



Full wwPDB EM Validation Report ⓘ

Jul 14, 2026 – 11:35 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
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) : 2.50

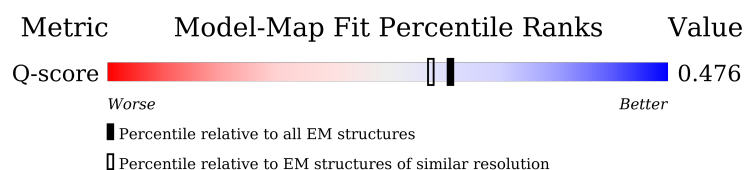
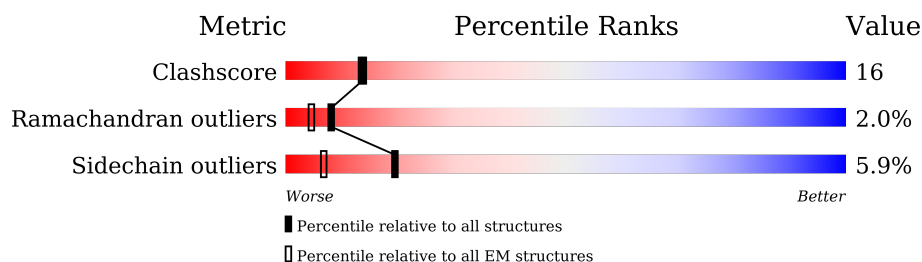
1 Overall quality at a glance

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.



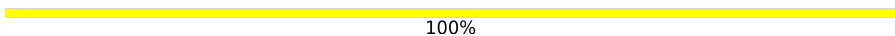
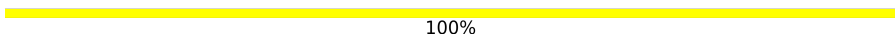
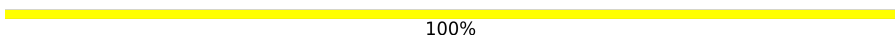
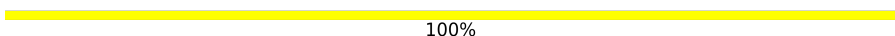
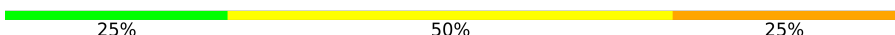
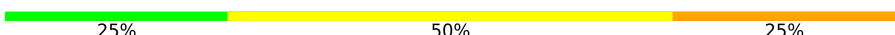
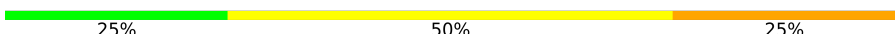
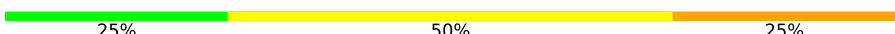
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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 ≥ 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	59% 36% 5%
2	B	9	56% 11% 33%
2	O	9	44% 22% 33%
2	b	9	44% 22% 33%

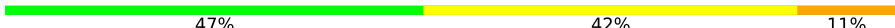
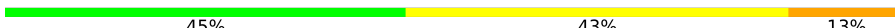
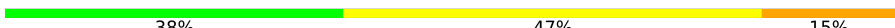
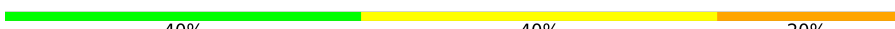
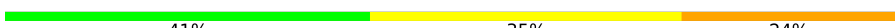
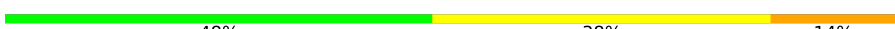
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Mol	Chain	Length	Quality of chain
2	o	9	
3	C	34	
3	P	34	
3	c	34	
3	p	34	
4	D	26	
4	Q	26	
4	d	26	
4	q	26	
5	E	2	
5	R	2	
5	e	2	
5	r	2	
6	F	4	
6	S	4	
6	f	4	
6	s	4	
7	G	22	
7	T	22	
7	g	22	
7	t	22	
8	H	20	
8	U	20	
8	h	20	
8	u	20	

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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		

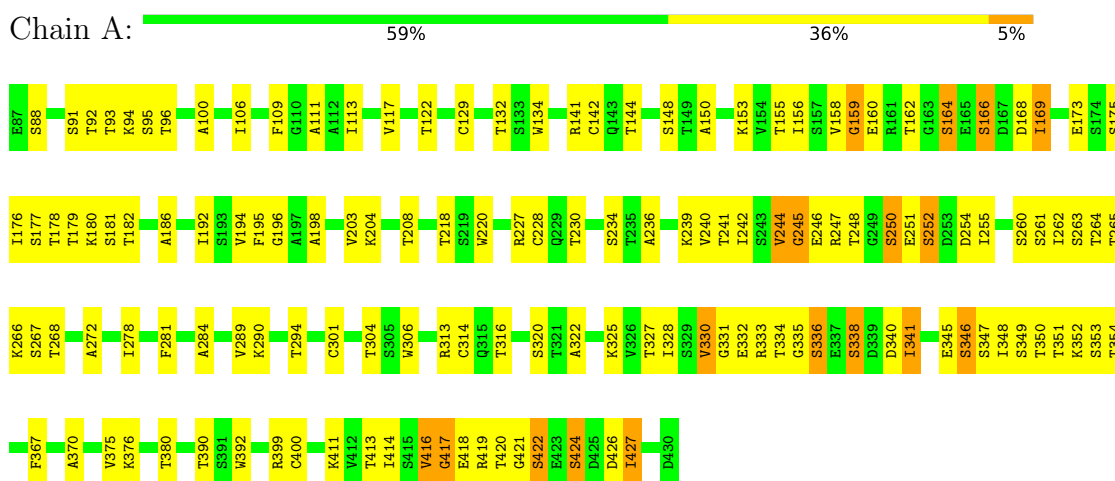
- Molecule 14 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)-alpha-L-arabinofuranose-(1-2)-[beta-D-xylopyranose-(1-3)-[alpha-L-arabinofuranose-(1-4)]beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-2)]beta-D-xylopyranose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

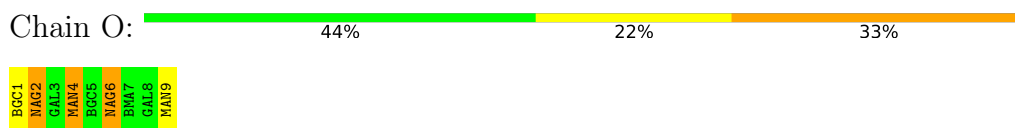
• Molecule 1: TLP-IPT



• 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

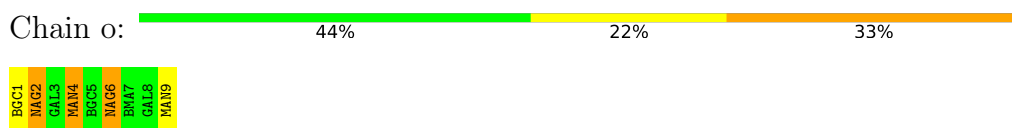


• Molecule 2: beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha

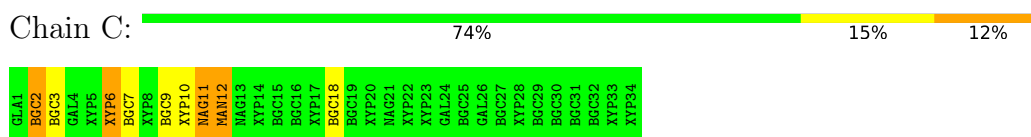
a-D-mannopyranose-(1-2)-[beta-D-galactopyranose-(1-2)-beta-D-mannopyranose-(1-3)]beta-D-galactopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- 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% 4%



• 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%

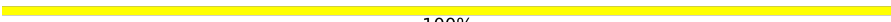


• Molecule 4: beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-4)]beta-D-mannopyranose-(1-2)-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-4)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-L-arabinofuranose-(1-5)-[beta-D-xylopyranose-(1-3)]alpha-L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

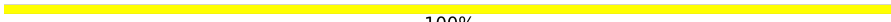


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose

Chain E:  100%

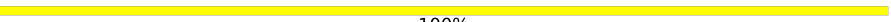
MAN1
NAG2

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

Chain R:  100%

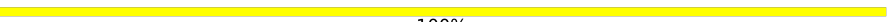
MAN1
NAG2

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

Chain e:  100%

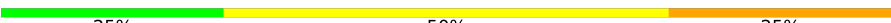
MAN1
NAG2

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

Chain r:  100%

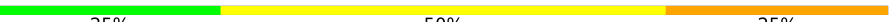
MAN1
NAG2

- 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%

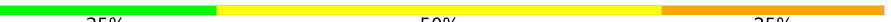
MAN1
GZL2
FUB3
NAG4

- 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%

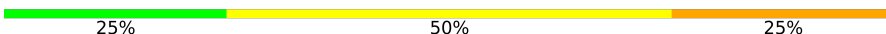
MAN1
GZL2
FUB3
NAG4

- 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: 



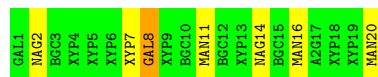
● Molecule 7: alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-4)-beta-D-xylopyranose-(1-4)-[alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-3)]beta-D-glucopyranose-(1-4)]beta-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-alpha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



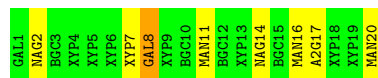
● Molecule 8: beta-D-glucopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]beta-D-xylopyranose-(1-3)-[beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-(1-4)]beta-D-galactopyranose-(1-2)-beta-D-xylopyranose-(1-3)-beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]b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



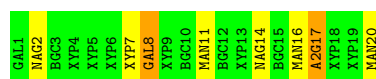
● Molecule 8: beta-D-glucopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]beta-D-xylopyranose-(1-3)-[beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-(1-4)]beta-D-galactopyranose-(1-2)-beta-D-xylopyranose-(1-3)-beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]b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



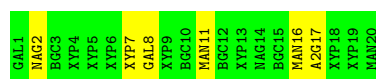
● Molecule 8: beta-D-glucopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]beta-D-xylopyranose-(1-3)-[beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-(1-4)]beta-D-galactopyranose-(1-2)-beta-D-xylopyranose-(1-3)-beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]b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



- 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: 



- 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

Chain I: 



- 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

Chain V: 



- 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

Chain i: 



- 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%



- 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%



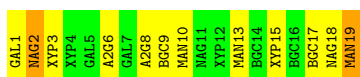
- Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-glucopyranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-[beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-4)]beta-D-galactopyranose-(1-3)-[beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)-[beta-D-xylopyranose-(1-2)]beta-D-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



- 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%



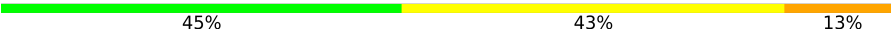
- Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-glucopyranose-(1-4)-[2-acetamido-2-deoxy-b

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:  47% 42% 11%



● 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:  45% 43% 13%



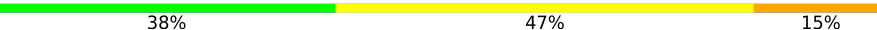
● Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-mannopyranose-(1-6)-beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-D-galactopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-[alph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

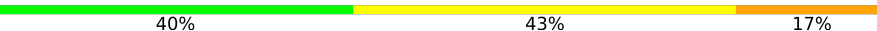
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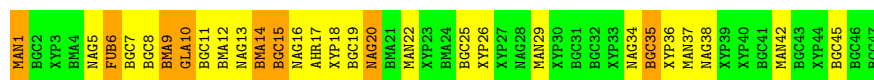
● Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-mannopyranose-(1-6)-beta-D-glucopyranose-(1-2)-[beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)-alpha-L-arabinofuranose-(1-3)]alpha-D-galactopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-[alpha-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	NAN22	XYF23	BMA24	BGC25	XYF26	XYF27	NAG28	NAN29	XYF30	BGC31	BGC32	XYF33	NAG34	BGC35	XYF36	NAN37	NAG38	XYF39	XYF40	BGC41	NAN42	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



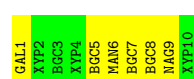
- Molecule 12: beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]beta-D-glucopyranose-(1-3)-[beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-3)-beta-D-galactopyranose



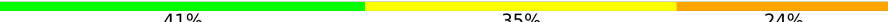
- Molecule 12: beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-xylopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]beta-D-glucopyranose-(1-3)-[beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-3)-beta-D-galactopyranose



- 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

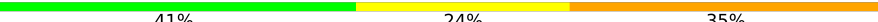


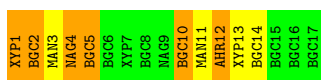
- Molecule 13: beta-D-glucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-xylopyranose-(1-4)-[beta-D-glucopyranose-(1-2)]alpha-D-mannopyranose-(1-3)]beta-D-glucopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)]2-acetamido-2-deoxy-beta-D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



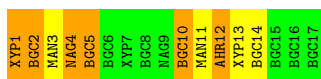
• Molecule 13: beta-D-glucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta a-D-xylopyranose-(1-4)-[beta-D-glucopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-glucopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)]2-acetamido-2-deoxy-bet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

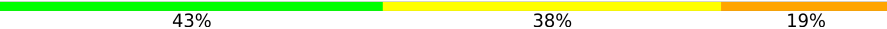


• Molecule 13: beta-D-glucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta a-D-xylopyranose-(1-4)-[beta-D-glucopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-glucopyranose-(1-4)-[alpha-L-arabinofuranose-(1-2)]beta-D-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)]2-acetamido-2-deoxy-bet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



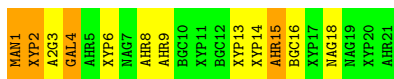
• Molecule 14: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)-alpha-L-arabinofuranose-(1-2)-[beta-D-xylopyranose-(1-3)-[alpha-L-arabinofuranose-(1-4)]beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-2)]beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-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



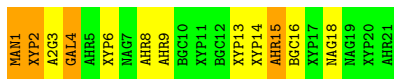
• Molecule 14: alpha-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-3)-alpha-L-arabinofuranose-(1-2)-[beta-D-xylopyranose-(1-3)-[alpha-L-arabinofuranose-(1-4)]beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-4)-[beta-D-glucopyranose-(1-2)]beta-D-xylopyranose-(1-2)-beta-D-glucopyranose-(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, BGC, MAN, A2G, BMA, XYP, NAG, GAL, GZL, GLA, AHR

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.

All (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
4:Q:25:BGC:H6C1	9:i:5:BGC:O3	1.67	0.95
4:d:25:BGC:H6C1	9:v:5:BGC:O3	1.69	0.93
1:A:164:SER:HB3	12:L:1:GAL:O2	1.72	0.91
1:A:93:THR:HG23	1:A:168:ASP:OD2	1.72	0.90
1:A:250:SER:HB3	12:Y:1:GAL:O2	1.72	0.90
1:A:336:SER:HB3	12:l:1:GAL:O2	1.72	0.90
1:A:351:THR:HG23	1:A:426:ASP:OD2	1.72	0.89
1:A:422:SER:HB3	12:y:1:GAL:O2	1.72	0.88
1:A:265:THR:HG23	1:A:340:ASP:OD2	1.72	0.88
3:c:18:BGC:O6	14:n:18:NAG:H83	1.78	0.84
3:P:18:BGC:O6	14:a:18:NAG:H83	1.78	0.83
3:C:18:BGC:O6	14:N:18:NAG:H83	1.78	0.82
3:p:18:BGC:O6	14:0:18:NAG:H83	1.78	0.82
1:A:192:ILE:HD11	1:A:255:ILE:HG21	1.62	0.82
8:H:8:GAL:O6	7:T:16:NAG:H83	1.83	0.79
1:A:150:ALA:HB2	1:A:247:ARG:HD2	1.63	0.79
8:U:20:MAN:H62	11:k:45:BGC:O3	1.83	0.78
1:A:100:ALA:HB2	1:A:198:ALA:HA	1.67	0.76
13:M:5:BGC:C1	13:M:12:HRH:C4	2.63	0.76
1:A:322:ALA:HB2	1:A:419:ARG:HD2	1.67	0.76
1:A:186:ALA:HB2	1:A:284:ALA:HA	1.68	0.76
1:A:236:ALA:HB2	1:A:333:ARG:HD2	1.66	0.76
11:K:1:MAN:C6	11:K:6:FUB:C5	2.65	0.75
1:A:265:THR:OG1	1:A:268:THR:HG22	1.87	0.74
11:k:1:MAN:C6	11:k:6:FUB:C5	2.65	0.74
11:x:1:MAN:C6	11:x:6:FUB:C5	2.65	0.74
1:A:320:SER:OG	1:A:376:LYS:HE2	1.87	0.74
11:X:1:MAN:C6	11:X:6:FUB:C5	2.65	0.74
8:h:8:GAL:O6	7:t:16:NAG:H83	1.87	0.74
1:A:351:THR:CG2	1:A:426:ASP:OD2	2.36	0.74
1:A:265:THR:CG2	1:A:340:ASP:OD2	2.36	0.73
8:U:8:GAL:O6	7:g:16:NAG:C7	2.37	0.73
3:C:12:MAN:H61	14:N:14:XYP:O3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:THR:CG2	1:A:168:ASP:OD2	2.36	0.73
1:A:351:THR:OG1	1:A:354:THR:HG22	1.88	0.73
1:A:179:THR:OG1	1:A:182:THR:HG22	1.87	0.72
7:G:8:MAN:O6	8:H:2:NAG:H82	1.90	0.72
7:t:8:MAN:O6	8:u:2:NAG:H82	1.90	0.72
1:A:93:THR:OG1	1:A:96:THR:HG22	1.88	0.72
4:Q:13:FUB:C2	6:S:3:FUB:O3	2.38	0.72
13:Z:5:BGC:H3	13:Z:12:AHR:C2	2.20	0.72
7:g:8:MAN:O6	8:h:2:NAG:H82	1.90	0.72
1:A:148:SER:OG	1:A:204:LYS:HE2	1.90	0.71
1:A:260:SER:OG	1:A:328:ILE:CG2	2.38	0.71
3:P:12:MAN:H61	14:a:14:XYP:O3	1.90	0.71
4:d:13:FUB:C2	6:f:3:FUB:O3	2.38	0.71
4:D:13:FUB:C2	6:F:3:FUB:O3	2.38	0.70
7:T:8:MAN:O6	8:U:2:NAG:H82	1.90	0.70
8:U:8:GAL:O6	7:g:16:NAG:N2	2.24	0.70
4:q:13:FUB:C2	6:s:3:FUB:O3	2.38	0.70
8:U:8:GAL:O6	7:g:16:NAG:H83	1.92	0.70
1:A:272:ALA:HB2	1:A:370:ALA:HA	1.74	0.70
10:J:18:NAG:H3	12:Y:8:BGC:O3	1.92	0.69
1:A:186:ALA:CB	1:A:284:ALA:HA	2.22	0.69
1:A:100:ALA:CB	1:A:198:ALA:HA	2.22	0.69
1:A:153:LYS:HD3	1:A:166:SER:HB2	1.76	0.68
13:M:5:BGC:C1	13:M:12:AHR:O4	2.41	0.68
1:A:239:LYS:HD3	1:A:252:SER:HB2	1.76	0.67
1:A:325:LYS:HD3	1:A:338:SER:HB2	1.76	0.67
1:A:411:LYS:HD3	1:A:424:SER:HB2	1.76	0.67
1:A:234:SER:OG	1:A:290:LYS:HE2	1.95	0.67
3:c:12:MAN:H61	14:n:14:XYP:O3	1.95	0.67
8:H:8:GAL:O6	7:T:16:NAG:C7	2.43	0.66
1:A:88:SER:HB2	1:A:113:ILE:HG12	1.78	0.66
3:p:12:MAN:H61	14:0:14:XYP:O3	1.95	0.66
1:A:272:ALA:CB	1:A:370:ALA:HA	2.25	0.65
8:h:8:GAL:O6	7:t:16:NAG:C7	2.45	0.65
1:A:88:SER:CB	1:A:113:ILE:HG12	2.28	0.64
13:Z:5:BGC:C1	13:Z:12:AHR:C4	2.75	0.63
7:G:2:BGC:H6C2	7:G:3:A2G:C5	2.29	0.63
13:m:5:BGC:H3	13:m:12:AHR:C2	2.28	0.63
7:T:2:BGC:H6C2	7:T:3:A2G:C5	2.29	0.62
7:t:2:BGC:H6C2	7:t:3:A2G:C5	2.29	0.62
8:H:8:GAL:O6	7:T:16:NAG:C8	2.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:2:BGC:O3	3:c:3:BGC:C1	2.48	0.62
1:A:261:SER:O	1:A:262:ILE:HG12	2.00	0.61
7:g:2:BGC:H6C2	7:g:3:A2G:C5	2.29	0.61
3:p:2:BGC:O3	3:p:3:BGC:C1	2.48	0.61
3:p:18:BGC:O6	14:0:18:NAG:C8	2.49	0.61
3:C:2:BGC:O3	3:C:3:BGC:C1	2.48	0.61
3:c:18:BGC:O6	14:n:18:NAG:C8	2.49	0.60
3:P:2:BGC:O3	3:P:3:BGC:C1	2.48	0.60
3:P:18:BGC:O6	14:a:18:NAG:C8	2.49	0.60
10:J:17:BGC:O3	11:X:16:NAG:H2	2.00	0.60
10:W:18:NAG:H3	12:l:8:BGC:O3	2.01	0.60
14:a:13:XYP:C5	10:j:10:MAN:O2	2.50	0.60
1:A:177:SER:HB3	1:A:178:THR:HG23	1.84	0.59
1:A:91:SER:HB3	1:A:92:THR:HG23	1.84	0.59
2:o:1:BGC:O6	13:z:13:XYP:C5	2.51	0.59
10:w:19:MAN:H61	14:0:16:BGC:O4	2.03	0.59
8:h:8:GAL:O6	7:t:16:NAG:N2	2.36	0.59
2:B:1:BGC:O6	13:M:13:XYP:C5	2.51	0.59
8:H:8:GAL:O6	7:T:16:NAG:N2	2.36	0.58
2:O:1:BGC:O6	13:Z:13:XYP:C5	2.51	0.58
10:W:17:BGC:O3	11:k:16:NAG:H2	2.03	0.58
1:A:263:SER:HB3	1:A:264:THR:HG23	1.84	0.58
2:b:1:BGC:O6	13:m:13:XYP:C5	2.51	0.58
1:A:349:SER:HB3	1:A:350:THR:HG23	1.84	0.58
8:h:8:GAL:O6	7:t:16:NAG:C8	2.52	0.57
8:H:20:MAN:H62	11:X:45:BGC:O3	2.04	0.57
10:j:19:MAN:H61	14:n:16:BGC:O4	2.04	0.57
13:m:4:NAG:C1	13:m:4:NAG:O7	2.53	0.57
8:U:8:GAL:O6	7:g:16:NAG:C8	2.51	0.57
13:z:4:NAG:C1	13:z:4:NAG:O7	2.53	0.57
3:C:18:BGC:O6	14:N:18:NAG:C8	2.49	0.57
1:A:182:THR:HA	1:A:255:ILE:HG22	1.86	0.57
8:H:14:NAG:H61	7:T:21:XYP:O4	2.05	0.56
10:J:19:MAN:C2	11:X:47:BGC:HB	2.18	0.56
13:Z:4:NAG:C1	13:Z:4:NAG:O7	2.53	0.56
1:A:180:LYS:HG3	1:A:195:PHE:HE2	1.71	0.56
1:A:347:SER:O	1:A:348:ILE:HG12	2.06	0.56
1:A:352:LYS:HG3	1:A:367:PHE:HE2	1.70	0.56
13:M:4:NAG:C1	13:M:4:NAG:O7	2.53	0.56
4:Q:25:BGC:H6C1	9:i:5:BGC:HC	1.69	0.56
10:W:19:MAN:H2	11:k:47:BGC:O2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LYS:HG3	1:A:281:PHE:HE2	1.71	0.55
13:Z:5:BGC:C3	13:Z:12:HR:A:C2	2.84	0.55
1:A:336:SER:CB	12:l:1:GAL:O2	2.52	0.55
3:P:10:XYP:O3	14:a:6:XYP:C5	2.55	0.55
1:A:94:LYS:HG3	1:A:109:PHE:HE2	1.70	0.55
1:A:164:SER:CB	12:L:1:GAL:O2	2.52	0.55
10:W:19:MAN:C2	11:k:47:BGC:O2	2.55	0.55
3:c:10:XYP:O3	14:n:6:XYP:C5	2.54	0.55
3:p:10:XYP:O3	14:0:6:XYP:C5	2.54	0.55
1:A:176:ILE:HG22	1:A:251:GLU:OE1	2.07	0.55
3:C:10:XYP:O3	14:N:6:XYP:C5	2.54	0.55
1:A:250:SER:CB	12:Y:1:GAL:O2	2.52	0.54
10:J:19:MAN:C2	11:X:47:BGC:O2	2.55	0.54
13:M:5:BGC:H3	13:M:12:HR:A:C2	2.37	0.54
14:N:1:MAN:H61	14:N:2:XYP:O5	2.07	0.54
14:n:1:MAN:H61	14:n:2:XYP:O5	2.07	0.54
1:A:208:THR:HB	1:A:242:ILE:HD12	1.89	0.54
1:A:122:THR:HB	1:A:156:ILE:HD12	1.89	0.54
1:A:380:THR:HB	1:A:414:ILE:HD12	1.89	0.53
10:J:19:MAN:O2	11:X:47:BGC:O2	2.26	0.53
8:U:20:MAN:C6	11:k:45:BGC:O3	2.54	0.53
14:0:1:MAN:H61	14:0:2:XYP:O5	2.07	0.53
1:A:176:ILE:HD13	1:A:240:VAL:HG12	1.91	0.53
1:A:177:SER:HA	13:Z:4:NAG:O7	2.09	0.53
1:A:294:THR:HB	1:A:328:ILE:HD12	1.89	0.53
11:X:20:NAG:H83	11:X:26:XYP:O2	2.09	0.53
8:h:14:NAG:H61	7:t:21:XYP:O4	2.09	0.53
1:A:349:SER:HA	13:z:4:NAG:O7	2.09	0.53
11:K:20:NAG:H83	11:K:26:XYP:O2	2.09	0.52
11:x:20:NAG:H83	11:x:26:XYP:O2	2.09	0.52
11:k:20:NAG:H83	11:k:26:XYP:O2	2.09	0.52
1:A:263:SER:HA	13:m:4:NAG:O7	2.09	0.52
10:w:2:NAG:H4	10:w:19:MAN:H3	1.91	0.52
2:O:4:MAN:H62	2:O:6:NAG:C7	2.40	0.52
2:b:4:MAN:H62	2:b:6:NAG:C7	2.40	0.52
1:A:91:SER:HA	13:M:4:NAG:O7	2.09	0.52
1:A:422:SER:CB	12:y:1:GAL:O2	2.52	0.52
14:N:4:GAL:H61	14:N:16:BGC:H4	1.92	0.52
1:A:234:SER:HB2	1:A:330:VAL:HG22	1.91	0.51
10:J:2:NAG:H4	10:J:19:MAN:H3	1.91	0.51
2:B:4:MAN:H62	2:B:6:NAG:C7	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:20:MAN:H62	11:x:45:BGC:O3	2.11	0.51
14:n:4:GAL:H61	14:n:16:BGC:H4	1.92	0.51
1:A:266:LYS:HG3	1:A:281:PHE:CE2	2.45	0.51
1:A:180:LYS:HG3	1:A:195:PHE:CE2	2.45	0.51
7:G:2:BGC:C6	7:G:3:A2G:C5	2.89	0.51
1:A:352:LYS:HG3	1:A:367:PHE:CE2	2.45	0.51
4:d:25:BGC:H6C1	9:v:5:BGC:HC	1.72	0.51
1:A:169:ILE:O	1:A:169:ILE:HG13	2.10	0.51
7:T:2:BGC:C6	7:T:3:A2G:C5	2.89	0.51
14:0:4:GAL:H61	14:0:16:BGC:H4	1.92	0.51
1:A:192:ILE:CD1	1:A:255:ILE:HG21	2.37	0.51
1:A:427:ILE:HG13	1:A:427:ILE:O	2.10	0.51
13:Z:5:BGC:C1	13:Z:12:AHR:O4	2.58	0.51
14:a:4:GAL:H61	14:a:16:BGC:H4	1.92	0.51
1:A:88:SER:HA	1:A:111:ALA:O	2.11	0.51
1:A:94:LYS:HG3	1:A:109:PHE:CE2	2.45	0.51
10:j:2:NAG:H4	10:j:19:MAN:H3	1.91	0.51
2:o:4:MAN:H62	2:o:6:NAG:C7	2.40	0.51
1:A:341:ILE:HG13	1:A:341:ILE:O	2.11	0.50
1:A:422:SER:HB3	12:y:1:GAL:HO2	1.74	0.50
2:o:1:BGC:H6C2	2:o:2:NAG:C7	2.42	0.50
7:g:2:BGC:C6	7:g:3:A2G:C5	2.89	0.50
2:O:1:BGC:H6C2	2:O:2:NAG:C7	2.42	0.50
7:t:2:BGC:C6	7:t:3:A2G:C5	2.89	0.50
1:A:234:SER:HB2	1:A:330:VAL:CG2	2.42	0.50
14:N:15:AHR:O5	8:U:17:A2G:H8A	2.11	0.50
2:B:1:BGC:H6C2	2:B:2:NAG:C7	2.42	0.50
1:A:148:SER:HB2	1:A:244:VAL:CG2	2.41	0.49
1:A:148:SER:HB2	1:A:244:VAL:HG22	1.93	0.49
1:A:345:GLU:HG2	1:A:419:ARG:HB3	1.93	0.49
1:A:417:GLY:C	1:A:418:GLU:HG3	2.37	0.49
2:b:1:BGC:H6C2	2:b:2:NAG:C7	2.42	0.49
14:n:15:AHR:O5	8:u:17:A2G:H8A	2.12	0.49
1:A:417:GLY:O	1:A:418:GLU:HG3	2.13	0.49
4:D:23:BGC:O2	9:V:6:MAN:H61	2.12	0.49
1:A:175:SER:O	1:A:196:GLY:HA3	2.11	0.49
8:U:8:GAL:C6	7:g:16:NAG:H83	2.43	0.49
4:D:25:BGC:H6C1	9:V:5:BGC:HC	1.73	0.48
10:J:19:MAN:H2	11:X:47:BGC:O2	2.13	0.48
10:W:19:MAN:O2	11:k:47:BGC:O2	2.31	0.48
13:m:5:BGC:C1	13:m:12:AHR:C4	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:SER:HB2	1:A:416:VAL:CG2	2.44	0.48
8:H:14:NAG:C6	7:T:21:XYP:O4	2.62	0.48
13:M:5:BGC:H2	13:M:13:XYP:O5	2.14	0.48
4:d:13:FUB:O2	6:f:3:FUB:O3	2.32	0.48
1:A:320:SER:HB2	1:A:416:VAL:HG22	1.94	0.48
10:W:19:MAN:HO2	11:k:47:BGC:C2	2.27	0.48
4:Q:13:FUB:O2	6:S:3:FUB:O3	2.32	0.48
13:z:5:BGC:H2	13:z:13:XYP:O5	2.14	0.48
13:Z:5:BGC:H2	13:Z:13:XYP:O5	2.14	0.48
13:m:5:BGC:H2	13:m:13:XYP:O5	2.14	0.48
4:D:13:FUB:O2	6:F:3:FUB:O3	2.32	0.47
13:m:5:BGC:C3	13:m:12:AHR:C2	2.93	0.47
4:q:13:FUB:O2	6:s:3:FUB:O3	2.32	0.47
1:A:260:SER:OG	1:A:328:ILE:HG23	2.15	0.47
1:A:129:CYS:HB3	1:A:142:CYS:HB2	1.73	0.47
1:A:245:GLY:C	1:A:246:GLU:HG3	2.39	0.47
1:A:346:SER:O	1:A:421:GLY:HA3	2.14	0.47
8:H:8:GAL:C6	7:T:16:NAG:H83	2.43	0.47
10:J:19:MAN:HO2	11:X:47:BGC:C2	2.28	0.47
1:A:352:LYS:HE2	1:A:367:PHE:CE2	2.50	0.47
1:A:266:LYS:HE2	1:A:281:PHE:CE2	2.50	0.47
14:N:13:XYP:C5	10:W:10:MAN:O2	2.63	0.47
3:P:9:BGC:H6C2	3:P:10:XYP:O5	2.15	0.47
1:A:94:LYS:HE2	1:A:109:PHE:CE2	2.50	0.47
1:A:180:LYS:HE2	1:A:195:PHE:CE2	2.50	0.47
3:C:9:BGC:H6C2	3:C:10:XYP:O5	2.15	0.46
13:z:5:BGC:C1	13:z:12:AHR:C4	2.93	0.46
14:N:14:XYP:O4	11:k:41:BGC:O3	2.25	0.46
11:k:9:BMA:H3	11:k:10:GLA:H5	1.97	0.46
3:p:9:BGC:H6C2	3:p:10:XYP:O5	2.15	0.46
11:x:9:BMA:H3	11:x:10:GLA:H5	1.97	0.46
1:A:88:SER:HB3	1:A:113:ILE:HG12	1.98	0.46
3:c:9:BGC:H6C2	3:c:10:XYP:O5	2.15	0.45
11:K:9:BMA:H3	11:K:10:GLA:H5	1.97	0.45
11:X:5:NAG:H82	11:X:34:NAG:H83	1.99	0.45
1:A:182:THR:HG22	1:A:255:ILE:HG22	1.97	0.45
11:X:9:BMA:H3	11:X:10:GLA:H5	1.97	0.45
1:A:390:THR:HA	1:A:400:CYS:HA	1.99	0.45
1:A:390:THR:HG23	1:A:400:CYS:HB3	1.99	0.45
10:J:17:BGC:O3	11:X:16:NAG:C1	2.65	0.45
11:k:5:NAG:H82	11:k:34:NAG:H83	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:p:9:BGC:H6C2	3:p:10:XYP:C1	2.47	0.45
3:c:9:BGC:H6C2	3:c:10:XYP:C1	2.47	0.45
3:C:6:XYP:O3	3:C:11:NAG:H4	2.17	0.45
13:m:4:NAG:H62	13:m:12:AHR:O4	2.16	0.45
13:z:5:BGC:C1	13:z:12:AHR:O4	2.65	0.45
11:K:5:NAG:H82	11:K:34:NAG:H83	1.99	0.45
1:A:176:ILE:HG23	1:A:194:VAL:CG1	2.47	0.45
1:A:304:THR:HA	1:A:314:CYS:HA	1.98	0.45
1:A:327:THR:CG2	1:A:334:THR:CG2	2.96	0.45
8:U:14:NAG:H61	7:g:21:XYP:O4	2.17	0.45
1:A:346:SER:HB2	1:A:414:ILE:HG21	1.99	0.44
11:K:35:BGC:H5	11:K:36:XYP:O5	2.17	0.44
11:x:5:NAG:H82	11:x:34:NAG:H83	1.99	0.44
11:X:35:BGC:H5	11:X:36:XYP:O5	2.17	0.44
11:k:35:BGC:H5	11:k:36:XYP:O5	2.17	0.44
11:x:35:BGC:H5	11:x:36:XYP:O5	2.17	0.44
14:a:1:MAN:H61	14:a:2:XYP:O5	2.18	0.44
1:A:413:THR:CG2	1:A:420:THR:CG2	2.96	0.44
3:C:9:BGC:H6C2	3:C:10:XYP:C1	2.47	0.44
13:M:4:NAG:O4	13:M:12:AHR:O4	2.36	0.44
1:A:132:THR:HA	1:A:142:CYS:HA	1.98	0.44
1:A:218:THR:HA	1:A:228:CYS:HA	1.99	0.44
3:P:9:BGC:H6C2	3:P:10:XYP:C1	2.47	0.44
1:A:304:THR:HG23	1:A:314:CYS:HB3	1.99	0.44
1:A:132:THR:HG23	1:A:142:CYS:HB3	1.99	0.44
1:A:241:THR:CG2	1:A:248:THR:CG2	2.96	0.44
3:c:25:BGC:O2	13:z:12:AHR:O3	2.30	0.44
1:A:100:ALA:HB2	1:A:198:ALA:CA	2.44	0.43
1:A:155:THR:CG2	1:A:162:THR:CG2	2.96	0.43
1:A:218:THR:HG23	1:A:228:CYS:HB3	1.99	0.43
1:A:186:ALA:HB2	1:A:284:ALA:CA	2.45	0.43
8:h:8:GAL:C6	7:t:16:NAG:H83	2.46	0.43
11:x:36:XYP:O2	11:x:37:MAN:O5	2.37	0.43
1:A:260:SER:O	1:A:335:GLY:HA3	2.18	0.43
1:A:227:ARG:HH12	5:R:2:NAG:HN2	1.66	0.43
1:A:313:ARG:HH12	5:e:2:NAG:HN2	1.66	0.43
8:h:14:NAG:C6	7:t:21:XYP:O4	2.66	0.43
11:k:36:XYP:O2	11:k:37:MAN:O5	2.37	0.43
1:A:186:ALA:HB3	1:A:284:ALA:HA	2.01	0.43
1:A:331:GLY:C	1:A:332:GLU:HG3	2.44	0.42
11:x:14:BMA:O3	11:x:15:BGC:O5	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:17:BGC:O3	11:X:16:NAG:C2	2.65	0.42
10:j:15:XYP:C5	11:x:15:BGC:O4	2.67	0.42
11:K:36:XYP:O2	11:K:37:MAN:O5	2.37	0.42
1:A:254:ASP:HB3	1:A:255:ILE:H	1.58	0.42
1:A:141:ARG:HH12	5:E:2:NAG:HN2	1.66	0.42
11:X:36:XYP:O2	11:X:37:MAN:O5	2.37	0.42
14:a:15:AHR:O5	8:h:17:A2G:H8A	2.19	0.42
14:n:13:XYP:C5	10:w:10:MAN:O2	2.67	0.42
1:A:272:ALA:HB3	1:A:370:ALA:HA	2.01	0.42
1:A:203:VAL:HG22	1:A:220:TRP:CE3	2.55	0.42
7:T:2:BGC:H5	7:T:16:NAG:H61	2.02	0.42
1:A:289:VAL:HG22	1:A:306:TRP:CE3	2.55	0.41
1:A:399:ARG:HH12	5:r:2:NAG:HN2	1.66	0.41
7:G:2:BGC:H5	7:G:16:NAG:H61	2.02	0.41
13:m:1:XYP:O3	13:m:2:BGC:C1	2.68	0.41
1:A:159:GLY:C	1:A:160:GLU:HG3	2.45	0.41
1:A:301:CYS:HB3	1:A:314:CYS:HB2	1.73	0.41
1:A:375:VAL:HG22	1:A:392:TRP:CE3	2.55	0.41
13:Z:5:BGC:O3	13:Z:10:BGC:O5	2.39	0.41
13:z:1:XYP:O3	13:z:2:BGC:C1	2.68	0.41
1:A:248:THR:OG1	11:X:1:MAN:H3	2.21	0.41
1:A:332:GLU:HB2	10:W:1:GAL:H62	2.02	0.41
1:A:420:THR:OG1	11:x:1:MAN:H3	2.21	0.41
7:g:2:BGC:H5	7:g:16:NAG:H61	2.02	0.41
10:J:19:MAN:C6	14:N:16:BGC:O4	2.69	0.41
7:t:2:BGC:H5	7:t:16:NAG:H61	2.02	0.41
1:A:162:THR:OG1	11:K:1:MAN:H3	2.21	0.41
13:M:5:BGC:O3	13:M:10:BGC:O5	2.39	0.41
4:d:11:MAN:H61	4:d:19:BGC:O3	2.21	0.41
10:J:2:NAG:H4	10:J:19:MAN:C3	2.49	0.41
1:A:100:ALA:HB3	1:A:198:ALA:HA	2.02	0.41
1:A:106:ILE:HG21	1:A:144:THR:HG23	2.03	0.41
1:A:117:VAL:HG22	1:A:134:TRP:CE3	2.55	0.41
4:D:11:MAN:H61	4:D:19:BGC:O3	2.21	0.41
7:G:2:BGC:H6C1	7:G:3:A2G:O6	2.21	0.41
1:A:254:ASP:O	14:a:1:MAN:H5	2.21	0.41
4:Q:11:MAN:H61	4:Q:19:BGC:O3	2.21	0.41
1:A:192:ILE:HG21	1:A:230:THR:HG23	2.03	0.40
1:A:278:ILE:HG21	1:A:316:THR:HG23	2.03	0.40
1:A:418:GLU:HB2	10:j:1:GAL:H62	2.03	0.40
10:W:18:NAG:H83	12:l:5:BGC:O3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:z:5:BGC:O3	13:z:10:BGC:O5	2.39	0.40
1:A:331:GLY:O	1:A:332:GLU:HG3	2.22	0.40
13:Z:1:XYP:O3	13:Z:2:BGC:C1	2.68	0.40
7:t:2:BGC:H6C1	7:t:3:A2G:O6	2.21	0.40
1:A:156:ILE:HD12	1:A:156:ILE:HA	1.92	0.40
1:A:242:ILE:HD12	1:A:242:ILE:HA	1.92	0.40
7:G:4:BGC:H2	7:G:5:BGC:O2	2.22	0.40
7:T:4:BGC:H2	7:T:5:BGC:O2	2.22	0.40
4:q:11:MAN:H61	4:q:19:BGC:O3	2.21	0.40
1:A:176:ILE:HG21	1:A:240:VAL:CG1	2.52	0.40
1:A:182:THR:HB	1:A:255:ILE:HA	2.03	0.40
10:W:19:MAN:H62	14:a:16:BGC:O4	2.21	0.40
7:g:2:BGC:H6C1	7:g:3:A2G:O6	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	342/344 (99%)	306 (90%)	29 (8%)	7 (2%)	6	27

All (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
1	A	159	GLY
1	A	245	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	288/288 (100%)	271 (94%)	17 (6%)	18	46

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	VAL
1	A	164	SER
1	A	166	SER
1	A	169	ILE
1	A	173	GLU
1	A	244	VAL
1	A	250	SER
1	A	252	SER
1	A	330	VAL
1	A	336	SER
1	A	338	SER
1	A	341	ILE
1	A	346	SER
1	A	416	VAL
1	A	422	SER
1	A	424	SER
1	A	427	ILE

