



# wwPDB EM Validation Summary Report ⓘ

Jun 15, 2026 – 03:29 PM JST

PDB ID : 21NR / pdb\_000021nr  
EMDB ID : EMD-67848  
Title : Cryo-EM structure of TLP-IPT  
Authors : Yan, N.; Li, Z.; Wang, T.  
Deposited on : 2025-12-21  
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

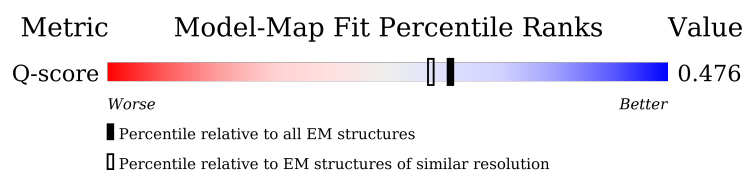
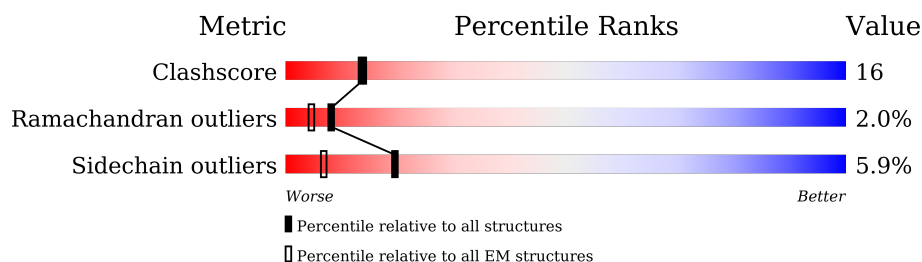
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 Å.

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












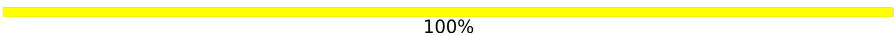
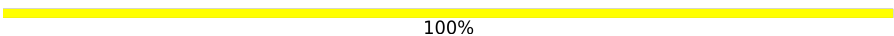
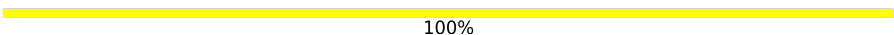
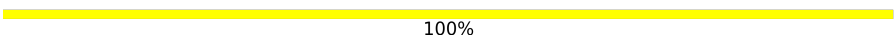
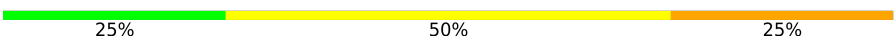
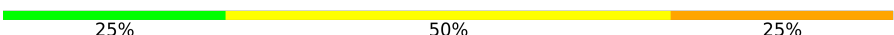
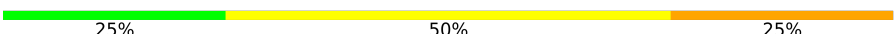
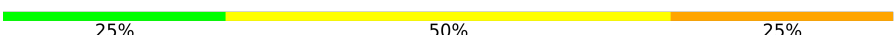








Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 ( 2.80 - 3.80 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>59%</div> <div>36%</div> <div>5%</div> </div>
2	B	9	<div> <div>56%</div> <div>11%</div> <div>33%</div> </div>
2	O	9	<div> <div>44%</div> <div>22%</div> <div>33%</div> </div>
2	b	9	<div> <div>44%</div> <div>22%</div> <div>33%</div> </div>










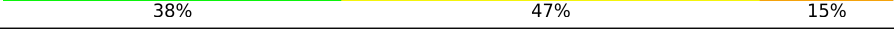



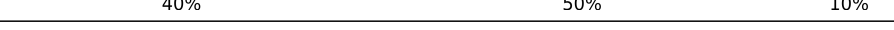



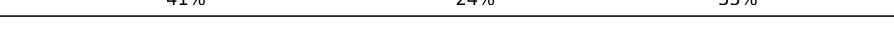
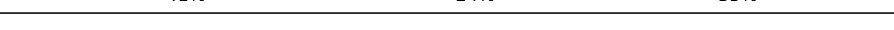


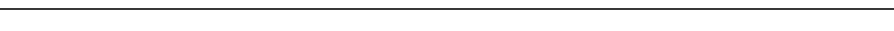


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Mol	Chain	Length	Quality of chain
2	o	9	
3	C	34	
3	P	34	
3	c	34	
3	p	34	
4	D	26	
4	Q	26	
4	d	26	
4	q	26	
5	E	2	
5	R	2	
5	e	2	
5	r	2	
6	F	4	
6	S	4	
6	f	4	
6	s	4	
7	G	22	
7	T	22	
7	g	22	
7	t	22	
8	H	20	
8	U	20	
8	h	20	
8	u	20	

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Mol	Chain	Length	Quality of chain
9	I	10	 60% 40%
9	V	10	 50% 40% 10%
9	i	10	 50% 50%
9	v	10	 60% 40%
10	J	19	 58% 26% 16%
10	W	19	 47% 42% 11%
10	j	19	 37% 53% 11%
10	w	19	 47% 42% 11%
11	K	47	 45% 43% 13%
11	X	47	 38% 47% 15%
11	k	47	 38% 47% 15%
11	x	47	 40% 43% 17%
12	L	10	 40% 60%
12	Y	10	 40% 50% 10%
12	l	10	 40% 40% 20%
12	y	10	 40% 60%
13	M	17	 41% 35% 24%
13	Z	17	 41% 24% 35%
13	m	17	 41% 24% 35%
13	z	17	 41% 24% 35%
14	0	21	 48% 38% 14%
14	N	21	 43% 38% 19%
14	a	21	 43% 38% 19%
14	n	21	 43% 38% 19%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MAN	J	19	-	-	X	-
13	BGC	Z	5	-	-	X	-

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 12836 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-IPT.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	344	Total	C	N	O	S	0	0
			2412	1416	400	588	8		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	9	Total	C	N	O	0	0
			105	58	2	45		
2	O	9	Total	C	N	O	0	0
			105	58	2	45		
2	b	9	Total	C	N	O	0	0
			105	58	2	45		
2	o	9	Total	C	N	O	0	0
			105	58	2	45		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	34	Total	C	N	O	0	0
			359	198	3	158		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	P	34	Total	C	N	O	0	0
			359	198	3	158		
3	c	34	Total	C	N	O	0	0
			359	198	3	158		
3	p	34	Total	C	N	O	0	0
			359	198	3	158		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	26	Total	C	N	O	0	0
			274	151	2	121		
4	Q	26	Total	C	N	O	0	0
			274	151	2	121		
4	d	26	Total	C	N	O	0	0
			274	151	2	121		
4	q	26	Total	C	N	O	0	0
			274	151	2	121		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	2	Total	C	N	O	0	0
			25	14	1	10		
5	R	2	Total	C	N	O	0	0
			25	14	1	10		
5	e	2	Total	C	N	O	0	0
			25	14	1	10		
5	r	2	Total	C	N	O	0	0
			25	14	1	10		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-5)-beta-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-alpha-D-mannopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	4	Total	C	N	O	0	0
			45	25	1	19		
6	S	4	Total	C	N	O	0	0
			45	25	1	19		
6	f	4	Total	C	N	O	0	0
			45	25	1	19		
6	s	4	Total	C	N	O	0	0
			45	25	1	19		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	22	Total	C	N	O	0	0
			237	131	3	103		
7	T	22	Total	C	N	O	0	0
			237	131	3	103		
7	g	22	Total	C	N	O	0	0
			237	131	3	103		
7	t	22	Total	C	N	O	0	0
			237	131	3	103		

- Molecule 8 is an oligosaccharide called beta-D-glucopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]beta-D-xylopyranose-(1-3)-[beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-(1-4)]beta-D-galactopyranose-(1-2)-beta-D-xylopyranose-(1-3)-beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)-beta-D-xylopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-galactopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	20	Total	C	N	O	0	0
			213	118	3	92		
8	U	20	Total	C	N	O	0	0
			213	118	3	92		

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Mol	Chain	Residues	Atoms				AltConf	Trace
8	h	20	Total	C	N	O	0	0
			213	118	3	92		
8	u	20	Total	C	N	O	0	0
			213	118	3	92		

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-3)][alpha-D-mannopyranose-(1-4)]beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-3)][beta-D-xylopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-4)]beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	10	Total	C	N	O	0	0
			109	60	1	48		
9	V	10	Total	C	N	O	0	0
			109	60	1	48		
9	i	10	Total	C	N	O	0	0
			109	60	1	48		
9	v	10	Total	C	N	O	0	0
			109	60	1	48		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-glucopyranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-[beta-D-xylopyranose-(1-2)][alpha-D-mannopyranose-(1-4)]beta-D-galactopyranose-(1-3)-[beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-[beta-D-xylopyranose-(1-2)][beta-D-glucopyranose-(1-4)]beta-D-galactopyranose-(1-3)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-beta-D-glucopyranose-(1-4)]beta-D-xylopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	19	Total	C	N	O	0	0
			216	120	5	91		
10	W	19	Total	C	N	O	0	0
			216	120	5	91		
10	j	19	Total	C	N	O	0	0
			216	120	5	91		
10	w	19	Total	C	N	O	0	0
			216	120	5	91		

- Molecule 11 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-mannopyranose-(1-6)-beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-D-galactopyranose

-(1-3)-[beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-mannopyranose-(1-4)-[beta-D-xylopyranose-(1-2)-[beta-D-xylopyranose-(1-4)]beta-D-glucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-4)]beta-D-xylopyranose-(1-3)-alpha-D-mannopyranose-(1-2)]beta-D-xylopyranose-(1-3)]beta-D-glucopyranose-(1-6)-beta-D-glucopyranose-(1-2)-beta-L-arabinofuranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)]beta-D-glucopyranose-(1-3)]beta-D-xylopyranose-(1-4)]beta-D-mannopyranose-(1-2)-[beta-D-glucopyranose-(1-4)-beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-3)-[beta-D-xylopyranose-(1-3)-[beta-D-glucopyranose-(1-4)]beta-D-glucopyranose-(1-6)]beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-4)]beta-D-glucopyranose-(1-6)-[beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	47	Total	C	N	O	0	0
			512	283	7	222		
11	X	47	Total	C	N	O	0	0
			512	283	7	222		
11	k	47	Total	C	N	O	0	0
			512	283	7	222		
11	x	47	Total	C	N	O	0	0
			512	283	7	222		

- Molecule 12 is an oligosaccharide called beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]beta-D-glucopyranose-(1-3)-[beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-3)-beta-D-galactopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	10	Total	C	N	O	0	0
			107	59	1	47		
12	Y	10	Total	C	N	O	0	0
			107	59	1	47		
12	l	10	Total	C	N	O	0	0
			107	59	1	47		
12	y	10	Total	C	N	O	0	0
			107	59	1	47		

- Molecule 13 is an oligosaccharide called beta-D-glucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-xylopyranose-(1-4)-[beta-D-glucopyranose-(1-2)]alpha-D-mannopyranose-(1-3)]beta-D-glucopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-beta-D-glucopyranose-(1-2)-beta-D-x

xylopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	17	Total	C	N	O	0	0
			185	102	2	81		
13	Z	17	Total	C	N	O	0	0
			185	102	2	81		
13	m	17	Total	C	N	O	0	0
			185	102	2	81		
13	z	17	Total	C	N	O	0	0
			185	102	2	81		

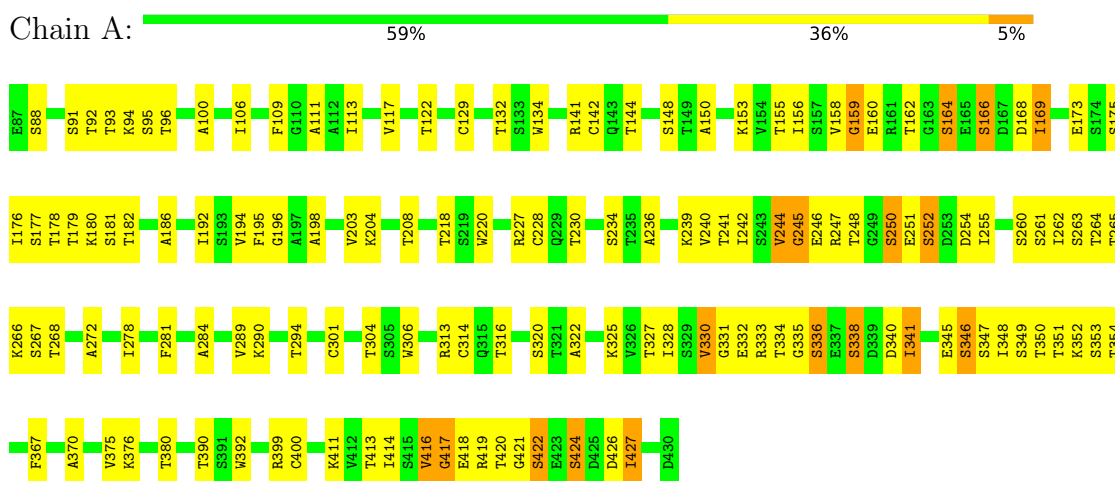
- Molecule 14 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)-alpha-L-arabinofuranose-(1-2)-[beta-D-xylopyranose-(1-3)-[alpha-L-arabinofuranose-(1-4)]beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-2)]beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-(1-3)]|beta-D-xylopyranose-(1-6)]beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)]|alpha-L-arabinofuranose-(1-2)-beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-4)-alpha-D-mannopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	21	Total	C	N	O	0	0
			219	122	4	93		
14	a	21	Total	C	N	O	0	0
			219	122	4	93		
14	n	21	Total	C	N	O	0	0
			219	122	4	93		
14	o	21	Total	C	N	O	0	0
			219	122	4	93		

### 3 Residue-property plots

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

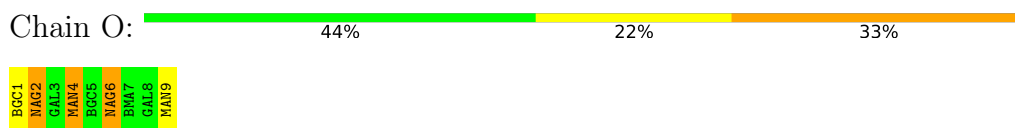
- Molecule 1: TLP-IPT



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



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

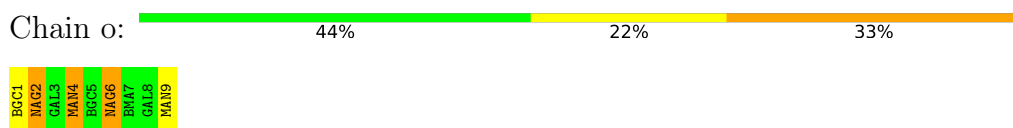


- Molecule 2: beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha

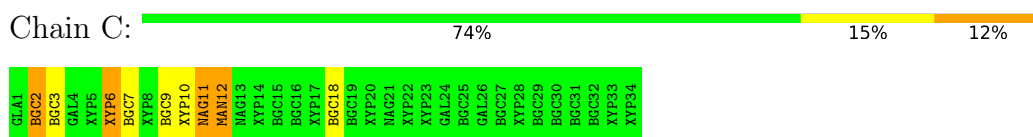
a-D-mannopyranose-(1-2)-[beta-D-galactopyranose-(1-2)-beta-D-mannopyranose-(1-3)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



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



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



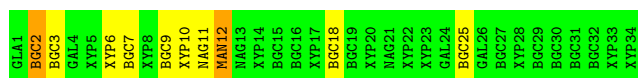
- Molecule 3: beta-D-xylopyranose-(1-4)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]alpha-D-mannopyranose-(1-4)]beta-D-xylopyranose-(1-3)-beta-D-xylopyranose-(1-4)-[beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)-[beta-D-xylopyranose-(1-4)-beta-D-glucopyranose-(1-4)]2-acetam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





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

Chain c: 71% 24% 6%



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

Chain p: 74% 21% 6%



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

Chain D: 50% 46%



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

Chain Q: 54% 42%



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

Chain d: 54% 42%



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

Chain q: 58% 38%

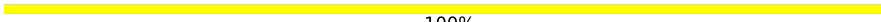


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose

Chain E:  100%

MAN1  
NAG2

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

Chain R:  100%

MAN1  
NAG2

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

Chain e:  100%

MAN1  
NAG2

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

Chain r:  100%

MAN1  
NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-5)-beta-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-alpha-D-mannopyranose

Chain F:  25% 50% 25%

MAN1  
GZL2  
FUB3  
NAG4

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-5)-beta-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-alpha-D-mannopyranose

Chain S:  25% 50% 25%

MAN1  
GZL2  
FUB3  
NAG4

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-5)-beta-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-alpha-D-mannopyranose

Chain f:  25% 50% 25%

MAN1  
GZL2  
FUB3  
NAG4



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-5)-beta-L-arabinofuranose-(1-3)-beta-D-galactofuranose-(1-2)-alpha-D-mannopyranose

Chain s: 



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

Chain G: 



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

Chain T: 



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

Chain g: 



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

Chain t:  55% 32% 14%

XYP1	BGC2	A2G3	BGC4	BGC5	XYP6	A2G7	MAN8	MAN9	MAN10	MAN11	BGC12	BGC13	XYP14	MAN15	BGC16	BGC17	BGC18	XYP19	XYP20	XYP21	XYP22
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● Molecule 8: beta-D-glucopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]beta-D-xylopyranose-(1-3)-[beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-(1-4)]beta-D-galactopyranose-(1-2)-beta-D-xylopyranose-(1-3)-beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)-beta-D-xylopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain H:  65% 30% 5%

GAL1	MAG2	BGC3	XYP4	XYP5	XYP6	XYP7	GAL8	XYP9	BGC10	MAN11	BGC12	XYP13	MAG14	BGC15	MAN16	A2G17	XYP18	XYP19	MAN20
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● Molecule 8: beta-D-glucopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]beta-D-xylopyranose-(1-3)-[beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-(1-4)]beta-D-galactopyranose-(1-2)-beta-D-xylopyranose-(1-3)-beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)-beta-D-xylopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-galactopyranose

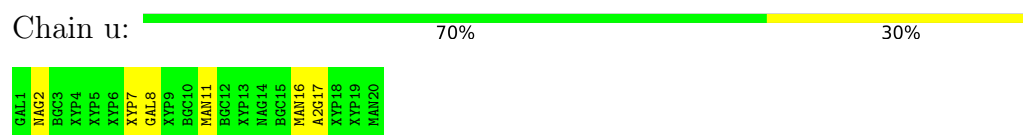
Chain U:  60% 35% 5%

GAL1	MAG2	BGC3	XYP4	XYP5	XYP6	XYP7	GAL8	XYP9	BGC10	MAN11	BGC12	XYP13	MAG14	BGC15	MAN16	A2G17	XYP18	XYP19	MAN20
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● Molecule 8: beta-D-glucopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]beta-D-xylopyranose-(1-3)-[beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-(1-4)]beta-D-galactopyranose-(1-2)-beta-D-xylopyranose-(1-3)-beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)-beta-D-xylopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-galactopyranose



- Molecule 8: beta-D-glucopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]beta-D-xylopyranose-(1-3)-[beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-(1-4)]beta-D-galactopyranose-(1-2)-beta-D-xylopyranose-(1-3)-beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)-beta-D-xylopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-galactopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-3)][alpha-D-mannopyranose-(1-4)]beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-3)][beta-D-xylopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-4)]beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-3)][alpha-D-mannopyranose-(1-4)]beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-3)][beta-D-xylopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-4)]beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-3)][alpha-D-mannopyranose-(1-4)]beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-3)][beta-D-xylopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-4)]beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-3)][alpha

a-D-mannopyranose-(1-4)]beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-3)]beta-D-xylopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-4)]beta-D-glucopyranose

Chain v:  60% 40%

BGC1  
MAN2  
BGC3  
NAG4  
BGC5  
MAN6  
BGC7  
XYP8  
XYP9  
BGC10

• Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-glucopyranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-[beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-4)]beta-D-galactopyranose-(1-3)-[beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-[beta-D-xylopyranose-(1-2)]beta-D-glucopyranose-(1-4)]beta-D-galactopyranose-(1-3)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-beta-D-glucopyranose-(1-4)]beta-D-xylopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain J:  58% 26% 16%

GAL1  
NAG2  
XYP3  
XYP4  
GAL5  
A2G6  
GAL7  
A2G8  
BGC9  
MAN10  
NAG11  
XYP12  
MAN13  
BGC14  
XYP15  
BGC16  
BGC17  
NAG18  
MAN19

• Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-glucopyranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-[beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-4)]beta-D-galactopyranose-(1-3)-[beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-[beta-D-xylopyranose-(1-2)]beta-D-glucopyranose-(1-4)]beta-D-galactopyranose-(1-3)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-beta-D-glucopyranose-(1-4)]beta-D-xylopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain W:  47% 42% 11%

GAL1  
NAG2  
XYP3  
XYP4  
GAL5  
A2G6  
GAL7  
A2G8  
BGC9  
MAN10  
NAG11  
XYP12  
MAN13  
BGC14  
XYP15  
BGC16  
BGC17  
NAG18  
MAN19

• Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-glucopyranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-[beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-4)]beta-D-galactopyranose-(1-3)-[beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-[beta-D-xylopyranose-(1-2)]beta-D-glucopyranose-(1-4)]beta-D-galactopyranose-(1-3)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-beta-D-glucopyranose-(1-4)]beta-D-xylopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain j:  37% 53% 11%

GAL1  
NAG2  
XYP3  
XYP4  
GAL5  
A2G6  
GAL7  
A2G8  
BGC9  
MAN10  
NAG11  
XYP12  
MAN13  
BGC14  
XYP15  
BGC16  
BGC17  
NAG18  
MAN19

• Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-glucopyranose-(1-4)-[2-acetamido-2-deoxy-b

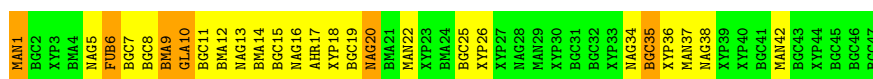
eta-D-glucopyranose-(1-3)]2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-[beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-4)]beta-D-galactopyranose-(1-3)-[beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-[beta-D-xylopyranose-(1-2)]beta-D-glucopyranose-(1-4)]beta-D-galactopyranose-(1-3)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-beta-D-glucopyranose-(1-4)]beta-D-xylopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain w: 




● Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-mannopyranose-(1-6)-beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-D-galactopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-mannopyranose-(1-4)-[beta-D-xylopyranose-(1-2)-[beta-D-xylopyranose-(1-4)]beta-D-glucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-4)]beta-D-xylopyranose-(1-3)-alpha-D-mannopyranose-(1-2)]beta-D-xylopyranose-(1-3)]beta-D-glucopyranose-(1-6)-beta-D-glucopyranose-(1-2)-beta-L-arabinofuranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)]beta-D-glucopyranose-(1-3)]beta-D-xylopyranose-(1-4)]beta-D-mannopyranose-(1-2)-[beta-D-glucopyranose-(1-4)-beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-3)-[beta-D-xylopyranose-(1-3)-[beta-D-glucopyranose-(1-4)]beta-D-glucopyranose-(1-6)]beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-4)]beta-D-glucopyranose-(1-6)-[beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose

Chain K: 



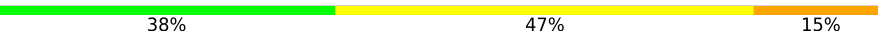
● Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-mannopyranose-(1-6)-beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-D-galactopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-mannopyranose-(1-4)-[beta-D-xylopyranose-(1-2)-[beta-D-xylopyranose-(1-4)]beta-D-glucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-4)]beta-D-xylopyranose-(1-3)-alpha-D-mannopyranose-(1-2)]beta-D-xylopyranose-(1-3)]beta-D-glucopyranose-(1-6)-beta-D-glucopyranose-(1-2)-beta-L-arabinofuranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)]beta-D-glucopyranose-(1-3)]beta-D-xylopyranose-(1-4)]beta-D-mannopyranose-(1-2)-[beta-D-glucopyranose-(1-4)-beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-3)-[beta-D-xylopyranose-(1-3)-[beta-D-glucopyranose-(1-4)]beta-D-glucopyranose-(1-6)]beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-4)]beta-D-glucopyranose-(1-6)-[beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose

e-(1-6)]beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-4)]beta-D-glucopyranose-(1-6)-[beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose

Chain X:  38% 47% 15%

MAN1	BGC2	XYF3	BMA4	NAG5	FUB6	BGC7	BGC8	BMA9	GLA10	BGC11	BMA12	NAG13	BMA14	BGC15	NAG16	AHR17	XYF18	BGC19	NAG20	BMA21	MAN22	XYF23	BMA24	BGC25	XYF26	XYF27	NAG28	MAN29	XYF30	BGC31	BGC32	XYF33	NAG34	BGC35	XYF36	MAN37	NAG38	XYF39	XYF40	BGC41	MAN42	BGC43	XYF44	BGC45	BGC46	BGC47
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● Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-mannopyranose-(1-6)-beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-D-galactopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-mannopyranose-(1-4)-[beta-D-xylopyranose-(1-2)-[beta-D-xylopyranose-(1-4)]beta-D-glucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-4)]beta-D-xylopyranose-(1-3)-alpha-D-mannopyranose-(1-2)]beta-D-xylopyranose-(1-3)]beta-D-glucopyranose-(1-6)-beta-D-glucopyranose-(1-2)-beta-L-arabinofuranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)]beta-D-glucopyranose-(1-3)]beta-D-xylopyranose-(1-4)]beta-D-mannopyranose-(1-2)-[beta-D-glucopyranose-(1-4)-beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-3)-[beta-D-xylopyranose-(1-3)-[beta-D-glucopyranose-(1-4)]beta-D-glucopyranose-(1-6)]beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-4)]beta-D-glucopyranose-(1-6)-[beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose

Chain k:  38% 47% 15%

MAN1	BGC2	XYF3	BMA4	NAG5	FUB6	BGC7	BGC8	BMA9	GLA10	BGC11	BMA12	NAG13	BMA14	BGC15	NAG16	AHR17	XYF18	BGC19	NAG20	BMA21	MAN22	XYF23	BMA24	BGC25	XYF26	XYF27	NAG28	MAN29	XYF30	BGC31	BGC32	XYF33	NAG34	BGC35	XYF36	MAN37	NAG38	XYF39	XYF40	BGC41	MAN42	BGC43	XYF44	BGC45	BGC46	BGC47
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● Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-mannopyranose-(1-6)-beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-D-galactopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-mannopyranose-(1-4)-[beta-D-xylopyranose-(1-2)-[beta-D-xylopyranose-(1-4)]beta-D-glucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-4)]beta-D-xylopyranose-(1-3)-alpha-D-mannopyranose-(1-2)]beta-D-xylopyranose-(1-3)]beta-D-glucopyranose-(1-6)-beta-D-glucopyranose-(1-2)-beta-L-arabinofuranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)]beta-D-glucopyranose-(1-3)]beta-D-xylopyranose-(1-4)]beta-D-mannopyranose-(1-2)-[beta-D-glucopyranose-(1-4)-beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-3)-[beta-D-xylopyranose-(1-3)-[beta-D-glucopyranose-(1-4)]beta-D-glucopyranose-(1-6)]beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-4)]beta-D-glucopyranose-(1-6)-[beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose

Chain x:  40% 43% 17%





- Molecule 12: beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]beta-D-glucopyranose-(1-3)-[beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-3)-beta-D-galactopyranose



- Molecule 12: beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]beta-D-glucopyranose-(1-3)-[beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-3)-beta-D-galactopyranose



- Molecule 12: beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]beta-D-glucopyranose-(1-3)-[beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-3)-beta-D-galactopyranose



- Molecule 12: beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]beta-D-glucopyranose-(1-3)-[beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-3)-beta-D-galactopyranose



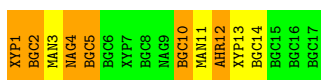
- Molecule 13: beta-D-glucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-xylopyranose-(1-4)-[beta-D-glucopyranose-(1-2)]alpha-D-mannopyranose-(1-3)]beta-D-glucopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose

Chain M:  41% 35% 24%



• Molecule 13: beta-D-glucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta a-D-xylopyranose-(1-4)-[beta-D-glucopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-glucopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose

Chain Z:  41% 24% 35%



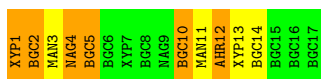
• Molecule 13: beta-D-glucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta a-D-xylopyranose-(1-4)-[beta-D-glucopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-glucopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose

Chain m:  41% 24% 35%



• Molecule 13: beta-D-glucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta a-D-xylopyranose-(1-4)-[beta-D-glucopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-glucopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose

Chain z:  41% 24% 35%



• Molecule 14: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)-alpha-L-arabinofuranose-(1-2)-[beta-D-xylopyranose-(1-3)-[alpha-L-arabinofuranose-(1-4)]beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-2)]beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-(1-3)][beta-D-xylopyranose-(1-6)]beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)][alpha-L-arabinofuranose-(1-2)-beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-4)-alpha-D-mannopyranose

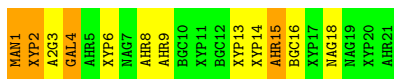


Chain N:  43% 38% 19%



• Molecule 14: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)-alpha-L-arabinofuranose-(1-2)-[beta-D-xylopyranose-(1-3)-[alpha-L-arabinofuranose-(1-4)]beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-2)]beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-(1-3)][beta-D-xylopyranose-(1-6)]beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)][alpha-L-arabinofuranose-(1-2)-beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-4)-alpha-D-mannopyranose

Chain a:  43% 38% 19%



• Molecule 14: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)-alpha-L-arabinofuranose-(1-2)-[beta-D-xylopyranose-(1-3)-[alpha-L-arabinofuranose-(1-4)]beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-2)]beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-(1-3)][beta-D-xylopyranose-(1-6)]beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)][alpha-L-arabinofuranose-(1-2)-beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-4)-alpha-D-mannopyranose

Chain n:  43% 38% 19%



• Molecule 14: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)-alpha-L-arabinofuranose-(1-2)-[beta-D-xylopyranose-(1-3)-[alpha-L-arabinofuranose-(1-4)]beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-2)]beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-(1-3)][beta-D-xylopyranose-(1-6)]beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)][alpha-L-arabinofuranose-(1-2)-beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-4)-alpha-D-mannopyranose

Chain 0:  48% 38% 14%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=85.1°, rise=32.7 Å, axial sym=C1	Depositor
Number of segments used	70391	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.456	Depositor
Minimum map value	-1.176	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.073	Depositor
Recommended contour level	0.202	Depositor
Map size (Å)	421.59363, 421.59363, 421.59363	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	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: FUB, A2G, BGC, AHR, GAL, XYP, BMA, GLA, GZL, MAN, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.03	0/2427	0.97	0/3277

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	2412	0	2235	135	0
2	B	105	0	88	3	0
2	O	105	0	88	3	0
2	b	105	0	88	3	0
2	o	105	0	88	3	0
3	C	359	0	206	8	0
3	P	359	0	206	7	0
3	c	359	0	206	8	0
3	p	359	0	206	7	0
4	D	274	0	160	6	0
4	Q	274	0	160	5	0
4	d	274	0	160	5	0
4	q	274	0	160	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	25	0	22	1	0
5	R	25	0	22	1	0
5	e	25	0	22	1	0
5	r	25	0	22	1	0
6	F	45	0	30	2	0
6	S	45	0	30	2	0
6	f	45	0	30	2	0
6	s	45	0	30	2	0
7	G	237	0	142	6	0
7	T	237	0	142	12	0
7	g	237	0	142	11	0
7	t	237	0	142	12	0
8	H	213	0	117	9	0
8	U	213	0	117	10	0
8	h	213	0	117	10	0
8	u	213	0	117	2	0
9	I	109	0	75	0	0
9	V	109	0	75	3	0
9	i	109	0	75	2	0
9	v	109	0	75	2	0
10	J	216	0	148	12	0
10	W	216	0	148	10	0
10	j	216	0	148	5	0
10	w	216	0	148	3	0
11	K	512	0	325	8	0
11	X	512	0	325	17	0
11	k	512	0	325	15	0
11	x	512	0	325	11	0
12	L	107	0	67	2	0
12	Y	107	0	67	3	0
12	l	107	0	67	4	0
12	y	107	0	67	3	0
13	M	185	0	124	9	0
13	Z	185	0	124	10	0
13	m	185	0	124	9	0
13	z	185	0	124	9	0
14	0	219	0	92	7	0
14	N	219	0	92	10	0
14	a	219	0	92	10	0
14	n	219	0	92	9	0
All	All	12836	0	8619	338	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 16.

The worst 5 of 338 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)
11:x:1:MAN:H62	11:x:6:FUB:C5	1.92	1.00
11:k:1:MAN:H62	11:k:6:FUB:C5	1.92	1.00
11:K:1:MAN:H62	11:K:6:FUB:C5	1.91	0.99
11:X:1:MAN:H62	11:X:6:FUB:C5	1.91	0.99
4:D:25:BGC:H6C1	9:V:5:BGC:O3	1.63	0.98

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	342/344 (99%)	306 (90%)	29 (8%)	7 (2%)	6	27

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	SER
1	A	181	SER
1	A	267	SER
1	A	353	SER
1	A	417	GLY

### 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	288/288 (100%)	271 (94%)	17 (6%)	18	46

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	SER
1	A	427	ILE
1	A	252	SER
1	A	330	VAL
1	A	336	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	229	GLN
1	A	315	GLN
1	A	401	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

