3:a:4:NGA:H3	3:a:16:BMA:H2	2.02	0.41
3:y:4:NGA:H3	3:y:16:BMA:H2	2.02	0.41
3:U:4:NGA:H3	3:U:16:BMA:H2	2.02	0.41
3:s:4:NGA:H3	3:s:16:BMA:H2	2.02	0.40
4:Y:16:HR:O3	3:a:1:FUB:O3	2.38	0.40
3:L:4:NGA:H3	3:L:16:BMA:H2	2.02	0.40
3:1:4:NGA:H3	3:1:16:BMA:H2	2.02	0.40
3:d:4:NGA:H3	3:d:16:BMA:H2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	53/72 (74%)	52 (98%)	1 (2%)	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	36/36 (100%)	35 (97%)	1 (3%)	38	61

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

18 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	A1D9O	A	21	1	8,9,10	0.96	0	6,12,14	1.47	1 (16%)
1	A1D9O	A	37	1	8,9,10	0.89	0	6,12,14	1.30	1 (16%)
1	A1D9O	A	53	1	8,9,10	0.93	0	6,12,14	1.29	0
1	A1D9O	A	69	1	8,9,10	0.86	0	6,12,14	1.51	1 (16%)
1	A1D9O	A	45	1	8,9,10	1.03	0	6,12,14	1.47	1 (16%)
1	A1D9O	A	1	1	8,9,10	0.90	0	6,12,14	1.01	0
1	A1D9O	A	5	1	8,9,10	0.92	0	6,12,14	1.34	0
1	A1D9O	A	29	1	8,9,10	0.94	0	6,12,14	1.20	0
1	A1D9O	A	41	1	8,9,10	0.90	0	6,12,14	1.14	0
1	A1D9O	A	57	1	8,9,10	0.85	0	6,12,14	1.48	1 (16%)
1	A1D9O	A	61	1	8,9,10	0.91	0	6,12,14	1.06	0
1	A1D9O	A	65	1	8,9,10	0.88	0	6,12,14	1.51	1 (16%)
1	A1D9O	A	13	1	8,9,10	0.89	0	6,12,14	1.55	1 (16%)
1	A1D9O	A	25	1	8,9,10	0.93	0	6,12,14	1.08	0
1	A1D9O	A	33	1	8,9,10	0.91	0	6,12,14	1.06	0
1	A1D9O	A	17	1	8,9,10	0.91	0	6,12,14	1.19	0
1	A1D9O	A	9	1	8,9,10	0.98	0	6,12,14	1.51	1 (16%)
1	A1D9O	A	49	1	8,9,10	0.87	0	6,12,14	1.36	1 (16%)

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
1	A1D9O	A	21	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	37	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	53	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	69	1	-	0/1/15/17	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A1D9O	A	45	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	1	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	5	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	29	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	41	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	57	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	61	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	65	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	13	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	25	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	33	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	17	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	9	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	49	1	-	0/1/15/17	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	A1D9O	CD-CG-CB	2.82	106.37	103.40
1	A	13	A1D9O	CD-CG-CB	2.72	106.26	103.40
1	A	9	A1D9O	OD2-CB-CA	-2.59	105.29	111.78
1	A	49	A1D9O	CD-CG-CB	2.55	106.07	103.40
1	A	65	A1D9O	CD-CG-CB	2.52	106.05	103.40
1	A	57	A1D9O	CD-CG-CB	2.26	105.78	103.40
1	A	21	A1D9O	CD-CG-CB	2.25	105.76	103.40
1	A	37	A1D9O	CD-CG-CB	2.09	105.59	103.40
1	A	45	A1D9O	CD-CG-CB	2.03	105.54	103.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