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	1,14	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	1,3	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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	1,4	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
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	1,5	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	1,6	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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	1,11	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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	1,14	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	1,3	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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	1,4	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%)
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	1,5	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	1,6	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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	1,11	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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	1,14	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
3	GLA	c	1	1,3	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	1,4	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
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	1,5	11,11,12	0.22	0	15,15,17	0.77	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	e	2	5	14,14,15	0.27	0	17,19,21	0.65	0
6	MAN	f	1	1,6	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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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	1,11	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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	1,14	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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	1,3	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	1,4	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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	1,5	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	1,6	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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BGC	w	9	10	11,11,12	0.81	1 (9%)	15,15,17	0.90	1 (6%)
11	MAN	x	1	1,11	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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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	1,14	-	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
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	1,3	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	1,4	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,5	-	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	1,6	-	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,11	-	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	M	9	13	-	2/6/23/26	0/1/1/1
14	MAN	N	1	1,14	-	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
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	1,3	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	1,4	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,5	-	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	1,6	-	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,11	-	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	MAN	a	1	1,14	-	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
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	1,3	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	1,4	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,5	-	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	1,6	-	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,11	-	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	MAN	n	1	1,14	-	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
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	1,3	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	1,4	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,5	-	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	1,6	-	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,11	-	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (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
6	s	2	GZL	O4-C4	-7.19	1.27	1.43
6	f	2	GZL	O4-C4	-7.18	1.27	1.43
6	S	2	GZL	O4-C4	-7.18	1.27	1.43
6	f	2	GZL	C3-C4	6.44	1.67	1.52
6	S	2	GZL	C3-C4	6.43	1.67	1.52
6	s	2	GZL	C3-C4	6.43	1.67	1.52
6	F	2	GZL	C3-C4	6.41	1.67	1.52
6	S	2	GZL	C1-C2	4.94	1.60	1.51
6	F	2	GZL	C1-C2	4.94	1.60	1.51
6	s	2	GZL	C1-C2	4.92	1.60	1.51
6	f	2	GZL	C1-C2	4.92	1.60	1.51
6	S	2	GZL	O4-C1	4.00	1.52	1.43
6	F	2	GZL	O4-C1	3.99	1.52	1.43
6	s	2	GZL	O4-C1	3.99	1.52	1.43
6	f	2	GZL	O4-C1	3.94	1.52	1.43
6	s	2	GZL	O2-C2	3.83	1.51	1.43
6	f	2	GZL	O2-C2	3.83	1.51	1.43
6	S	2	GZL	O2-C2	3.82	1.51	1.43
6	F	2	GZL	O2-C2	3.81	1.51	1.43
13	M	5	BGC	C2-C3	-3.00	1.48	1.52
13	m	5	BGC	C2-C3	-2.96	1.48	1.52
13	Z	5	BGC	C2-C3	-2.95	1.48	1.52
13	z	5	BGC	C2-C3	-2.92	1.48	1.52
10	w	19	MAN	C2-C3	-2.80	1.48	1.52
10	j	19	MAN	C2-C3	-2.77	1.48	1.52
13	Z	2	BGC	C2-C3	-2.69	1.48	1.52
10	W	19	MAN	C2-C3	-2.63	1.48	1.52
13	m	2	BGC	C2-C3	-2.63	1.48	1.52
13	z	2	BGC	C2-C3	-2.62	1.48	1.52
13	M	2	BGC	C2-C3	-2.59	1.48	1.52
10	J	19	MAN	C2-C3	-2.46	1.48	1.52
4	q	11	MAN	C2-C3	-2.40	1.49	1.52
4	D	11	MAN	C2-C3	-2.36	1.49	1.52
12	L	8	BGC	C2-C3	-2.36	1.49	1.52
4	Q	11	MAN	C2-C3	-2.36	1.49	1.52
4	d	11	MAN	C2-C3	-2.33	1.49	1.52
10	w	9	BGC	C2-C3	-2.31	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	9	BGC	C2-C3	-2.28	1.49	1.52
12	Y	8	BGC	C2-C3	-2.28	1.49	1.52
10	W	9	BGC	C2-C3	-2.28	1.49	1.52
10	j	9	BGC	C2-C3	-2.24	1.49	1.52
7	t	1	XYP	O5-C1	-2.20	1.38	1.42
7	G	1	XYP	O5-C1	-2.17	1.38	1.42
7	T	1	XYP	O5-C1	-2.17	1.38	1.42
2	B	6	NAG	O5-C1	-2.16	1.40	1.43
2	o	6	NAG	O5-C1	-2.14	1.40	1.43
2	O	6	NAG	O5-C1	-2.13	1.40	1.43
6	s	2	GZL	O3-C3	2.13	1.48	1.43
7	g	1	XYP	O5-C1	-2.13	1.38	1.42
6	f	2	GZL	O3-C3	2.12	1.48	1.43
6	S	2	GZL	O3-C3	2.11	1.47	1.43
2	b	6	NAG	O5-C1	-2.11	1.40	1.43
6	F	2	GZL	O3-C3	2.10	1.47	1.43
13	z	2	BGC	C1-C2	-2.07	1.47	1.52
11	X	12	BMA	O5-C1	-2.05	1.40	1.43
13	m	2	BGC	C1-C2	-2.05	1.47	1.52
11	X	11	BGC	C2-C3	-2.04	1.49	1.52
13	M	2	BGC	C1-C2	-2.03	1.47	1.52
11	k	12	BMA	O5-C1	-2.03	1.40	1.43
13	Z	2	BGC	C1-C2	-2.03	1.47	1.52
11	x	12	BMA	O5-C1	-2.02	1.40	1.43
11	K	12	BMA	O5-C1	-2.02	1.40	1.43

All (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
10	j	3	XYP	C1-C2-C3	7.78	119.23	109.67
14	0	1	MAN	C2-C3-C4	-6.85	99.05	110.89
14	a	1	MAN	C2-C3-C4	-6.84	99.06	110.89
14	n	1	MAN	C2-C3-C4	-6.82	99.09	110.89
14	N	1	MAN	C2-C3-C4	-6.80	99.13	110.89
7	G	1	XYP	C5-C4-C3	6.62	117.81	109.67
7	g	1	XYP	C5-C4-C3	6.62	117.80	109.67
7	T	1	XYP	C5-C4-C3	6.59	117.77	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	t	1	XYP	C5-C4-C3	6.56	117.73	109.67
11	K	12	BMA	C1-O5-C5	-6.54	103.33	112.19
11	X	12	BMA	C1-O5-C5	-6.54	103.33	112.19
11	k	12	BMA	C1-O5-C5	-6.52	103.36	112.19
11	x	12	BMA	C1-O5-C5	-6.51	103.37	112.19
13	m	2	BGC	O3-C3-C2	-6.48	97.59	109.99
13	Z	2	BGC	O3-C3-C2	-6.47	97.60	109.99
13	M	2	BGC	O3-C3-C2	-6.47	97.61	109.99
12	y	5	BGC	C1-C2-C3	6.47	117.62	109.67
13	z	2	BGC	O3-C3-C2	-6.47	97.61	109.99
12	L	5	BGC	C1-C2-C3	6.46	117.60	109.67
12	l	5	BGC	C1-C2-C3	6.45	117.60	109.67
12	Y	5	BGC	C1-C2-C3	6.42	117.55	109.67
11	X	9	BMA	C1-C2-C3	6.19	117.27	109.67
11	K	9	BMA	C1-C2-C3	6.17	117.25	109.67
11	x	9	BMA	C1-C2-C3	6.15	117.22	109.67
11	k	9	BMA	C1-C2-C3	6.14	117.21	109.67
11	k	9	BMA	C2-C3-C4	-6.00	100.52	110.89
11	x	9	BMA	C2-C3-C4	-5.99	100.52	110.89
11	X	9	BMA	C2-C3-C4	-5.99	100.53	110.89
11	K	9	BMA	C2-C3-C4	-5.99	100.54	110.89
11	k	12	BMA	C1-C2-C3	5.57	116.51	109.67
11	x	12	BMA	C1-C2-C3	5.57	116.51	109.67
11	K	12	BMA	C1-C2-C3	5.56	116.50	109.67
11	X	12	BMA	C1-C2-C3	5.56	116.50	109.67
14	a	1	MAN	C3-C4-C5	-5.54	100.36	110.24
14	0	1	MAN	C3-C4-C5	-5.53	100.38	110.24
14	N	1	MAN	C3-C4-C5	-5.52	100.39	110.24
14	n	1	MAN	C3-C4-C5	-5.49	100.44	110.24
12	y	8	BGC	C1-C2-C3	4.99	115.80	109.67
12	L	7	BGC	C1-C2-C3	4.98	115.79	109.67
12	Y	7	BGC	C1-C2-C3	4.98	115.79	109.67
12	y	7	BGC	C1-C2-C3	4.97	115.78	109.67
12	l	7	BGC	C1-C2-C3	4.95	115.76	109.67
10	j	17	BGC	C1-C2-C3	4.85	115.62	109.67
11	X	11	BGC	O5-C1-C2	-4.80	103.37	110.77
11	k	11	BGC	O5-C1-C2	-4.78	103.39	110.77
11	x	11	BGC	O5-C1-C2	-4.76	103.42	110.77
11	K	11	BGC	O5-C1-C2	-4.75	103.45	110.77
13	m	5	BGC	O5-C1-C2	-4.72	103.48	110.77
13	z	5	BGC	O5-C1-C2	-4.72	103.49	110.77
13	Z	5	BGC	O5-C1-C2	-4.70	103.52	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	5	BGC	O5-C1-C2	-4.70	103.52	110.77
12	Y	9	NAG	C1-O5-C5	4.53	118.33	112.19
12	L	9	NAG	C1-O5-C5	4.51	118.30	112.19
12	l	9	NAG	C1-O5-C5	4.49	118.28	112.19
12	y	9	NAG	C1-O5-C5	4.49	118.27	112.19
13	m	14	BGC	C1-O5-C5	-4.38	106.25	112.19
13	M	14	BGC	C1-O5-C5	-4.38	106.25	112.19
11	K	20	NAG	C2-N2-C7	-4.35	116.71	122.90
11	X	20	NAG	C2-N2-C7	-4.34	116.72	122.90
11	k	20	NAG	C2-N2-C7	-4.34	116.72	122.90
13	z	14	BGC	C1-O5-C5	-4.34	106.31	112.19
10	w	2	NAG	C4-C3-C2	-4.34	104.66	111.02
11	x	20	NAG	C2-N2-C7	-4.34	116.73	122.90
13	Z	14	BGC	C1-O5-C5	-4.33	106.32	112.19
10	J	2	NAG	C4-C3-C2	-4.33	104.67	111.02
10	W	2	NAG	C4-C3-C2	-4.33	104.67	111.02
13	m	4	NAG	C3-C4-C5	-4.31	102.55	110.24
13	M	4	NAG	C3-C4-C5	-4.31	102.55	110.24
10	j	2	NAG	C4-C3-C2	-4.31	104.71	111.02
13	Z	4	NAG	C3-C4-C5	-4.31	102.56	110.24
13	z	4	NAG	C3-C4-C5	-4.30	102.57	110.24
10	j	3	XYP	C4-C3-C2	4.28	116.00	110.92
10	j	17	BGC	O5-C1-C2	4.20	117.25	110.77
12	l	8	BGC	O5-C1-C2	4.18	117.22	110.77
10	w	3	XYP	C4-C3-C2	4.14	115.84	110.92
4	d	7	NAG	C4-C3-C2	-4.04	105.09	111.02
4	Q	7	NAG	C4-C3-C2	-4.03	105.11	111.02
4	q	7	NAG	C4-C3-C2	-4.02	105.12	111.02
4	D	7	NAG	C4-C3-C2	-4.01	105.13	111.02
13	M	2	BGC	O5-C1-C2	-3.95	104.67	110.77
13	Z	2	BGC	O5-C1-C2	-3.94	104.69	110.77
13	m	2	BGC	O5-C1-C2	-3.94	104.69	110.77
3	p	12	MAN	C1-C2-C3	3.94	114.50	109.67
13	z	2	BGC	O5-C1-C2	-3.93	104.71	110.77
6	F	2	GZL	C5-C4-C3	-3.90	110.65	115.86
6	S	2	GZL	C5-C4-C3	-3.89	110.65	115.86
3	C	12	MAN	C1-C2-C3	3.89	114.44	109.67
6	s	2	GZL	C5-C4-C3	-3.88	110.67	115.86
6	f	2	GZL	C5-C4-C3	-3.87	110.69	115.86
14	0	1	MAN	O5-C5-C4	-3.86	101.45	110.83
14	n	1	MAN	O5-C5-C4	-3.85	101.47	110.83
14	N	1	MAN	O5-C5-C4	-3.84	101.48	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	1	MAN	O5-C5-C4	-3.84	101.49	110.83
10	w	17	BGC	C1-C2-C3	3.77	114.30	109.67
13	z	1	XYP	O2-C2-C3	3.76	117.68	110.14
13	m	1	XYP	O2-C2-C3	3.76	117.67	110.14
13	Z	1	XYP	O2-C2-C3	3.75	117.66	110.14
13	z	12	AHR	C1-C2-C3	3.75	107.35	101.63
13	M	1	XYP	O2-C2-C3	3.74	117.63	110.14
14	a	1	MAN	O4-C4-C5	3.69	118.45	109.30
14	N	1	MAN	O4-C4-C5	3.68	118.43	109.30
13	m	12	AHR	C1-C2-C3	3.67	107.22	101.63
14	0	1	MAN	O4-C4-C5	3.66	118.39	109.30
11	k	13	NAG	O3-C3-C2	3.66	117.04	109.47
11	K	13	NAG	O3-C3-C2	3.66	117.04	109.47
14	n	1	MAN	O4-C4-C5	3.66	118.38	109.30
13	M	14	BGC	C3-C4-C5	3.65	116.75	110.24
11	X	13	NAG	O3-C3-C2	3.65	117.02	109.47
13	z	14	BGC	C3-C4-C5	3.64	116.74	110.24
11	x	13	NAG	O3-C3-C2	3.64	117.00	109.47
13	Z	14	BGC	C3-C4-C5	3.64	116.73	110.24
13	m	14	BGC	C3-C4-C5	3.63	116.71	110.24
13	m	2	BGC	C1-C2-C3	-3.62	105.21	109.67
13	z	2	BGC	C1-C2-C3	-3.61	105.22	109.67
13	M	2	BGC	C1-C2-C3	-3.61	105.23	109.67
13	Z	5	BGC	O4-C4-C3	-3.61	102.01	110.35
3	P	12	MAN	C1-C2-C3	3.61	114.10	109.67
13	m	5	BGC	O4-C4-C3	-3.60	102.02	110.35
13	M	5	BGC	O4-C4-C3	-3.60	102.02	110.35
13	z	5	BGC	O4-C4-C3	-3.60	102.02	110.35
13	Z	2	BGC	C1-C2-C3	-3.56	105.29	109.67
11	x	8	BGC	O5-C1-C2	-3.52	105.34	110.77
12	l	7	BGC	C2-C3-C4	3.52	116.98	110.89
13	Z	12	AHR	C1-C2-C3	3.52	106.98	101.63
11	X	19	BGC	C1-C2-C3	3.51	113.98	109.67
11	k	8	BGC	O5-C1-C2	-3.51	105.35	110.77
11	K	19	BGC	C1-C2-C3	3.51	113.98	109.67
11	k	19	BGC	C1-C2-C3	3.50	113.97	109.67
11	x	19	BGC	C1-C2-C3	3.50	113.97	109.67
11	X	8	BGC	O5-C1-C2	-3.50	105.37	110.77
12	y	7	BGC	C2-C3-C4	3.50	116.95	110.89
3	c	12	MAN	C1-C2-C3	3.49	113.96	109.67
12	Y	7	BGC	C2-C3-C4	3.49	116.94	110.89
12	L	7	BGC	C2-C3-C4	3.49	116.94	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	11	BGC	C1-O5-C5	3.48	116.91	112.19
11	K	8	BGC	O5-C1-C2	-3.48	105.40	110.77
11	k	11	BGC	C1-O5-C5	3.46	116.88	112.19
11	K	7	BGC	C1-C2-C3	-3.45	105.43	109.67
11	X	11	BGC	C1-O5-C5	3.45	116.86	112.19
11	x	11	BGC	C1-O5-C5	3.44	116.86	112.19
11	X	7	BGC	C1-C2-C3	-3.44	105.44	109.67
11	k	7	BGC	C1-C2-C3	-3.43	105.45	109.67
11	x	7	BGC	C1-C2-C3	-3.42	105.47	109.67
10	j	6	A2G	C4-C3-C2	3.42	116.02	111.02
14	0	1	MAN	C1-C2-C3	-3.41	105.47	109.67
14	n	1	MAN	C1-C2-C3	-3.41	105.47	109.67
13	M	12	AHR	C1-C2-C3	3.40	106.81	101.63
14	N	1	MAN	C1-C2-C3	-3.40	105.49	109.67
12	Y	5	BGC	C2-C3-C4	3.39	116.76	110.89
11	K	13	NAG	O3-C3-C4	-3.39	102.51	110.35
10	J	6	A2G	C4-C3-C2	3.39	115.98	111.02
12	y	5	BGC	C2-C3-C4	3.39	116.75	110.89
10	w	6	A2G	C4-C3-C2	3.39	115.98	111.02
14	a	1	MAN	C1-C2-C3	-3.38	105.51	109.67
4	Q	6	BMA	C1-O5-C5	-3.38	107.62	112.19
4	Q	7	NAG	O5-C1-C2	-3.37	105.96	111.29
4	q	6	BMA	C1-O5-C5	-3.37	107.62	112.19
7	t	16	NAG	C1-O5-C5	3.37	116.76	112.19
4	d	7	NAG	O5-C1-C2	-3.37	105.97	111.29
10	W	6	A2G	C4-C3-C2	3.37	115.95	111.02
11	x	13	NAG	O3-C3-C4	-3.37	102.56	110.35
12	l	5	BGC	C2-C3-C4	3.37	116.72	110.89
7	T	1	XYP	C4-C3-C2	3.36	114.92	110.92
11	X	13	NAG	O3-C3-C4	-3.36	102.57	110.35
7	T	16	NAG	C1-O5-C5	3.36	116.75	112.19
4	D	7	NAG	O5-C1-C2	-3.36	105.98	111.29
11	k	13	NAG	O3-C3-C4	-3.36	102.58	110.35
10	j	19	MAN	O2-C2-C3	-3.36	103.41	110.14
4	d	6	BMA	C1-O5-C5	-3.36	107.64	112.19
7	G	1	XYP	C4-C3-C2	3.36	114.91	110.92
4	D	6	BMA	C1-O5-C5	-3.35	107.65	112.19
7	g	16	NAG	C1-O5-C5	3.35	116.73	112.19
7	G	16	NAG	C1-O5-C5	3.35	116.73	112.19
7	t	1	XYP	C4-C3-C2	3.35	114.89	110.92
7	g	1	XYP	C4-C3-C2	3.34	114.89	110.92
12	L	5	BGC	C2-C3-C4	3.34	116.67	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	p	6	XYP	O2-C2-C3	3.34	116.82	110.14
3	c	6	XYP	O2-C2-C3	3.34	116.82	110.14
3	C	6	XYP	O2-C2-C3	3.33	116.81	110.14
4	q	7	NAG	O5-C1-C2	-3.33	106.03	111.29
11	x	10	GLA	C1-O5-C5	-3.31	107.70	112.19
10	w	19	MAN	O2-C2-C3	-3.31	103.50	110.14
3	P	6	XYP	O2-C2-C3	3.30	116.75	110.14
11	K	10	GLA	C1-O5-C5	-3.30	107.72	112.19
11	k	10	GLA	C1-O5-C5	-3.29	107.73	112.19
11	X	10	GLA	C1-O5-C5	-3.28	107.74	112.19
12	L	6	MAN	O5-C1-C2	-3.28	105.71	110.77
12	Y	6	MAN	O5-C1-C2	-3.27	105.72	110.77
13	M	2	BGC	O3-C3-C4	3.26	117.88	110.35
12	l	6	MAN	O5-C1-C2	-3.25	105.76	110.77
12	y	6	MAN	O5-C1-C2	-3.24	105.77	110.77
10	j	6	A2G	O4-C4-C3	3.24	117.83	110.35
10	J	6	A2G	O4-C4-C3	3.23	117.82	110.35
10	W	6	A2G	O4-C4-C3	3.23	117.82	110.35
10	w	6	A2G	O4-C4-C3	3.23	117.82	110.35
13	z	2	BGC	O3-C3-C4	3.23	117.82	110.35
13	Z	2	BGC	O3-C3-C4	3.22	117.80	110.35
13	m	2	BGC	O3-C3-C4	3.22	117.80	110.35
12	y	8	BGC	O5-C1-C2	3.22	115.74	110.77
13	M	10	BGC	C1-O5-C5	3.21	116.55	112.19
13	m	10	BGC	C1-O5-C5	3.21	116.54	112.19
13	z	10	BGC	C1-O5-C5	3.19	116.51	112.19
13	Z	10	BGC	C1-O5-C5	3.16	116.47	112.19
13	Z	14	BGC	C2-C3-C4	3.15	116.35	110.89
11	K	11	BGC	C1-C2-C3	-3.15	105.80	109.67
13	m	14	BGC	C2-C3-C4	3.15	116.34	110.89
13	z	14	BGC	C2-C3-C4	3.14	116.33	110.89
13	M	14	BGC	C2-C3-C4	3.12	116.30	110.89
11	X	11	BGC	C1-C2-C3	-3.12	105.83	109.67
10	j	18	NAG	C1-O5-C5	3.12	116.42	112.19
11	x	11	BGC	C1-C2-C3	-3.12	105.84	109.67
11	k	11	BGC	C1-C2-C3	-3.11	105.84	109.67
10	J	19	MAN	C1-C2-C3	3.10	113.47	109.67
11	k	16	NAG	C1-O5-C5	-3.04	108.08	112.19
11	X	16	NAG	C1-O5-C5	-3.03	108.09	112.19
11	K	16	NAG	C1-O5-C5	-3.03	108.09	112.19
11	k	17	AHR	C1-C2-C3	3.03	106.24	101.63
11	x	17	AHR	C1-C2-C3	3.03	106.24	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	17	AHR	C1-C2-C3	3.02	106.23	101.63
11	X	17	AHR	C1-C2-C3	3.01	106.22	101.63
11	x	16	NAG	C1-O5-C5	-3.00	108.13	112.19
11	K	15	BGC	C1-C2-C3	2.98	113.33	109.67
3	p	2	BGC	O5-C1-C2	-2.96	106.20	110.77
3	c	2	BGC	O5-C1-C2	-2.95	106.21	110.77
11	k	14	BMA	C2-C3-C4	-2.95	105.79	110.89
3	C	2	BGC	O5-C1-C2	-2.95	106.22	110.77
13	m	10	BGC	O5-C5-C6	2.95	111.82	107.20
11	k	9	BMA	O5-C5-C4	-2.95	103.66	110.83
13	M	10	BGC	O5-C5-C6	2.94	111.82	107.20
11	K	14	BMA	C2-C3-C4	-2.94	105.80	110.89
11	X	9	BMA	O5-C5-C4	-2.94	103.68	110.83
11	K	9	BMA	O5-C5-C4	-2.93	103.69	110.83
13	z	10	BGC	O5-C5-C6	2.93	111.79	107.20
3	P	2	BGC	O5-C1-C2	-2.93	106.25	110.77
2	O	6	NAG	C2-N2-C7	-2.92	118.74	122.90
2	O	6	NAG	C1-O5-C5	-2.92	108.24	112.19
2	B	6	NAG	C2-N2-C7	-2.92	118.75	122.90
11	x	9	BMA	O5-C5-C4	-2.92	103.73	110.83
11	X	20	NAG	O4-C4-C5	2.91	116.53	109.30
13	Z	10	BGC	O5-C5-C6	2.91	111.77	107.20
11	x	14	BMA	C2-C3-C4	-2.91	105.86	110.89
11	K	20	NAG	O4-C4-C5	2.91	116.52	109.30
2	B	6	NAG	C1-O5-C5	-2.90	108.26	112.19
11	X	14	BMA	C2-C3-C4	-2.90	105.88	110.89
3	P	11	NAG	C2-N2-C7	2.90	127.03	122.90
10	W	18	NAG	C1-O5-C5	2.89	116.11	112.19
2	o	6	NAG	C2-N2-C7	-2.89	118.78	122.90
2	o	6	NAG	C1-O5-C5	-2.89	108.27	112.19
11	x	20	NAG	O4-C4-C5	2.89	116.48	109.30
11	k	20	NAG	O4-C4-C5	2.89	116.48	109.30
13	z	5	BGC	C3-C4-C5	-2.89	105.08	110.24
2	b	6	NAG	C1-O5-C5	-2.89	108.28	112.19
2	b	6	NAG	C2-N2-C7	-2.88	118.80	122.90
13	m	5	BGC	C3-C4-C5	-2.88	105.11	110.24
13	Z	5	BGC	C3-C4-C5	-2.88	105.11	110.24
13	M	5	BGC	C3-C4-C5	-2.87	105.12	110.24
8	h	16	MAN	C1-O5-C5	2.86	116.07	112.19
14	a	4	GAL	C1-C2-C3	2.85	113.17	109.67
14	N	4	GAL	C1-C2-C3	2.85	113.17	109.67
8	U	16	MAN	C1-O5-C5	2.84	116.04	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	u	16	MAN	C1-O5-C5	2.84	116.04	112.19
14	0	4	GAL	C1-C2-C3	2.83	113.14	109.67
8	H	16	MAN	C1-O5-C5	2.81	116.00	112.19
14	n	4	GAL	C1-C2-C3	2.81	113.12	109.67
10	j	19	MAN	C1-C2-C3	2.80	113.11	109.67
10	W	19	MAN	C1-C2-C3	2.79	113.10	109.67
11	X	15	BGC	C1-C2-C3	2.79	113.09	109.67
10	j	17	BGC	C3-C4-C5	-2.79	105.27	110.24
3	p	11	NAG	C2-N2-C7	2.78	126.86	122.90
10	w	17	BGC	O5-C1-C2	2.78	115.06	110.77
11	k	11	BGC	C2-C3-C4	-2.76	106.11	110.89
7	t	7	A2G	C1-O5-C5	2.76	115.93	112.19
11	x	11	BGC	C2-C3-C4	-2.74	106.15	110.89
11	X	13	NAG	C1-O5-C5	-2.74	108.48	112.19
11	k	13	NAG	C1-O5-C5	-2.74	108.48	112.19
11	X	11	BGC	C2-C3-C4	-2.73	106.16	110.89
11	x	13	NAG	C1-O5-C5	-2.73	108.49	112.19
11	K	13	NAG	C1-O5-C5	-2.73	108.49	112.19
7	g	7	A2G	C1-O5-C5	2.73	115.89	112.19
12	l	8	BGC	C1-O5-C5	2.73	115.89	112.19
7	G	7	A2G	C1-O5-C5	2.72	115.88	112.19
11	K	11	BGC	C2-C3-C4	-2.72	106.19	110.89
11	K	20	NAG	O5-C1-C2	-2.72	106.99	111.29
10	J	2	NAG	C1-O5-C5	2.71	115.87	112.19
7	T	7	A2G	C1-O5-C5	2.70	115.86	112.19
11	X	20	NAG	O5-C1-C2	-2.69	107.03	111.29
11	x	20	NAG	O5-C1-C2	-2.69	107.04	111.29
2	O	6	NAG	C4-C3-C2	-2.68	107.08	111.02
10	W	2	NAG	C1-O5-C5	2.68	115.82	112.19
11	k	20	NAG	O5-C1-C2	-2.68	107.06	111.29
2	b	6	NAG	C4-C3-C2	-2.67	107.10	111.02
10	w	19	MAN	C1-C2-C3	2.67	112.94	109.67
2	o	6	NAG	C4-C3-C2	-2.67	107.11	111.02
10	j	2	NAG	C1-O5-C5	2.66	115.80	112.19
10	w	2	NAG	C1-O5-C5	2.66	115.79	112.19
7	G	16	NAG	O5-C1-C2	2.66	115.48	111.29
11	K	11	BGC	O5-C5-C6	2.65	111.36	107.20
2	B	6	NAG	C4-C3-C2	-2.65	107.13	111.02
11	K	35	BGC	O2-C2-C3	-2.64	104.84	110.14
13	m	1	XYP	C4-C3-C2	-2.64	107.78	110.92
11	X	35	BGC	O2-C2-C3	-2.64	104.85	110.14
13	M	1	XYP	C4-C3-C2	-2.64	107.79	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	x	35	BGC	O2-C2-C3	-2.63	104.86	110.14
11	k	11	BGC	O5-C5-C6	2.63	111.32	107.20
11	k	35	BGC	O2-C2-C3	-2.63	104.88	110.14
7	T	16	NAG	O5-C1-C2	2.62	115.43	111.29
7	g	16	NAG	O5-C1-C2	2.61	115.42	111.29
11	X	8	BGC	O3-C3-C4	-2.61	104.31	110.35
11	x	11	BGC	O5-C5-C6	2.61	111.29	107.20
11	X	11	BGC	O5-C5-C6	2.61	111.29	107.20
13	Z	1	XYP	C4-C3-C2	-2.61	107.83	110.92
7	t	16	NAG	O5-C1-C2	2.60	115.40	111.29
13	z	14	BGC	O5-C1-C2	-2.60	106.76	110.77
11	x	8	BGC	O3-C3-C4	-2.60	104.34	110.35
13	z	10	BGC	C6-C5-C4	-2.60	106.92	113.00
11	X	7	BGC	C6-C5-C4	-2.59	106.93	113.00
13	z	1	XYP	C4-C3-C2	-2.59	107.84	110.92
11	K	8	BGC	O3-C3-C4	-2.59	104.37	110.35
11	x	7	BGC	C6-C5-C4	-2.59	106.95	113.00
11	k	8	BGC	O3-C3-C4	-2.59	104.37	110.35
12	L	5	BGC	O2-C2-C3	-2.58	104.97	110.14
13	Z	10	BGC	C6-C5-C4	-2.58	106.96	113.00
3	c	2	BGC	C1-C2-C3	-2.58	106.50	109.67
11	k	7	BGC	C6-C5-C4	-2.58	106.97	113.00
12	l	5	BGC	O2-C2-C3	-2.58	104.98	110.14
13	M	10	BGC	C6-C5-C4	-2.58	106.97	113.00
13	m	10	BGC	C6-C5-C4	-2.58	106.97	113.00
11	K	7	BGC	C6-C5-C4	-2.57	106.97	113.00
12	Y	5	BGC	O2-C2-C3	-2.57	104.99	110.14
13	m	14	BGC	O5-C1-C2	-2.57	106.80	110.77
12	y	5	BGC	O4-C4-C5	-2.57	102.93	109.30
12	Y	5	BGC	O4-C4-C5	-2.56	102.95	109.30
3	P	2	BGC	C1-C2-C3	-2.56	106.52	109.67
12	L	5	BGC	O4-C4-C5	-2.56	102.95	109.30
11	K	12	BMA	O5-C5-C4	-2.56	104.61	110.83
13	M	14	BGC	O5-C1-C2	-2.55	106.83	110.77
3	p	2	BGC	C1-C2-C3	-2.55	106.53	109.67
3	C	2	BGC	C1-C2-C3	-2.55	106.53	109.67
13	Z	14	BGC	O5-C1-C2	-2.55	106.84	110.77
12	y	5	BGC	O2-C2-C3	-2.55	105.03	110.14
12	l	5	BGC	O4-C4-C5	-2.54	102.98	109.30
10	w	18	NAG	O5-C1-C2	2.54	115.30	111.29
11	X	12	BMA	O5-C5-C4	-2.54	104.66	110.83
11	x	12	BMA	O5-C5-C4	-2.54	104.66	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	6	MAN	C1-C2-C3	2.52	112.77	109.67
12	L	8	BGC	C1-O5-C5	2.52	115.61	112.19
11	x	16	NAG	O5-C5-C6	2.52	111.16	107.20
11	k	12	BMA	O5-C5-C4	-2.52	104.70	110.83
11	x	20	NAG	O4-C4-C3	-2.52	104.53	110.35
11	X	20	NAG	O4-C4-C3	-2.51	104.53	110.35
12	y	8	BGC	O5-C5-C4	-2.51	104.71	110.83
11	K	16	NAG	O5-C5-C6	2.50	111.13	107.20
11	k	20	NAG	O4-C4-C3	-2.50	104.57	110.35
11	X	16	NAG	O5-C5-C6	2.50	111.12	107.20
13	m	5	BGC	C2-C3-C4	-2.50	106.57	110.89
11	k	16	NAG	O5-C5-C6	2.50	111.12	107.20
3	C	11	NAG	C2-N2-C7	2.50	126.46	122.90
11	K	20	NAG	O4-C4-C3	-2.50	104.57	110.35
12	Y	8	BGC	O5-C1-C2	2.49	114.62	110.77
13	Z	5	BGC	C2-C3-C4	-2.49	106.59	110.89
13	z	5	BGC	C2-C3-C4	-2.49	106.59	110.89
13	M	5	BGC	C2-C3-C4	-2.48	106.61	110.89
10	W	9	BGC	C1-O5-C5	2.45	115.50	112.19
7	T	3	A2G	C1-O5-C5	2.44	115.50	112.19
10	j	9	BGC	C1-O5-C5	2.44	115.50	112.19
10	w	17	BGC	C3-C4-C5	-2.44	105.89	110.24
14	a	3	A2G	O5-C1-C2	2.43	115.13	111.29
7	g	3	A2G	C1-O5-C5	2.43	115.48	112.19
10	J	9	BGC	C1-O5-C5	2.42	115.48	112.19
14	0	3	A2G	O5-C1-C2	2.42	115.12	111.29
10	w	9	BGC	C1-O5-C5	2.42	115.48	112.19
11	k	13	NAG	O5-C5-C4	-2.42	104.93	110.83
11	x	13	NAG	O5-C5-C4	-2.42	104.93	110.83
7	t	3	A2G	C1-O5-C5	2.42	115.47	112.19
11	K	13	NAG	O5-C5-C4	-2.42	104.94	110.83
7	G	3	A2G	C1-O5-C5	2.41	115.46	112.19
11	X	13	NAG	O5-C5-C4	-2.41	104.96	110.83
14	n	3	A2G	O5-C1-C2	2.41	115.09	111.29
10	W	19	MAN	C1-O5-C5	2.41	115.45	112.19
14	N	3	A2G	O5-C1-C2	2.41	115.09	111.29
10	J	18	NAG	C1-O5-C5	2.40	115.45	112.19
8	h	16	MAN	C1-C2-C3	2.39	112.60	109.67
10	J	8	A2G	O5-C1-C2	-2.39	107.52	111.29
13	Z	5	BGC	O4-C4-C5	2.38	115.22	109.30
13	M	5	BGC	O4-C4-C5	2.38	115.20	109.30
13	m	2	BGC	C3-C4-C5	-2.37	106.01	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	16	MAN	C1-C2-C3	2.37	112.58	109.67
8	u	16	MAN	C1-C2-C3	2.37	112.58	109.67
13	m	5	BGC	O4-C4-C5	2.37	115.17	109.30
13	z	5	BGC	O4-C4-C5	2.37	115.17	109.30
8	U	16	MAN	C1-C2-C3	2.36	112.57	109.67
10	j	8	A2G	O5-C1-C2	-2.36	107.55	111.29
13	Z	14	BGC	O4-C4-C3	-2.36	104.89	110.35
13	m	14	BGC	O4-C4-C3	-2.36	104.89	110.35
13	M	14	BGC	O4-C4-C3	-2.36	104.89	110.35
13	z	2	BGC	C3-C4-C5	-2.36	106.03	110.24
2	o	6	NAG	O5-C1-C2	-2.36	107.57	111.29
13	Z	2	BGC	C3-C4-C5	-2.36	106.03	110.24
13	z	14	BGC	O4-C4-C3	-2.35	104.91	110.35
10	w	8	A2G	O5-C1-C2	-2.35	107.58	111.29
12	Y	5	BGC	O3-C3-C2	-2.35	105.50	109.99
12	l	5	BGC	O3-C3-C2	-2.35	105.50	109.99
3	c	11	NAG	C2-N2-C7	2.34	126.24	122.90
2	b	6	NAG	O5-C1-C2	-2.34	107.59	111.29
12	y	5	BGC	O3-C3-C2	-2.34	105.52	109.99
11	k	15	BGC	C1-C2-C3	2.33	112.54	109.67
11	K	16	NAG	O5-C1-C2	-2.33	107.60	111.29
12	L	5	BGC	O3-C3-C2	-2.33	105.52	109.99
10	W	8	A2G	O5-C1-C2	-2.33	107.60	111.29
13	M	2	BGC	C3-C4-C5	-2.33	106.09	110.24
10	W	18	NAG	O5-C1-C2	2.33	114.96	111.29
11	k	16	NAG	O5-C1-C2	-2.33	107.62	111.29
11	x	16	NAG	O5-C1-C2	-2.32	107.62	111.29
11	k	13	NAG	C1-C2-N2	-2.32	106.53	110.49
11	X	16	NAG	O5-C1-C2	-2.32	107.63	111.29
10	j	19	MAN	C1-O5-C5	2.31	115.32	112.19
2	O	6	NAG	O5-C1-C2	-2.31	107.64	111.29
11	K	13	NAG	C1-C2-N2	-2.30	106.56	110.49
11	X	13	NAG	C1-C2-N2	-2.30	106.56	110.49
2	B	6	NAG	O5-C1-C2	-2.30	107.66	111.29
10	j	17	BGC	C1-O5-C5	2.29	115.29	112.19
11	x	13	NAG	C1-C2-N2	-2.29	106.58	110.49
9	I	6	MAN	C1-C2-C3	2.29	112.48	109.67
12	Y	8	BGC	C1-O5-C5	2.28	115.28	112.19
10	j	6	A2G	C2-N2-C7	2.27	126.14	122.90
11	x	14	BMA	O5-C1-C2	-2.27	107.27	110.77
13	m	5	BGC	C1-O5-C5	-2.27	109.12	112.19
10	w	6	A2G	C2-N2-C7	2.27	126.13	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Z	5	BGC	C1-O5-C5	-2.26	109.13	112.19
13	M	5	BGC	C1-O5-C5	-2.26	109.13	112.19
10	J	19	MAN	O2-C2-C3	-2.25	105.62	110.14
6	s	2	GZL	C1-C2-C3	2.25	105.06	101.63
11	X	14	BMA	O5-C1-C2	-2.25	107.30	110.77
10	w	18	NAG	C1-O5-C5	2.25	115.24	112.19
6	f	2	GZL	C1-C2-C3	2.25	105.06	101.63
11	k	14	BMA	O5-C1-C2	-2.25	107.31	110.77
10	W	6	A2G	C2-N2-C7	2.25	126.10	122.90
13	z	5	BGC	C1-O5-C5	-2.24	109.16	112.19
6	F	2	GZL	C1-C2-C3	2.24	105.04	101.63
10	w	3	XYP	C5-C4-C3	2.24	112.41	109.67
11	X	6	FUB	O2-C2-C1	2.23	117.62	110.97
11	k	6	FUB	O2-C2-C1	2.23	117.62	110.97
11	x	6	FUB	O2-C2-C1	2.23	117.60	110.97
14	0	2	XYP	C1-C2-C3	2.23	112.40	109.67
6	S	2	GZL	C1-C2-C3	2.22	105.02	101.63
11	K	6	FUB	O2-C2-C1	2.22	117.59	110.97
11	K	14	BMA	O5-C1-C2	-2.22	107.34	110.77
10	J	6	A2G	C2-N2-C7	2.22	126.07	122.90
11	X	7	BGC	O5-C1-C2	-2.22	107.34	110.77
14	N	2	XYP	C1-C2-C3	2.21	112.38	109.67
8	H	7	XYP	C1-C2-C3	2.21	112.38	109.67
11	x	7	BGC	O5-C1-C2	-2.21	107.36	110.77
14	n	2	XYP	C1-C2-C3	2.21	112.38	109.67
8	u	7	XYP	C1-C2-C3	2.21	112.38	109.67
7	t	1	XYP	O3-C3-C2	2.20	114.21	109.99
10	W	18	NAG	C2-N2-C7	-2.20	119.77	122.90
11	K	42	MAN	C1-C2-C3	2.20	112.37	109.67
11	K	7	BGC	O5-C1-C2	-2.20	107.37	110.77
7	G	1	XYP	O3-C3-C2	2.20	114.21	109.99
7	g	1	XYP	O3-C3-C2	2.20	114.21	109.99
3	C	7	BGC	C1-O5-C5	2.20	115.17	112.19
11	k	7	BGC	O5-C1-C2	-2.20	107.38	110.77
11	K	1	MAN	C1-C2-C3	2.20	112.37	109.67
14	a	2	XYP	C1-C2-C3	2.20	112.37	109.67
3	p	7	BGC	C1-O5-C5	2.20	115.17	112.19
4	D	22	FUB	C1-C2-C3	2.19	104.97	101.63
3	P	7	BGC	C1-O5-C5	2.19	115.16	112.19
3	c	7	BGC	C1-O5-C5	2.19	115.16	112.19
4	Q	7	NAG	C2-N2-C7	-2.19	119.79	122.90
14	a	8	AHR	C1-C2-C3	2.19	104.96	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	7	XYP	C1-C2-C3	2.18	112.35	109.67
10	j	17	BGC	O5-C5-C4	-2.18	105.52	110.83
4	d	7	NAG	C2-N2-C7	-2.18	119.80	122.90
13	z	14	BGC	O2-C2-C3	-2.18	105.77	110.14
4	d	22	FUB	C1-C2-C3	2.18	104.95	101.63
11	X	1	MAN	C1-C2-C3	2.18	112.34	109.67
4	D	7	NAG	C2-N2-C7	-2.18	119.80	122.90
12	L	8	BGC	O5-C1-C2	2.18	114.13	110.77
11	x	1	MAN	C1-C2-C3	2.18	112.34	109.67
11	k	1	MAN	C1-C2-C3	2.17	112.34	109.67
11	x	42	MAN	C1-C2-C3	2.17	112.34	109.67
4	q	7	NAG	C2-N2-C7	-2.17	119.81	122.90
11	X	42	MAN	C1-C2-C3	2.17	112.34	109.67
11	x	15	BGC	C1-C2-C3	2.17	112.34	109.67
8	U	7	XYP	C1-C2-C3	2.17	112.33	109.67
10	J	18	NAG	C1-C2-N2	-2.17	106.78	110.49
14	0	8	AHR	C1-C2-C3	2.17	104.93	101.63
13	m	14	BGC	O2-C2-C3	-2.17	105.80	110.14
4	q	22	FUB	C1-C2-C3	2.16	104.93	101.63
7	T	1	XYP	O3-C3-C2	2.16	114.14	109.99
4	Q	22	FUB	C1-C2-C3	2.16	104.92	101.63
9	I	2	MAN	C1-C2-C3	2.16	112.32	109.67
13	M	14	BGC	O2-C2-C3	-2.16	105.81	110.14
13	Z	14	BGC	O2-C2-C3	-2.16	105.81	110.14
11	k	42	MAN	C1-C2-C3	2.16	112.32	109.67
14	n	8	AHR	C1-C2-C3	2.15	104.91	101.63
4	Q	2	AHR	C1-C2-C3	2.15	104.90	101.63
14	N	8	AHR	C1-C2-C3	2.15	104.90	101.63
13	z	5	BGC	C1-C2-C3	-2.15	107.03	109.67
4	Q	26	AHR	C1-C2-C3	2.14	104.90	101.63
4	d	2	AHR	C1-C2-C3	2.14	104.89	101.63
9	v	3	BGC	O2-C2-C3	2.14	114.42	110.14
9	V	2	MAN	C1-C2-C3	2.14	112.29	109.67
10	w	19	MAN	C1-O5-C5	2.14	115.09	112.19
9	I	3	BGC	O2-C2-C3	2.13	114.41	110.14
4	D	26	AHR	C1-C2-C3	2.13	104.88	101.63
2	B	2	NAG	C4-C3-C2	-2.13	107.89	111.02
7	t	8	MAN	C1-O5-C5	2.13	115.08	112.19
9	i	3	BGC	O2-C2-C3	2.13	114.41	110.14
6	F	3	FUB	C1-C2-C3	2.13	104.87	101.63
7	G	8	MAN	C1-O5-C5	2.13	115.07	112.19
7	T	8	MAN	C1-O5-C5	2.12	115.07	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	s	3	FUB	C1-C2-C3	2.12	104.86	101.63
13	Z	5	BGC	C1-C2-C3	-2.12	107.06	109.67
11	K	6	FUB	C1-C2-C3	-2.12	98.40	101.63
6	s	1	MAN	C1-C2-C3	2.12	112.27	109.67
13	M	5	BGC	C1-C2-C3	-2.12	107.06	109.67
9	v	4	NAG	C1-O5-C5	2.12	115.06	112.19
11	K	38	NAG	C1-O5-C5	2.12	115.06	112.19
4	D	17	AHR	C1-C2-C3	2.12	104.85	101.63
8	u	11	MAN	C1-C2-C3	2.12	112.27	109.67
4	Q	17	AHR	C1-C2-C3	2.12	104.85	101.63
6	f	1	MAN	C1-C2-C3	2.11	112.27	109.67
11	K	18	XYP	C1-C2-C3	2.11	112.26	109.67
9	V	3	BGC	O2-C2-C3	2.11	114.37	110.14
14	a	15	AHR	C1-C2-C3	2.11	104.85	101.63
6	S	3	FUB	C1-C2-C3	2.11	104.85	101.63
4	q	26	AHR	C1-C2-C3	2.11	104.85	101.63
11	X	38	NAG	C1-O5-C5	2.11	115.05	112.19
8	H	11	MAN	C1-C2-C3	2.11	112.26	109.67
4	d	26	AHR	C1-C2-C3	2.11	104.84	101.63
9	i	4	NAG	C1-O5-C5	2.11	115.05	112.19
13	m	5	BGC	C1-C2-C3	-2.11	107.08	109.67
8	U	11	MAN	C1-C2-C3	2.11	112.25	109.67
9	v	2	MAN	C1-C2-C3	2.11	112.25	109.67
6	f	3	FUB	C1-C2-C3	2.11	104.84	101.63
7	g	8	MAN	C1-O5-C5	2.10	115.04	112.19
4	q	17	AHR	C1-C2-C3	2.10	104.83	101.63
11	k	6	FUB	C1-C2-C3	-2.10	98.43	101.63
2	b	2	NAG	C4-C3-C2	-2.10	107.94	111.02
11	x	6	FUB	C1-C2-C3	-2.10	98.43	101.63
2	O	2	NAG	C4-C3-C2	-2.10	107.94	111.02
4	D	2	AHR	C1-C2-C3	2.10	104.83	101.63
11	x	38	NAG	C1-O5-C5	2.10	115.03	112.19
7	t	10	MAN	C1-O5-C5	2.10	115.03	112.19
2	o	2	NAG	C4-C3-C2	-2.10	107.95	111.02
7	g	10	MAN	C1-O5-C5	2.10	115.03	112.19
9	I	4	NAG	C1-O5-C5	2.09	115.03	112.19
4	q	2	AHR	C1-C2-C3	2.09	104.82	101.63
8	H	8	GAL	C1-C2-C3	2.09	112.24	109.67
3	C	12	MAN	O5-C5-C4	-2.09	105.74	110.83
9	i	2	MAN	C1-C2-C3	2.09	112.24	109.67
6	F	1	MAN	C1-C2-C3	2.09	112.23	109.67
7	t	15	MAN	C1-C2-C3	2.09	112.23	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	10	MAN	C1-O5-C5	2.09	115.02	112.19
14	0	15	AHR	C1-C2-C3	2.09	104.81	101.63
14	N	15	AHR	C1-C2-C3	2.09	104.81	101.63
11	X	6	FUB	C1-C2-C3	-2.09	98.45	101.63
6	S	1	MAN	C1-C2-C3	2.09	112.23	109.67
11	x	18	XYP	C1-C2-C3	2.09	112.23	109.67
8	h	11	MAN	C1-C2-C3	2.09	112.23	109.67
11	X	8	BGC	O5-C5-C6	2.08	110.47	107.20
11	k	38	NAG	C1-O5-C5	2.08	115.01	112.19
4	d	18	MAN	C1-C2-C3	2.08	112.22	109.67
14	n	3	A2G	O3-C3-C2	-2.08	105.17	109.47
8	h	8	GAL	C1-C2-C3	2.08	112.22	109.67
11	k	8	BGC	O5-C5-C6	2.08	110.46	107.20
8	H	11	MAN	C1-O5-C5	2.07	115.00	112.19
11	k	18	XYP	C1-C2-C3	2.07	112.21	109.67
14	N	3	A2G	O3-C3-C2	-2.07	105.18	109.47
4	Q	18	MAN	C1-C2-C3	2.07	112.21	109.67
9	V	4	NAG	C1-O5-C5	2.07	115.00	112.19
8	U	8	GAL	C1-C2-C3	2.07	112.21	109.67
7	T	15	MAN	C1-C2-C3	2.06	112.20	109.67
4	d	17	AHR	C1-C2-C3	2.06	104.77	101.63
13	Z	3	MAN	C1-C2-C3	2.06	112.20	109.67
7	g	15	MAN	C1-C2-C3	2.06	112.20	109.67
13	m	3	MAN	C1-C2-C3	2.06	112.20	109.67
14	n	15	AHR	C1-C2-C3	2.06	104.77	101.63
8	u	8	GAL	C1-C2-C3	2.06	112.20	109.67
10	j	3	XYP	C5-C4-C3	2.06	112.20	109.67
4	q	18	MAN	C1-C2-C3	2.06	112.19	109.67
13	z	11	MAN	C1-C2-C3	2.06	112.19	109.67
11	x	22	MAN	C1-O5-C5	2.06	114.98	112.19
7	T	11	MAN	C1-C2-C3	2.06	112.19	109.67
2	b	4	MAN	C1-C2-C3	2.05	112.19	109.67
11	X	22	MAN	C1-O5-C5	2.05	114.97	112.19
14	a	3	A2G	O3-C3-C2	-2.05	105.22	109.47
11	x	8	BGC	O5-C5-C6	2.05	110.42	107.20
7	t	3	A2G	C2-N2-C7	-2.05	119.98	122.90
5	R	1	MAN	C1-C2-C3	2.05	112.19	109.67
13	z	3	MAN	C1-C2-C3	2.05	112.19	109.67
14	0	3	A2G	O3-C3-C2	-2.05	105.23	109.47
7	G	15	MAN	C1-C2-C3	2.05	112.18	109.67
13	Z	11	MAN	C1-C2-C3	2.05	112.18	109.67
10	J	13	MAN	C1-C2-C3	2.05	112.18	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	3	MAN	C1-C2-C3	2.05	112.18	109.67
8	U	7	XYP	O2-C2-C3	2.05	114.24	110.14
7	G	10	MAN	C1-O5-C5	2.04	114.96	112.19
4	D	12	AHR	C1-C2-C3	2.04	104.74	101.63
2	O	4	MAN	C1-C2-C3	2.04	112.18	109.67
11	X	18	XYP	C1-C2-C3	2.04	112.17	109.67
13	M	11	MAN	C1-C2-C3	2.04	112.17	109.67
4	D	18	MAN	C1-C2-C3	2.04	112.17	109.67
7	T	3	A2G	C2-N2-C7	-2.04	120.00	122.90
13	m	11	MAN	C1-C2-C3	2.04	112.17	109.67
5	r	1	MAN	C1-C2-C3	2.04	112.17	109.67
7	G	3	A2G	C2-N2-C7	-2.03	120.01	122.90
2	b	9	MAN	C1-C2-C3	2.03	112.17	109.67
7	g	11	MAN	C1-C2-C3	2.03	112.16	109.67
7	g	3	A2G	C2-N2-C7	-2.03	120.01	122.90
10	W	13	MAN	C1-C2-C3	2.03	112.16	109.67
10	w	13	MAN	C1-C2-C3	2.03	112.16	109.67
11	X	29	MAN	C1-C2-C3	2.03	112.16	109.67
8	u	11	MAN	C1-O5-C5	2.03	114.94	112.19
8	H	7	XYP	O2-C2-C3	2.03	114.20	110.14
8	u	7	XYP	O2-C2-C3	2.03	114.20	110.14
8	U	11	MAN	C1-O5-C5	2.03	114.94	112.19
11	K	8	BGC	O5-C5-C6	2.03	110.38	107.20
7	g	15	MAN	C1-O5-C5	2.03	114.94	112.19
11	k	22	MAN	C1-O5-C5	2.03	114.94	112.19
12	y	7	BGC	C1-O5-C5	-2.02	109.45	112.19
11	x	25	BGC	C1-C2-C3	2.02	112.15	109.67
11	x	29	MAN	C1-C2-C3	2.02	112.15	109.67
4	q	12	AHR	C1-C2-C3	2.02	104.71	101.63
7	t	11	MAN	C1-C2-C3	2.02	112.15	109.67
13	m	13	XYP	C1-C2-C3	2.02	112.15	109.67
4	Q	12	AHR	C1-C2-C3	2.02	104.71	101.63
11	k	29	MAN	C1-C2-C3	2.02	112.15	109.67
10	j	13	MAN	C1-C2-C3	2.02	112.15	109.67
7	T	9	MAN	C1-O5-C5	2.02	114.93	112.19
10	W	13	MAN	C1-O5-C5	2.02	114.93	112.19
11	X	25	BGC	C1-C2-C3	2.02	112.15	109.67
12	L	7	BGC	C1-O5-C5	-2.02	109.46	112.19
7	T	15	MAN	C1-O5-C5	2.02	114.92	112.19
14	N	9	AHR	C1-C2-C3	2.02	104.70	101.63
5	e	1	MAN	C1-C2-C3	2.02	112.14	109.67
12	Y	7	BGC	C1-O5-C5	-2.01	109.46	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	1	MAN	C1-O5-C5	2.01	114.92	112.19
4	d	12	AHR	C1-C2-C3	2.01	104.69	101.63
8	h	7	XYP	O2-C2-C3	2.01	114.16	110.14
12	L	8	BGC	C3-C4-C5	-2.01	106.65	110.24
2	O	9	MAN	C1-C2-C3	2.01	112.14	109.67
2	o	4	MAN	C1-C2-C3	2.01	112.14	109.67
5	E	1	MAN	C1-C2-C3	2.01	112.14	109.67
4	Q	18	MAN	C1-O5-C5	2.01	114.91	112.19
8	h	17	A2G	O5-C1-C2	2.01	114.46	111.29
10	W	8	A2G	C2-N2-C7	-2.01	120.05	122.90
11	K	25	BGC	C1-C2-C3	2.01	112.13	109.67
11	K	22	MAN	C1-O5-C5	2.01	114.91	112.19
2	o	9	MAN	C1-C2-C3	2.01	112.13	109.67
8	h	11	MAN	C1-O5-C5	2.00	114.91	112.19
2	B	4	MAN	C1-C2-C3	2.00	112.13	109.67
14	n	9	AHR	C1-C2-C3	2.00	104.68	101.63
14	0	9	AHR	C1-C2-C3	2.00	104.68	101.63
9	i	6	MAN	C1-C2-C3	2.00	112.13	109.67
13	m	10	BGC	C2-C3-C4	-2.00	107.43	110.89
14	a	9	AHR	C1-C2-C3	2.00	104.68	101.63

