



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 03:01 PM BST

PDB ID : 5JU6
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

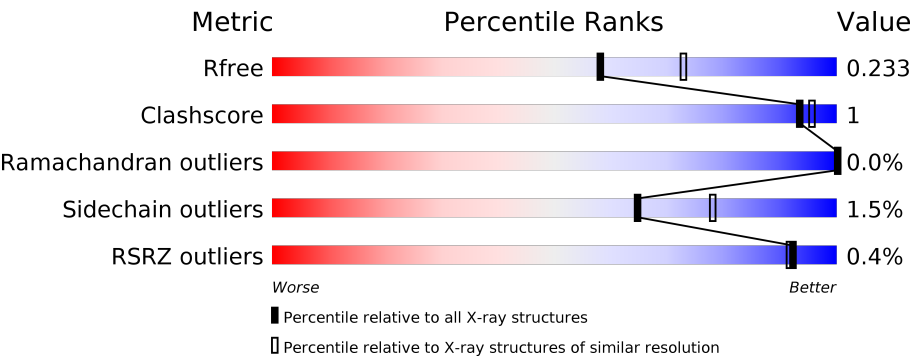
1 Overall quality at a glance i

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.




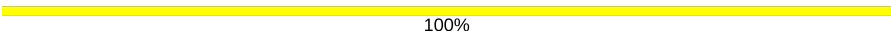
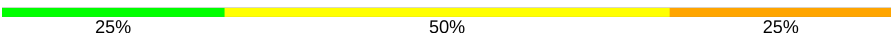
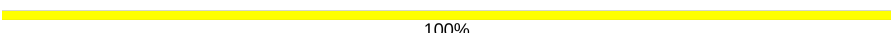
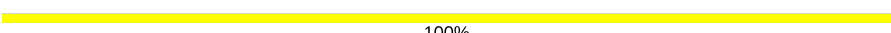
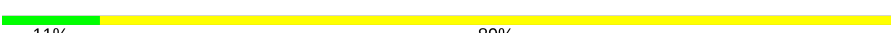
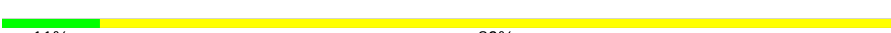




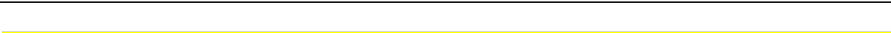


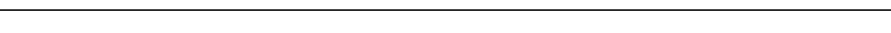


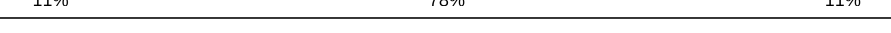

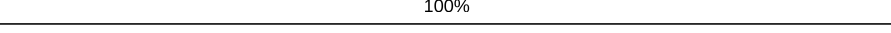

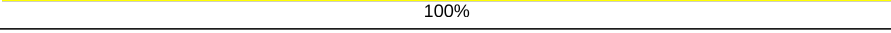
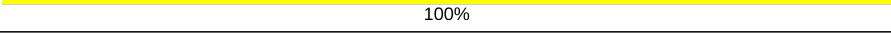
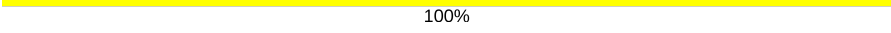

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	<div><div></div><div>93%</div><div></div></div>
1	B	857	<div><div>%</div><div>91%</div><div>6%</div></div>
1	C	857	<div><div></div><div>92%</div><div>5%</div></div>
1	D	857	<div><div></div><div>92%</div><div>5%</div></div>
2	E	5	<div><div>20%</div><div>60%</div><div>20%</div></div>
2	M	5	<div><div>20%</div><div>80%</div></div>

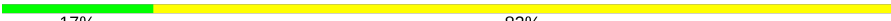
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Mol	Chain	Length	Quality of chain
3	F	7	 14%86%
4	G	4	 100%
4	L	4	 25%50%25%
4	N	4	 100%
4	c	4	 100%
5	H	9	 11%89%
5	V	9	 11%89%
6	I	4	 100%
7	J	9	 11%89%
8	K	2	 50%50%
8	R	2	 100%
8	Y	2	 100%
9	O	10	 20%80%
9	d	10	 10%90%
10	P	5	 20%80%
11	Q	10	 30%70%
12	S	9	 11%78%11%
13	T	8	 13%88%
13	b	8	 100%
14	U	5	 40%60%
15	W	3	 100%
15	Z	3	 100%
15	e	3	 100%
16	X	8	 25%75%
16	f	8	 25%75%

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Mol	Chain	Length	Quality of chain
17	a	6	 <div>17% 83%</div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	N	4	-	-	-	X

2 Entry composition [i](#)

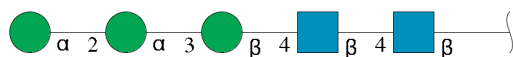
There are 21 unique types of molecules in this entry. The entry contains 29503 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

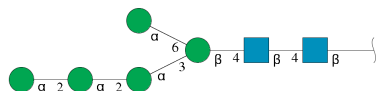
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	835	Total	C	N	O	S	0	0	0
			6373	4018	1093	1239	23			
1	B	835	Total	C	N	O	S	0	1	0
			6379	4021	1094	1241	23			
1	C	835	Total	C	N	O	S	0	3	0
			6388	4028	1095	1242	23			
1	D	835	Total	C	N	O	S	0	2	0
			6382	4023	1094	1241	24			

- 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.



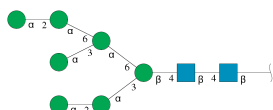
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	7	Total	C	N	O	0	0	0
			83	46	2	35			

- 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.



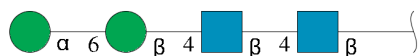
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	L	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	N	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	c	4	Total	C	N	O	0	0	0
			50	28	2	20			

- 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.



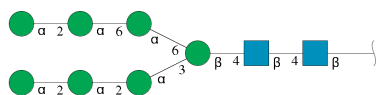
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	9	Total	C	N	O	0	0	0
			105	58	2	45			
5	V	9	Total	C	N	O	0	0	0
			105	58	2	45			

- 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.



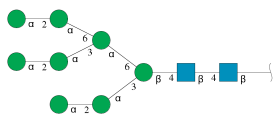
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	J	9	Total	C	N	O	0	0	0
			105	58	2	45			

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



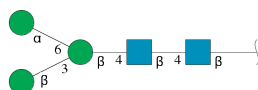
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



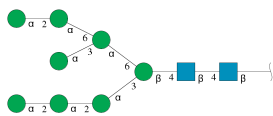
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	O	10	Total	C	N	O	0	0	0
			116	64	2	50			
9	d	10	Total	C	N	O	0	0	0
			116	64	2	50			

- 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.



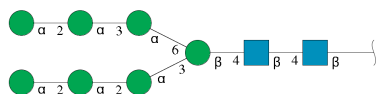
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	P	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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-(1-3)]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.



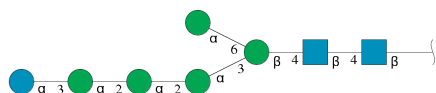
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	Q	10	Total	C	N	O	0	0	0
			116	64	2	50			

- 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-(1-6)-[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.



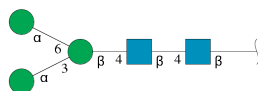
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	S	9	Total	C	N	O	0	0	0
			105	58	2	45			

- 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.



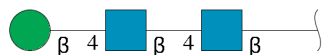
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	T	8	Total	C	N	O	0	0	0
			94	52	2	40			
13	b	8	Total	C	N	O	0	0	0
			94	52	2	40			

- 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.



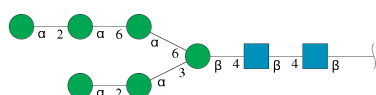
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	U	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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.



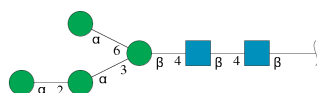
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	W	3	Total	C	N	O	0	0	0
			39	22	2	15			
15	Z	3	Total	C	N	O	0	0	0
			39	22	2	15			
15	e	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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.



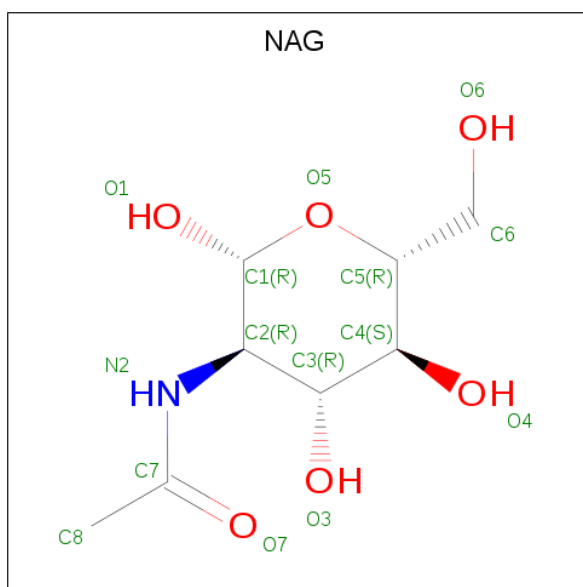
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	X	8	Total	C	N	O	0	0	0
			94	52	2	40			
16	f	8	Total	C	N	O	0	0	0
			94	52	2	40			

- 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 (three-letter code: NAG) (formula: C₈H₁₅NO₆).



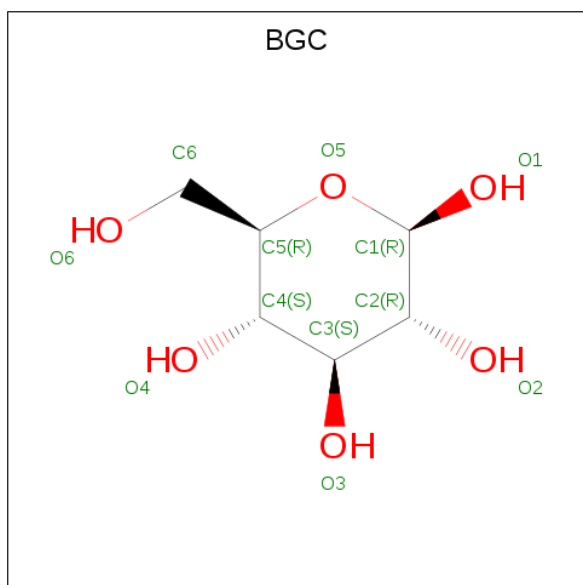
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	N	O	0	0
			14	8	1	5		
18	A	1	Total	C	N	O	0	0
			14	8	1	5		
18	A	1	Total	C	N	O	0	0
			14	8	1	5		
18	A	1	Total	C	N	O	0	0
			14	8	1	5		
18	A	1	Total	C	N	O	0	0
			14	8	1	5		
18	B	1	Total	C	N	O	0	0
			14	8	1	5		
18	B	1	Total	C	N	O	0	0
			14	8	1	5		
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 (three-letter code: 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 (three-letter code: MAN) (formula: C₆H₁₂O₆).



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

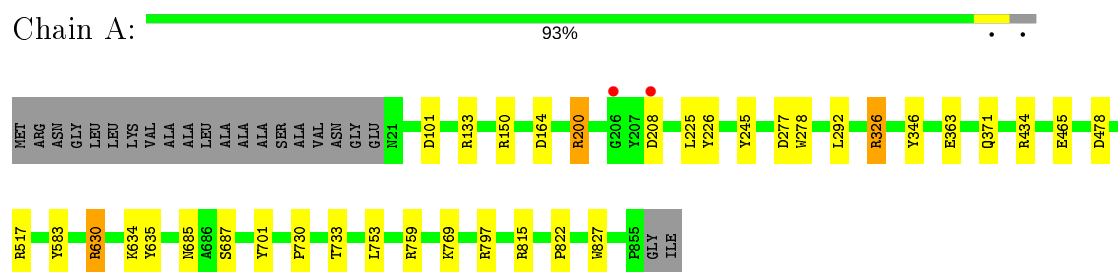
- Molecule 21 is water.

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		

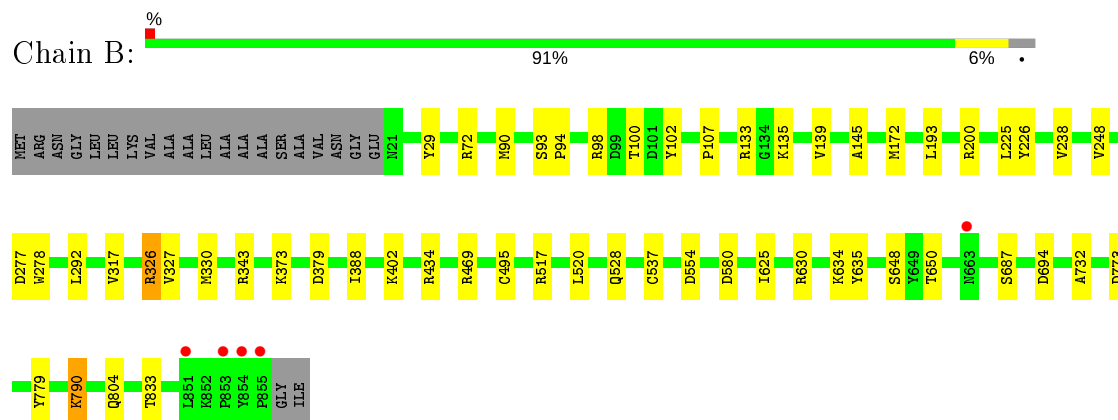
3 Residue-property plots [i](#)

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.

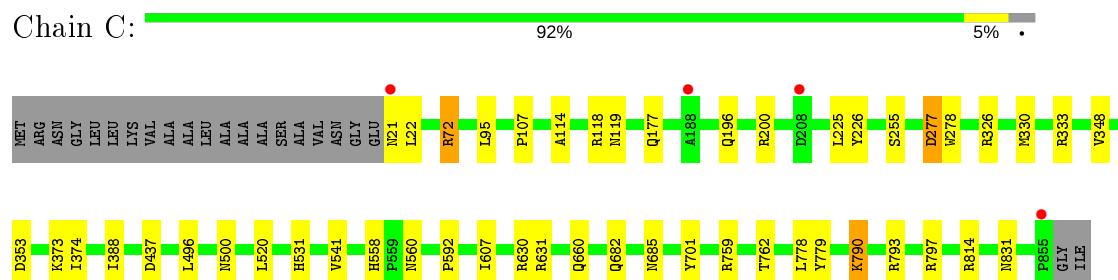
- Molecule 1: Beta-glucosidase



- Molecule 1: Beta-glucosidase

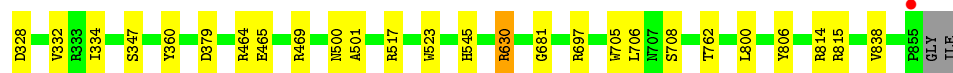


- Molecule 1: Beta-glucosidase

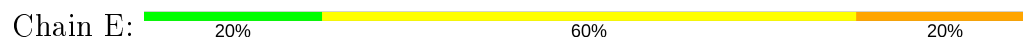


- Molecule 1: Beta-glucosidase





- 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



- 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



- 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




- 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



- 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



- 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%

MAG1
MAG2
BGL3
MAN4

- 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:  100%


MAG1
MAG2
BGL3
MAN4

- 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%

MAG1
MAG2
BGL3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

- 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:  11% 89%

MAG1
MAG2
BGL3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

- 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%

MAG1
MAG2
BGL3
MAN4

- 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:  11% 89%

MAG1
MAG2
BGL3
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:  50% 50%

NAG1
NAG2

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

Chain R:  100%

NAG1
NAG2

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

Chain Y:  100%

NAG1
NAG2

- 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

Chain O:  20% 80%

NAG1
NAG2
MAN3
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

Chain d:  10% 90%

NAG1
NAG2
MAN3
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

Chain P:  20% 80%



- 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: 30% 70%



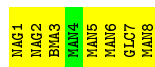
- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 11% 78% 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: 13% 88%



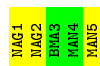
- Molecule 13: alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 100%



- 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 U: 40% 60%



- 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:  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 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

Chain a:  17% 83%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

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 48.04 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (118.51-2.20) 99.9 (48.04-2.20)	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)	0.33 , 36.2	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: GLC, BGC, NAG, BMA, MAN

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	0.74	0/6549	0.86	16/8954 (0.2%)
1	B	0.73	0/6555	0.87	14/8962 (0.2%)
1	C	0.74	0/6574	0.85	11/8988 (0.1%)
1	D	0.77	0/6561	0.86	14/8970 (0.2%)
All	All	0.74	0/26239	0.86	55/35874 (0.2%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	ARG	NE-CZ-NH2	-10.85	114.87	120.30
1	A	326	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	B	326	ARG	NE-CZ-NH1	9.67	125.13	120.30
1	B	72	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	A	326	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	D	630	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	A	630	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	C	814	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	C	118	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	A	759	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	434	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	630	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	D	464	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	B	517	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	343	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	D	517	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	517	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	434	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	D	133	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	C	631	ARG	NE-CZ-NH2	-6.08	117.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	72	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	797	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	434	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	D	814	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	133	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	517	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	200	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	D	200	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	101	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	469	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	D	133	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	D	815	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	580	ASP	CB-CG-OD1	5.57	123.31	118.30
1	C	793	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	D	200	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	D	123	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	200	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	98	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	C	814	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	D	630	ARG	CG-CD-NE	-5.44	100.37	111.80
1	A	815	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	B	98	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	101	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	200	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	C	277	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	478	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	150	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	82	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	C	333	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	773	ASP	CB-CG-OD1	5.07	122.86	118.30
1	C	631	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	D	517	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	200	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	517	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	C	797	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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	12	0
1	B	6379	0	6039	22	0
1	C	6388	0	6048	20	0
1	D	6382	0	6040	19	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
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	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	73	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 1.

