



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:29 AM UTC

PDB ID : 5JU6 / pdb_00005ju6
Title : Structural and Functional Studies of Glycoside Hydrolase Family 3 beta-Glucosidase Cel3A from the Moderately Thermophilic Fungus *Rasamsonia emersonii*
Authors : Gudmundsson, M.; Sandgren, M.; Karkehabadi, S.
Deposited on : 2016-05-10
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

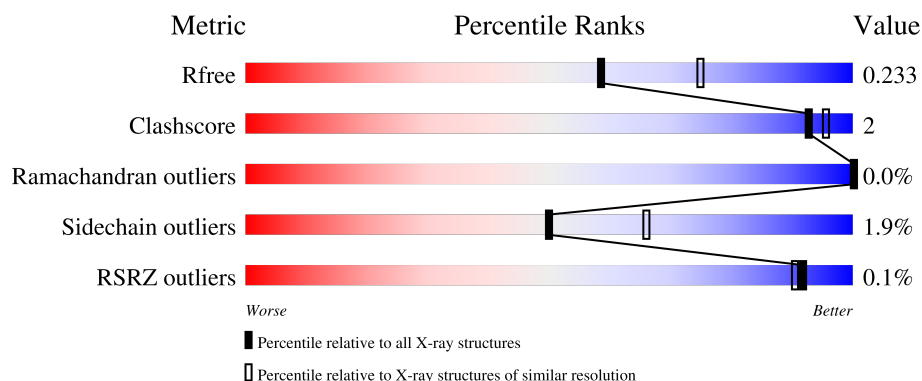
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

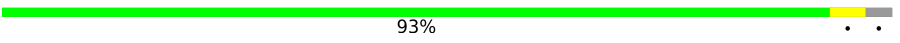
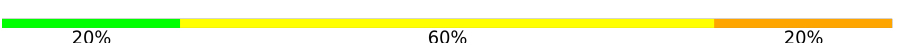
The reported resolution of this entry is 2.20 Å.

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



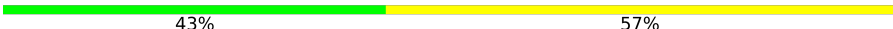
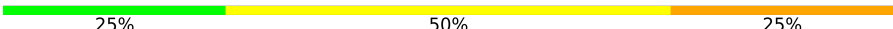
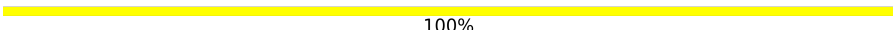
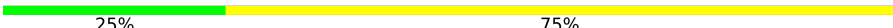
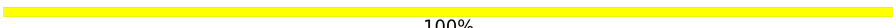
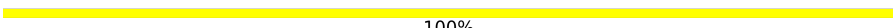
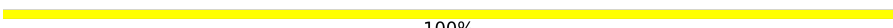
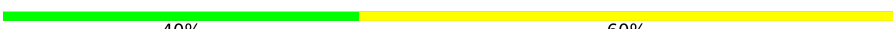
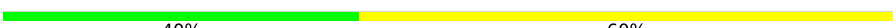
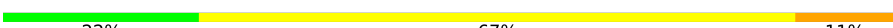
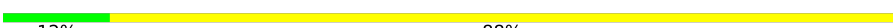
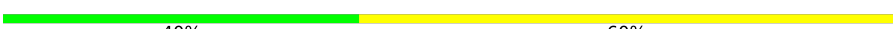
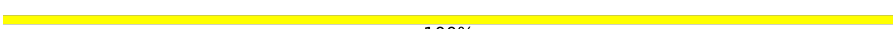
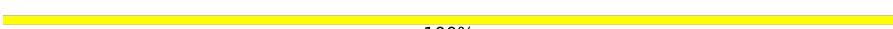
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	857	 93% 6%
1	B	857	 91% 7%
1	C	857	 91% 7%
1	D	857	 91% 7%
2	E	5	 20% 60% 20%

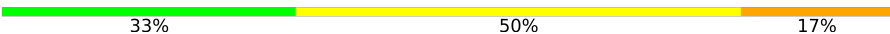
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Mol	Chain	Length	Quality of chain
2	M	5	 20% 80%
3	F	7	 43% 57%
4	G	4	 100%
4	L	4	 25% 50% 25%
4	N	4	 100%
4	c	4	 25% 75%
5	H	9	 11% 89%
5	V	9	 22% 78%
6	I	4	 100%
7	J	9	 33% 67%
8	K	2	 100%
8	R	2	 100%
8	Y	2	 50% 50%
9	O	10	 30% 70%
9	d	10	 40% 60%
10	P	5	 60% 40%
11	Q	10	 40% 60%
12	S	9	 22% 67% 11%
13	T	8	 12% 88%
13	b	8	 12% 88%
14	U	5	 40% 60%
15	W	3	 33% 67%
15	Z	3	 100%
15	e	3	 100%
16	X	8	 25% 75%

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Mol	Chain	Length	Quality of chain
16	f	8	 25% 75%
17	a	6	 33% 50% 17%

2 Entry composition [i](#)

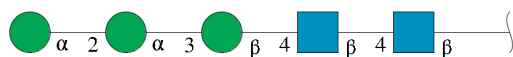
There are 21 unique types of molecules in this entry. The entry contains 29503 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-glucosidase.

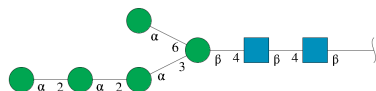
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	835	Total	C	N	O	S	0	0	0
			6373	4018	1093	1239	23			
1	B	835	Total	C	N	O	S	0	1	0
			6379	4021	1094	1241	23			
1	C	835	Total	C	N	O	S	0	3	0
			6388	4028	1095	1242	23			
1	D	835	Total	C	N	O	S	0	2	0
			6382	4023	1094	1241	24			

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



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

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



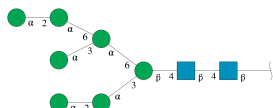
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	7	Total	C	N	O	0	0	0
			83	46	2	35			

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



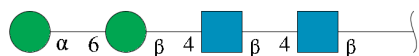
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	L	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	N	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	c	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



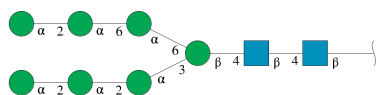
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	9	Total	C	N	O	0	0	0
			105	58	2	45			
5	V	9	Total	C	N	O	0	0	0
			105	58	2	45			

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



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

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



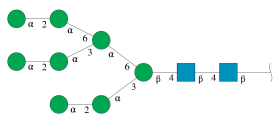
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	J	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



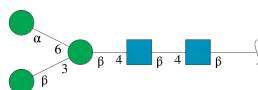
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



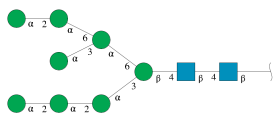
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	O	10	Total	C	N	O	0	0	0
			116	64	2	50			
9	d	10	Total	C	N	O	0	0	0
			116	64	2	50			

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



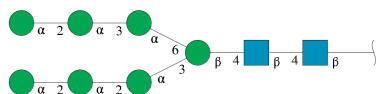
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	P	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



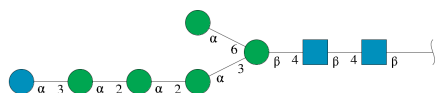
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	Q	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



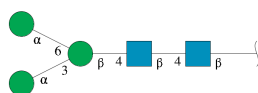
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	S	9	Total	C	N	O	0	0	0
			105	58	2	45			

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



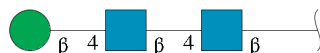
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	T	8	Total	C	N	O	0	0	0
			94	52	2	40			
13	b	8	Total	C	N	O	0	0	0
			94	52	2	40			

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



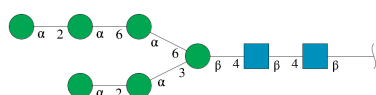
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	U	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 15 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



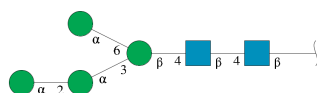
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	W	3	Total	C	N	O	0	0	0
			39	22	2	15			
15	Z	3	Total	C	N	O	0	0	0
			39	22	2	15			
15	e	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 16 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	X	8	Total	C	N	O	0	0	0
			94	52	2	40			
16	f	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 17 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	a	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 18 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



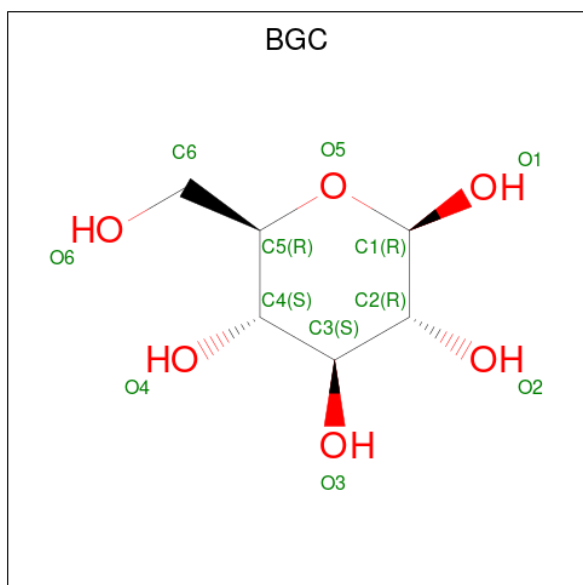
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	N	O	0	0
			14	8	1	5		
18	A	1	Total	C	N	O	0	0
			14	8	1	5		
18	A	1	Total	C	N	O	0	0
			14	8	1	5		
18	A	1	Total	C	N	O	0	0
			14	8	1	5		
18	B	1	Total	C	N	O	0	0
			14	8	1	5		
18	B	1	Total	C	N	O	0	0
			14	8	1	5		
18	B	1	Total	C	N	O	0	0
			14	8	1	5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

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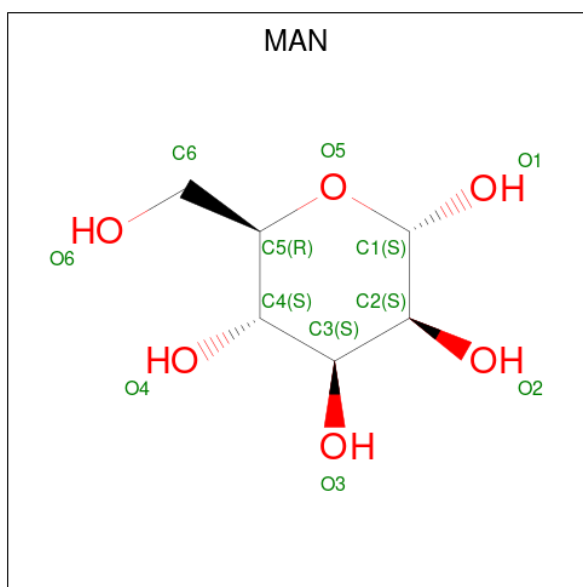
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	N	O	0	0
			14	8	1	5		
18	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 19 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			12	6	6		
19	B	1	Total	C	O	0	0
			12	6	6		
19	C	1	Total	C	O	0	0
			12	6	6		
19	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 20 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			11	6	5		

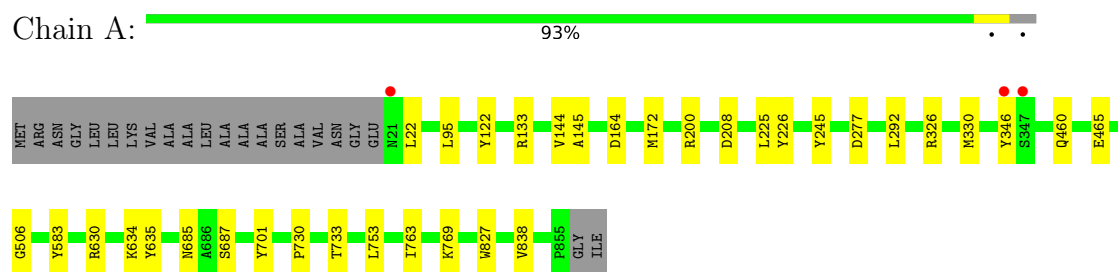
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	431	Total	O	0	0
			431	431		
21	B	399	Total	O	0	1
			400	400		
21	C	441	Total	O	0	0
			441	441		
21	D	432	Total	O	0	0
			432	432		

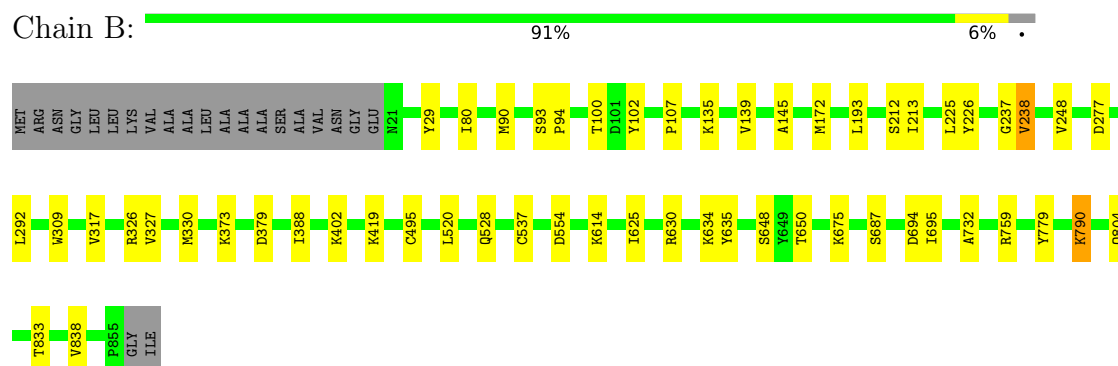
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

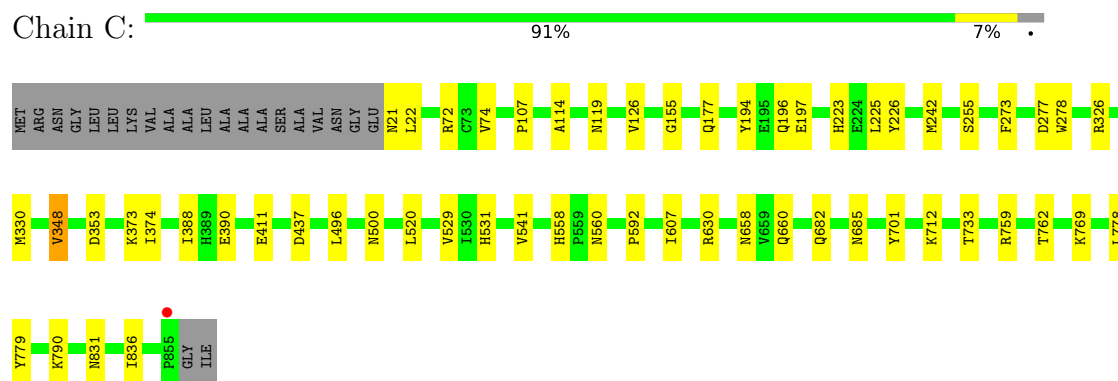
- Molecule 1: Beta-glucosidase



- Molecule 1: Beta-glucosidase



- Molecule 1: Beta-glucosidase

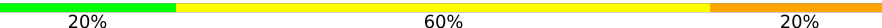


- Molecule 1: Beta-glucosidase

Chain D:  91% 6%



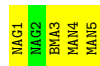
- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  20% 60% 20%

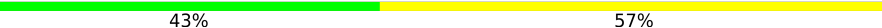


- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  20% 80%

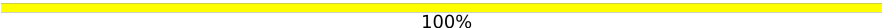


- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  43% 57%

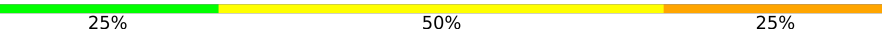


- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%



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

Chain L:  25% 50% 25%



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

Chain N: 100%



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

Chain c: 25% 75%



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

Chain H: 11% 89%



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

Chain V: 22% 78%

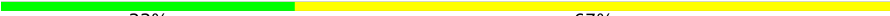


- Molecule 6: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%

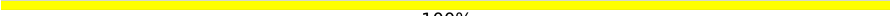


- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  33% 67%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

MAG1
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%

MAG1
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  50% 50%

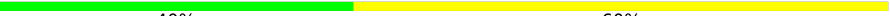
MAG1
MAG2

- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  30% 70%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  40% 60%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

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

nose

Chain P:  60% 40%



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

Chain Q:  40% 60%



- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  22% 67% 11%

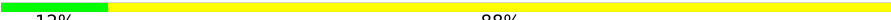


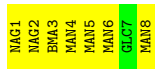
- Molecule 13: alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  12% 88%

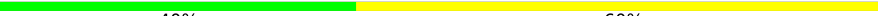


- Molecule 14: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  12% 88%



- Molecule 15: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  40% 60%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 15: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  33% 67%

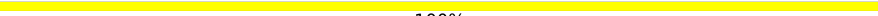
MAG1
MAG2
BMA3

- Molecule 15: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%

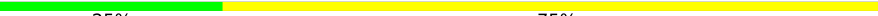
MAG1
MAG2
BMA3

- Molecule 15: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  100%

MAG1
MAG2
BMA3

- Molecule 16: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  25% 75%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

- Molecule 16: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  25% 75%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

- Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.29Å 148.63Å 196.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.51 – 2.20 118.51 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (118.51-2.20) 99.9 (118.51-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0155, REFMAC 5.8.0155	Depositor
R, R_{free}	0.173 , 0.228 0.180 , 0.233	Depositor DCC
R_{free} test set	10215 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.990	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	29503	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, GLC, MAN, NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.99	1/6549 (0.0%)	1.00	3/8954 (0.0%)
1	B	0.99	2/6555 (0.0%)	1.03	2/8962 (0.0%)
1	C	0.99	2/6574 (0.0%)	1.03	7/8988 (0.1%)
1	D	1.03	0/6561	1.02	2/8970 (0.0%)
All	All	1.00	5/26239 (0.0%)	1.02	14/35874 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	309	TRP	CA-C	6.52	1.57	1.53
1	A	122	TYR	C-O	-5.57	1.17	1.24
1	B	80	ILE	CA-C	5.26	1.58	1.52
1	C	273	PHE	N-CA	5.09	1.51	1.45
1	C	390	GLU	C-O	-5.03	1.18	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	348	VAL	N-CA-C	-7.03	103.43	109.19
1	C	348	VAL	CA-C-N	-6.76	112.82	119.78
1	C	348	VAL	C-N-CA	-6.76	112.82	119.78
1	C	155	GLY	N-CA-C	6.60	121.89	113.24
1	C	126	VAL	CB-CA-C	-5.95	104.36	111.97
1	A	144	VAL	N-CA-C	5.84	116.22	107.51
1	D	714	SER	N-CA-C	5.71	118.28	111.71
1	B	419	LYS	N-CA-C	5.56	118.06	111.33
1	A	506	GLY	N-CA-C	5.51	120.73	114.67
1	C	529	VAL	CB-CA-C	-5.46	104.98	111.97
1	B	695	ILE	N-CA-C	5.30	116.87	109.55
1	D	630	ARG	CG-CD-NE	-5.29	100.37	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	MET	N-CA-C	-5.12	105.61	111.14
1	C	223	HIS	N-CA-C	5.04	116.58	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	6373	0	6031	14	0
1	B	6379	0	6039	23	0
1	C	6388	0	6048	22	0
1	D	6382	0	6040	23	0
2	E	61	0	52	1	0
2	M	61	0	52	0	0
3	F	83	0	70	0	0
4	G	50	0	43	0	0
4	L	50	0	43	1	0
4	N	50	0	43	0	0
4	c	50	0	43	0	0
5	H	105	0	88	0	0
5	V	105	0	88	0	0
6	I	50	0	43	0	0
7	J	105	0	88	0	0
8	K	28	0	25	0	0
8	R	28	0	25	0	0
8	Y	28	0	25	0	0
9	O	116	0	97	0	0
9	d	116	0	97	0	0
10	P	61	0	52	0	0
11	Q	116	0	97	0	0
12	S	105	0	88	1	0
13	T	94	0	79	0	0
13	b	94	0	79	0	0
14	U	61	0	52	0	0
15	W	39	0	34	0	0

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Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	Z	39	0	34	0	0
15	e	39	0	34	0	0
16	X	94	0	79	0	0
16	f	94	0	79	0	0
17	a	72	0	61	1	0
18	A	70	0	65	1	0
18	B	42	0	39	0	0
18	C	42	0	39	0	0
18	D	70	0	65	0	0
19	A	12	0	12	1	0
19	B	12	0	12	1	0
19	C	12	0	12	1	0
19	D	12	0	12	1	0
20	B	11	0	10	1	0
21	A	431	0	0	1	0
21	B	400	0	0	2	0
21	C	441	0	0	5	0
21	D	432	0	0	6	0
All	All	29503	0	26114	82	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 2.

All (82) 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)
1:C:196:GLN:HE22	1:C:607:ILE:H	1.30	0.79
1:B:804:GLN:HE22	1:C:348:VAL:HG12	1.54	0.73
20:B:905:MAN:C1	4:L:4:MAN:O2	2.41	0.68
1:D:360:TYR:O	21:D:1001:HOH:O	2.13	0.67
1:B:225:LEU:HD23	1:B:226:TYR:CZ	2.31	0.65
1:C:119:ASN:ND2	21:C:1002:HOH:O	2.28	0.65
1:A:277:ASP:OD1	19:A:946:BGC:H1	1.96	0.64
1:C:660:GLN:NE2	21:C:1003:HOH:O	2.31	0.63
1:A:465:GLU:HG2	1:A:583:TYR:CE2	2.34	0.62
1:A:145:ALA:HB2	1:A:172:MET:HE2	1.82	0.62
1:D:277:ASP:OD1	19:D:945:BGC:H1	2.02	0.60
1:D:311:THR:OG1	1:D:705:TRP:O	2.17	0.59
1:B:495:CYS:SG	1:B:537:CYS:SG	3.00	0.58
1:B:225:LEU:HD23	1:B:226:TYR:CE2	2.38	0.57
1:A:164:ASP:OD1	1:A:630:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:762:THR:HG21	1:D:838:VAL:HG11	1.87	0.56
1:C:630:ARG:NH1	21:C:1001:HOH:O	2.22	0.56
1:B:277:ASP:OD1	19:B:945:BGC:H1	2.06	0.55
1:B:193:LEU:HD12	1:B:248:VAL:HG13	1.87	0.55
1:C:558:HIS:HD2	1:C:560:ASN:H	1.52	0.55
1:B:648:SER:OG	1:B:650:THR:O	2.25	0.54
1:D:102:TYR:HB3	1:D:379:ASP:HA	1.90	0.53
1:D:500:ASN:HB2	1:D:545:HIS:O	2.09	0.52
1:D:800:LEU:HD21	1:D:806:TYR:HB2	1.91	0.52
1:C:778:LEU:HD23	1:C:778:LEU:C	2.35	0.51
1:C:701:TYR:CZ	12:S:2:NAG:H82	2.46	0.51
1:D:145:ALA:HB2	1:D:172:MET:HE2	1.92	0.51
1:D:630:ARG:HD3	21:D:1003:HOH:O	2.10	0.50
1:C:496:LEU:HD23	1:C:541:VAL:HB	1.94	0.49
1:D:681:GLY:HA3	21:D:1128:HOH:O	2.12	0.49
1:D:697:ARG:HD3	21:D:1291:HOH:O	2.12	0.49
1:C:225:LEU:HD23	1:C:226:TYR:CE2	2.48	0.49
1:C:277:ASP:OD1	19:C:951:BGC:H1	2.13	0.49
1:D:285:VAL:HA	1:D:322:ILE:HD11	1.95	0.49
1:C:107:PRO:HD3	1:C:388:ILE:HG23	1.95	0.48
1:A:225:LEU:HD23	1:A:226:TYR:CE2	2.49	0.47
1:B:528:GLN:HB2	21:B:1372:HOH:O	2.15	0.47
1:B:634:LYS:HD3	1:B:635:TYR:CE1	2.50	0.46
1:D:273:PHE:CD1	1:D:334:ILE:HA	2.50	0.46
1:B:625:ILE:O	1:B:630:ARG:HD3	2.16	0.46
1:C:779:TYR:HB3	1:C:790:LYS:HB2	1.99	0.45
1:A:634:LYS:HD3	1:A:635:TYR:CE2	2.52	0.45
1:B:93:SER:HB2	1:B:94:PRO:CD	2.47	0.45
1:B:779:TYR:HB3	1:B:790:LYS:HB2	1.99	0.45
1:D:701:TYR:CZ	17:a:2:NAG:H82	2.52	0.45
1:B:292:LEU:O	1:B:326:ARG:NH2	2.50	0.44
1:D:37:GLN:NE2	21:D:1023:HOH:O	2.49	0.44
1:B:29:TYR:HB3	1:B:732:ALA:HA	2.00	0.44
1:D:95:LEU:C	1:D:95:LEU:HD12	2.43	0.44
1:A:730:PRO:HB3	18:A:945:NAG:H82	2.00	0.44
1:D:243[B]:CYS:SG	1:D:276:THR:HA	2.58	0.43
1:B:145:ALA:HB2	1:B:172:MET:SD	2.58	0.43
1:B:326:ARG:O	1:B:330:MET:HG3	2.18	0.43
1:D:465:GLU:OE1	1:D:469:ARG:NH2	2.51	0.43
1:A:701:TYR:CZ	2:E:2:NAG:H82	2.54	0.43
21:B:1313:HOH:O	1:C:759:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:MET:HE2	1:C:278:TRP:HZ3	1.84	0.43
1:D:31:SER:HA	1:D:261:ASN:ND2	2.34	0.43
1:A:733:THR:CG2	21:A:1351:HOH:O	2.66	0.43
1:B:90:MET:HG3	1:B:139:VAL:HB	2.00	0.43
1:B:107:PRO:HD3	1:B:388:ILE:HG23	2.01	0.43
1:C:630:ARG:HD2	21:C:1001:HOH:O	2.18	0.43
1:A:292:LEU:O	1:A:326:ARG:NH2	2.52	0.42
1:C:353:ASP:HB2	1:C:374:ILE:HB	2.01	0.42
1:D:328:ASP:O	1:D:332:VAL:HG23	2.18	0.42
1:C:21:ASN:HB3	21:C:1322:HOH:O	2.20	0.42
1:B:317:VAL:HG21	1:B:327:VAL:HG21	2.02	0.42
1:D:250:ASN:ND2	21:D:1011:HOH:O	2.44	0.42
1:B:212:SER:O	1:B:213:ILE:C	2.62	0.41
1:B:102:TYR:HB3	1:B:379:ASP:HA	2.02	0.41
1:A:753:LEU:HD21	1:A:827:TRP:HB2	2.01	0.41
1:A:200:ARG:O	1:A:245:TYR:HB3	2.19	0.41
1:D:132:HIS:O	1:D:133:ARG:C	2.64	0.41
1:B:237:GLY:O	1:B:238:VAL:C	2.63	0.41
1:C:114:ALA:HB2	1:C:592:PRO:HD3	2.02	0.41
1:C:194:TYR:OH	1:C:197:GLU:OE2	2.34	0.41
1:C:437:ASP:OD2	1:C:500:ASN:OD1	2.39	0.41
1:D:501:ALA:HA	1:D:523:TRP:CD1	2.55	0.40
1:B:100:THR:HG21	1:B:135:LYS:HE3	2.04	0.40
1:A:95:LEU:HD12	1:A:95:LEU:C	2.46	0.40
1:A:133:ARG:HD2	1:A:346:TYR:CD1	2.56	0.40
1:C:326:ARG:O	1:C:330:MET:HG3	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	833/857 (97%)	804 (96%)	29 (4%)	0	100	100
1	B	834/857 (97%)	802 (96%)	31 (4%)	1 (0%)	48	57
1	C	836/857 (98%)	807 (96%)	29 (4%)	0	100	100
1	D	835/857 (97%)	800 (96%)	35 (4%)	0	100	100
All	All	3338/3428 (97%)	3213 (96%)	124 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	694	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	672/685 (98%)	664 (99%)	8 (1%)	63	78
1	B	673/685 (98%)	661 (98%)	12 (2%)	51	68
1	C	675/685 (98%)	656 (97%)	19 (3%)	38	52
1	D	674/685 (98%)	661 (98%)	13 (2%)	50	66
All	All	2694/2740 (98%)	2642 (98%)	52 (2%)	50	66

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	208	ASP
1	A	460	GLN
1	A	685	ASN
1	A	687	SER
1	A	763	ILE
1	A	769	LYS
1	A	838	VAL
1	B	238	VAL
1	B	373	LYS

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Mol	Chain	Res	Type
1	B	402	LYS
1	B	520	LEU
1	B	554	ASP
1	B	614	LYS
1	B	675	LYS
1	B	687	SER
1	B	759	ARG
1	B	790	LYS
1	B	833	THR
1	B	838	VAL
1	C	22	LEU
1	C	72	ARG
1	C	74	VAL
1	C	177	GLN
1	C	255	SER
1	C	373	LYS
1	C	411	GLU
1	C	520	LEU
1	C	531[A]	HIS
1	C	531[B]	HIS
1	C	658	ASN
1	C	682	GLN
1	C	685	ASN
1	C	712	LYS
1	C	733	THR
1	C	762	THR
1	C	769	LYS
1	C	831	ASN
1	C	836	ILE
1	D	83	LEU
1	D	88	LEU
1	D	123	ARG
1	D	204	GLN
1	D	324	GLU
1	D	347	SER
1	D	411	GLU
1	D	520	LEU
1	D	532	ASN
1	D	651	THR
1	D	706	LEU
1	D	708	SER
1	D	789	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	45	GLN
1	A	103	ASN
1	A	216	ASN
1	A	246	ASN
1	A	250	ASN
1	A	369	GLN
1	A	460	GLN
1	A	558	HIS
1	A	612	ASN
1	A	618	GLN
1	A	619	GLN
1	A	636	ASN
1	A	658	ASN
1	A	738	GLN
1	A	777	GLN
1	A	805	GLN
1	B	45	GLN
1	B	49	GLN
1	B	91	GLN
1	B	261	ASN
1	B	369	GLN
1	B	383	ASN
1	B	528	GLN
1	B	531	HIS
1	B	619	GLN
1	B	658	ASN
1	B	685	ASN
1	B	716	ASN
1	B	804	GLN
1	C	37	GLN
1	C	53	GLN
1	C	103	ASN
1	C	140	GLN
1	C	177	GLN
1	C	196	GLN
1	C	261	ASN
1	C	491	GLN
1	C	539	ASN
1	C	558	HIS
1	C	612	ASN

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Mol	Chain	Res	Type
1	C	618	GLN
1	C	660	GLN
1	D	37	GLN
1	D	45	GLN
1	D	49	GLN
1	D	103	ASN
1	D	177	GLN
1	D	261	ASN
1	D	282	HIS
1	D	371	GLN
1	D	470	ASN
1	D	491	GLN
1	D	528	GLN
1	D	587	ASN
1	D	656	GLN
1	D	685	ASN
1	D	716	ASN
1	D	805	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 ⓘ