There are no chirality outliers.

All (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
3	c	21	NAG	O7-C7-N2-C2
3	p	11	NAG	O7-C7-N2-C2
3	p	21	NAG	C8-C7-N2-C2
3	p	21	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	R	2	NAG	C8-C7-N2-C2
5	R	2	NAG	O7-C7-N2-C2
5	e	2	NAG	C8-C7-N2-C2
5	e	2	NAG	O7-C7-N2-C2
5	r	2	NAG	C8-C7-N2-C2
5	r	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	F	2	GZL	C3-C4-C5-C6
6	F	2	GZL	O4-C4-C5-C6
6	F	2	GZL	C3-C4-C5-O5
6	F	2	GZL	O4-C4-C5-O5
6	S	2	GZL	C3-C4-C5-C6
6	S	2	GZL	O4-C4-C5-C6
6	S	2	GZL	C3-C4-C5-O5
6	S	2	GZL	O4-C4-C5-O5
6	f	2	GZL	C3-C4-C5-C6
6	f	2	GZL	O4-C4-C5-C6
6	f	2	GZL	C3-C4-C5-O5
6	f	2	GZL	O4-C4-C5-O5
6	s	2	GZL	C3-C4-C5-C6
6	s	2	GZL	O4-C4-C5-C6
6	s	2	GZL	C3-C4-C5-O5
6	s	2	GZL	O4-C4-C5-O5
8	H	2	NAG	C3-C2-N2-C7
8	H	2	NAG	C8-C7-N2-C2
8	H	2	NAG	O7-C7-N2-C2
8	H	14	NAG	C8-C7-N2-C2
8	H	14	NAG	O7-C7-N2-C2
8	U	2	NAG	C3-C2-N2-C7
8	U	2	NAG	C8-C7-N2-C2
8	U	2	NAG	O7-C7-N2-C2
8	U	14	NAG	C8-C7-N2-C2
8	U	14	NAG	O7-C7-N2-C2
8	h	2	NAG	C3-C2-N2-C7
8	h	2	NAG	C8-C7-N2-C2
8	h	2	NAG	O7-C7-N2-C2
8	h	14	NAG	C8-C7-N2-C2
8	h	14	NAG	O7-C7-N2-C2
8	u	2	NAG	C3-C2-N2-C7
8	u	2	NAG	C8-C7-N2-C2
8	u	2	NAG	O7-C7-N2-C2
8	u	14	NAG	C8-C7-N2-C2
8	u	14	NAG	O7-C7-N2-C2
9	I	4	NAG	C3-C2-N2-C7
9	I	4	NAG	C8-C7-N2-C2
9	I	4	NAG	O7-C7-N2-C2
9	V	4	NAG	C3-C2-N2-C7
9	V	4	NAG	C8-C7-N2-C2
9	V	4	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
9	i	4	NAG	C3-C2-N2-C7
9	i	4	NAG	C8-C7-N2-C2
9	i	4	NAG	O7-C7-N2-C2
9	v	4	NAG	C3-C2-N2-C7
9	v	4	NAG	C8-C7-N2-C2
9	v	4	NAG	O7-C7-N2-C2
10	J	11	NAG	C8-C7-N2-C2
10	J	11	NAG	O7-C7-N2-C2
10	J	18	NAG	C8-C7-N2-C2
10	J	18	NAG	O7-C7-N2-C2
10	W	11	NAG	C8-C7-N2-C2
10	W	11	NAG	O7-C7-N2-C2
10	W	18	NAG	C8-C7-N2-C2
10	W	18	NAG	O7-C7-N2-C2
10	j	11	NAG	C8-C7-N2-C2
10	j	11	NAG	O7-C7-N2-C2
10	j	18	NAG	C8-C7-N2-C2
10	j	18	NAG	O7-C7-N2-C2
10	w	11	NAG	C8-C7-N2-C2
10	w	11	NAG	O7-C7-N2-C2
10	w	18	NAG	C8-C7-N2-C2
10	w	18	NAG	O7-C7-N2-C2
11	K	5	NAG	C8-C7-N2-C2
11	K	5	NAG	O7-C7-N2-C2
11	K	16	NAG	C8-C7-N2-C2
11	K	16	NAG	O7-C7-N2-C2
11	K	20	NAG	O7-C7-N2-C2
11	K	28	NAG	C8-C7-N2-C2
11	K	28	NAG	O7-C7-N2-C2
11	K	34	NAG	C8-C7-N2-C2
11	K	34	NAG	O7-C7-N2-C2
11	X	5	NAG	C8-C7-N2-C2
11	X	5	NAG	O7-C7-N2-C2
11	X	16	NAG	C8-C7-N2-C2
11	X	16	NAG	O7-C7-N2-C2
11	X	20	NAG	O7-C7-N2-C2
11	X	28	NAG	C8-C7-N2-C2
11	X	28	NAG	O7-C7-N2-C2
11	X	34	NAG	C8-C7-N2-C2
11	X	34	NAG	O7-C7-N2-C2
11	k	5	NAG	C8-C7-N2-C2
11	k	5	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
11	k	16	NAG	C8-C7-N2-C2
11	k	16	NAG	O7-C7-N2-C2
11	k	20	NAG	O7-C7-N2-C2
11	k	28	NAG	C8-C7-N2-C2
11	k	28	NAG	O7-C7-N2-C2
11	k	34	NAG	C8-C7-N2-C2
11	k	34	NAG	O7-C7-N2-C2
11	x	5	NAG	C8-C7-N2-C2
11	x	5	NAG	O7-C7-N2-C2
11	x	16	NAG	C8-C7-N2-C2
11	x	16	NAG	O7-C7-N2-C2
11	x	20	NAG	O7-C7-N2-C2
11	x	28	NAG	C8-C7-N2-C2
11	x	28	NAG	O7-C7-N2-C2
11	x	34	NAG	C8-C7-N2-C2
11	x	34	NAG	O7-C7-N2-C2
12	L	9	NAG	C8-C7-N2-C2
12	L	9	NAG	O7-C7-N2-C2
12	Y	9	NAG	C8-C7-N2-C2
12	Y	9	NAG	O7-C7-N2-C2
12	l	9	NAG	C8-C7-N2-C2
12	l	9	NAG	O7-C7-N2-C2
12	y	9	NAG	C8-C7-N2-C2
12	y	9	NAG	O7-C7-N2-C2
13	M	9	NAG	C8-C7-N2-C2
13	M	9	NAG	O7-C7-N2-C2
13	Z	9	NAG	C8-C7-N2-C2
13	Z	9	NAG	O7-C7-N2-C2
13	m	9	NAG	C8-C7-N2-C2
13	m	9	NAG	O7-C7-N2-C2
13	z	9	NAG	C8-C7-N2-C2
13	z	9	NAG	O7-C7-N2-C2
14	N	7	NAG	C3-C2-N2-C7
14	N	7	NAG	C8-C7-N2-C2
14	N	7	NAG	O7-C7-N2-C2
14	N	18	NAG	C8-C7-N2-C2
14	N	18	NAG	O7-C7-N2-C2
14	N	19	NAG	C3-C2-N2-C7
14	N	19	NAG	C8-C7-N2-C2
14	N	19	NAG	O7-C7-N2-C2
14	a	7	NAG	C3-C2-N2-C7
14	a	7	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
14	a	7	NAG	O7-C7-N2-C2
14	a	18	NAG	C8-C7-N2-C2
14	a	18	NAG	O7-C7-N2-C2
14	a	19	NAG	C3-C2-N2-C7
14	a	19	NAG	C8-C7-N2-C2
14	a	19	NAG	O7-C7-N2-C2
14	n	7	NAG	C3-C2-N2-C7
14	n	7	NAG	C8-C7-N2-C2
14	n	7	NAG	O7-C7-N2-C2
14	n	18	NAG	C8-C7-N2-C2
14	n	18	NAG	O7-C7-N2-C2
14	n	19	NAG	C3-C2-N2-C7
14	n	19	NAG	C8-C7-N2-C2
14	n	19	NAG	O7-C7-N2-C2
14	0	7	NAG	C3-C2-N2-C7
14	0	7	NAG	C8-C7-N2-C2
14	0	7	NAG	O7-C7-N2-C2
14	0	18	NAG	C8-C7-N2-C2
14	0	18	NAG	O7-C7-N2-C2
14	0	19	NAG	C3-C2-N2-C7
14	0	19	NAG	C8-C7-N2-C2
14	0	19	NAG	O7-C7-N2-C2
3	p	11	NAG	C8-C7-N2-C2
4	D	14	NAG	C8-C7-N2-C2
4	D	14	NAG	O7-C7-N2-C2
4	Q	14	NAG	C8-C7-N2-C2
4	Q	14	NAG	O7-C7-N2-C2
4	d	14	NAG	C8-C7-N2-C2
4	d	14	NAG	O7-C7-N2-C2
4	q	14	NAG	C8-C7-N2-C2
4	q	14	NAG	O7-C7-N2-C2
11	K	20	NAG	C8-C7-N2-C2
11	K	38	NAG	C8-C7-N2-C2
11	K	38	NAG	O7-C7-N2-C2
11	X	20	NAG	C8-C7-N2-C2
11	X	38	NAG	C8-C7-N2-C2
11	X	38	NAG	O7-C7-N2-C2
11	k	20	NAG	C8-C7-N2-C2
11	k	38	NAG	C8-C7-N2-C2
11	k	38	NAG	O7-C7-N2-C2
11	x	20	NAG	C8-C7-N2-C2
11	x	38	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
11	x	38	NAG	O7-C7-N2-C2
2	B	6	NAG	O5-C5-C6-O6
2	O	6	NAG	O5-C5-C6-O6
2	b	6	NAG	O5-C5-C6-O6
2	o	6	NAG	O5-C5-C6-O6
14	N	12	BGC	O5-C5-C6-O6
14	a	12	BGC	O5-C5-C6-O6
3	c	11	NAG	C1-C2-N2-C7
11	K	11	BGC	O5-C5-C6-O6
11	X	11	BGC	O5-C5-C6-O6
11	k	11	BGC	O5-C5-C6-O6
11	x	11	BGC	O5-C5-C6-O6
13	M	5	BGC	O5-C5-C6-O6
13	Z	5	BGC	O5-C5-C6-O6
13	m	5	BGC	O5-C5-C6-O6
13	z	5	BGC	O5-C5-C6-O6
11	K	12	BMA	C4-C5-C6-O6
11	X	12	BMA	C4-C5-C6-O6
11	k	12	BMA	C4-C5-C6-O6
11	x	12	BMA	C4-C5-C6-O6
4	D	13	FUB	C3-C4-C5-O5
4	D	16	FUB	C3-C4-C5-O5
4	Q	13	FUB	C3-C4-C5-O5
4	Q	16	FUB	C3-C4-C5-O5
4	d	13	FUB	C3-C4-C5-O5
4	d	16	FUB	C3-C4-C5-O5
4	q	13	FUB	C3-C4-C5-O5
4	q	16	FUB	C3-C4-C5-O5
8	H	20	MAN	O5-C5-C6-O6
8	U	20	MAN	O5-C5-C6-O6
8	h	20	MAN	O5-C5-C6-O6
8	u	20	MAN	O5-C5-C6-O6
12	L	6	MAN	O5-C5-C6-O6
12	Y	6	MAN	O5-C5-C6-O6
12	l	6	MAN	O5-C5-C6-O6
12	y	6	MAN	O5-C5-C6-O6
3	C	11	NAG	C8-C7-N2-C2
3	P	11	NAG	C8-C7-N2-C2
14	N	1	MAN	O5-C5-C6-O6
14	a	1	MAN	O5-C5-C6-O6
14	n	1	MAN	O5-C5-C6-O6
14	0	1	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
12	L	7	BGC	O5-C5-C6-O6
12	Y	7	BGC	O5-C5-C6-O6
12	l	7	BGC	O5-C5-C6-O6
12	y	7	BGC	O5-C5-C6-O6
2	B	6	NAG	C4-C5-C6-O6
10	J	6	A2G	C4-C5-C6-O6
10	W	6	A2G	C4-C5-C6-O6
10	j	6	A2G	C4-C5-C6-O6
10	w	6	A2G	C4-C5-C6-O6
4	D	16	FUB	O4-C4-C5-O5
4	Q	16	FUB	O4-C4-C5-O5
4	d	16	FUB	O4-C4-C5-O5
4	q	16	FUB	O4-C4-C5-O5
4	D	11	MAN	O5-C5-C6-O6
4	Q	11	MAN	O5-C5-C6-O6
4	d	11	MAN	O5-C5-C6-O6
4	q	11	MAN	O5-C5-C6-O6
10	J	11	NAG	O5-C5-C6-O6
10	W	11	NAG	O5-C5-C6-O6
10	j	11	NAG	O5-C5-C6-O6
10	w	11	NAG	O5-C5-C6-O6
2	O	6	NAG	C4-C5-C6-O6
2	b	6	NAG	C4-C5-C6-O6
2	o	6	NAG	C4-C5-C6-O6
11	K	11	BGC	C4-C5-C6-O6
11	X	11	BGC	C4-C5-C6-O6
11	k	11	BGC	C4-C5-C6-O6
11	x	11	BGC	C4-C5-C6-O6
13	M	5	BGC	C4-C5-C6-O6
13	Z	5	BGC	C4-C5-C6-O6
13	m	5	BGC	C4-C5-C6-O6
13	z	5	BGC	C4-C5-C6-O6
14	N	12	BGC	C4-C5-C6-O6
4	D	7	NAG	O5-C5-C6-O6
4	D	8	BGC	O5-C5-C6-O6
4	Q	7	NAG	O5-C5-C6-O6
4	d	7	NAG	O5-C5-C6-O6
4	q	7	NAG	O5-C5-C6-O6
10	J	10	MAN	O5-C5-C6-O6
10	W	10	MAN	O5-C5-C6-O6
10	j	10	MAN	O5-C5-C6-O6
10	w	10	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	d	8	BGC	O5-C5-C6-O6
10	J	6	A2G	O5-C5-C6-O6
10	W	6	A2G	O5-C5-C6-O6
10	j	6	A2G	O5-C5-C6-O6
10	w	6	A2G	O5-C5-C6-O6
11	K	37	MAN	O5-C5-C6-O6
11	X	37	MAN	O5-C5-C6-O6
11	k	37	MAN	O5-C5-C6-O6
11	x	37	MAN	O5-C5-C6-O6
10	J	10	MAN	C4-C5-C6-O6
10	W	10	MAN	C4-C5-C6-O6
10	j	10	MAN	C4-C5-C6-O6
10	w	10	MAN	C4-C5-C6-O6
12	L	7	BGC	C4-C5-C6-O6
12	Y	7	BGC	C4-C5-C6-O6
12	l	7	BGC	C4-C5-C6-O6
12	y	7	BGC	C4-C5-C6-O6
14	N	21	AHR	O4-C4-C5-O5
14	a	21	AHR	O4-C4-C5-O5
14	n	21	AHR	O4-C4-C5-O5
14	0	21	AHR	O4-C4-C5-O5
3	P	11	NAG	O7-C7-N2-C2
6	F	4	NAG	C8-C7-N2-C2
6	S	4	NAG	C8-C7-N2-C2
6	f	4	NAG	C8-C7-N2-C2
6	s	4	NAG	C8-C7-N2-C2
7	G	3	A2G	C8-C7-N2-C2
7	T	3	A2G	C8-C7-N2-C2
7	g	3	A2G	C8-C7-N2-C2
7	t	3	A2G	C8-C7-N2-C2
4	Q	8	BGC	O5-C5-C6-O6
4	q	8	BGC	O5-C5-C6-O6
11	K	9	BMA	O5-C5-C6-O6
11	X	9	BMA	O5-C5-C6-O6
11	k	9	BMA	O5-C5-C6-O6
11	x	9	BMA	O5-C5-C6-O6
14	a	12	BGC	C4-C5-C6-O6
3	C	11	NAG	C1-C2-N2-C7
3	P	11	NAG	C1-C2-N2-C7
3	p	11	NAG	C1-C2-N2-C7
4	D	14	NAG	C1-C2-N2-C7
4	Q	14	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	d	14	NAG	C1-C2-N2-C7
4	q	14	NAG	C1-C2-N2-C7
11	K	28	NAG	C1-C2-N2-C7
11	X	28	NAG	C1-C2-N2-C7
11	k	28	NAG	C1-C2-N2-C7
11	x	28	NAG	C1-C2-N2-C7
13	M	4	NAG	C1-C2-N2-C7
13	Z	4	NAG	C1-C2-N2-C7
13	m	4	NAG	C1-C2-N2-C7
13	z	4	NAG	C1-C2-N2-C7
11	K	16	NAG	O5-C5-C6-O6
11	X	16	NAG	O5-C5-C6-O6
11	k	16	NAG	O5-C5-C6-O6
11	x	16	NAG	O5-C5-C6-O6
10	J	11	NAG	C4-C5-C6-O6
10	W	11	NAG	C4-C5-C6-O6
10	j	11	NAG	C4-C5-C6-O6
10	w	11	NAG	C4-C5-C6-O6
11	K	19	BGC	C4-C5-C6-O6
11	X	19	BGC	C4-C5-C6-O6
11	k	19	BGC	C4-C5-C6-O6
11	x	19	BGC	C4-C5-C6-O6
4	D	13	FUB	O4-C4-C5-O5
4	Q	13	FUB	O4-C4-C5-O5
4	d	13	FUB	O4-C4-C5-O5
4	q	13	FUB	O4-C4-C5-O5
4	D	11	MAN	C4-C5-C6-O6
4	Q	11	MAN	C4-C5-C6-O6
4	d	11	MAN	C4-C5-C6-O6
4	q	11	MAN	C4-C5-C6-O6
11	K	16	NAG	C4-C5-C6-O6
11	X	16	NAG	C4-C5-C6-O6
11	k	16	NAG	C4-C5-C6-O6
11	x	16	NAG	C4-C5-C6-O6
12	L	6	MAN	C4-C5-C6-O6
12	Y	6	MAN	C4-C5-C6-O6
12	l	6	MAN	C4-C5-C6-O6
12	y	6	MAN	C4-C5-C6-O6
11	K	37	MAN	C4-C5-C6-O6
11	X	37	MAN	C4-C5-C6-O6
11	k	37	MAN	C4-C5-C6-O6
11	x	37	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	11	NAG	O7-C7-N2-C2
3	c	11	NAG	C8-C7-N2-C2
6	F	4	NAG	O7-C7-N2-C2
6	S	4	NAG	O7-C7-N2-C2
6	f	4	NAG	O7-C7-N2-C2
6	s	4	NAG	O7-C7-N2-C2
14	N	1	MAN	C4-C5-C6-O6
14	a	1	MAN	C4-C5-C6-O6
14	n	1	MAN	C4-C5-C6-O6
14	0	1	MAN	C4-C5-C6-O6
3	c	11	NAG	O5-C5-C6-O6
4	D	7	NAG	C4-C5-C6-O6
4	Q	7	NAG	C4-C5-C6-O6
4	d	7	NAG	C4-C5-C6-O6
4	q	7	NAG	C4-C5-C6-O6
3	C	11	NAG	O5-C5-C6-O6
11	K	20	NAG	O5-C5-C6-O6
11	X	20	NAG	O5-C5-C6-O6
11	k	20	NAG	O5-C5-C6-O6
11	x	20	NAG	O5-C5-C6-O6
11	K	9	BMA	C4-C5-C6-O6
11	X	9	BMA	C4-C5-C6-O6
11	k	9	BMA	C4-C5-C6-O6
11	x	9	BMA	C4-C5-C6-O6
7	G	16	NAG	O5-C5-C6-O6
7	T	16	NAG	O5-C5-C6-O6
7	g	16	NAG	O5-C5-C6-O6
7	t	16	NAG	O5-C5-C6-O6
3	c	11	NAG	C4-C5-C6-O6
7	G	3	A2G	O7-C7-N2-C2
7	T	3	A2G	O7-C7-N2-C2
7	g	3	A2G	O7-C7-N2-C2
7	t	3	A2G	O7-C7-N2-C2
11	K	19	BGC	O5-C5-C6-O6
11	X	19	BGC	O5-C5-C6-O6
11	k	19	BGC	O5-C5-C6-O6
11	x	19	BGC	O5-C5-C6-O6
3	p	11	NAG	O5-C5-C6-O6
3	C	11	NAG	C4-C5-C6-O6
8	H	20	MAN	C4-C5-C6-O6
8	U	20	MAN	C4-C5-C6-O6
8	h	20	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	u	20	MAN	C4-C5-C6-O6
3	P	2	BGC	O5-C5-C6-O6
3	c	2	BGC	O5-C5-C6-O6
3	p	2	BGC	O5-C5-C6-O6
11	K	20	NAG	C4-C5-C6-O6
11	X	20	NAG	C4-C5-C6-O6
11	x	20	NAG	C4-C5-C6-O6
14	N	21	AHR	C3-C4-C5-O5
14	a	21	AHR	C3-C4-C5-O5
14	n	21	AHR	C3-C4-C5-O5
14	0	21	AHR	C3-C4-C5-O5
3	C	2	BGC	O5-C5-C6-O6
11	k	20	NAG	C4-C5-C6-O6
3	P	11	NAG	O5-C5-C6-O6
3	c	11	NAG	O7-C7-N2-C2
11	X	12	BMA	O5-C5-C6-O6
11	k	12	BMA	O5-C5-C6-O6
11	x	12	BMA	O5-C5-C6-O6
10	W	8	A2G	O5-C5-C6-O6
10	j	8	A2G	O5-C5-C6-O6
10	w	8	A2G	O5-C5-C6-O6
10	J	8	A2G	O5-C5-C6-O6
11	K	12	BMA	O5-C5-C6-O6
14	N	18	NAG	O5-C5-C6-O6
14	a	18	NAG	O5-C5-C6-O6
14	n	18	NAG	O5-C5-C6-O6
14	0	18	NAG	O5-C5-C6-O6
3	C	13	NAG	C8-C7-N2-C2
3	P	13	NAG	C8-C7-N2-C2
3	c	13	NAG	C8-C7-N2-C2
3	p	13	NAG	C8-C7-N2-C2
10	j	19	MAN	C4-C5-C6-O6
11	K	14	BMA	O5-C5-C6-O6
11	K	21	BMA	O5-C5-C6-O6
11	X	14	BMA	O5-C5-C6-O6
11	X	21	BMA	O5-C5-C6-O6
11	k	14	BMA	O5-C5-C6-O6
11	k	21	BMA	O5-C5-C6-O6
11	x	14	BMA	O5-C5-C6-O6
11	x	21	BMA	O5-C5-C6-O6
11	K	6	FUB	O4-C4-C5-O5
11	X	6	FUB	O4-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
11	k	6	FUB	O4-C4-C5-O5
11	x	6	FUB	O4-C4-C5-O5
11	X	28	NAG	O5-C5-C6-O6
11	k	28	NAG	O5-C5-C6-O6
11	x	28	NAG	O5-C5-C6-O6
11	K	28	NAG	O5-C5-C6-O6
14	N	19	NAG	C1-C2-N2-C7
14	a	19	NAG	C1-C2-N2-C7
14	n	19	NAG	C1-C2-N2-C7
14	0	19	NAG	C1-C2-N2-C7
11	K	13	NAG	C4-C5-C6-O6
11	X	13	NAG	C4-C5-C6-O6
11	k	13	NAG	C4-C5-C6-O6
11	x	13	NAG	C4-C5-C6-O6
14	N	7	NAG	C1-C2-N2-C7
14	a	7	NAG	C1-C2-N2-C7
14	n	7	NAG	C1-C2-N2-C7
14	0	7	NAG	C1-C2-N2-C7
11	X	34	NAG	O5-C5-C6-O6
11	k	34	NAG	O5-C5-C6-O6
11	x	34	NAG	O5-C5-C6-O6
11	K	34	NAG	O5-C5-C6-O6
11	K	1	MAN	O5-C5-C6-O6
11	X	1	MAN	O5-C5-C6-O6
11	k	1	MAN	O5-C5-C6-O6
11	x	1	MAN	O5-C5-C6-O6
3	p	11	NAG	C4-C5-C6-O6
9	I	4	NAG	C1-C2-N2-C7
9	V	4	NAG	C1-C2-N2-C7
9	i	4	NAG	C1-C2-N2-C7
9	v	4	NAG	C1-C2-N2-C7
10	J	7	GAL	O5-C5-C6-O6
10	W	7	GAL	O5-C5-C6-O6
10	j	7	GAL	O5-C5-C6-O6
10	w	7	GAL	O5-C5-C6-O6
3	C	7	BGC	O5-C5-C6-O6
3	P	7	BGC	O5-C5-C6-O6
3	c	7	BGC	O5-C5-C6-O6
3	p	7	BGC	O5-C5-C6-O6
4	D	5	BGC	O5-C5-C6-O6
4	D	20	BGC	O5-C5-C6-O6
4	Q	5	BGC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	Q	20	BGC	O5-C5-C6-O6
4	d	5	BGC	O5-C5-C6-O6
4	d	20	BGC	O5-C5-C6-O6
4	q	5	BGC	O5-C5-C6-O6
4	q	20	BGC	O5-C5-C6-O6
7	G	7	A2G	O5-C5-C6-O6
7	T	7	A2G	O5-C5-C6-O6
7	g	7	A2G	O5-C5-C6-O6
7	t	7	A2G	O5-C5-C6-O6
11	K	31	BGC	O5-C5-C6-O6
11	X	31	BGC	O5-C5-C6-O6
11	k	31	BGC	O5-C5-C6-O6
11	x	31	BGC	O5-C5-C6-O6
7	G	18	BGC	O5-C5-C6-O6
7	T	18	BGC	O5-C5-C6-O6
7	g	18	BGC	O5-C5-C6-O6
3	C	19	BGC	O5-C5-C6-O6
3	P	19	BGC	O5-C5-C6-O6
3	c	19	BGC	O5-C5-C6-O6
3	p	19	BGC	O5-C5-C6-O6
7	t	18	BGC	O5-C5-C6-O6
8	H	17	A2G	O5-C5-C6-O6
8	U	17	A2G	O5-C5-C6-O6
8	h	17	A2G	O5-C5-C6-O6
8	u	17	A2G	O5-C5-C6-O6
3	P	11	NAG	C4-C5-C6-O6
4	D	3	BGC	O5-C5-C6-O6
4	Q	3	BGC	O5-C5-C6-O6
4	d	3	BGC	O5-C5-C6-O6
4	q	3	BGC	O5-C5-C6-O6
14	a	3	A2G	O5-C5-C6-O6
14	N	3	A2G	O5-C5-C6-O6
14	n	3	A2G	O5-C5-C6-O6
14	o	3	A2G	O5-C5-C6-O6
10	w	19	MAN	C4-C5-C6-O6
3	C	13	NAG	O7-C7-N2-C2
3	P	13	NAG	O7-C7-N2-C2
3	c	13	NAG	O7-C7-N2-C2
3	p	13	NAG	O7-C7-N2-C2
12	Y	5	BGC	C4-C5-C6-O6
12	l	5	BGC	C4-C5-C6-O6
12	y	5	BGC	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	G	9	MAN	O5-C5-C6-O6
7	T	9	MAN	O5-C5-C6-O6
7	g	9	MAN	O5-C5-C6-O6
7	t	9	MAN	O5-C5-C6-O6
11	K	25	BGC	O5-C5-C6-O6
11	X	25	BGC	O5-C5-C6-O6
11	k	25	BGC	O5-C5-C6-O6
11	x	25	BGC	O5-C5-C6-O6
12	L	9	NAG	O5-C5-C6-O6
12	l	9	NAG	O5-C5-C6-O6
12	y	9	NAG	O5-C5-C6-O6
12	L	5	BGC	C4-C5-C6-O6
4	D	18	MAN	O5-C5-C6-O6
4	Q	18	MAN	O5-C5-C6-O6
4	d	18	MAN	O5-C5-C6-O6
4	q	18	MAN	O5-C5-C6-O6
11	x	47	BGC	O5-C5-C6-O6
12	Y	9	NAG	O5-C5-C6-O6
7	T	3	A2G	C4-C5-C6-O6
7	g	3	A2G	C4-C5-C6-O6
7	G	3	A2G	C4-C5-C6-O6
7	t	3	A2G	C4-C5-C6-O6
12	L	5	BGC	O5-C5-C6-O6
12	Y	5	BGC	O5-C5-C6-O6
12	l	5	BGC	O5-C5-C6-O6
12	y	5	BGC	O5-C5-C6-O6
11	K	28	NAG	C3-C2-N2-C7
11	X	28	NAG	C3-C2-N2-C7
11	k	28	NAG	C3-C2-N2-C7
11	x	28	NAG	C3-C2-N2-C7
6	F	2	GZL	C4-C5-C6-O6
6	S	2	GZL	C4-C5-C6-O6
6	f	2	GZL	C4-C5-C6-O6
6	s	2	GZL	C4-C5-C6-O6
3	p	2	BGC	C4-C5-C6-O6
3	C	2	BGC	C4-C5-C6-O6
3	P	2	BGC	C4-C5-C6-O6
3	c	2	BGC	C4-C5-C6-O6
7	T	16	NAG	C4-C5-C6-O6
7	g	16	NAG	C4-C5-C6-O6
7	G	16	NAG	C4-C5-C6-O6
7	t	16	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	j	19	MAN	O5-C5-C6-O6
4	d	8	BGC	C4-C5-C6-O6
4	D	8	BGC	C4-C5-C6-O6
4	q	8	BGC	C4-C5-C6-O6
4	Q	8	BGC	C4-C5-C6-O6
7	G	8	MAN	C4-C5-C6-O6
7	T	8	MAN	C4-C5-C6-O6
7	g	8	MAN	C4-C5-C6-O6
7	t	8	MAN	C4-C5-C6-O6
7	T	8	MAN	O5-C5-C6-O6
7	g	8	MAN	O5-C5-C6-O6
7	G	8	MAN	O5-C5-C6-O6
7	t	8	MAN	O5-C5-C6-O6
3	P	11	NAG	C3-C2-N2-C7
3	c	11	NAG	C3-C2-N2-C7
3	p	11	NAG	C3-C2-N2-C7
4	D	14	NAG	C3-C2-N2-C7
4	Q	14	NAG	C3-C2-N2-C7
4	d	14	NAG	C3-C2-N2-C7
4	q	14	NAG	C3-C2-N2-C7
10	w	19	MAN	O5-C5-C6-O6
11	K	6	FUB	C3-C4-C5-O5
11	X	6	FUB	C3-C4-C5-O5
11	x	6	FUB	C3-C4-C5-O5
11	k	6	FUB	C3-C4-C5-O5
12	L	9	NAG	C1-C2-N2-C7
12	Y	9	NAG	C1-C2-N2-C7
12	l	9	NAG	C1-C2-N2-C7
12	y	9	NAG	C1-C2-N2-C7
4	D	17	AHR	O4-C4-C5-O5
4	Q	17	AHR	O4-C4-C5-O5
4	d	17	AHR	O4-C4-C5-O5
4	q	17	AHR	O4-C4-C5-O5
2	B	2	NAG	C8-C7-N2-C2
2	O	2	NAG	C8-C7-N2-C2
2	b	2	NAG	C8-C7-N2-C2
2	o	2	NAG	C8-C7-N2-C2
8	H	2	NAG	C1-C2-N2-C7
8	U	2	NAG	C1-C2-N2-C7
8	h	2	NAG	C1-C2-N2-C7
8	u	2	NAG	C1-C2-N2-C7
3	C	11	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
13	M	2	BGC	C4-C5-C6-O6
13	Z	2	BGC	C4-C5-C6-O6
13	m	2	BGC	C4-C5-C6-O6
13	z	2	BGC	C4-C5-C6-O6
7	g	3	A2G	O5-C5-C6-O6
7	T	3	A2G	O5-C5-C6-O6
7	G	3	A2G	O5-C5-C6-O6
7	t	3	A2G	O5-C5-C6-O6
2	B	2	NAG	O7-C7-N2-C2
2	O	2	NAG	O7-C7-N2-C2
2	o	2	NAG	O7-C7-N2-C2

There are no ring outliers.