All (73) 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: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: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
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:701:TYR:CZ	12:S:2:NAG:H82	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:495:CYS:HG	1:B:537:CYS:CB	2.27	0.48
1:C:107:PRO:HD3	1:C:388:ILE:HG23	1.95	0.48
1:B:495:CYS:SG	1:B:537:CYS:SG	3.00	0.47
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:C:778:LEU:HD23	1:C:778:LEU:C	2.35	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: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: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
21:B:1313:HOH:O	1:C:759:ARG:HD3	2.18	0.43
1:D:31:SER:HA	1:D:261:ASN:ND2	2.34	0.43
1:A:701:TYR:CZ	2:E:2:NAG:H82	2.54	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ARG:O	1:A:245:TYR:HB3	2.19	0.41
1:C:437:ASP:OD2	1:C:500:ASN:OD1	2.39	0.41
1:C:114:ALA:HB2	1:C:592:PRO:HD3	2.02	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: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%)	51	60
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 [i](#)

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%)	71	83
1	B	673/685 (98%)	664 (99%)	9 (1%)	69	81
1	C	675/685 (98%)	660 (98%)	15 (2%)	52	65
1	D	674/685 (98%)	665 (99%)	9 (1%)	69	81
All	All	2694/2740 (98%)	2653 (98%)	41 (2%)	65	78

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	ASP
1	A	278	TRP
1	A	363	GLU
1	A	371	GLN
1	A	685	ASN
1	A	687	SER
1	A	769	LYS
1	A	822	PRO
1	B	238	VAL
1	B	278	TRP
1	B	373	LYS
1	B	402	LYS
1	B	520	LEU
1	B	554	ASP
1	B	687	SER
1	B	790	LYS
1	B	833	THR
1	C	22	LEU
1	C	72	ARG
1	C	95	LEU
1	C	177	GLN
1	C	255	SER
1	C	278	TRP
1	C	373	LYS
1	C	520	LEU
1	C	531[A]	HIS
1	C	531[B]	HIS
1	C	682	GLN
1	C	685	ASN
1	C	762	THR

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Mol	Chain	Res	Type
1	C	790	LYS
1	C	831	ASN
1	D	83	LEU
1	D	88	LEU
1	D	123	ARG
1	D	200	ARG
1	D	204	GLN
1	D	278	TRP
1	D	347	SER
1	D	706	LEU
1	D	708	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	157	ASN
1	A	246	ASN
1	A	369	GLN
1	A	371	GLN
1	A	460	GLN
1	A	539	ASN
1	A	558	HIS
1	A	612	ASN
1	A	636	ASN
1	A	777	GLN
1	A	844	ASN
1	B	45	GLN
1	B	91	GLN
1	B	157	ASN
1	B	261	ASN
1	B	369	GLN
1	B	463	GLN
1	B	619	GLN
1	B	716	ASN
1	B	804	GLN
1	B	844	ASN
1	C	37	GLN
1	C	119	ASN
1	C	132	HIS
1	C	140	GLN
1	C	177	GLN

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Mol	Chain	Res	Type
1	C	196	GLN
1	C	261	ASN
1	C	463	GLN
1	C	491	GLN
1	C	539	ASN
1	C	558	HIS
1	C	612	ASN
1	C	618	GLN
1	C	660	GLN
1	D	37	GLN
1	D	45	GLN
1	D	132	HIS
1	D	216	ASN
1	D	250	ASN
1	D	261	ASN
1	D	282	HIS
1	D	371	GLN
1	D	463	GLN
1	D	470	ASN
1	D	491	GLN
1	D	618	GLN
1	D	656	GLN
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	1,2	14,14,15	0.49	0	17,19,21	1.05	1 (5%)
2	NAG	E	2	2	14,14,15	0.66	0	17,19,21	1.30	1 (5%)
2	BMA	E	3	2	11,11,12	1.05	1 (9%)	15,15,17	1.81	5 (33%)
2	MAN	E	4	2	11,11,12	0.44	0	15,15,17	1.50	2 (13%)
2	MAN	E	5	2	11,11,12	0.66	0	15,15,17	0.85	0
3	NAG	F	1	1,3	14,14,15	0.76	0	17,19,21	1.40	2 (11%)
3	NAG	F	2	3	14,14,15	0.54	0	17,19,21	0.72	0
3	BMA	F	3	3	11,11,12	0.23	0	15,15,17	1.45	3 (20%)
3	MAN	F	4	3	11,11,12	0.91	1 (9%)	15,15,17	1.31	2 (13%)
3	MAN	F	5	3	11,11,12	0.79	0	15,15,17	1.42	1 (6%)
3	MAN	F	6	3	11,11,12	0.75	0	15,15,17	1.12	1 (6%)
3	MAN	F	7	3	11,11,12	1.41	2 (18%)	15,15,17	2.07	6 (40%)
4	NAG	G	1	1,4	14,14,15	0.69	0	17,19,21	1.57	4 (23%)
4	NAG	G	2	4	14,14,15	0.61	0	17,19,21	1.26	1 (5%)
4	BMA	G	3	4	11,11,12	0.61	0	15,15,17	2.52	7 (46%)
4	MAN	G	4	4	11,11,12	0.97	0	15,15,17	1.63	2 (13%)
5	NAG	H	1	1,5	14,14,15	0.40	0	17,19,21	0.97	1 (5%)
5	NAG	H	2	5	14,14,15	0.96	1 (7%)	17,19,21	1.14	1 (5%)
5	BMA	H	3	5	11,11,12	0.67	0	15,15,17	0.92	0
5	MAN	H	4	5	11,11,12	0.51	0	15,15,17	1.40	3 (20%)
5	MAN	H	5	5	11,11,12	0.60	0	15,15,17	1.45	3 (20%)
5	MAN	H	6	5	11,11,12	0.72	0	15,15,17	1.43	3 (20%)
5	MAN	H	7	5	11,11,12	1.03	0	15,15,17	1.69	4 (26%)
5	MAN	H	8	5	11,11,12	0.62	0	15,15,17	1.85	5 (33%)
5	MAN	H	9	5	11,11,12	0.96	1 (9%)	15,15,17	1.46	3 (20%)
6	NAG	I	1	1,6	14,14,15	0.79	0	17,19,21	0.88	1 (5%)
6	NAG	I	2	6	14,14,15	0.61	0	17,19,21	1.64	2 (11%)
6	BMA	I	3	6	11,11,12	0.77	0	15,15,17	1.28	2 (13%)
6	MAN	I	4	6	11,11,12	0.86	0	15,15,17	1.48	1 (6%)
7	NAG	J	1	1,7	14,14,15	0.66	0	17,19,21	0.92	0
7	NAG	J	2	7	14,14,15	0.43	0	17,19,21	1.33	1 (5%)
7	BMA	J	3	7	11,11,12	0.70	0	15,15,17	1.43	3 (20%)
7	MAN	J	4	7	11,11,12	0.47	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
7	MAN	J	5	7	11,11,12	1.05	0	15,15,17	1.51	4 (26%)
7	MAN	J	6	7	11,11,12	0.91	1 (9%)	15,15,17	1.03	1 (6%)
7	MAN	J	7	7	11,11,12	0.95	0	15,15,17	1.59	1 (6%)
7	MAN	J	8	7	11,11,12	0.52	0	15,15,17	1.64	3 (20%)
7	MAN	J	9	7	11,11,12	0.58	0	15,15,17	1.24	2 (13%)
8	NAG	K	1	1,8	14,14,15	0.42	0	17,19,21	1.35	1 (5%)
8	NAG	K	2	8	14,14,15	0.50	0	17,19,21	1.03	0
4	NAG	L	1	1,4	14,14,15	0.60	0	17,19,21	0.92	0
4	NAG	L	2	4	14,14,15	0.50	0	17,19,21	1.20	2 (11%)
4	BMA	L	3	4	11,11,12	0.39	0	15,15,17	1.14	2 (13%)
4	MAN	L	4	4	11,11,12	0.69	0	15,15,17	1.47	3 (20%)
2	NAG	M	1	1,2	14,14,15	0.41	0	17,19,21	1.68	4 (23%)
2	NAG	M	2	2	14,14,15	0.51	0	17,19,21	1.04	0
2	BMA	M	3	2	11,11,12	0.48	0	15,15,17	1.78	4 (26%)
2	MAN	M	4	2	11,11,12	0.91	1 (9%)	15,15,17	1.60	4 (26%)
2	MAN	M	5	2	11,11,12	0.84	1 (9%)	15,15,17	1.93	5 (33%)
4	NAG	N	1	1,4	14,14,15	0.73	0	17,19,21	1.41	4 (23%)
4	NAG	N	2	4	14,14,15	0.65	0	17,19,21	2.01	5 (29%)
4	BMA	N	3	4	11,11,12	0.90	0	15,15,17	1.27	2 (13%)
4	MAN	N	4	4	11,11,12	0.91	0	15,15,17	1.31	2 (13%)
9	NAG	O	1	1,9	14,14,15	0.74	0	17,19,21	1.23	2 (11%)
9	MAN	O	10	9	11,11,12	1.03	0	15,15,17	1.70	5 (33%)
9	NAG	O	2	9	14,14,15	0.60	0	17,19,21	1.14	1 (5%)
9	BMA	O	3	9	11,11,12	0.45	0	15,15,17	0.85	0
9	MAN	O	4	9	11,11,12	0.53	0	15,15,17	1.09	2 (13%)
9	MAN	O	5	9	11,11,12	1.07	0	15,15,17	1.71	3 (20%)
9	MAN	O	6	9	11,11,12	0.94	0	15,15,17	1.18	2 (13%)
9	MAN	O	7	9	11,11,12	0.78	0	15,15,17	1.21	2 (13%)
9	MAN	O	8	9	11,11,12	0.61	0	15,15,17	1.85	5 (33%)
9	MAN	O	9	9	11,11,12	0.64	0	15,15,17	1.02	0
10	NAG	P	1	1,10	14,14,15	0.67	0	17,19,21	1.18	2 (11%)
10	NAG	P	2	10	14,14,15	0.65	0	17,19,21	1.01	0
10	BMA	P	3	10	11,11,12	0.69	0	15,15,17	1.36	1 (6%)
10	BMA	P	4	10	11,11,12	0.93	0	15,15,17	1.41	1 (6%)
10	MAN	P	5	10	11,11,12	0.95	0	15,15,17	1.47	4 (26%)
11	NAG	Q	1	1,11	14,14,15	0.57	0	17,19,21	1.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	MAN	Q	10	11	11,11,12	0.78	0	15,15,17	1.52	4 (26%)
11	NAG	Q	2	11	14,14,15	0.62	0	17,19,21	1.24	1 (5%)
11	BMA	Q	3	11	11,11,12	0.69	0	15,15,17	0.78	0
11	MAN	Q	4	11	11,11,12	0.64	0	15,15,17	1.45	2 (13%)
11	MAN	Q	5	11	11,11,12	0.89	0	15,15,17	1.49	4 (26%)
11	MAN	Q	6	11	11,11,12	0.77	0	15,15,17	1.13	0
11	MAN	Q	7	11	11,11,12	0.70	0	15,15,17	2.37	7 (46%)
11	MAN	Q	8	11	11,11,12	0.62	0	15,15,17	1.22	2 (13%)
11	MAN	Q	9	11	11,11,12	0.97	0	15,15,17	1.11	1 (6%)
8	NAG	R	1	1,8	14,14,15	0.75	0	17,19,21	1.74	3 (17%)
8	NAG	R	2	8	14,14,15	0.72	0	17,19,21	1.77	4 (23%)
12	NAG	S	1	1,12	14,14,15	0.45	0	17,19,21	1.05	1 (5%)
12	NAG	S	2	12	14,14,15	0.47	0	17,19,21	1.23	2 (11%)
12	BMA	S	3	12	11,11,12	0.61	0	15,15,17	1.33	2 (13%)
12	MAN	S	4	12	11,11,12	0.54	0	15,15,17	0.82	0
12	MAN	S	5	12	11,11,12	0.77	0	15,15,17	1.48	3 (20%)
12	MAN	S	6	12	11,11,12	1.06	1 (9%)	15,15,17	1.69	5 (33%)
12	MAN	S	7	12	11,11,12	1.08	1 (9%)	15,15,17	1.43	2 (13%)
12	MAN	S	8	12	11,11,12	0.93	0	15,15,17	1.24	1 (6%)
12	MAN	S	9	12	11,11,12	0.93	1 (9%)	15,15,17	1.25	2 (13%)
13	NAG	T	1	1,13	14,14,15	0.73	0	17,19,21	1.81	6 (35%)
13	NAG	T	2	13	14,14,15	0.77	0	17,19,21	1.10	1 (5%)
13	BMA	T	3	13	11,11,12	0.59	0	15,15,17	2.03	5 (33%)
13	MAN	T	4	13	11,11,12	0.59	0	15,15,17	1.09	0
13	MAN	T	5	13	11,11,12	0.79	0	15,15,17	1.17	1 (6%)
13	MAN	T	6	13	11,11,12	1.31	1 (9%)	15,15,17	1.62	3 (20%)
13	GLC	T	7	13	11,11,12	1.06	1 (9%)	15,15,17	1.82	3 (20%)
13	MAN	T	8	13	11,11,12	1.28	2 (18%)	15,15,17	1.73	4 (26%)
14	NAG	U	1	1,14	14,14,15	0.47	0	17,19,21	1.46	4 (23%)
14	NAG	U	2	14	14,14,15	0.46	0	17,19,21	1.62	3 (17%)
14	BMA	U	3	14	11,11,12	0.67	0	15,15,17	1.08	0
14	MAN	U	4	14	11,11,12	0.60	0	15,15,17	1.02	0
14	MAN	U	5	14	11,11,12	1.01	1 (9%)	15,15,17	1.47	3 (20%)
5	NAG	V	1	1,5	14,14,15	0.48	0	17,19,21	1.40	2 (11%)
5	NAG	V	2	5	14,14,15	0.47	0	17,19,21	1.01	0
5	BMA	V	3	5	11,11,12	0.81	1 (9%)	15,15,17	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	V	4	5	11,11,12	0.69	0	15,15,17	1.11	1 (6%)
5	MAN	V	5	5	11,11,12	0.58	0	15,15,17	1.20	1 (6%)
5	MAN	V	6	5	11,11,12	0.63	0	15,15,17	1.18	2 (13%)
5	MAN	V	7	5	11,11,12	0.67	0	15,15,17	1.37	3 (20%)
5	MAN	V	8	5	11,11,12	0.62	0	15,15,17	1.45	4 (26%)
5	MAN	V	9	5	11,11,12	1.00	1 (9%)	15,15,17	1.35	2 (13%)
15	NAG	W	1	1,15	14,14,15	0.63	0	17,19,21	1.52	3 (17%)
15	NAG	W	2	15	14,14,15	0.55	0	17,19,21	1.42	2 (11%)
15	BMA	W	3	15	11,11,12	0.67	0	15,15,17	1.20	1 (6%)
16	NAG	X	1	1,16	14,14,15	0.78	0	17,19,21	1.91	6 (35%)
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	0.65	0	15,15,17	1.44	3 (20%)
16	MAN	X	4	16	11,11,12	0.66	0	15,15,17	0.97	0
16	MAN	X	5	16	11,11,12	0.82	1 (9%)	15,15,17	1.53	2 (13%)
16	MAN	X	6	16	11,11,12	0.71	0	15,15,17	1.07	2 (13%)
16	MAN	X	7	16	11,11,12	0.63	0	15,15,17	0.83	0
16	MAN	X	8	16	11,11,12	1.19	1 (9%)	15,15,17	1.87	4 (26%)
8	NAG	Y	1	1,8	14,14,15	0.42	0	17,19,21	1.03	1 (5%)
8	NAG	Y	2	8	14,14,15	0.72	0	17,19,21	1.65	5 (29%)
15	NAG	Z	1	1,15	14,14,15	0.65	0	17,19,21	1.66	4 (23%)
15	NAG	Z	2	15	14,14,15	0.68	0	17,19,21	1.59	4 (23%)
15	BMA	Z	3	15	11,11,12	0.87	0	15,15,17	1.20	2 (13%)
17	NAG	a	1	1,17	14,14,15	0.59	0	17,19,21	1.41	3 (17%)
17	NAG	a	2	17	14,14,15	0.43	0	17,19,21	1.27	2 (11%)
17	BMA	a	3	17	11,11,12	0.61	0	15,15,17	1.01	1 (6%)
17	MAN	a	4	17	11,11,12	0.63	0	15,15,17	1.48	2 (13%)
17	MAN	a	5	17	11,11,12	0.83	0	15,15,17	1.06	1 (6%)
17	MAN	a	6	17	11,11,12	0.65	0	15,15,17	0.77	0
13	NAG	b	1	1,13	14,14,15	0.77	1 (7%)	17,19,21	1.14	1 (5%)
13	NAG	b	2	13	14,14,15	0.57	0	17,19,21	1.14	2 (11%)
13	BMA	b	3	13	11,11,12	0.63	0	15,15,17	1.32	2 (13%)
13	MAN	b	4	13	11,11,12	1.07	0	15,15,17	1.24	1 (6%)
13	MAN	b	5	13	11,11,12	0.59	0	15,15,17	1.17	1 (6%)
13	MAN	b	6	13	11,11,12	0.81	1 (9%)	15,15,17	1.42	2 (13%)
13	GLC	b	7	13	11,11,12	0.71	0	15,15,17	1.28	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	MAN	b	8	13	11,11,12	1.28	1 (9%)	15,15,17	1.83	4 (26%)
4	NAG	c	1	1,4	14,14,15	0.57	0	17,19,21	1.41	3 (17%)
4	NAG	c	2	4	14,14,15	0.86	0	17,19,21	1.87	4 (23%)
4	BMA	c	3	4	11,11,12	0.72	0	15,15,17	1.84	6 (40%)
4	MAN	c	4	4	11,11,12	0.78	0	15,15,17	1.04	1 (6%)
9	NAG	d	1	1,9	14,14,15	0.56	0	17,19,21	1.37	2 (11%)
9	MAN	d	10	9	11,11,12	0.71	0	15,15,17	1.30	2 (13%)
9	NAG	d	2	9	14,14,15	0.76	0	17,19,21	1.27	1 (5%)
9	BMA	d	3	9	11,11,12	0.77	0	15,15,17	1.07	0
9	MAN	d	4	9	11,11,12	0.54	0	15,15,17	1.11	1 (6%)
9	MAN	d	5	9	11,11,12	0.75	0	15,15,17	1.27	1 (6%)
9	MAN	d	6	9	11,11,12	0.71	0	15,15,17	0.98	1 (6%)
9	MAN	d	7	9	11,11,12	0.91	0	15,15,17	1.16	2 (13%)
9	MAN	d	8	9	11,11,12	0.61	0	15,15,17	1.37	2 (13%)
9	MAN	d	9	9	11,11,12	0.62	0	15,15,17	1.34	2 (13%)
15	NAG	e	1	1,15	14,14,15	0.76	0	17,19,21	1.13	2 (11%)
15	NAG	e	2	15	14,14,15	0.51	0	17,19,21	1.27	2 (11%)
15	BMA	e	3	15	11,11,12	0.68	0	15,15,17	1.30	3 (20%)
16	NAG	f	1	1,16	14,14,15	0.52	0	17,19,21	1.24	3 (17%)
16	NAG	f	2	16	14,14,15	0.84	1 (7%)	17,19,21	1.30	2 (11%)
16	BMA	f	3	16	11,11,12	0.51	0	15,15,17	0.91	0
16	MAN	f	4	16	11,11,12	0.69	0	15,15,17	0.86	0
16	MAN	f	5	16	11,11,12	0.91	0	15,15,17	1.46	1 (6%)
16	MAN	f	6	16	11,11,12	0.85	0	15,15,17	1.35	2 (13%)
16	MAN	f	7	16	11,11,12	0.82	0	15,15,17	1.02	1 (6%)
16	MAN	f	8	16	11,11,12	0.63	0	15,15,17	1.48	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	1,2	-	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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	M	1	1,2	-	0/6/23/26	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	1,4	-	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
4	MAN	N	4	4	-	2/2/19/22	0/1/1/1
9	NAG	O	1	1,9	-	0/6/23/26	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	1,10	-	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	1,11	-	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	1,12	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,13	-	1/6/23/26	0/1/1/1
13	NAG	T	2	13	-	0/6/23/26	0/1/1/1
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	1,14	-	0/6/23/26	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	1,5	-	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	1,15	-	0/6/23/26	0/1/1/1
15	NAG	W	2	15	-	0/6/23/26	0/1/1/1
15	BMA	W	3	15	-	0/2/19/22	0/1/1/1
16	NAG	X	1	1,16	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	Y	2	8	-	0/6/23/26	0/1/1/1
15	NAG	Z	1	1,15	-	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	1,17	-	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
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	1,13	-	0/6/23/26	0/1/1/1
13	NAG	b	2	13	-	2/6/23/26	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	1,4	-	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	1,9	-	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	1,15	-	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	1,16	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	6	MAN	C2-C3	3.63	1.57	1.52
12	S	6	MAN	C2-C3	2.77	1.56	1.52
13	b	8	MAN	C2-C3	2.64	1.56	1.52
5	V	9	MAN	C2-C3	2.47	1.56	1.52
2	M	4	MAN	C2-C3	2.42	1.56	1.52
2	E	3	BMA	C2-C3	2.40	1.56	1.52
14	U	5	MAN	C2-C3	2.37	1.56	1.52
13	T	8	MAN	C1-C2	2.35	1.57	1.52
5	H	9	MAN	C2-C3	2.33	1.55	1.52
16	X	8	MAN	C2-C3	2.28	1.55	1.52
16	f	2	NAG	C1-C2	-2.25	1.49	1.52
2	M	5	MAN	C2-C3	2.24	1.55	1.52
13	b	6	MAN	C2-C3	2.23	1.55	1.52
5	H	2	NAG	O5-C1	-2.22	1.40	1.43
3	F	7	MAN	C4-C5	2.22	1.57	1.53
5	V	3	BMA	O5-C1	-2.20	1.40	1.43
13	b	1	NAG	O5-C1	-2.19	1.40	1.43
13	T	8	MAN	C2-C3	2.18	1.55	1.52
12	S	9	MAN	C2-C3	2.16	1.55	1.52
13	T	7	GLC	C1-C2	2.12	1.57	1.52
16	X	5	MAN	C1-C2	2.04	1.56	1.52
3	F	7	MAN	C2-C3	2.04	1.55	1.52
7	J	6	MAN	C2-C3	2.04	1.55	1.52
3	F	4	MAN	C2-C3	2.03	1.55	1.52
12	S	7	MAN	C2-C3	2.03	1.55	1.52