166 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	E	1	2,1	14,14,15	0.50	0	17,19,21	1.09	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	2	2	14,14,15	0.65	0	17,19,21	1.28	1 (5%)
2	BMA	E	3	2	11,11,12	1.03	1 (9%)	15,15,17	1.60	5 (33%)
2	MAN	E	4	2	11,11,12	0.43	0	15,15,17	1.34	1 (6%)
2	MAN	E	5	2	11,11,12	0.65	0	15,15,17	0.79	0
3	NAG	F	1	3,1	14,14,15	0.75	0	17,19,21	1.47	2 (11%)
3	NAG	F	2	3	14,14,15	0.53	0	17,19,21	0.72	0
3	BMA	F	3	3	11,11,12	0.24	0	15,15,17	1.19	1 (6%)
3	MAN	F	4	3	11,11,12	0.89	0	15,15,17	1.18	0
3	MAN	F	5	3	11,11,12	0.78	0	15,15,17	1.36	1 (6%)
3	MAN	F	6	3	11,11,12	0.74	0	15,15,17	0.99	0
3	MAN	F	7	3	11,11,12	1.38	1 (9%)	15,15,17	1.89	6 (40%)
4	NAG	G	1	4,1	14,14,15	0.68	0	17,19,21	1.56	4 (23%)
4	NAG	G	2	4	14,14,15	0.59	0	17,19,21	1.30	1 (5%)
4	BMA	G	3	4	11,11,12	0.59	0	15,15,17	2.33	7 (46%)
4	MAN	G	4	4	11,11,12	0.96	0	15,15,17	1.54	1 (6%)
5	NAG	H	1	5,1	14,14,15	0.39	0	17,19,21	1.00	1 (5%)
5	NAG	H	2	5	14,14,15	0.95	1 (7%)	17,19,21	1.15	1 (5%)
5	BMA	H	3	5	11,11,12	0.65	0	15,15,17	0.88	0
5	MAN	H	4	5	11,11,12	0.50	0	15,15,17	1.31	3 (20%)
5	MAN	H	5	5	11,11,12	0.57	0	15,15,17	1.32	1 (6%)
5	MAN	H	6	5	11,11,12	0.70	0	15,15,17	1.26	2 (13%)
5	MAN	H	7	5	11,11,12	1.01	0	15,15,17	1.54	4 (26%)
5	MAN	H	8	5	11,11,12	0.62	0	15,15,17	1.71	3 (20%)
5	MAN	H	9	5	11,11,12	0.94	1 (9%)	15,15,17	1.35	2 (13%)
6	NAG	I	1	6,1	14,14,15	0.78	0	17,19,21	0.89	1 (5%)
6	NAG	I	2	6	14,14,15	0.62	0	17,19,21	1.72	2 (11%)
6	BMA	I	3	6	11,11,12	0.76	0	15,15,17	1.09	2 (13%)
6	MAN	I	4	6	11,11,12	0.83	0	15,15,17	1.43	1 (6%)
7	NAG	J	1	7,1	14,14,15	0.66	0	17,19,21	0.94	0
7	NAG	J	2	7	14,14,15	0.44	0	17,19,21	1.33	2 (11%)
7	BMA	J	3	7	11,11,12	0.67	0	15,15,17	1.35	1 (6%)
7	MAN	J	4	7	11,11,12	0.46	0	15,15,17	1.24	1 (6%)
7	MAN	J	5	7	11,11,12	1.03	0	15,15,17	1.34	3 (20%)
7	MAN	J	6	7	11,11,12	0.89	0	15,15,17	0.86	0
7	MAN	J	7	7	11,11,12	0.94	0	15,15,17	1.41	1 (6%)
7	MAN	J	8	7	11,11,12	0.52	0	15,15,17	1.45	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	J	9	7	11,11,12	0.58	0	15,15,17	1.01	0
8	NAG	K	1	1,8	14,14,15	0.42	0	17,19,21	1.33	1 (5%)
8	NAG	K	2	8	14,14,15	0.52	0	17,19,21	1.04	1 (5%)
4	NAG	L	1	4,1	14,14,15	0.61	0	17,19,21	0.92	0
4	NAG	L	2	4	14,14,15	0.50	0	17,19,21	1.13	1 (5%)
4	BMA	L	3	4	11,11,12	0.39	0	15,15,17	0.96	1 (6%)
4	MAN	L	4	4	11,11,12	0.67	0	15,15,17	1.31	1 (6%)
2	NAG	M	1	2,1	14,14,15	0.42	0	17,19,21	1.70	5 (29%)
2	NAG	M	2	2	14,14,15	0.49	0	17,19,21	1.06	0
2	BMA	M	3	2	11,11,12	0.47	0	15,15,17	1.55	3 (20%)
2	MAN	M	4	2	11,11,12	0.89	1 (9%)	15,15,17	1.45	3 (20%)
2	MAN	M	5	2	11,11,12	0.82	1 (9%)	15,15,17	1.75	5 (33%)
4	NAG	N	1	4,1	14,14,15	0.74	0	17,19,21	1.37	3 (17%)
4	NAG	N	2	4	14,14,15	0.65	0	17,19,21	1.97	4 (23%)
4	BMA	N	3	4	11,11,12	0.89	0	15,15,17	1.17	1 (6%)
4	MAN	N	4	4	11,11,12	0.88	0	15,15,17	1.13	2 (13%)
9	NAG	O	1	9,1	14,14,15	0.77	0	17,19,21	1.22	2 (11%)
9	MAN	O	10	9	11,11,12	1.01	0	15,15,17	1.59	4 (26%)
9	NAG	O	2	9	14,14,15	0.62	0	17,19,21	1.15	1 (5%)
9	BMA	O	3	9	11,11,12	0.44	0	15,15,17	0.80	0
9	MAN	O	4	9	11,11,12	0.52	0	15,15,17	1.00	2 (13%)
9	MAN	O	5	9	11,11,12	1.06	0	15,15,17	1.44	1 (6%)
9	MAN	O	6	9	11,11,12	0.92	0	15,15,17	0.96	0
9	MAN	O	7	9	11,11,12	0.77	0	15,15,17	1.14	1 (6%)
9	MAN	O	8	9	11,11,12	0.59	0	15,15,17	1.77	4 (26%)
9	MAN	O	9	9	11,11,12	0.63	0	15,15,17	0.91	0
10	NAG	P	1	10,1	14,14,15	0.67	0	17,19,21	1.21	2 (11%)
10	NAG	P	2	10	14,14,15	0.68	0	17,19,21	0.98	0
10	BMA	P	3	10	11,11,12	0.67	0	15,15,17	1.19	0
10	BMA	P	4	10	11,11,12	0.92	0	15,15,17	1.20	0
10	MAN	P	5	10	11,11,12	0.93	0	15,15,17	1.23	3 (20%)
11	NAG	Q	1	11,1	14,14,15	0.57	0	17,19,21	1.19	0
11	MAN	Q	10	11	11,11,12	0.77	0	15,15,17	1.47	4 (26%)
11	NAG	Q	2	11	14,14,15	0.62	0	17,19,21	1.26	4 (23%)
11	BMA	Q	3	11	11,11,12	0.67	0	15,15,17	0.75	0
11	MAN	Q	4	11	11,11,12	0.64	0	15,15,17	1.12	2 (13%)
11	MAN	Q	5	11	11,11,12	0.87	0	15,15,17	1.39	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	MAN	Q	6	11	11,11,12	0.75	0	15,15,17	1.04	0
11	MAN	Q	7	11	11,11,12	0.69	0	15,15,17	2.10	7 (46%)
11	MAN	Q	8	11	11,11,12	0.60	0	15,15,17	1.12	1 (6%)
11	MAN	Q	9	11	11,11,12	0.96	0	15,15,17	0.98	0
8	NAG	R	1	1,8	14,14,15	0.76	0	17,19,21	1.79	3 (17%)
8	NAG	R	2	8	14,14,15	0.74	0	17,19,21	1.79	4 (23%)
12	NAG	S	1	12,1	14,14,15	0.47	0	17,19,21	1.05	1 (5%)
12	NAG	S	2	12	14,14,15	0.46	0	17,19,21	1.24	2 (11%)
12	BMA	S	3	12	11,11,12	0.60	0	15,15,17	1.18	2 (13%)
12	MAN	S	4	12	11,11,12	0.53	0	15,15,17	0.73	0
12	MAN	S	5	12	11,11,12	0.76	0	15,15,17	1.34	3 (20%)
12	MAN	S	6	12	11,11,12	1.04	1 (9%)	15,15,17	1.50	3 (20%)
12	MAN	S	7	12	11,11,12	1.06	0	15,15,17	1.26	2 (13%)
12	MAN	S	8	12	11,11,12	0.91	0	15,15,17	1.09	0
12	MAN	S	9	12	11,11,12	0.92	1 (9%)	15,15,17	1.01	0
13	NAG	T	1	13,1	14,14,15	0.74	0	17,19,21	1.86	7 (41%)
13	NAG	T	2	13	14,14,15	0.77	0	17,19,21	1.12	1 (5%)
13	BMA	T	3	13	11,11,12	0.59	0	15,15,17	1.78	5 (33%)
13	MAN	T	4	13	11,11,12	0.59	0	15,15,17	0.95	0
13	MAN	T	5	13	11,11,12	0.77	0	15,15,17	1.04	1 (6%)
13	MAN	T	6	13	11,11,12	1.28	1 (9%)	15,15,17	1.50	2 (13%)
13	GLC	T	7	13	11,11,12	1.03	1 (9%)	15,15,17	1.55	1 (6%)
13	MAN	T	8	13	11,11,12	1.24	2 (18%)	15,15,17	1.55	3 (20%)
14	NAG	U	1	14,1	14,14,15	0.48	0	17,19,21	1.51	4 (23%)
14	NAG	U	2	14	14,14,15	0.46	0	17,19,21	1.64	3 (17%)
14	BMA	U	3	14	11,11,12	0.66	0	15,15,17	1.00	0
14	MAN	U	4	14	11,11,12	0.59	0	15,15,17	0.99	0
14	MAN	U	5	14	11,11,12	0.99	1 (9%)	15,15,17	1.34	2 (13%)
5	NAG	V	1	5,1	14,14,15	0.48	0	17,19,21	1.43	2 (11%)
5	NAG	V	2	5	14,14,15	0.47	0	17,19,21	0.99	0
5	BMA	V	3	5	11,11,12	0.77	1 (9%)	15,15,17	0.93	0
5	MAN	V	4	5	11,11,12	0.68	0	15,15,17	1.02	1 (6%)
5	MAN	V	5	5	11,11,12	0.57	0	15,15,17	1.15	1 (6%)
5	MAN	V	6	5	11,11,12	0.62	0	15,15,17	1.03	1 (6%)
5	MAN	V	7	5	11,11,12	0.66	0	15,15,17	1.18	0
5	MAN	V	8	5	11,11,12	0.62	0	15,15,17	1.28	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	V	9	5	11,11,12	0.98	1 (9%)	15,15,17	1.29	2 (13%)
15	NAG	W	1	15,1	14,14,15	0.66	0	17,19,21	1.54	3 (17%)
15	NAG	W	2	15	14,14,15	0.55	0	17,19,21	1.44	2 (11%)
15	BMA	W	3	15	11,11,12	0.66	0	15,15,17	1.04	0
16	NAG	X	1	16,1	14,14,15	0.78	0	17,19,21	1.93	5 (29%)
16	NAG	X	2	16	14,14,15	0.44	0	17,19,21	1.78	4 (23%)
16	BMA	X	3	16	11,11,12	0.63	0	15,15,17	1.28	3 (20%)
16	MAN	X	4	16	11,11,12	0.65	0	15,15,17	0.94	0
16	MAN	X	5	16	11,11,12	0.79	0	15,15,17	1.38	2 (13%)
16	MAN	X	6	16	11,11,12	0.70	0	15,15,17	0.95	1 (6%)
16	MAN	X	7	16	11,11,12	0.61	0	15,15,17	0.73	0
16	MAN	X	8	16	11,11,12	1.17	1 (9%)	15,15,17	1.57	3 (20%)
8	NAG	Y	1	1,8	14,14,15	0.42	0	17,19,21	1.01	0
8	NAG	Y	2	8	14,14,15	0.74	0	17,19,21	1.65	4 (23%)
15	NAG	Z	1	15,1	14,14,15	0.65	0	17,19,21	1.64	4 (23%)
15	NAG	Z	2	15	14,14,15	0.68	0	17,19,21	1.61	4 (23%)
15	BMA	Z	3	15	11,11,12	0.86	0	15,15,17	0.96	1 (6%)
17	NAG	a	1	17,1	14,14,15	0.61	0	17,19,21	1.45	3 (17%)
17	NAG	a	2	17	14,14,15	0.43	0	17,19,21	1.23	2 (11%)
17	BMA	a	3	17	11,11,12	0.61	0	15,15,17	0.97	1 (6%)
17	MAN	a	4	17	11,11,12	0.63	0	15,15,17	1.42	2 (13%)
17	MAN	a	5	17	11,11,12	0.82	0	15,15,17	0.95	0
17	MAN	a	6	17	11,11,12	0.64	0	15,15,17	0.63	0
13	NAG	b	1	13,1	14,14,15	0.75	1 (7%)	17,19,21	1.10	1 (5%)
13	NAG	b	2	13	14,14,15	0.57	0	17,19,21	1.16	2 (11%)
13	BMA	b	3	13	11,11,12	0.62	0	15,15,17	1.24	1 (6%)
13	MAN	b	4	13	11,11,12	1.06	0	15,15,17	1.02	1 (6%)
13	MAN	b	5	13	11,11,12	0.57	0	15,15,17	1.11	1 (6%)
13	MAN	b	6	13	11,11,12	0.79	1 (9%)	15,15,17	1.24	1 (6%)
13	GLC	b	7	13	11,11,12	0.69	0	15,15,17	1.16	0
13	MAN	b	8	13	11,11,12	1.25	1 (9%)	15,15,17	1.57	3 (20%)
4	NAG	c	1	4,1	14,14,15	0.58	0	17,19,21	1.39	2 (11%)
4	NAG	c	2	4	14,14,15	0.85	0	17,19,21	1.92	3 (17%)
4	BMA	c	3	4	11,11,12	0.72	0	15,15,17	1.76	5 (33%)
4	MAN	c	4	4	11,11,12	0.77	0	15,15,17	0.80	0
9	NAG	d	1	9,1	14,14,15	0.56	0	17,19,21	1.38	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MAN	d	10	9	11,11,12	0.70	0	15,15,17	1.28	2 (13%)
9	NAG	d	2	9	14,14,15	0.77	0	17,19,21	1.28	1 (5%)
9	BMA	d	3	9	11,11,12	0.76	0	15,15,17	1.04	0
9	MAN	d	4	9	11,11,12	0.54	0	15,15,17	0.99	0
9	MAN	d	5	9	11,11,12	0.73	0	15,15,17	1.14	0
9	MAN	d	6	9	11,11,12	0.70	0	15,15,17	0.83	0
9	MAN	d	7	9	11,11,12	0.89	0	15,15,17	1.02	1 (6%)
9	MAN	d	8	9	11,11,12	0.60	0	15,15,17	1.15	2 (13%)
9	MAN	d	9	9	11,11,12	0.62	0	15,15,17	1.20	2 (13%)
15	NAG	e	1	15,1	14,14,15	0.79	1 (7%)	17,19,21	1.15	2 (11%)
15	NAG	e	2	15	14,14,15	0.51	0	17,19,21	1.28	2 (11%)
15	BMA	e	3	15	11,11,12	0.68	0	15,15,17	1.11	1 (6%)
16	NAG	f	1	16,1	14,14,15	0.52	0	17,19,21	1.24	2 (11%)
16	NAG	f	2	16	14,14,15	0.88	1 (7%)	17,19,21	1.29	2 (11%)
16	BMA	f	3	16	11,11,12	0.48	0	15,15,17	0.86	0
16	MAN	f	4	16	11,11,12	0.67	0	15,15,17	0.83	0
16	MAN	f	5	16	11,11,12	0.88	0	15,15,17	1.31	1 (6%)
16	MAN	f	6	16	11,11,12	0.83	0	15,15,17	1.26	2 (13%)
16	MAN	f	7	16	11,11,12	0.81	0	15,15,17	0.89	1 (6%)
16	MAN	f	8	16	11,11,12	0.61	0	15,15,17	1.43	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	1/2/19/22	0/1/1/1
4	MAN	G	4	4	-	1/2/19/22	0/1/1/1
5	NAG	H	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	MAN	H	5	5	-	0/2/19/22	0/1/1/1
5	MAN	H	6	5	-	0/2/19/22	0/1/1/1
5	MAN	H	7	5	-	0/2/19/22	0/1/1/1
5	MAN	H	8	5	-	0/2/19/22	0/1/1/1
5	MAN	H	9	5	-	2/2/19/22	0/1/1/1
6	NAG	I	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	BMA	I	3	6	-	2/2/19/22	0/1/1/1
6	MAN	I	4	6	-	0/2/19/22	0/1/1/1
7	NAG	J	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	BMA	J	3	7	-	0/2/19/22	0/1/1/1
7	MAN	J	4	7	-	0/2/19/22	0/1/1/1
7	MAN	J	5	7	-	2/2/19/22	0/1/1/1
7	MAN	J	6	7	-	2/2/19/22	0/1/1/1
7	MAN	J	7	7	-	0/2/19/22	0/1/1/1
7	MAN	J	8	7	-	0/2/19/22	0/1/1/1
7	MAN	J	9	7	-	0/2/19/22	0/1/1/1
8	NAG	K	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	K	2	8	-	0/6/23/26	0/1/1/1
4	NAG	L	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	BMA	L	3	4	-	2/2/19/22	0/1/1/1
4	MAN	L	4	4	-	2/2/19/22	0/1/1/1
2	NAG	M	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	M	2	2	-	1/6/23/26	0/1/1/1
2	BMA	M	3	2	-	0/2/19/22	0/1/1/1
2	MAN	M	4	2	-	0/2/19/22	0/1/1/1
2	MAN	M	5	2	-	0/2/19/22	0/1/1/1
4	NAG	N	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	1/6/23/26	0/1/1/1
4	BMA	N	3	4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	N	4	4	-	2/2/19/22	0/1/1/1
9	NAG	O	1	9,1	-	1/6/23/26	0/1/1/1
9	MAN	O	10	9	-	0/2/19/22	0/1/1/1
9	NAG	O	2	9	-	0/6/23/26	0/1/1/1
9	BMA	O	3	9	-	0/2/19/22	0/1/1/1
9	MAN	O	4	9	-	0/2/19/22	0/1/1/1
9	MAN	O	5	9	-	0/2/19/22	0/1/1/1
9	MAN	O	6	9	-	2/2/19/22	0/1/1/1
9	MAN	O	7	9	-	2/2/19/22	0/1/1/1
9	MAN	O	8	9	-	0/2/19/22	0/1/1/1
9	MAN	O	9	9	-	2/2/19/22	0/1/1/1
10	NAG	P	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	P	2	10	-	0/6/23/26	0/1/1/1
10	BMA	P	3	10	-	1/2/19/22	0/1/1/1
10	BMA	P	4	10	-	2/2/19/22	0/1/1/1
10	MAN	P	5	10	-	0/2/19/22	0/1/1/1
11	NAG	Q	1	11,1	-	0/6/23/26	0/1/1/1
11	MAN	Q	10	11	-	2/2/19/22	0/1/1/1
11	NAG	Q	2	11	-	0/6/23/26	0/1/1/1
11	BMA	Q	3	11	-	0/2/19/22	0/1/1/1
11	MAN	Q	4	11	-	0/2/19/22	0/1/1/1
11	MAN	Q	5	11	-	2/2/19/22	0/1/1/1
11	MAN	Q	6	11	-	0/2/19/22	0/1/1/1
11	MAN	Q	7	11	-	0/2/19/22	0/1/1/1
11	MAN	Q	8	11	-	2/2/19/22	0/1/1/1
11	MAN	Q	9	11	-	0/2/19/22	0/1/1/1
8	NAG	R	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	R	2	8	-	2/6/23/26	0/1/1/1
12	NAG	S	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	S	2	12	-	0/6/23/26	0/1/1/1
12	BMA	S	3	12	-	2/2/19/22	0/1/1/1
12	MAN	S	4	12	-	0/2/19/22	0/1/1/1
12	MAN	S	5	12	-	2/2/19/22	0/1/1/1
12	MAN	S	6	12	-	0/2/19/22	0/1/1/1
12	MAN	S	7	12	-	1/2/19/22	0/1/1/1
12	MAN	S	8	12	-	0/2/19/22	0/1/1/1
12	MAN	S	9	12	-	0/2/19/22	0/1/1/1
13	NAG	T	1	13,1	-	1/6/23/26	0/1/1/1
13	NAG	T	2	13	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BMA	T	3	13	-	2/2/19/22	0/1/1/1
13	MAN	T	4	13	-	0/2/19/22	0/1/1/1
13	MAN	T	5	13	-	0/2/19/22	0/1/1/1
13	MAN	T	6	13	-	1/2/19/22	0/1/1/1
13	GLC	T	7	13	-	2/2/19/22	0/1/1/1
13	MAN	T	8	13	-	2/2/19/22	0/1/1/1
14	NAG	U	1	14,1	-	1/6/23/26	0/1/1/1
14	NAG	U	2	14	-	0/6/23/26	0/1/1/1
14	BMA	U	3	14	-	0/2/19/22	0/1/1/1
14	MAN	U	4	14	-	1/2/19/22	0/1/1/1
14	MAN	U	5	14	-	2/2/19/22	0/1/1/1
5	NAG	V	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	V	2	5	-	0/6/23/26	0/1/1/1
5	BMA	V	3	5	-	0/2/19/22	0/1/1/1
5	MAN	V	4	5	-	1/2/19/22	0/1/1/1
5	MAN	V	5	5	-	0/2/19/22	0/1/1/1
5	MAN	V	6	5	-	0/2/19/22	0/1/1/1
5	MAN	V	7	5	-	2/2/19/22	0/1/1/1
5	MAN	V	8	5	-	0/2/19/22	0/1/1/1
5	MAN	V	9	5	-	2/2/19/22	0/1/1/1
15	NAG	W	1	15,1	-	1/6/23/26	0/1/1/1
15	NAG	W	2	15	-	0/6/23/26	0/1/1/1
15	BMA	W	3	15	-	1/2/19/22	0/1/1/1
16	NAG	X	1	16,1	-	0/6/23/26	0/1/1/1
16	NAG	X	2	16	-	0/6/23/26	0/1/1/1
16	BMA	X	3	16	-	0/2/19/22	0/1/1/1
16	MAN	X	4	16	-	0/2/19/22	0/1/1/1
16	MAN	X	5	16	-	2/2/19/22	0/1/1/1
16	MAN	X	6	16	-	2/2/19/22	0/1/1/1
16	MAN	X	7	16	-	2/2/19/22	0/1/1/1
16	MAN	X	8	16	-	2/2/19/22	0/1/1/1
8	NAG	Y	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	0/6/23/26	0/1/1/1
15	NAG	Z	1	15,1	-	0/6/23/26	0/1/1/1
15	NAG	Z	2	15	-	0/6/23/26	0/1/1/1
15	BMA	Z	3	15	-	0/2/19/22	0/1/1/1
17	NAG	a	1	17,1	-	0/6/23/26	0/1/1/1
17	NAG	a	2	17	-	0/6/23/26	0/1/1/1
17	BMA	a	3	17	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MAN	a	4	17	-	2/2/19/22	0/1/1/1
17	MAN	a	5	17	-	0/2/19/22	0/1/1/1
17	MAN	a	6	17	-	1/2/19/22	0/1/1/1
13	NAG	b	1	13,1	-	1/6/23/26	0/1/1/1
13	NAG	b	2	13	-	3/6/23/26	0/1/1/1
13	BMA	b	3	13	-	0/2/19/22	0/1/1/1
13	MAN	b	4	13	-	0/2/19/22	0/1/1/1
13	MAN	b	5	13	-	0/2/19/22	0/1/1/1
13	MAN	b	6	13	-	1/2/19/22	0/1/1/1
13	GLC	b	7	13	-	1/2/19/22	0/1/1/1
13	MAN	b	8	13	-	2/2/19/22	0/1/1/1
4	NAG	c	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	c	2	4	-	0/6/23/26	0/1/1/1
4	BMA	c	3	4	-	2/2/19/22	0/1/1/1
4	MAN	c	4	4	-	1/2/19/22	0/1/1/1
9	NAG	d	1	9,1	-	0/6/23/26	0/1/1/1
9	MAN	d	10	9	-	2/2/19/22	0/1/1/1
9	NAG	d	2	9	-	1/6/23/26	0/1/1/1
9	BMA	d	3	9	-	0/2/19/22	0/1/1/1
9	MAN	d	4	9	-	0/2/19/22	0/1/1/1
9	MAN	d	5	9	-	0/2/19/22	0/1/1/1
9	MAN	d	6	9	-	0/2/19/22	0/1/1/1
9	MAN	d	7	9	-	0/2/19/22	0/1/1/1
9	MAN	d	8	9	-	0/2/19/22	0/1/1/1
9	MAN	d	9	9	-	1/2/19/22	0/1/1/1
15	NAG	e	1	15,1	-	0/6/23/26	0/1/1/1
15	NAG	e	2	15	-	0/6/23/26	0/1/1/1
15	BMA	e	3	15	-	2/2/19/22	0/1/1/1
16	NAG	f	1	16,1	-	0/6/23/26	0/1/1/1
16	NAG	f	2	16	-	0/6/23/26	0/1/1/1
16	BMA	f	3	16	-	0/2/19/22	0/1/1/1
16	MAN	f	4	16	-	0/2/19/22	0/1/1/1
16	MAN	f	5	16	-	2/2/19/22	0/1/1/1
16	MAN	f	6	16	-	2/2/19/22	0/1/1/1
16	MAN	f	7	16	-	0/2/19/22	0/1/1/1
16	MAN	f	8	16	-	0/2/19/22	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	6	MAN	C2-C3	3.50	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	S	6	MAN	C2-C3	2.68	1.56	1.52
13	b	8	MAN	C2-C3	2.55	1.56	1.52
16	f	2	NAG	C1-C2	-2.48	1.49	1.52
5	V	9	MAN	C2-C3	2.39	1.56	1.52
2	M	4	MAN	C2-C3	2.35	1.56	1.52
2	E	3	BMA	C2-C3	2.33	1.56	1.52
14	U	5	MAN	C2-C3	2.29	1.56	1.52
5	H	9	MAN	C2-C3	2.26	1.55	1.52
13	T	8	MAN	C1-C2	2.24	1.57	1.52
16	X	8	MAN	C2-C3	2.21	1.55	1.52
3	F	7	MAN	C4-C5	2.20	1.57	1.53
2	M	5	MAN	C2-C3	2.17	1.55	1.52
13	b	6	MAN	C2-C3	2.16	1.55	1.52
15	e	1	NAG	C1-C2	2.14	1.55	1.52
13	T	8	MAN	C2-C3	2.12	1.55	1.52
5	H	2	NAG	O5-C1	-2.10	1.40	1.43
12	S	9	MAN	C2-C3	2.10	1.55	1.52
5	V	3	BMA	O5-C1	-2.08	1.40	1.43
13	b	1	NAG	O5-C1	-2.07	1.40	1.43
13	T	7	GLC	C1-C2	2.02	1.57	1.52