964 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
14	MAN	0	1	14,1	11,11,12	0.85	0	15,15,17	2.95	5 (33%)
14	BGC	0	10	14	11,11,12	0.20	0	15,15,17	0.50	0
14	XYP	0	11	14	9,9,10	0.18	0	10,12,14	0.50	0
14	BGC	0	12	14	11,11,12	0.18	0	15,15,17	0.56	0
14	XYP	0	13	14	9,9,10	0.17	0	10,12,14	0.60	0
14	XYP	0	14	14	9,9,10	0.18	0	10,12,14	0.62	0
14	AHR	0	15	14	9,9,10	0.57	0	10,12,14	1.01	1 (10%)
14	BGC	0	16	14	11,11,12	0.18	0	15,15,17	0.55	0
14	XYP	0	17	14	9,9,10	0.20	0	10,12,14	0.64	0
14	NAG	0	18	14	14,14,15	0.28	0	17,19,21	0.66	0
14	NAG	0	19	14	14,14,15	0.34	0	17,19,21	0.84	0
14	XYP	0	2	14	9,9,10	0.19	0	10,12,14	0.91	1 (10%)
14	XYP	0	20	14	9,9,10	0.30	0	10,12,14	0.58	0
14	AHR	0	21	14	9,9,10	0.51	0	10,12,14	0.77	0
14	A2G	0	3	14	14,14,15	0.40	0	17,19,21	0.88	2 (11%)
14	GAL	0	4	14	11,11,12	0.22	0	15,15,17	0.87	1 (6%)
14	AHR	0	5	14	9,9,10	0.50	0	10,12,14	0.77	0
14	XYP	0	6	14	9,9,10	0.19	0	10,12,14	0.76	0
14	NAG	0	7	14	14,14,15	0.32	0	17,19,21	0.70	0
14	AHR	0	8	14	9,9,10	0.59	0	10,12,14	1.04	1 (10%)
14	AHR	0	9	14	9,9,10	0.58	0	10,12,14	1.00	1 (10%)
2	BGC	B	1	2,1	11,11,12	0.35	0	15,15,17	0.61	0
2	NAG	B	2	2	14,14,15	0.29	0	17,19,21	0.85	1 (5%)
2	GAL	B	3	2	11,11,12	0.18	0	15,15,17	0.60	0
2	MAN	B	4	2	11,11,12	0.24	0	15,15,17	0.78	1 (6%)
2	BGC	B	5	2	11,11,12	0.19	0	15,15,17	0.56	0
2	NAG	B	6	2	14,14,15	0.88	1 (7%)	17,19,21	1.40	4 (23%)
2	BMA	B	7	2	11,11,12	0.22	0	15,15,17	0.74	0
2	GAL	B	8	2	11,11,12	0.16	0	15,15,17	0.63	0
2	MAN	B	9	2	11,11,12	0.21	0	15,15,17	0.78	0
3	GLA	C	1	3,1	11,11,12	0.18	0	15,15,17	0.63	0
3	XYP	C	10	3	9,9,10	0.30	0	10,12,14	0.57	0
3	NAG	C	11	3	14,14,15	0.51	0	17,19,21	1.06	1 (5%)
3	MAN	C	12	3	11,11,12	0.36	0	15,15,17	1.37	2 (13%)
3	NAG	C	13	3	14,14,15	0.29	0	17,19,21	0.70	0
3	XYP	C	14	3	9,9,10	0.19	0	10,12,14	0.60	0
3	BGC	C	15	3	11,11,12	0.18	0	15,15,17	0.56	0
3	BGC	C	16	3	11,11,12	0.18	0	15,15,17	0.57	0
3	XYP	C	17	3	9,9,10	0.20	0	10,12,14	0.63	0
3	BGC	C	18	3	11,11,12	0.19	0	15,15,17	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BGC	C	19	3	11,11,12	0.20	0	15,15,17	0.58	0
3	BGC	C	2	3	11,11,12	0.70	0	15,15,17	1.24	2 (13%)
3	XYP	C	20	3	9,9,10	0.18	0	10,12,14	0.61	0
3	NAG	C	21	3	14,14,15	0.28	0	17,19,21	0.73	0
3	XYP	C	22	3	9,9,10	0.18	0	10,12,14	0.53	0
3	XYP	C	23	3	9,9,10	0.19	0	10,12,14	0.57	0
3	GAL	C	24	3	11,11,12	0.18	0	15,15,17	0.58	0
3	BGC	C	25	3	11,11,12	0.20	0	15,15,17	0.64	0
3	GAL	C	26	3	11,11,12	0.17	0	15,15,17	0.57	0
3	BGC	C	27	3	11,11,12	0.17	0	15,15,17	0.57	0
3	XYP	C	28	3	9,9,10	0.19	0	10,12,14	0.62	0
3	BGC	C	29	3	11,11,12	0.18	0	15,15,17	0.57	0
3	BGC	C	3	3	11,11,12	0.18	0	15,15,17	0.47	0
3	BGC	C	30	3	11,11,12	0.19	0	15,15,17	0.58	0
3	BGC	C	31	3	11,11,12	0.21	0	15,15,17	0.58	0
3	BGC	C	32	3	11,11,12	0.20	0	15,15,17	0.57	0
3	XYP	C	33	3	9,9,10	0.19	0	10,12,14	0.61	0
3	XYP	C	34	3	9,9,10	0.16	0	10,12,14	0.61	0
3	GAL	C	4	3	11,11,12	0.16	0	15,15,17	0.59	0
3	XYP	C	5	3	9,9,10	0.18	0	10,12,14	0.60	0
3	XYP	C	6	3	9,9,10	0.19	0	10,12,14	1.24	1 (10%)
3	BGC	C	7	3	11,11,12	0.19	0	15,15,17	0.82	1 (6%)
3	XYP	C	8	3	9,9,10	0.21	0	10,12,14	0.54	0
3	BGC	C	9	3	11,11,12	0.20	0	15,15,17	0.53	0
4	MAN	D	1	4,1	11,11,12	0.21	0	15,15,17	0.78	0
4	XYP	D	10	4	9,9,10	0.17	0	10,12,14	0.61	0
4	MAN	D	11	4	11,11,12	0.80	1 (9%)	15,15,17	0.80	0
4	AHR	D	12	4	9,9,10	0.58	0	10,12,14	1.03	1 (10%)
4	FUB	D	13	4	9,9,10	0.52	0	10,12,14	0.57	0
4	NAG	D	14	4	14,14,15	0.30	0	17,19,21	0.65	0
4	XYP	D	15	4	9,9,10	0.24	0	10,12,14	0.70	0
4	FUB	D	16	4	9,9,10	0.57	0	10,12,14	0.94	0
4	AHR	D	17	4	9,9,10	0.58	0	10,12,14	1.03	1 (10%)
4	MAN	D	18	4	11,11,12	0.22	0	15,15,17	0.80	1 (6%)
4	BGC	D	19	4	11,11,12	0.18	0	15,15,17	0.57	0
4	AHR	D	2	4	9,9,10	0.59	0	10,12,14	1.03	1 (10%)
4	BGC	D	20	4	11,11,12	0.19	0	15,15,17	0.60	0
4	BGC	D	21	4	11,11,12	0.18	0	15,15,17	0.58	0
4	FUB	D	22	4	9,9,10	0.58	0	10,12,14	1.05	1 (10%)
4	BGC	D	23	4	11,11,12	0.20	0	15,15,17	0.60	0
4	BGC	D	24	4	11,11,12	0.19	0	15,15,17	0.58	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BGC	D	25	4	11,11,12	0.18	0	15,15,17	0.58	0
4	AHR	D	26	4	9,9,10	0.58	0	10,12,14	1.03	1 (10%)
4	BGC	D	3	4	11,11,12	0.21	0	15,15,17	0.60	0
4	MAN	D	4	4	11,11,12	0.23	0	15,15,17	0.76	0
4	BGC	D	5	4	11,11,12	0.19	0	15,15,17	0.73	0
4	BMA	D	6	4	11,11,12	0.41	0	15,15,17	1.14	1 (6%)
4	NAG	D	7	4	14,14,15	0.77	0	17,19,21	1.59	3 (17%)
4	BGC	D	8	4	11,11,12	0.63	0	15,15,17	0.77	0
4	BGC	D	9	4	11,11,12	0.20	0	15,15,17	0.55	0
5	MAN	E	1	5,1	11,11,12	0.22	0	15,15,17	0.77	1 (6%)
5	NAG	E	2	5	14,14,15	0.28	0	17,19,21	0.65	0
6	MAN	F	1	6,1	11,11,12	0.24	0	15,15,17	0.79	1 (6%)
6	GZL	F	2	6	11,11,12	6.70	7 (63%)	14,15,17	1.43	2 (14%)
6	FUB	F	3	6	9,9,10	0.55	0	10,12,14	1.03	1 (10%)
6	NAG	F	4	6	14,14,15	0.28	0	17,19,21	0.63	0
7	XYP	G	1	7	9,9,10	0.84	1 (11%)	10,12,14	2.58	3 (30%)
7	MAN	G	10	7	11,11,12	0.51	0	15,15,17	0.86	1 (6%)
7	MAN	G	11	7	11,11,12	0.22	0	15,15,17	0.77	0
7	BGC	G	12	7	11,11,12	0.19	0	15,15,17	0.55	0
7	BGC	G	13	7	11,11,12	0.20	0	15,15,17	0.57	0
7	XYP	G	14	7	9,9,10	0.19	0	10,12,14	0.60	0
7	MAN	G	15	7	11,11,12	0.22	0	15,15,17	0.80	1 (6%)
7	NAG	G	16	7	14,14,15	0.39	0	17,19,21	1.23	2 (11%)
7	BGC	G	17	7	11,11,12	0.18	0	15,15,17	0.52	0
7	BGC	G	18	7	11,11,12	0.22	0	15,15,17	0.58	0
7	XYP	G	19	7	9,9,10	0.20	0	10,12,14	0.61	0
7	BGC	G	2	7	11,11,12	0.18	0	15,15,17	0.57	0
7	XYP	G	20	7	9,9,10	0.31	0	10,12,14	0.58	0
7	XYP	G	21	7	9,9,10	0.39	0	10,12,14	0.66	0
7	XYP	G	22	7	9,9,10	0.26	0	10,12,14	0.71	0
7	A2G	G	3	7	14,14,15	0.42	0	17,19,21	1.02	2 (11%)
7	BGC	G	4	7	11,11,12	0.20	0	15,15,17	0.61	0
7	BGC	G	5	7	11,11,12	0.18	0	15,15,17	0.67	0
7	XYP	G	6	7	9,9,10	0.19	0	10,12,14	0.60	0
7	A2G	G	7	7	14,14,15	0.44	0	17,19,21	0.95	1 (5%)
7	MAN	G	8	7	11,11,12	0.47	0	15,15,17	0.84	1 (6%)
7	MAN	G	9	7	11,11,12	0.23	0	15,15,17	0.79	0
8	GAL	H	1	8	11,11,12	0.17	0	15,15,17	0.63	0
8	BGC	H	10	8	11,11,12	0.21	0	15,15,17	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	MAN	H	11	8	11,11,12	0.21	0	15,15,17	0.82	2 (13%)
8	BGC	H	12	8	11,11,12	0.19	0	15,15,17	0.56	0
8	XYP	H	13	8	9,9,10	0.19	0	10,12,14	0.61	0
8	NAG	H	14	8	14,14,15	0.28	0	17,19,21	0.55	0
8	BGC	H	15	8	11,11,12	0.20	0	15,15,17	0.57	0
8	MAN	H	16	8	11,11,12	0.45	0	15,15,17	0.98	2 (13%)
8	A2G	H	17	8	14,14,15	0.40	0	17,19,21	0.69	0
8	XYP	H	18	8	9,9,10	0.18	0	10,12,14	0.60	0
8	XYP	H	19	8	9,9,10	0.19	0	10,12,14	0.61	0
8	NAG	H	2	8	14,14,15	0.28	0	17,19,21	0.72	0
8	MAN	H	20	8	11,11,12	0.52	0	15,15,17	0.59	0
8	BGC	H	3	8	11,11,12	0.19	0	15,15,17	0.72	0
8	XYP	H	4	8	9,9,10	0.18	0	10,12,14	0.70	0
8	XYP	H	5	8	9,9,10	0.20	0	10,12,14	0.55	0
8	XYP	H	6	8	9,9,10	0.21	0	10,12,14	0.52	0
8	XYP	H	7	8	9,9,10	0.19	0	10,12,14	1.03	2 (20%)
8	GAL	H	8	8	11,11,12	0.22	0	15,15,17	0.64	1 (6%)
8	XYP	H	9	8	9,9,10	0.19	0	10,12,14	0.58	0
9	BGC	I	1	9,1	11,11,12	0.17	0	15,15,17	0.59	0
9	BGC	I	10	9	11,11,12	0.20	0	15,15,17	0.58	0
9	MAN	I	2	9	11,11,12	0.22	0	15,15,17	0.96	1 (6%)
9	BGC	I	3	9	11,11,12	0.25	0	15,15,17	0.88	1 (6%)
9	NAG	I	4	9	14,14,15	0.36	0	17,19,21	0.88	1 (5%)
9	BGC	I	5	9	11,11,12	0.18	0	15,15,17	0.54	0
9	MAN	I	6	9	11,11,12	0.49	0	15,15,17	0.79	1 (6%)
9	BGC	I	7	9	11,11,12	0.20	0	15,15,17	0.57	0
9	XYP	I	8	9	9,9,10	0.18	0	10,12,14	0.60	0
9	XYP	I	9	9	9,9,10	0.19	0	10,12,14	0.60	0
10	GAL	J	1	10	11,11,12	0.16	0	15,15,17	0.64	0
10	MAN	J	10	10	11,11,12	0.58	0	15,15,17	0.59	0
10	NAG	J	11	10	14,14,15	0.60	0	17,19,21	0.90	0
10	XYP	J	12	10	9,9,10	0.18	0	10,12,14	0.62	0
10	MAN	J	13	10	11,11,12	0.20	0	15,15,17	0.80	1 (6%)
10	BGC	J	14	10	11,11,12	0.19	0	15,15,17	0.52	0
10	XYP	J	15	10	9,9,10	0.20	0	10,12,14	0.59	0
10	BGC	J	16	10	11,11,12	0.19	0	15,15,17	0.55	0
10	BGC	J	17	10	11,11,12	0.20	0	15,15,17	0.56	0
10	NAG	J	18	10	14,14,15	0.58	0	17,19,21	1.39	2 (11%)
10	MAN	J	19	10	11,11,12	0.95	1 (9%)	15,15,17	1.28	2 (13%)
10	NAG	J	2	10	14,14,15	0.31	0	17,19,21	1.52	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	XYP	J	3	10	9,9,10	0.19	0	10,12,14	0.58	0
10	XYP	J	4	10	9,9,10	0.19	0	10,12,14	0.57	0
10	GAL	J	5	10	11,11,12	0.17	0	15,15,17	0.60	0
10	A2G	J	6	10	14,14,15	0.42	0	17,19,21	1.48	3 (17%)
10	GAL	J	7	10	11,11,12	0.18	0	15,15,17	0.58	0
10	A2G	J	8	10	14,14,15	0.46	0	17,19,21	1.07	1 (5%)
10	BGC	J	9	10	11,11,12	0.81	1 (9%)	15,15,17	0.90	1 (6%)
11	MAN	K	1	11,1	11,11,12	0.26	0	15,15,17	0.84	1 (6%)
11	GLA	K	10	11	11,11,12	0.41	0	15,15,17	1.13	1 (6%)
11	BGC	K	11	11	11,11,12	0.76	0	15,15,17	2.13	5 (33%)
11	BMA	K	12	11	11,11,12	1.01	1 (9%)	15,15,17	2.48	3 (20%)
11	NAG	K	13	11	14,14,15	0.85	0	17,19,21	1.71	5 (29%)
11	BMA	K	14	11	11,11,12	0.75	0	15,15,17	2.44	3 (20%)
11	BGC	K	15	11	11,11,12	0.69	0	15,15,17	1.05	1 (6%)
11	NAG	K	16	11	14,14,15	0.80	0	17,19,21	1.32	3 (17%)
11	AHR	K	17	11	9,9,10	0.62	0	10,12,14	1.08	1 (10%)
11	XYP	K	18	11	9,9,10	0.26	0	10,12,14	1.13	1 (10%)
11	BGC	K	19	11	11,11,12	0.40	0	15,15,17	1.13	1 (6%)
11	BGC	K	2	11	11,11,12	0.19	0	15,15,17	0.62	0
11	NAG	K	20	11	14,14,15	0.80	0	17,19,21	1.70	4 (23%)
11	BMA	K	21	11	11,11,12	0.21	0	15,15,17	0.53	0
11	MAN	K	22	11	11,11,12	0.21	0	15,15,17	0.79	1 (6%)
11	XYP	K	23	11	9,9,10	0.20	0	10,12,14	0.60	0
11	BMA	K	24	11	11,11,12	0.23	0	15,15,17	0.80	0
11	BGC	K	25	11	11,11,12	0.22	0	15,15,17	0.82	1 (6%)
11	XYP	K	26	11	9,9,10	0.23	0	10,12,14	0.60	0
11	XYP	K	27	11	9,9,10	0.19	0	10,12,14	0.64	0
11	NAG	K	28	11	14,14,15	0.30	0	17,19,21	0.61	0
11	MAN	K	29	11	11,11,12	0.22	0	15,15,17	0.79	0
11	XYP	K	3	11	9,9,10	0.19	0	10,12,14	0.60	0
11	XYP	K	30	11	9,9,10	0.21	0	10,12,14	0.62	0
11	BGC	K	31	11	11,11,12	0.19	0	15,15,17	0.61	0
11	BGC	K	32	11	11,11,12	0.18	0	15,15,17	0.58	0
11	XYP	K	33	11	9,9,10	0.21	0	10,12,14	0.61	0
11	NAG	K	34	11	14,14,15	0.26	0	17,19,21	0.56	0
11	BGC	K	35	11	11,11,12	0.20	0	15,15,17	0.95	1 (6%)
11	XYP	K	36	11	9,9,10	0.38	0	10,12,14	0.49	0
11	MAN	K	37	11	11,11,12	0.37	0	15,15,17	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NAG	K	38	11	14,14,15	0.29	0	17,19,21	0.72	1 (5%)
11	XYP	K	39	11	9,9,10	0.19	0	10,12,14	0.60	0
11	BMA	K	4	11	11,11,12	0.24	0	15,15,17	0.43	0
11	XYP	K	40	11	9,9,10	0.18	0	10,12,14	0.63	0
11	BGC	K	41	11	11,11,12	0.19	0	15,15,17	0.59	0
11	MAN	K	42	11	11,11,12	0.22	0	15,15,17	0.82	1 (6%)
11	BGC	K	43	11	11,11,12	0.19	0	15,15,17	0.56	0
11	XYP	K	44	11	9,9,10	0.18	0	10,12,14	0.62	0
11	BGC	K	45	11	11,11,12	0.19	0	15,15,17	0.57	0
11	BGC	K	46	11	11,11,12	0.21	0	15,15,17	0.55	0
11	BGC	K	47	11	11,11,12	0.19	0	15,15,17	0.57	0
11	NAG	K	5	11	14,14,15	0.32	0	17,19,21	0.61	0
11	FUB	K	6	11	9,9,10	0.61	0	10,12,14	1.14	2 (20%)
11	BGC	K	7	11	11,11,12	0.46	0	15,15,17	1.56	3 (20%)
11	BGC	K	8	11	11,11,12	0.85	0	15,15,17	1.46	3 (20%)
11	BMA	K	9	11	11,11,12	0.87	0	15,15,17	2.56	3 (20%)
12	GAL	L	1	12	11,11,12	0.18	0	15,15,17	0.63	0
12	XYP	L	10	12	9,9,10	0.18	0	10,12,14	0.62	0
12	XYP	L	2	12	9,9,10	0.19	0	10,12,14	0.64	0
12	BGC	L	3	12	11,11,12	0.21	0	15,15,17	0.53	0
12	XYP	L	4	12	9,9,10	0.19	0	10,12,14	0.62	0
12	BGC	L	5	12	11,11,12	0.81	0	15,15,17	2.33	5 (33%)
12	MAN	L	6	12	11,11,12	0.80	0	15,15,17	1.36	1 (6%)
12	BGC	L	7	12	11,11,12	0.64	0	15,15,17	1.97	3 (20%)
12	BGC	L	8	12	11,11,12	0.90	1 (9%)	15,15,17	1.22	3 (20%)
12	NAG	L	9	12	14,14,15	0.55	0	17,19,21	1.39	1 (5%)
13	XYP	M	1	13	9,9,10	0.32	0	10,12,14	1.55	2 (20%)
13	BGC	M	10	13	11,11,12	0.63	0	15,15,17	1.56	3 (20%)
13	MAN	M	11	13	11,11,12	0.23	0	15,15,17	0.79	1 (6%)
13	AHR	M	12	13	9,9,10	0.71	0	10,12,14	1.43	1 (10%)
13	XYP	M	13	13	9,9,10	0.29	0	10,12,14	0.87	0
13	BGC	M	14	13	11,11,12	0.72	0	15,15,17	2.10	6 (40%)
13	BGC	M	15	13	11,11,12	0.53	0	15,15,17	1.08	0
13	BGC	M	16	13	11,11,12	0.18	0	15,15,17	0.53	0
13	BGC	M	17	13	11,11,12	0.20	0	15,15,17	0.56	0
13	BGC	M	2	13	11,11,12	1.21	2 (18%)	15,15,17	2.51	5 (33%)
13	MAN	M	3	13	11,11,12	0.22	0	15,15,17	0.83	1 (6%)
13	NAG	M	4	13	14,14,15	0.88	0	17,19,21	1.56	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	BGC	M	5	13	11,11,12	1.13	1 (9%)	15,15,17	2.19	7 (46%)
13	BGC	M	6	13	11,11,12	0.18	0	15,15,17	0.63	0
13	XYP	M	7	13	9,9,10	0.17	0	10,12,14	0.59	0
13	BGC	M	8	13	11,11,12	0.20	0	15,15,17	0.58	0
13	NAG	M	9	13	14,14,15	0.30	0	17,19,21	0.64	0
14	MAN	N	1	14,1	11,11,12	0.86	0	15,15,17	2.94	5 (33%)
14	BGC	N	10	14	11,11,12	0.20	0	15,15,17	0.50	0
14	XYP	N	11	14	9,9,10	0.20	0	10,12,14	0.49	0
14	BGC	N	12	14	11,11,12	0.18	0	15,15,17	0.56	0
14	XYP	N	13	14	9,9,10	0.17	0	10,12,14	0.60	0
14	XYP	N	14	14	9,9,10	0.18	0	10,12,14	0.61	0
14	AHR	N	15	14	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
14	BGC	N	16	14	11,11,12	0.18	0	15,15,17	0.55	0
14	XYP	N	17	14	9,9,10	0.19	0	10,12,14	0.65	0
14	NAG	N	18	14	14,14,15	0.26	0	17,19,21	0.66	0
14	NAG	N	19	14	14,14,15	0.33	0	17,19,21	0.84	0
14	XYP	N	2	14	9,9,10	0.20	0	10,12,14	0.91	1 (10%)
14	XYP	N	20	14	9,9,10	0.31	0	10,12,14	0.56	0
14	AHR	N	21	14	9,9,10	0.51	0	10,12,14	0.77	0
14	A2G	N	3	14	14,14,15	0.40	0	17,19,21	0.89	2 (11%)
14	GAL	N	4	14	11,11,12	0.22	0	15,15,17	0.87	1 (6%)
14	AHR	N	5	14	9,9,10	0.51	0	10,12,14	0.78	0
14	XYP	N	6	14	9,9,10	0.19	0	10,12,14	0.76	0
14	NAG	N	7	14	14,14,15	0.32	0	17,19,21	0.70	0
14	AHR	N	8	14	9,9,10	0.59	0	10,12,14	1.03	1 (10%)
14	AHR	N	9	14	9,9,10	0.60	0	10,12,14	1.00	1 (10%)
2	BGC	O	1	2,1	11,11,12	0.33	0	15,15,17	0.61	0
2	NAG	O	2	2	14,14,15	0.29	0	17,19,21	0.85	1 (5%)
2	GAL	O	3	2	11,11,12	0.17	0	15,15,17	0.60	0
2	MAN	O	4	2	11,11,12	0.23	0	15,15,17	0.78	1 (6%)
2	BGC	O	5	2	11,11,12	0.20	0	15,15,17	0.57	0
2	NAG	O	6	2	14,14,15	0.88	1 (7%)	17,19,21	1.40	4 (23%)
2	BMA	O	7	2	11,11,12	0.22	0	15,15,17	0.73	0
2	GAL	O	8	2	11,11,12	0.17	0	15,15,17	0.61	0
2	MAN	O	9	2	11,11,12	0.22	0	15,15,17	0.79	1 (6%)
3	GLA	P	1	3,1	11,11,12	0.18	0	15,15,17	0.63	0
3	XYP	P	10	3	9,9,10	0.30	0	10,12,14	0.58	0
3	NAG	P	11	3	14,14,15	0.53	0	17,19,21	1.12	1 (5%)
3	MAN	P	12	3	11,11,12	0.34	0	15,15,17	1.31	1 (6%)
3	NAG	P	13	3	14,14,15	0.30	0	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	XYP	P	14	3	9,9,10	0.18	0	10,12,14	0.60	0
3	BGC	P	15	3	11,11,12	0.19	0	15,15,17	0.56	0
3	BGC	P	16	3	11,11,12	0.19	0	15,15,17	0.57	0
3	XYP	P	17	3	9,9,10	0.19	0	10,12,14	0.63	0
3	BGC	P	18	3	11,11,12	0.18	0	15,15,17	0.47	0
3	BGC	P	19	3	11,11,12	0.20	0	15,15,17	0.58	0
3	BGC	P	2	3	11,11,12	0.71	0	15,15,17	1.24	2 (13%)
3	XYP	P	20	3	9,9,10	0.19	0	10,12,14	0.60	0
3	NAG	P	21	3	14,14,15	0.28	0	17,19,21	0.73	0
3	XYP	P	22	3	9,9,10	0.18	0	10,12,14	0.53	0
3	XYP	P	23	3	9,9,10	0.18	0	10,12,14	0.57	0
3	GAL	P	24	3	11,11,12	0.17	0	15,15,17	0.58	0
3	BGC	P	25	3	11,11,12	0.19	0	15,15,17	0.65	0
3	GAL	P	26	3	11,11,12	0.17	0	15,15,17	0.57	0
3	BGC	P	27	3	11,11,12	0.20	0	15,15,17	0.58	0
3	XYP	P	28	3	9,9,10	0.18	0	10,12,14	0.62	0
3	BGC	P	29	3	11,11,12	0.17	0	15,15,17	0.59	0
3	BGC	P	3	3	11,11,12	0.18	0	15,15,17	0.47	0
3	BGC	P	30	3	11,11,12	0.20	0	15,15,17	0.57	0
3	BGC	P	31	3	11,11,12	0.21	0	15,15,17	0.58	0
3	BGC	P	32	3	11,11,12	0.19	0	15,15,17	0.57	0
3	XYP	P	33	3	9,9,10	0.19	0	10,12,14	0.61	0
3	XYP	P	34	3	9,9,10	0.18	0	10,12,14	0.60	0
3	GAL	P	4	3	11,11,12	0.16	0	15,15,17	0.59	0
3	XYP	P	5	3	9,9,10	0.18	0	10,12,14	0.59	0
3	XYP	P	6	3	9,9,10	0.21	0	10,12,14	1.23	1 (10%)
3	BGC	P	7	3	11,11,12	0.21	0	15,15,17	0.82	1 (6%)
3	XYP	P	8	3	9,9,10	0.20	0	10,12,14	0.53	0
3	BGC	P	9	3	11,11,12	0.21	0	15,15,17	0.54	0
4	MAN	Q	1	4,1	11,11,12	0.21	0	15,15,17	0.78	0
4	XYP	Q	10	4	9,9,10	0.18	0	10,12,14	0.60	0
4	MAN	Q	11	4	11,11,12	0.80	1 (9%)	15,15,17	0.79	0
4	AHR	Q	12	4	9,9,10	0.60	0	10,12,14	1.02	1 (10%)
4	FUB	Q	13	4	9,9,10	0.53	0	10,12,14	0.57	0
4	NAG	Q	14	4	14,14,15	0.31	0	17,19,21	0.65	0
4	XYP	Q	15	4	9,9,10	0.26	0	10,12,14	0.71	0
4	FUB	Q	16	4	9,9,10	0.58	0	10,12,14	0.94	0
4	AHR	Q	17	4	9,9,10	0.59	0	10,12,14	1.03	1 (10%)
4	MAN	Q	18	4	11,11,12	0.22	0	15,15,17	0.81	2 (13%)
4	BGC	Q	19	4	11,11,12	0.20	0	15,15,17	0.56	0
4	AHR	Q	2	4	9,9,10	0.57	0	10,12,14	1.03	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BGC	Q	20	4	11,11,12	0.19	0	15,15,17	0.60	0
4	BGC	Q	21	4	11,11,12	0.19	0	15,15,17	0.58	0
4	FUB	Q	22	4	9,9,10	0.55	0	10,12,14	1.04	1 (10%)
4	BGC	Q	23	4	11,11,12	0.19	0	15,15,17	0.60	0
4	BGC	Q	24	4	11,11,12	0.19	0	15,15,17	0.58	0
4	BGC	Q	25	4	11,11,12	0.19	0	15,15,17	0.57	0
4	AHR	Q	26	4	9,9,10	0.59	0	10,12,14	1.03	1 (10%)
4	BGC	Q	3	4	11,11,12	0.20	0	15,15,17	0.59	0
4	MAN	Q	4	4	11,11,12	0.22	0	15,15,17	0.77	0
4	BGC	Q	5	4	11,11,12	0.20	0	15,15,17	0.72	0
4	BMA	Q	6	4	11,11,12	0.40	0	15,15,17	1.14	1 (6%)
4	NAG	Q	7	4	14,14,15	0.77	0	17,19,21	1.59	3 (17%)
4	BGC	Q	8	4	11,11,12	0.64	0	15,15,17	0.77	0
4	BGC	Q	9	4	11,11,12	0.19	0	15,15,17	0.56	0
5	MAN	R	1	5,1	11,11,12	0.22	0	15,15,17	0.78	1 (6%)
5	NAG	R	2	5	14,14,15	0.28	0	17,19,21	0.65	0
6	MAN	S	1	6,1	11,11,12	0.24	0	15,15,17	0.78	1 (6%)
6	GZL	S	2	6	11,11,12	6.71	7 (63%)	14,15,17	1.43	2 (14%)
6	FUB	S	3	6	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
6	NAG	S	4	6	14,14,15	0.27	0	17,19,21	0.64	0
7	XYP	T	1	7	9,9,10	0.86	1 (11%)	10,12,14	2.57	3 (30%)
7	MAN	T	10	7	11,11,12	0.52	0	15,15,17	0.87	1 (6%)
7	MAN	T	11	7	11,11,12	0.21	0	15,15,17	0.79	1 (6%)
7	BGC	T	12	7	11,11,12	0.21	0	15,15,17	0.56	0
7	BGC	T	13	7	11,11,12	0.20	0	15,15,17	0.57	0
7	XYP	T	14	7	9,9,10	0.19	0	10,12,14	0.61	0
7	MAN	T	15	7	11,11,12	0.21	0	15,15,17	0.81	2 (13%)
7	NAG	T	16	7	14,14,15	0.39	0	17,19,21	1.23	2 (11%)
7	BGC	T	17	7	11,11,12	0.18	0	15,15,17	0.53	0
7	BGC	T	18	7	11,11,12	0.22	0	15,15,17	0.59	0
7	XYP	T	19	7	9,9,10	0.19	0	10,12,14	0.61	0
7	BGC	T	2	7	11,11,12	0.17	0	15,15,17	0.57	0
7	XYP	T	20	7	9,9,10	0.28	0	10,12,14	0.59	0
7	XYP	T	21	7	9,9,10	0.40	0	10,12,14	0.65	0
7	XYP	T	22	7	9,9,10	0.26	0	10,12,14	0.71	0
7	A2G	T	3	7	14,14,15	0.42	0	17,19,21	1.03	2 (11%)
7	BGC	T	4	7	11,11,12	0.20	0	15,15,17	0.61	0
7	BGC	T	5	7	11,11,12	0.17	0	15,15,17	0.67	0
7	XYP	T	6	7	9,9,10	0.19	0	10,12,14	0.61	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	A2G	T	7	7	14,14,15	0.44	0	17,19,21	0.94	1 (5%)
7	MAN	T	8	7	11,11,12	0.46	0	15,15,17	0.84	1 (6%)
7	MAN	T	9	7	11,11,12	0.21	0	15,15,17	0.80	1 (6%)
8	GAL	U	1	8	11,11,12	0.18	0	15,15,17	0.63	0
8	BGC	U	10	8	11,11,12	0.20	0	15,15,17	0.59	0
8	MAN	U	11	8	11,11,12	0.22	0	15,15,17	0.81	2 (13%)
8	BGC	U	12	8	11,11,12	0.20	0	15,15,17	0.57	0
8	XYP	U	13	8	9,9,10	0.20	0	10,12,14	0.59	0
8	NAG	U	14	8	14,14,15	0.29	0	17,19,21	0.56	0
8	BGC	U	15	8	11,11,12	0.18	0	15,15,17	0.57	0
8	MAN	U	16	8	11,11,12	0.44	0	15,15,17	0.98	2 (13%)
8	A2G	U	17	8	14,14,15	0.40	0	17,19,21	0.69	0
8	XYP	U	18	8	9,9,10	0.19	0	10,12,14	0.60	0
8	XYP	U	19	8	9,9,10	0.19	0	10,12,14	0.62	0
8	NAG	U	2	8	14,14,15	0.29	0	17,19,21	0.72	0
8	MAN	U	20	8	11,11,12	0.54	0	15,15,17	0.59	0
8	BGC	U	3	8	11,11,12	0.18	0	15,15,17	0.72	0
8	XYP	U	4	8	9,9,10	0.19	0	10,12,14	0.69	0
8	XYP	U	5	8	9,9,10	0.20	0	10,12,14	0.55	0
8	XYP	U	6	8	9,9,10	0.20	0	10,12,14	0.53	0
8	XYP	U	7	8	9,9,10	0.21	0	10,12,14	1.02	2 (20%)
8	GAL	U	8	8	11,11,12	0.21	0	15,15,17	0.64	1 (6%)
8	XYP	U	9	8	9,9,10	0.19	0	10,12,14	0.58	0
9	BGC	V	1	9,1	11,11,12	0.17	0	15,15,17	0.58	0
9	BGC	V	10	9	11,11,12	0.20	0	15,15,17	0.57	0
9	MAN	V	2	9	11,11,12	0.21	0	15,15,17	0.96	1 (6%)
9	BGC	V	3	9	11,11,12	0.25	0	15,15,17	0.87	1 (6%)
9	NAG	V	4	9	14,14,15	0.36	0	17,19,21	0.88	1 (5%)
9	BGC	V	5	9	11,11,12	0.19	0	15,15,17	0.54	0
9	MAN	V	6	9	11,11,12	0.49	0	15,15,17	0.79	1 (6%)
9	BGC	V	7	9	11,11,12	0.21	0	15,15,17	0.57	0
9	XYP	V	8	9	9,9,10	0.19	0	10,12,14	0.60	0
9	XYP	V	9	9	9,9,10	0.18	0	10,12,14	0.61	0
10	GAL	W	1	10	11,11,12	0.16	0	15,15,17	0.64	0
10	MAN	W	10	10	11,11,12	0.58	0	15,15,17	0.59	0
10	NAG	W	11	10	14,14,15	0.60	0	17,19,21	0.89	0
10	XYP	W	12	10	9,9,10	0.18	0	10,12,14	0.64	0
10	MAN	W	13	10	11,11,12	0.19	0	15,15,17	0.80	2 (13%)
10	BGC	W	14	10	11,11,12	0.19	0	15,15,17	0.54	0
10	XYP	W	15	10	9,9,10	0.20	0	10,12,14	0.60	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	BGC	W	16	10	11,11,12	0.19	0	15,15,17	0.55	0
10	BGC	W	17	10	11,11,12	0.19	0	15,15,17	0.57	0
10	NAG	W	18	10	14,14,15	0.61	0	17,19,21	1.36	3 (17%)
10	MAN	W	19	10	11,11,12	0.99	1 (9%)	15,15,17	1.26	2 (13%)
10	NAG	W	2	10	14,14,15	0.32	0	17,19,21	1.52	2 (11%)
10	XYP	W	3	10	9,9,10	0.18	0	10,12,14	0.60	0
10	XYP	W	4	10	9,9,10	0.19	0	10,12,14	0.56	0
10	GAL	W	5	10	11,11,12	0.16	0	15,15,17	0.62	0
10	A2G	W	6	10	14,14,15	0.42	0	17,19,21	1.48	3 (17%)
10	GAL	W	7	10	11,11,12	0.19	0	15,15,17	0.58	0
10	A2G	W	8	10	14,14,15	0.46	0	17,19,21	1.07	2 (11%)
10	BGC	W	9	10	11,11,12	0.80	1 (9%)	15,15,17	0.91	1 (6%)
11	MAN	X	1	11,1	11,11,12	0.25	0	15,15,17	0.84	1 (6%)
11	GLA	X	10	11	11,11,12	0.41	0	15,15,17	1.13	1 (6%)
11	BGC	X	11	11	11,11,12	0.78	1 (9%)	15,15,17	2.13	5 (33%)
11	BMA	X	12	11	11,11,12	1.03	1 (9%)	15,15,17	2.48	3 (20%)
11	NAG	X	13	11	14,14,15	0.87	0	17,19,21	1.71	5 (29%)
11	BMA	X	14	11	11,11,12	0.75	0	15,15,17	2.43	3 (20%)
11	BGC	X	15	11	11,11,12	0.77	0	15,15,17	1.08	1 (6%)
11	NAG	X	16	11	14,14,15	0.79	0	17,19,21	1.32	3 (17%)
11	AHR	X	17	11	9,9,10	0.63	0	10,12,14	1.08	1 (10%)
11	XYP	X	18	11	9,9,10	0.26	0	10,12,14	1.11	1 (10%)
11	BGC	X	19	11	11,11,12	0.39	0	15,15,17	1.13	1 (6%)
11	BGC	X	2	11	11,11,12	0.20	0	15,15,17	0.63	0
11	NAG	X	20	11	14,14,15	0.80	0	17,19,21	1.69	4 (23%)
11	BMA	X	21	11	11,11,12	0.22	0	15,15,17	0.54	0
11	MAN	X	22	11	11,11,12	0.21	0	15,15,17	0.79	1 (6%)
11	XYP	X	23	11	9,9,10	0.19	0	10,12,14	0.60	0
11	BMA	X	24	11	11,11,12	0.22	0	15,15,17	0.80	0
11	BGC	X	25	11	11,11,12	0.21	0	15,15,17	0.82	1 (6%)
11	XYP	X	26	11	9,9,10	0.23	0	10,12,14	0.59	0
11	XYP	X	27	11	9,9,10	0.19	0	10,12,14	0.63	0
11	NAG	X	28	11	14,14,15	0.30	0	17,19,21	0.61	0
11	MAN	X	29	11	11,11,12	0.22	0	15,15,17	0.80	1 (6%)
11	XYP	X	3	11	9,9,10	0.20	0	10,12,14	0.61	0
11	XYP	X	30	11	9,9,10	0.19	0	10,12,14	0.62	0
11	BGC	X	31	11	11,11,12	0.18	0	15,15,17	0.61	0
11	BGC	X	32	11	11,11,12	0.18	0	15,15,17	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	XYP	X	33	11	9,9,10	0.19	0	10,12,14	0.63	0
11	NAG	X	34	11	14,14,15	0.27	0	17,19,21	0.56	0
11	BGC	X	35	11	11,11,12	0.19	0	15,15,17	0.95	1 (6%)
11	XYP	X	36	11	9,9,10	0.39	0	10,12,14	0.50	0
11	MAN	X	37	11	11,11,12	0.37	0	15,15,17	0.73	0
11	NAG	X	38	11	14,14,15	0.30	0	17,19,21	0.72	1 (5%)
11	XYP	X	39	11	9,9,10	0.19	0	10,12,14	0.60	0
11	BMA	X	4	11	11,11,12	0.25	0	15,15,17	0.43	0
11	XYP	X	40	11	9,9,10	0.18	0	10,12,14	0.62	0
11	BGC	X	41	11	11,11,12	0.18	0	15,15,17	0.58	0
11	MAN	X	42	11	11,11,12	0.21	0	15,15,17	0.81	1 (6%)
11	BGC	X	43	11	11,11,12	0.20	0	15,15,17	0.56	0
11	XYP	X	44	11	9,9,10	0.17	0	10,12,14	0.63	0
11	BGC	X	45	11	11,11,12	0.19	0	15,15,17	0.57	0
11	BGC	X	46	11	11,11,12	0.19	0	15,15,17	0.55	0
11	BGC	X	47	11	11,11,12	0.19	0	15,15,17	0.57	0
11	NAG	X	5	11	14,14,15	0.33	0	17,19,21	0.61	0
11	FUB	X	6	11	9,9,10	0.59	0	10,12,14	1.14	2 (20%)
11	BGC	X	7	11	11,11,12	0.46	0	15,15,17	1.56	3 (20%)
11	BGC	X	8	11	11,11,12	0.85	0	15,15,17	1.47	3 (20%)
11	BMA	X	9	11	11,11,12	0.86	0	15,15,17	2.57	3 (20%)
12	GAL	Y	1	12	11,11,12	0.19	0	15,15,17	0.62	0
12	XYP	Y	10	12	9,9,10	0.19	0	10,12,14	0.61	0
12	XYP	Y	2	12	9,9,10	0.18	0	10,12,14	0.65	0
12	BGC	Y	3	12	11,11,12	0.21	0	15,15,17	0.54	0
12	XYP	Y	4	12	9,9,10	0.18	0	10,12,14	0.62	0
12	BGC	Y	5	12	11,11,12	0.81	0	15,15,17	2.32	5 (33%)
12	MAN	Y	6	12	11,11,12	0.80	0	15,15,17	1.36	1 (6%)
12	BGC	Y	7	12	11,11,12	0.64	0	15,15,17	1.97	3 (20%)
12	BGC	Y	8	12	11,11,12	0.89	1 (9%)	15,15,17	1.17	2 (13%)
12	NAG	Y	9	12	14,14,15	0.56	0	17,19,21	1.39	1 (5%)
13	XYP	Z	1	13	9,9,10	0.32	0	10,12,14	1.55	2 (20%)
13	BGC	Z	10	13	11,11,12	0.63	0	15,15,17	1.55	3 (20%)
13	MAN	Z	11	13	11,11,12	0.24	0	15,15,17	0.79	1 (6%)
13	AHR	Z	12	13	9,9,10	0.73	0	10,12,14	1.47	1 (10%)
13	XYP	Z	13	13	9,9,10	0.29	0	10,12,14	0.88	0
13	BGC	Z	14	13	11,11,12	0.72	0	15,15,17	2.10	6 (40%)
13	BGC	Z	15	13	11,11,12	0.53	0	15,15,17	1.07	0
13	BGC	Z	16	13	11,11,12	0.20	0	15,15,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	BGC	Z	17	13	11,11,12	0.20	0	15,15,17	0.56	0
13	BGC	Z	2	13	11,11,12	1.23	2 (18%)	15,15,17	2.50	5 (33%)
13	MAN	Z	3	13	11,11,12	0.21	0	15,15,17	0.84	1 (6%)
13	NAG	Z	4	13	14,14,15	0.88	0	17,19,21	1.56	1 (5%)
13	BGC	Z	5	13	11,11,12	1.12	1 (9%)	15,15,17	2.19	7 (46%)
13	BGC	Z	6	13	11,11,12	0.17	0	15,15,17	0.63	0
13	XYP	Z	7	13	9,9,10	0.18	0	10,12,14	0.59	0
13	BGC	Z	8	13	11,11,12	0.19	0	15,15,17	0.57	0
13	NAG	Z	9	13	14,14,15	0.31	0	17,19,21	0.64	0
14	MAN	a	1	14,1	11,11,12	0.84	0	15,15,17	2.95	5 (33%)
14	BGC	a	10	14	11,11,12	0.21	0	15,15,17	0.51	0
14	XYP	a	11	14	9,9,10	0.20	0	10,12,14	0.49	0
14	BGC	a	12	14	11,11,12	0.17	0	15,15,17	0.56	0
14	XYP	a	13	14	9,9,10	0.17	0	10,12,14	0.61	0
14	XYP	a	14	14	9,9,10	0.18	0	10,12,14	0.61	0
14	AHR	a	15	14	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
14	BGC	a	16	14	11,11,12	0.17	0	15,15,17	0.55	0
14	XYP	a	17	14	9,9,10	0.19	0	10,12,14	0.64	0
14	NAG	a	18	14	14,14,15	0.27	0	17,19,21	0.66	0
14	NAG	a	19	14	14,14,15	0.33	0	17,19,21	0.84	0
14	XYP	a	2	14	9,9,10	0.20	0	10,12,14	0.91	1 (10%)
14	XYP	a	20	14	9,9,10	0.31	0	10,12,14	0.57	0
14	AHR	a	21	14	9,9,10	0.51	0	10,12,14	0.77	0
14	A2G	a	3	14	14,14,15	0.37	0	17,19,21	0.89	2 (11%)
14	GAL	a	4	14	11,11,12	0.21	0	15,15,17	0.88	1 (6%)
14	AHR	a	5	14	9,9,10	0.51	0	10,12,14	0.77	0
14	XYP	a	6	14	9,9,10	0.19	0	10,12,14	0.77	0
14	NAG	a	7	14	14,14,15	0.31	0	17,19,21	0.71	0
14	AHR	a	8	14	9,9,10	0.58	0	10,12,14	1.03	1 (10%)
14	AHR	a	9	14	9,9,10	0.59	0	10,12,14	1.01	1 (10%)
2	BGC	b	1	2,1	11,11,12	0.34	0	15,15,17	0.61	0
2	NAG	b	2	2	14,14,15	0.30	0	17,19,21	0.85	1 (5%)
2	GAL	b	3	2	11,11,12	0.17	0	15,15,17	0.59	0
2	MAN	b	4	2	11,11,12	0.23	0	15,15,17	0.78	1 (6%)
2	BGC	b	5	2	11,11,12	0.19	0	15,15,17	0.56	0
2	NAG	b	6	2	14,14,15	0.87	1 (7%)	17,19,21	1.40	4 (23%)
2	BMA	b	7	2	11,11,12	0.21	0	15,15,17	0.74	0
2	GAL	b	8	2	11,11,12	0.16	0	15,15,17	0.62	0
2	MAN	b	9	2	11,11,12	0.21	0	15,15,17	0.79	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GLA	c	1	3,1	11,11,12	0.18	0	15,15,17	0.64	0
3	XYP	c	10	3	9,9,10	0.29	0	10,12,14	0.58	0
3	NAG	c	11	3	14,14,15	0.51	0	17,19,21	1.04	1 (5%)
3	MAN	c	12	3	11,11,12	0.34	0	15,15,17	1.26	1 (6%)
3	NAG	c	13	3	14,14,15	0.29	0	17,19,21	0.69	0
3	XYP	c	14	3	9,9,10	0.17	0	10,12,14	0.59	0
3	BGC	c	15	3	11,11,12	0.18	0	15,15,17	0.57	0
3	BGC	c	16	3	11,11,12	0.20	0	15,15,17	0.57	0
3	XYP	c	17	3	9,9,10	0.20	0	10,12,14	0.62	0
3	BGC	c	18	3	11,11,12	0.20	0	15,15,17	0.48	0
3	BGC	c	19	3	11,11,12	0.19	0	15,15,17	0.57	0
3	BGC	c	2	3	11,11,12	0.71	0	15,15,17	1.24	2 (13%)
3	XYP	c	20	3	9,9,10	0.18	0	10,12,14	0.60	0
3	NAG	c	21	3	14,14,15	0.28	0	17,19,21	0.74	0
3	XYP	c	22	3	9,9,10	0.19	0	10,12,14	0.54	0
3	XYP	c	23	3	9,9,10	0.19	0	10,12,14	0.57	0
3	GAL	c	24	3	11,11,12	0.18	0	15,15,17	0.57	0
3	BGC	c	25	3	11,11,12	0.20	0	15,15,17	0.65	0
3	GAL	c	26	3	11,11,12	0.17	0	15,15,17	0.57	0
3	BGC	c	27	3	11,11,12	0.18	0	15,15,17	0.57	0
3	XYP	c	28	3	9,9,10	0.18	0	10,12,14	0.61	0
3	BGC	c	29	3	11,11,12	0.18	0	15,15,17	0.57	0
3	BGC	c	3	3	11,11,12	0.18	0	15,15,17	0.46	0
3	BGC	c	30	3	11,11,12	0.19	0	15,15,17	0.57	0
3	BGC	c	31	3	11,11,12	0.19	0	15,15,17	0.58	0
3	BGC	c	32	3	11,11,12	0.20	0	15,15,17	0.56	0
3	XYP	c	33	3	9,9,10	0.19	0	10,12,14	0.61	0
3	XYP	c	34	3	9,9,10	0.17	0	10,12,14	0.60	0
3	GAL	c	4	3	11,11,12	0.15	0	15,15,17	0.59	0
3	XYP	c	5	3	9,9,10	0.18	0	10,12,14	0.59	0
3	XYP	c	6	3	9,9,10	0.20	0	10,12,14	1.23	1 (10%)
3	BGC	c	7	3	11,11,12	0.20	0	15,15,17	0.81	1 (6%)
3	XYP	c	8	3	9,9,10	0.20	0	10,12,14	0.53	0
3	BGC	c	9	3	11,11,12	0.21	0	15,15,17	0.53	0
4	MAN	d	1	4,1	11,11,12	0.21	0	15,15,17	0.79	0
4	XYP	d	10	4	9,9,10	0.18	0	10,12,14	0.61	0
4	MAN	d	11	4	11,11,12	0.79	1 (9%)	15,15,17	0.80	0
4	AHR	d	12	4	9,9,10	0.58	0	10,12,14	1.03	1 (10%)
4	FUB	d	13	4	9,9,10	0.53	0	10,12,14	0.57	0
4	NAG	d	14	4	14,14,15	0.30	0	17,19,21	0.64	0
4	XYP	d	15	4	9,9,10	0.24	0	10,12,14	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FUB	d	16	4	9,9,10	0.58	0	10,12,14	0.95	0
4	AHR	d	17	4	9,9,10	0.60	0	10,12,14	1.02	1 (10%)
4	MAN	d	18	4	11,11,12	0.21	0	15,15,17	0.81	1 (6%)
4	BGC	d	19	4	11,11,12	0.20	0	15,15,17	0.57	0
4	AHR	d	2	4	9,9,10	0.58	0	10,12,14	1.03	1 (10%)
4	BGC	d	20	4	11,11,12	0.19	0	15,15,17	0.60	0
4	BGC	d	21	4	11,11,12	0.19	0	15,15,17	0.57	0
4	FUB	d	22	4	9,9,10	0.58	0	10,12,14	1.05	1 (10%)
4	BGC	d	23	4	11,11,12	0.19	0	15,15,17	0.61	0
4	BGC	d	24	4	11,11,12	0.19	0	15,15,17	0.59	0
4	BGC	d	25	4	11,11,12	0.19	0	15,15,17	0.58	0
4	AHR	d	26	4	9,9,10	0.60	0	10,12,14	1.03	1 (10%)
4	BGC	d	3	4	11,11,12	0.21	0	15,15,17	0.59	0
4	MAN	d	4	4	11,11,12	0.23	0	15,15,17	0.76	0
4	BGC	d	5	4	11,11,12	0.19	0	15,15,17	0.72	0
4	BMA	d	6	4	11,11,12	0.41	0	15,15,17	1.14	1 (6%)
4	NAG	d	7	4	14,14,15	0.76	0	17,19,21	1.59	3 (17%)
4	BGC	d	8	4	11,11,12	0.64	0	15,15,17	0.77	0
4	BGC	d	9	4	11,11,12	0.19	0	15,15,17	0.54	0
5	MAN	e	1	5,1	11,11,12	0.22	0	15,15,17	0.77	1 (6%)
5	NAG	e	2	5	14,14,15	0.27	0	17,19,21	0.65	0
6	MAN	f	1	6,1	11,11,12	0.24	0	15,15,17	0.79	1 (6%)
6	GZL	f	2	6	11,11,12	6.71	7 (63%)	14,15,17	1.42	2 (14%)
6	FUB	f	3	6	9,9,10	0.57	0	10,12,14	1.03	1 (10%)
6	NAG	f	4	6	14,14,15	0.27	0	17,19,21	0.63	0
7	XYP	g	1	7	9,9,10	0.83	1 (11%)	10,12,14	2.58	3 (30%)
7	MAN	g	10	7	11,11,12	0.51	0	15,15,17	0.88	1 (6%)
7	MAN	g	11	7	11,11,12	0.21	0	15,15,17	0.78	1 (6%)
7	BGC	g	12	7	11,11,12	0.21	0	15,15,17	0.56	0
7	BGC	g	13	7	11,11,12	0.20	0	15,15,17	0.58	0
7	XYP	g	14	7	9,9,10	0.17	0	10,12,14	0.60	0
7	MAN	g	15	7	11,11,12	0.20	0	15,15,17	0.81	2 (13%)
7	NAG	g	16	7	14,14,15	0.38	0	17,19,21	1.23	2 (11%)
7	BGC	g	17	7	11,11,12	0.17	0	15,15,17	0.52	0
7	BGC	g	18	7	11,11,12	0.22	0	15,15,17	0.58	0
7	XYP	g	19	7	9,9,10	0.18	0	10,12,14	0.61	0
7	BGC	g	2	7	11,11,12	0.18	0	15,15,17	0.57	0
7	XYP	g	20	7	9,9,10	0.30	0	10,12,14	0.58	0
7	XYP	g	21	7	9,9,10	0.39	0	10,12,14	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	XYP	g	22	7	9,9,10	0.26	0	10,12,14	0.71	0
7	A2G	g	3	7	14,14,15	0.42	0	17,19,21	1.02	2 (11%)
7	BGC	g	4	7	11,11,12	0.19	0	15,15,17	0.61	0
7	BGC	g	5	7	11,11,12	0.19	0	15,15,17	0.67	0
7	XYP	g	6	7	9,9,10	0.19	0	10,12,14	0.61	0
7	A2G	g	7	7	14,14,15	0.44	0	17,19,21	0.94	1 (5%)
7	MAN	g	8	7	11,11,12	0.47	0	15,15,17	0.84	1 (6%)
7	MAN	g	9	7	11,11,12	0.22	0	15,15,17	0.80	0
8	GAL	h	1	8	11,11,12	0.17	0	15,15,17	0.63	0
8	BGC	h	10	8	11,11,12	0.19	0	15,15,17	0.59	0
8	MAN	h	11	8	11,11,12	0.23	0	15,15,17	0.80	2 (13%)
8	BGC	h	12	8	11,11,12	0.20	0	15,15,17	0.56	0
8	XYP	h	13	8	9,9,10	0.19	0	10,12,14	0.60	0
8	NAG	h	14	8	14,14,15	0.28	0	17,19,21	0.56	0
8	BGC	h	15	8	11,11,12	0.19	0	15,15,17	0.58	0
8	MAN	h	16	8	11,11,12	0.44	0	15,15,17	0.99	2 (13%)
8	A2G	h	17	8	14,14,15	0.40	0	17,19,21	0.69	1 (5%)
8	XYP	h	18	8	9,9,10	0.19	0	10,12,14	0.60	0
8	XYP	h	19	8	9,9,10	0.18	0	10,12,14	0.61	0
8	NAG	h	2	8	14,14,15	0.28	0	17,19,21	0.72	0
8	MAN	h	20	8	11,11,12	0.53	0	15,15,17	0.59	0
8	BGC	h	3	8	11,11,12	0.18	0	15,15,17	0.72	0
8	XYP	h	4	8	9,9,10	0.19	0	10,12,14	0.69	0
8	XYP	h	5	8	9,9,10	0.19	0	10,12,14	0.56	0
8	XYP	h	6	8	9,9,10	0.20	0	10,12,14	0.53	0
8	XYP	h	7	8	9,9,10	0.20	0	10,12,14	1.01	2 (20%)
8	GAL	h	8	8	11,11,12	0.22	0	15,15,17	0.64	1 (6%)
8	XYP	h	9	8	9,9,10	0.19	0	10,12,14	0.57	0
9	BGC	i	1	9,1	11,11,12	0.17	0	15,15,17	0.59	0
9	BGC	i	10	9	11,11,12	0.20	0	15,15,17	0.57	0
9	MAN	i	2	9	11,11,12	0.23	0	15,15,17	0.95	1 (6%)
9	BGC	i	3	9	11,11,12	0.24	0	15,15,17	0.87	1 (6%)
9	NAG	i	4	9	14,14,15	0.37	0	17,19,21	0.88	1 (5%)
9	BGC	i	5	9	11,11,12	0.20	0	15,15,17	0.54	0
9	MAN	i	6	9	11,11,12	0.49	0	15,15,17	0.66	1 (6%)
9	BGC	i	7	9	11,11,12	0.19	0	15,15,17	0.57	0
9	XYP	i	8	9	9,9,10	0.20	0	10,12,14	0.59	0
9	XYP	i	9	9	9,9,10	0.18	0	10,12,14	0.59	0
10	GAL	j	1	10	11,11,12	0.16	0	15,15,17	0.64	0
10	MAN	j	10	10	11,11,12	0.59	0	15,15,17	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	NAG	j	11	10	14,14,15	0.61	0	17,19,21	0.90	0
10	XYP	j	12	10	9,9,10	0.19	0	10,12,14	0.63	0
10	MAN	j	13	10	11,11,12	0.20	0	15,15,17	0.79	1 (6%)
10	BGC	j	14	10	11,11,12	0.19	0	15,15,17	0.53	0
10	XYP	j	15	10	9,9,10	0.21	0	10,12,14	0.59	0
10	BGC	j	16	10	11,11,12	0.18	0	15,15,17	0.55	0
10	BGC	j	17	10	11,11,12	0.67	0	15,15,17	2.03	5 (33%)
10	NAG	j	18	10	14,14,15	0.61	0	17,19,21	1.23	1 (5%)
10	MAN	j	19	10	11,11,12	1.01	1 (9%)	15,15,17	1.45	3 (20%)
10	NAG	j	2	10	14,14,15	0.33	0	17,19,21	1.51	2 (11%)
10	XYP	j	3	10	9,9,10	0.57	0	10,12,14	2.98	3 (30%)
10	XYP	j	4	10	9,9,10	0.17	0	10,12,14	0.56	0
10	GAL	j	5	10	11,11,12	0.16	0	15,15,17	0.61	0
10	A2G	j	6	10	14,14,15	0.42	0	17,19,21	1.49	3 (17%)
10	GAL	j	7	10	11,11,12	0.18	0	15,15,17	0.58	0
10	A2G	j	8	10	14,14,15	0.46	0	17,19,21	1.07	1 (5%)
10	BGC	j	9	10	11,11,12	0.79	1 (9%)	15,15,17	0.91	1 (6%)
11	MAN	k	1	11,1	11,11,12	0.24	0	15,15,17	0.84	2 (13%)
11	GLA	k	10	11	11,11,12	0.41	0	15,15,17	1.13	1 (6%)
11	BGC	k	11	11	11,11,12	0.76	0	15,15,17	2.14	5 (33%)
11	BMA	k	12	11	11,11,12	1.03	1 (9%)	15,15,17	2.47	3 (20%)
11	NAG	k	13	11	14,14,15	0.85	0	17,19,21	1.72	5 (29%)
11	BMA	k	14	11	11,11,12	0.73	0	15,15,17	2.44	3 (20%)
11	BGC	k	15	11	11,11,12	0.73	0	15,15,17	0.95	1 (6%)
11	NAG	k	16	11	14,14,15	0.80	0	17,19,21	1.32	3 (17%)
11	AHR	k	17	11	9,9,10	0.64	0	10,12,14	1.08	1 (10%)
11	XYP	k	18	11	9,9,10	0.25	0	10,12,14	1.12	1 (10%)
11	BGC	k	19	11	11,11,12	0.40	0	15,15,17	1.12	1 (6%)
11	BGC	k	2	11	11,11,12	0.20	0	15,15,17	0.62	0
11	NAG	k	20	11	14,14,15	0.80	0	17,19,21	1.69	4 (23%)
11	BMA	k	21	11	11,11,12	0.21	0	15,15,17	0.53	0
11	MAN	k	22	11	11,11,12	0.21	0	15,15,17	0.78	1 (6%)
11	XYP	k	23	11	9,9,10	0.20	0	10,12,14	0.61	0
11	BMA	k	24	11	11,11,12	0.22	0	15,15,17	0.81	0
11	BGC	k	25	11	11,11,12	0.23	0	15,15,17	0.82	0
11	XYP	k	26	11	9,9,10	0.23	0	10,12,14	0.60	0
11	XYP	k	27	11	9,9,10	0.20	0	10,12,14	0.63	0
11	NAG	k	28	11	14,14,15	0.29	0	17,19,21	0.61	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	MAN	k	29	11	11,11,12	0.22	0	15,15,17	0.80	1 (6%)
11	XYP	k	3	11	9,9,10	0.18	0	10,12,14	0.61	0
11	XYP	k	30	11	9,9,10	0.19	0	10,12,14	0.61	0
11	BGC	k	31	11	11,11,12	0.19	0	15,15,17	0.61	0
11	BGC	k	32	11	11,11,12	0.18	0	15,15,17	0.57	0
11	XYP	k	33	11	9,9,10	0.20	0	10,12,14	0.61	0
11	NAG	k	34	11	14,14,15	0.27	0	17,19,21	0.56	0
11	BGC	k	35	11	11,11,12	0.20	0	15,15,17	0.94	1 (6%)
11	XYP	k	36	11	9,9,10	0.39	0	10,12,14	0.49	0
11	MAN	k	37	11	11,11,12	0.38	0	15,15,17	0.73	0
11	NAG	k	38	11	14,14,15	0.28	0	17,19,21	0.71	1 (5%)
11	XYP	k	39	11	9,9,10	0.20	0	10,12,14	0.60	0
11	BMA	k	4	11	11,11,12	0.25	0	15,15,17	0.43	0
11	XYP	k	40	11	9,9,10	0.18	0	10,12,14	0.63	0
11	BGC	k	41	11	11,11,12	0.19	0	15,15,17	0.58	0
11	MAN	k	42	11	11,11,12	0.22	0	15,15,17	0.81	1 (6%)
11	BGC	k	43	11	11,11,12	0.19	0	15,15,17	0.56	0
11	XYP	k	44	11	9,9,10	0.18	0	10,12,14	0.62	0
11	BGC	k	45	11	11,11,12	0.19	0	15,15,17	0.58	0
11	BGC	k	46	11	11,11,12	0.21	0	15,15,17	0.54	0
11	BGC	k	47	11	11,11,12	0.18	0	15,15,17	0.57	0
11	NAG	k	5	11	14,14,15	0.32	0	17,19,21	0.63	0
11	FUB	k	6	11	9,9,10	0.61	0	10,12,14	1.14	2 (20%)
11	BGC	k	7	11	11,11,12	0.47	0	15,15,17	1.56	3 (20%)
11	BGC	k	8	11	11,11,12	0.85	0	15,15,17	1.47	3 (20%)
11	BMA	k	9	11	11,11,12	0.87	0	15,15,17	2.56	3 (20%)
12	GAL	l	1	12	11,11,12	0.19	0	15,15,17	0.62	0
12	XYP	l	10	12	9,9,10	0.19	0	10,12,14	0.61	0
12	XYP	l	2	12	9,9,10	0.18	0	10,12,14	0.63	0
12	BGC	l	3	12	11,11,12	0.20	0	15,15,17	0.54	0
12	XYP	l	4	12	9,9,10	0.16	0	10,12,14	0.62	0
12	BGC	l	5	12	11,11,12	0.81	0	15,15,17	2.33	5 (33%)
12	MAN	l	6	12	11,11,12	0.80	0	15,15,17	1.36	1 (6%)
12	BGC	l	7	12	11,11,12	0.64	0	15,15,17	1.97	2 (13%)
12	BGC	l	8	12	11,11,12	0.84	0	15,15,17	1.55	2 (13%)
12	NAG	l	9	12	14,14,15	0.56	0	17,19,21	1.39	1 (5%)
13	XYP	m	1	13	9,9,10	0.34	0	10,12,14	1.55	2 (20%)
13	BGC	m	10	13	11,11,12	0.63	0	15,15,17	1.56	4 (26%)
13	MAN	m	11	13	11,11,12	0.21	0	15,15,17	0.79	1 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	AHR	m	12	13	9,9,10	0.70	0	10,12,14	1.48	1 (10%)
13	XYP	m	13	13	9,9,10	0.28	0	10,12,14	0.89	1 (10%)
13	BGC	m	14	13	11,11,12	0.71	0	15,15,17	2.10	6 (40%)
13	BGC	m	15	13	11,11,12	0.53	0	15,15,17	1.08	0
13	BGC	m	16	13	11,11,12	0.19	0	15,15,17	0.52	0
13	BGC	m	17	13	11,11,12	0.20	0	15,15,17	0.56	0
13	BGC	m	2	13	11,11,12	1.23	2 (18%)	15,15,17	2.51	5 (33%)
13	MAN	m	3	13	11,11,12	0.21	0	15,15,17	0.84	1 (6%)
13	NAG	m	4	13	14,14,15	0.90	0	17,19,21	1.55	1 (5%)
13	BGC	m	5	13	11,11,12	1.13	1 (9%)	15,15,17	2.19	7 (46%)
13	BGC	m	6	13	11,11,12	0.17	0	15,15,17	0.63	0
13	XYP	m	7	13	9,9,10	0.18	0	10,12,14	0.59	0
13	BGC	m	8	13	11,11,12	0.20	0	15,15,17	0.57	0
13	NAG	m	9	13	14,14,15	0.29	0	17,19,21	0.63	0
14	MAN	n	1	14,1	11,11,12	0.85	0	15,15,17	2.94	5 (33%)
14	BGC	n	10	14	11,11,12	0.22	0	15,15,17	0.50	0
14	XYP	n	11	14	9,9,10	0.19	0	10,12,14	0.49	0
14	BGC	n	12	14	11,11,12	0.18	0	15,15,17	0.56	0
14	XYP	n	13	14	9,9,10	0.17	0	10,12,14	0.60	0
14	XYP	n	14	14	9,9,10	0.16	0	10,12,14	0.62	0
14	AHR	n	15	14	9,9,10	0.59	0	10,12,14	1.01	1 (10%)
14	BGC	n	16	14	11,11,12	0.17	0	15,15,17	0.55	0
14	XYP	n	17	14	9,9,10	0.20	0	10,12,14	0.65	0
14	NAG	n	18	14	14,14,15	0.27	0	17,19,21	0.66	0
14	NAG	n	19	14	14,14,15	0.35	0	17,19,21	0.84	0
14	XYP	n	2	14	9,9,10	0.20	0	10,12,14	0.91	1 (10%)
14	XYP	n	20	14	9,9,10	0.30	0	10,12,14	0.56	0
14	AHR	n	21	14	9,9,10	0.52	0	10,12,14	0.77	0
14	A2G	n	3	14	14,14,15	0.40	0	17,19,21	0.89	2 (11%)
14	GAL	n	4	14	11,11,12	0.23	0	15,15,17	0.87	1 (6%)
14	AHR	n	5	14	9,9,10	0.51	0	10,12,14	0.77	0
14	XYP	n	6	14	9,9,10	0.19	0	10,12,14	0.75	0
14	NAG	n	7	14	14,14,15	0.32	0	17,19,21	0.70	0
14	AHR	n	8	14	9,9,10	0.60	0	10,12,14	1.03	1 (10%)
14	AHR	n	9	14	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
2	BGC	o	1	2,1	11,11,12	0.34	0	15,15,17	0.61	0
2	NAG	o	2	2	14,14,15	0.28	0	17,19,21	0.86	1 (5%)
2	GAL	o	3	2	11,11,12	0.17	0	15,15,17	0.59	0
2	MAN	o	4	2	11,11,12	0.24	0	15,15,17	0.78	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BGC	o	5	2	11,11,12	0.20	0	15,15,17	0.56	0
2	NAG	o	6	2	14,14,15	0.87	1 (7%)	17,19,21	1.40	4 (23%)
2	BMA	o	7	2	11,11,12	0.21	0	15,15,17	0.74	0
2	GAL	o	8	2	11,11,12	0.17	0	15,15,17	0.62	0
2	MAN	o	9	2	11,11,12	0.21	0	15,15,17	0.79	1 (6%)
3	GLA	p	1	3,1	11,11,12	0.18	0	15,15,17	0.63	0
3	XYP	p	10	3	9,9,10	0.31	0	10,12,14	0.58	0
3	NAG	p	11	3	14,14,15	0.47	0	17,19,21	1.10	1 (5%)
3	MAN	p	12	3	11,11,12	0.32	0	15,15,17	1.34	1 (6%)
3	NAG	p	13	3	14,14,15	0.29	0	17,19,21	0.70	0
3	XYP	p	14	3	9,9,10	0.17	0	10,12,14	0.60	0
3	BGC	p	15	3	11,11,12	0.18	0	15,15,17	0.56	0
3	BGC	p	16	3	11,11,12	0.19	0	15,15,17	0.58	0
3	XYP	p	17	3	9,9,10	0.18	0	10,12,14	0.62	0
3	BGC	p	18	3	11,11,12	0.18	0	15,15,17	0.48	0
3	BGC	p	19	3	11,11,12	0.20	0	15,15,17	0.58	0
3	BGC	p	2	3	11,11,12	0.70	0	15,15,17	1.24	2 (13%)
3	XYP	p	20	3	9,9,10	0.19	0	10,12,14	0.60	0
3	NAG	p	21	3	14,14,15	0.29	0	17,19,21	0.74	0
3	XYP	p	22	3	9,9,10	0.20	0	10,12,14	0.53	0
3	XYP	p	23	3	9,9,10	0.18	0	10,12,14	0.57	0
3	GAL	p	24	3	11,11,12	0.19	0	15,15,17	0.57	0
3	BGC	p	25	3	11,11,12	0.20	0	15,15,17	0.64	0
3	GAL	p	26	3	11,11,12	0.18	0	15,15,17	0.57	0
3	BGC	p	27	3	11,11,12	0.18	0	15,15,17	0.57	0
3	XYP	p	28	3	9,9,10	0.18	0	10,12,14	0.62	0
3	BGC	p	29	3	11,11,12	0.17	0	15,15,17	0.59	0
3	BGC	p	3	3	11,11,12	0.18	0	15,15,17	0.47	0
3	BGC	p	30	3	11,11,12	0.18	0	15,15,17	0.58	0
3	BGC	p	31	3	11,11,12	0.20	0	15,15,17	0.58	0
3	BGC	p	32	3	11,11,12	0.19	0	15,15,17	0.57	0
3	XYP	p	33	3	9,9,10	0.18	0	10,12,14	0.61	0
3	XYP	p	34	3	9,9,10	0.16	0	10,12,14	0.61	0
3	GAL	p	4	3	11,11,12	0.15	0	15,15,17	0.59	0
3	XYP	p	5	3	9,9,10	0.18	0	10,12,14	0.59	0
3	XYP	p	6	3	9,9,10	0.20	0	10,12,14	1.23	1 (10%)
3	BGC	p	7	3	11,11,12	0.21	0	15,15,17	0.82	1 (6%)
3	XYP	p	8	3	9,9,10	0.20	0	10,12,14	0.54	0
3	BGC	p	9	3	11,11,12	0.20	0	15,15,17	0.54	0
4	MAN	q	1	4,1	11,11,12	0.21	0	15,15,17	0.79	0
4	XYP	q	10	4	9,9,10	0.18	0	10,12,14	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	q	11	4	11,11,12	0.81	1 (9%)	15,15,17	0.80	0
4	AHR	q	12	4	9,9,10	0.60	0	10,12,14	1.03	1 (10%)
4	FUB	q	13	4	9,9,10	0.52	0	10,12,14	0.56	0
4	NAG	q	14	4	14,14,15	0.31	0	17,19,21	0.64	0