All (360) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	7	GLC	C1-C2-C3	5.77	116.76	109.67
13	T	3	BMA	O5-C5-C6	5.72	116.17	107.20
11	Q	7	MAN	O5-C5-C6	5.13	115.25	107.20
6	I	2	NAG	C2-N2-C7	5.02	130.04	122.90
4	G	4	MAN	C1-O5-C5	4.84	118.76	112.19
8	R	1	NAG	C1-O5-C5	4.76	118.64	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	6	MAN	O2-C2-C3	4.74	119.62	110.14
16	X	5	MAN	O2-C2-C1	4.68	118.73	109.15
4	G	3	BMA	O5-C5-C6	-4.66	99.90	107.20
8	K	1	NAG	C1-O5-C5	4.65	118.49	112.19
14	U	2	NAG	C1-O5-C5	4.46	118.23	112.19
2	M	1	NAG	C1-O5-C5	4.45	118.23	112.19
8	R	2	NAG	O5-C1-C2	-4.38	104.37	111.29
11	Q	4	MAN	O5-C1-C2	-4.29	104.14	110.77
13	b	8	MAN	O5-C5-C6	4.24	113.86	107.20
6	I	4	MAN	C1-O5-C5	4.21	117.90	112.19
9	O	5	MAN	O5-C5-C6	4.20	113.80	107.20
16	X	8	MAN	C1-C2-C3	-3.99	104.76	109.67
4	N	2	NAG	O4-C4-C3	-3.97	101.17	110.35
9	O	8	MAN	C1-O5-C5	3.93	117.52	112.19
13	b	4	MAN	O5-C5-C6	3.93	113.37	107.20
2	M	5	MAN	O5-C5-C6	3.91	113.33	107.20
4	c	2	NAG	C8-C7-N2	-3.90	109.50	116.10
15	Z	2	NAG	C1-O5-C5	3.88	117.45	112.19
4	N	2	NAG	C8-C7-N2	-3.88	109.53	116.10
2	E	3	BMA	O5-C5-C6	3.84	113.22	107.20
8	Y	2	NAG	C1-O5-C5	3.75	117.27	112.19
16	f	5	MAN	O2-C2-C1	3.74	116.81	109.15
4	G	3	BMA	C1-C2-C3	3.74	114.26	109.67
17	a	4	MAN	C1-O5-C5	3.73	117.25	112.19
3	F	7	MAN	C1-C2-C3	3.66	114.17	109.67
9	O	8	MAN	C6-C5-C4	-3.64	104.48	113.00
4	G	3	BMA	C3-C4-C5	3.63	116.72	110.24
2	M	3	BMA	O5-C1-C2	-3.63	105.17	110.77
16	X	2	NAG	O4-C4-C3	-3.62	101.99	110.35
7	J	7	MAN	C1-C2-C3	3.61	114.11	109.67
15	Z	1	NAG	O3-C3-C2	-3.61	102.00	109.47
4	c	2	NAG	C2-N2-C7	3.60	128.04	122.90
4	G	3	BMA	C1-O5-C5	3.60	117.07	112.19
9	d	2	NAG	C1-C2-N2	-3.58	104.37	110.49
5	V	1	NAG	O3-C3-C2	-3.54	102.13	109.47
16	X	2	NAG	C1-C2-N2	3.54	116.53	110.49
5	H	7	MAN	C1-C2-C3	-3.52	105.33	109.67
4	c	2	NAG	O7-C7-N2	3.52	128.43	121.95
9	d	8	MAN	O5-C1-C2	-3.46	105.43	110.77
8	R	1	NAG	C1-C2-N2	-3.45	104.59	110.49
12	S	7	MAN	O5-C5-C6	3.44	112.59	107.20
13	T	8	MAN	C1-O5-C5	3.43	116.85	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	d	1	NAG	O4-C4-C5	-3.43	100.78	109.30
13	b	8	MAN	C1-O5-C5	3.43	116.84	112.19
2	M	5	MAN	O2-C2-C3	3.43	117.00	110.14
3	F	7	MAN	O5-C5-C6	3.42	112.57	107.20
16	X	1	NAG	O3-C3-C2	-3.42	102.40	109.47
15	Z	1	NAG	C1-O5-C5	3.39	116.79	112.19
5	H	8	MAN	C6-C5-C4	-3.39	105.06	113.00
16	X	8	MAN	O5-C5-C6	3.37	112.48	107.20
12	S	5	MAN	O2-C2-C3	-3.36	103.41	110.14
4	L	4	MAN	O5-C5-C6	3.36	112.46	107.20
3	F	5	MAN	C1-O5-C5	3.35	116.73	112.19
9	d	9	MAN	O4-C4-C3	-3.33	102.64	110.35
7	J	8	MAN	O5-C1-C2	-3.30	105.67	110.77
6	I	3	BMA	O5-C5-C6	3.27	112.33	107.20
4	c	3	BMA	O2-C2-C3	3.26	116.66	110.14
16	X	3	BMA	O5-C1-C2	-3.25	105.75	110.77
3	F	1	NAG	C2-N2-C7	3.25	127.53	122.90
9	O	10	MAN	C3-C4-C5	3.21	115.97	110.24
9	O	2	NAG	C1-C2-N2	-3.20	105.03	110.49
5	V	8	MAN	O2-C2-C3	3.19	116.53	110.14
13	T	1	NAG	O7-C7-N2	3.19	127.81	121.95
15	W	2	NAG	C2-N2-C7	3.18	127.44	122.90
5	H	8	MAN	C1-O5-C5	3.17	116.49	112.19
12	S	6	MAN	O3-C3-C2	3.16	116.05	109.99
7	J	8	MAN	C1-O5-C5	3.15	116.46	112.19
11	Q	7	MAN	C1-C2-C3	-3.15	105.79	109.67
13	T	8	MAN	C1-C2-C3	3.15	113.53	109.67
14	U	1	NAG	C1-C2-N2	-3.13	105.14	110.49
2	E	2	NAG	O3-C3-C2	-3.12	103.00	109.47
4	c	3	BMA	O4-C4-C3	-3.11	103.15	110.35
16	X	1	NAG	O4-C4-C5	-3.11	101.57	109.30
16	f	7	MAN	O2-C2-C1	3.09	115.47	109.15
10	P	5	MAN	O5-C1-C2	-3.09	106.01	110.77
3	F	3	BMA	O5-C1-C2	-3.08	106.01	110.77
12	S	3	BMA	O5-C5-C6	3.08	112.03	107.20
15	Z	3	BMA	O5-C5-C6	3.05	111.99	107.20
4	G	3	BMA	O4-C4-C3	-3.04	103.33	110.35
4	G	3	BMA	O3-C3-C4	-3.04	103.33	110.35
15	W	1	NAG	O7-C7-N2	3.03	127.52	121.95
11	Q	7	MAN	C3-C4-C5	-3.03	104.84	110.24
9	O	8	MAN	O3-C3-C4	-3.03	103.35	110.35
5	V	5	MAN	C1-O5-C5	3.00	116.26	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	6	MAN	O5-C1-C2	-3.00	106.15	110.77
4	N	3	BMA	C3-C4-C5	2.99	115.57	110.24
10	P	4	BMA	O5-C1-C2	-2.99	106.16	110.77
4	L	2	NAG	O4-C4-C5	-2.98	101.89	109.30
16	X	1	NAG	C2-N2-C7	2.98	127.15	122.90
7	J	9	MAN	O5-C1-C2	-2.98	106.17	110.77
5	V	9	MAN	C1-O5-C5	2.98	116.23	112.19
7	J	4	MAN	O2-C2-C3	-2.97	104.18	110.14
7	J	5	MAN	O2-C2-C1	2.97	115.23	109.15
3	F	1	NAG	C1-C2-N2	2.96	115.54	110.49
2	M	4	MAN	O2-C2-C3	2.96	116.06	110.14
7	J	4	MAN	O5-C1-C2	-2.94	106.24	110.77
9	d	10	MAN	O2-C2-C3	2.94	116.02	110.14
5	V	9	MAN	O2-C2-C3	2.93	116.02	110.14
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
3	F	7	MAN	O4-C4-C5	2.92	116.55	109.30
8	Y	2	NAG	C1-C2-N2	2.92	115.47	110.49
12	S	9	MAN	O5-C1-C2	-2.91	106.27	110.77
16	f	8	MAN	C3-C4-C5	2.91	115.43	110.24
4	N	1	NAG	O5-C1-C2	-2.91	106.70	111.29
17	a	2	NAG	O3-C3-C2	-2.90	103.46	109.47
5	H	7	MAN	O2-C2-C3	2.90	115.95	110.14
11	Q	10	MAN	C3-C4-C5	2.90	115.41	110.24
11	Q	7	MAN	O3-C3-C2	2.90	115.54	109.99
8	R	2	NAG	C1-O5-C5	2.89	116.11	112.19
4	G	1	NAG	C1-C2-N2	-2.89	105.56	110.49
5	V	7	MAN	O5-C1-C2	-2.88	106.32	110.77
13	b	3	BMA	O4-C4-C3	-2.88	103.69	110.35
5	H	9	MAN	C2-C3-C4	2.87	115.87	110.89
16	f	6	MAN	O4-C4-C5	2.87	116.42	109.30
13	T	1	NAG	C2-N2-C7	2.87	126.98	122.90
16	f	1	NAG	O3-C3-C2	-2.86	103.55	109.47
4	N	4	MAN	O5-C5-C6	2.86	111.69	107.20
5	H	4	MAN	O2-C2-C1	2.85	114.98	109.15
16	X	8	MAN	O2-C2-C3	2.84	115.83	110.14
9	d	8	MAN	C6-C5-C4	-2.81	106.41	113.00
16	f	2	NAG	O5-C1-C2	-2.80	106.87	111.29
13	b	6	MAN	O2-C2-C3	2.79	115.72	110.14
5	H	7	MAN	O2-C2-C1	2.78	114.85	109.15
2	E	4	MAN	O5-C1-C2	-2.78	106.47	110.77
11	Q	10	MAN	C1-O5-C5	-2.78	108.42	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	d	7	MAN	O5-C1-C2	-2.78	106.48	110.77
16	X	8	MAN	O5-C1-C2	-2.77	106.49	110.77
4	c	4	MAN	O5-C1-C2	-2.77	106.49	110.77
2	M	5	MAN	O3-C3-C2	2.77	115.31	109.99
7	J	6	MAN	O5-C5-C6	2.77	111.55	107.20
14	U	5	MAN	C1-C2-C3	2.75	113.05	109.67
16	f	1	NAG	O4-C4-C5	-2.75	102.46	109.30
15	W	1	NAG	C2-N2-C7	2.75	126.81	122.90
3	F	3	BMA	O5-C5-C6	2.74	111.50	107.20
13	T	1	NAG	C4-C3-C2	-2.74	107.00	111.02
17	a	1	NAG	O4-C4-C5	-2.74	102.50	109.30
6	I	2	NAG	O7-C7-N2	2.73	126.98	121.95
5	H	9	MAN	O5-C5-C6	2.73	111.49	107.20
13	T	7	GLC	O5-C5-C6	2.72	111.47	107.20
11	Q	7	MAN	O2-C2-C3	2.71	115.57	110.14
10	P	5	MAN	O5-C5-C6	2.71	111.45	107.20
2	M	5	MAN	C1-O5-C5	2.71	115.86	112.19
9	O	1	NAG	O4-C4-C5	-2.69	102.61	109.30
13	T	3	BMA	O4-C4-C3	-2.68	104.15	110.35
2	E	3	BMA	O2-C2-C1	2.68	114.64	109.15
9	O	10	MAN	O5-C5-C6	2.68	111.40	107.20
7	J	2	NAG	O4-C4-C3	-2.67	104.18	110.35
17	a	2	NAG	O4-C4-C5	-2.65	102.71	109.30
13	T	8	MAN	O5-C5-C6	2.65	111.36	107.20
13	b	6	MAN	O5-C1-C2	-2.65	106.69	110.77
12	S	1	NAG	C2-N2-C7	2.64	126.66	122.90
13	T	2	NAG	O5-C1-C2	-2.64	107.13	111.29
12	S	5	MAN	O2-C2-C1	2.63	114.53	109.15
9	O	6	MAN	O5-C1-C2	-2.63	106.72	110.77
5	H	8	MAN	O5-C5-C6	2.62	111.32	107.20
16	X	6	MAN	O5-C5-C6	2.62	111.31	107.20
2	M	4	MAN	O2-C2-C1	-2.61	103.81	109.15
5	H	4	MAN	O6-C6-C5	-2.59	102.39	111.29
15	Z	2	NAG	C4-C3-C2	-2.59	107.22	111.02
2	M	4	MAN	O5-C5-C6	2.58	111.25	107.20
11	Q	7	MAN	O5-C5-C4	-2.58	104.55	110.83
10	P	3	BMA	O5-C1-C2	-2.58	106.80	110.77
12	S	6	MAN	O2-C2-C1	-2.57	103.89	109.15
11	Q	5	MAN	O4-C4-C5	2.57	115.67	109.30
16	X	1	NAG	O7-C7-C8	-2.57	117.29	122.06
2	E	3	BMA	C6-C5-C4	2.56	119.01	113.00
13	T	1	NAG	C1-C2-N2	2.56	114.87	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	e	3	BMA	C1-C2-C3	-2.55	106.53	109.67
5	V	8	MAN	O5-C5-C6	2.55	111.20	107.20
4	L	3	BMA	O5-C5-C6	2.55	111.20	107.20
12	S	3	BMA	O5-C5-C4	-2.54	104.64	110.83
7	J	5	MAN	O5-C5-C6	2.52	111.16	107.20
11	Q	8	MAN	O4-C4-C3	-2.52	104.52	110.35
11	Q	7	MAN	C1-O5-C5	2.52	115.61	112.19
13	T	1	NAG	O7-C7-C8	-2.52	117.38	122.06
12	S	7	MAN	O2-C2-C3	2.52	115.18	110.14
2	M	4	MAN	O3-C3-C2	2.51	114.81	109.99
9	d	9	MAN	C1-C2-C3	2.49	112.73	109.67
16	X	2	NAG	C1-O5-C5	-2.48	108.83	112.19
14	U	2	NAG	O7-C7-N2	2.47	126.50	121.95
15	W	2	NAG	O7-C7-N2	2.47	126.49	121.95
14	U	1	NAG	C1-O5-C5	2.47	115.54	112.19
4	G	2	NAG	C2-N2-C7	2.47	126.41	122.90
13	b	8	MAN	C1-C2-C3	2.46	112.69	109.67
4	N	2	NAG	O5-C5-C6	2.46	111.06	107.20
4	c	1	NAG	C1-C2-N2	-2.46	106.29	110.49
16	f	8	MAN	C1-O5-C5	-2.45	108.88	112.19
4	N	1	NAG	O5-C5-C6	2.45	111.04	107.20
4	N	4	MAN	C1-C2-C3	2.44	112.67	109.67
9	d	6	MAN	O5-C1-C2	-2.44	107.01	110.77
13	b	8	MAN	O5-C1-C2	-2.44	107.01	110.77
2	M	3	BMA	O5-C5-C6	2.43	111.02	107.20
16	f	2	NAG	O4-C4-C3	-2.43	104.72	110.35
13	T	3	BMA	C1-O5-C5	2.43	115.49	112.19
9	d	4	MAN	O5-C5-C6	2.43	111.02	107.20
3	F	7	MAN	C6-C5-C4	2.43	118.70	113.00
15	Z	2	NAG	O4-C4-C5	2.43	115.32	109.30
12	S	6	MAN	O5-C1-C2	-2.42	107.03	110.77
2	M	3	BMA	O4-C4-C3	-2.42	104.75	110.35
4	c	3	BMA	C3-C4-C5	2.42	114.55	110.24
17	a	1	NAG	C1-C2-N2	-2.42	106.36	110.49
5	H	5	MAN	O5-C1-C2	-2.41	107.04	110.77
5	V	6	MAN	C6-C5-C4	-2.41	107.35	113.00
2	E	1	NAG	C1-C2-N2	-2.40	106.39	110.49
12	S	5	MAN	O4-C4-C3	-2.40	104.81	110.35
4	L	2	NAG	O5-C5-C6	2.39	110.95	107.20
16	X	3	BMA	C1-O5-C5	2.39	115.43	112.19
13	T	6	MAN	O3-C3-C2	2.39	114.57	109.99
2	M	1	NAG	C2-N2-C7	2.39	126.30	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	2	NAG	C1-C2-N2	-2.38	106.42	110.49
4	G	1	NAG	O5-C1-C2	-2.38	107.53	111.29
9	d	7	MAN	C1-O5-C5	2.38	115.42	112.19
4	c	3	BMA	O2-C2-C1	-2.37	104.30	109.15
16	X	2	NAG	O5-C5-C6	2.37	110.91	107.20
13	T	1	NAG	O5-C5-C6	-2.36	103.50	107.20
5	V	1	NAG	C1-C2-N2	2.36	114.52	110.49
5	H	7	MAN	O3-C3-C4	2.36	115.81	110.35
2	M	5	MAN	C6-C5-C4	-2.36	107.47	113.00
10	P	5	MAN	O3-C3-C2	2.36	114.51	109.99
3	F	7	MAN	C2-C3-C4	-2.36	106.82	110.89
9	O	10	MAN	C2-C3-C4	2.36	114.97	110.89
5	H	9	MAN	O2-C2-C3	2.36	114.86	110.14
5	V	6	MAN	O5-C1-C2	-2.35	107.14	110.77
2	M	1	NAG	O5-C1-C2	-2.35	107.58	111.29
14	U	2	NAG	O4-C4-C5	-2.35	103.47	109.30
15	e	2	NAG	C2-N2-C7	2.34	126.24	122.90
7	J	5	MAN	C1-O5-C5	2.34	115.36	112.19
15	W	3	BMA	O5-C5-C6	2.34	110.87	107.20
13	T	3	BMA	O5-C5-C4	-2.34	105.13	110.83
9	O	7	MAN	O2-C2-C3	-2.34	105.45	110.14
16	X	1	NAG	O7-C7-N2	2.33	126.23	121.95
11	Q	5	MAN	C1-O5-C5	2.33	115.35	112.19
3	F	7	MAN	O3-C3-C2	2.32	114.44	109.99
2	E	4	MAN	C1-O5-C5	2.32	115.34	112.19
15	Z	1	NAG	O7-C7-N2	2.32	126.22	121.95
5	H	6	MAN	O2-C2-C3	-2.32	105.50	110.14
13	T	8	MAN	O2-C2-C1	2.32	113.89	109.15
5	V	4	MAN	O6-C6-C5	-2.31	103.36	111.29
17	a	3	BMA	C3-C4-C5	2.31	114.35	110.24
15	e	1	NAG	C1-O5-C5	2.30	115.31	112.19
15	e	3	BMA	O5-C5-C6	2.30	110.81	107.20
16	X	5	MAN	O2-C2-C3	-2.30	105.54	110.14
4	G	1	NAG	C4-C3-C2	-2.29	107.66	111.02
15	W	1	NAG	C8-C7-N2	-2.28	112.24	116.10
11	Q	5	MAN	O3-C3-C2	2.27	114.35	109.99
9	O	8	MAN	O4-C4-C5	2.27	114.94	109.30
16	f	8	MAN	O4-C4-C5	-2.27	103.66	109.30
4	N	1	NAG	C1-C2-N2	-2.27	106.62	110.49
11	Q	2	NAG	O4-C4-C3	-2.26	105.12	110.35
6	I	3	BMA	O5-C5-C4	-2.26	105.33	110.83
9	O	10	MAN	O2-C2-C3	2.26	114.66	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	S	9	MAN	O5-C5-C6	2.26	110.74	107.20
13	b	2	NAG	O3-C3-C2	-2.25	104.80	109.47
14	U	1	NAG	O4-C4-C5	-2.25	103.72	109.30
4	G	3	BMA	O2-C2-C1	-2.25	104.56	109.15
5	H	5	MAN	O2-C2-C3	-2.25	105.64	110.14
9	O	8	MAN	O5-C1-C2	-2.24	107.31	110.77
9	O	4	MAN	O6-C6-C5	-2.24	103.61	111.29
14	U	5	MAN	O4-C4-C5	2.24	114.86	109.30
12	S	6	MAN	C1-C2-C3	2.24	112.42	109.67
4	c	3	BMA	C1-O5-C5	2.24	115.22	112.19
5	H	6	MAN	C1-O5-C5	2.24	115.22	112.19
7	J	3	BMA	C1-O5-C5	2.24	115.22	112.19
8	Y	2	NAG	C6-C5-C4	-2.23	107.78	113.00
2	E	3	BMA	O5-C5-C4	-2.23	105.40	110.83
15	e	3	BMA	O2-C2-C1	2.23	113.71	109.15
12	S	2	NAG	C2-N2-C7	-2.22	119.74	122.90
8	R	1	NAG	C2-N2-C7	2.22	126.06	122.90
4	N	2	NAG	O4-C4-C5	2.22	114.81	109.30
7	J	3	BMA	C1-C2-C3	2.22	112.39	109.67
12	S	6	MAN	O2-C2-C3	2.22	114.58	110.14
11	Q	10	MAN	O2-C2-C3	2.21	114.57	110.14
9	O	5	MAN	C1-C2-C3	-2.21	106.95	109.67
10	P	1	NAG	C2-N2-C7	2.21	126.05	122.90
17	a	1	NAG	C2-N2-C7	2.20	126.04	122.90
10	P	5	MAN	C1-O5-C5	2.20	115.17	112.19
13	b	2	NAG	C4-C3-C2	-2.19	107.80	111.02
13	T	3	BMA	O2-C2-C3	2.19	114.53	110.14
15	Z	1	NAG	O5-C5-C4	-2.18	105.52	110.83
5	H	1	NAG	C1-C2-N2	-2.18	106.76	110.49
8	Y	2	NAG	O5-C1-C2	-2.18	107.85	111.29
4	N	1	NAG	C1-O5-C5	2.17	115.13	112.19
11	Q	4	MAN	O2-C2-C3	-2.17	105.79	110.14
8	Y	2	NAG	O5-C5-C6	2.17	110.60	107.20
11	Q	10	MAN	O4-C4-C3	-2.16	105.35	110.35
5	V	7	MAN	C1-C2-C3	-2.16	107.01	109.67
14	U	1	NAG	O5-C1-C2	-2.16	107.88	111.29
2	M	1	NAG	C4-C3-C2	-2.16	107.85	111.02
3	F	6	MAN	O3-C3-C2	2.15	114.12	109.99
14	U	5	MAN	O3-C3-C2	2.15	114.11	109.99
10	P	1	NAG	C1-O5-C5	2.15	115.10	112.19
13	T	6	MAN	O5-C5-C6	2.15	110.57	107.20
15	Z	2	NAG	C1-C2-N2	2.14	114.15	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	e	1	NAG	O3-C3-C4	-2.14	105.41	110.35
4	N	3	BMA	O5-C1-C2	-2.14	107.47	110.77
5	H	8	MAN	O4-C4-C3	-2.14	105.41	110.35
5	H	5	MAN	O2-C2-C1	2.14	113.52	109.15
16	X	1	NAG	O5-C5-C6	-2.13	103.86	107.20
5	H	4	MAN	C1-O5-C5	2.13	115.08	112.19
9	O	1	NAG	O3-C3-C2	-2.13	105.07	109.47
4	c	1	NAG	O5-C5-C6	2.12	110.52	107.20
7	J	5	MAN	O3-C3-C4	2.11	115.22	110.35
16	X	6	MAN	C3-C4-C5	2.11	114.00	110.24
16	X	3	BMA	O6-C6-C5	-2.10	104.09	111.29
15	Z	3	BMA	O5-C1-C2	-2.10	107.53	110.77
9	O	10	MAN	O4-C4-C5	-2.09	104.10	109.30
9	d	10	MAN	C3-C4-C5	2.09	113.97	110.24
13	b	5	MAN	O4-C4-C5	2.09	114.49	109.30
5	V	8	MAN	O5-C1-C2	-2.09	107.55	110.77
11	Q	9	MAN	C6-C5-C4	-2.09	108.12	113.00
12	S	8	MAN	O2-C2-C1	2.09	113.42	109.15
17	a	4	MAN	O3-C3-C4	-2.08	105.53	110.35
5	H	8	MAN	O2-C2-C1	2.08	113.41	109.15
5	V	8	MAN	O4-C4-C3	-2.08	105.55	110.35
16	f	6	MAN	C2-C3-C4	-2.08	107.30	110.89
8	R	2	NAG	O4-C4-C5	2.08	114.45	109.30
9	d	5	MAN	O5-C1-C2	-2.08	107.57	110.77
8	R	2	NAG	O3-C3-C4	-2.07	105.56	110.35
9	O	7	MAN	O5-C5-C6	-2.07	103.96	107.20
4	G	4	MAN	O5-C1-C2	-2.06	107.59	110.77
13	b	7	GLC	C6-C5-C4	2.06	117.83	113.00
11	Q	5	MAN	O5-C5-C6	2.06	110.44	107.20
6	I	1	NAG	O4-C4-C5	-2.06	104.18	109.30
4	G	1	NAG	O4-C4-C5	-2.06	104.19	109.30
2	M	3	BMA	O3-C3-C4	-2.06	105.59	110.35
9	O	4	MAN	O3-C3-C4	-2.06	105.59	110.35
9	d	1	NAG	O3-C3-C4	2.05	115.10	110.35
12	S	2	NAG	C4-C3-C2	-2.05	108.01	111.02
4	c	3	BMA	O3-C3-C2	2.05	113.93	109.99
4	L	4	MAN	O2-C2-C3	2.04	114.23	110.14
5	V	7	MAN	O2-C2-C3	2.03	114.20	110.14
7	J	3	BMA	O2-C2-C1	-2.03	105.00	109.15
13	b	1	NAG	C4-C3-C2	-2.03	108.05	111.02
13	T	5	MAN	O4-C4-C5	2.03	114.33	109.30
17	a	5	MAN	O5-C5-C6	2.02	110.38	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	O	5	MAN	O5-C1-C2	-2.02	107.65	110.77
3	F	3	BMA	C6-C5-C4	-2.02	108.27	113.00
3	F	4	MAN	O5-C1-C2	-2.02	107.65	110.77
7	J	8	MAN	O3-C3-C2	2.02	113.86	109.99
2	E	3	BMA	C1-O5-C5	-2.02	109.45	112.19
9	O	6	MAN	C1-C2-C3	2.02	112.15	109.67
4	L	4	MAN	O3-C3-C4	-2.02	105.69	110.35
4	L	3	BMA	O5-C5-C4	-2.02	105.92	110.83
4	c	2	NAG	C6-C5-C4	-2.02	108.28	113.00
16	f	1	NAG	O3-C3-C4	2.02	115.01	110.35
13	b	3	BMA	O3-C3-C2	-2.01	106.14	109.99
7	J	4	MAN	O4-C4-C3	-2.01	105.70	110.35
11	Q	8	MAN	O2-C2-C1	2.01	113.27	109.15
7	J	9	MAN	O5-C5-C6	2.01	110.36	107.20
13	T	7	GLC	O2-C2-C3	-2.01	106.12	110.14
15	e	2	NAG	C8-C7-N2	-2.00	112.71	116.10
3	F	4	MAN	O2-C2-C1	-2.00	105.06	109.15
8	Y	1	NAG	O3-C3-C2	-2.00	105.33	109.47