936 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	AHR	0	1	2	9,9,10	0.53	0	11,12,14	0.86	0
2	FUB	0	2	2	9,9,10	0.58	0	11,12,14	0.97	0
2	FUB	0	3	2	9,9,10	0.55	0	11,12,14	0.95	0
2	GAL	0	4	2	11,11,12	0.18	0	15,15,17	0.55	0
2	AHR	0	5	2	9,9,10	0.54	0	11,12,14	0.97	0
2	FUB	0	6	2	9,9,10	0.56	0	11,12,14	0.92	0
2	AHR	0	7	2	9,9,10	0.56	0	11,12,14	0.94	0
3	FUB	1	1	3	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
3	AHR	1	10	3	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
3	AHR	1	11	3	9,9,10	0.55	0	11,12,14	0.99	0
3	AHR	1	12	3	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
3	AHR	1	13	3	9,9,10	0.55	0	11,12,14	0.99	1 (9%)
3	AHR	1	14	3	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
3	MAN	1	15	3	11,11,12	0.22	0	15,15,17	0.74	1 (6%)
3	BMA	1	16	3	11,11,12	0.25	0	15,15,17	0.69	0
3	BMA	1	17	3	11,11,12	0.19	0	15,15,17	0.75	1 (6%)
3	MAN	1	18	3	11,11,12	0.22	0	15,15,17	0.72	0
3	AHR	1	19	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	BMA	1	2	3	11,11,12	0.24	0	15,15,17	0.73	0
3	BMA	1	20	3	11,11,12	0.22	0	15,15,17	0.60	0
3	AHR	1	21	3	9,9,10	0.55	0	11,12,14	0.96	0
3	AHR	1	22	3	9,9,10	0.52	0	11,12,14	1.01	1 (9%)
3	AHR	1	23	3	9,9,10	0.54	0	11,12,14	0.97	0
3	AHR	1	24	3	9,9,10	0.53	0	11,12,14	0.88	0
3	FUB	1	25	3	9,9,10	0.52	0	11,12,14	1.01	1 (9%)
3	AHR	1	26	3	9,9,10	0.58	0	11,12,14	1.01	1 (9%)
3	FUB	1	27	3	9,9,10	0.53	0	11,12,14	1.11	1 (9%)
3	AHR	1	28	3	9,9,10	0.56	0	11,12,14	0.94	0
3	AHR	1	29	3	9,9,10	0.52	0	11,12,14	0.92	0
3	BMA	1	3	3	11,11,12	0.42	0	15,15,17	0.66	0
3	NGA	1	4	3	14,14,15	0.83	0	17,19,21	1.00	0
3	MAN	1	5	3	11,11,12	0.23	0	15,15,17	0.76	0
3	MAN	1	6	3	11,11,12	0.23	0	15,15,17	0.77	1 (6%)
3	MAN	1	7	3	11,11,12	0.21	0	15,15,17	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GAL	1	8	3	11,11,12	0.16	0	15,15,17	0.75	0
3	MAN	1	9	3	11,11,12	0.21	0	15,15,17	0.81	1 (6%)
4	GAL	2	1	4	11,11,12	0.18	0	15,15,17	0.63	0
4	AHR	2	10	4	9,9,10	0.55	0	11,12,14	0.92	0
4	FUB	2	11	4	9,9,10	0.58	0	11,12,14	1.01	1 (9%)
4	AHR	2	12	4	9,9,10	0.55	0	11,12,14	0.96	0
4	MAN	2	13	4	11,11,12	0.23	0	15,15,17	1.05	1 (6%)
4	MAN	2	14	4	11,11,12	0.24	0	15,15,17	0.73	0
4	MAN	2	15	4	11,11,12	0.24	0	15,15,17	0.72	0
4	AHR	2	16	4	9,9,10	0.54	0	11,12,14	0.94	0
4	BMA	2	2	4	11,11,12	0.24	0	15,15,17	0.71	0
4	BGC	2	3	4	11,11,12	0.18	0	15,15,17	0.52	0
4	AHR	2	4	4	9,9,10	0.52	0	11,12,14	1.03	1 (9%)
4	MAN	2	5	4	11,11,12	0.21	0	15,15,17	0.72	0
4	AHR	2	6	4	9,9,10	0.55	0	11,12,14	0.88	0
4	AHR	2	7	4	9,9,10	0.56	0	11,12,14	0.94	0
4	AHR	2	8	4	9,9,10	0.56	0	11,12,14	1.01	1 (9%)
4	AHR	2	9	4	9,9,10	0.55	0	11,12,14	0.93	0
2	AHR	B	1	2	9,9,10	0.54	0	11,12,14	0.88	0
2	FUB	B	2	2	9,9,10	0.57	0	11,12,14	0.97	0
2	FUB	B	3	2	9,9,10	0.57	0	11,12,14	0.95	0
2	GAL	B	4	2	11,11,12	0.19	0	15,15,17	0.57	0
2	AHR	B	5	2	9,9,10	0.52	0	11,12,14	0.96	0
2	FUB	B	6	2	9,9,10	0.56	0	11,12,14	0.93	0
2	AHR	B	7	2	9,9,10	0.57	0	11,12,14	0.95	0
3	FUB	C	1	3	9,9,10	0.52	0	11,12,14	1.01	1 (9%)
3	AHR	C	10	3	9,9,10	0.53	0	11,12,14	0.97	0
3	AHR	C	11	3	9,9,10	0.57	0	11,12,14	0.98	1 (9%)
3	AHR	C	12	3	9,9,10	0.56	0	11,12,14	0.99	1 (9%)
3	AHR	C	13	3	9,9,10	0.55	0	11,12,14	0.98	0
3	AHR	C	14	3	9,9,10	0.55	0	11,12,14	0.99	1 (9%)
3	MAN	C	15	3	11,11,12	0.23	0	15,15,17	0.73	1 (6%)
3	BMA	C	16	3	11,11,12	0.23	0	15,15,17	0.75	0
3	BMA	C	17	3	11,11,12	0.20	0	15,15,17	0.76	1 (6%)
3	MAN	C	18	3	11,11,12	0.22	0	15,15,17	0.74	0
3	AHR	C	19	3	9,9,10	0.54	0	11,12,14	0.97	1 (9%)
3	BMA	C	2	3	11,11,12	0.25	0	15,15,17	0.69	0
3	BMA	C	20	3	11,11,12	0.21	0	15,15,17	0.78	0
3	AHR	C	21	3	9,9,10	0.56	0	11,12,14	0.97	0
3	AHR	C	22	3	9,9,10	0.52	0	11,12,14	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AHR	C	23	3	9,9,10	0.57	0	11,12,14	0.89	0
3	AHR	C	24	3	9,9,10	0.55	0	11,12,14	0.93	0
3	FUB	C	25	3	9,9,10	0.55	0	11,12,14	0.99	1 (9%)
3	AHR	C	26	3	9,9,10	0.52	0	11,12,14	0.97	1 (9%)
3	FUB	C	27	3	9,9,10	0.55	0	11,12,14	1.11	1 (9%)
3	AHR	C	28	3	9,9,10	0.57	0	11,12,14	0.97	0
3	AHR	C	29	3	9,9,10	0.57	0	11,12,14	0.92	0
3	BMA	C	3	3	11,11,12	0.47	0	15,15,17	0.92	0
3	NGA	C	4	3	14,14,15	0.85	0	17,19,21	1.15	1 (5%)
3	MAN	C	5	3	11,11,12	0.59	0	15,15,17	2.09	5 (33%)
3	MAN	C	6	3	11,11,12	0.23	0	15,15,17	0.78	1 (6%)
3	MAN	C	7	3	11,11,12	0.21	0	15,15,17	0.73	0
3	GAL	C	8	3	11,11,12	0.17	0	15,15,17	0.79	0
3	MAN	C	9	3	11,11,12	0.22	0	15,15,17	0.86	2 (13%)
4	GAL	D	1	4	11,11,12	0.21	0	15,15,17	0.59	0
4	AHR	D	10	4	9,9,10	0.56	0	11,12,14	0.94	0
4	FUB	D	11	4	9,9,10	0.57	0	11,12,14	0.99	0
4	AHR	D	12	4	9,9,10	0.55	0	11,12,14	0.95	0
4	MAN	D	13	4	11,11,12	0.23	0	15,15,17	1.16	1 (6%)
4	MAN	D	14	4	11,11,12	0.36	0	15,15,17	1.15	2 (13%)
4	MAN	D	15	4	11,11,12	0.24	0	15,15,17	0.75	1 (6%)
4	AHR	D	16	4	9,9,10	0.57	0	11,12,14	0.93	0
4	BMA	D	2	4	11,11,12	0.25	0	15,15,17	0.64	0
4	BGC	D	3	4	11,11,12	0.23	0	15,15,17	0.53	0
4	AHR	D	4	4	9,9,10	0.54	0	11,12,14	1.05	1 (9%)
4	MAN	D	5	4	11,11,12	0.20	0	15,15,17	0.72	0
4	AHR	D	6	4	9,9,10	0.54	0	11,12,14	0.83	0
4	AHR	D	7	4	9,9,10	0.58	0	11,12,14	0.91	0
4	AHR	D	8	4	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
4	AHR	D	9	4	9,9,10	0.54	0	11,12,14	0.94	0
2	AHR	E	1	2	9,9,10	0.56	0	11,12,14	0.86	0
2	FUB	E	2	2	9,9,10	0.57	0	11,12,14	0.97	0
2	FUB	E	3	2	9,9,10	0.56	0	11,12,14	0.95	0
2	GAL	E	4	2	11,11,12	0.18	0	15,15,17	0.55	0
2	AHR	E	5	2	9,9,10	0.55	0	11,12,14	0.98	1 (9%)
2	FUB	E	6	2	9,9,10	0.57	0	11,12,14	0.92	0
2	AHR	E	7	2	9,9,10	0.55	0	11,12,14	0.96	0
3	FUB	F	1	3	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
3	AHR	F	10	3	9,9,10	0.55	0	11,12,14	1.00	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AHR	F	11	3	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
3	AHR	F	12	3	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
3	AHR	F	13	3	9,9,10	0.54	0	11,12,14	1.00	0
3	AHR	F	14	3	9,9,10	0.56	0	11,12,14	0.99	1 (9%)
3	MAN	F	15	3	11,11,12	0.22	0	15,15,17	0.74	1 (6%)
3	BMA	F	16	3	11,11,12	0.24	0	15,15,17	0.70	0
3	BMA	F	17	3	11,11,12	0.20	0	15,15,17	0.76	1 (6%)
3	MAN	F	18	3	11,11,12	0.21	0	15,15,17	0.73	0
3	AHR	F	19	3	9,9,10	0.53	0	11,12,14	0.98	1 (9%)
3	BMA	F	2	3	11,11,12	0.23	0	15,15,17	0.73	0
3	BMA	F	20	3	11,11,12	0.22	0	15,15,17	0.61	0
3	AHR	F	21	3	9,9,10	0.56	0	11,12,14	0.95	0
3	AHR	F	22	3	9,9,10	0.57	0	11,12,14	1.02	1 (9%)
3	AHR	F	23	3	9,9,10	0.56	0	11,12,14	0.97	0
3	AHR	F	24	3	9,9,10	0.54	0	11,12,14	0.88	0
3	FUB	F	25	3	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
3	AHR	F	26	3	9,9,10	0.54	0	11,12,14	1.01	1 (9%)
3	FUB	F	27	3	9,9,10	0.55	0	11,12,14	1.11	1 (9%)
3	AHR	F	28	3	9,9,10	0.54	0	11,12,14	0.95	0
3	AHR	F	29	3	9,9,10	0.54	0	11,12,14	0.92	0
3	BMA	F	3	3	11,11,12	0.43	0	15,15,17	0.66	0
3	NGA	F	4	3	14,14,15	0.82	0	17,19,21	1.00	0
3	MAN	F	5	3	11,11,12	0.23	0	15,15,17	0.77	0
3	MAN	F	6	3	11,11,12	0.22	0	15,15,17	0.77	1 (6%)
3	MAN	F	7	3	11,11,12	0.21	0	15,15,17	0.72	0
3	GAL	F	8	3	11,11,12	0.16	0	15,15,17	0.75	0
3	MAN	F	9	3	11,11,12	0.22	0	15,15,17	0.82	2 (13%)
4	GAL	G	1	4	11,11,12	0.20	0	15,15,17	0.62	0
4	AHR	G	10	4	9,9,10	0.58	0	11,12,14	0.94	0
4	FUB	G	11	4	9,9,10	0.56	0	11,12,14	1.01	1 (9%)
4	AHR	G	12	4	9,9,10	0.55	0	11,12,14	0.96	0
4	MAN	G	13	4	11,11,12	0.22	0	15,15,17	1.05	1 (6%)
4	MAN	G	14	4	11,11,12	0.22	0	15,15,17	0.74	0
4	MAN	G	15	4	11,11,12	0.21	0	15,15,17	0.73	1 (6%)
4	AHR	G	16	4	9,9,10	0.55	0	11,12,14	0.94	0
4	BMA	G	2	4	11,11,12	0.24	0	15,15,17	0.71	0
4	BGC	G	3	4	11,11,12	0.18	0	15,15,17	0.53	0
4	AHR	G	4	4	9,9,10	0.53	0	11,12,14	1.04	1 (9%)
4	MAN	G	5	4	11,11,12	0.21	0	15,15,17	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AHR	G	6	4	9,9,10	0.57	0	11,12,14	0.87	0
4	AHR	G	7	4	9,9,10	0.54	0	11,12,14	0.94	0
4	AHR	G	8	4	9,9,10	0.54	0	11,12,14	1.01	1 (9%)
4	AHR	G	9	4	9,9,10	0.56	0	11,12,14	0.93	0
2	AHR	H	1	2	9,9,10	0.53	0	11,12,14	0.87	0
2	FUB	H	2	2	9,9,10	0.57	0	11,12,14	0.96	0
2	FUB	H	3	2	9,9,10	0.55	0	11,12,14	0.94	0
2	GAL	H	4	2	11,11,12	0.18	0	15,15,17	0.56	0
2	AHR	H	5	2	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
2	FUB	H	6	2	9,9,10	0.56	0	11,12,14	0.92	0
2	AHR	H	7	2	9,9,10	0.54	0	11,12,14	0.95	0
3	FUB	I	1	3	9,9,10	0.51	0	11,12,14	0.99	1 (9%)
3	AHR	I	10	3	9,9,10	0.56	0	11,12,14	1.00	1 (9%)
3	AHR	I	11	3	9,9,10	0.54	0	11,12,14	0.99	0
3	AHR	I	12	3	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
3	AHR	I	13	3	9,9,10	0.55	0	11,12,14	1.00	1 (9%)
3	AHR	I	14	3	9,9,10	0.53	0	11,12,14	0.99	1 (9%)
3	MAN	I	15	3	11,11,12	0.23	0	15,15,17	0.74	1 (6%)
3	BMA	I	16	3	11,11,12	0.24	0	15,15,17	0.69	0
3	BMA	I	17	3	11,11,12	0.19	0	15,15,17	0.75	1 (6%)
3	MAN	I	18	3	11,11,12	0.21	0	15,15,17	0.73	0
3	AHR	I	19	3	9,9,10	0.55	0	11,12,14	0.98	0
3	BMA	I	2	3	11,11,12	0.24	0	15,15,17	0.73	0
3	BMA	I	20	3	11,11,12	0.22	0	15,15,17	0.62	0
3	AHR	I	21	3	9,9,10	0.53	0	11,12,14	0.95	0
3	AHR	I	22	3	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
3	AHR	I	23	3	9,9,10	0.56	0	11,12,14	0.97	0
3	AHR	I	24	3	9,9,10	0.53	0	11,12,14	0.89	0
3	FUB	I	25	3	9,9,10	0.54	0	11,12,14	1.00	0
3	AHR	I	26	3	9,9,10	0.56	0	11,12,14	1.01	1 (9%)
3	FUB	I	27	3	9,9,10	0.54	0	11,12,14	1.10	1 (9%)
3	AHR	I	28	3	9,9,10	0.55	0	11,12,14	0.93	0
3	AHR	I	29	3	9,9,10	0.54	0	11,12,14	0.92	0
3	BMA	I	3	3	11,11,12	0.41	0	15,15,17	0.67	0
3	NGA	I	4	3	14,14,15	0.82	0	17,19,21	1.00	0
3	MAN	I	5	3	11,11,12	0.22	0	15,15,17	0.76	0
3	MAN	I	6	3	11,11,12	0.22	0	15,15,17	0.77	1 (6%)
3	MAN	I	7	3	11,11,12	0.21	0	15,15,17	0.73	0
3	GAL	I	8	3	11,11,12	0.17	0	15,15,17	0.74	0
3	MAN	I	9	3	11,11,12	0.20	0	15,15,17	0.81	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GAL	J	1	4	11,11,12	0.22	0	15,15,17	0.63	0
4	AHR	J	10	4	9,9,10	0.53	0	11,12,14	0.93	0
4	FUB	J	11	4	9,9,10	0.55	0	11,12,14	1.00	1 (9%)
4	AHR	J	12	4	9,9,10	0.56	0	11,12,14	0.96	0
4	MAN	J	13	4	11,11,12	0.22	0	15,15,17	1.04	1 (6%)
4	MAN	J	14	4	11,11,12	0.24	0	15,15,17	0.74	0
4	MAN	J	15	4	11,11,12	0.22	0	15,15,17	0.74	1 (6%)
4	AHR	J	16	4	9,9,10	0.55	0	11,12,14	0.94	0
4	BMA	J	2	4	11,11,12	0.25	0	15,15,17	0.70	0
4	BGC	J	3	4	11,11,12	0.19	0	15,15,17	0.53	0
4	AHR	J	4	4	9,9,10	0.52	0	11,12,14	1.04	1 (9%)
4	MAN	J	5	4	11,11,12	0.20	0	15,15,17	0.71	0
4	AHR	J	6	4	9,9,10	0.55	0	11,12,14	0.87	0
4	AHR	J	7	4	9,9,10	0.53	0	11,12,14	0.95	0
4	AHR	J	8	4	9,9,10	0.57	0	11,12,14	1.01	1 (9%)
4	AHR	J	9	4	9,9,10	0.54	0	11,12,14	0.94	0
2	AHR	K	1	2	9,9,10	0.54	0	11,12,14	0.88	0
2	FUB	K	2	2	9,9,10	0.59	0	11,12,14	0.97	0
2	FUB	K	3	2	9,9,10	0.55	0	11,12,14	0.94	0
2	GAL	K	4	2	11,11,12	0.18	0	15,15,17	0.55	0
2	AHR	K	5	2	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
2	FUB	K	6	2	9,9,10	0.55	0	11,12,14	0.92	0
2	AHR	K	7	2	9,9,10	0.56	0	11,12,14	0.94	0
3	FUB	L	1	3	9,9,10	0.55	0	11,12,14	0.99	1 (9%)
3	AHR	L	10	3	9,9,10	0.55	0	11,12,14	0.98	1 (9%)
3	AHR	L	11	3	9,9,10	0.56	0	11,12,14	0.98	0
3	AHR	L	12	3	9,9,10	0.53	0	11,12,14	1.03	1 (9%)
3	AHR	L	13	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	AHR	L	14	3	9,9,10	0.55	0	11,12,14	0.98	1 (9%)
3	MAN	L	15	3	11,11,12	0.23	0	15,15,17	0.74	1 (6%)
3	BMA	L	16	3	11,11,12	0.24	0	15,15,17	0.70	0
3	BMA	L	17	3	11,11,12	0.20	0	15,15,17	0.76	1 (6%)
3	MAN	L	18	3	11,11,12	0.21	0	15,15,17	0.73	0
3	AHR	L	19	3	9,9,10	0.55	0	11,12,14	0.99	1 (9%)
3	BMA	L	2	3	11,11,12	0.23	0	15,15,17	0.72	0
3	BMA	L	20	3	11,11,12	0.21	0	15,15,17	0.61	0
3	AHR	L	21	3	9,9,10	0.55	0	11,12,14	0.94	0
3	AHR	L	22	3	9,9,10	0.54	0	11,12,14	1.01	1 (9%)
3	AHR	L	23	3	9,9,10	0.54	0	11,12,14	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AHR	L	24	3	9,9,10	0.54	0	11,12,14	0.88	0
3	FUB	L	25	3	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
3	AHR	L	26	3	9,9,10	0.58	0	11,12,14	1.01	1 (9%)
3	FUB	L	27	3	9,9,10	0.53	0	11,12,14	1.11	1 (9%)
3	AHR	L	28	3	9,9,10	0.57	0	11,12,14	0.94	0
3	AHR	L	29	3	9,9,10	0.56	0	11,12,14	0.92	0
3	BMA	L	3	3	11,11,12	0.43	0	15,15,17	0.66	0
3	NGA	L	4	3	14,14,15	0.82	0	17,19,21	1.01	0
3	MAN	L	5	3	11,11,12	0.22	0	15,15,17	0.77	1 (6%)
3	MAN	L	6	3	11,11,12	0.23	0	15,15,17	0.77	1 (6%)
3	MAN	L	7	3	11,11,12	0.20	0	15,15,17	0.73	0
3	GAL	L	8	3	11,11,12	0.18	0	15,15,17	0.73	0
3	MAN	L	9	3	11,11,12	0.21	0	15,15,17	0.81	1 (6%)
4	GAL	M	1	4	11,11,12	0.19	0	15,15,17	0.62	0
4	AHR	M	10	4	9,9,10	0.55	0	11,12,14	0.94	0
4	FUB	M	11	4	9,9,10	0.57	0	11,12,14	1.01	1 (9%)
4	AHR	M	12	4	9,9,10	0.55	0	11,12,14	0.97	0
4	MAN	M	13	4	11,11,12	0.23	0	15,15,17	1.05	1 (6%)
4	MAN	M	14	4	11,11,12	0.24	0	15,15,17	0.74	0
4	MAN	M	15	4	11,11,12	0.23	0	15,15,17	0.74	1 (6%)
4	AHR	M	16	4	9,9,10	0.52	0	11,12,14	0.95	0
4	BMA	M	2	4	11,11,12	0.22	0	15,15,17	0.71	0
4	BGC	M	3	4	11,11,12	0.19	0	15,15,17	0.53	0
4	AHR	M	4	4	9,9,10	0.54	0	11,12,14	1.03	1 (9%)
4	MAN	M	5	4	11,11,12	0.21	0	15,15,17	0.70	0
4	AHR	M	6	4	9,9,10	0.55	0	11,12,14	0.87	0
4	AHR	M	7	4	9,9,10	0.55	0	11,12,14	0.93	0
4	AHR	M	8	4	9,9,10	0.53	0	11,12,14	1.01	1 (9%)
4	AHR	M	9	4	9,9,10	0.57	0	11,12,14	0.94	0
2	AHR	N	1	2	9,9,10	0.53	0	11,12,14	0.87	0
2	FUB	N	2	2	9,9,10	0.58	0	11,12,14	0.96	0
2	FUB	N	3	2	9,9,10	0.54	0	11,12,14	0.94	0
2	GAL	N	4	2	11,11,12	0.17	0	15,15,17	0.55	0
2	AHR	N	5	2	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
2	FUB	N	6	2	9,9,10	0.56	0	11,12,14	0.92	0
2	AHR	N	7	2	9,9,10	0.56	0	11,12,14	0.94	0
3	FUB	O	1	3	9,9,10	0.55	0	11,12,14	1.00	1 (9%)
3	AHR	O	10	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	AHR	O	11	3	9,9,10	0.53	0	11,12,14	1.00	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AHR	O	12	3	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
3	AHR	O	13	3	9,9,10	0.55	0	11,12,14	0.99	1 (9%)
3	AHR	O	14	3	9,9,10	0.56	0	11,12,14	0.99	1 (9%)
3	MAN	O	15	3	11,11,12	0.20	0	15,15,17	0.74	1 (6%)
3	BMA	O	16	3	11,11,12	0.25	0	15,15,17	0.69	0
3	BMA	O	17	3	11,11,12	0.18	0	15,15,17	0.76	1 (6%)
3	MAN	O	18	3	11,11,12	0.21	0	15,15,17	0.73	0
3	AHR	O	19	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	BMA	O	2	3	11,11,12	0.25	0	15,15,17	0.73	0
3	BMA	O	20	3	11,11,12	0.22	0	15,15,17	0.61	0
3	AHR	O	21	3	9,9,10	0.53	0	11,12,14	0.95	0
3	AHR	O	22	3	9,9,10	0.56	0	11,12,14	1.01	1 (9%)
3	AHR	O	23	3	9,9,10	0.57	0	11,12,14	0.97	0
3	AHR	O	24	3	9,9,10	0.56	0	11,12,14	0.87	0
3	FUB	O	25	3	9,9,10	0.52	0	11,12,14	0.99	1 (9%)
3	AHR	O	26	3	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
3	FUB	O	27	3	9,9,10	0.56	0	11,12,14	1.11	1 (9%)
3	AHR	O	28	3	9,9,10	0.56	0	11,12,14	0.93	0
3	AHR	O	29	3	9,9,10	0.54	0	11,12,14	0.91	0
3	BMA	O	3	3	11,11,12	0.42	0	15,15,17	0.66	0
3	NGA	O	4	3	14,14,15	0.82	0	17,19,21	1.00	0
3	MAN	O	5	3	11,11,12	0.23	0	15,15,17	0.75	0
3	MAN	O	6	3	11,11,12	0.24	0	15,15,17	0.76	1 (6%)
3	MAN	O	7	3	11,11,12	0.22	0	15,15,17	0.73	0
3	GAL	O	8	3	11,11,12	0.17	0	15,15,17	0.74	0
3	MAN	O	9	3	11,11,12	0.24	0	15,15,17	0.81	1 (6%)
4	GAL	P	1	4	11,11,12	0.19	0	15,15,17	0.62	0
4	AHR	P	10	4	9,9,10	0.54	0	11,12,14	0.93	0
4	FUB	P	11	4	9,9,10	0.56	0	11,12,14	1.01	1 (9%)
4	AHR	P	12	4	9,9,10	0.56	0	11,12,14	0.96	0
4	MAN	P	13	4	11,11,12	0.24	0	15,15,17	1.05	1 (6%)
4	MAN	P	14	4	11,11,12	0.24	0	15,15,17	0.74	0
4	MAN	P	15	4	11,11,12	0.22	0	15,15,17	0.73	1 (6%)
4	AHR	P	16	4	9,9,10	0.54	0	11,12,14	0.93	0
4	BMA	P	2	4	11,11,12	0.23	0	15,15,17	0.70	0
4	BGC	P	3	4	11,11,12	0.20	0	15,15,17	0.52	0
4	AHR	P	4	4	9,9,10	0.54	0	11,12,14	1.03	1 (9%)
4	MAN	P	5	4	11,11,12	0.22	0	15,15,17	0.71	0
4	AHR	P	6	4	9,9,10	0.55	0	11,12,14	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AHR	P	7	4	9,9,10	0.56	0	11,12,14	0.93	0
4	AHR	P	8	4	9,9,10	0.56	0	11,12,14	1.00	1 (9%)
4	AHR	P	9	4	9,9,10	0.55	0	11,12,14	0.93	0
2	AHR	Q	1	2	9,9,10	0.53	0	11,12,14	0.86	0
2	FUB	Q	2	2	9,9,10	0.60	0	11,12,14	0.98	0
2	FUB	Q	3	2	9,9,10	0.55	0	11,12,14	0.95	0
2	GAL	Q	4	2	11,11,12	0.18	0	15,15,17	0.56	0
2	AHR	Q	5	2	9,9,10	0.53	0	11,12,14	0.99	1 (9%)
2	FUB	Q	6	2	9,9,10	0.54	0	11,12,14	0.92	0
2	AHR	Q	7	2	9,9,10	0.54	0	11,12,14	0.94	0
3	FUB	R	1	3	9,9,10	0.51	0	11,12,14	0.99	1 (9%)
3	AHR	R	10	3	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
3	AHR	R	11	3	9,9,10	0.56	0	11,12,14	0.99	1 (9%)
3	AHR	R	12	3	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
3	AHR	R	13	3	9,9,10	0.53	0	11,12,14	0.99	0
3	AHR	R	14	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	MAN	R	15	3	11,11,12	0.23	0	15,15,17	0.73	1 (6%)
3	BMA	R	16	3	11,11,12	0.26	0	15,15,17	0.69	0
3	BMA	R	17	3	11,11,12	0.19	0	15,15,17	0.75	1 (6%)
3	MAN	R	18	3	11,11,12	0.21	0	15,15,17	0.73	0
3	AHR	R	19	3	9,9,10	0.55	0	11,12,14	0.98	0
3	BMA	R	2	3	11,11,12	0.25	0	15,15,17	0.72	0
3	BMA	R	20	3	11,11,12	0.21	0	15,15,17	0.62	0
3	AHR	R	21	3	9,9,10	0.54	0	11,12,14	0.95	0
3	AHR	R	22	3	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
3	AHR	R	23	3	9,9,10	0.58	0	11,12,14	0.96	0
3	AHR	R	24	3	9,9,10	0.54	0	11,12,14	0.87	0
3	FUB	R	25	3	9,9,10	0.54	0	11,12,14	0.99	0
3	AHR	R	26	3	9,9,10	0.54	0	11,12,14	1.01	1 (9%)
3	FUB	R	27	3	9,9,10	0.54	0	11,12,14	1.11	1 (9%)
3	AHR	R	28	3	9,9,10	0.57	0	11,12,14	0.94	0
3	AHR	R	29	3	9,9,10	0.56	0	11,12,14	0.92	0
3	BMA	R	3	3	11,11,12	0.42	0	15,15,17	0.66	0
3	NGA	R	4	3	14,14,15	0.85	0	17,19,21	1.01	0
3	MAN	R	5	3	11,11,12	0.21	0	15,15,17	0.77	0
3	MAN	R	6	3	11,11,12	0.23	0	15,15,17	0.76	1 (6%)
3	MAN	R	7	3	11,11,12	0.21	0	15,15,17	0.73	0
3	GAL	R	8	3	11,11,12	0.17	0	15,15,17	0.74	0
3	MAN	R	9	3	11,11,12	0.20	0	15,15,17	0.80	1 (6%)
4	GAL	S	1	4	11,11,12	0.20	0	15,15,17	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AHR	S	10	4	9,9,10	0.55	0	11,12,14	0.93	0
4	FUB	S	11	4	9,9,10	0.56	0	11,12,14	1.01	1 (9%)
4	AHR	S	12	4	9,9,10	0.57	0	11,12,14	0.95	0
4	MAN	S	13	4	11,11,12	0.21	0	15,15,17	1.05	1 (6%)
4	MAN	S	14	4	11,11,12	0.24	0	15,15,17	0.75	1 (6%)
4	MAN	S	15	4	11,11,12	0.25	0	15,15,17	0.74	0
4	AHR	S	16	4	9,9,10	0.55	0	11,12,14	0.94	0
4	BMA	S	2	4	11,11,12	0.24	0	15,15,17	0.71	0
4	BGC	S	3	4	11,11,12	0.17	0	15,15,17	0.53	0
4	AHR	S	4	4	9,9,10	0.53	0	11,12,14	1.04	1 (9%)
4	MAN	S	5	4	11,11,12	0.21	0	15,15,17	0.70	0
4	AHR	S	6	4	9,9,10	0.56	0	11,12,14	0.87	0
4	AHR	S	7	4	9,9,10	0.54	0	11,12,14	0.94	0
4	AHR	S	8	4	9,9,10	0.56	0	11,12,14	1.00	1 (9%)
4	AHR	S	9	4	9,9,10	0.54	0	11,12,14	0.93	0
2	AHR	T	1	2	9,9,10	0.54	0	11,12,14	0.86	0
2	FUB	T	2	2	9,9,10	0.56	0	11,12,14	0.97	0
2	FUB	T	3	2	9,9,10	0.57	0	11,12,14	0.95	0
2	GAL	T	4	2	11,11,12	0.18	0	15,15,17	0.55	0
2	AHR	T	5	2	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
2	FUB	T	6	2	9,9,10	0.55	0	11,12,14	0.91	0
2	AHR	T	7	2	9,9,10	0.55	0	11,12,14	0.95	0
3	FUB	U	1	3	9,9,10	0.51	0	11,12,14	1.00	1 (9%)
3	AHR	U	10	3	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
3	AHR	U	11	3	9,9,10	0.55	0	11,12,14	0.99	0
3	AHR	U	12	3	9,9,10	0.54	0	11,12,14	1.03	1 (9%)
3	AHR	U	13	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	AHR	U	14	3	9,9,10	0.56	0	11,12,14	0.99	1 (9%)
3	MAN	U	15	3	11,11,12	0.24	0	15,15,17	0.73	0
3	BMA	U	16	3	11,11,12	0.25	0	15,15,17	0.69	0
3	BMA	U	17	3	11,11,12	0.20	0	15,15,17	0.76	1 (6%)
3	MAN	U	18	3	11,11,12	0.20	0	15,15,17	0.74	0
3	AHR	U	19	3	9,9,10	0.56	0	11,12,14	0.99	1 (9%)
3	BMA	U	2	3	11,11,12	0.25	0	15,15,17	0.72	0
3	BMA	U	20	3	11,11,12	0.22	0	15,15,17	0.62	0
3	AHR	U	21	3	9,9,10	0.55	0	11,12,14	0.95	0
3	AHR	U	22	3	9,9,10	0.52	0	11,12,14	1.02	1 (9%)
3	AHR	U	23	3	9,9,10	0.58	0	11,12,14	0.97	0
3	AHR	U	24	3	9,9,10	0.57	0	11,12,14	0.88	0
3	FUB	U	25	3	9,9,10	0.54	0	11,12,14	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AHR	U	26	3	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
3	FUB	U	27	3	9,9,10	0.55	0	11,12,14	1.10	1 (9%)
3	AHR	U	28	3	9,9,10	0.53	0	11,12,14	0.94	0
3	AHR	U	29	3	9,9,10	0.55	0	11,12,14	0.92	0
3	BMA	U	3	3	11,11,12	0.42	0	15,15,17	0.66	0
3	NGA	U	4	3	14,14,15	0.82	0	17,19,21	1.00	0
3	MAN	U	5	3	11,11,12	0.22	0	15,15,17	0.76	0
3	MAN	U	6	3	11,11,12	0.24	0	15,15,17	0.75	1 (6%)
3	MAN	U	7	3	11,11,12	0.21	0	15,15,17	0.74	0
3	GAL	U	8	3	11,11,12	0.18	0	15,15,17	0.73	0
3	MAN	U	9	3	11,11,12	0.22	0	15,15,17	0.82	1 (6%)
4	GAL	V	1	4	11,11,12	0.20	0	15,15,17	0.63	0
4	AHR	V	10	4	9,9,10	0.54	0	11,12,14	0.93	0
4	FUB	V	11	4	9,9,10	0.55	0	11,12,14	1.00	1 (9%)
4	AHR	V	12	4	9,9,10	0.55	0	11,12,14	0.96	0
4	MAN	V	13	4	11,11,12	0.23	0	15,15,17	1.05	1 (6%)
4	MAN	V	14	4	11,11,12	0.22	0	15,15,17	0.75	1 (6%)
4	MAN	V	15	4	11,11,12	0.23	0	15,15,17	0.74	1 (6%)
4	AHR	V	16	4	9,9,10	0.55	0	11,12,14	0.94	0
4	BMA	V	2	4	11,11,12	0.23	0	15,15,17	0.71	0
4	BGC	V	3	4	11,11,12	0.19	0	15,15,17	0.52	0
4	AHR	V	4	4	9,9,10	0.55	0	11,12,14	1.03	1 (9%)
4	MAN	V	5	4	11,11,12	0.20	0	15,15,17	0.71	0
4	AHR	V	6	4	9,9,10	0.54	0	11,12,14	0.88	0
4	AHR	V	7	4	9,9,10	0.56	0	11,12,14	0.93	0
4	AHR	V	8	4	9,9,10	0.54	0	11,12,14	1.01	1 (9%)
4	AHR	V	9	4	9,9,10	0.53	0	11,12,14	0.93	0
2	AHR	W	1	2	9,9,10	0.53	0	11,12,14	0.87	0
2	FUB	W	2	2	9,9,10	0.58	0	11,12,14	0.97	0
2	FUB	W	3	2	9,9,10	0.55	0	11,12,14	0.94	0
2	GAL	W	4	2	11,11,12	0.17	0	15,15,17	0.56	0
2	AHR	W	5	2	9,9,10	0.55	0	11,12,14	0.98	1 (9%)
2	FUB	W	6	2	9,9,10	0.56	0	11,12,14	0.92	0
2	AHR	W	7	2	9,9,10	0.55	0	11,12,14	0.94	0
3	FUB	X	1	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	AHR	X	10	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	AHR	X	11	3	9,9,10	0.56	0	11,12,14	0.99	1 (9%)
3	AHR	X	12	3	9,9,10	0.54	0	11,12,14	1.03	1 (9%)
3	AHR	X	13	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AHR	X	14	3	9,9,10	0.55	0	11,12,14	1.00	1 (9%)
3	MAN	X	15	3	11,11,12	0.22	0	15,15,17	0.73	0
3	BMA	X	16	3	11,11,12	0.24	0	15,15,17	0.69	0
3	BMA	X	17	3	11,11,12	0.20	0	15,15,17	0.74	1 (6%)
3	MAN	X	18	3	11,11,12	0.22	0	15,15,17	0.74	0
3	AHR	X	19	3	9,9,10	0.55	0	11,12,14	0.99	1 (9%)
3	BMA	X	2	3	11,11,12	0.24	0	15,15,17	0.72	0
3	BMA	X	20	3	11,11,12	0.21	0	15,15,17	0.61	0
3	AHR	X	21	3	9,9,10	0.55	0	11,12,14	0.96	0
3	AHR	X	22	3	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
3	AHR	X	23	3	9,9,10	0.57	0	11,12,14	0.97	0
3	AHR	X	24	3	9,9,10	0.56	0	11,12,14	0.89	0
3	FUB	X	25	3	9,9,10	0.53	0	11,12,14	1.00	0
3	AHR	X	26	3	9,9,10	0.56	0	11,12,14	1.02	1 (9%)
3	FUB	X	27	3	9,9,10	0.54	0	11,12,14	1.11	1 (9%)
3	AHR	X	28	3	9,9,10	0.53	0	11,12,14	0.95	0
3	AHR	X	29	3	9,9,10	0.53	0	11,12,14	0.92	0
3	BMA	X	3	3	11,11,12	0.42	0	15,15,17	0.67	0
3	NGA	X	4	3	14,14,15	0.82	0	17,19,21	1.00	0
3	MAN	X	5	3	11,11,12	0.21	0	15,15,17	0.76	0
3	MAN	X	6	3	11,11,12	0.23	0	15,15,17	0.77	1 (6%)
3	MAN	X	7	3	11,11,12	0.21	0	15,15,17	0.73	0
3	GAL	X	8	3	11,11,12	0.16	0	15,15,17	0.74	0
3	MAN	X	9	3	11,11,12	0.21	0	15,15,17	0.81	1 (6%)
4	GAL	Y	1	4	11,11,12	0.19	0	15,15,17	0.62	0
4	AHR	Y	10	4	9,9,10	0.56	0	11,12,14	0.93	0
4	FUB	Y	11	4	9,9,10	0.55	0	11,12,14	1.00	1 (9%)
4	AHR	Y	12	4	9,9,10	0.55	0	11,12,14	0.96	0
4	MAN	Y	13	4	11,11,12	0.24	0	15,15,17	1.05	1 (6%)
4	MAN	Y	14	4	11,11,12	0.22	0	15,15,17	0.75	1 (6%)
4	MAN	Y	15	4	11,11,12	0.23	0	15,15,17	0.74	1 (6%)
4	AHR	Y	16	4	9,9,10	0.54	0	11,12,14	0.94	0
4	BMA	Y	2	4	11,11,12	0.24	0	15,15,17	0.70	0
4	BGC	Y	3	4	11,11,12	0.19	0	15,15,17	0.52	0
4	AHR	Y	4	4	9,9,10	0.52	0	11,12,14	1.04	1 (9%)
4	MAN	Y	5	4	11,11,12	0.20	0	15,15,17	0.71	0
4	AHR	Y	6	4	9,9,10	0.54	0	11,12,14	0.88	0
4	AHR	Y	7	4	9,9,10	0.57	0	11,12,14	0.93	0
4	AHR	Y	8	4	9,9,10	0.53	0	11,12,14	1.01	1 (9%)
4	AHR	Y	9	4	9,9,10	0.53	0	11,12,14	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AHR	Z	1	2	9,9,10	0.55	0	11,12,14	0.87	0
2	FUB	Z	2	2	9,9,10	0.58	0	11,12,14	0.97	0
2	FUB	Z	3	2	9,9,10	0.56	0	11,12,14	0.95	0
2	GAL	Z	4	2	11,11,12	0.19	0	15,15,17	0.56	0
2	AHR	Z	5	2	9,9,10	0.53	0	11,12,14	0.99	1 (9%)
2	FUB	Z	6	2	9,9,10	0.57	0	11,12,14	0.92	0
2	AHR	Z	7	2	9,9,10	0.55	0	11,12,14	0.95	0
3	FUB	a	1	3	9,9,10	0.55	0	11,12,14	0.98	1 (9%)
3	AHR	a	10	3	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
3	AHR	a	11	3	9,9,10	0.56	0	11,12,14	0.98	1 (9%)
3	AHR	a	12	3	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
3	AHR	a	13	3	9,9,10	0.53	0	11,12,14	0.99	1 (9%)
3	AHR	a	14	3	9,9,10	0.56	0	11,12,14	0.99	1 (9%)
3	MAN	a	15	3	11,11,12	0.20	0	15,15,17	0.74	1 (6%)
3	BMA	a	16	3	11,11,12	0.25	0	15,15,17	0.69	0
3	BMA	a	17	3	11,11,12	0.20	0	15,15,17	0.76	1 (6%)
3	MAN	a	18	3	11,11,12	0.22	0	15,15,17	0.73	0
3	AHR	a	19	3	9,9,10	0.53	0	11,12,14	0.99	1 (9%)
3	BMA	a	2	3	11,11,12	0.26	0	15,15,17	0.72	0
3	BMA	a	20	3	11,11,12	0.21	0	15,15,17	0.61	0
3	AHR	a	21	3	9,9,10	0.57	0	11,12,14	0.95	0
3	AHR	a	22	3	9,9,10	0.56	0	11,12,14	1.00	1 (9%)
3	AHR	a	23	3	9,9,10	0.59	0	11,12,14	0.97	0
3	AHR	a	24	3	9,9,10	0.53	0	11,12,14	0.88	0
3	FUB	a	25	3	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
3	AHR	a	26	3	9,9,10	0.58	0	11,12,14	1.01	1 (9%)
3	FUB	a	27	3	9,9,10	0.56	0	11,12,14	1.11	1 (9%)
3	AHR	a	28	3	9,9,10	0.57	0	11,12,14	0.94	0
3	AHR	a	29	3	9,9,10	0.54	0	11,12,14	0.91	0
3	BMA	a	3	3	11,11,12	0.40	0	15,15,17	0.66	0
3	NGA	a	4	3	14,14,15	0.82	0	17,19,21	1.00	0
3	MAN	a	5	3	11,11,12	0.21	0	15,15,17	0.76	0
3	MAN	a	6	3	11,11,12	0.23	0	15,15,17	0.77	1 (6%)
3	MAN	a	7	3	11,11,12	0.22	0	15,15,17	0.73	0
3	GAL	a	8	3	11,11,12	0.16	0	15,15,17	0.74	0
3	MAN	a	9	3	11,11,12	0.20	0	15,15,17	0.82	1 (6%)
4	GAL	b	1	4	11,11,12	0.19	0	15,15,17	0.62	0
4	AHR	b	10	4	9,9,10	0.57	0	11,12,14	0.94	0
4	FUB	b	11	4	9,9,10	0.55	0	11,12,14	1.01	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AHR	b	12	4	9,9,10	0.54	0	11,12,14	0.96	0
4	MAN	b	13	4	11,11,12	0.22	0	15,15,17	1.05	1 (6%)
4	MAN	b	14	4	11,11,12	0.23	0	15,15,17	0.75	1 (6%)
4	MAN	b	15	4	11,11,12	0.25	0	15,15,17	0.72	0
4	AHR	b	16	4	9,9,10	0.54	0	11,12,14	0.94	0
4	BMA	b	2	4	11,11,12	0.24	0	15,15,17	0.71	0
4	BGC	b	3	4	11,11,12	0.18	0	15,15,17	0.54	0
4	AHR	b	4	4	9,9,10	0.54	0	11,12,14	1.04	1 (9%)
4	MAN	b	5	4	11,11,12	0.21	0	15,15,17	0.72	0
4	AHR	b	6	4	9,9,10	0.56	0	11,12,14	0.87	0
4	AHR	b	7	4	9,9,10	0.56	0	11,12,14	0.93	0
4	AHR	b	8	4	9,9,10	0.54	0	11,12,14	1.01	1 (9%)
4	AHR	b	9	4	9,9,10	0.55	0	11,12,14	0.93	0
2	AHR	c	1	2	9,9,10	0.55	0	11,12,14	0.86	0
2	FUB	c	2	2	9,9,10	0.57	0	11,12,14	0.96	0
2	FUB	c	3	2	9,9,10	0.54	0	11,12,14	0.95	0
2	GAL	c	4	2	11,11,12	0.18	0	15,15,17	0.56	0
2	AHR	c	5	2	9,9,10	0.55	0	11,12,14	0.98	1 (9%)
2	FUB	c	6	2	9,9,10	0.55	0	11,12,14	0.93	0
2	AHR	c	7	2	9,9,10	0.54	0	11,12,14	0.94	0
3	FUB	d	1	3	9,9,10	0.53	0	11,12,14	0.99	1 (9%)
3	AHR	d	10	3	9,9,10	0.56	0	11,12,14	1.00	1 (9%)
3	AHR	d	11	3	9,9,10	0.56	0	11,12,14	0.98	1 (9%)
3	AHR	d	12	3	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
3	AHR	d	13	3	9,9,10	0.55	0	11,12,14	1.00	1 (9%)
3	AHR	d	14	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	MAN	d	15	3	11,11,12	0.22	0	15,15,17	0.73	1 (6%)
3	BMA	d	16	3	11,11,12	0.24	0	15,15,17	0.70	0
3	BMA	d	17	3	11,11,12	0.19	0	15,15,17	0.76	1 (6%)
3	MAN	d	18	3	11,11,12	0.21	0	15,15,17	0.73	0
3	AHR	d	19	3	9,9,10	0.55	0	11,12,14	1.00	1 (9%)
3	BMA	d	2	3	11,11,12	0.25	0	15,15,17	0.73	0
3	BMA	d	20	3	11,11,12	0.20	0	15,15,17	0.61	0
3	AHR	d	21	3	9,9,10	0.57	0	11,12,14	0.94	0
3	AHR	d	22	3	9,9,10	0.57	0	11,12,14	1.02	1 (9%)
3	AHR	d	23	3	9,9,10	0.52	0	11,12,14	0.97	0
3	AHR	d	24	3	9,9,10	0.55	0	11,12,14	0.87	0
3	FUB	d	25	3	9,9,10	0.55	0	11,12,14	1.00	0
3	AHR	d	26	3	9,9,10	0.55	0	11,12,14	1.01	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUB	d	27	3	9,9,10	0.52	0	11,12,14	1.11	1 (9%)
3	AHR	d	28	3	9,9,10	0.55	0	11,12,14	0.93	0
3	AHR	d	29	3	9,9,10	0.55	0	11,12,14	0.91	0
3	BMA	d	3	3	11,11,12	0.41	0	15,15,17	0.66	0
3	NGA	d	4	3	14,14,15	0.82	0	17,19,21	1.00	0
3	MAN	d	5	3	11,11,12	0.22	0	15,15,17	0.76	0
3	MAN	d	6	3	11,11,12	0.23	0	15,15,17	0.77	1 (6%)
3	MAN	d	7	3	11,11,12	0.21	0	15,15,17	0.75	0
3	GAL	d	8	3	11,11,12	0.16	0	15,15,17	0.74	0
3	MAN	d	9	3	11,11,12	0.20	0	15,15,17	0.81	1 (6%)
4	GAL	e	1	4	11,11,12	0.20	0	15,15,17	0.62	0
4	AHR	e	10	4	9,9,10	0.56	0	11,12,14	0.93	0
4	FUB	e	11	4	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
4	AHR	e	12	4	9,9,10	0.55	0	11,12,14	0.96	0
4	MAN	e	13	4	11,11,12	0.21	0	15,15,17	1.04	1 (6%)
4	MAN	e	14	4	11,11,12	0.24	0	15,15,17	0.74	0
4	MAN	e	15	4	11,11,12	0.22	0	15,15,17	0.73	0
4	AHR	e	16	4	9,9,10	0.55	0	11,12,14	0.93	0
4	BMA	e	2	4	11,11,12	0.21	0	15,15,17	0.70	0
4	BGC	e	3	4	11,11,12	0.20	0	15,15,17	0.53	0
4	AHR	e	4	4	9,9,10	0.55	0	11,12,14	1.04	1 (9%)
4	MAN	e	5	4	11,11,12	0.21	0	15,15,17	0.70	0
4	AHR	e	6	4	9,9,10	0.57	0	11,12,14	0.88	0
4	AHR	e	7	4	9,9,10	0.55	0	11,12,14	0.95	0
4	AHR	e	8	4	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
4	AHR	e	9	4	9,9,10	0.53	0	11,12,14	0.93	0
2	AHR	f	1	2	9,9,10	0.54	0	11,12,14	0.87	0
2	FUB	f	2	2	9,9,10	0.58	0	11,12,14	0.96	0
2	FUB	f	3	2	9,9,10	0.56	0	11,12,14	0.95	0
2	GAL	f	4	2	11,11,12	0.17	0	15,15,17	0.56	0
2	AHR	f	5	2	9,9,10	0.55	0	11,12,14	0.97	1 (9%)
2	FUB	f	6	2	9,9,10	0.56	0	11,12,14	0.93	0
2	AHR	f	7	2	9,9,10	0.55	0	11,12,14	0.95	0
3	FUB	g	1	3	9,9,10	0.50	0	11,12,14	1.00	1 (9%)
3	AHR	g	10	3	9,9,10	0.55	0	11,12,14	0.99	1 (9%)
3	AHR	g	11	3	9,9,10	0.52	0	11,12,14	0.99	1 (9%)
3	AHR	g	12	3	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
3	AHR	g	13	3	9,9,10	0.54	0	11,12,14	0.99	0
3	AHR	g	14	3	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
3	MAN	g	15	3	11,11,12	0.23	0	15,15,17	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	g	16	3	11,11,12	0.25	0	15,15,17	0.69	0
3	BMA	g	17	3	11,11,12	0.19	0	15,15,17	0.76	1 (6%)
3	MAN	g	18	3	11,11,12	0.20	0	15,15,17	0.73	0
3	AHR	g	19	3	9,9,10	0.55	0	11,12,14	0.98	1 (9%)
3	BMA	g	2	3	11,11,12	0.24	0	15,15,17	0.73	0
3	BMA	g	20	3	11,11,12	0.22	0	15,15,17	0.61	0
3	AHR	g	21	3	9,9,10	0.56	0	11,12,14	0.94	0
3	AHR	g	22	3	9,9,10	0.53	0	11,12,14	1.01	1 (9%)
3	AHR	g	23	3	9,9,10	0.55	0	11,12,14	0.97	0
3	AHR	g	24	3	9,9,10	0.54	0	11,12,14	0.89	0
3	FUB	g	25	3	9,9,10	0.54	0	11,12,14	0.98	0
3	AHR	g	26	3	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
3	FUB	g	27	3	9,9,10	0.55	0	11,12,14	1.11	1 (9%)
3	AHR	g	28	3	9,9,10	0.55	0	11,12,14	0.92	0
3	AHR	g	29	3	9,9,10	0.54	0	11,12,14	0.92	0
3	BMA	g	3	3	11,11,12	0.42	0	15,15,17	0.67	0
3	NGA	g	4	3	14,14,15	0.83	0	17,19,21	1.01	0
3	MAN	g	5	3	11,11,12	0.21	0	15,15,17	0.77	1 (6%)
3	MAN	g	6	3	11,11,12	0.25	0	15,15,17	0.76	1 (6%)
3	MAN	g	7	3	11,11,12	0.21	0	15,15,17	0.73	0
3	GAL	g	8	3	11,11,12	0.16	0	15,15,17	0.74	0
3	MAN	g	9	3	11,11,12	0.21	0	15,15,17	0.80	1 (6%)
4	GAL	h	1	4	11,11,12	0.19	0	15,15,17	0.62	0
4	AHR	h	10	4	9,9,10	0.56	0	11,12,14	0.93	0
4	FUB	h	11	4	9,9,10	0.55	0	11,12,14	1.00	1 (9%)
4	AHR	h	12	4	9,9,10	0.55	0	11,12,14	0.95	0
4	MAN	h	13	4	11,11,12	0.23	0	15,15,17	1.05	1 (6%)
4	MAN	h	14	4	11,11,12	0.21	0	15,15,17	0.75	1 (6%)
4	MAN	h	15	4	11,11,12	0.25	0	15,15,17	0.74	0
4	AHR	h	16	4	9,9,10	0.53	0	11,12,14	0.93	0
4	BMA	h	2	4	11,11,12	0.25	0	15,15,17	0.71	0
4	BGC	h	3	4	11,11,12	0.18	0	15,15,17	0.51	0
4	AHR	h	4	4	9,9,10	0.53	0	11,12,14	1.03	1 (9%)
4	MAN	h	5	4	11,11,12	0.21	0	15,15,17	0.71	0
4	AHR	h	6	4	9,9,10	0.54	0	11,12,14	0.87	0
4	AHR	h	7	4	9,9,10	0.56	0	11,12,14	0.94	0
4	AHR	h	8	4	9,9,10	0.54	0	11,12,14	1.01	1 (9%)
4	AHR	h	9	4	9,9,10	0.57	0	11,12,14	0.93	0
2	AHR	i	1	2	9,9,10	0.53	0	11,12,14	0.86	0
2	FUB	i	2	2	9,9,10	0.58	0	11,12,14	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FUB	i	3	2	9,9,10	0.54	0	11,12,14	0.96	0
2	GAL	i	4	2	11,11,12	0.17	0	15,15,17	0.55	0
2	AHR	i	5	2	9,9,10	0.55	0	11,12,14	0.97	0
2	FUB	i	6	2	9,9,10	0.55	0	11,12,14	0.92	0
2	AHR	i	7	2	9,9,10	0.55	0	11,12,14	0.94	0
3	FUB	j	1	3	9,9,10	0.53	0	11,12,14	0.99	1 (9%)
3	AHR	j	10	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	AHR	j	11	3	9,9,10	0.56	0	11,12,14	1.00	1 (9%)
3	AHR	j	12	3	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
3	AHR	j	13	3	9,9,10	0.56	0	11,12,14	0.99	1 (9%)
3	AHR	j	14	3	9,9,10	0.55	0	11,12,14	0.98	1 (9%)
3	MAN	j	15	3	11,11,12	0.23	0	15,15,17	0.73	0
3	BMA	j	16	3	11,11,12	0.24	0	15,15,17	0.70	0
3	BMA	j	17	3	11,11,12	0.20	0	15,15,17	0.76	1 (6%)
3	MAN	j	18	3	11,11,12	0.22	0	15,15,17	0.72	0
3	AHR	j	19	3	9,9,10	0.57	0	11,12,14	0.97	0
3	BMA	j	2	3	11,11,12	0.25	0	15,15,17	0.72	0
3	BMA	j	20	3	11,11,12	0.21	0	15,15,17	0.61	0
3	AHR	j	21	3	9,9,10	0.57	0	11,12,14	0.94	0
3	AHR	j	22	3	9,9,10	0.56	0	11,12,14	1.02	1 (9%)
3	AHR	j	23	3	9,9,10	0.56	0	11,12,14	0.97	0
3	AHR	j	24	3	9,9,10	0.55	0	11,12,14	0.89	0
3	FUB	j	25	3	9,9,10	0.54	0	11,12,14	0.99	0
3	AHR	j	26	3	9,9,10	0.56	0	11,12,14	1.02	1 (9%)
3	FUB	j	27	3	9,9,10	0.53	0	11,12,14	1.11	1 (9%)
3	AHR	j	28	3	9,9,10	0.57	0	11,12,14	0.92	0
3	AHR	j	29	3	9,9,10	0.54	0	11,12,14	0.92	0
3	BMA	j	3	3	11,11,12	0.40	0	15,15,17	0.67	0
3	NGA	j	4	3	14,14,15	0.83	0	17,19,21	1.01	0
3	MAN	j	5	3	11,11,12	0.22	0	15,15,17	0.76	0
3	MAN	j	6	3	11,11,12	0.24	0	15,15,17	0.76	1 (6%)
3	MAN	j	7	3	11,11,12	0.20	0	15,15,17	0.73	0
3	GAL	j	8	3	11,11,12	0.17	0	15,15,17	0.74	0
3	MAN	j	9	3	11,11,12	0.22	0	15,15,17	0.82	1 (6%)
4	GAL	k	1	4	11,11,12	0.19	0	15,15,17	0.62	0
4	AHR	k	10	4	9,9,10	0.55	0	11,12,14	0.94	0
4	FUB	k	11	4	9,9,10	0.54	0	11,12,14	1.01	1 (9%)
4	AHR	k	12	4	9,9,10	0.54	0	11,12,14	0.96	0
4	MAN	k	13	4	11,11,12	0.23	0	15,15,17	1.05	1 (6%)
4	MAN	k	14	4	11,11,12	0.23	0	15,15,17	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	k	15	4	11,11,12	0.23	0	15,15,17	0.74	1 (6%)
4	AHR	k	16	4	9,9,10	0.53	0	11,12,14	0.94	0
4	BMA	k	2	4	11,11,12	0.26	0	15,15,17	0.70	0
4	BGC	k	3	4	11,11,12	0.20	0	15,15,17	0.52	0
4	AHR	k	4	4	9,9,10	0.52	0	11,12,14	1.03	1 (9%)
4	MAN	k	5	4	11,11,12	0.20	0	15,15,17	0.72	0
4	AHR	k	6	4	9,9,10	0.52	0	11,12,14	0.88	0
4	AHR	k	7	4	9,9,10	0.57	0	11,12,14	0.93	0
4	AHR	k	8	4	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
4	AHR	k	9	4	9,9,10	0.56	0	11,12,14	0.93	0
2	AHR	l	1	2	9,9,10	0.53	0	11,12,14	0.86	0
2	FUB	l	2	2	9,9,10	0.58	0	11,12,14	0.96	0
2	FUB	l	3	2	9,9,10	0.53	0	11,12,14	0.95	0
2	GAL	l	4	2	11,11,12	0.18	0	15,15,17	0.56	0
2	AHR	l	5	2	9,9,10	0.54	0	11,12,14	0.97	0
2	FUB	l	6	2	9,9,10	0.56	0	11,12,14	0.92	0
2	AHR	l	7	2	9,9,10	0.56	0	11,12,14	0.96	0
3	FUB	m	1	3	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
3	AHR	m	10	3	9,9,10	0.52	0	11,12,14	0.99	1 (9%)
3	AHR	m	11	3	9,9,10	0.53	0	11,12,14	0.99	1 (9%)
3	AHR	m	12	3	9,9,10	0.56	0	11,12,14	1.02	1 (9%)
3	AHR	m	13	3	9,9,10	0.56	0	11,12,14	0.99	0
3	AHR	m	14	3	9,9,10	0.54	0	11,12,14	0.98	0
3	MAN	m	15	3	11,11,12	0.24	0	15,15,17	0.74	1 (6%)
3	BMA	m	16	3	11,11,12	0.24	0	15,15,17	0.70	0
3	BMA	m	17	3	11,11,12	0.18	0	15,15,17	0.76	1 (6%)
3	MAN	m	18	3	11,11,12	0.21	0	15,15,17	0.73	0
3	AHR	m	19	3	9,9,10	0.53	0	11,12,14	0.99	1 (9%)
3	BMA	m	2	3	11,11,12	0.25	0	15,15,17	0.72	0
3	BMA	m	20	3	11,11,12	0.23	0	15,15,17	0.61	0
3	AHR	m	21	3	9,9,10	0.55	0	11,12,14	0.94	0
3	AHR	m	22	3	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
3	AHR	m	23	3	9,9,10	0.55	0	11,12,14	0.96	0
3	AHR	m	24	3	9,9,10	0.54	0	11,12,14	0.89	0
3	FUB	m	25	3	9,9,10	0.52	0	11,12,14	1.01	1 (9%)
3	AHR	m	26	3	9,9,10	0.56	0	11,12,14	1.01	1 (9%)
3	FUB	m	27	3	9,9,10	0.56	0	11,12,14	1.12	1 (9%)
3	AHR	m	28	3	9,9,10	0.56	0	11,12,14	0.94	0
3	AHR	m	29	3	9,9,10	0.54	0	11,12,14	0.92	0
3	BMA	m	3	3	11,11,12	0.41	0	15,15,17	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NGA	m	4	3	14,14,15	0.82	0	17,19,21	1.00	0
3	MAN	m	5	3	11,11,12	0.20	0	15,15,17	0.76	0
3	MAN	m	6	3	11,11,12	0.23	0	15,15,17	0.76	1 (6%)
3	MAN	m	7	3	11,11,12	0.23	0	15,15,17	0.74	0
3	GAL	m	8	3	11,11,12	0.16	0	15,15,17	0.74	0
3	MAN	m	9	3	11,11,12	0.20	0	15,15,17	0.82	1 (6%)
4	GAL	n	1	4	11,11,12	0.21	0	15,15,17	0.61	0
4	AHR	n	10	4	9,9,10	0.55	0	11,12,14	0.93	0
4	FUB	n	11	4	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
4	AHR	n	12	4	9,9,10	0.55	0	11,12,14	0.96	0
4	MAN	n	13	4	11,11,12	0.24	0	15,15,17	1.05	1 (6%)
4	MAN	n	14	4	11,11,12	0.21	0	15,15,17	0.74	1 (6%)
4	MAN	n	15	4	11,11,12	0.23	0	15,15,17	0.73	0
4	AHR	n	16	4	9,9,10	0.54	0	11,12,14	0.93	0
4	BMA	n	2	4	11,11,12	0.24	0	15,15,17	0.70	0
4	BGC	n	3	4	11,11,12	0.19	0	15,15,17	0.53	0
4	AHR	n	4	4	9,9,10	0.51	0	11,12,14	1.04	1 (9%)
4	MAN	n	5	4	11,11,12	0.22	0	15,15,17	0.70	0
4	AHR	n	6	4	9,9,10	0.55	0	11,12,14	0.87	0
4	AHR	n	7	4	9,9,10	0.55	0	11,12,14	0.95	0
4	AHR	n	8	4	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
4	AHR	n	9	4	9,9,10	0.56	0	11,12,14	0.94	0
2	AHR	o	1	2	9,9,10	0.54	0	11,12,14	0.87	0
2	FUB	o	2	2	9,9,10	0.56	0	11,12,14	0.96	0
2	FUB	o	3	2	9,9,10	0.54	0	11,12,14	0.97	0
2	GAL	o	4	2	11,11,12	0.17	0	15,15,17	0.55	0
2	AHR	o	5	2	9,9,10	0.54	0	11,12,14	0.98	1 (9%)
2	FUB	o	6	2	9,9,10	0.56	0	11,12,14	0.92	0
2	AHR	o	7	2	9,9,10	0.54	0	11,12,14	0.95	0
3	FUB	p	1	3	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
3	AHR	p	10	3	9,9,10	0.56	0	11,12,14	0.99	1 (9%)
3	AHR	p	11	3	9,9,10	0.56	0	11,12,14	0.98	1 (9%)
3	AHR	p	12	3	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
3	AHR	p	13	3	9,9,10	0.56	0	11,12,14	0.98	0
3	AHR	p	14	3	9,9,10	0.55	0	11,12,14	0.98	0
3	MAN	p	15	3	11,11,12	0.23	0	15,15,17	0.73	0
3	BMA	p	16	3	11,11,12	0.23	0	15,15,17	0.70	0
3	BMA	p	17	3	11,11,12	0.19	0	15,15,17	0.77	1 (6%)
3	MAN	p	18	3	11,11,12	0.20	0	15,15,17	0.74	0
3	AHR	p	19	3	9,9,10	0.56	0	11,12,14	1.00	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	p	2	3	11,11,12	0.24	0	15,15,17	0.73	0
3	BMA	p	20	3	11,11,12	0.22	0	15,15,17	0.61	0
3	AHR	p	21	3	9,9,10	0.54	0	11,12,14	0.96	0
3	AHR	p	22	3	9,9,10	0.53	0	11,12,14	1.02	1 (9%)
3	AHR	p	23	3	9,9,10	0.56	0	11,12,14	0.98	0
3	AHR	p	24	3	9,9,10	0.53	0	11,12,14	0.89	0
3	FUB	p	25	3	9,9,10	0.55	0	11,12,14	1.00	0
3	AHR	p	26	3	9,9,10	0.56	0	11,12,14	1.02	1 (9%)
3	FUB	p	27	3	9,9,10	0.52	0	11,12,14	1.10	1 (9%)
3	AHR	p	28	3	9,9,10	0.57	0	11,12,14	0.94	0
3	AHR	p	29	3	9,9,10	0.53	0	11,12,14	0.92	0
3	BMA	p	3	3	11,11,12	0.40	0	15,15,17	0.67	0
3	NGA	p	4	3	14,14,15	0.82	0	17,19,21	1.00	0
3	MAN	p	5	3	11,11,12	0.22	0	15,15,17	0.76	0
3	MAN	p	6	3	11,11,12	0.24	0	15,15,17	0.76	1 (6%)
3	MAN	p	7	3	11,11,12	0.21	0	15,15,17	0.72	0
3	GAL	p	8	3	11,11,12	0.16	0	15,15,17	0.74	0
3	MAN	p	9	3	11,11,12	0.22	0	15,15,17	0.82	1 (6%)
4	GAL	q	1	4	11,11,12	0.19	0	15,15,17	0.62	0
4	AHR	q	10	4	9,9,10	0.55	0	11,12,14	0.94	0
4	FUB	q	11	4	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
4	AHR	q	12	4	9,9,10	0.56	0	11,12,14	0.96	0
4	MAN	q	13	4	11,11,12	0.24	0	15,15,17	1.05	1 (6%)
4	MAN	q	14	4	11,11,12	0.23	0	15,15,17	0.73	0
4	MAN	q	15	4	11,11,12	0.24	0	15,15,17	0.73	0
4	AHR	q	16	4	9,9,10	0.53	0	11,12,14	0.93	0
4	BMA	q	2	4	11,11,12	0.24	0	15,15,17	0.71	0
4	BGC	q	3	4	11,11,12	0.20	0	15,15,17	0.52	0
4	AHR	q	4	4	9,9,10	0.53	0	11,12,14	1.03	1 (9%)
4	MAN	q	5	4	11,11,12	0.22	0	15,15,17	0.71	0
4	AHR	q	6	4	9,9,10	0.56	0	11,12,14	0.88	0
4	AHR	q	7	4	9,9,10	0.58	0	11,12,14	0.95	0
4	AHR	q	8	4	9,9,10	0.56	0	11,12,14	1.00	1 (9%)
4	AHR	q	9	4	9,9,10	0.54	0	11,12,14	0.93	0
2	AHR	r	1	2	9,9,10	0.54	0	11,12,14	0.86	0
2	FUB	r	2	2	9,9,10	0.59	0	11,12,14	0.96	0
2	FUB	r	3	2	9,9,10	0.54	0	11,12,14	0.95	0
2	GAL	r	4	2	11,11,12	0.17	0	15,15,17	0.55	0
2	AHR	r	5	2	9,9,10	0.54	0	11,12,14	0.97	1 (9%)
2	FUB	r	6	2	9,9,10	0.55	0	11,12,14	0.92	0
2	AHR	r	7	2	9,9,10	0.55	0	11,12,14	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUB	s	1	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	AHR	s	10	3	9,9,10	0.55	0	11,12,14	0.99	1 (9%)
3	AHR	s	11	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	AHR	s	12	3	9,9,10	0.53	0	11,12,14	1.01	1 (9%)
3	AHR	s	13	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	AHR	s	14	3	9,9,10	0.53	0	11,12,14	1.00	1 (9%)
3	MAN	s	15	3	11,11,12	0.21	0	15,15,17	0.74	1 (6%)
3	BMA	s	16	3	11,11,12	0.25	0	15,15,17	0.68	0