4	XYP	q	15	4	9,9,10	0.24	0	10,12,14	0.71	0
4	FUB	q	16	4	9,9,10	0.57	0	10,12,14	0.94	0
4	AHR	q	17	4	9,9,10	0.58	0	10,12,14	1.03	1 (10%)
4	MAN	q	18	4	11,11,12	0.21	0	15,15,17	0.80	1 (6%)
4	BGC	q	19	4	11,11,12	0.20	0	15,15,17	0.56	0
4	AHR	q	2	4	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
4	BGC	q	20	4	11,11,12	0.20	0	15,15,17	0.61	0
4	BGC	q	21	4	11,11,12	0.19	0	15,15,17	0.58	0
4	FUB	q	22	4	9,9,10	0.57	0	10,12,14	1.04	1 (10%)
4	BGC	q	23	4	11,11,12	0.20	0	15,15,17	0.60	0
4	BGC	q	24	4	11,11,12	0.20	0	15,15,17	0.58	0
4	BGC	q	25	4	11,11,12	0.18	0	15,15,17	0.57	0
4	AHR	q	26	4	9,9,10	0.59	0	10,12,14	1.02	1 (10%)
4	BGC	q	3	4	11,11,12	0.20	0	15,15,17	0.59	0
4	MAN	q	4	4	11,11,12	0.22	0	15,15,17	0.77	0
4	BGC	q	5	4	11,11,12	0.18	0	15,15,17	0.73	0
4	BMA	q	6	4	11,11,12	0.41	0	15,15,17	1.14	1 (6%)
4	NAG	q	7	4	14,14,15	0.77	0	17,19,21	1.58	3 (17%)
4	BGC	q	8	4	11,11,12	0.63	0	15,15,17	0.77	0
4	BGC	q	9	4	11,11,12	0.18	0	15,15,17	0.55	0
5	MAN	r	1	5,1	11,11,12	0.22	0	15,15,17	0.78	1 (6%)
5	NAG	r	2	5	14,14,15	0.28	0	17,19,21	0.64	0
6	MAN	s	1	6,1	11,11,12	0.23	0	15,15,17	0.79	1 (6%)
6	GZL	s	2	6	11,11,12	6.71	7 (63%)	14,15,17	1.43	2 (14%)
6	FUB	s	3	6	9,9,10	0.56	0	10,12,14	1.03	1 (10%)
6	NAG	s	4	6	14,14,15	0.28	0	17,19,21	0.63	0
7	XYP	t	1	7	9,9,10	0.86	1 (11%)	10,12,14	2.57	3 (30%)
7	MAN	t	10	7	11,11,12	0.51	0	15,15,17	0.87	1 (6%)
7	MAN	t	11	7	11,11,12	0.22	0	15,15,17	0.77	1 (6%)
7	BGC	t	12	7	11,11,12	0.19	0	15,15,17	0.56	0
7	BGC	t	13	7	11,11,12	0.19	0	15,15,17	0.57	0
7	XYP	t	14	7	9,9,10	0.19	0	10,12,14	0.61	0
7	MAN	t	15	7	11,11,12	0.21	0	15,15,17	0.81	1 (6%)
7	NAG	t	16	7	14,14,15	0.38	0	17,19,21	1.23	2 (11%)
7	BGC	t	17	7	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
7	BGC	t	18	7	11,11,12	0.22	0	15,15,17	0.59	0
7	XYP	t	19	7	9,9,10	0.20	0	10,12,14	0.62	0
7	BGC	t	2	7	11,11,12	0.19	0	15,15,17	0.57	0
7	XYP	t	20	7	9,9,10	0.30	0	10,12,14	0.59	0
7	XYP	t	21	7	9,9,10	0.41	0	10,12,14	0.66	0
7	XYP	t	22	7	9,9,10	0.25	0	10,12,14	0.72	0
7	A2G	t	3	7	14,14,15	0.42	0	17,19,21	1.03	2 (11%)
7	BGC	t	4	7	11,11,12	0.20	0	15,15,17	0.61	0
7	BGC	t	5	7	11,11,12	0.18	0	15,15,17	0.67	0
7	XYP	t	6	7	9,9,10	0.19	0	10,12,14	0.61	0
7	A2G	t	7	7	14,14,15	0.43	0	17,19,21	0.95	1 (5%)
7	MAN	t	8	7	11,11,12	0.48	0	15,15,17	0.84	1 (6%)
7	MAN	t	9	7	11,11,12	0.23	0	15,15,17	0.79	0
8	GAL	u	1	8	11,11,12	0.16	0	15,15,17	0.63	0
8	BGC	u	10	8	11,11,12	0.20	0	15,15,17	0.60	0
8	MAN	u	11	8	11,11,12	0.22	0	15,15,17	0.81	2 (13%)
8	BGC	u	12	8	11,11,12	0.20	0	15,15,17	0.56	0
8	XYP	u	13	8	9,9,10	0.18	0	10,12,14	0.60	0
8	NAG	u	14	8	14,14,15	0.29	0	17,19,21	0.56	0
8	BGC	u	15	8	11,11,12	0.19	0	15,15,17	0.57	0
8	MAN	u	16	8	11,11,12	0.45	0	15,15,17	0.98	2 (13%)
8	A2G	u	17	8	14,14,15	0.39	0	17,19,21	0.68	0
8	XYP	u	18	8	9,9,10	0.17	0	10,12,14	0.61	0
8	XYP	u	19	8	9,9,10	0.19	0	10,12,14	0.61	0
8	NAG	u	2	8	14,14,15	0.28	0	17,19,21	0.72	0
8	MAN	u	20	8	11,11,12	0.53	0	15,15,17	0.59	0
8	BGC	u	3	8	11,11,12	0.17	0	15,15,17	0.73	0
8	XYP	u	4	8	9,9,10	0.19	0	10,12,14	0.69	0
8	XYP	u	5	8	9,9,10	0.20	0	10,12,14	0.56	0
8	XYP	u	6	8	9,9,10	0.22	0	10,12,14	0.53	0
8	XYP	u	7	8	9,9,10	0.19	0	10,12,14	1.02	2 (20%)
8	GAL	u	8	8	11,11,12	0.22	0	15,15,17	0.64	1 (6%)
8	XYP	u	9	8	9,9,10	0.19	0	10,12,14	0.59	0
9	BGC	v	1	9,1	11,11,12	0.17	0	15,15,17	0.58	0
9	BGC	v	10	9	11,11,12	0.21	0	15,15,17	0.59	0
9	MAN	v	2	9	11,11,12	0.23	0	15,15,17	0.95	1 (6%)
9	BGC	v	3	9	11,11,12	0.24	0	15,15,17	0.88	1 (6%)
9	NAG	v	4	9	14,14,15	0.37	0	17,19,21	0.88	1 (5%)
9	BGC	v	5	9	11,11,12	0.19	0	15,15,17	0.53	0
9	MAN	v	6	9	11,11,12	0.45	0	15,15,17	0.59	0
9	BGC	v	7	9	11,11,12	0.19	0	15,15,17	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	XYP	v	8	9	9,9,10	0.19	0	10,12,14	0.60	0
9	XYP	v	9	9	9,9,10	0.17	0	10,12,14	0.60	0
10	GAL	w	1	10	11,11,12	0.15	0	15,15,17	0.64	0
10	MAN	w	10	10	11,11,12	0.58	0	15,15,17	0.59	0
10	NAG	w	11	10	14,14,15	0.60	0	17,19,21	0.90	0
10	XYP	w	12	10	9,9,10	0.20	0	10,12,14	0.62	0
10	MAN	w	13	10	11,11,12	0.20	0	15,15,17	0.80	1 (6%)
10	BGC	w	14	10	11,11,12	0.21	0	15,15,17	0.52	0
10	XYP	w	15	10	9,9,10	0.18	0	10,12,14	0.60	0
10	BGC	w	16	10	11,11,12	0.18	0	15,15,17	0.55	0
10	BGC	w	17	10	11,11,12	0.62	0	15,15,17	1.57	3 (20%)
10	NAG	w	18	10	14,14,15	0.65	0	17,19,21	1.12	2 (11%)
10	MAN	w	19	10	11,11,12	1.00	1 (9%)	15,15,17	1.40	3 (20%)
10	NAG	w	2	10	14,14,15	0.31	0	17,19,21	1.52	2 (11%)
10	XYP	w	3	10	9,9,10	0.59	0	10,12,14	3.02	3 (30%)
10	XYP	w	4	10	9,9,10	0.18	0	10,12,14	0.57	0
10	GAL	w	5	10	11,11,12	0.16	0	15,15,17	0.61	0
10	A2G	w	6	10	14,14,15	0.43	0	17,19,21	1.48	3 (17%)
10	GAL	w	7	10	11,11,12	0.18	0	15,15,17	0.58	0
10	A2G	w	8	10	14,14,15	0.46	0	17,19,21	1.07	1 (5%)
10	BGC	w	9	10	11,11,12	0.81	1 (9%)	15,15,17	0.90	1 (6%)
11	MAN	x	1	11,1	11,11,12	0.25	0	15,15,17	0.84	1 (6%)
11	GLA	x	10	11	11,11,12	0.42	0	15,15,17	1.13	1 (6%)
11	BGC	x	11	11	11,11,12	0.77	0	15,15,17	2.13	5 (33%)
11	BMA	x	12	11	11,11,12	1.02	1 (9%)	15,15,17	2.47	3 (20%)
11	NAG	x	13	11	14,14,15	0.86	0	17,19,21	1.71	5 (29%)
11	BMA	x	14	11	11,11,12	0.73	0	15,15,17	2.43	3 (20%)
11	BGC	x	15	11	11,11,12	0.79	0	15,15,17	0.93	1 (6%)
11	NAG	x	16	11	14,14,15	0.80	0	17,19,21	1.32	3 (17%)
11	AHR	x	17	11	9,9,10	0.62	0	10,12,14	1.08	1 (10%)
11	XYP	x	18	11	9,9,10	0.25	0	10,12,14	1.12	1 (10%)
11	BGC	x	19	11	11,11,12	0.39	0	15,15,17	1.12	1 (6%)
11	BGC	x	2	11	11,11,12	0.21	0	15,15,17	0.62	0
11	NAG	x	20	11	14,14,15	0.80	0	17,19,21	1.69	4 (23%)
11	BMA	x	21	11	11,11,12	0.22	0	15,15,17	0.54	0
11	MAN	x	22	11	11,11,12	0.21	0	15,15,17	0.79	1 (6%)
11	XYP	x	23	11	9,9,10	0.20	0	10,12,14	0.61	0
11	BMA	x	24	11	11,11,12	0.22	0	15,15,17	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	BGC	x	25	11	11,11,12	0.21	0	15,15,17	0.82	1 (6%)
11	XYP	x	26	11	9,9,10	0.23	0	10,12,14	0.59	0
11	XYP	x	27	11	9,9,10	0.19	0	10,12,14	0.65	0
11	NAG	x	28	11	14,14,15	0.31	0	17,19,21	0.61	0
11	MAN	x	29	11	11,11,12	0.22	0	15,15,17	0.80	1 (6%)
11	XYP	x	3	11	9,9,10	0.19	0	10,12,14	0.61	0
11	XYP	x	30	11	9,9,10	0.19	0	10,12,14	0.63	0
11	BGC	x	31	11	11,11,12	0.18	0	15,15,17	0.62	0
11	BGC	x	32	11	11,11,12	0.18	0	15,15,17	0.58	0
11	XYP	x	33	11	9,9,10	0.18	0	10,12,14	0.62	0
11	NAG	x	34	11	14,14,15	0.27	0	17,19,21	0.56	0
11	BGC	x	35	11	11,11,12	0.20	0	15,15,17	0.95	1 (6%)
11	XYP	x	36	11	9,9,10	0.40	0	10,12,14	0.50	0
11	MAN	x	37	11	11,11,12	0.37	0	15,15,17	0.72	0
11	NAG	x	38	11	14,14,15	0.31	0	17,19,21	0.71	1 (5%)
11	XYP	x	39	11	9,9,10	0.18	0	10,12,14	0.61	0
11	BMA	x	4	11	11,11,12	0.25	0	15,15,17	0.44	0
11	XYP	x	40	11	9,9,10	0.18	0	10,12,14	0.62	0
11	BGC	x	41	11	11,11,12	0.19	0	15,15,17	0.59	0
11	MAN	x	42	11	11,11,12	0.22	0	15,15,17	0.81	1 (6%)
11	BGC	x	43	11	11,11,12	0.20	0	15,15,17	0.55	0
11	XYP	x	44	11	9,9,10	0.18	0	10,12,14	0.63	0
11	BGC	x	45	11	11,11,12	0.18	0	15,15,17	0.58	0
11	BGC	x	46	11	11,11,12	0.19	0	15,15,17	0.56	0
11	BGC	x	47	11	11,11,12	0.54	0	15,15,17	0.81	0
11	NAG	x	5	11	14,14,15	0.33	0	17,19,21	0.62	0
11	FUB	x	6	11	9,9,10	0.61	0	10,12,14	1.14	2 (20%)
11	BGC	x	7	11	11,11,12	0.47	0	15,15,17	1.56	3 (20%)
11	BGC	x	8	11	11,11,12	0.84	0	15,15,17	1.47	3 (20%)
11	BMA	x	9	11	11,11,12	0.87	0	15,15,17	2.56	3 (20%)
12	GAL	y	1	12	11,11,12	0.20	0	15,15,17	0.62	0
12	XYP	y	10	12	9,9,10	0.19	0	10,12,14	0.61	0
12	XYP	y	2	12	9,9,10	0.19	0	10,12,14	0.65	0
12	BGC	y	3	12	11,11,12	0.21	0	15,15,17	0.54	0
12	XYP	y	4	12	9,9,10	0.17	0	10,12,14	0.63	0
12	BGC	y	5	12	11,11,12	0.80	0	15,15,17	2.33	5 (33%)
12	MAN	y	6	12	11,11,12	0.81	0	15,15,17	1.35	1 (6%)
12	BGC	y	7	12	11,11,12	0.63	0	15,15,17	1.97	3 (20%)
12	BGC	y	8	12	11,11,12	0.53	0	15,15,17	1.77	3 (20%)
12	NAG	y	9	12	14,14,15	0.56	0	17,19,21	1.38	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	XYP	z	1	13	9,9,10	0.34	0	10,12,14	1.54	2 (20%)
13	BGC	z	10	13	11,11,12	0.64	0	15,15,17	1.55	3 (20%)
13	MAN	z	11	13	11,11,12	0.24	0	15,15,17	0.79	1 (6%)
13	AHR	z	12	13	9,9,10	0.62	0	10,12,14	1.42	1 (10%)
13	XYP	z	13	13	9,9,10	0.28	0	10,12,14	0.88	0
13	BGC	z	14	13	11,11,12	0.71	0	15,15,17	2.10	6 (40%)
13	BGC	z	15	13	11,11,12	0.52	0	15,15,17	1.07	0
13	BGC	z	16	13	11,11,12	0.19	0	15,15,17	0.53	0
13	BGC	z	17	13	11,11,12	0.21	0	15,15,17	0.55	0
13	BGC	z	2	13	11,11,12	1.22	2 (18%)	15,15,17	2.50	5 (33%)
13	MAN	z	3	13	11,11,12	0.20	0	15,15,17	0.83	1 (6%)
13	NAG	z	4	13	14,14,15	0.87	0	17,19,21	1.55	1 (5%)
13	BGC	z	5	13	11,11,12	1.12	1 (9%)	15,15,17	2.20	7 (46%)
13	BGC	z	6	13	11,11,12	0.18	0	15,15,17	0.62	0
13	XYP	z	7	13	9,9,10	0.17	0	10,12,14	0.60	0
13	BGC	z	8	13	11,11,12	0.20	0	15,15,17	0.58	0
13	NAG	z	9	13	14,14,15	0.30	0	17,19,21	0.65	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
14	MAN	0	1	14,1	-	2/2/19/22	0/1/1/1
14	BGC	0	10	14	-	0/2/19/22	0/1/1/1
14	XYP	0	11	14	-	-	0/1/1/1
14	BGC	0	12	14	-	0/2/19/22	0/1/1/1
14	XYP	0	13	14	-	-	0/1/1/1
14	XYP	0	14	14	-	-	0/1/1/1
14	AHR	0	15	14	-	0/2/15/18	0/1/1/1
14	BGC	0	16	14	-	0/2/19/22	0/1/1/1
14	XYP	0	17	14	-	-	0/1/1/1
14	NAG	0	18	14	-	3/6/23/26	0/1/1/1
14	NAG	0	19	14	-	4/6/23/26	0/1/1/1
14	XYP	0	2	14	-	-	0/1/1/1
14	XYP	0	20	14	-	-	0/1/1/1
14	AHR	0	21	14	-	2/2/15/18	0/1/1/1
14	A2G	0	3	14	-	1/6/23/26	0/1/1/1
14	GAL	0	4	14	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	AHR	0	5	14	-	0/2/15/18	0/1/1/1
14	XYP	0	6	14	-	-	0/1/1/1
14	NAG	0	7	14	-	4/6/23/26	0/1/1/1
14	AHR	0	8	14	-	0/2/15/18	0/1/1/1
14	AHR	0	9	14	-	0/2/15/18	0/1/1/1
2	BGC	B	1	2,1	-	0/2/19/22	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	GAL	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	B	5	2	-	0/2/19/22	0/1/1/1
2	NAG	B	6	2	-	2/6/23/26	0/1/1/1
2	BMA	B	7	2	-	0/2/19/22	0/1/1/1
2	GAL	B	8	2	-	0/2/19/22	0/1/1/1
2	MAN	B	9	2	-	0/2/19/22	0/1/1/1
3	GLA	C	1	3,1	-	0/2/19/22	0/1/1/1
3	XYP	C	10	3	-	-	0/1/1/1
3	NAG	C	11	3	-	6/6/23/26	0/1/1/1
3	MAN	C	12	3	-	0/2/19/22	0/1/1/1
3	NAG	C	13	3	-	2/6/23/26	0/1/1/1
3	XYP	C	14	3	-	-	0/1/1/1
3	BGC	C	15	3	-	0/2/19/22	0/1/1/1
3	BGC	C	16	3	-	0/2/19/22	0/1/1/1
3	XYP	C	17	3	-	-	0/1/1/1
3	BGC	C	18	3	-	0/2/19/22	0/1/1/1
3	BGC	C	19	3	-	1/2/19/22	0/1/1/1
3	BGC	C	2	3	-	2/2/19/22	0/1/1/1
3	XYP	C	20	3	-	-	0/1/1/1
3	NAG	C	21	3	-	2/6/23/26	0/1/1/1
3	XYP	C	22	3	-	-	0/1/1/1
3	XYP	C	23	3	-	-	0/1/1/1
3	GAL	C	24	3	-	0/2/19/22	0/1/1/1
3	BGC	C	25	3	-	0/2/19/22	0/1/1/1
3	GAL	C	26	3	-	0/2/19/22	0/1/1/1
3	BGC	C	27	3	-	0/2/19/22	0/1/1/1
3	XYP	C	28	3	-	-	0/1/1/1
3	BGC	C	29	3	-	0/2/19/22	0/1/1/1
3	BGC	C	3	3	-	0/2/19/22	0/1/1/1
3	BGC	C	30	3	-	0/2/19/22	0/1/1/1
3	BGC	C	31	3	-	0/2/19/22	0/1/1/1
3	BGC	C	32	3	-	0/2/19/22	0/1/1/1
3	XYP	C	33	3	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	XYP	C	34	3	-	-	0/1/1/1
3	GAL	C	4	3	-	0/2/19/22	0/1/1/1
3	XYP	C	5	3	-	-	0/1/1/1
3	XYP	C	6	3	-	-	0/1/1/1
3	BGC	C	7	3	-	1/2/19/22	0/1/1/1
3	XYP	C	8	3	-	-	0/1/1/1
3	BGC	C	9	3	-	0/2/19/22	0/1/1/1
4	MAN	D	1	4,1	-	0/2/19/22	0/1/1/1
4	XYP	D	10	4	-	-	0/1/1/1
4	MAN	D	11	4	-	2/2/19/22	0/1/1/1
4	AHR	D	12	4	-	0/2/15/18	0/1/1/1
4	FUB	D	13	4	-	2/2/15/18	0/1/1/1
4	NAG	D	14	4	-	4/6/23/26	0/1/1/1
4	XYP	D	15	4	-	-	0/1/1/1
4	FUB	D	16	4	-	2/2/15/18	0/1/1/1
4	AHR	D	17	4	-	1/2/15/18	0/1/1/1
4	MAN	D	18	4	-	1/2/19/22	0/1/1/1
4	BGC	D	19	4	-	0/2/19/22	0/1/1/1
4	AHR	D	2	4	-	0/2/15/18	0/1/1/1
4	BGC	D	20	4	-	1/2/19/22	0/1/1/1
4	BGC	D	21	4	-	0/2/19/22	0/1/1/1
4	FUB	D	22	4	-	0/2/15/18	0/1/1/1
4	BGC	D	23	4	-	0/2/19/22	0/1/1/1
4	BGC	D	24	4	-	0/2/19/22	0/1/1/1
4	BGC	D	25	4	-	0/2/19/22	0/1/1/1
4	AHR	D	26	4	-	0/2/15/18	0/1/1/1
4	BGC	D	3	4	-	1/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	BGC	D	5	4	-	1/2/19/22	0/1/1/1
4	BMA	D	6	4	-	0/2/19/22	0/1/1/1
4	NAG	D	7	4	-	2/6/23/26	0/1/1/1
4	BGC	D	8	4	-	2/2/19/22	0/1/1/1
4	BGC	D	9	4	-	0/2/19/22	0/1/1/1
5	MAN	E	1	5,1	-	0/2/19/22	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
6	MAN	F	1	6,1	-	0/2/19/22	0/1/1/1
6	GZL	F	2	6	-	5/6/19/22	0/1/1/1
6	FUB	F	3	6	-	0/2/15/18	0/1/1/1
6	NAG	F	4	6	-	2/6/23/26	0/1/1/1
7	XYP	G	1	7	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	G	10	7	-	0/2/19/22	0/1/1/1
7	MAN	G	11	7	-	0/2/19/22	0/1/1/1
7	BGC	G	12	7	-	0/2/19/22	0/1/1/1
7	BGC	G	13	7	-	0/2/19/22	0/1/1/1
7	XYP	G	14	7	-	-	0/1/1/1
7	MAN	G	15	7	-	0/2/19/22	0/1/1/1
7	NAG	G	16	7	-	2/6/23/26	0/1/1/1
7	BGC	G	17	7	-	0/2/19/22	0/1/1/1
7	BGC	G	18	7	-	1/2/19/22	0/1/1/1
7	XYP	G	19	7	-	-	0/1/1/1
7	BGC	G	2	7	-	0/2/19/22	0/1/1/1
7	XYP	G	20	7	-	-	0/1/1/1
7	XYP	G	21	7	-	-	0/1/1/1
7	XYP	G	22	7	-	-	0/1/1/1
7	A2G	G	3	7	-	4/6/23/26	0/1/1/1
7	BGC	G	4	7	-	0/2/19/22	0/1/1/1
7	BGC	G	5	7	-	0/2/19/22	0/1/1/1
7	XYP	G	6	7	-	-	0/1/1/1
7	A2G	G	7	7	-	1/6/23/26	0/1/1/1
7	MAN	G	8	7	-	2/2/19/22	0/1/1/1
7	MAN	G	9	7	-	1/2/19/22	0/1/1/1
8	GAL	H	1	8	-	0/2/19/22	0/1/1/1
8	BGC	H	10	8	-	0/2/19/22	0/1/1/1
8	MAN	H	11	8	-	0/2/19/22	0/1/1/1
8	BGC	H	12	8	-	0/2/19/22	0/1/1/1
8	XYP	H	13	8	-	-	0/1/1/1
8	NAG	H	14	8	-	2/6/23/26	0/1/1/1
8	BGC	H	15	8	-	0/2/19/22	0/1/1/1
8	MAN	H	16	8	-	0/2/19/22	0/1/1/1
8	A2G	H	17	8	-	1/6/23/26	0/1/1/1
8	XYP	H	18	8	-	-	0/1/1/1
8	XYP	H	19	8	-	-	0/1/1/1
8	NAG	H	2	8	-	4/6/23/26	0/1/1/1
8	MAN	H	20	8	-	2/2/19/22	0/1/1/1
8	BGC	H	3	8	-	0/2/19/22	0/1/1/1
8	XYP	H	4	8	-	-	0/1/1/1
8	XYP	H	5	8	-	-	0/1/1/1
8	XYP	H	6	8	-	-	0/1/1/1
8	XYP	H	7	8	-	-	0/1/1/1
8	GAL	H	8	8	-	0/2/19/22	0/1/1/1
8	XYP	H	9	8	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BGC	I	1	9,1	-	0/2/19/22	0/1/1/1
9	BGC	I	10	9	-	0/2/19/22	0/1/1/1
9	MAN	I	2	9	-	0/2/19/22	0/1/1/1
9	BGC	I	3	9	-	0/2/19/22	0/1/1/1
9	NAG	I	4	9	-	4/6/23/26	0/1/1/1
9	BGC	I	5	9	-	0/2/19/22	0/1/1/1
9	MAN	I	6	9	-	0/2/19/22	0/1/1/1
9	BGC	I	7	9	-	0/2/19/22	0/1/1/1
9	XYP	I	8	9	-	-	0/1/1/1
9	XYP	I	9	9	-	-	0/1/1/1
10	GAL	J	1	10	-	0/2/19/22	0/1/1/1
10	MAN	J	10	10	-	2/2/19/22	0/1/1/1
10	NAG	J	11	10	-	4/6/23/26	0/1/1/1
10	XYP	J	12	10	-	-	0/1/1/1
10	MAN	J	13	10	-	0/2/19/22	0/1/1/1
10	BGC	J	14	10	-	0/2/19/22	0/1/1/1
10	XYP	J	15	10	-	-	0/1/1/1
10	BGC	J	16	10	-	0/2/19/22	0/1/1/1
10	BGC	J	17	10	-	0/2/19/22	0/1/1/1
10	NAG	J	18	10	-	2/6/23/26	0/1/1/1
10	MAN	J	19	10	-	0/2/19/22	0/1/1/1
10	NAG	J	2	10	-	0/6/23/26	0/1/1/1
10	XYP	J	3	10	-	-	0/1/1/1
10	XYP	J	4	10	-	-	0/1/1/1
10	GAL	J	5	10	-	0/2/19/22	0/1/1/1
10	A2G	J	6	10	-	2/6/23/26	0/1/1/1
10	GAL	J	7	10	-	1/2/19/22	0/1/1/1
10	A2G	J	8	10	-	1/6/23/26	0/1/1/1
10	BGC	J	9	10	-	0/2/19/22	0/1/1/1
11	MAN	K	1	11,1	-	1/2/19/22	0/1/1/1
11	GLA	K	10	11	-	0/2/19/22	0/1/1/1
11	BGC	K	11	11	-	2/2/19/22	0/1/1/1
11	BMA	K	12	11	-	2/2/19/22	0/1/1/1
11	NAG	K	13	11	-	1/6/23/26	0/1/1/1
11	BMA	K	14	11	-	1/2/19/22	0/1/1/1
11	BGC	K	15	11	-	0/2/19/22	0/1/1/1
11	NAG	K	16	11	-	4/6/23/26	0/1/1/1
11	AHR	K	17	11	-	0/2/15/18	0/1/1/1
11	XYP	K	18	11	-	-	0/1/1/1
11	BGC	K	19	11	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BGC	K	2	11	-	0/2/19/22	0/1/1/1
11	NAG	K	20	11	-	4/6/23/26	0/1/1/1
11	BMA	K	21	11	-	1/2/19/22	0/1/1/1
11	MAN	K	22	11	-	0/2/19/22	0/1/1/1
11	XYP	K	23	11	-	-	0/1/1/1
11	BMA	K	24	11	-	0/2/19/22	0/1/1/1
11	BGC	K	25	11	-	1/2/19/22	0/1/1/1
11	XYP	K	26	11	-	-	0/1/1/1
11	XYP	K	27	11	-	-	0/1/1/1
11	NAG	K	28	11	-	5/6/23/26	0/1/1/1
11	MAN	K	29	11	-	0/2/19/22	0/1/1/1
11	XYP	K	3	11	-	-	0/1/1/1
11	XYP	K	30	11	-	-	0/1/1/1
11	BGC	K	31	11	-	1/2/19/22	0/1/1/1
11	BGC	K	32	11	-	0/2/19/22	0/1/1/1
11	XYP	K	33	11	-	-	0/1/1/1
11	NAG	K	34	11	-	3/6/23/26	0/1/1/1
11	BGC	K	35	11	-	0/2/19/22	0/1/1/1
11	XYP	K	36	11	-	-	0/1/1/1
11	MAN	K	37	11	-	2/2/19/22	0/1/1/1
11	NAG	K	38	11	-	2/6/23/26	0/1/1/1
11	XYP	K	39	11	-	-	0/1/1/1
11	BMA	K	4	11	-	0/2/19/22	0/1/1/1
11	XYP	K	40	11	-	-	0/1/1/1
11	BGC	K	41	11	-	0/2/19/22	0/1/1/1
11	MAN	K	42	11	-	0/2/19/22	0/1/1/1
11	BGC	K	43	11	-	0/2/19/22	0/1/1/1
11	XYP	K	44	11	-	-	0/1/1/1
11	BGC	K	45	11	-	0/2/19/22	0/1/1/1
11	BGC	K	46	11	-	0/2/19/22	0/1/1/1
11	BGC	K	47	11	-	0/2/19/22	0/1/1/1
11	NAG	K	5	11	-	2/6/23/26	0/1/1/1
11	FUB	K	6	11	-	2/2/15/18	0/1/1/1
11	BGC	K	7	11	-	0/2/19/22	0/1/1/1
11	BGC	K	8	11	-	0/2/19/22	0/1/1/1
11	BMA	K	9	11	-	2/2/19/22	0/1/1/1
12	GAL	L	1	12	-	0/2/19/22	0/1/1/1
12	XYP	L	10	12	-	-	0/1/1/1
12	XYP	L	2	12	-	-	0/1/1/1
12	BGC	L	3	12	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	XYP	L	4	12	-	-	0/1/1/1
12	BGC	L	5	12	-	2/2/19/22	0/1/1/1
12	MAN	L	6	12	-	2/2/19/22	0/1/1/1
12	BGC	L	7	12	-	2/2/19/22	0/1/1/1
12	BGC	L	8	12	-	0/2/19/22	0/1/1/1
12	NAG	L	9	12	-	4/6/23/26	0/1/1/1
13	XYP	M	1	13	-	-	0/1/1/1
13	BGC	M	10	13	-	0/2/19/22	0/1/1/1
13	MAN	M	11	13	-	0/2/19/22	0/1/1/1
13	AHR	M	12	13	-	0/2/15/18	0/1/1/1
13	XYP	M	13	13	-	-	0/1/1/1
13	BGC	M	14	13	-	0/2/19/22	0/1/1/1
13	BGC	M	15	13	-	0/2/19/22	0/1/1/1
13	BGC	M	16	13	-	0/2/19/22	0/1/1/1
13	BGC	M	17	13	-	0/2/19/22	0/1/1/1
13	BGC	M	2	13	-	1/2/19/22	0/1/1/1
13	MAN	M	3	13	-	0/2/19/22	0/1/1/1
13	NAG	M	4	13	-	1/6/23/26	0/1/1/1
13	BGC	M	5	13	-	2/2/19/22	0/1/1/1
13	BGC	M	6	13	-	0/2/19/22	0/1/1/1
13	XYP	M	7	13	-	-	0/1/1/1
13	BGC	M	8	13	-	0/2/19/22	0/1/1/1
13	NAG	M	9	13	-	2/6/23/26	0/1/1/1
14	MAN	N	1	14,1	-	2/2/19/22	0/1/1/1
14	BGC	N	10	14	-	0/2/19/22	0/1/1/1
14	XYP	N	11	14	-	-	0/1/1/1
14	BGC	N	12	14	-	2/2/19/22	0/1/1/1
14	XYP	N	13	14	-	-	0/1/1/1
14	XYP	N	14	14	-	-	0/1/1/1
14	AHR	N	15	14	-	0/2/15/18	0/1/1/1
14	BGC	N	16	14	-	0/2/19/22	0/1/1/1
14	XYP	N	17	14	-	-	0/1/1/1
14	NAG	N	18	14	-	3/6/23/26	0/1/1/1
14	NAG	N	19	14	-	4/6/23/26	0/1/1/1
14	XYP	N	2	14	-	-	0/1/1/1
14	XYP	N	20	14	-	-	0/1/1/1
14	AHR	N	21	14	-	2/2/15/18	0/1/1/1
14	A2G	N	3	14	-	1/6/23/26	0/1/1/1
14	GAL	N	4	14	-	0/2/19/22	0/1/1/1
14	AHR	N	5	14	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	XYP	N	6	14	-	-	0/1/1/1
14	NAG	N	7	14	-	4/6/23/26	0/1/1/1
14	AHR	N	8	14	-	0/2/15/18	0/1/1/1
14	AHR	N	9	14	-	0/2/15/18	0/1/1/1
2	BGC	O	1	2,1	-	0/2/19/22	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
2	GAL	O	3	2	-	0/2/19/22	0/1/1/1
2	MAN	O	4	2	-	0/2/19/22	0/1/1/1
2	BGC	O	5	2	-	0/2/19/22	0/1/1/1
2	NAG	O	6	2	-	2/6/23/26	0/1/1/1
2	BMA	O	7	2	-	0/2/19/22	0/1/1/1
2	GAL	O	8	2	-	0/2/19/22	0/1/1/1
2	MAN	O	9	2	-	0/2/19/22	0/1/1/1
3	GLA	P	1	3,1	-	0/2/19/22	0/1/1/1
3	XYP	P	10	3	-	-	0/1/1/1
3	NAG	P	11	3	-	6/6/23/26	0/1/1/1
3	MAN	P	12	3	-	0/2/19/22	0/1/1/1
3	NAG	P	13	3	-	2/6/23/26	0/1/1/1
3	XYP	P	14	3	-	-	0/1/1/1
3	BGC	P	15	3	-	0/2/19/22	0/1/1/1
3	BGC	P	16	3	-	0/2/19/22	0/1/1/1
3	XYP	P	17	3	-	-	0/1/1/1
3	BGC	P	18	3	-	0/2/19/22	0/1/1/1
3	BGC	P	19	3	-	1/2/19/22	0/1/1/1
3	BGC	P	2	3	-	2/2/19/22	0/1/1/1
3	XYP	P	20	3	-	-	0/1/1/1
3	NAG	P	21	3	-	2/6/23/26	0/1/1/1
3	XYP	P	22	3	-	-	0/1/1/1
3	XYP	P	23	3	-	-	0/1/1/1
3	GAL	P	24	3	-	0/2/19/22	0/1/1/1
3	BGC	P	25	3	-	0/2/19/22	0/1/1/1
3	GAL	P	26	3	-	0/2/19/22	0/1/1/1
3	BGC	P	27	3	-	0/2/19/22	0/1/1/1
3	XYP	P	28	3	-	-	0/1/1/1
3	BGC	P	29	3	-	0/2/19/22	0/1/1/1
3	BGC	P	3	3	-	0/2/19/22	0/1/1/1
3	BGC	P	30	3	-	0/2/19/22	0/1/1/1
3	BGC	P	31	3	-	0/2/19/22	0/1/1/1
3	BGC	P	32	3	-	0/2/19/22	0/1/1/1
3	XYP	P	33	3	-	-	0/1/1/1
3	XYP	P	34	3	-	-	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	T	11	7	-	0/2/19/22	0/1/1/1
7	BGC	T	12	7	-	0/2/19/22	0/1/1/1
7	BGC	T	13	7	-	0/2/19/22	0/1/1/1
7	XYP	T	14	7	-	-	0/1/1/1
7	MAN	T	15	7	-	0/2/19/22	0/1/1/1
7	NAG	T	16	7	-	2/6/23/26	0/1/1/1
7	BGC	T	17	7	-	0/2/19/22	0/1/1/1
7	BGC	T	18	7	-	1/2/19/22	0/1/1/1
7	XYP	T	19	7	-	-	0/1/1/1
7	BGC	T	2	7	-	0/2/19/22	0/1/1/1
7	XYP	T	20	7	-	-	0/1/1/1
7	XYP	T	21	7	-	-	0/1/1/1
7	XYP	T	22	7	-	-	0/1/1/1
7	A2G	T	3	7	-	4/6/23/26	0/1/1/1
7	BGC	T	4	7	-	0/2/19/22	0/1/1/1
7	BGC	T	5	7	-	0/2/19/22	0/1/1/1
7	XYP	T	6	7	-	-	0/1/1/1
7	A2G	T	7	7	-	1/6/23/26	0/1/1/1
7	MAN	T	8	7	-	2/2/19/22	0/1/1/1
7	MAN	T	9	7	-	1/2/19/22	0/1/1/1
8	GAL	U	1	8	-	0/2/19/22	0/1/1/1
8	BGC	U	10	8	-	0/2/19/22	0/1/1/1
8	MAN	U	11	8	-	0/2/19/22	0/1/1/1
8	BGC	U	12	8	-	0/2/19/22	0/1/1/1
8	XYP	U	13	8	-	-	0/1/1/1
8	NAG	U	14	8	-	2/6/23/26	0/1/1/1
8	BGC	U	15	8	-	0/2/19/22	0/1/1/1
8	MAN	U	16	8	-	0/2/19/22	0/1/1/1
8	A2G	U	17	8	-	1/6/23/26	0/1/1/1
8	XYP	U	18	8	-	-	0/1/1/1
8	XYP	U	19	8	-	-	0/1/1/1
8	NAG	U	2	8	-	4/6/23/26	0/1/1/1
8	MAN	U	20	8	-	2/2/19/22	0/1/1/1
8	BGC	U	3	8	-	0/2/19/22	0/1/1/1
8	XYP	U	4	8	-	-	0/1/1/1
8	XYP	U	5	8	-	-	0/1/1/1
8	XYP	U	6	8	-	-	0/1/1/1
8	XYP	U	7	8	-	-	0/1/1/1
8	GAL	U	8	8	-	0/2/19/22	0/1/1/1
8	XYP	U	9	8	-	-	0/1/1/1
9	BGC	V	1	9,1	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BGC	V	10	9	-	0/2/19/22	0/1/1/1
9	MAN	V	2	9	-	0/2/19/22	0/1/1/1
9	BGC	V	3	9	-	0/2/19/22	0/1/1/1
9	NAG	V	4	9	-	4/6/23/26	0/1/1/1
9	BGC	V	5	9	-	0/2/19/22	0/1/1/1
9	MAN	V	6	9	-	0/2/19/22	0/1/1/1
9	BGC	V	7	9	-	0/2/19/22	0/1/1/1
9	XYP	V	8	9	-	-	0/1/1/1
9	XYP	V	9	9	-	-	0/1/1/1
10	GAL	W	1	10	-	0/2/19/22	0/1/1/1
10	MAN	W	10	10	-	2/2/19/22	0/1/1/1
10	NAG	W	11	10	-	4/6/23/26	0/1/1/1
10	XYP	W	12	10	-	-	0/1/1/1
10	MAN	W	13	10	-	0/2/19/22	0/1/1/1
10	BGC	W	14	10	-	0/2/19/22	0/1/1/1
10	XYP	W	15	10	-	-	0/1/1/1
10	BGC	W	16	10	-	0/2/19/22	0/1/1/1
10	BGC	W	17	10	-	0/2/19/22	0/1/1/1
10	NAG	W	18	10	-	2/6/23/26	0/1/1/1
10	MAN	W	19	10	-	0/2/19/22	0/1/1/1
10	NAG	W	2	10	-	0/6/23/26	0/1/1/1
10	XYP	W	3	10	-	-	0/1/1/1
10	XYP	W	4	10	-	-	0/1/1/1
10	GAL	W	5	10	-	0/2/19/22	0/1/1/1
10	A2G	W	6	10	-	2/6/23/26	0/1/1/1
10	GAL	W	7	10	-	1/2/19/22	0/1/1/1
10	A2G	W	8	10	-	1/6/23/26	0/1/1/1
10	BGC	W	9	10	-	0/2/19/22	0/1/1/1
11	MAN	X	1	11,1	-	1/2/19/22	0/1/1/1
11	GLA	X	10	11	-	0/2/19/22	0/1/1/1
11	BGC	X	11	11	-	2/2/19/22	0/1/1/1
11	BMA	X	12	11	-	2/2/19/22	0/1/1/1
11	NAG	X	13	11	-	1/6/23/26	0/1/1/1
11	BMA	X	14	11	-	1/2/19/22	0/1/1/1
11	BGC	X	15	11	-	0/2/19/22	0/1/1/1
11	NAG	X	16	11	-	4/6/23/26	0/1/1/1
11	AHR	X	17	11	-	0/2/15/18	0/1/1/1
11	XYP	X	18	11	-	-	0/1/1/1
11	BGC	X	19	11	-	2/2/19/22	0/1/1/1
11	BGC	X	2	11	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	X	20	11	-	4/6/23/26	0/1/1/1
11	BMA	X	21	11	-	1/2/19/22	0/1/1/1
11	MAN	X	22	11	-	0/2/19/22	0/1/1/1
11	XYP	X	23	11	-	-	0/1/1/1
11	BMA	X	24	11	-	0/2/19/22	0/1/1/1
11	BGC	X	25	11	-	1/2/19/22	0/1/1/1
11	XYP	X	26	11	-	-	0/1/1/1
11	XYP	X	27	11	-	-	0/1/1/1
11	NAG	X	28	11	-	5/6/23/26	0/1/1/1
11	MAN	X	29	11	-	0/2/19/22	0/1/1/1
11	XYP	X	3	11	-	-	0/1/1/1
11	XYP	X	30	11	-	-	0/1/1/1
11	BGC	X	31	11	-	1/2/19/22	0/1/1/1
11	BGC	X	32	11	-	0/2/19/22	0/1/1/1
11	XYP	X	33	11	-	-	0/1/1/1
11	NAG	X	34	11	-	3/6/23/26	0/1/1/1
11	BGC	X	35	11	-	0/2/19/22	0/1/1/1
11	XYP	X	36	11	-	-	0/1/1/1
11	MAN	X	37	11	-	2/2/19/22	0/1/1/1
11	NAG	X	38	11	-	2/6/23/26	0/1/1/1
11	XYP	X	39	11	-	-	0/1/1/1
11	BMA	X	4	11	-	0/2/19/22	0/1/1/1
11	XYP	X	40	11	-	-	0/1/1/1
11	BGC	X	41	11	-	0/2/19/22	0/1/1/1
11	MAN	X	42	11	-	0/2/19/22	0/1/1/1
11	BGC	X	43	11	-	0/2/19/22	0/1/1/1
11	XYP	X	44	11	-	-	0/1/1/1
11	BGC	X	45	11	-	0/2/19/22	0/1/1/1
11	BGC	X	46	11	-	0/2/19/22	0/1/1/1
11	BGC	X	47	11	-	0/2/19/22	0/1/1/1
11	NAG	X	5	11	-	2/6/23/26	0/1/1/1
11	FUB	X	6	11	-	2/2/15/18	0/1/1/1
11	BGC	X	7	11	-	0/2/19/22	0/1/1/1
11	BGC	X	8	11	-	0/2/19/22	0/1/1/1
11	BMA	X	9	11	-	2/2/19/22	0/1/1/1
12	GAL	Y	1	12	-	0/2/19/22	0/1/1/1
12	XYP	Y	10	12	-	-	0/1/1/1
12	XYP	Y	2	12	-	-	0/1/1/1
12	BGC	Y	3	12	-	0/2/19/22	0/1/1/1
12	XYP	Y	4	12	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BGC	Y	5	12	-	2/2/19/22	0/1/1/1
12	MAN	Y	6	12	-	2/2/19/22	0/1/1/1
12	BGC	Y	7	12	-	2/2/19/22	0/1/1/1
12	BGC	Y	8	12	-	0/2/19/22	0/1/1/1
12	NAG	Y	9	12	-	4/6/23/26	0/1/1/1
13	XYP	Z	1	13	-	-	0/1/1/1
13	BGC	Z	10	13	-	0/2/19/22	0/1/1/1
13	MAN	Z	11	13	-	0/2/19/22	0/1/1/1
13	AHR	Z	12	13	-	0/2/15/18	0/1/1/1
13	XYP	Z	13	13	-	-	0/1/1/1
13	BGC	Z	14	13	-	0/2/19/22	0/1/1/1
13	BGC	Z	15	13	-	0/2/19/22	0/1/1/1
13	BGC	Z	16	13	-	0/2/19/22	0/1/1/1
13	BGC	Z	17	13	-	0/2/19/22	0/1/1/1
13	BGC	Z	2	13	-	1/2/19/22	0/1/1/1
13	MAN	Z	3	13	-	0/2/19/22	0/1/1/1
13	NAG	Z	4	13	-	1/6/23/26	0/1/1/1
13	BGC	Z	5	13	-	2/2/19/22	0/1/1/1
13	BGC	Z	6	13	-	0/2/19/22	0/1/1/1
13	XYP	Z	7	13	-	-	0/1/1/1
13	BGC	Z	8	13	-	0/2/19/22	0/1/1/1
13	NAG	Z	9	13	-	2/6/23/26	0/1/1/1
14	MAN	a	1	14,1	-	2/2/19/22	0/1/1/1
14	BGC	a	10	14	-	0/2/19/22	0/1/1/1
14	XYP	a	11	14	-	-	0/1/1/1
14	BGC	a	12	14	-	2/2/19/22	0/1/1/1
14	XYP	a	13	14	-	-	0/1/1/1
14	XYP	a	14	14	-	-	0/1/1/1
14	AHR	a	15	14	-	0/2/15/18	0/1/1/1
14	BGC	a	16	14	-	0/2/19/22	0/1/1/1
14	XYP	a	17	14	-	-	0/1/1/1
14	NAG	a	18	14	-	3/6/23/26	0/1/1/1
14	NAG	a	19	14	-	4/6/23/26	0/1/1/1
14	XYP	a	2	14	-	-	0/1/1/1
14	XYP	a	20	14	-	-	0/1/1/1
14	AHR	a	21	14	-	2/2/15/18	0/1/1/1
14	A2G	a	3	14	-	1/6/23/26	0/1/1/1
14	GAL	a	4	14	-	0/2/19/22	0/1/1/1
14	AHR	a	5	14	-	0/2/15/18	0/1/1/1
14	XYP	a	6	14	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	a	7	14	-	4/6/23/26	0/1/1/1
14	AHR	a	8	14	-	0/2/15/18	0/1/1/1
14	AHR	a	9	14	-	0/2/15/18	0/1/1/1
2	BGC	b	1	2,1	-	0/2/19/22	0/1/1/1
2	NAG	b	2	2	-	1/6/23/26	0/1/1/1
2	GAL	b	3	2	-	0/2/19/22	0/1/1/1
2	MAN	b	4	2	-	0/2/19/22	0/1/1/1
2	BGC	b	5	2	-	0/2/19/22	0/1/1/1
2	NAG	b	6	2	-	2/6/23/26	0/1/1/1
2	BMA	b	7	2	-	0/2/19/22	0/1/1/1
2	GAL	b	8	2	-	0/2/19/22	0/1/1/1
2	MAN	b	9	2	-	0/2/19/22	0/1/1/1
3	GLA	c	1	3,1	-	0/2/19/22	0/1/1/1
3	XYP	c	10	3	-	-	0/1/1/1
3	NAG	c	11	3	-	6/6/23/26	0/1/1/1
3	MAN	c	12	3	-	0/2/19/22	0/1/1/1
3	NAG	c	13	3	-	2/6/23/26	0/1/1/1
3	XYP	c	14	3	-	-	0/1/1/1
3	BGC	c	15	3	-	0/2/19/22	0/1/1/1
3	BGC	c	16	3	-	0/2/19/22	0/1/1/1
3	XYP	c	17	3	-	-	0/1/1/1
3	BGC	c	18	3	-	0/2/19/22	0/1/1/1
3	BGC	c	19	3	-	1/2/19/22	0/1/1/1
3	BGC	c	2	3	-	2/2/19/22	0/1/1/1
3	XYP	c	20	3	-	-	0/1/1/1
3	NAG	c	21	3	-	2/6/23/26	0/1/1/1
3	XYP	c	22	3	-	-	0/1/1/1
3	XYP	c	23	3	-	-	0/1/1/1
3	GAL	c	24	3	-	0/2/19/22	0/1/1/1
3	BGC	c	25	3	-	0/2/19/22	0/1/1/1
3	GAL	c	26	3	-	0/2/19/22	0/1/1/1
3	BGC	c	27	3	-	0/2/19/22	0/1/1/1
3	XYP	c	28	3	-	-	0/1/1/1
3	BGC	c	29	3	-	0/2/19/22	0/1/1/1
3	BGC	c	3	3	-	0/2/19/22	0/1/1/1
3	BGC	c	30	3	-	0/2/19/22	0/1/1/1
3	BGC	c	31	3	-	0/2/19/22	0/1/1/1
3	BGC	c	32	3	-	0/2/19/22	0/1/1/1
3	XYP	c	33	3	-	-	0/1/1/1
3	XYP	c	34	3	-	-	0/1/1/1
3	GAL	c	4	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	XYP	c	5	3	-	-	0/1/1/1
3	XYP	c	6	3	-	-	0/1/1/1
3	BGC	c	7	3	-	1/2/19/22	0/1/1/1
3	XYP	c	8	3	-	-	0/1/1/1
3	BGC	c	9	3	-	0/2/19/22	0/1/1/1
4	MAN	d	1	4,1	-	0/2/19/22	0/1/1/1
4	XYP	d	10	4	-	-	0/1/1/1
4	MAN	d	11	4	-	2/2/19/22	0/1/1/1
4	AHR	d	12	4	-	0/2/15/18	0/1/1/1
4	FUB	d	13	4	-	2/2/15/18	0/1/1/1
4	NAG	d	14	4	-	4/6/23/26	0/1/1/1
4	XYP	d	15	4	-	-	0/1/1/1
4	FUB	d	16	4	-	2/2/15/18	0/1/1/1
4	AHR	d	17	4	-	1/2/15/18	0/1/1/1
4	MAN	d	18	4	-	1/2/19/22	0/1/1/1
4	BGC	d	19	4	-	0/2/19/22	0/1/1/1
4	AHR	d	2	4	-	0/2/15/18	0/1/1/1
4	BGC	d	20	4	-	1/2/19/22	0/1/1/1
4	BGC	d	21	4	-	0/2/19/22	0/1/1/1
4	FUB	d	22	4	-	0/2/15/18	0/1/1/1
4	BGC	d	23	4	-	0/2/19/22	0/1/1/1
4	BGC	d	24	4	-	0/2/19/22	0/1/1/1
4	BGC	d	25	4	-	0/2/19/22	0/1/1/1
4	AHR	d	26	4	-	0/2/15/18	0/1/1/1
4	BGC	d	3	4	-	1/2/19/22	0/1/1/1
4	MAN	d	4	4	-	0/2/19/22	0/1/1/1
4	BGC	d	5	4	-	1/2/19/22	0/1/1/1
4	BMA	d	6	4	-	0/2/19/22	0/1/1/1
4	NAG	d	7	4	-	2/6/23/26	0/1/1/1
4	BGC	d	8	4	-	2/2/19/22	0/1/1/1
4	BGC	d	9	4	-	0/2/19/22	0/1/1/1
5	MAN	e	1	5,1	-	0/2/19/22	0/1/1/1
5	NAG	e	2	5	-	2/6/23/26	0/1/1/1
6	MAN	f	1	6,1	-	0/2/19/22	0/1/1/1
6	GZL	f	2	6	-	5/6/19/22	0/1/1/1
6	FUB	f	3	6	-	0/2/15/18	0/1/1/1
6	NAG	f	4	6	-	2/6/23/26	0/1/1/1
7	XYP	g	1	7	-	-	0/1/1/1
7	MAN	g	10	7	-	0/2/19/22	0/1/1/1
7	MAN	g	11	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BGC	g	12	7	-	0/2/19/22	0/1/1/1
7	BGC	g	13	7	-	0/2/19/22	0/1/1/1
7	XYP	g	14	7	-	-	0/1/1/1
7	MAN	g	15	7	-	0/2/19/22	0/1/1/1
7	NAG	g	16	7	-	2/6/23/26	0/1/1/1
7	BGC	g	17	7	-	0/2/19/22	0/1/1/1
7	BGC	g	18	7	-	1/2/19/22	0/1/1/1
7	XYP	g	19	7	-	-	0/1/1/1
7	BGC	g	2	7	-	0/2/19/22	0/1/1/1
7	XYP	g	20	7	-	-	0/1/1/1
7	XYP	g	21	7	-	-	0/1/1/1
7	XYP	g	22	7	-	-	0/1/1/1
7	A2G	g	3	7	-	4/6/23/26	0/1/1/1
7	BGC	g	4	7	-	0/2/19/22	0/1/1/1
7	BGC	g	5	7	-	0/2/19/22	0/1/1/1
7	XYP	g	6	7	-	-	0/1/1/1
7	A2G	g	7	7	-	1/6/23/26	0/1/1/1
7	MAN	g	8	7	-	2/2/19/22	0/1/1/1
7	MAN	g	9	7	-	1/2/19/22	0/1/1/1
8	GAL	h	1	8	-	0/2/19/22	0/1/1/1
8	BGC	h	10	8	-	0/2/19/22	0/1/1/1
8	MAN	h	11	8	-	0/2/19/22	0/1/1/1
8	BGC	h	12	8	-	0/2/19/22	0/1/1/1
8	XYP	h	13	8	-	-	0/1/1/1
8	NAG	h	14	8	-	2/6/23/26	0/1/1/1
8	BGC	h	15	8	-	0/2/19/22	0/1/1/1
8	MAN	h	16	8	-	0/2/19/22	0/1/1/1
8	A2G	h	17	8	-	1/6/23/26	0/1/1/1
8	XYP	h	18	8	-	-	0/1/1/1
8	XYP	h	19	8	-	-	0/1/1/1
8	NAG	h	2	8	-	4/6/23/26	0/1/1/1
8	MAN	h	20	8	-	2/2/19/22	0/1/1/1
8	BGC	h	3	8	-	0/2/19/22	0/1/1/1
8	XYP	h	4	8	-	-	0/1/1/1
8	XYP	h	5	8	-	-	0/1/1/1
8	XYP	h	6	8	-	-	0/1/1/1
8	XYP	h	7	8	-	-	0/1/1/1
8	GAL	h	8	8	-	0/2/19/22	0/1/1/1
8	XYP	h	9	8	-	-	0/1/1/1
9	BGC	i	1	9,1	-	0/2/19/22	0/1/1/1
9	BGC	i	10	9	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	i	2	9	-	0/2/19/22	0/1/1/1
9	BGC	i	3	9	-	0/2/19/22	0/1/1/1
9	NAG	i	4	9	-	4/6/23/26	0/1/1/1
9	BGC	i	5	9	-	0/2/19/22	0/1/1/1
9	MAN	i	6	9	-	0/2/19/22	0/1/1/1
9	BGC	i	7	9	-	0/2/19/22	0/1/1/1
9	XYP	i	8	9	-	-	0/1/1/1
9	XYP	i	9	9	-	-	0/1/1/1
10	GAL	j	1	10	-	0/2/19/22	0/1/1/1
10	MAN	j	10	10	-	2/2/19/22	0/1/1/1
10	NAG	j	11	10	-	4/6/23/26	0/1/1/1
10	XYP	j	12	10	-	-	0/1/1/1
10	MAN	j	13	10	-	0/2/19/22	0/1/1/1
10	BGC	j	14	10	-	0/2/19/22	0/1/1/1
10	XYP	j	15	10	-	-	0/1/1/1
10	BGC	j	16	10	-	0/2/19/22	0/1/1/1
10	BGC	j	17	10	-	0/2/19/22	0/1/1/1
10	NAG	j	18	10	-	2/6/23/26	0/1/1/1
10	MAN	j	19	10	-	2/2/19/22	0/1/1/1
10	NAG	j	2	10	-	0/6/23/26	0/1/1/1
10	XYP	j	3	10	-	-	0/1/1/1
10	XYP	j	4	10	-	-	0/1/1/1
10	GAL	j	5	10	-	0/2/19/22	0/1/1/1
10	A2G	j	6	10	-	2/6/23/26	0/1/1/1
10	GAL	j	7	10	-	1/2/19/22	0/1/1/1
10	A2G	j	8	10	-	1/6/23/26	0/1/1/1
10	BGC	j	9	10	-	0/2/19/22	0/1/1/1
11	MAN	k	1	11,1	-	1/2/19/22	0/1/1/1
11	GLA	k	10	11	-	0/2/19/22	0/1/1/1
11	BGC	k	11	11	-	2/2/19/22	0/1/1/1
11	BMA	k	12	11	-	2/2/19/22	0/1/1/1
11	NAG	k	13	11	-	1/6/23/26	0/1/1/1
11	BMA	k	14	11	-	1/2/19/22	0/1/1/1
11	BGC	k	15	11	-	0/2/19/22	0/1/1/1
11	NAG	k	16	11	-	4/6/23/26	0/1/1/1
11	AHR	k	17	11	-	0/2/15/18	0/1/1/1
11	XYP	k	18	11	-	-	0/1/1/1
11	BGC	k	19	11	-	2/2/19/22	0/1/1/1
11	BGC	k	2	11	-	0/2/19/22	0/1/1/1
11	NAG	k	20	11	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BMA	k	21	11	-	1/2/19/22	0/1/1/1
11	MAN	k	22	11	-	0/2/19/22	0/1/1/1
11	XYP	k	23	11	-	-	0/1/1/1
11	BMA	k	24	11	-	0/2/19/22	0/1/1/1
11	BGC	k	25	11	-	1/2/19/22	0/1/1/1
11	XYP	k	26	11	-	-	0/1/1/1
11	XYP	k	27	11	-	-	0/1/1/1
11	NAG	k	28	11	-	5/6/23/26	0/1/1/1
11	MAN	k	29	11	-	0/2/19/22	0/1/1/1
11	XYP	k	3	11	-	-	0/1/1/1
11	XYP	k	30	11	-	-	0/1/1/1
11	BGC	k	31	11	-	1/2/19/22	0/1/1/1
11	BGC	k	32	11	-	0/2/19/22	0/1/1/1
11	XYP	k	33	11	-	-	0/1/1/1
11	NAG	k	34	11	-	3/6/23/26	0/1/1/1
11	BGC	k	35	11	-	0/2/19/22	0/1/1/1
11	XYP	k	36	11	-	-	0/1/1/1
11	MAN	k	37	11	-	2/2/19/22	0/1/1/1
11	NAG	k	38	11	-	2/6/23/26	0/1/1/1
11	XYP	k	39	11	-	-	0/1/1/1
11	BMA	k	4	11	-	0/2/19/22	0/1/1/1
11	XYP	k	40	11	-	-	0/1/1/1
11	BGC	k	41	11	-	0/2/19/22	0/1/1/1
11	MAN	k	42	11	-	0/2/19/22	0/1/1/1
11	BGC	k	43	11	-	0/2/19/22	0/1/1/1
11	XYP	k	44	11	-	-	0/1/1/1
11	BGC	k	45	11	-	0/2/19/22	0/1/1/1
11	BGC	k	46	11	-	0/2/19/22	0/1/1/1
11	BGC	k	47	11	-	0/2/19/22	0/1/1/1
11	NAG	k	5	11	-	2/6/23/26	0/1/1/1
11	FUB	k	6	11	-	2/2/15/18	0/1/1/1
11	BGC	k	7	11	-	0/2/19/22	0/1/1/1
11	BGC	k	8	11	-	0/2/19/22	0/1/1/1
11	BMA	k	9	11	-	2/2/19/22	0/1/1/1
12	GAL	l	1	12	-	0/2/19/22	0/1/1/1
12	XYP	l	10	12	-	-	0/1/1/1
12	XYP	l	2	12	-	-	0/1/1/1
12	BGC	l	3	12	-	0/2/19/22	0/1/1/1
12	XYP	l	4	12	-	-	0/1/1/1
12	BGC	l	5	12	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	l	6	12	-	2/2/19/22	0/1/1/1
12	BGC	l	7	12	-	2/2/19/22	0/1/1/1
12	BGC	l	8	12	-	0/2/19/22	0/1/1/1
12	NAG	l	9	12	-	4/6/23/26	0/1/1/1
13	XYP	m	1	13	-	-	0/1/1/1
13	BGC	m	10	13	-	0/2/19/22	0/1/1/1
13	MAN	m	11	13	-	0/2/19/22	0/1/1/1
13	AHR	m	12	13	-	0/2/15/18	0/1/1/1
13	XYP	m	13	13	-	-	0/1/1/1
13	BGC	m	14	13	-	0/2/19/22	0/1/1/1
13	BGC	m	15	13	-	0/2/19/22	0/1/1/1
13	BGC	m	16	13	-	0/2/19/22	0/1/1/1
13	BGC	m	17	13	-	0/2/19/22	0/1/1/1
13	BGC	m	2	13	-	1/2/19/22	0/1/1/1
13	MAN	m	3	13	-	0/2/19/22	0/1/1/1
13	NAG	m	4	13	-	1/6/23/26	0/1/1/1
13	BGC	m	5	13	-	2/2/19/22	0/1/1/1
13	BGC	m	6	13	-	0/2/19/22	0/1/1/1
13	XYP	m	7	13	-	-	0/1/1/1
13	BGC	m	8	13	-	0/2/19/22	0/1/1/1
13	NAG	m	9	13	-	2/6/23/26	0/1/1/1
14	MAN	n	1	14,1	-	2/2/19/22	0/1/1/1
14	BGC	n	10	14	-	0/2/19/22	0/1/1/1
14	XYP	n	11	14	-	-	0/1/1/1
14	BGC	n	12	14	-	0/2/19/22	0/1/1/1
14	XYP	n	13	14	-	-	0/1/1/1
14	XYP	n	14	14	-	-	0/1/1/1
14	AHR	n	15	14	-	0/2/15/18	0/1/1/1
14	BGC	n	16	14	-	0/2/19/22	0/1/1/1
14	XYP	n	17	14	-	-	0/1/1/1
14	NAG	n	18	14	-	3/6/23/26	0/1/1/1
14	NAG	n	19	14	-	4/6/23/26	0/1/1/1
14	XYP	n	2	14	-	-	0/1/1/1
14	XYP	n	20	14	-	-	0/1/1/1
14	AHR	n	21	14	-	2/2/15/18	0/1/1/1
14	A2G	n	3	14	-	1/6/23/26	0/1/1/1
14	GAL	n	4	14	-	0/2/19/22	0/1/1/1
14	AHR	n	5	14	-	0/2/15/18	0/1/1/1
14	XYP	n	6	14	-	-	0/1/1/1
14	NAG	n	7	14	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	AHR	n	8	14	-	0/2/15/18	0/1/1/1
14	AHR	n	9	14	-	0/2/15/18	0/1/1/1
2	BGC	o	1	2,1	-	0/2/19/22	0/1/1/1
2	NAG	o	2	2	-	2/6/23/26	0/1/1/1
2	GAL	o	3	2	-	0/2/19/22	0/1/1/1
2	MAN	o	4	2	-	0/2/19/22	0/1/1/1
2	BGC	o	5	2	-	0/2/19/22	0/1/1/1
2	NAG	o	6	2	-	2/6/23/26	0/1/1/1
2	BMA	o	7	2	-	0/2/19/22	0/1/1/1
2	GAL	o	8	2	-	0/2/19/22	0/1/1/1
2	MAN	o	9	2	-	0/2/19/22	0/1/1/1
3	GLA	p	1	3,1	-	0/2/19/22	0/1/1/1
3	XYP	p	10	3	-	-	0/1/1/1
3	NAG	p	11	3	-	6/6/23/26	0/1/1/1
3	MAN	p	12	3	-	0/2/19/22	0/1/1/1
3	NAG	p	13	3	-	2/6/23/26	0/1/1/1
3	XYP	p	14	3	-	-	0/1/1/1
3	BGC	p	15	3	-	0/2/19/22	0/1/1/1
3	BGC	p	16	3	-	0/2/19/22	0/1/1/1
3	XYP	p	17	3	-	-	0/1/1/1
3	BGC	p	18	3	-	0/2/19/22	0/1/1/1
3	BGC	p	19	3	-	1/2/19/22	0/1/1/1
3	BGC	p	2	3	-	2/2/19/22	0/1/1/1
3	XYP	p	20	3	-	-	0/1/1/1
3	NAG	p	21	3	-	2/6/23/26	0/1/1/1
3	XYP	p	22	3	-	-	0/1/1/1
3	XYP	p	23	3	-	-	0/1/1/1
3	GAL	p	24	3	-	0/2/19/22	0/1/1/1
3	BGC	p	25	3	-	0/2/19/22	0/1/1/1
3	GAL	p	26	3	-	0/2/19/22	0/1/1/1
3	BGC	p	27	3	-	0/2/19/22	0/1/1/1
3	XYP	p	28	3	-	-	0/1/1/1
3	BGC	p	29	3	-	0/2/19/22	0/1/1/1
3	BGC	p	3	3	-	0/2/19/22	0/1/1/1
3	BGC	p	30	3	-	0/2/19/22	0/1/1/1
3	BGC	p	31	3	-	0/2/19/22	0/1/1/1
3	BGC	p	32	3	-	0/2/19/22	0/1/1/1
3	XYP	p	33	3	-	-	0/1/1/1
3	XYP	p	34	3	-	-	0/1/1/1
3	GAL	p	4	3	-	0/2/19/22	0/1/1/1
3	XYP	p	5	3	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	XYP	p	6	3	-	-	0/1/1/1
3	BGC	p	7	3	-	1/2/19/22	0/1/1/1
3	XYP	p	8	3	-	-	0/1/1/1
3	BGC	p	9	3	-	0/2/19/22	0/1/1/1
4	MAN	q	1	4,1	-	0/2/19/22	0/1/1/1
4	XYP	q	10	4	-	-	0/1/1/1
4	MAN	q	11	4	-	2/2/19/22	0/1/1/1
4	AHR	q	12	4	-	0/2/15/18	0/1/1/1
4	FUB	q	13	4	-	2/2/15/18	0/1/1/1
4	NAG	q	14	4	-	4/6/23/26	0/1/1/1
4	XYP	q	15	4	-	-	0/1/1/1
4	FUB	q	16	4	-	2/2/15/18	0/1/1/1
4	AHR	q	17	4	-	1/2/15/18	0/1/1/1
4	MAN	q	18	4	-	1/2/19/22	0/1/1/1
4	BGC	q	19	4	-	0/2/19/22	0/1/1/1
4	AHR	q	2	4	-	0/2/15/18	0/1/1/1
4	BGC	q	20	4	-	1/2/19/22	0/1/1/1
4	BGC	q	21	4	-	0/2/19/22	0/1/1/1
4	FUB	q	22	4	-	0/2/15/18	0/1/1/1
4	BGC	q	23	4	-	0/2/19/22	0/1/1/1
4	BGC	q	24	4	-	0/2/19/22	0/1/1/1
4	BGC	q	25	4	-	0/2/19/22	0/1/1/1
4	AHR	q	26	4	-	0/2/15/18	0/1/1/1
4	BGC	q	3	4	-	1/2/19/22	0/1/1/1
4	MAN	q	4	4	-	0/2/19/22	0/1/1/1
4	BGC	q	5	4	-	1/2/19/22	0/1/1/1
4	BMA	q	6	4	-	0/2/19/22	0/1/1/1
4	NAG	q	7	4	-	2/6/23/26	0/1/1/1
4	BGC	q	8	4	-	2/2/19/22	0/1/1/1
4	BGC	q	9	4	-	0/2/19/22	0/1/1/1
5	MAN	r	1	5,1	-	0/2/19/22	0/1/1/1
5	NAG	r	2	5	-	2/6/23/26	0/1/1/1
6	MAN	s	1	6,1	-	0/2/19/22	0/1/1/1
6	GZL	s	2	6	-	5/6/19/22	0/1/1/1
6	FUB	s	3	6	-	0/2/15/18	0/1/1/1
6	NAG	s	4	6	-	2/6/23/26	0/1/1/1
7	XYP	t	1	7	-	-	0/1/1/1
7	MAN	t	10	7	-	0/2/19/22	0/1/1/1
7	MAN	t	11	7	-	0/2/19/22	0/1/1/1
7	BGC	t	12	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BGC	t	13	7	-	0/2/19/22	0/1/1/1
7	XYP	t	14	7	-	-	0/1/1/1
7	MAN	t	15	7	-	0/2/19/22	0/1/1/1
7	NAG	t	16	7	-	2/6/23/26	0/1/1/1
7	BGC	t	17	7	-	0/2/19/22	0/1/1/1
7	BGC	t	18	7	-	1/2/19/22	0/1/1/1
7	XYP	t	19	7	-	-	0/1/1/1
7	BGC	t	2	7	-	0/2/19/22	0/1/1/1
7	XYP	t	20	7	-	-	0/1/1/1
7	XYP	t	21	7	-	-	0/1/1/1
7	XYP	t	22	7	-	-	0/1/1/1
7	A2G	t	3	7	-	4/6/23/26	0/1/1/1
7	BGC	t	4	7	-	0/2/19/22	0/1/1/1
7	BGC	t	5	7	-	0/2/19/22	0/1/1/1
7	XYP	t	6	7	-	-	0/1/1/1
7	A2G	t	7	7	-	1/6/23/26	0/1/1/1
7	MAN	t	8	7	-	2/2/19/22	0/1/1/1
7	MAN	t	9	7	-	1/2/19/22	0/1/1/1
8	GAL	u	1	8	-	0/2/19/22	0/1/1/1
8	BGC	u	10	8	-	0/2/19/22	0/1/1/1
8	MAN	u	11	8	-	0/2/19/22	0/1/1/1
8	BGC	u	12	8	-	0/2/19/22	0/1/1/1
8	XYP	u	13	8	-	-	0/1/1/1
8	NAG	u	14	8	-	2/6/23/26	0/1/1/1
8	BGC	u	15	8	-	0/2/19/22	0/1/1/1
8	MAN	u	16	8	-	0/2/19/22	0/1/1/1
8	A2G	u	17	8	-	1/6/23/26	0/1/1/1
8	XYP	u	18	8	-	-	0/1/1/1
8	XYP	u	19	8	-	-	0/1/1/1
8	NAG	u	2	8	-	4/6/23/26	0/1/1/1
8	MAN	u	20	8	-	2/2/19/22	0/1/1/1
8	BGC	u	3	8	-	0/2/19/22	0/1/1/1
8	XYP	u	4	8	-	-	0/1/1/1
8	XYP	u	5	8	-	-	0/1/1/1
8	XYP	u	6	8	-	-	0/1/1/1
8	XYP	u	7	8	-	-	0/1/1/1
8	GAL	u	8	8	-	0/2/19/22	0/1/1/1
8	XYP	u	9	8	-	-	0/1/1/1
9	BGC	v	1	9,1	-	0/2/19/22	0/1/1/1
9	BGC	v	10	9	-	0/2/19/22	0/1/1/1
9	MAN	v	2	9	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BGC	v	3	9	-	0/2/19/22	0/1/1/1
9	NAG	v	4	9	-	4/6/23/26	0/1/1/1
9	BGC	v	5	9	-	0/2/19/22	0/1/1/1
9	MAN	v	6	9	-	0/2/19/22	0/1/1/1
9	BGC	v	7	9	-	0/2/19/22	0/1/1/1
9	XYP	v	8	9	-	-	0/1/1/1
9	XYP	v	9	9	-	-	0/1/1/1
10	GAL	w	1	10	-	0/2/19/22	0/1/1/1
10	MAN	w	10	10	-	2/2/19/22	0/1/1/1
10	NAG	w	11	10	-	4/6/23/26	0/1/1/1
10	XYP	w	12	10	-	-	0/1/1/1
10	MAN	w	13	10	-	0/2/19/22	0/1/1/1
10	BGC	w	14	10	-	0/2/19/22	0/1/1/1
10	XYP	w	15	10	-	-	0/1/1/1
10	BGC	w	16	10	-	0/2/19/22	0/1/1/1
10	BGC	w	17	10	-	0/2/19/22	0/1/1/1
10	NAG	w	18	10	-	2/6/23/26	0/1/1/1
10	MAN	w	19	10	-	2/2/19/22	0/1/1/1
10	NAG	w	2	10	-	0/6/23/26	0/1/1/1
10	XYP	w	3	10	-	-	0/1/1/1
10	XYP	w	4	10	-	-	0/1/1/1
10	GAL	w	5	10	-	0/2/19/22	0/1/1/1
10	A2G	w	6	10	-	2/6/23/26	0/1/1/1
10	GAL	w	7	10	-	1/2/19/22	0/1/1/1
10	A2G	w	8	10	-	1/6/23/26	0/1/1/1
10	BGC	w	9	10	-	0/2/19/22	0/1/1/1
11	MAN	x	1	11,1	-	1/2/19/22	0/1/1/1
11	GLA	x	10	11	-	0/2/19/22	0/1/1/1
11	BGC	x	11	11	-	2/2/19/22	0/1/1/1
11	BMA	x	12	11	-	2/2/19/22	0/1/1/1
11	NAG	x	13	11	-	1/6/23/26	0/1/1/1
11	BMA	x	14	11	-	1/2/19/22	0/1/1/1
11	BGC	x	15	11	-	0/2/19/22	0/1/1/1
11	NAG	x	16	11	-	4/6/23/26	0/1/1/1
11	AHR	x	17	11	-	0/2/15/18	0/1/1/1
11	XYP	x	18	11	-	-	0/1/1/1
11	BGC	x	19	11	-	2/2/19/22	0/1/1/1
11	BGC	x	2	11	-	0/2/19/22	0/1/1/1
11	NAG	x	20	11	-	4/6/23/26	0/1/1/1
11	BMA	x	21	11	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	x	22	11	-	0/2/19/22	0/1/1/1
11	XYP	x	23	11	-	-	0/1/1/1
11	BMA	x	24	11	-	0/2/19/22	0/1/1/1
11	BGC	x	25	11	-	1/2/19/22	0/1/1/1
11	XYP	x	26	11	-	-	0/1/1/1
11	XYP	x	27	11	-	-	0/1/1/1
11	NAG	x	28	11	-	5/6/23/26	0/1/1/1
11	MAN	x	29	11	-	0/2/19/22	0/1/1/1
11	XYP	x	3	11	-	-	0/1/1/1
11	XYP	x	30	11	-	-	0/1/1/1
11	BGC	x	31	11	-	1/2/19/22	0/1/1/1
11	BGC	x	32	11	-	0/2/19/22	0/1/1/1
11	XYP	x	33	11	-	-	0/1/1/1
11	NAG	x	34	11	-	3/6/23/26	0/1/1/1
11	BGC	x	35	11	-	0/2/19/22	0/1/1/1
11	XYP	x	36	11	-	-	0/1/1/1
11	MAN	x	37	11	-	2/2/19/22	0/1/1/1
11	NAG	x	38	11	-	2/6/23/26	0/1/1/1
11	XYP	x	39	11	-	-	0/1/1/1
11	BMA	x	4	11	-	0/2/19/22	0/1/1/1
11	XYP	x	40	11	-	-	0/1/1/1
11	BGC	x	41	11	-	0/2/19/22	0/1/1/1
11	MAN	x	42	11	-	0/2/19/22	0/1/1/1
11	BGC	x	43	11	-	0/2/19/22	0/1/1/1
11	XYP	x	44	11	-	-	0/1/1/1
11	BGC	x	45	11	-	0/2/19/22	0/1/1/1
11	BGC	x	46	11	-	0/2/19/22	0/1/1/1
11	BGC	x	47	11	-	1/2/19/22	0/1/1/1
11	NAG	x	5	11	-	2/6/23/26	0/1/1/1
11	FUB	x	6	11	-	2/2/15/18	0/1/1/1
11	BGC	x	7	11	-	0/2/19/22	0/1/1/1
11	BGC	x	8	11	-	0/2/19/22	0/1/1/1
11	BMA	x	9	11	-	2/2/19/22	0/1/1/1
12	GAL	y	1	12	-	0/2/19/22	0/1/1/1
12	XYP	y	10	12	-	-	0/1/1/1
12	XYP	y	2	12	-	-	0/1/1/1
12	BGC	y	3	12	-	0/2/19/22	0/1/1/1
12	XYP	y	4	12	-	-	0/1/1/1
12	BGC	y	5	12	-	2/2/19/22	0/1/1/1
12	MAN	y	6	12	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BGC	y	7	12	-	2/2/19/22	0/1/1/1
12	BGC	y	8	12	-	0/2/19/22	0/1/1/1
12	NAG	y	9	12	-	4/6/23/26	0/1/1/1
13	XYP	z	1	13	-	-	0/1/1/1
13	BGC	z	10	13	-	0/2/19/22	0/1/1/1
13	MAN	z	11	13	-	0/2/19/22	0/1/1/1
13	AHR	z	12	13	-	0/2/15/18	0/1/1/1
13	XYP	z	13	13	-	-	0/1/1/1
13	BGC	z	14	13	-	0/2/19/22	0/1/1/1
13	BGC	z	15	13	-	0/2/19/22	0/1/1/1
13	BGC	z	16	13	-	0/2/19/22	0/1/1/1
13	BGC	z	17	13	-	0/2/19/22	0/1/1/1
13	BGC	z	2	13	-	1/2/19/22	0/1/1/1
13	MAN	z	3	13	-	0/2/19/22	0/1/1/1
13	NAG	z	4	13	-	1/6/23/26	0/1/1/1
13	BGC	z	5	13	-	2/2/19/22	0/1/1/1
13	BGC	z	6	13	-	0/2/19/22	0/1/1/1
13	XYP	z	7	13	-	-	0/1/1/1
13	BGC	z	8	13	-	0/2/19/22	0/1/1/1
13	NAG	z	9	13	-	2/6/23/26	0/1/1/1