There are no chirality outliers.

All (100) torsion outliers are listed below:

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

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

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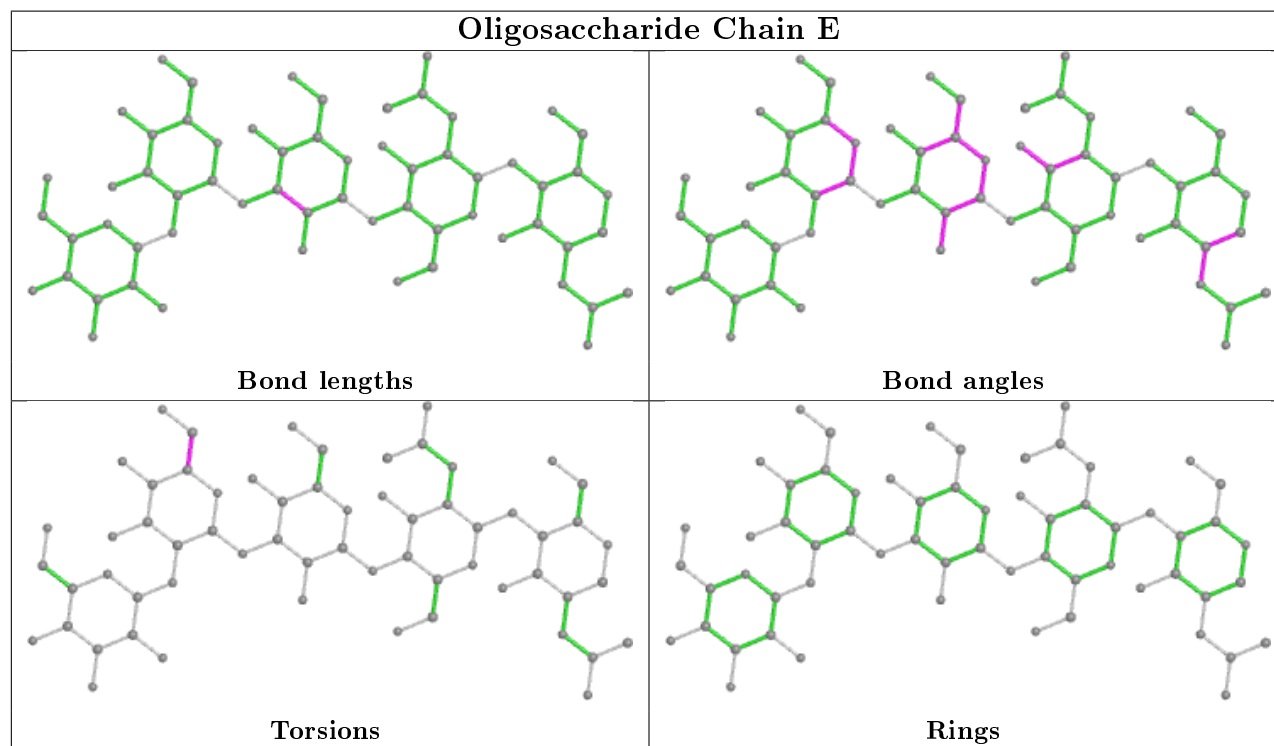
Mol	Chain	Res	Type	Atoms
3	F	5	MAN	O5-C5-C6-O6
17	a	6	MAN	O5-C5-C6-O6
9	O	6	MAN	C4-C5-C6-O6
9	O	9	MAN	O5-C5-C6-O6
13	b	6	MAN	O5-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
17	a	4	MAN	C4-C5-C6-O6
14	U	4	MAN	O5-C5-C6-O6
4	c	4	MAN	O5-C5-C6-O6
9	d	2	NAG	O5-C5-C6-O6
14	U	5	MAN	C4-C5-C6-O6
5	V	9	MAN	C4-C5-C6-O6
17	a	4	MAN	O5-C5-C6-O6
16	X	7	MAN	O5-C5-C6-O6
9	O	7	MAN	C4-C5-C6-O6
12	S	3	BMA	O5-C5-C6-O6
9	d	9	MAN	C4-C5-C6-O6
12	S	5	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
12	S	5	MAN	O5-C5-C6-O6
11	Q	8	MAN	O5-C5-C6-O6
7	J	6	MAN	C4-C5-C6-O6
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

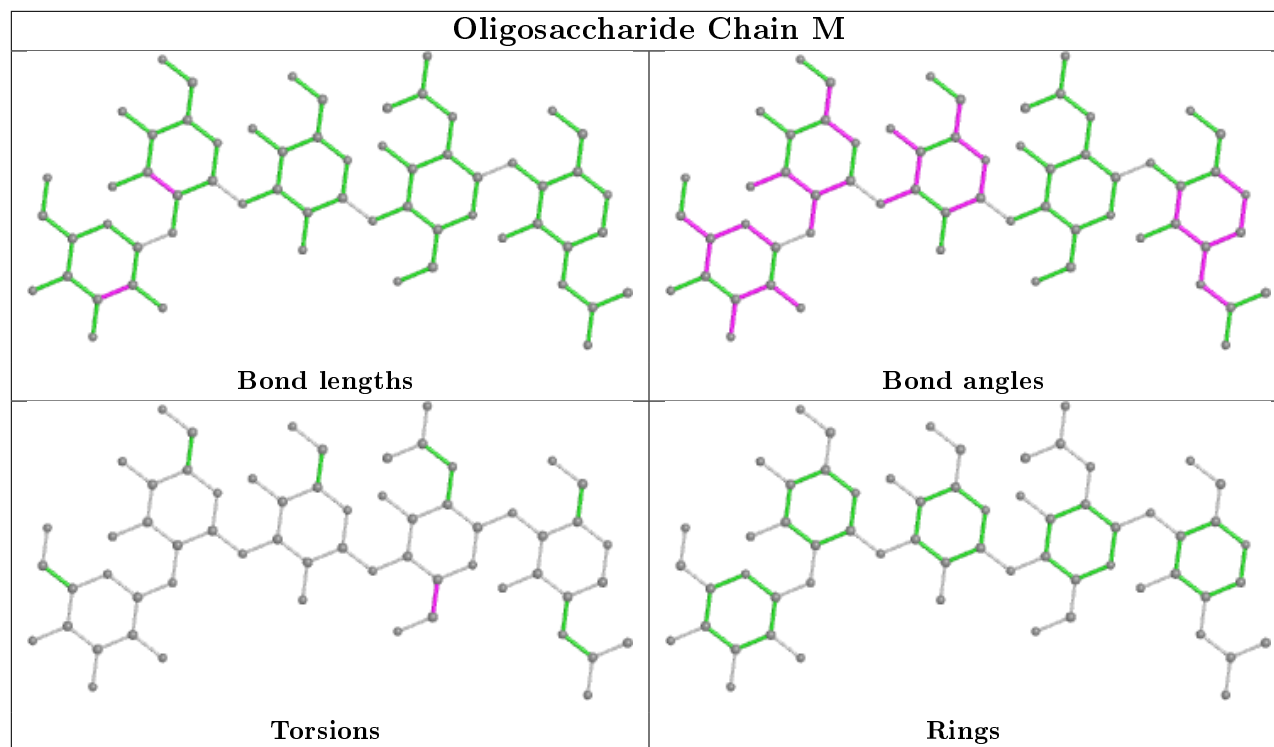
There are no ring outliers.