All (284) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	2	NAG	C2-N2-C7	5.33	130.04	122.90
4	G	4	MAN	C1-O5-C5	4.90	118.76	112.19
13	T	7	GLC	C1-C2-C3	4.89	116.76	109.64
8	R	1	NAG	C1-O5-C5	4.82	118.64	112.19
8	K	1	NAG	C1-O5-C5	4.71	118.49	112.19
13	T	6	MAN	O2-C2-C3	4.57	119.62	110.15
14	U	2	NAG	C1-O5-C5	4.51	118.23	112.19
2	M	1	NAG	C1-O5-C5	4.51	118.23	112.19
8	R	2	NAG	O5-C1-C2	-4.47	104.37	111.29
13	T	3	BMA	O5-C5-C6	4.37	116.17	107.66
6	I	4	MAN	C1-O5-C5	4.26	117.90	112.19
16	X	5	MAN	O2-C2-C1	4.15	118.73	109.22
4	c	2	NAG	C8-C7-N2	-3.99	109.50	116.12
4	G	3	BMA	O5-C5-C6	-3.99	99.90	107.66
9	O	8	MAN	C1-O5-C5	3.98	117.52	112.19
4	N	2	NAG	C8-C7-N2	-3.98	109.53	116.12
15	Z	2	NAG	C1-O5-C5	3.93	117.45	112.19
4	N	2	NAG	O4-C4-C3	-3.91	101.17	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Q	7	MAN	O5-C5-C6	3.90	115.25	107.66
16	X	2	NAG	C1-C2-N2	3.87	116.53	110.43
9	d	2	NAG	C1-C2-N2	-3.85	104.37	110.43
4	c	2	NAG	C2-N2-C7	3.83	128.04	122.90
8	Y	2	NAG	C1-O5-C5	3.79	117.27	112.19
17	a	4	MAN	C1-O5-C5	3.78	117.25	112.19
8	R	1	NAG	C1-C2-N2	-3.71	104.59	110.43
4	c	2	NAG	O7-C7-N2	3.65	128.43	121.98
4	G	3	BMA	C1-O5-C5	3.64	117.07	112.19
4	G	3	BMA	C3-C4-C5	3.58	116.72	110.23
15	Z	1	NAG	O3-C3-C2	-3.56	102.00	109.40
16	X	2	NAG	O4-C4-C3	-3.56	101.99	110.38
5	V	1	NAG	O3-C3-C2	-3.50	102.13	109.40
9	O	8	MAN	C6-C5-C4	-3.48	104.48	113.02
13	T	8	MAN	C1-O5-C5	3.48	116.85	112.19
13	b	8	MAN	C1-O5-C5	3.47	116.84	112.19
9	d	1	NAG	O4-C4-C5	-3.47	100.78	109.32
3	F	1	NAG	C2-N2-C7	3.45	127.53	122.90
15	Z	1	NAG	C1-O5-C5	3.44	116.79	112.19
9	O	2	NAG	C1-C2-N2	-3.43	105.03	110.43
3	F	5	MAN	C1-O5-C5	3.39	116.73	112.19
15	W	2	NAG	C2-N2-C7	3.39	127.44	122.90
16	X	1	NAG	O3-C3-C2	-3.37	102.40	109.40
14	U	1	NAG	C1-C2-N2	-3.36	105.14	110.43
16	X	8	MAN	C1-C2-C3	-3.35	104.76	109.64
16	f	5	MAN	O2-C2-C1	3.31	116.81	109.22
2	M	5	MAN	O2-C2-C3	3.31	117.00	110.15
13	T	1	NAG	O7-C7-N2	3.30	127.81	121.98
9	d	9	MAN	O4-C4-C3	-3.28	102.64	110.38
12	S	5	MAN	O2-C2-C3	-3.26	103.41	110.15
5	H	8	MAN	C6-C5-C4	-3.24	105.06	113.02
3	F	1	NAG	C1-C2-N2	3.24	115.54	110.43
5	H	8	MAN	C1-O5-C5	3.21	116.49	112.19
8	Y	2	NAG	C1-C2-N2	3.20	115.47	110.43
7	J	8	MAN	C1-O5-C5	3.19	116.46	112.19
13	b	8	MAN	O5-C5-C6	3.18	113.86	107.66
16	X	1	NAG	C2-N2-C7	3.17	127.15	122.90
4	G	3	BMA	C1-C2-C3	3.17	114.26	109.64
9	O	10	MAN	C3-C4-C5	3.17	115.97	110.23
9	O	5	MAN	O5-C5-C6	3.15	113.80	107.66
16	X	1	NAG	O4-C4-C5	-3.15	101.57	109.32
4	c	3	BMA	O2-C2-C3	3.14	116.66	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	W	1	NAG	O7-C7-N2	3.13	127.52	121.98
3	F	7	MAN	C1-C2-C3	3.11	114.17	109.64
4	G	1	NAG	C1-C2-N2	-3.09	105.56	110.43
2	E	2	NAG	O3-C3-C2	-3.08	103.00	109.40
5	V	8	MAN	O2-C2-C3	3.08	116.53	110.15
7	J	7	MAN	C1-C2-C3	3.07	114.11	109.64
4	c	3	BMA	O4-C4-C3	-3.07	103.15	110.38
13	T	1	NAG	C2-N2-C7	3.05	126.98	122.90
5	V	5	MAN	C1-O5-C5	3.04	116.26	112.19
4	L	2	NAG	O4-C4-C5	-3.02	101.89	109.32
5	V	9	MAN	C1-O5-C5	3.01	116.23	112.19
4	G	3	BMA	O4-C4-C3	-2.99	103.33	110.38
4	G	3	BMA	O3-C3-C4	-2.99	103.33	110.38
9	O	8	MAN	O3-C3-C4	-2.98	103.35	110.38
11	Q	7	MAN	C3-C4-C5	-2.97	104.84	110.23
4	N	1	NAG	O5-C1-C2	-2.97	106.70	111.29
5	H	7	MAN	C1-C2-C3	-2.96	105.33	109.64
4	N	3	BMA	C3-C4-C5	2.94	115.57	110.23
12	S	6	MAN	O3-C3-C2	2.94	116.05	110.05
3	F	7	MAN	O4-C4-C5	2.93	116.55	109.32
13	b	4	MAN	O5-C5-C6	2.93	113.37	107.66
4	N	2	NAG	C4-C3-C2	2.93	115.31	111.02
4	c	1	NAG	C4-C3-C2	-2.93	106.73	111.02
8	R	2	NAG	C1-O5-C5	2.93	116.11	112.19
15	W	1	NAG	C2-N2-C7	2.92	126.81	122.90
2	M	5	MAN	O5-C5-C6	2.91	113.33	107.66
7	J	4	MAN	O2-C2-C3	-2.88	104.18	110.15
16	f	6	MAN	O4-C4-C5	2.88	116.42	109.32
16	f	8	MAN	C3-C4-C5	2.87	115.43	110.23
17	a	2	NAG	O3-C3-C2	-2.86	103.46	109.40
2	E	3	BMA	O5-C5-C6	2.86	113.22	107.66
11	Q	10	MAN	C3-C4-C5	2.86	115.41	110.23
16	f	2	NAG	O5-C1-C2	-2.85	106.87	111.29
2	M	4	MAN	O2-C2-C3	2.85	116.06	110.15
5	H	9	MAN	C2-C3-C4	2.85	115.87	110.86
13	b	3	BMA	O4-C4-C3	-2.83	103.69	110.38
9	d	10	MAN	O2-C2-C3	2.83	116.02	110.15
5	V	9	MAN	O2-C2-C3	2.83	116.02	110.15
6	I	2	NAG	O7-C7-N2	2.83	126.98	121.98
16	f	1	NAG	O3-C3-C2	-2.82	103.55	109.40
13	T	1	NAG	C1-C2-N2	2.81	114.87	110.43
11	Q	10	MAN	C1-O5-C5	-2.81	108.42	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	S	1	NAG	C2-N2-C7	2.80	126.66	122.90
5	H	7	MAN	O2-C2-C3	2.80	115.95	110.15
11	Q	4	MAN	O5-C1-C2	-2.79	104.14	110.79
16	f	1	NAG	O4-C4-C5	-2.79	102.46	109.32
17	a	1	NAG	O4-C4-C5	-2.77	102.50	109.32
2	M	5	MAN	C1-O5-C5	2.74	115.86	112.19
16	X	8	MAN	O2-C2-C3	2.74	115.83	110.15
13	T	1	NAG	C4-C3-C2	-2.74	107.00	111.02
16	f	7	MAN	O2-C2-C1	2.73	115.47	109.22
9	O	1	NAG	O4-C4-C5	-2.73	102.61	109.32
13	T	2	NAG	O5-C1-C2	-2.69	107.13	111.29
13	b	6	MAN	O2-C2-C3	2.69	115.72	110.15
9	d	8	MAN	C6-C5-C4	-2.69	106.41	113.02
11	Q	7	MAN	O3-C3-C2	2.69	115.54	110.05
17	a	2	NAG	O4-C4-C5	-2.69	102.71	109.32
16	X	1	NAG	O7-C7-C8	-2.67	117.29	122.05
13	T	8	MAN	C1-C2-C3	2.67	113.53	109.64
11	Q	7	MAN	C1-C2-C3	-2.64	105.79	109.64
13	T	3	BMA	O4-C4-C3	-2.64	104.15	110.38
7	J	2	NAG	O4-C4-C3	-2.63	104.18	110.38
4	c	1	NAG	C1-C2-N2	-2.63	106.29	110.43
5	H	4	MAN	O6-C6-C5	-2.63	102.39	111.33
13	T	1	NAG	O7-C7-C8	-2.62	117.38	122.05
7	J	5	MAN	O2-C2-C1	2.62	115.23	109.22
4	G	2	NAG	C2-N2-C7	2.62	126.41	122.90
11	Q	7	MAN	O2-C2-C3	2.62	115.57	110.15
5	V	1	NAG	C1-C2-N2	2.60	114.52	110.43
15	Z	2	NAG	C4-C3-C2	-2.59	107.22	111.02
17	a	1	NAG	C1-C2-N2	-2.59	106.36	110.43
11	Q	7	MAN	O5-C5-C4	-2.58	104.55	110.83
11	Q	5	MAN	O4-C4-C5	2.58	115.67	109.32
2	M	5	MAN	O3-C3-C2	2.57	115.31	110.05
2	E	1	NAG	C1-C2-N2	-2.57	106.39	110.43
14	U	2	NAG	O7-C7-N2	2.56	126.50	121.98
15	W	2	NAG	O7-C7-N2	2.55	126.49	121.98
11	Q	7	MAN	C1-O5-C5	2.55	115.61	112.19
5	H	2	NAG	C1-C2-N2	-2.55	106.42	110.43
12	S	3	BMA	O5-C5-C4	-2.54	104.64	110.83
2	M	1	NAG	C2-N2-C7	2.54	126.30	122.90
12	S	7	MAN	O5-C5-C6	2.53	112.59	107.66
3	F	7	MAN	O5-C5-C6	2.52	112.57	107.66
5	H	4	MAN	O2-C2-C1	2.51	114.98	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	X	2	NAG	C1-O5-C5	-2.50	108.83	112.19
14	U	1	NAG	C1-O5-C5	2.50	115.54	112.19
15	e	2	NAG	C2-N2-C7	2.49	126.24	122.90
11	Q	8	MAN	O4-C4-C3	-2.49	104.52	110.38
16	X	8	MAN	O5-C5-C6	2.47	112.48	107.66
16	f	8	MAN	C1-O5-C5	-2.47	108.88	112.19
4	L	4	MAN	O5-C5-C6	2.47	112.46	107.66
13	T	3	BMA	C1-O5-C5	2.46	115.49	112.19
5	H	7	MAN	O2-C2-C1	2.46	114.85	109.22
2	E	3	BMA	C6-C5-C4	2.44	119.01	113.02
15	Z	2	NAG	O4-C4-C5	2.44	115.32	109.32
4	G	1	NAG	O5-C1-C2	-2.43	107.53	111.29
12	S	7	MAN	O2-C2-C3	2.43	115.18	110.15
16	X	3	BMA	C1-O5-C5	2.42	115.43	112.19
4	N	1	NAG	C1-C2-N2	-2.42	106.62	110.43
9	d	7	MAN	C1-O5-C5	2.41	115.42	112.19
16	X	1	NAG	O7-C7-N2	2.41	126.23	121.98
2	M	1	NAG	O5-C1-C2	-2.40	107.58	111.29
16	f	2	NAG	O4-C4-C3	-2.40	104.72	110.38
6	I	3	BMA	O5-C5-C6	2.40	112.33	107.66
15	Z	1	NAG	O7-C7-N2	2.40	126.22	121.98
2	M	3	BMA	O4-C4-C3	-2.39	104.75	110.38
4	c	3	BMA	C3-C4-C5	2.38	114.55	110.23
14	U	2	NAG	O4-C4-C5	-2.38	103.47	109.32
7	J	5	MAN	C1-O5-C5	2.37	115.36	112.19
2	E	3	BMA	O2-C2-C1	2.37	114.64	109.22
2	M	4	MAN	O2-C2-C1	-2.36	103.81	109.22
12	S	5	MAN	O4-C4-C3	-2.36	104.81	110.38
8	R	1	NAG	C2-N2-C7	2.36	126.06	122.90
15	Z	2	NAG	C1-C2-N2	2.36	114.15	110.43
12	S	2	NAG	C2-N2-C7	-2.36	119.74	122.90
11	Q	5	MAN	C1-O5-C5	2.36	115.35	112.19
2	M	3	BMA	O5-C1-C2	-2.35	105.17	110.79
2	E	4	MAN	C1-O5-C5	2.35	115.34	112.19
10	P	1	NAG	C2-N2-C7	2.35	126.05	122.90
17	a	1	NAG	C2-N2-C7	2.34	126.04	122.90
5	V	4	MAN	O6-C6-C5	-2.34	103.36	111.33
13	T	3	BMA	O5-C5-C4	-2.34	105.13	110.83
14	U	5	MAN	C1-C2-C3	2.34	113.05	109.64
15	W	1	NAG	C8-C7-N2	-2.34	112.24	116.12
9	O	10	MAN	C2-C3-C4	2.34	114.97	110.86
12	S	6	MAN	O2-C2-C1	-2.33	103.89	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1	NAG	C1-C2-N2	-2.33	106.76	110.43
15	e	1	NAG	C1-O5-C5	2.33	115.31	112.19
2	M	4	MAN	O3-C3-C2	2.33	114.81	110.05
12	S	5	MAN	O2-C2-C1	2.32	114.53	109.22
3	F	7	MAN	C6-C5-C4	2.31	118.70	113.02
5	V	6	MAN	C6-C5-C4	-2.31	107.35	113.02
5	H	7	MAN	O3-C3-C4	2.30	115.81	110.38
3	F	7	MAN	C2-C3-C4	-2.30	106.82	110.86
16	f	8	MAN	O4-C4-C5	-2.30	103.66	109.32
4	G	1	NAG	C4-C3-C2	-2.29	107.66	111.02
9	O	8	MAN	O4-C4-C5	2.28	114.94	109.32
14	U	1	NAG	O4-C4-C5	-2.28	103.72	109.32
17	a	3	BMA	C3-C4-C5	2.27	114.35	110.23
5	H	9	MAN	O2-C2-C3	2.27	114.86	110.15
9	O	4	MAN	O6-C6-C5	-2.27	103.61	111.33
9	O	7	MAN	O2-C2-C3	-2.27	105.45	110.15
4	c	3	BMA	C1-O5-C5	2.27	115.22	112.19
5	H	6	MAN	C1-O5-C5	2.27	115.22	112.19
7	J	3	BMA	C1-O5-C5	2.26	115.22	112.19
6	I	3	BMA	O5-C5-C4	-2.26	105.33	110.83
2	M	5	MAN	C6-C5-C4	-2.26	107.47	113.02
9	d	8	MAN	O5-C1-C2	-2.25	105.43	110.79
5	H	6	MAN	O2-C2-C3	-2.25	105.50	110.15
14	U	5	MAN	O4-C4-C5	2.25	114.86	109.32
12	S	3	BMA	O5-C5-C6	2.24	112.03	107.66
11	Q	2	NAG	O4-C4-C3	-2.23	105.12	110.38
10	P	5	MAN	C1-O5-C5	2.23	115.17	112.19
2	E	3	BMA	O5-C5-C4	-2.23	105.40	110.83
16	X	5	MAN	O2-C2-C3	-2.23	105.54	110.15
4	N	2	NAG	O4-C4-C5	2.23	114.81	109.32
8	Y	2	NAG	O5-C1-C2	-2.23	107.85	111.29
15	Z	3	BMA	O5-C5-C6	2.22	111.99	107.66
13	T	6	MAN	O3-C3-C2	2.21	114.57	110.05
13	b	2	NAG	O3-C3-C2	-2.21	104.80	109.40
14	U	1	NAG	O5-C1-C2	-2.21	107.88	111.29
4	N	1	NAG	C1-O5-C5	2.20	115.13	112.19
13	b	2	NAG	C4-C3-C2	-2.19	107.80	111.02
10	P	5	MAN	O3-C3-C2	2.18	114.51	110.05
15	Z	1	NAG	O5-C5-C4	-2.18	105.52	110.83
5	H	5	MAN	O2-C2-C3	-2.18	105.64	110.15
9	O	10	MAN	O2-C2-C3	2.18	114.66	110.15
10	P	1	NAG	C1-O5-C5	2.17	115.10	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1	NAG	C4-C3-C2	-2.16	107.85	111.02
5	H	4	MAN	C1-O5-C5	2.16	115.08	112.19
4	c	3	BMA	O2-C2-C1	-2.15	104.30	109.22
3	F	7	MAN	O3-C3-C2	2.15	114.44	110.05
7	J	8	MAN	O5-C1-C2	-2.15	105.67	110.79
13	T	1	NAG	O5-C5-C6	-2.14	103.50	107.66
15	e	3	BMA	C1-C2-C3	-2.14	106.53	109.64
12	S	6	MAN	O2-C2-C3	2.14	114.58	110.15
8	Y	2	NAG	C6-C5-C4	-2.14	107.78	113.02
11	Q	10	MAN	O2-C2-C3	2.13	114.57	110.15
11	Q	10	MAN	O4-C4-C3	-2.13	105.35	110.38
16	X	3	BMA	O6-C6-C5	-2.13	104.09	111.33
9	O	10	MAN	O4-C4-C5	-2.12	104.10	109.32
9	d	9	MAN	C1-C2-C3	2.12	112.73	109.64
13	T	3	BMA	O2-C2-C3	2.12	114.53	110.15
16	X	3	BMA	O5-C1-C2	-2.11	105.75	110.79
15	e	1	NAG	O3-C3-C4	-2.11	105.41	110.38
5	H	8	MAN	O4-C4-C3	-2.11	105.41	110.38
11	Q	4	MAN	O2-C2-C3	-2.10	105.79	110.15
11	Q	5	MAN	O3-C3-C2	2.10	114.35	110.05
13	b	5	MAN	O4-C4-C5	2.10	114.49	109.32
2	M	1	NAG	C1-C2-N2	2.10	113.74	110.43
11	Q	2	NAG	C1-C2-N2	2.10	113.73	110.43
13	b	8	MAN	C1-C2-C3	2.09	112.69	109.64
6	I	1	NAG	O4-C4-C5	-2.09	104.18	109.32
9	O	1	NAG	O3-C3-C2	-2.09	105.07	109.40
4	G	1	NAG	O4-C4-C5	-2.09	104.19	109.32
8	R	2	NAG	O4-C4-C5	2.08	114.45	109.32
4	N	4	MAN	C1-C2-C3	2.08	112.67	109.64
16	X	6	MAN	C3-C4-C5	2.08	114.00	110.23
16	X	2	NAG	O7-C7-C8	-2.07	118.36	122.05
4	N	4	MAN	O5-C5-C6	2.07	111.69	107.66
9	d	10	MAN	C3-C4-C5	2.06	113.97	110.23
7	J	5	MAN	O3-C3-C4	2.06	115.22	110.38
15	e	2	NAG	C8-C7-N2	-2.06	112.71	116.12
17	a	4	MAN	O3-C3-C4	-2.05	105.53	110.38
12	S	2	NAG	C4-C3-C2	-2.05	108.01	111.02
5	V	8	MAN	O4-C4-C3	-2.05	105.55	110.38
8	R	2	NAG	O3-C3-C4	-2.04	105.56	110.38
8	K	2	NAG	C2-N2-C7	2.04	125.64	122.90
4	G	3	BMA	O2-C2-C1	-2.04	104.56	109.22
13	T	8	MAN	O2-C2-C1	2.04	113.89	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	BMA	C1-O5-C5	-2.04	109.45	112.19
13	T	5	MAN	O4-C4-C5	2.03	114.33	109.32
2	M	3	BMA	O3-C3-C4	-2.03	105.59	110.38
9	O	4	MAN	O3-C3-C4	-2.03	105.59	110.38
13	b	1	NAG	C4-C3-C2	-2.03	108.05	111.02
13	T	1	NAG	C1-O5-C5	2.03	114.90	112.19
16	f	6	MAN	C2-C3-C4	-2.02	107.30	110.86
4	L	3	BMA	O5-C5-C4	-2.02	105.92	110.83
7	J	2	NAG	O6-C6-C5	-2.01	104.47	111.33
10	P	5	MAN	O5-C1-C2	-2.00	106.01	110.79
9	d	1	NAG	O3-C3-C4	2.00	115.10	110.38
3	F	3	BMA	O5-C1-C2	-2.00	106.01	110.79
11	Q	2	NAG	C1-O5-C5	-2.00	109.50	112.19
11	Q	2	NAG	O7-C7-N2	2.00	125.52	121.98

There are no chirality outliers.

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	Q	5	MAN	O5-C5-C6-O6
6	I	3	BMA	O5-C5-C6-O6
16	f	5	MAN	O5-C5-C6-O6
5	V	7	MAN	O5-C5-C6-O6
15	e	3	BMA	O5-C5-C6-O6
16	f	6	MAN	O5-C5-C6-O6
17	a	3	BMA	C4-C5-C6-O6
16	X	6	MAN	O5-C5-C6-O6
16	f	5	MAN	C4-C5-C6-O6
3	F	7	MAN	O5-C5-C6-O6
4	L	4	MAN	O5-C5-C6-O6
6	I	3	BMA	C4-C5-C6-O6
16	X	8	MAN	O5-C5-C6-O6
4	c	3	BMA	C4-C5-C6-O6
5	V	7	MAN	C4-C5-C6-O6
10	P	4	BMA	C4-C5-C6-O6
11	Q	5	MAN	C4-C5-C6-O6
4	c	3	BMA	O5-C5-C6-O6
9	d	10	MAN	O5-C5-C6-O6
4	L	3	BMA	O5-C5-C6-O6
4	L	4	MAN	C4-C5-C6-O6
15	e	3	BMA	C4-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	R	2	NAG	O5-C5-C6-O6
4	N	3	BMA	O5-C5-C6-O6
11	Q	10	MAN	O5-C5-C6-O6
13	T	7	GLC	O5-C5-C6-O6
4	L	3	BMA	C4-C5-C6-O6
4	N	3	BMA	C4-C5-C6-O6
5	H	9	MAN	C4-C5-C6-O6
8	R	2	NAG	C4-C5-C6-O6
11	Q	10	MAN	C4-C5-C6-O6
7	J	5	MAN	O5-C5-C6-O6
13	b	2	NAG	C4-C5-C6-O6
16	X	6	MAN	C4-C5-C6-O6
17	a	3	BMA	O5-C5-C6-O6
16	f	6	MAN	C4-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
16	X	5	MAN	O5-C5-C6-O6
3	F	7	MAN	C4-C5-C6-O6
13	T	7	GLC	C4-C5-C6-O6
10	P	4	BMA	O5-C5-C6-O6
16	X	8	MAN	C4-C5-C6-O6
13	T	3	BMA	O5-C5-C6-O6
16	X	5	MAN	C4-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
4	N	4	MAN	O5-C5-C6-O6
5	H	9	MAN	O5-C5-C6-O6
14	U	5	MAN	O5-C5-C6-O6
13	b	2	NAG	O5-C5-C6-O6
13	T	3	BMA	C4-C5-C6-O6
9	d	10	MAN	C4-C5-C6-O6
5	V	9	MAN	O5-C5-C6-O6
13	b	8	MAN	O5-C5-C6-O6
2	E	4	MAN	C4-C5-C6-O6
13	T	8	MAN	O5-C5-C6-O6
12	S	3	BMA	C4-C5-C6-O6
3	F	5	MAN	O5-C5-C6-O6
7	J	5	MAN	C4-C5-C6-O6
9	O	9	MAN	C4-C5-C6-O6
7	J	6	MAN	O5-C5-C6-O6
17	a	6	MAN	O5-C5-C6-O6
16	X	7	MAN	C4-C5-C6-O6
9	O	6	MAN	C4-C5-C6-O6
9	O	9	MAN	O5-C5-C6-O6

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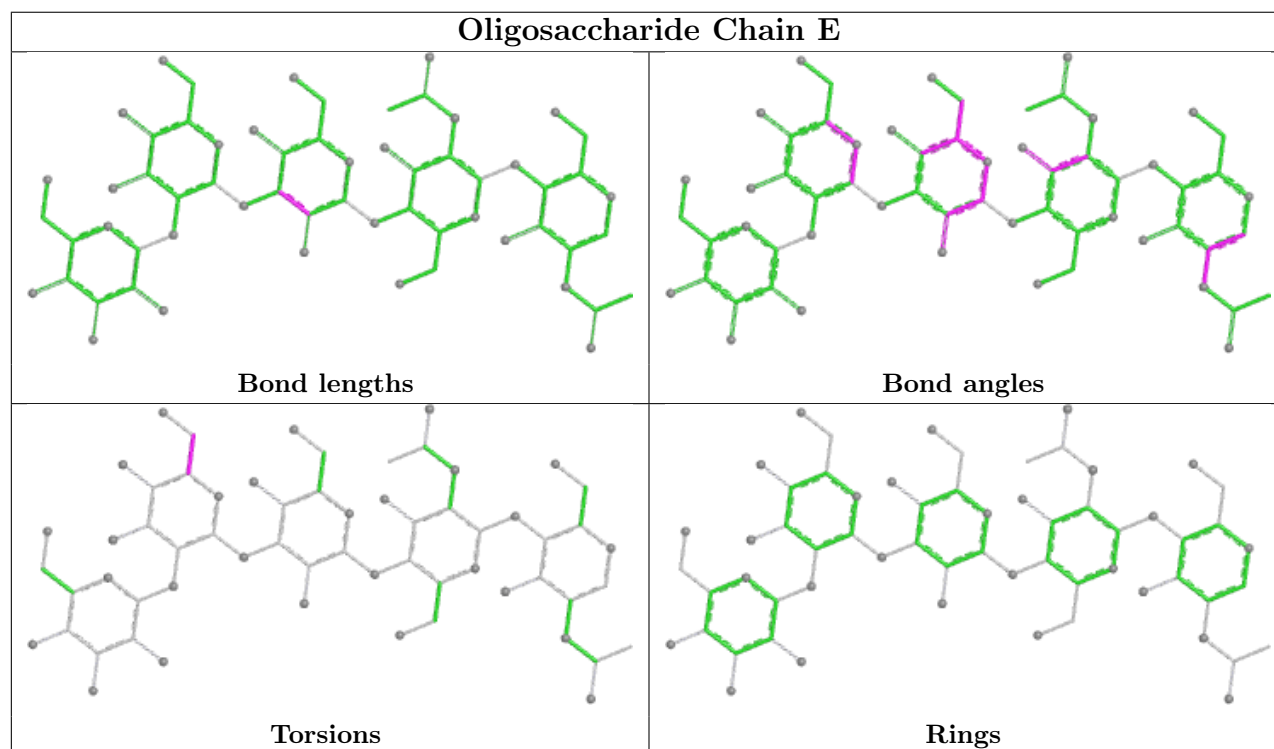
Mol	Chain	Res	Type	Atoms
13	b	6	MAN	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6
14	U	4	MAN	O5-C5-C6-O6
17	a	4	MAN	C4-C5-C6-O6
4	c	4	MAN	O5-C5-C6-O6
9	d	2	NAG	O5-C5-C6-O6
5	V	9	MAN	C4-C5-C6-O6
14	U	5	MAN	C4-C5-C6-O6
17	a	4	MAN	O5-C5-C6-O6
16	X	7	MAN	O5-C5-C6-O6
12	S	3	BMA	O5-C5-C6-O6
9	O	7	MAN	C4-C5-C6-O6
12	S	5	MAN	C4-C5-C6-O6
9	d	9	MAN	C4-C5-C6-O6
13	T	6	MAN	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
9	O	6	MAN	O5-C5-C6-O6
5	V	4	MAN	C4-C5-C6-O6
13	b	8	MAN	C4-C5-C6-O6
4	N	4	MAN	C4-C5-C6-O6
11	Q	8	MAN	C4-C5-C6-O6
12	S	1	NAG	O5-C5-C6-O6
7	J	6	MAN	C4-C5-C6-O6
12	S	5	MAN	O5-C5-C6-O6
11	Q	8	MAN	O5-C5-C6-O6
2	M	1	NAG	C1-C2-N2-C7
9	O	1	NAG	C1-C2-N2-C7
13	b	1	NAG	C1-C2-N2-C7
13	b	2	NAG	C1-C2-N2-C7
15	W	1	NAG	C1-C2-N2-C7
12	S	1	NAG	C4-C5-C6-O6
13	T	8	MAN	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
13	b	7	GLC	C4-C5-C6-O6
13	T	1	NAG	C4-C5-C6-O6
10	P	3	BMA	O5-C5-C6-O6
12	S	7	MAN	C4-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
9	O	7	MAN	O5-C5-C6-O6
14	U	1	NAG	C4-C5-C6-O6
15	W	3	BMA	C4-C5-C6-O6

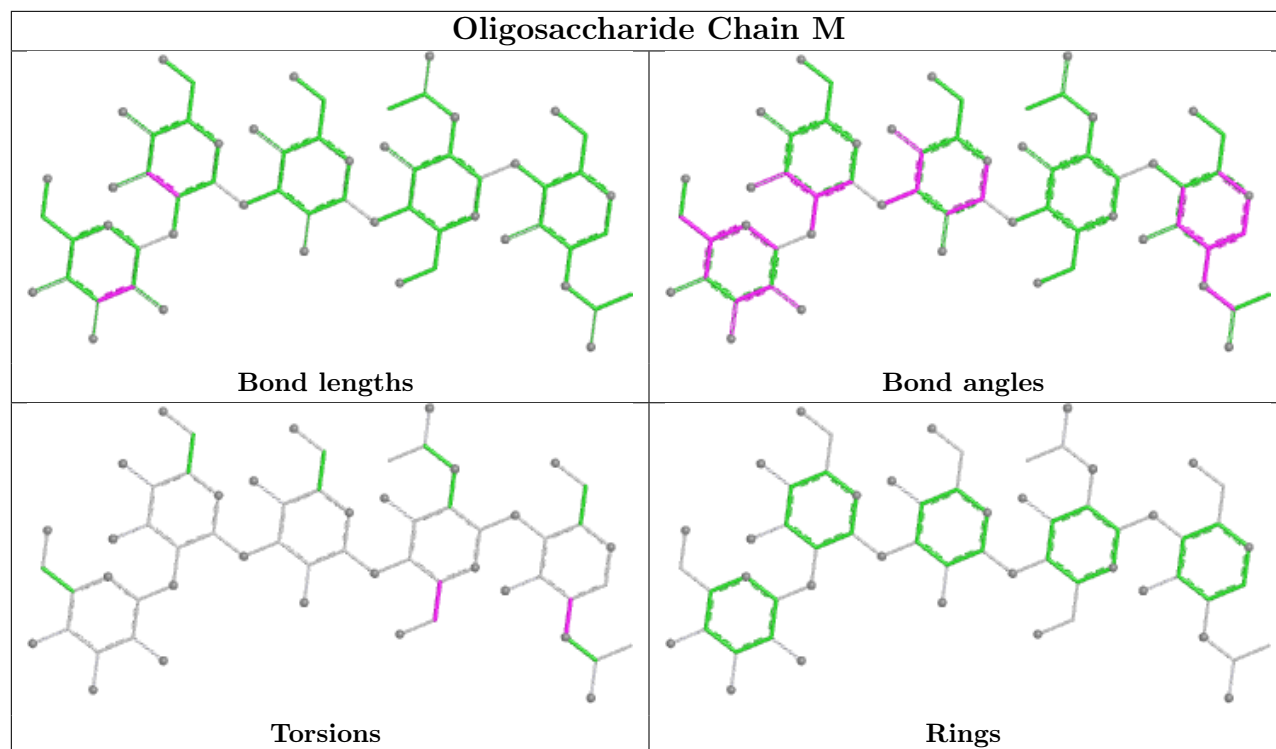
There are no ring outliers.

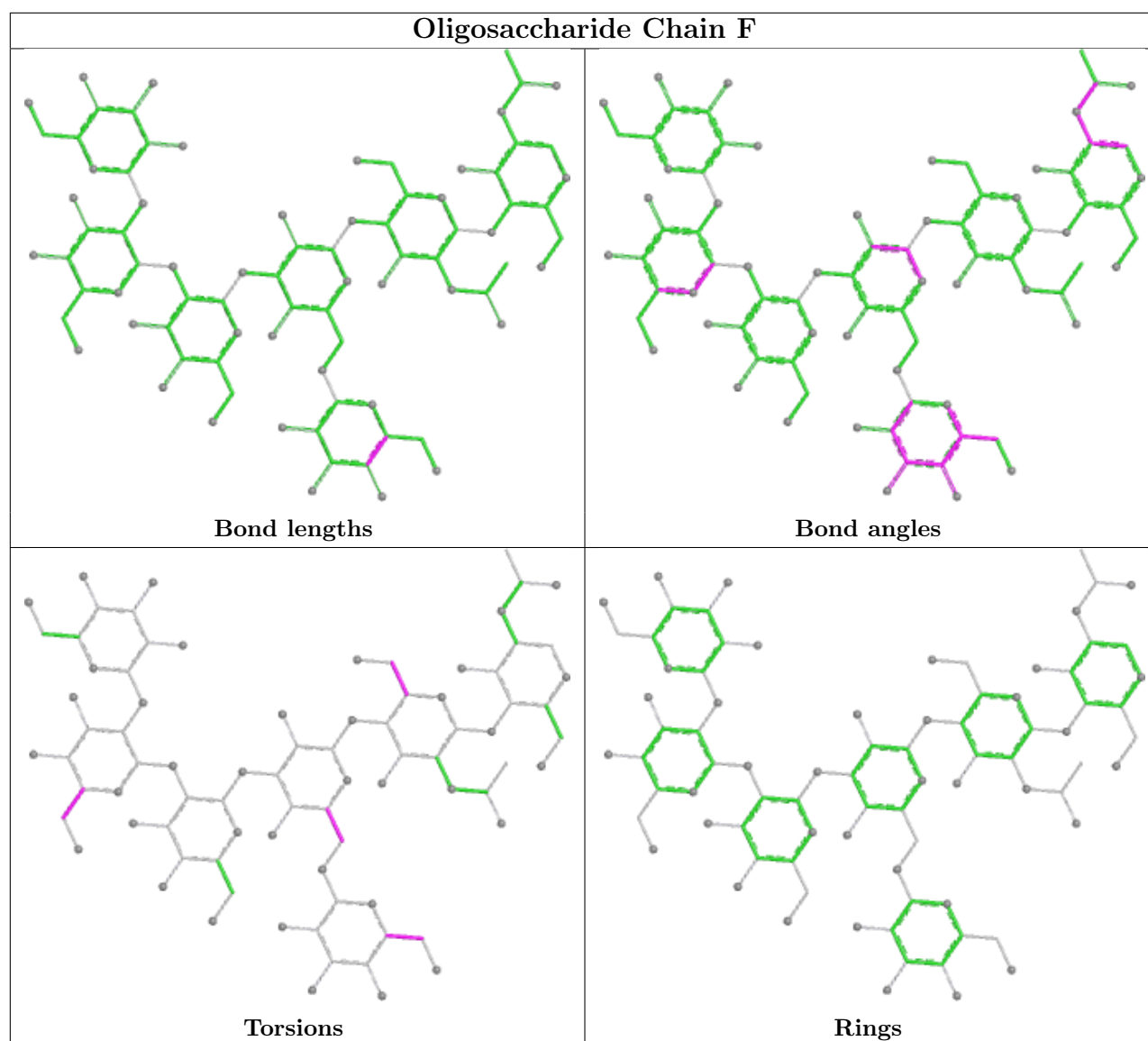
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	4	MAN	1	0
12	S	2	NAG	1	0
17	a	2	NAG	1	0
2	E	2	NAG	1	0

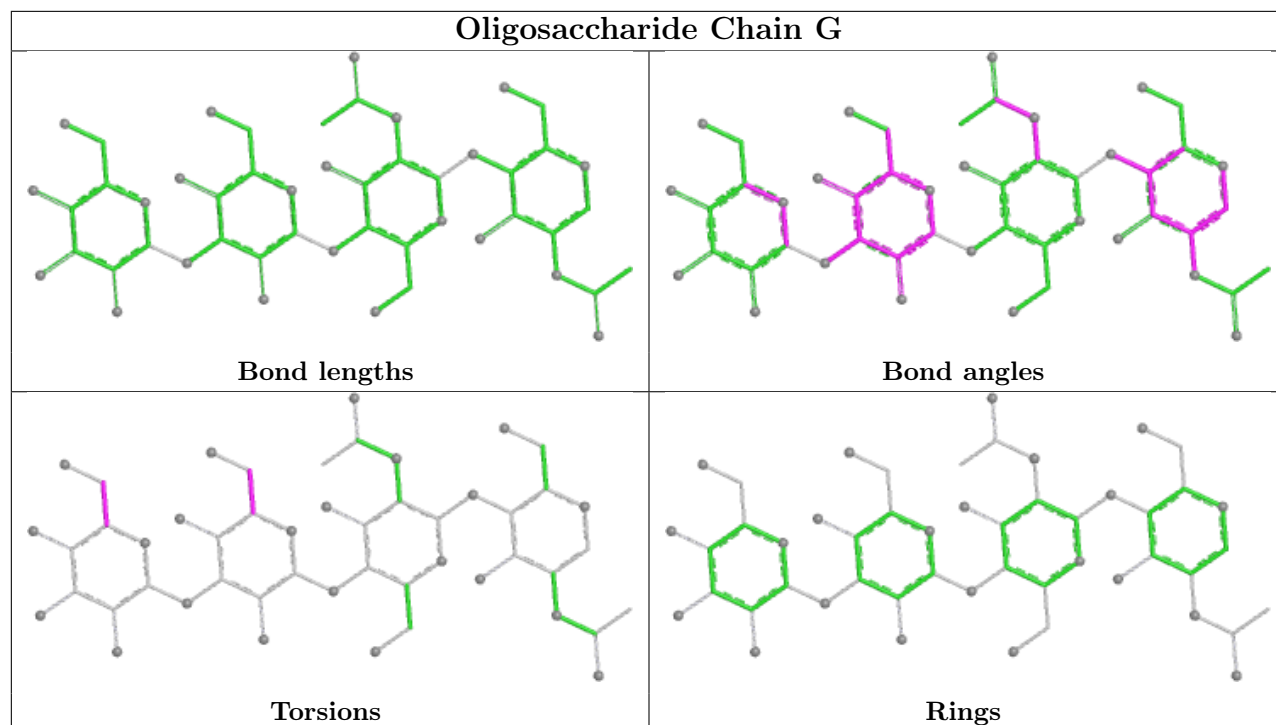
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