3	BMA	s	17	3	11,11,12	0.20	0	15,15,17	0.76	1 (6%)
3	MAN	s	18	3	11,11,12	0.22	0	15,15,17	0.73	0
3	AHR	s	19	3	9,9,10	0.55	0	11,12,14	0.99	1 (9%)
3	BMA	s	2	3	11,11,12	0.25	0	15,15,17	0.73	0
3	BMA	s	20	3	11,11,12	0.21	0	15,15,17	0.62	0
3	AHR	s	21	3	9,9,10	0.57	0	11,12,14	0.94	0
3	AHR	s	22	3	9,9,10	0.54	0	11,12,14	1.03	1 (9%)
3	AHR	s	23	3	9,9,10	0.57	0	11,12,14	0.98	0
3	AHR	s	24	3	9,9,10	0.56	0	11,12,14	0.87	0
3	FUB	s	25	3	9,9,10	0.56	0	11,12,14	0.99	0
3	AHR	s	26	3	9,9,10	0.54	0	11,12,14	1.01	1 (9%)
3	FUB	s	27	3	9,9,10	0.57	0	11,12,14	1.10	1 (9%)
3	AHR	s	28	3	9,9,10	0.54	0	11,12,14	0.94	0
3	AHR	s	29	3	9,9,10	0.55	0	11,12,14	0.92	0
3	BMA	s	3	3	11,11,12	0.41	0	15,15,17	0.67	0
3	NGA	s	4	3	14,14,15	0.82	0	17,19,21	1.01	0
3	MAN	s	5	3	11,11,12	0.22	0	15,15,17	0.77	1 (6%)
3	MAN	s	6	3	11,11,12	0.25	0	15,15,17	0.76	1 (6%)
3	MAN	s	7	3	11,11,12	0.21	0	15,15,17	0.74	0
3	GAL	s	8	3	11,11,12	0.16	0	15,15,17	0.75	0
3	MAN	s	9	3	11,11,12	0.20	0	15,15,17	0.82	2 (13%)
4	GAL	t	1	4	11,11,12	0.19	0	15,15,17	0.62	0
4	AHR	t	10	4	9,9,10	0.56	0	11,12,14	0.93	0
4	FUB	t	11	4	9,9,10	0.56	0	11,12,14	1.01	1 (9%)
4	AHR	t	12	4	9,9,10	0.56	0	11,12,14	0.96	0
4	MAN	t	13	4	11,11,12	0.24	0	15,15,17	1.04	1 (6%)
4	MAN	t	14	4	11,11,12	0.23	0	15,15,17	0.74	0
4	MAN	t	15	4	11,11,12	0.23	0	15,15,17	0.73	0
4	AHR	t	16	4	9,9,10	0.55	0	11,12,14	0.93	0
4	BMA	t	2	4	11,11,12	0.26	0	15,15,17	0.70	0
4	BGC	t	3	4	11,11,12	0.17	0	15,15,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AHR	t	4	4	9,9,10	0.53	0	11,12,14	1.05	1 (9%)
4	MAN	t	5	4	11,11,12	0.21	0	15,15,17	0.71	0
4	AHR	t	6	4	9,9,10	0.53	0	11,12,14	0.88	0
4	AHR	t	7	4	9,9,10	0.55	0	11,12,14	0.93	0
4	AHR	t	8	4	9,9,10	0.55	0	11,12,14	0.99	1 (9%)
4	AHR	t	9	4	9,9,10	0.55	0	11,12,14	0.94	0
2	AHR	u	1	2	9,9,10	0.54	0	11,12,14	0.86	0
2	FUB	u	2	2	9,9,10	0.57	0	11,12,14	0.97	0
2	FUB	u	3	2	9,9,10	0.54	0	11,12,14	0.95	0
2	GAL	u	4	2	11,11,12	0.18	0	15,15,17	0.55	0
2	AHR	u	5	2	9,9,10	0.53	0	11,12,14	0.98	1 (9%)
2	FUB	u	6	2	9,9,10	0.56	0	11,12,14	0.93	0
2	AHR	u	7	2	9,9,10	0.55	0	11,12,14	0.95	0
3	FUB	v	1	3	9,9,10	0.50	0	11,12,14	1.00	1 (9%)
3	AHR	v	10	3	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
3	AHR	v	11	3	9,9,10	0.55	0	11,12,14	0.99	1 (9%)
3	AHR	v	12	3	9,9,10	0.56	0	11,12,14	1.02	1 (9%)
3	AHR	v	13	3	9,9,10	0.54	0	11,12,14	0.99	1 (9%)
3	AHR	v	14	3	9,9,10	0.55	0	11,12,14	0.99	1 (9%)
3	MAN	v	15	3	11,11,12	0.23	0	15,15,17	0.73	0
3	BMA	v	16	3	11,11,12	0.24	0	15,15,17	0.68	0
3	BMA	v	17	3	11,11,12	0.20	0	15,15,17	0.77	1 (6%)
3	MAN	v	18	3	11,11,12	0.21	0	15,15,17	0.73	0
3	AHR	v	19	3	9,9,10	0.53	0	11,12,14	0.98	1 (9%)
3	BMA	v	2	3	11,11,12	0.25	0	15,15,17	0.73	0
3	BMA	v	20	3	11,11,12	0.22	0	15,15,17	0.61	0
3	AHR	v	21	3	9,9,10	0.54	0	11,12,14	0.95	0
3	AHR	v	22	3	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
3	AHR	v	23	3	9,9,10	0.57	0	11,12,14	0.97	0
3	AHR	v	24	3	9,9,10	0.55	0	11,12,14	0.88	0
3	FUB	v	25	3	9,9,10	0.52	0	11,12,14	1.00	0
3	AHR	v	26	3	9,9,10	0.54	0	11,12,14	1.02	1 (9%)
3	FUB	v	27	3	9,9,10	0.53	0	11,12,14	1.11	1 (9%)
3	AHR	v	28	3	9,9,10	0.54	0	11,12,14	0.93	0
3	AHR	v	29	3	9,9,10	0.56	0	11,12,14	0.93	0
3	BMA	v	3	3	11,11,12	0.42	0	15,15,17	0.67	0
3	NGA	v	4	3	14,14,15	0.82	0	17,19,21	1.00	0
3	MAN	v	5	3	11,11,12	0.22	0	15,15,17	0.76	0
3	MAN	v	6	3	11,11,12	0.23	0	15,15,17	0.77	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	v	7	3	11,11,12	0.22	0	15,15,17	0.73	0
3	GAL	v	8	3	11,11,12	0.17	0	15,15,17	0.74	0
3	MAN	v	9	3	11,11,12	0.22	0	15,15,17	0.82	2 (13%)
4	GAL	w	1	4	11,11,12	0.19	0	15,15,17	0.62	0
4	AHR	w	10	4	9,9,10	0.57	0	11,12,14	0.94	0
4	FUB	w	11	4	9,9,10	0.56	0	11,12,14	1.01	1 (9%)
4	AHR	w	12	4	9,9,10	0.57	0	11,12,14	0.96	0
4	MAN	w	13	4	11,11,12	0.23	0	15,15,17	1.05	1 (6%)
4	MAN	w	14	4	11,11,12	0.22	0	15,15,17	0.75	1 (6%)
4	MAN	w	15	4	11,11,12	0.25	0	15,15,17	0.73	0
4	AHR	w	16	4	9,9,10	0.54	0	11,12,14	0.94	0
4	BMA	w	2	4	11,11,12	0.25	0	15,15,17	0.70	0
4	BGC	w	3	4	11,11,12	0.18	0	15,15,17	0.53	0
4	AHR	w	4	4	9,9,10	0.54	0	11,12,14	1.03	1 (9%)
4	MAN	w	5	4	11,11,12	0.20	0	15,15,17	0.71	0
4	AHR	w	6	4	9,9,10	0.54	0	11,12,14	0.87	0
4	AHR	w	7	4	9,9,10	0.56	0	11,12,14	0.94	0
4	AHR	w	8	4	9,9,10	0.53	0	11,12,14	1.01	1 (9%)
4	AHR	w	9	4	9,9,10	0.54	0	11,12,14	0.93	0
2	AHR	x	1	2	9,9,10	0.54	0	11,12,14	0.87	0
2	FUB	x	2	2	9,9,10	0.59	0	11,12,14	0.96	0
2	FUB	x	3	2	9,9,10	0.55	0	11,12,14	0.95	0
2	GAL	x	4	2	11,11,12	0.17	0	15,15,17	0.56	0
2	AHR	x	5	2	9,9,10	0.53	0	11,12,14	0.97	1 (9%)
2	FUB	x	6	2	9,9,10	0.56	0	11,12,14	0.91	0
2	AHR	x	7	2	9,9,10	0.56	0	11,12,14	0.95	0
3	FUB	y	1	3	9,9,10	0.54	0	11,12,14	1.00	1 (9%)
3	AHR	y	10	3	9,9,10	0.55	0	11,12,14	1.00	1 (9%)
3	AHR	y	11	3	9,9,10	0.57	0	11,12,14	0.99	0
3	AHR	y	12	3	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
3	AHR	y	13	3	9,9,10	0.56	0	11,12,14	0.98	1 (9%)
3	AHR	y	14	3	9,9,10	0.56	0	11,12,14	0.98	1 (9%)
3	MAN	y	15	3	11,11,12	0.24	0	15,15,17	0.74	1 (6%)
3	BMA	y	16	3	11,11,12	0.24	0	15,15,17	0.70	0
3	BMA	y	17	3	11,11,12	0.19	0	15,15,17	0.76	1 (6%)
3	MAN	y	18	3	11,11,12	0.21	0	15,15,17	0.73	0
3	AHR	y	19	3	9,9,10	0.54	0	11,12,14	0.98	0
3	BMA	y	2	3	11,11,12	0.24	0	15,15,17	0.73	0
3	BMA	y	20	3	11,11,12	0.22	0	15,15,17	0.61	0
3	AHR	y	21	3	9,9,10	0.57	0	11,12,14	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AHR	y	22	3	9,9,10	0.55	0	11,12,14	1.02	1 (9%)
3	AHR	y	23	3	9,9,10	0.55	0	11,12,14	0.97	0
3	AHR	y	24	3	9,9,10	0.55	0	11,12,14	0.88	0
3	FUB	y	25	3	9,9,10	0.53	0	11,12,14	1.00	0
3	AHR	y	26	3	9,9,10	0.55	0	11,12,14	1.01	1 (9%)
3	FUB	y	27	3	9,9,10	0.53	0	11,12,14	1.10	1 (9%)
3	AHR	y	28	3	9,9,10	0.53	0	11,12,14	0.94	0
3	AHR	y	29	3	9,9,10	0.57	0	11,12,14	0.91	0
3	BMA	y	3	3	11,11,12	0.41	0	15,15,17	0.66	0
3	NGA	y	4	3	14,14,15	0.81	0	17,19,21	1.00	0
3	MAN	y	5	3	11,11,12	0.21	0	15,15,17	0.76	0
3	MAN	y	6	3	11,11,12	0.24	0	15,15,17	0.75	1 (6%)
3	MAN	y	7	3	11,11,12	0.21	0	15,15,17	0.73	0
3	GAL	y	8	3	11,11,12	0.16	0	15,15,17	0.74	0
3	MAN	y	9	3	11,11,12	0.22	0	15,15,17	0.82	2 (13%)
4	GAL	z	1	4	11,11,12	0.18	0	15,15,17	0.63	0
4	AHR	z	10	4	9,9,10	0.56	0	11,12,14	0.93	0
4	FUB	z	11	4	9,9,10	0.58	0	11,12,14	1.02	1 (9%)
4	AHR	z	12	4	9,9,10	0.55	0	11,12,14	0.96	0
4	MAN	z	13	4	11,11,12	0.23	0	15,15,17	1.05	1 (6%)
4	MAN	z	14	4	11,11,12	0.23	0	15,15,17	0.73	0
4	MAN	z	15	4	11,11,12	0.25	0	15,15,17	0.73	0
4	AHR	z	16	4	9,9,10	0.55	0	11,12,14	0.94	0
4	BMA	z	2	4	11,11,12	0.23	0	15,15,17	0.70	0
4	BGC	z	3	4	11,11,12	0.19	0	15,15,17	0.54	0
4	AHR	z	4	4	9,9,10	0.52	0	11,12,14	1.03	1 (9%)
4	MAN	z	5	4	11,11,12	0.21	0	15,15,17	0.72	0
4	AHR	z	6	4	9,9,10	0.57	0	11,12,14	0.87	0
4	AHR	z	7	4	9,9,10	0.55	0	11,12,14	0.94	0
4	AHR	z	8	4	9,9,10	0.55	0	11,12,14	1.00	1 (9%)
4	AHR	z	9	4	9,9,10	0.54	0	11,12,14	0.92	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	AHR	0	1	2	-	0/2/15/18	0/1/1/1
2	FUB	0	2	2	-	0/2/15/18	0/1/1/1
2	FUB	0	3	2	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	0	4	2	-	0/2/19/22	0/1/1/1
2	AHR	0	5	2	-	0/2/15/18	0/1/1/1
2	FUB	0	6	2	-	0/2/15/18	0/1/1/1
2	AHR	0	7	2	-	0/2/15/18	0/1/1/1
3	FUB	1	1	3	-	0/2/15/18	0/1/1/1
3	AHR	1	10	3	-	0/2/15/18	0/1/1/1
3	AHR	1	11	3	-	0/2/15/18	0/1/1/1
3	AHR	1	12	3	-	0/2/15/18	0/1/1/1
3	AHR	1	13	3	-	0/2/15/18	0/1/1/1
3	AHR	1	14	3	-	0/2/15/18	0/1/1/1
3	MAN	1	15	3	-	0/2/19/22	0/1/1/1
3	BMA	1	16	3	-	0/2/19/22	0/1/1/1
3	BMA	1	17	3	-	1/2/19/22	0/1/1/1
3	MAN	1	18	3	-	0/2/19/22	0/1/1/1
3	AHR	1	19	3	-	0/2/15/18	0/1/1/1
3	BMA	1	2	3	-	2/2/19/22	0/1/1/1
3	BMA	1	20	3	-	1/2/19/22	0/1/1/1
3	AHR	1	21	3	-	0/2/15/18	0/1/1/1
3	AHR	1	22	3	-	0/2/15/18	0/1/1/1
3	AHR	1	23	3	-	0/2/15/18	0/1/1/1
3	AHR	1	24	3	-	0/2/15/18	0/1/1/1
3	FUB	1	25	3	-	0/2/15/18	0/1/1/1
3	AHR	1	26	3	-	0/2/15/18	0/1/1/1
3	FUB	1	27	3	-	0/2/15/18	0/1/1/1
3	AHR	1	28	3	-	0/2/15/18	0/1/1/1
3	AHR	1	29	3	-	0/2/15/18	0/1/1/1
3	BMA	1	3	3	-	0/2/19/22	0/1/1/1
3	NGA	1	4	3	-	2/6/23/26	0/1/1/1
3	MAN	1	5	3	-	0/2/19/22	0/1/1/1
3	MAN	1	6	3	-	0/2/19/22	0/1/1/1
3	MAN	1	7	3	-	0/2/19/22	0/1/1/1
3	GAL	1	8	3	-	1/2/19/22	0/1/1/1
3	MAN	1	9	3	-	0/2/19/22	0/1/1/1
4	GAL	2	1	4	-	0/2/19/22	0/1/1/1
4	AHR	2	10	4	-	0/2/15/18	0/1/1/1
4	FUB	2	11	4	-	0/2/15/18	0/1/1/1
4	AHR	2	12	4	-	0/2/15/18	0/1/1/1
4	MAN	2	13	4	-	0/2/19/22	0/1/1/1
4	MAN	2	14	4	-	0/2/19/22	0/1/1/1
4	MAN	2	15	4	-	0/2/19/22	0/1/1/1
4	AHR	2	16	4	-	0/2/15/18	0/1/1/1
4	BMA	2	2	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BGC	2	3	4	-	0/2/19/22	0/1/1/1
4	AHR	2	4	4	-	0/2/15/18	0/1/1/1
4	MAN	2	5	4	-	0/2/19/22	0/1/1/1
4	AHR	2	6	4	-	0/2/15/18	0/1/1/1
4	AHR	2	7	4	-	0/2/15/18	0/1/1/1
4	AHR	2	8	4	-	0/2/15/18	0/1/1/1
4	AHR	2	9	4	-	0/2/15/18	0/1/1/1
2	AHR	B	1	2	-	0/2/15/18	0/1/1/1
2	FUB	B	2	2	-	0/2/15/18	0/1/1/1
2	FUB	B	3	2	-	0/2/15/18	0/1/1/1
2	GAL	B	4	2	-	0/2/19/22	0/1/1/1
2	AHR	B	5	2	-	0/2/15/18	0/1/1/1
2	FUB	B	6	2	-	0/2/15/18	0/1/1/1
2	AHR	B	7	2	-	0/2/15/18	0/1/1/1
3	FUB	C	1	3	-	0/2/15/18	0/1/1/1
3	AHR	C	10	3	-	0/2/15/18	0/1/1/1
3	AHR	C	11	3	-	0/2/15/18	0/1/1/1
3	AHR	C	12	3	-	0/2/15/18	0/1/1/1
3	AHR	C	13	3	-	0/2/15/18	0/1/1/1
3	AHR	C	14	3	-	0/2/15/18	0/1/1/1
3	MAN	C	15	3	-	0/2/19/22	0/1/1/1
3	BMA	C	16	3	-	1/2/19/22	0/1/1/1
3	BMA	C	17	3	-	1/2/19/22	0/1/1/1
3	MAN	C	18	3	-	0/2/19/22	0/1/1/1
3	AHR	C	19	3	-	0/2/15/18	0/1/1/1
3	BMA	C	2	3	-	2/2/19/22	0/1/1/1
3	BMA	C	20	3	-	2/2/19/22	0/1/1/1
3	AHR	C	21	3	-	0/2/15/18	0/1/1/1
3	AHR	C	22	3	-	0/2/15/18	0/1/1/1
3	AHR	C	23	3	-	0/2/15/18	0/1/1/1
3	AHR	C	24	3	-	0/2/15/18	0/1/1/1
3	FUB	C	25	3	-	0/2/15/18	0/1/1/1
3	AHR	C	26	3	-	0/2/15/18	0/1/1/1
3	FUB	C	27	3	-	0/2/15/18	0/1/1/1
3	AHR	C	28	3	-	0/2/15/18	0/1/1/1
3	AHR	C	29	3	-	0/2/15/18	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	NGA	C	4	3	-	2/6/23/26	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
3	MAN	C	7	3	-	0/2/19/22	0/1/1/1
3	GAL	C	8	3	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	C	9	3	-	0/2/19/22	0/1/1/1
4	GAL	D	1	4	-	2/2/19/22	0/1/1/1
4	AHR	D	10	4	-	0/2/15/18	0/1/1/1
4	FUB	D	11	4	-	0/2/15/18	0/1/1/1
4	AHR	D	12	4	-	0/2/15/18	0/1/1/1
4	MAN	D	13	4	-	0/2/19/22	0/1/1/1
4	MAN	D	14	4	-	2/2/19/22	0/1/1/1
4	MAN	D	15	4	-	0/2/19/22	0/1/1/1
4	AHR	D	16	4	-	0/2/15/18	0/1/1/1
4	BMA	D	2	4	-	0/2/19/22	0/1/1/1
4	BGC	D	3	4	-	0/2/19/22	0/1/1/1
4	AHR	D	4	4	-	0/2/15/18	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
4	AHR	D	6	4	-	0/2/15/18	0/1/1/1
4	AHR	D	7	4	-	0/2/15/18	0/1/1/1
4	AHR	D	8	4	-	0/2/15/18	0/1/1/1
4	AHR	D	9	4	-	0/2/15/18	0/1/1/1
2	AHR	E	1	2	-	0/2/15/18	0/1/1/1
2	FUB	E	2	2	-	0/2/15/18	0/1/1/1
2	FUB	E	3	2	-	0/2/15/18	0/1/1/1
2	GAL	E	4	2	-	0/2/19/22	0/1/1/1
2	AHR	E	5	2	-	0/2/15/18	0/1/1/1
2	FUB	E	6	2	-	0/2/15/18	0/1/1/1
2	AHR	E	7	2	-	0/2/15/18	0/1/1/1
3	FUB	F	1	3	-	0/2/15/18	0/1/1/1
3	AHR	F	10	3	-	0/2/15/18	0/1/1/1
3	AHR	F	11	3	-	0/2/15/18	0/1/1/1
3	AHR	F	12	3	-	0/2/15/18	0/1/1/1
3	AHR	F	13	3	-	0/2/15/18	0/1/1/1
3	AHR	F	14	3	-	0/2/15/18	0/1/1/1
3	MAN	F	15	3	-	0/2/19/22	0/1/1/1
3	BMA	F	16	3	-	0/2/19/22	0/1/1/1
3	BMA	F	17	3	-	1/2/19/22	0/1/1/1
3	MAN	F	18	3	-	0/2/19/22	0/1/1/1
3	AHR	F	19	3	-	0/2/15/18	0/1/1/1
3	BMA	F	2	3	-	2/2/19/22	0/1/1/1
3	BMA	F	20	3	-	1/2/19/22	0/1/1/1
3	AHR	F	21	3	-	0/2/15/18	0/1/1/1
3	AHR	F	22	3	-	0/2/15/18	0/1/1/1
3	AHR	F	23	3	-	0/2/15/18	0/1/1/1
3	AHR	F	24	3	-	0/2/15/18	0/1/1/1
3	FUB	F	25	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AHR	F	26	3	-	0/2/15/18	0/1/1/1
3	FUB	F	27	3	-	0/2/15/18	0/1/1/1
3	AHR	F	28	3	-	0/2/15/18	0/1/1/1
3	AHR	F	29	3	-	0/2/15/18	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	NGA	F	4	3	-	2/6/23/26	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
3	MAN	F	6	3	-	0/2/19/22	0/1/1/1
3	MAN	F	7	3	-	0/2/19/22	0/1/1/1
3	GAL	F	8	3	-	1/2/19/22	0/1/1/1
3	MAN	F	9	3	-	0/2/19/22	0/1/1/1
4	GAL	G	1	4	-	0/2/19/22	0/1/1/1
4	AHR	G	10	4	-	0/2/15/18	0/1/1/1
4	FUB	G	11	4	-	0/2/15/18	0/1/1/1
4	AHR	G	12	4	-	0/2/15/18	0/1/1/1
4	MAN	G	13	4	-	0/2/19/22	0/1/1/1
4	MAN	G	14	4	-	0/2/19/22	0/1/1/1
4	MAN	G	15	4	-	0/2/19/22	0/1/1/1
4	AHR	G	16	4	-	0/2/15/18	0/1/1/1
4	BMA	G	2	4	-	0/2/19/22	0/1/1/1
4	BGC	G	3	4	-	0/2/19/22	0/1/1/1
4	AHR	G	4	4	-	0/2/15/18	0/1/1/1
4	MAN	G	5	4	-	0/2/19/22	0/1/1/1
4	AHR	G	6	4	-	0/2/15/18	0/1/1/1
4	AHR	G	7	4	-	0/2/15/18	0/1/1/1
4	AHR	G	8	4	-	0/2/15/18	0/1/1/1
4	AHR	G	9	4	-	0/2/15/18	0/1/1/1
2	AHR	H	1	2	-	0/2/15/18	0/1/1/1
2	FUB	H	2	2	-	0/2/15/18	0/1/1/1
2	FUB	H	3	2	-	0/2/15/18	0/1/1/1
2	GAL	H	4	2	-	0/2/19/22	0/1/1/1
2	AHR	H	5	2	-	0/2/15/18	0/1/1/1
2	FUB	H	6	2	-	0/2/15/18	0/1/1/1
2	AHR	H	7	2	-	0/2/15/18	0/1/1/1
3	FUB	I	1	3	-	0/2/15/18	0/1/1/1
3	AHR	I	10	3	-	0/2/15/18	0/1/1/1
3	AHR	I	11	3	-	0/2/15/18	0/1/1/1
3	AHR	I	12	3	-	0/2/15/18	0/1/1/1
3	AHR	I	13	3	-	0/2/15/18	0/1/1/1
3	AHR	I	14	3	-	0/2/15/18	0/1/1/1
3	MAN	I	15	3	-	0/2/19/22	0/1/1/1
3	BMA	I	16	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	I	17	3	-	1/2/19/22	0/1/1/1
3	MAN	I	18	3	-	0/2/19/22	0/1/1/1
3	AHR	I	19	3	-	0/2/15/18	0/1/1/1
3	BMA	I	2	3	-	2/2/19/22	0/1/1/1
3	BMA	I	20	3	-	1/2/19/22	0/1/1/1
3	AHR	I	21	3	-	0/2/15/18	0/1/1/1
3	AHR	I	22	3	-	0/2/15/18	0/1/1/1
3	AHR	I	23	3	-	0/2/15/18	0/1/1/1
3	AHR	I	24	3	-	0/2/15/18	0/1/1/1
3	FUB	I	25	3	-	0/2/15/18	0/1/1/1
3	AHR	I	26	3	-	0/2/15/18	0/1/1/1
3	FUB	I	27	3	-	0/2/15/18	0/1/1/1
3	AHR	I	28	3	-	0/2/15/18	0/1/1/1
3	AHR	I	29	3	-	0/2/15/18	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
3	NGA	I	4	3	-	2/6/23/26	0/1/1/1
3	MAN	I	5	3	-	0/2/19/22	0/1/1/1
3	MAN	I	6	3	-	0/2/19/22	0/1/1/1
3	MAN	I	7	3	-	0/2/19/22	0/1/1/1
3	GAL	I	8	3	-	1/2/19/22	0/1/1/1
3	MAN	I	9	3	-	0/2/19/22	0/1/1/1
4	GAL	J	1	4	-	0/2/19/22	0/1/1/1
4	AHR	J	10	4	-	0/2/15/18	0/1/1/1
4	FUB	J	11	4	-	0/2/15/18	0/1/1/1
4	AHR	J	12	4	-	0/2/15/18	0/1/1/1
4	MAN	J	13	4	-	0/2/19/22	0/1/1/1
4	MAN	J	14	4	-	0/2/19/22	0/1/1/1
4	MAN	J	15	4	-	0/2/19/22	0/1/1/1
4	AHR	J	16	4	-	0/2/15/18	0/1/1/1
4	BMA	J	2	4	-	0/2/19/22	0/1/1/1
4	BGC	J	3	4	-	0/2/19/22	0/1/1/1
4	AHR	J	4	4	-	0/2/15/18	0/1/1/1
4	MAN	J	5	4	-	0/2/19/22	0/1/1/1
4	AHR	J	6	4	-	0/2/15/18	0/1/1/1
4	AHR	J	7	4	-	0/2/15/18	0/1/1/1
4	AHR	J	8	4	-	0/2/15/18	0/1/1/1
4	AHR	J	9	4	-	0/2/15/18	0/1/1/1
2	AHR	K	1	2	-	0/2/15/18	0/1/1/1
2	FUB	K	2	2	-	0/2/15/18	0/1/1/1
2	FUB	K	3	2	-	0/2/15/18	0/1/1/1
2	GAL	K	4	2	-	0/2/19/22	0/1/1/1
2	AHR	K	5	2	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUB	K	6	2	-	0/2/15/18	0/1/1/1
2	AHR	K	7	2	-	0/2/15/18	0/1/1/1
3	FUB	L	1	3	-	0/2/15/18	0/1/1/1
3	AHR	L	10	3	-	0/2/15/18	0/1/1/1
3	AHR	L	11	3	-	0/2/15/18	0/1/1/1
3	AHR	L	12	3	-	0/2/15/18	0/1/1/1
3	AHR	L	13	3	-	0/2/15/18	0/1/1/1
3	AHR	L	14	3	-	0/2/15/18	0/1/1/1
3	MAN	L	15	3	-	0/2/19/22	0/1/1/1
3	BMA	L	16	3	-	0/2/19/22	0/1/1/1
3	BMA	L	17	3	-	1/2/19/22	0/1/1/1
3	MAN	L	18	3	-	0/2/19/22	0/1/1/1
3	AHR	L	19	3	-	0/2/15/18	0/1/1/1
3	BMA	L	2	3	-	2/2/19/22	0/1/1/1
3	BMA	L	20	3	-	1/2/19/22	0/1/1/1
3	AHR	L	21	3	-	0/2/15/18	0/1/1/1
3	AHR	L	22	3	-	0/2/15/18	0/1/1/1
3	AHR	L	23	3	-	0/2/15/18	0/1/1/1
3	AHR	L	24	3	-	0/2/15/18	0/1/1/1
3	FUB	L	25	3	-	0/2/15/18	0/1/1/1
3	AHR	L	26	3	-	0/2/15/18	0/1/1/1
3	FUB	L	27	3	-	0/2/15/18	0/1/1/1
3	AHR	L	28	3	-	0/2/15/18	0/1/1/1
3	AHR	L	29	3	-	0/2/15/18	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1
3	NGA	L	4	3	-	2/6/23/26	0/1/1/1
3	MAN	L	5	3	-	0/2/19/22	0/1/1/1
3	MAN	L	6	3	-	0/2/19/22	0/1/1/1
3	MAN	L	7	3	-	0/2/19/22	0/1/1/1
3	GAL	L	8	3	-	1/2/19/22	0/1/1/1
3	MAN	L	9	3	-	0/2/19/22	0/1/1/1
4	GAL	M	1	4	-	0/2/19/22	0/1/1/1
4	AHR	M	10	4	-	0/2/15/18	0/1/1/1
4	FUB	M	11	4	-	0/2/15/18	0/1/1/1
4	AHR	M	12	4	-	0/2/15/18	0/1/1/1
4	MAN	M	13	4	-	0/2/19/22	0/1/1/1
4	MAN	M	14	4	-	0/2/19/22	0/1/1/1
4	MAN	M	15	4	-	0/2/19/22	0/1/1/1
4	AHR	M	16	4	-	0/2/15/18	0/1/1/1
4	BMA	M	2	4	-	0/2/19/22	0/1/1/1
4	BGC	M	3	4	-	0/2/19/22	0/1/1/1
4	AHR	M	4	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	M	5	4	-	0/2/19/22	0/1/1/1
4	AHR	M	6	4	-	0/2/15/18	0/1/1/1
4	AHR	M	7	4	-	0/2/15/18	0/1/1/1
4	AHR	M	8	4	-	0/2/15/18	0/1/1/1
4	AHR	M	9	4	-	0/2/15/18	0/1/1/1
2	AHR	N	1	2	-	0/2/15/18	0/1/1/1
2	FUB	N	2	2	-	0/2/15/18	0/1/1/1
2	FUB	N	3	2	-	0/2/15/18	0/1/1/1
2	GAL	N	4	2	-	0/2/19/22	0/1/1/1
2	AHR	N	5	2	-	0/2/15/18	0/1/1/1
2	FUB	N	6	2	-	0/2/15/18	0/1/1/1
2	AHR	N	7	2	-	0/2/15/18	0/1/1/1
3	FUB	O	1	3	-	0/2/15/18	0/1/1/1
3	AHR	O	10	3	-	0/2/15/18	0/1/1/1
3	AHR	O	11	3	-	0/2/15/18	0/1/1/1
3	AHR	O	12	3	-	0/2/15/18	0/1/1/1
3	AHR	O	13	3	-	0/2/15/18	0/1/1/1
3	AHR	O	14	3	-	0/2/15/18	0/1/1/1
3	MAN	O	15	3	-	0/2/19/22	0/1/1/1
3	BMA	O	16	3	-	0/2/19/22	0/1/1/1
3	BMA	O	17	3	-	1/2/19/22	0/1/1/1
3	MAN	O	18	3	-	0/2/19/22	0/1/1/1
3	AHR	O	19	3	-	0/2/15/18	0/1/1/1
3	BMA	O	2	3	-	2/2/19/22	0/1/1/1
3	BMA	O	20	3	-	1/2/19/22	0/1/1/1
3	AHR	O	21	3	-	0/2/15/18	0/1/1/1
3	AHR	O	22	3	-	0/2/15/18	0/1/1/1
3	AHR	O	23	3	-	0/2/15/18	0/1/1/1
3	AHR	O	24	3	-	0/2/15/18	0/1/1/1
3	FUB	O	25	3	-	0/2/15/18	0/1/1/1
3	AHR	O	26	3	-	0/2/15/18	0/1/1/1
3	FUB	O	27	3	-	0/2/15/18	0/1/1/1
3	AHR	O	28	3	-	0/2/15/18	0/1/1/1
3	AHR	O	29	3	-	0/2/15/18	0/1/1/1
3	BMA	O	3	3	-	0/2/19/22	0/1/1/1
3	NGA	O	4	3	-	2/6/23/26	0/1/1/1
3	MAN	O	5	3	-	0/2/19/22	0/1/1/1
3	MAN	O	6	3	-	0/2/19/22	0/1/1/1
3	MAN	O	7	3	-	0/2/19/22	0/1/1/1
3	GAL	O	8	3	-	1/2/19/22	0/1/1/1
3	MAN	O	9	3	-	0/2/19/22	0/1/1/1
4	GAL	P	1	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AHR	P	10	4	-	0/2/15/18	0/1/1/1
4	FUB	P	11	4	-	0/2/15/18	0/1/1/1
4	AHR	P	12	4	-	0/2/15/18	0/1/1/1
4	MAN	P	13	4	-	0/2/19/22	0/1/1/1
4	MAN	P	14	4	-	0/2/19/22	0/1/1/1
4	MAN	P	15	4	-	0/2/19/22	0/1/1/1
4	AHR	P	16	4	-	0/2/15/18	0/1/1/1
4	BMA	P	2	4	-	0/2/19/22	0/1/1/1
4	BGC	P	3	4	-	0/2/19/22	0/1/1/1
4	AHR	P	4	4	-	0/2/15/18	0/1/1/1
4	MAN	P	5	4	-	0/2/19/22	0/1/1/1
4	AHR	P	6	4	-	0/2/15/18	0/1/1/1
4	AHR	P	7	4	-	0/2/15/18	0/1/1/1
4	AHR	P	8	4	-	0/2/15/18	0/1/1/1
4	AHR	P	9	4	-	0/2/15/18	0/1/1/1
2	AHR	Q	1	2	-	0/2/15/18	0/1/1/1
2	FUB	Q	2	2	-	0/2/15/18	0/1/1/1
2	FUB	Q	3	2	-	0/2/15/18	0/1/1/1
2	GAL	Q	4	2	-	0/2/19/22	0/1/1/1
2	AHR	Q	5	2	-	0/2/15/18	0/1/1/1
2	FUB	Q	6	2	-	0/2/15/18	0/1/1/1
2	AHR	Q	7	2	-	0/2/15/18	0/1/1/1
3	FUB	R	1	3	-	0/2/15/18	0/1/1/1
3	AHR	R	10	3	-	0/2/15/18	0/1/1/1
3	AHR	R	11	3	-	0/2/15/18	0/1/1/1
3	AHR	R	12	3	-	0/2/15/18	0/1/1/1
3	AHR	R	13	3	-	0/2/15/18	0/1/1/1
3	AHR	R	14	3	-	0/2/15/18	0/1/1/1
3	MAN	R	15	3	-	0/2/19/22	0/1/1/1
3	BMA	R	16	3	-	0/2/19/22	0/1/1/1
3	BMA	R	17	3	-	1/2/19/22	0/1/1/1
3	MAN	R	18	3	-	0/2/19/22	0/1/1/1
3	AHR	R	19	3	-	0/2/15/18	0/1/1/1
3	BMA	R	2	3	-	2/2/19/22	0/1/1/1
3	BMA	R	20	3	-	1/2/19/22	0/1/1/1
3	AHR	R	21	3	-	0/2/15/18	0/1/1/1
3	AHR	R	22	3	-	0/2/15/18	0/1/1/1
3	AHR	R	23	3	-	0/2/15/18	0/1/1/1
3	AHR	R	24	3	-	0/2/15/18	0/1/1/1
3	FUB	R	25	3	-	0/2/15/18	0/1/1/1
3	AHR	R	26	3	-	0/2/15/18	0/1/1/1
3	FUB	R	27	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AHR	R	28	3	-	0/2/15/18	0/1/1/1
3	AHR	R	29	3	-	0/2/15/18	0/1/1/1
3	BMA	R	3	3	-	0/2/19/22	0/1/1/1
3	NGA	R	4	3	-	2/6/23/26	0/1/1/1
3	MAN	R	5	3	-	0/2/19/22	0/1/1/1
3	MAN	R	6	3	-	0/2/19/22	0/1/1/1
3	MAN	R	7	3	-	0/2/19/22	0/1/1/1
3	GAL	R	8	3	-	1/2/19/22	0/1/1/1
3	MAN	R	9	3	-	0/2/19/22	0/1/1/1
4	GAL	S	1	4	-	0/2/19/22	0/1/1/1
4	AHR	S	10	4	-	0/2/15/18	0/1/1/1
4	FUB	S	11	4	-	0/2/15/18	0/1/1/1
4	AHR	S	12	4	-	0/2/15/18	0/1/1/1
4	MAN	S	13	4	-	0/2/19/22	0/1/1/1
4	MAN	S	14	4	-	0/2/19/22	0/1/1/1
4	MAN	S	15	4	-	0/2/19/22	0/1/1/1
4	AHR	S	16	4	-	0/2/15/18	0/1/1/1
4	BMA	S	2	4	-	0/2/19/22	0/1/1/1
4	BGC	S	3	4	-	0/2/19/22	0/1/1/1
4	AHR	S	4	4	-	0/2/15/18	0/1/1/1
4	MAN	S	5	4	-	0/2/19/22	0/1/1/1
4	AHR	S	6	4	-	0/2/15/18	0/1/1/1
4	AHR	S	7	4	-	0/2/15/18	0/1/1/1
4	AHR	S	8	4	-	0/2/15/18	0/1/1/1
4	AHR	S	9	4	-	0/2/15/18	0/1/1/1
2	AHR	T	1	2	-	0/2/15/18	0/1/1/1
2	FUB	T	2	2	-	0/2/15/18	0/1/1/1
2	FUB	T	3	2	-	0/2/15/18	0/1/1/1
2	GAL	T	4	2	-	0/2/19/22	0/1/1/1
2	AHR	T	5	2	-	0/2/15/18	0/1/1/1
2	FUB	T	6	2	-	0/2/15/18	0/1/1/1
2	AHR	T	7	2	-	0/2/15/18	0/1/1/1
3	FUB	U	1	3	-	0/2/15/18	0/1/1/1
3	AHR	U	10	3	-	0/2/15/18	0/1/1/1
3	AHR	U	11	3	-	0/2/15/18	0/1/1/1
3	AHR	U	12	3	-	0/2/15/18	0/1/1/1
3	AHR	U	13	3	-	0/2/15/18	0/1/1/1
3	AHR	U	14	3	-	0/2/15/18	0/1/1/1
3	MAN	U	15	3	-	0/2/19/22	0/1/1/1
3	BMA	U	16	3	-	0/2/19/22	0/1/1/1
3	BMA	U	17	3	-	1/2/19/22	0/1/1/1
3	MAN	U	18	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AHR	U	19	3	-	0/2/15/18	0/1/1/1
3	BMA	U	2	3	-	2/2/19/22	0/1/1/1
3	BMA	U	20	3	-	1/2/19/22	0/1/1/1
3	AHR	U	21	3	-	0/2/15/18	0/1/1/1
3	AHR	U	22	3	-	0/2/15/18	0/1/1/1
3	AHR	U	23	3	-	0/2/15/18	0/1/1/1
3	AHR	U	24	3	-	0/2/15/18	0/1/1/1
3	FUB	U	25	3	-	0/2/15/18	0/1/1/1
3	AHR	U	26	3	-	0/2/15/18	0/1/1/1
3	FUB	U	27	3	-	0/2/15/18	0/1/1/1
3	AHR	U	28	3	-	0/2/15/18	0/1/1/1
3	AHR	U	29	3	-	0/2/15/18	0/1/1/1
3	BMA	U	3	3	-	0/2/19/22	0/1/1/1
3	NGA	U	4	3	-	2/6/23/26	0/1/1/1
3	MAN	U	5	3	-	0/2/19/22	0/1/1/1
3	MAN	U	6	3	-	0/2/19/22	0/1/1/1
3	MAN	U	7	3	-	0/2/19/22	0/1/1/1
3	GAL	U	8	3	-	1/2/19/22	0/1/1/1
3	MAN	U	9	3	-	0/2/19/22	0/1/1/1
4	GAL	V	1	4	-	0/2/19/22	0/1/1/1
4	AHR	V	10	4	-	0/2/15/18	0/1/1/1
4	FUB	V	11	4	-	0/2/15/18	0/1/1/1
4	AHR	V	12	4	-	0/2/15/18	0/1/1/1
4	MAN	V	13	4	-	0/2/19/22	0/1/1/1
4	MAN	V	14	4	-	0/2/19/22	0/1/1/1
4	MAN	V	15	4	-	0/2/19/22	0/1/1/1
4	AHR	V	16	4	-	0/2/15/18	0/1/1/1
4	BMA	V	2	4	-	0/2/19/22	0/1/1/1
4	BGC	V	3	4	-	0/2/19/22	0/1/1/1
4	AHR	V	4	4	-	0/2/15/18	0/1/1/1
4	MAN	V	5	4	-	0/2/19/22	0/1/1/1
4	AHR	V	6	4	-	0/2/15/18	0/1/1/1
4	AHR	V	7	4	-	0/2/15/18	0/1/1/1
4	AHR	V	8	4	-	0/2/15/18	0/1/1/1
4	AHR	V	9	4	-	0/2/15/18	0/1/1/1
2	AHR	W	1	2	-	0/2/15/18	0/1/1/1
2	FUB	W	2	2	-	0/2/15/18	0/1/1/1
2	FUB	W	3	2	-	0/2/15/18	0/1/1/1
2	GAL	W	4	2	-	0/2/19/22	0/1/1/1
2	AHR	W	5	2	-	0/2/15/18	0/1/1/1
2	FUB	W	6	2	-	0/2/15/18	0/1/1/1
2	AHR	W	7	2	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	X	1	3	-	0/2/15/18	0/1/1/1
3	AHR	X	10	3	-	0/2/15/18	0/1/1/1
3	AHR	X	11	3	-	0/2/15/18	0/1/1/1
3	AHR	X	12	3	-	0/2/15/18	0/1/1/1
3	AHR	X	13	3	-	0/2/15/18	0/1/1/1
3	AHR	X	14	3	-	0/2/15/18	0/1/1/1
3	MAN	X	15	3	-	0/2/19/22	0/1/1/1
3	BMA	X	16	3	-	0/2/19/22	0/1/1/1
3	BMA	X	17	3	-	1/2/19/22	0/1/1/1
3	MAN	X	18	3	-	0/2/19/22	0/1/1/1
3	AHR	X	19	3	-	0/2/15/18	0/1/1/1
3	BMA	X	2	3	-	2/2/19/22	0/1/1/1
3	BMA	X	20	3	-	1/2/19/22	0/1/1/1
3	AHR	X	21	3	-	0/2/15/18	0/1/1/1
3	AHR	X	22	3	-	0/2/15/18	0/1/1/1
3	AHR	X	23	3	-	0/2/15/18	0/1/1/1
3	AHR	X	24	3	-	0/2/15/18	0/1/1/1
3	FUB	X	25	3	-	0/2/15/18	0/1/1/1
3	AHR	X	26	3	-	0/2/15/18	0/1/1/1
3	FUB	X	27	3	-	0/2/15/18	0/1/1/1
3	AHR	X	28	3	-	0/2/15/18	0/1/1/1
3	AHR	X	29	3	-	0/2/15/18	0/1/1/1
3	BMA	X	3	3	-	0/2/19/22	0/1/1/1
3	NGA	X	4	3	-	2/6/23/26	0/1/1/1
3	MAN	X	5	3	-	0/2/19/22	0/1/1/1
3	MAN	X	6	3	-	0/2/19/22	0/1/1/1
3	MAN	X	7	3	-	0/2/19/22	0/1/1/1
3	GAL	X	8	3	-	1/2/19/22	0/1/1/1
3	MAN	X	9	3	-	0/2/19/22	0/1/1/1
4	GAL	Y	1	4	-	0/2/19/22	0/1/1/1
4	AHR	Y	10	4	-	0/2/15/18	0/1/1/1
4	FUB	Y	11	4	-	0/2/15/18	0/1/1/1
4	AHR	Y	12	4	-	0/2/15/18	0/1/1/1
4	MAN	Y	13	4	-	0/2/19/22	0/1/1/1
4	MAN	Y	14	4	-	0/2/19/22	0/1/1/1
4	MAN	Y	15	4	-	0/2/19/22	0/1/1/1
4	AHR	Y	16	4	-	0/2/15/18	0/1/1/1
4	BMA	Y	2	4	-	0/2/19/22	0/1/1/1
4	BGC	Y	3	4	-	0/2/19/22	0/1/1/1
4	AHR	Y	4	4	-	0/2/15/18	0/1/1/1
4	MAN	Y	5	4	-	0/2/19/22	0/1/1/1
4	AHR	Y	6	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AHR	Y	7	4	-	0/2/15/18	0/1/1/1
4	AHR	Y	8	4	-	0/2/15/18	0/1/1/1
4	AHR	Y	9	4	-	0/2/15/18	0/1/1/1
2	AHR	Z	1	2	-	0/2/15/18	0/1/1/1
2	FUB	Z	2	2	-	0/2/15/18	0/1/1/1
2	FUB	Z	3	2	-	0/2/15/18	0/1/1/1
2	GAL	Z	4	2	-	0/2/19/22	0/1/1/1
2	AHR	Z	5	2	-	0/2/15/18	0/1/1/1
2	FUB	Z	6	2	-	0/2/15/18	0/1/1/1
2	AHR	Z	7	2	-	0/2/15/18	0/1/1/1
3	FUB	a	1	3	-	0/2/15/18	0/1/1/1
3	AHR	a	10	3	-	0/2/15/18	0/1/1/1
3	AHR	a	11	3	-	0/2/15/18	0/1/1/1
3	AHR	a	12	3	-	0/2/15/18	0/1/1/1
3	AHR	a	13	3	-	0/2/15/18	0/1/1/1
3	AHR	a	14	3	-	0/2/15/18	0/1/1/1
3	MAN	a	15	3	-	0/2/19/22	0/1/1/1
3	BMA	a	16	3	-	0/2/19/22	0/1/1/1
3	BMA	a	17	3	-	1/2/19/22	0/1/1/1
3	MAN	a	18	3	-	0/2/19/22	0/1/1/1
3	AHR	a	19	3	-	0/2/15/18	0/1/1/1
3	BMA	a	2	3	-	2/2/19/22	0/1/1/1
3	BMA	a	20	3	-	1/2/19/22	0/1/1/1
3	AHR	a	21	3	-	0/2/15/18	0/1/1/1
3	AHR	a	22	3	-	0/2/15/18	0/1/1/1
3	AHR	a	23	3	-	0/2/15/18	0/1/1/1
3	AHR	a	24	3	-	0/2/15/18	0/1/1/1
3	FUB	a	25	3	-	0/2/15/18	0/1/1/1
3	AHR	a	26	3	-	0/2/15/18	0/1/1/1
3	FUB	a	27	3	-	0/2/15/18	0/1/1/1
3	AHR	a	28	3	-	0/2/15/18	0/1/1/1
3	AHR	a	29	3	-	0/2/15/18	0/1/1/1
3	BMA	a	3	3	-	0/2/19/22	0/1/1/1
3	NGA	a	4	3	-	2/6/23/26	0/1/1/1
3	MAN	a	5	3	-	0/2/19/22	0/1/1/1
3	MAN	a	6	3	-	0/2/19/22	0/1/1/1
3	MAN	a	7	3	-	0/2/19/22	0/1/1/1
3	GAL	a	8	3	-	1/2/19/22	0/1/1/1
3	MAN	a	9	3	-	0/2/19/22	0/1/1/1
4	GAL	b	1	4	-	0/2/19/22	0/1/1/1
4	AHR	b	10	4	-	0/2/15/18	0/1/1/1
4	FUB	b	11	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AHR	b	12	4	-	0/2/15/18	0/1/1/1
4	MAN	b	13	4	-	0/2/19/22	0/1/1/1
4	MAN	b	14	4	-	0/2/19/22	0/1/1/1
4	MAN	b	15	4	-	0/2/19/22	0/1/1/1
4	AHR	b	16	4	-	0/2/15/18	0/1/1/1
4	BMA	b	2	4	-	0/2/19/22	0/1/1/1
4	BGC	b	3	4	-	0/2/19/22	0/1/1/1
4	AHR	b	4	4	-	0/2/15/18	0/1/1/1
4	MAN	b	5	4	-	0/2/19/22	0/1/1/1
4	AHR	b	6	4	-	0/2/15/18	0/1/1/1
4	AHR	b	7	4	-	0/2/15/18	0/1/1/1
4	AHR	b	8	4	-	0/2/15/18	0/1/1/1
4	AHR	b	9	4	-	0/2/15/18	0/1/1/1
2	AHR	c	1	2	-	0/2/15/18	0/1/1/1
2	FUB	c	2	2	-	0/2/15/18	0/1/1/1
2	FUB	c	3	2	-	0/2/15/18	0/1/1/1
2	GAL	c	4	2	-	0/2/19/22	0/1/1/1
2	AHR	c	5	2	-	0/2/15/18	0/1/1/1
2	FUB	c	6	2	-	0/2/15/18	0/1/1/1
2	AHR	c	7	2	-	0/2/15/18	0/1/1/1
3	FUB	d	1	3	-	0/2/15/18	0/1/1/1
3	AHR	d	10	3	-	0/2/15/18	0/1/1/1
3	AHR	d	11	3	-	0/2/15/18	0/1/1/1
3	AHR	d	12	3	-	0/2/15/18	0/1/1/1
3	AHR	d	13	3	-	0/2/15/18	0/1/1/1
3	AHR	d	14	3	-	0/2/15/18	0/1/1/1
3	MAN	d	15	3	-	0/2/19/22	0/1/1/1
3	BMA	d	16	3	-	0/2/19/22	0/1/1/1
3	BMA	d	17	3	-	1/2/19/22	0/1/1/1
3	MAN	d	18	3	-	0/2/19/22	0/1/1/1
3	AHR	d	19	3	-	0/2/15/18	0/1/1/1
3	BMA	d	2	3	-	2/2/19/22	0/1/1/1
3	BMA	d	20	3	-	1/2/19/22	0/1/1/1
3	AHR	d	21	3	-	0/2/15/18	0/1/1/1
3	AHR	d	22	3	-	0/2/15/18	0/1/1/1
3	AHR	d	23	3	-	0/2/15/18	0/1/1/1
3	AHR	d	24	3	-	0/2/15/18	0/1/1/1
3	FUB	d	25	3	-	0/2/15/18	0/1/1/1
3	AHR	d	26	3	-	0/2/15/18	0/1/1/1
3	FUB	d	27	3	-	0/2/15/18	0/1/1/1
3	AHR	d	28	3	-	0/2/15/18	0/1/1/1
3	AHR	d	29	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	d	3	3	-	0/2/19/22	0/1/1/1
3	NGA	d	4	3	-	2/6/23/26	0/1/1/1
3	MAN	d	5	3	-	0/2/19/22	0/1/1/1
3	MAN	d	6	3	-	0/2/19/22	0/1/1/1
3	MAN	d	7	3	-	0/2/19/22	0/1/1/1
3	GAL	d	8	3	-	1/2/19/22	0/1/1/1
3	MAN	d	9	3	-	0/2/19/22	0/1/1/1
4	GAL	e	1	4	-	0/2/19/22	0/1/1/1
4	AHR	e	10	4	-	0/2/15/18	0/1/1/1
4	FUB	e	11	4	-	0/2/15/18	0/1/1/1
4	AHR	e	12	4	-	0/2/15/18	0/1/1/1
4	MAN	e	13	4	-	0/2/19/22	0/1/1/1
4	MAN	e	14	4	-	0/2/19/22	0/1/1/1
4	MAN	e	15	4	-	0/2/19/22	0/1/1/1
4	AHR	e	16	4	-	0/2/15/18	0/1/1/1
4	BMA	e	2	4	-	0/2/19/22	0/1/1/1
4	BGC	e	3	4	-	0/2/19/22	0/1/1/1
4	AHR	e	4	4	-	0/2/15/18	0/1/1/1
4	MAN	e	5	4	-	0/2/19/22	0/1/1/1
4	AHR	e	6	4	-	0/2/15/18	0/1/1/1
4	AHR	e	7	4	-	0/2/15/18	0/1/1/1
4	AHR	e	8	4	-	0/2/15/18	0/1/1/1
4	AHR	e	9	4	-	0/2/15/18	0/1/1/1
2	AHR	f	1	2	-	0/2/15/18	0/1/1/1
2	FUB	f	2	2	-	0/2/15/18	0/1/1/1
2	FUB	f	3	2	-	0/2/15/18	0/1/1/1
2	GAL	f	4	2	-	0/2/19/22	0/1/1/1
2	AHR	f	5	2	-	0/2/15/18	0/1/1/1
2	FUB	f	6	2	-	0/2/15/18	0/1/1/1
2	AHR	f	7	2	-	0/2/15/18	0/1/1/1
3	FUB	g	1	3	-	0/2/15/18	0/1/1/1
3	AHR	g	10	3	-	0/2/15/18	0/1/1/1
3	AHR	g	11	3	-	0/2/15/18	0/1/1/1
3	AHR	g	12	3	-	0/2/15/18	0/1/1/1
3	AHR	g	13	3	-	0/2/15/18	0/1/1/1
3	AHR	g	14	3	-	0/2/15/18	0/1/1/1
3	MAN	g	15	3	-	0/2/19/22	0/1/1/1
3	BMA	g	16	3	-	0/2/19/22	0/1/1/1
3	BMA	g	17	3	-	1/2/19/22	0/1/1/1
3	MAN	g	18	3	-	0/2/19/22	0/1/1/1
3	AHR	g	19	3	-	0/2/15/18	0/1/1/1
3	BMA	g	2	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	g	20	3	-	1/2/19/22	0/1/1/1
3	AHR	g	21	3	-	0/2/15/18	0/1/1/1
3	AHR	g	22	3	-	0/2/15/18	0/1/1/1
3	AHR	g	23	3	-	0/2/15/18	0/1/1/1
3	AHR	g	24	3	-	0/2/15/18	0/1/1/1
3	FUB	g	25	3	-	0/2/15/18	0/1/1/1
3	AHR	g	26	3	-	0/2/15/18	0/1/1/1
3	FUB	g	27	3	-	0/2/15/18	0/1/1/1
3	AHR	g	28	3	-	0/2/15/18	0/1/1/1
3	AHR	g	29	3	-	0/2/15/18	0/1/1/1
3	BMA	g	3	3	-	0/2/19/22	0/1/1/1
3	NGA	g	4	3	-	2/6/23/26	0/1/1/1
3	MAN	g	5	3	-	0/2/19/22	0/1/1/1
3	MAN	g	6	3	-	0/2/19/22	0/1/1/1
3	MAN	g	7	3	-	0/2/19/22	0/1/1/1
3	GAL	g	8	3	-	1/2/19/22	0/1/1/1
3	MAN	g	9	3	-	0/2/19/22	0/1/1/1
4	GAL	h	1	4	-	0/2/19/22	0/1/1/1
4	AHR	h	10	4	-	0/2/15/18	0/1/1/1
4	FUB	h	11	4	-	0/2/15/18	0/1/1/1
4	AHR	h	12	4	-	0/2/15/18	0/1/1/1
4	MAN	h	13	4	-	0/2/19/22	0/1/1/1
4	MAN	h	14	4	-	0/2/19/22	0/1/1/1
4	MAN	h	15	4	-	0/2/19/22	0/1/1/1
4	AHR	h	16	4	-	0/2/15/18	0/1/1/1
4	BMA	h	2	4	-	0/2/19/22	0/1/1/1
4	BGC	h	3	4	-	0/2/19/22	0/1/1/1
4	AHR	h	4	4	-	0/2/15/18	0/1/1/1
4	MAN	h	5	4	-	0/2/19/22	0/1/1/1
4	AHR	h	6	4	-	0/2/15/18	0/1/1/1
4	AHR	h	7	4	-	0/2/15/18	0/1/1/1
4	AHR	h	8	4	-	0/2/15/18	0/1/1/1
4	AHR	h	9	4	-	0/2/15/18	0/1/1/1
2	AHR	i	1	2	-	0/2/15/18	0/1/1/1
2	FUB	i	2	2	-	0/2/15/18	0/1/1/1
2	FUB	i	3	2	-	0/2/15/18	0/1/1/1
2	GAL	i	4	2	-	0/2/19/22	0/1/1/1
2	AHR	i	5	2	-	0/2/15/18	0/1/1/1
2	FUB	i	6	2	-	0/2/15/18	0/1/1/1
2	AHR	i	7	2	-	0/2/15/18	0/1/1/1
3	FUB	j	1	3	-	0/2/15/18	0/1/1/1
3	AHR	j	10	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AHR	j	11	3	-	0/2/15/18	0/1/1/1
3	AHR	j	12	3	-	0/2/15/18	0/1/1/1
3	AHR	j	13	3	-	0/2/15/18	0/1/1/1
3	AHR	j	14	3	-	0/2/15/18	0/1/1/1
3	MAN	j	15	3	-	0/2/19/22	0/1/1/1
3	BMA	j	16	3	-	0/2/19/22	0/1/1/1
3	BMA	j	17	3	-	1/2/19/22	0/1/1/1
3	MAN	j	18	3	-	0/2/19/22	0/1/1/1
3	AHR	j	19	3	-	0/2/15/18	0/1/1/1
3	BMA	j	2	3	-	2/2/19/22	0/1/1/1
3	BMA	j	20	3	-	1/2/19/22	0/1/1/1
3	AHR	j	21	3	-	0/2/15/18	0/1/1/1
3	AHR	j	22	3	-	0/2/15/18	0/1/1/1
3	AHR	j	23	3	-	0/2/15/18	0/1/1/1
3	AHR	j	24	3	-	0/2/15/18	0/1/1/1
3	FUB	j	25	3	-	0/2/15/18	0/1/1/1
3	AHR	j	26	3	-	0/2/15/18	0/1/1/1
3	FUB	j	27	3	-	0/2/15/18	0/1/1/1
3	AHR	j	28	3	-	0/2/15/18	0/1/1/1
3	AHR	j	29	3	-	0/2/15/18	0/1/1/1
3	BMA	j	3	3	-	0/2/19/22	0/1/1/1
3	NGA	j	4	3	-	2/6/23/26	0/1/1/1
3	MAN	j	5	3	-	0/2/19/22	0/1/1/1
3	MAN	j	6	3	-	0/2/19/22	0/1/1/1
3	MAN	j	7	3	-	0/2/19/22	0/1/1/1
3	GAL	j	8	3	-	1/2/19/22	0/1/1/1
3	MAN	j	9	3	-	0/2/19/22	0/1/1/1
4	GAL	k	1	4	-	0/2/19/22	0/1/1/1
4	AHR	k	10	4	-	0/2/15/18	0/1/1/1
4	FUB	k	11	4	-	0/2/15/18	0/1/1/1
4	AHR	k	12	4	-	0/2/15/18	0/1/1/1
4	MAN	k	13	4	-	0/2/19/22	0/1/1/1
4	MAN	k	14	4	-	0/2/19/22	0/1/1/1
4	MAN	k	15	4	-	0/2/19/22	0/1/1/1
4	AHR	k	16	4	-	0/2/15/18	0/1/1/1
4	BMA	k	2	4	-	0/2/19/22	0/1/1/1
4	BGC	k	3	4	-	0/2/19/22	0/1/1/1
4	AHR	k	4	4	-	0/2/15/18	0/1/1/1
4	MAN	k	5	4	-	0/2/19/22	0/1/1/1
4	AHR	k	6	4	-	0/2/15/18	0/1/1/1
4	AHR	k	7	4	-	0/2/15/18	0/1/1/1
4	AHR	k	8	4	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AHR	k	9	4	-	0/2/15/18	0/1/1/1
2	AHR	l	1	2	-	0/2/15/18	0/1/1/1
2	FUB	l	2	2	-	0/2/15/18	0/1/1/1
2	FUB	l	3	2	-	0/2/15/18	0/1/1/1
2	GAL	l	4	2	-	0/2/19/22	0/1/1/1
2	AHR	l	5	2	-	0/2/15/18	0/1/1/1
2	FUB	l	6	2	-	0/2/15/18	0/1/1/1
2	AHR	l	7	2	-	0/2/15/18	0/1/1/1
3	FUB	m	1	3	-	0/2/15/18	0/1/1/1
3	AHR	m	10	3	-	0/2/15/18	0/1/1/1
3	AHR	m	11	3	-	0/2/15/18	0/1/1/1
3	AHR	m	12	3	-	0/2/15/18	0/1/1/1
3	AHR	m	13	3	-	0/2/15/18	0/1/1/1
3	AHR	m	14	3	-	0/2/15/18	0/1/1/1
3	MAN	m	15	3	-	0/2/19/22	0/1/1/1
3	BMA	m	16	3	-	0/2/19/22	0/1/1/1
3	BMA	m	17	3	-	1/2/19/22	0/1/1/1
3	MAN	m	18	3	-	0/2/19/22	0/1/1/1
3	AHR	m	19	3	-	0/2/15/18	0/1/1/1
3	BMA	m	2	3	-	2/2/19/22	0/1/1/1
3	BMA	m	20	3	-	1/2/19/22	0/1/1/1
3	AHR	m	21	3	-	0/2/15/18	0/1/1/1
3	AHR	m	22	3	-	0/2/15/18	0/1/1/1
3	AHR	m	23	3	-	0/2/15/18	0/1/1/1
3	AHR	m	24	3	-	0/2/15/18	0/1/1/1
3	FUB	m	25	3	-	0/2/15/18	0/1/1/1
3	AHR	m	26	3	-	0/2/15/18	0/1/1/1
3	FUB	m	27	3	-	0/2/15/18	0/1/1/1
3	AHR	m	28	3	-	0/2/15/18	0/1/1/1
3	AHR	m	29	3	-	0/2/15/18	0/1/1/1
3	BMA	m	3	3	-	0/2/19/22	0/1/1/1
3	NGA	m	4	3	-	2/6/23/26	0/1/1/1
3	MAN	m	5	3	-	0/2/19/22	0/1/1/1
3	MAN	m	6	3	-	0/2/19/22	0/1/1/1
3	MAN	m	7	3	-	0/2/19/22	0/1/1/1
3	GAL	m	8	3	-	1/2/19/22	0/1/1/1
3	MAN	m	9	3	-	0/2/19/22	0/1/1/1
4	GAL	n	1	4	-	0/2/19/22	0/1/1/1
4	AHR	n	10	4	-	0/2/15/18	0/1/1/1
4	FUB	n	11	4	-	0/2/15/18	0/1/1/1
4	AHR	n	12	4	-	0/2/15/18	0/1/1/1
4	MAN	n	13	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	n	14	4	-	0/2/19/22	0/1/1/1
4	MAN	n	15	4	-	0/2/19/22	0/1/1/1
4	AHR	n	16	4	-	0/2/15/18	0/1/1/1
4	BMA	n	2	4	-	0/2/19/22	0/1/1/1
4	BGC	n	3	4	-	0/2/19/22	0/1/1/1
4	AHR	n	4	4	-	0/2/15/18	0/1/1/1
4	MAN	n	5	4	-	0/2/19/22	0/1/1/1
4	AHR	n	6	4	-	0/2/15/18	0/1/1/1
4	AHR	n	7	4	-	0/2/15/18	0/1/1/1
4	AHR	n	8	4	-	0/2/15/18	0/1/1/1
4	AHR	n	9	4	-	0/2/15/18	0/1/1/1
2	AHR	o	1	2	-	0/2/15/18	0/1/1/1
2	FUB	o	2	2	-	0/2/15/18	0/1/1/1
2	FUB	o	3	2	-	0/2/15/18	0/1/1/1
2	GAL	o	4	2	-	0/2/19/22	0/1/1/1
2	AHR	o	5	2	-	0/2/15/18	0/1/1/1
2	FUB	o	6	2	-	0/2/15/18	0/1/1/1
2	AHR	o	7	2	-	0/2/15/18	0/1/1/1
3	FUB	p	1	3	-	0/2/15/18	0/1/1/1
3	AHR	p	10	3	-	0/2/15/18	0/1/1/1
3	AHR	p	11	3	-	0/2/15/18	0/1/1/1
3	AHR	p	12	3	-	0/2/15/18	0/1/1/1
3	AHR	p	13	3	-	0/2/15/18	0/1/1/1
3	AHR	p	14	3	-	0/2/15/18	0/1/1/1
3	MAN	p	15	3	-	0/2/19/22	0/1/1/1
3	BMA	p	16	3	-	0/2/19/22	0/1/1/1
3	BMA	p	17	3	-	1/2/19/22	0/1/1/1
3	MAN	p	18	3	-	0/2/19/22	0/1/1/1
3	AHR	p	19	3	-	0/2/15/18	0/1/1/1
3	BMA	p	2	3	-	2/2/19/22	0/1/1/1
3	BMA	p	20	3	-	1/2/19/22	0/1/1/1
3	AHR	p	21	3	-	0/2/15/18	0/1/1/1
3	AHR	p	22	3	-	0/2/15/18	0/1/1/1
3	AHR	p	23	3	-	0/2/15/18	0/1/1/1
3	AHR	p	24	3	-	0/2/15/18	0/1/1/1
3	FUB	p	25	3	-	0/2/15/18	0/1/1/1
3	AHR	p	26	3	-	0/2/15/18	0/1/1/1
3	FUB	p	27	3	-	0/2/15/18	0/1/1/1
3	AHR	p	28	3	-	0/2/15/18	0/1/1/1
3	AHR	p	29	3	-	0/2/15/18	0/1/1/1
3	BMA	p	3	3	-	0/2/19/22	0/1/1/1
3	NGA	p	4	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	p	5	3	-	0/2/19/22	0/1/1/1
3	MAN	p	6	3	-	0/2/19/22	0/1/1/1
3	MAN	p	7	3	-	0/2/19/22	0/1/1/1
3	GAL	p	8	3	-	1/2/19/22	0/1/1/1
3	MAN	p	9	3	-	0/2/19/22	0/1/1/1
4	GAL	q	1	4	-	0/2/19/22	0/1/1/1
4	AHR	q	10	4	-	0/2/15/18	0/1/1/1
4	FUB	q	11	4	-	0/2/15/18	0/1/1/1
4	AHR	q	12	4	-	0/2/15/18	0/1/1/1
4	MAN	q	13	4	-	0/2/19/22	0/1/1/1
4	MAN	q	14	4	-	0/2/19/22	0/1/1/1
4	MAN	q	15	4	-	0/2/19/22	0/1/1/1
4	AHR	q	16	4	-	0/2/15/18	0/1/1/1
4	BMA	q	2	4	-	0/2/19/22	0/1/1/1
4	BGC	q	3	4	-	0/2/19/22	0/1/1/1
4	AHR	q	4	4	-	0/2/15/18	0/1/1/1
4	MAN	q	5	4	-	0/2/19/22	0/1/1/1
4	AHR	q	6	4	-	0/2/15/18	0/1/1/1
4	AHR	q	7	4	-	0/2/15/18	0/1/1/1
4	AHR	q	8	4	-	0/2/15/18	0/1/1/1
4	AHR	q	9	4	-	0/2/15/18	0/1/1/1
2	AHR	r	1	2	-	0/2/15/18	0/1/1/1
2	FUB	r	2	2	-	0/2/15/18	0/1/1/1
2	FUB	r	3	2	-	0/2/15/18	0/1/1/1
2	GAL	r	4	2	-	0/2/19/22	0/1/1/1
2	AHR	r	5	2	-	0/2/15/18	0/1/1/1
2	FUB	r	6	2	-	0/2/15/18	0/1/1/1
2	AHR	r	7	2	-	0/2/15/18	0/1/1/1
3	FUB	s	1	3	-	0/2/15/18	0/1/1/1
3	AHR	s	10	3	-	0/2/15/18	0/1/1/1
3	AHR	s	11	3	-	0/2/15/18	0/1/1/1
3	AHR	s	12	3	-	0/2/15/18	0/1/1/1
3	AHR	s	13	3	-	0/2/15/18	0/1/1/1
3	AHR	s	14	3	-	0/2/15/18	0/1/1/1
3	MAN	s	15	3	-	0/2/19/22	0/1/1/1
3	BMA	s	16	3	-	0/2/19/22	0/1/1/1
3	BMA	s	17	3	-	1/2/19/22	0/1/1/1
3	MAN	s	18	3	-	0/2/19/22	0/1/1/1
3	AHR	s	19	3	-	0/2/15/18	0/1/1/1
3	BMA	s	2	3	-	2/2/19/22	0/1/1/1
3	BMA	s	20	3	-	1/2/19/22	0/1/1/1
3	AHR	s	21	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AHR	s	22	3	-	0/2/15/18	0/1/1/1
3	AHR	s	23	3	-	0/2/15/18	0/1/1/1
3	AHR	s	24	3	-	0/2/15/18	0/1/1/1
3	FUB	s	25	3	-	0/2/15/18	0/1/1/1
3	AHR	s	26	3	-	0/2/15/18	0/1/1/1
3	FUB	s	27	3	-	0/2/15/18	0/1/1/1
3	AHR	s	28	3	-	0/2/15/18	0/1/1/1
3	AHR	s	29	3	-	0/2/15/18	0/1/1/1
3	BMA	s	3	3	-	0/2/19/22	0/1/1/1
3	NGA	s	4	3	-	2/6/23/26	0/1/1/1
3	MAN	s	5	3	-	0/2/19/22	0/1/1/1
3	MAN	s	6	3	-	0/2/19/22	0/1/1/1
3	MAN	s	7	3	-	0/2/19/22	0/1/1/1
3	GAL	s	8	3	-	1/2/19/22	0/1/1/1
3	MAN	s	9	3	-	0/2/19/22	0/1/1/1
4	GAL	t	1	4	-	0/2/19/22	0/1/1/1
4	AHR	t	10	4	-	0/2/15/18	0/1/1/1
4	FUB	t	11	4	-	0/2/15/18	0/1/1/1
4	AHR	t	12	4	-	0/2/15/18	0/1/1/1
4	MAN	t	13	4	-	0/2/19/22	0/1/1/1
4	MAN	t	14	4	-	0/2/19/22	0/1/1/1
4	MAN	t	15	4	-	0/2/19/22	0/1/1/1
4	AHR	t	16	4	-	0/2/15/18	0/1/1/1
4	BMA	t	2	4	-	0/2/19/22	0/1/1/1
4	BGC	t	3	4	-	0/2/19/22	0/1/1/1
4	AHR	t	4	4	-	0/2/15/18	0/1/1/1
4	MAN	t	5	4	-	0/2/19/22	0/1/1/1
4	AHR	t	6	4	-	0/2/15/18	0/1/1/1
4	AHR	t	7	4	-	0/2/15/18	0/1/1/1
4	AHR	t	8	4	-	0/2/15/18	0/1/1/1
4	AHR	t	9	4	-	0/2/15/18	0/1/1/1
2	AHR	u	1	2	-	0/2/15/18	0/1/1/1
2	FUB	u	2	2	-	0/2/15/18	0/1/1/1
2	FUB	u	3	2	-	0/2/15/18	0/1/1/1
2	GAL	u	4	2	-	0/2/19/22	0/1/1/1
2	AHR	u	5	2	-	0/2/15/18	0/1/1/1
2	FUB	u	6	2	-	0/2/15/18	0/1/1/1
2	AHR	u	7	2	-	0/2/15/18	0/1/1/1
3	FUB	v	1	3	-	0/2/15/18	0/1/1/1
3	AHR	v	10	3	-	0/2/15/18	0/1/1/1
3	AHR	v	11	3	-	0/2/15/18	0/1/1/1
3	AHR	v	12	3	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AHR	v	13	3	-	0/2/15/18	0/1/1/1
3	AHR	v	14	3	-	0/2/15/18	0/1/1/1
3	MAN	v	15	3	-	0/2/19/22	0/1/1/1
3	BMA	v	16	3	-	0/2/19/22	0/1/1/1
3	BMA	v	17	3	-	1/2/19/22	0/1/1/1
3	MAN	v	18	3	-	0/2/19/22	0/1/1/1
3	AHR	v	19	3	-	0/2/15/18	0/1/1/1
3	BMA	v	2	3	-	2/2/19/22	0/1/1/1
3	BMA	v	20	3	-	1/2/19/22	0/1/1/1
3	AHR	v	21	3	-	0/2/15/18	0/1/1/1
3	AHR	v	22	3	-	0/2/15/18	0/1/1/1
3	AHR	v	23	3	-	0/2/15/18	0/1/1/1
3	AHR	v	24	3	-	0/2/15/18	0/1/1/1
3	FUB	v	25	3	-	0/2/15/18	0/1/1/1
3	AHR	v	26	3	-	0/2/15/18	0/1/1/1
3	FUB	v	27	3	-	0/2/15/18	0/1/1/1
3	AHR	v	28	3	-	0/2/15/18	0/1/1/1
3	AHR	v	29	3	-	0/2/15/18	0/1/1/1
3	BMA	v	3	3	-	0/2/19/22	0/1/1/1
3	NGA	v	4	3	-	2/6/23/26	0/1/1/1
3	MAN	v	5	3	-	0/2/19/22	0/1/1/1
3	MAN	v	6	3	-	0/2/19/22	0/1/1/1
3	MAN	v	7	3	-	0/2/19/22	0/1/1/1
3	GAL	v	8	3	-	1/2/19/22	0/1/1/1
3	MAN	v	9	3	-	0/2/19/22	0/1/1/1
4	GAL	w	1	4	-	0/2/19/22	0/1/1/1
4	AHR	w	10	4	-	0/2/15/18	0/1/1/1
4	FUB	w	11	4	-	0/2/15/18	0/1/1/1
4	AHR	w	12	4	-	0/2/15/18	0/1/1/1
4	MAN	w	13	4	-	0/2/19/22	0/1/1/1
4	MAN	w	14	4	-	0/2/19/22	0/1/1/1
4	MAN	w	15	4	-	0/2/19/22	0/1/1/1
4	AHR	w	16	4	-	0/2/15/18	0/1/1/1
4	BMA	w	2	4	-	0/2/19/22	0/1/1/1
4	BGC	w	3	4	-	0/2/19/22	0/1/1/1
4	AHR	w	4	4	-	0/2/15/18	0/1/1/1
4	MAN	w	5	4	-	0/2/19/22	0/1/1/1
4	AHR	w	6	4	-	0/2/15/18	0/1/1/1
4	AHR	w	7	4	-	0/2/15/18	0/1/1/1
4	AHR	w	8	4	-	0/2/15/18	0/1/1/1
4	AHR	w	9	4	-	0/2/15/18	0/1/1/1
2	AHR	x	1	2	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUB	x	2	2	-	0/2/15/18	0/1/1/1
2	FUB	x	3	2	-	0/2/15/18	0/1/1/1
2	GAL	x	4	2	-	0/2/19/22	0/1/1/1
2	AHR	x	5	2	-	0/2/15/18	0/1/1/1
2	FUB	x	6	2	-	0/2/15/18	0/1/1/1
2	AHR	x	7	2	-	0/2/15/18	0/1/1/1
3	FUB	y	1	3	-	0/2/15/18	0/1/1/1
3	AHR	y	10	3	-	0/2/15/18	0/1/1/1
3	AHR	y	11	3	-	0/2/15/18	0/1/1/1
3	AHR	y	12	3	-	0/2/15/18	0/1/1/1
3	AHR	y	13	3	-	0/2/15/18	0/1/1/1
3	AHR	y	14	3	-	0/2/15/18	0/1/1/1
3	MAN	y	15	3	-	0/2/19/22	0/1/1/1
3	BMA	y	16	3	-	0/2/19/22	0/1/1/1
3	BMA	y	17	3	-	1/2/19/22	0/1/1/1
3	MAN	y	18	3	-	0/2/19/22	0/1/1/1
3	AHR	y	19	3	-	0/2/15/18	0/1/1/1
3	BMA	y	2	3	-	2/2/19/22	0/1/1/1
3	BMA	y	20	3	-	1/2/19/22	0/1/1/1
3	AHR	y	21	3	-	0/2/15/18	0/1/1/1
3	AHR	y	22	3	-	0/2/15/18	0/1/1/1
3	AHR	y	23	3	-	0/2/15/18	0/1/1/1
3	AHR	y	24	3	-	0/2/15/18	0/1/1/1
3	FUB	y	25	3	-	0/2/15/18	0/1/1/1
3	AHR	y	26	3	-	0/2/15/18	0/1/1/1
3	FUB	y	27	3	-	0/2/15/18	0/1/1/1
3	AHR	y	28	3	-	0/2/15/18	0/1/1/1
3	AHR	y	29	3	-	0/2/15/18	0/1/1/1
3	BMA	y	3	3	-	0/2/19/22	0/1/1/1
3	NGA	y	4	3	-	2/6/23/26	0/1/1/1
3	MAN	y	5	3	-	0/2/19/22	0/1/1/1
3	MAN	y	6	3	-	0/2/19/22	0/1/1/1
3	MAN	y	7	3	-	0/2/19/22	0/1/1/1
3	GAL	y	8	3	-	1/2/19/22	0/1/1/1
3	MAN	y	9	3	-	0/2/19/22	0/1/1/1
4	GAL	z	1	4	-	0/2/19/22	0/1/1/1
4	AHR	z	10	4	-	0/2/15/18	0/1/1/1
4	FUB	z	11	4	-	0/2/15/18	0/1/1/1
4	AHR	z	12	4	-	0/2/15/18	0/1/1/1
4	MAN	z	13	4	-	0/2/19/22	0/1/1/1
4	MAN	z	14	4	-	0/2/19/22	0/1/1/1
4	MAN	z	15	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AHR	z	16	4	-	0/2/15/18	0/1/1/1
4	BMA	z	2	4	-	0/2/19/22	0/1/1/1
4	BGC	z	3	4	-	0/2/19/22	0/1/1/1
4	AHR	z	4	4	-	0/2/15/18	0/1/1/1
4	MAN	z	5	4	-	0/2/19/22	0/1/1/1
4	AHR	z	6	4	-	0/2/15/18	0/1/1/1
4	AHR	z	7	4	-	0/2/15/18	0/1/1/1
4	AHR	z	8	4	-	0/2/15/18	0/1/1/1
4	AHR	z	9	4	-	0/2/15/18	0/1/1/1