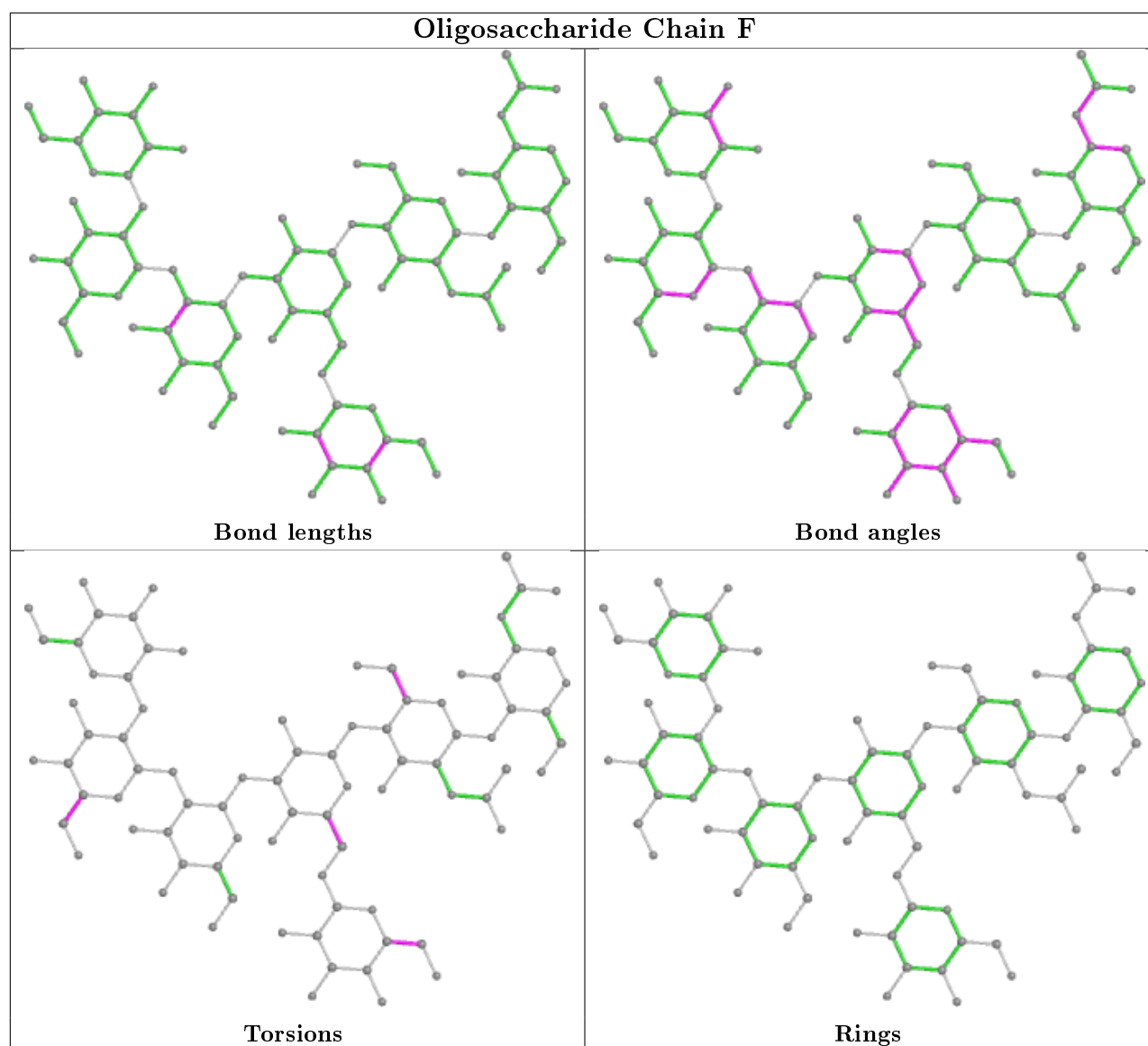
3 monomers are involved in 3 short contacts:

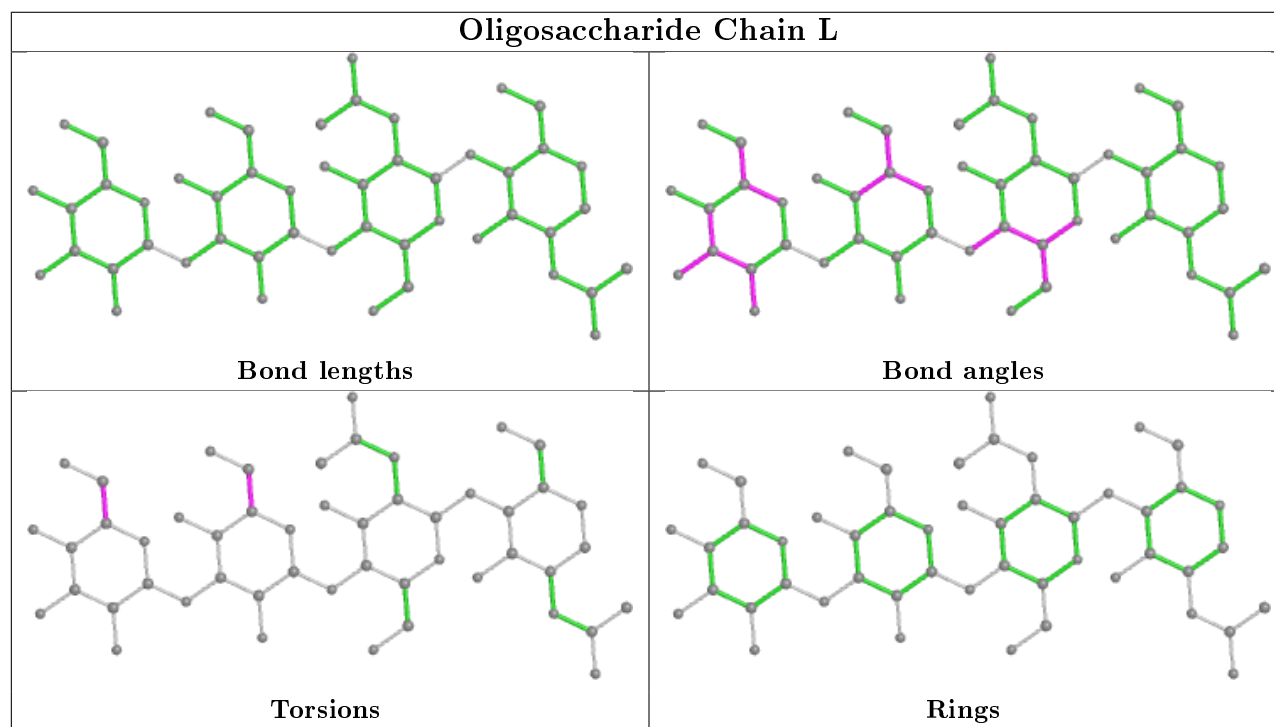
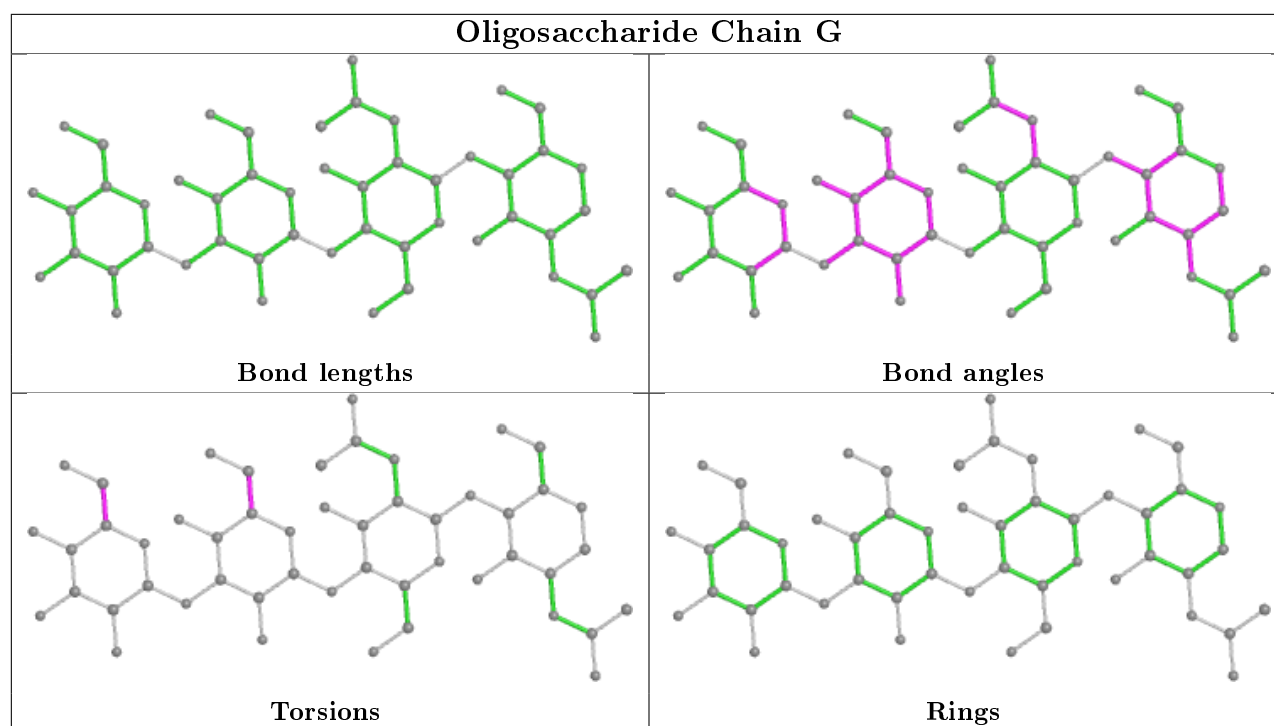
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
4	L	4	MAN	1	0
12	S	2	NAG	1	0

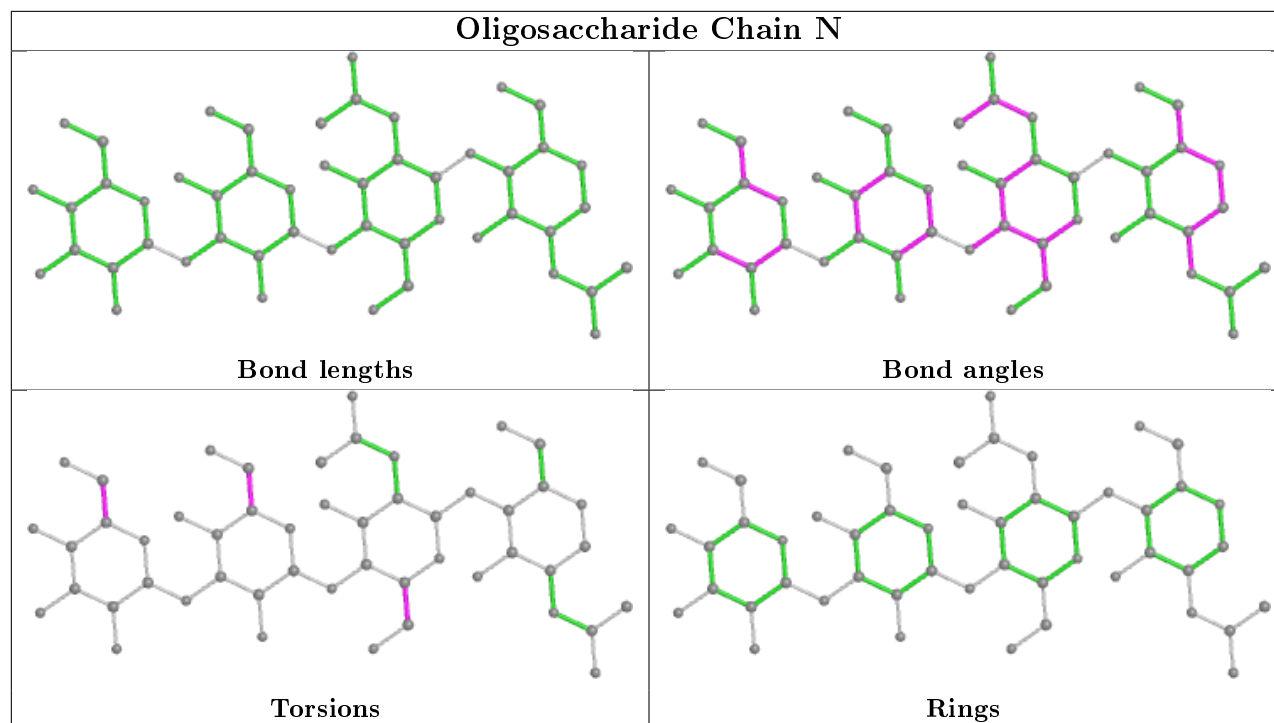
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