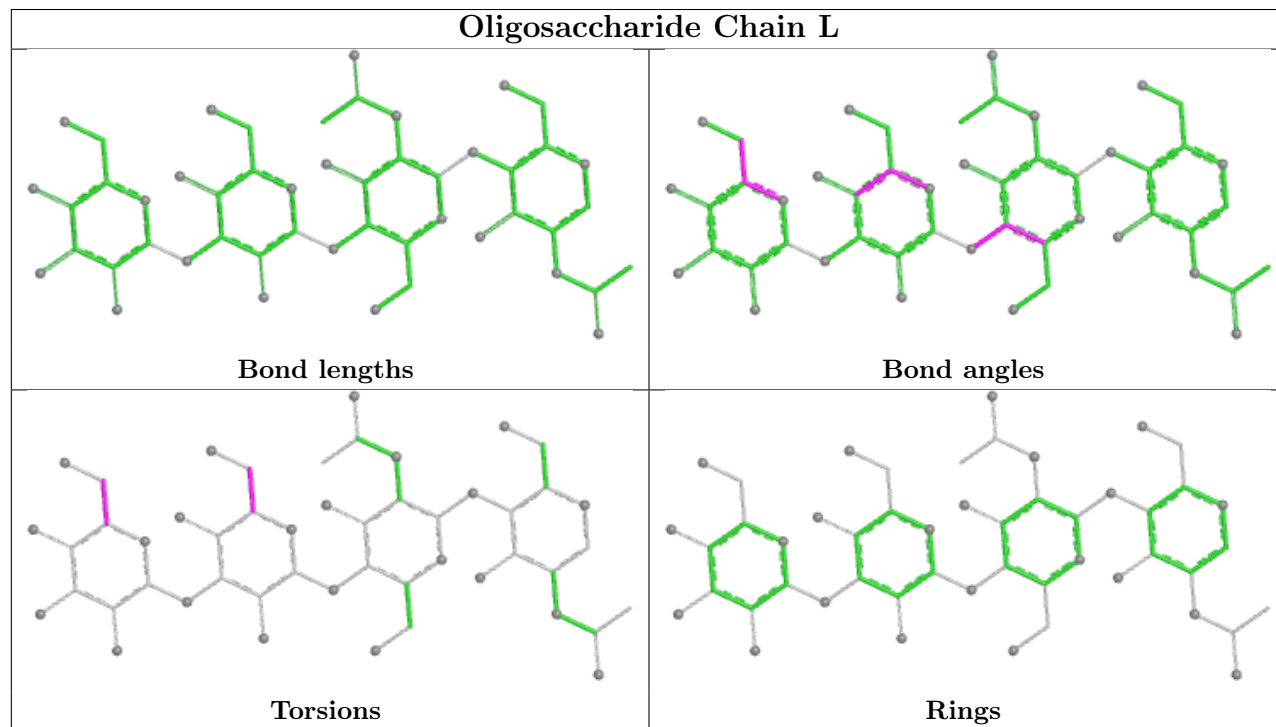


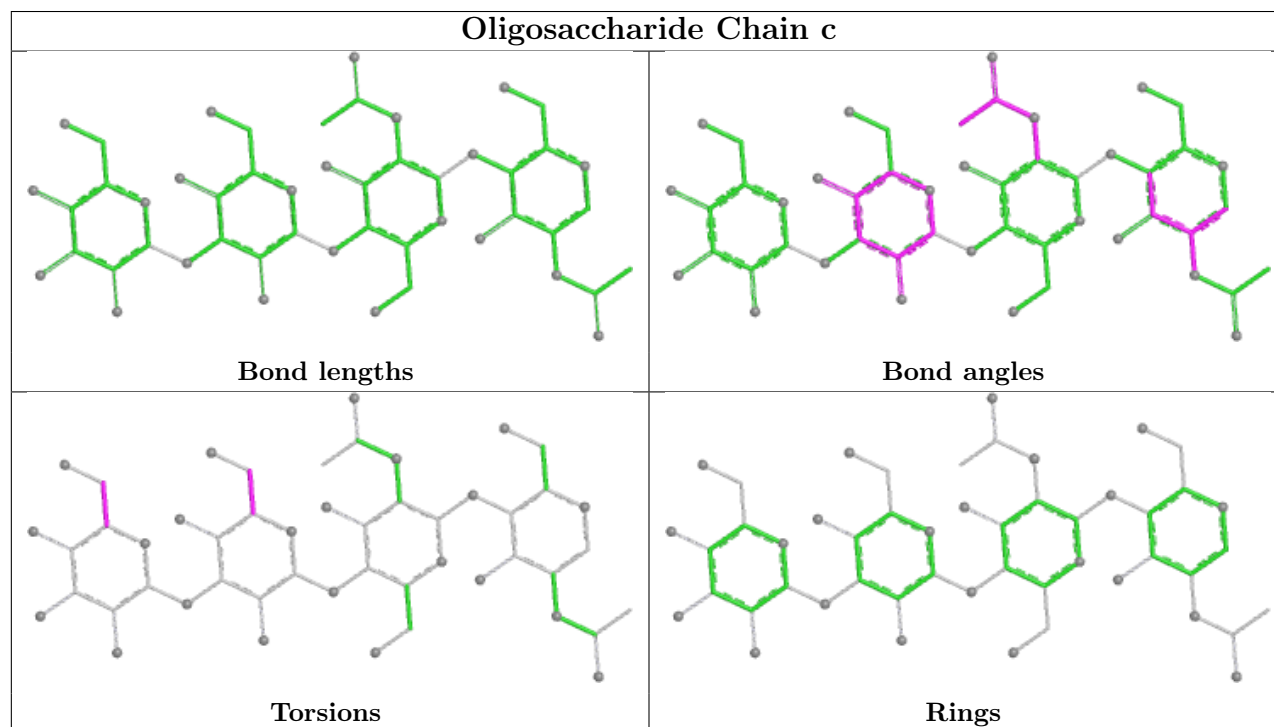
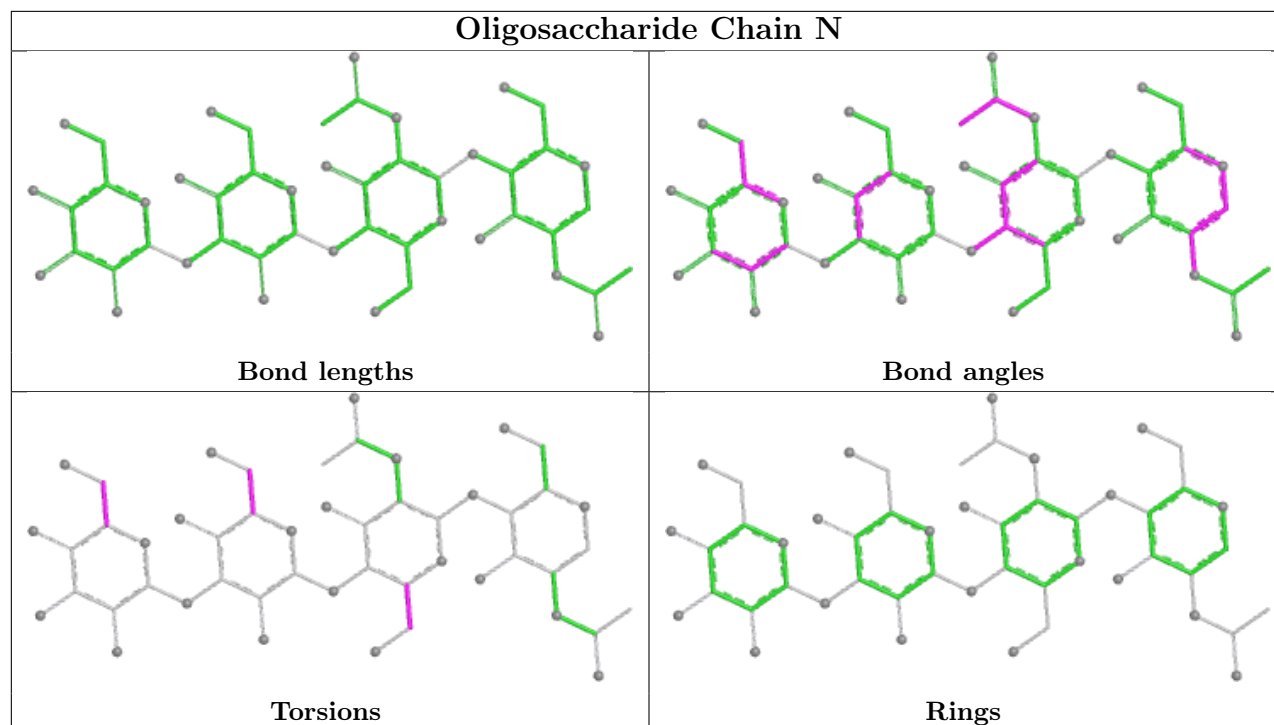