There are no bond length outliers.

All (350) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	MAN	C1-C2-C3	4.34	115.96	109.64
3	C	5	MAN	O5-C5-C4	-4.17	100.69	110.83
4	D	13	MAN	O2-C2-C3	2.97	116.30	110.15
3	C	5	MAN	C3-C4-C5	2.77	115.26	110.23
3	j	27	FUB	C1-C2-C3	2.71	105.96	101.63
3	g	27	FUB	C1-C2-C3	2.68	105.92	101.63
3	X	27	FUB	C1-C2-C3	2.68	105.91	101.63
3	d	27	FUB	C1-C2-C3	2.67	105.90	101.63
3	L	27	FUB	C1-C2-C3	2.67	105.90	101.63
3	m	27	FUB	C1-C2-C3	2.66	105.89	101.63
3	C	27	FUB	C1-C2-C3	2.66	105.88	101.63
3	O	27	FUB	C1-C2-C3	2.65	105.86	101.63
3	v	27	FUB	C1-C2-C3	2.65	105.86	101.63
3	R	27	FUB	C1-C2-C3	2.65	105.86	101.63
3	a	27	FUB	C1-C2-C3	2.64	105.86	101.63
3	l	27	FUB	C1-C2-C3	2.64	105.85	101.63
3	F	27	FUB	C1-C2-C3	2.64	105.85	101.63
3	s	27	FUB	C1-C2-C3	2.63	105.83	101.63
3	p	27	FUB	C1-C2-C3	2.61	105.80	101.63
3	U	27	FUB	C1-C2-C3	2.61	105.80	101.63
3	I	27	FUB	C1-C2-C3	2.60	105.79	101.63
3	y	27	FUB	C1-C2-C3	2.60	105.78	101.63
4	D	4	AHR	C1-C2-C3	2.53	105.68	101.63
3	C	5	MAN	C2-C3-C4	2.53	115.31	110.86
3	C	9	MAN	C1-O5-C5	2.45	115.47	112.19
4	t	4	AHR	C1-C2-C3	2.43	105.51	101.63
4	G	4	AHR	C1-C2-C3	2.42	105.50	101.63
3	v	17	BMA	C1-O5-C5	2.42	115.43	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	4	AHR	C1-C2-C3	2.42	105.49	101.63
4	P	4	AHR	C1-C2-C3	2.41	105.49	101.63
4	e	4	AHR	C1-C2-C3	2.41	105.48	101.63
4	n	4	AHR	C1-C2-C3	2.41	105.48	101.63
4	k	4	AHR	C1-C2-C3	2.41	105.47	101.63
4	D	14	MAN	O5-C5-C4	-2.40	104.98	110.83
4	b	4	AHR	C1-C2-C3	2.40	105.47	101.63
4	J	4	AHR	C1-C2-C3	2.40	105.46	101.63
4	z	4	AHR	C1-C2-C3	2.40	105.46	101.63
4	h	4	AHR	C1-C2-C3	2.40	105.46	101.63
3	O	17	BMA	C1-O5-C5	2.40	115.40	112.19
3	p	17	BMA	C1-O5-C5	2.40	115.40	112.19
4	Y	4	AHR	C1-C2-C3	2.40	105.46	101.63
4	w	4	AHR	C1-C2-C3	2.39	105.45	101.63
3	j	17	BMA	C1-O5-C5	2.39	115.39	112.19
4	q	4	AHR	C1-C2-C3	2.39	105.45	101.63
3	m	17	BMA	C1-O5-C5	2.39	115.39	112.19
3	F	17	BMA	C1-O5-C5	2.39	115.38	112.19
3	L	17	BMA	C1-O5-C5	2.38	115.37	112.19
3	a	17	BMA	C1-O5-C5	2.38	115.37	112.19
4	2	4	AHR	C1-C2-C3	2.38	105.43	101.63
3	d	17	BMA	C1-O5-C5	2.38	115.37	112.19
3	y	17	BMA	C1-O5-C5	2.37	115.37	112.19
4	M	4	AHR	C1-C2-C3	2.37	105.42	101.63
4	V	4	AHR	C1-C2-C3	2.37	105.42	101.63
3	g	17	BMA	C1-O5-C5	2.37	115.36	112.19
3	s	17	BMA	C1-O5-C5	2.37	115.36	112.19
3	U	17	BMA	C1-O5-C5	2.37	115.36	112.19
3	R	17	BMA	C1-O5-C5	2.37	115.36	112.19
3	X	17	BMA	C1-O5-C5	2.33	115.31	112.19
3	I	17	BMA	C1-O5-C5	2.33	115.31	112.19
3	l	17	BMA	C1-O5-C5	2.33	115.31	112.19
3	p	9	MAN	C1-O5-C5	2.33	115.30	112.19
3	j	9	MAN	C1-O5-C5	2.32	115.29	112.19
4	q	13	MAN	O2-C2-C3	2.32	114.95	110.15
4	G	13	MAN	O2-C2-C3	2.31	114.94	110.15
3	a	9	MAN	C1-O5-C5	2.31	115.29	112.19
4	b	13	MAN	O2-C2-C3	2.31	114.93	110.15
3	C	5	MAN	O5-C5-C6	2.31	112.15	107.66
4	z	13	MAN	O2-C2-C3	2.30	114.92	110.15
3	m	9	MAN	C1-O5-C5	2.30	115.27	112.19
3	C	4	NGA	C3-C4-C5	-2.30	106.06	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	9	MAN	C1-O5-C5	2.30	115.27	112.19
4	P	13	MAN	O2-C2-C3	2.30	114.91	110.15
3	L	9	MAN	C1-O5-C5	2.30	115.27	112.19
4	h	13	MAN	O2-C2-C3	2.30	114.91	110.15
4	Y	13	MAN	O2-C2-C3	2.29	114.90	110.15
4	M	13	MAN	O2-C2-C3	2.29	114.89	110.15
3	I	9	MAN	C1-O5-C5	2.29	115.25	112.19
4	2	13	MAN	O2-C2-C3	2.29	114.89	110.15
3	F	9	MAN	C1-O5-C5	2.29	115.25	112.19
4	t	13	MAN	O2-C2-C3	2.29	114.89	110.15
4	w	13	MAN	O2-C2-C3	2.29	114.89	110.15
3	O	9	MAN	C1-O5-C5	2.28	115.25	112.19
4	n	13	MAN	O2-C2-C3	2.28	114.88	110.15
3	v	9	MAN	C1-O5-C5	2.28	115.25	112.19
3	g	9	MAN	C1-O5-C5	2.28	115.24	112.19
3	s	9	MAN	C1-O5-C5	2.28	115.24	112.19
4	J	13	MAN	O2-C2-C3	2.28	114.88	110.15
4	k	13	MAN	O2-C2-C3	2.28	114.87	110.15
4	e	13	MAN	O2-C2-C3	2.28	114.87	110.15
4	V	13	MAN	O2-C2-C3	2.28	114.86	110.15
3	y	9	MAN	C1-O5-C5	2.27	115.23	112.19
4	S	13	MAN	O2-C2-C3	2.27	114.86	110.15
3	g	1	FUB	C1-C2-C3	2.27	105.26	101.63
3	O	1	FUB	C1-C2-C3	2.26	105.24	101.63
3	R	9	MAN	C1-O5-C5	2.26	115.21	112.19
3	d	9	MAN	C1-O5-C5	2.26	115.21	112.19
3	X	9	MAN	C1-O5-C5	2.25	115.20	112.19
3	l	9	MAN	C1-O5-C5	2.25	115.20	112.19
3	C	1	FUB	C1-C2-C3	2.25	105.22	101.63
3	m	1	FUB	C1-C2-C3	2.24	105.22	101.63
3	p	1	FUB	C1-C2-C3	2.24	105.22	101.63
3	v	1	FUB	C1-C2-C3	2.24	105.22	101.63
3	X	12	AHR	C1-C2-C3	2.24	105.21	101.63
3	F	1	FUB	C1-C2-C3	2.24	105.20	101.63
3	y	1	FUB	C1-C2-C3	2.24	105.20	101.63
3	L	1	FUB	C1-C2-C3	2.23	105.20	101.63
3	I	1	FUB	C1-C2-C3	2.23	105.20	101.63
3	U	1	FUB	C1-C2-C3	2.23	105.20	101.63
3	l	1	FUB	C1-C2-C3	2.23	105.19	101.63
3	L	12	AHR	C1-C2-C3	2.23	105.19	101.63
3	R	12	AHR	C1-C2-C3	2.23	105.19	101.63
3	s	1	FUB	C1-C2-C3	2.22	105.18	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	j	1	FUB	C1-C2-C3	2.22	105.18	101.63
3	d	1	FUB	C1-C2-C3	2.22	105.17	101.63
3	v	12	AHR	C1-C2-C3	2.22	105.17	101.63
3	I	12	AHR	C1-C2-C3	2.22	105.17	101.63
3	p	12	AHR	C1-C2-C3	2.21	105.17	101.63
3	X	1	FUB	C1-C2-C3	2.21	105.17	101.63
3	R	1	FUB	C1-C2-C3	2.21	105.17	101.63
3	a	1	FUB	C1-C2-C3	2.21	105.16	101.63
3	F	12	AHR	C1-C2-C3	2.21	105.16	101.63
3	O	12	AHR	C1-C2-C3	2.20	105.15	101.63
3	l	12	AHR	C1-C2-C3	2.20	105.15	101.63
3	U	12	AHR	C1-C2-C3	2.20	105.14	101.63
3	a	12	AHR	C1-C2-C3	2.20	105.14	101.63
3	d	12	AHR	C1-C2-C3	2.19	105.13	101.63
3	g	12	AHR	C1-C2-C3	2.19	105.13	101.63
3	s	12	AHR	C1-C2-C3	2.18	105.12	101.63
3	m	12	AHR	C1-C2-C3	2.18	105.11	101.63
3	X	26	AHR	C1-C2-C3	2.18	105.11	101.63
3	C	6	MAN	C1-O5-C5	2.18	115.10	112.19
3	j	26	AHR	C1-C2-C3	2.17	105.11	101.63
4	D	14	MAN	C3-C4-C5	-2.17	106.29	110.23
3	j	12	AHR	C1-C2-C3	2.17	105.10	101.63
3	v	26	AHR	C1-C2-C3	2.17	105.09	101.63
3	R	26	AHR	C1-C2-C3	2.16	105.09	101.63
3	y	12	AHR	C1-C2-C3	2.16	105.08	101.63
3	y	26	AHR	C1-C2-C3	2.16	105.08	101.63
3	F	26	AHR	C1-C2-C3	2.16	105.08	101.63
3	L	6	MAN	C1-O5-C5	2.15	115.07	112.19
3	d	26	AHR	C1-C2-C3	2.15	105.07	101.63
3	s	26	AHR	C1-C2-C3	2.15	105.07	101.63
3	O	26	AHR	C1-C2-C3	2.15	105.06	101.63
3	p	26	AHR	C1-C2-C3	2.14	105.06	101.63
3	I	6	MAN	C1-O5-C5	2.14	115.06	112.19
3	v	6	MAN	C1-O5-C5	2.14	115.06	112.19
4	D	8	AHR	C1-C2-C3	2.14	105.05	101.63
3	U	26	AHR	C1-C2-C3	2.14	105.05	101.63
3	L	26	AHR	C1-C2-C3	2.14	105.05	101.63
3	d	6	MAN	C1-O5-C5	2.14	115.05	112.19
3	a	26	AHR	C1-C2-C3	2.13	105.04	101.63
3	m	26	AHR	C1-C2-C3	2.13	105.03	101.63
3	m	6	MAN	C1-O5-C5	2.13	115.03	112.19
3	y	22	AHR	C1-C2-C3	2.12	105.02	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	6	MAN	C1-O5-C5	2.12	115.03	112.19
3	v	22	AHR	C1-C2-C3	2.12	105.02	101.63
4	2	8	AHR	C1-C2-C3	2.12	105.02	101.63
3	j	6	MAN	C1-O5-C5	2.12	115.03	112.19
3	g	26	AHR	C1-C2-C3	2.12	105.02	101.63
3	1	6	MAN	C1-O5-C5	2.12	115.03	112.19
3	X	6	MAN	C1-O5-C5	2.12	115.03	112.19
3	F	6	MAN	C1-O5-C5	2.12	115.02	112.19
3	I	26	AHR	C1-C2-C3	2.11	105.01	101.63
3	1	26	AHR	C1-C2-C3	2.11	105.01	101.63
3	j	22	AHR	C1-C2-C3	2.11	105.00	101.63
4	b	8	AHR	C1-C2-C3	2.11	105.00	101.63
3	U	6	MAN	C1-O5-C5	2.11	115.01	112.19
3	R	10	AHR	C1-C2-C3	2.11	105.00	101.63
4	M	8	AHR	C1-C2-C3	2.11	105.00	101.63
3	I	22	AHR	C1-C2-C3	2.10	104.99	101.63
4	Y	8	AHR	C1-C2-C3	2.10	104.99	101.63
4	q	8	AHR	C1-C2-C3	2.10	104.99	101.63
3	g	6	MAN	C1-O5-C5	2.10	115.00	112.19
3	1	22	AHR	C1-C2-C3	2.10	104.98	101.63
3	R	22	AHR	C1-C2-C3	2.10	104.98	101.63
4	V	8	AHR	C1-C2-C3	2.10	104.98	101.63
4	h	8	AHR	C1-C2-C3	2.10	104.98	101.63
3	C	17	BMA	C1-O5-C5	2.09	114.99	112.19
3	s	6	MAN	C1-O5-C5	2.09	114.99	112.19
3	X	10	AHR	C1-C2-C3	2.09	104.97	101.63
3	O	6	MAN	C1-O5-C5	2.09	114.99	112.19
3	F	10	AHR	C1-C2-C3	2.09	104.97	101.63
4	k	8	AHR	C1-C2-C3	2.09	104.97	101.63
3	y	6	MAN	C1-O5-C5	2.09	114.98	112.19
3	g	22	AHR	C1-C2-C3	2.09	104.97	101.63
3	d	10	AHR	C1-C2-C3	2.09	104.97	101.63
3	y	10	AHR	C1-C2-C3	2.09	104.97	101.63
3	1	10	AHR	C1-C2-C3	2.09	104.97	101.63
4	w	8	AHR	C1-C2-C3	2.09	104.96	101.63
3	F	22	AHR	C1-C2-C3	2.09	104.96	101.63
3	p	22	AHR	C1-C2-C3	2.09	104.96	101.63
3	d	19	AHR	C1-C2-C3	2.08	104.96	101.63
3	R	6	MAN	C1-O5-C5	2.08	114.98	112.19
3	C	25	FUB	C1-C2-C3	2.08	104.96	101.63
3	C	14	AHR	C1-C2-C3	2.08	104.95	101.63
3	d	22	AHR	C1-C2-C3	2.08	104.95	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	s	22	AHR	C1-C2-C3	2.08	104.95	101.63
3	p	6	MAN	C1-O5-C5	2.08	114.97	112.19
3	U	22	AHR	C1-C2-C3	2.08	104.95	101.63
3	m	22	AHR	C1-C2-C3	2.08	104.95	101.63
4	P	8	AHR	C1-C2-C3	2.08	104.95	101.63
3	O	22	AHR	C1-C2-C3	2.08	104.95	101.63
4	G	8	AHR	C1-C2-C3	2.08	104.95	101.63
4	J	8	AHR	C1-C2-C3	2.08	104.95	101.63
3	U	10	AHR	C1-C2-C3	2.08	104.95	101.63
4	e	8	AHR	C1-C2-C3	2.08	104.95	101.63
4	n	8	AHR	C1-C2-C3	2.07	104.95	101.63
3	a	10	AHR	C1-C2-C3	2.07	104.94	101.63
3	X	22	AHR	C1-C2-C3	2.07	104.94	101.63
4	S	8	AHR	C1-C2-C3	2.07	104.94	101.63
3	L	22	AHR	C1-C2-C3	2.07	104.94	101.63
4	t	8	AHR	C1-C2-C3	2.06	104.93	101.63
4	z	8	AHR	C1-C2-C3	2.06	104.92	101.63
3	a	22	AHR	C1-C2-C3	2.06	104.92	101.63
3	g	10	AHR	C1-C2-C3	2.06	104.92	101.63
3	m	25	FUB	C1-C2-C3	2.06	104.92	101.63
2	H	5	AHR	C1-C2-C3	2.06	104.92	101.63
3	I	10	AHR	C1-C2-C3	2.06	104.92	101.63
4	w	11	FUB	C1-C2-C3	2.06	104.92	101.63
3	s	14	AHR	C1-C2-C3	2.06	104.92	101.63
3	v	10	AHR	C1-C2-C3	2.05	104.91	101.63
2	Z	5	AHR	C1-C2-C3	2.05	104.91	101.63
3	C	9	MAN	C1-C2-C3	2.05	112.63	109.64
2	K	5	AHR	C1-C2-C3	2.05	104.91	101.63
3	L	10	AHR	C1-C2-C3	2.05	104.91	101.63
3	s	15	MAN	C1-O5-C5	2.05	114.94	112.19
4	J	15	MAN	C1-O5-C5	2.05	114.94	112.19
4	t	11	FUB	C1-C2-C3	2.05	104.91	101.63
4	D	15	MAN	C1-O5-C5	2.05	114.93	112.19
3	O	11	AHR	C1-C2-C3	2.05	104.91	101.63
3	s	11	AHR	C1-C2-C3	2.05	104.90	101.63
3	O	15	MAN	C1-O5-C5	2.05	114.93	112.19
3	m	10	AHR	C1-C2-C3	2.05	104.90	101.63
3	s	10	AHR	C1-C2-C3	2.05	104.90	101.63
3	O	10	AHR	C1-C2-C3	2.05	104.90	101.63
3	U	19	AHR	C1-C2-C3	2.04	104.90	101.63
4	z	11	FUB	C1-C2-C3	2.04	104.90	101.63
3	U	14	AHR	C1-C2-C3	2.04	104.90	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	g	11	AHR	C1-C2-C3	2.04	104.90	101.63
4	2	11	FUB	C1-C2-C3	2.04	104.90	101.63
4	e	11	FUB	C1-C2-C3	2.04	104.90	101.63
3	a	19	AHR	C1-C2-C3	2.04	104.89	101.63
4	S	14	MAN	C1-O5-C5	2.04	114.92	112.19
4	h	14	MAN	C1-O5-C5	2.04	114.92	112.19
2	u	5	AHR	C1-C2-C3	2.04	104.89	101.63
4	P	11	FUB	C1-C2-C3	2.04	104.89	101.63
3	p	10	AHR	C1-C2-C3	2.04	104.89	101.63
3	O	13	AHR	C1-C2-C3	2.04	104.89	101.63
2	N	5	AHR	C1-C2-C3	2.04	104.89	101.63
2	Q	5	AHR	C1-C2-C3	2.04	104.89	101.63
3	v	11	AHR	C1-C2-C3	2.04	104.88	101.63
4	n	11	FUB	C1-C2-C3	2.04	104.88	101.63
3	j	11	AHR	C1-C2-C3	2.03	104.88	101.63
3	a	15	MAN	C1-O5-C5	2.03	114.91	112.19
3	X	13	AHR	C1-C2-C3	2.03	104.88	101.63
3	d	13	AHR	C1-C2-C3	2.03	104.88	101.63
3	m	19	AHR	C1-C2-C3	2.03	104.88	101.63
3	C	11	AHR	C1-C2-C3	2.03	104.87	101.63
4	G	11	FUB	C1-C2-C3	2.03	104.87	101.63
3	m	15	MAN	C1-O5-C5	2.03	114.91	112.19
3	C	12	AHR	C1-C2-C3	2.03	104.87	101.63
3	F	25	FUB	C1-C2-C3	2.03	104.87	101.63
3	p	19	AHR	C1-C2-C3	2.03	104.87	101.63
2	E	5	AHR	C1-C2-C3	2.03	104.87	101.63
3	L	5	MAN	C1-O5-C5	2.03	114.90	112.19
3	F	11	AHR	C1-C2-C3	2.03	104.87	101.63
3	O	25	FUB	C1-C2-C3	2.03	104.87	101.63
3	X	14	AHR	C1-C2-C3	2.03	104.87	101.63
3	d	14	AHR	C1-C2-C3	2.03	104.87	101.63
3	s	13	AHR	C1-C2-C3	2.03	104.87	101.63
4	S	11	FUB	C1-C2-C3	2.03	104.87	101.63
4	M	15	MAN	C1-O5-C5	2.03	114.90	112.19
3	v	14	AHR	C1-C2-C3	2.03	104.87	101.63
3	1	25	FUB	C1-C2-C3	2.03	104.87	101.63
3	X	19	AHR	C1-C2-C3	2.03	104.87	101.63
3	v	13	AHR	C1-C2-C3	2.03	104.87	101.63
3	y	9	MAN	C1-C2-C3	2.03	112.59	109.64
4	V	14	MAN	C1-O5-C5	2.03	114.90	112.19
3	R	14	AHR	C1-C2-C3	2.02	104.87	101.63
3	m	11	AHR	C1-C2-C3	2.02	104.87	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	y	14	AHR	C1-C2-C3	2.02	104.86	101.63
4	M	11	FUB	C1-C2-C3	2.02	104.86	101.63
3	L	15	MAN	C1-O5-C5	2.02	114.90	112.19
3	U	13	AHR	C1-C2-C3	2.02	104.86	101.63
3	s	19	AHR	C1-C2-C3	2.02	104.86	101.63
3	l	19	AHR	C1-C2-C3	2.02	104.86	101.63
4	n	14	MAN	C1-O5-C5	2.02	114.90	112.19
3	R	15	MAN	C1-O5-C5	2.02	114.90	112.19
4	k	11	FUB	C1-C2-C3	2.02	104.86	101.63
3	a	25	FUB	C1-C2-C3	2.02	104.86	101.63
2	o	5	AHR	C1-C2-C3	2.02	104.86	101.63
3	j	10	AHR	C1-C2-C3	2.02	104.86	101.63
2	f	5	AHR	C1-C2-C3	2.02	104.86	101.63
2	x	5	AHR	C1-C2-C3	2.02	104.86	101.63
2	W	5	AHR	C1-C2-C3	2.02	104.86	101.63
4	J	11	FUB	C1-C2-C3	2.02	104.86	101.63
3	l	15	MAN	C1-O5-C5	2.02	114.89	112.19
4	b	14	MAN	C1-O5-C5	2.02	114.89	112.19
3	L	13	AHR	C1-C2-C3	2.02	104.86	101.63
2	r	5	AHR	C1-C2-C3	2.02	104.85	101.63
3	O	14	AHR	C1-C2-C3	2.02	104.85	101.63
2	T	5	AHR	C1-C2-C3	2.02	104.85	101.63
4	V	15	MAN	C1-O5-C5	2.02	114.89	112.19
3	I	14	AHR	C1-C2-C3	2.02	104.85	101.63
3	L	25	FUB	C1-C2-C3	2.02	104.85	101.63
4	V	11	FUB	C1-C2-C3	2.02	104.85	101.63
3	j	14	AHR	C1-C2-C3	2.02	104.85	101.63
3	O	19	AHR	C1-C2-C3	2.01	104.85	101.63
3	j	13	AHR	C1-C2-C3	2.01	104.85	101.63
3	a	13	AHR	C1-C2-C3	2.01	104.85	101.63
3	F	9	MAN	C1-C2-C3	2.01	112.58	109.64
3	F	19	AHR	C1-C2-C3	2.01	104.85	101.63
3	d	15	MAN	C1-O5-C5	2.01	114.88	112.19
3	v	9	MAN	C1-C2-C3	2.01	112.57	109.64
4	h	11	FUB	C1-C2-C3	2.01	104.84	101.63
4	G	15	MAN	C1-O5-C5	2.01	114.88	112.19
3	L	19	AHR	C1-C2-C3	2.01	104.84	101.63
3	v	19	AHR	C1-C2-C3	2.01	104.84	101.63
3	l	14	AHR	C1-C2-C3	2.01	104.84	101.63
4	q	11	FUB	C1-C2-C3	2.01	104.84	101.63
4	Y	14	MAN	C1-O5-C5	2.01	114.88	112.19
3	I	13	AHR	C1-C2-C3	2.01	104.84	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	11	AHR	C1-C2-C3	2.01	104.84	101.63
3	y	15	MAN	C1-O5-C5	2.01	114.88	112.19
3	a	14	AHR	C1-C2-C3	2.01	104.84	101.63
3	d	11	AHR	C1-C2-C3	2.01	104.84	101.63
3	l	13	AHR	C1-C2-C3	2.01	104.84	101.63
4	Y	11	FUB	C1-C2-C3	2.01	104.84	101.63
3	C	26	AHR	C1-C2-C3	2.01	104.84	101.63
3	L	14	AHR	C1-C2-C3	2.01	104.84	101.63
3	g	19	AHR	C1-C2-C3	2.01	104.84	101.63
3	s	5	MAN	C1-O5-C5	2.01	114.88	112.19
3	s	9	MAN	C1-C2-C3	2.01	112.56	109.64
4	b	11	FUB	C1-C2-C3	2.00	104.83	101.63
3	C	15	MAN	C1-O5-C5	2.00	114.87	112.19
4	k	15	MAN	C1-O5-C5	2.00	114.87	112.19
3	F	14	AHR	C1-C2-C3	2.00	104.83	101.63
3	y	13	AHR	C1-C2-C3	2.00	104.83	101.63
3	g	14	AHR	C1-C2-C3	2.00	104.83	101.63
4	P	15	MAN	C1-O5-C5	2.00	114.87	112.19
4	w	14	MAN	C1-O5-C5	2.00	114.87	112.19
2	c	5	AHR	C1-C2-C3	2.00	104.83	101.63
3	C	19	AHR	C1-C2-C3	2.00	104.83	101.63
4	Y	15	MAN	C1-O5-C5	2.00	114.87	112.19
3	R	11	AHR	C1-C2-C3	2.00	104.83	101.63
3	p	11	AHR	C1-C2-C3	2.00	104.83	101.63
3	I	15	MAN	C1-O5-C5	2.00	114.87	112.19
3	g	5	MAN	C1-O5-C5	2.00	114.87	112.19
3	X	11	AHR	C1-C2-C3	2.00	104.83	101.63
3	F	15	MAN	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	BMA	O5-C5-C6-O6
3	I	2	BMA	O5-C5-C6-O6
3	L	2	BMA	O5-C5-C6-O6
3	O	2	BMA	O5-C5-C6-O6
3	R	2	BMA	O5-C5-C6-O6
3	U	2	BMA	O5-C5-C6-O6
3	X	2	BMA	O5-C5-C6-O6
3	a	2	BMA	O5-C5-C6-O6
3	d	2	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	g	2	BMA	O5-C5-C6-O6
3	j	2	BMA	O5-C5-C6-O6
3	m	2	BMA	O5-C5-C6-O6
3	p	2	BMA	O5-C5-C6-O6
3	s	2	BMA	O5-C5-C6-O6
3	v	2	BMA	O5-C5-C6-O6
3	y	2	BMA	O5-C5-C6-O6
3	1	2	BMA	O5-C5-C6-O6
3	C	2	BMA	O5-C5-C6-O6
3	C	4	NGA	O5-C5-C6-O6
3	F	4	NGA	O5-C5-C6-O6
3	I	4	NGA	O5-C5-C6-O6
3	L	4	NGA	O5-C5-C6-O6
3	O	4	NGA	O5-C5-C6-O6
3	R	4	NGA	O5-C5-C6-O6
3	U	4	NGA	O5-C5-C6-O6
3	X	4	NGA	O5-C5-C6-O6
3	a	4	NGA	O5-C5-C6-O6
3	d	4	NGA	O5-C5-C6-O6
3	g	4	NGA	O5-C5-C6-O6
3	j	4	NGA	O5-C5-C6-O6
3	m	4	NGA	O5-C5-C6-O6
3	p	4	NGA	O5-C5-C6-O6
3	s	4	NGA	O5-C5-C6-O6
3	v	4	NGA	O5-C5-C6-O6
3	y	4	NGA	O5-C5-C6-O6
3	1	4	NGA	O5-C5-C6-O6
3	F	4	NGA	C4-C5-C6-O6
3	I	4	NGA	C4-C5-C6-O6
3	L	4	NGA	C4-C5-C6-O6
3	O	4	NGA	C4-C5-C6-O6
3	R	4	NGA	C4-C5-C6-O6
3	U	4	NGA	C4-C5-C6-O6
3	X	4	NGA	C4-C5-C6-O6
3	a	4	NGA	C4-C5-C6-O6
3	d	4	NGA	C4-C5-C6-O6
3	g	4	NGA	C4-C5-C6-O6
3	j	4	NGA	C4-C5-C6-O6
3	m	4	NGA	C4-C5-C6-O6
3	p	4	NGA	C4-C5-C6-O6
3	s	4	NGA	C4-C5-C6-O6
3	v	4	NGA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	y	4	NGA	C4-C5-C6-O6
3	1	4	NGA	C4-C5-C6-O6
3	C	4	NGA	C4-C5-C6-O6
4	D	14	MAN	C4-C5-C6-O6
3	C	20	BMA	O5-C5-C6-O6
4	D	14	MAN	O5-C5-C6-O6
3	C	2	BMA	C4-C5-C6-O6
3	F	2	BMA	C4-C5-C6-O6
3	I	2	BMA	C4-C5-C6-O6
3	L	2	BMA	C4-C5-C6-O6
3	O	2	BMA	C4-C5-C6-O6
3	R	2	BMA	C4-C5-C6-O6
3	U	2	BMA	C4-C5-C6-O6
3	X	2	BMA	C4-C5-C6-O6
3	a	2	BMA	C4-C5-C6-O6
3	d	2	BMA	C4-C5-C6-O6
3	g	2	BMA	C4-C5-C6-O6
3	j	2	BMA	C4-C5-C6-O6
3	m	2	BMA	C4-C5-C6-O6
3	p	2	BMA	C4-C5-C6-O6
3	s	2	BMA	C4-C5-C6-O6
3	v	2	BMA	C4-C5-C6-O6
3	y	2	BMA	C4-C5-C6-O6
3	1	2	BMA	C4-C5-C6-O6
3	C	20	BMA	C4-C5-C6-O6
3	L	8	GAL	O5-C5-C6-O6
3	O	8	GAL	O5-C5-C6-O6
3	R	8	GAL	O5-C5-C6-O6
3	1	8	GAL	O5-C5-C6-O6
3	F	8	GAL	O5-C5-C6-O6
3	U	8	GAL	O5-C5-C6-O6
3	X	8	GAL	O5-C5-C6-O6
3	j	8	GAL	O5-C5-C6-O6
3	p	8	GAL	O5-C5-C6-O6
3	v	8	GAL	O5-C5-C6-O6
3	I	8	GAL	O5-C5-C6-O6
3	a	8	GAL	O5-C5-C6-O6
3	d	8	GAL	O5-C5-C6-O6
3	g	8	GAL	O5-C5-C6-O6
3	m	8	GAL	O5-C5-C6-O6
3	s	8	GAL	O5-C5-C6-O6
3	y	8	GAL	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	8	GAL	O5-C5-C6-O6
3	F	17	BMA	O5-C5-C6-O6
3	I	17	BMA	O5-C5-C6-O6
3	L	17	BMA	O5-C5-C6-O6
3	O	17	BMA	O5-C5-C6-O6
3	R	17	BMA	O5-C5-C6-O6
3	U	17	BMA	O5-C5-C6-O6
3	X	17	BMA	O5-C5-C6-O6
3	a	17	BMA	O5-C5-C6-O6
3	d	17	BMA	O5-C5-C6-O6
3	g	17	BMA	O5-C5-C6-O6
3	j	17	BMA	O5-C5-C6-O6
3	m	17	BMA	O5-C5-C6-O6
3	p	17	BMA	O5-C5-C6-O6
3	s	17	BMA	O5-C5-C6-O6
3	v	17	BMA	O5-C5-C6-O6
3	y	17	BMA	O5-C5-C6-O6
3	1	17	BMA	O5-C5-C6-O6
3	C	17	BMA	O5-C5-C6-O6
3	C	16	BMA	O5-C5-C6-O6
3	F	20	BMA	O5-C5-C6-O6
3	p	20	BMA	O5-C5-C6-O6
3	I	20	BMA	O5-C5-C6-O6
3	L	20	BMA	O5-C5-C6-O6
3	O	20	BMA	O5-C5-C6-O6
3	R	20	BMA	O5-C5-C6-O6
3	U	20	BMA	O5-C5-C6-O6
3	X	20	BMA	O5-C5-C6-O6
3	a	20	BMA	O5-C5-C6-O6
3	d	20	BMA	O5-C5-C6-O6
3	g	20	BMA	O5-C5-C6-O6
3	j	20	BMA	O5-C5-C6-O6
3	m	20	BMA	O5-C5-C6-O6
3	s	20	BMA	O5-C5-C6-O6
3	v	20	BMA	O5-C5-C6-O6
3	y	20	BMA	O5-C5-C6-O6
3	1	20	BMA	O5-C5-C6-O6
4	D	1	GAL	C4-C5-C6-O6
4	D	1	GAL	O5-C5-C6-O6

There are no ring outliers.

129 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	e	16	AHR	1	0
3	L	1	FUB	1	0
3	v	16	BMA	1	0
3	a	5	MAN	1	0
3	R	4	NGA	1	0
3	F	16	BMA	1	0
3	j	11	AHR	1	0
3	d	5	MAN	1	0
3	U	16	BMA	1	0
4	J	16	AHR	1	0
4	n	14	MAN	1	0
4	b	14	MAN	3	0
3	s	6	MAN	1	0
4	b	13	MAN	3	0
4	k	1	GAL	1	0
3	O	4	NGA	1	0
3	d	16	BMA	1	0
3	a	16	BMA	1	0
3	v	5	MAN	1	0
3	X	4	NGA	1	0
4	k	5	MAN	1	0
3	y	4	NGA	1	0
3	F	6	MAN	1	0
3	I	11	AHR	1	0
3	L	16	BMA	1	0
3	v	4	NGA	1	0
3	U	5	MAN	1	0
3	R	17	BMA	1	0
4	z	14	MAN	1	0
3	p	5	MAN	1	0
3	s	11	AHR	1	0
2	o	4	GAL	1	0
3	I	17	BMA	1	0
3	O	6	MAN	1	0
3	j	5	MAN	1	0
3	I	4	NGA	1	0
4	k	13	MAN	1	0
3	y	17	BMA	1	0
3	g	6	MAN	1	0
3	s	4	NGA	1	0
3	l	5	MAN	1	0
3	p	11	AHR	1	0
4	t	14	MAN	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	h	16	AHR	1	0
4	n	13	MAN	1	0
3	l	1	FUB	1	0
3	d	17	BMA	1	0
2	T	4	GAL	1	0
3	a	4	NGA	1	0
4	S	5	MAN	1	0
3	I	6	MAN	1	0
4	k	14	MAN	1	0
3	d	4	NGA	1	0
4	V	5	MAN	1	0
3	a	17	BMA	1	0
3	R	6	MAN	1	0
4	w	5	MAN	1	0
3	g	16	BMA	1	0
3	X	5	MAN	1	0
3	m	4	NGA	1	0
3	U	4	NGA	1	0
4	J	5	MAN	1	0
3	v	17	BMA	1	0
3	L	5	MAN	1	0
3	X	17	BMA	1	0
3	y	5	MAN	1	0
4	G	16	AHR	1	0
2	o	6	FUB	1	0
3	d	6	MAN	1	0
4	z	5	MAN	1	0
3	g	5	MAN	1	0
3	y	16	BMA	1	0
3	p	4	NGA	1	0
3	j	24	AHR	1	0
3	p	16	BMA	1	0
3	y	6	MAN	1	0
3	p	6	MAN	1	0
3	j	17	BMA	1	0
4	z	13	MAN	1	0
3	s	16	BMA	1	0
3	O	5	MAN	1	0
3	O	16	BMA	1	0
3	m	17	BMA	1	0
4	b	5	MAN	1	0
3	l	4	NGA	1	0

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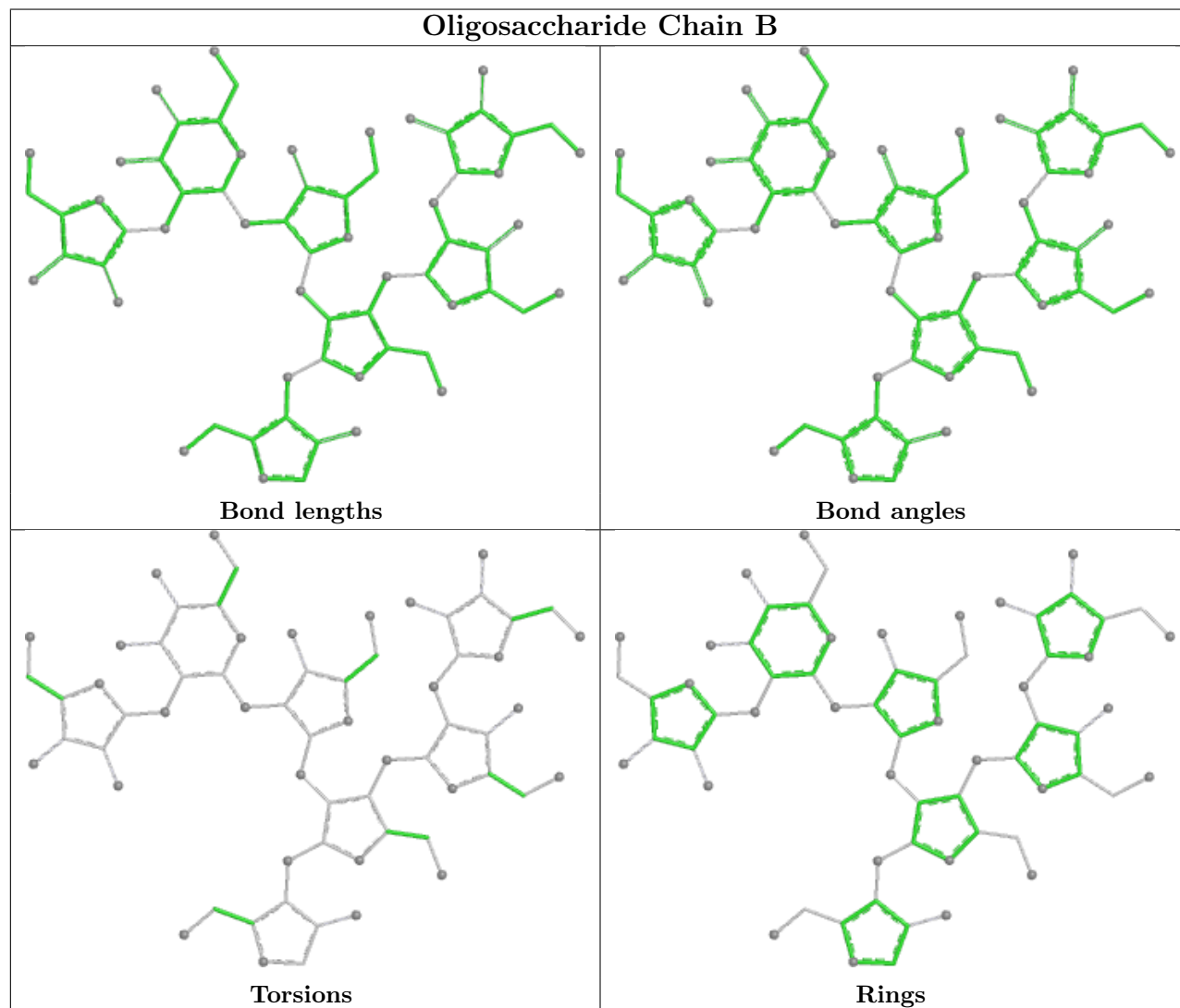
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	j	6	MAN	1	0
3	a	6	MAN	1	0
3	m	5	MAN	1	0
3	m	16	BMA	1	0
3	F	5	MAN	1	0
3	l	17	BMA	1	0
3	a	1	FUB	1	0
3	U	6	MAN	1	0
3	U	17	BMA	1	0
3	C	5	MAN	1	0
2	u	4	GAL	1	0
2	c	4	GAL	1	0
3	L	4	NGA	1	0
4	Y	16	AHR	1	0
4	n	5	MAN	1	0
4	M	5	MAN	2	0
4	e	5	MAN	1	0
3	L	17	BMA	2	0
3	l	6	MAN	1	0
3	R	5	MAN	1	0
3	R	16	BMA	1	0
3	X	16	BMA	1	0
3	m	6	MAN	1	0
3	v	6	MAN	1	0
3	F	4	NGA	1	0
2	x	4	GAL	1	0
3	a	11	AHR	1	0
3	d	1	FUB	1	0
4	Y	5	MAN	1	0
4	2	5	MAN	1	0
3	I	16	BMA	1	0
3	g	4	NGA	1	0
3	s	17	BMA	2	0
4	t	13	MAN	2	0
3	I	5	MAN	1	0
3	C	8	GAL	1	0
3	C	9	MAN	1	0
3	L	6	MAN	1	0
3	s	5	MAN	1	0
3	l	16	BMA	1	0
4	t	5	MAN	2	0
3	C	1	FUB	1	0