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	2	GZL	C2-C3	-18.44	1.23	1.53
6	f	2	GZL	C2-C3	-18.44	1.23	1.53
6	s	2	GZL	C2-C3	-18.42	1.24	1.53
6	F	2	GZL	C2-C3	-18.39	1.24	1.53
6	F	2	GZL	O4-C4	-7.20	1.27	1.43

The worst 5 of 663 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	14	BMA	C1-C2-C3	-7.98	99.86	109.67
11	x	14	BMA	C1-C2-C3	-7.96	99.89	109.67
11	k	14	BMA	C1-C2-C3	-7.94	99.91	109.67
11	X	14	BMA	C1-C2-C3	-7.92	99.92	109.67
10	w	3	XYP	C1-C2-C3	7.84	119.31	109.67

There are no chirality outliers.

5 of 616 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	21	NAG	C8-C7-N2-C2
3	C	21	NAG	O7-C7-N2-C2
3	P	21	NAG	C8-C7-N2-C2
3	P	21	NAG	O7-C7-N2-C2
3	c	21	NAG	C8-C7-N2-C2

There are no ring outliers.

247 monomers are involved in 226 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	0	18	NAG	2	0
14	n	14	XYP	1	0
13	z	12	AHR	3	0
14	N	15	AHR	1	0
13	M	13	XYP	2	0
11	X	26	XYP	1	0
7	g	3	A2G	3	0
5	R	2	NAG	1	0
7	t	8	MAN	1	0
10	W	10	MAN	1	0
11	x	20	NAG	1	0
13	M	5	BGC	5	0
3	C	9	BGC	2	0
2	o	6	NAG	1	0
13	z	2	BGC	1	0
11	X	37	MAN	1	0
7	g	16	NAG	6	0
10	J	19	MAN	8	0
4	d	13	FUB	2	0
7	g	2	BGC	4	0
7	t	2	BGC	4	0
14	0	14	XYP	1	0
4	q	11	MAN	1	0
6	S	3	FUB	2	0
7	t	3	A2G	3	0
7	T	16	NAG	6	0
11	k	47	BGC	4	0
13	z	1	XYP	1	0
8	H	2	NAG	1	0
14	a	6	XYP	1	0
11	X	34	NAG	1	0
3	P	3	BGC	1	0
11	K	20	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	n	13	XYP	1	0
4	D	23	BGC	1	0
7	G	5	BGC	1	0
2	B	2	NAG	1	0
3	p	2	BGC	1	0
13	M	4	NAG	3	0
3	p	18	BGC	2	0
11	K	1	MAN	3	0
12	l	8	BGC	1	0
10	j	19	MAN	2	0
11	K	6	FUB	2	0
14	n	1	MAN	1	0
11	k	37	MAN	1	0
11	X	47	BGC	5	0
11	x	10	GLA	1	0
7	G	16	NAG	1	0
13	m	12	AHR	4	0
6	f	3	FUB	2	0
7	G	3	A2G	3	0
2	B	4	MAN	1	0
3	P	9	BGC	2	0
14	a	15	AHR	1	0
8	h	2	NAG	1	0
14	n	18	NAG	2	0
3	c	2	BGC	1	0
6	F	3	FUB	2	0
8	H	14	NAG	2	0
7	G	4	BGC	1	0
2	b	6	NAG	1	0
11	x	37	MAN	1	0
2	o	1	BGC	2	0
4	D	25	BGC	2	0
11	k	34	NAG	1	0
13	Z	5	BGC	6	0
2	B	1	BGC	2	0
7	G	8	MAN	1	0
7	G	2	BGC	4	0
2	O	6	NAG	1	0
11	x	35	BGC	1	0
3	c	3	BGC	1	0
14	a	13	XYP	1	0
11	x	34	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	h	17	A2G	1	0
13	Z	10	BGC	1	0
13	m	4	NAG	3	0
13	m	5	BGC	4	0
8	U	14	NAG	1	0
7	T	21	XYP	2	0
10	W	1	GAL	1	0
7	T	4	BGC	1	0
4	Q	13	FUB	2	0
11	x	36	XYP	2	0
14	a	2	XYP	1	0
2	O	2	NAG	1	0
14	0	16	BGC	2	0
11	x	14	BMA	1	0
11	k	45	BGC	2	0
8	U	2	NAG	1	0
12	y	1	GAL	3	0
10	J	18	NAG	1	0
11	x	15	BGC	2	0
3	P	10	XYP	3	0
11	K	5	NAG	1	0
12	L	1	GAL	2	0
11	k	26	XYP	1	0
14	N	4	GAL	1	0
14	a	14	XYP	1	0
7	T	5	BGC	1	0
2	b	2	NAG	1	0
2	o	2	NAG	1	0
13	Z	2	BGC	1	0
4	d	25	BGC	2	0
12	l	5	BGC	1	0
13	Z	12	AHR	4	0
8	U	17	A2G	1	0
11	X	1	MAN	3	0
12	Y	1	GAL	2	0
10	w	10	MAN	1	0
11	x	26	XYP	1	0
11	X	16	NAG	3	0
10	w	2	NAG	1	0
11	K	9	BMA	1	0
8	u	2	NAG	1	0
12	Y	8	BGC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	h	8	GAL	5	0
3	C	11	NAG	1	0
12	l	1	GAL	2	0
14	N	1	MAN	1	0
11	k	10	GLA	1	0
11	X	9	BMA	1	0
9	V	5	BGC	2	0
3	P	12	MAN	1	0
4	d	19	BGC	1	0
3	c	12	MAN	1	0
7	t	16	NAG	6	0
7	g	21	XYP	1	0
8	u	17	A2G	1	0
14	n	4	GAL	1	0
9	V	6	MAN	1	0
9	i	5	BGC	2	0
4	Q	19	BGC	1	0
4	D	13	FUB	2	0
10	j	2	NAG	1	0
11	K	37	MAN	1	0
5	E	2	NAG	1	0
5	r	2	NAG	1	0
6	s	3	FUB	2	0
13	Z	1	XYP	1	0
2	b	1	BGC	2	0
14	N	16	BGC	2	0
4	q	19	BGC	1	0
10	J	17	BGC	3	0
14	n	6	XYP	1	0
3	p	9	BGC	2	0
11	K	34	NAG	1	0
11	k	41	BGC	1	0
13	M	10	BGC	1	0
8	h	14	NAG	2	0
4	d	11	MAN	1	0
14	N	18	NAG	2	0
4	Q	25	BGC	2	0
13	m	1	XYP	1	0
11	k	1	MAN	2	0
7	g	8	MAN	1	0
2	O	4	MAN	1	0
3	C	18	BGC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	Z	4	NAG	2	0
13	Z	13	XYP	2	0
13	z	13	XYP	2	0
11	X	10	GLA	1	0
3	p	12	MAN	1	0
14	0	6	XYP	1	0
11	K	36	XYP	2	0
11	x	1	MAN	3	0
4	D	11	MAN	1	0
9	v	5	BGC	2	0
13	m	2	BGC	1	0
11	x	45	BGC	1	0
3	c	10	XYP	3	0
11	K	26	XYP	1	0
4	q	13	FUB	2	0
14	N	13	XYP	1	0
10	j	10	MAN	1	0
11	K	35	BGC	1	0
10	j	15	XYP	1	0
14	0	4	GAL	1	0
2	b	4	MAN	1	0
2	o	4	MAN	1	0
7	T	8	MAN	1	0
11	X	6	FUB	2	0
8	H	20	MAN	1	0
13	z	4	NAG	2	0
8	H	8	GAL	5	0
8	h	20	MAN	1	0
3	C	3	BGC	1	0
2	B	6	NAG	1	0
11	k	16	NAG	1	0
8	U	20	MAN	2	0
3	C	2	BGC	1	0
10	w	19	MAN	2	0
11	X	35	BGC	1	0
7	T	3	A2G	2	0
4	D	19	BGC	1	0
14	a	4	GAL	1	0
14	N	14	XYP	2	0
13	m	13	XYP	2	0
11	X	5	NAG	1	0
14	0	2	XYP	1	0

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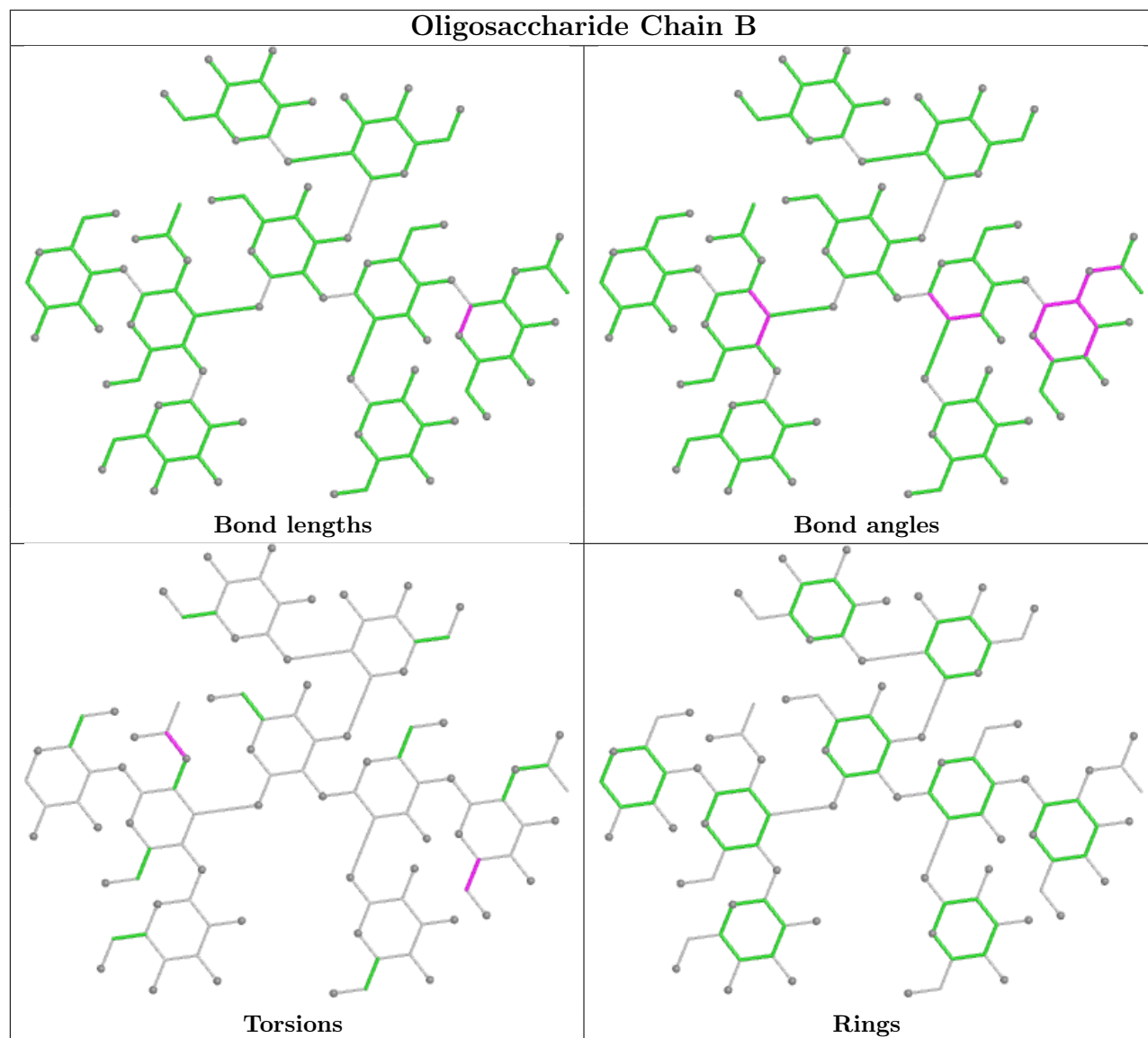
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	11	MAN	1	0
11	k	20	NAG	1	0
3	C	10	XYP	3	0
3	p	3	BGC	1	0
10	W	17	BGC	1	0
13	M	12	AHR	4	0
3	P	18	BGC	2	0
13	z	10	BGC	1	0
7	T	2	BGC	3	0
11	k	6	FUB	2	0
10	J	2	NAG	2	0
11	k	35	BGC	1	0
14	a	16	BGC	2	0
3	c	18	BGC	2	0
11	X	45	BGC	1	0
8	U	8	GAL	5	0
14	0	1	MAN	1	0
11	X	36	XYP	2	0
3	c	9	BGC	2	0
11	k	5	NAG	1	0
14	n	15	AHR	1	0
5	e	2	NAG	1	0
7	t	21	XYP	2	0
11	K	10	GLA	1	0
14	n	16	BGC	2	0
10	W	18	NAG	2	0
2	O	1	BGC	2	0
11	k	36	XYP	2	0
11	x	9	BMA	1	0
14	N	2	XYP	1	0
3	C	12	MAN	1	0
10	W	19	MAN	5	0
11	x	5	NAG	1	0
10	j	1	GAL	1	0
11	x	6	FUB	2	0
3	C	6	XYP	1	0
14	N	6	XYP	1	0
14	n	2	XYP	1	0
13	z	5	BGC	4	0
14	a	18	NAG	2	0
3	c	25	BGC	1	0
11	k	9	BMA	1	0

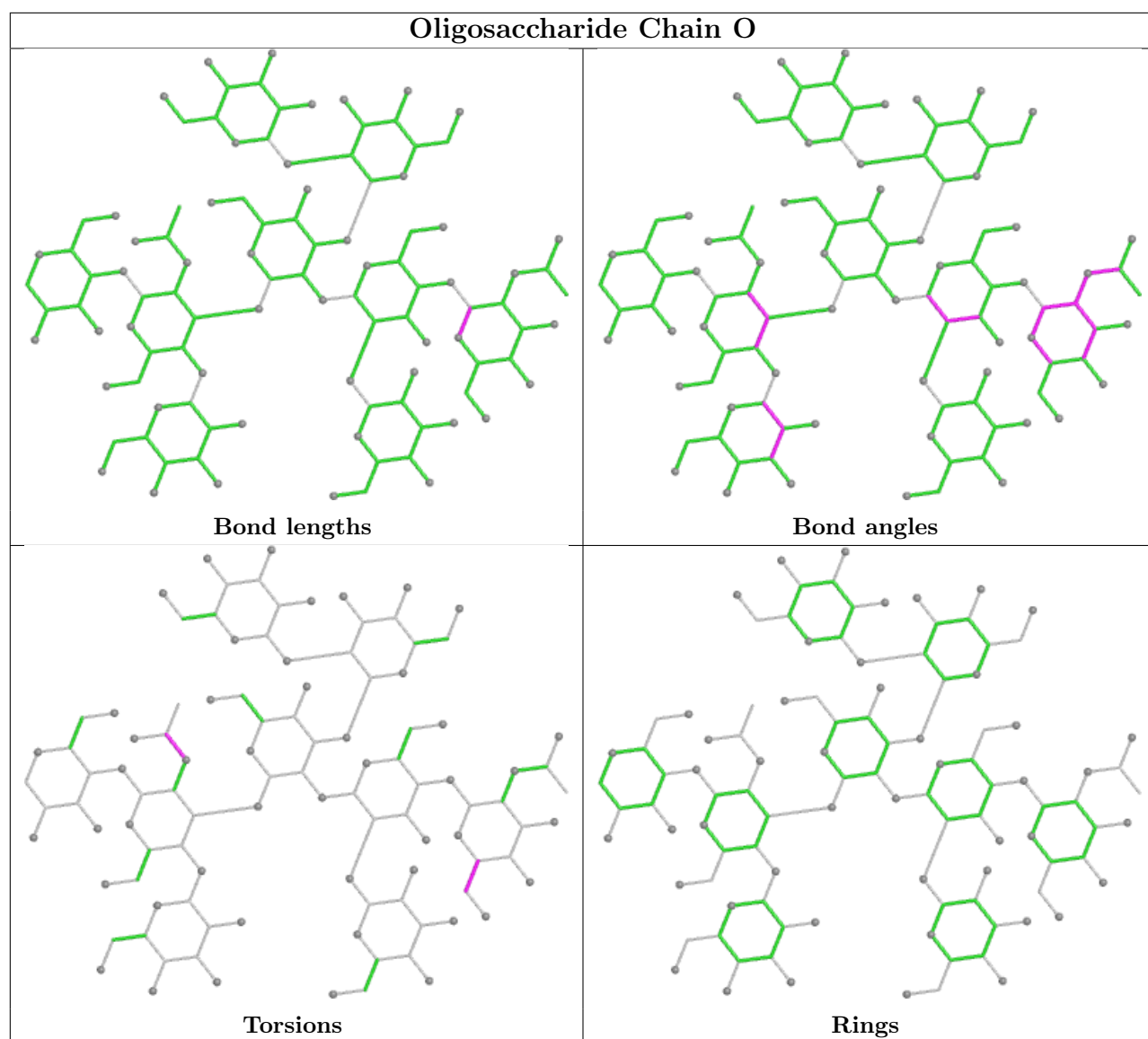
*Continued on next page...*

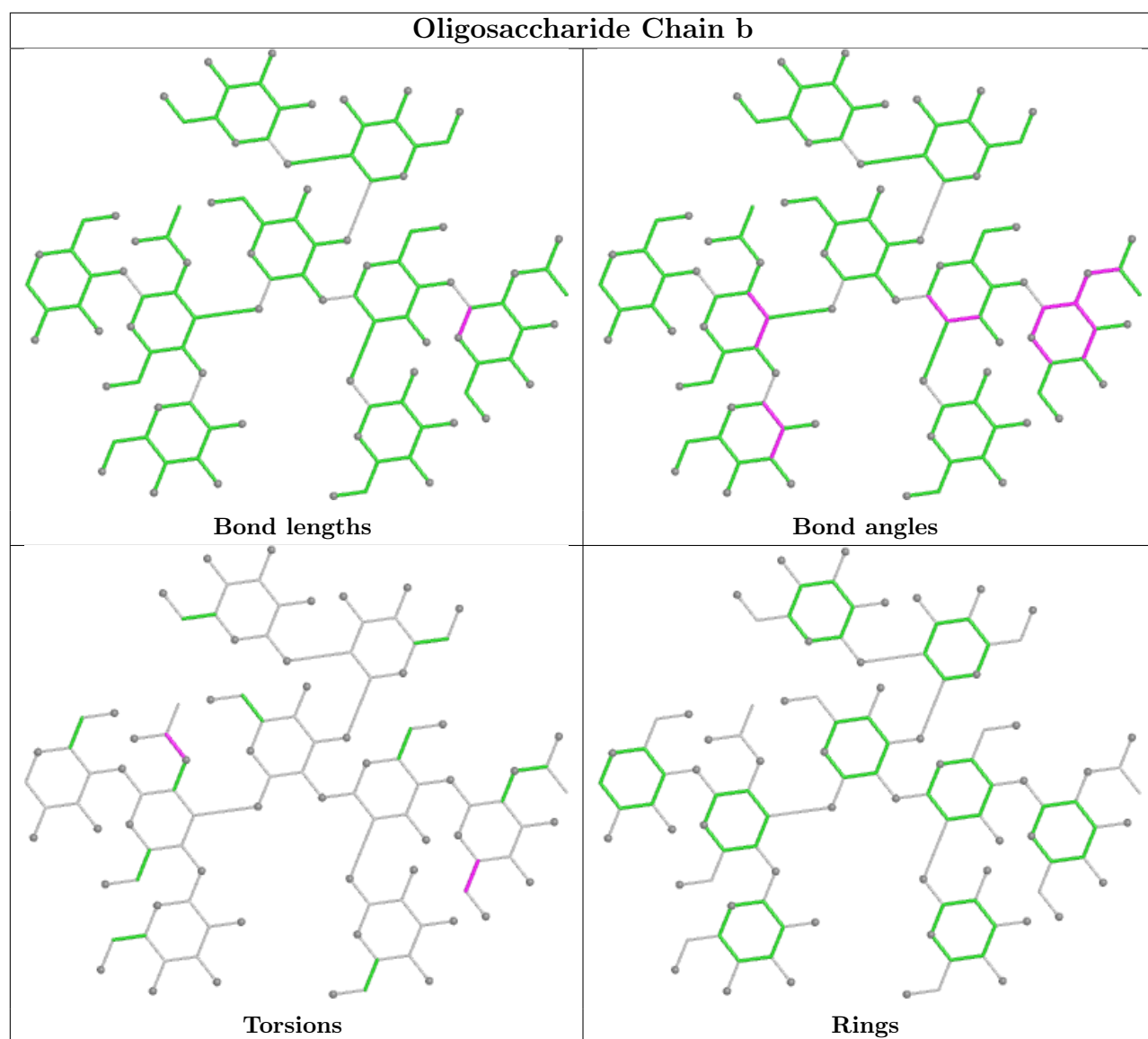
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	a	1	MAN	2	0
3	p	10	XYP	3	0
11	X	20	NAG	1	0
3	P	2	BGC	1	0

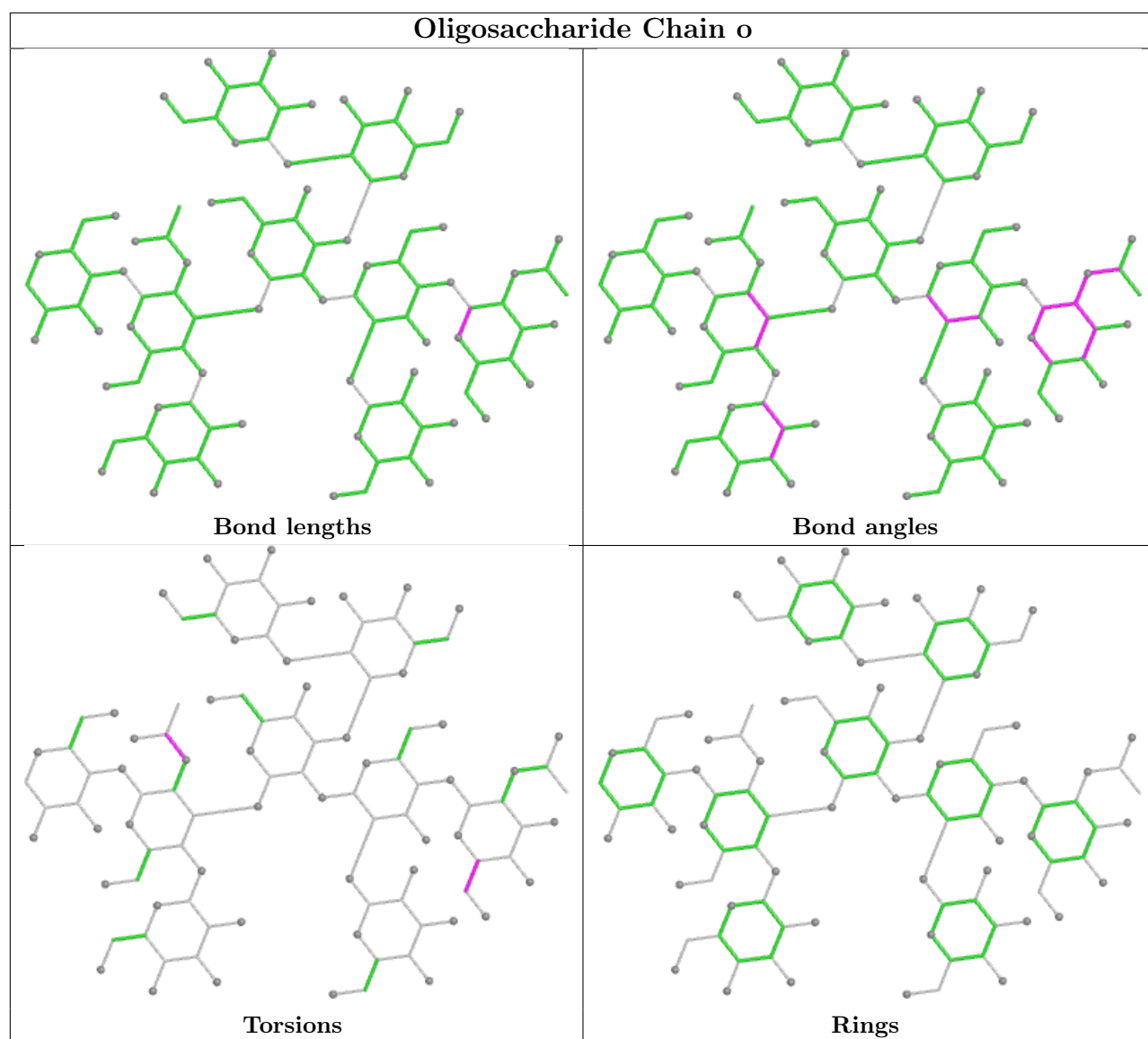
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