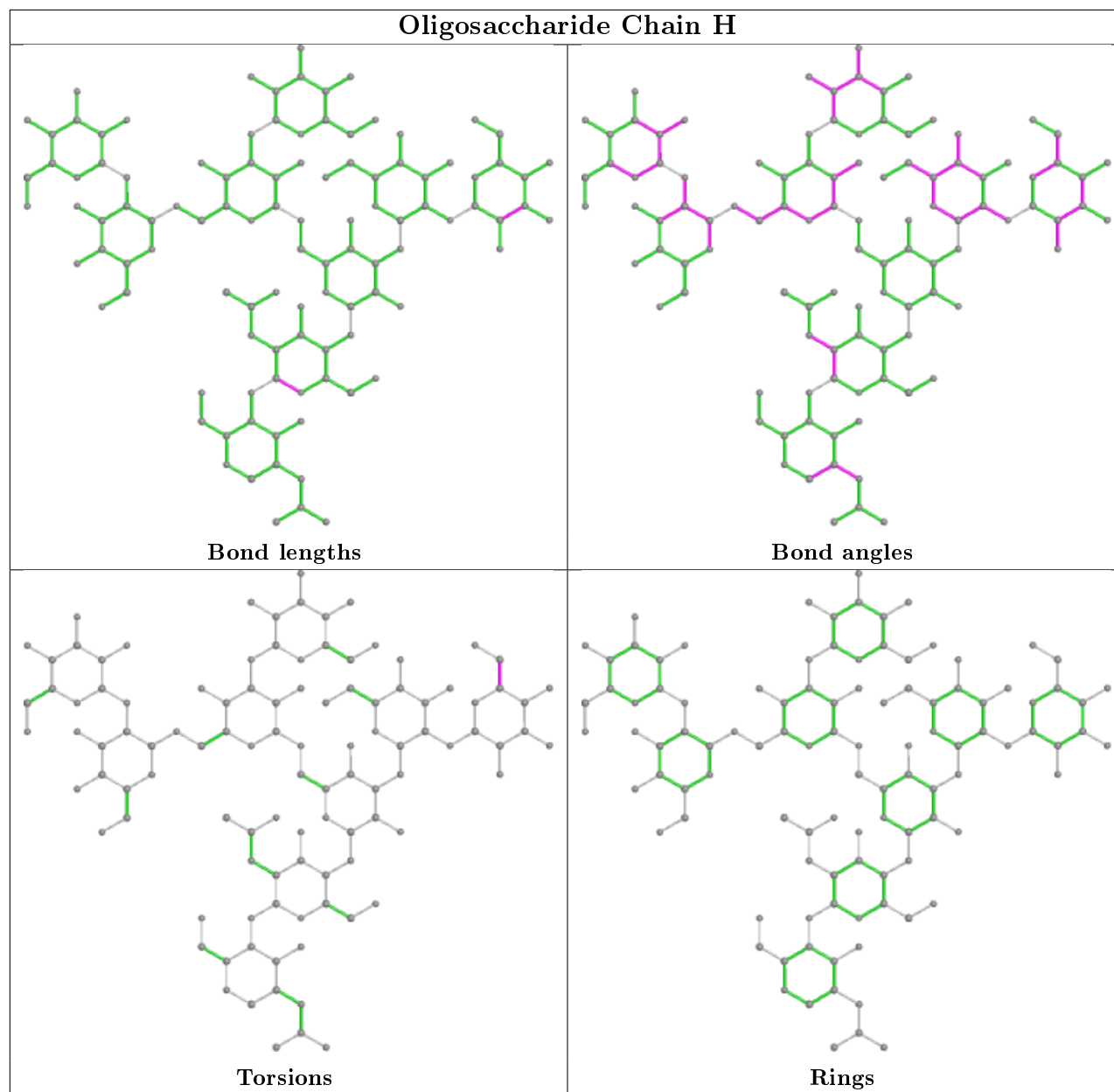


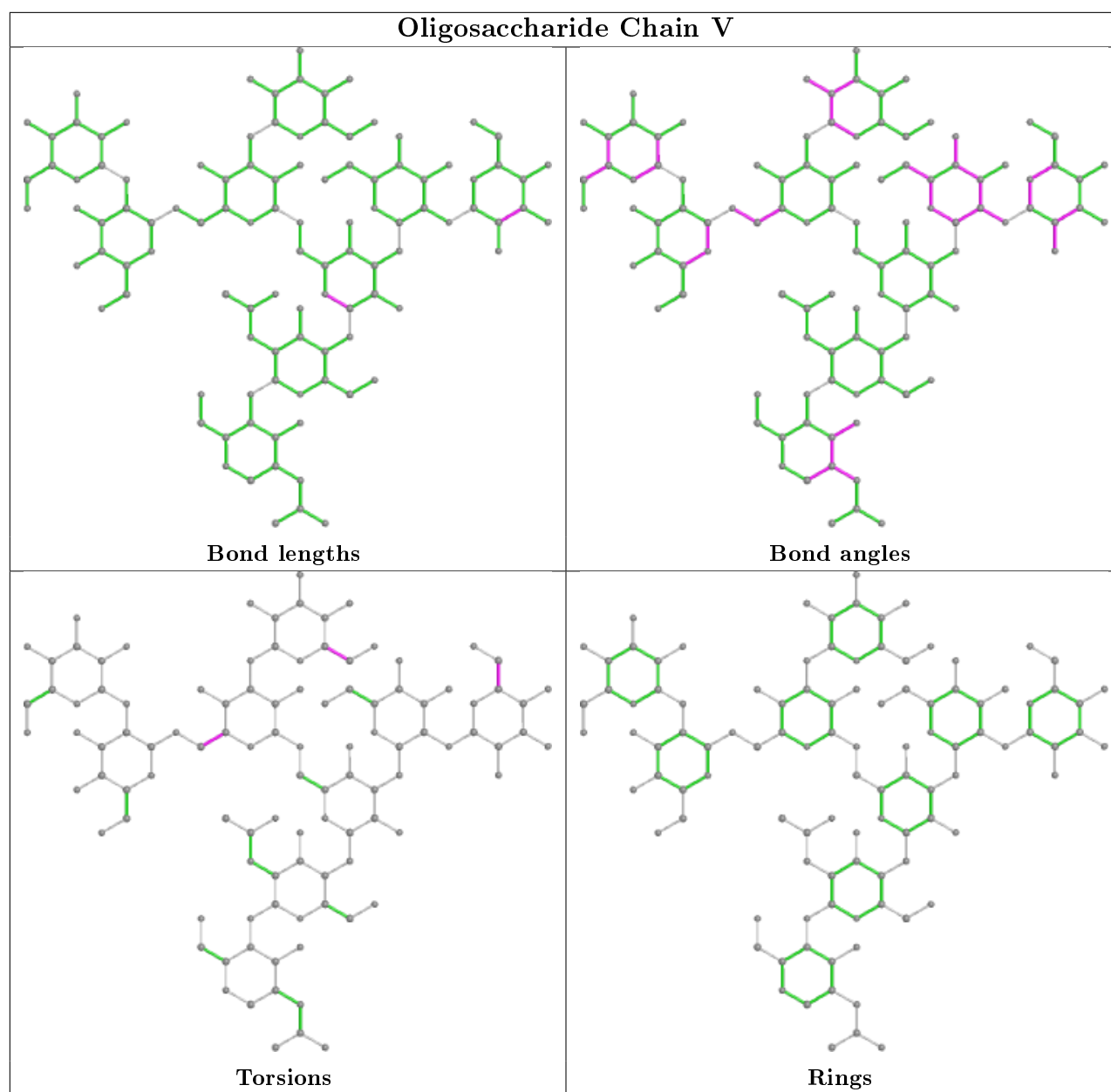


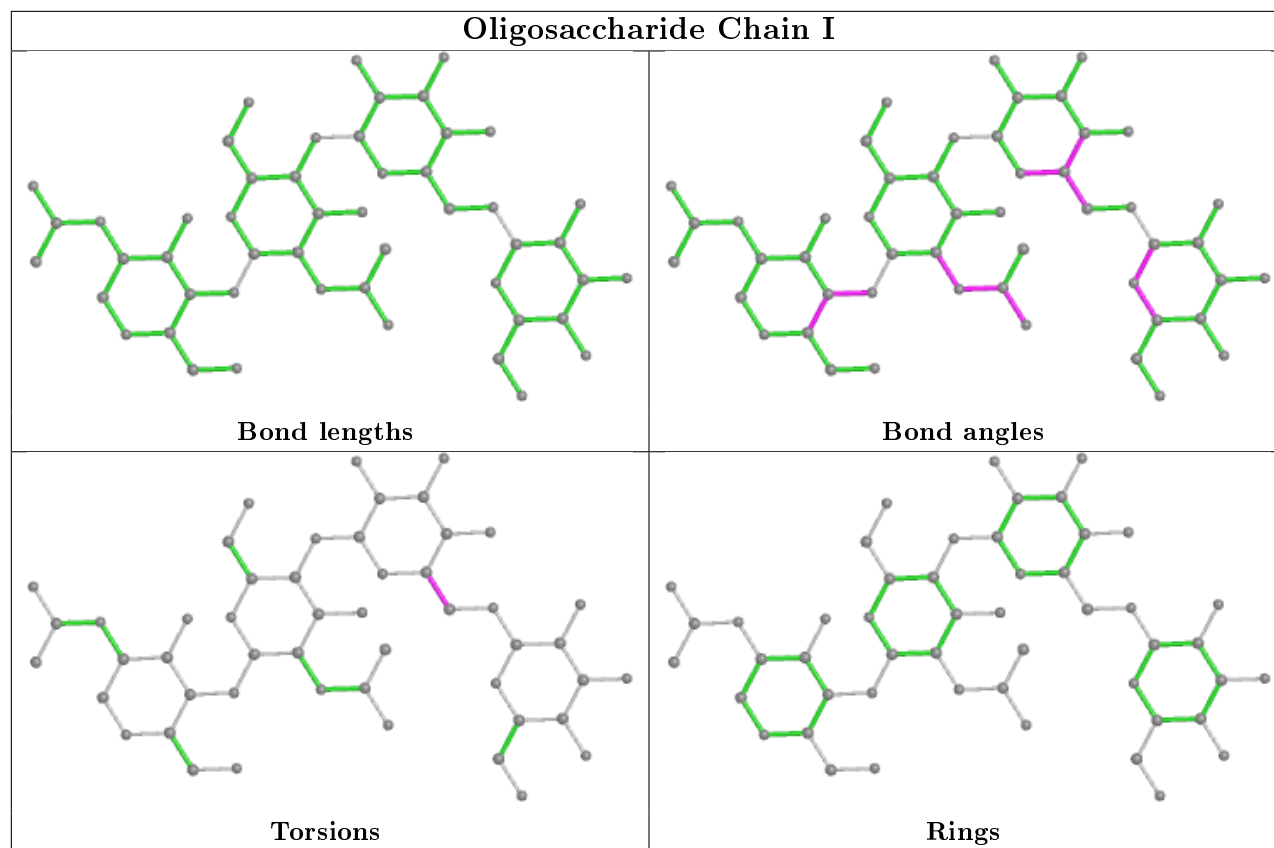


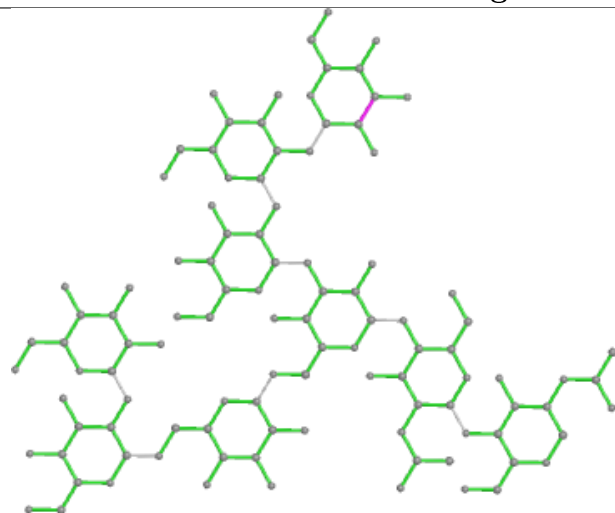
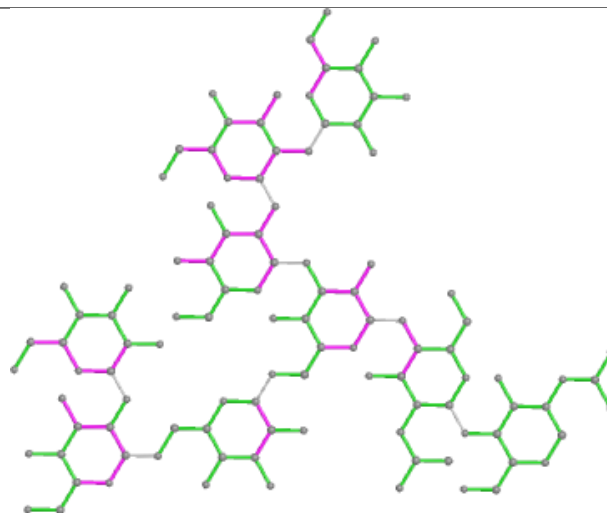
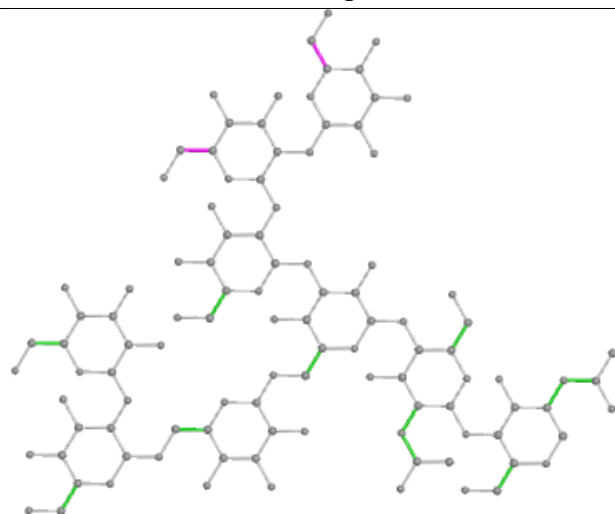
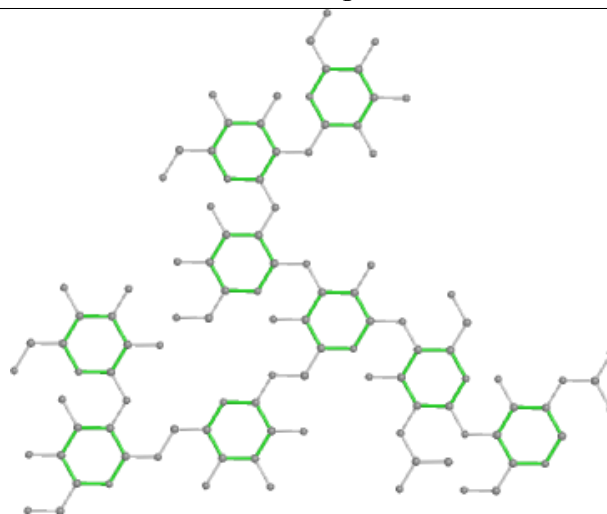