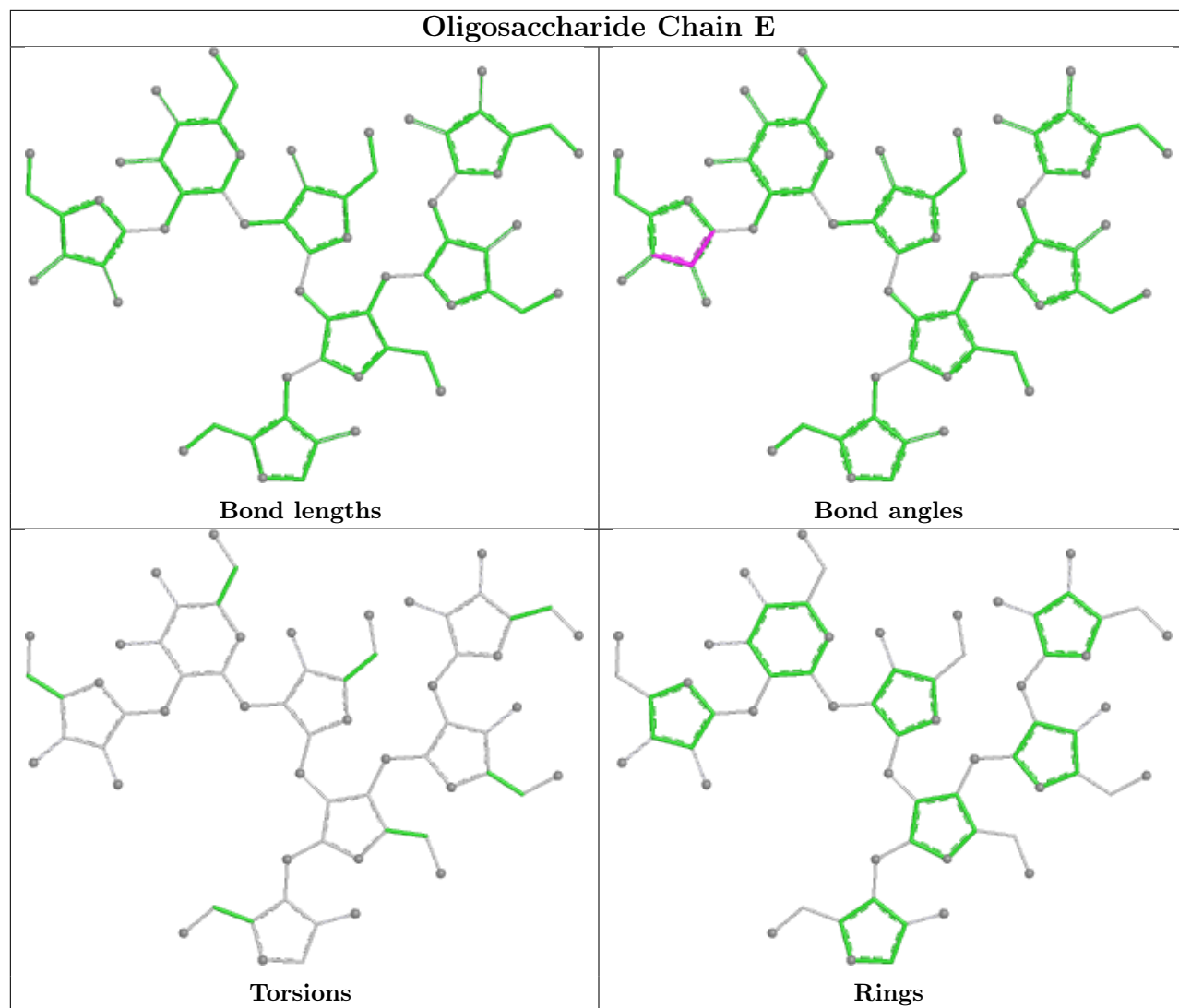
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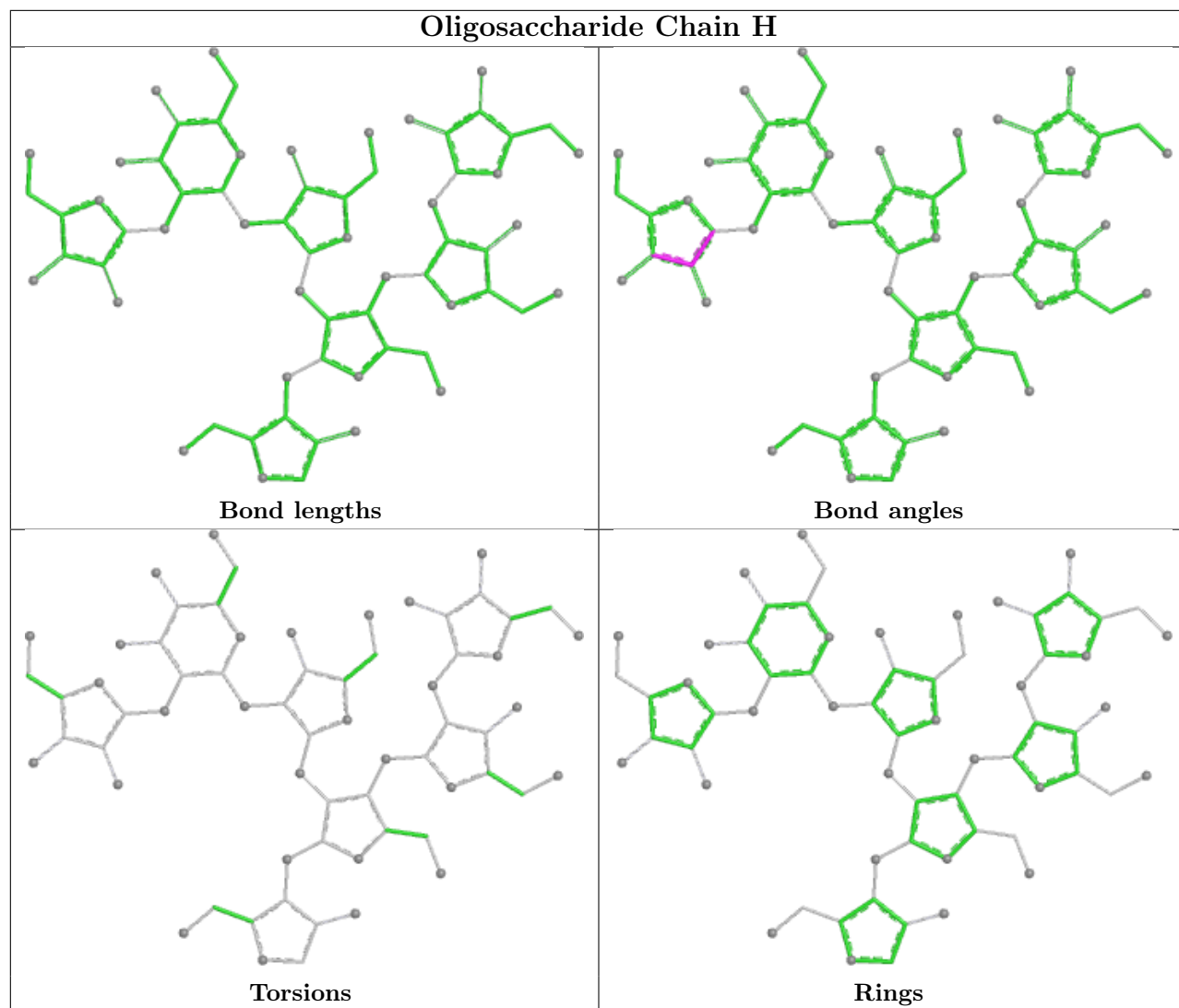
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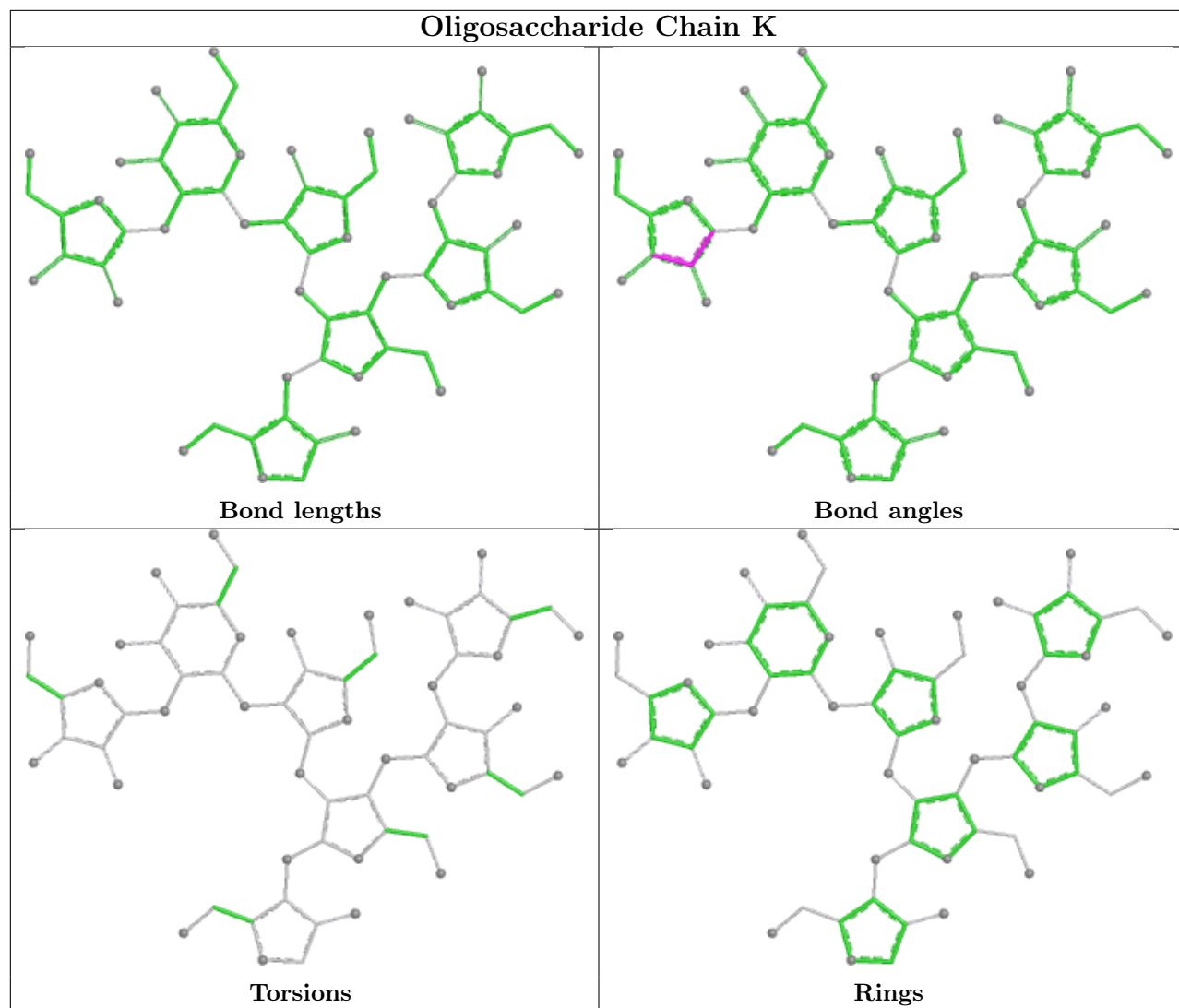
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	25	FUB	5	0
3	X	6	MAN	1	0

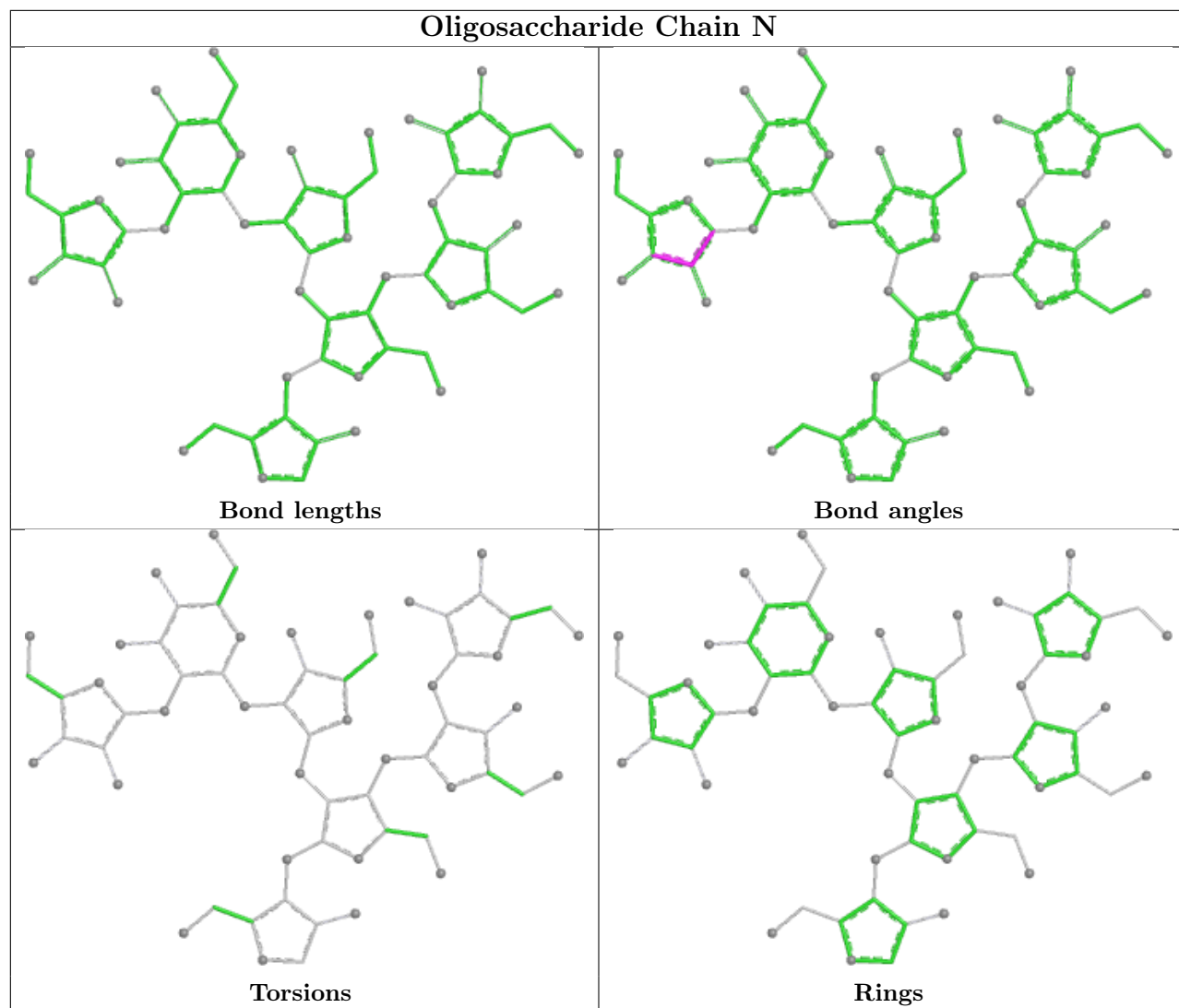
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