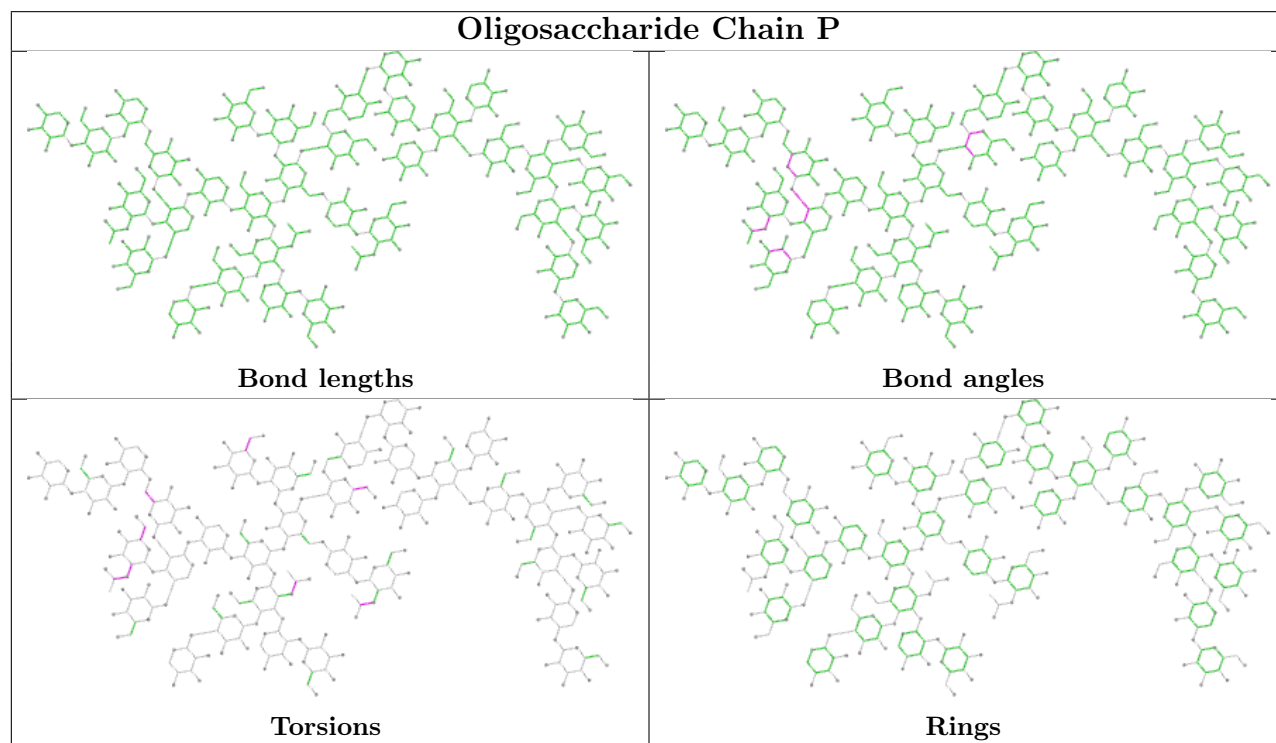
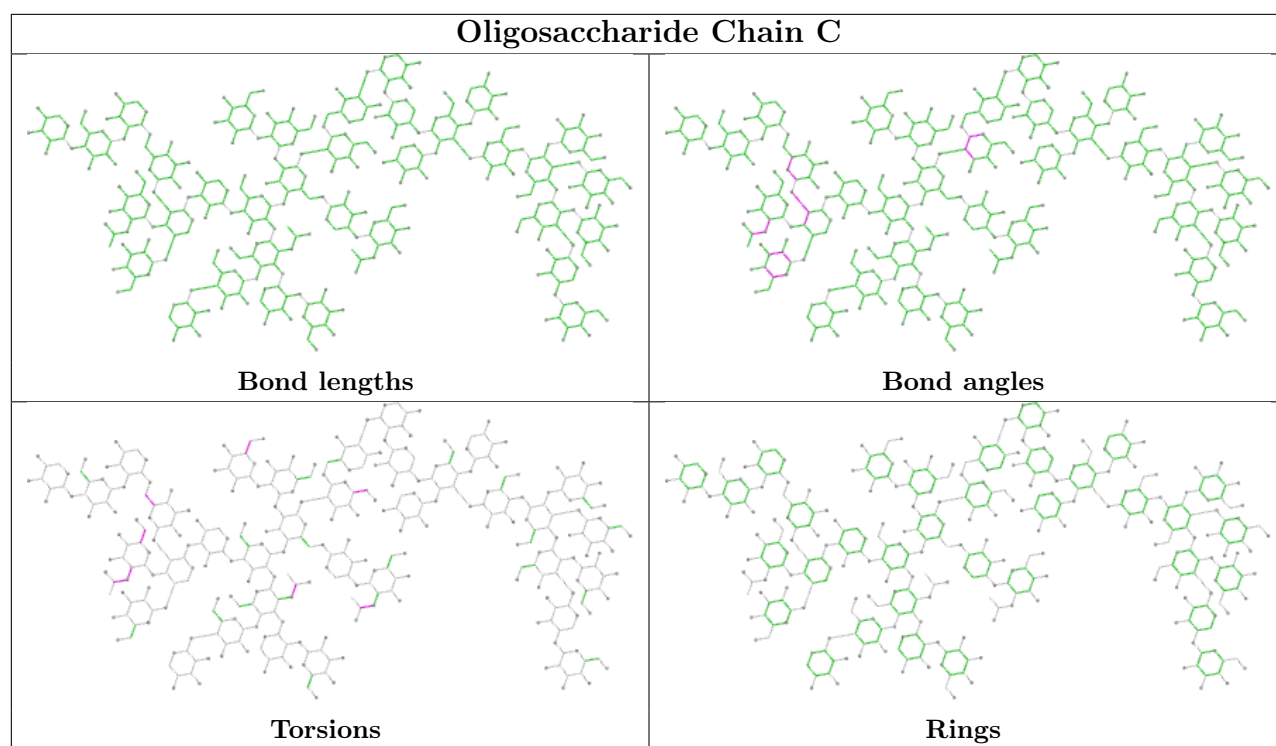


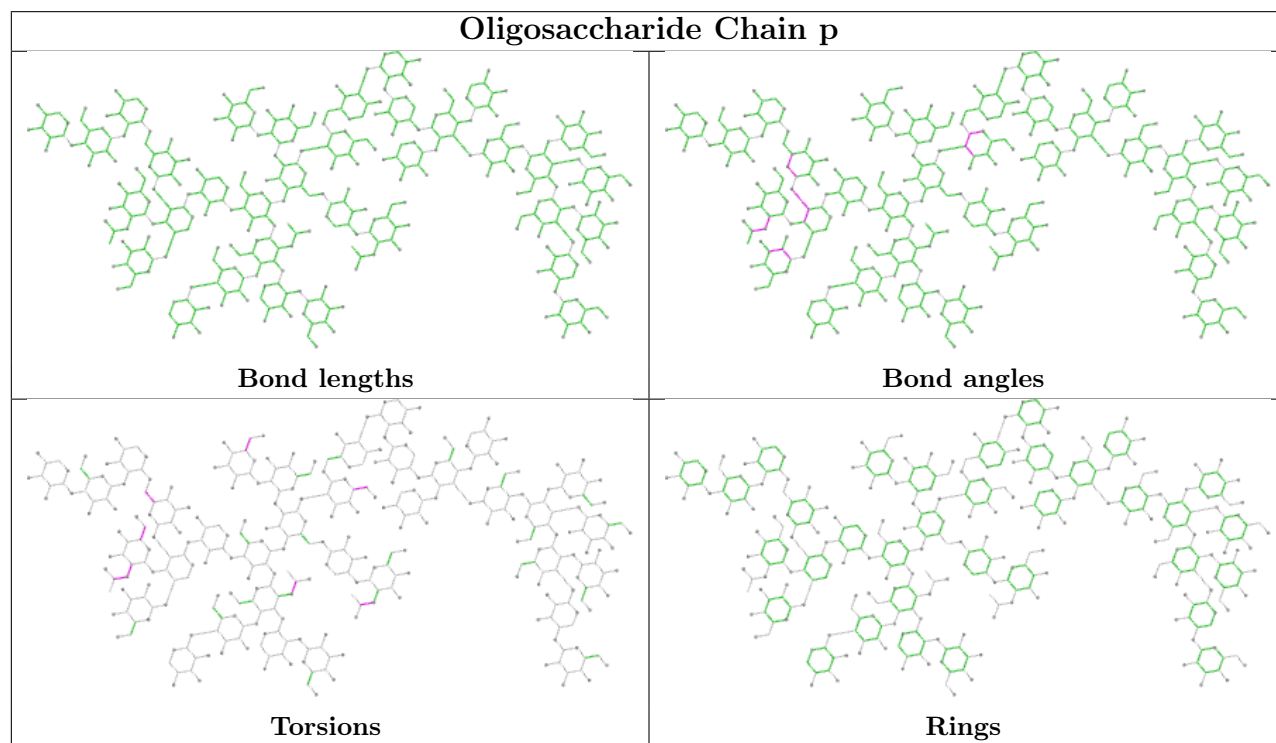
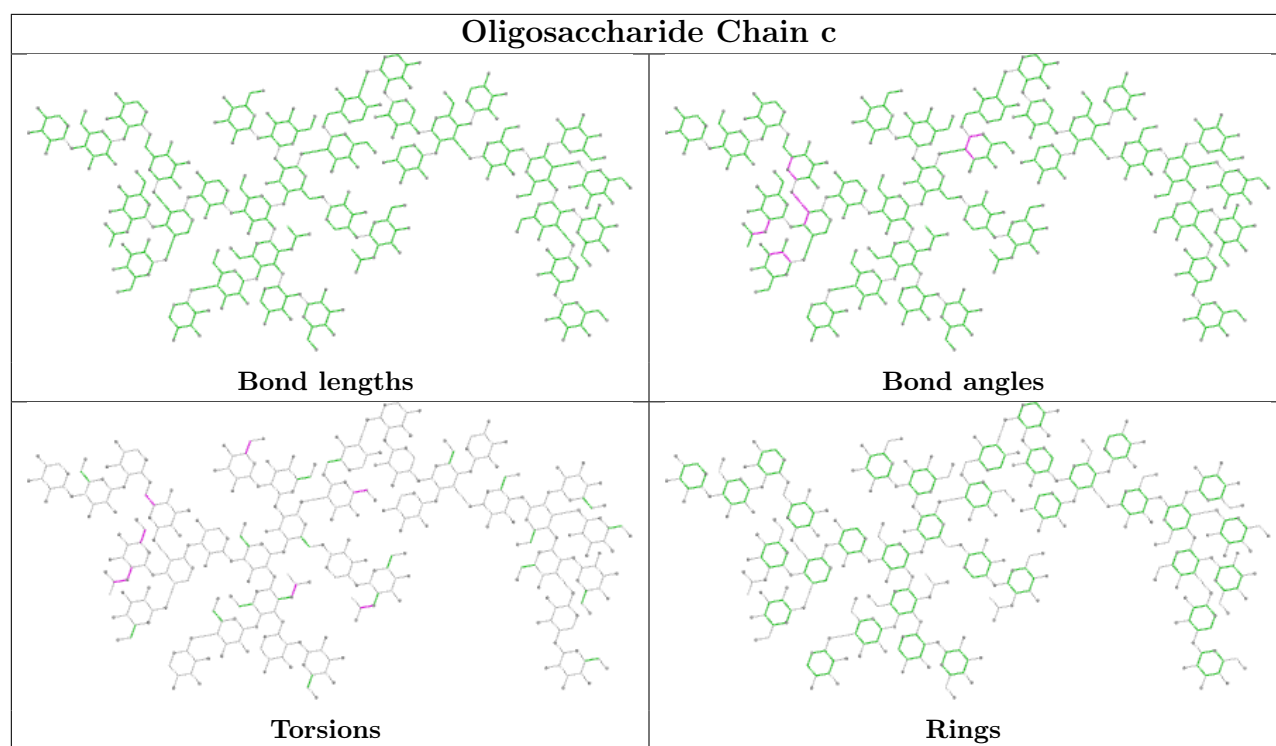


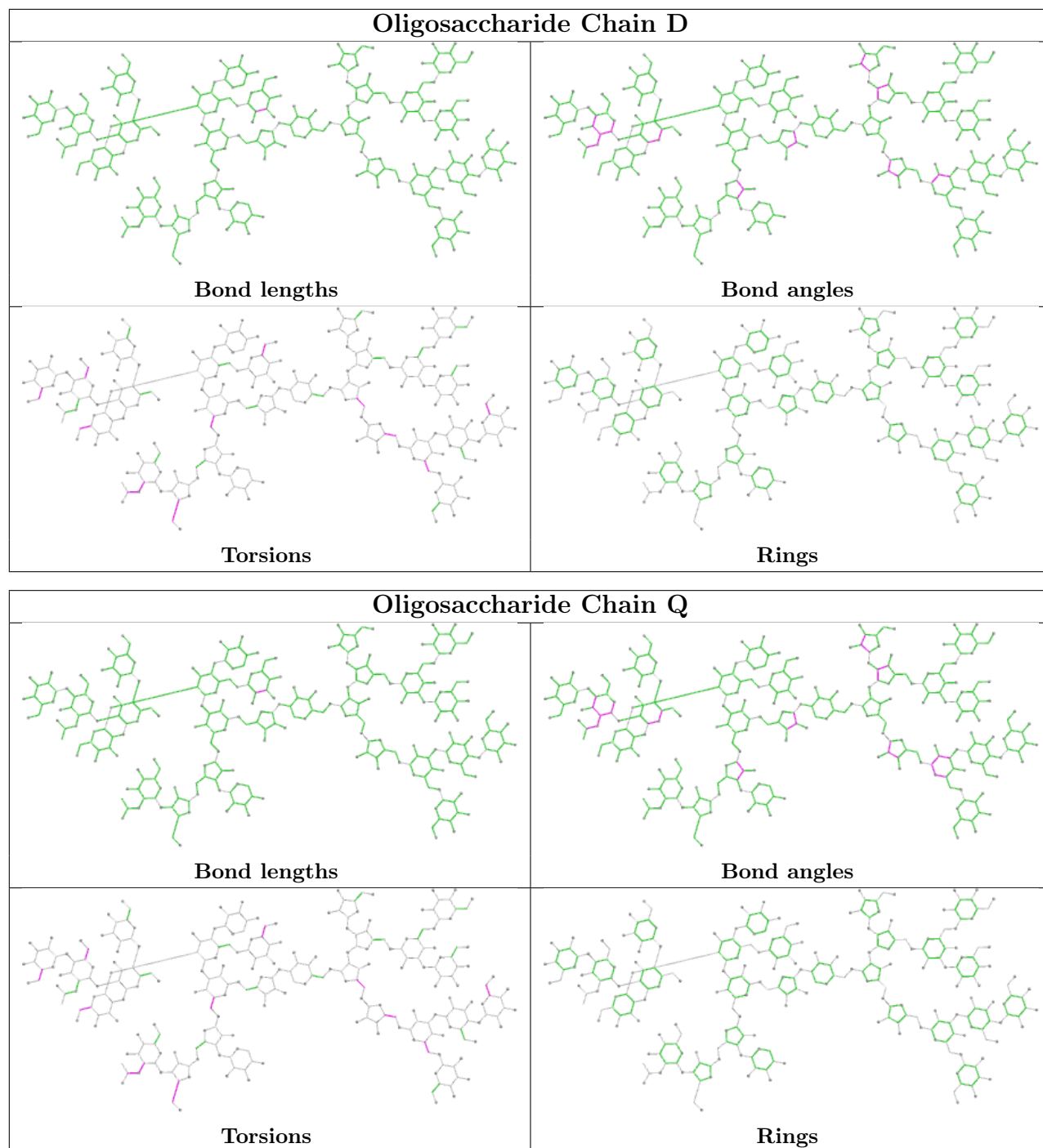


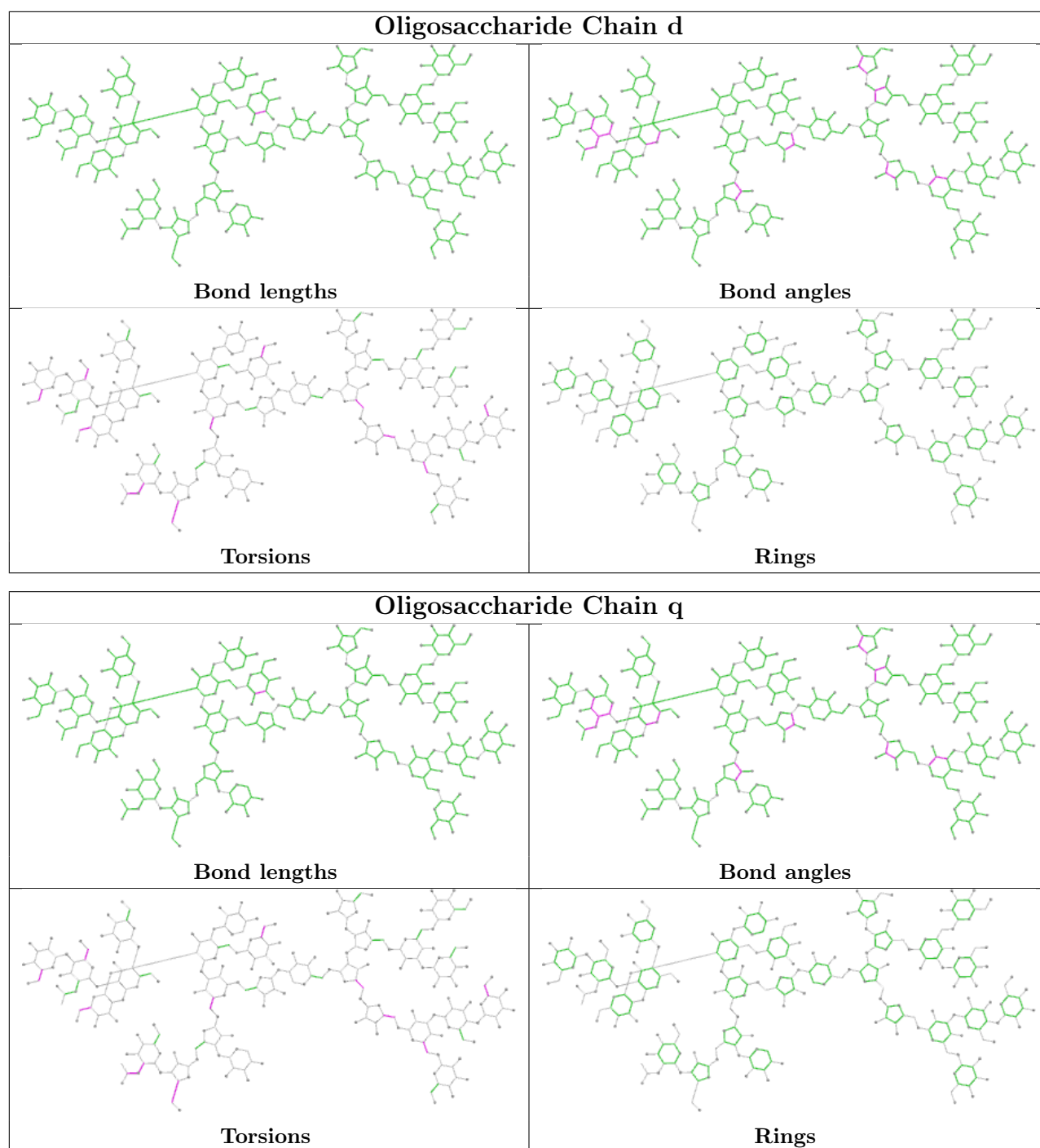


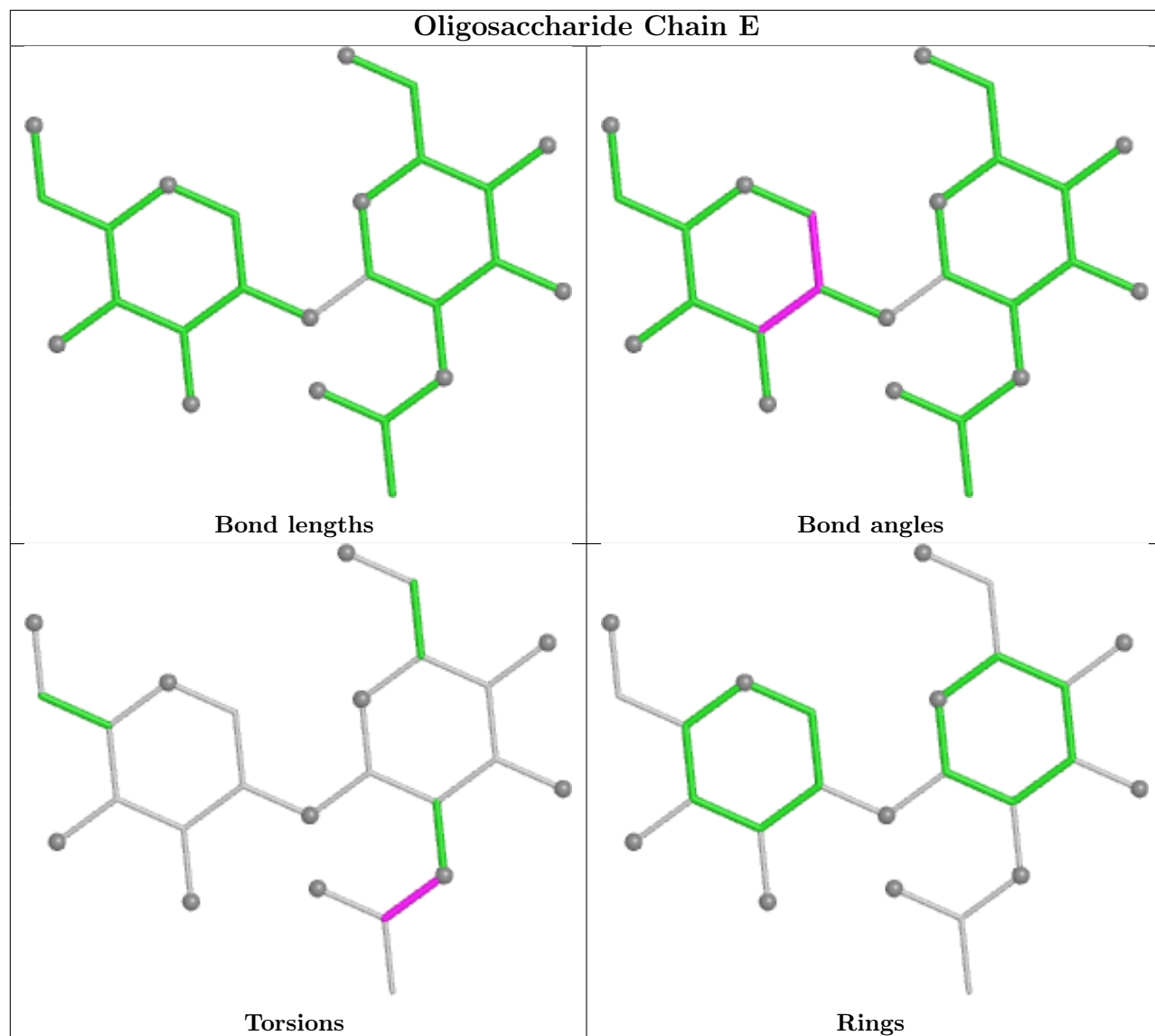


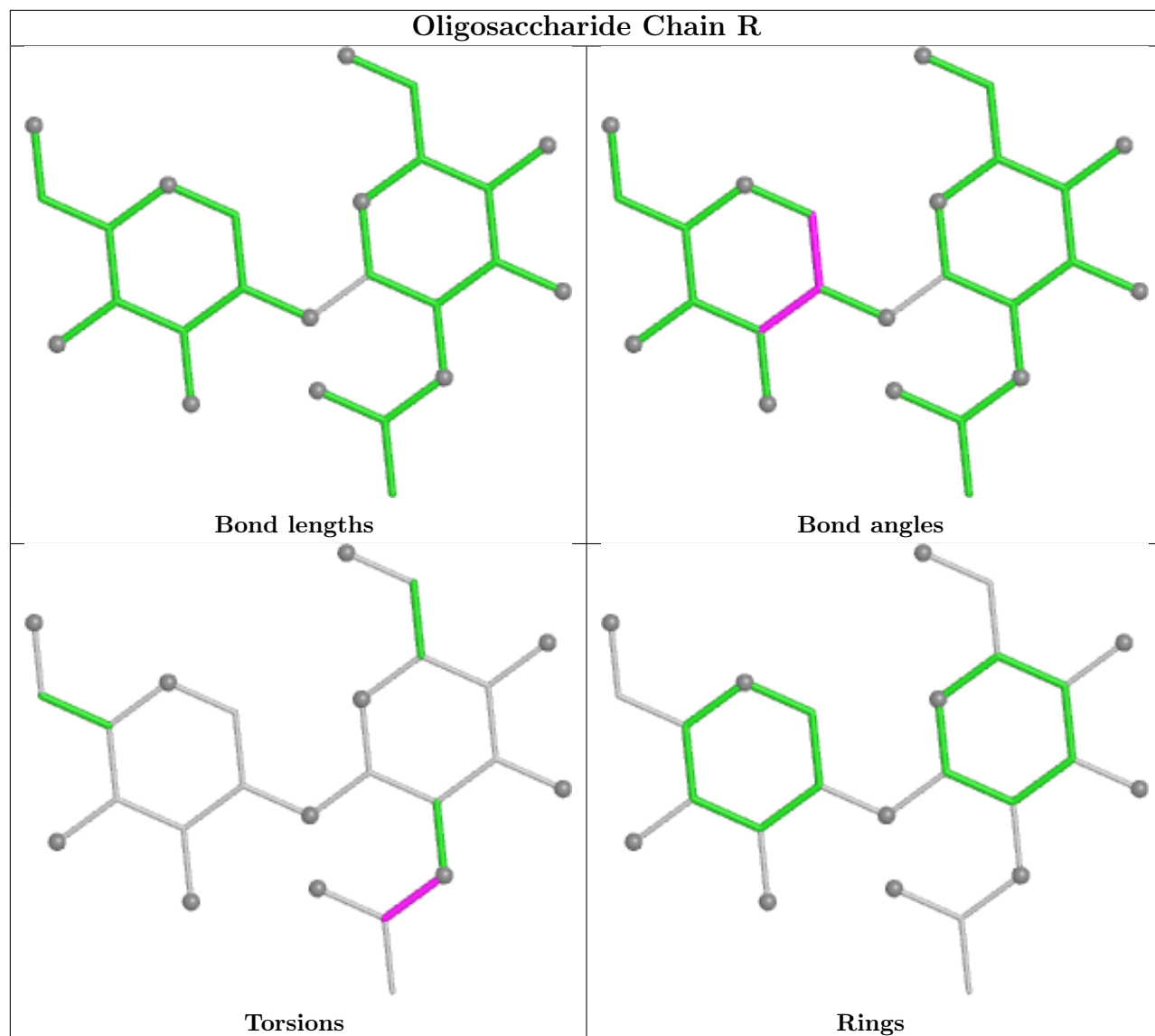


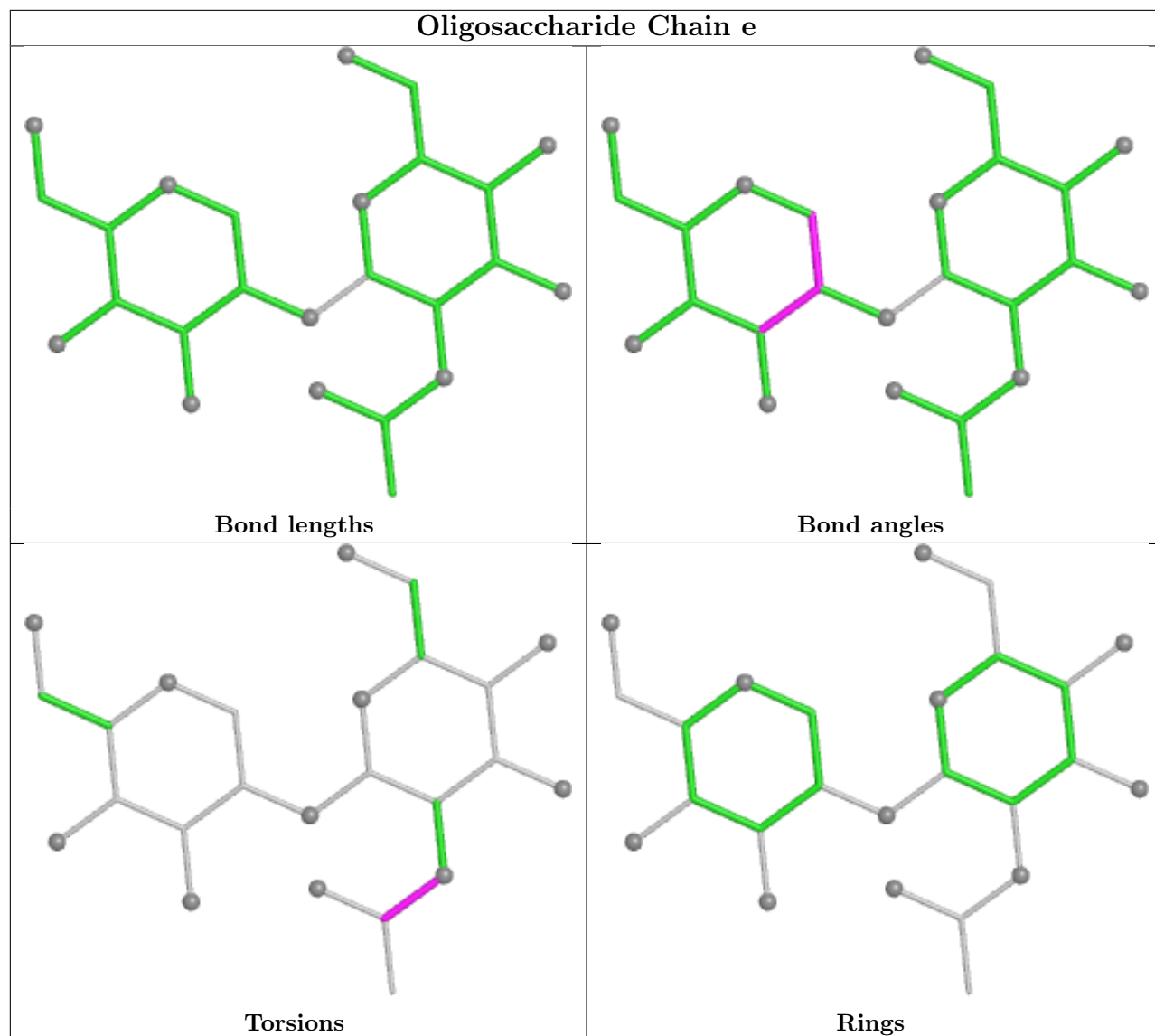




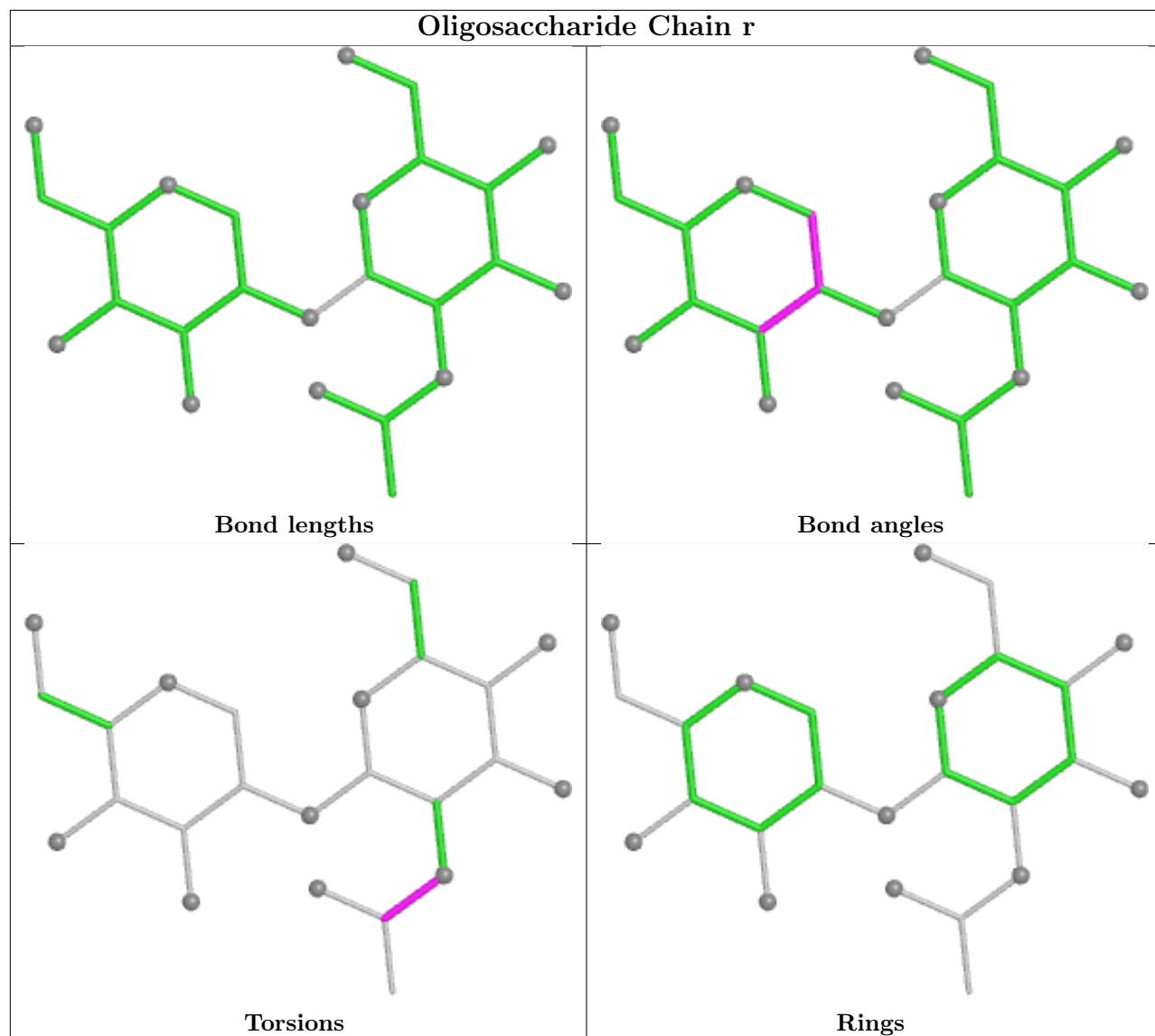


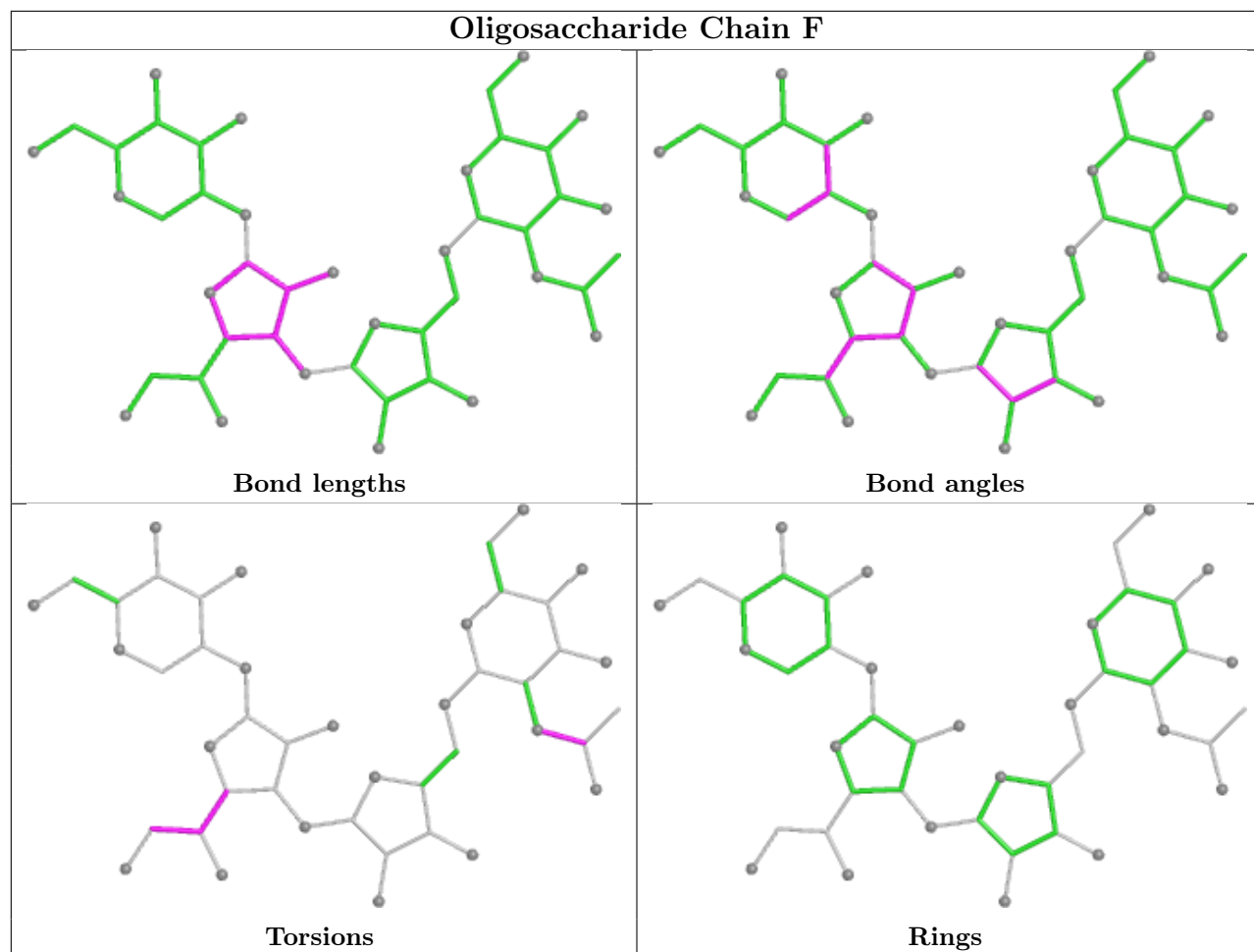


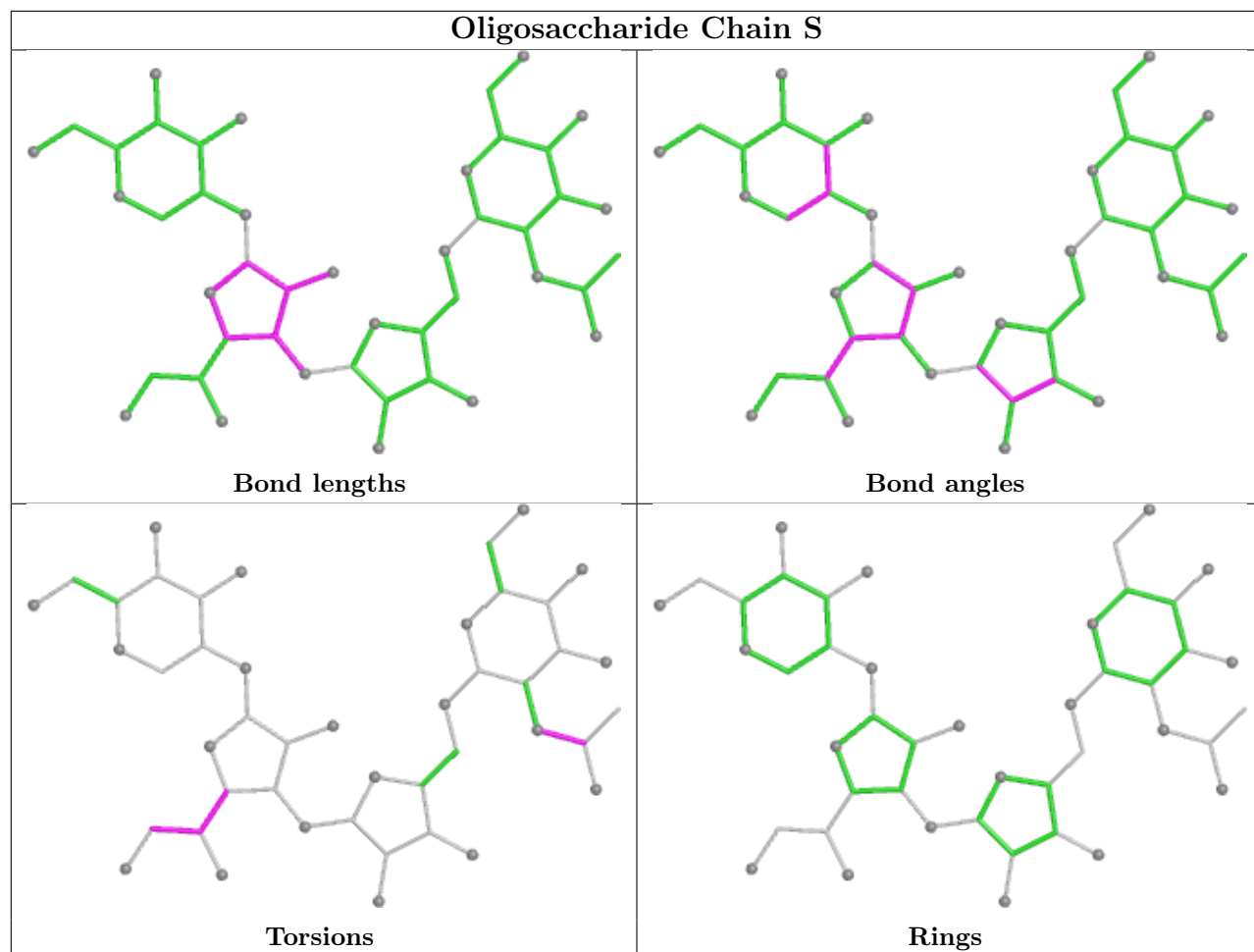


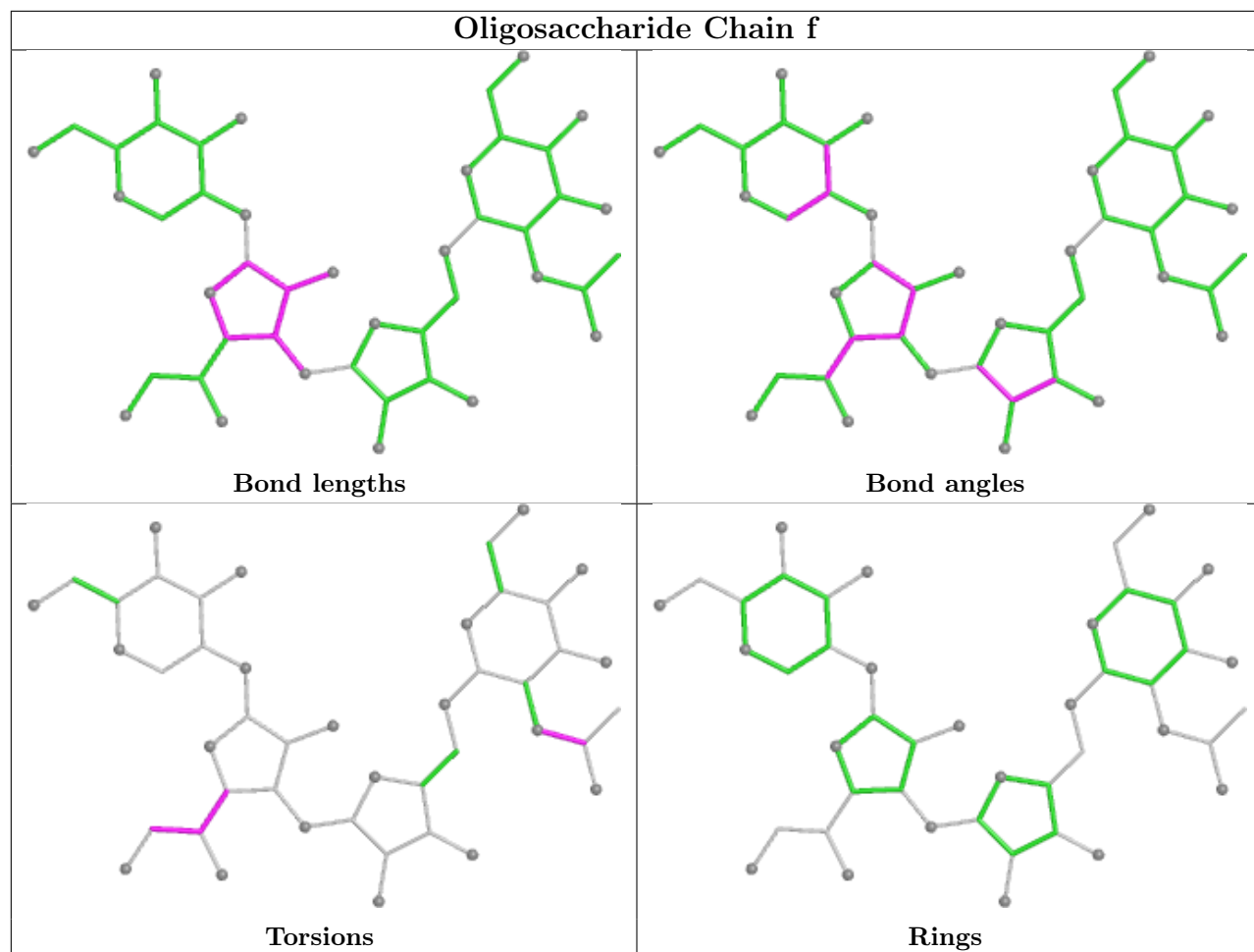


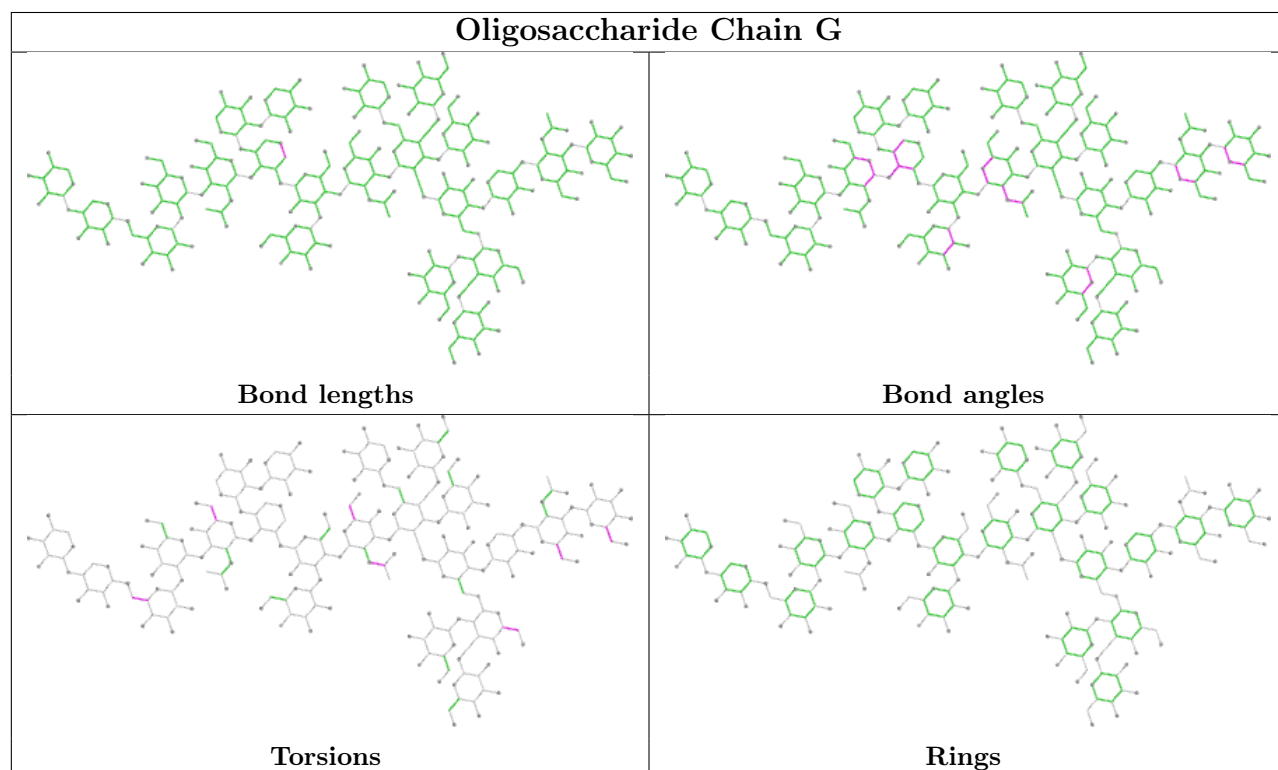
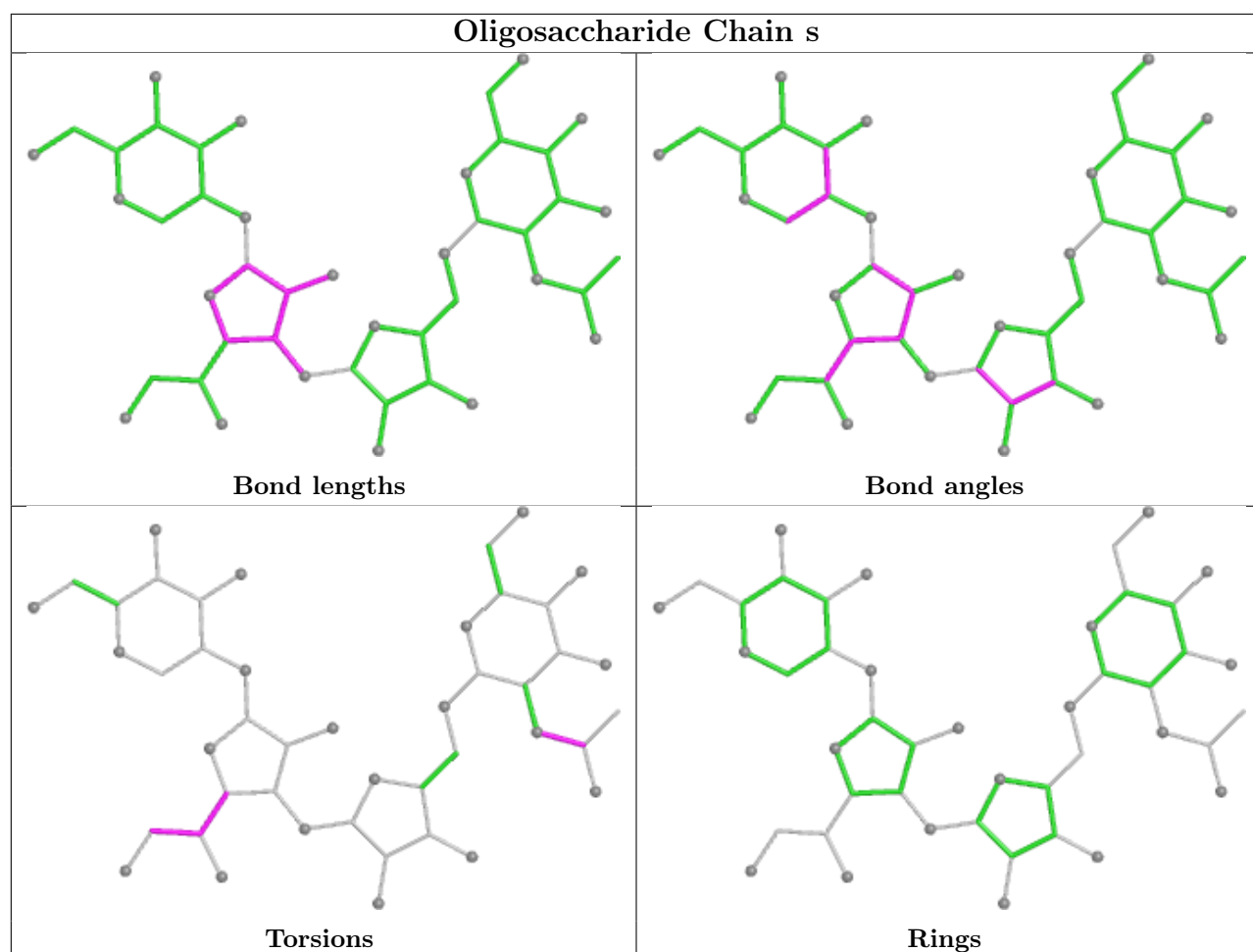