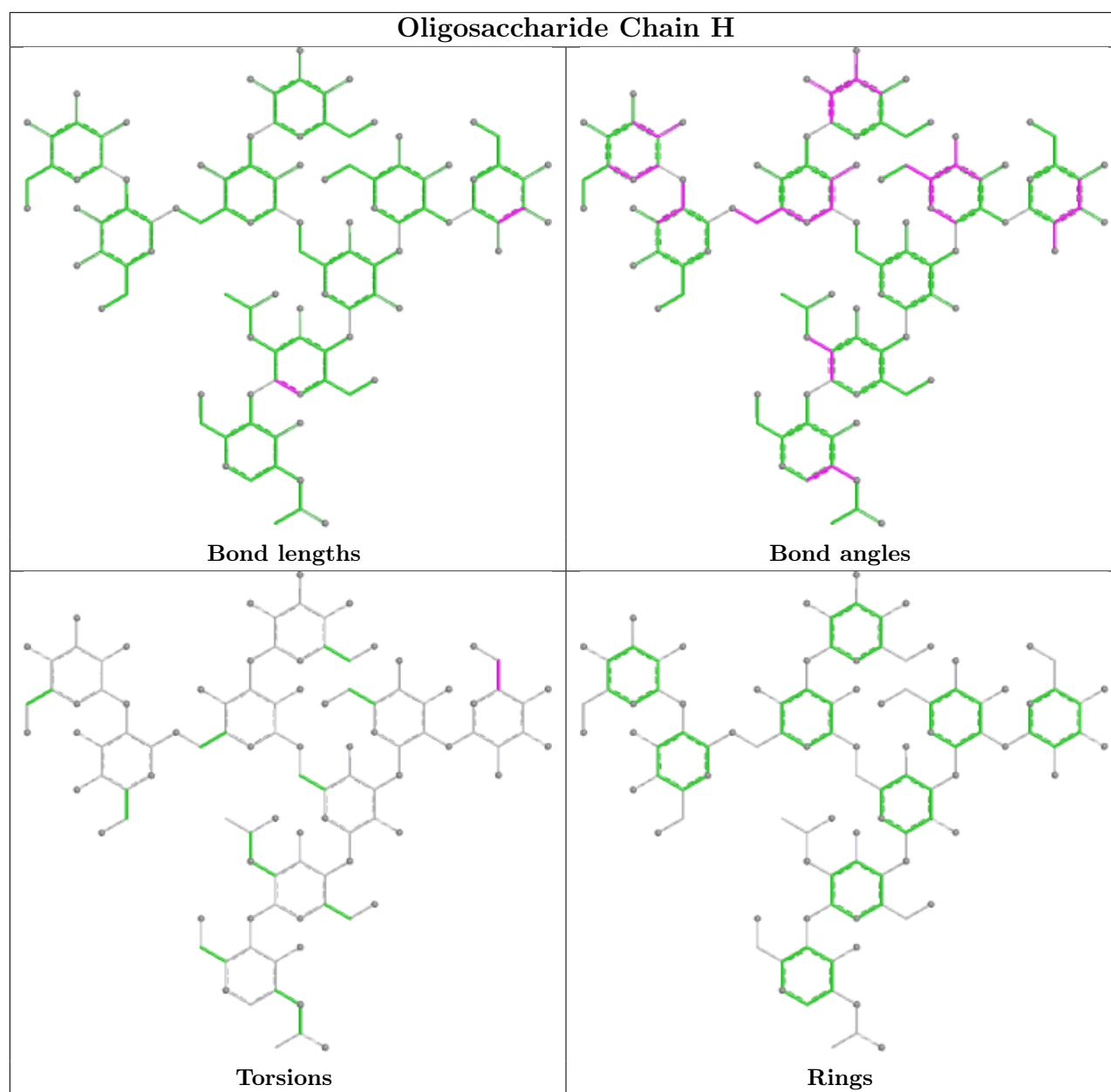
Oligosaccharide Chain G

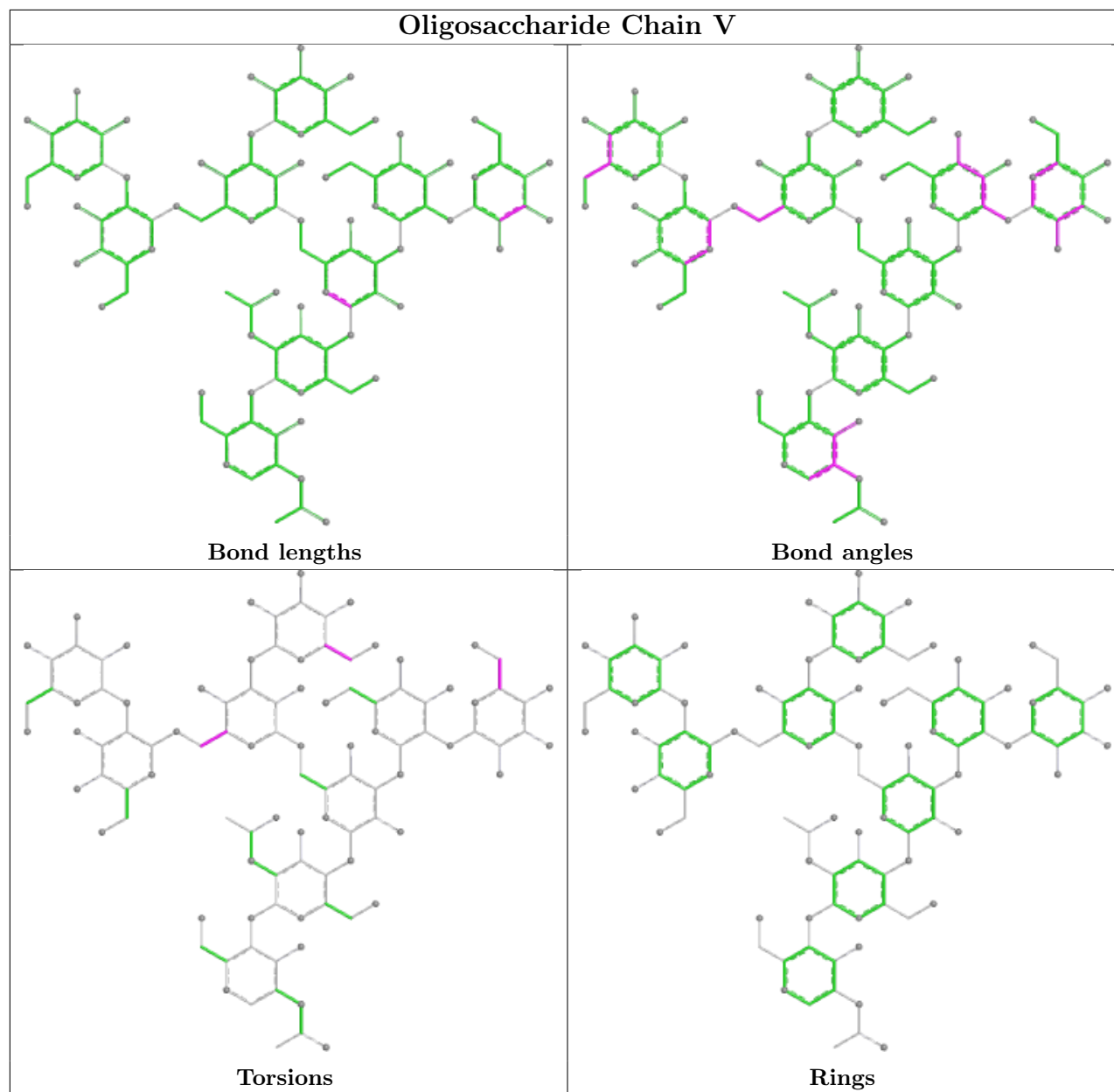


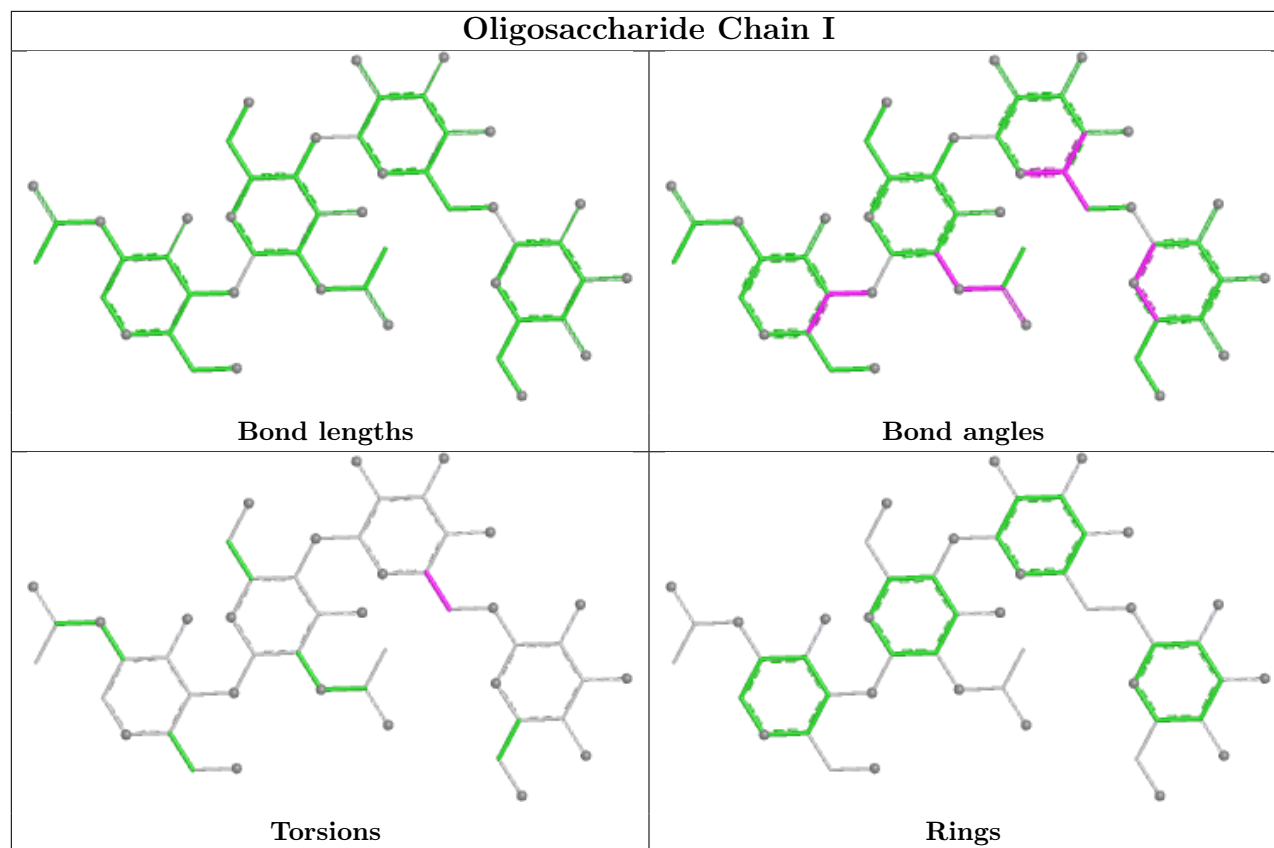
Oligosaccharide Chain L



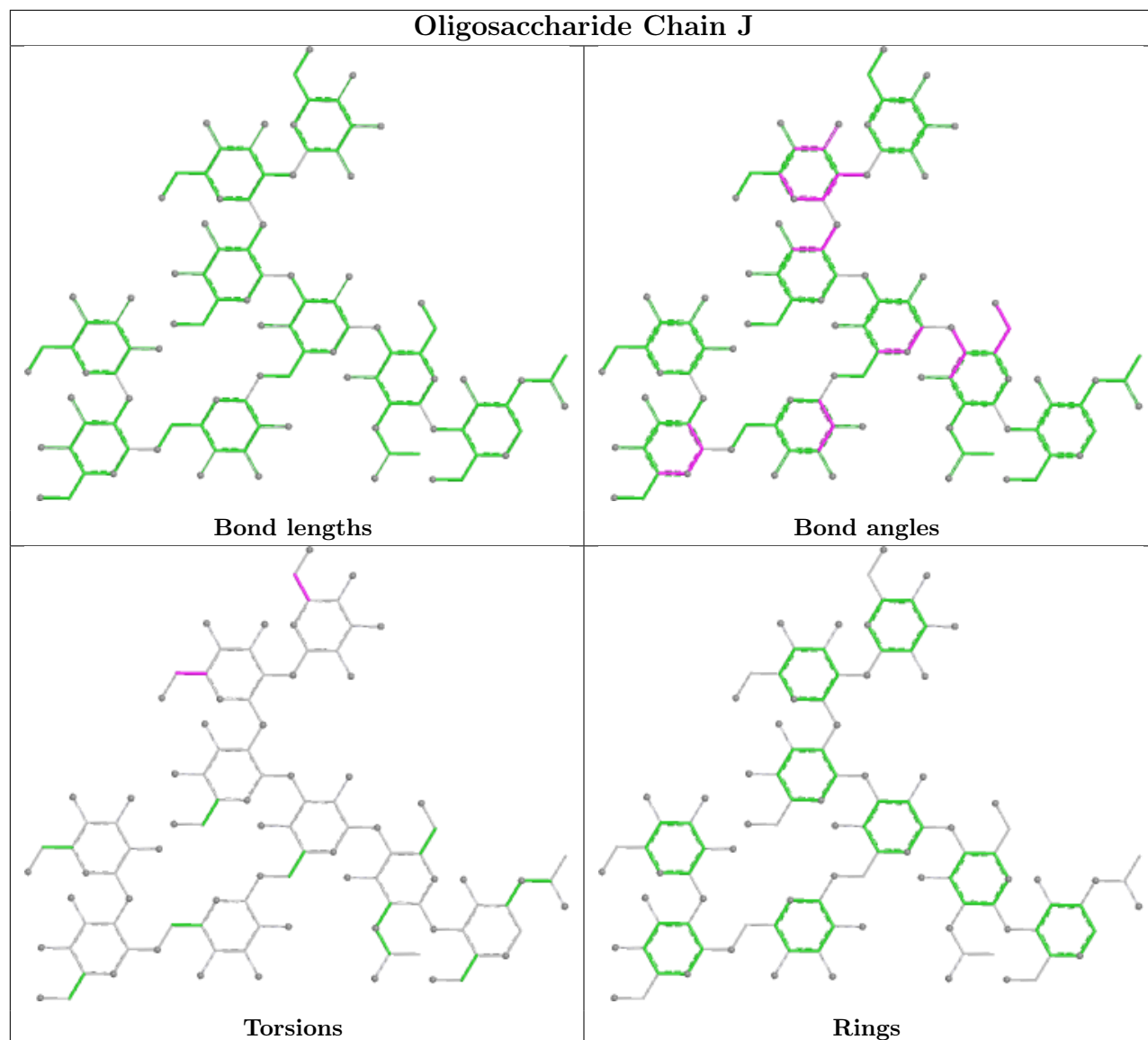


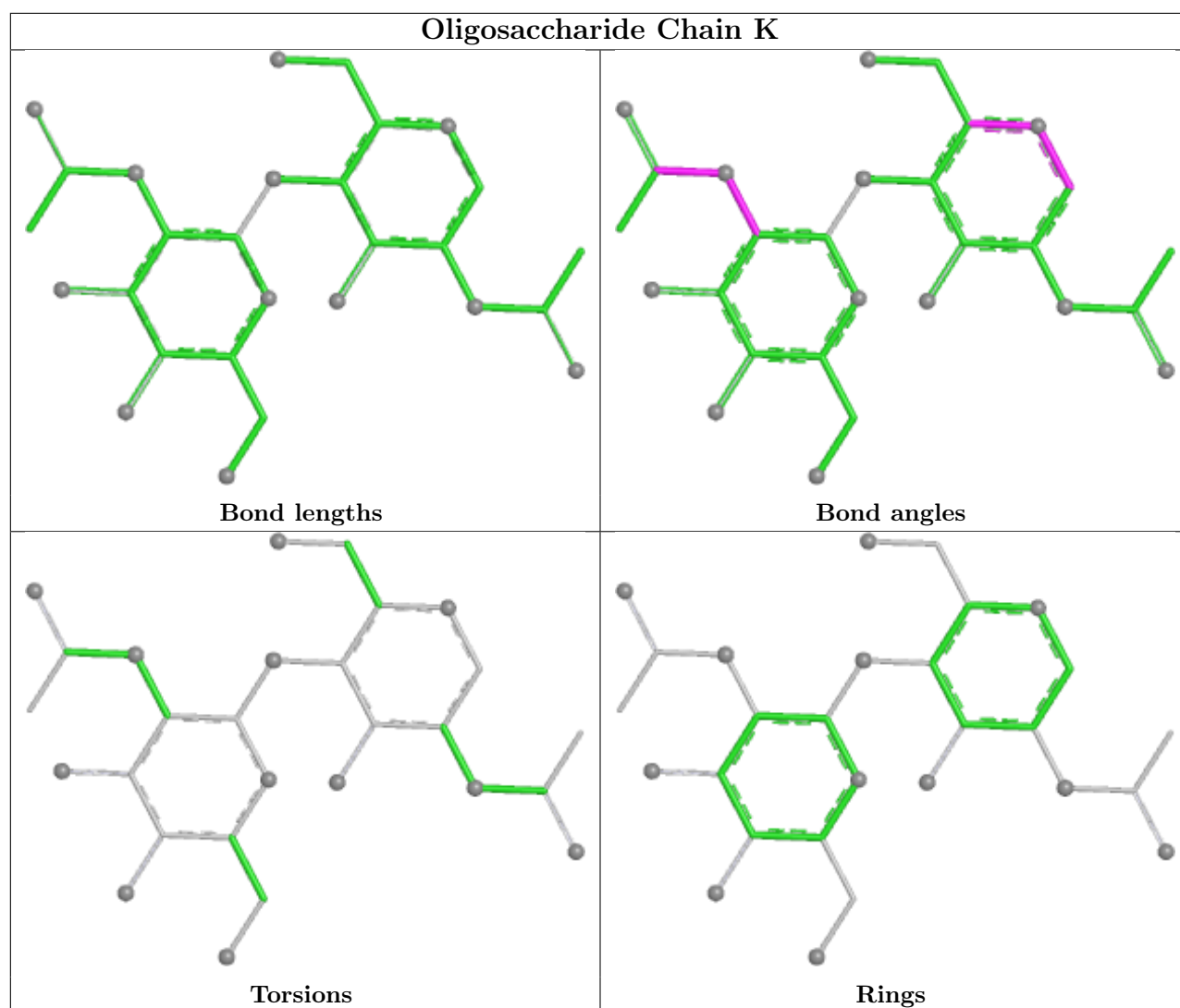


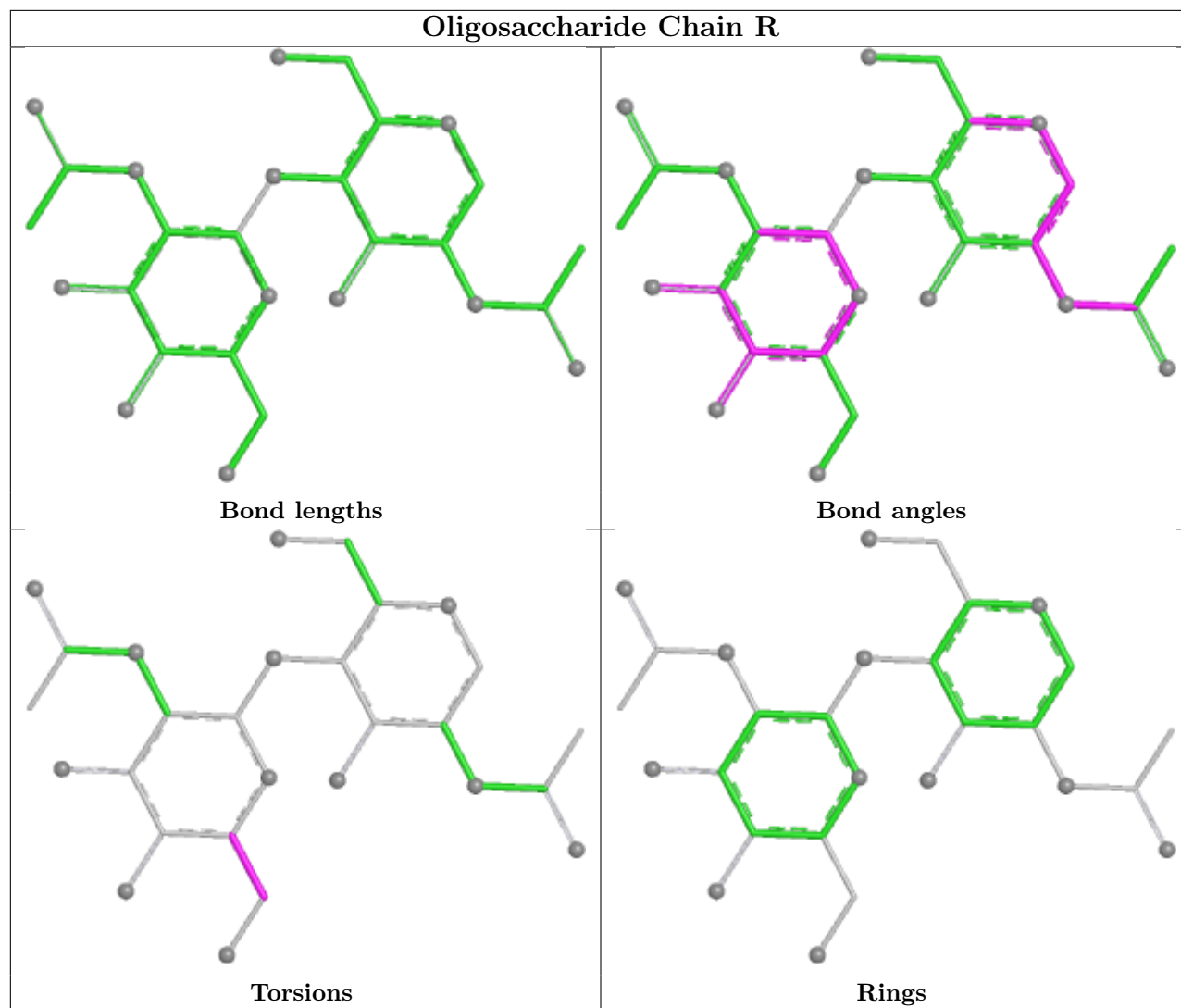


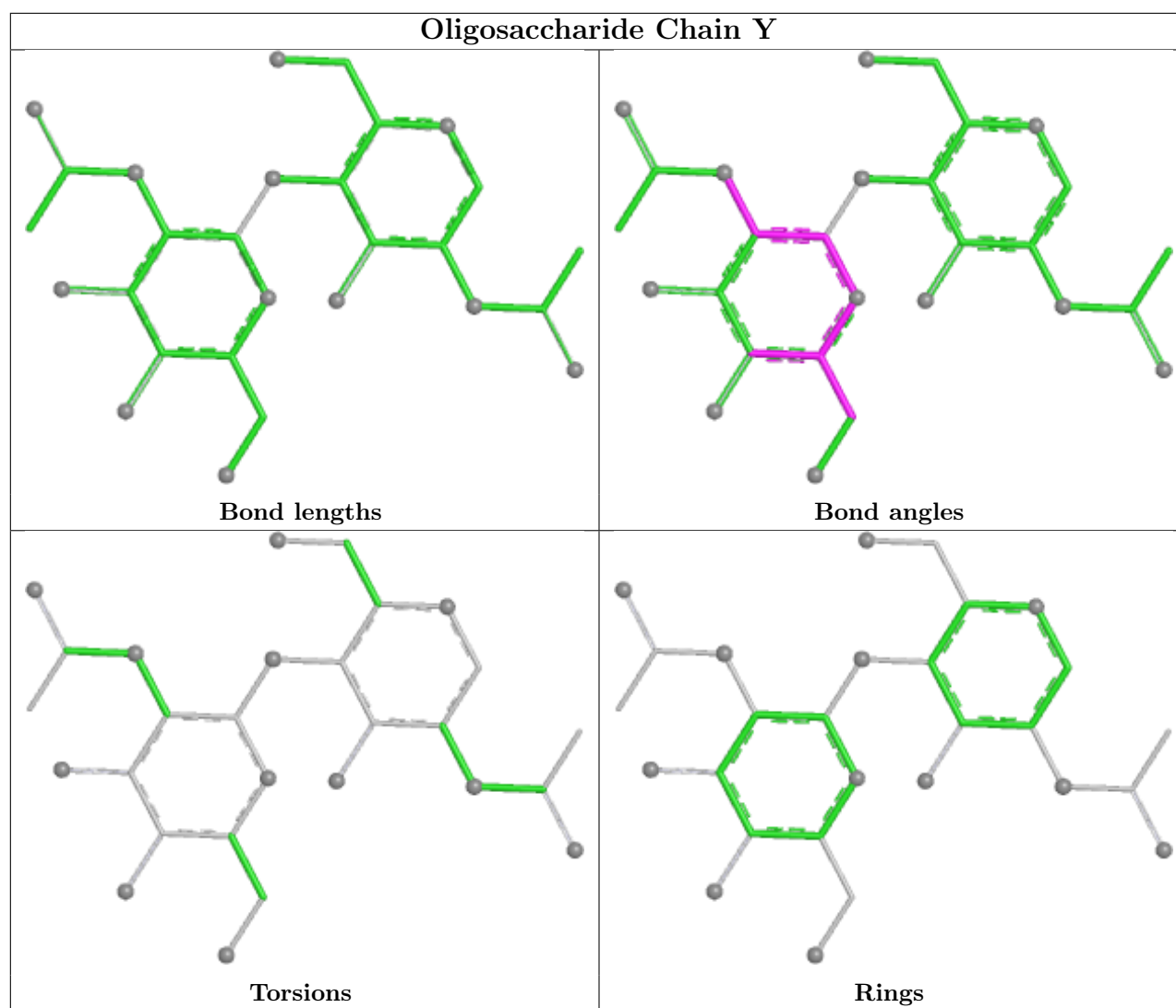


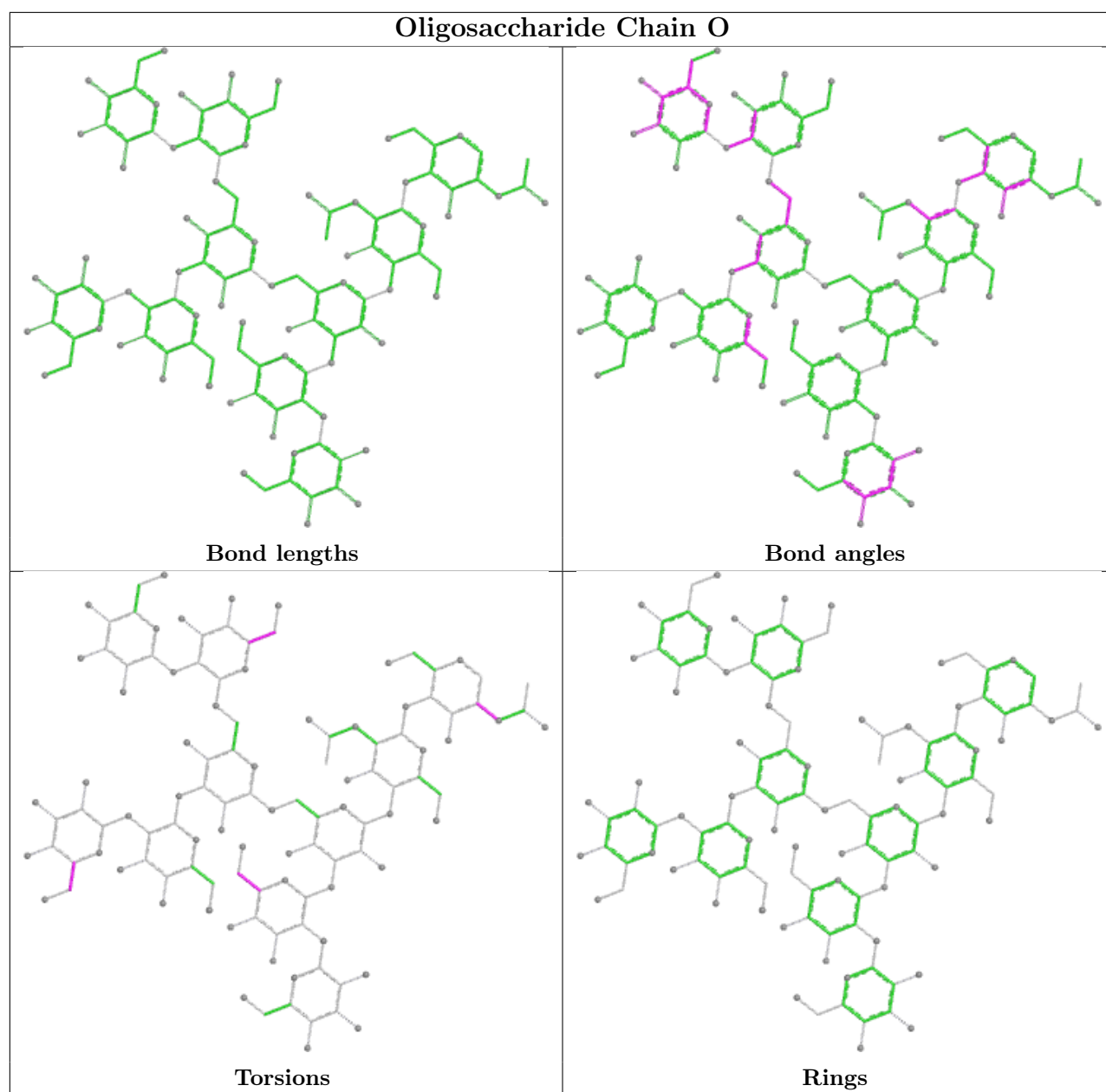
Oligosaccharide Chain J

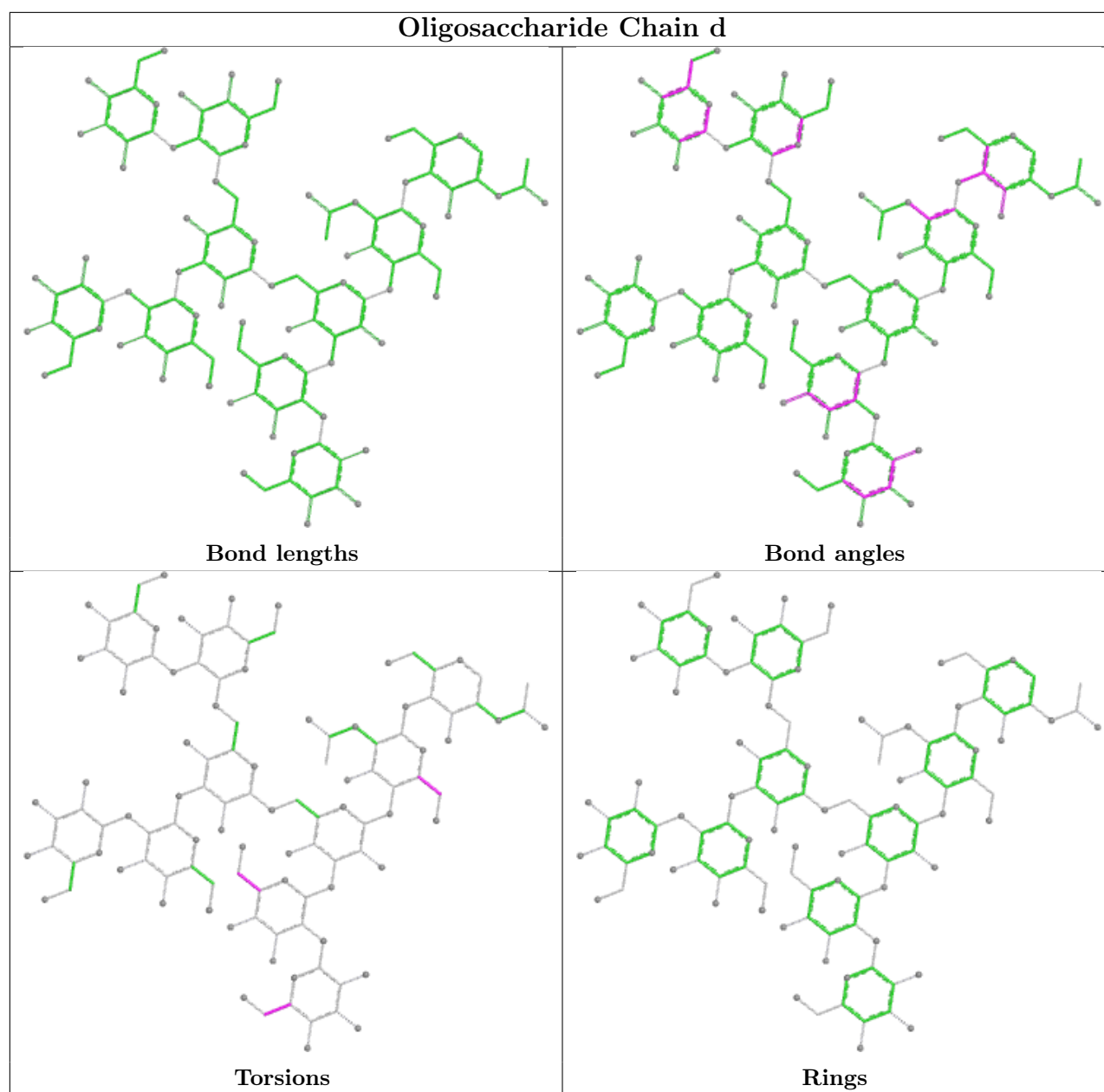


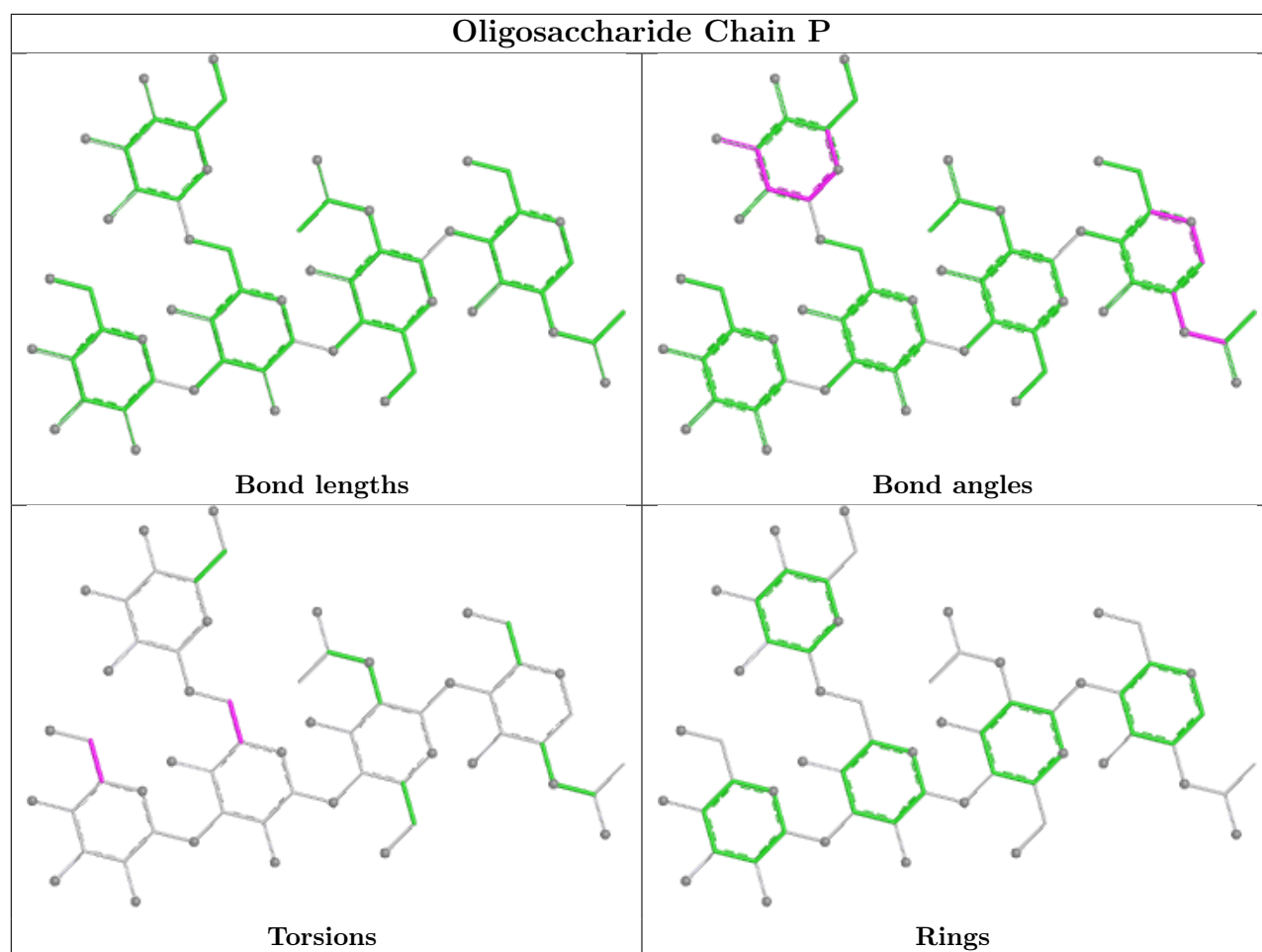


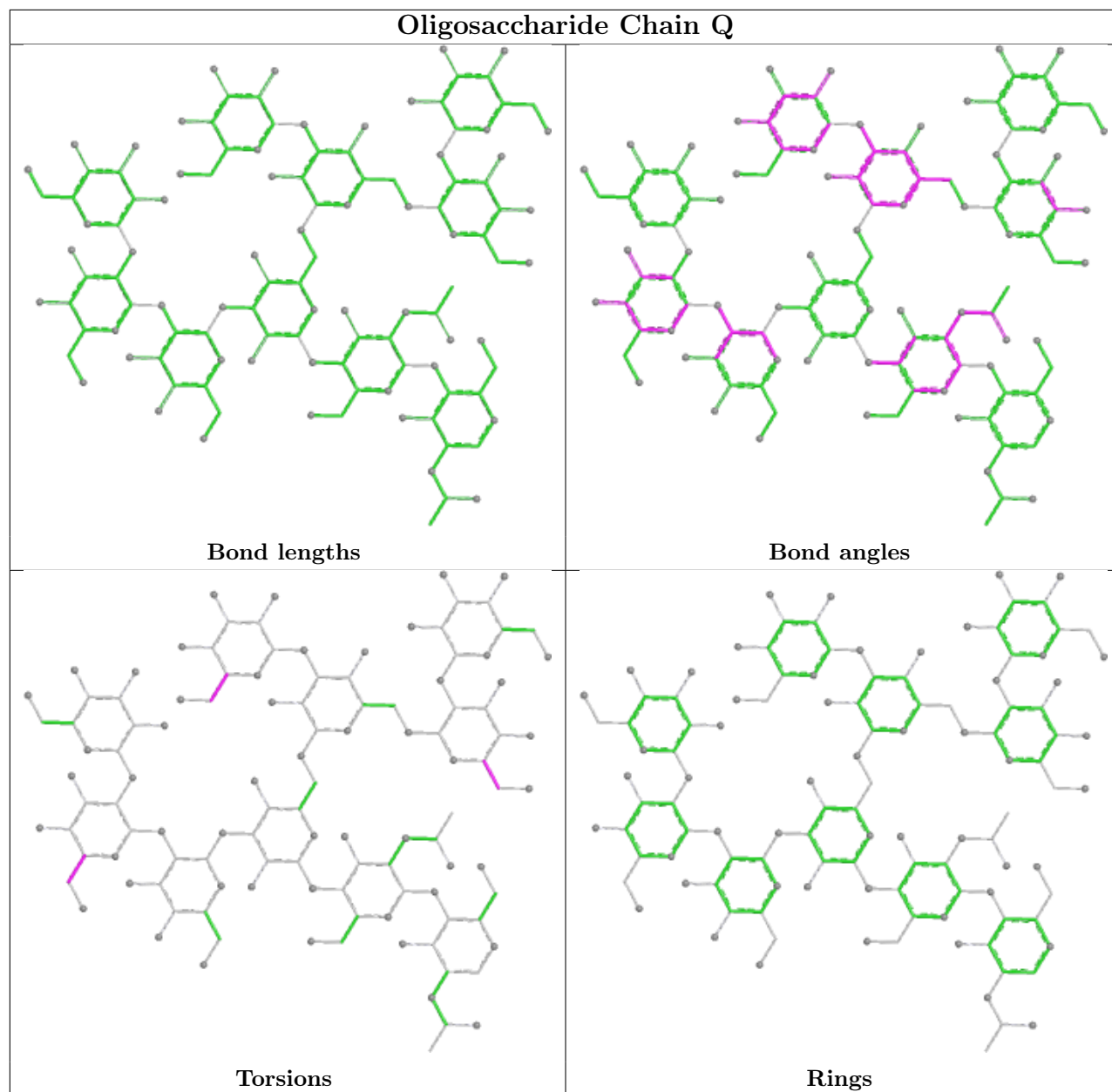


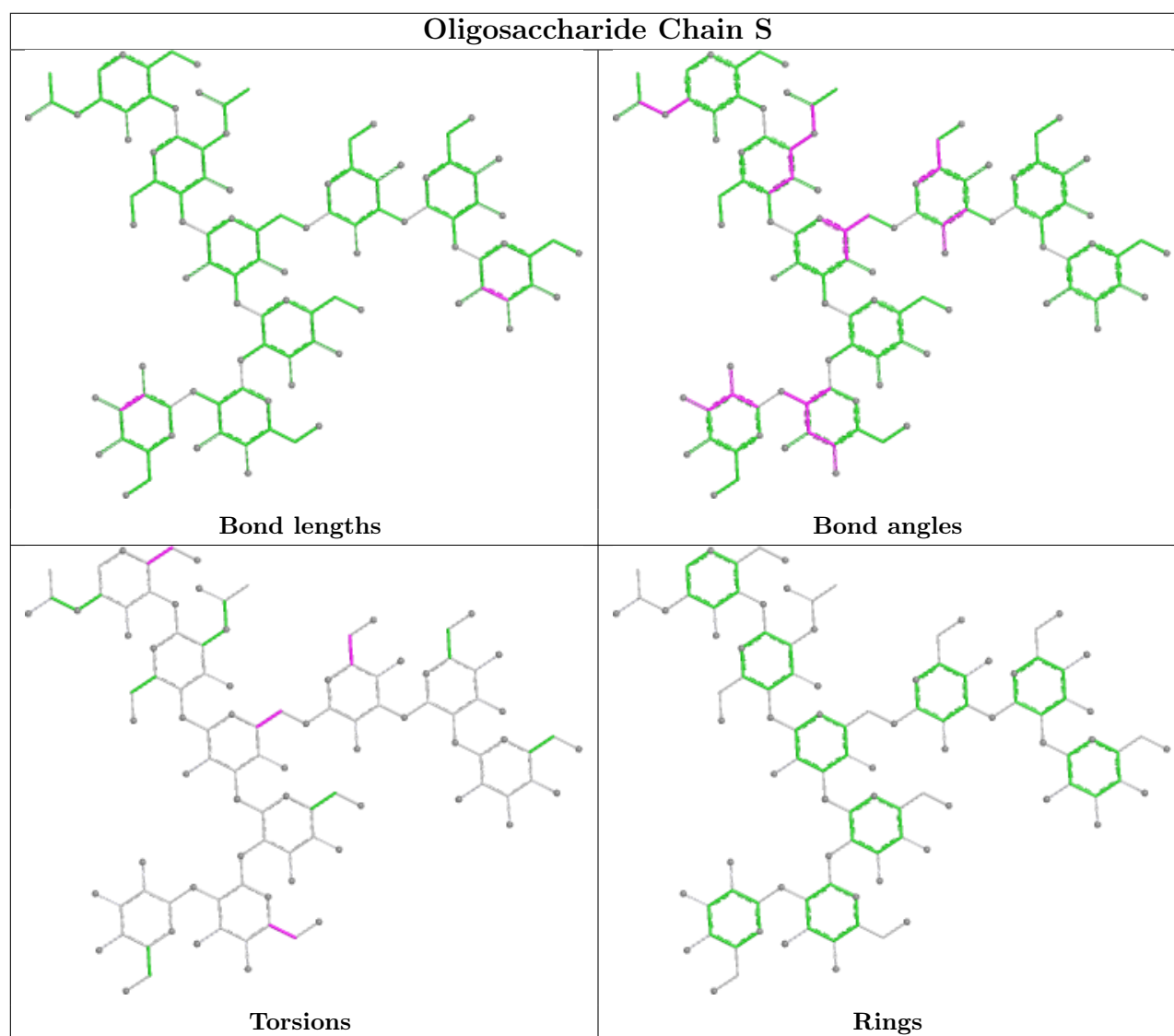




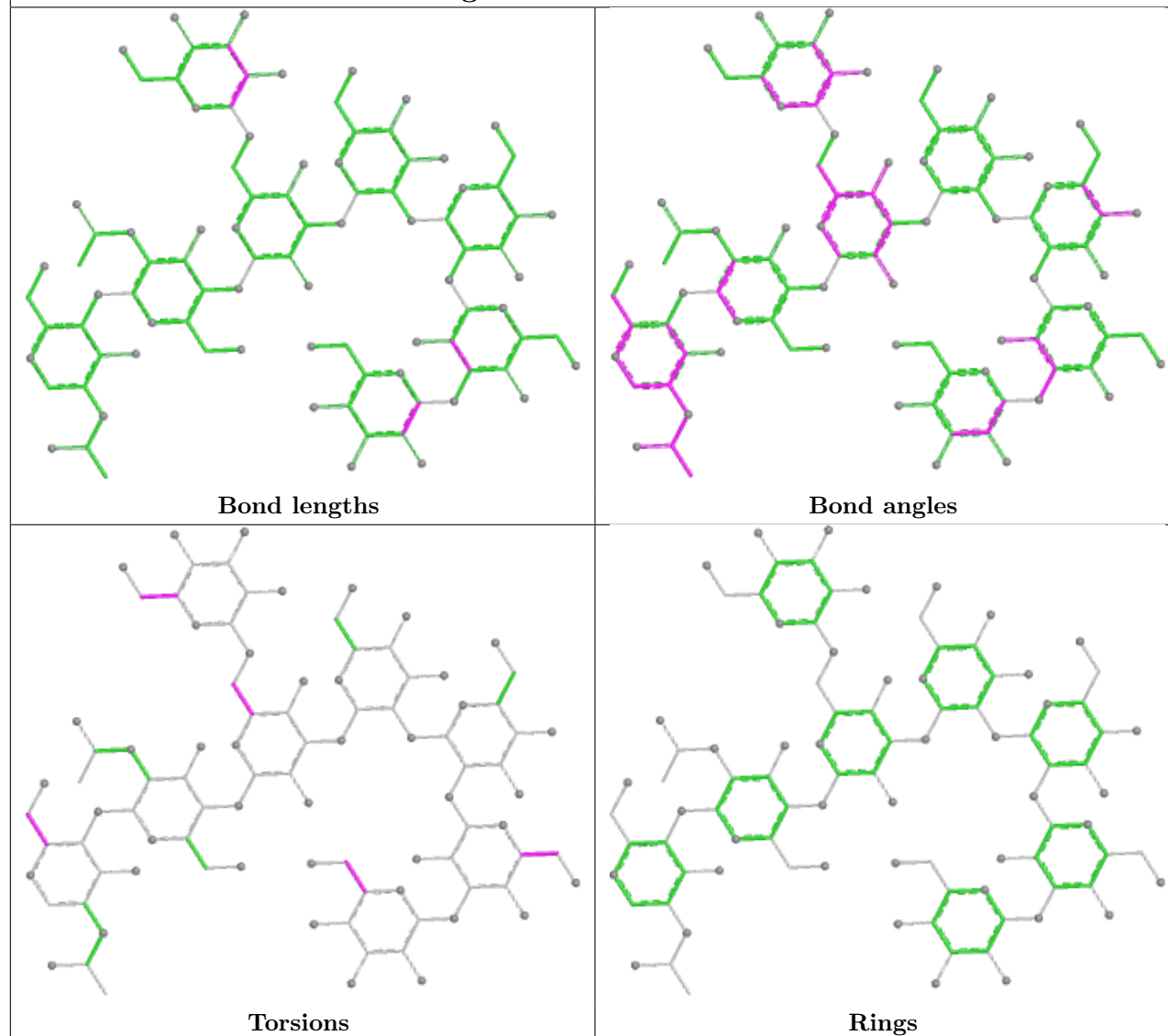


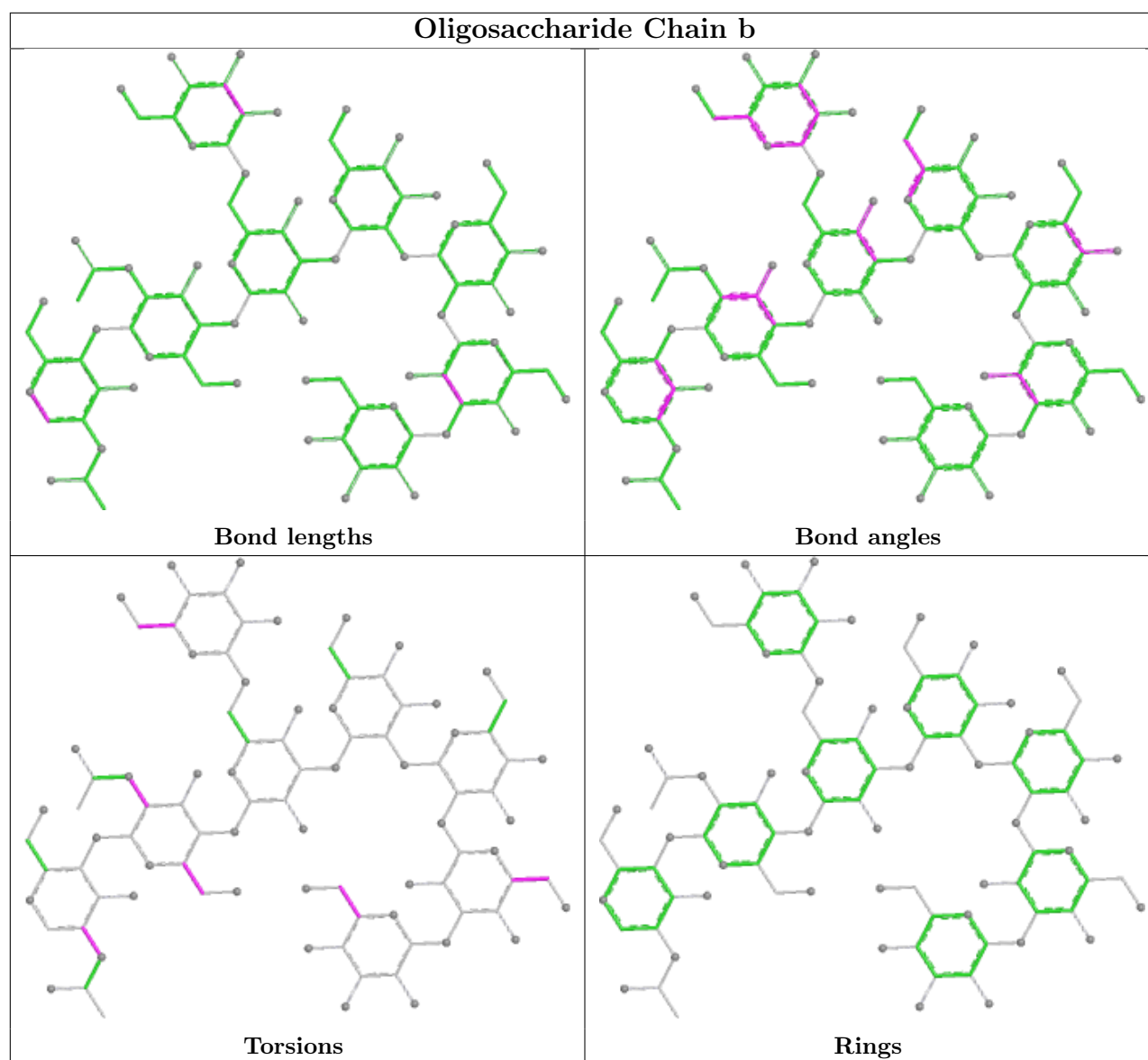




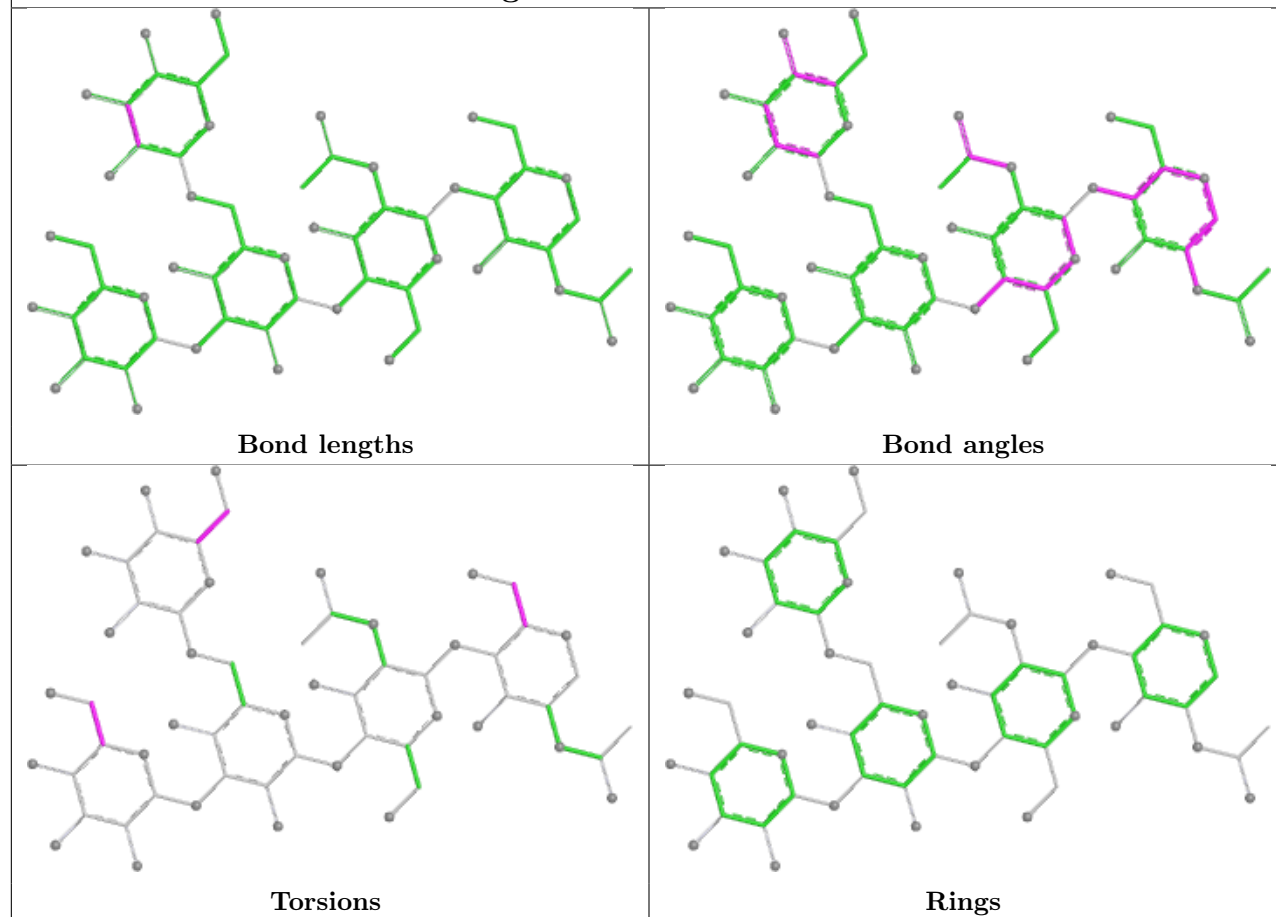


Oligosaccharide Chain T

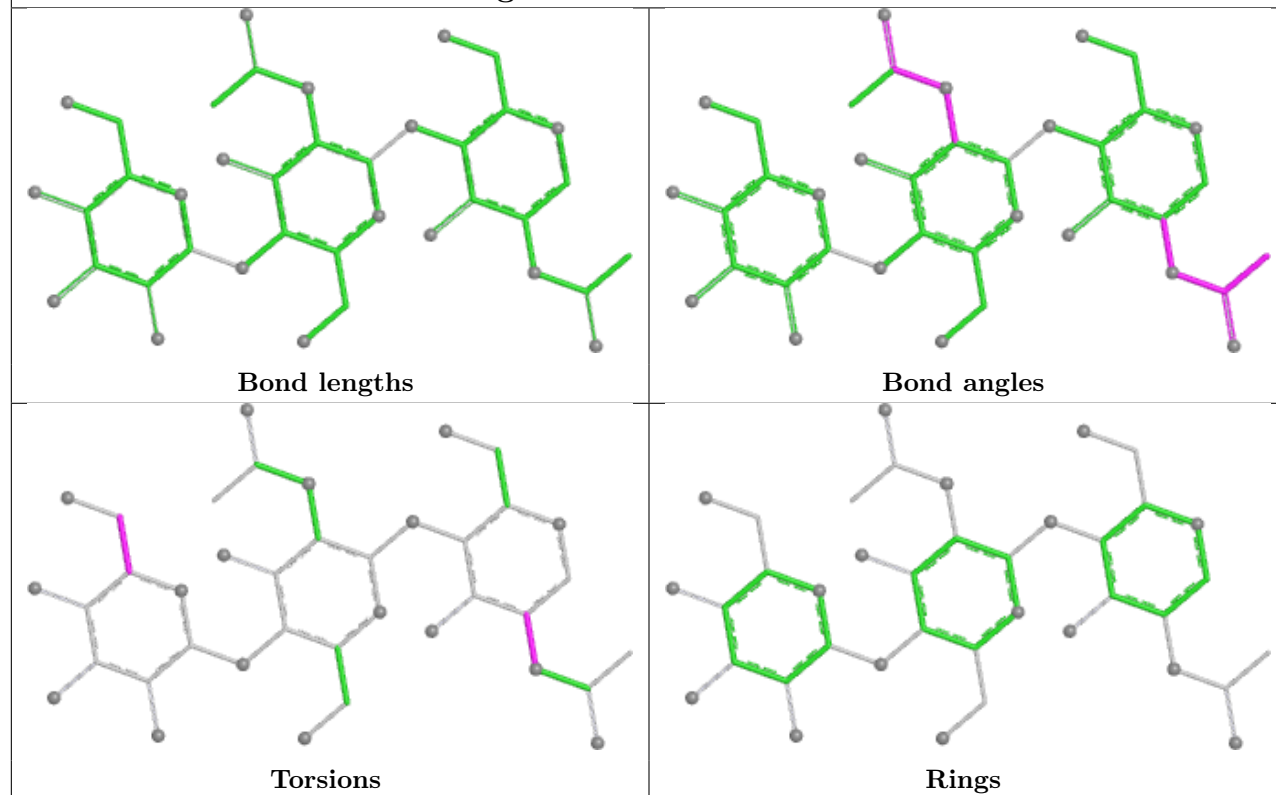


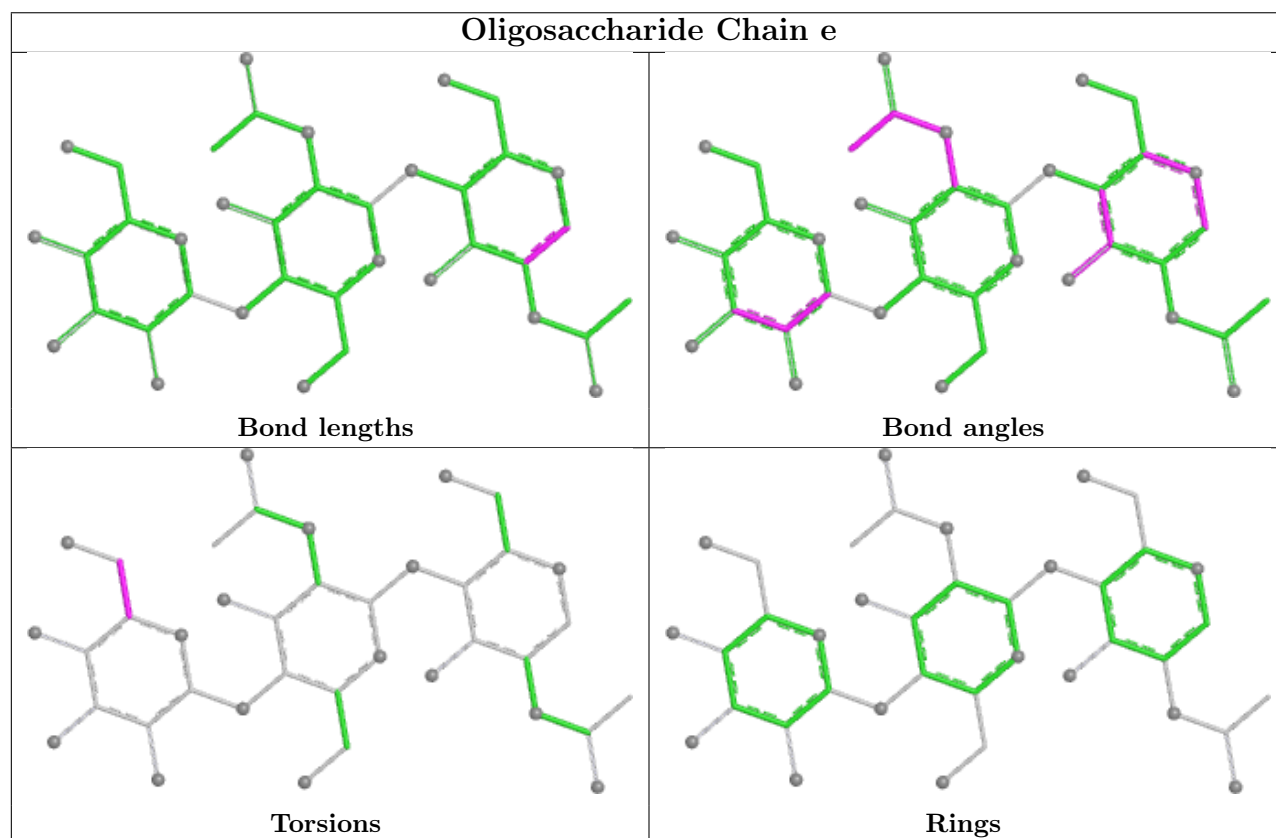
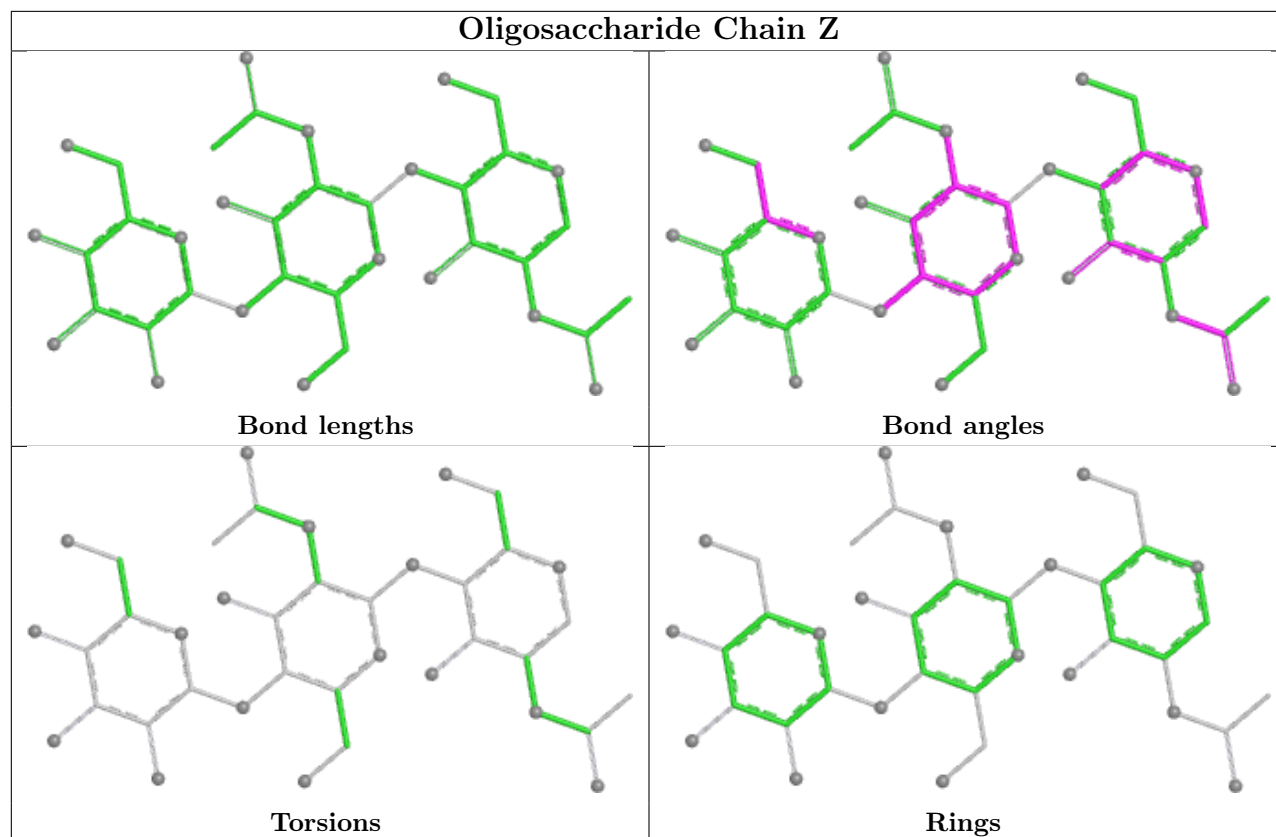


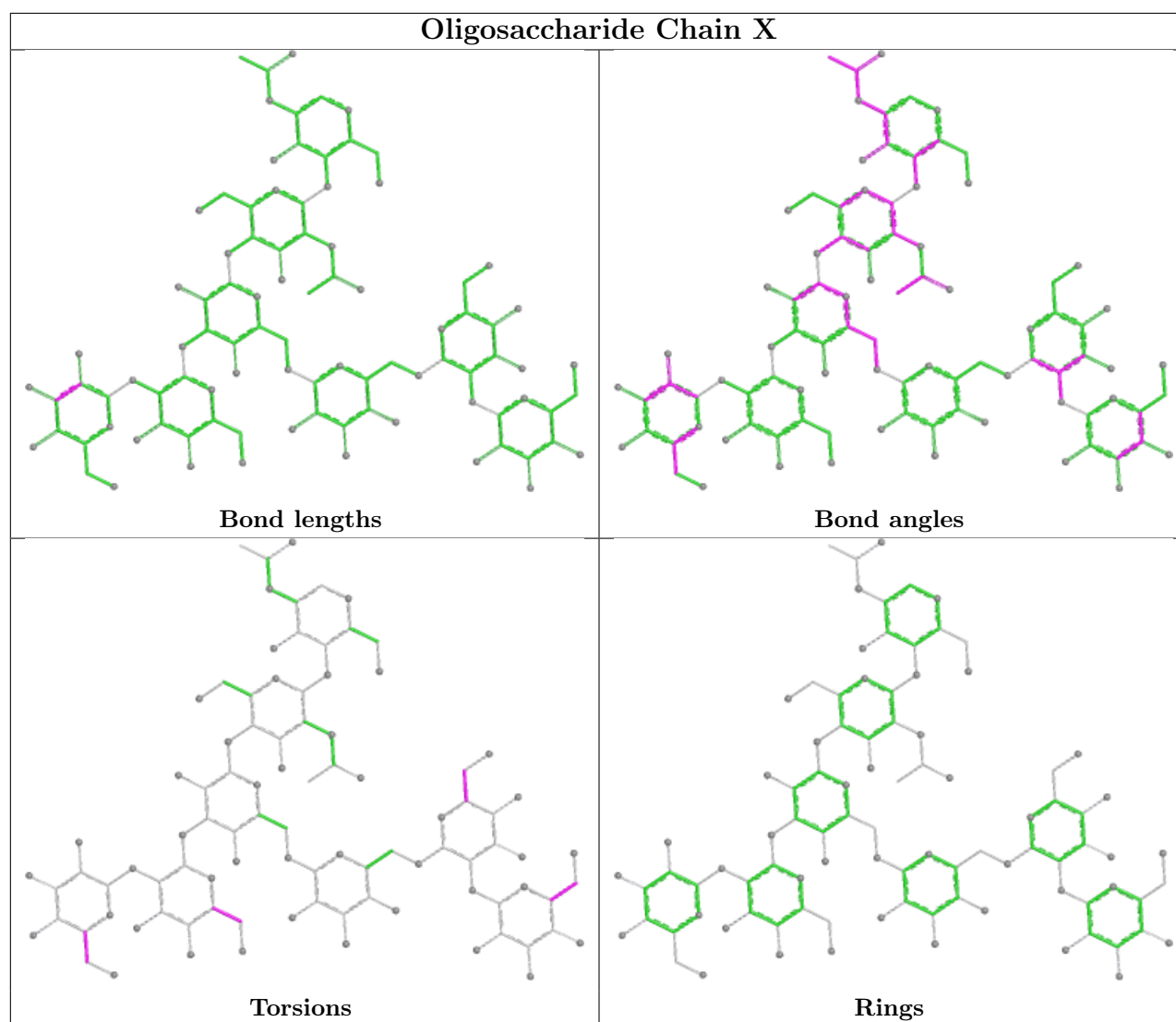
Oligosaccharide Chain U

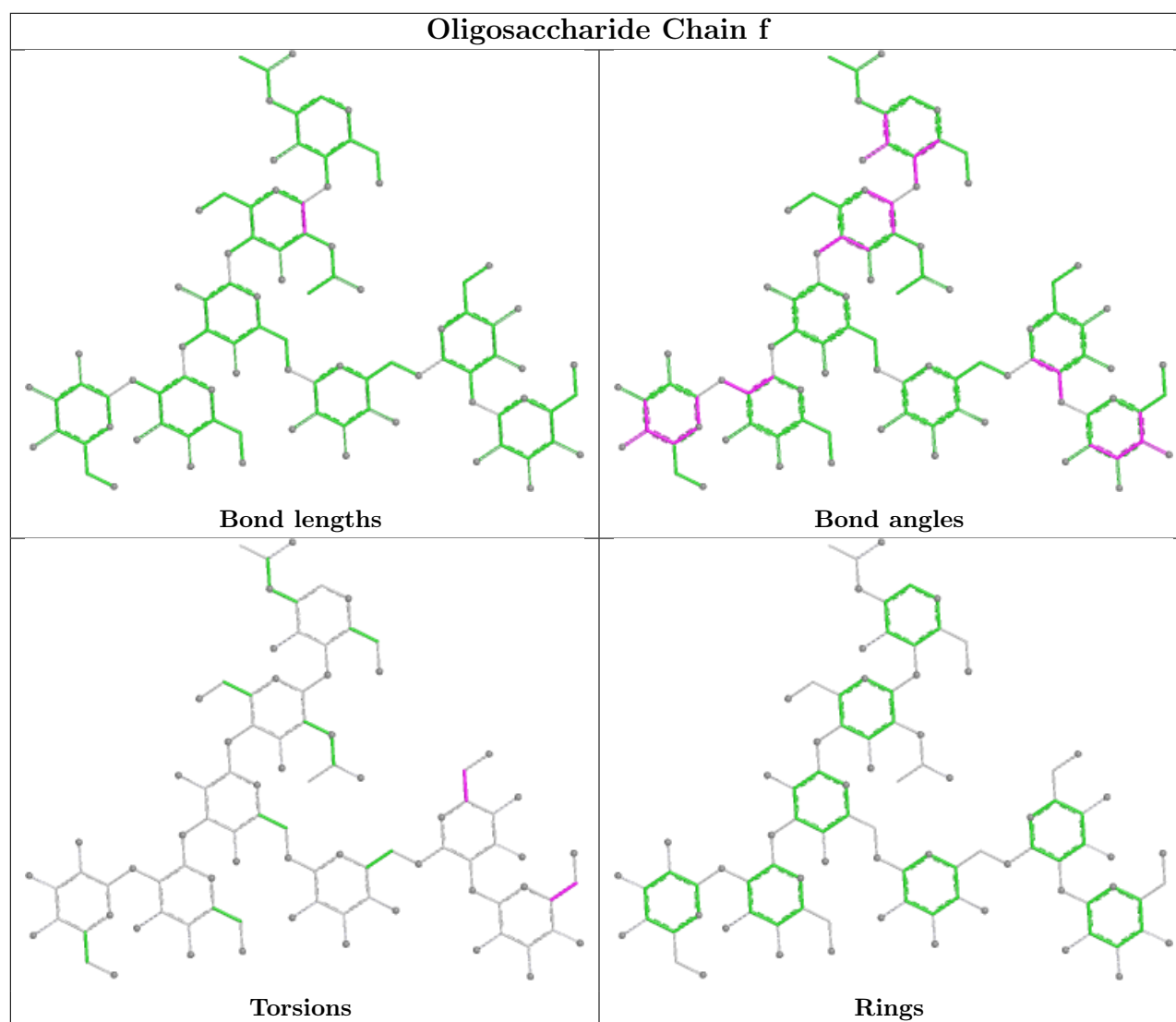


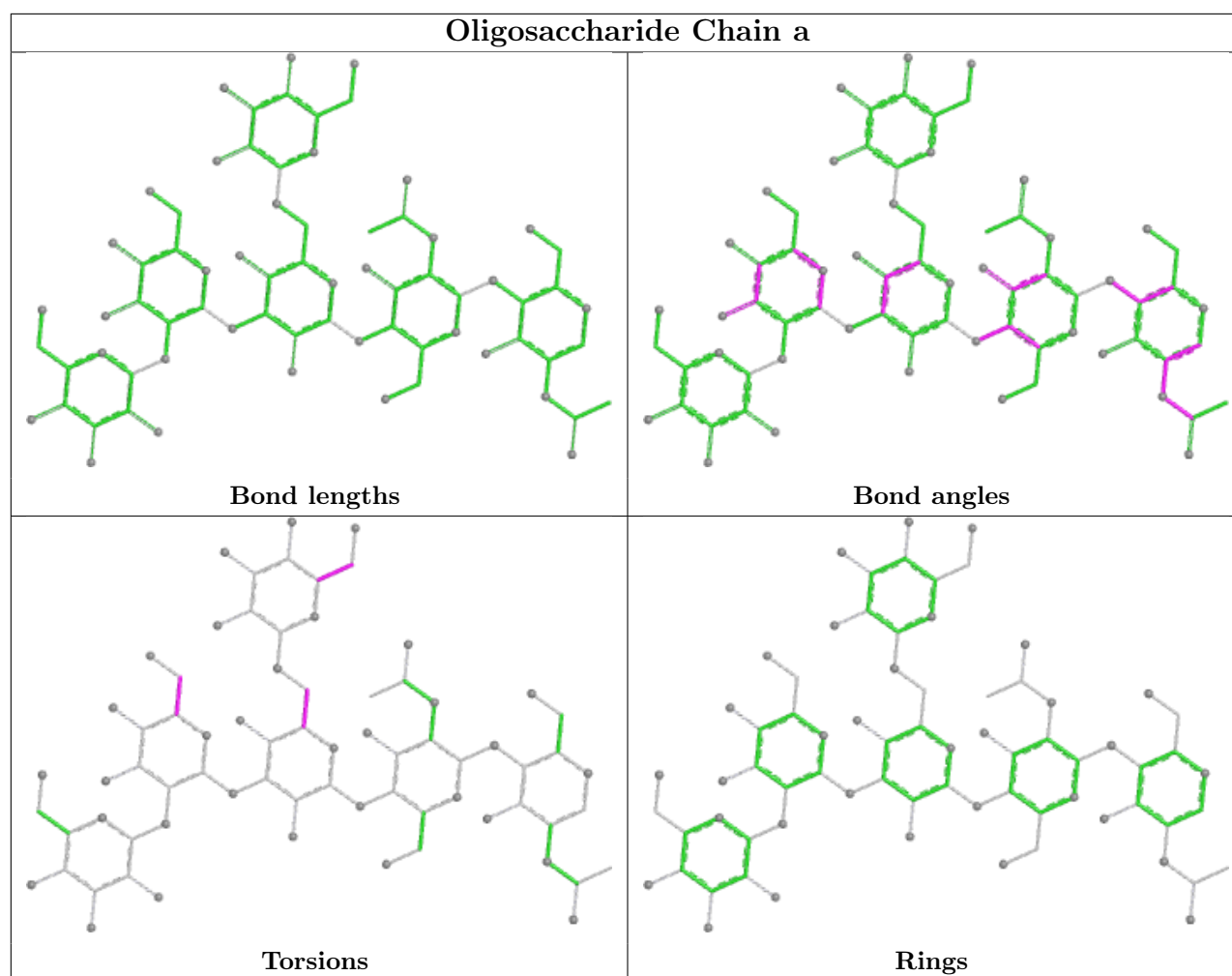
Oligosaccharide Chain W











5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	MAN	B	905	-	11,11,12	0.75	0	15,15,17	1.52	2 (13%)
18	NAG	D	942	1	14,14,15	1.02	1 (7%)	17,19,21	1.51	4 (23%)
19	BGC	D	945	-	12,12,12	0.84	0	17,17,17	1.23	3 (17%)
19	BGC	A	946	-	12,12,12	1.09	1 (8%)	17,17,17	1.14	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	NAG	C	935	1	14,14,15	0.80	0	17,19,21	1.33	4 (23%)
19	BGC	B	945	-	12,12,12	1.26	0	17,17,17	1.10	1 (5%)
18	NAG	A	945	1	14,14,15	0.74	0	17,19,21	1.44	3 (17%)
19	BGC	C	951	-	12,12,12	1.23	1 (8%)	17,17,17	1.40	2 (11%)
18	NAG	D	944	1	14,14,15	1.03	1 (7%)	17,19,21	1.89	5 (29%)
18	NAG	A	944	1	14,14,15	0.74	0	17,19,21	2.07	4 (23%)
18	NAG	C	944	1	14,14,15	0.93	0	17,19,21	2.06	6 (35%)
18	NAG	B	944	1	14,14,15	0.39	0	17,19,21	1.23	3 (17%)
18	NAG	D	941	1	14,14,15	0.55	0	17,19,21	1.20	1 (5%)
18	NAG	A	941	1	14,14,15	0.58	0	17,19,21	1.56	3 (17%)
18	NAG	C	950	1	14,14,15	0.70	0	17,19,21	1.02	2 (11%)
18	NAG	D	940	1	14,14,15	0.75	0	17,19,21	1.38	2 (11%)
18	NAG	B	943	1	14,14,15	0.58	0	17,19,21	1.20	1 (5%)
18	NAG	A	930	1	14,14,15	0.71	0	17,19,21	1.62	4 (23%)
18	NAG	A	940	1	14,14,15	0.88	0	17,19,21	1.32	1 (5%)
18	NAG	B	940	1	14,14,15	0.95	0	17,19,21	1.56	4 (23%)
18	NAG	D	943	1	14,14,15	0.58	0	17,19,21	1.67	4 (23%)

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
20	MAN	B	905	-	-	2/2/19/22	0/1/1/1
18	NAG	D	942	1	-	1/6/23/26	0/1/1/1
19	BGC	D	945	-	-	2/2/22/22	0/1/1/1
19	BGC	A	946	-	-	2/2/22/22	0/1/1/1
18	NAG	C	935	1	-	0/6/23/26	0/1/1/1
19	BGC	B	945	-	-	2/2/22/22	0/1/1/1
18	NAG	A	945	1	-	0/6/23/26	0/1/1/1
19	BGC	C	951	-	-	1/2/22/22	0/1/1/1
18	NAG	D	944	1	-	0/6/23/26	0/1/1/1
18	NAG	A	944	1	-	0/6/23/26	0/1/1/1
18	NAG	C	944	1	-	0/6/23/26	0/1/1/1
18	NAG	B	944	1	-	0/6/23/26	0/1/1/1
18	NAG	D	941	1	-	1/6/23/26	0/1/1/1
18	NAG	A	941	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	NAG	C	950	1	-	1/6/23/26	0/1/1/1
18	NAG	D	940	1	-	0/6/23/26	0/1/1/1
18	NAG	B	943	1	-	1/6/23/26	0/1/1/1
18	NAG	A	930	1	-	0/6/23/26	0/1/1/1
18	NAG	A	940	1	-	0/6/23/26	0/1/1/1
18	NAG	B	940	1	-	2/6/23/26	0/1/1/1
18	NAG	D	943	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	944	NAG	C1-C2	3.09	1.56	1.52
19	C	951	BGC	C1-C2	2.47	1.58	1.52
19	A	946	BGC	C1-C2	2.30	1.57	1.52
18	D	942	NAG	C3-C2	2.15	1.57	1.52

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	944	NAG	C1-O5-C5	4.77	118.58	112.19
18	D	944	NAG	C1-O5-C5	4.43	118.12	112.19
18	A	944	NAG	C1-C2-N2	-4.40	103.50	110.43
18	A	930	NAG	C1-C2-N2	3.97	116.69	110.43