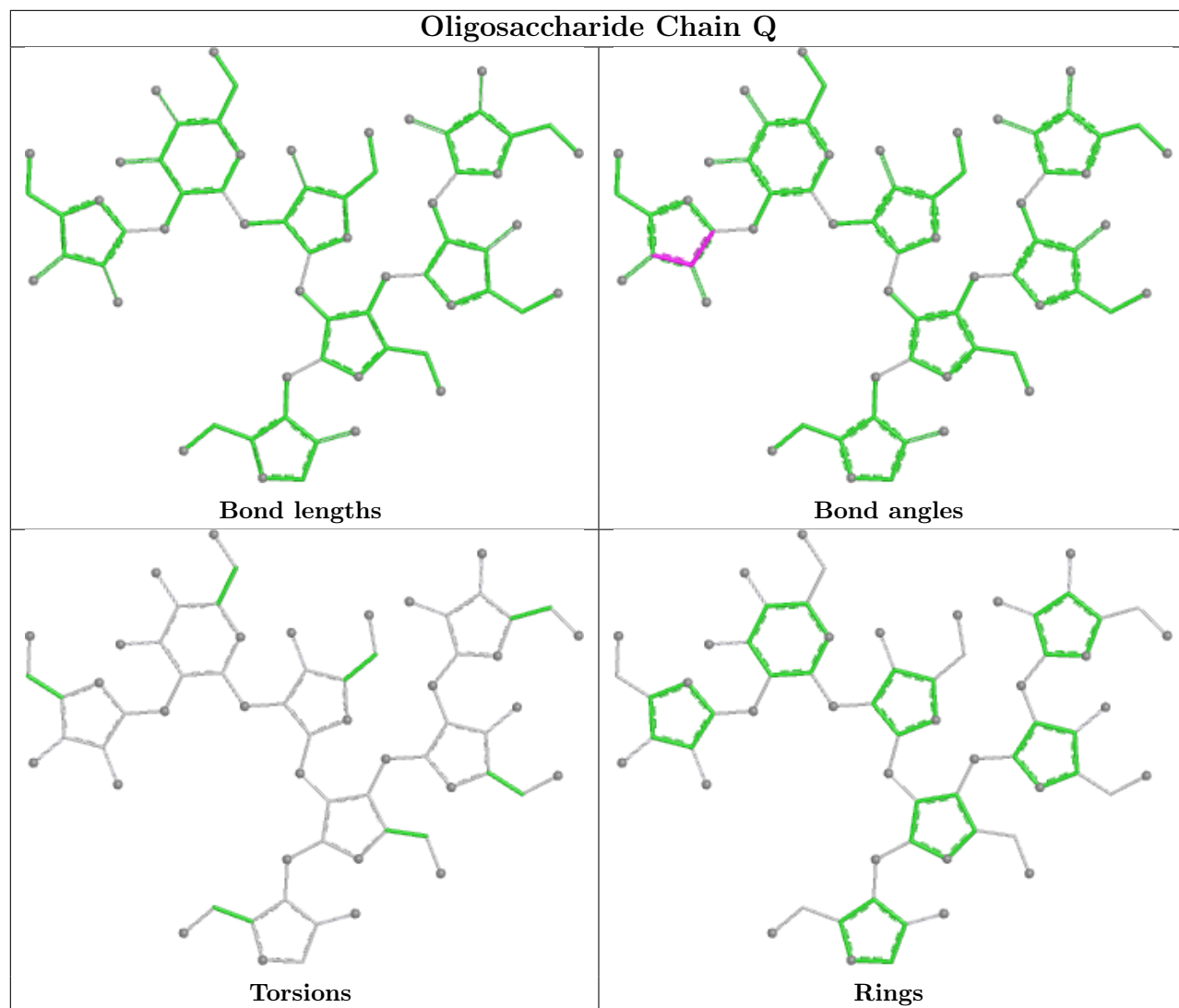


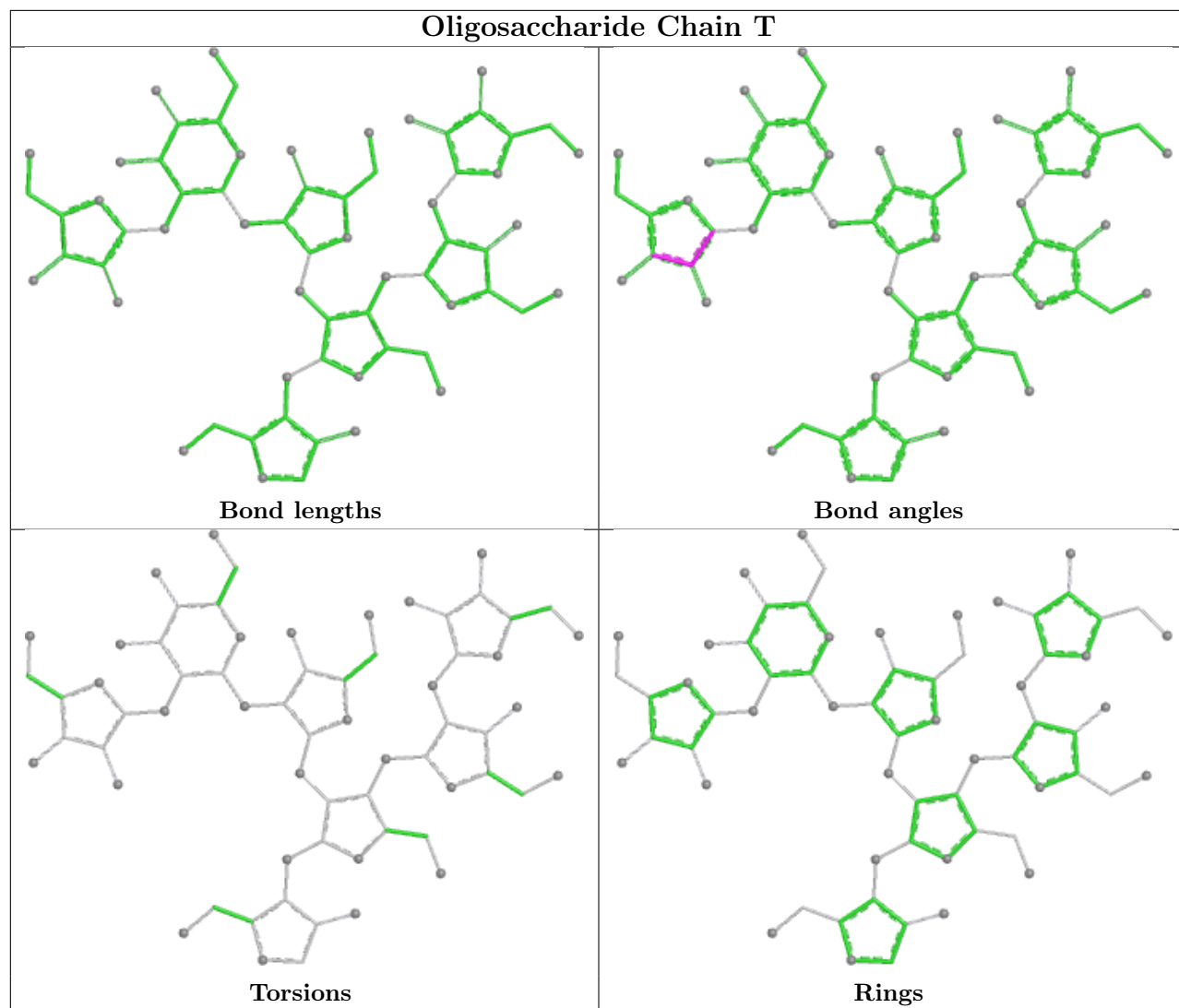


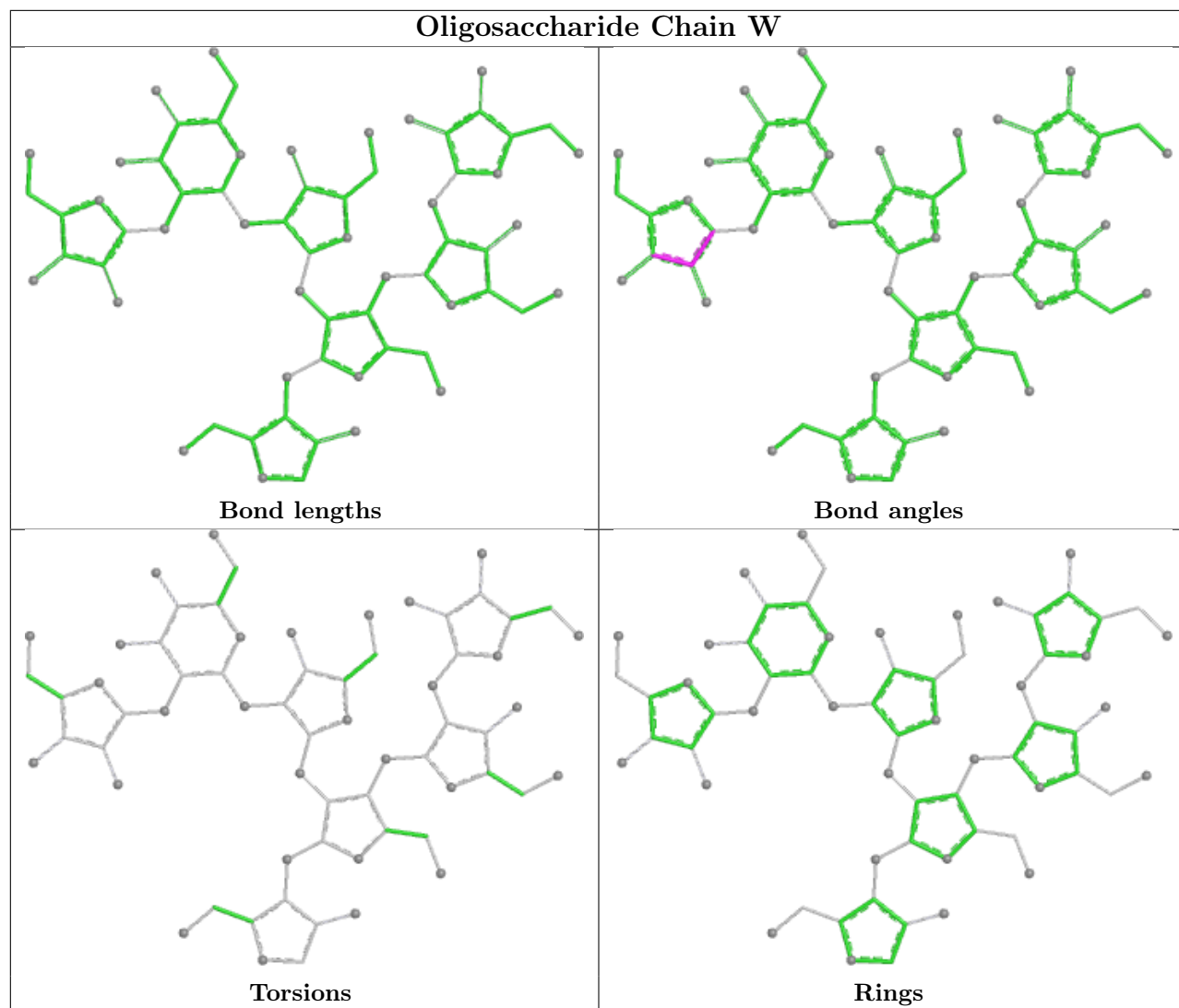


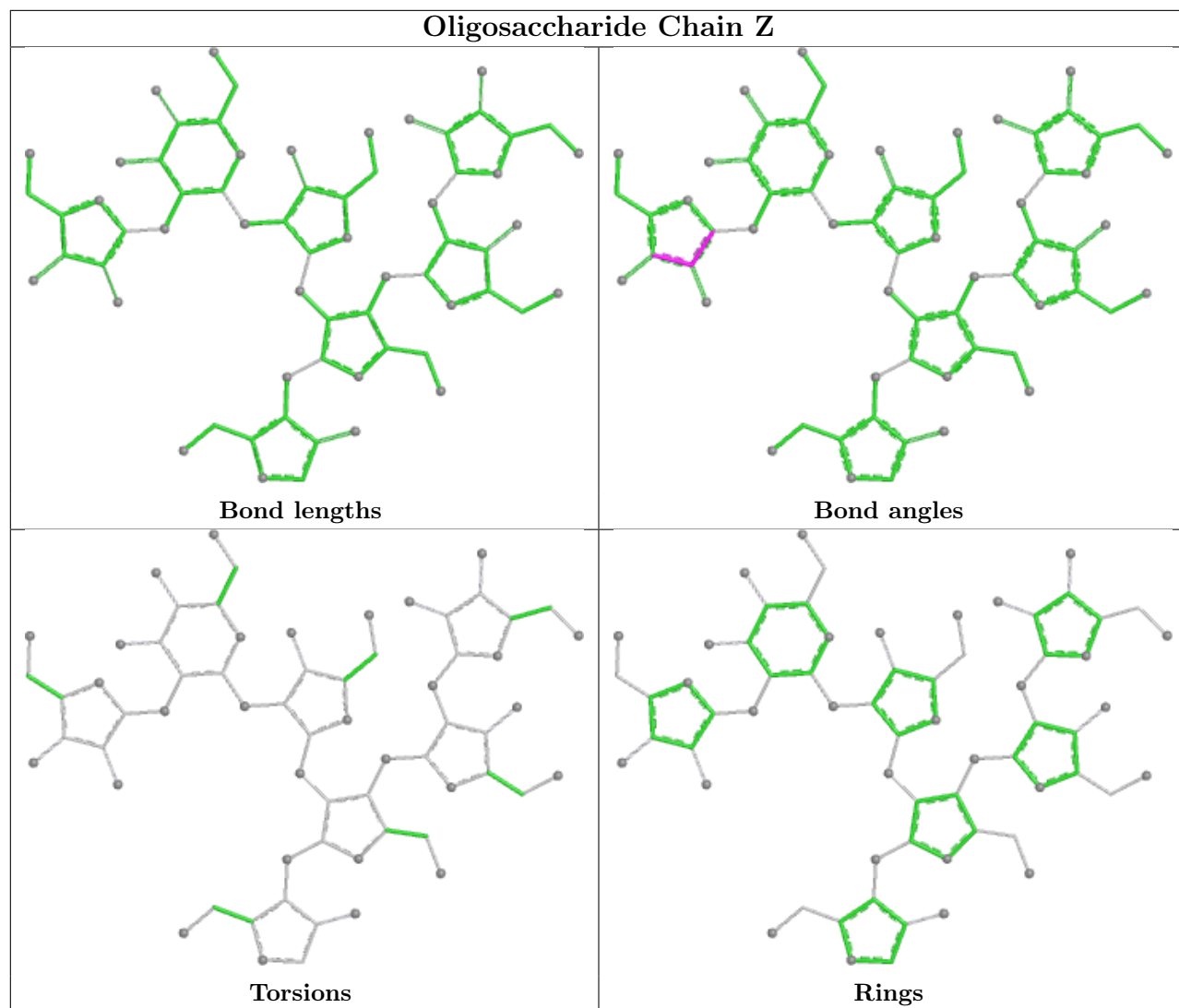


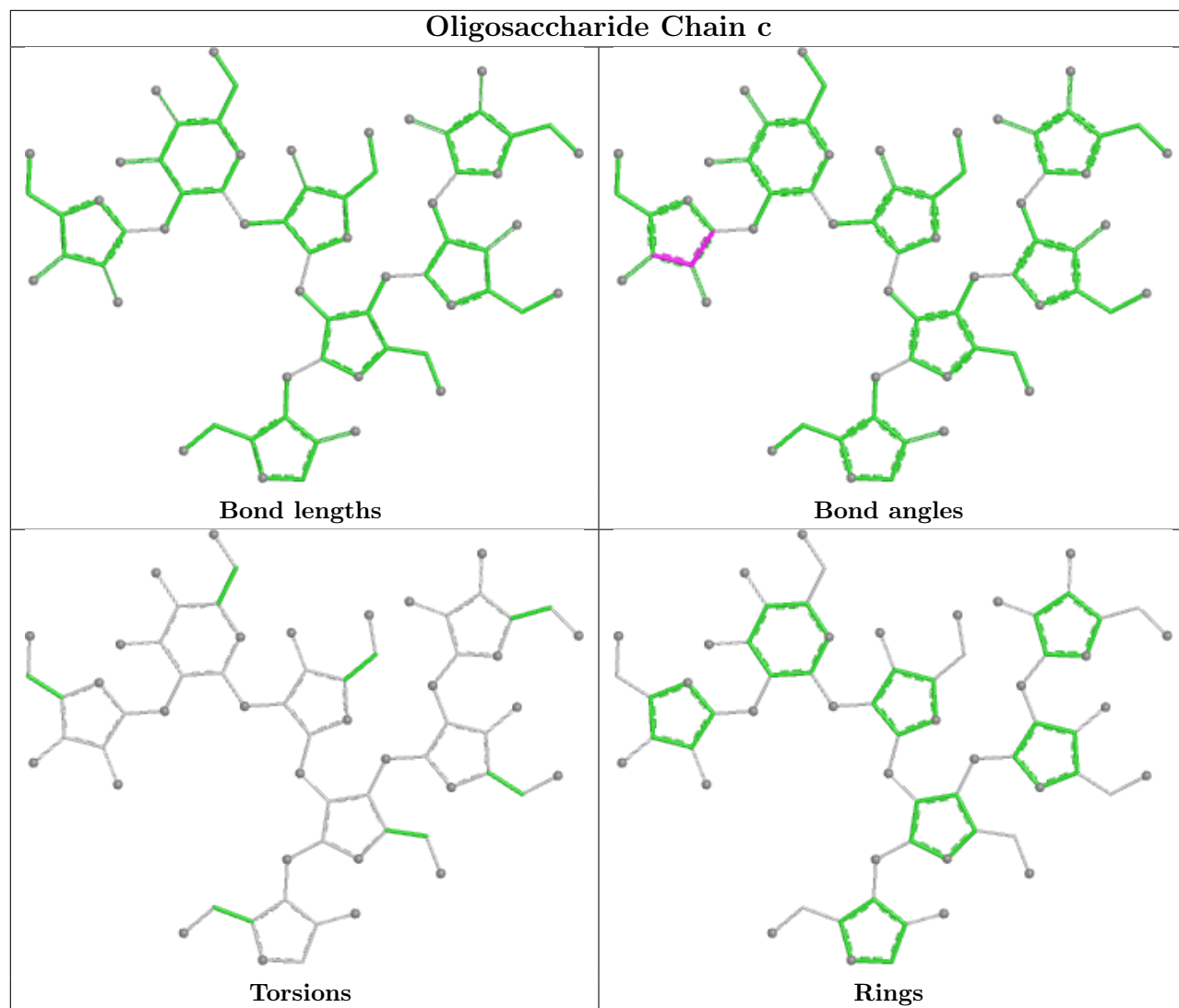


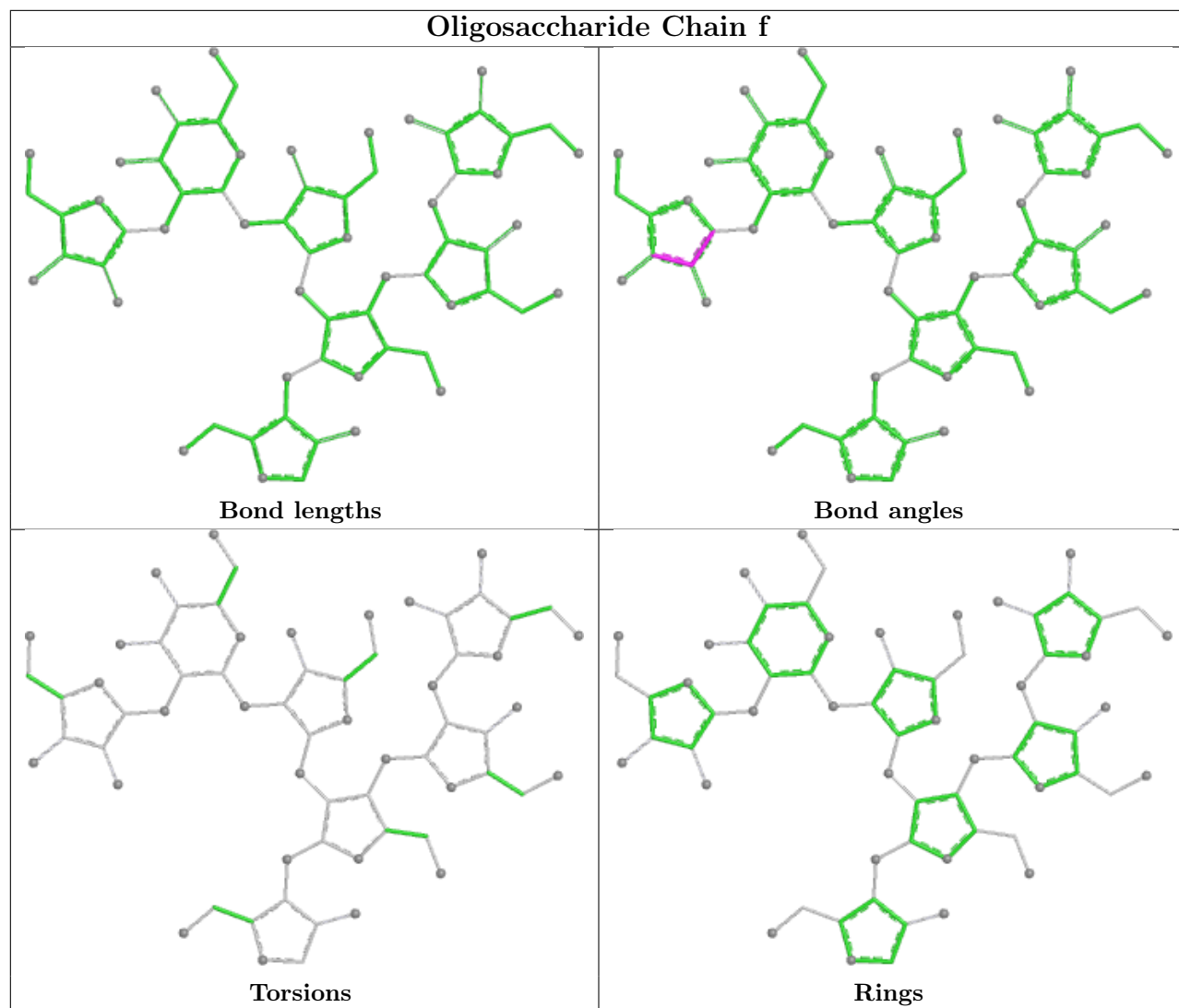


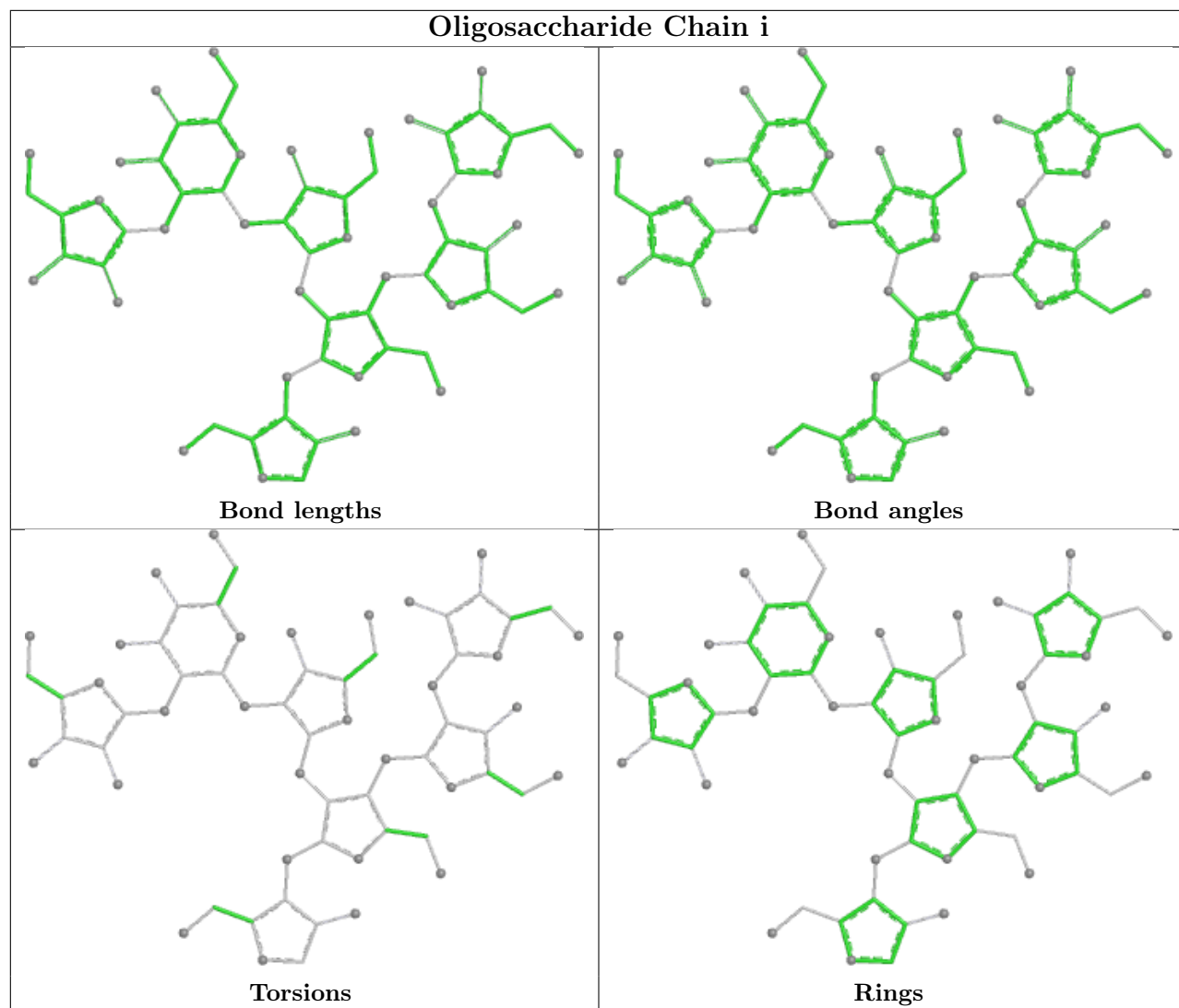


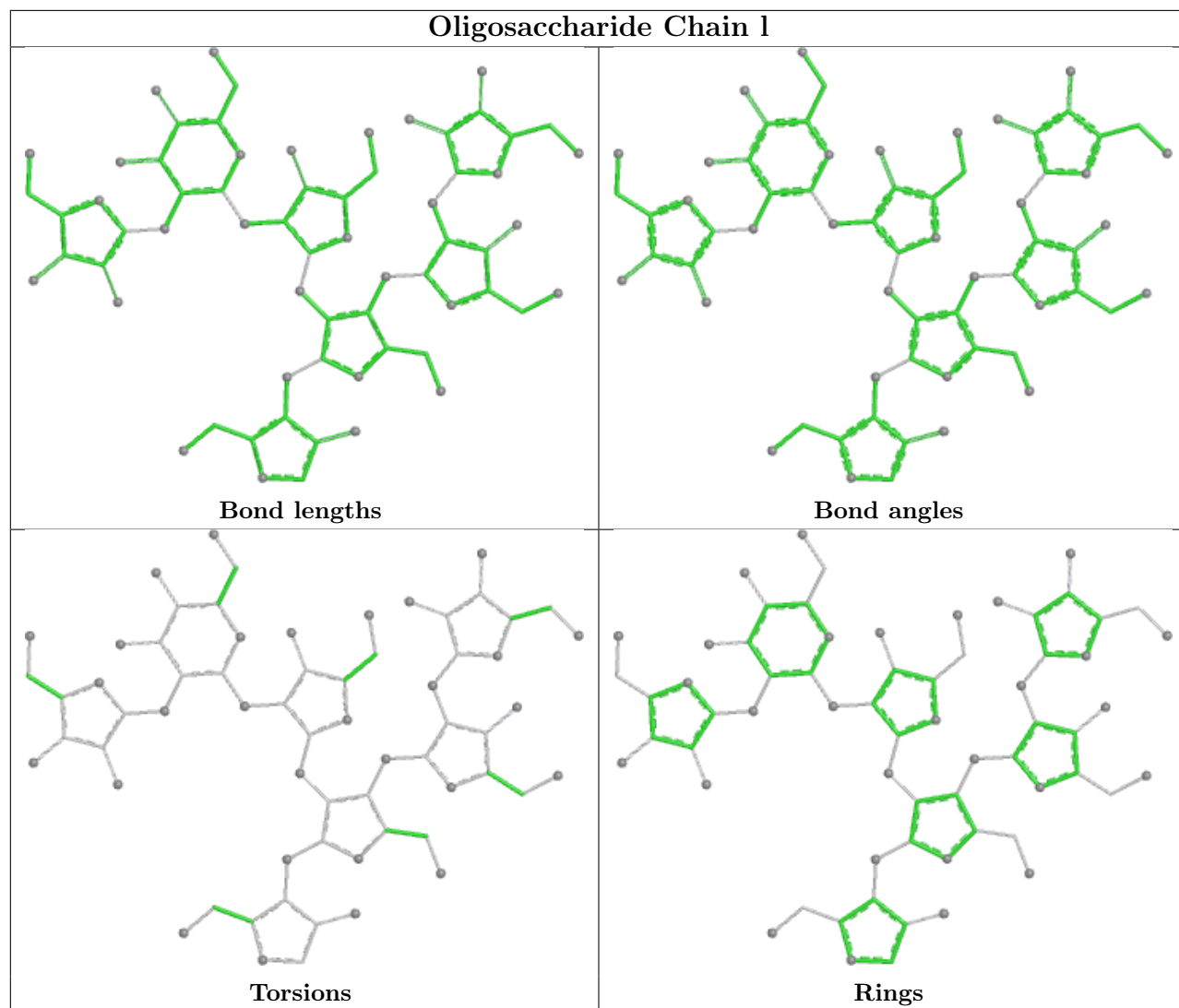


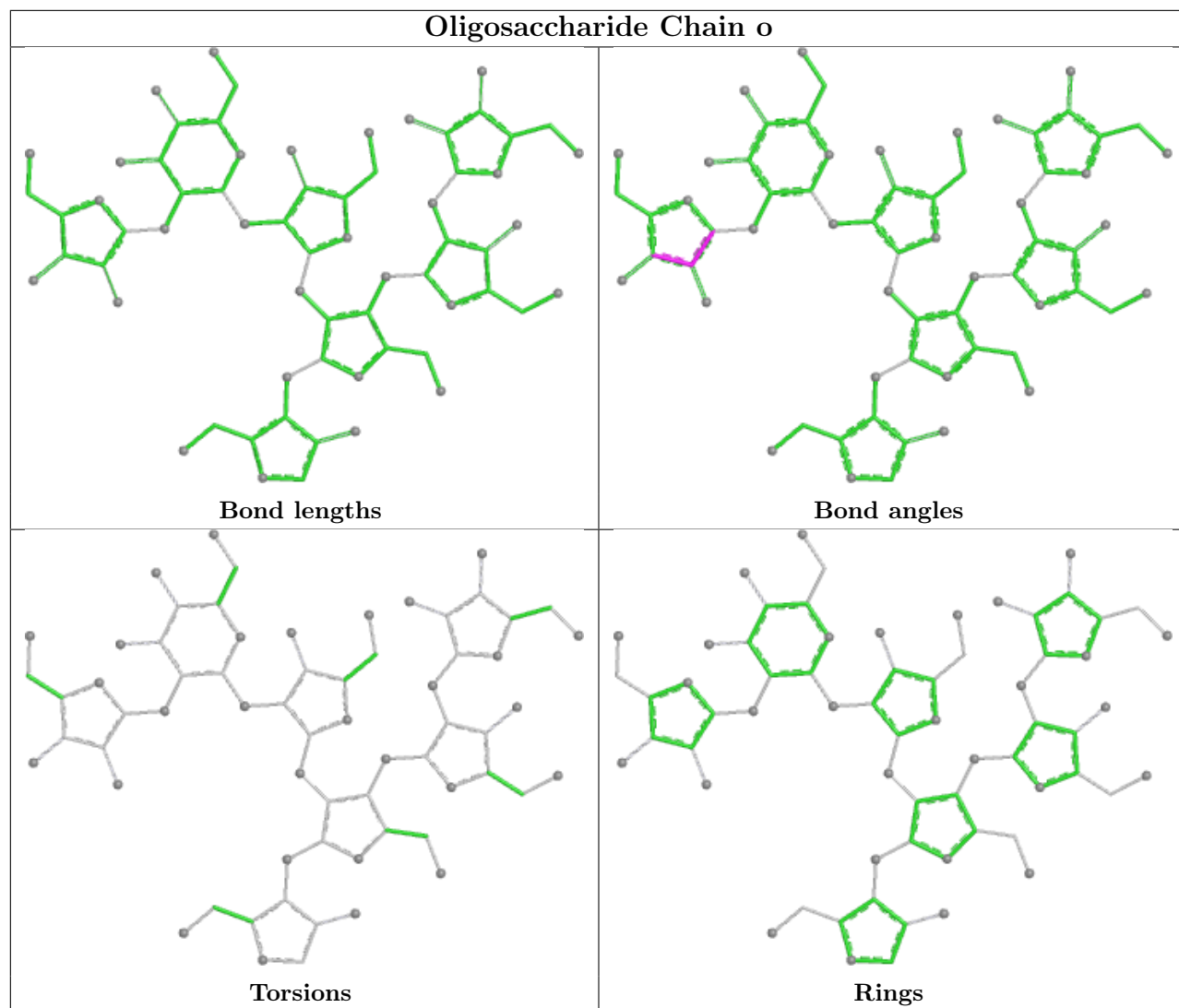


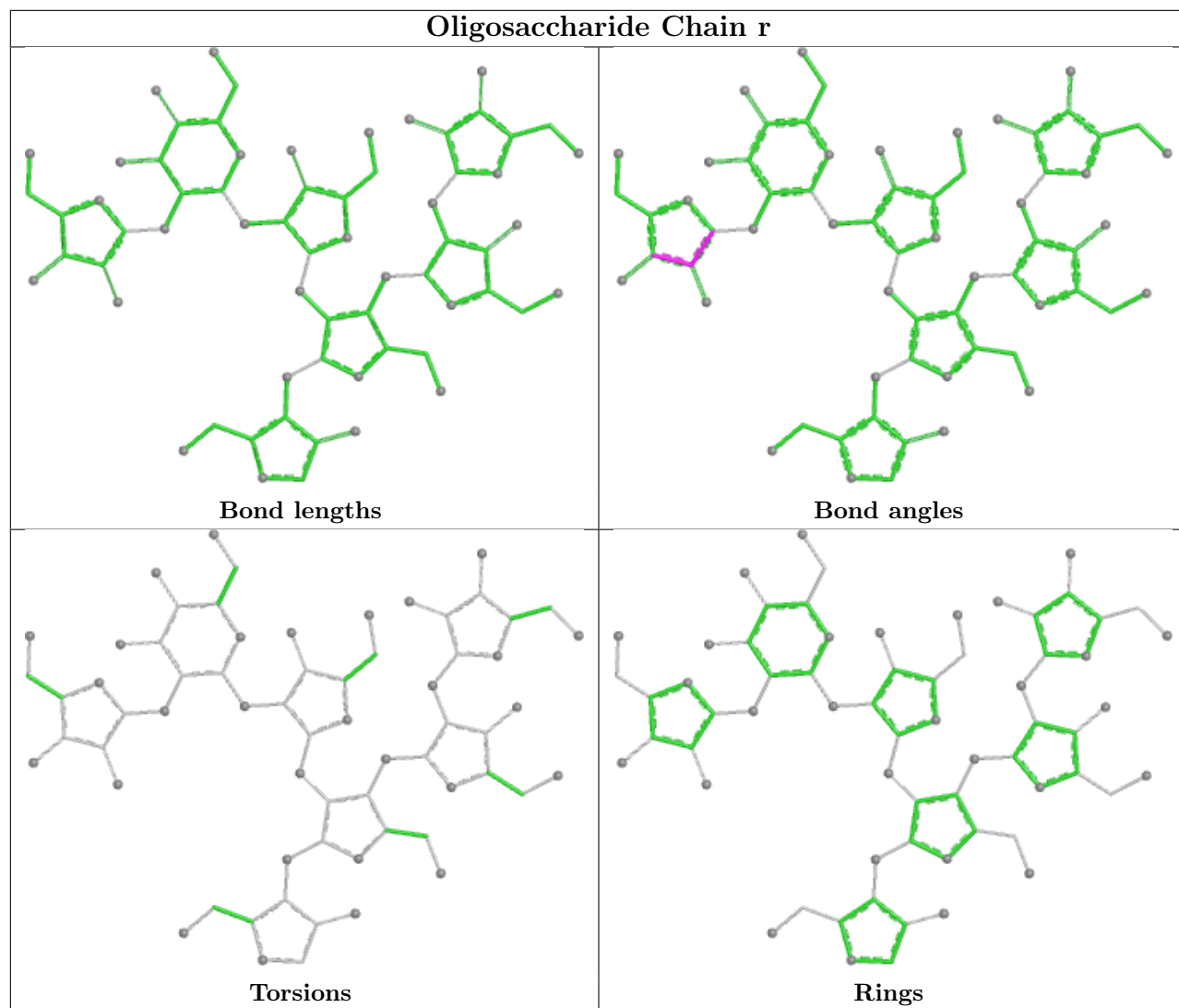


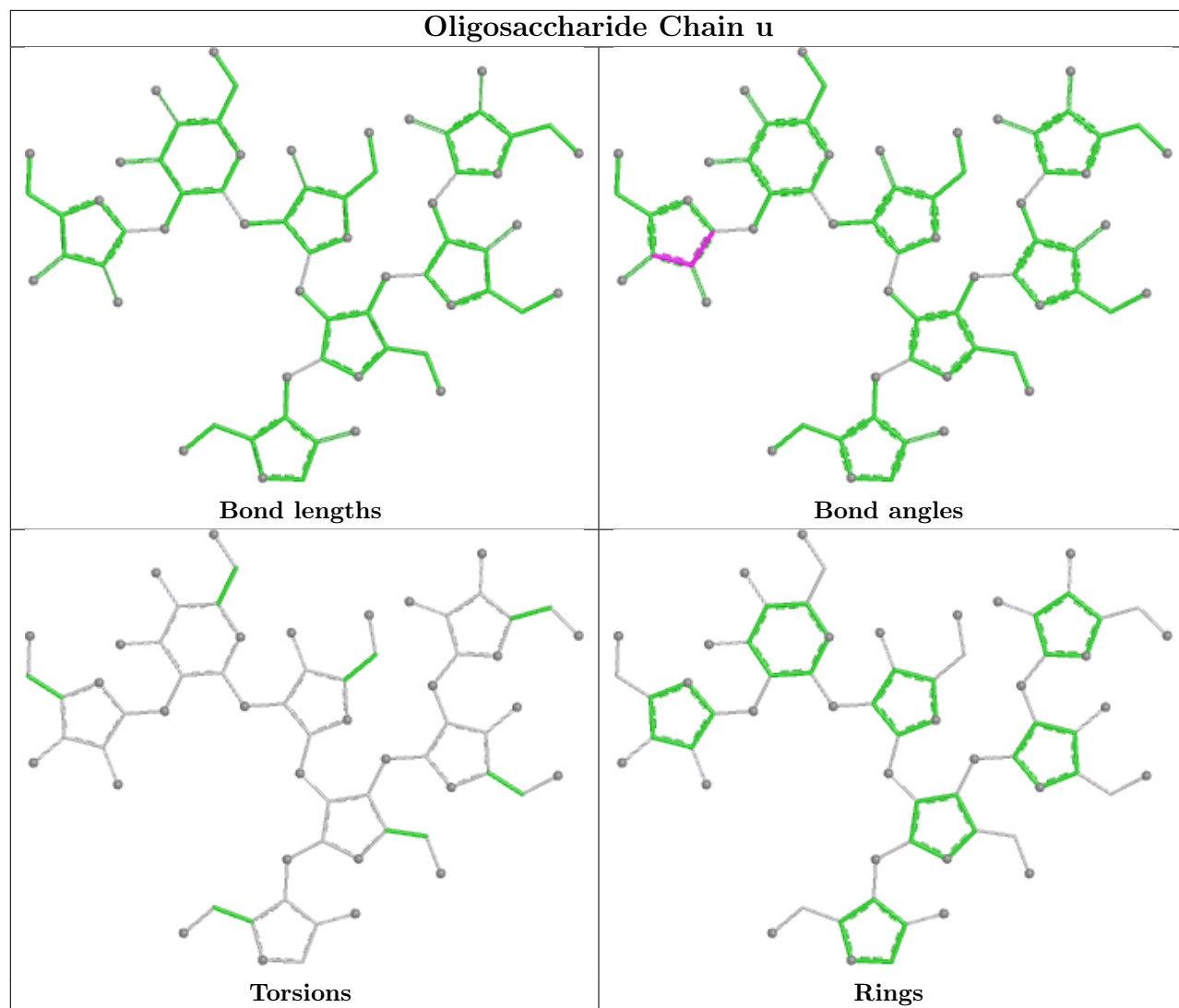


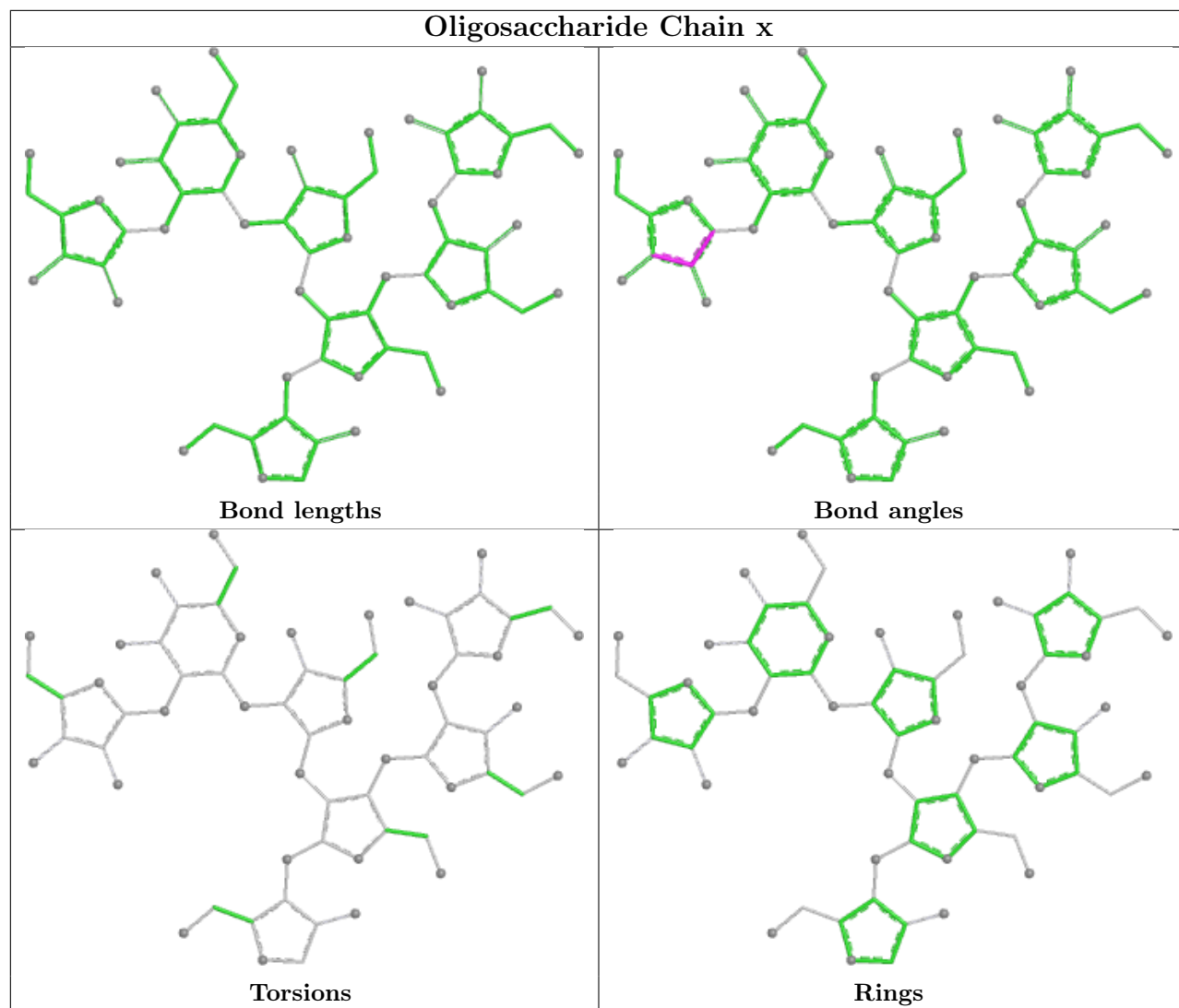


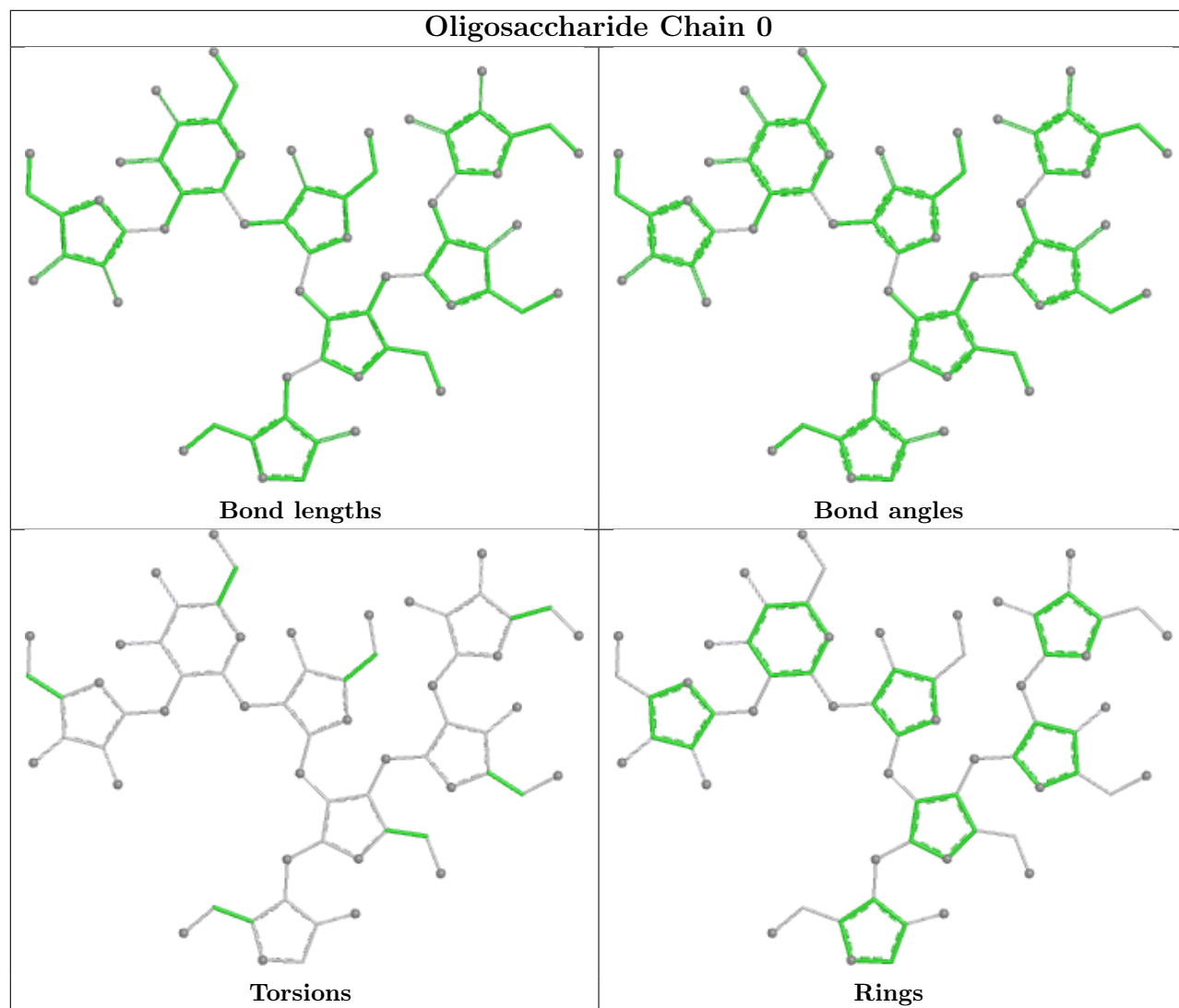


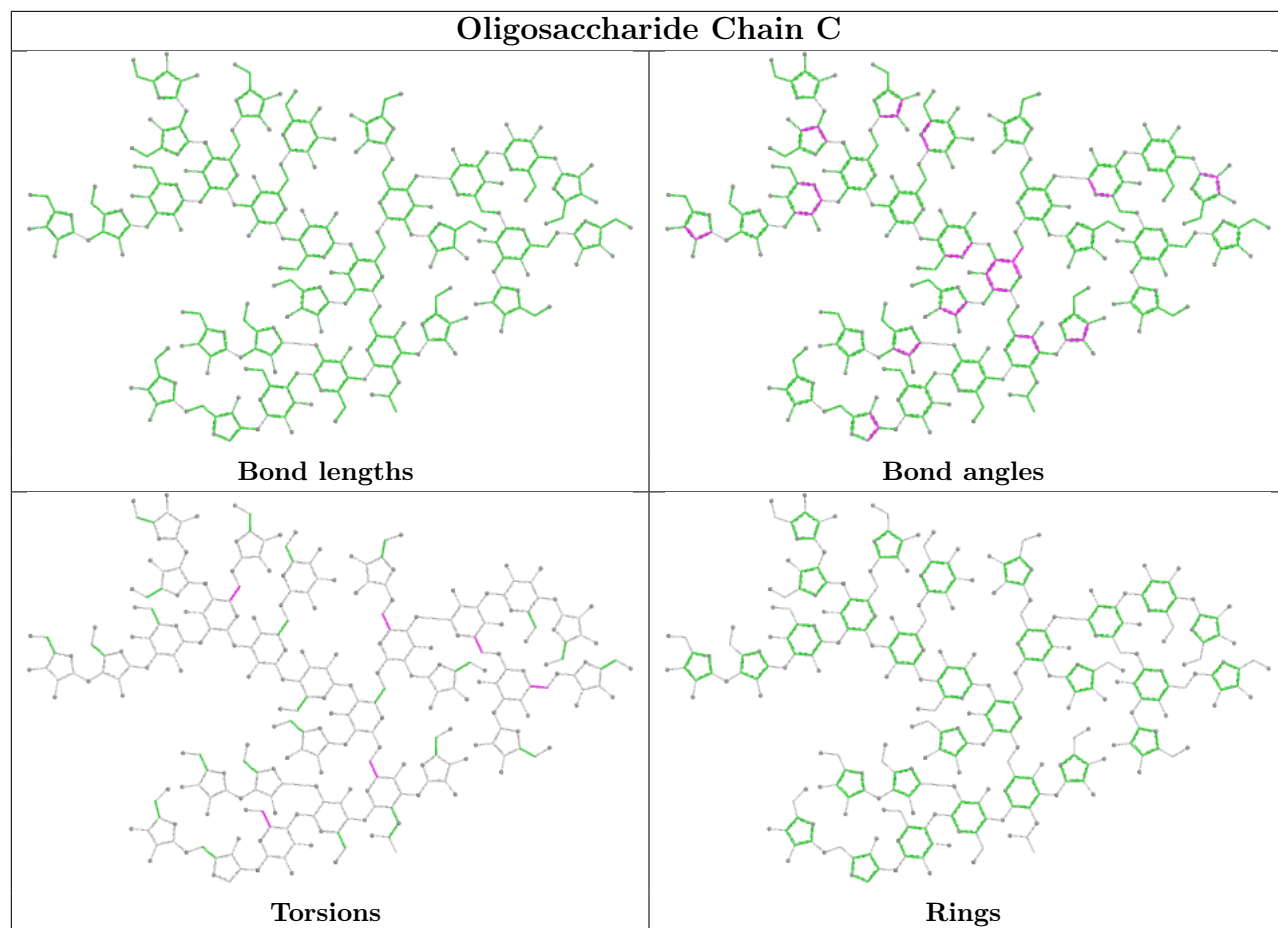


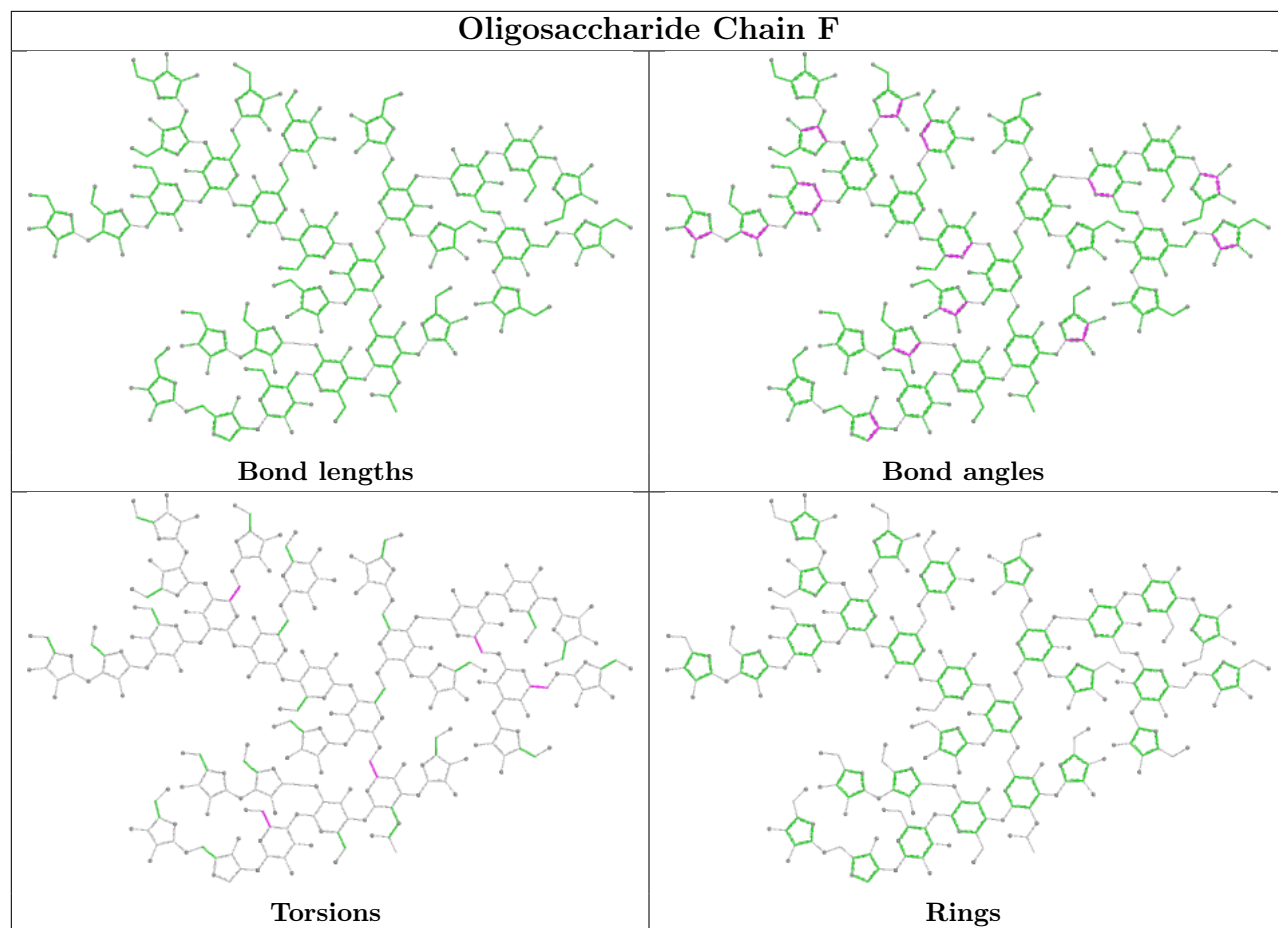


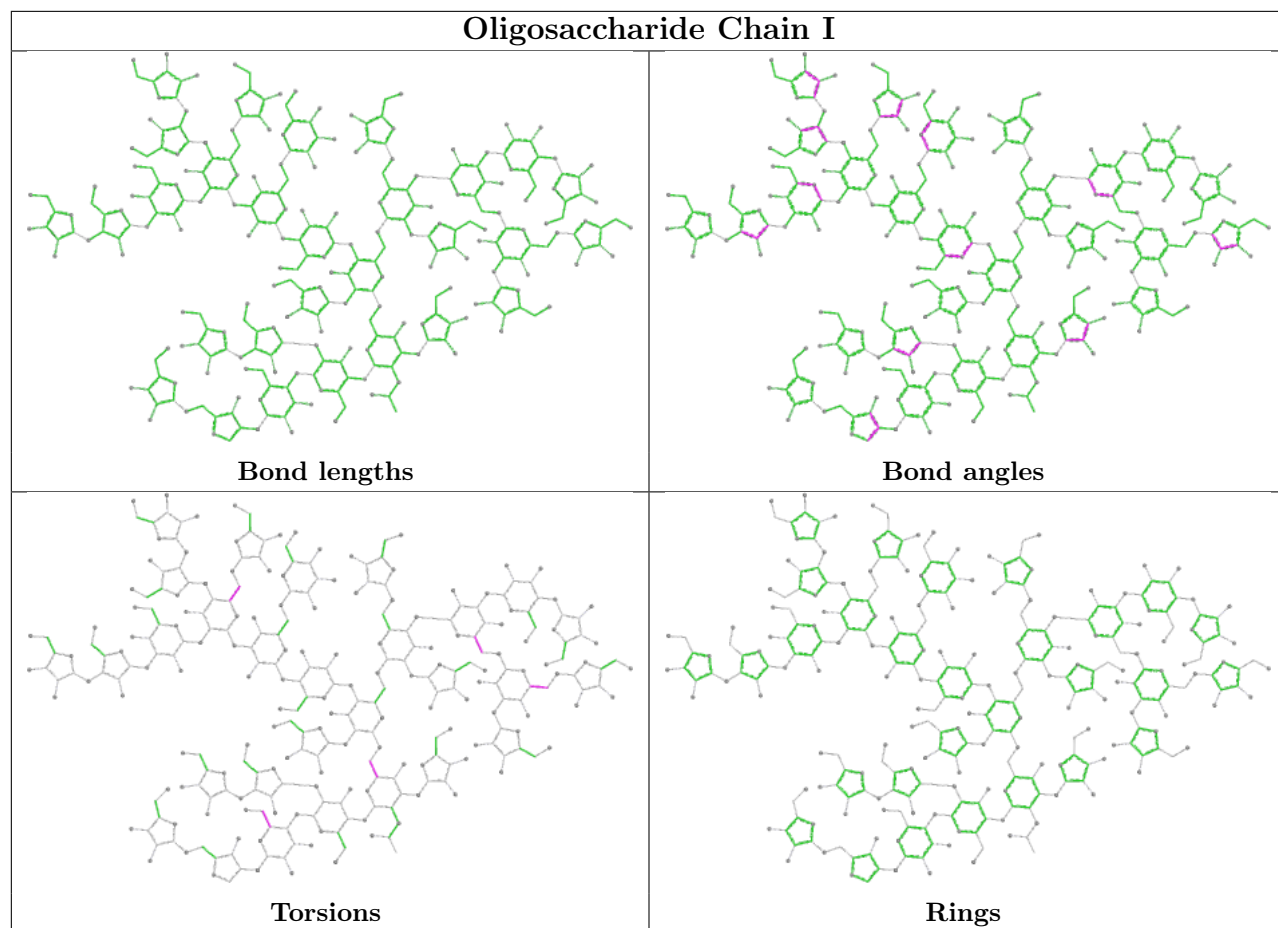


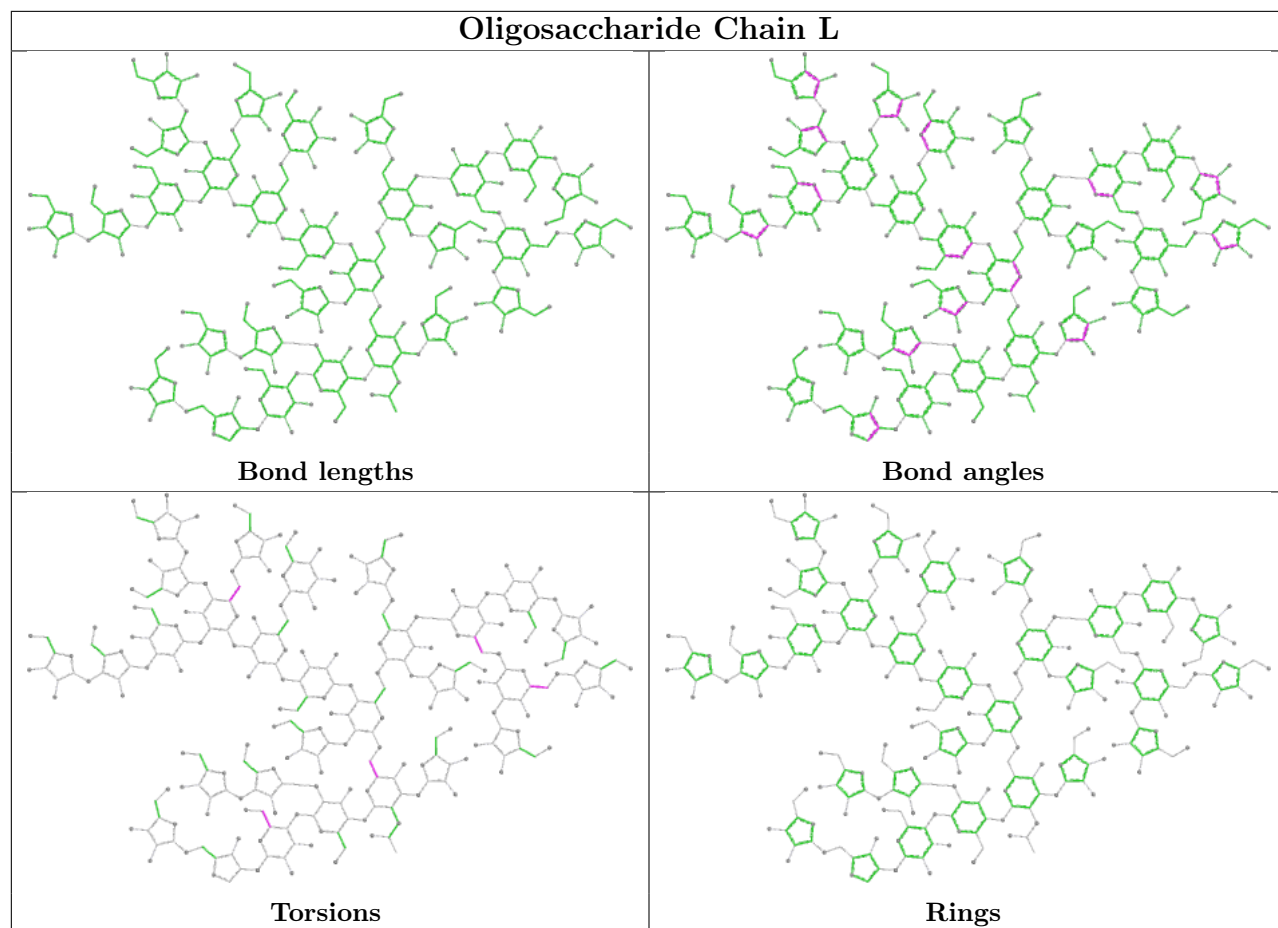


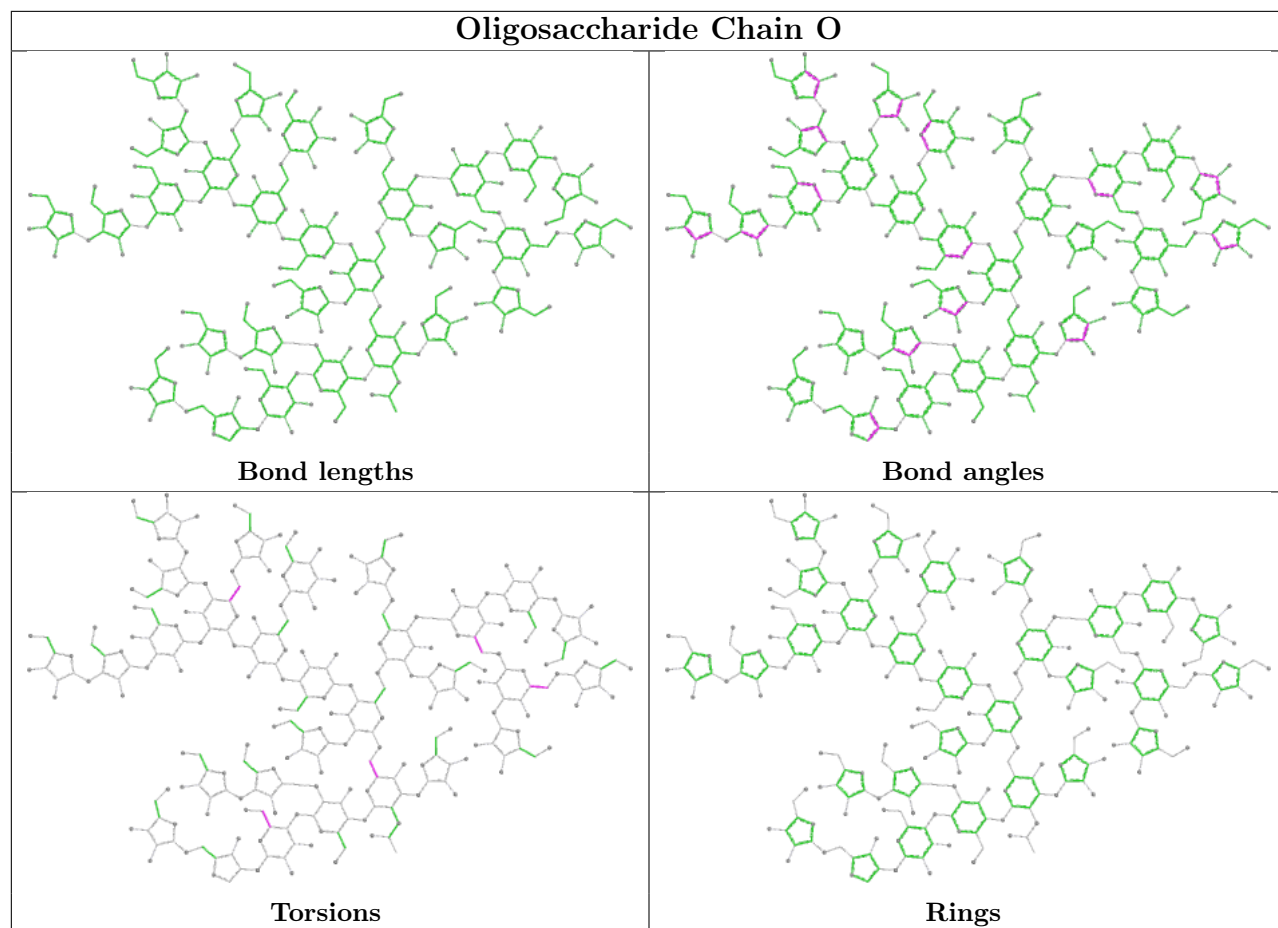