247 monomers are involved in 226 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	c	18	BGC	2	0
4	q	13	FUB	2	0
11	K	26	XYP	1	0
8	H	20	MAN	1	0
14	n	13	XYP	1	0
14	a	16	BGC	2	0
7	g	21	XYP	1	0
13	m	5	BGC	4	0
3	C	18	BGC	2	0
3	p	12	MAN	1	0
11	X	1	MAN	3	0
8	U	14	NAG	1	0
3	C	6	XYP	1	0
3	C	2	BGC	1	0
8	H	2	NAG	1	0
11	X	35	BGC	1	0
10	W	19	MAN	5	0
8	H	14	NAG	2	0
11	X	37	MAN	1	0
2	b	1	BGC	2	0
3	P	3	BGC	1	0
10	j	10	MAN	1	0
14	a	18	NAG	2	0
3	C	12	MAN	1	0
10	W	18	NAG	2	0
3	P	9	BGC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	X	26	XYP	1	0
7	g	3	A2G	3	0
11	k	35	BGC	1	0
10	w	10	MAN	1	0
7	t	8	MAN	1	0
7	G	2	BGC	4	0
13	Z	13	XYP	2	0
14	a	2	XYP	1	0
13	z	13	XYP	2	0
10	J	2	NAG	2	0
13	m	1	XYP	1	0
11	k	16	NAG	1	0
14	n	16	BGC	2	0
3	p	3	BGC	1	0
11	x	5	NAG	1	0
14	n	18	NAG	2	0
8	U	2	NAG	1	0
13	M	4	NAG	3	0
13	z	10	BGC	1	0
7	G	3	A2G	3	0
2	O	4	MAN	1	0
7	g	2	BGC	4	0
12	l	8	BGC	1	0
8	H	8	GAL	5	0
7	T	4	BGC	1	0
11	k	26	XYP	1	0
12	l	5	BGC	1	0
11	K	34	NAG	1	0
12	y	1	GAL	3	0
14	N	2	XYP	1	0
11	k	1	MAN	2	0
4	Q	13	FUB	2	0
5	E	2	NAG	1	0
11	K	35	BGC	1	0
13	M	10	BGC	1	0
6	f	3	FUB	2	0
14	n	15	AHR	1	0
13	m	4	NAG	3	0
10	w	2	NAG	1	0
12	Y	1	GAL	2	0
11	X	20	NAG	1	0
10	j	19	MAN	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	13	XYP	2	0
8	u	17	A2G	1	0
11	K	5	NAG	1	0
11	x	6	FUB	2	0
11	K	20	NAG	1	0
5	R	2	NAG	1	0
7	T	16	NAG	6	0
11	k	6	FUB	2	0
10	w	19	MAN	2	0
8	h	14	NAG	2	0
10	j	1	GAL	1	0
7	T	2	BGC	3	0
11	x	34	NAG	1	0
10	W	10	MAN	1	0
7	G	4	BGC	1	0
3	c	2	BGC	1	0
4	D	23	BGC	1	0
13	m	2	BGC	1	0
14	a	13	XYP	1	0
7	T	8	MAN	1	0
3	p	10	XYP	3	0
14	n	6	XYP	1	0
11	X	47	BGC	5	0
3	c	12	MAN	1	0
14	n	2	XYP	1	0
10	W	17	BGC	1	0
4	D	11	MAN	1	0
11	x	36	XYP	2	0
12	L	1	GAL	2	0
7	T	3	A2G	2	0
4	Q	19	BGC	1	0
10	j	15	XYP	1	0
8	h	8	GAL	5	0
11	x	9	BMA	1	0
10	J	17	BGC	3	0
11	X	10	GLA	1	0
14	N	13	XYP	1	0
3	P	12	MAN	1	0
11	x	35	BGC	1	0
14	a	15	AHR	1	0
13	Z	1	XYP	1	0
11	K	6	FUB	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	V	5	BGC	2	0
3	P	10	XYP	3	0
6	F	3	FUB	2	0
11	x	37	MAN	1	0
4	Q	25	BGC	2	0
2	b	4	MAN	1	0
4	D	13	FUB	2	0
2	b	6	NAG	1	0
9	i	5	BGC	2	0
11	k	47	BGC	4	0
5	r	2	NAG	1	0
2	b	2	NAG	1	0
14	N	6	XYP	1	0
13	z	4	NAG	2	0
14	N	4	GAL	1	0
7	G	8	MAN	1	0
11	x	10	GLA	1	0
7	t	3	A2G	3	0
2	o	1	BGC	2	0
11	K	36	XYP	2	0
11	k	10	GLA	1	0
13	Z	4	NAG	2	0
2	o	2	NAG	1	0
7	t	21	XYP	2	0
7	t	16	NAG	6	0
11	k	20	NAG	1	0
11	k	36	XYP	2	0
8	u	2	NAG	1	0
3	p	9	BGC	2	0
8	h	20	MAN	1	0
10	j	2	NAG	1	0
13	Z	2	BGC	1	0
14	n	1	MAN	1	0
11	K	37	MAN	1	0
11	x	45	BGC	1	0
14	0	1	MAN	1	0
14	N	15	AHR	1	0
3	C	3	BGC	1	0
4	d	13	FUB	2	0
4	d	25	BGC	2	0
2	B	4	MAN	1	0
9	v	5	BGC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	Z	5	BGC	6	0
2	B	6	NAG	1	0
8	U	17	A2G	1	0
3	p	18	BGC	2	0
12	l	1	GAL	2	0
2	o	6	NAG	1	0
11	x	15	BGC	2	0
8	h	2	NAG	1	0
14	0	4	GAL	1	0
3	c	10	XYP	3	0
3	p	2	BGC	1	0
2	B	2	NAG	1	0
11	X	9	BMA	1	0
4	q	11	MAN	1	0
14	N	1	MAN	1	0
13	M	12	AHR	4	0
14	a	4	GAL	1	0
11	K	10	GLA	1	0
3	C	10	XYP	3	0
4	d	11	MAN	1	0
11	X	45	BGC	1	0
13	z	1	XYP	1	0
11	K	9	BMA	1	0
3	c	9	BGC	2	0
3	C	9	BGC	2	0
7	T	5	BGC	1	0
12	Y	8	BGC	1	0
14	0	18	NAG	2	0
7	T	21	XYP	2	0
7	g	8	MAN	1	0
11	X	5	NAG	1	0
11	X	16	NAG	3	0
2	B	1	BGC	2	0
3	c	25	BGC	1	0
10	J	19	MAN	8	0
11	k	9	BMA	1	0
4	d	19	BGC	1	0
7	G	16	NAG	1	0
11	X	6	FUB	2	0
8	U	20	MAN	2	0
14	0	6	XYP	1	0
6	S	3	FUB	2	0

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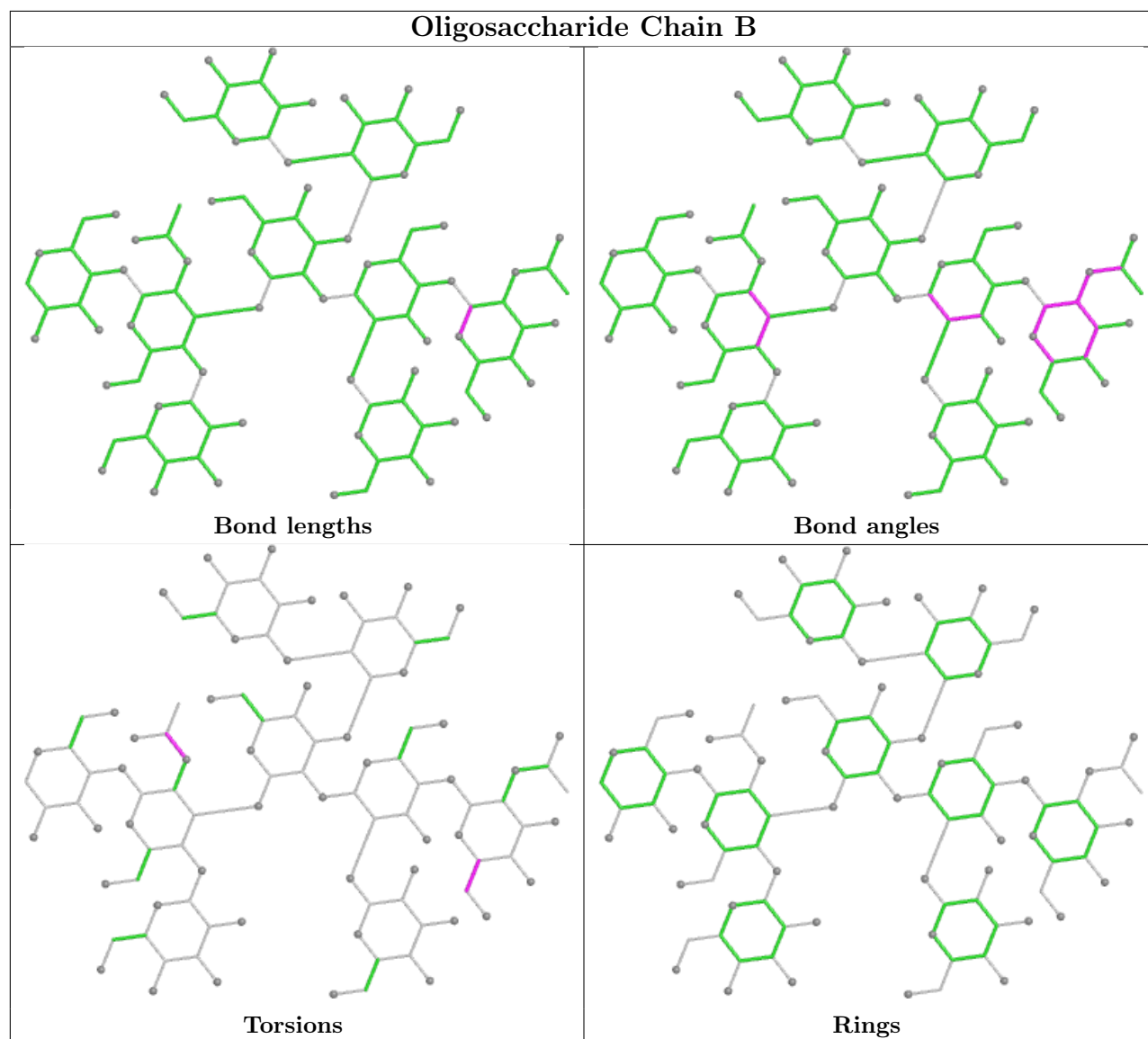
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	k	37	MAN	1	0
11	k	5	NAG	1	0
11	x	1	MAN	3	0
4	D	25	BGC	2	0
13	z	2	BGC	1	0
14	n	14	XYP	1	0
11	k	41	BGC	1	0
11	k	45	BGC	2	0
4	q	19	BGC	1	0
8	U	8	GAL	5	0
13	z	12	AHR	3	0
6	s	3	FUB	2	0
14	0	14	XYP	1	0
7	g	16	NAG	6	0
14	N	18	NAG	2	0
8	h	17	A2G	1	0
13	m	12	AHR	4	0
14	a	14	XYP	1	0
14	0	2	XYP	1	0
5	e	2	NAG	1	0
11	x	26	XYP	1	0
11	X	36	XYP	2	0
13	Z	12	AHR	4	0
3	c	3	BGC	1	0
4	D	19	BGC	1	0
7	t	2	BGC	4	0
11	x	20	NAG	1	0
2	O	6	NAG	1	0
13	m	13	XYP	2	0
10	J	18	NAG	1	0
14	a	6	XYP	1	0
3	P	18	BGC	2	0
2	O	1	BGC	2	0
14	N	16	BGC	2	0
2	o	4	MAN	1	0
14	n	4	GAL	1	0
11	X	34	NAG	1	0
4	Q	11	MAN	1	0
14	0	16	BGC	2	0
7	G	5	BGC	1	0
9	V	6	MAN	1	0
11	x	14	BMA	1	0

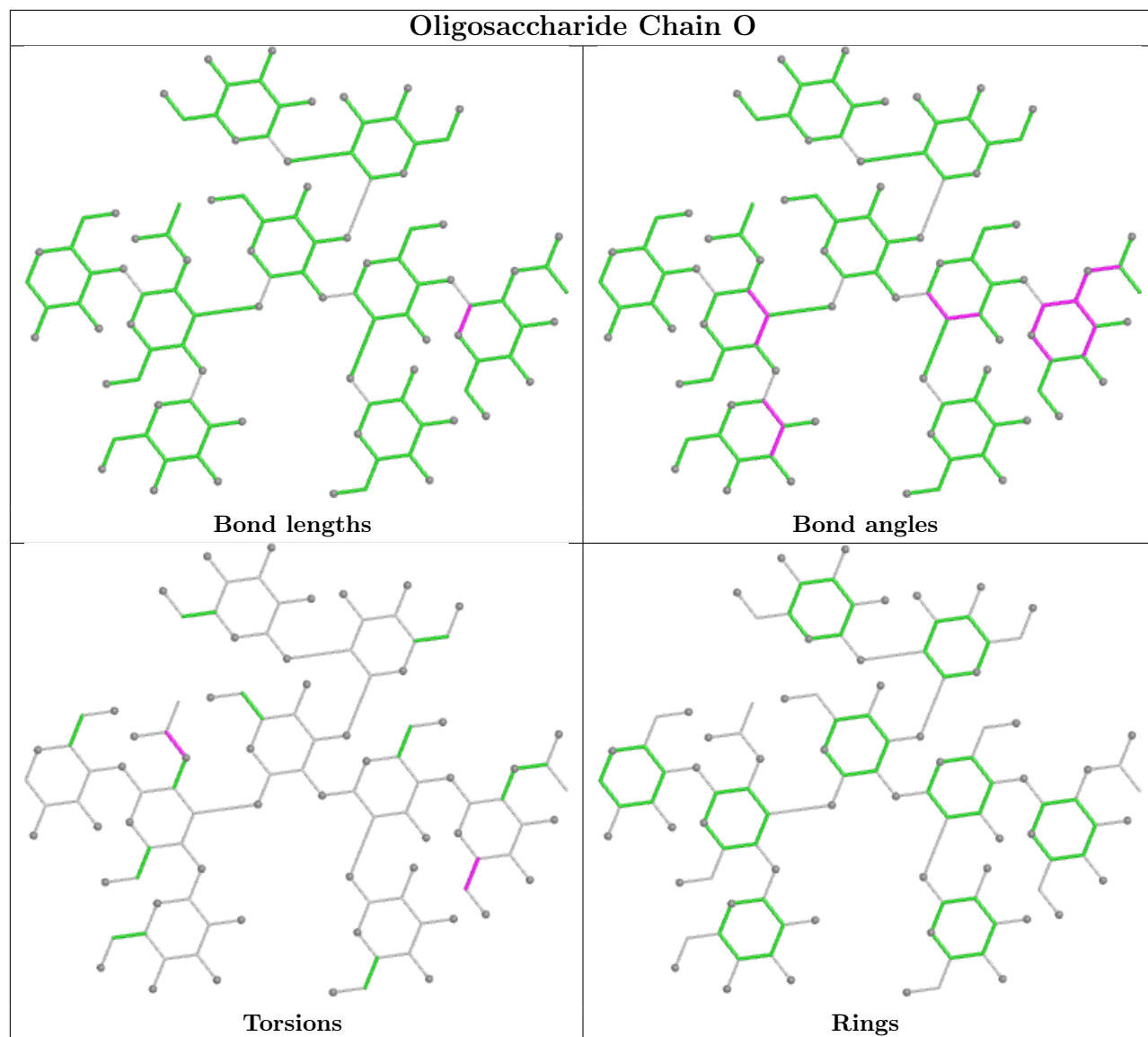
Continued on next page...

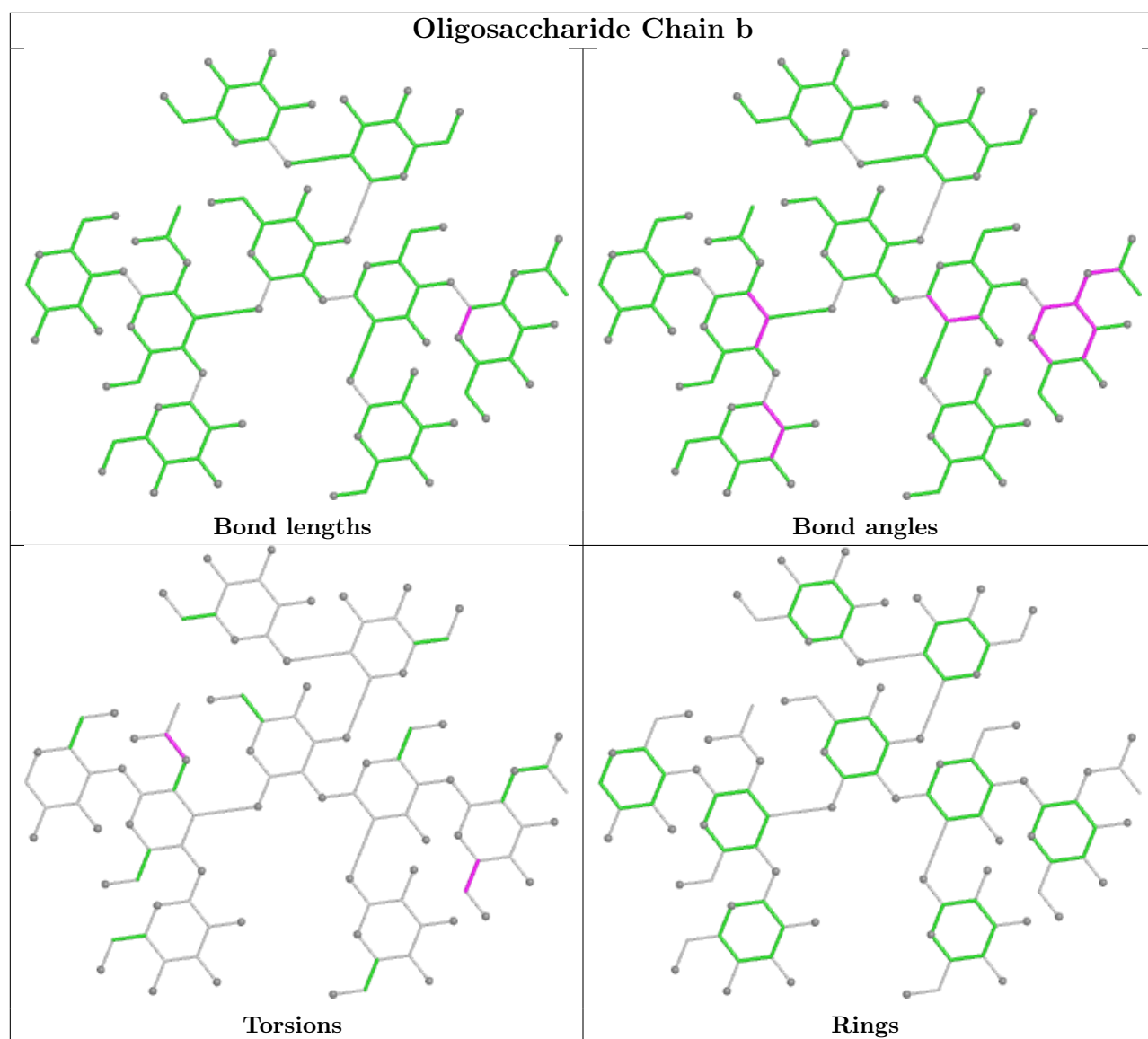
Continued from previous page...

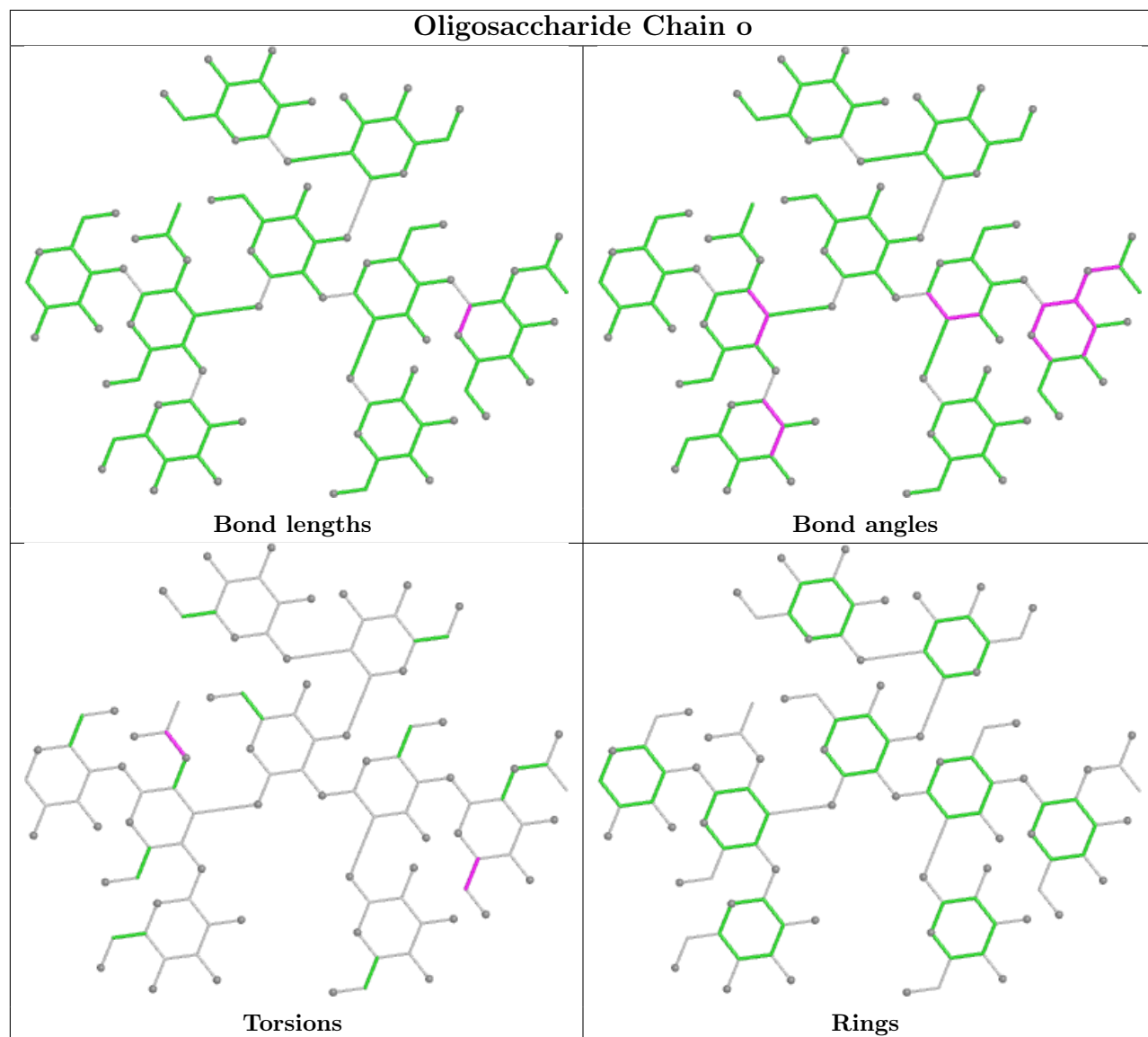
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	1	MAN	3	0
14	N	14	XYP	2	0
2	O	2	NAG	1	0
14	a	1	MAN	2	0
3	C	11	NAG	1	0
13	M	5	BGC	5	0
10	W	1	GAL	1	0
3	P	2	BGC	1	0
13	Z	10	BGC	1	0
11	k	34	NAG	1	0
13	z	5	BGC	4	0

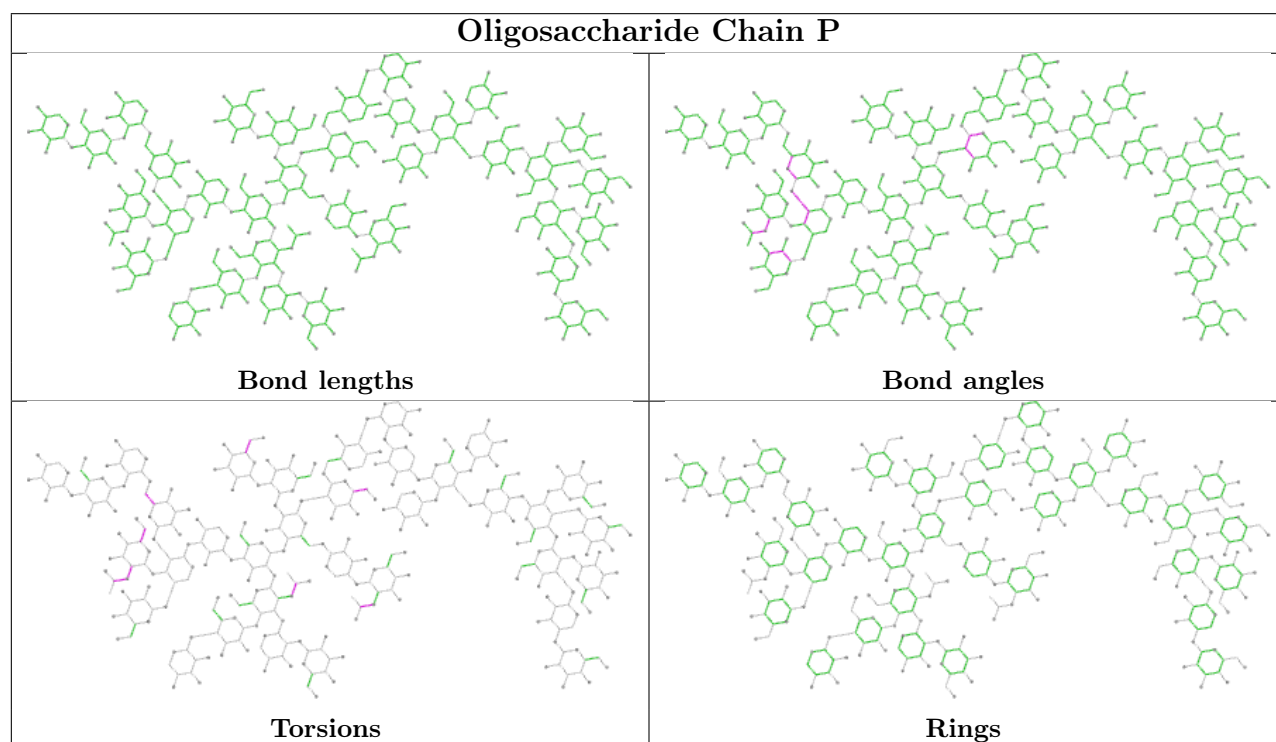
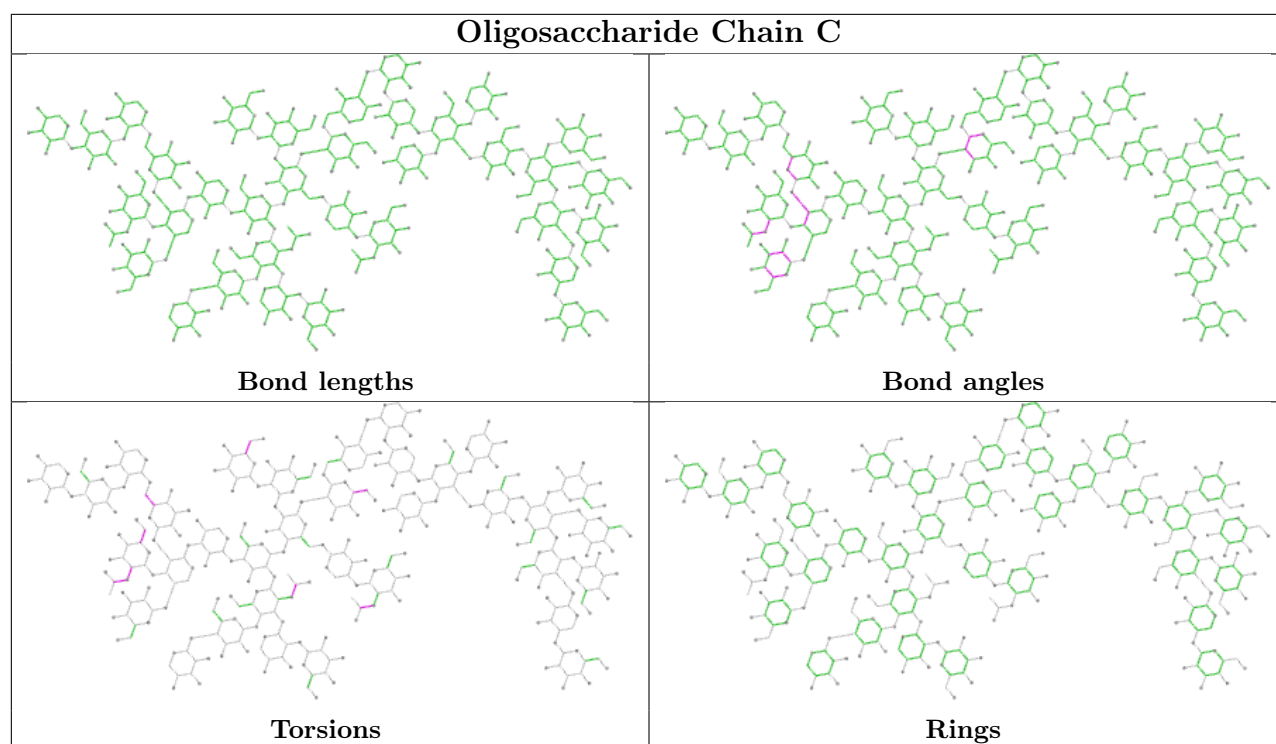
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

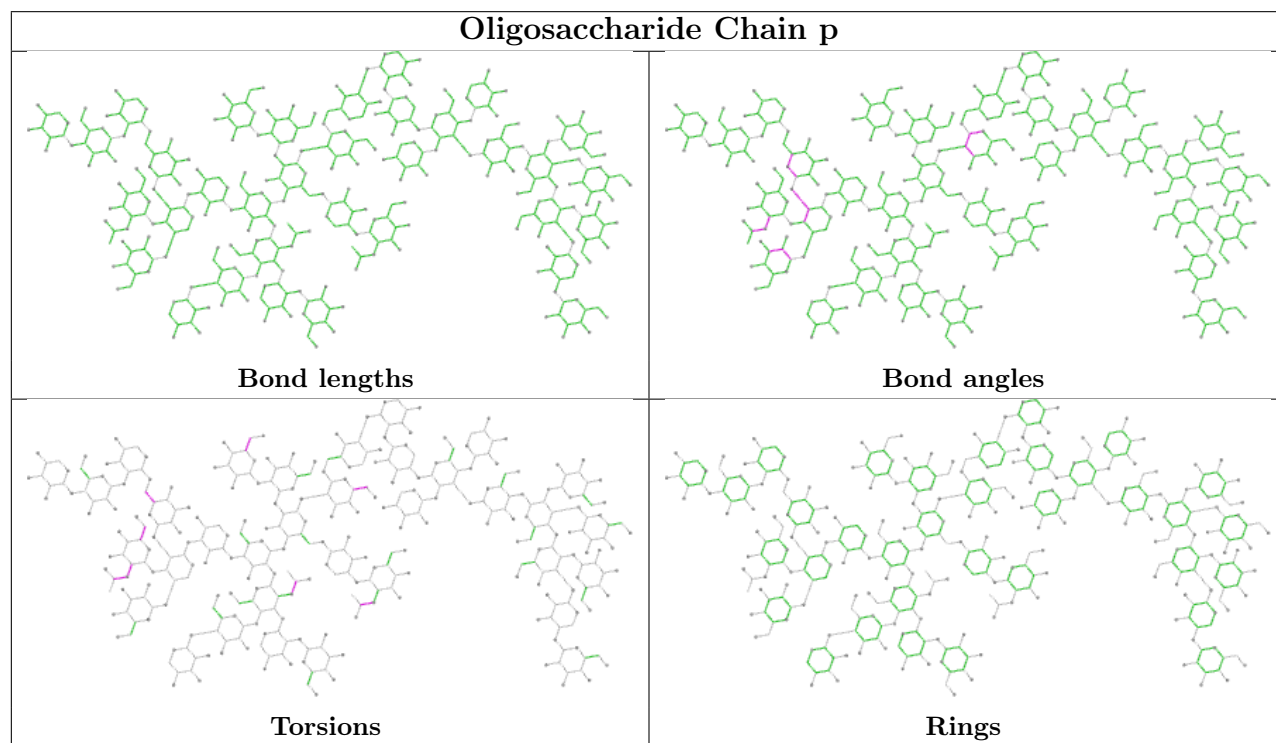
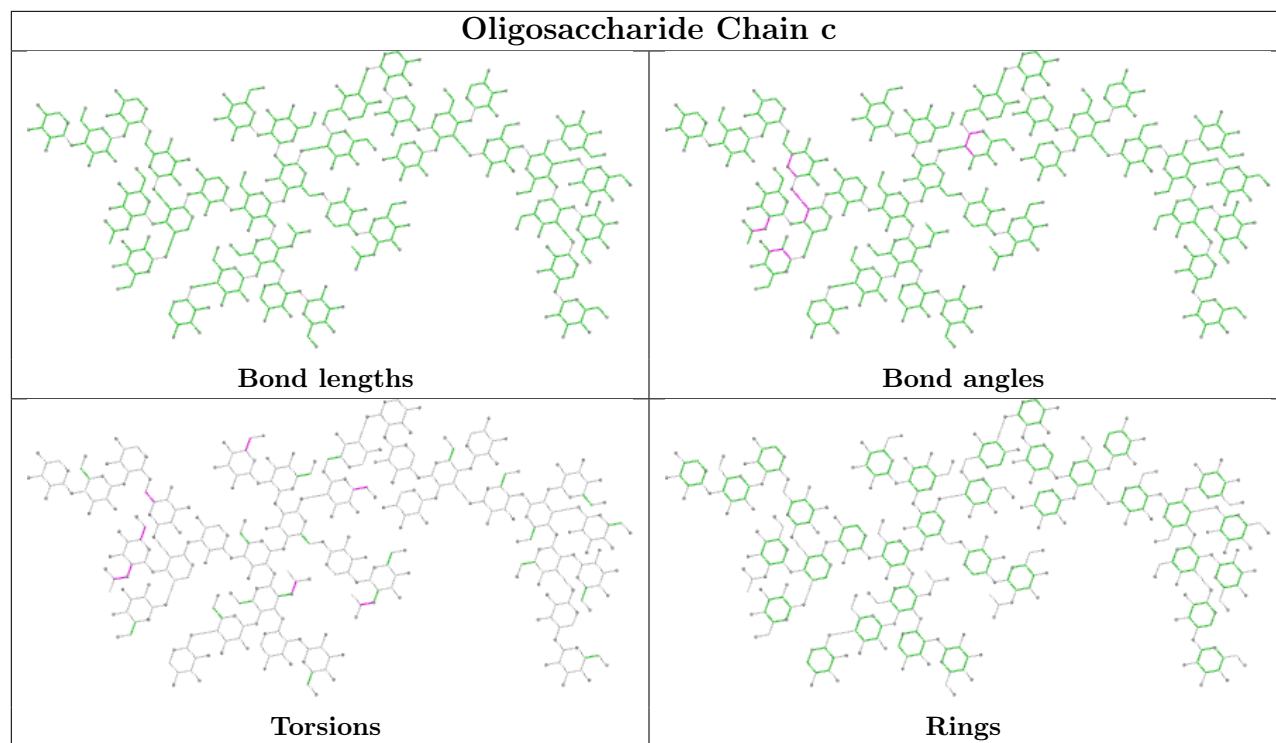