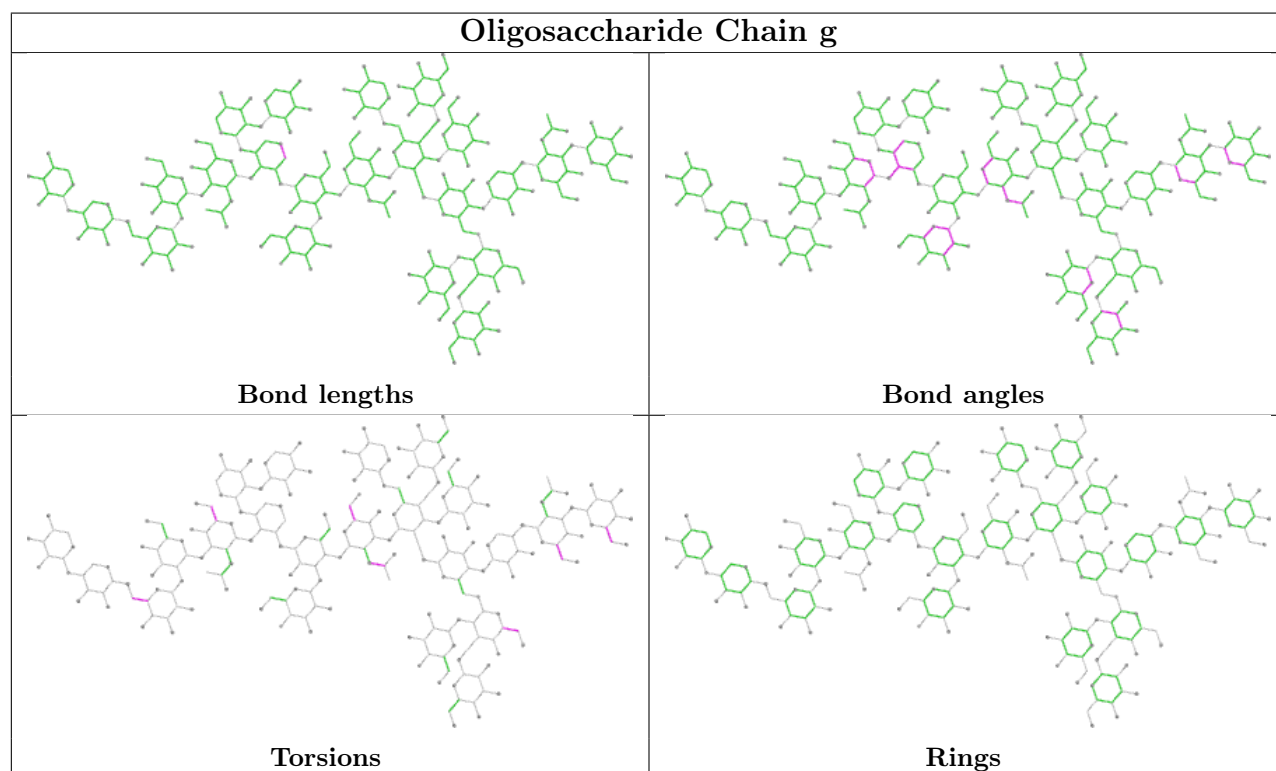
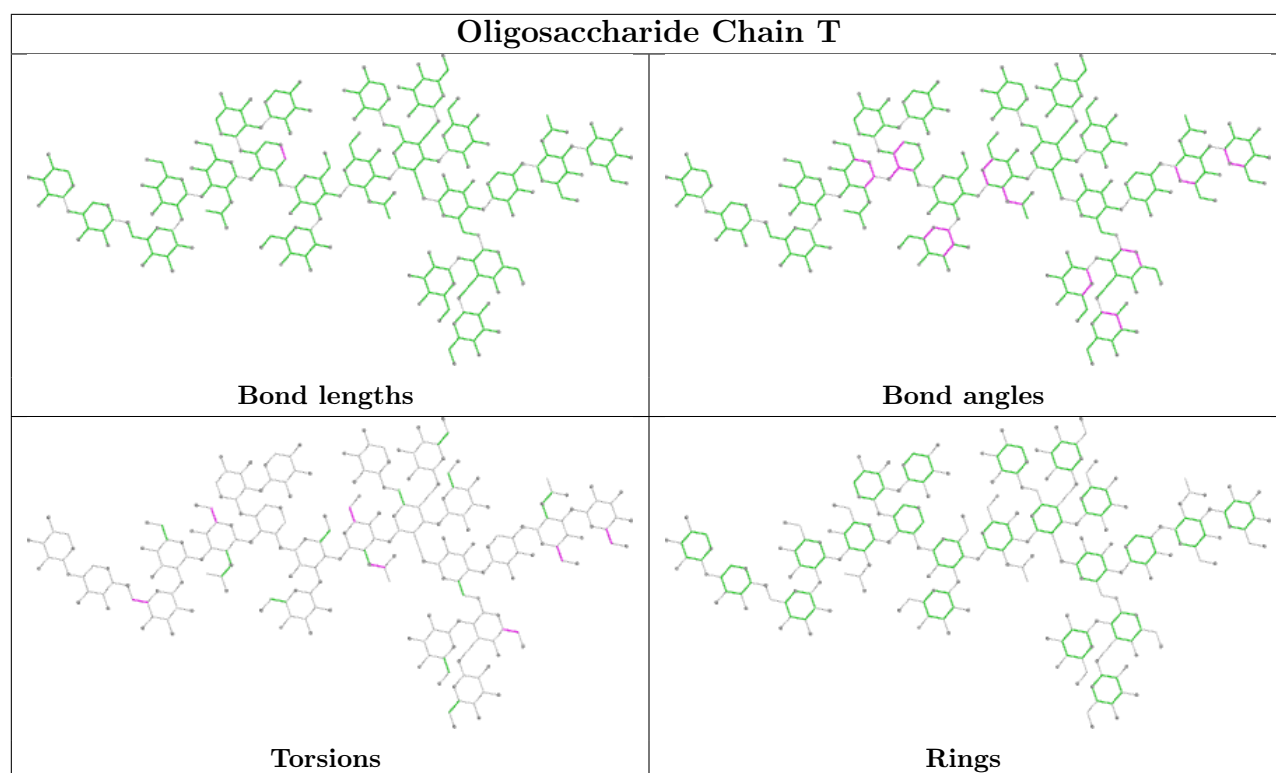


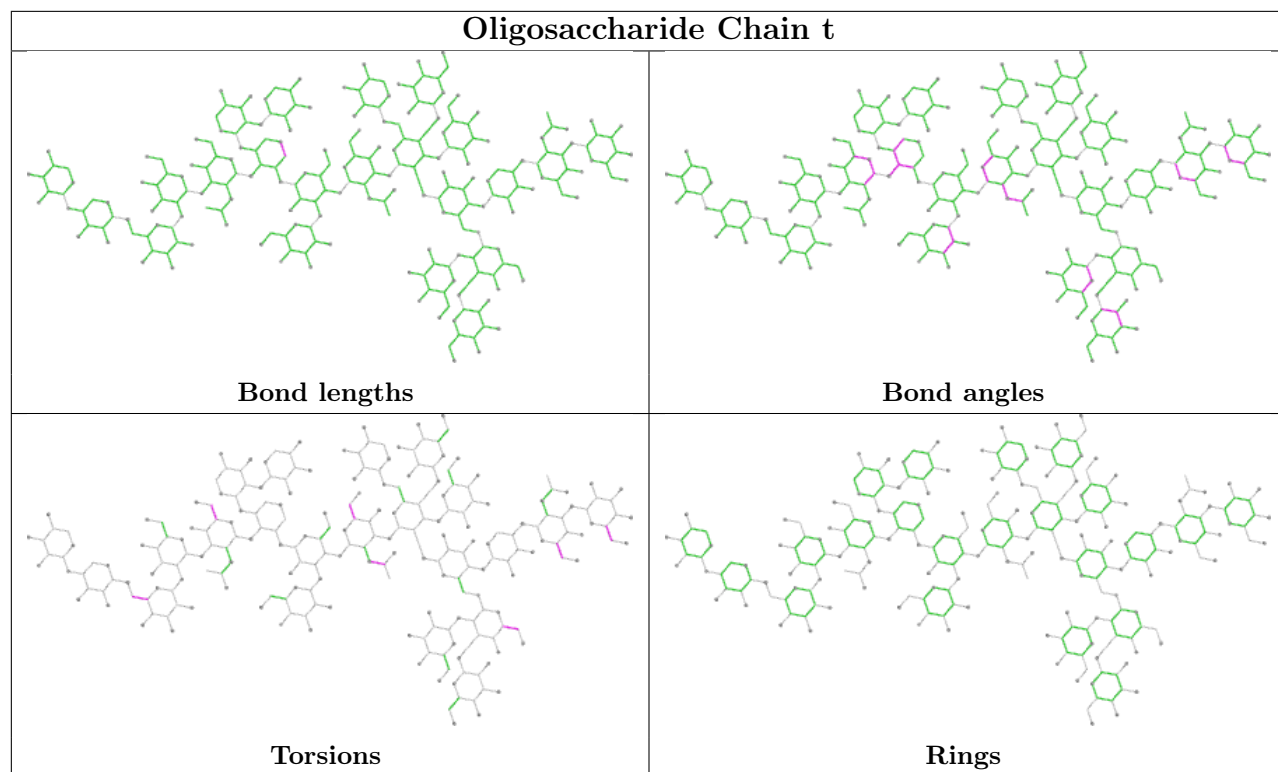


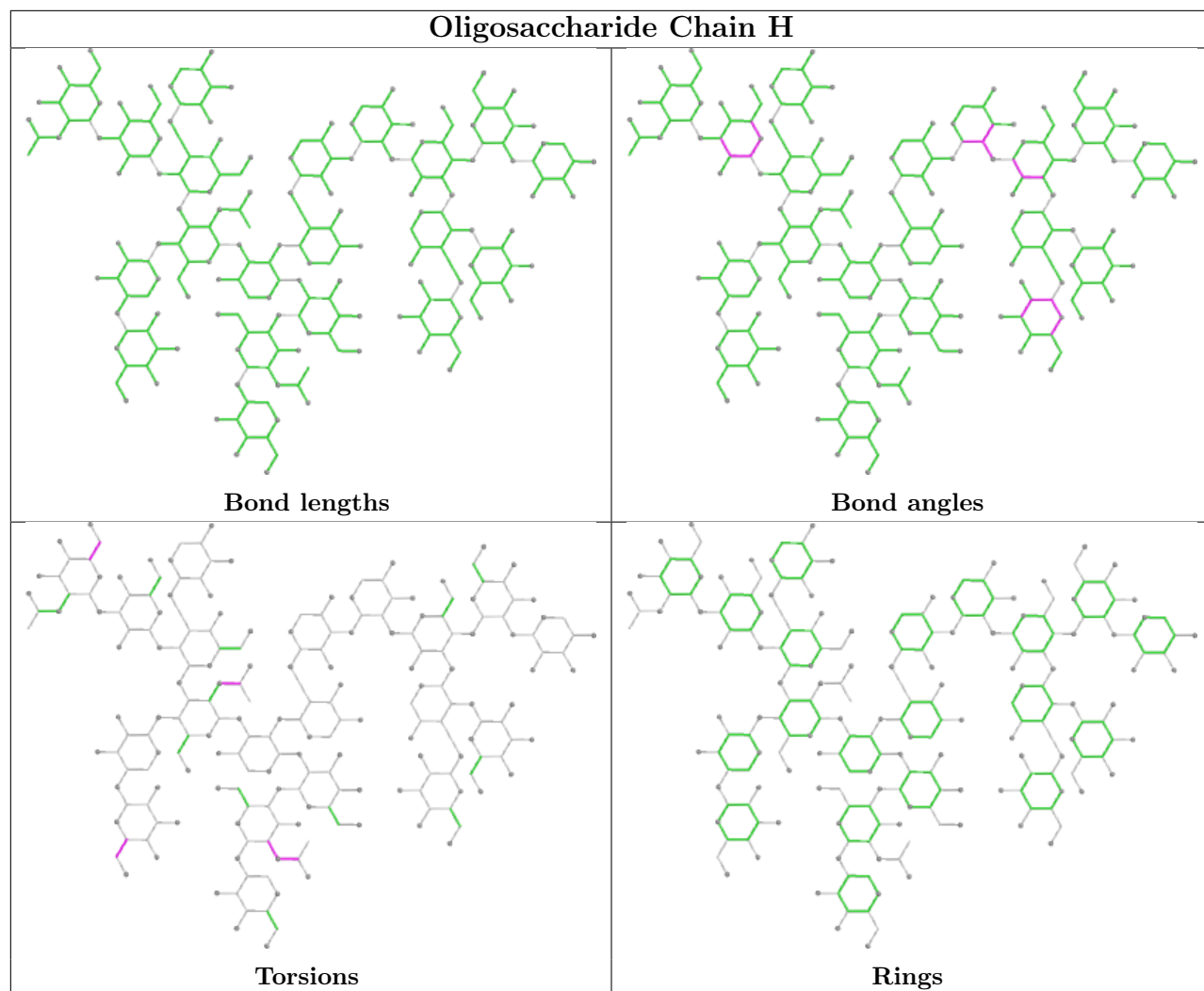




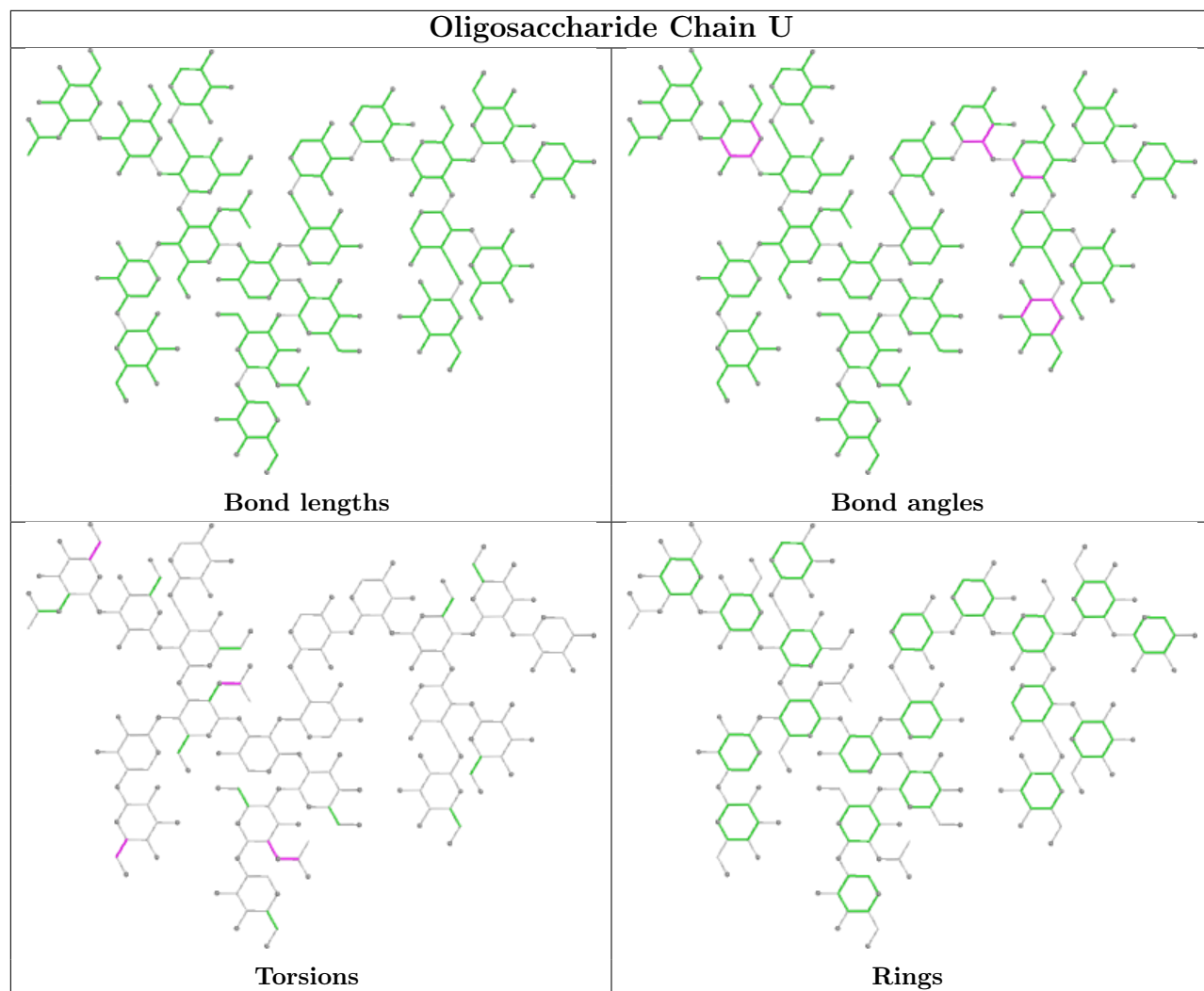


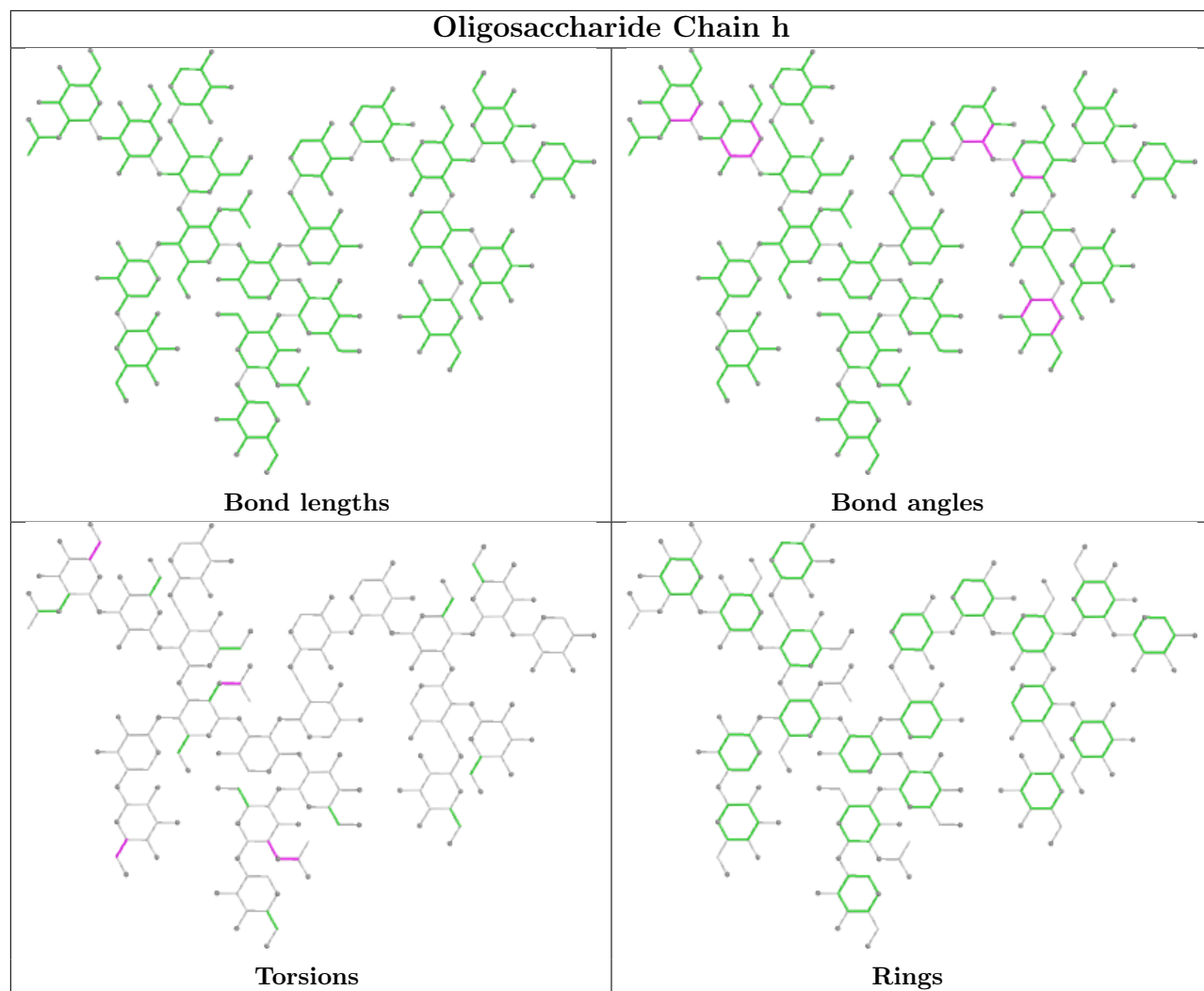


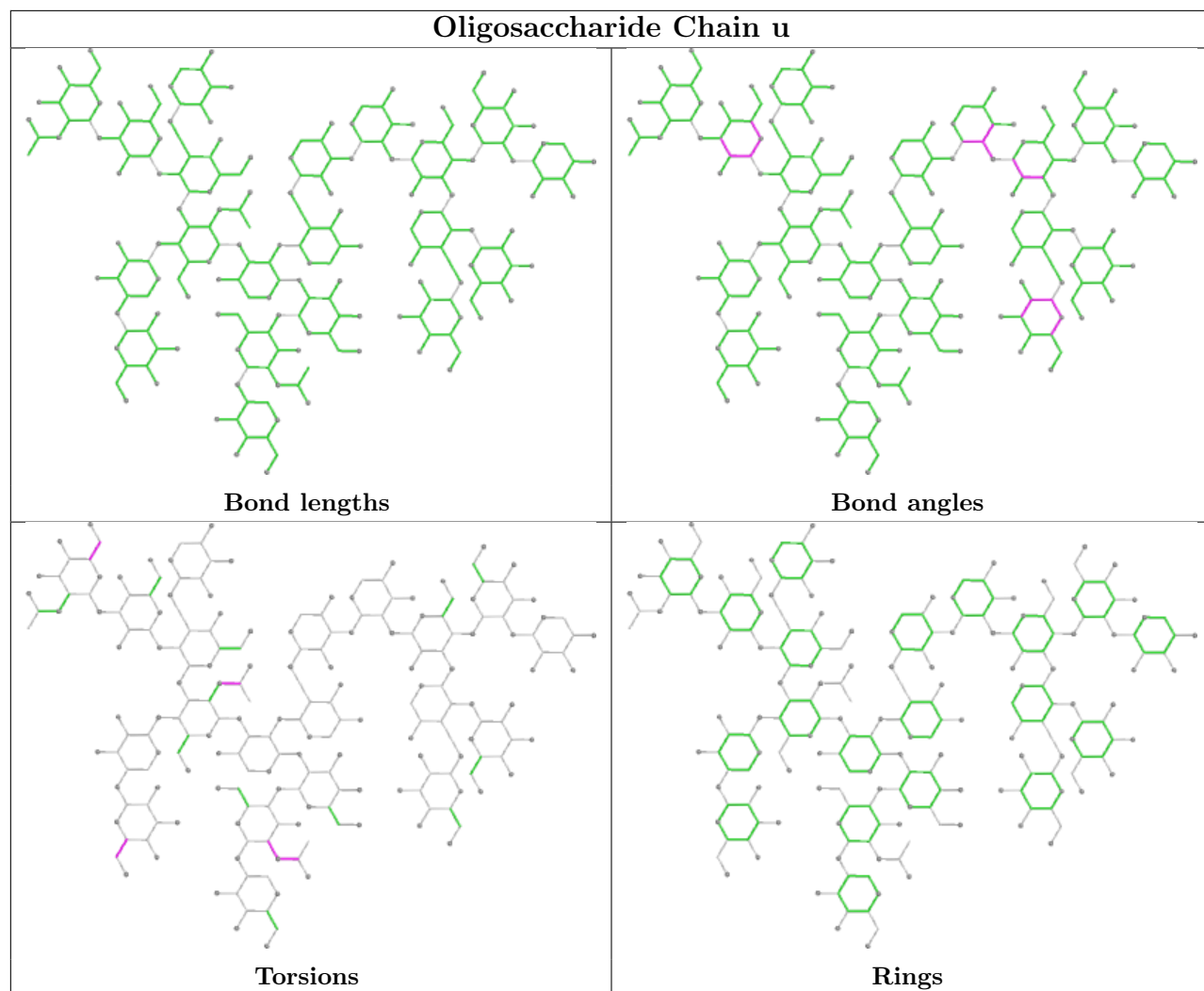


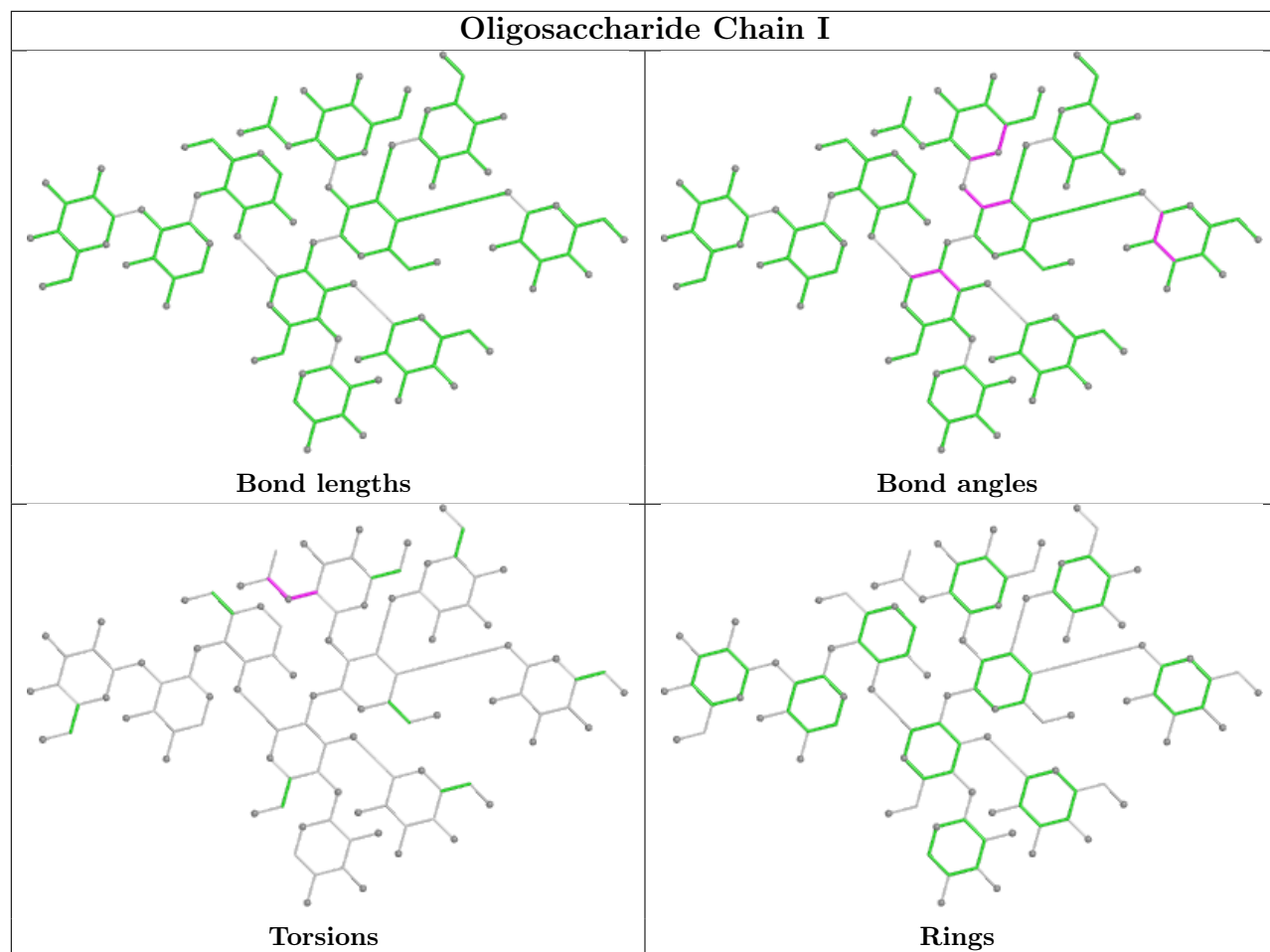


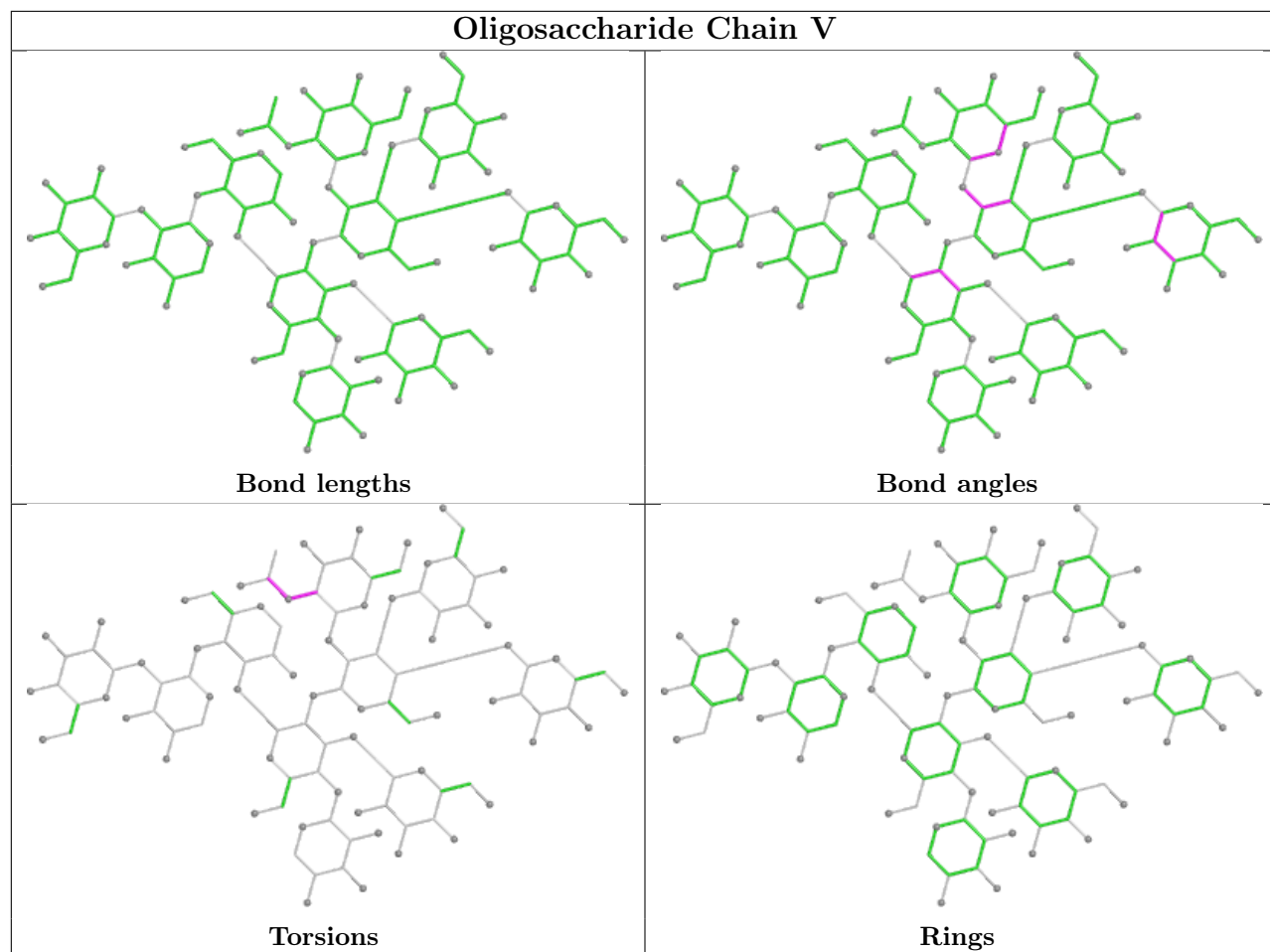


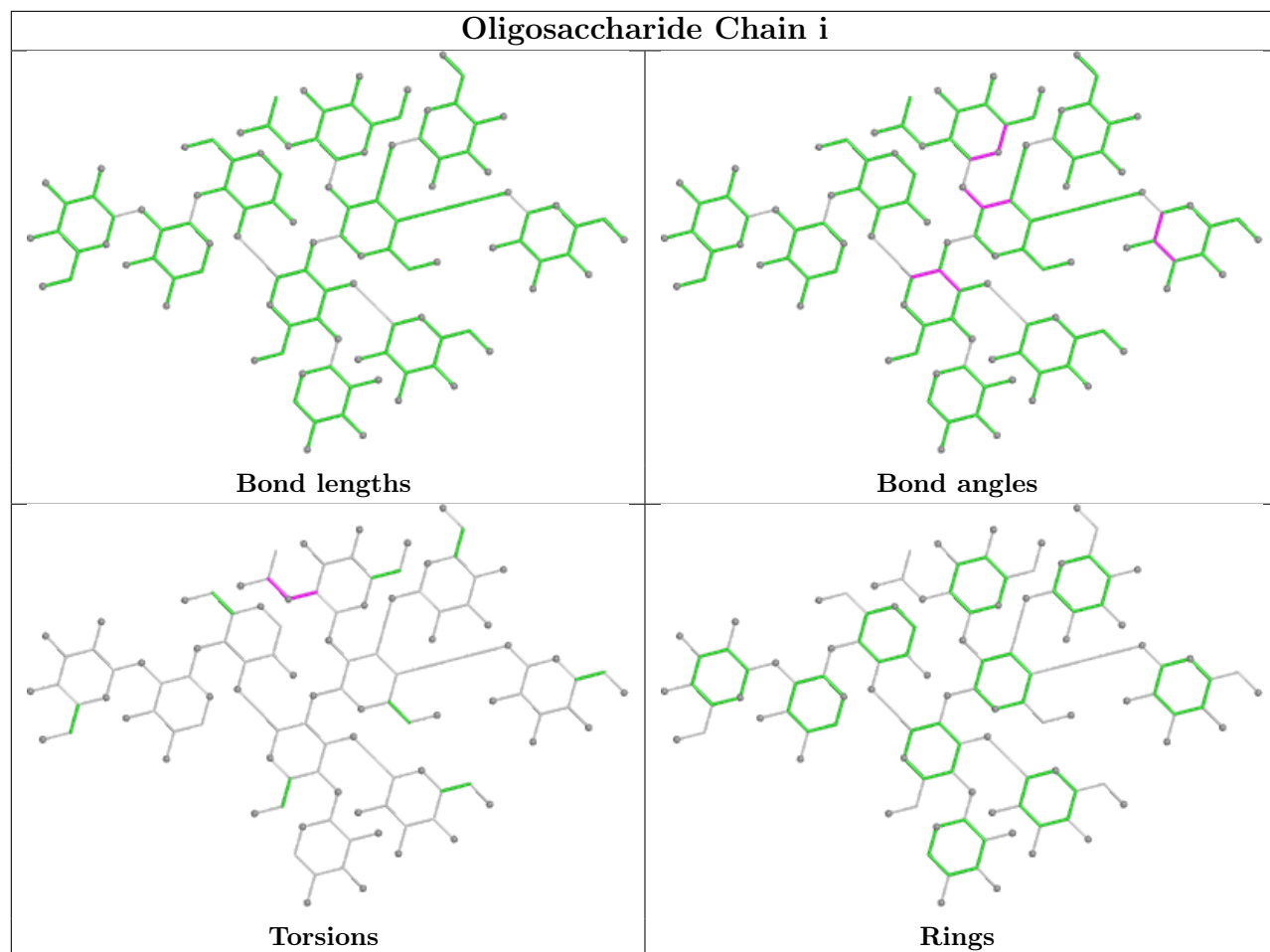


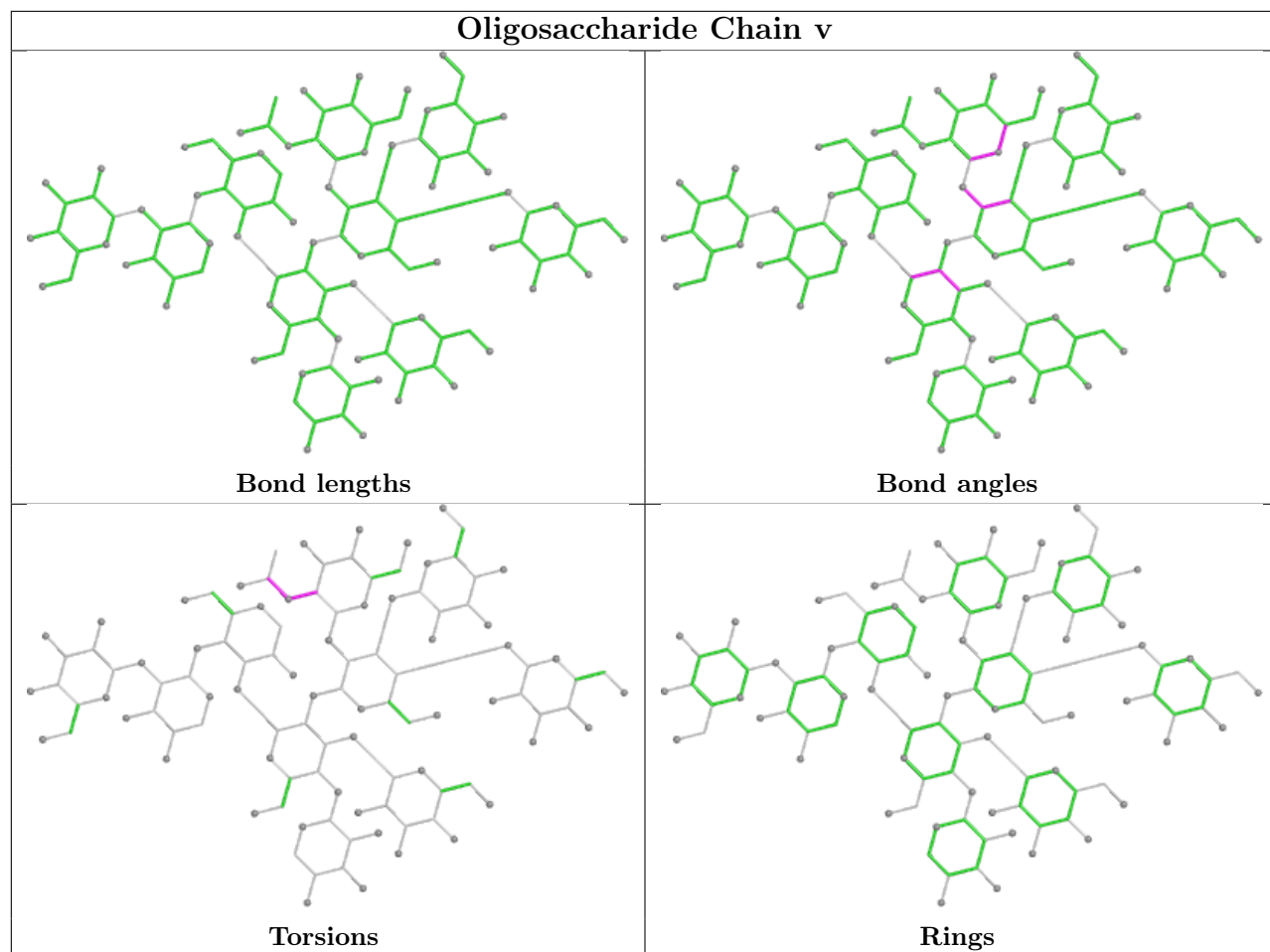


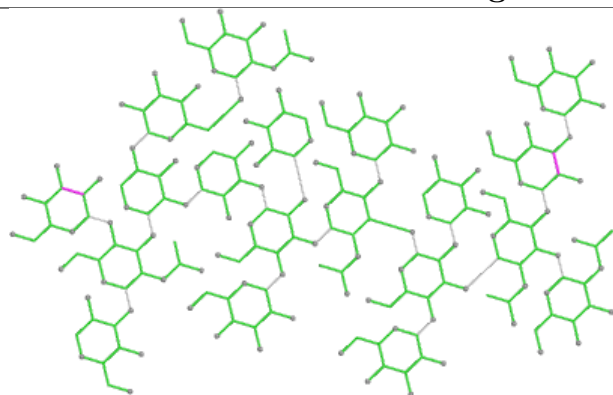
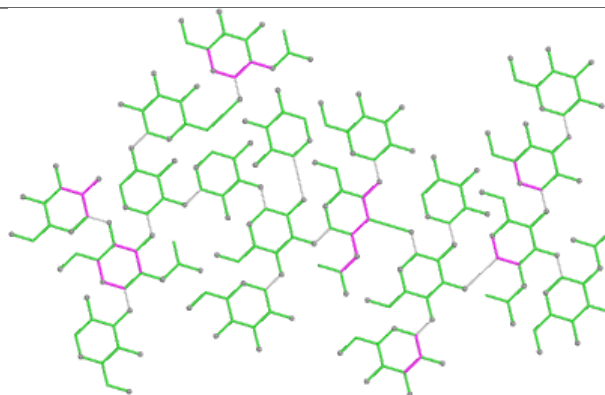
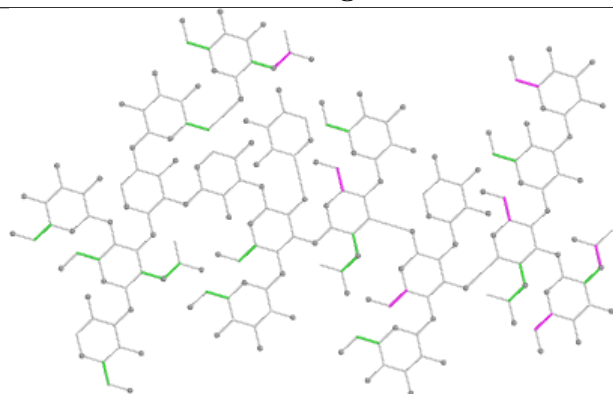
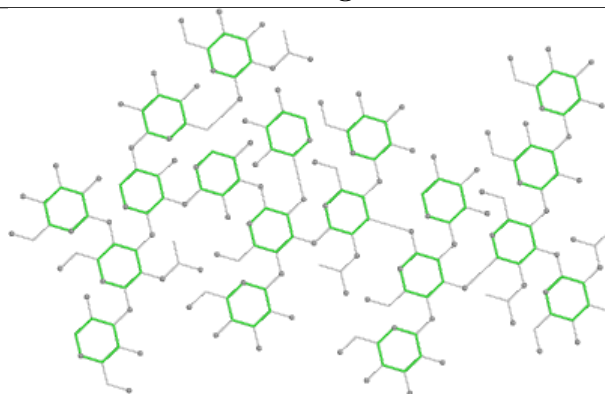