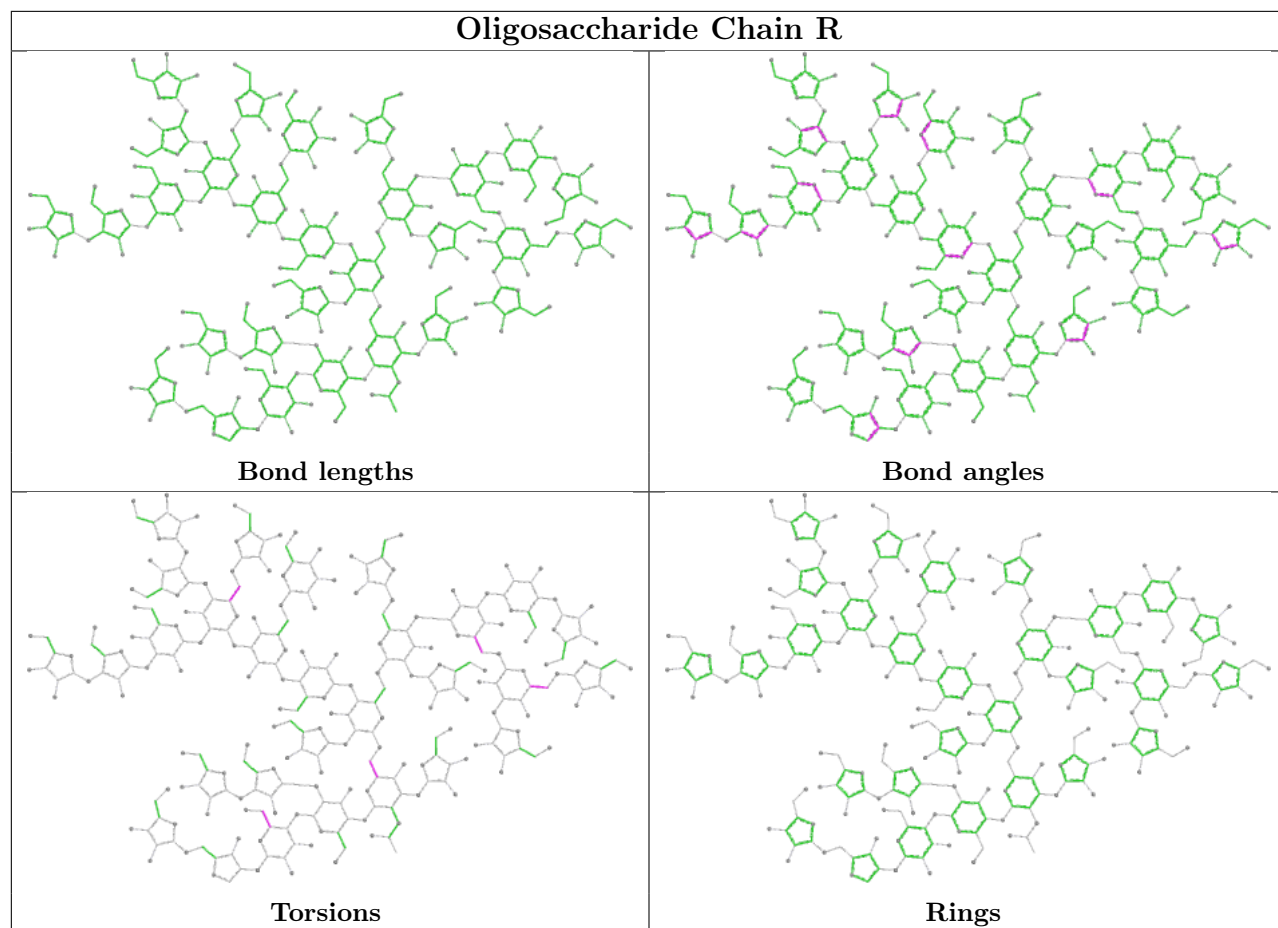


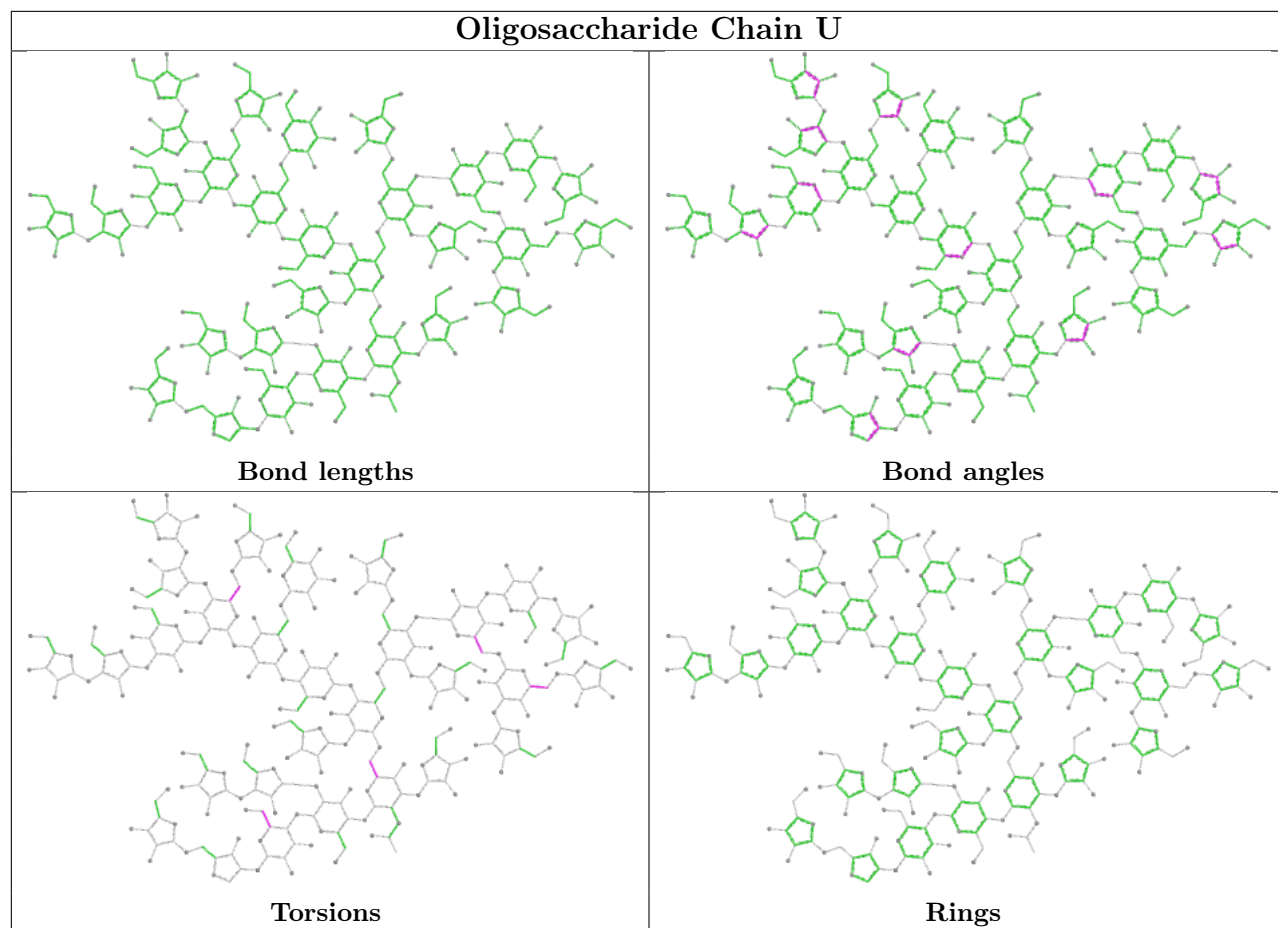


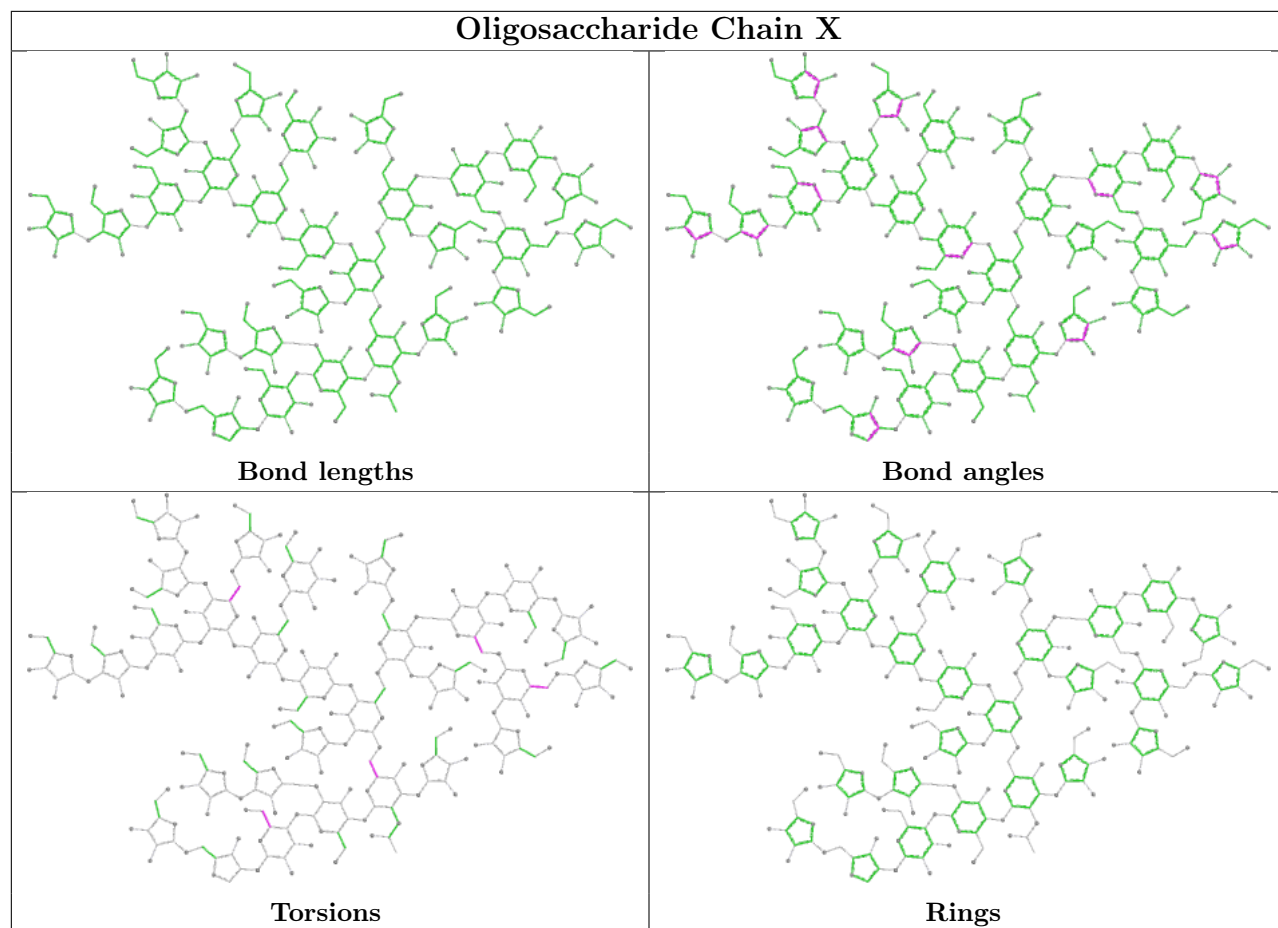


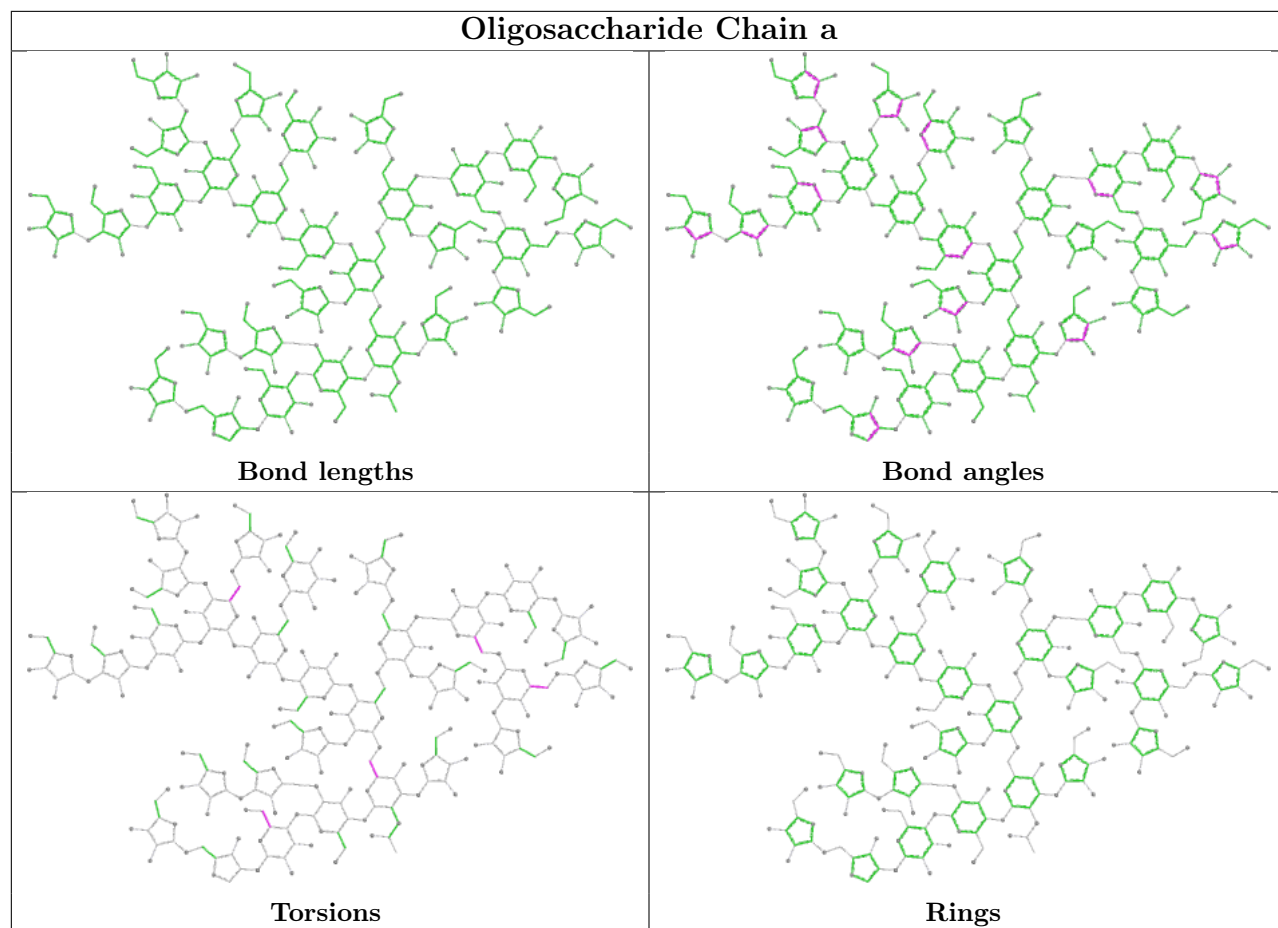


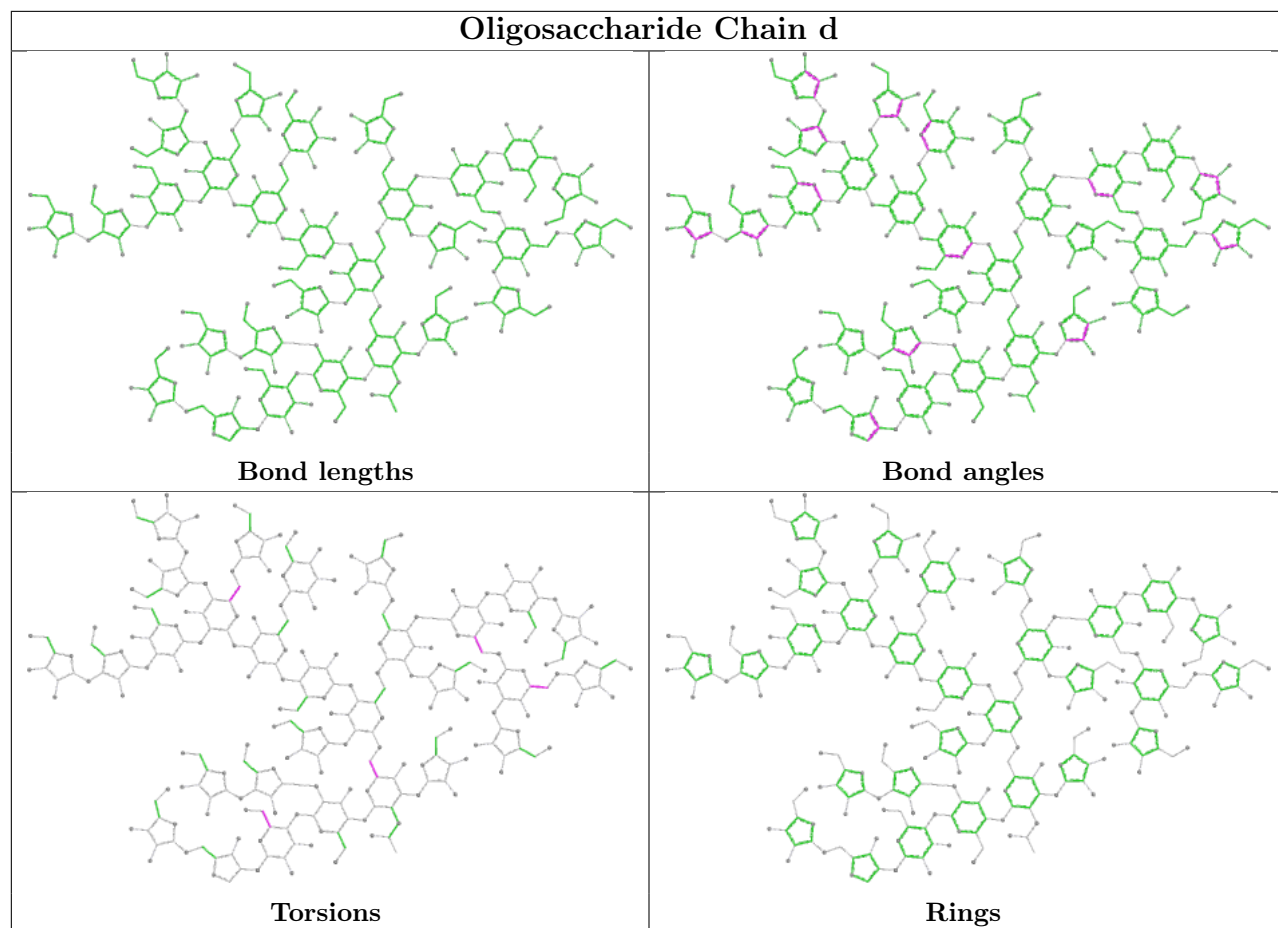


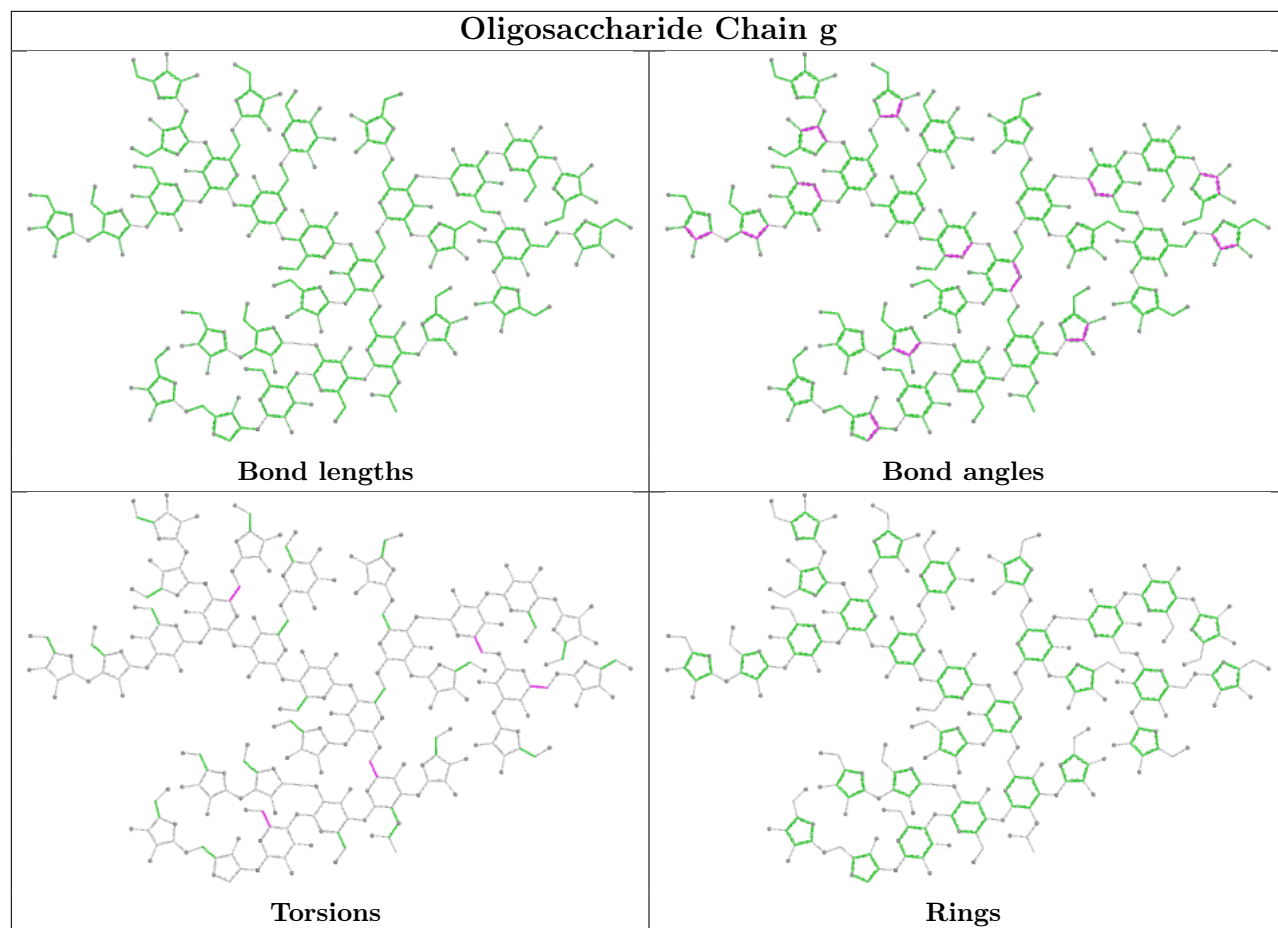


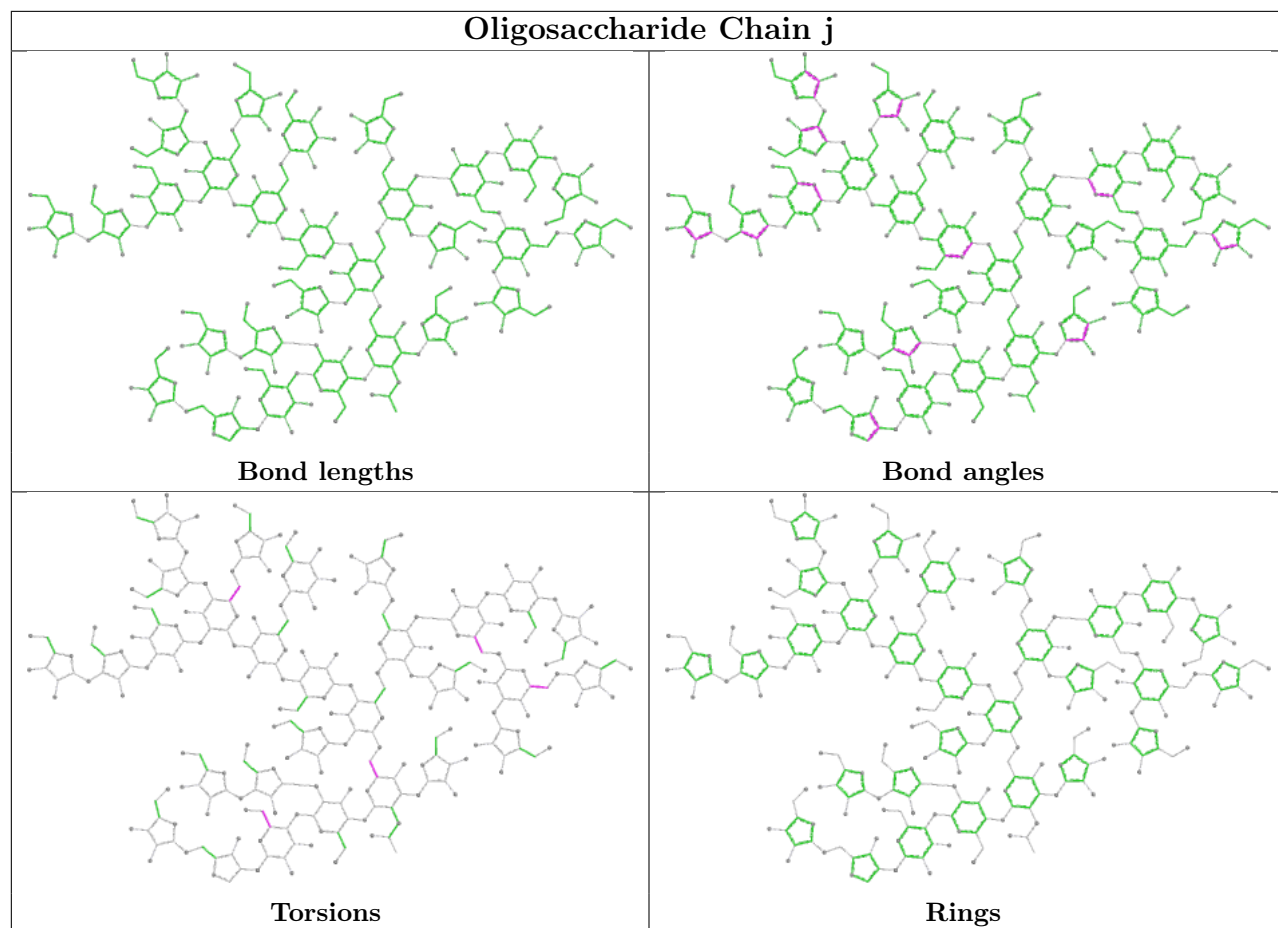


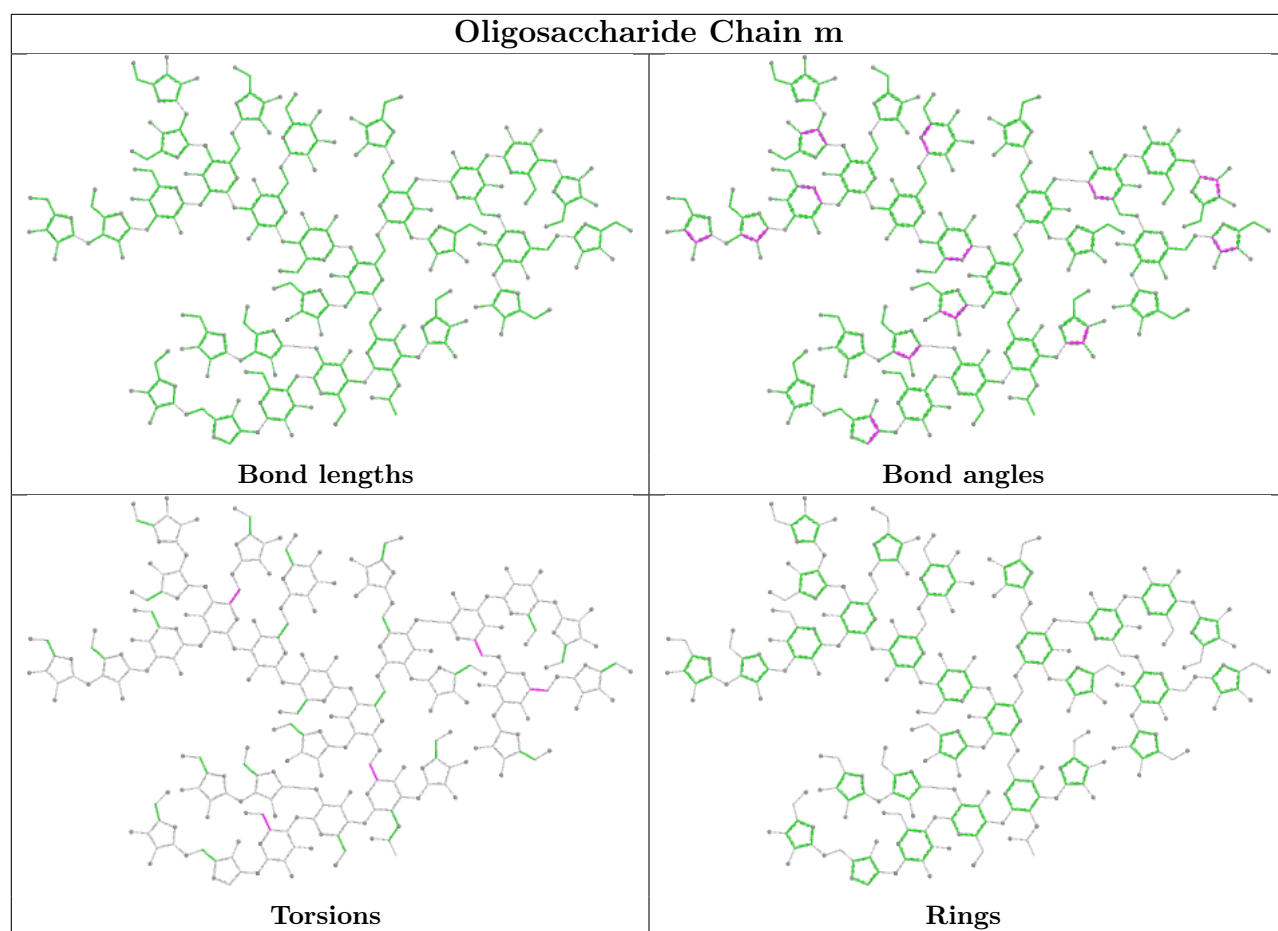


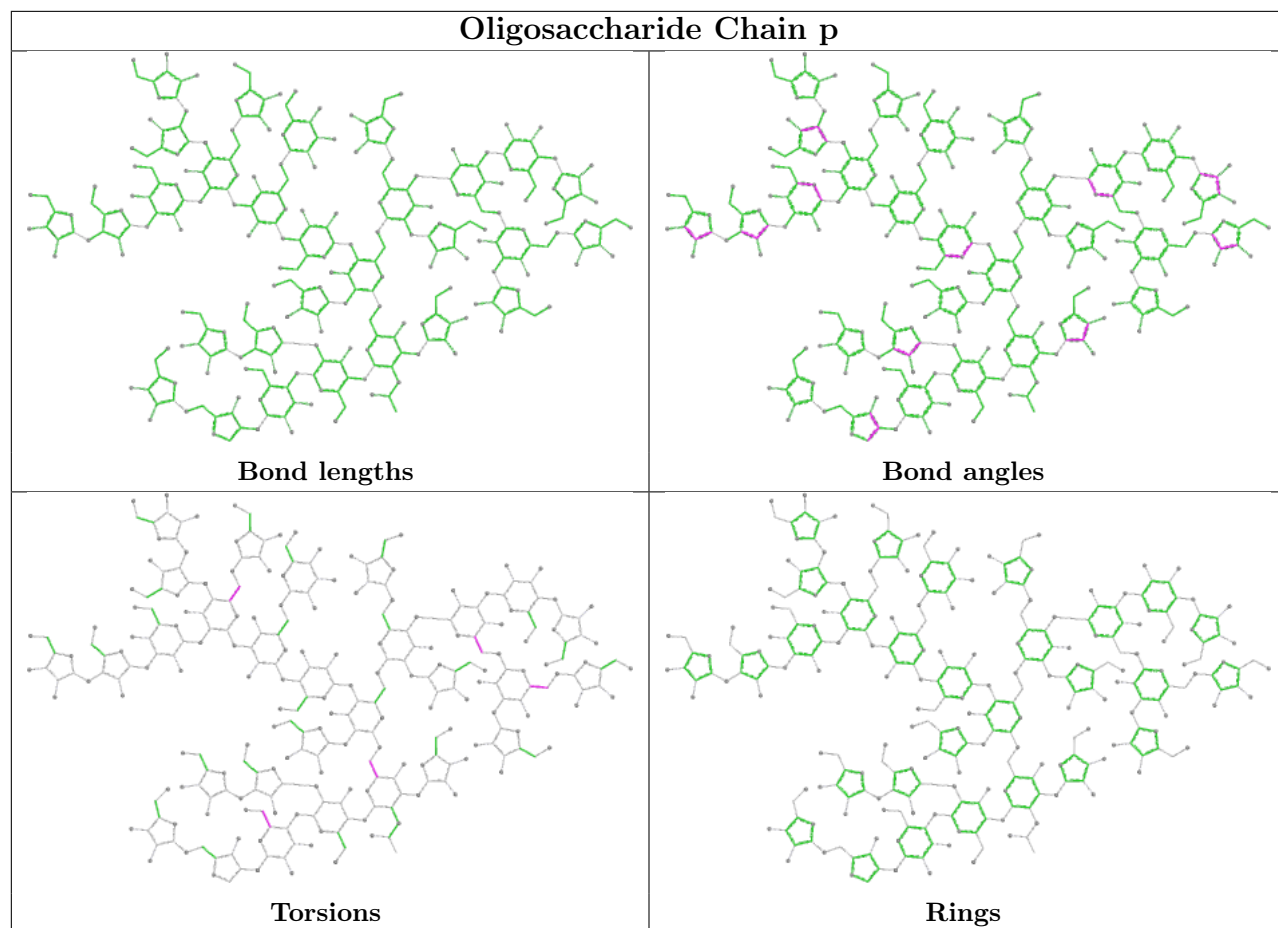


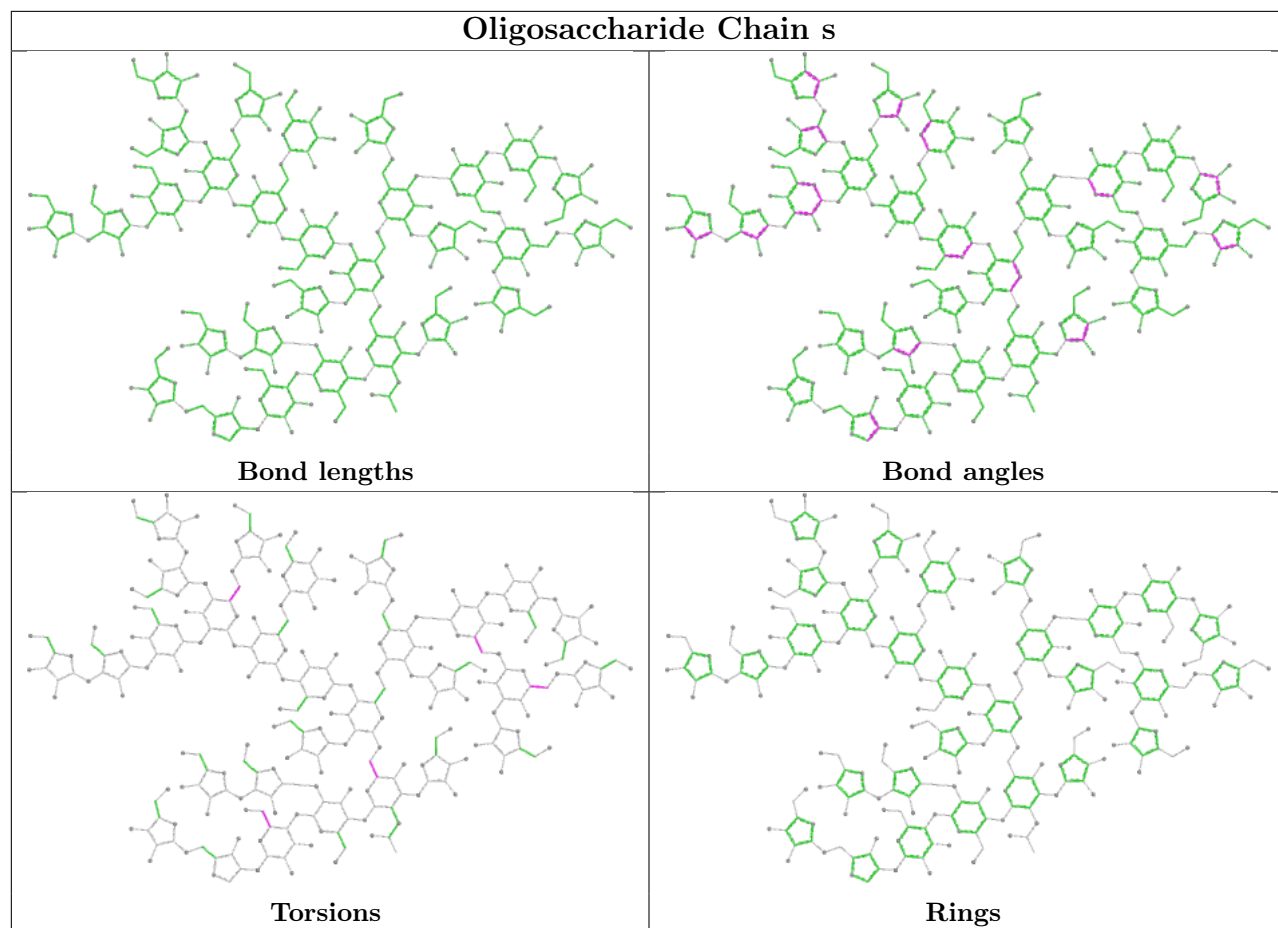


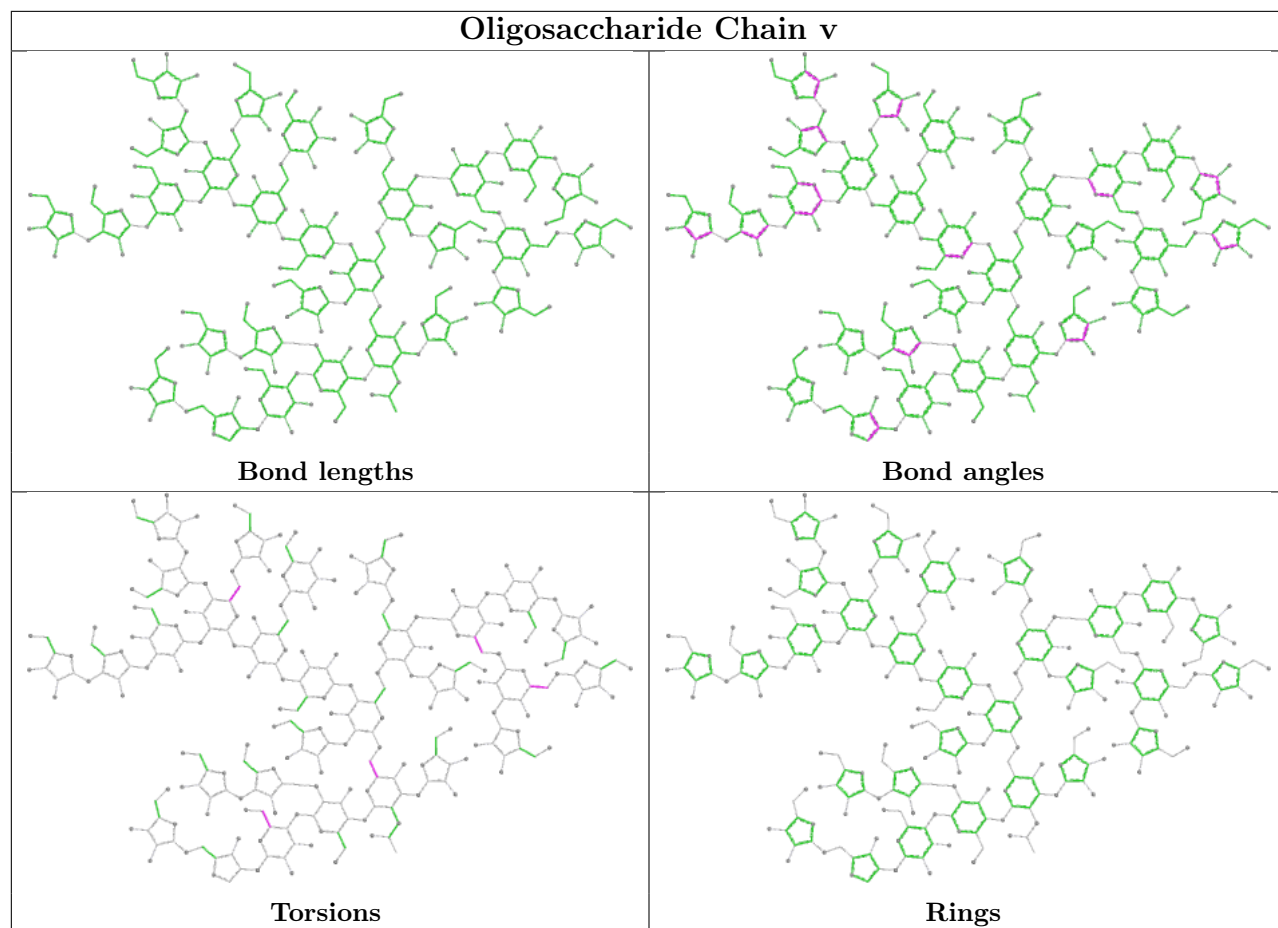


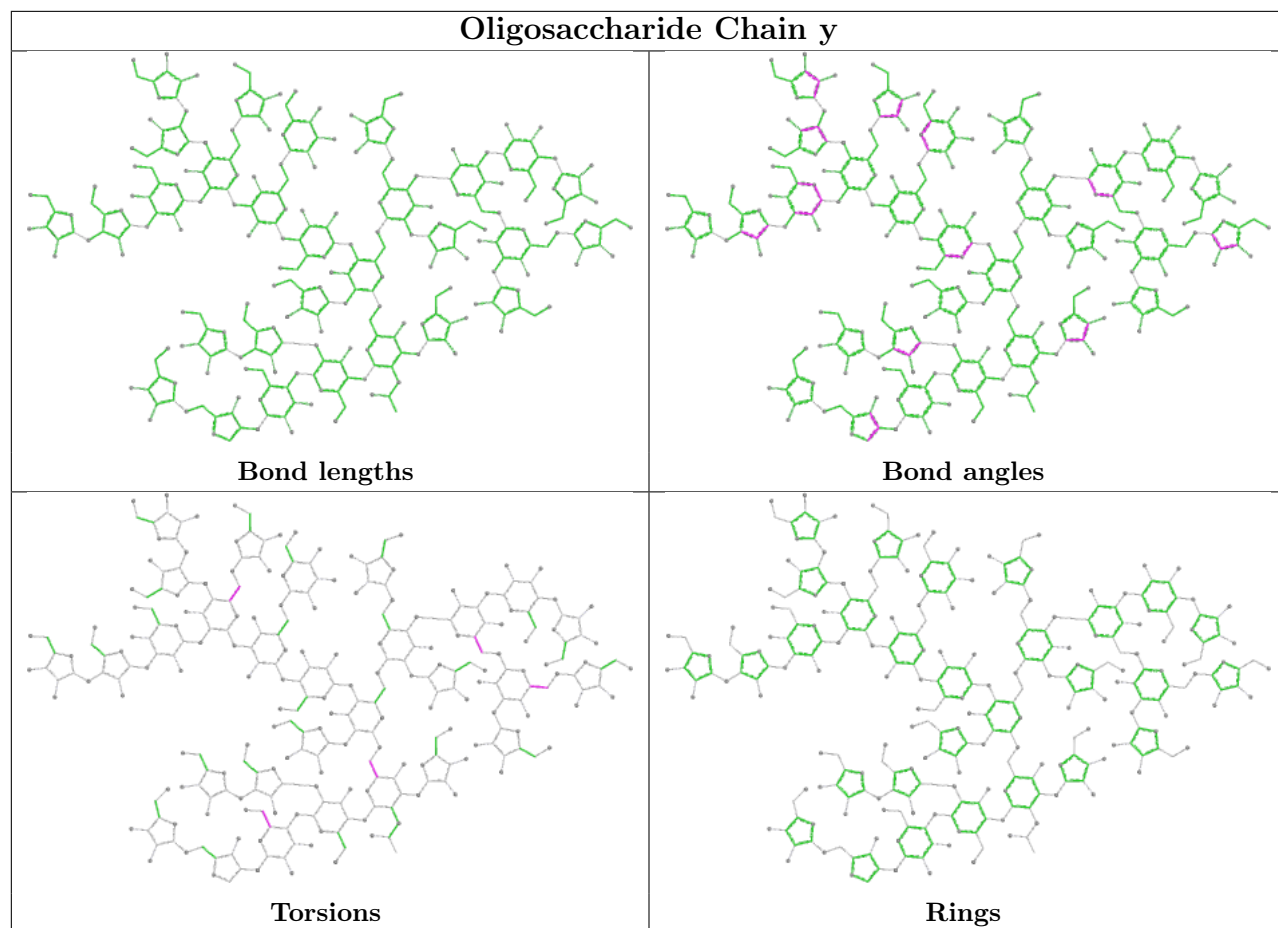


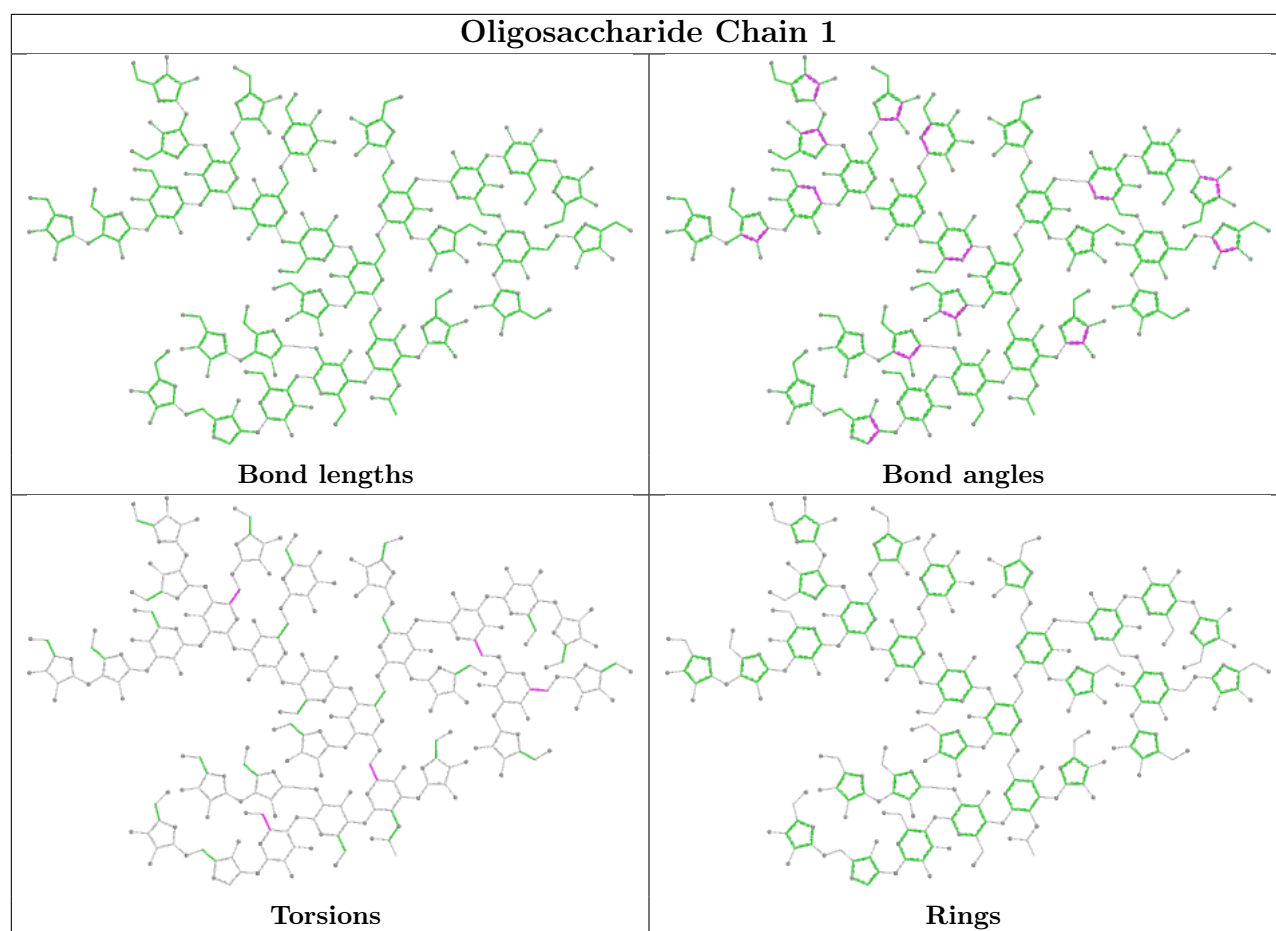


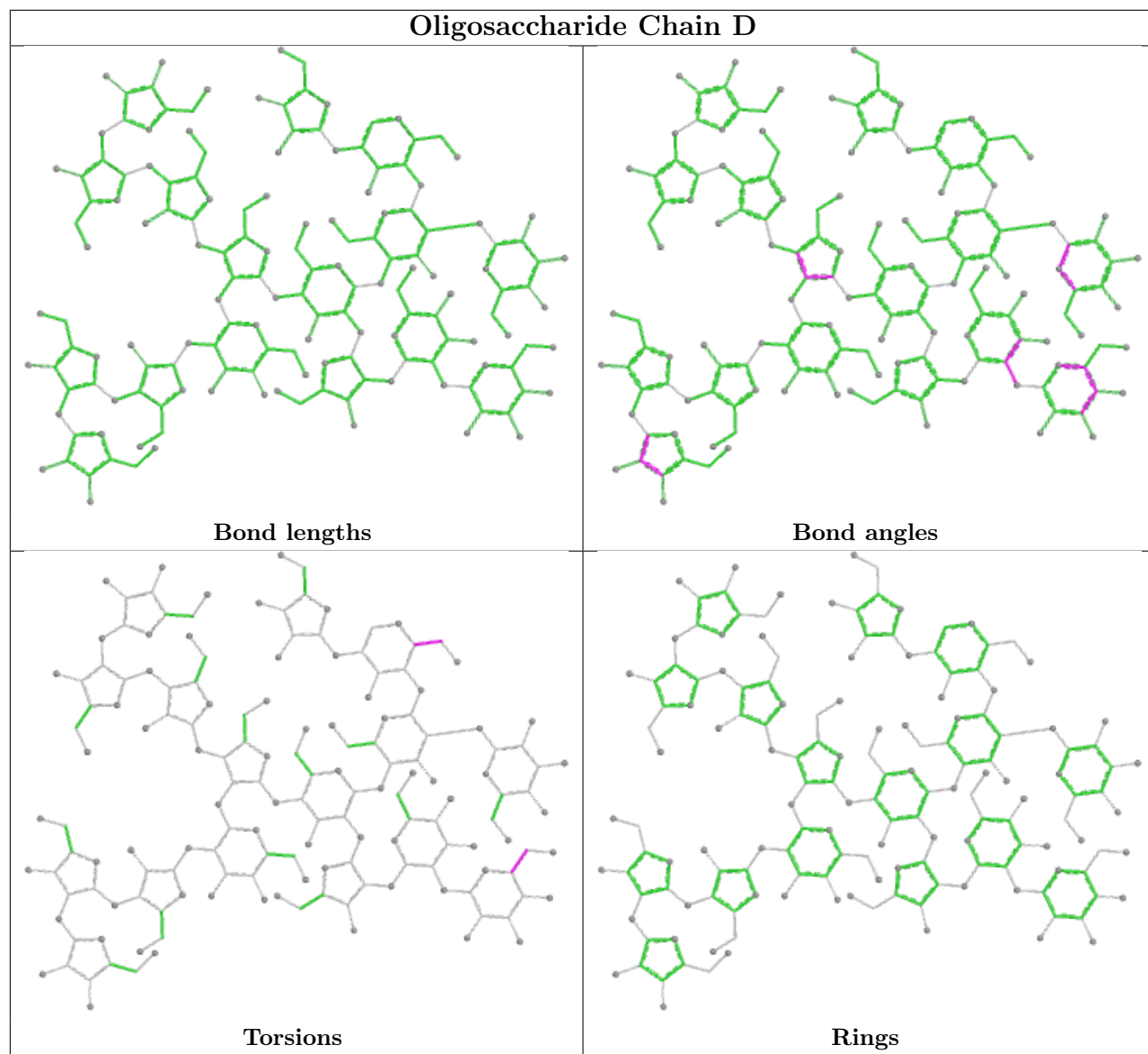


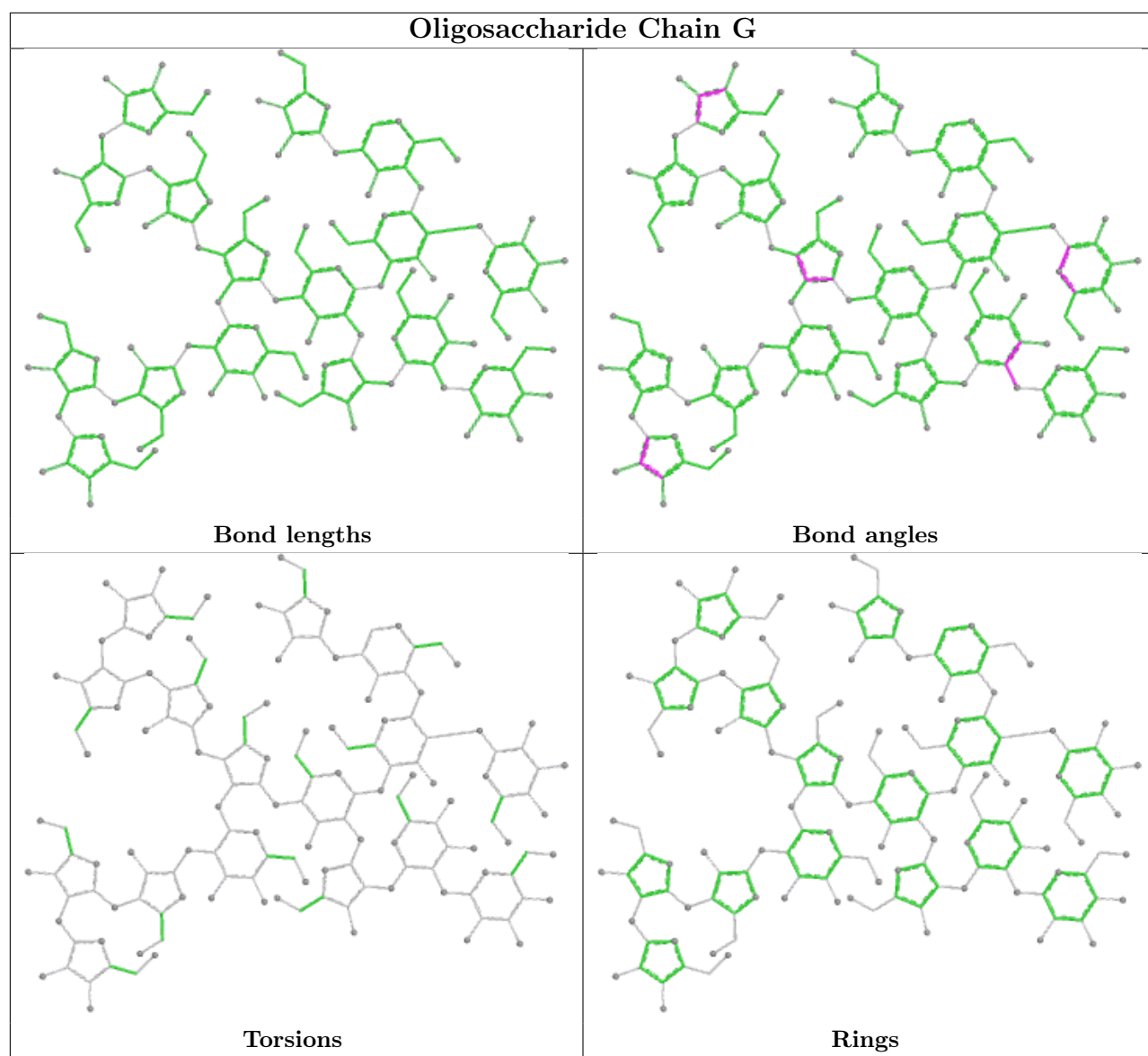


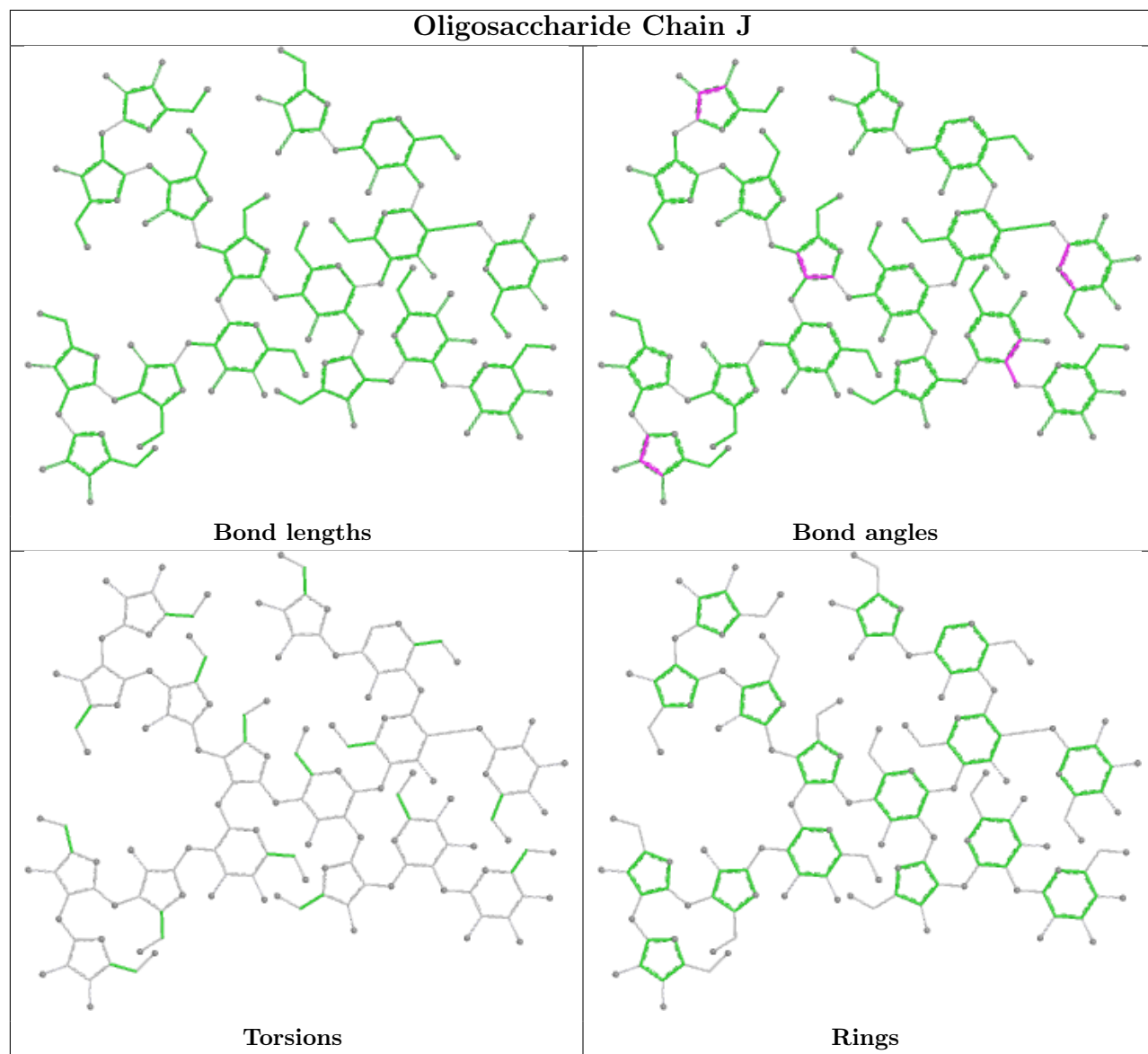


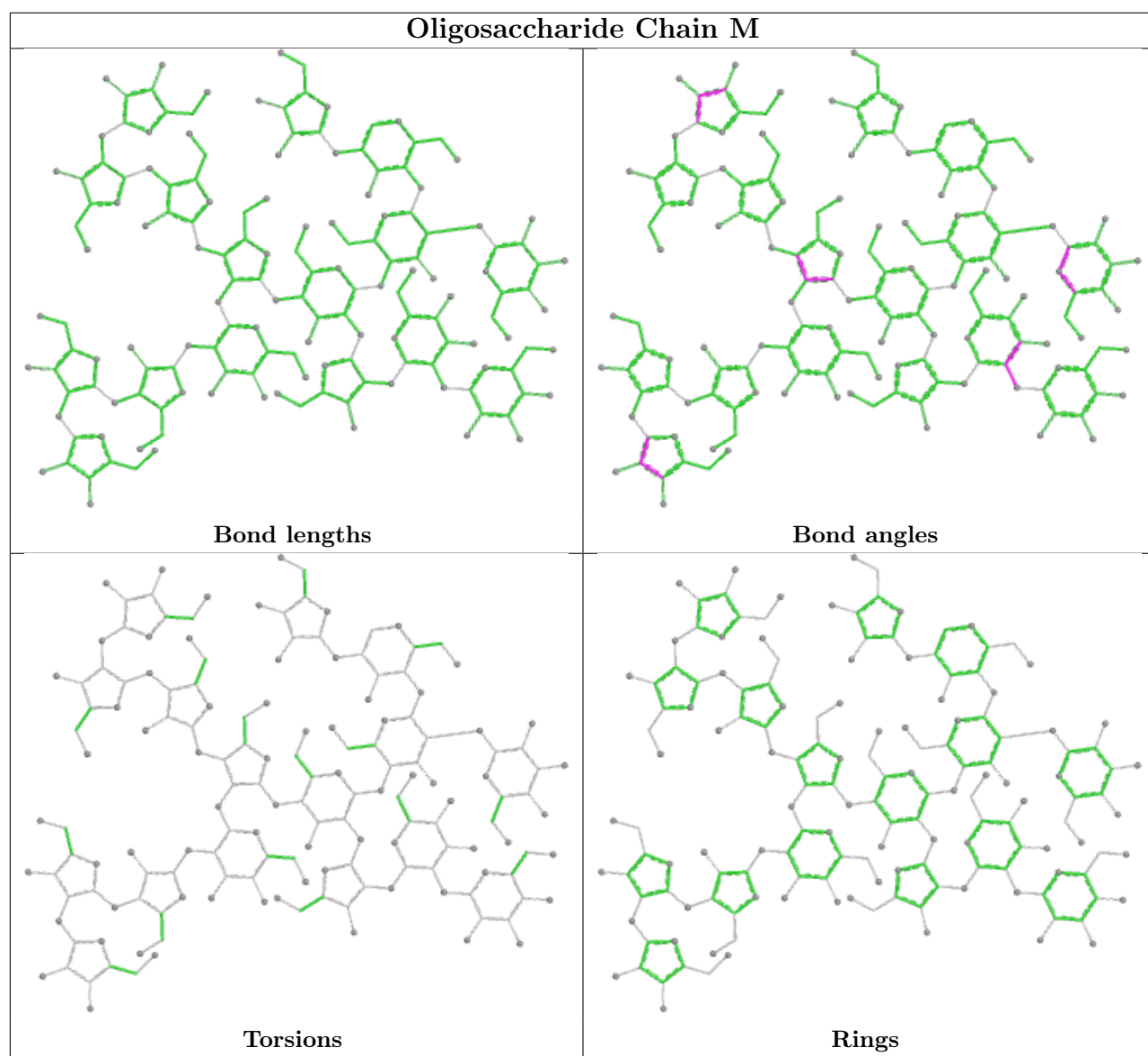


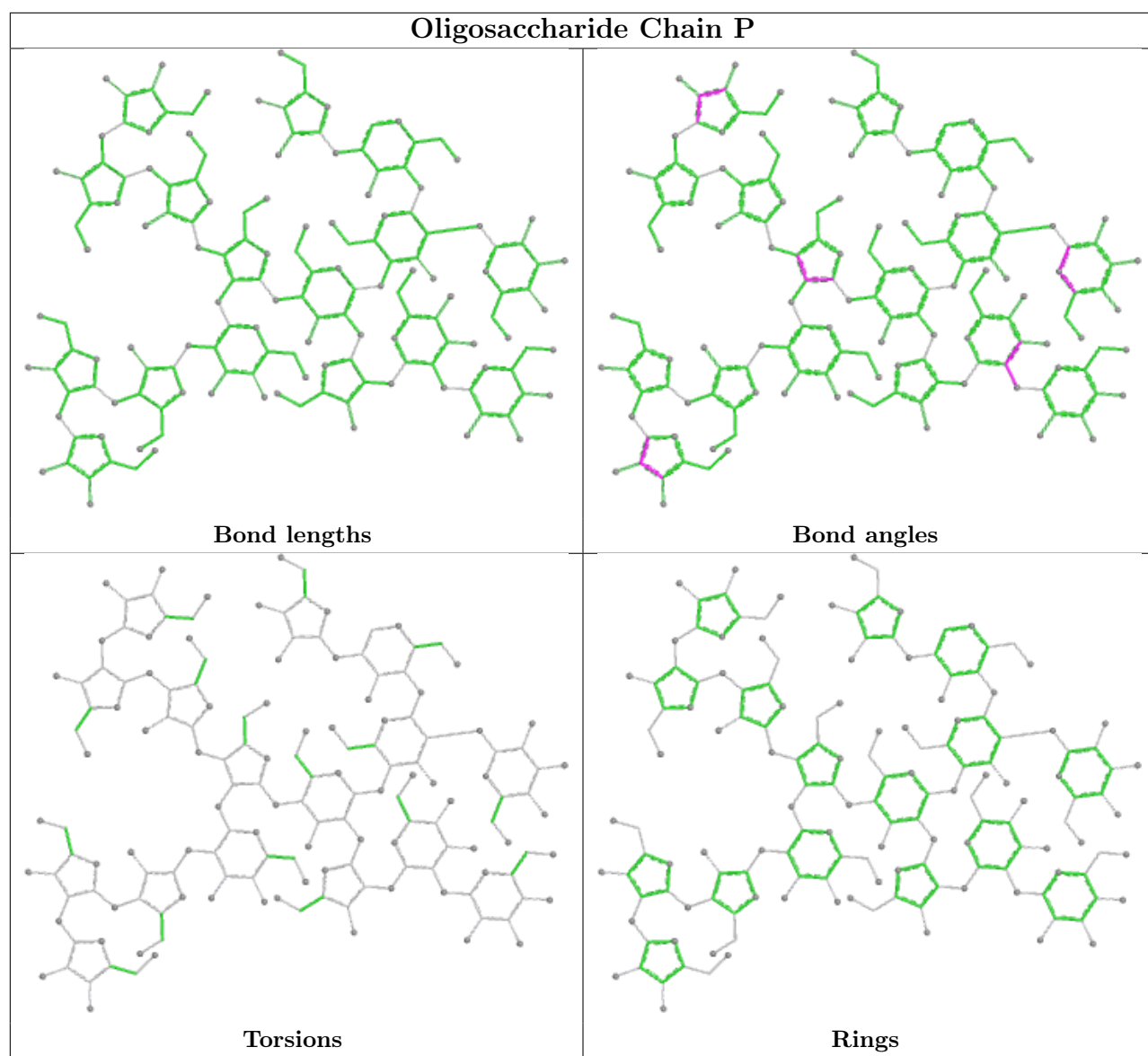