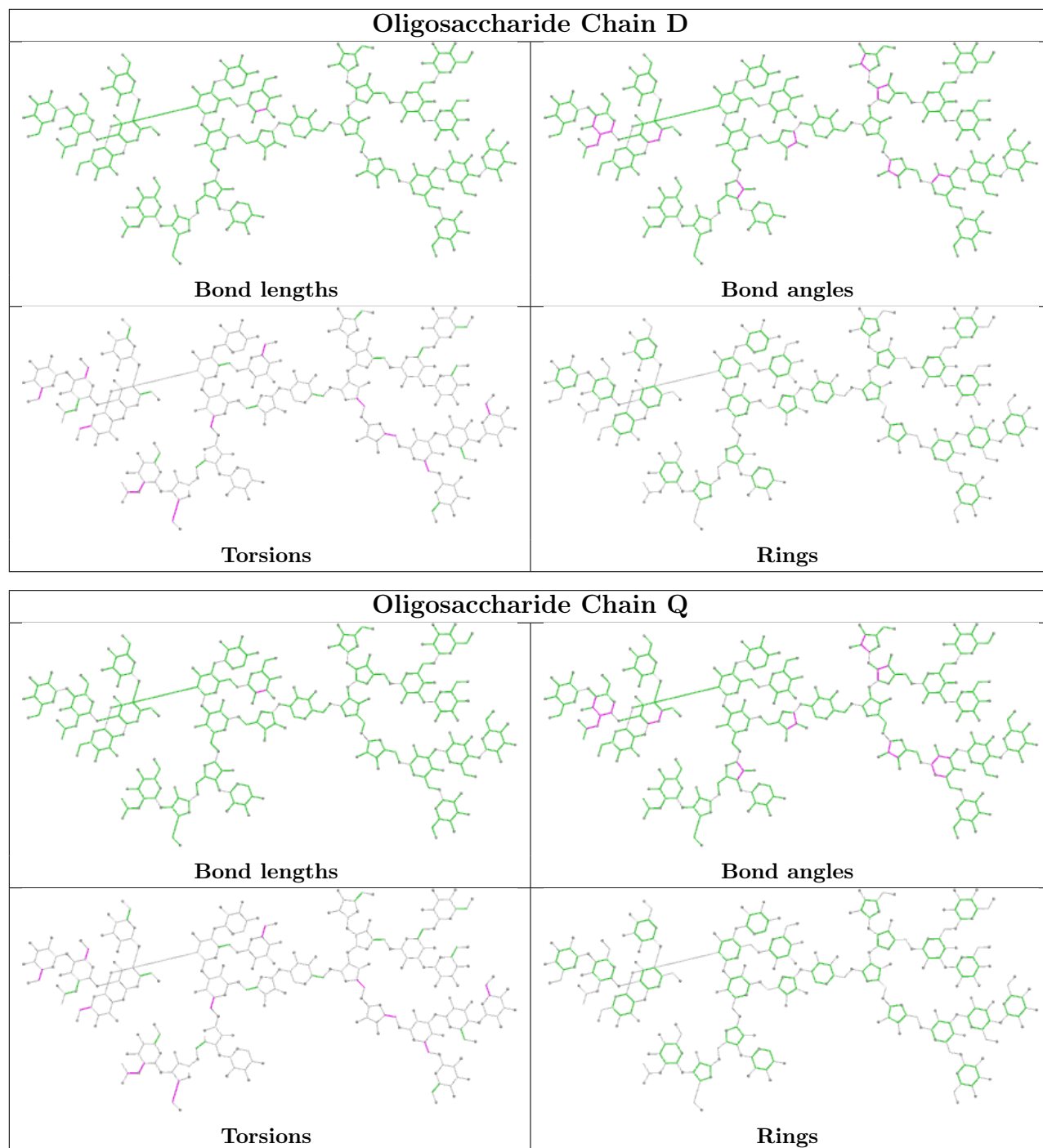


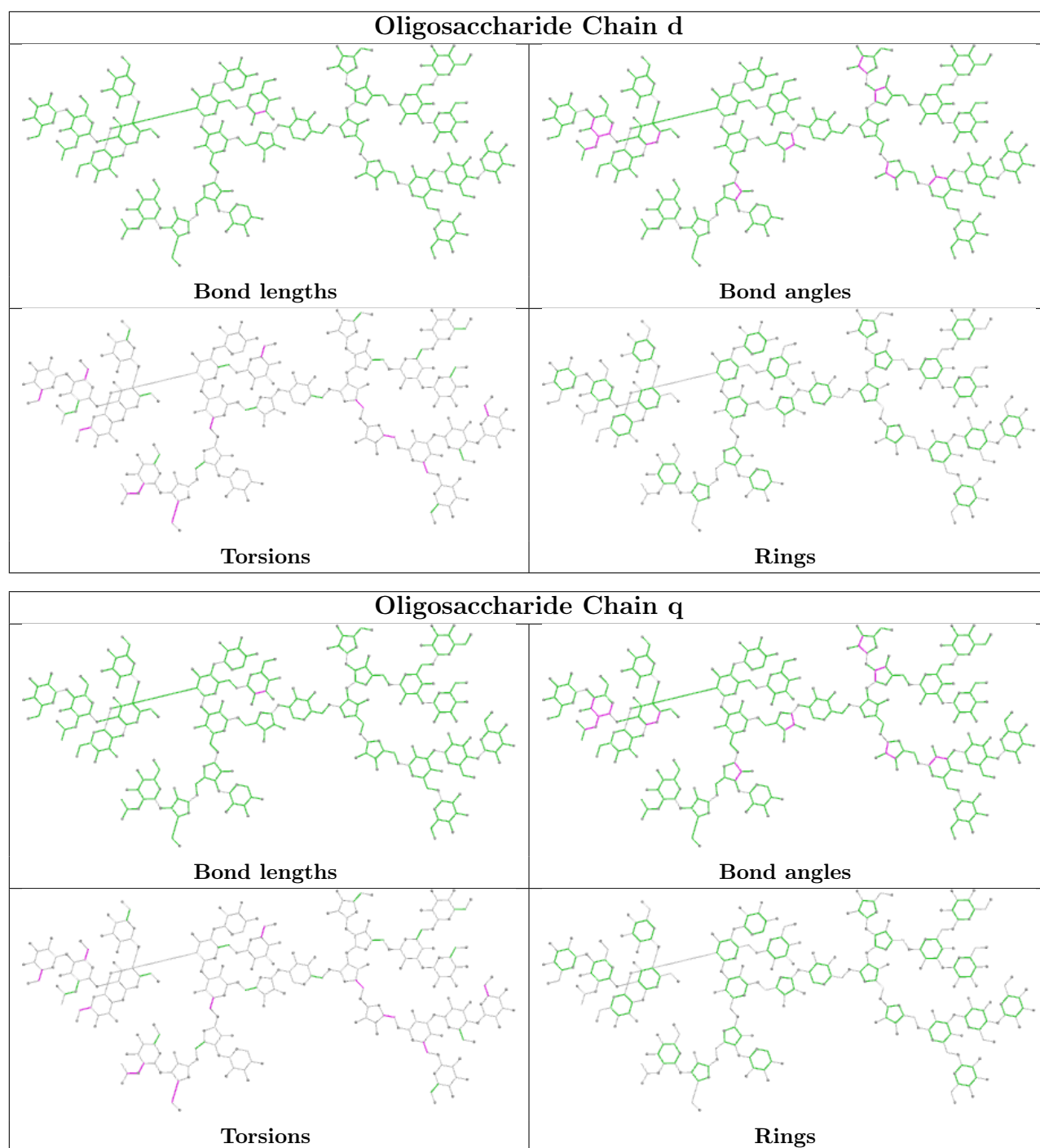


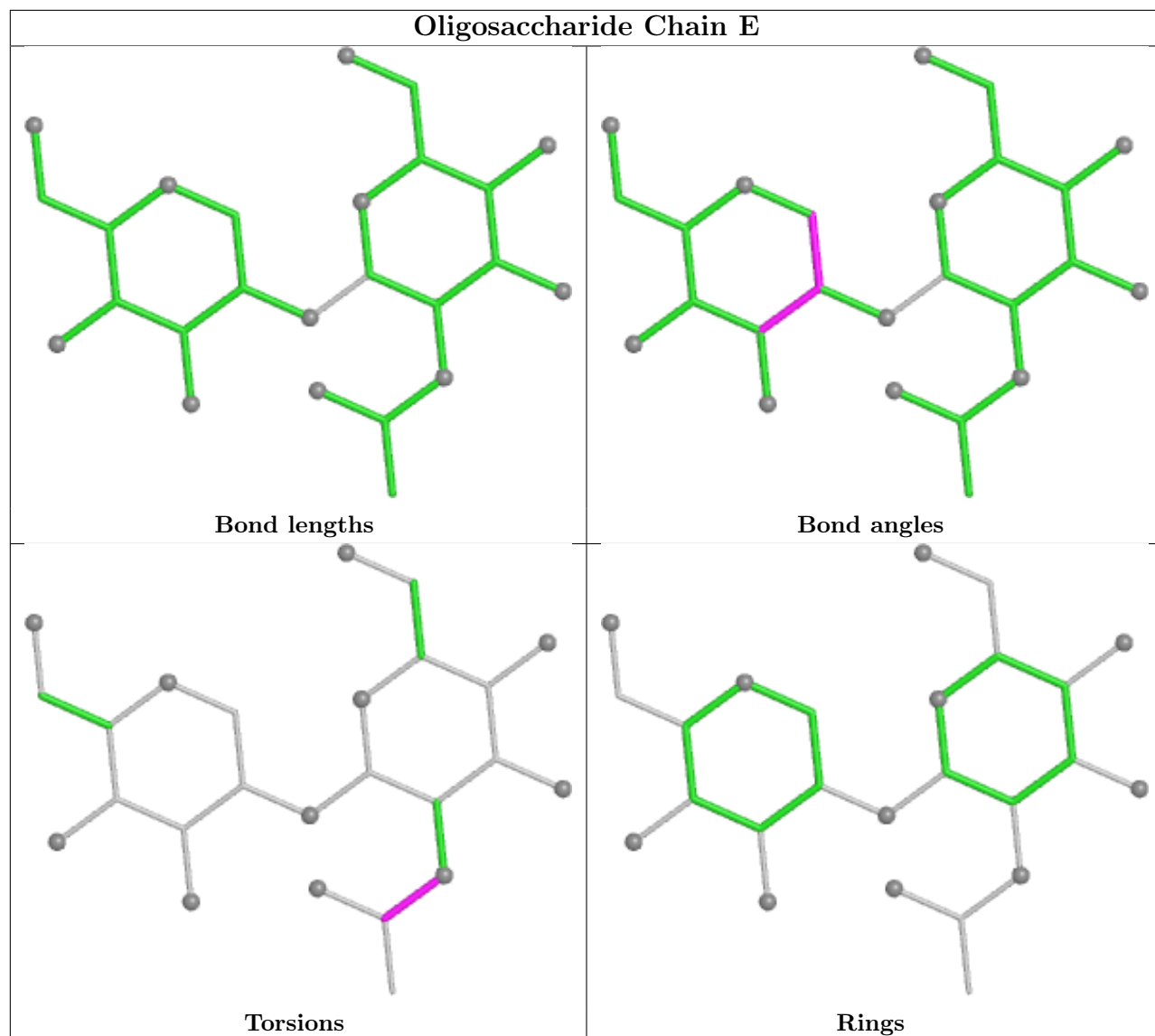


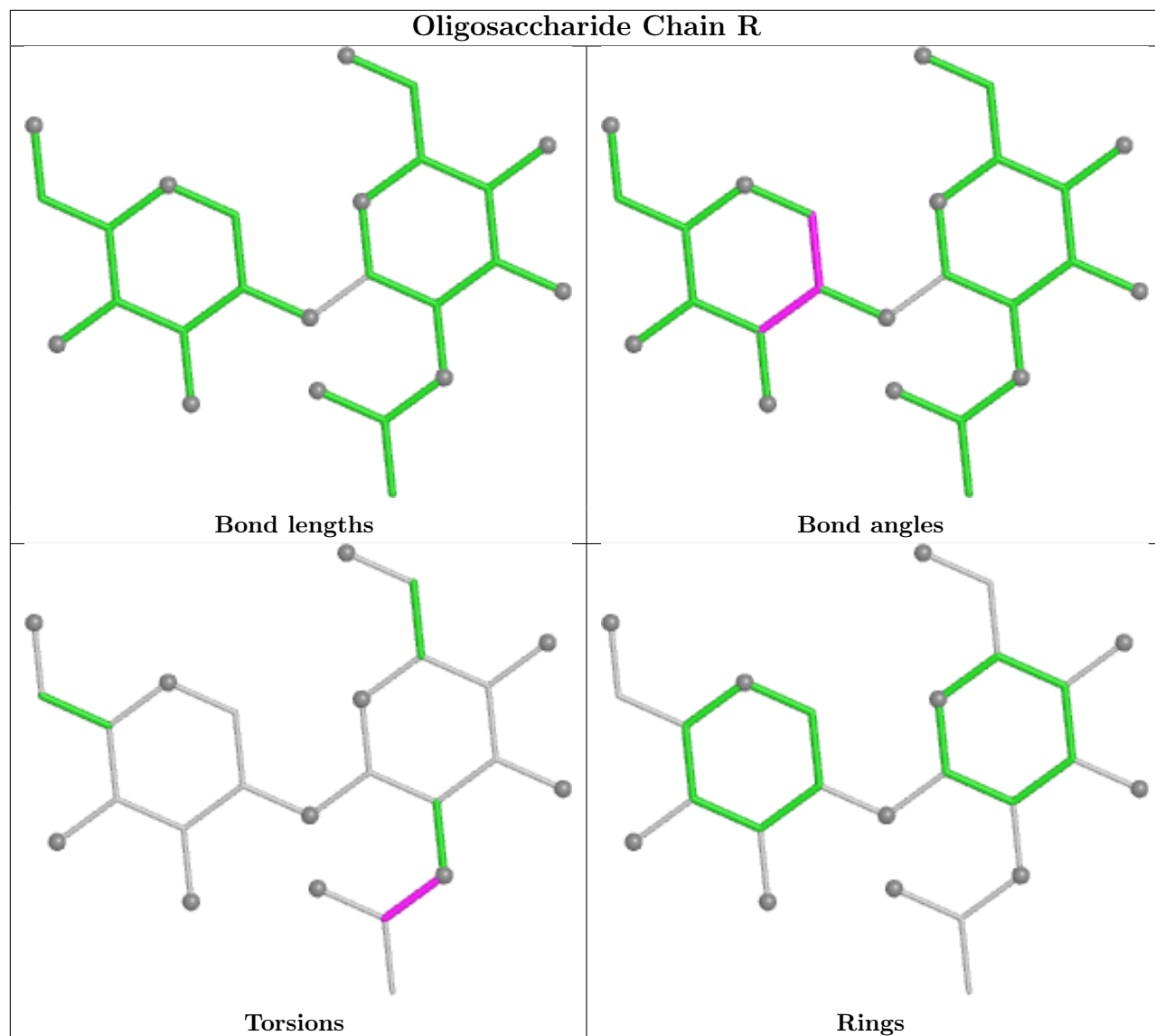


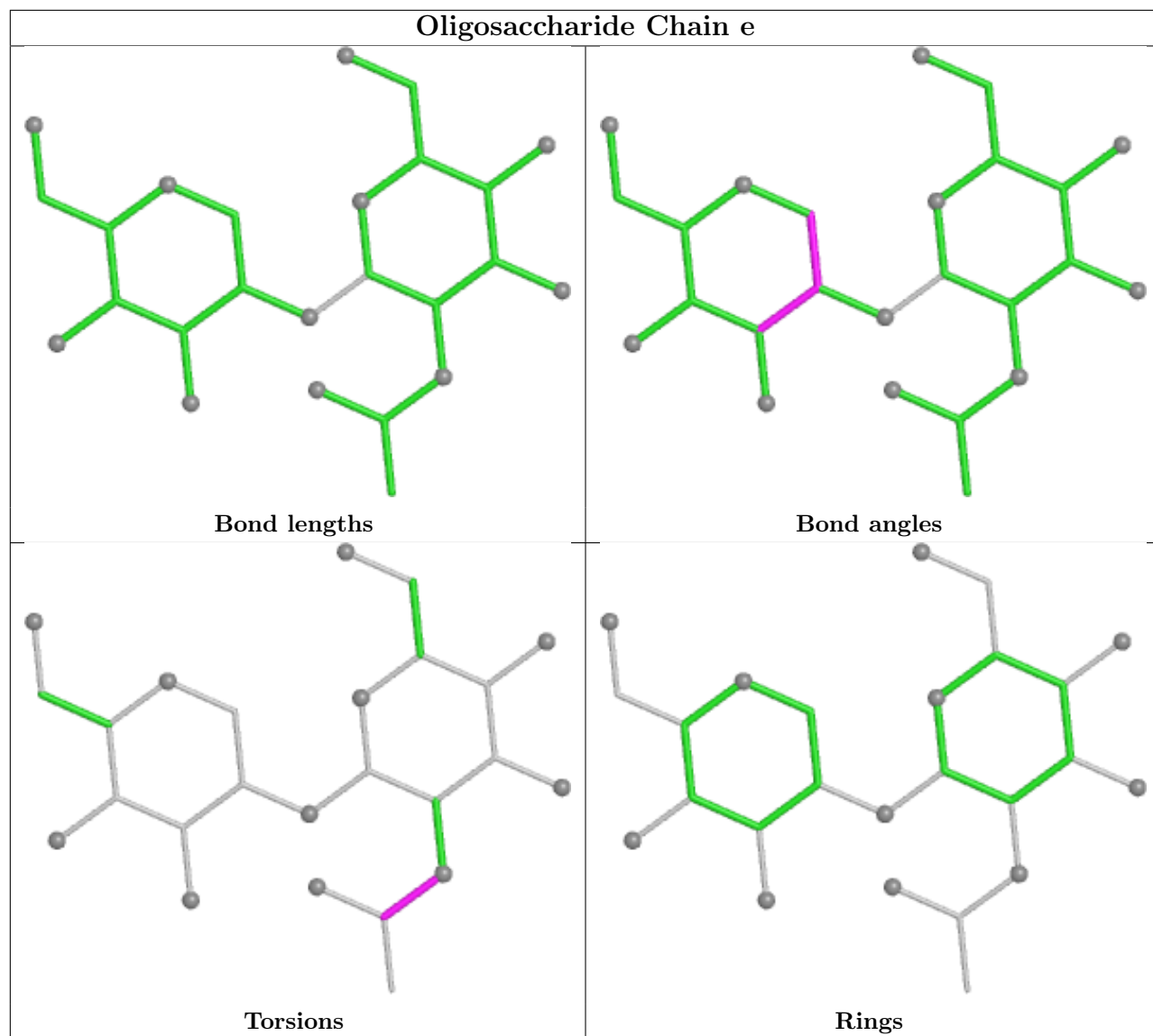


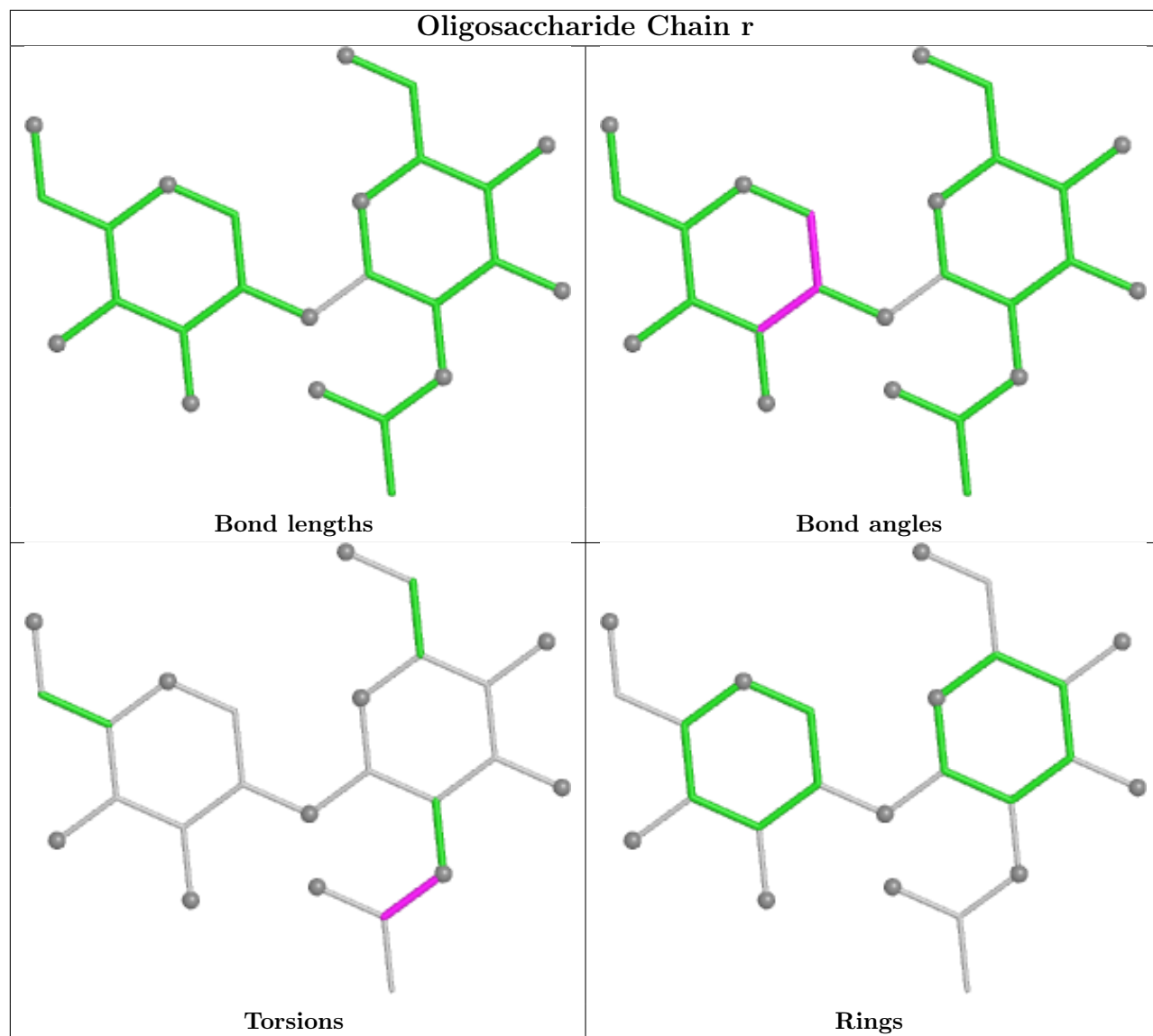


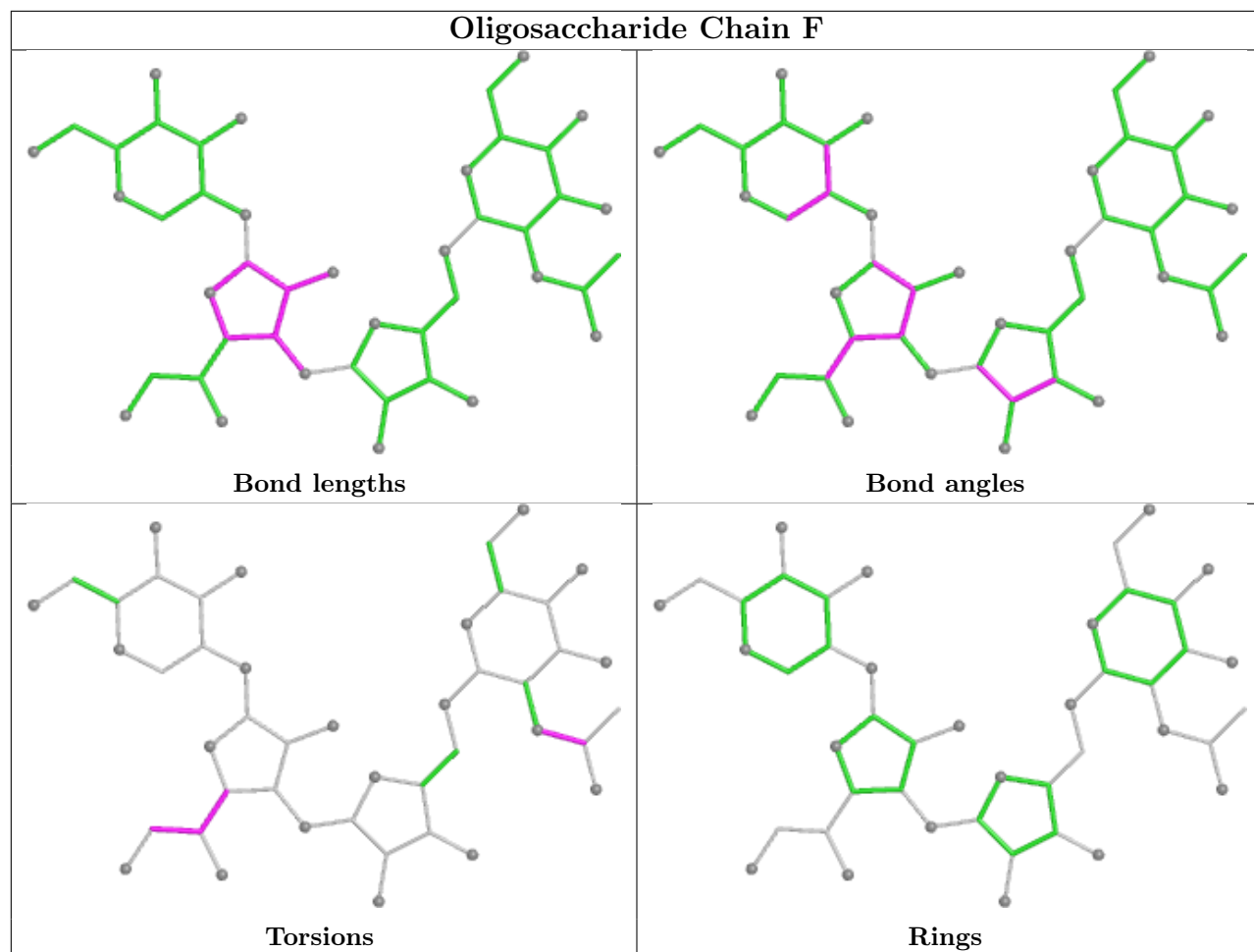


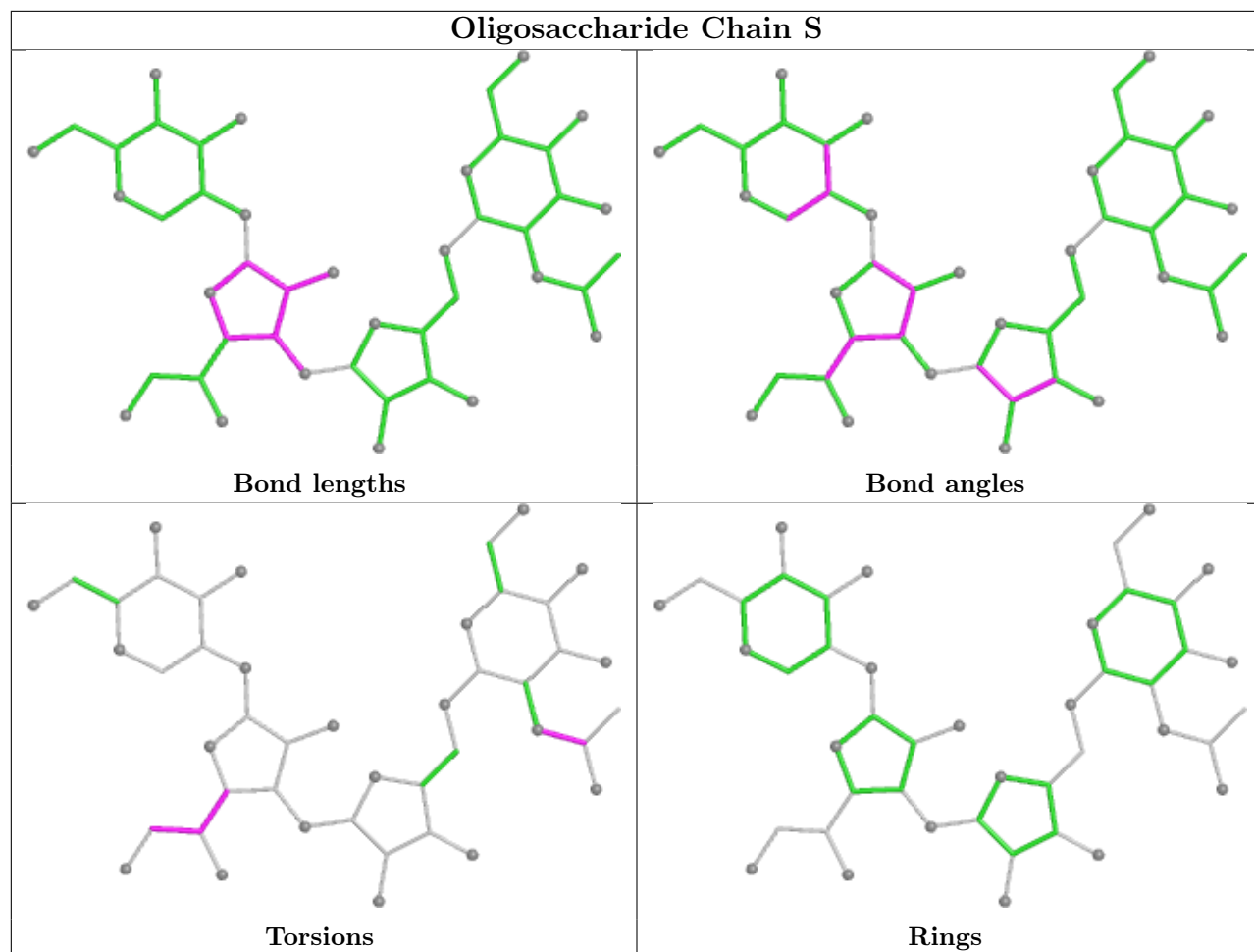


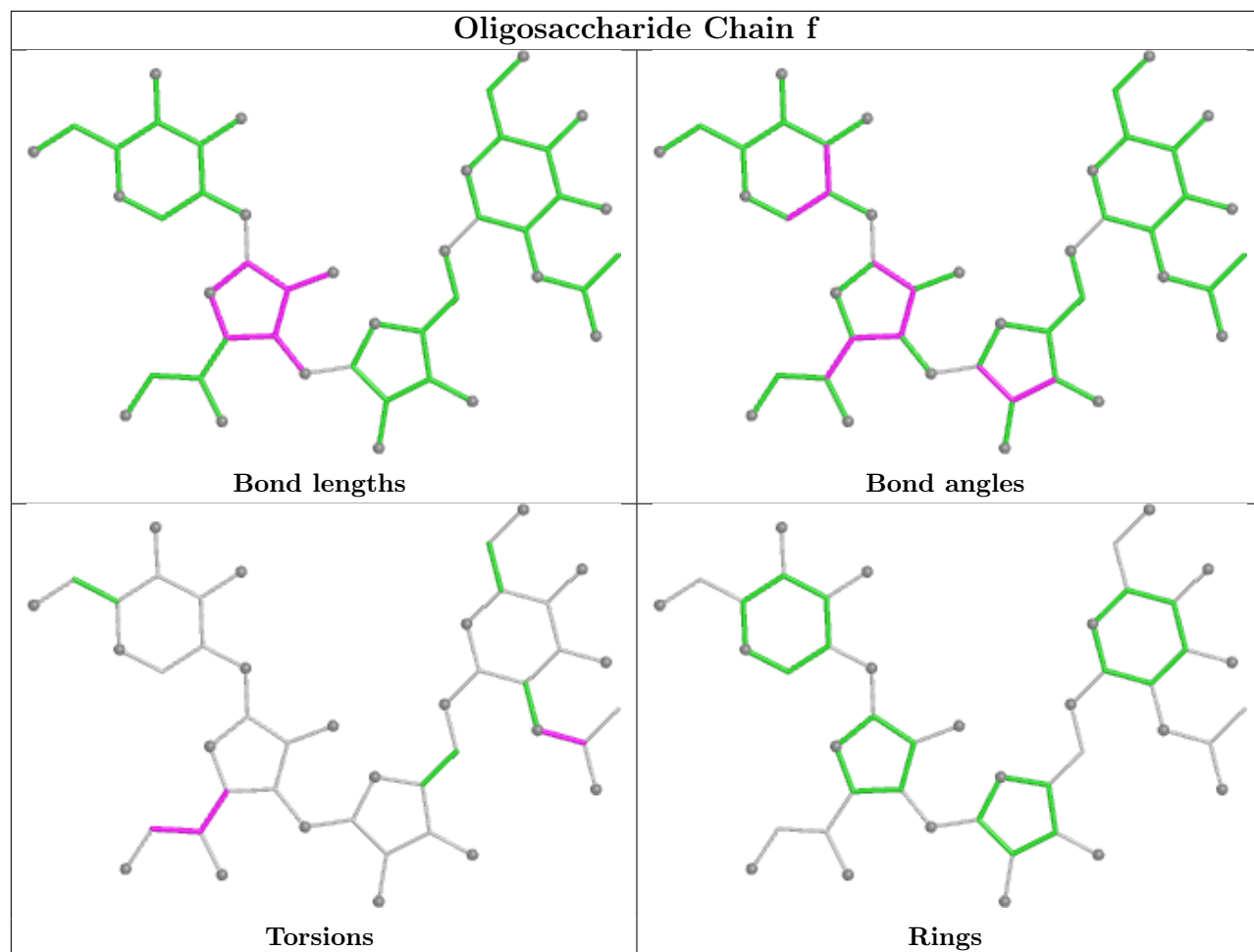


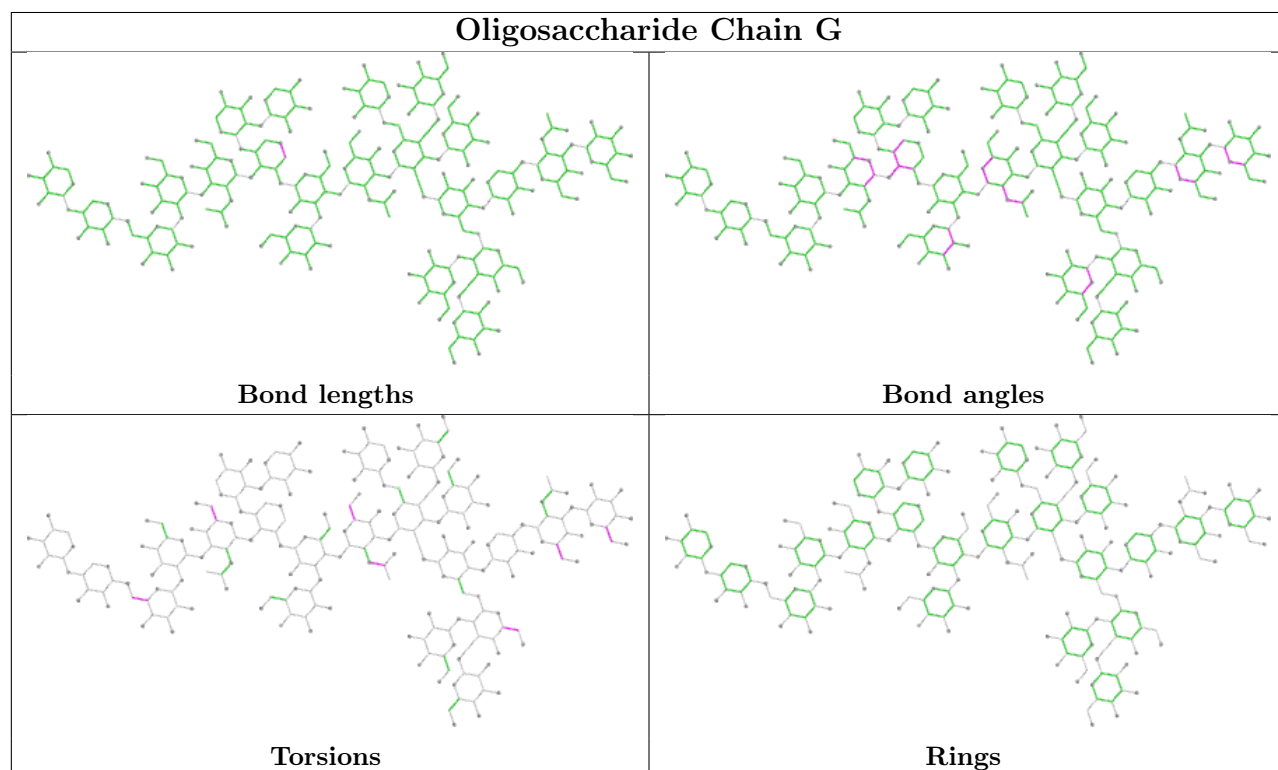
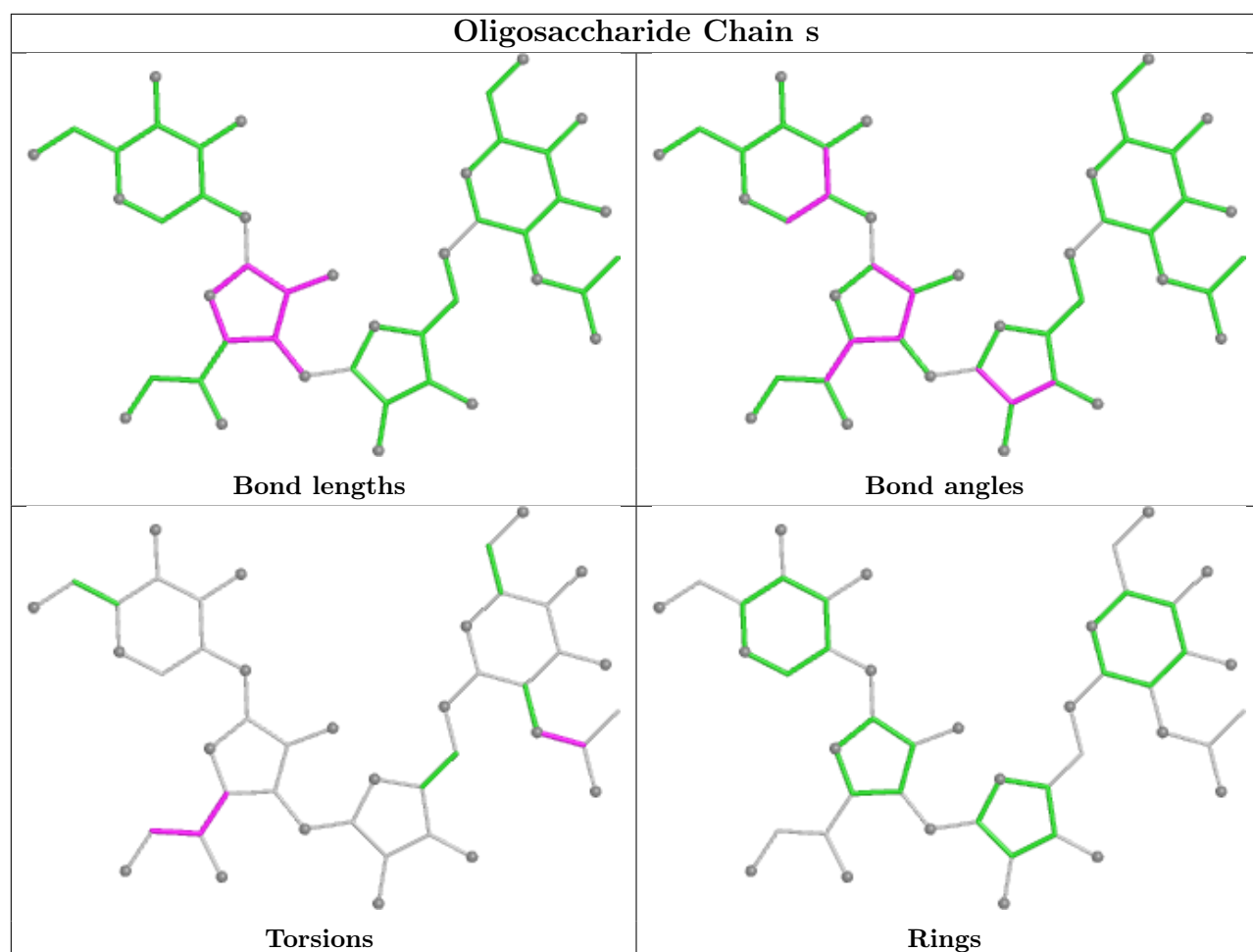


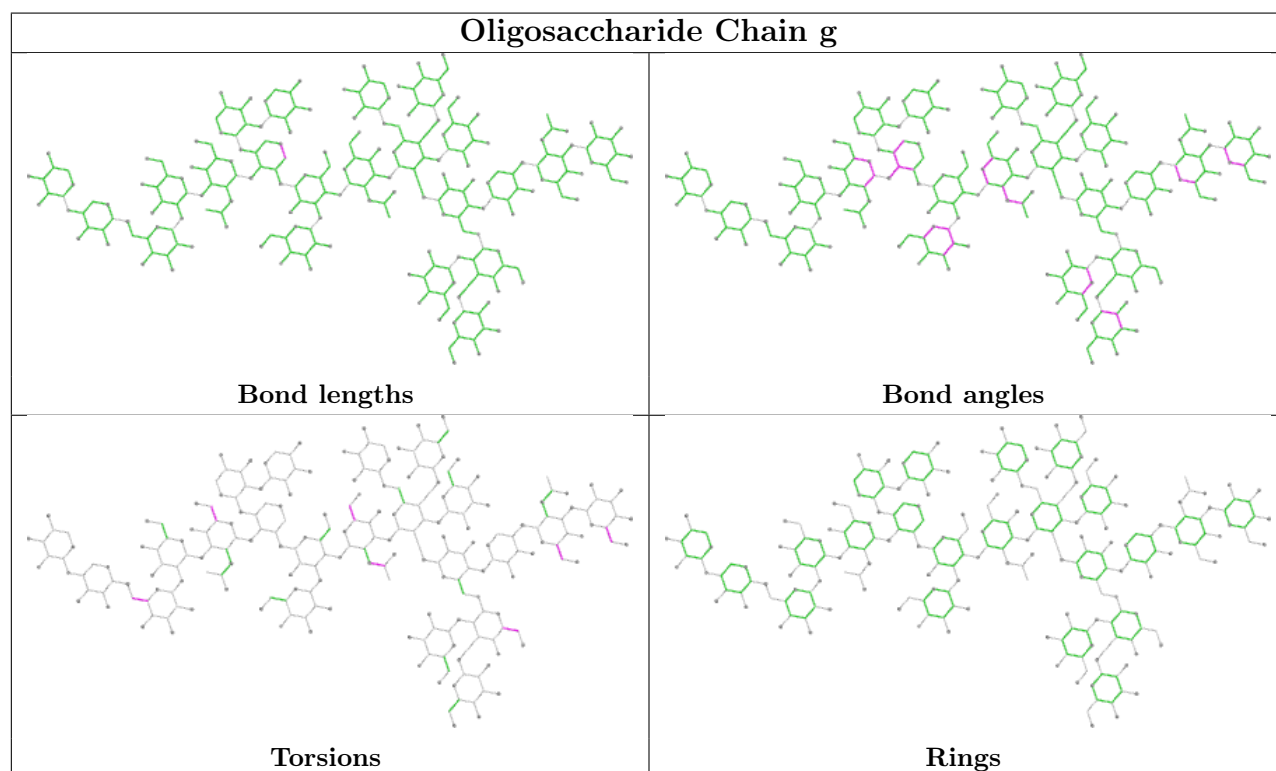
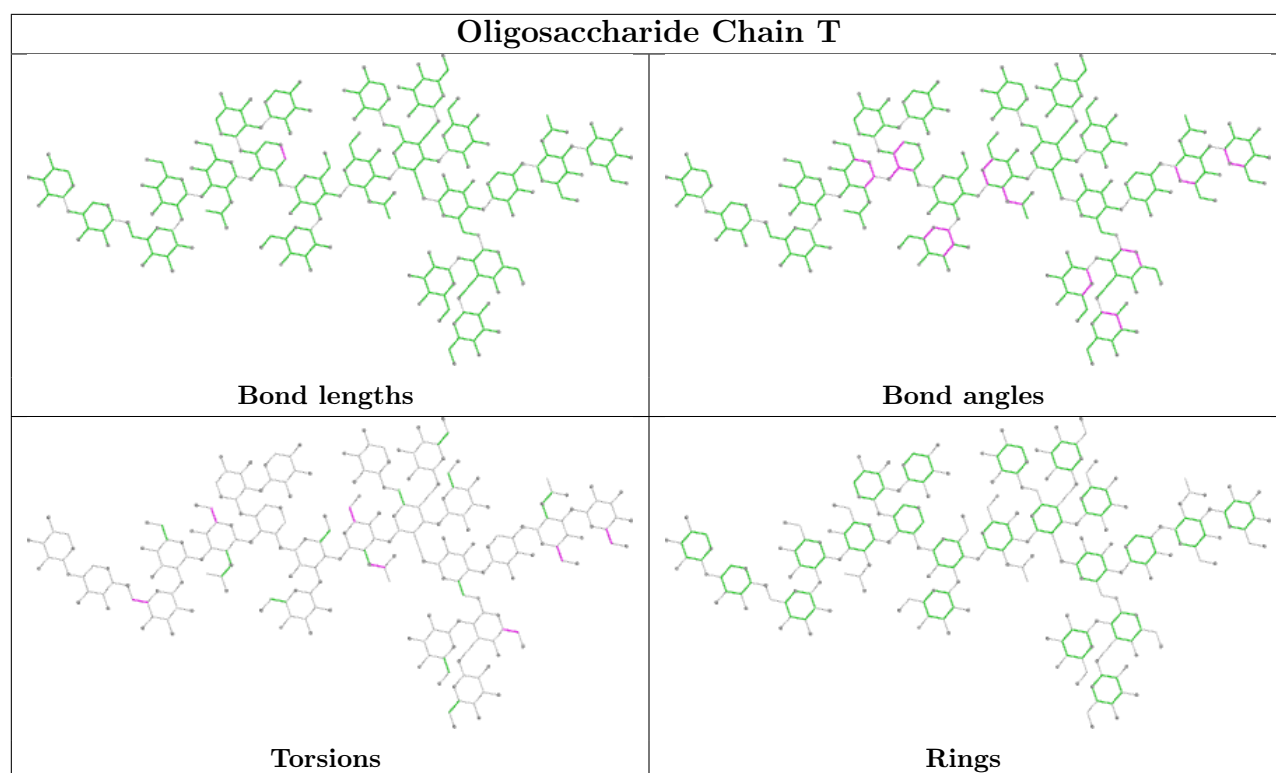