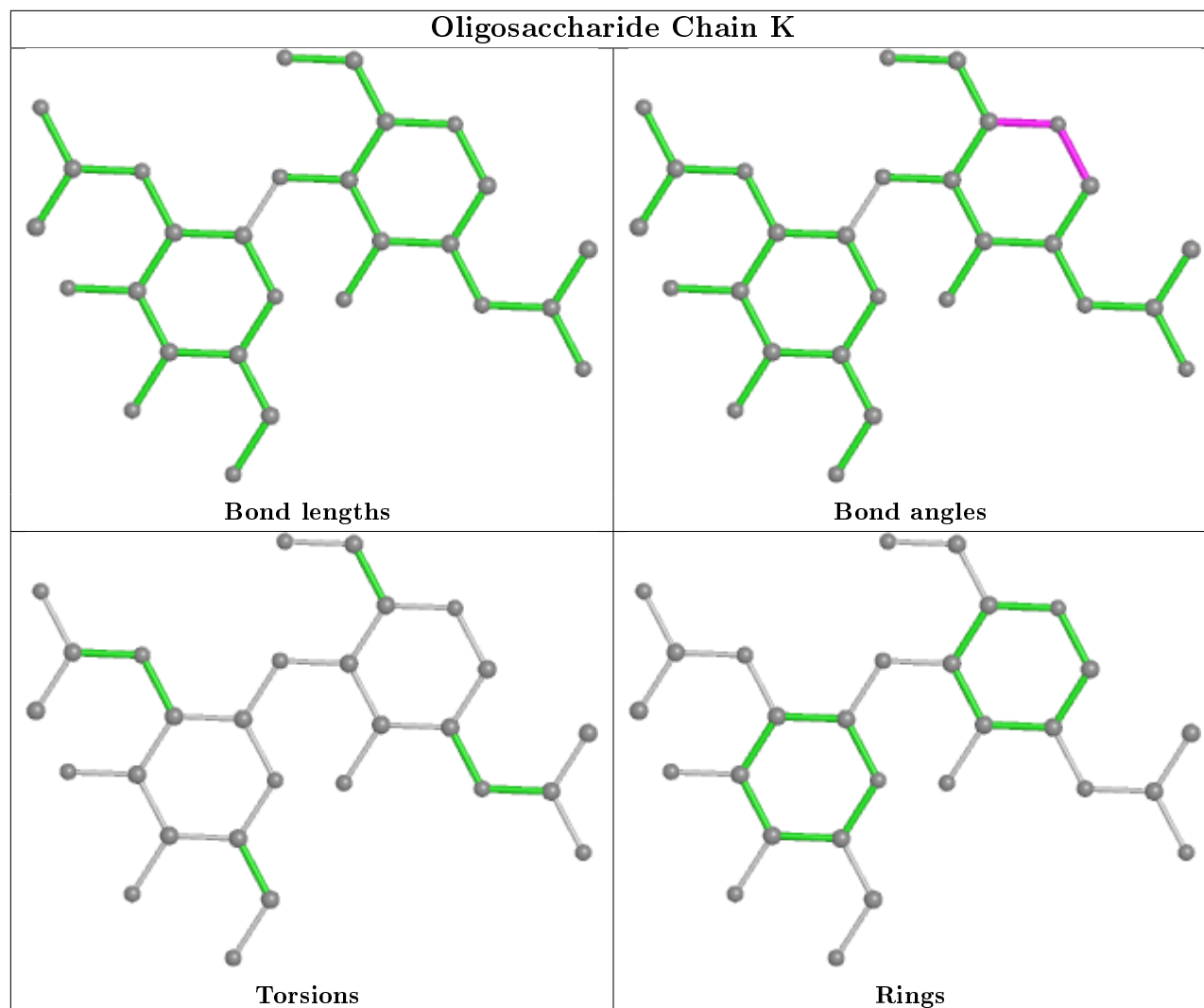


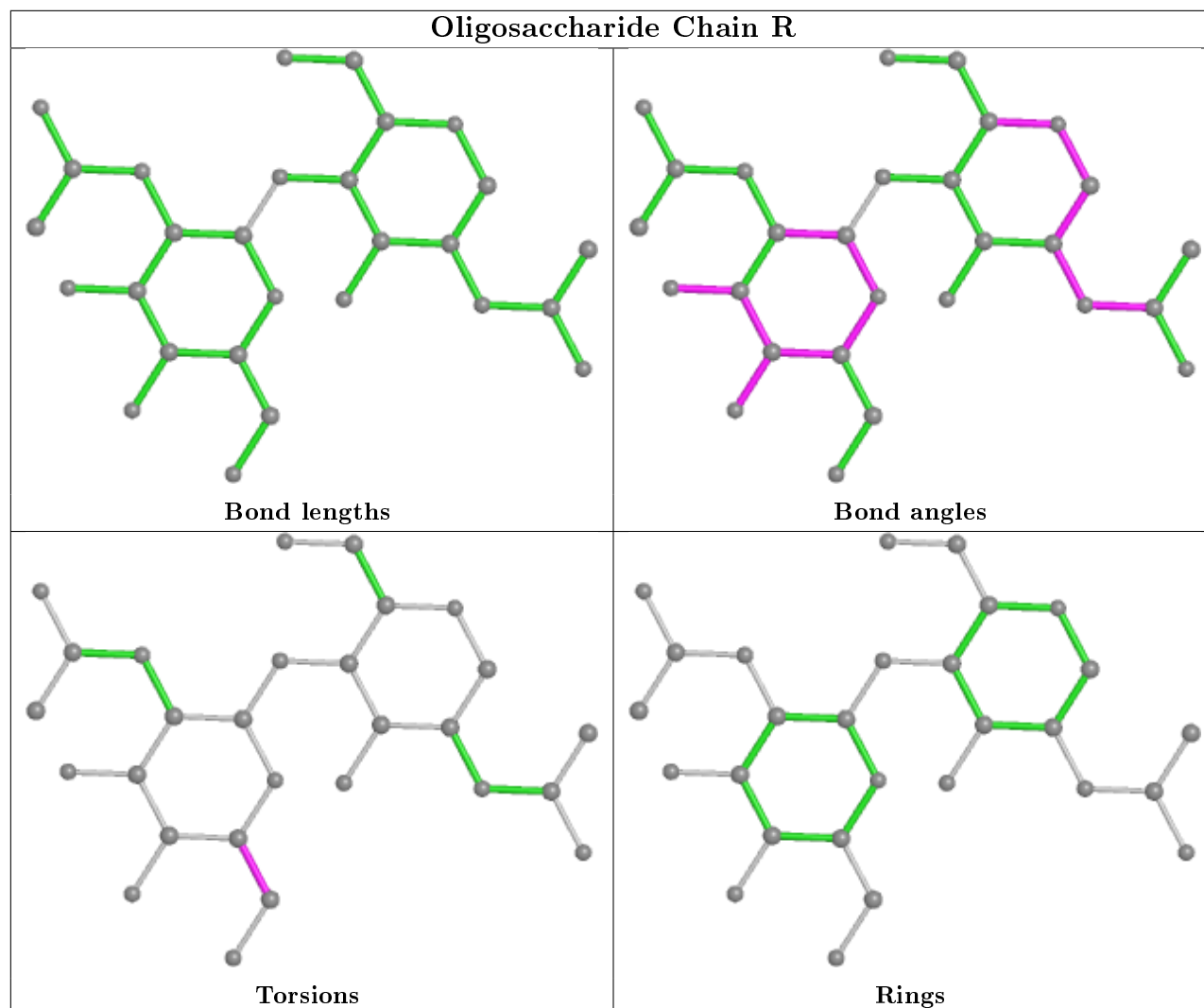


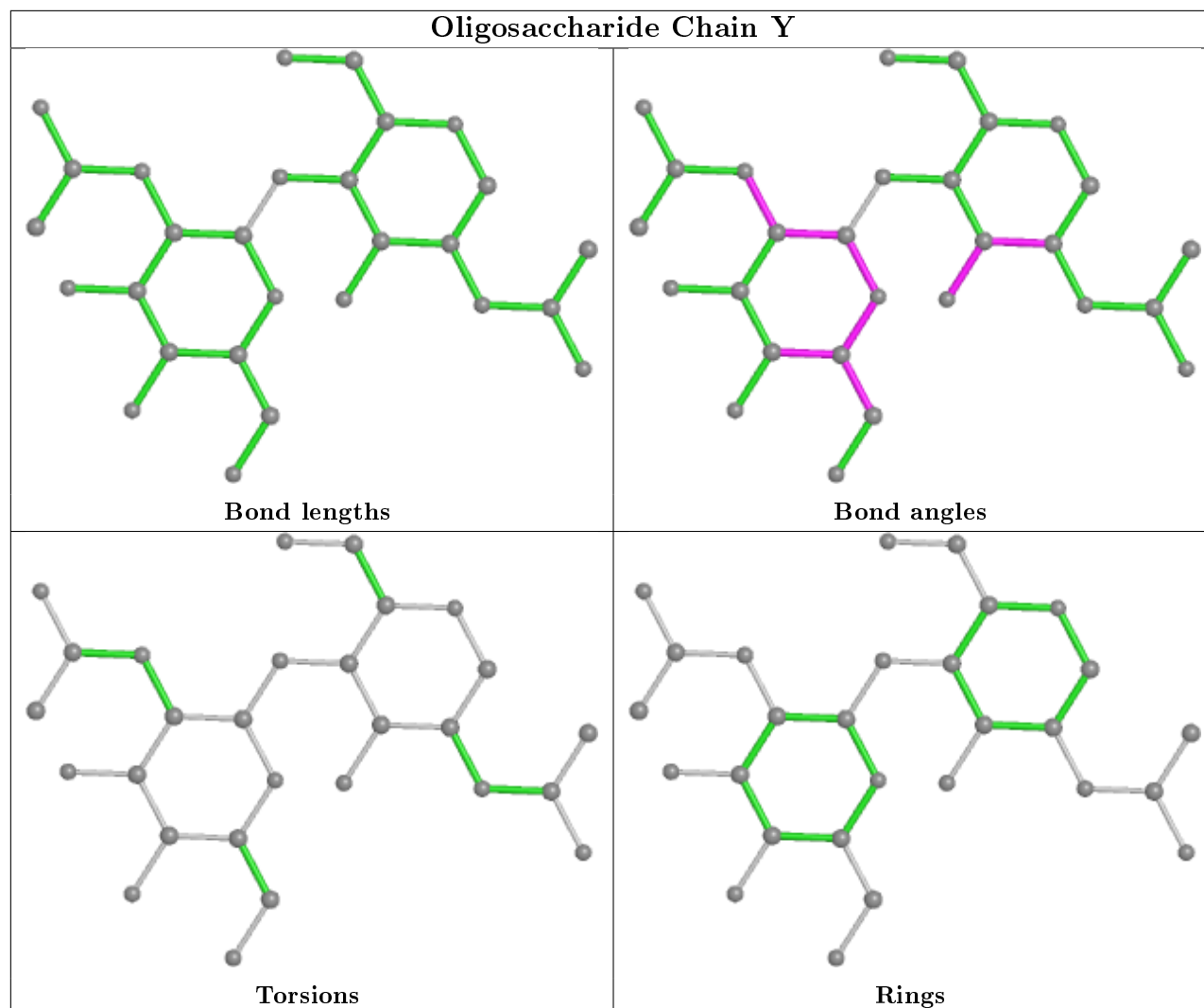


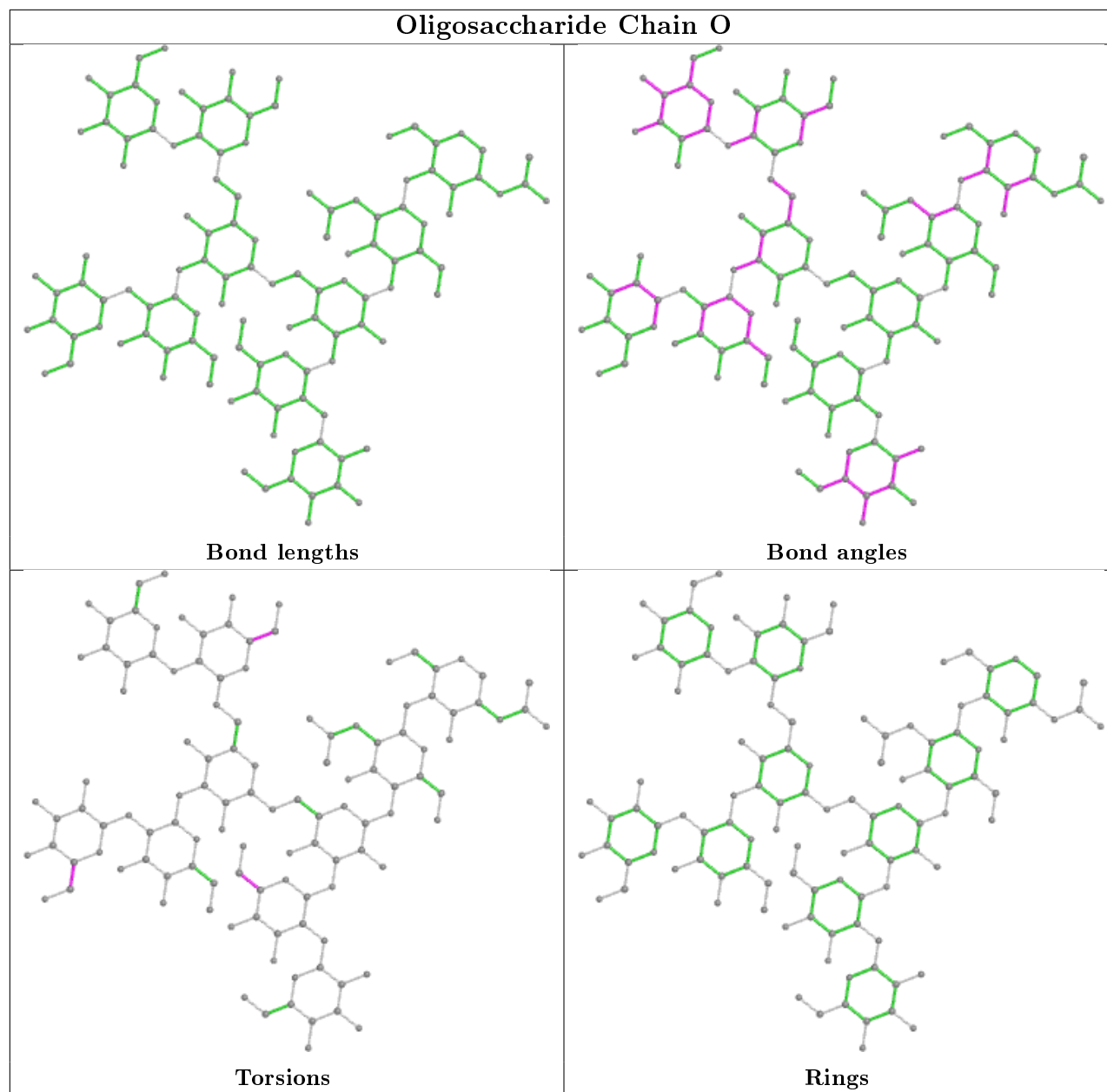


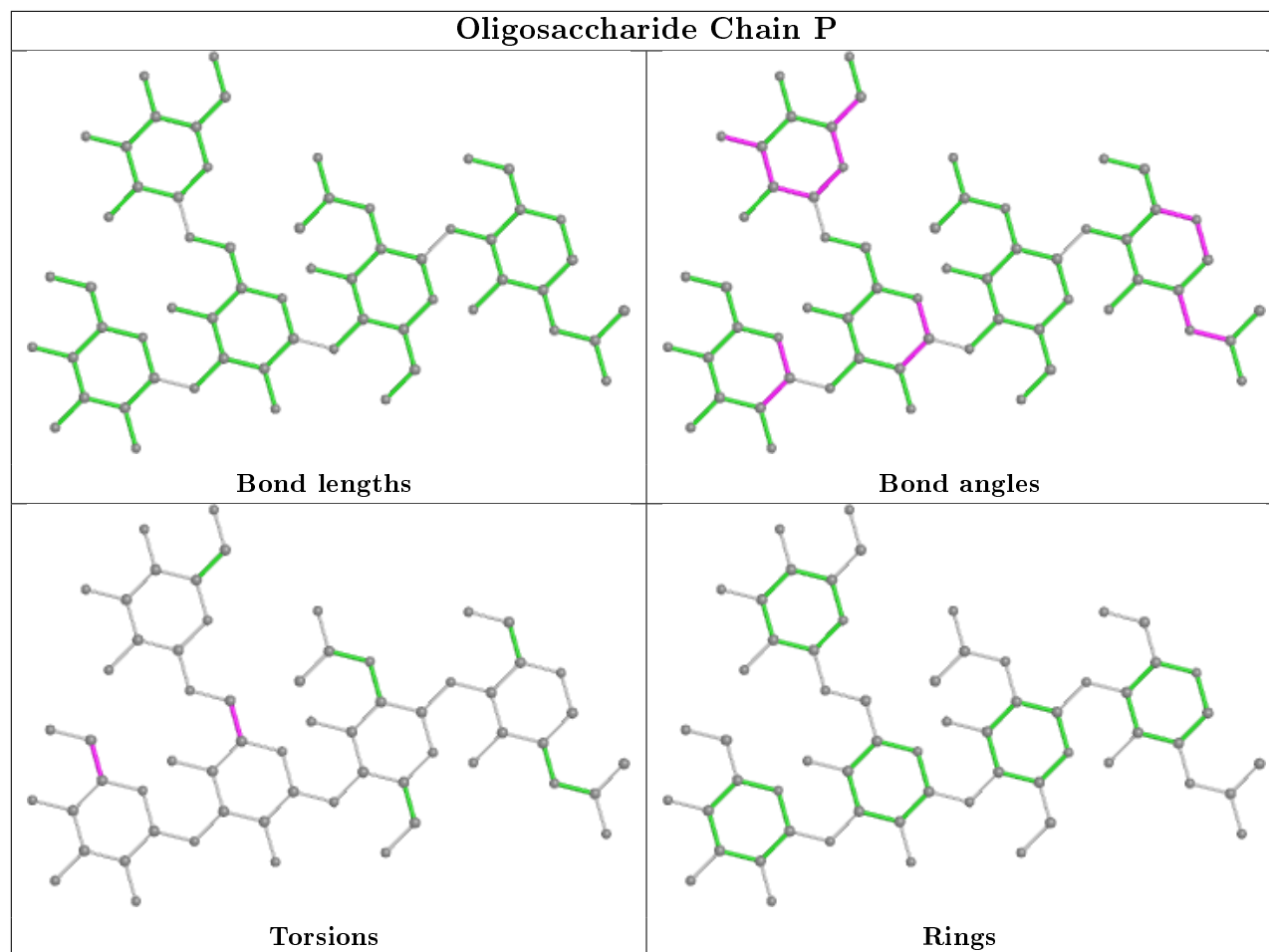
Oligosaccharide Chain J**Bond lengths****Bond angles****Torsions****Rings**

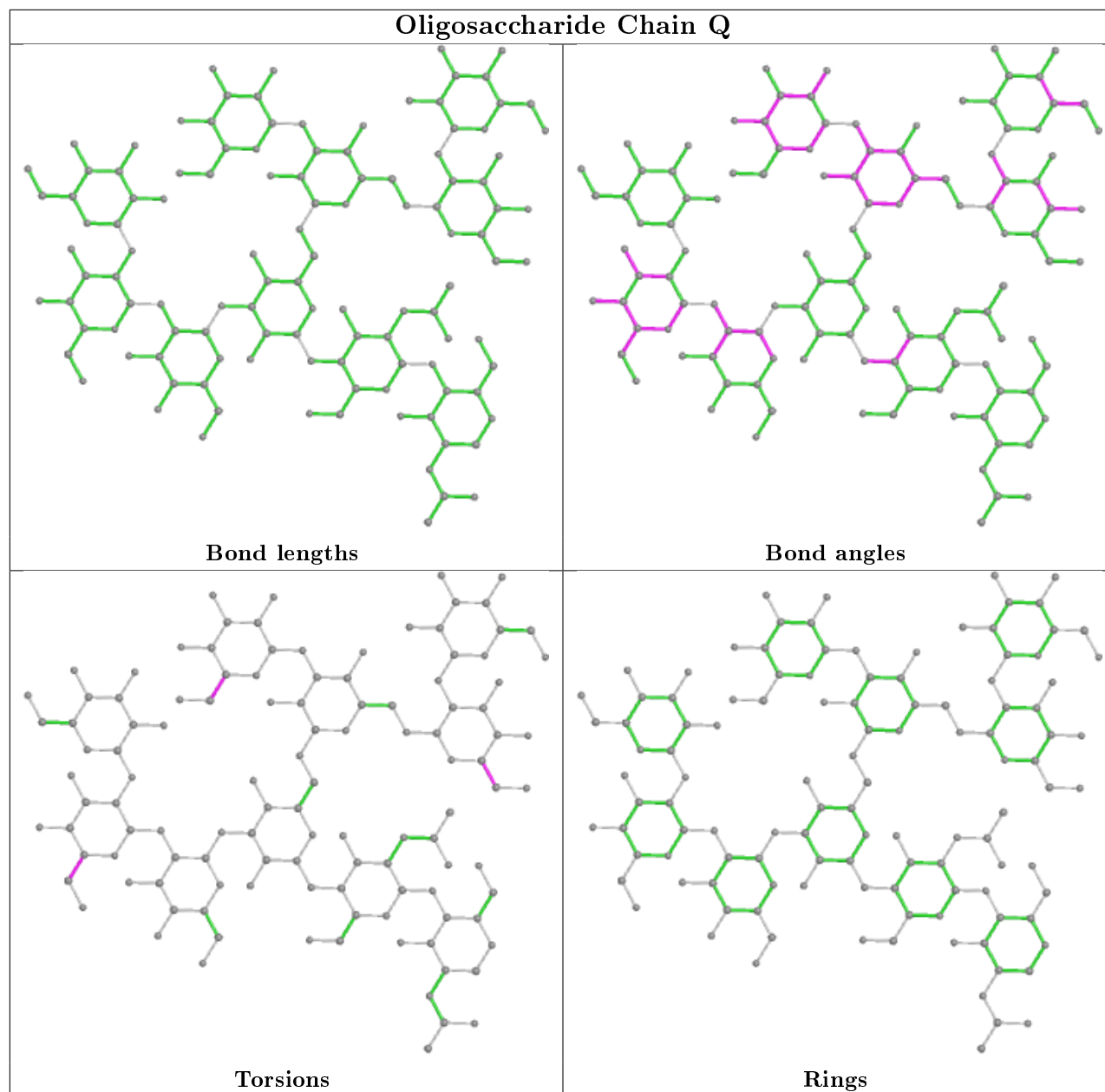


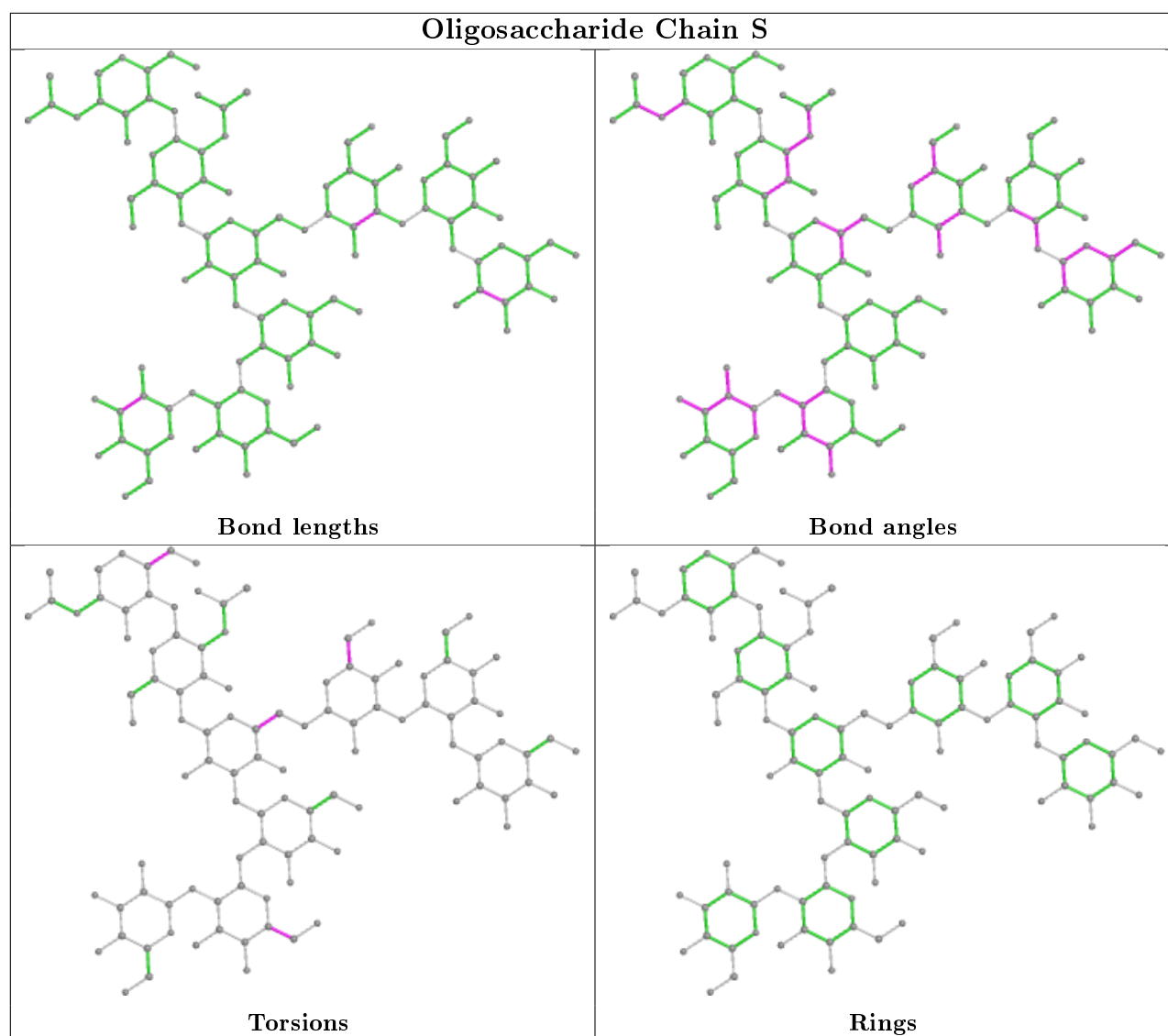


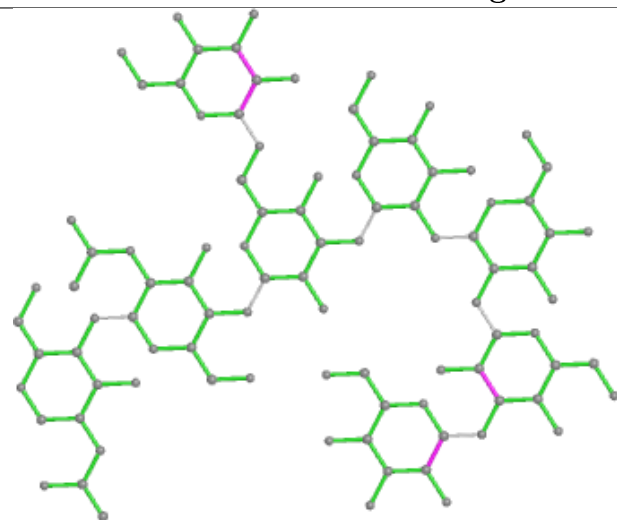
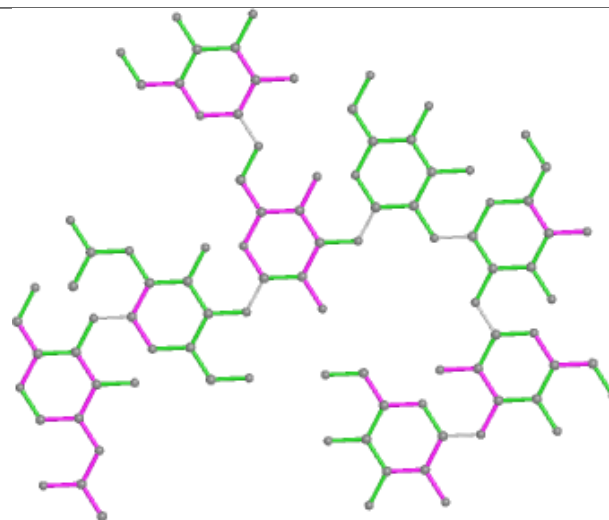
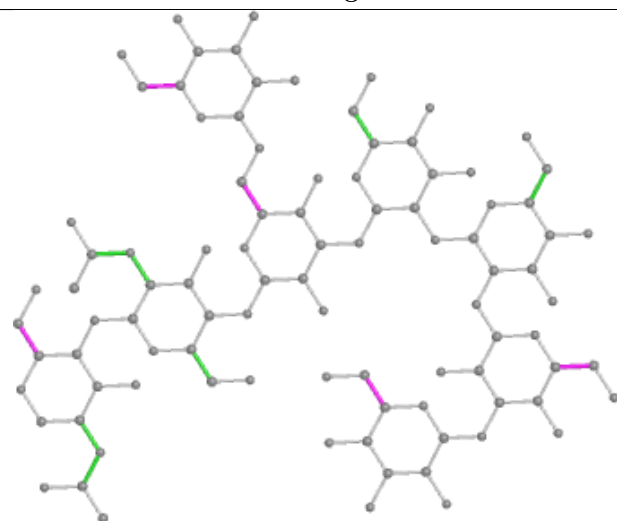
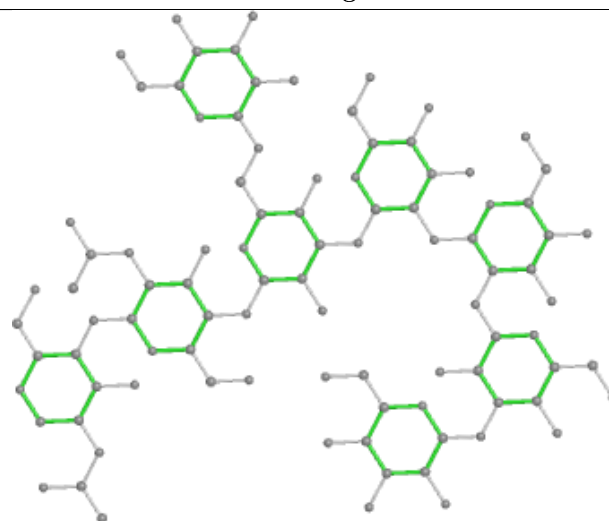