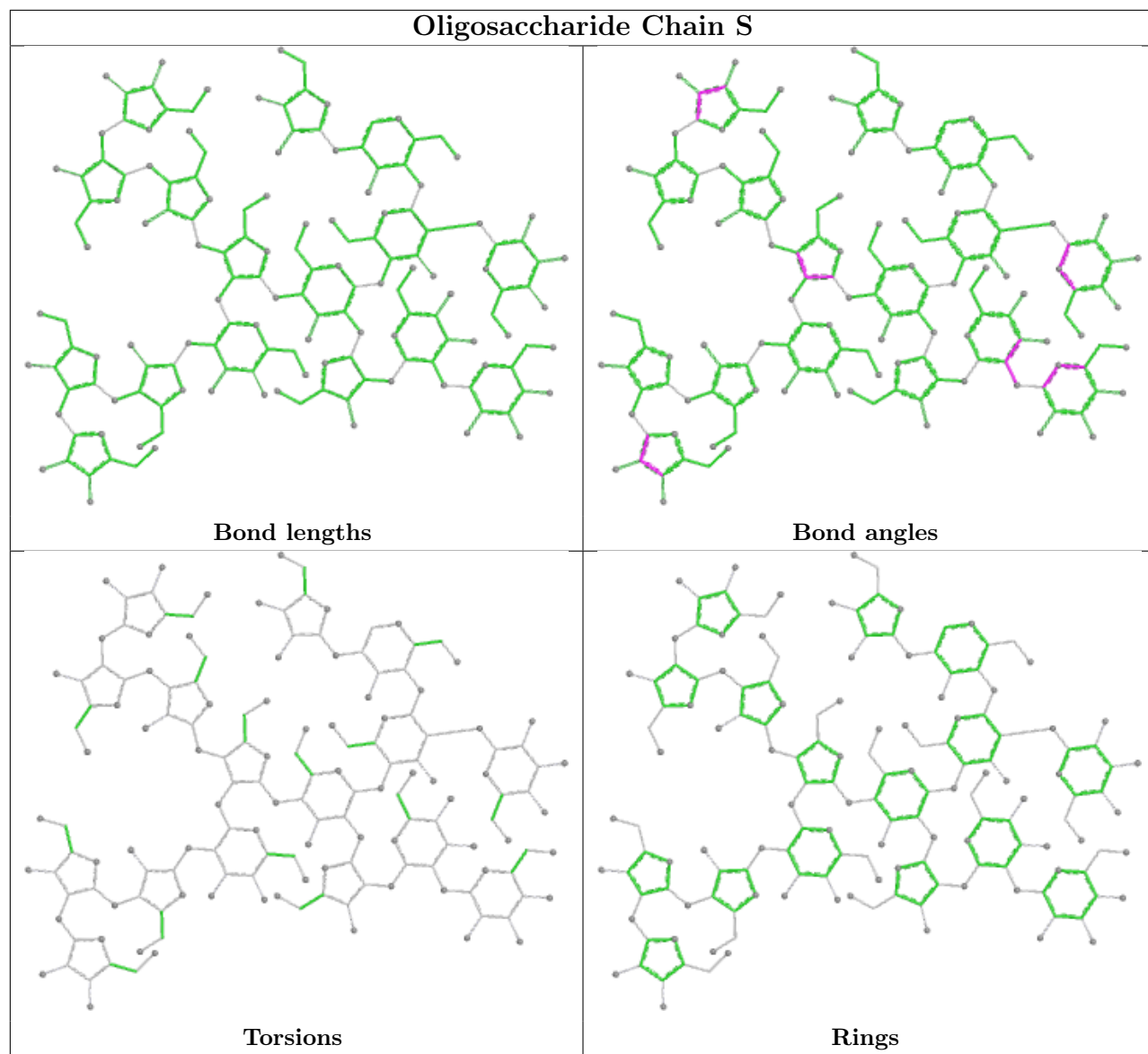


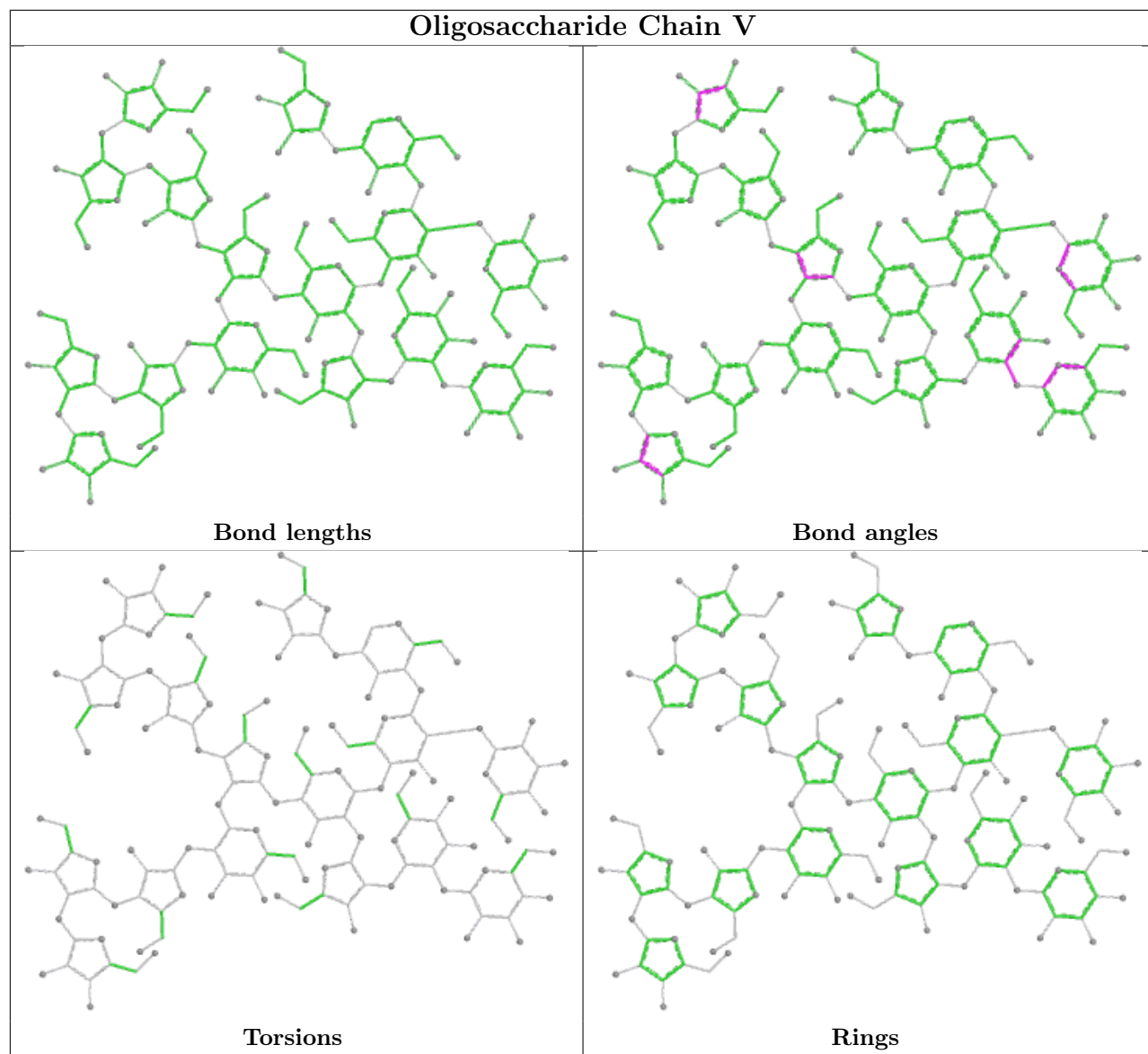


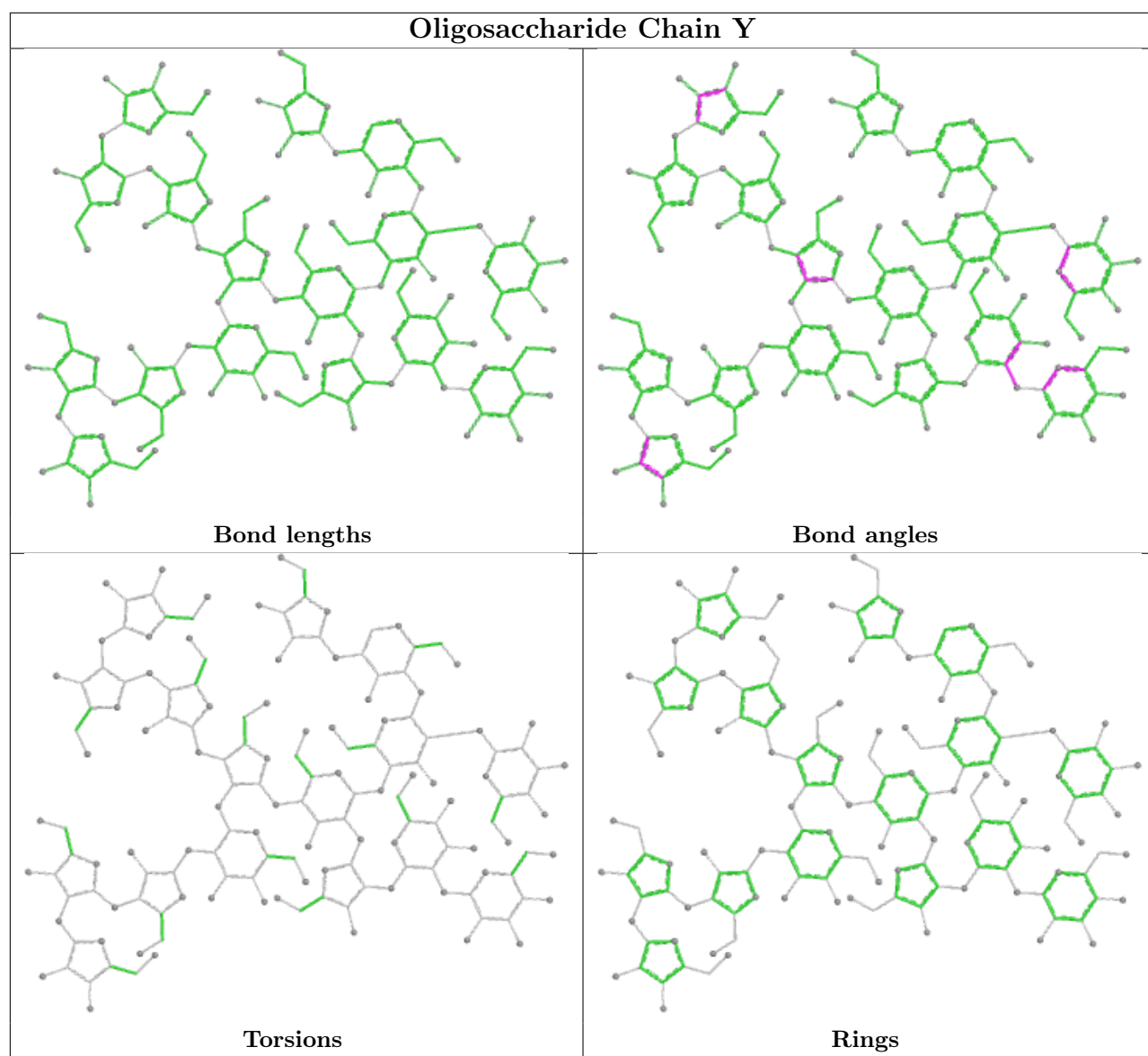


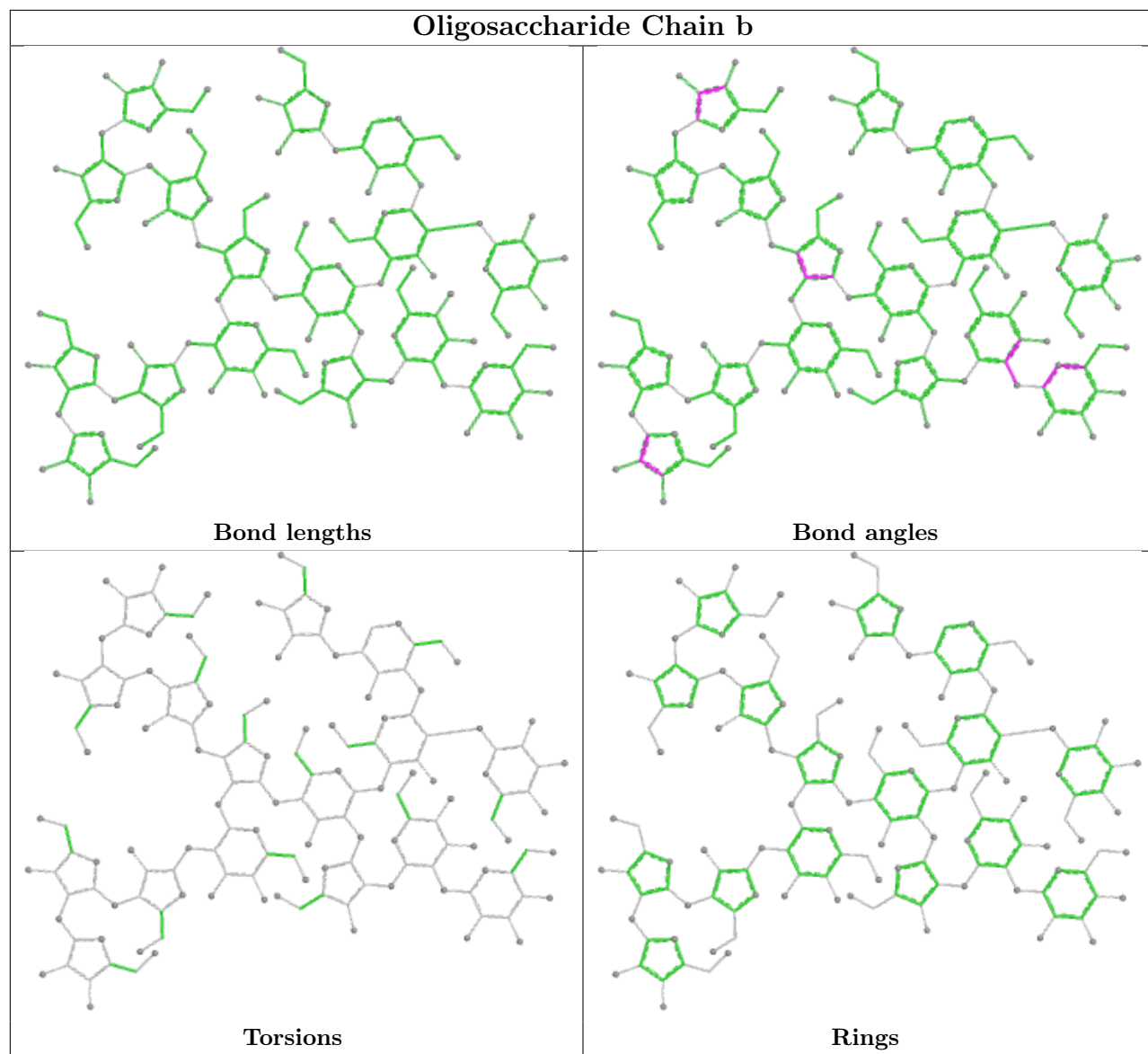


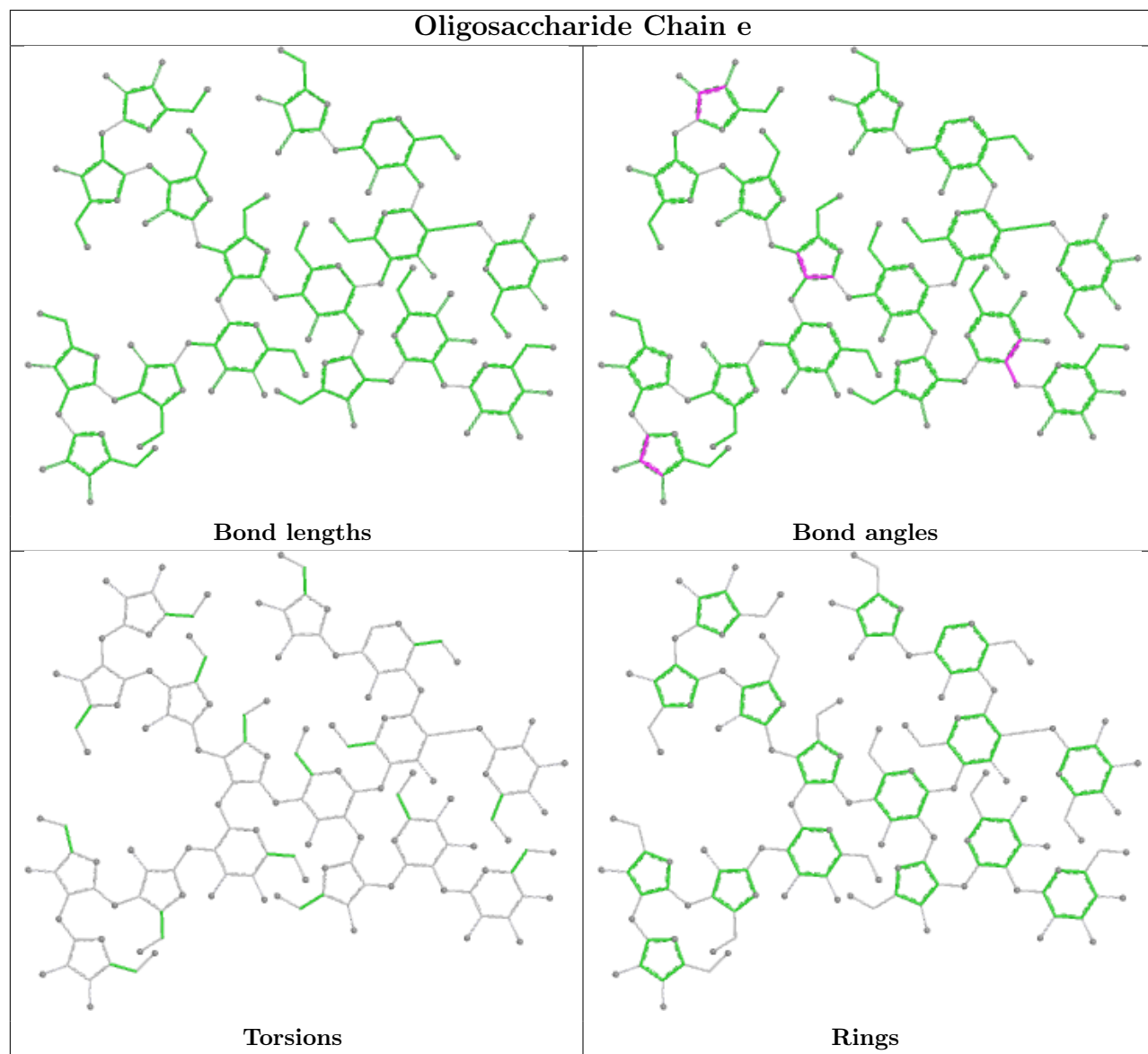


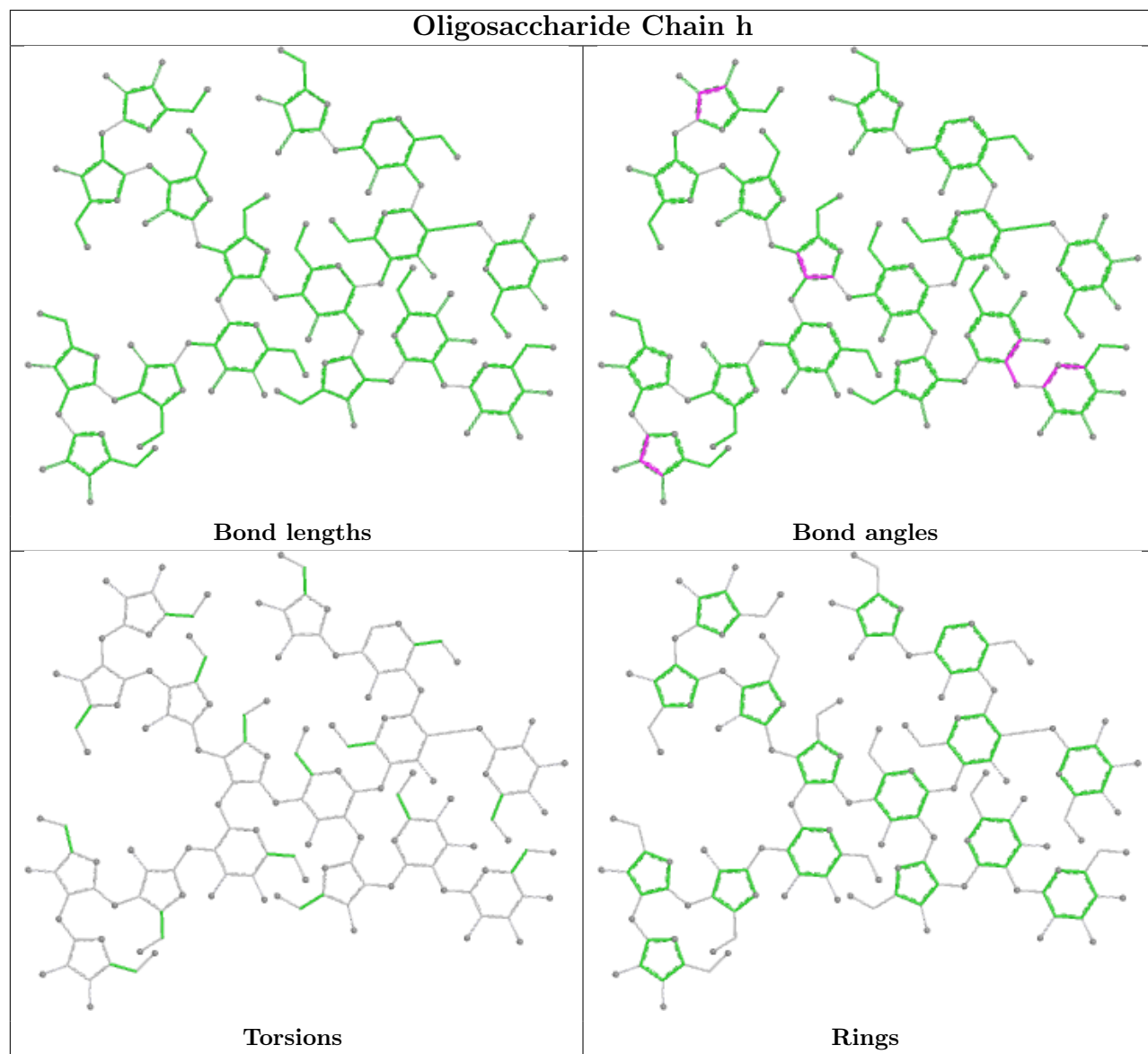


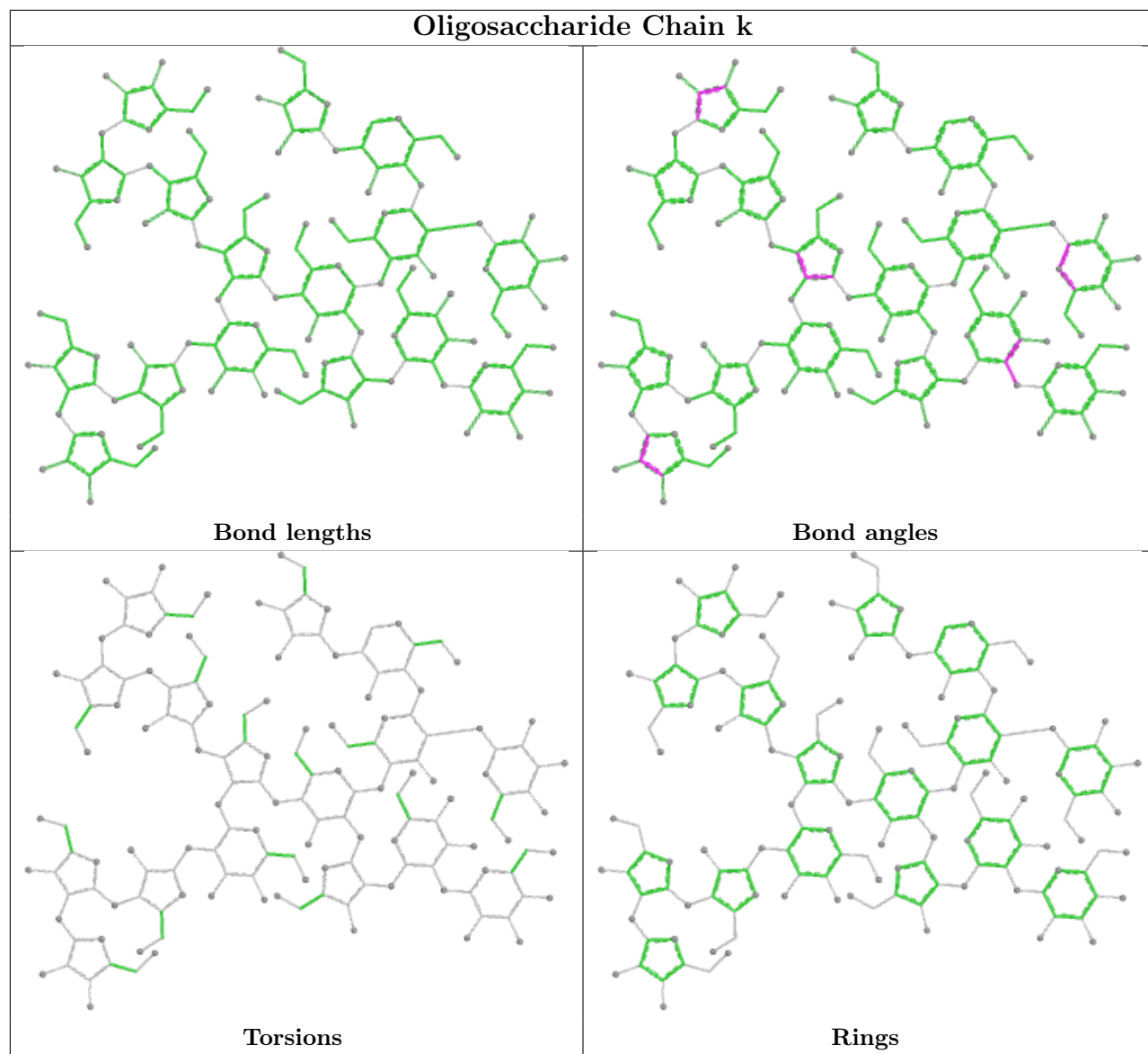


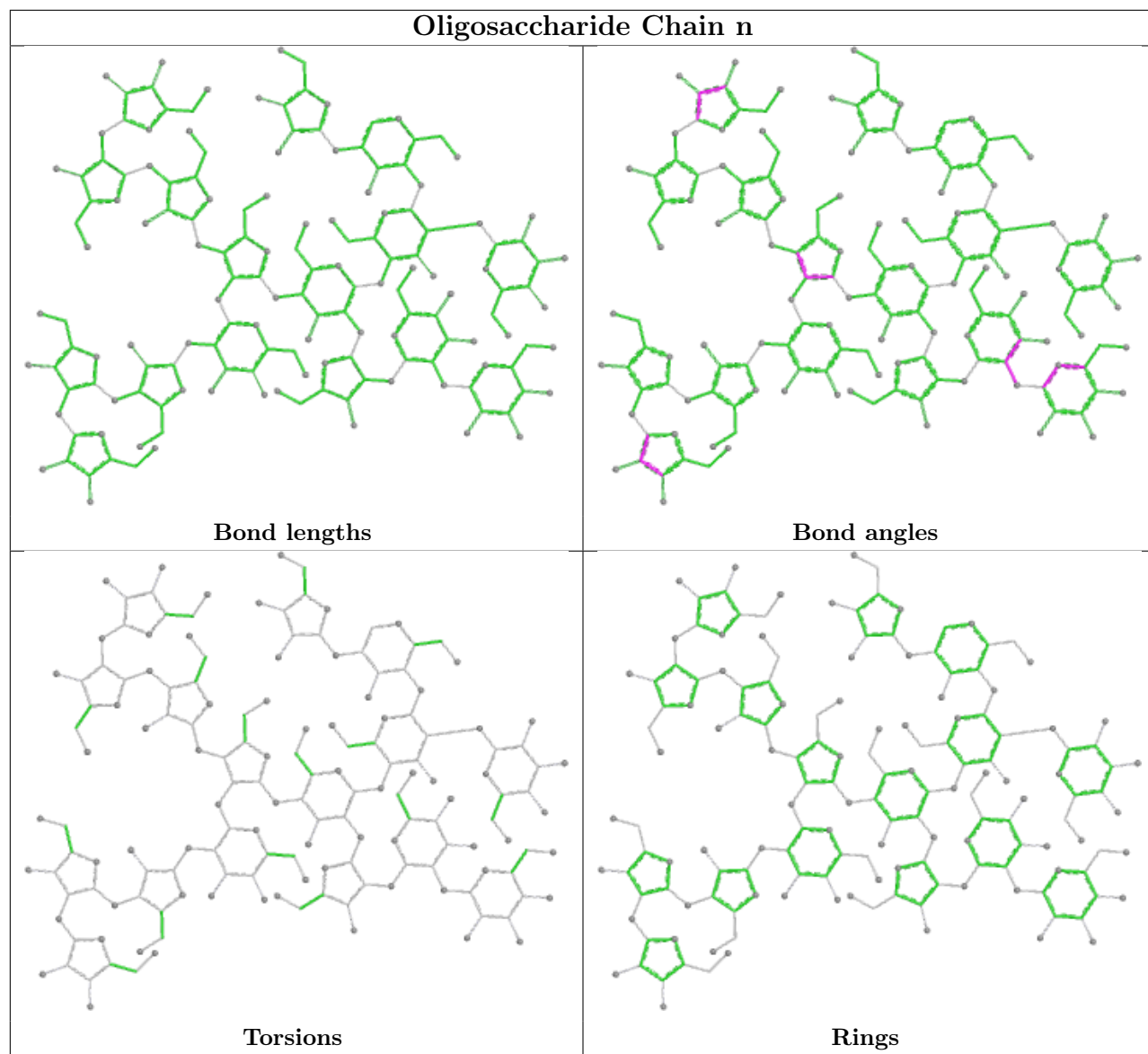


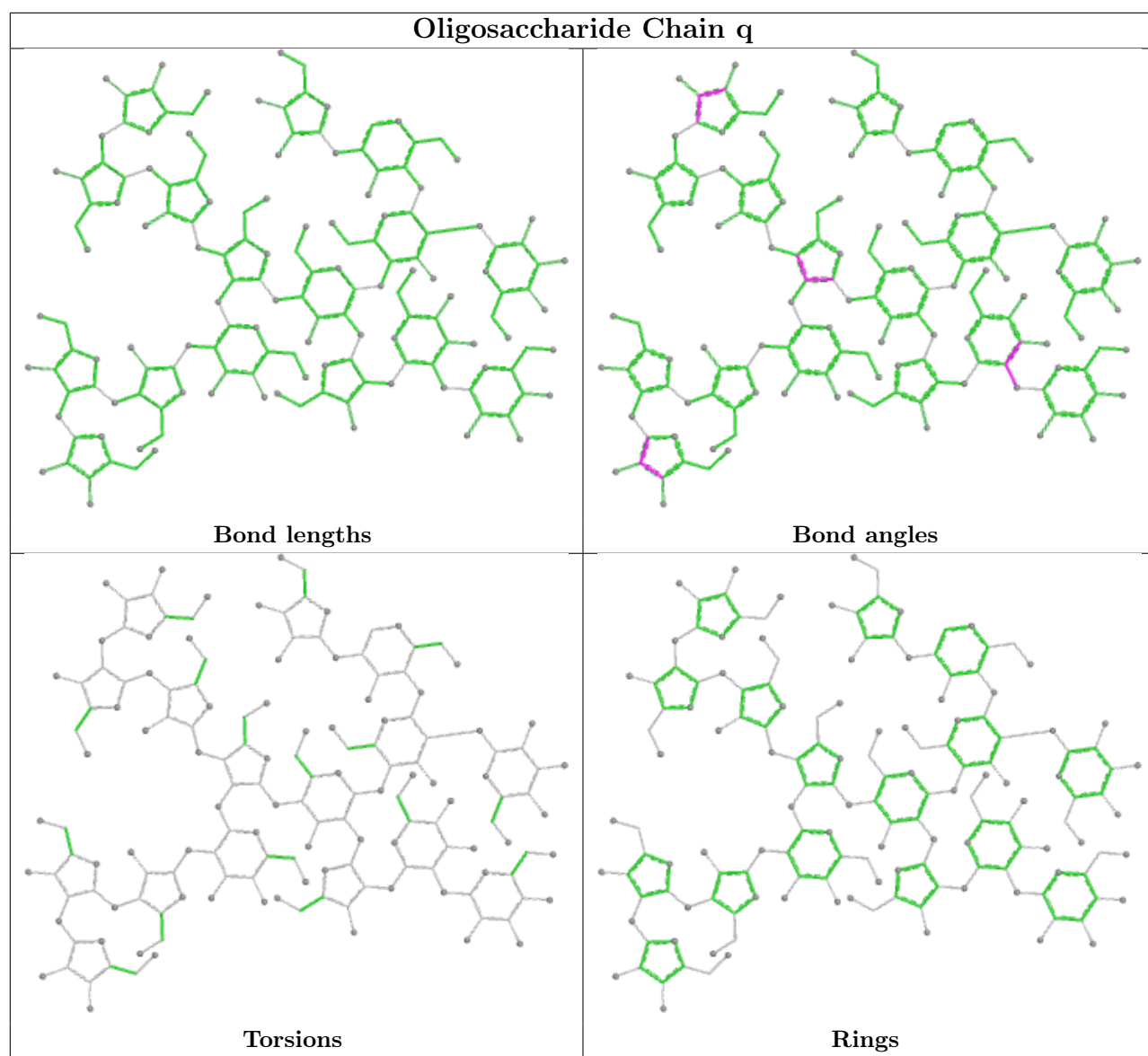


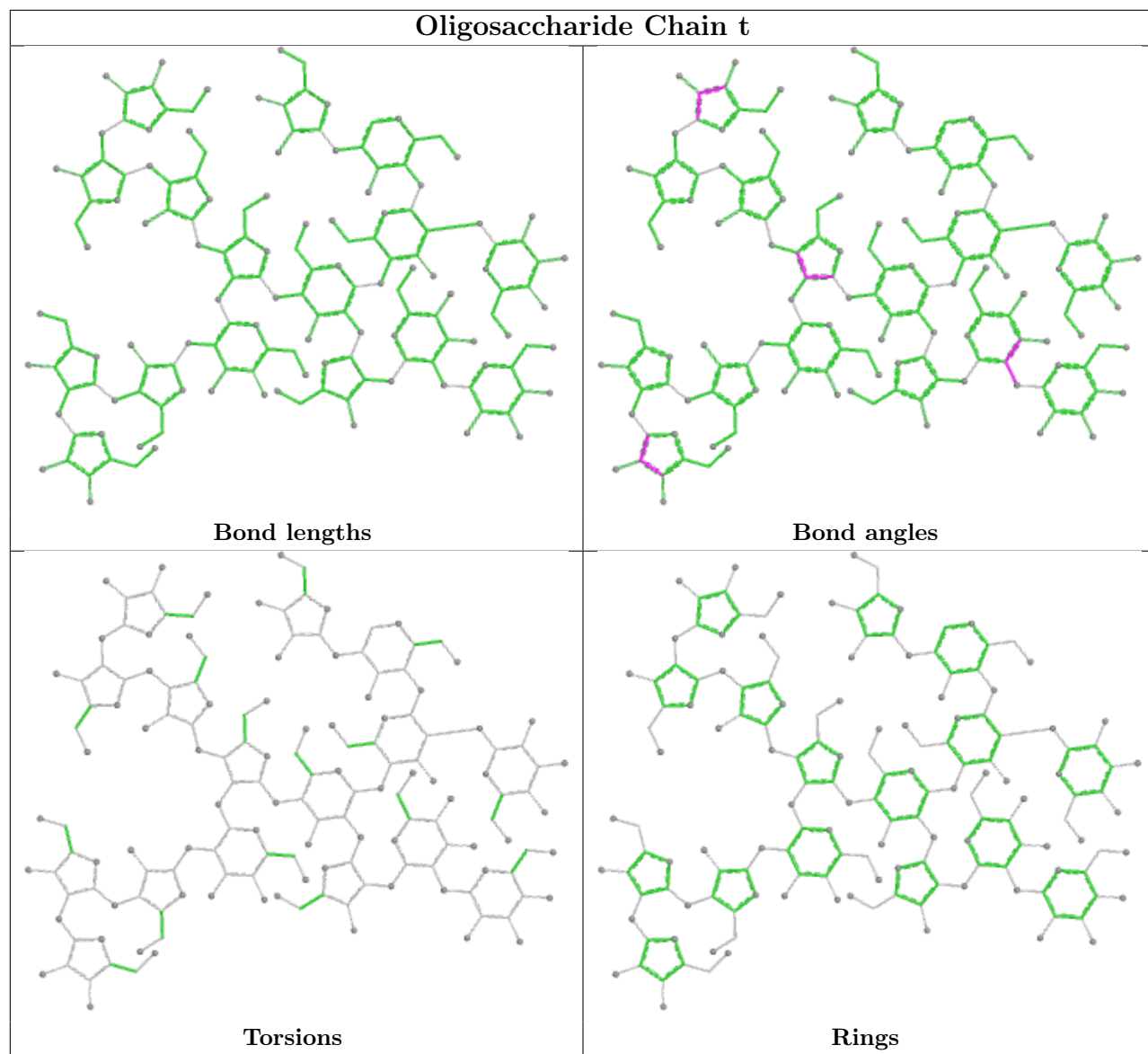


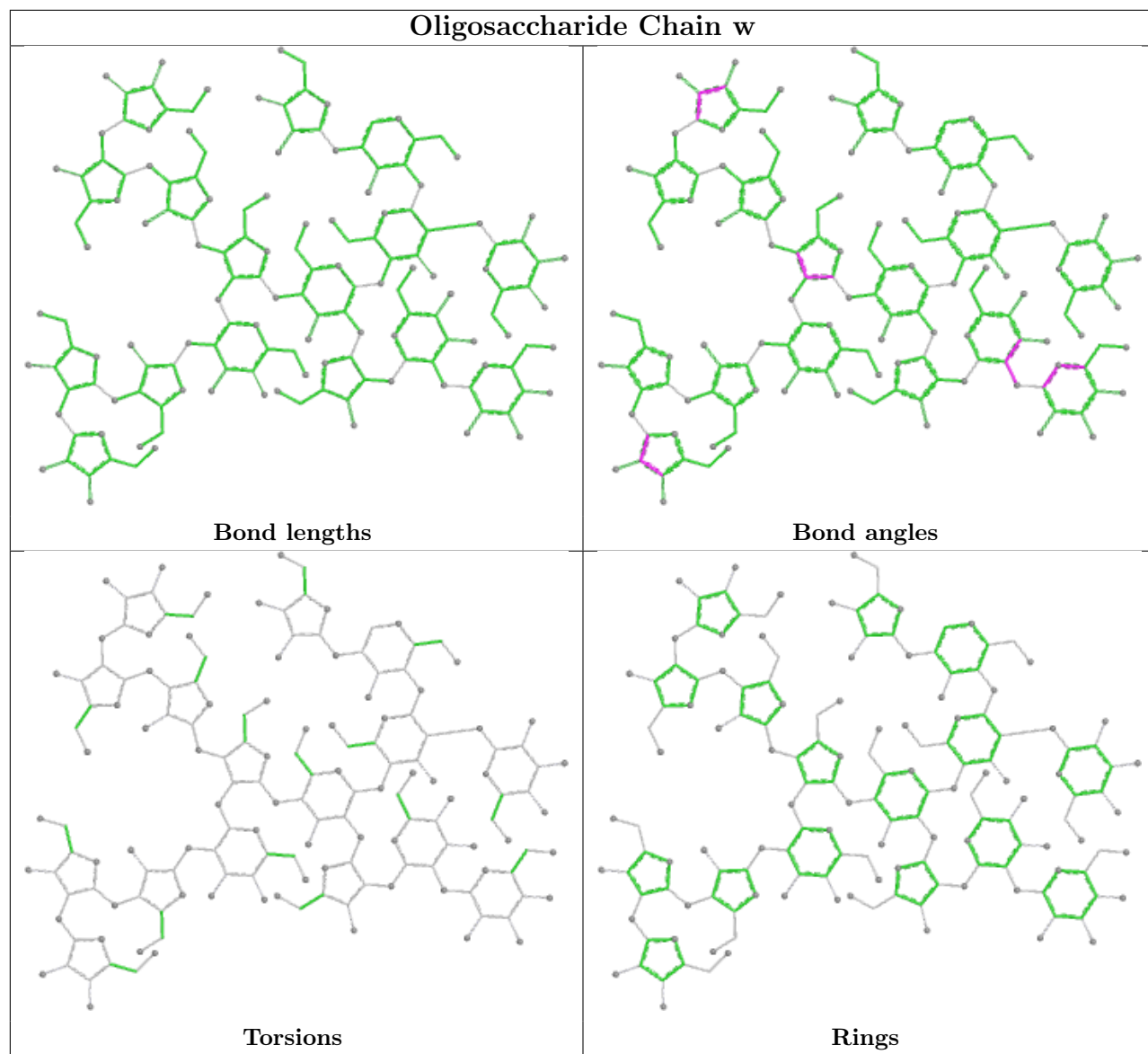


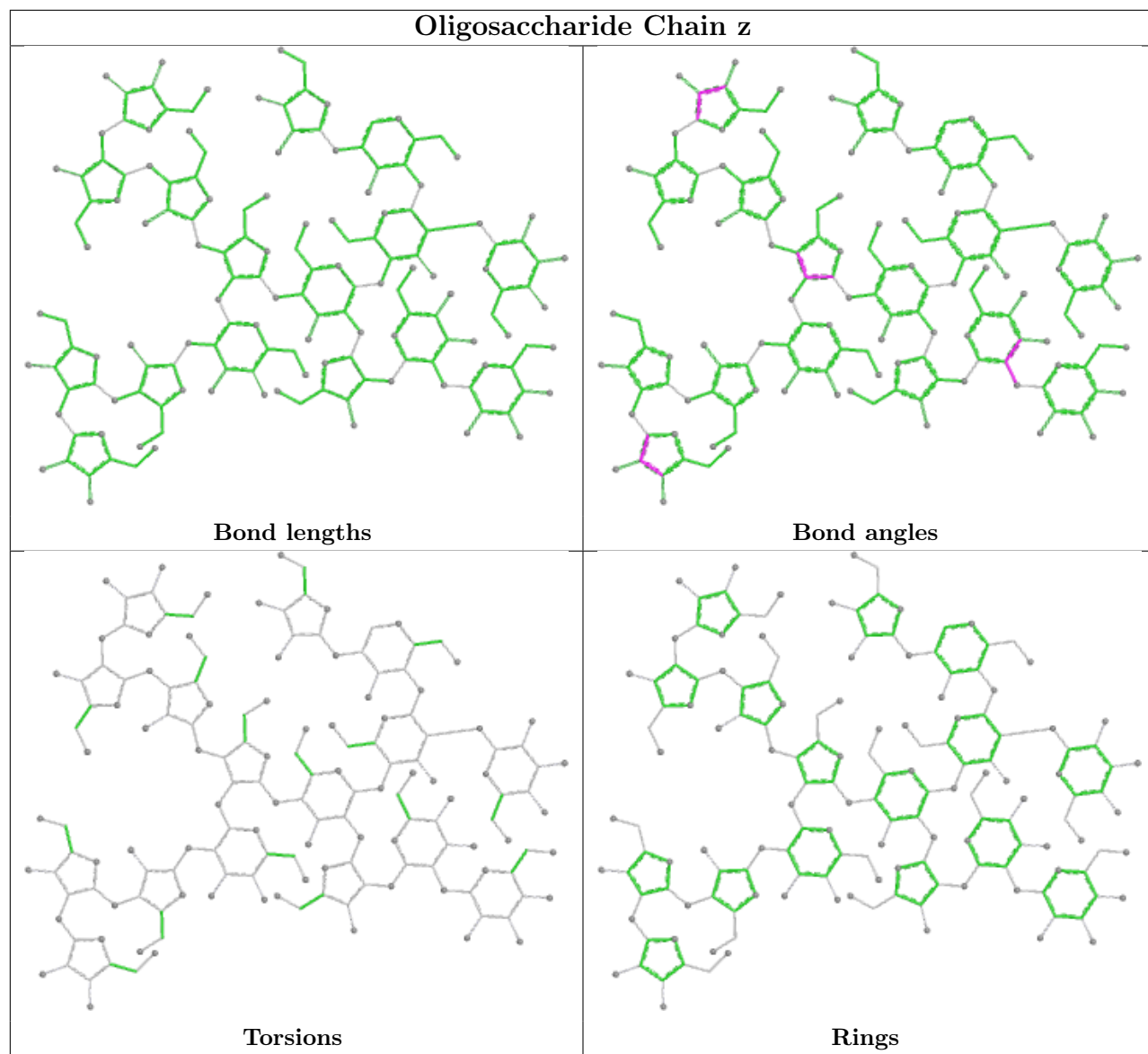


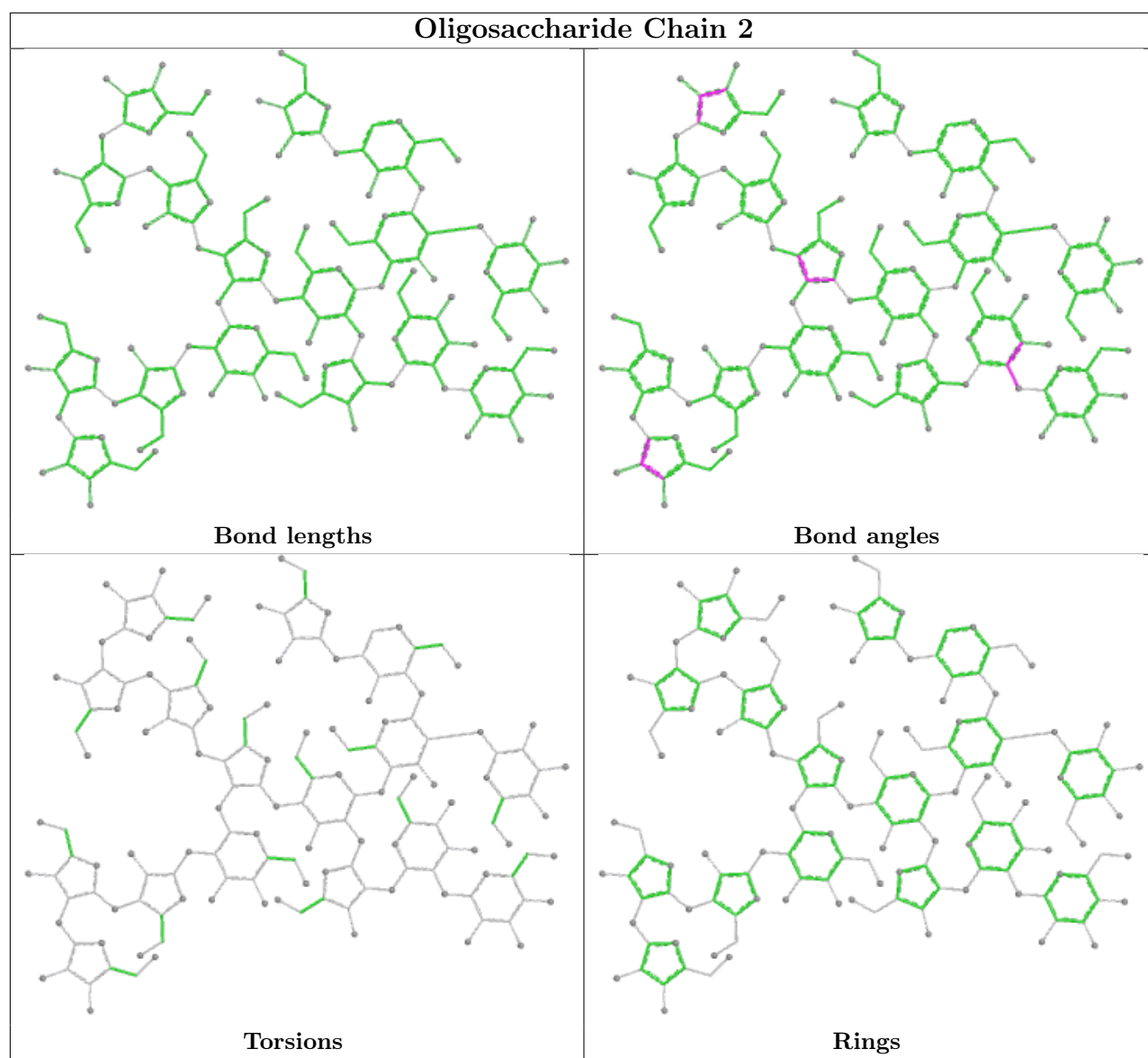












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

This section contains visualisations of the EMDB entry EMD-60659. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.