18	A	944	NAG	O5-C1-C2	-3.92	105.23	111.29
18	C	944	NAG	C3-C4-C5	-3.63	103.66	110.23
18	A	941	NAG	O5-C1-C2	-3.52	105.84	111.29
18	D	944	NAG	C2-N2-C7	3.45	127.52	122.90
18	C	944	NAG	O4-C4-C5	3.44	117.81	109.32
18	D	940	NAG	C1-C2-N2	-3.34	105.16	110.43
18	C	944	NAG	C1-O5-C5	3.25	116.54	112.19
20	B	905	MAN	O2-C2-C3	3.21	116.81	110.15
19	C	951	BGC	O1-C1-O5	-3.18	100.97	110.41
18	D	943	NAG	O5-C1-C2	-3.15	106.42	111.29
18	A	941	NAG	C1-C2-N2	-3.15	105.47	110.43
18	D	943	NAG	C1-O5-C5	3.15	116.40	112.19
18	B	940	NAG	C1-O5-C5	3.06	116.28	112.19
18	B	944	NAG	C1-O5-C5	2.96	116.15	112.19
18	C	944	NAG	O5-C1-C2	-2.95	106.73	111.29
18	D	941	NAG	O5-C1-C2	-2.93	106.75	111.29
18	D	942	NAG	O4-C4-C5	2.84	116.31	109.32
18	B	940	NAG	O5-C5-C6	2.83	113.17	107.66
18	B	943	NAG	C1-O5-C5	2.81	115.95	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	930	NAG	C1-O5-C5	2.80	115.94	112.19
18	C	944	NAG	O5-C5-C6	2.77	113.06	107.66
18	B	940	NAG	O5-C1-C2	-2.76	107.02	111.29
18	A	940	NAG	C1-O5-C5	2.75	115.87	112.19
19	C	951	BGC	C1-O5-C5	2.71	118.89	113.65
18	C	935	NAG	O5-C5-C6	2.66	112.85	107.66
19	D	945	BGC	O1-C1-O5	-2.66	102.51	110.41
18	A	941	NAG	C1-O5-C5	2.63	115.71	112.19
18	A	930	NAG	C6-C5-C4	-2.62	106.58	113.02
18	A	945	NAG	O4-C4-C3	-2.61	104.22	110.38
18	B	940	NAG	C3-C4-C5	-2.59	105.53	110.23
18	D	942	NAG	C1-C2-N2	-2.56	106.40	110.43
18	D	942	NAG	C1-O5-C5	2.55	115.60	112.19
18	D	943	NAG	C2-N2-C7	2.47	126.21	122.90
20	B	905	MAN	C2-C3-C4	2.43	115.14	110.86
18	D	944	NAG	C1-C2-N2	2.43	114.27	110.43
18	A	930	NAG	C2-N2-C7	2.42	126.14	122.90
18	D	940	NAG	O3-C3-C2	-2.40	104.42	109.40
18	C	935	NAG	O3-C3-C2	-2.33	104.56	109.40
18	C	935	NAG	C4-C3-C2	2.33	114.43	111.02
18	D	944	NAG	O5-C1-C2	-2.30	107.73	111.29
18	C	935	NAG	O5-C5-C4	-2.24	105.37	110.83
19	B	945	BGC	O4-C4-C5	2.24	114.83	109.32
18	A	945	NAG	C6-C5-C4	-2.22	107.56	113.02
18	C	950	NAG	C2-N2-C7	2.19	125.84	122.90
18	D	944	NAG	O4-C4-C5	2.18	114.70	109.32
18	C	950	NAG	C1-C2-N2	-2.18	107.00	110.43
19	A	946	BGC	O2-C2-C1	2.17	114.27	109.25
18	D	943	NAG	C3-C4-C5	-2.16	106.31	110.23
18	B	944	NAG	O6-C6-C5	-2.12	104.11	111.33
19	D	945	BGC	O3-C3-C4	-2.08	105.48	110.38
18	A	945	NAG	C3-C4-C5	2.06	113.97	110.23
18	D	942	NAG	C3-C4-C5	-2.05	106.51	110.23
18	C	944	NAG	C4-C3-C2	2.03	114.00	111.02
18	A	944	NAG	C3-C4-C5	-2.02	106.56	110.23
19	A	946	BGC	O4-C4-C5	2.02	114.29	109.32
18	B	944	NAG	C3-C4-C5	-2.00	106.60	110.23
19	D	945	BGC	O4-C4-C5	2.00	114.25	109.32

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	B	940	NAG	O5-C5-C6-O6
20	B	905	MAN	C4-C5-C6-O6
19	B	945	BGC	O5-C5-C6-O6
20	B	905	MAN	O5-C5-C6-O6
18	B	940	NAG	C4-C5-C6-O6
19	A	946	BGC	O5-C5-C6-O6
19	B	945	BGC	C4-C5-C6-O6
19	A	946	BGC	C4-C5-C6-O6
19	D	945	BGC	O5-C5-C6-O6
19	D	945	BGC	C4-C5-C6-O6
18	C	950	NAG	O5-C5-C6-O6
18	D	942	NAG	O5-C5-C6-O6
19	C	951	BGC	O5-C5-C6-O6
18	B	943	NAG	O5-C5-C6-O6
18	D	941	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	905	MAN	1	0
19	D	945	BGC	1	0
19	A	946	BGC	1	0
19	B	945	BGC	1	0
18	A	945	NAG	1	0
19	C	951	BGC	1	0

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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	835/857 (97%)	-0.39	3 (0%) 88 87	14, 25, 41, 69	7 (0%)
1	B	835/857 (97%)	-0.37	0 100 100	13, 26, 42, 77	10 (1%)
1	C	835/857 (97%)	-0.42	1 (0%) 92 90	11, 24, 40, 75	14 (1%)
1	D	835/857 (97%)	-0.45	1 (0%) 92 90	9, 23, 39, 79	10 (1%)
All	All	3340/3428 (97%)	-0.41	5 (0%) 92 90	9, 25, 40, 79	41 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	855	PRO	3.5
1	A	347	SER	3.4
1	C	855	PRO	2.3
1	A	21	ASN	2.2
1	A	346	TYR	2.1