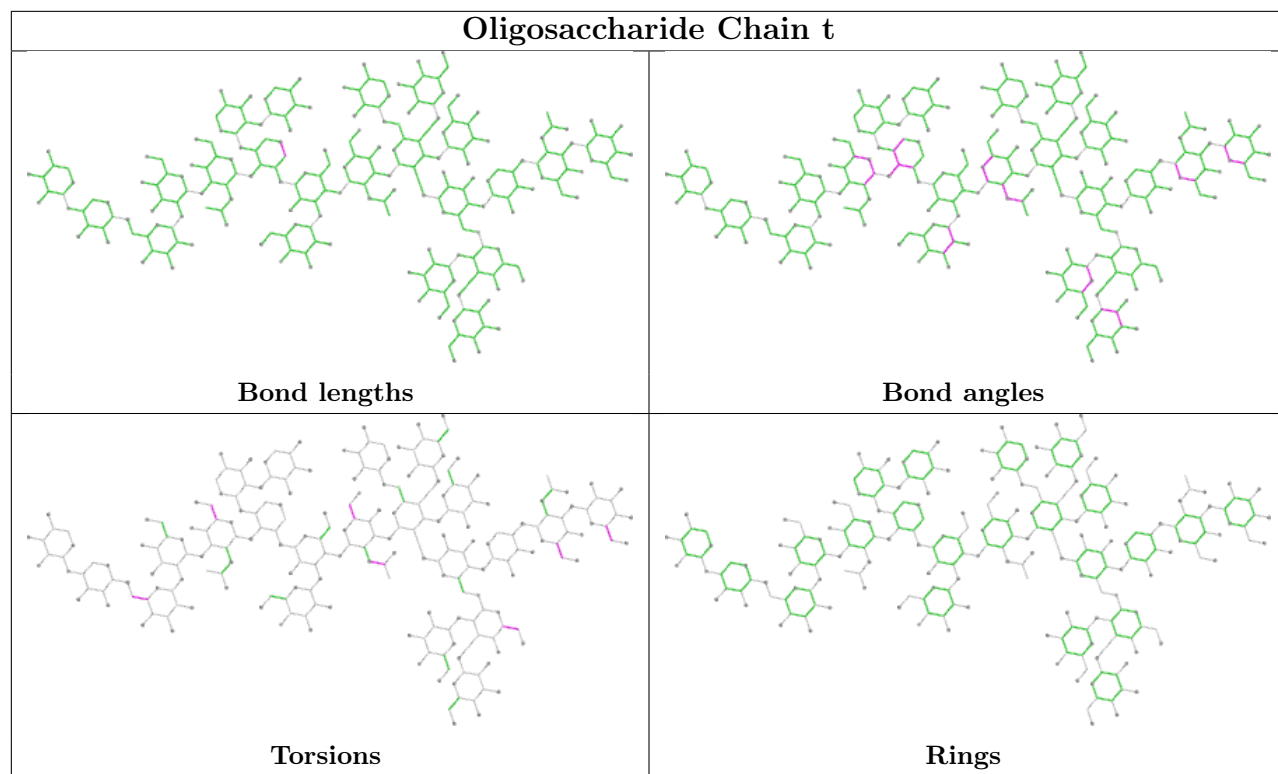


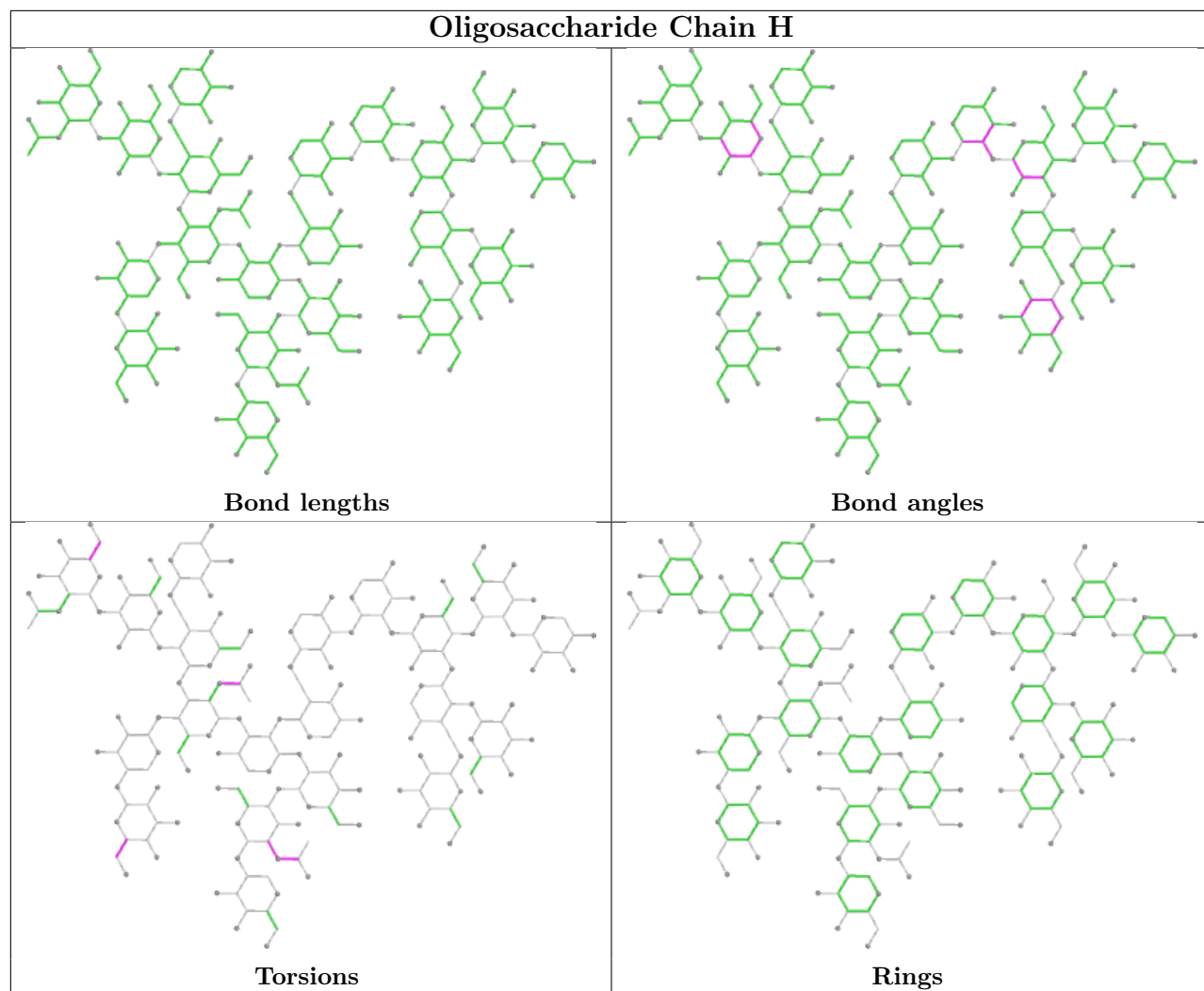


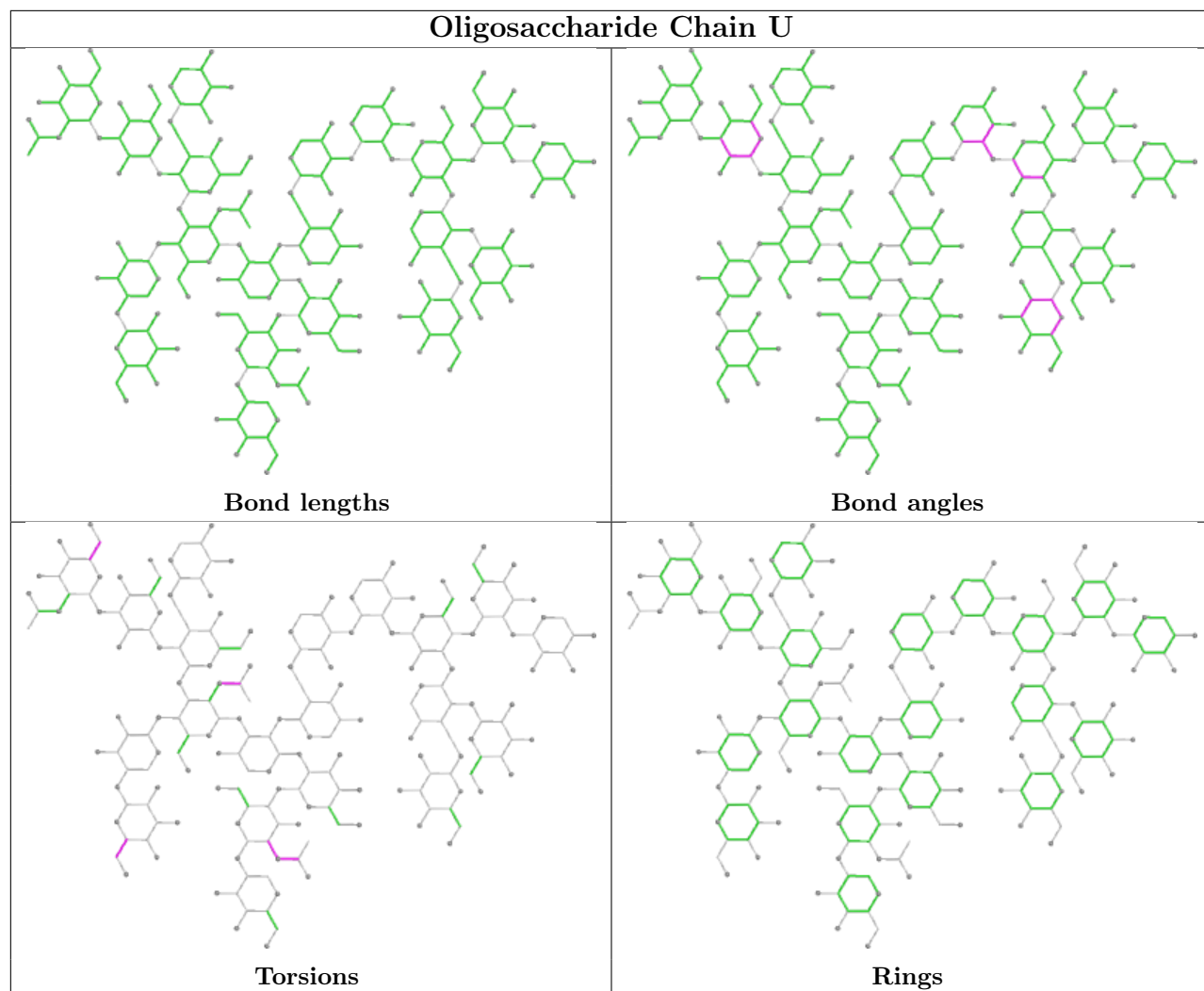


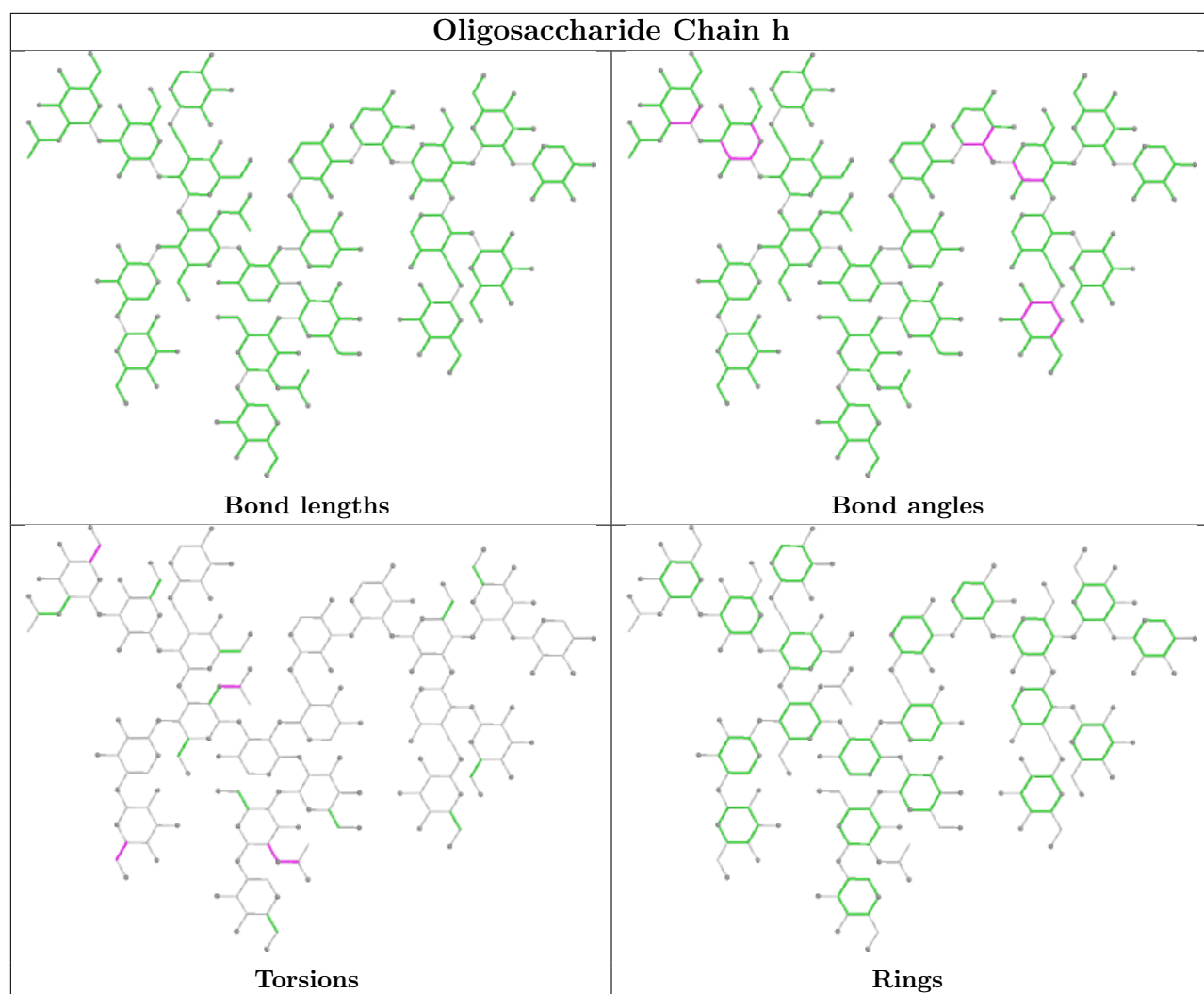


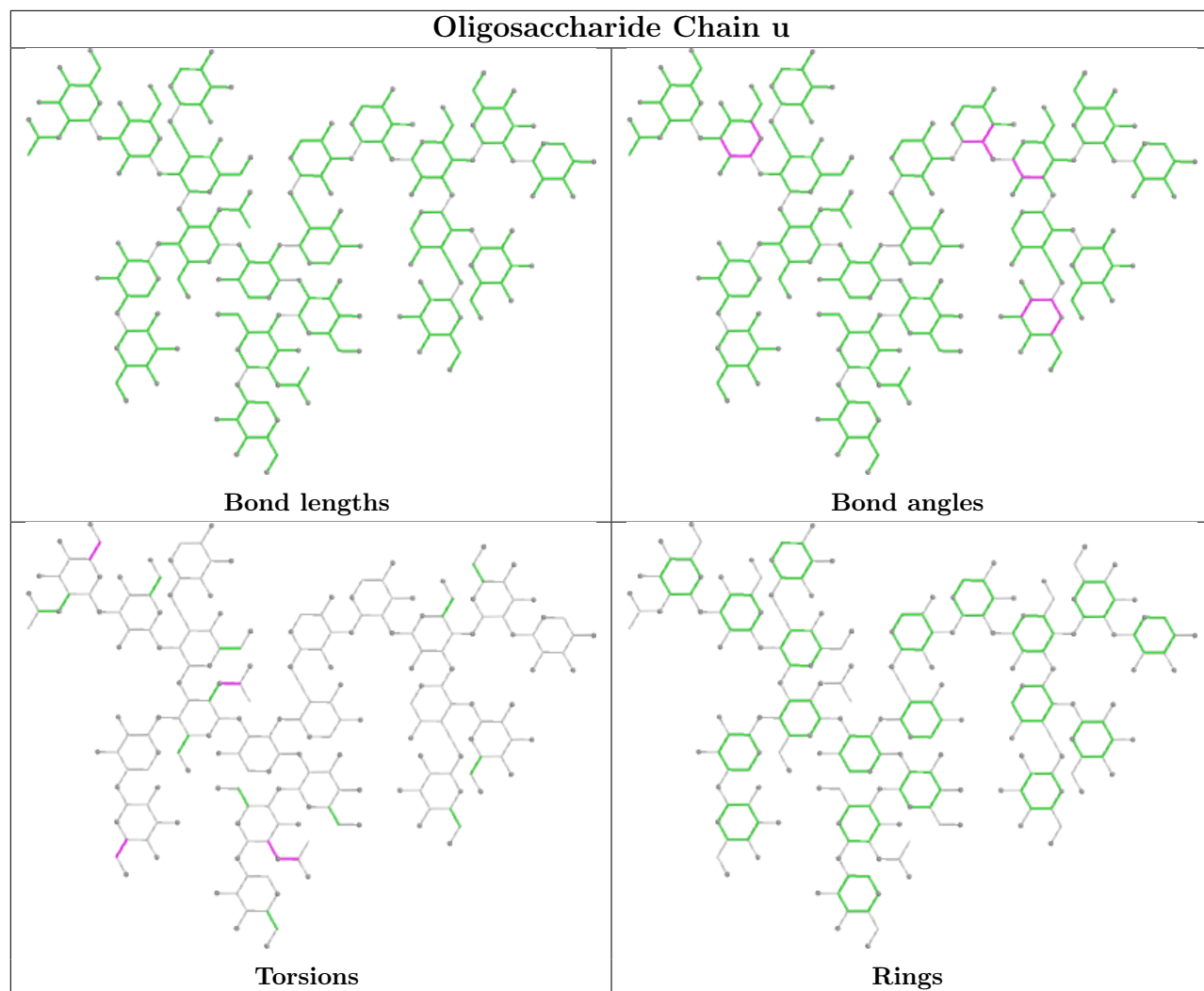


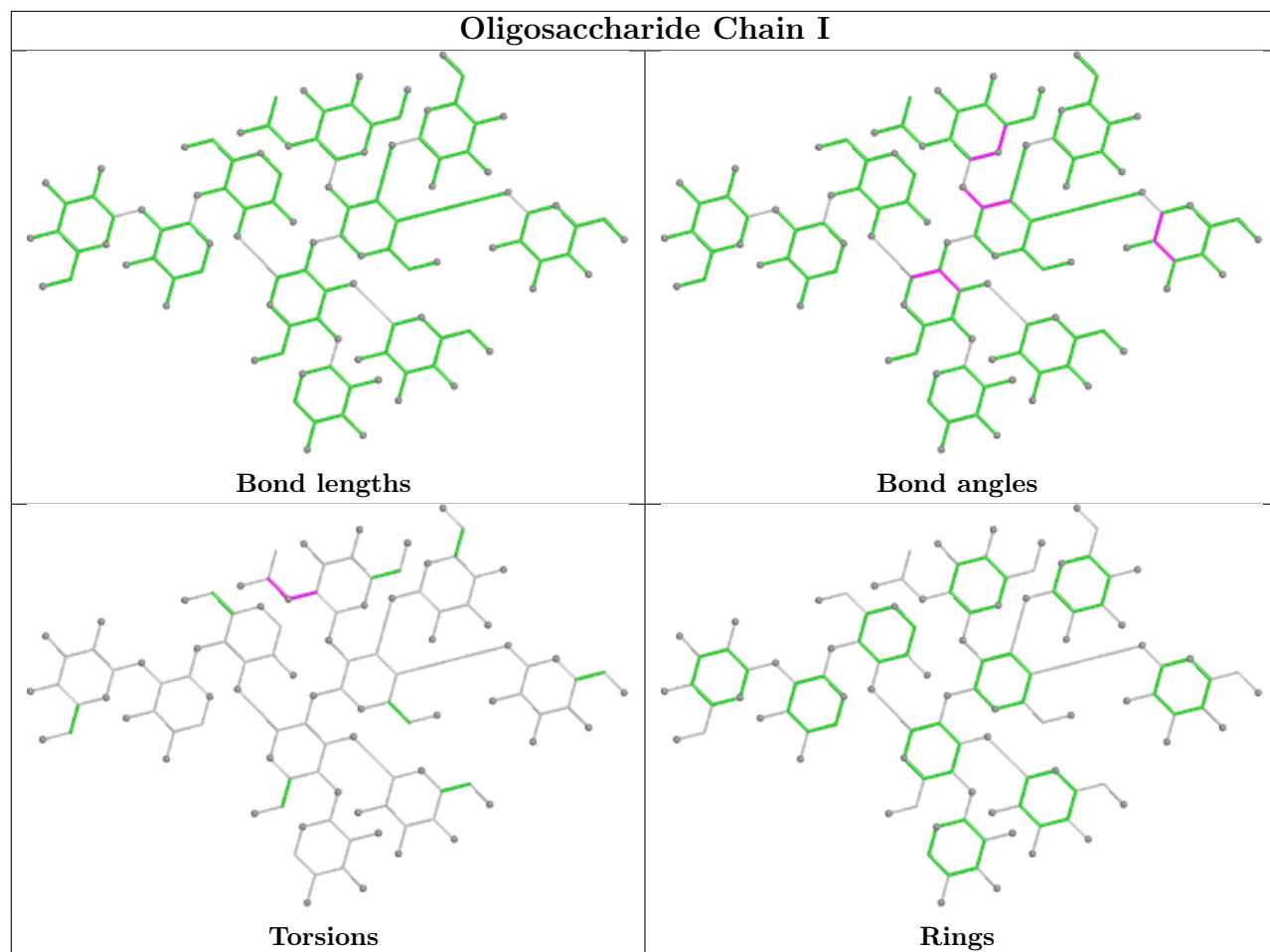


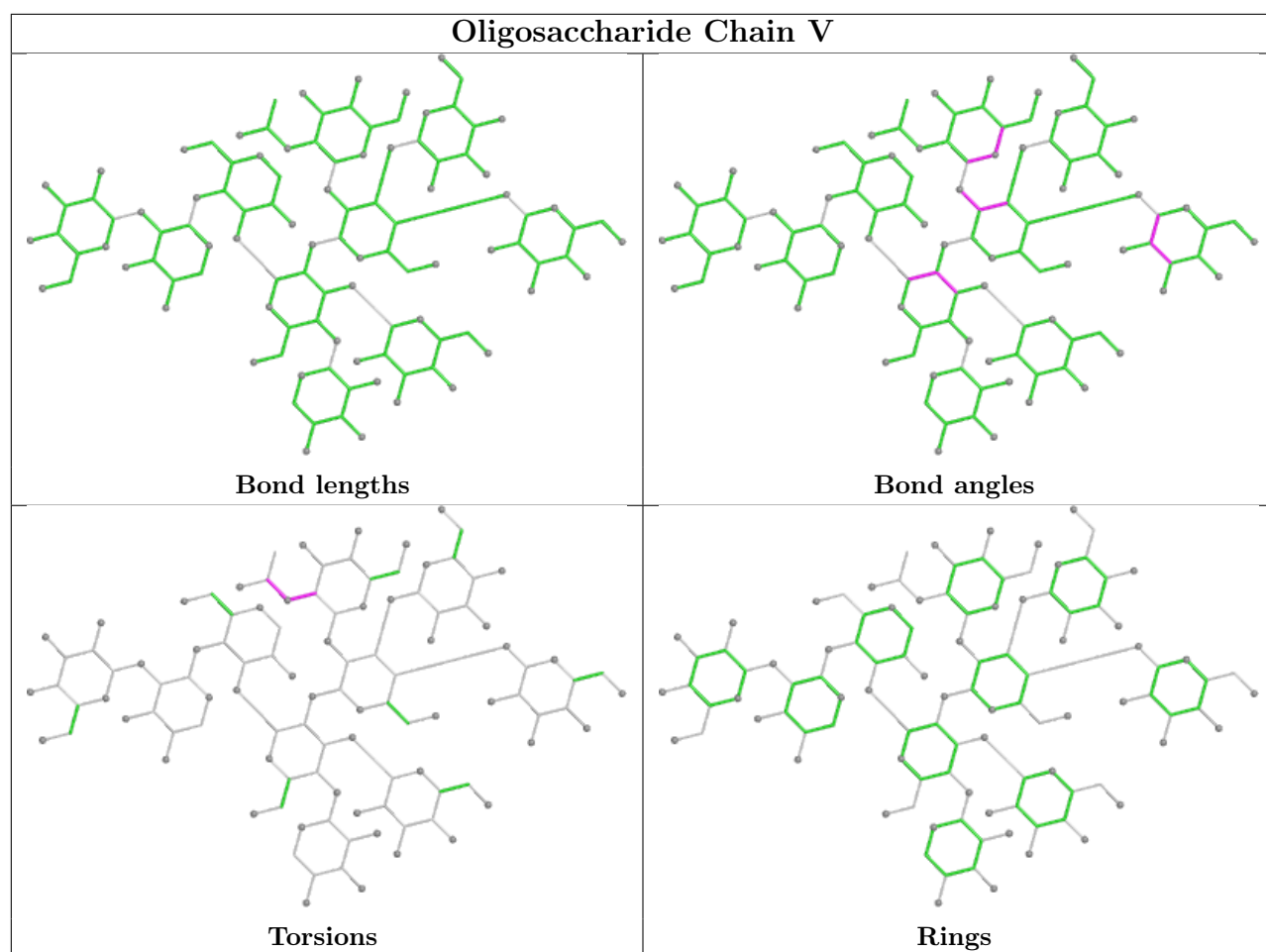


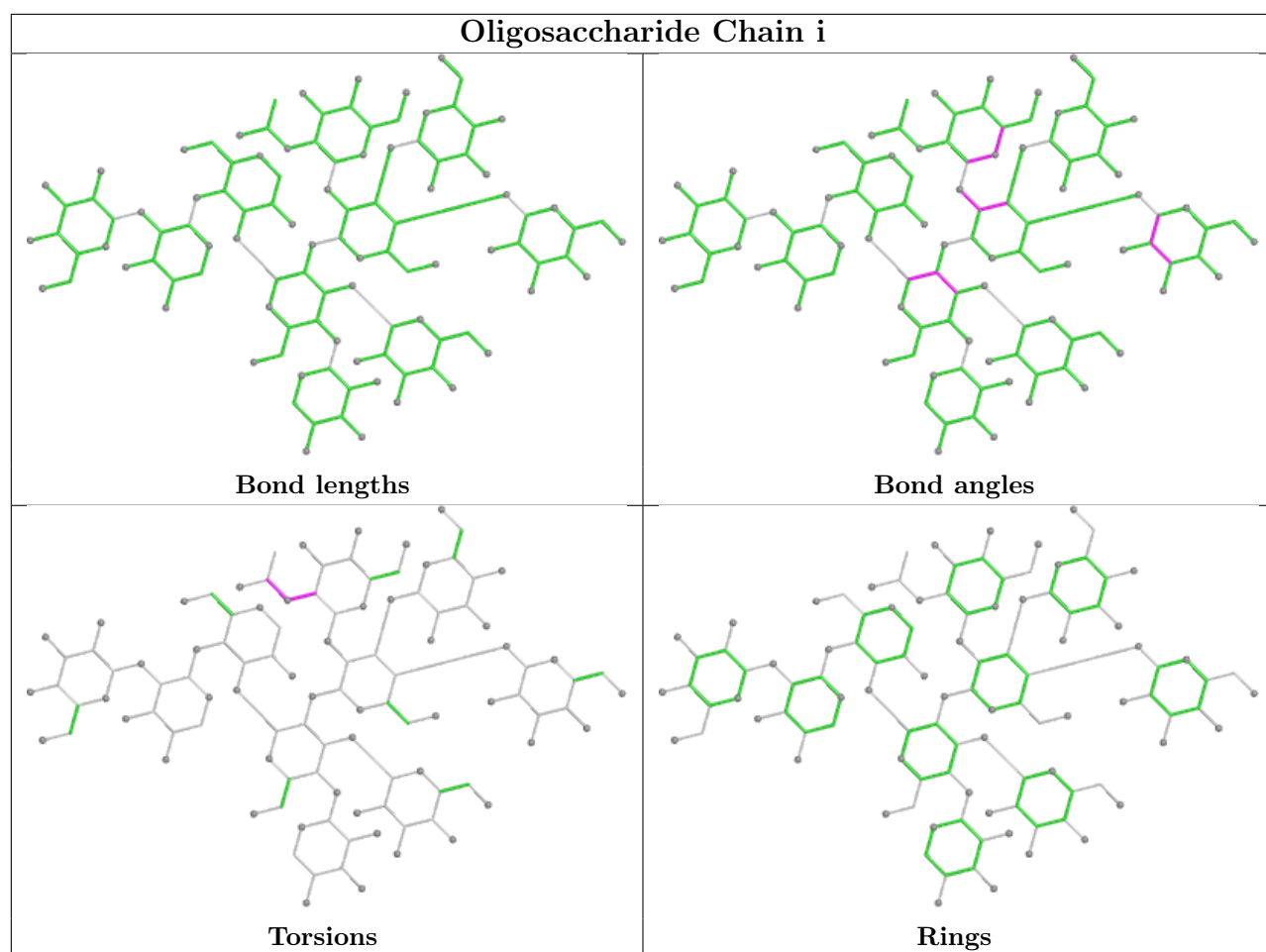


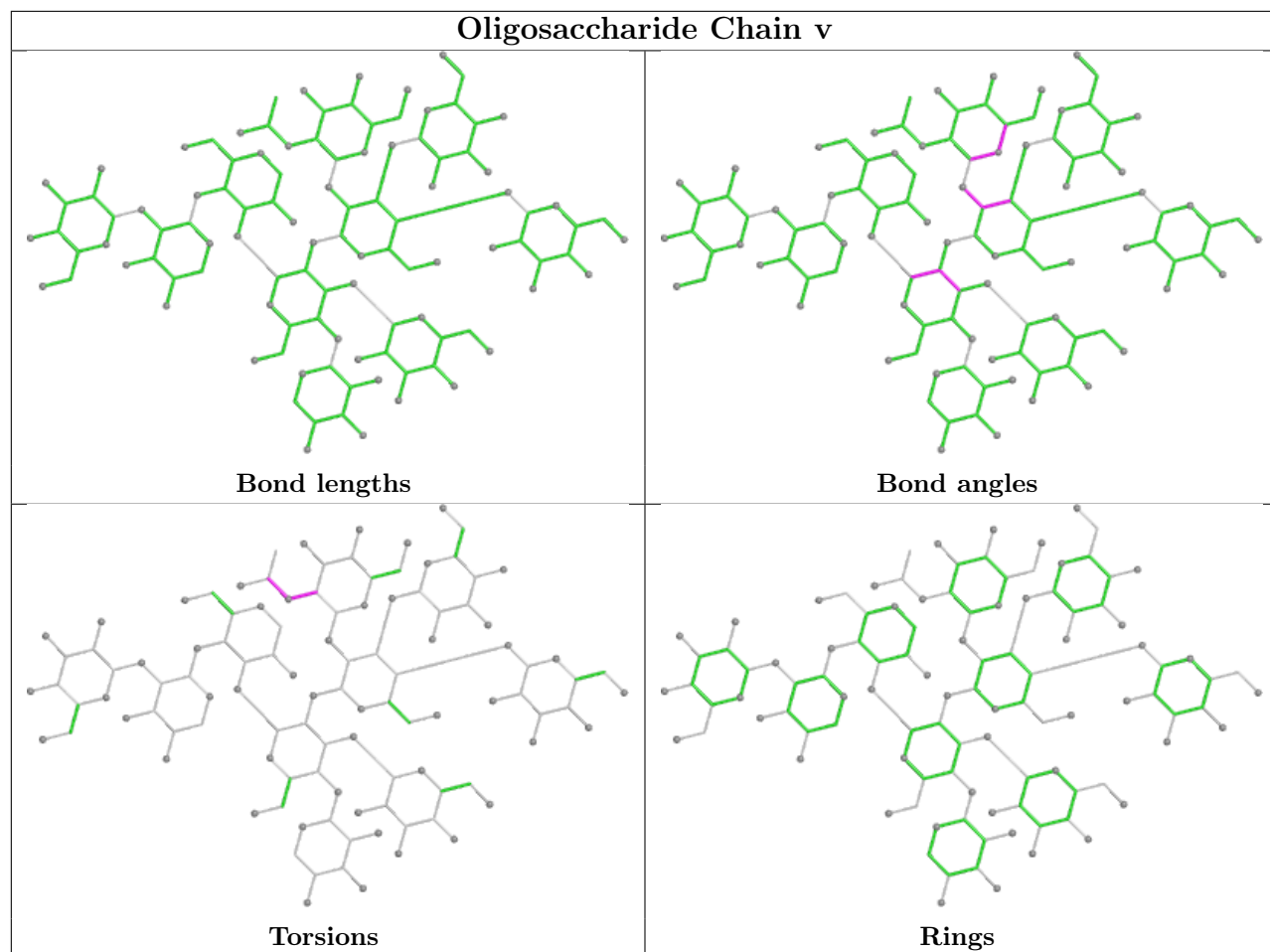


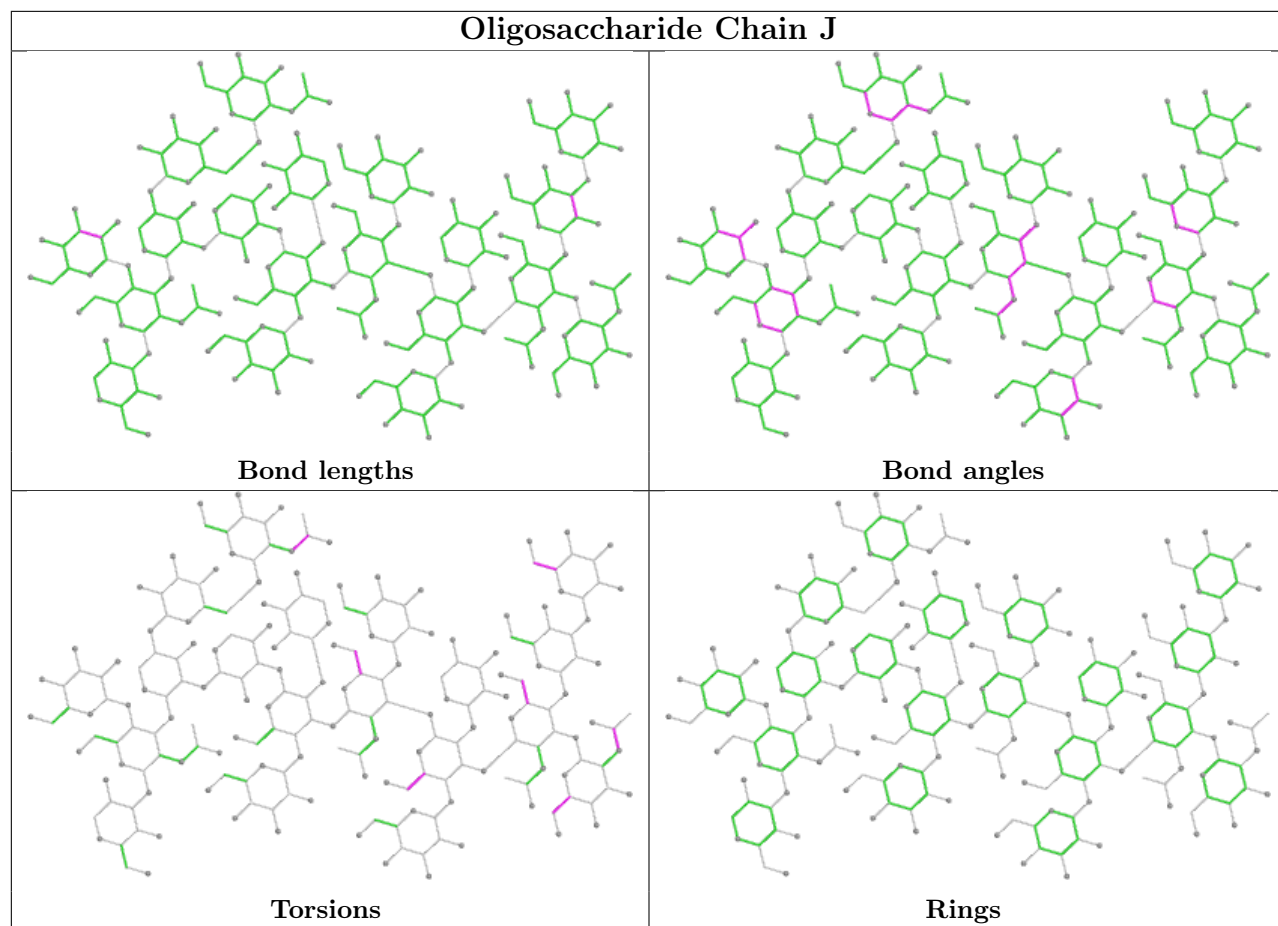


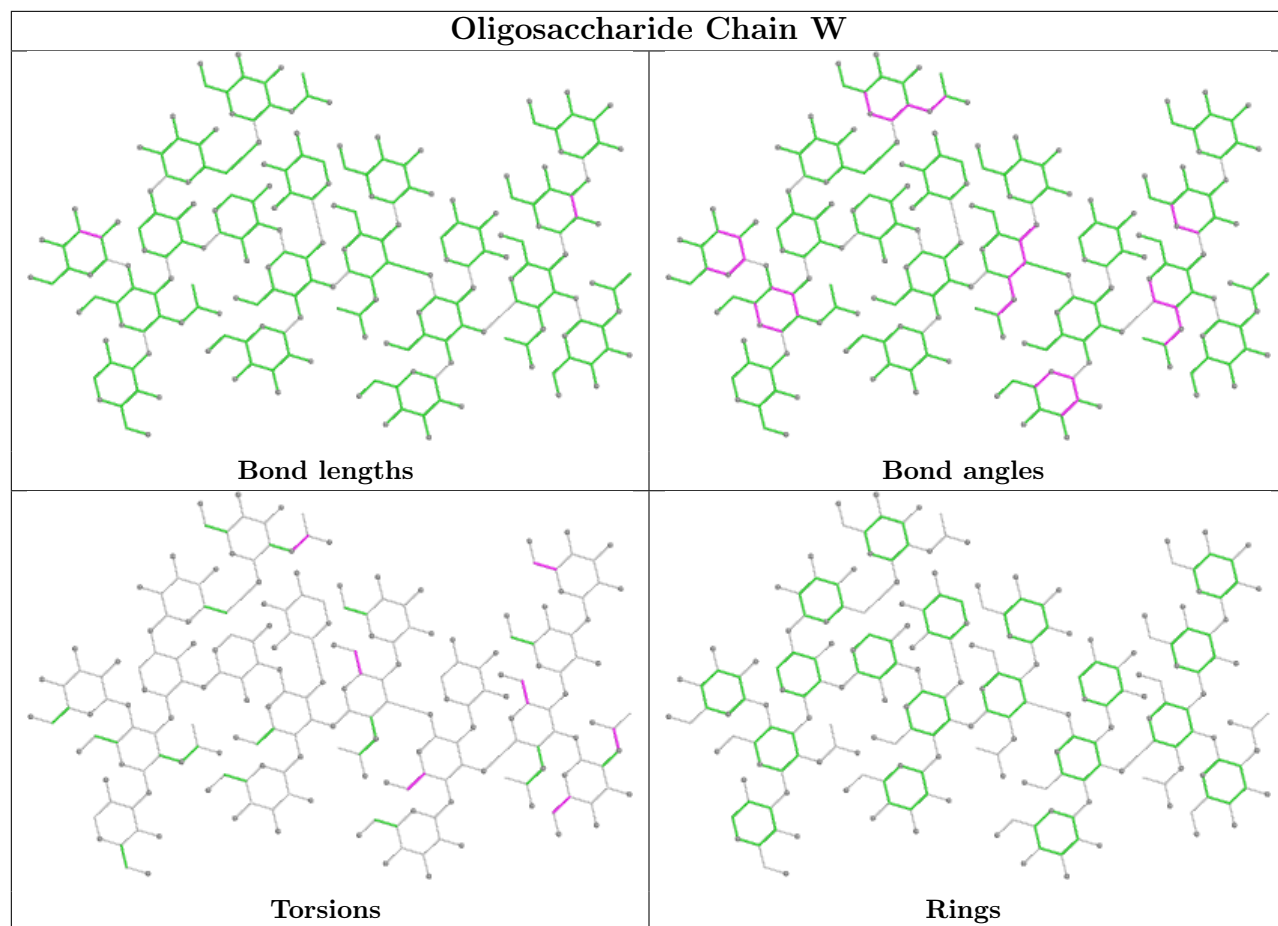


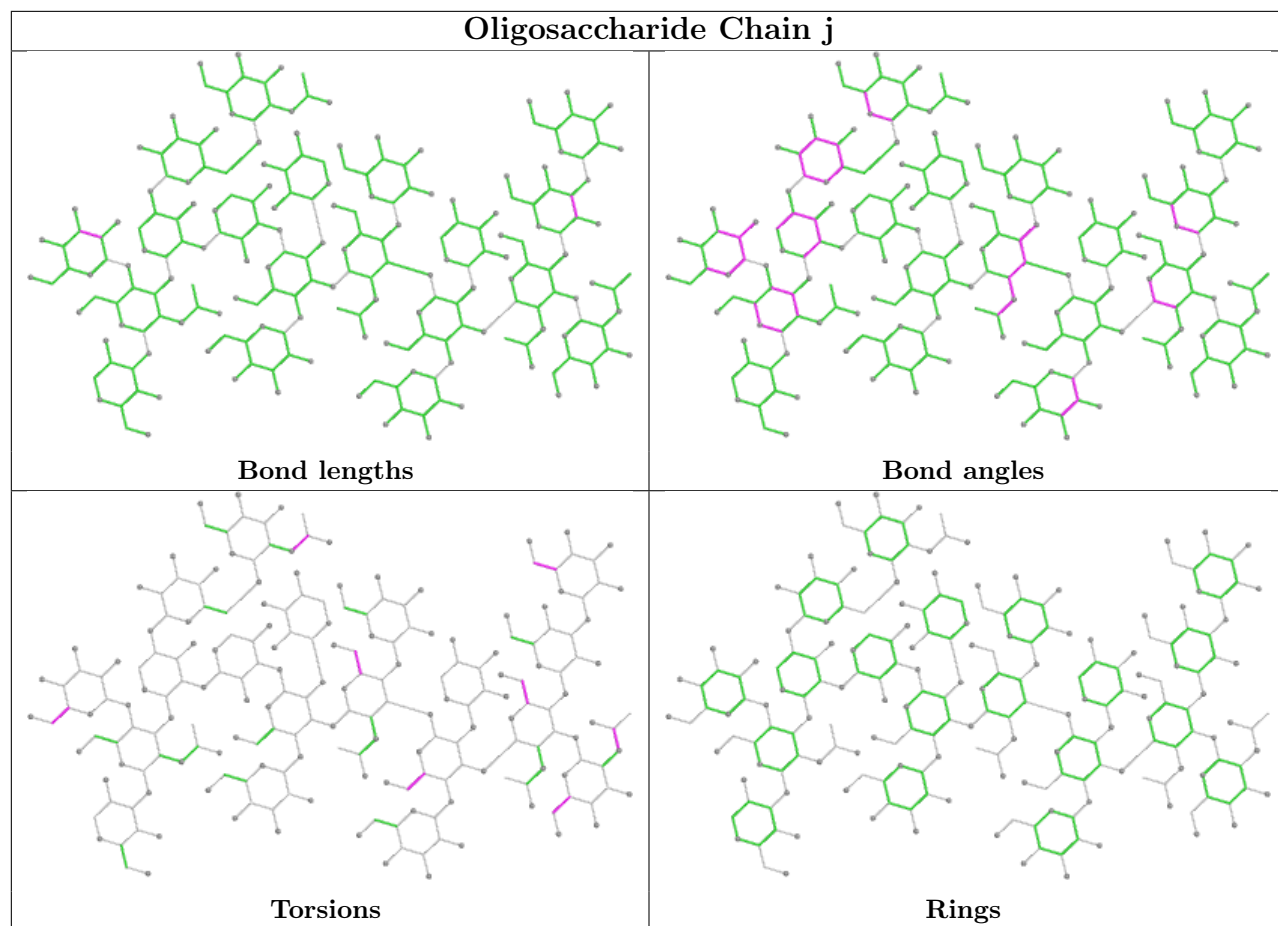


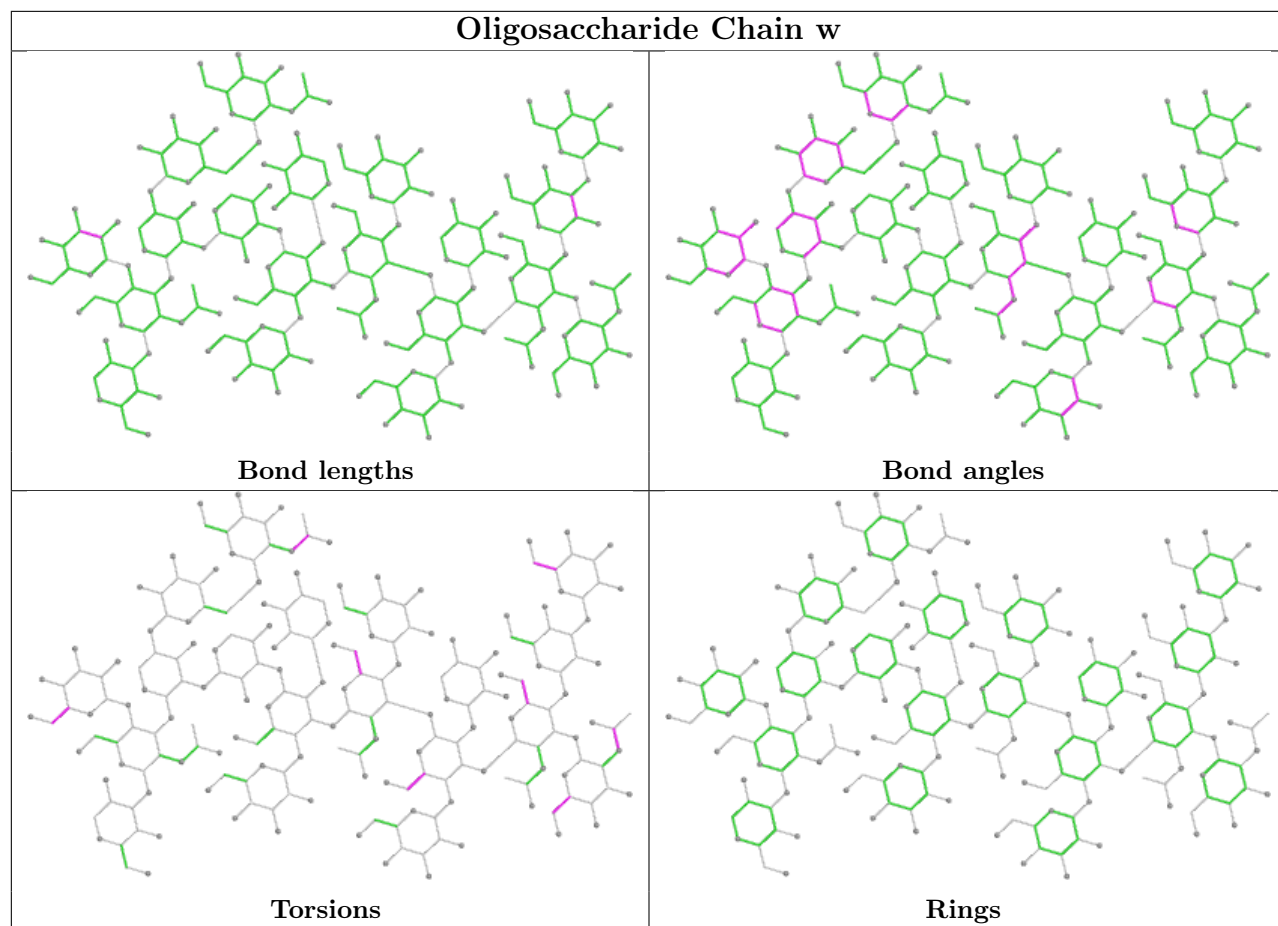


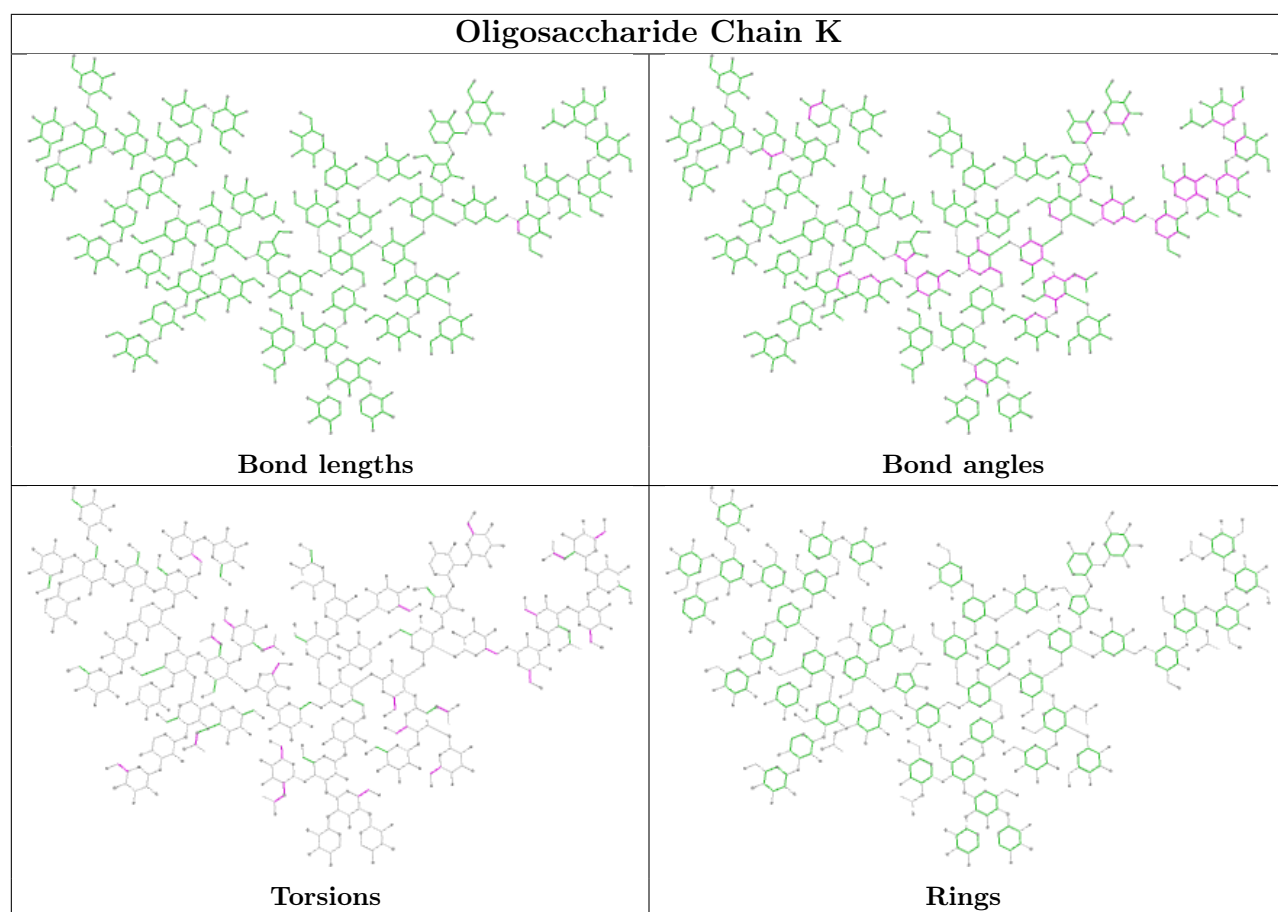


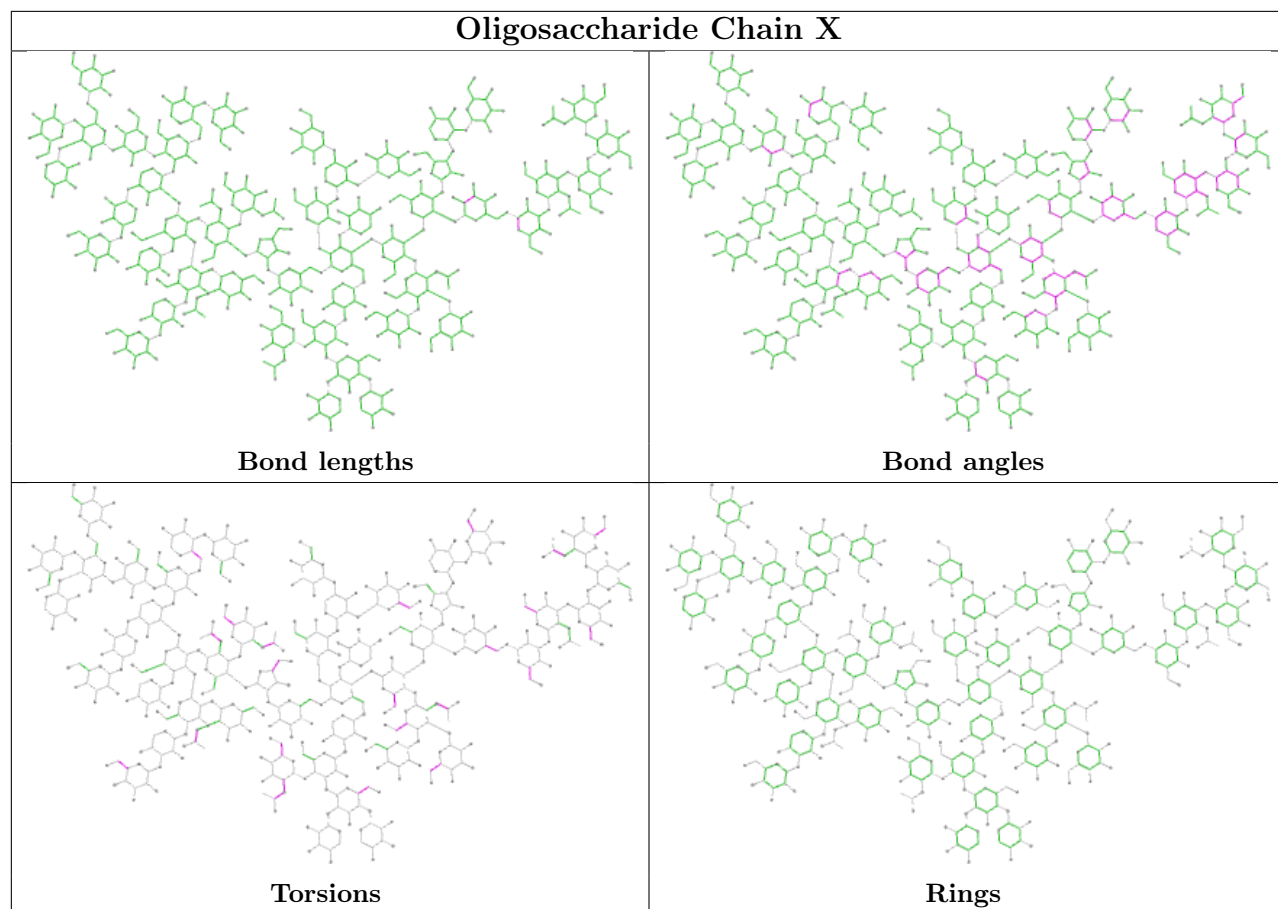


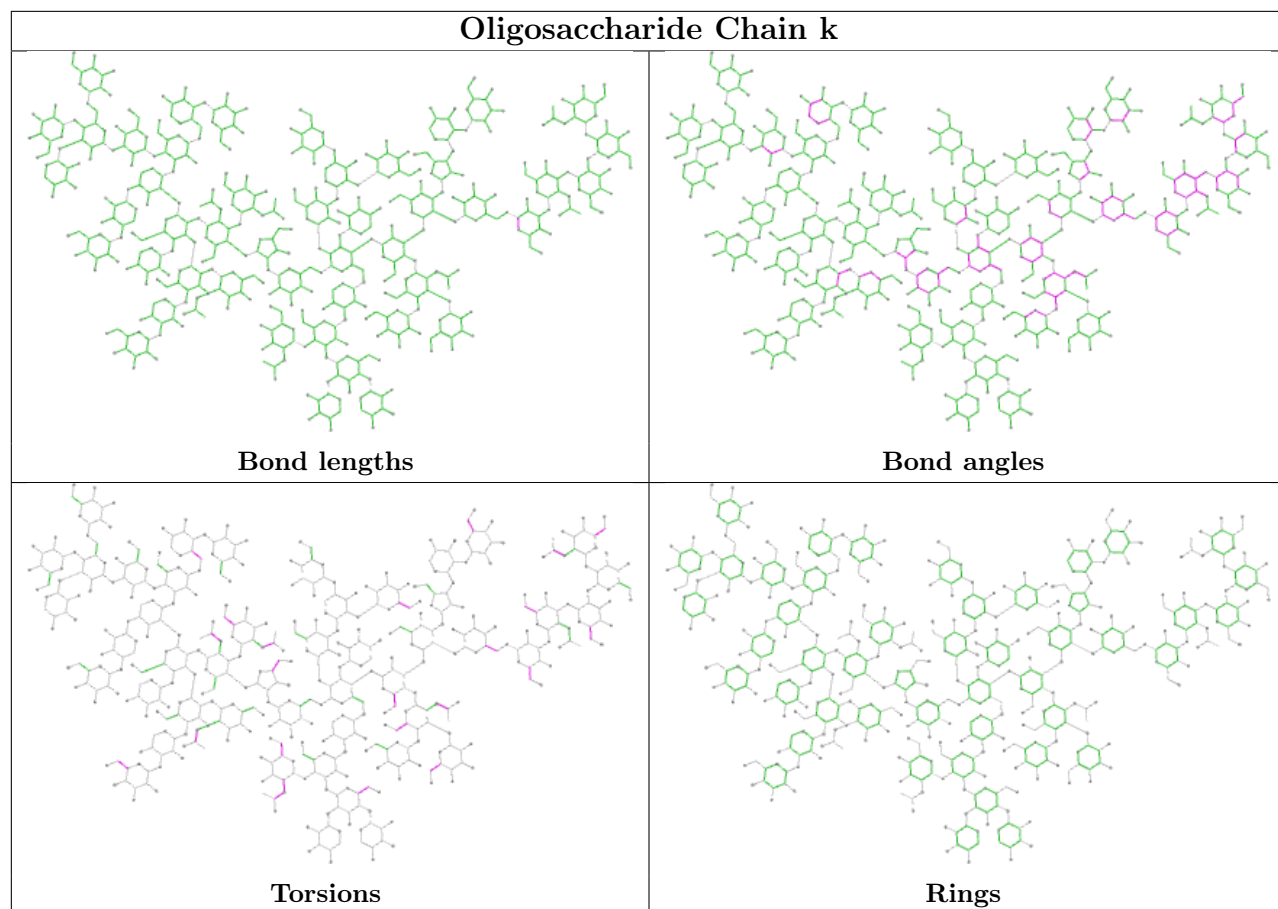