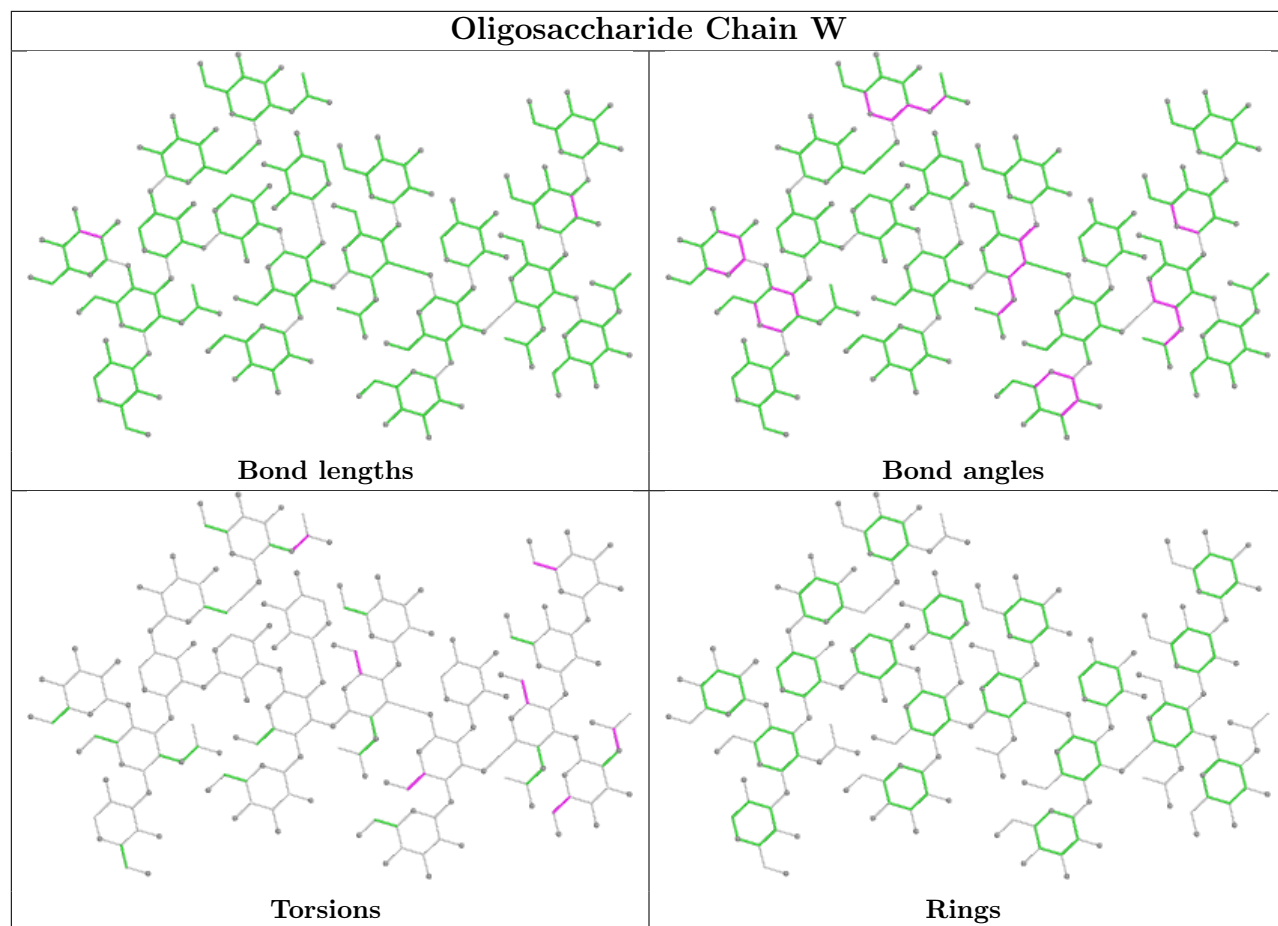


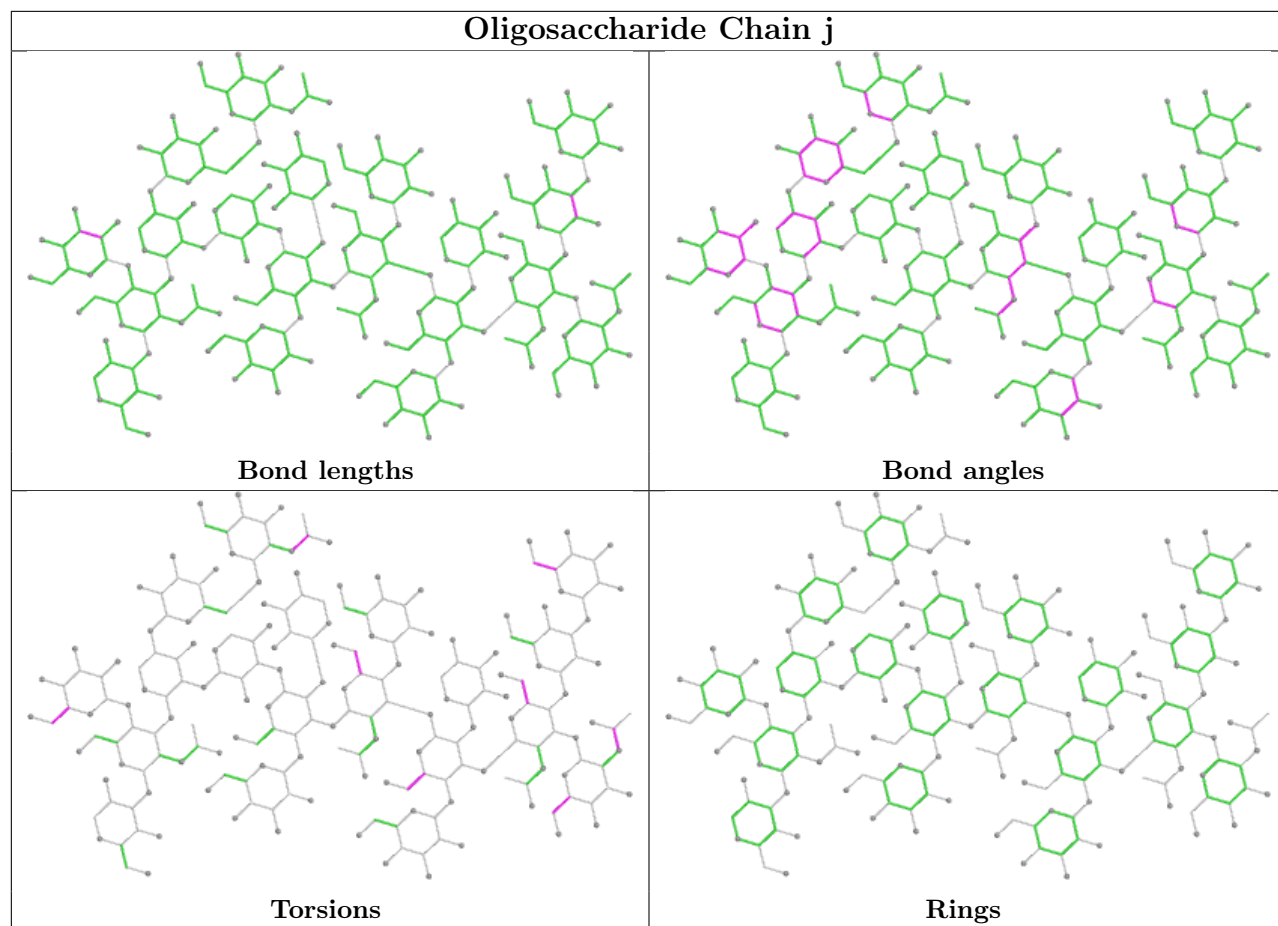


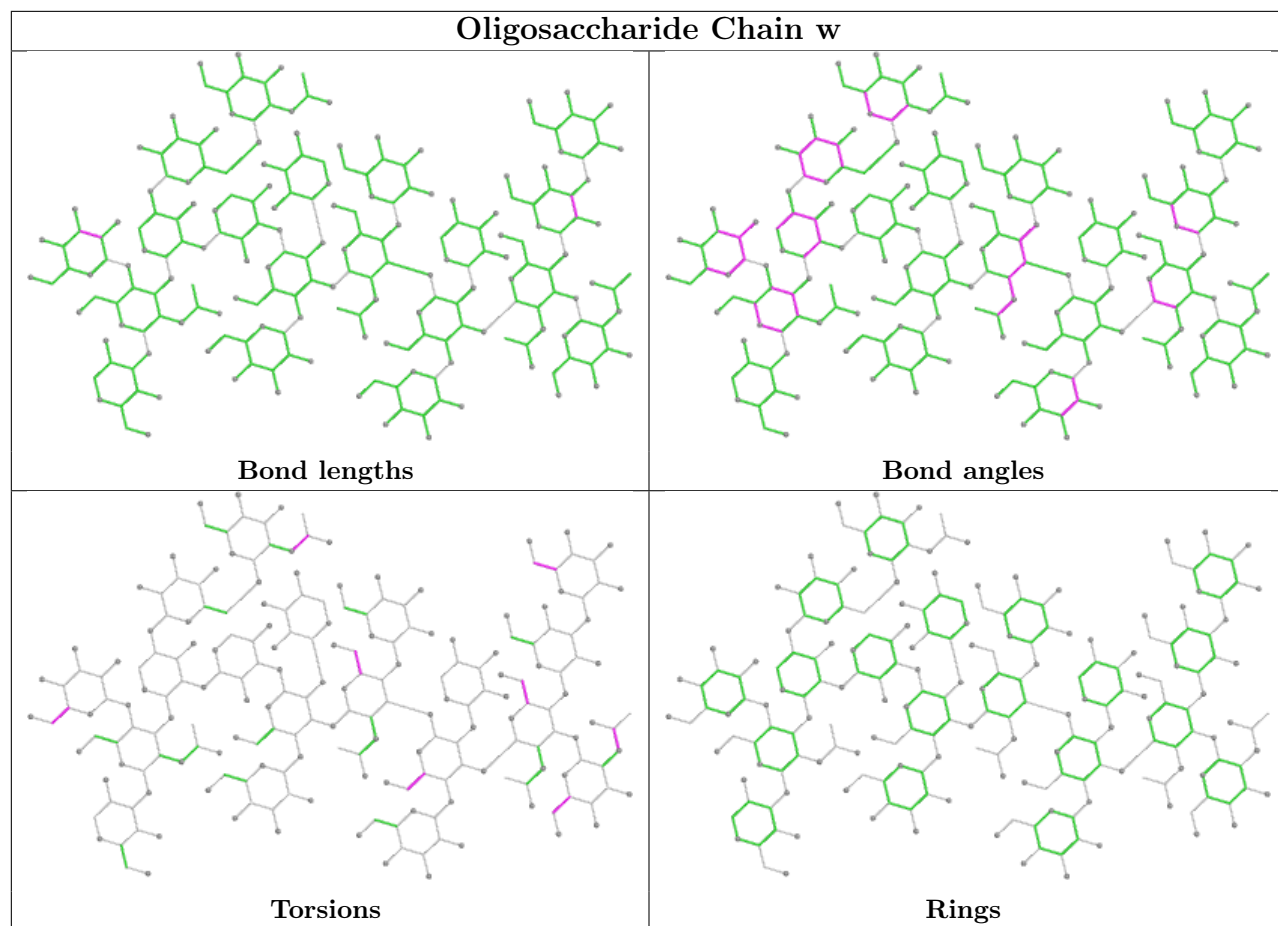


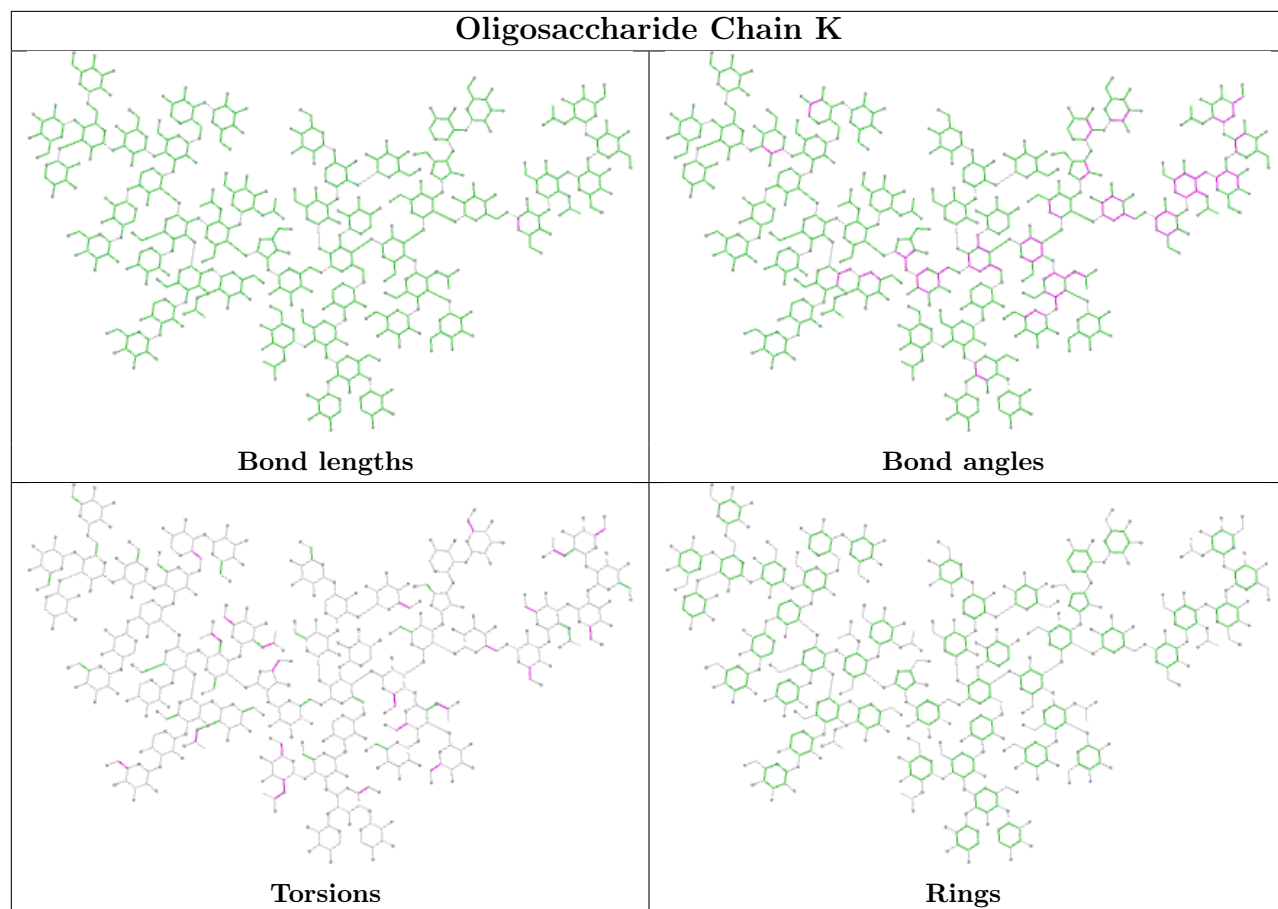
**Oligosaccharide Chain J****Bond lengths****Bond angles****Torsions****Rings**

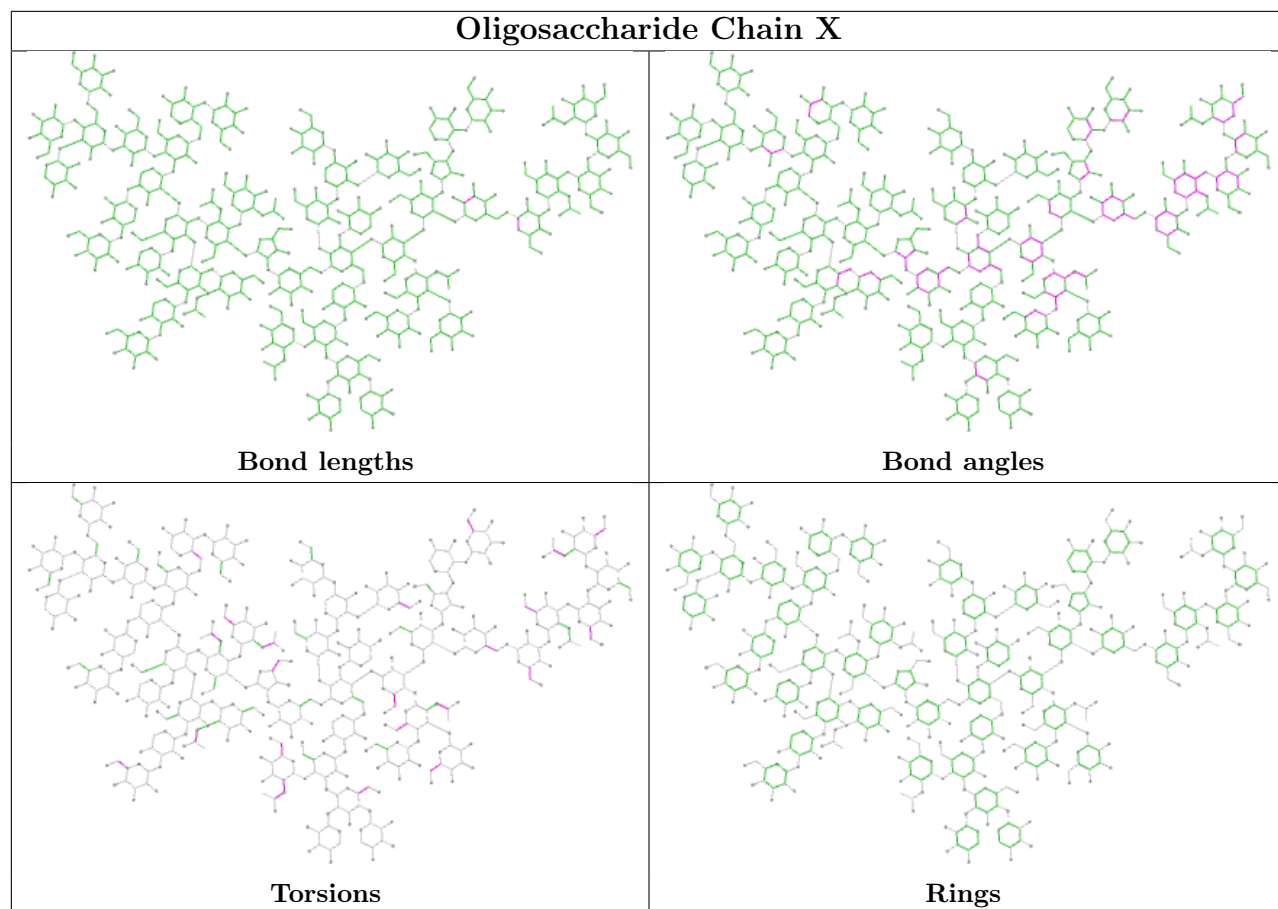


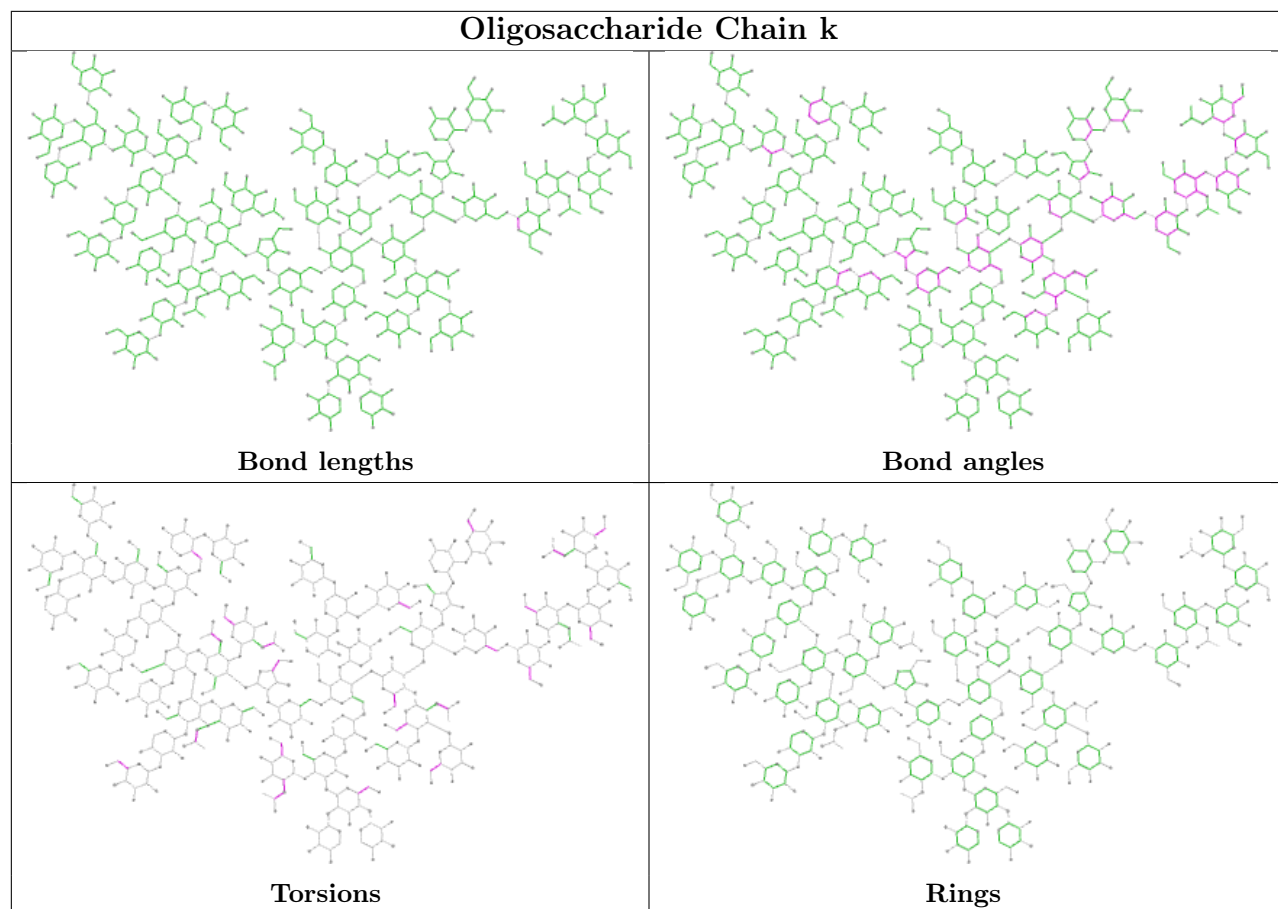


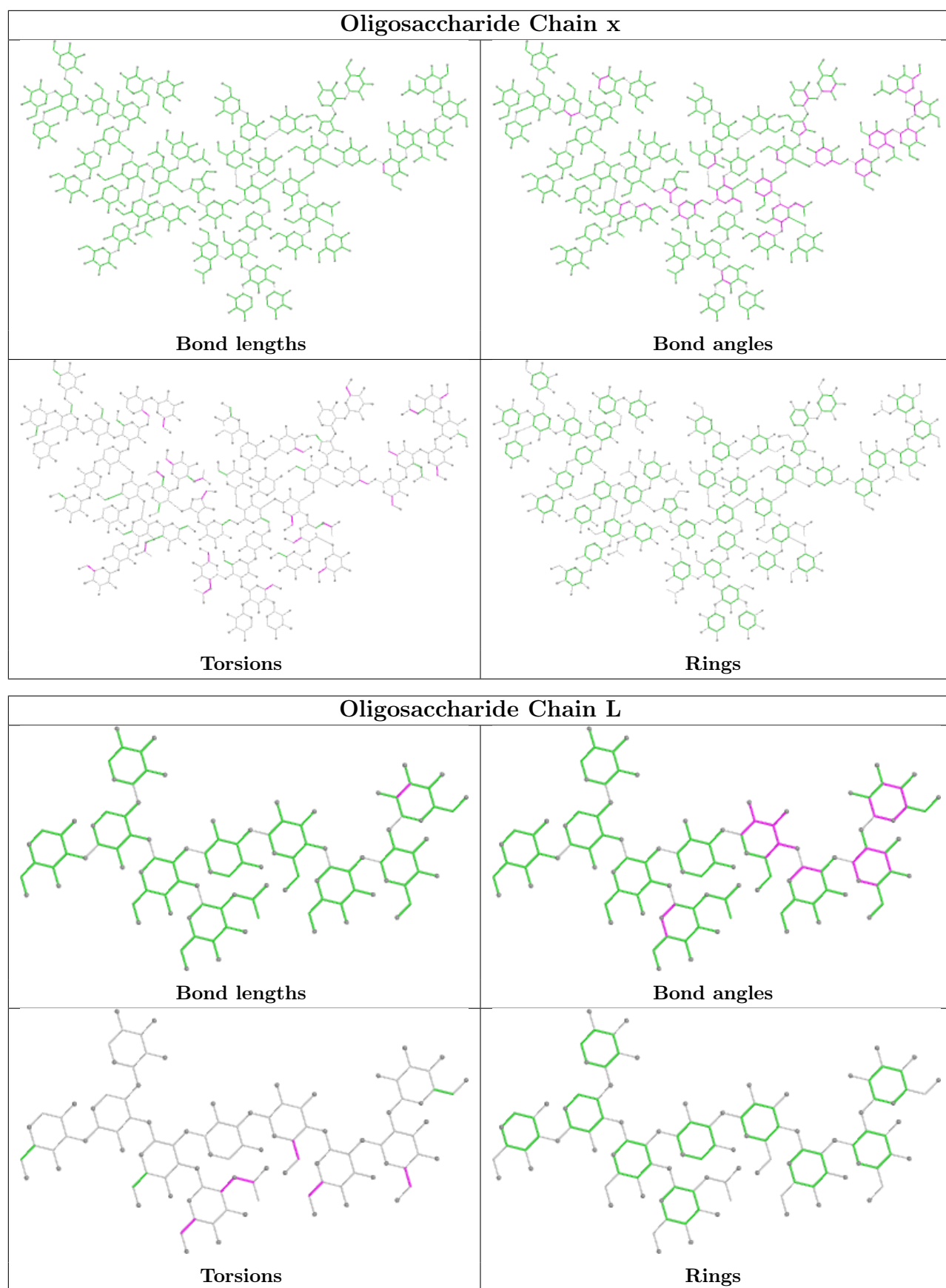


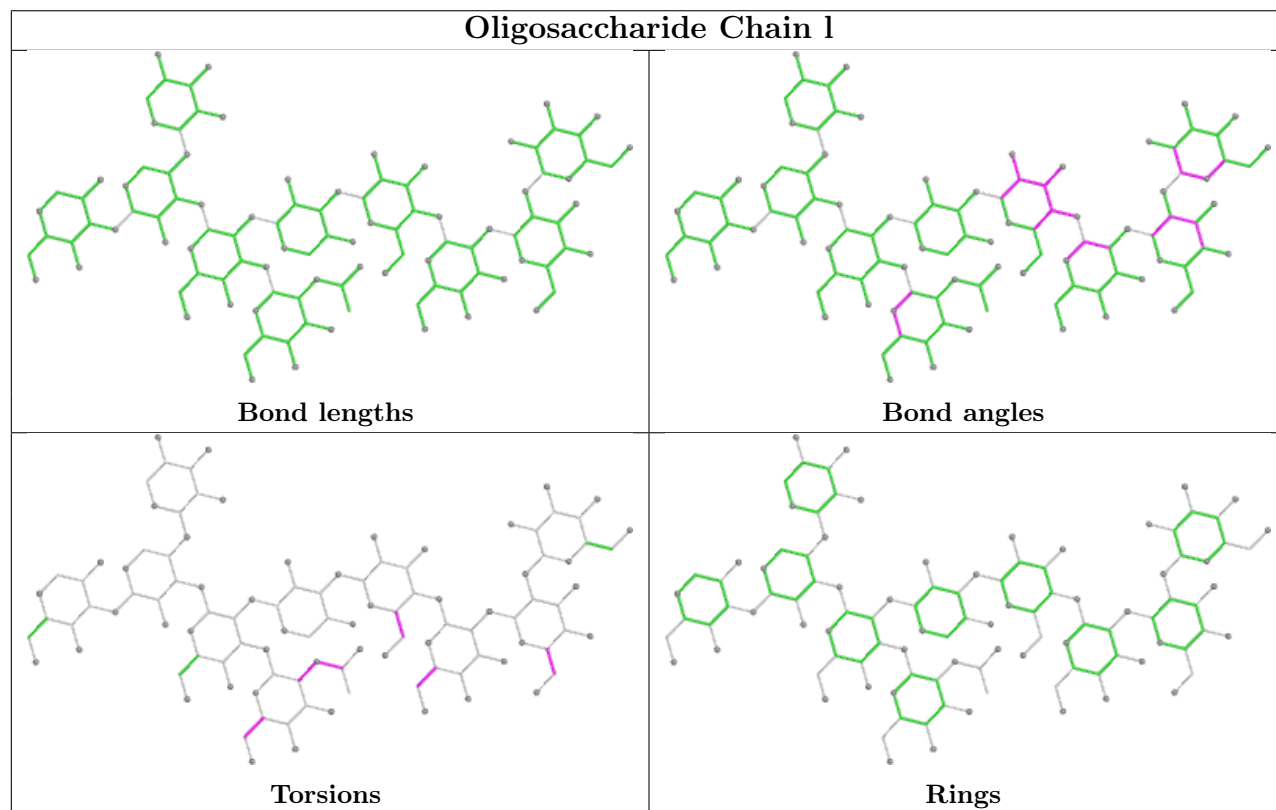
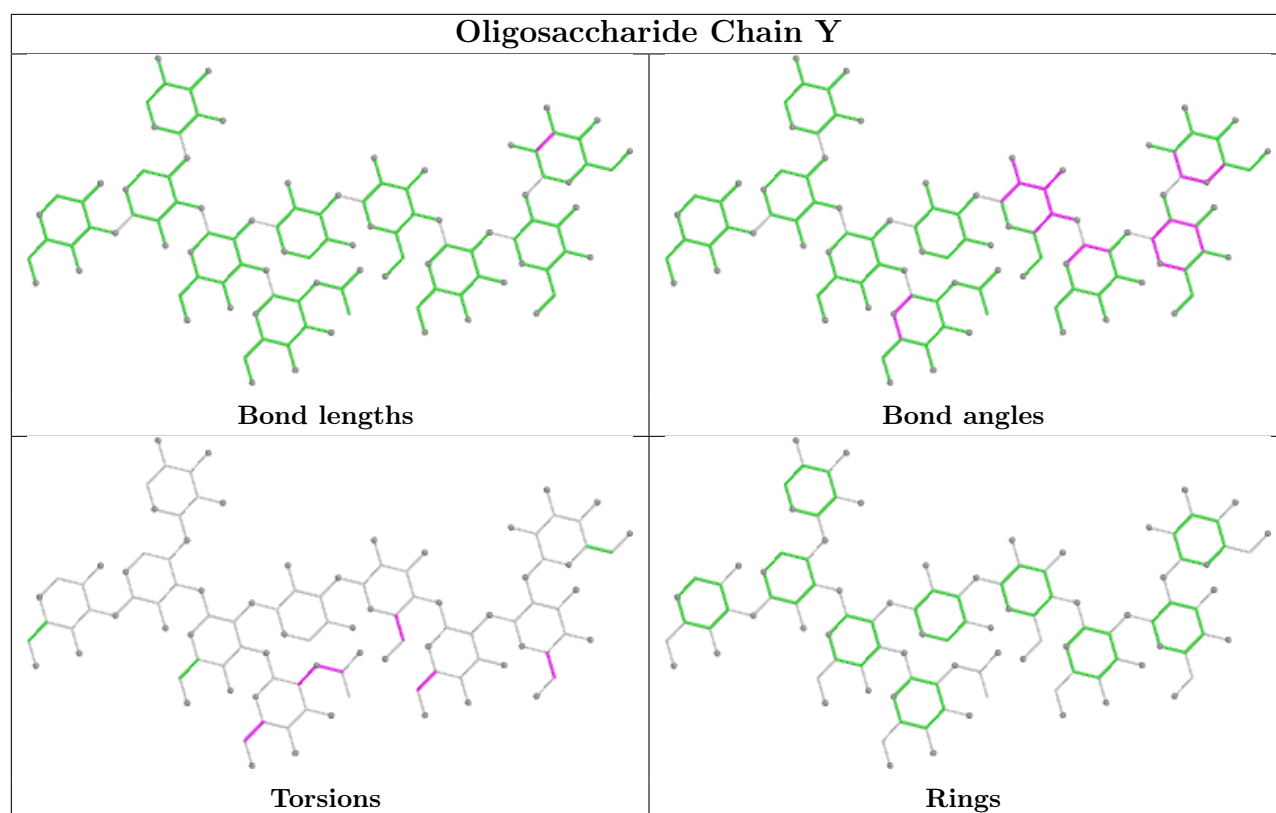