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	BMA	Z	3	11/12	0.42	0.19	82,110,119,119	0
6	MAN	I	4	11/12	0.48	0.18	89,98,103,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MAN	V	9	11/12	0.49	0.18	84,91,100,101	0
4	MAN	G	4	11/12	0.53	0.16	69,85,86,87	0
4	BMA	N	3	11/12	0.54	0.16	73,84,91,102	0
10	MAN	P	5	11/12	0.58	0.18	92,101,109,109	0
4	MAN	N	4	11/12	0.59	0.14	81,99,110,115	0
5	MAN	H	9	11/12	0.59	0.19	70,88,92,93	0
15	BMA	W	3	11/12	0.59	0.15	75,85,92,95	0
2	MAN	E	5	11/12	0.59	0.15	92,94,96,97	0
14	MAN	U	4	11/12	0.60	0.17	91,94,99,104	0
3	MAN	F	6	11/12	0.61	0.15	77,90,96,98	0
16	MAN	X	8	11/12	0.61	0.18	55,70,76,79	0
13	MAN	T	8	11/12	0.62	0.17	82,88,94,96	0
8	NAG	Y	2	14/15	0.63	0.16	67,82,96,100	0
10	BMA	P	4	11/12	0.64	0.18	78,85,94,99	0
6	BMA	I	3	11/12	0.67	0.14	71,77,91,102	0
3	MAN	F	7	11/12	0.68	0.18	56,75,83,84	0
11	MAN	Q	6	11/12	0.68	0.16	75,79,86,86	0
14	MAN	U	5	11/12	0.68	0.15	77,90,95,95	0
9	MAN	O	10	11/12	0.69	0.17	59,65,70,71	0
12	MAN	S	9	11/12	0.69	0.17	73,89,92,94	0
8	NAG	K	2	14/15	0.71	0.16	65,70,78,78	0
11	MAN	Q	5	11/12	0.71	0.15	80,82,86,87	0
8	NAG	R	2	14/15	0.72	0.16	53,66,79,80	0
4	BMA	G	3	11/12	0.72	0.14	60,70,79,81	0
7	MAN	J	6	11/12	0.73	0.15	76,85,89,90	0
12	MAN	S	6	11/12	0.74	0.15	59,68,74,76	0
11	MAN	Q	10	11/12	0.74	0.15	64,70,73,76	0
4	NAG	c	1	14/15	-	-	19,20,22,27	0
4	NAG	c	2	14/15	-	-	29,36,43,46	0
4	BMA	c	3	11/12	-	-	58,69,76,90	0
4	MAN	c	4	11/12	-	-	87,104,110,111	0
4	MAN	L	4	11/12	0.75	0.14	66,72,76,79	0
2	BMA	E	3	11/12	0.77	0.14	50,59,67,73	0
2	MAN	M	4	11/12	0.78	0.13	67,75,78,81	0
3	MAN	F	5	11/12	0.79	0.14	76,82,85,100	0
2	MAN	M	5	11/12	0.79	0.13	55,67,79,86	0
3	MAN	F	4	11/12	0.79	0.17	73,79,86,87	0
10	BMA	P	3	11/12	0.80	0.14	77,85,90,92	0
15	NAG	Z	2	14/15	0.80	0.17	55,77,93,106	0
12	MAN	S	8	11/12	0.80	0.12	72,76,79,84	0
8	NAG	Y	1	14/15	0.80	0.13	56,66,73,77	0
13	GLC	T	7	11/12	0.81	0.12	58,67,73,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BMA	L	3	11/12	0.82	0.12	55,66,73,73	0
5	MAN	H	7	11/12	0.83	0.13	43,53,59,65	0
5	MAN	V	7	11/12	0.83	0.13	47,52,53,60	0
7	MAN	J	5	11/12	0.84	0.12	57,65,70,71	0
2	MAN	E	4	11/12	0.84	0.10	60,70,76,77	0
2	BMA	M	3	11/12	0.85	0.11	45,54,57,67	0
14	BMA	U	3	11/12	0.87	0.11	62,70,78,83	0
12	MAN	S	7	11/12	0.87	0.11	57,63,65,71	0
7	MAN	J	4	11/12	0.87	0.10	43,49,57,57	0
11	MAN	Q	4	11/12	0.87	0.11	45,51,55,63	0
13	MAN	T	6	11/12	0.87	0.10	45,50,55,66	0
12	MAN	S	4	11/12	0.87	0.11	52,58,63,63	0
5	MAN	H	8	11/12	0.87	0.12	47,55,60,67	0
3	BMA	F	3	11/12	0.88	0.09	43,48,58,64	0
10	NAG	P	2	14/15	0.88	0.11	45,48,54,67	0
9	MAN	O	6	11/12	0.88	0.12	50,57,60,60	0
4	NAG	N	2	14/15	0.89	0.11	36,43,50,59	0
5	MAN	V	8	11/12	0.89	0.09	46,48,56,72	0
9	MAN	O	9	11/12	0.89	0.10	42,45,47,52	0
7	MAN	J	7	11/12	0.89	0.09	37,40,42,42	0
12	BMA	S	3	11/12	0.89	0.10	44,54,61,62	0
13	MAN	T	4	11/12	0.90	0.09	34,38,41,41	0
13	MAN	T	5	11/12	0.90	0.08	31,36,40,43	0
16	MAN	X	5	11/12	0.90	0.09	35,40,44,48	0
12	MAN	S	5	11/12	0.90	0.09	48,50,53,56	0
13	BMA	T	3	11/12	0.91	0.09	33,33,44,61	0
10	NAG	P	1	14/15	0.91	0.10	32,38,42,45	0
7	MAN	J	9	11/12	0.91	0.09	43,49,51,52	0
7	NAG	J	1	14/15	0.91	0.08	26,30,32,33	0
11	MAN	Q	8	11/12	0.91	0.09	43,49,53,57	0
7	BMA	J	3	11/12	0.91	0.08	33,34,37,38	0
16	MAN	X	7	11/12	0.91	0.08	46,49,52,59	0
7	MAN	J	8	11/12	0.91	0.08	40,44,47,47	0
11	MAN	Q	9	11/12	0.92	0.09	35,43,48,53	0
16	MAN	X	4	11/12	0.92	0.08	30,36,42,43	0
8	NAG	R	1	14/15	0.92	0.08	29,38,41,53	0
9	NAG	d	1	14/15	-	-	20,24,27,28	0
9	NAG	d	2	14/15	-	-	20,21,24,24	0
9	BMA	d	3	11/12	-	-	22,24,29,35	0
9	MAN	d	4	11/12	-	-	22,25,27,29	0
9	MAN	d	5	11/12	-	-	35,39,42,45	0
9	MAN	d	6	11/12	-	-	56,61,64,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	MAN	d	7	11/12	-	-	20,24,26,27	0
9	MAN	d	8	11/12	-	-	29,31,33,38	0
9	MAN	d	9	11/12	-	-	38,48,53,64	0
9	MAN	d	10	11/12	-	-	77,84,86,87	0
6	NAG	I	2	14/15	0.92	0.09	40,43,48,58	0
9	MAN	O	5	11/12	0.92	0.09	39,42,45,51	0
14	NAG	U	2	14/15	0.93	0.09	39,43,46,52	0
5	MAN	H	6	11/12	0.93	0.08	28,30,32,37	0
8	NAG	K	1	14/15	0.93	0.08	37,43,46,54	0
11	NAG	Q	1	14/15	0.93	0.07	24,27,32,33	0
16	MAN	X	6	11/12	0.93	0.08	34,39,43,44	0
15	NAG	W	2	14/15	0.93	0.09	40,44,50,64	0
11	MAN	Q	7	11/12	0.93	0.07	38,40,46,54	0
3	NAG	F	2	14/15	0.94	0.09	29,32,37,40	0
12	NAG	S	2	14/15	0.94	0.07	31,35,39,46	0
5	MAN	V	4	11/12	0.94	0.07	25,31,35,40	0
11	BMA	Q	3	11/12	0.94	0.07	29,32,36,44	0
5	NAG	V	2	14/15	0.95	0.07	21,26,29,29	0
7	NAG	J	2	14/15	0.95	0.06	24,28,31,32	0
9	NAG	O	2	14/15	0.95	0.07	23,26,27,27	0
9	MAN	O	4	11/12	0.95	0.07	27,28,34,36	0
5	BMA	V	3	11/12	0.95	0.06	26,30,33,37	0
4	NAG	G	2	14/15	0.95	0.08	29,35,41,46	0
9	MAN	O	7	11/12	0.95	0.07	24,25,29,29	0
5	MAN	V	5	11/12	0.95	0.07	22,24,26,29	0
15	NAG	W	1	14/15	0.95	0.07	30,33,35,35	0
5	MAN	V	6	11/12	0.95	0.06	25,27,29,33	0
2	NAG	M	2	14/15	0.95	0.07	34,37,41,45	0
15	NAG	Z	1	14/15	0.95	0.07	31,36,42,55	0
3	NAG	F	1	14/15	0.95	0.07	25,27,29,30	0
4	NAG	L	1	14/15	0.95	0.07	22,28,29,30	0
16	NAG	X	2	14/15	0.95	0.06	22,24,28,28	0
16	BMA	X	3	11/12	0.95	0.06	30,32,37,40	0
6	NAG	I	1	14/15	0.95	0.07	26,31,34,34	0
4	NAG	L	2	14/15	0.95	0.07	30,33,38,45	0
2	NAG	E	2	14/15	0.95	0.06	21,27,38,40	0
13	NAG	b	1	14/15	-	-	22,24,27,28	0
13	NAG	b	2	14/15	-	-	29,32,38,38	0
13	BMA	b	3	11/12	-	-	38,39,52,70	0
13	MAN	b	4	11/12	-	-	40,43,45,46	0
13	MAN	b	5	11/12	-	-	40,43,46,54	0
13	MAN	b	6	11/12	-	-	53,63,67,81	0

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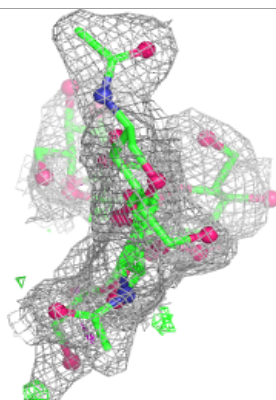
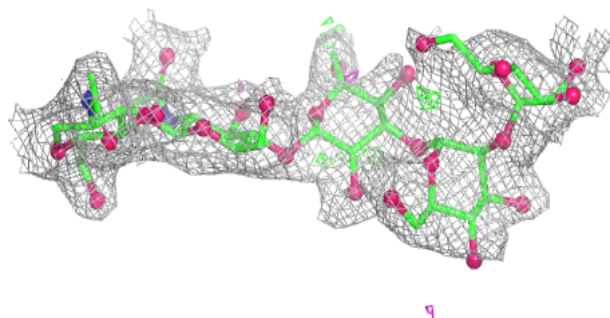
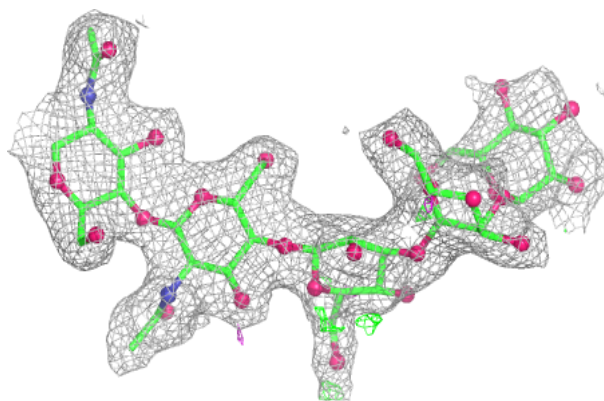
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	GLC	b	7	11/12	-	-	66,88,96,99	0
13	MAN	b	8	11/12	-	-	88,102,108,109	0
11	NAG	Q	2	14/15	0.95	0.07	22,24,26,27	0
2	NAG	M	1	14/15	0.95	0.06	27,28,29,31	0
9	BMA	O	3	11/12	0.96	0.06	27,28,31,35	0
13	NAG	T	2	14/15	0.96	0.06	25,27,30,31	0
5	MAN	H	4	11/12	0.96	0.06	27,29,33,40	0
5	MAN	H	5	11/12	0.96	0.05	18,21,23,24	0
12	NAG	S	1	14/15	0.96	0.06	24,25,28,28	0
4	NAG	G	1	14/15	0.96	0.06	20,22,27,27	0
16	NAG	X	1	14/15	0.96	0.05	23,25,28,30	0
5	NAG	H	1	14/15	0.96	0.06	24,25,28,29	0
9	MAN	O	8	11/12	0.96	0.06	26,27,31,36	0
15	NAG	e	1	14/15	-	-	31,32,34,37	0
15	NAG	e	2	14/15	-	-	36,43,49,60	0
15	BMA	e	3	11/12	-	-	72,81,84,86	0
14	NAG	U	1	14/15	0.96	0.07	24,29,32,34	0
5	NAG	H	2	14/15	0.96	0.06	21,24,30,31	0
5	BMA	H	3	11/12	0.96	0.06	26,28,31,40	0
9	NAG	O	1	14/15	0.96	0.06	25,26,27,28	0
5	NAG	V	1	14/15	0.96	0.07	25,27,32,34	0
13	NAG	T	1	14/15	0.97	0.06	18,21,23,24	0
2	NAG	E	1	14/15	0.97	0.05	22,24,27,30	0
4	NAG	N	1	14/15	0.97	0.05	22,25,27,30	0
16	NAG	f	1	14/15	-	-	23,25,30,30	0
16	NAG	f	2	14/15	-	-	22,25,30,33	0
16	BMA	f	3	11/12	-	-	29,34,37,42	0
16	MAN	f	4	11/12	-	-	39,42,46,47	0
16	MAN	f	5	11/12	-	-	39,43,45,46	0
16	MAN	f	6	11/12	-	-	39,43,46,47	0
16	MAN	f	7	11/12	-	-	55,59,65,67	0
16	MAN	f	8	11/12	-	-	70,83,92,93	0
17	NAG	a	1	14/15	-	-	21,23,25,26	0
17	NAG	a	2	14/15	-	-	22,28,34,41	0
17	BMA	a	3	11/12	-	-	44,65,82,84	0
17	MAN	a	4	11/12	-	-	71,79,88,90	0
17	MAN	a	5	11/12	-	-	74,94,99,100	0
17	MAN	a	6	11/12	-	-	67,78,86,89	0

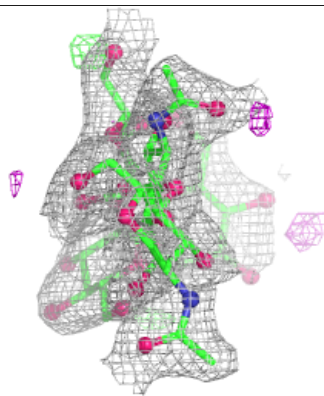
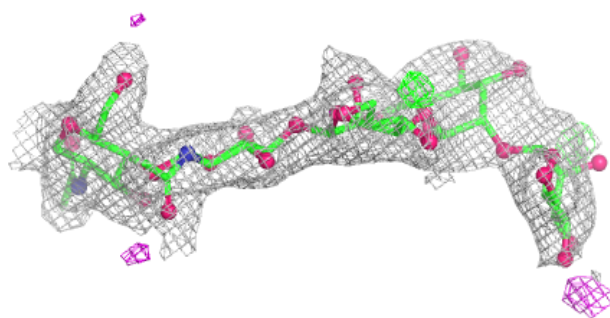
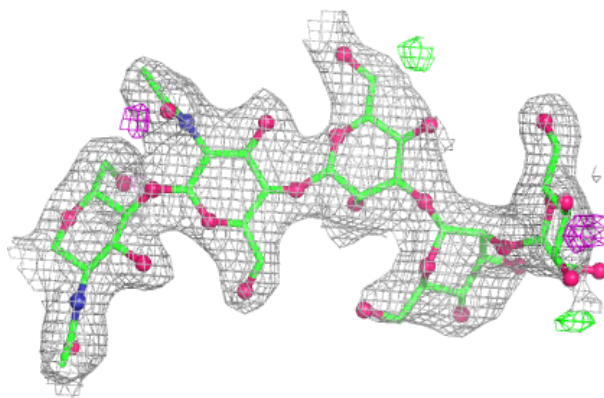
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

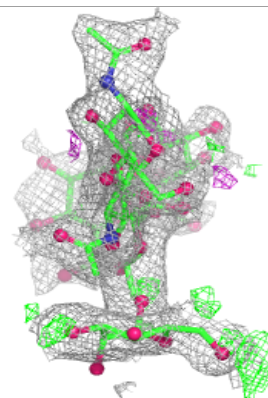
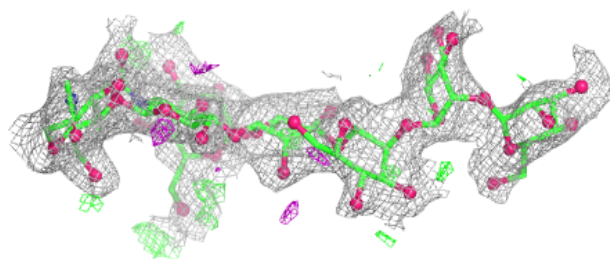
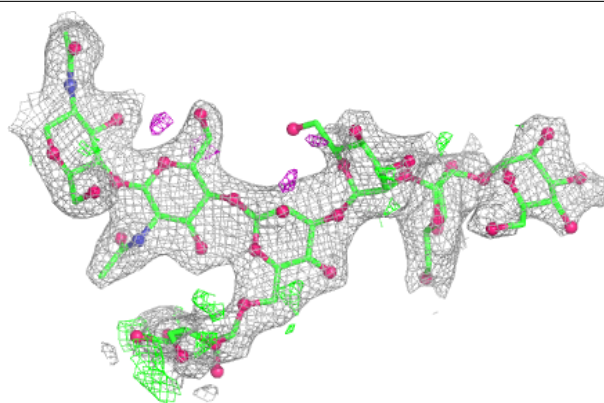
**Electron density around Chain M:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

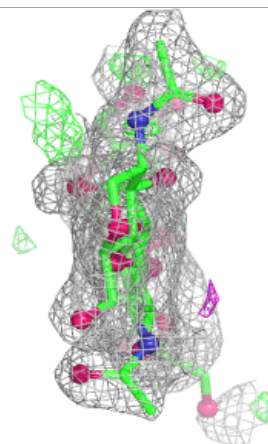
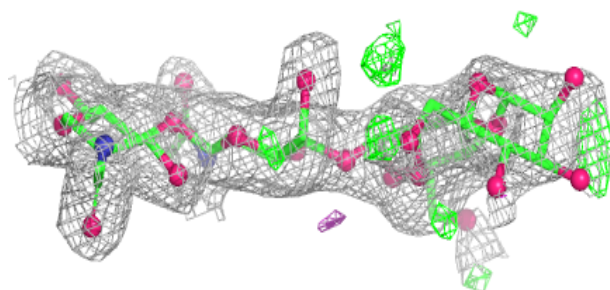
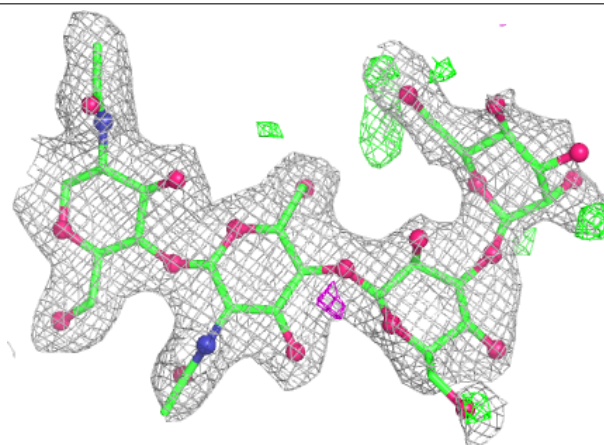


Electron density around Chain F:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

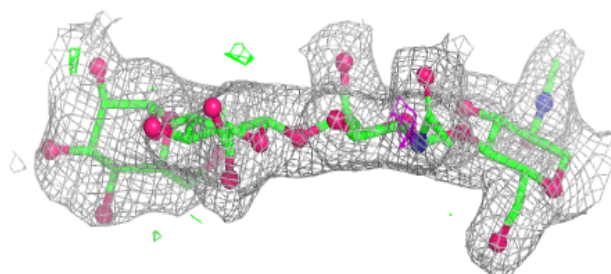
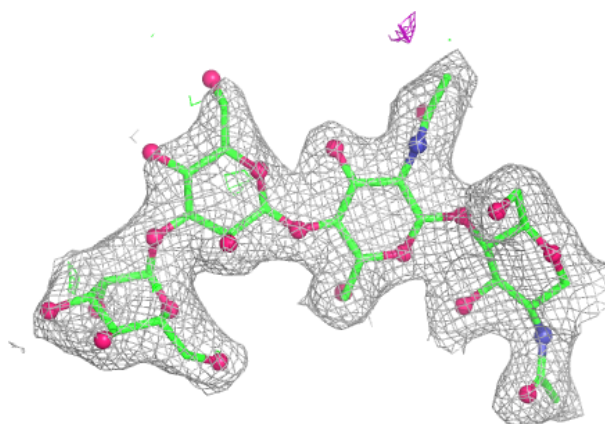
**Electron density around Chain G:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



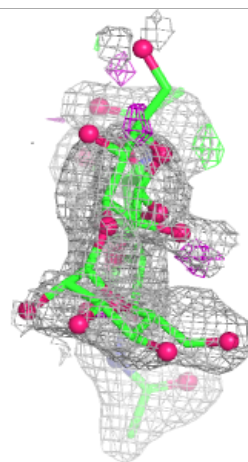
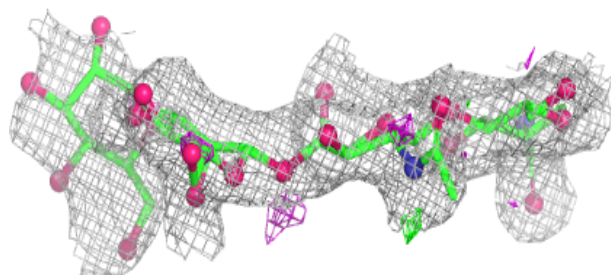
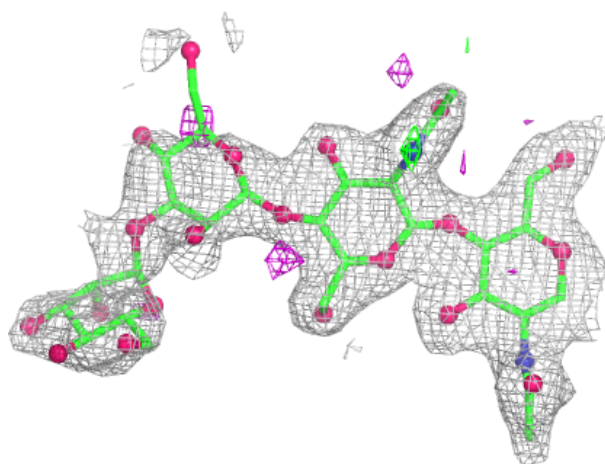
Electron density around Chain L:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



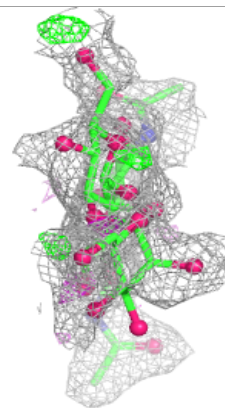
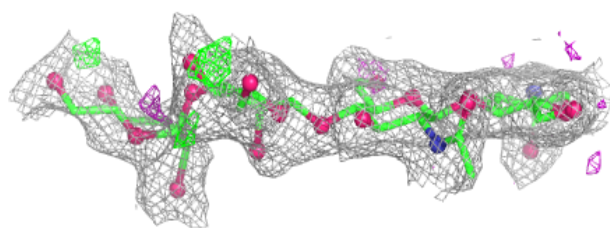
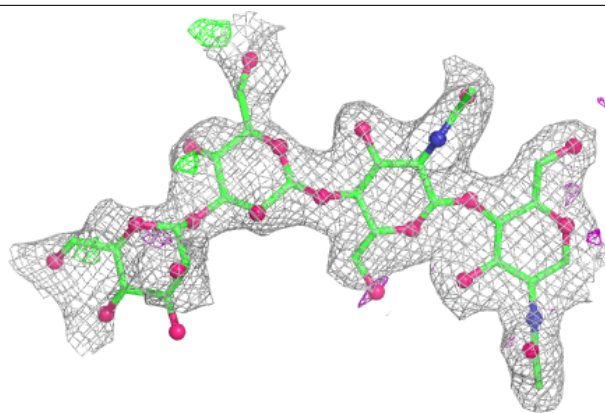
Electron density around Chain N:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



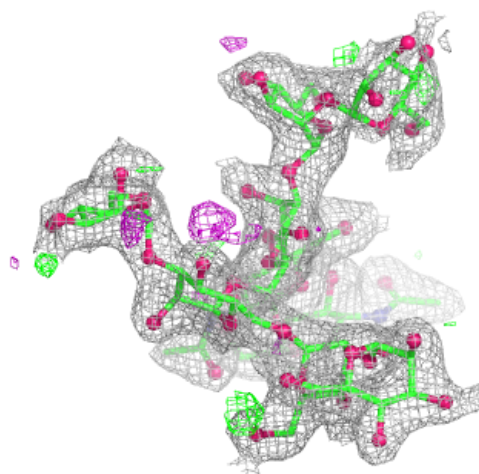
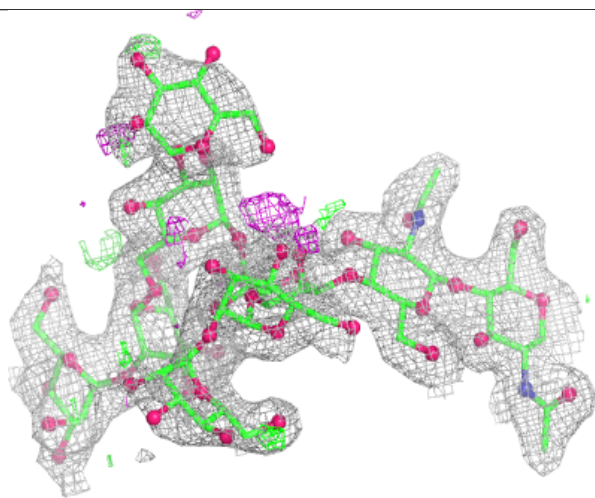
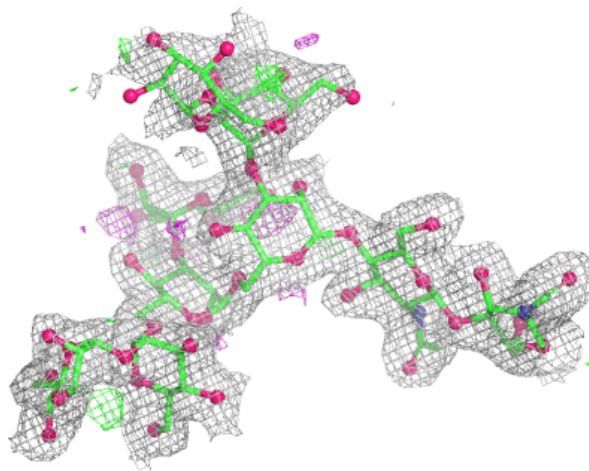
Electron density around Chain c:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



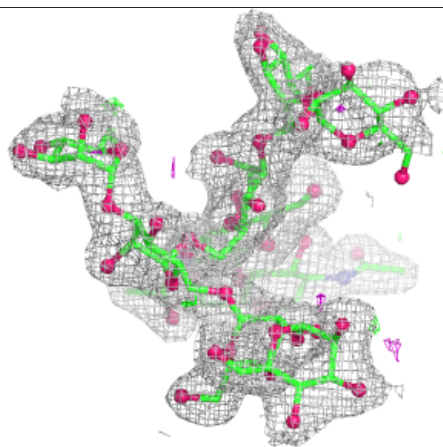
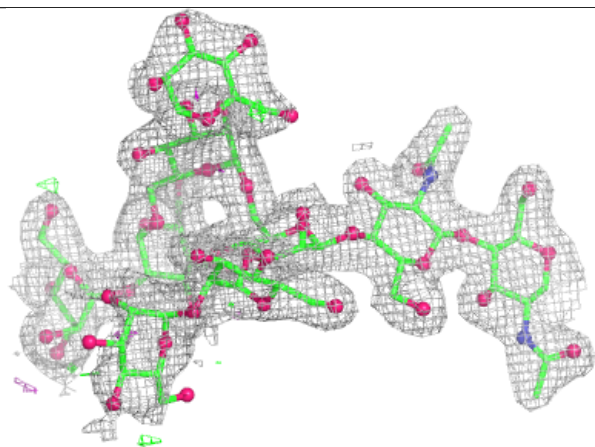
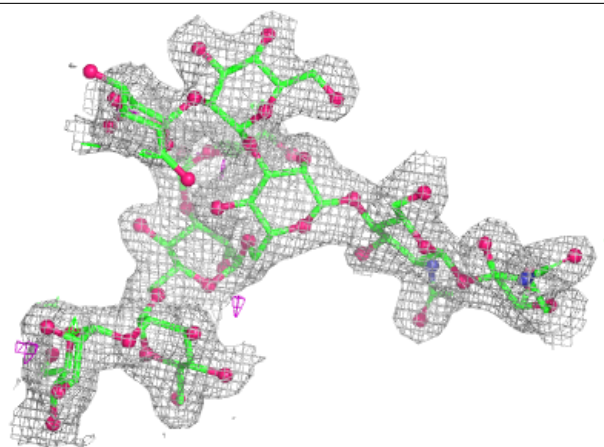
Electron density around Chain H:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



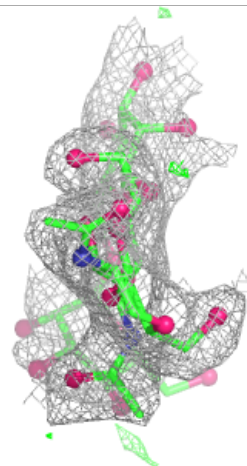
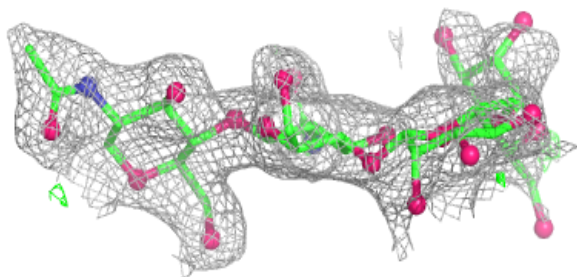
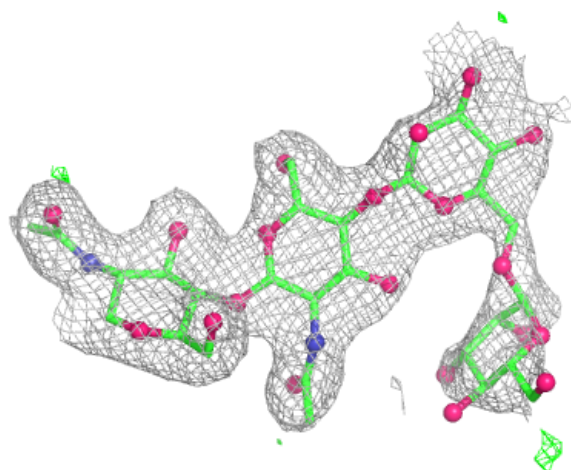
Electron density around Chain V:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



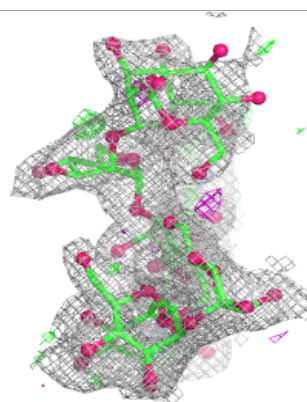
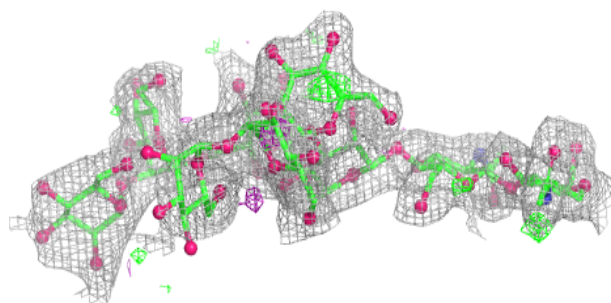
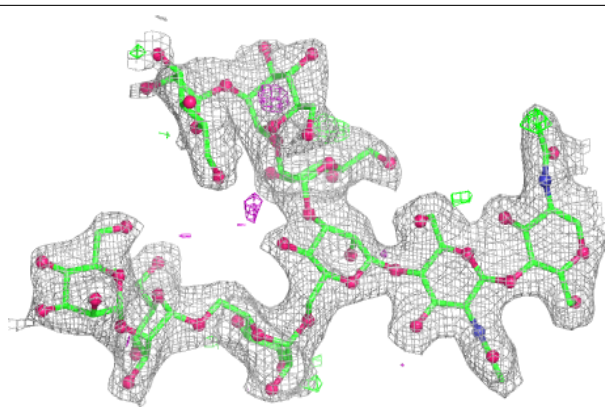
Electron density around Chain I:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



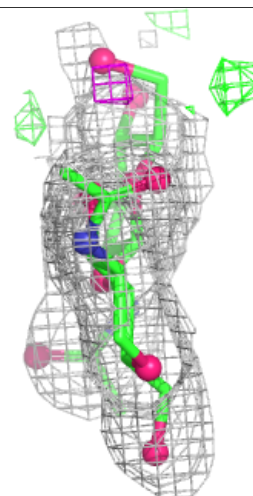
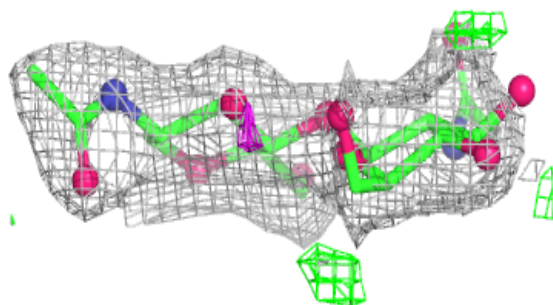
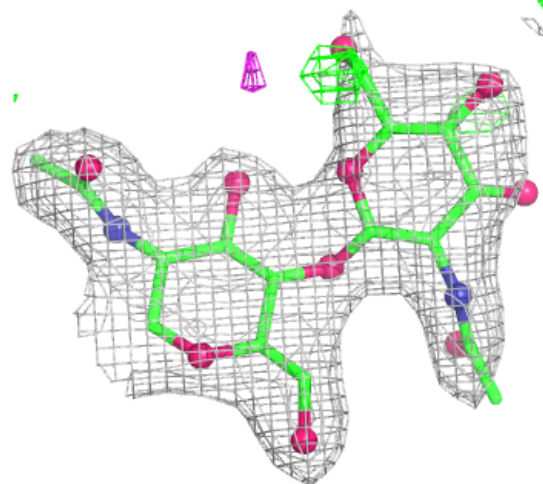
Electron density around Chain J:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



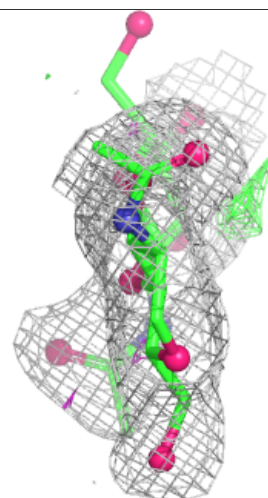
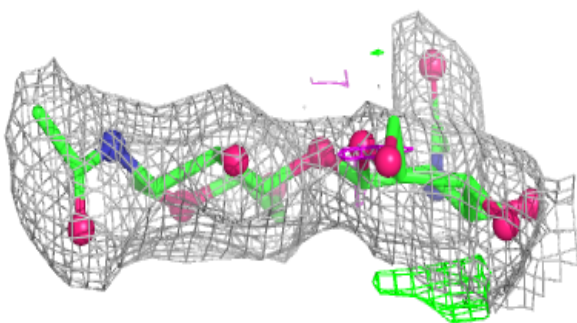
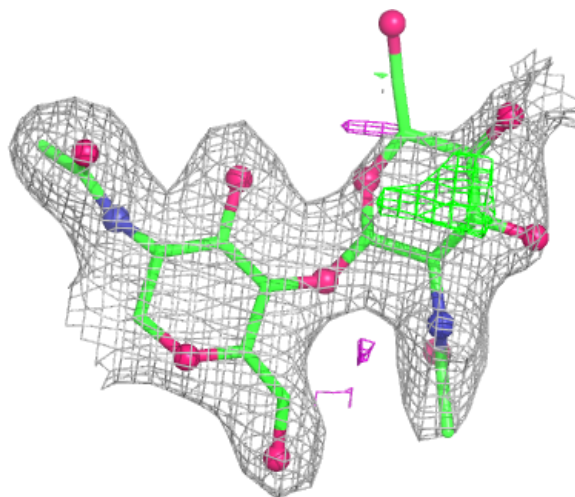
Electron density around Chain K:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