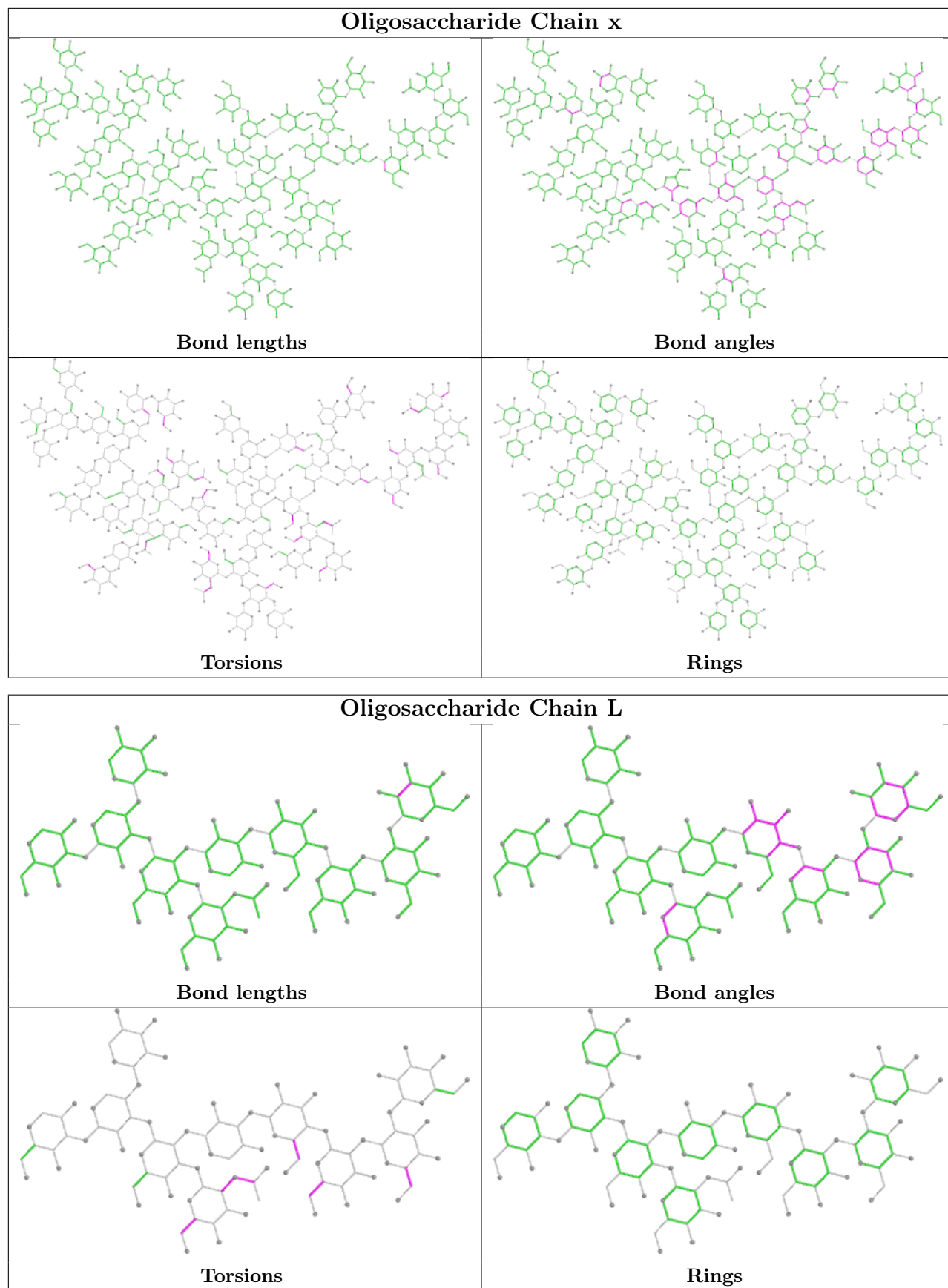


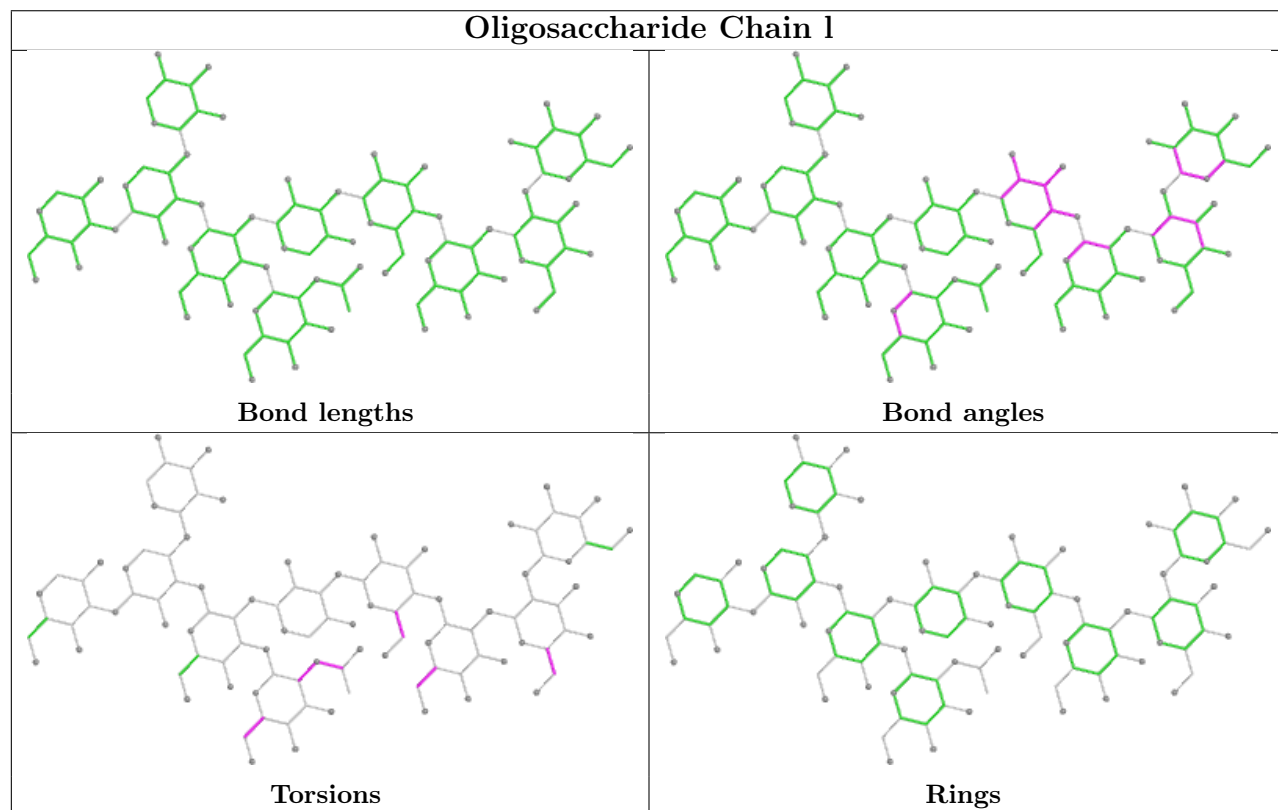
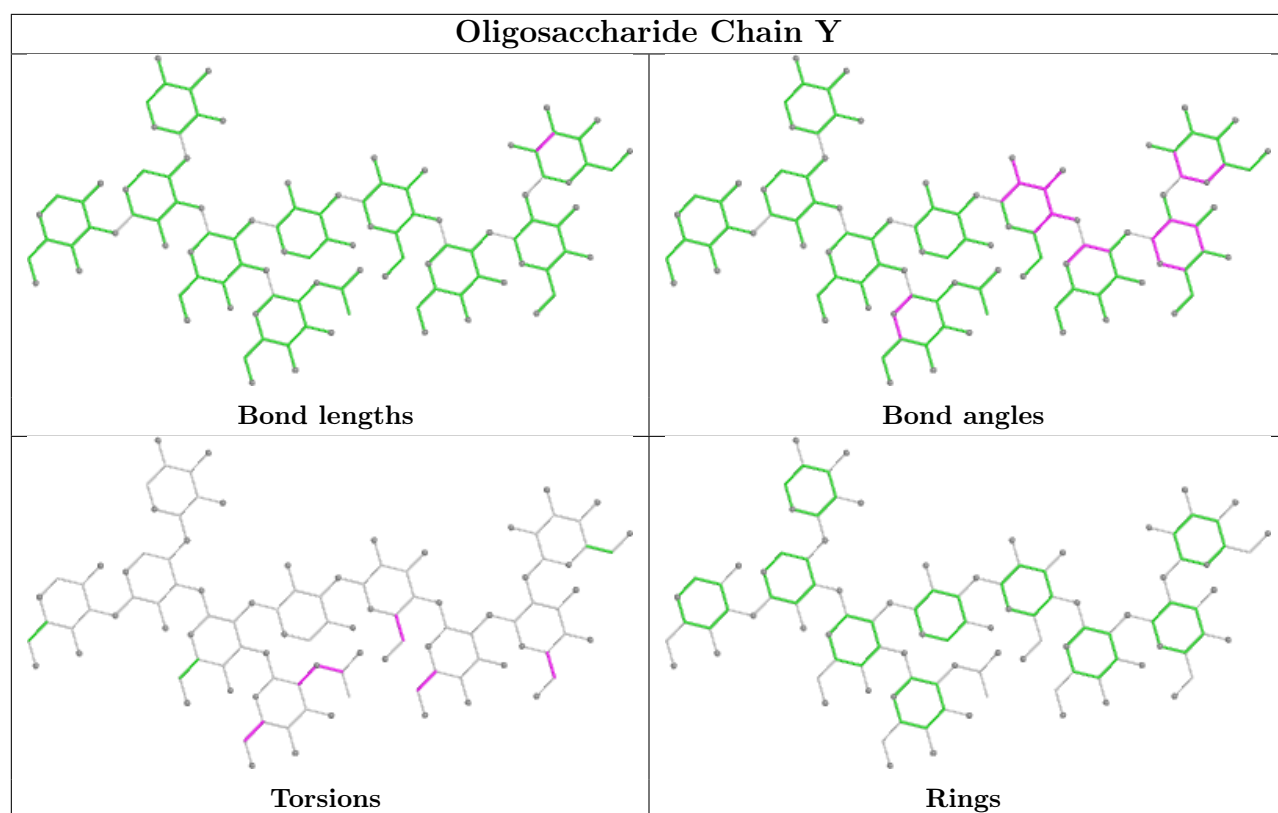


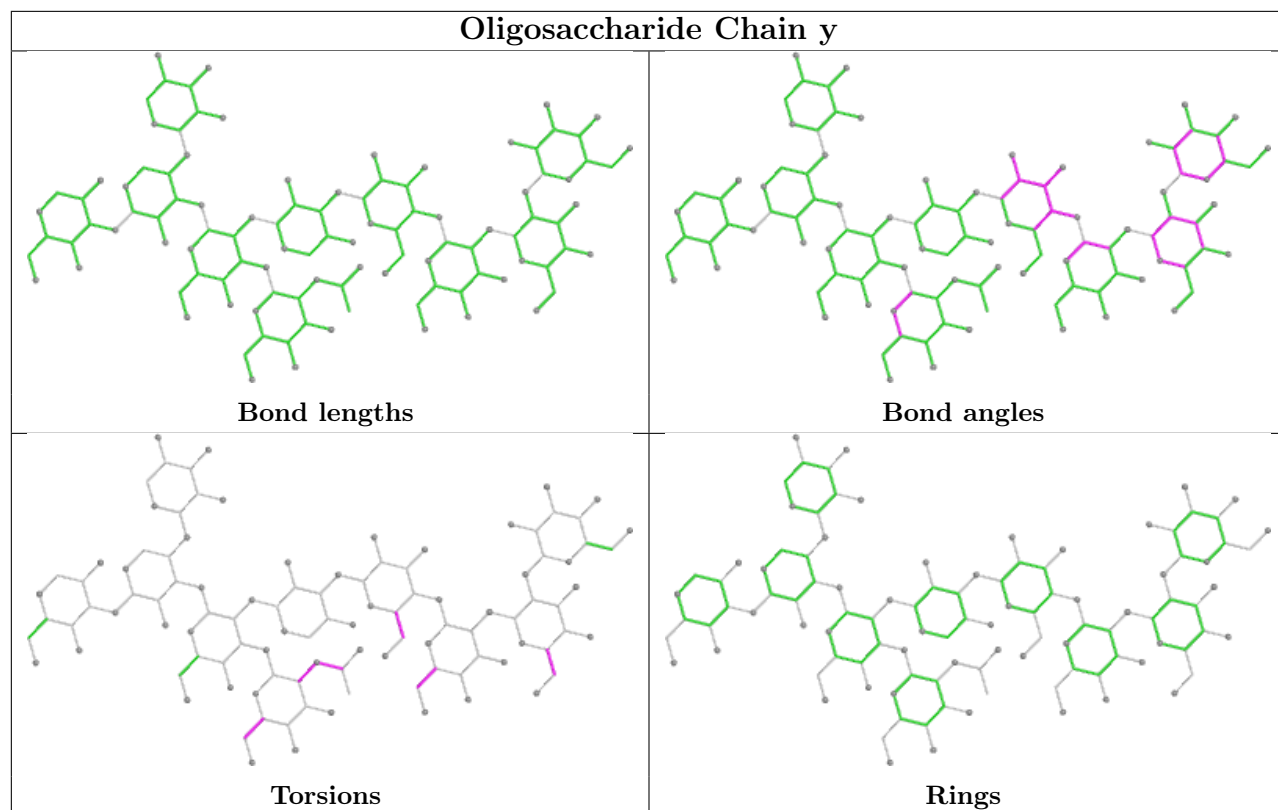


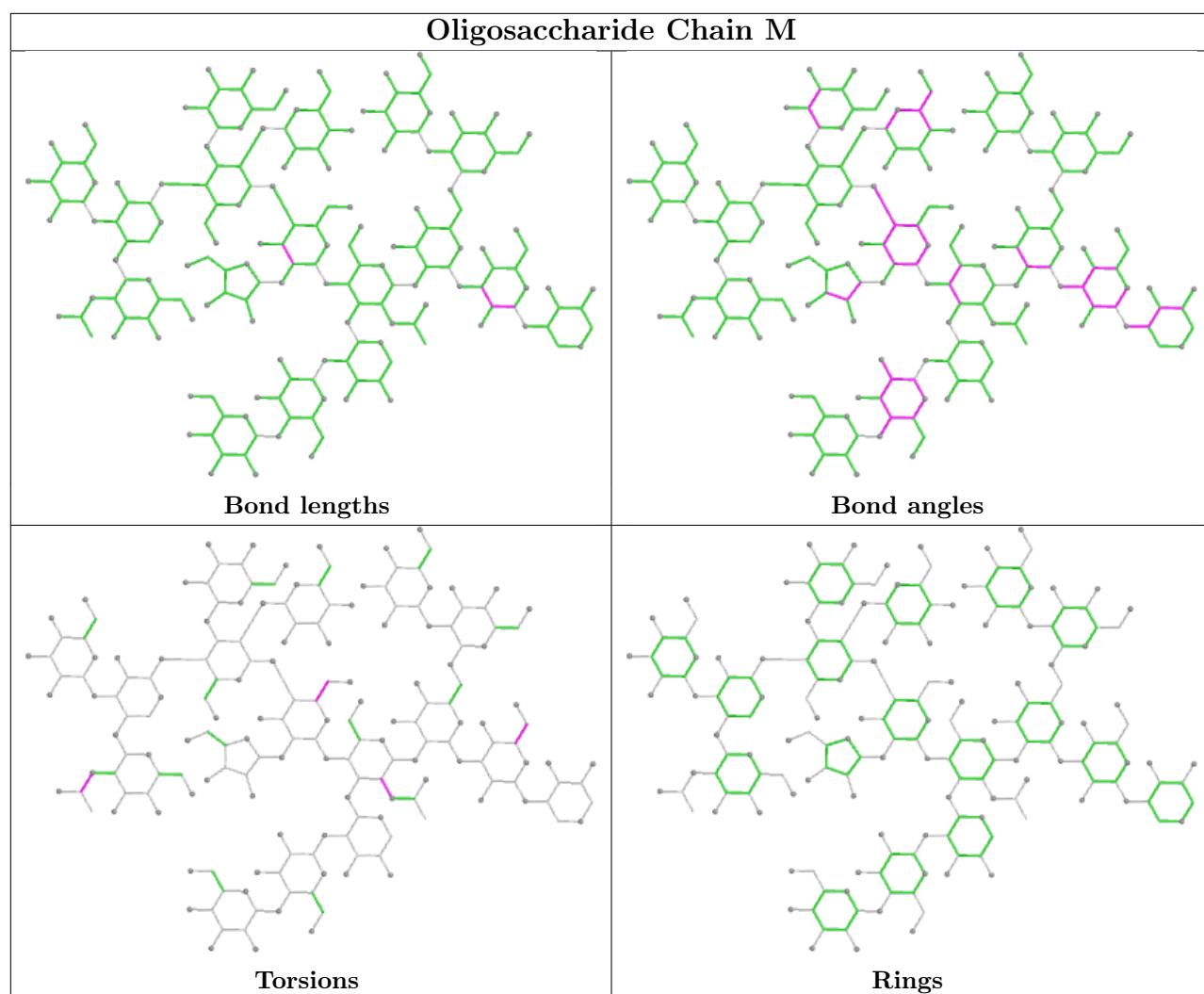


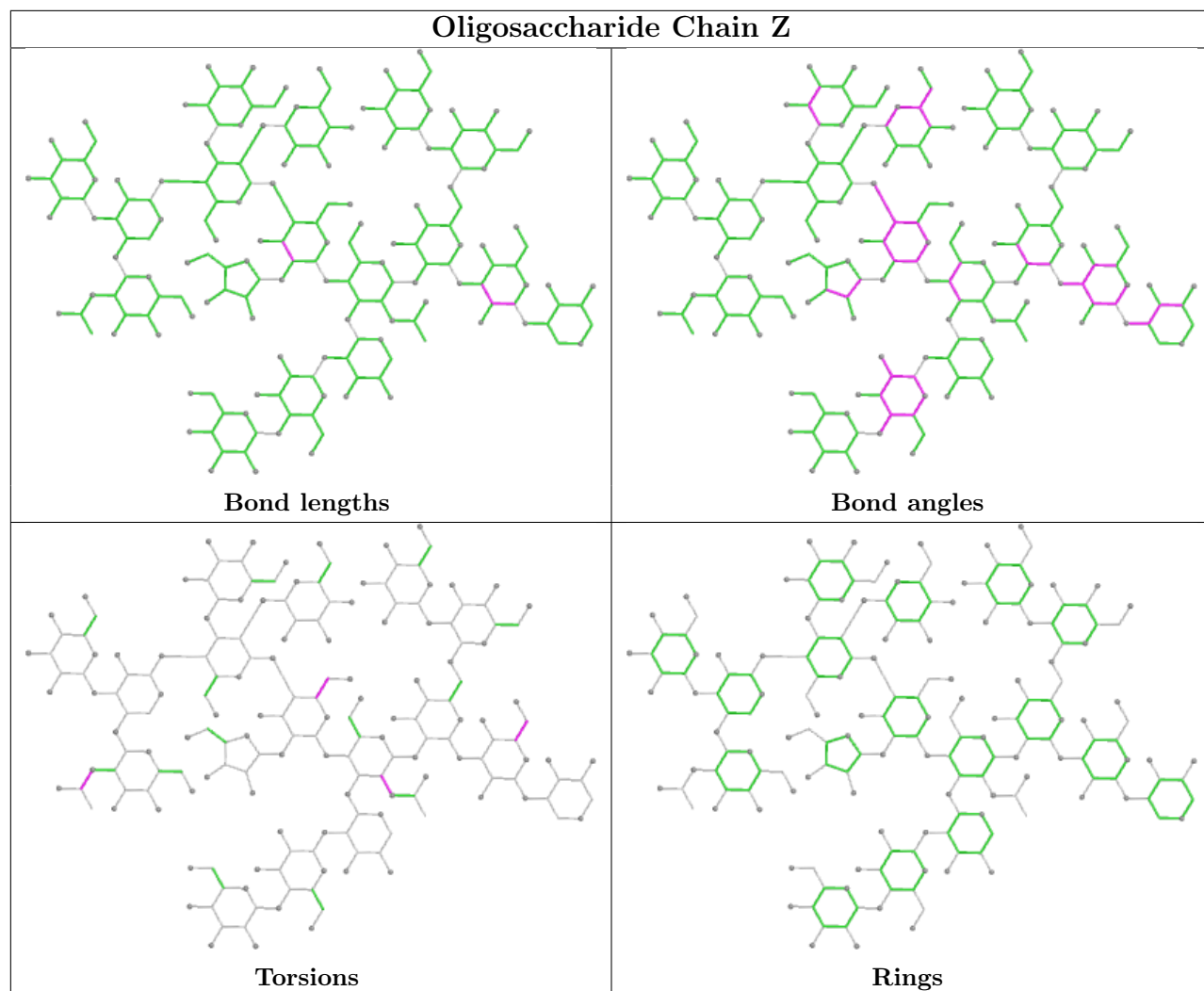


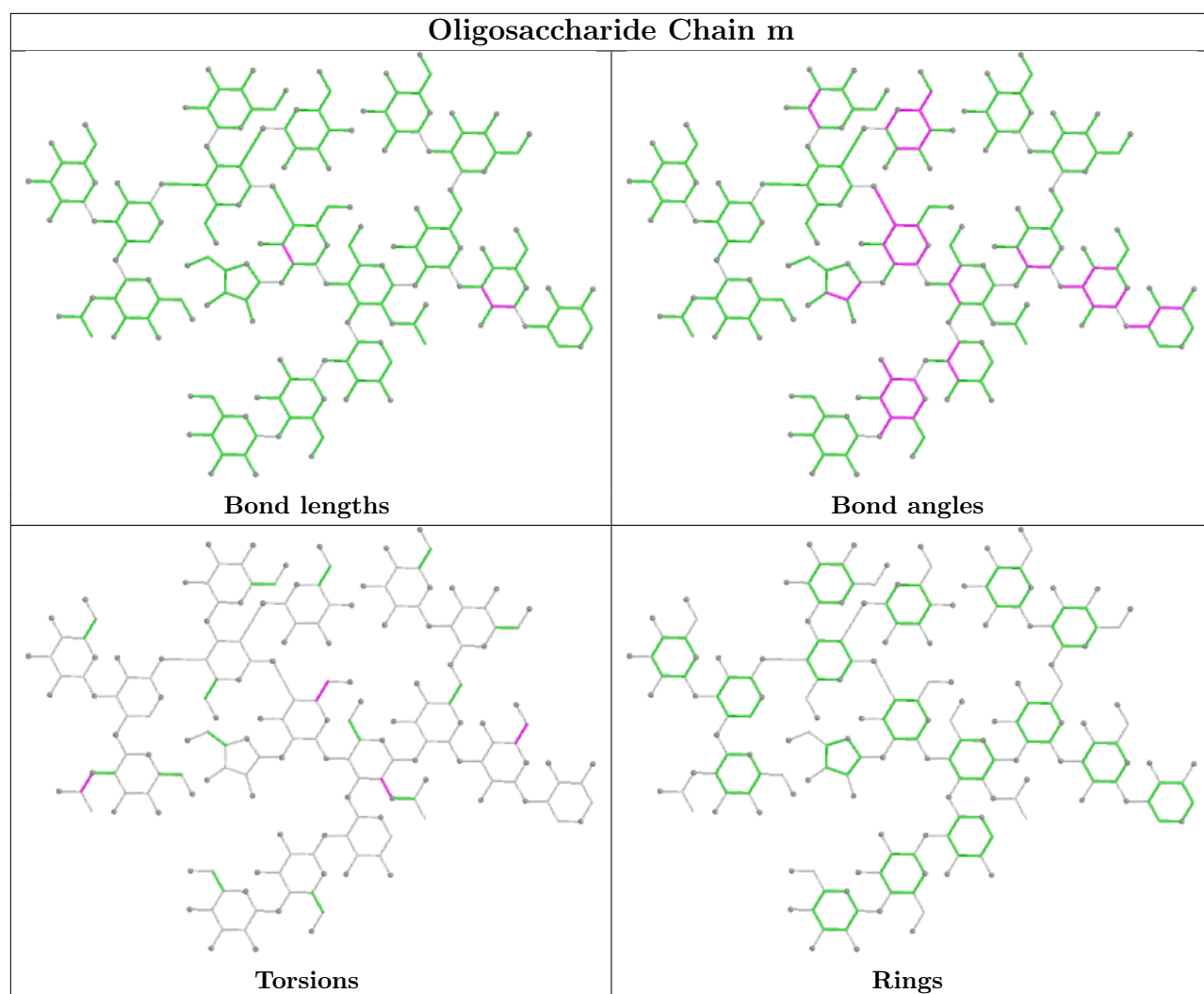


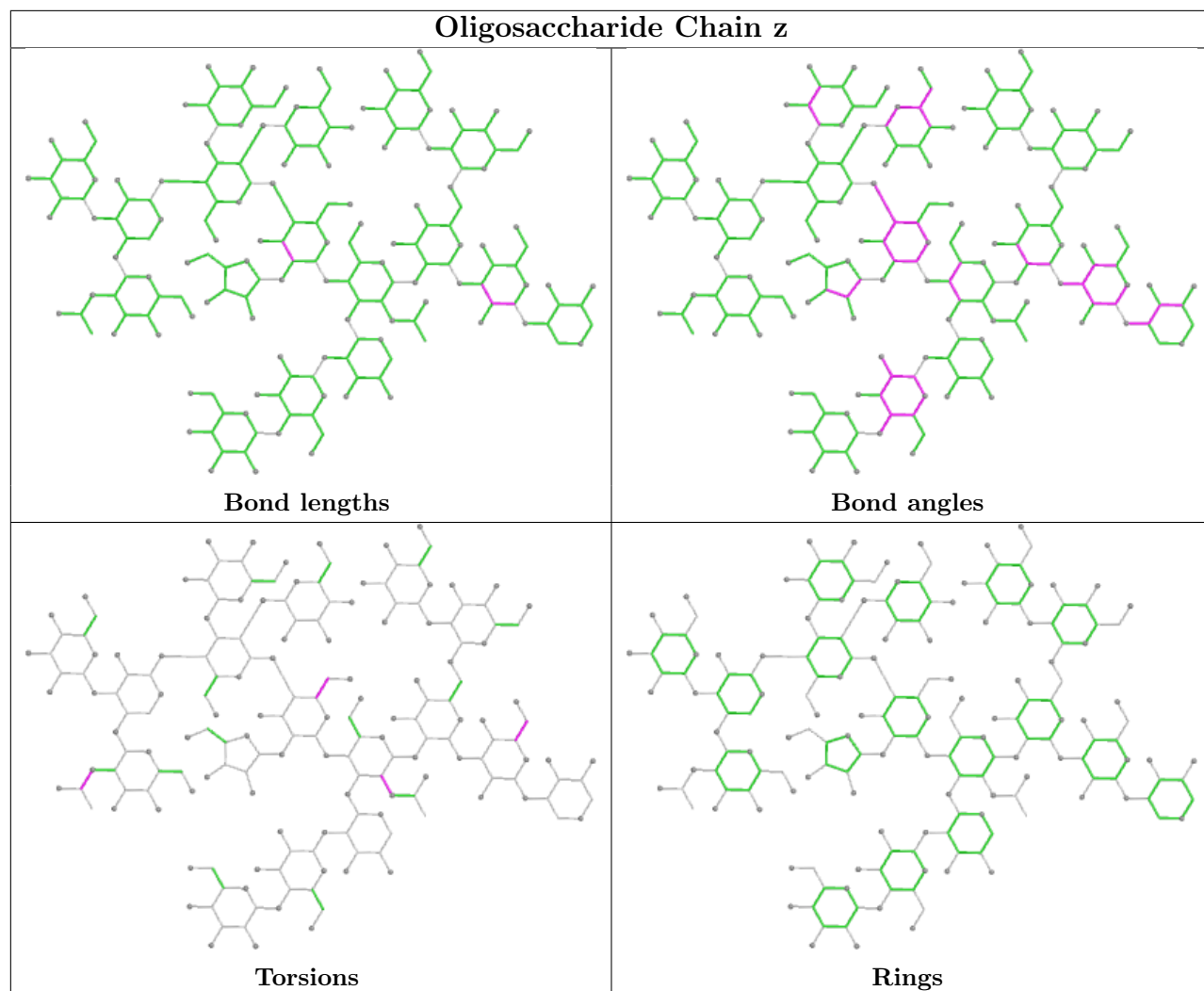


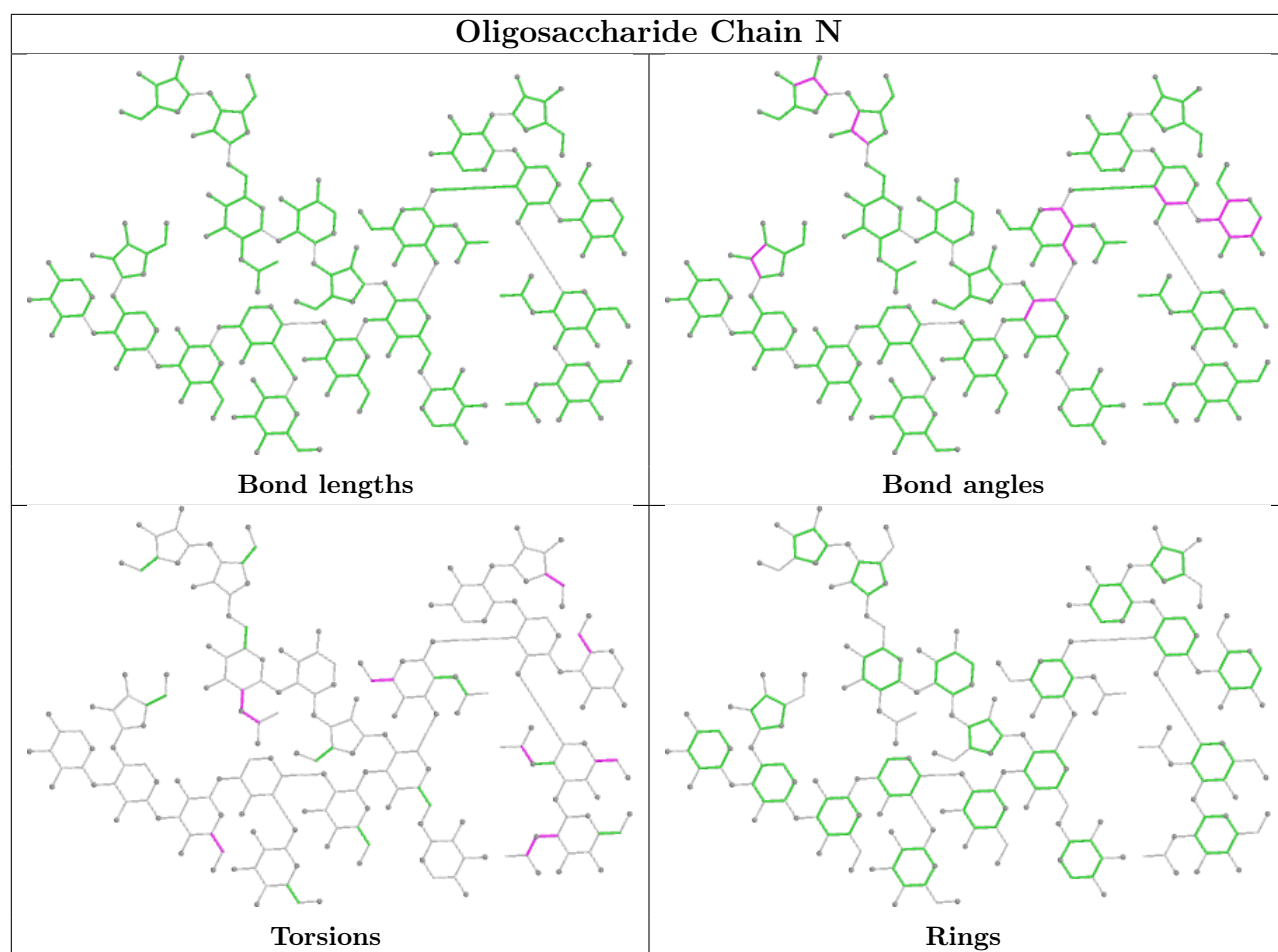


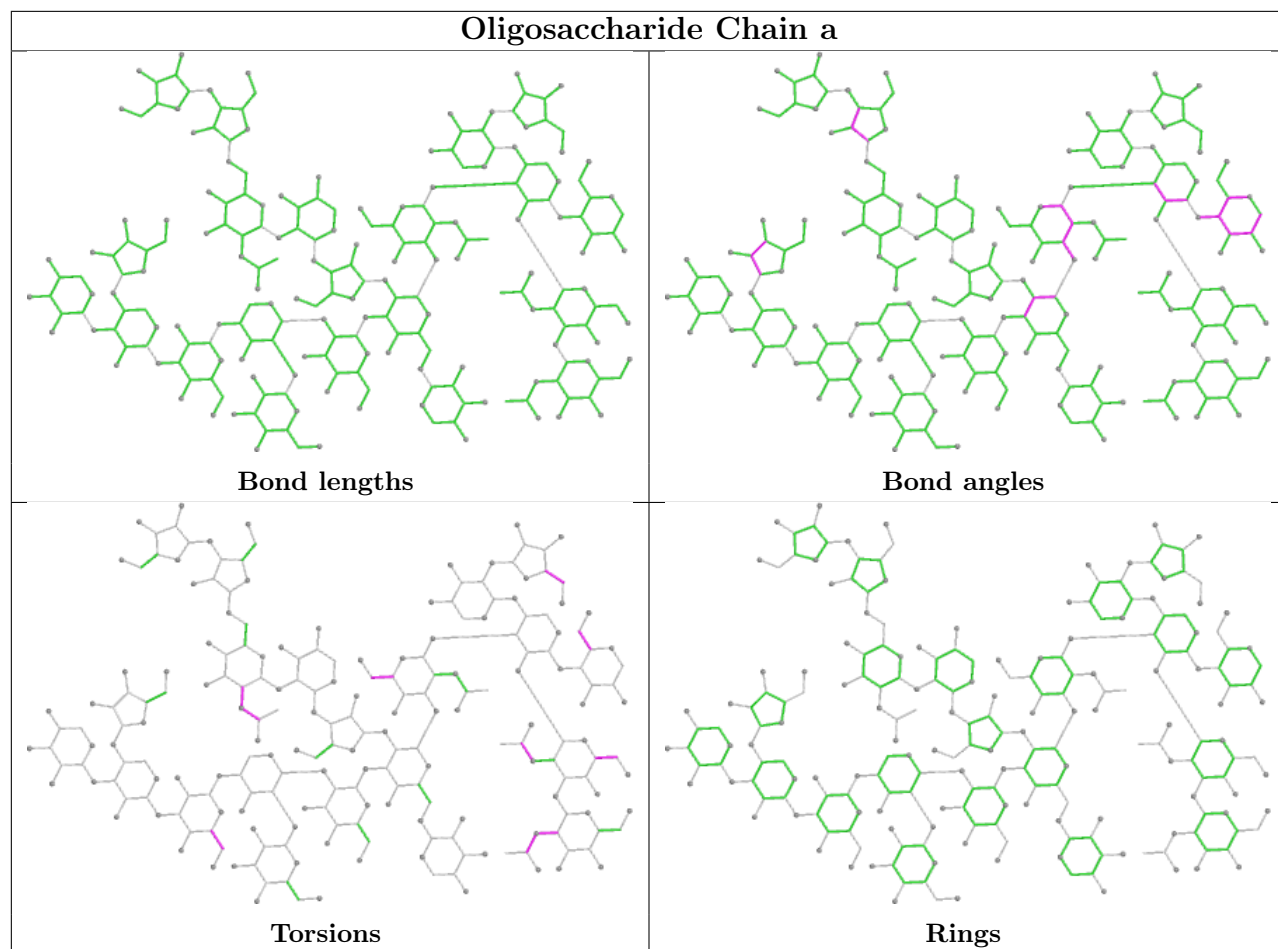


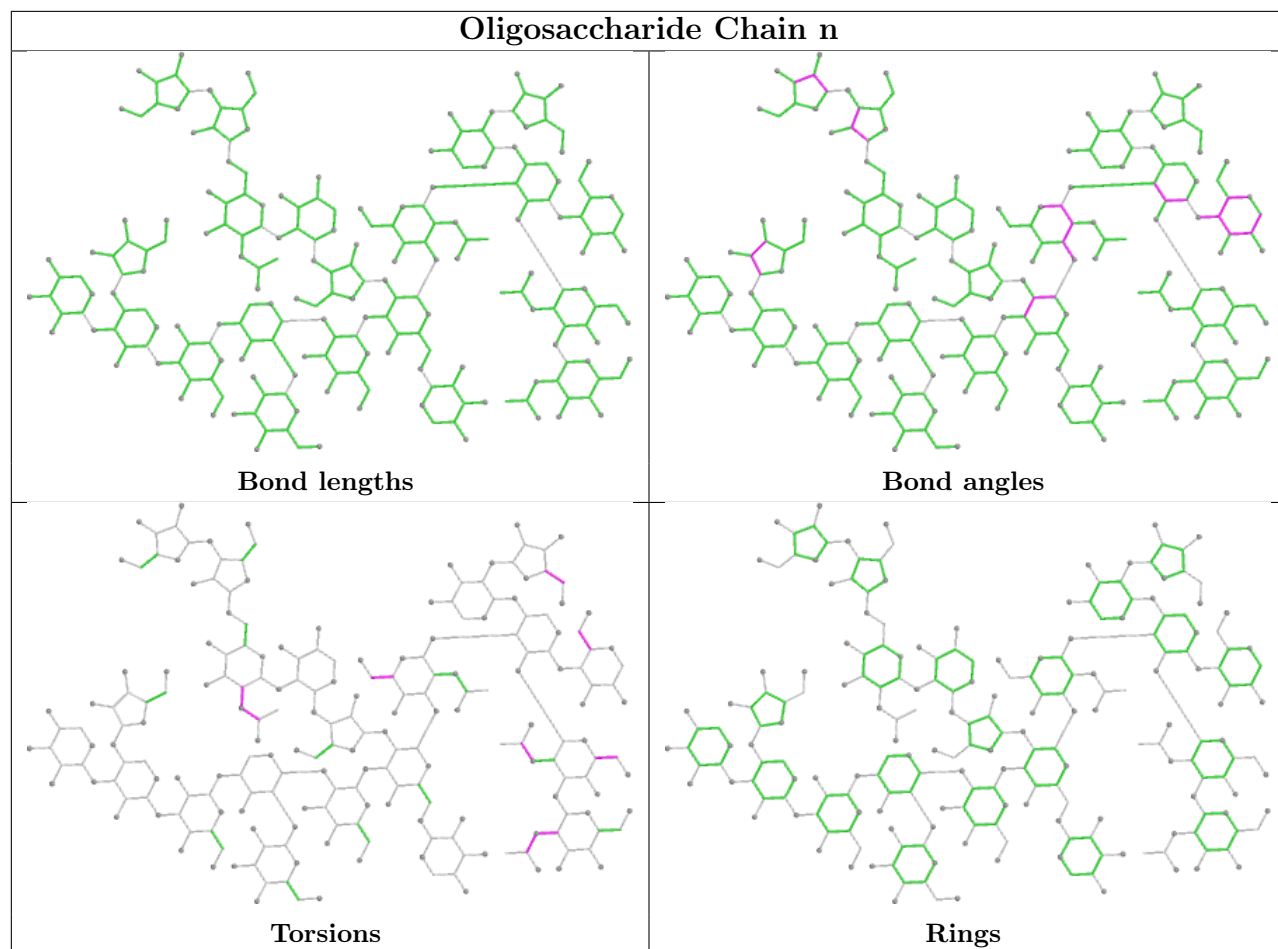


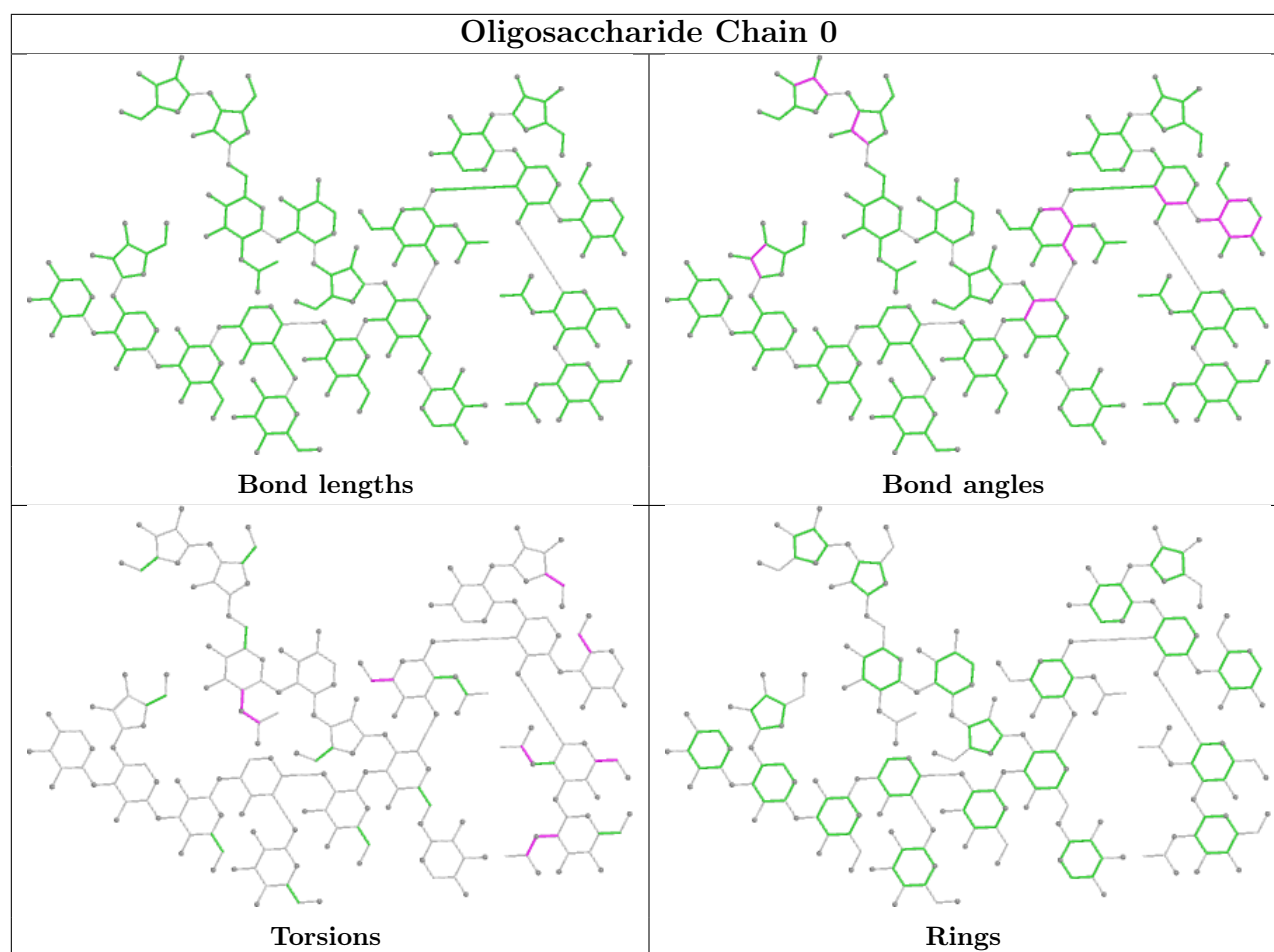












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

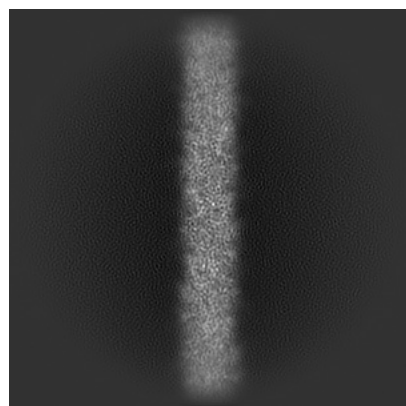
6 Map visualisation [i](#)

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.