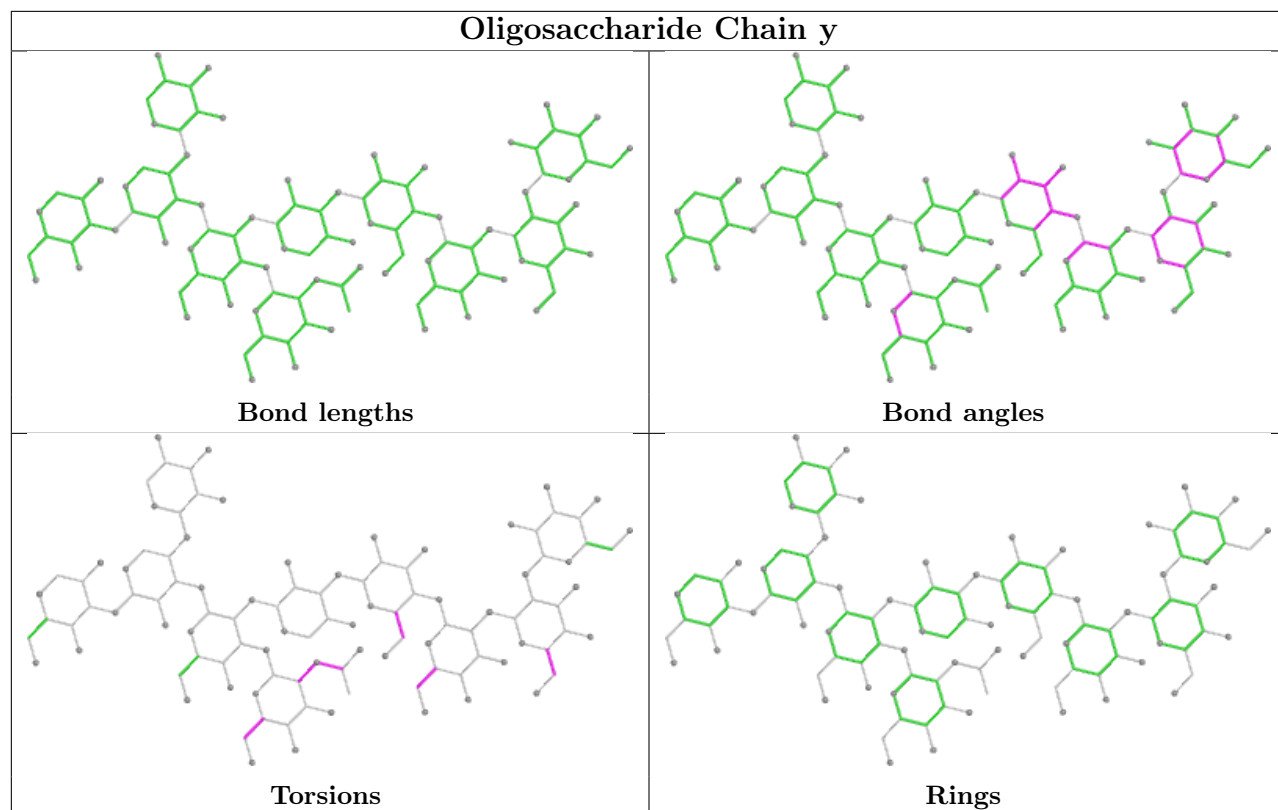


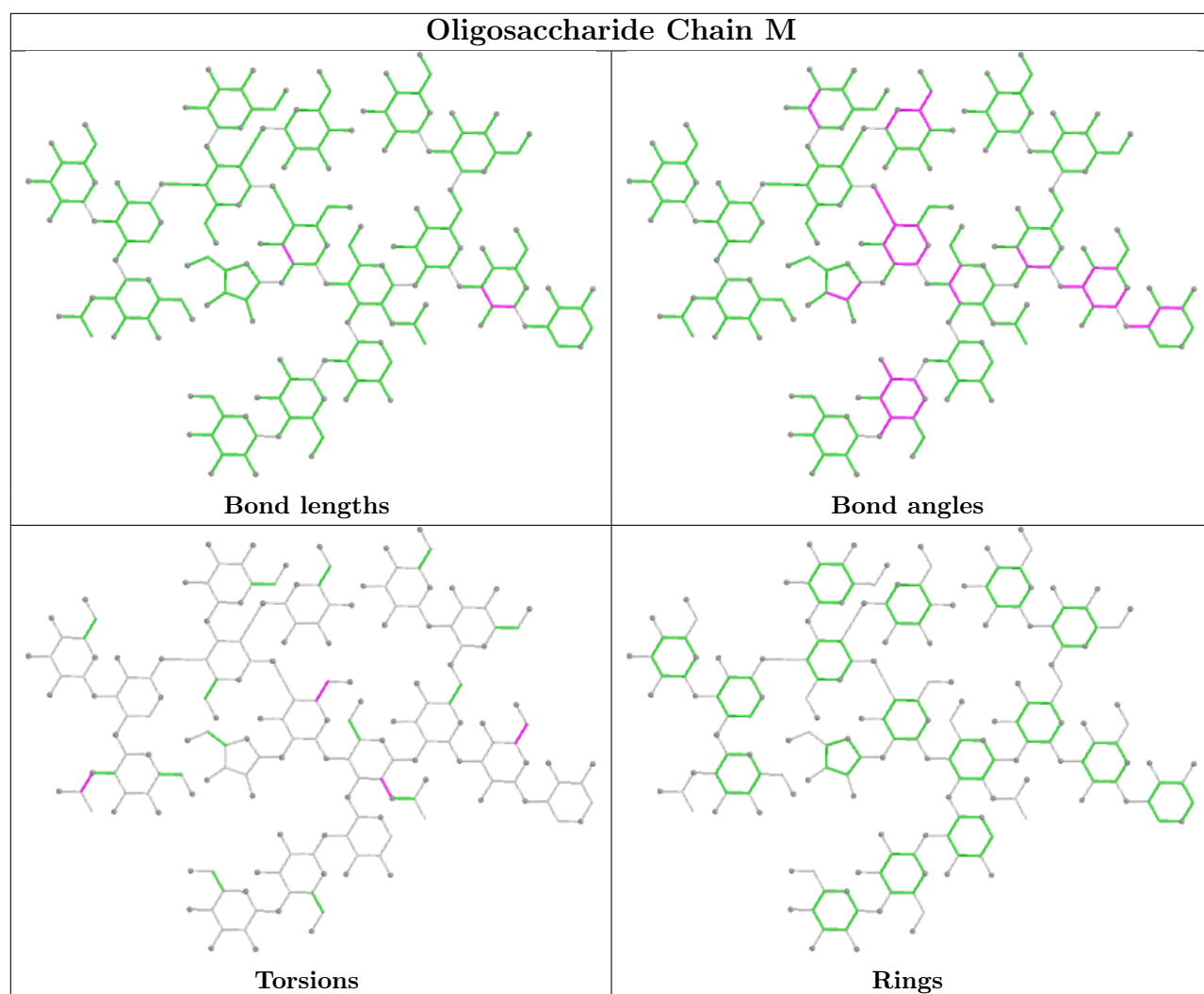


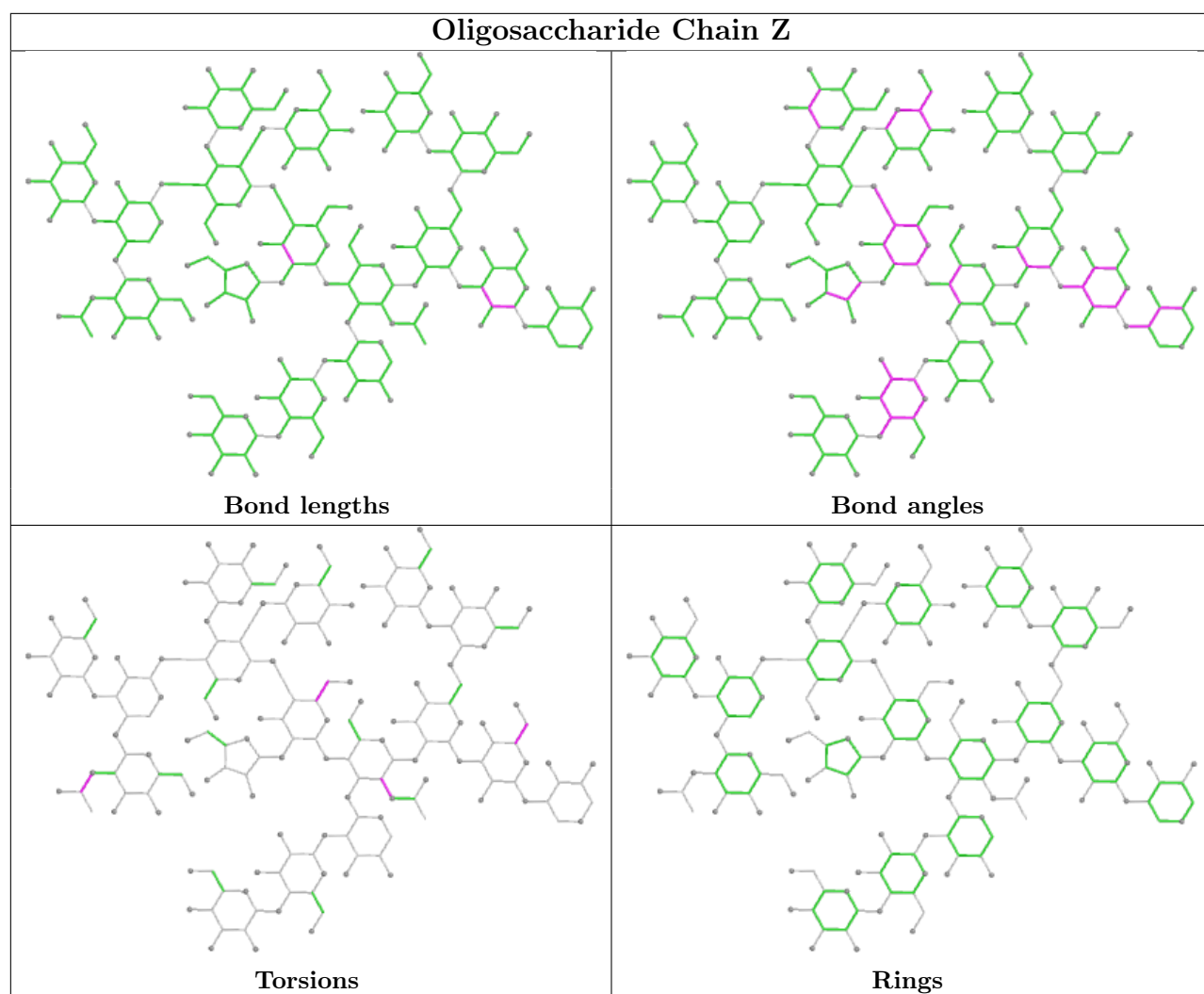


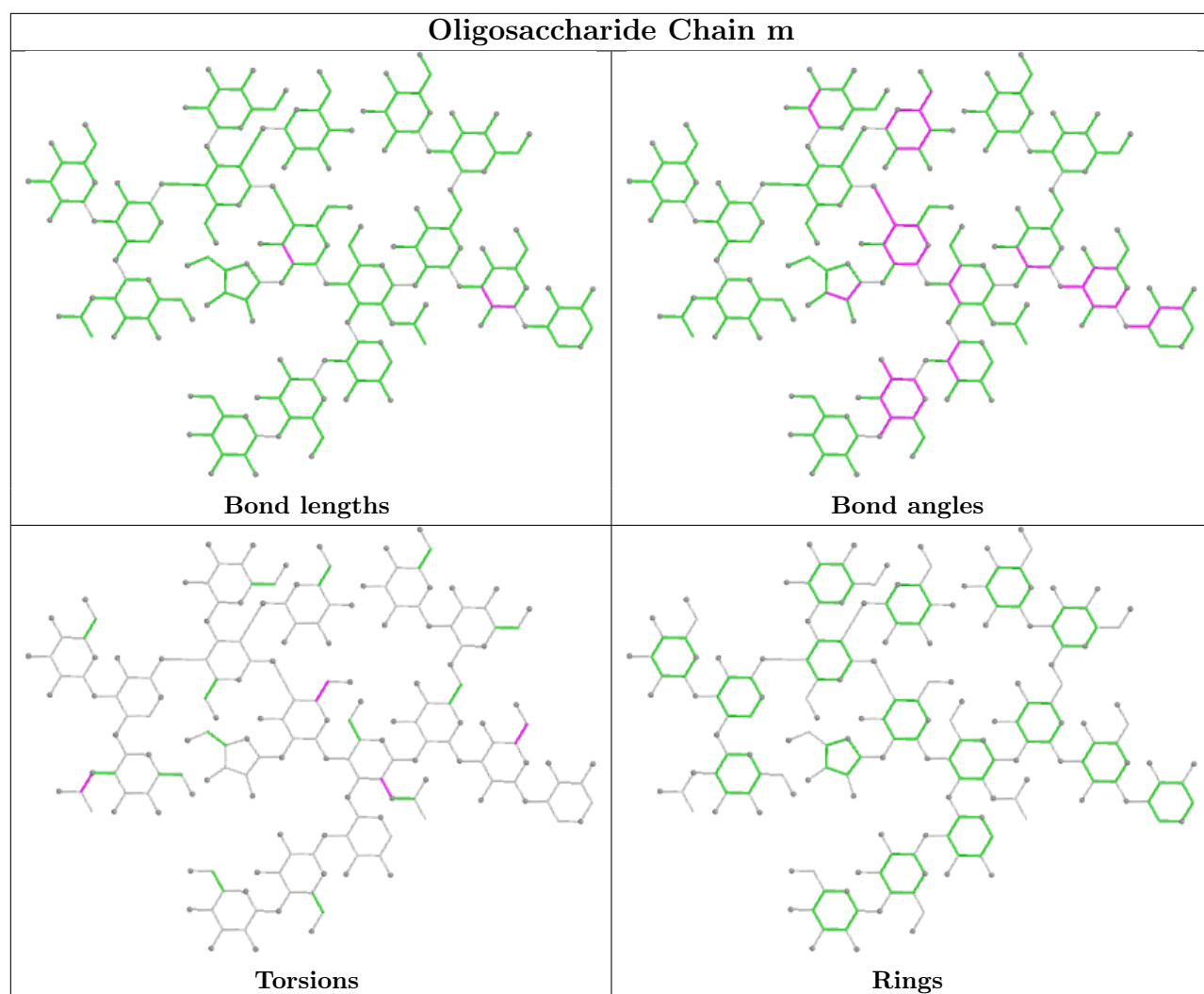


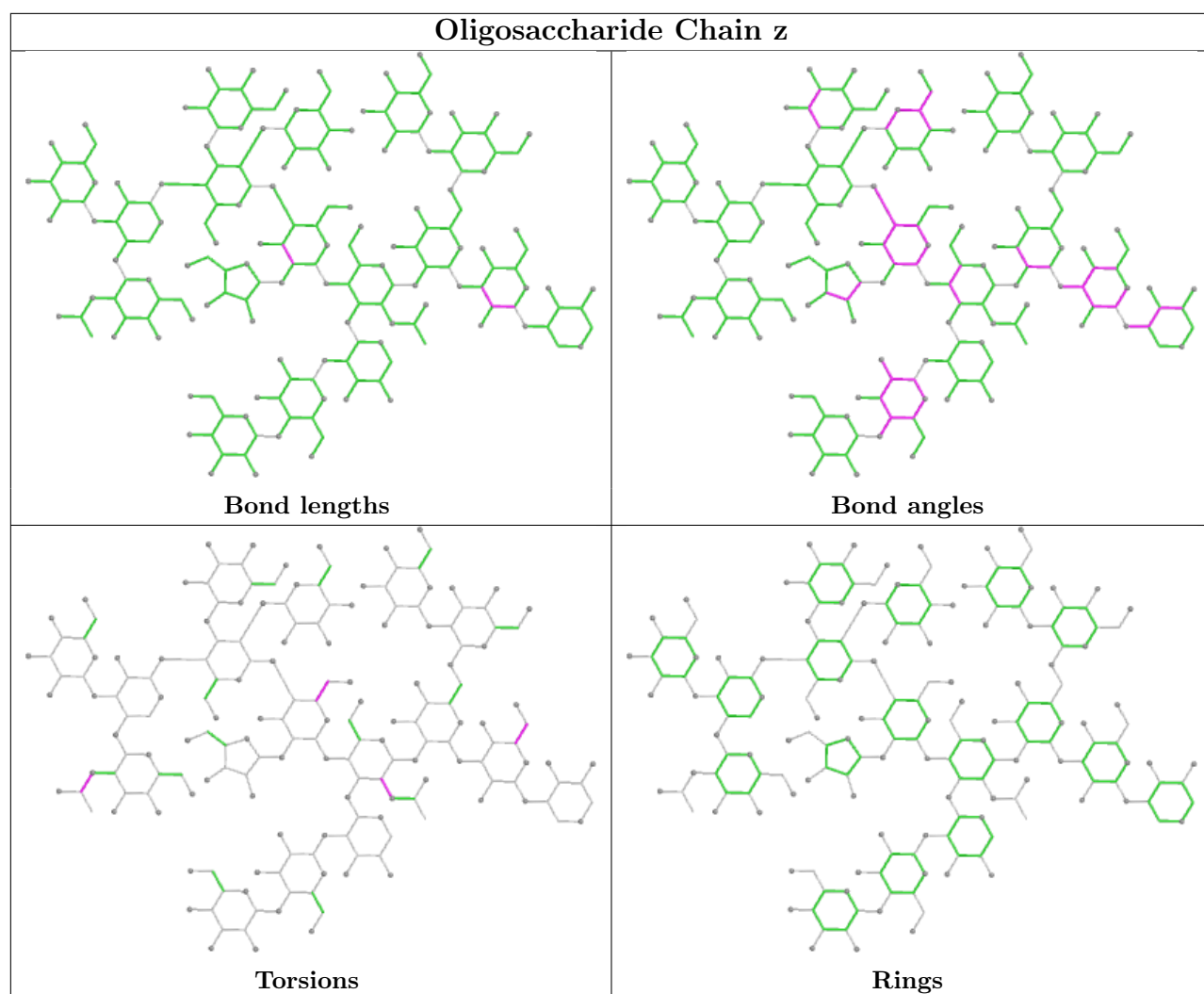


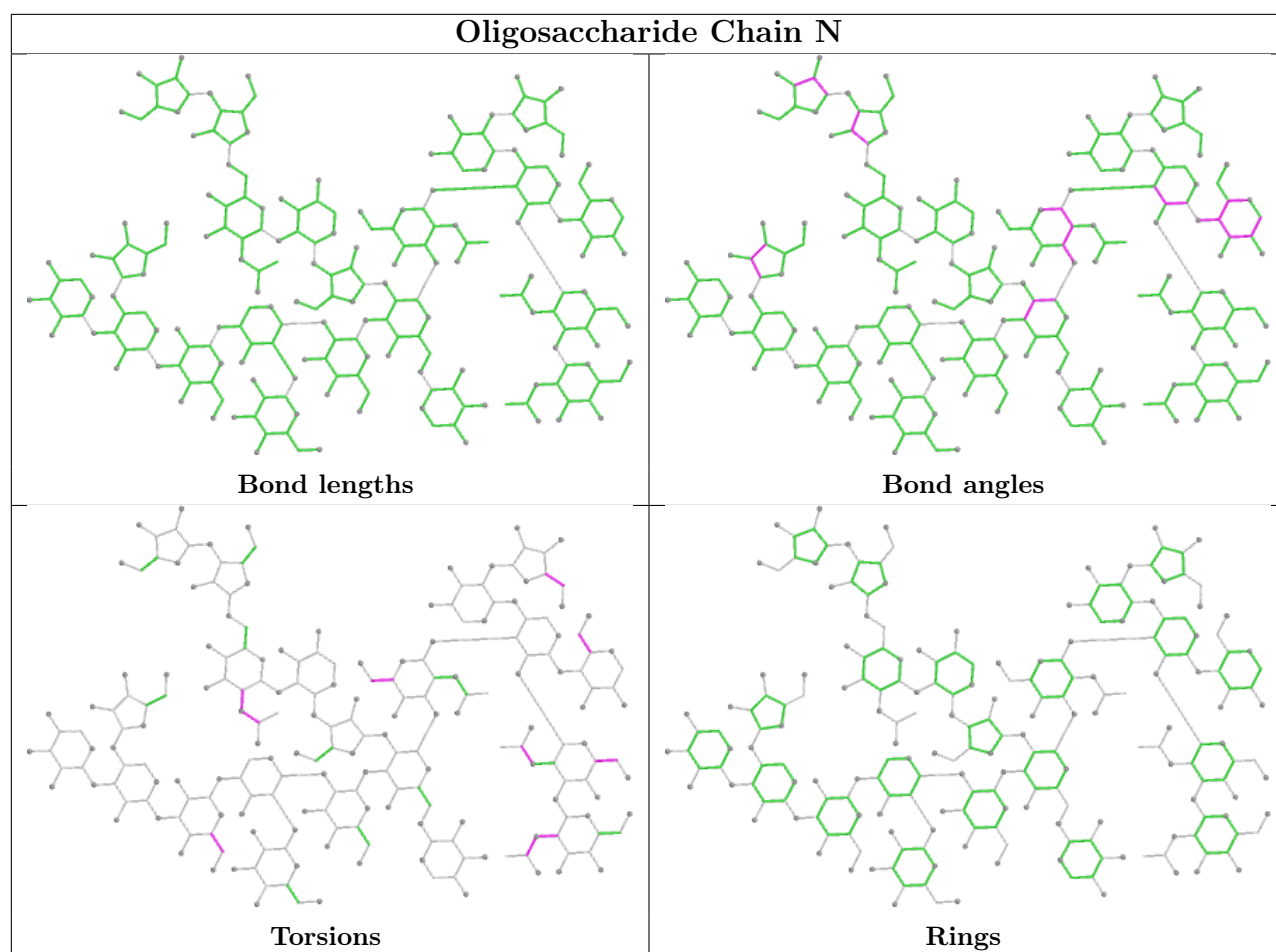


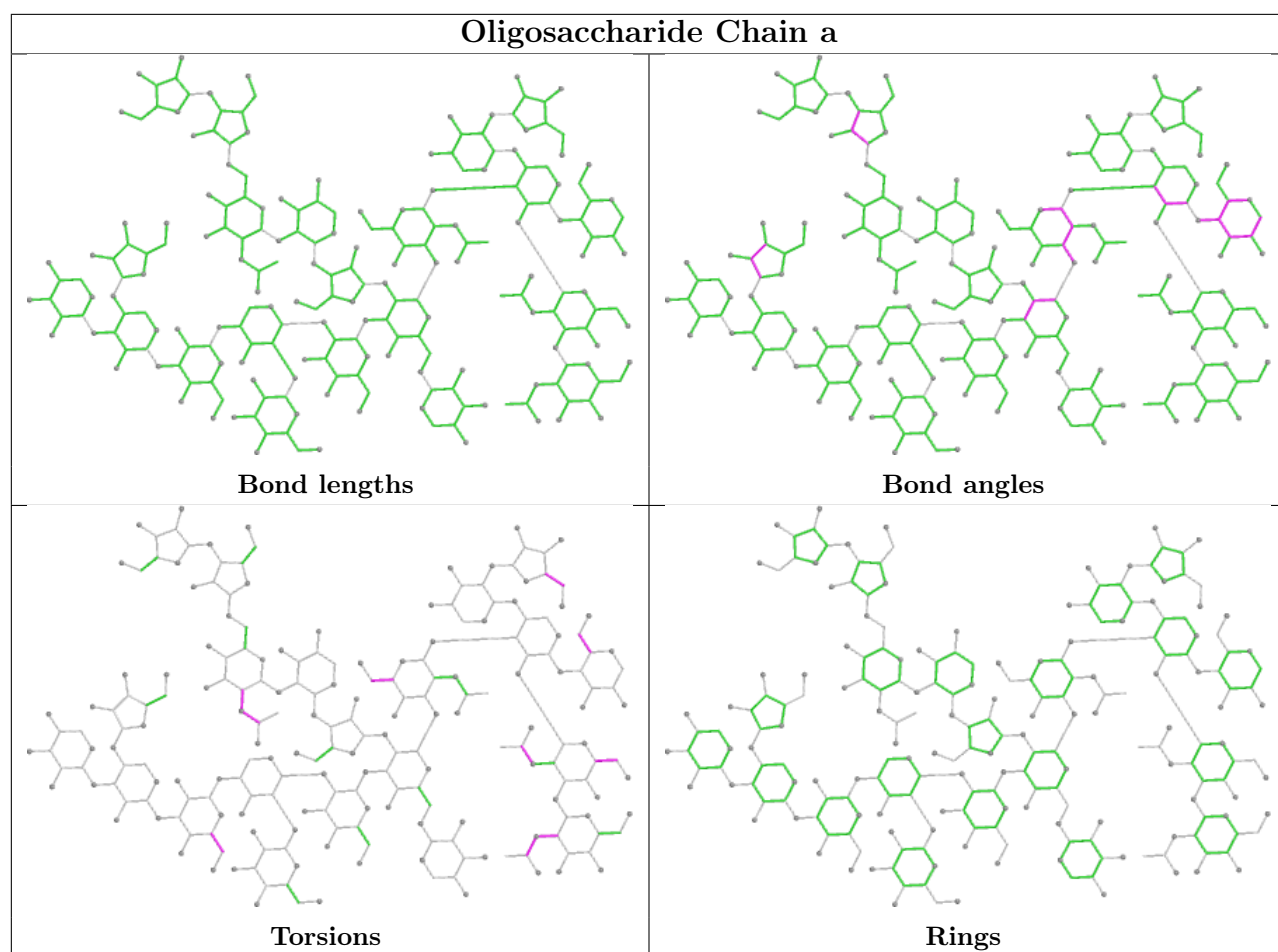


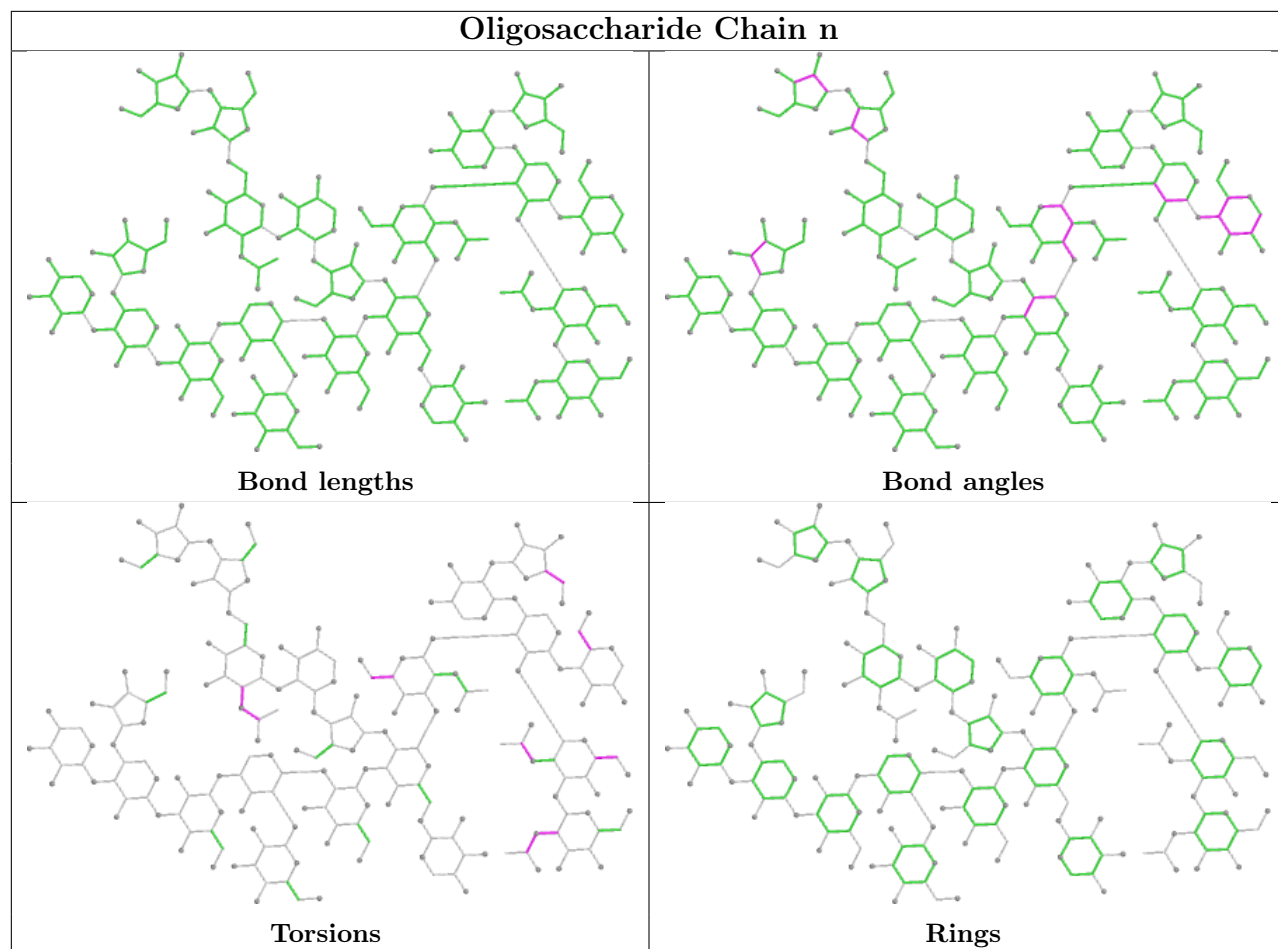




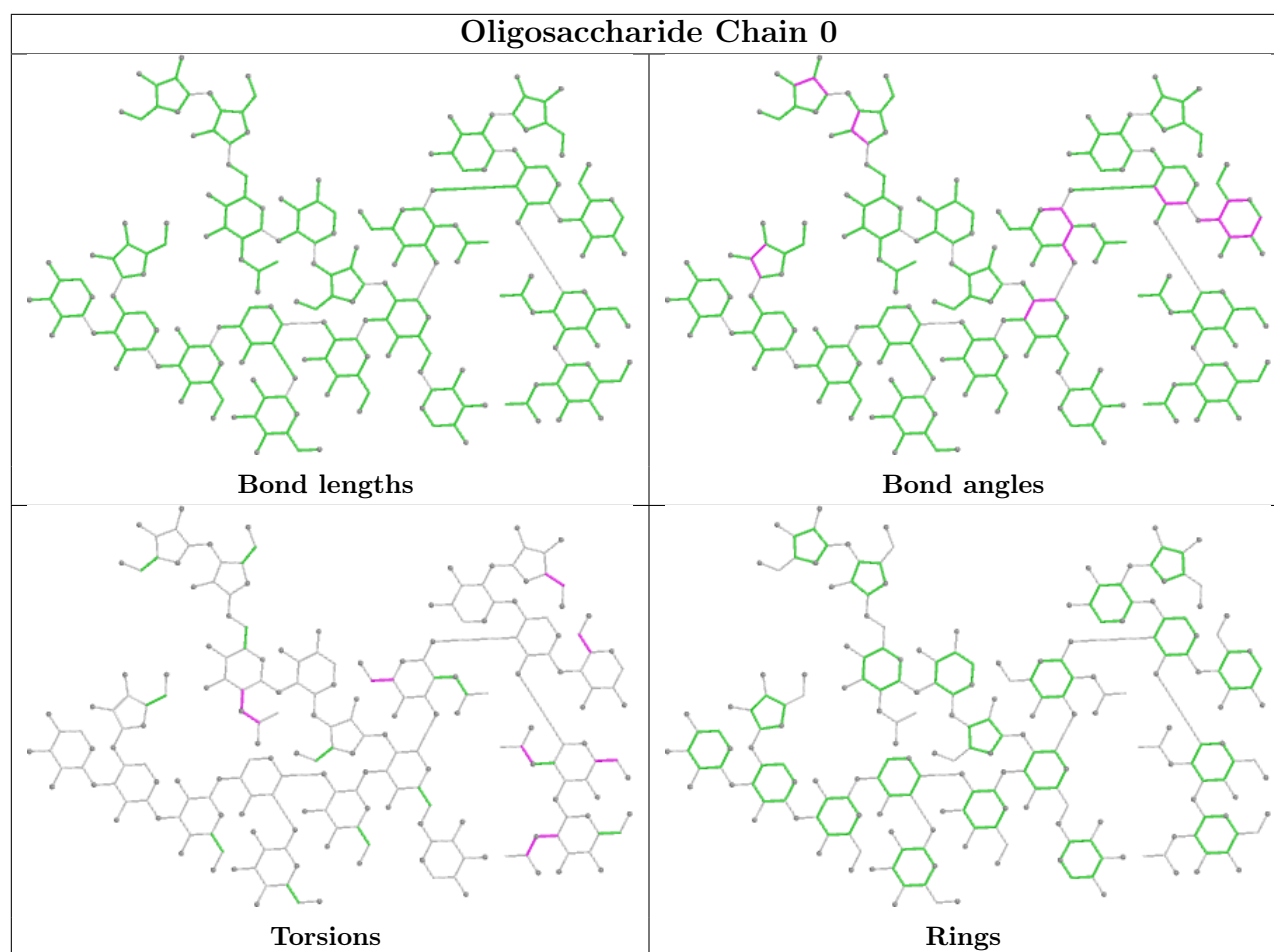












## 5.6 Ligand geometry [i](#)

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.

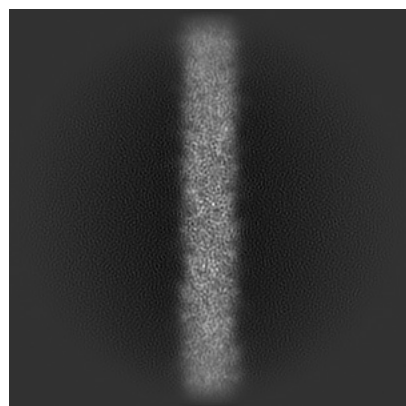
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67848. These allow visual inspection of the internal detail of the map and identification of artifacts.

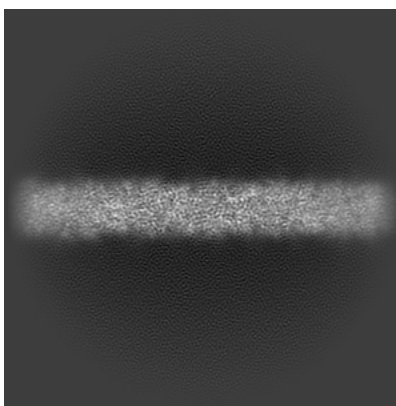
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

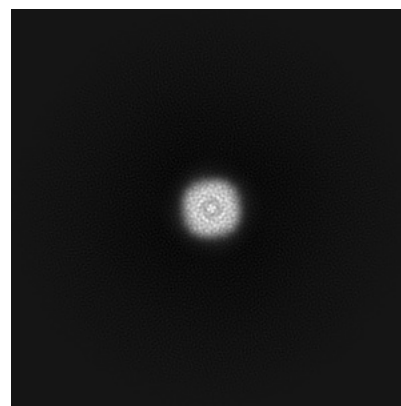
#### 6.1.1 Primary map



X

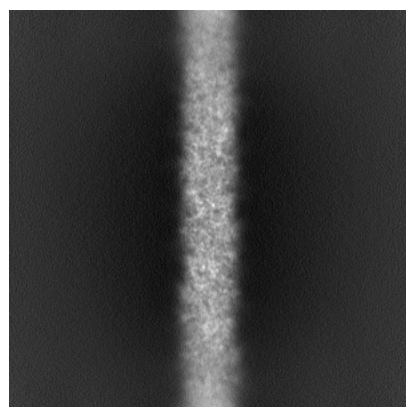


Y

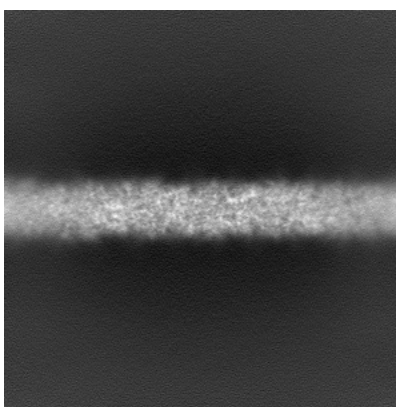


Z

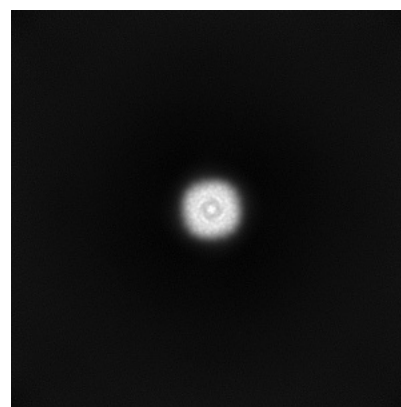
#### 6.1.2 Raw map



X



Y

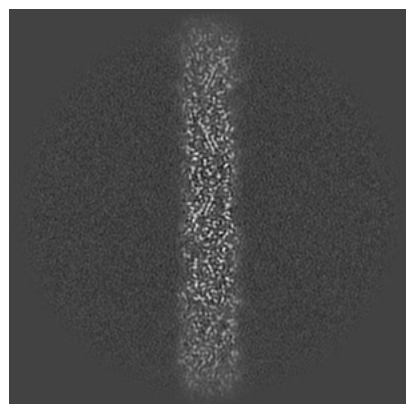


Z

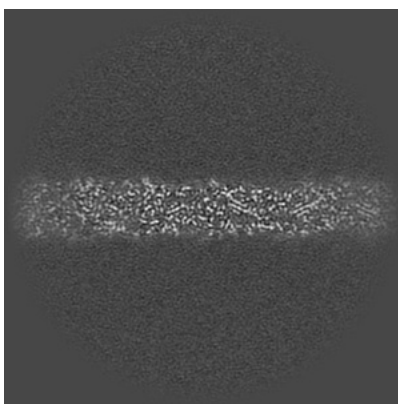
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

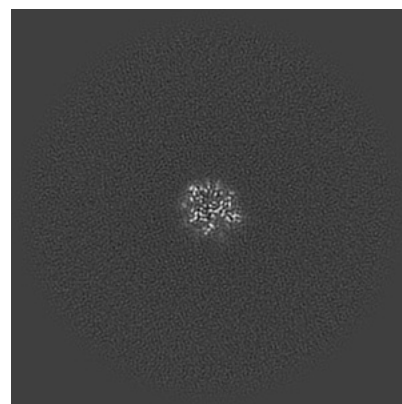
### 6.2.1 Primary map



X Index: 192

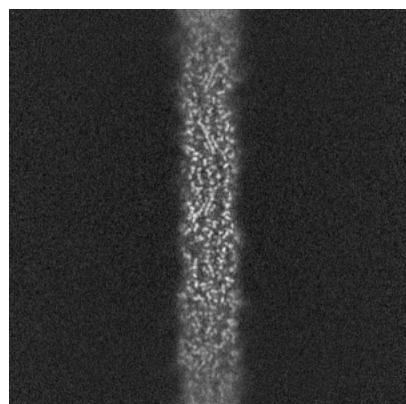


Y Index: 192

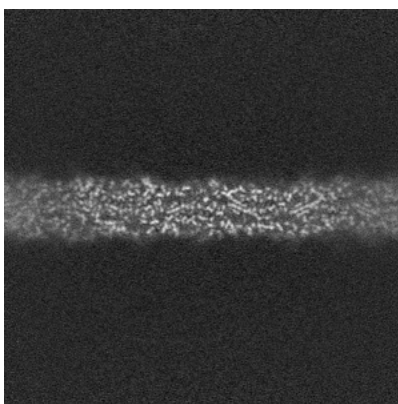


Z Index: 192

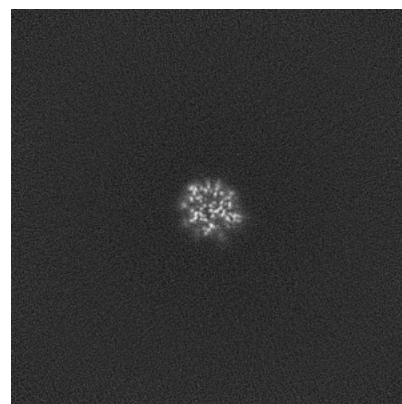
### 6.2.2 Raw map



X Index: 192



Y Index: 192

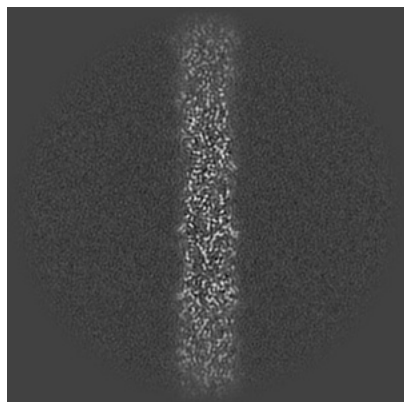


Z Index: 192

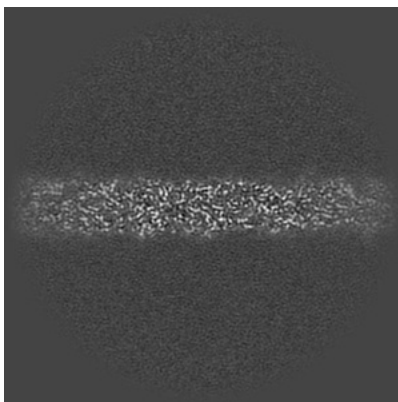
The images above show central slices of the map in three orthogonal directions.

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

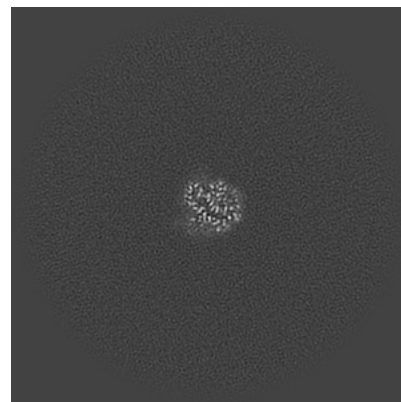
### 6.3.1 Primary map



X Index: 194

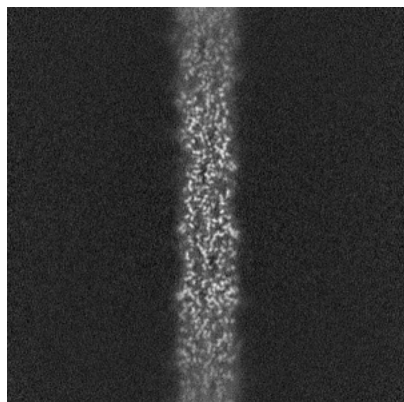


Y Index: 195

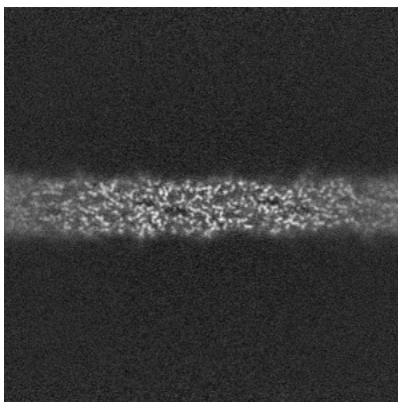


Z Index: 201

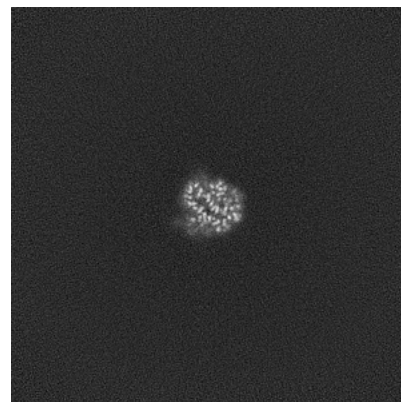
### 6.3.2 Raw map



X Index: 194



Y Index: 195



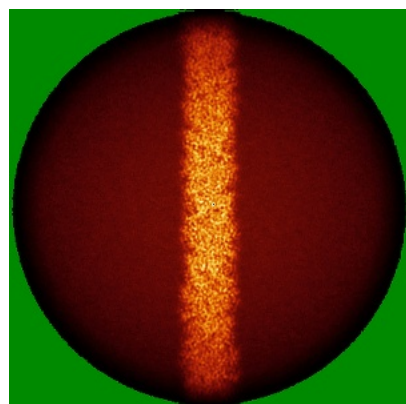
Z Index: 201

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

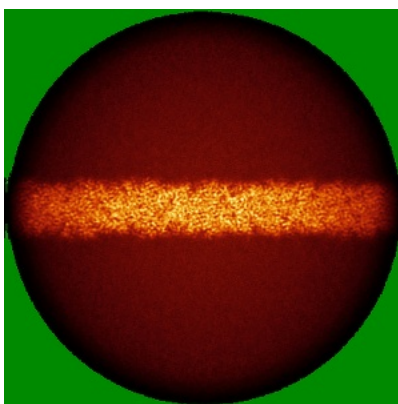


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

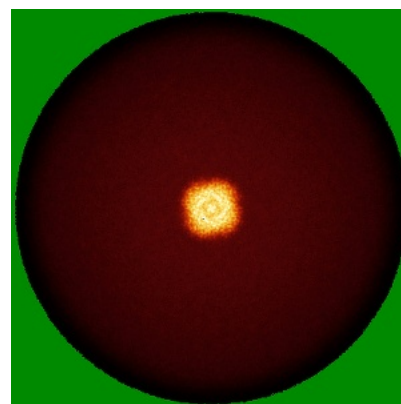
### 6.4.1 Primary map



X

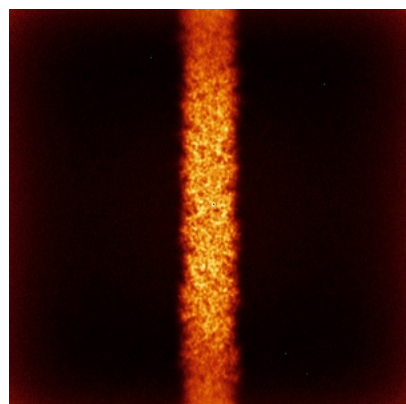


Y

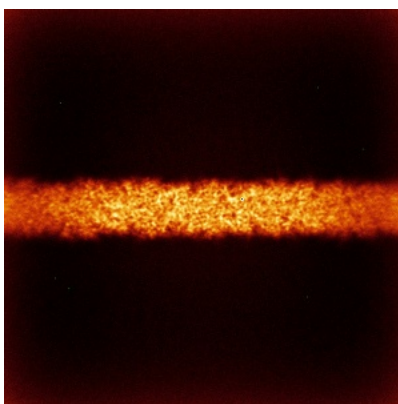


Z

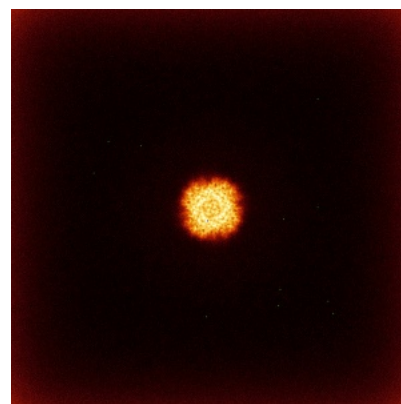
### 6.4.2 Raw map



X



Y

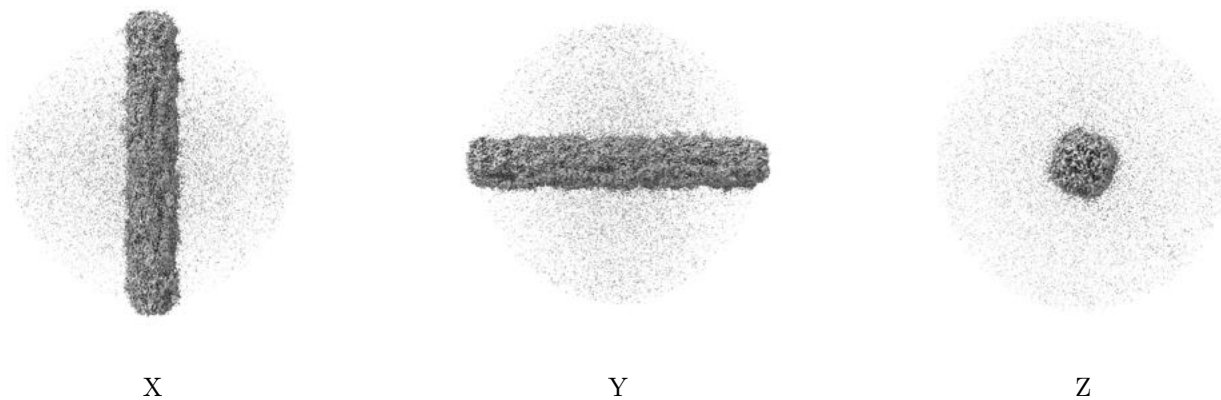


Z

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

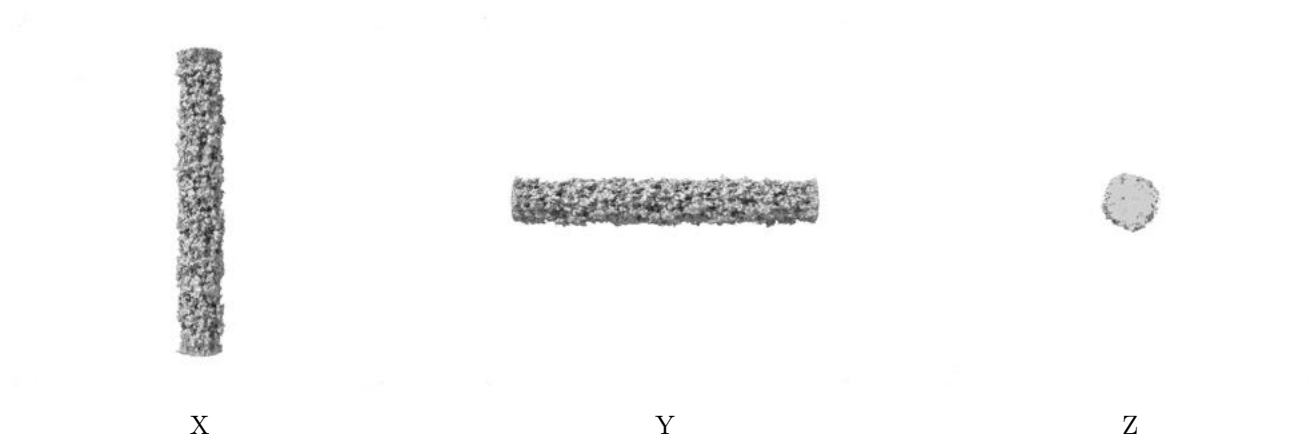
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.202. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

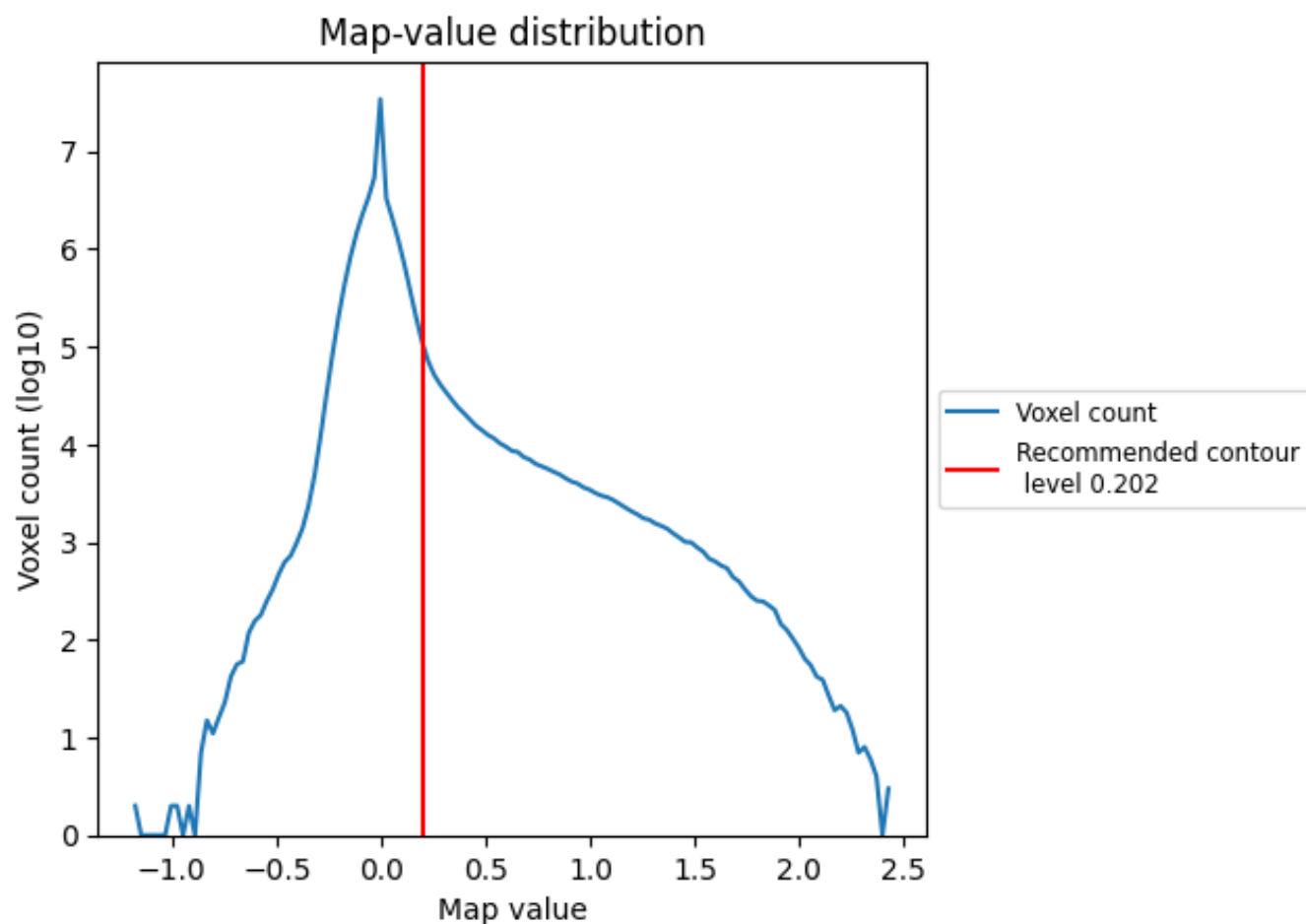
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

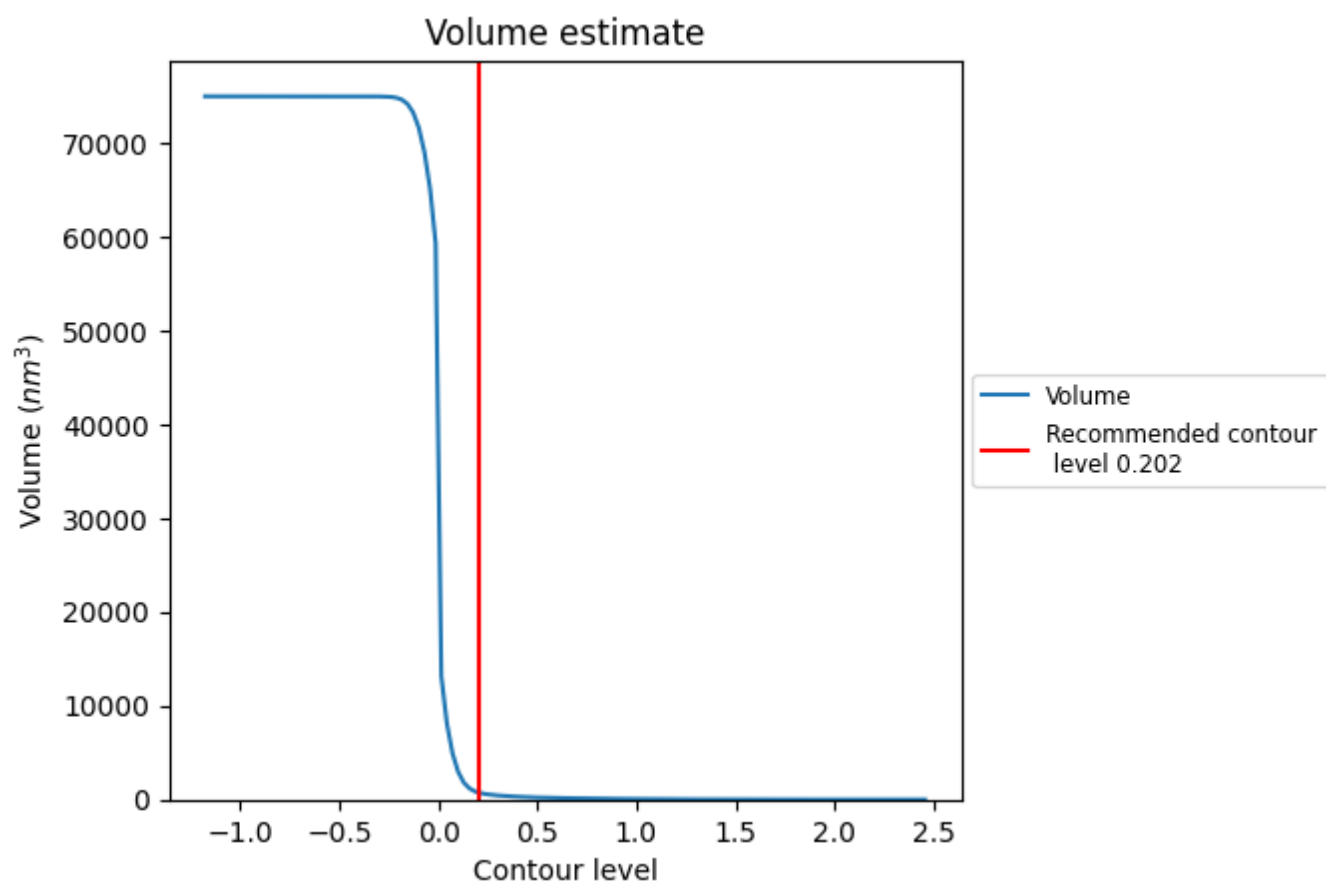
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

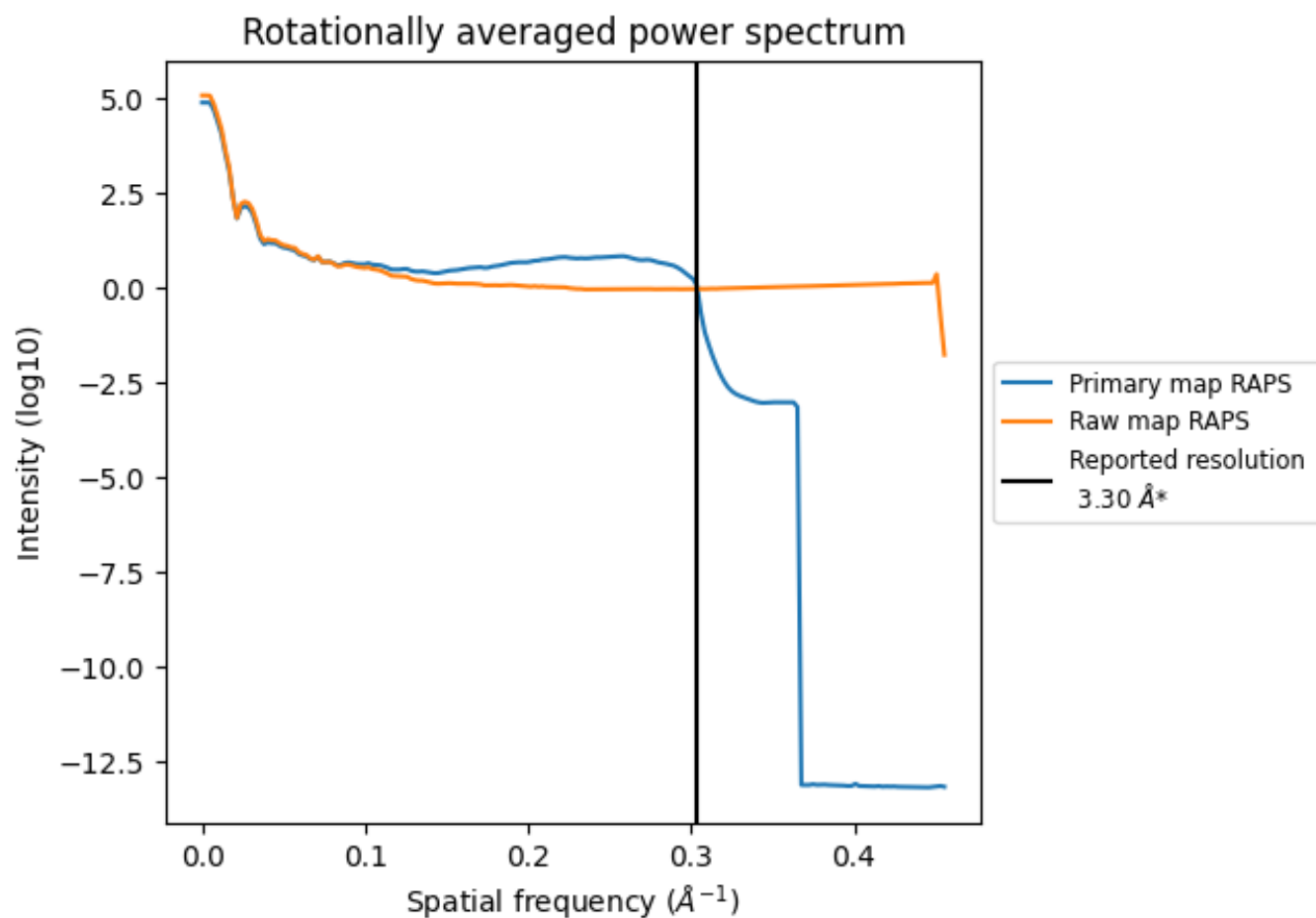


The volume at the recommended contour level is 763 nm<sup>3</sup>; this corresponds to an approximate mass of 689 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum ⓘ

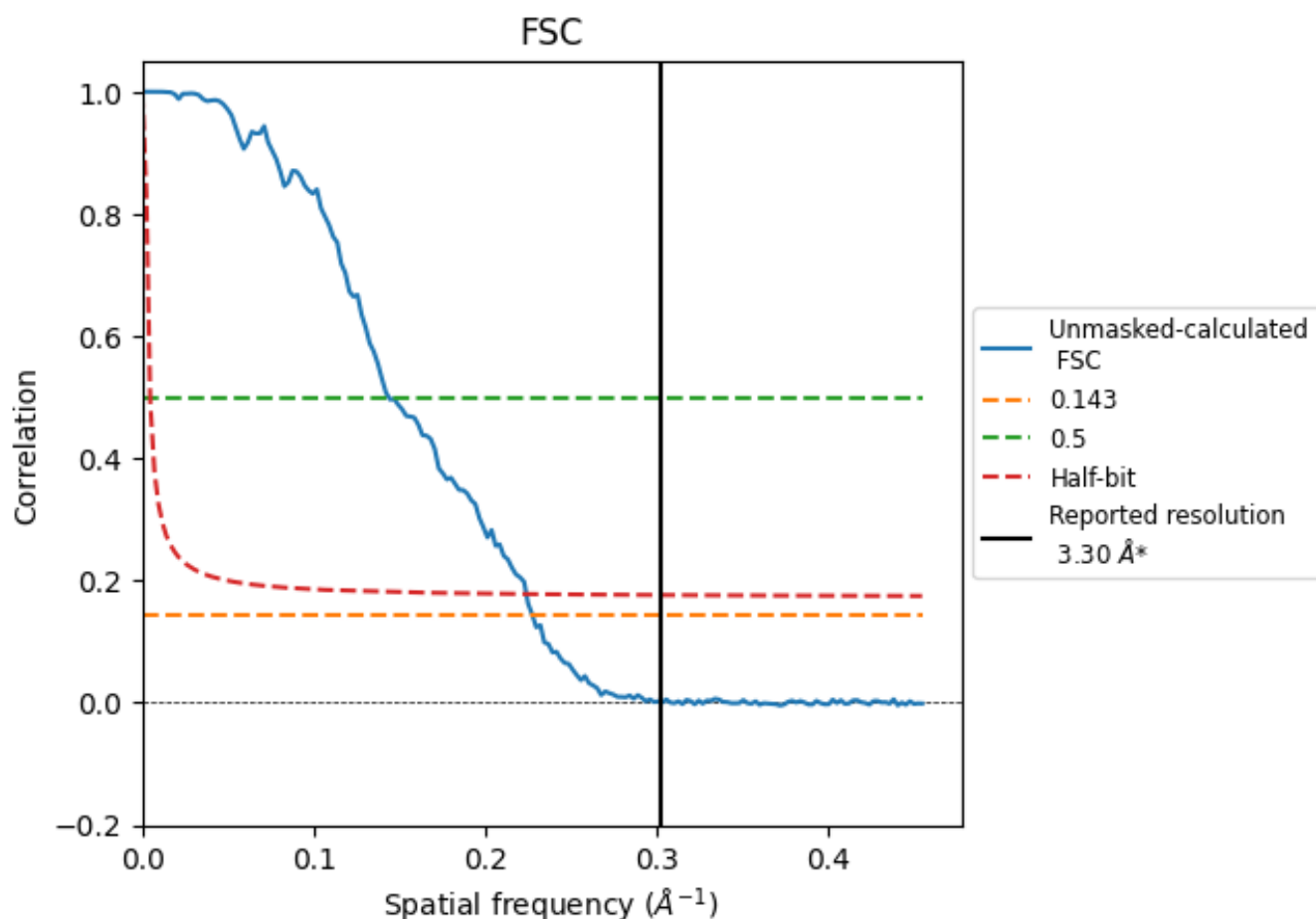


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

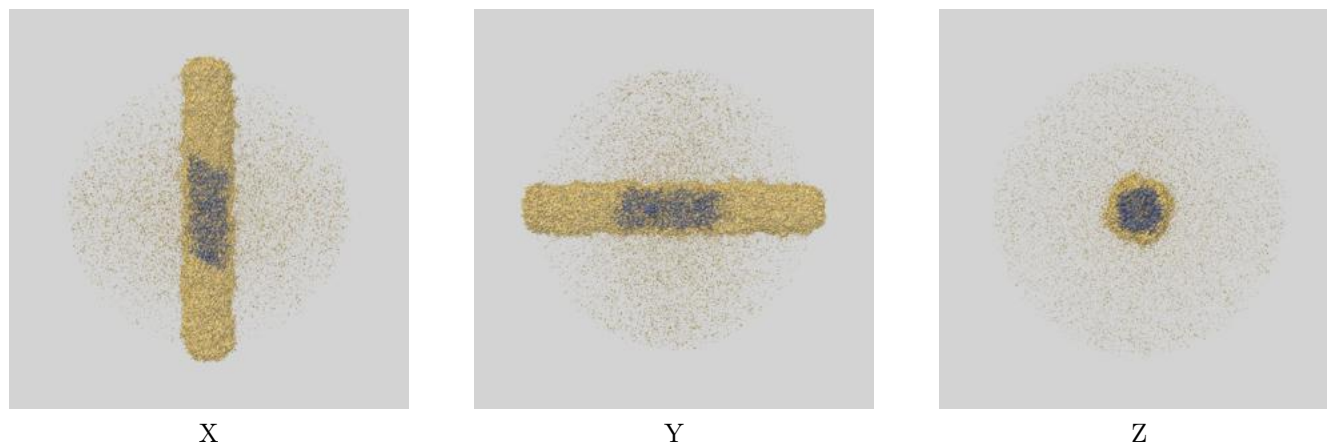
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.39	6.95	4.46

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.39 differs from the reported value 3.3 by more than 10 %

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

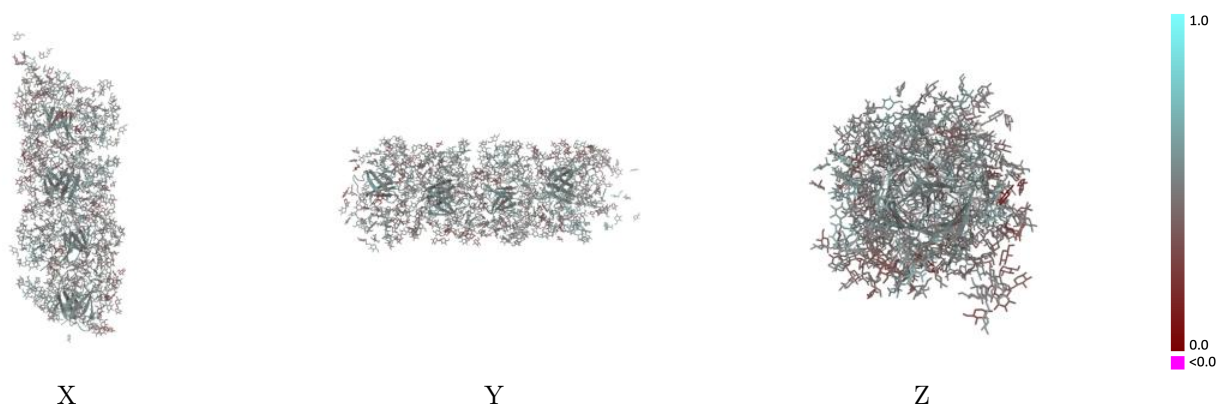
This section contains information regarding the fit between EMDB map EMD-67848 and PDB model 21NR. Per-residue inclusion information can be found in section [3](#) on page [12](#).

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



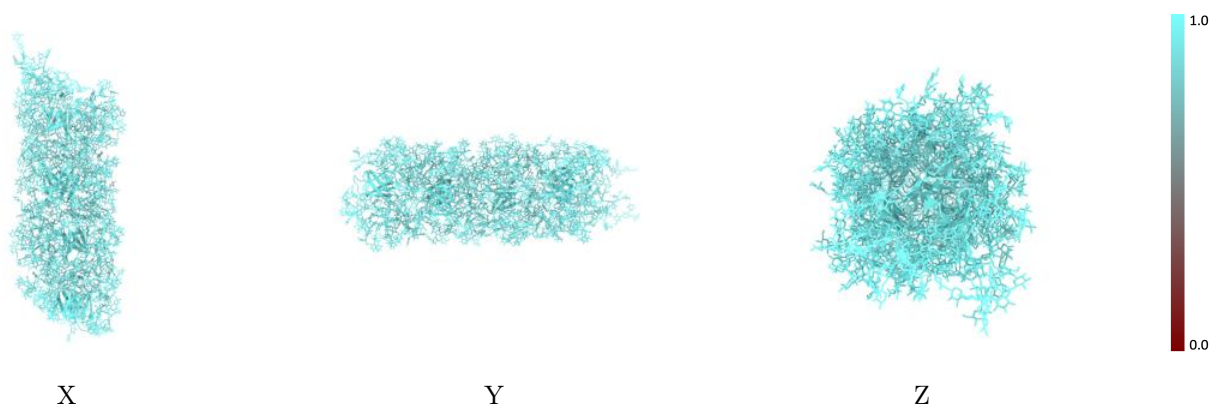
The images above show the 3D surface view of the map at the recommended contour level 0.202 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



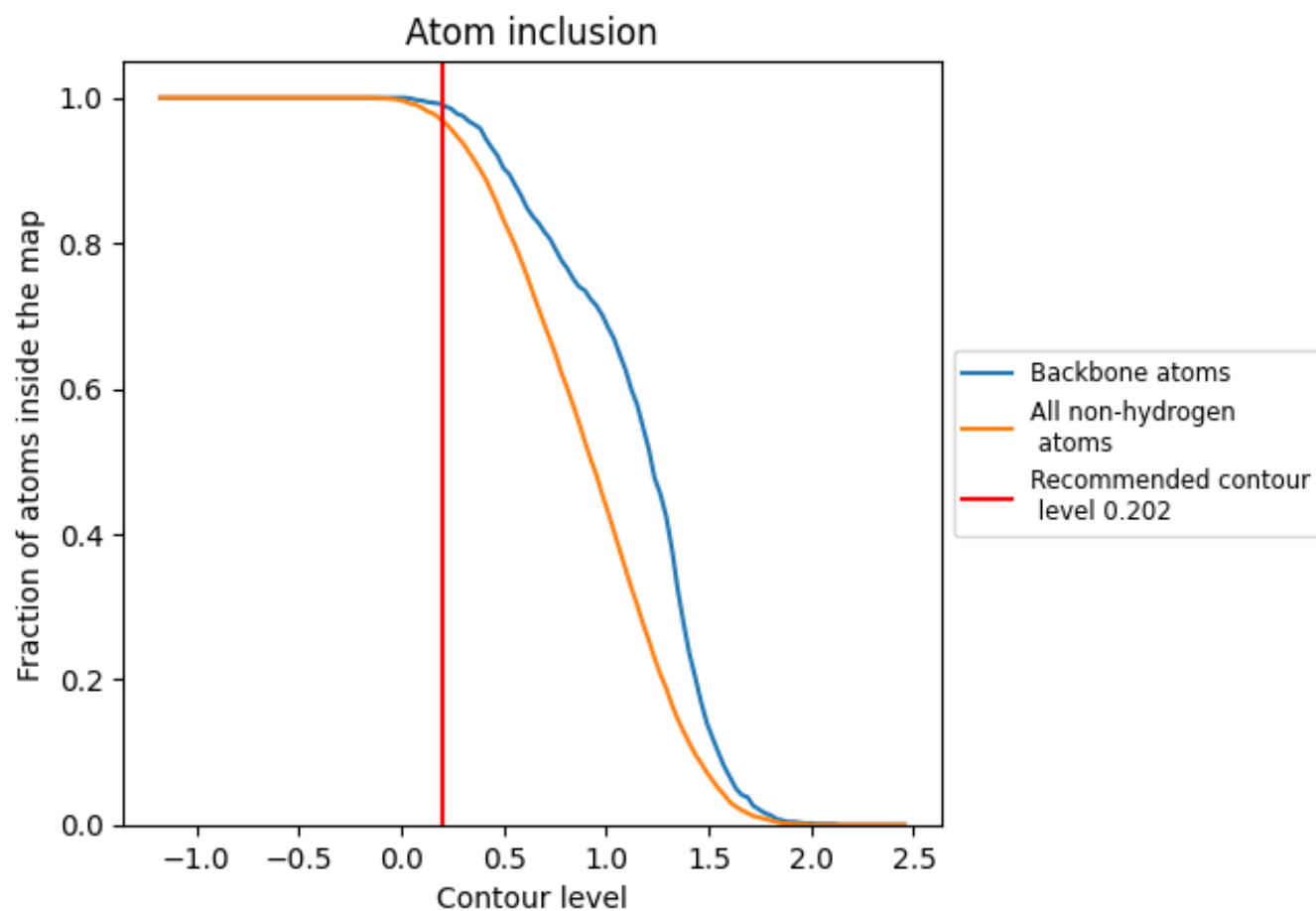
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.202).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ







































The table lists the average atom inclusion at the recommended contour level (0.202) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9680	 0.4760
0	 0.9590	 0.4280
A	 0.9840	 0.5300
B	 0.9520	 0.4810
C	 0.9530	 0.4450
D	 0.9560	 0.4360
E	 0.9600	 0.5040
F	 0.9780	 0.5000
G	 0.9540	 0.4260
H	 0.9480	 0.4370
I	 0.9540	 0.4530
J	 0.9860	 0.5050
K	 0.9790	 0.4850
L	 0.9530	 0.5200
M	 0.9950	 0.4920
N	 0.9500	 0.4400
O	 0.9430	 0.4730
P	 0.9530	 0.4480
Q	 0.9600	 0.4300
R	 0.9600	 0.4910
S	 0.9780	 0.4920
T	 0.9580	 0.4260
U	 0.9480	 0.4430
V	 0.9540	 0.4580
W	 0.9770	 0.4960
X	 0.9810	 0.4840
Y	 0.9440	 0.5110
Z	 0.9950	 0.4930
a	 0.9540	 0.4370
b	 0.9620	 0.4750
c	 0.9640	 0.4500
d	 0.9600	 0.4320
e	 0.9600	 0.4960
f	 0.9780	 0.4760
g	 0.9490	 0.4240



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Chain	Atom inclusion	Q-score
h	 0.9390	 0.4490
i	 0.9630	 0.4590
j	 0.9720	 0.5110
k	 0.9770	 0.4870
l	 0.9720	 0.5200
m	 0.9840	 0.4980
n	 0.9590	 0.4340
o	 0.9710	 0.4780
p	 0.9640	 0.4450
q	 0.9600	 0.4290
r	 1.0000	 0.5080
s	 0.9780	 0.4650
t	 0.9580	 0.4230
u	 0.9480	 0.4450
v	 0.9730	 0.4510
w	 0.9720	 0.5130
x	 0.9710	 0.4890
y	 0.9630	 0.5250
z	 0.9890	 0.4940