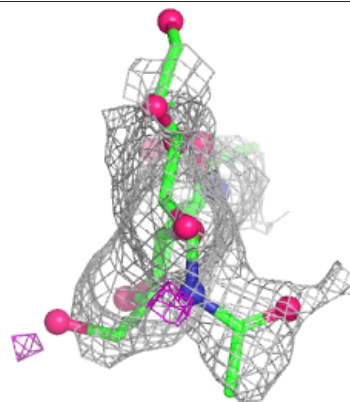
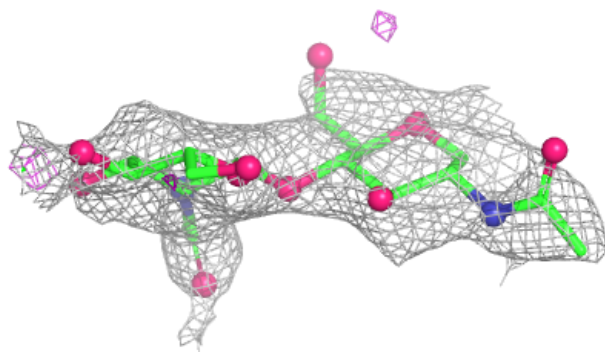
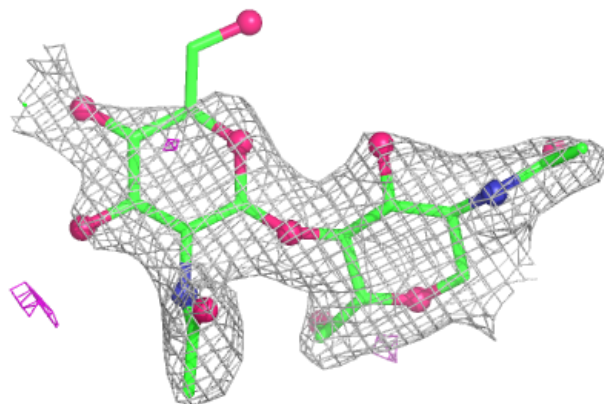
Electron density around Chain R:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



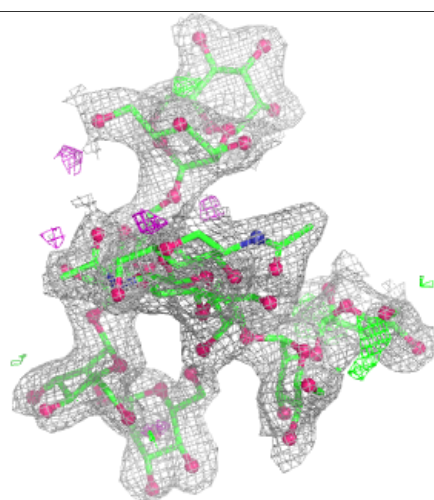
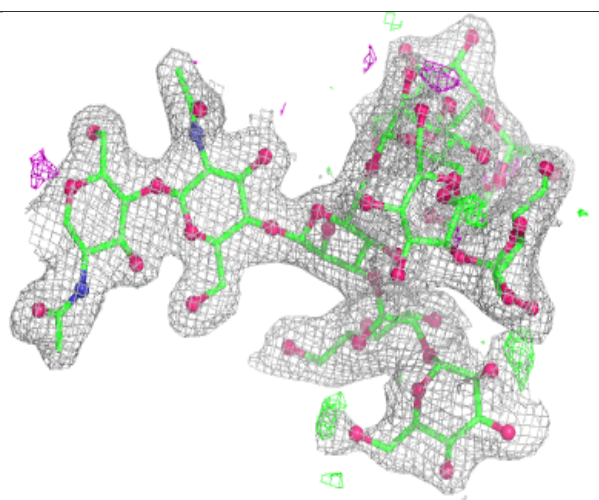
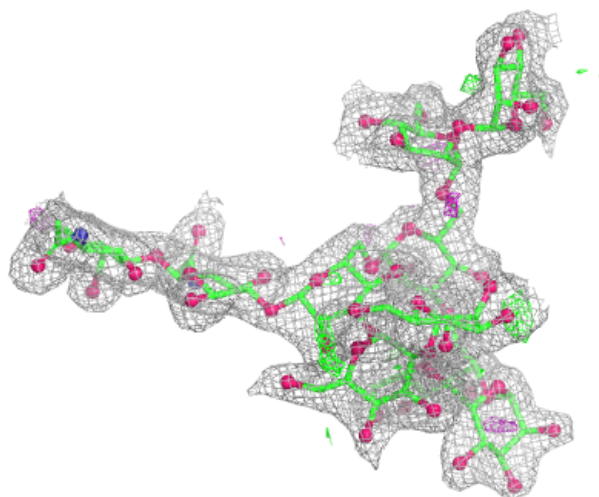
Electron density around Chain Y:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



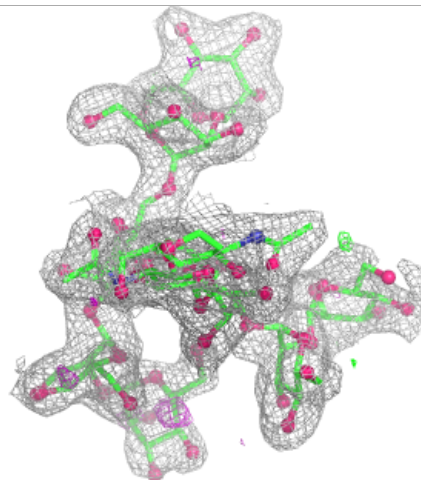
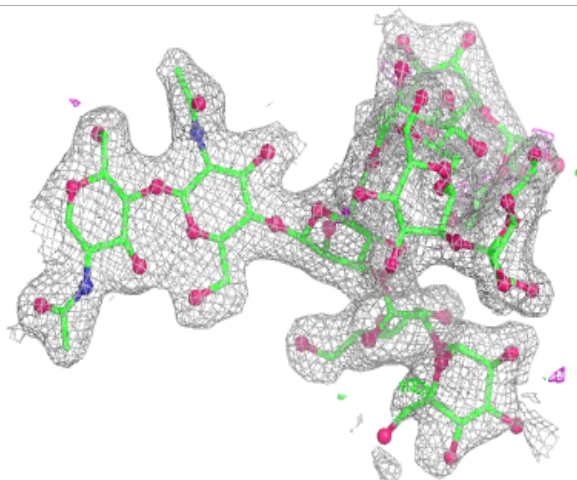
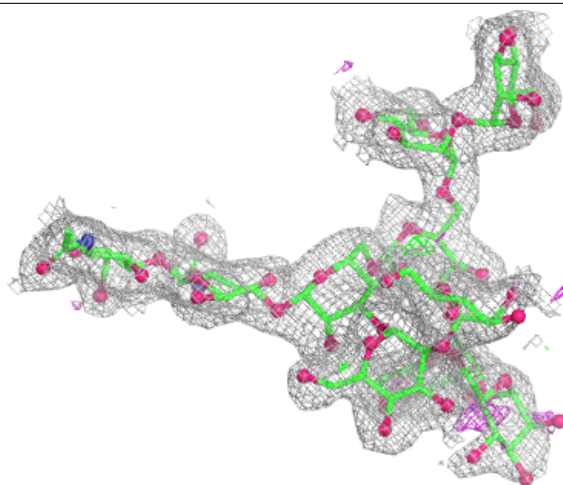
Electron density around Chain O:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



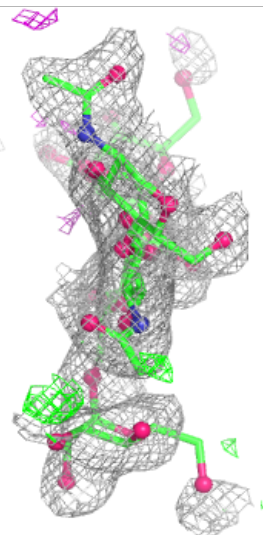
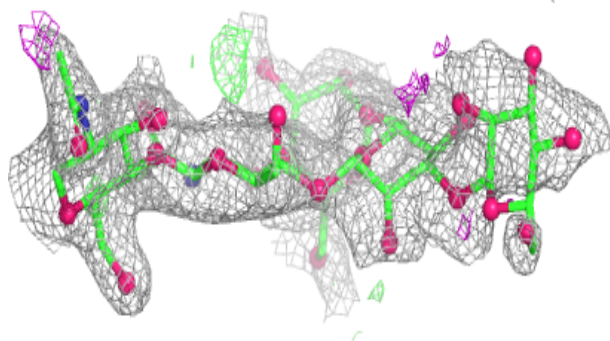
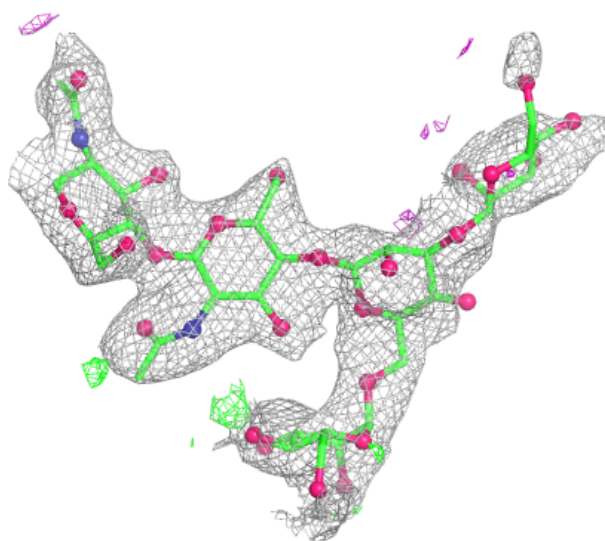
Electron density around Chain d:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



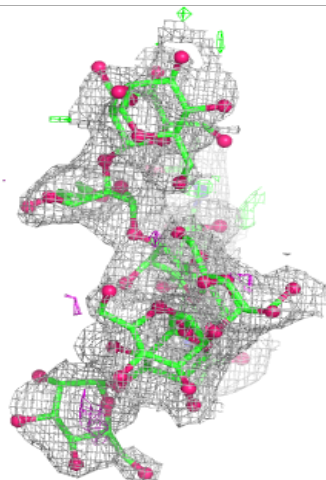
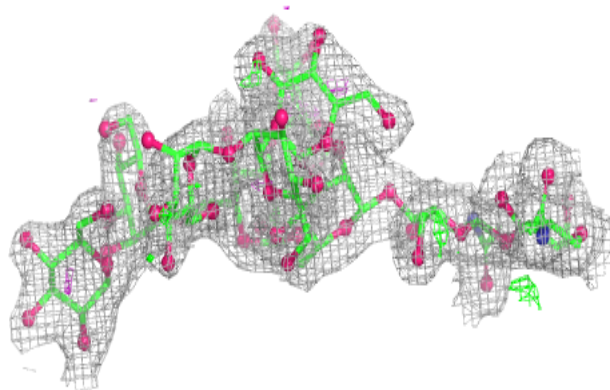
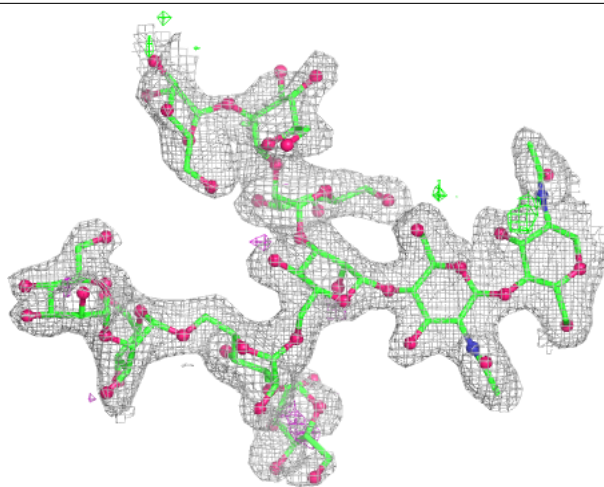
Electron density around Chain P:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



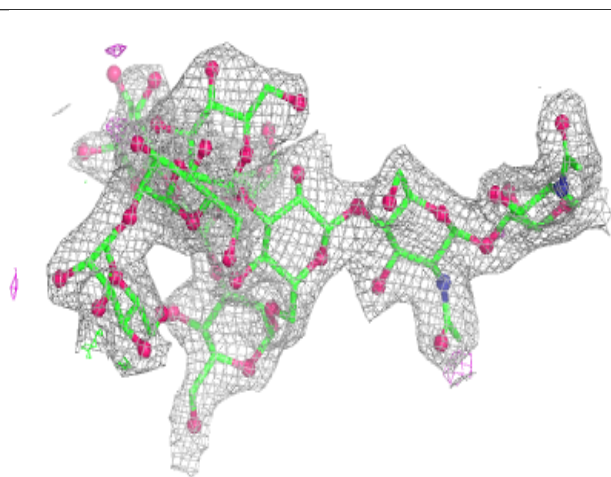
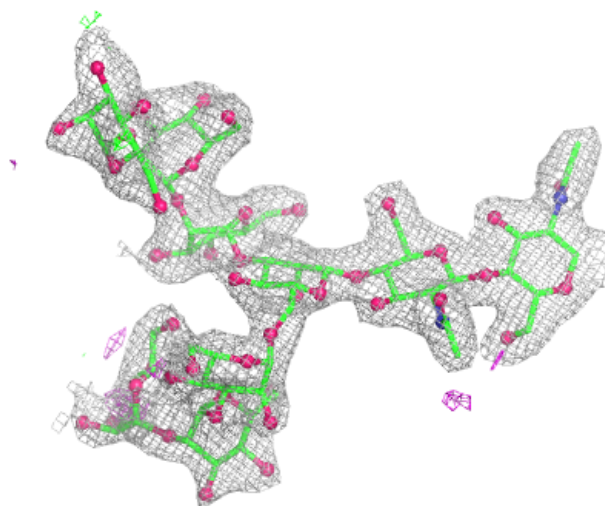
Electron density around Chain Q:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



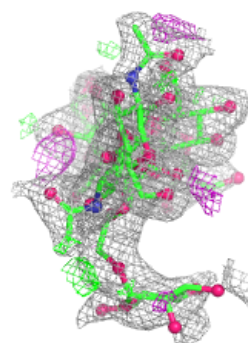
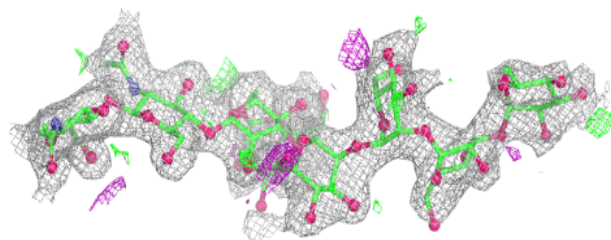
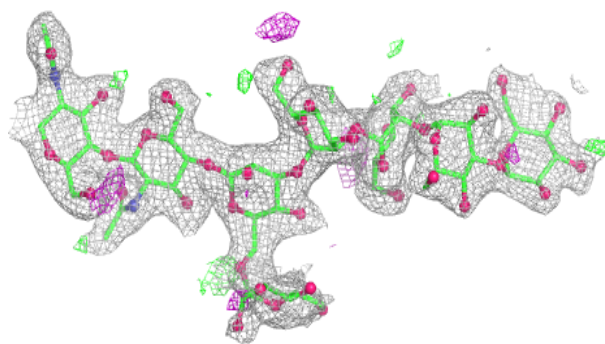
Electron density around Chain S:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

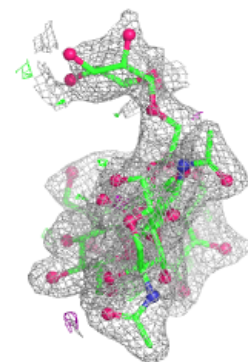
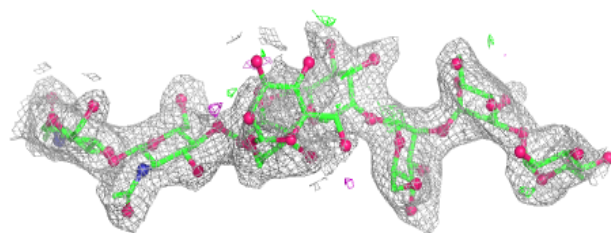
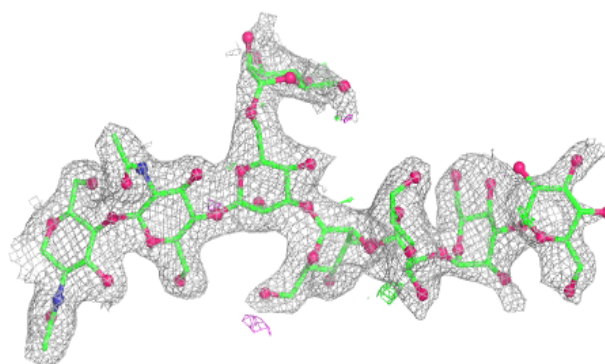


Electron density around Chain T:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

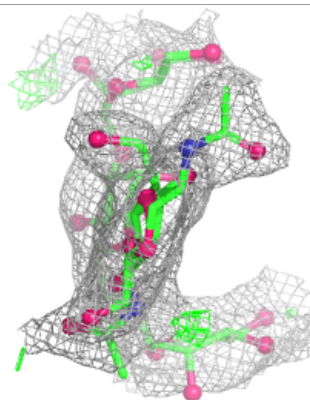
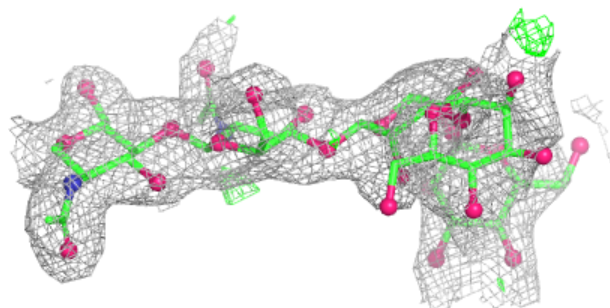
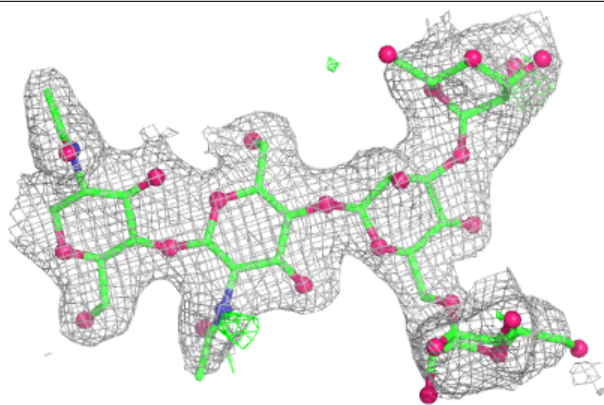
**Electron density around Chain b:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

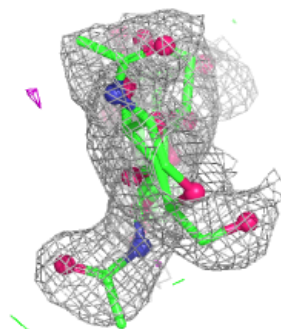
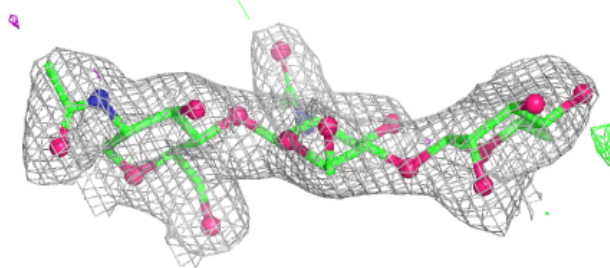
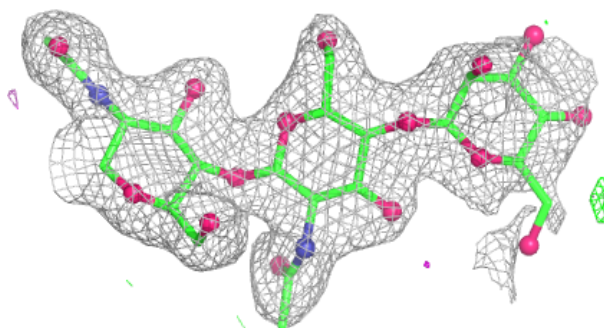


Electron density around Chain U:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

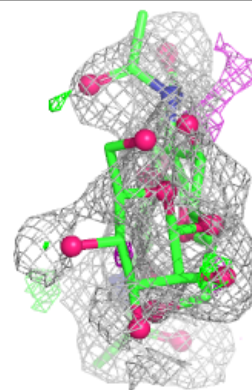
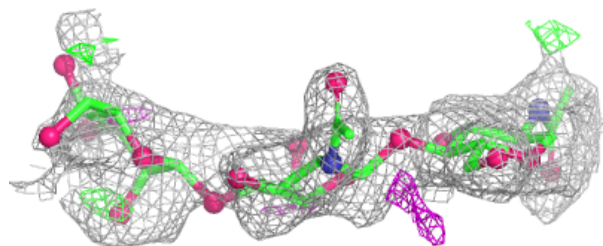
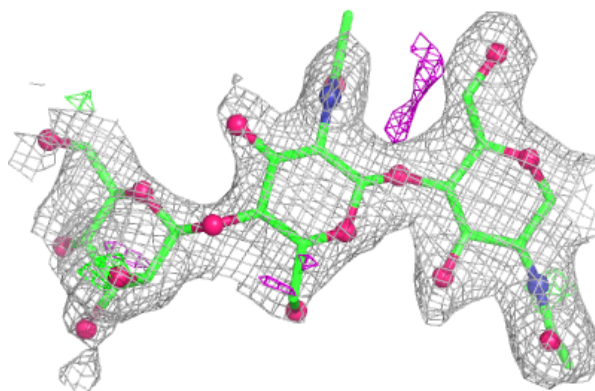
**Electron density around Chain W:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

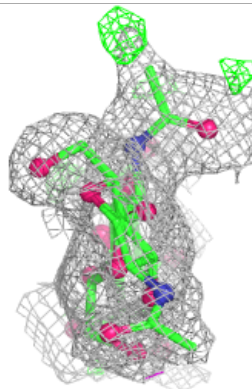
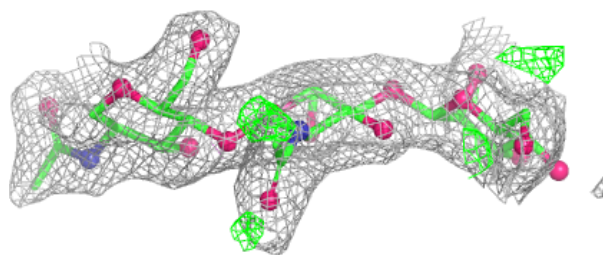
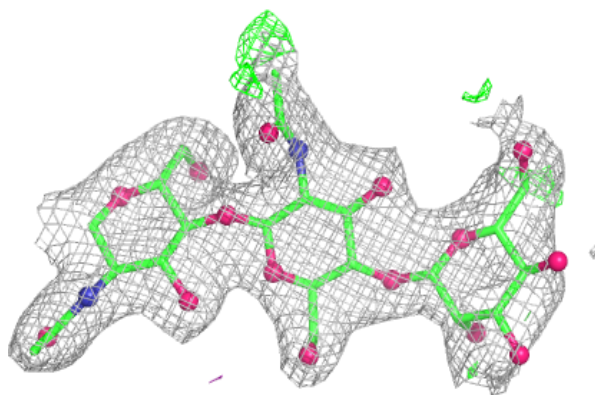


Electron density around Chain Z:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

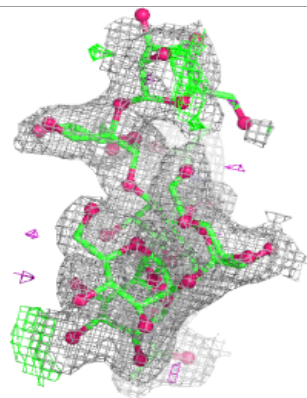
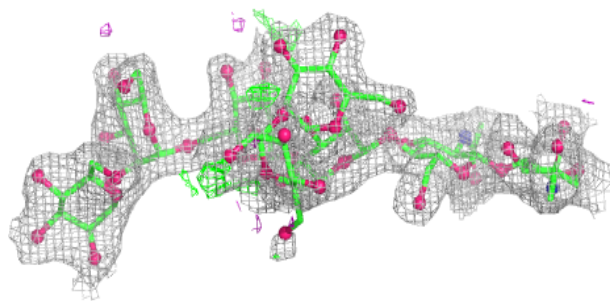
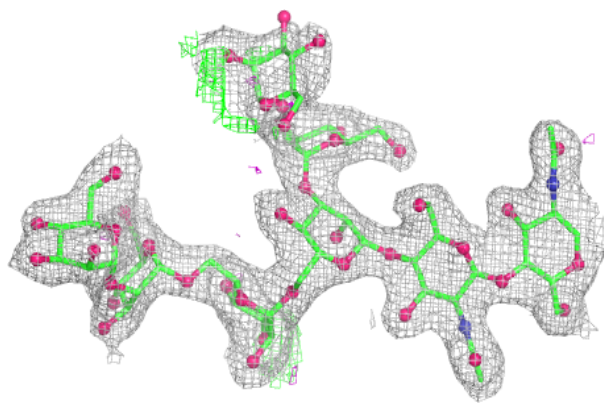
**Electron density around Chain e:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

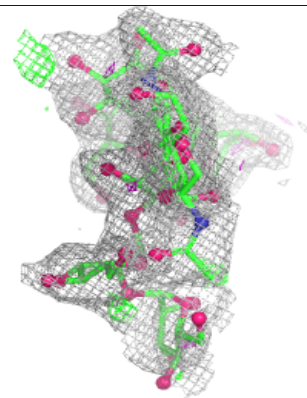
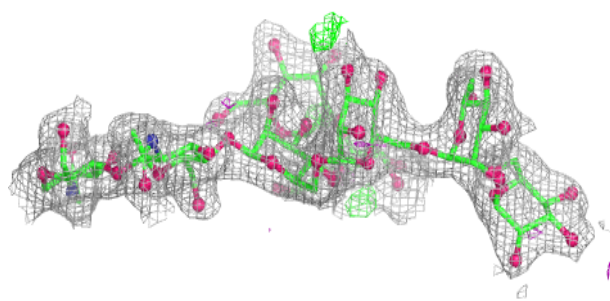
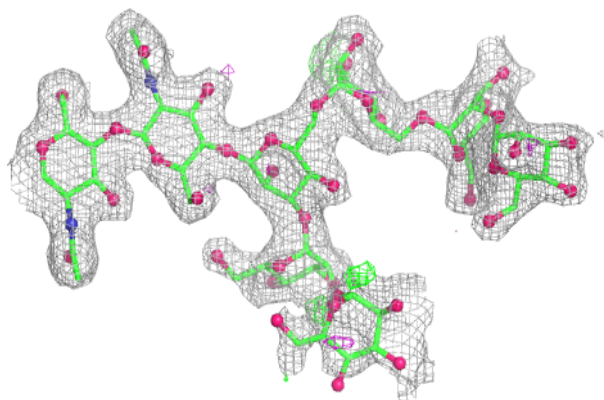


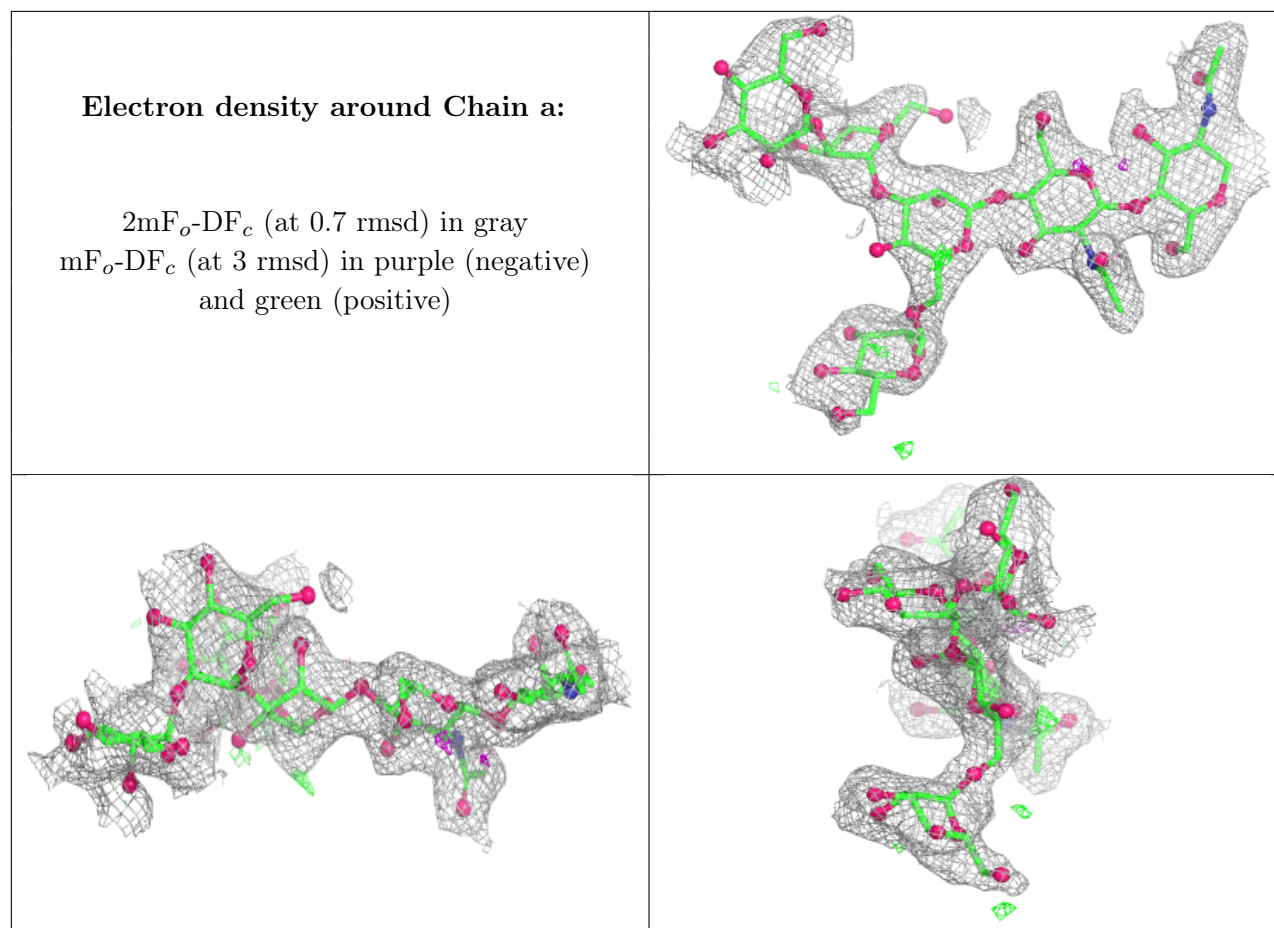
Electron density around Chain X:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain f:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	MAN	B	905	11/12	0.67	0.18	63,88,99,102	0
18	NAG	D	944	14/15	0.76	0.19	62,80,88,88	0
18	NAG	C	950	14/15	0.77	0.14	62,72,82,88	0
18	NAG	B	943	14/15	0.78	0.16	64,74,84,84	0
18	NAG	D	940	14/15	0.78	0.16	58,63,68,73	0
18	NAG	A	930	14/15	0.80	0.15	57,62,65,72	0
18	NAG	D	941	14/15	0.80	0.14	64,79,84,85	0
18	NAG	C	935	14/15	0.81	0.17	61,72,85,87	0
18	NAG	A	941	14/15	0.82	0.13	59,66,69,70	0
19	BGC	B	945	12/12	0.83	0.14	39,47,55,63	0
18	NAG	B	944	14/15	0.83	0.16	54,65,70,76	0
18	NAG	C	944	14/15	0.85	0.11	41,47,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	NAG	B	940	14/15	0.86	0.12	42,58,66,71	0
19	BGC	C	951	12/12	0.87	0.15	44,58,64,67	0
18	NAG	A	940	14/15	0.88	0.09	41,51,56,57	0
18	NAG	A	945	14/15	0.88	0.11	46,52,54,62	0
19	BGC	D	945	12/12	0.89	0.12	46,52,57,61	0
19	BGC	A	946	12/12	0.89	0.11	36,46,49,53	0
18	NAG	A	944	14/15	0.93	0.08	29,32,37,40	0
18	NAG	D	942	14/15	0.93	0.08	32,34,35,38	0
18	NAG	D	943	14/15	0.95	0.07	25,28,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.