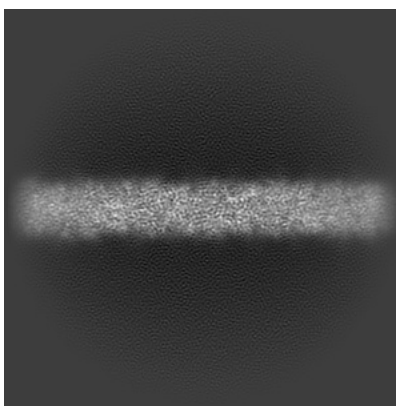
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

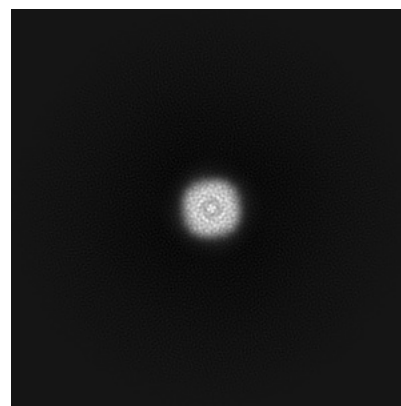
6.1.1 Primary map



X

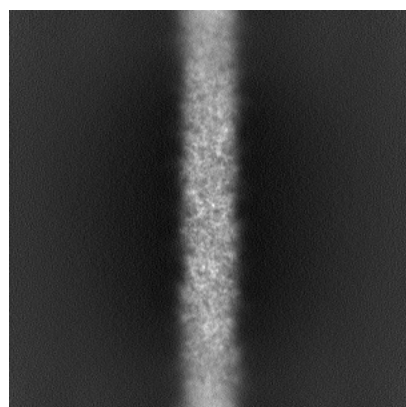


Y

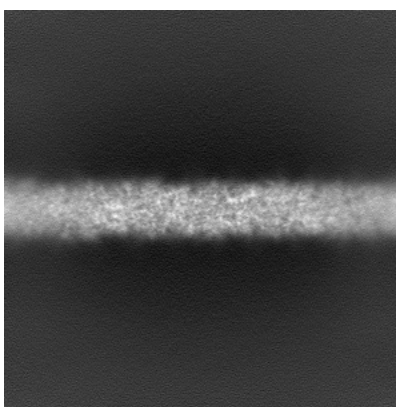


Z

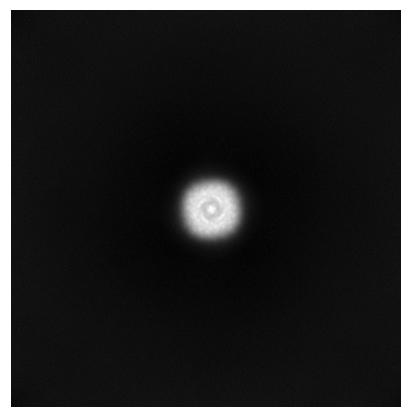
6.1.2 Raw map



X



Y

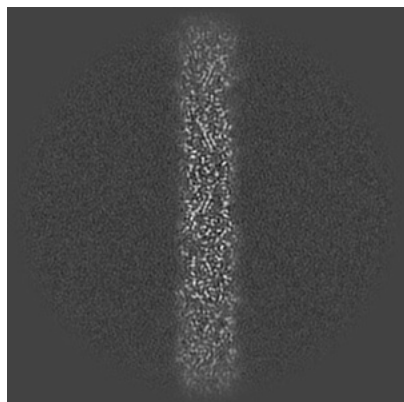


Z

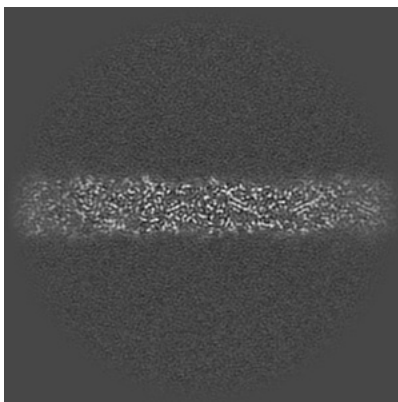
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

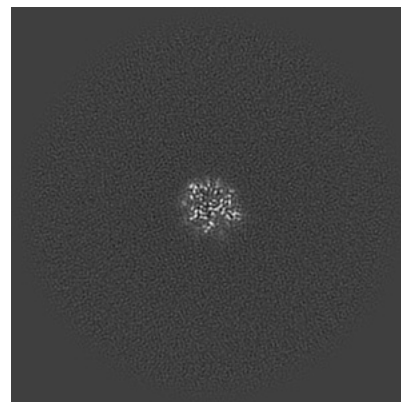
6.2.1 Primary map



X Index: 192

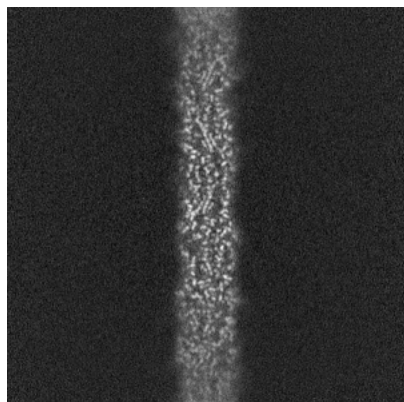


Y Index: 192

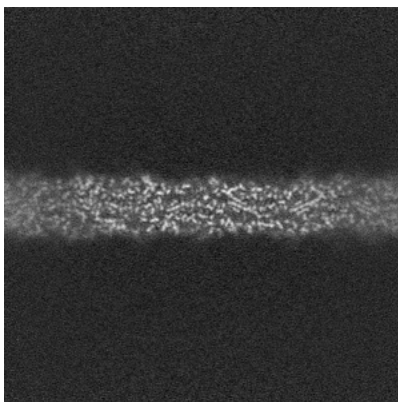


Z Index: 192

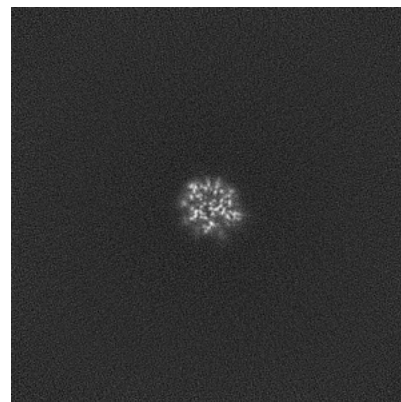
6.2.2 Raw map



X Index: 192



Y Index: 192

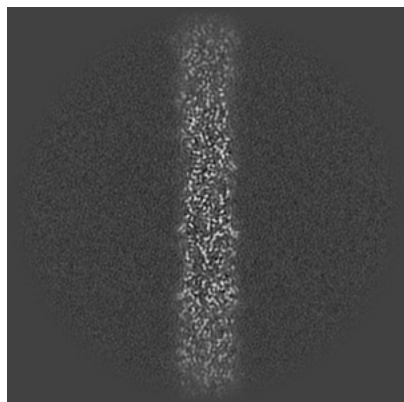


Z Index: 192

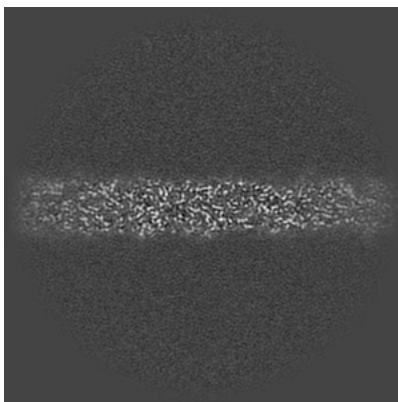
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

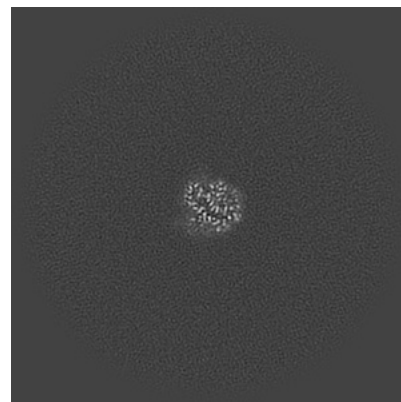
6.3.1 Primary map



X Index: 194

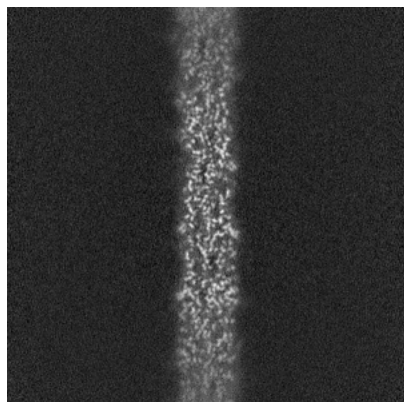


Y Index: 195

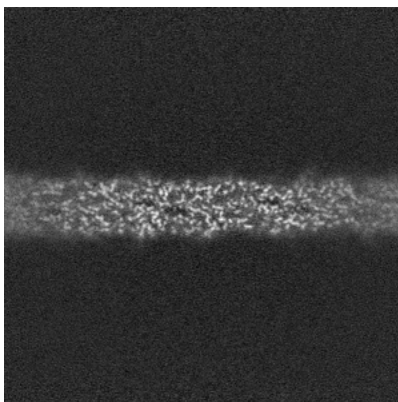


Z Index: 201

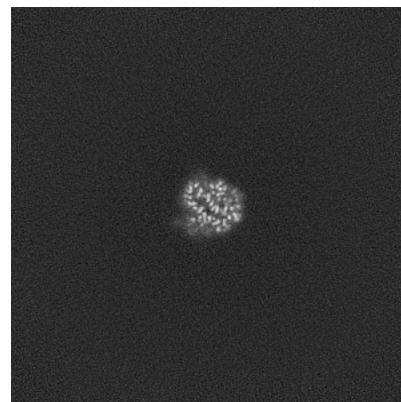
6.3.2 Raw map



X Index: 194



Y Index: 195

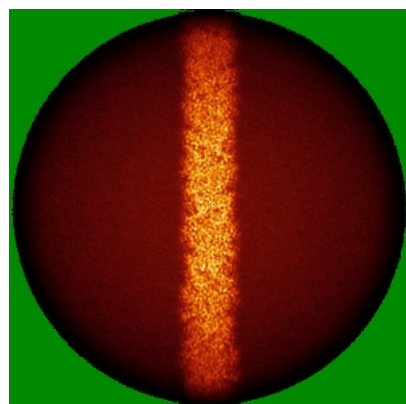


Z Index: 201

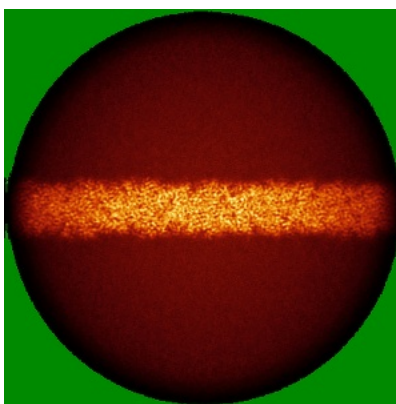
The images above show the largest variance slices of the map in three orthogonal directions.

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

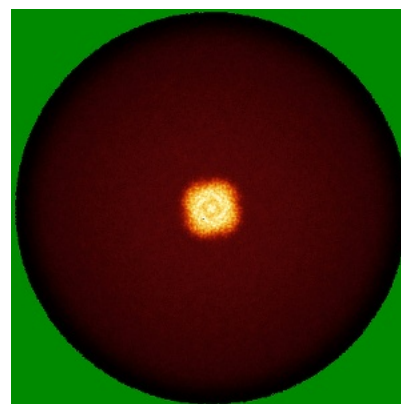
6.4.1 Primary map



X

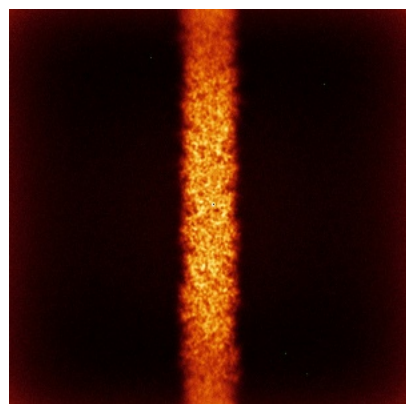


Y

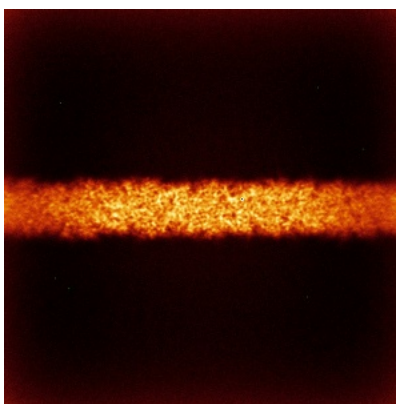


Z

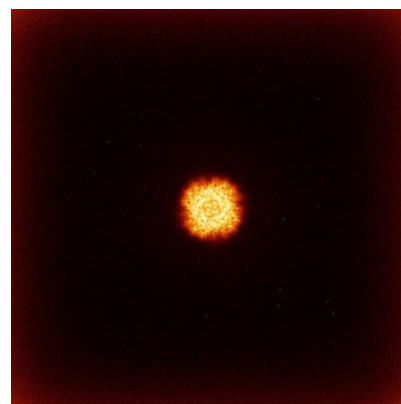
6.4.2 Raw map



X



Y

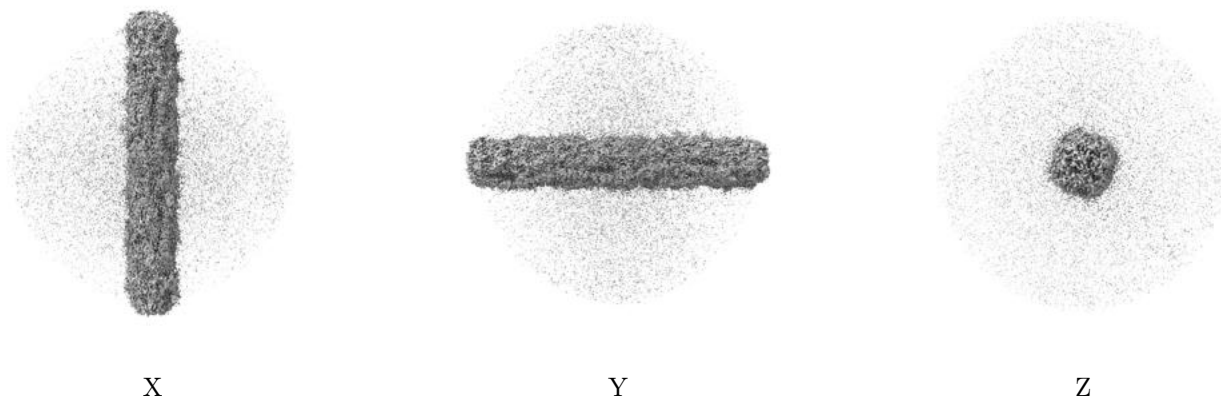


Z

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.

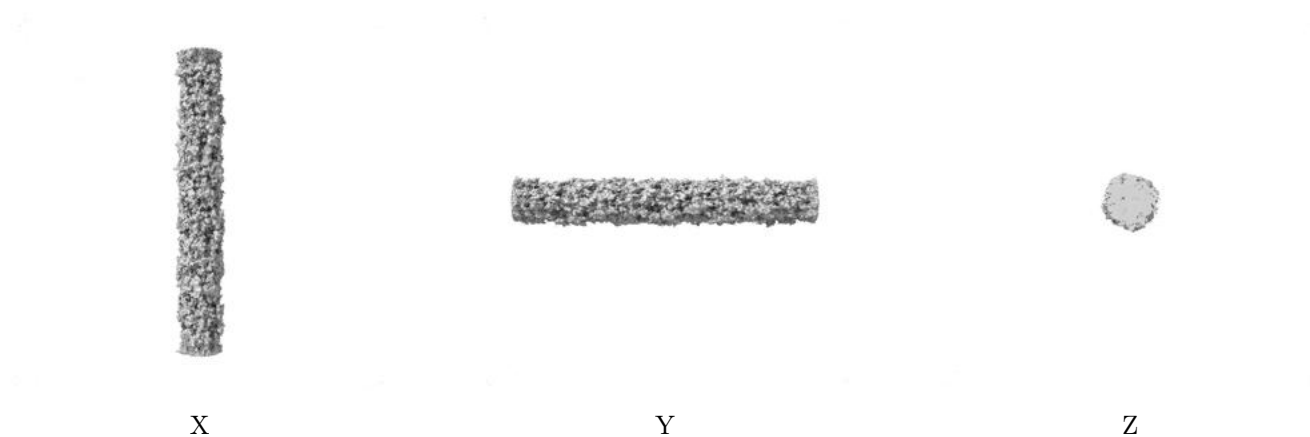
6.5 Orthogonal surface views [i](#)

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.

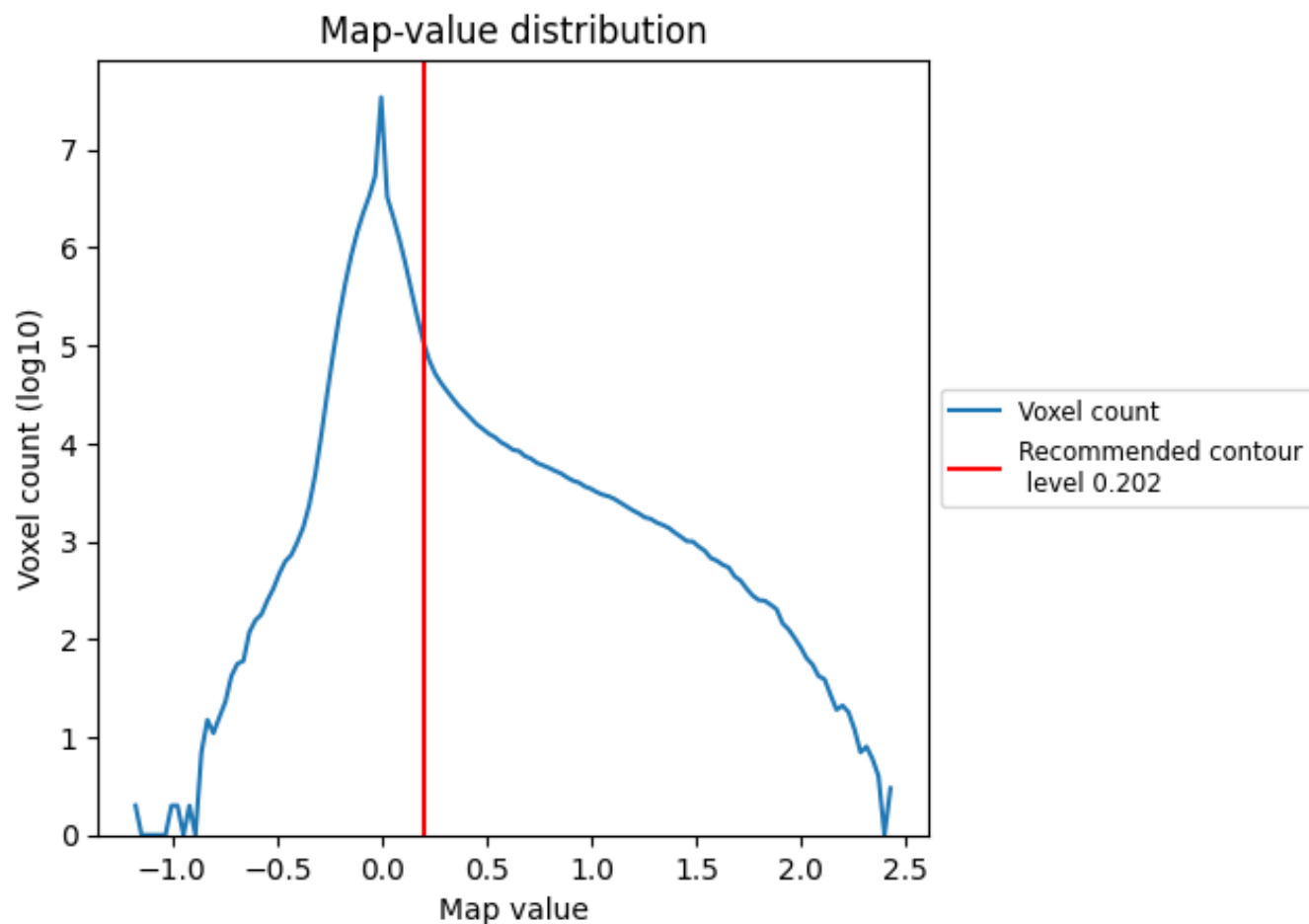
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

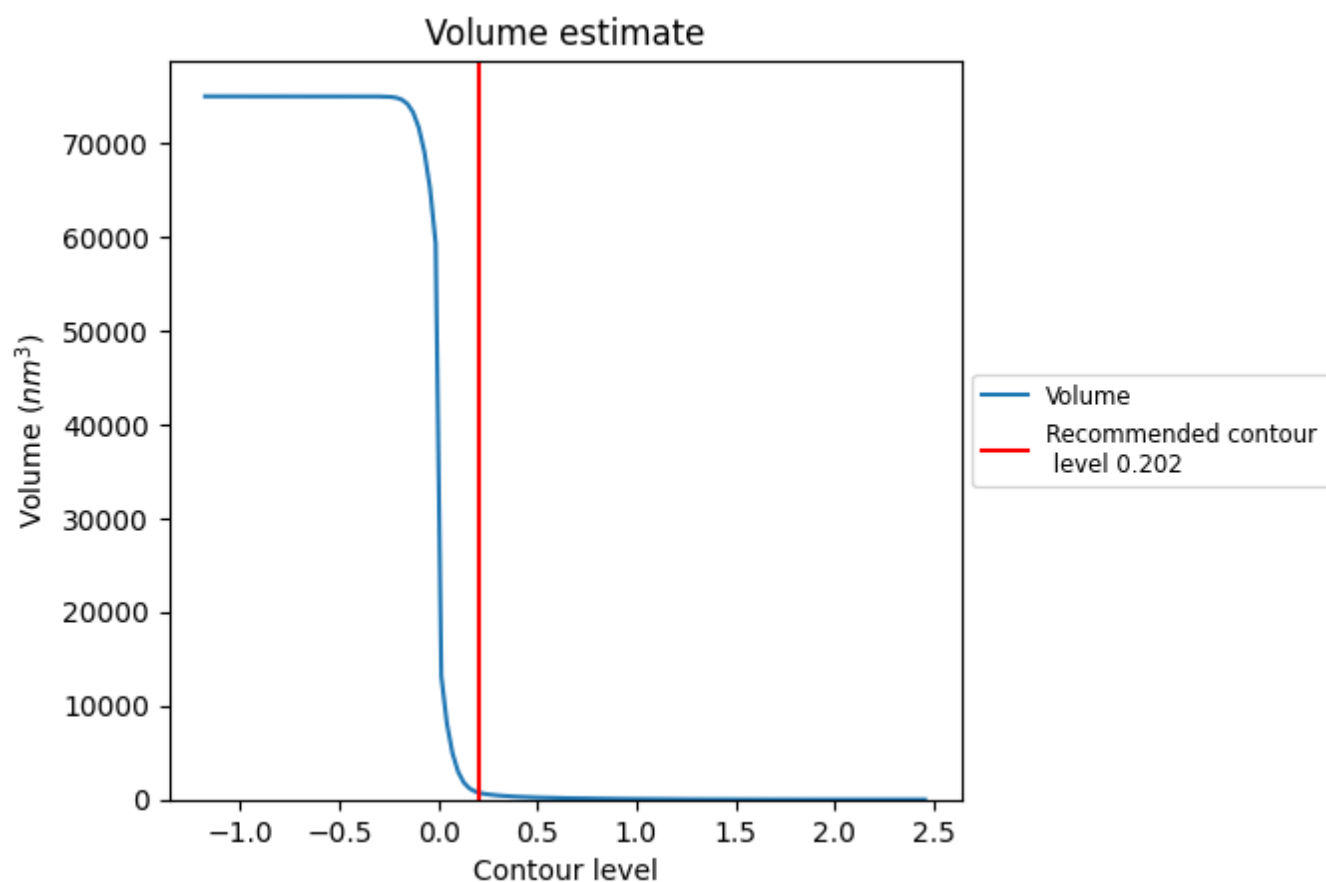
This section contains the results of statistical analysis of the map.

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.

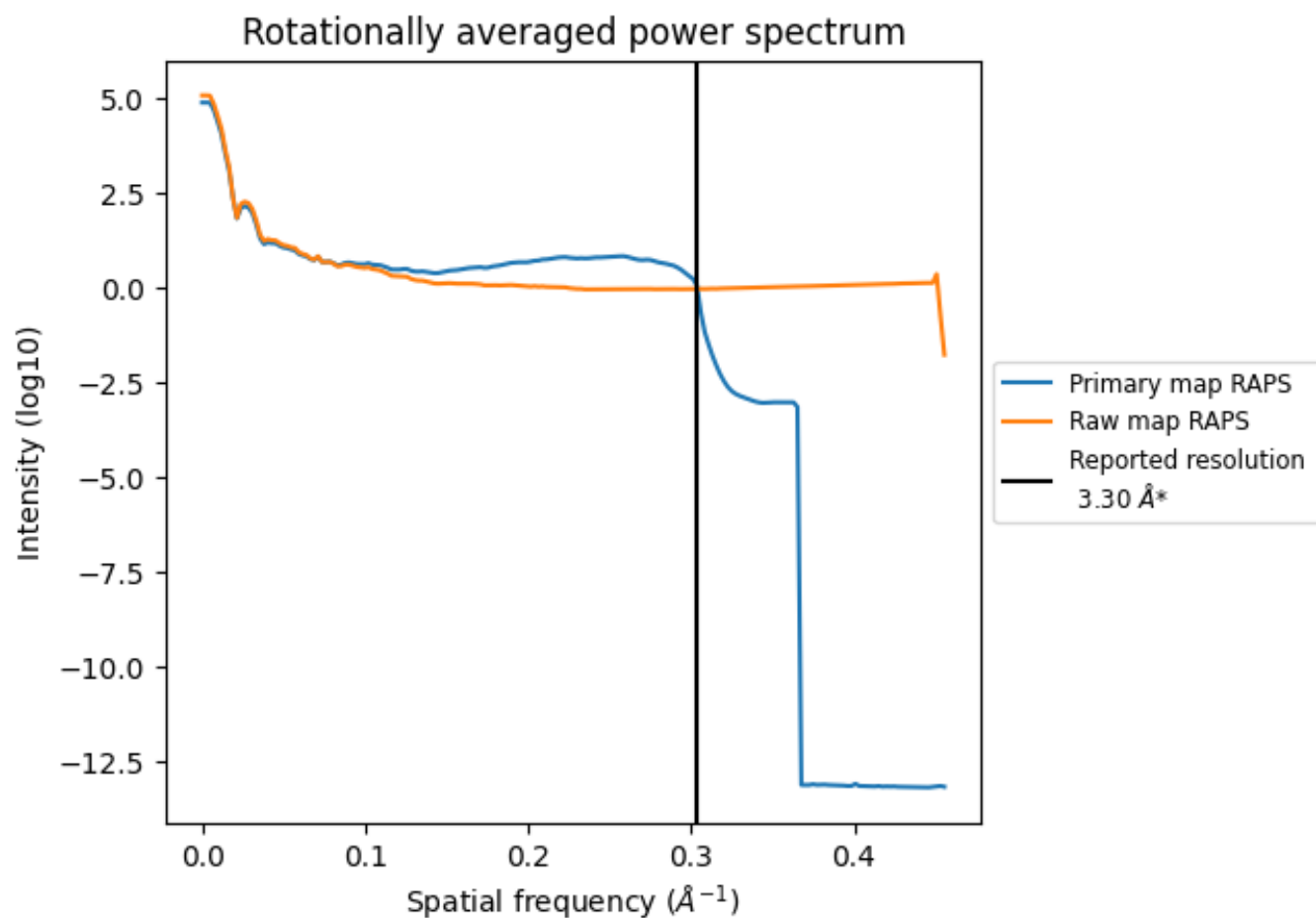
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 763 nm³; 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 ⓘ

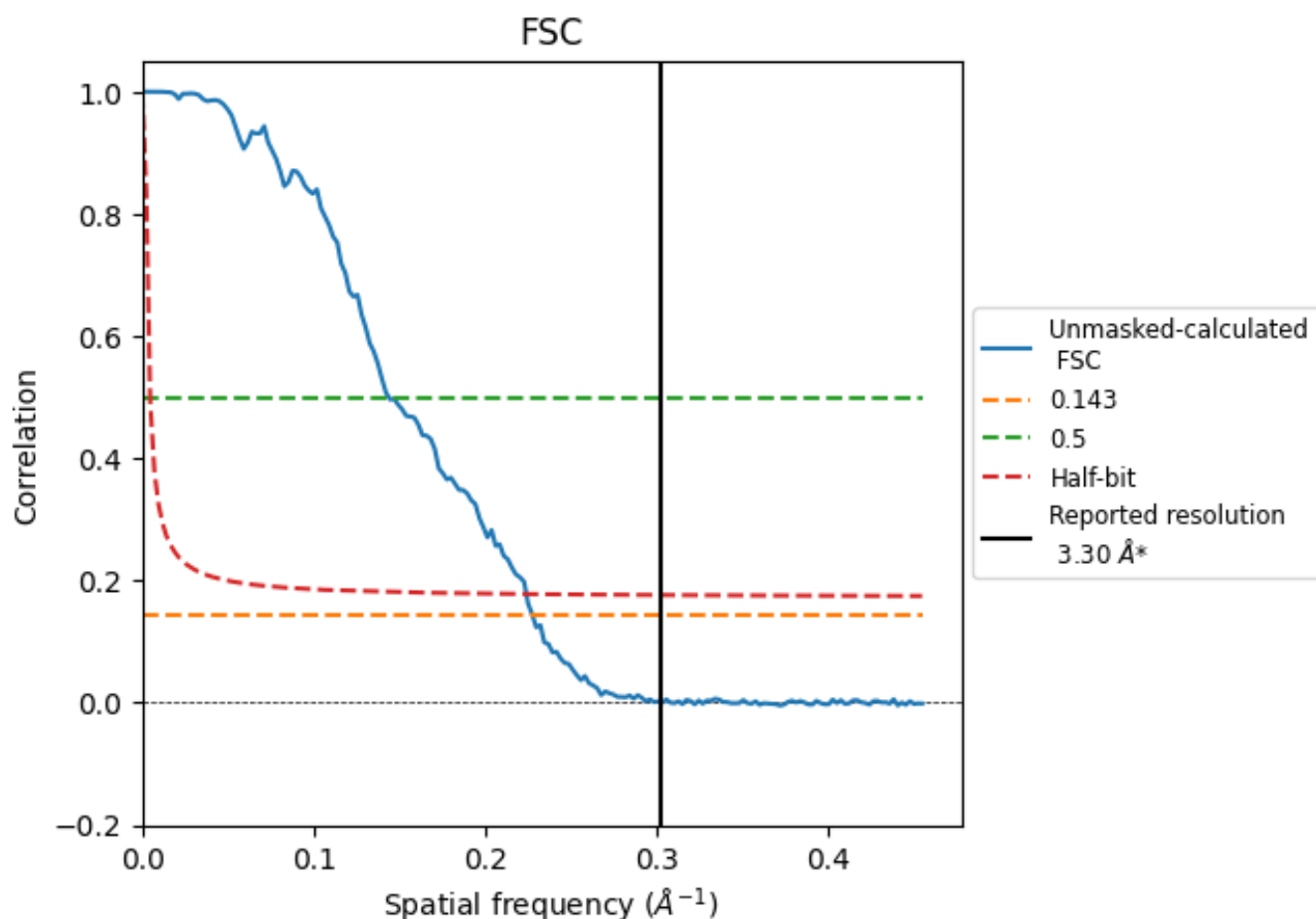


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

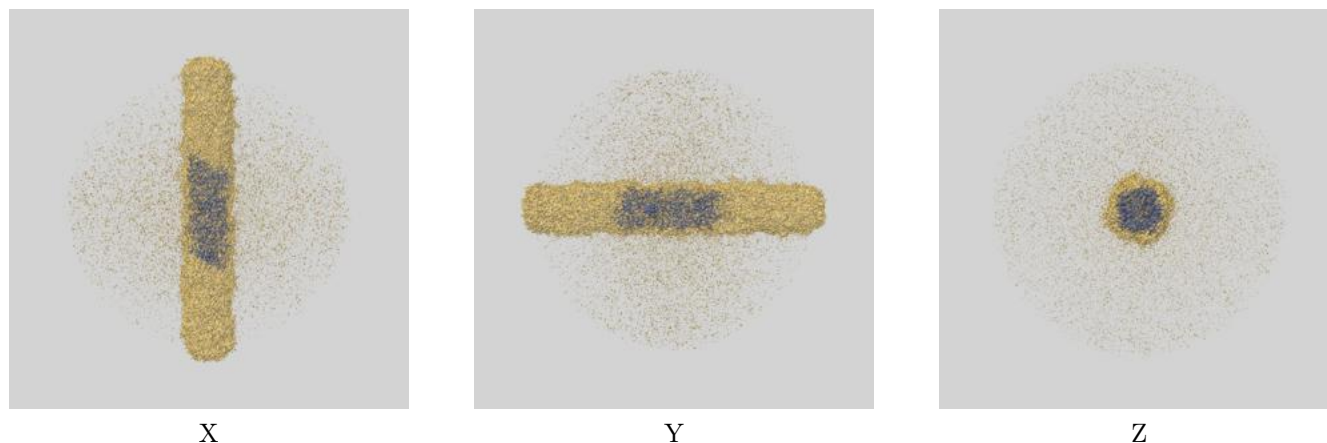
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.39	6.95	4.46

*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](#)

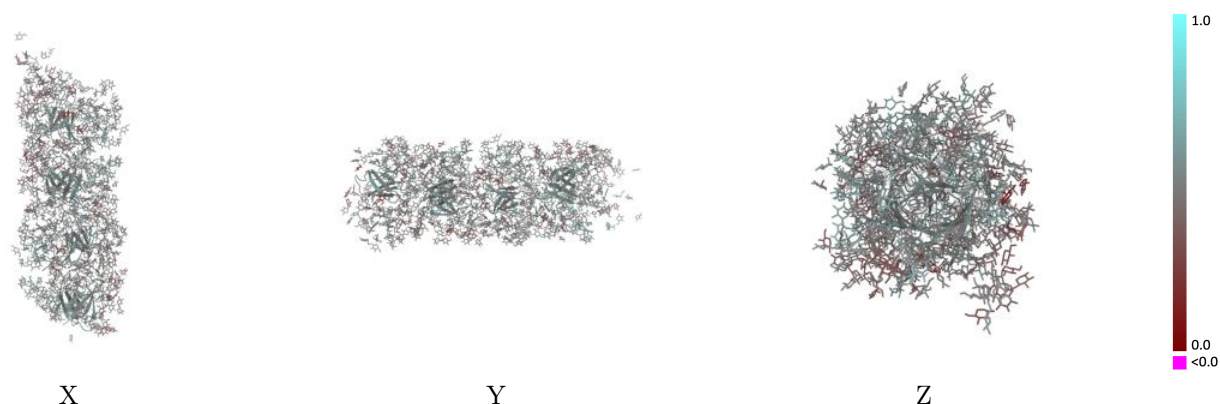
This section contains information regarding the fit between EMDB map EMD-67848 and PDB model 21NR. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



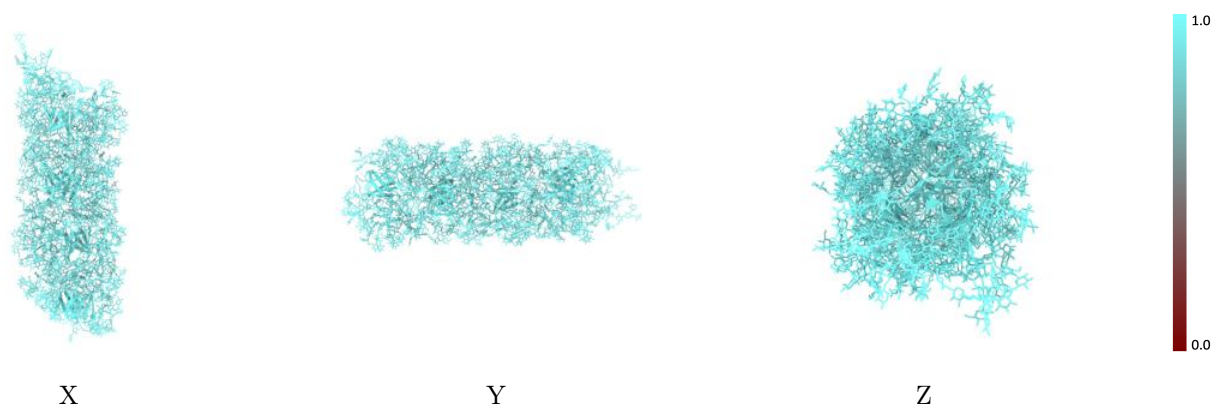
The images above show the 3D surface view of the map at the recommended contour level 0.202 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



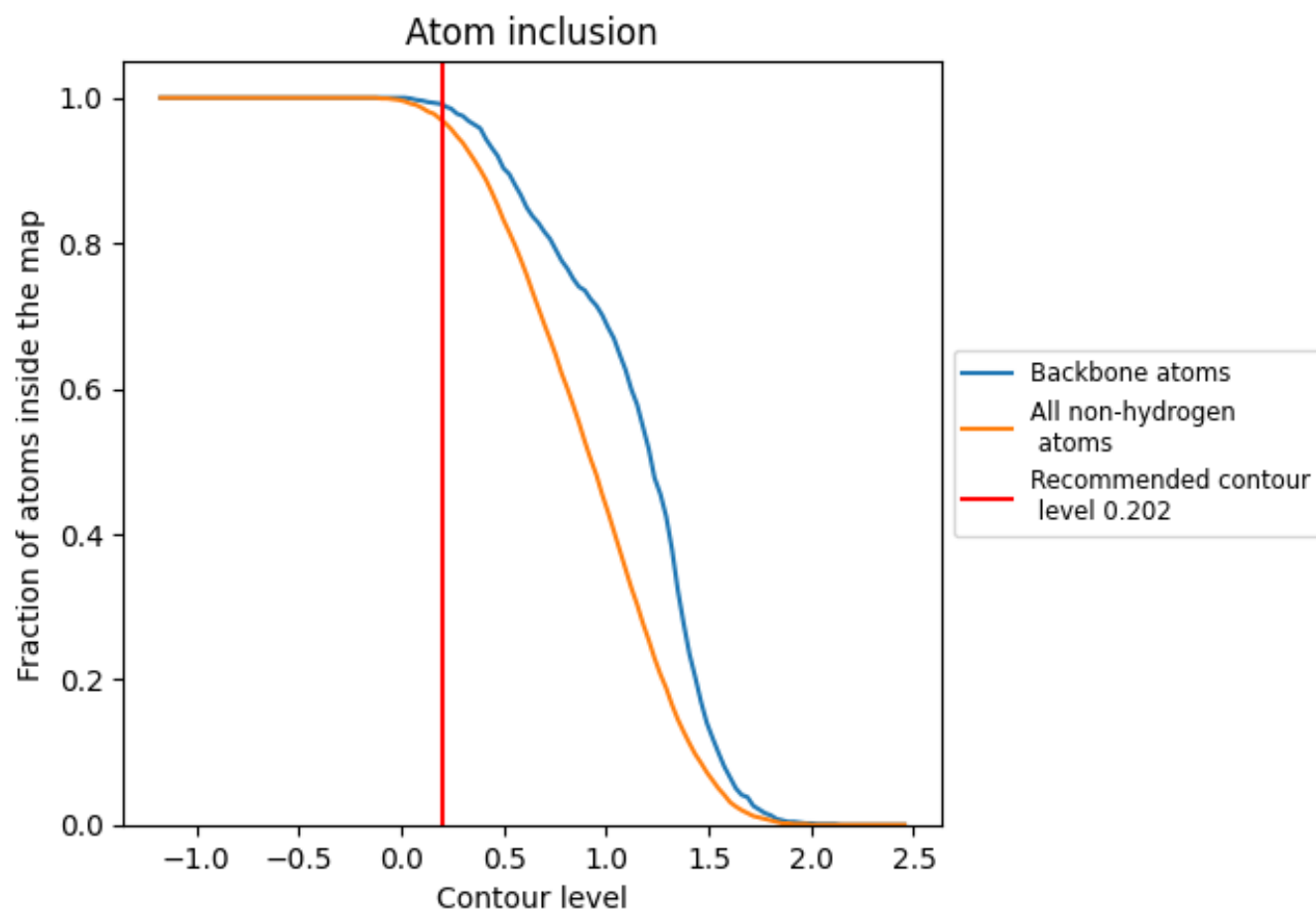
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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