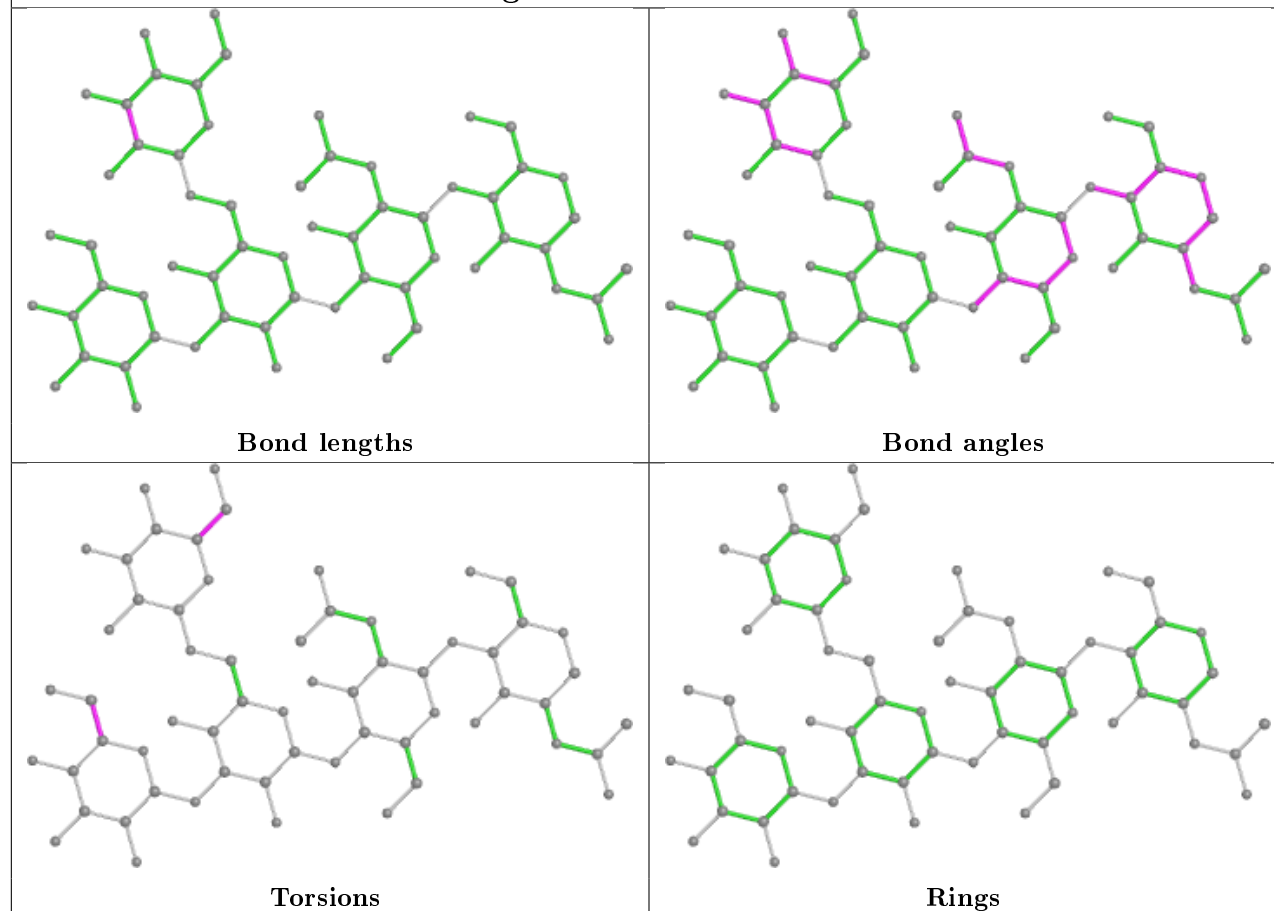




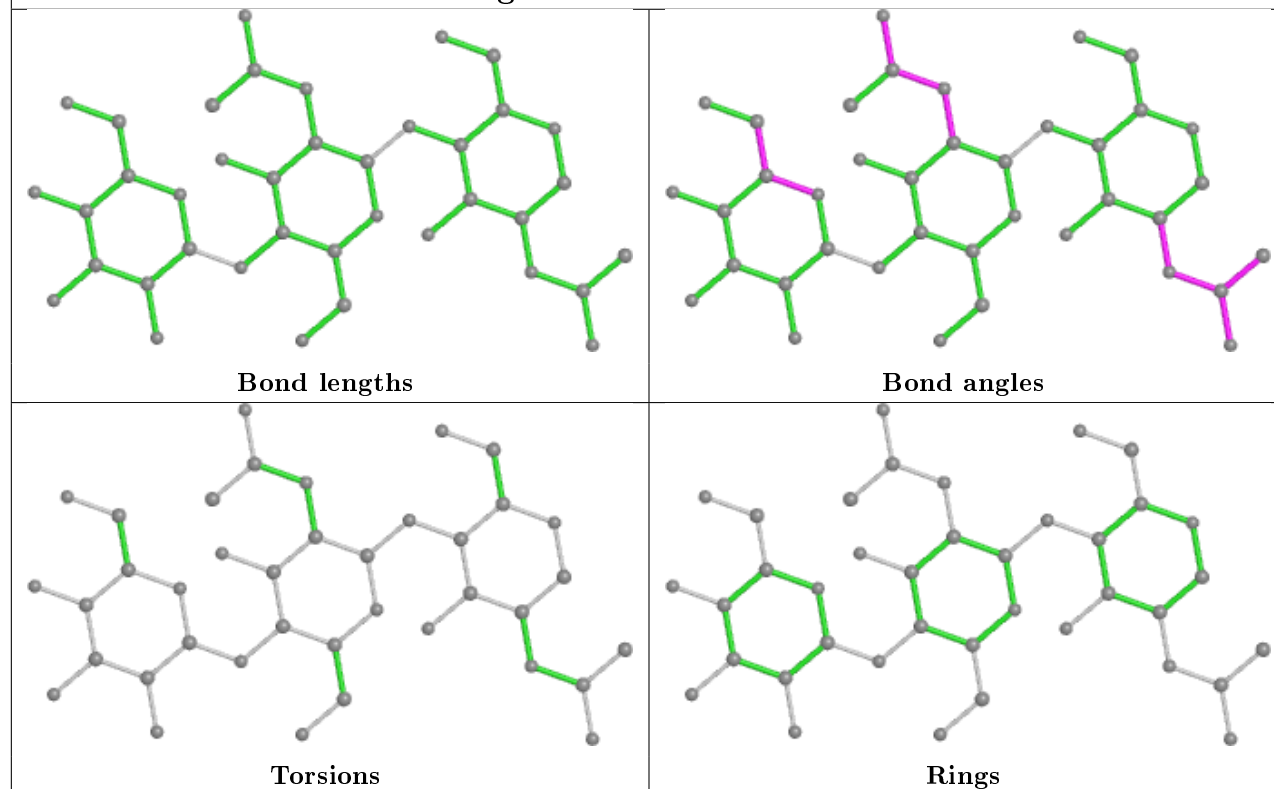


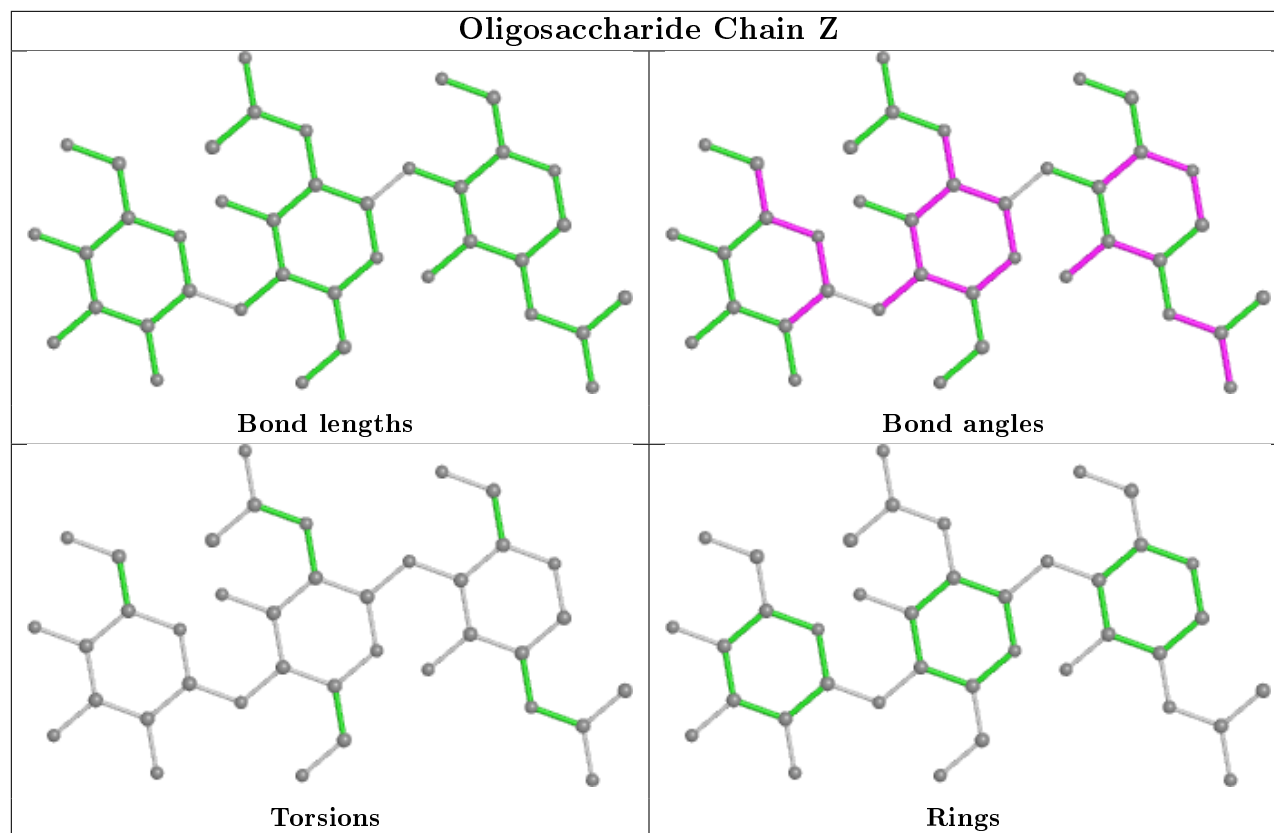
Oligosaccharide Chain T**Bond lengths****Bond angles****Torsions****Rings**

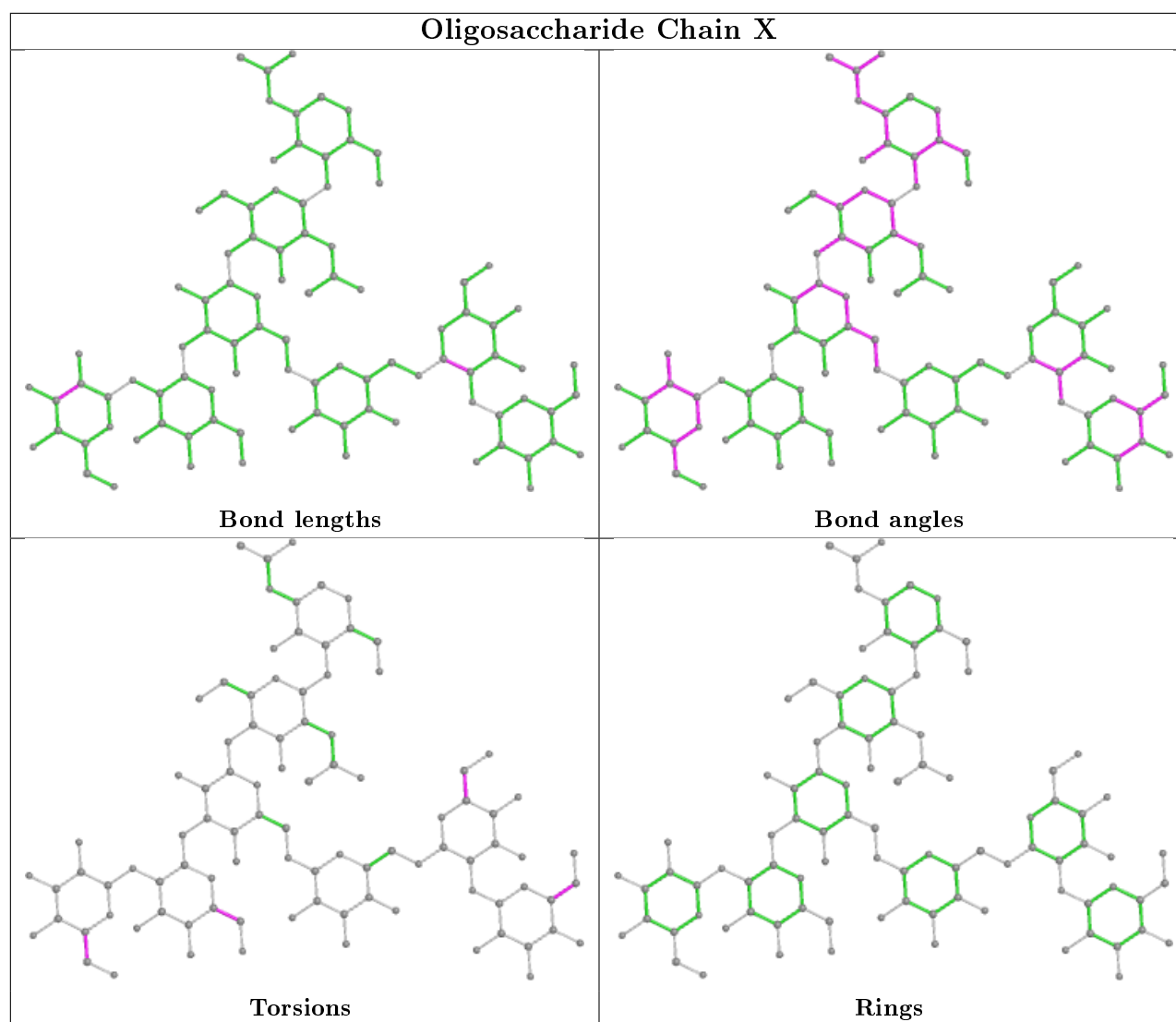
Oligosaccharide Chain U



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
18	NAG	C	944	1	14,14,15	0.94	0	17,19,21	2.14	6 (35%)
18	NAG	D	941	1	14,14,15	0.52	0	17,19,21	1.20	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	NAG	B	943	1	14,14,15	0.57	0	17,19,21	1.26	2 (11%)
18	NAG	A	930	1	14,14,15	0.68	0	17,19,21	1.57	4 (23%)
18	NAG	D	943	1	14,14,15	0.58	0	17,19,21	1.70	5 (29%)
18	NAG	A	944	1	14,14,15	0.73	0	17,19,21	2.01	4 (23%)
19	BGC	B	945	-	12,12,12	1.26	1 (8%)	17,17,17	1.10	1 (5%)
19	BGC	D	945	-	12,12,12	0.84	0	17,17,17	1.23	2 (11%)
18	NAG	B	944	1	14,14,15	0.39	0	17,19,21	1.21	3 (17%)
18	NAG	D	940	1	14,14,15	0.77	0	17,19,21	1.35	2 (11%)
18	NAG	C	950	1	14,14,15	0.68	0	17,19,21	0.99	2 (11%)
18	NAG	B	940	1	14,14,15	0.94	0	17,19,21	1.66	4 (23%)
19	BGC	A	946	-	12,12,12	1.09	1 (8%)	17,17,17	1.15	3 (17%)
18	NAG	D	944	1	14,14,15	0.97	1 (7%)	17,19,21	1.84	5 (29%)
18	NAG	C	935	1	14,14,15	0.80	0	17,19,21	1.45	4 (23%)
19	BGC	C	951	-	12,12,12	1.23	1 (8%)	17,17,17	1.41	2 (11%)
18	NAG	A	945	1	14,14,15	0.72	0	17,19,21	1.43	3 (17%)
20	MAN	B	905	-	11,11,12	0.77	0	15,15,17	1.67	3 (20%)
18	NAG	A	941	1	14,14,15	0.56	0	17,19,21	1.52	3 (17%)
18	NAG	D	942	1	14,14,15	1.02	1 (7%)	17,19,21	1.49	4 (23%)
18	NAG	A	940	1	14,14,15	0.88	0	17,19,21	1.36	2 (11%)

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
18	NAG	C	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	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	D	943	1	-	0/6/23/26	0/1/1/1
18	NAG	A	944	1	-	0/6/23/26	0/1/1/1
19	BGC	B	945	-	-	2/2/22/22	0/1/1/1
19	BGC	D	945	-	-	2/2/22/22	0/1/1/1
18	NAG	B	944	1	-	0/6/23/26	0/1/1/1
18	NAG	D	940	1	-	0/6/23/26	0/1/1/1
18	NAG	C	950	1	-	1/6/23/26	0/1/1/1
18	NAG	B	940	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BGC	A	946	-	-	2/2/22/22	0/1/1/1
18	NAG	D	944	1	-	0/6/23/26	0/1/1/1
18	NAG	C	935	1	-	0/6/23/26	0/1/1/1
19	BGC	C	951	-	-	1/2/22/22	0/1/1/1
18	NAG	A	945	1	-	0/6/23/26	0/1/1/1
20	MAN	B	905	-	-	2/2/19/22	0/1/1/1
18	NAG	A	941	1	-	0/6/23/26	0/1/1/1
18	NAG	D	942	1	-	1/6/23/26	0/1/1/1
18	NAG	A	940	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	944	NAG	C1-C2	2.82	1.56	1.52
19	C	951	BGC	C1-C2	2.40	1.58	1.52
19	A	946	BGC	C1-C2	2.24	1.57	1.52
18	D	942	NAG	C3-C2	2.12	1.57	1.52
19	B	945	BGC	C3-C2	2.00	1.57	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	944	NAG	C1-O5-C5	4.71	118.58	112.19
18	D	944	NAG	C1-O5-C5	4.38	118.12	112.19
18	A	944	NAG	C1-C2-N2	-4.09	103.50	110.49
18	A	944	NAG	O5-C1-C2	-3.83	105.23	111.29
18	B	940	NAG	O5-C5-C6	3.81	113.17	107.20
18	C	944	NAG	O5-C5-C6	3.73	113.06	107.20
18	C	944	NAG	C3-C4-C5	-3.69	103.66	110.24
18	A	930	NAG	C1-C2-N2	3.63	116.69	110.49
18	C	935	NAG	O5-C5-C6	3.60	112.85	107.20
18	A	941	NAG	O5-C1-C2	-3.45	105.84	111.29
18	C	944	NAG	O4-C4-C5	3.43	117.81	109.30
20	B	905	MAN	O2-C2-C3	3.33	116.81	110.14
18	D	944	NAG	C2-N2-C7	3.24	127.52	122.90
18	C	944	NAG	C1-O5-C5	3.21	116.54	112.19
19	C	951	BGC	O1-C1-O5	-3.14	100.97	110.38
18	D	940	NAG	C1-C2-N2	-3.12	105.16	110.49
18	D	943	NAG	C1-O5-C5	3.11	116.40	112.19
18	D	943	NAG	O5-C1-C2	-3.09	106.42	111.29
18	B	940	NAG	C1-O5-C5	3.02	116.28	112.19
18	A	941	NAG	C1-C2-N2	-2.94	105.47	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	944	NAG	C1-O5-C5	2.92	116.15	112.19
18	C	944	NAG	O5-C1-C2	-2.88	106.73	111.29
18	D	941	NAG	O5-C1-C2	-2.87	106.75	111.29
18	D	942	NAG	O4-C4-C5	2.82	116.31	109.30
18	B	943	NAG	C1-O5-C5	2.78	115.95	112.19
19	C	951	BGC	C1-O5-C5	2.77	118.89	113.66
18	A	930	NAG	C1-O5-C5	2.77	115.94	112.19
18	A	930	NAG	C6-C5-C4	-2.74	106.58	113.00
18	A	940	NAG	C1-O5-C5	2.71	115.87	112.19
18	B	940	NAG	O5-C1-C2	-2.70	107.02	111.29
18	A	945	NAG	O4-C4-C3	-2.65	104.22	110.35
18	B	940	NAG	C3-C4-C5	-2.64	105.53	110.24
19	D	945	BGC	O1-C1-O5	-2.62	102.51	110.38
20	B	905	MAN	O5-C1-C2	2.60	114.78	110.77
18	A	941	NAG	C1-O5-C5	2.60	115.71	112.19
18	D	942	NAG	C1-O5-C5	2.52	115.60	112.19
18	B	943	NAG	O5-C5-C6	2.50	111.13	107.20
20	B	905	MAN	C2-C3-C4	2.45	115.14	110.89
18	D	940	NAG	O3-C3-C2	-2.44	104.42	109.47
18	D	942	NAG	C1-C2-N2	-2.39	106.40	110.49
18	C	935	NAG	O3-C3-C2	-2.37	104.56	109.47
18	D	943	NAG	O5-C5-C6	2.35	110.89	107.20
18	C	935	NAG	C4-C3-C2	2.33	114.43	111.02
18	A	945	NAG	C6-C5-C4	-2.32	107.56	113.00
18	D	943	NAG	C2-N2-C7	2.32	126.21	122.90
18	A	930	NAG	C2-N2-C7	2.28	126.14	122.90
18	D	944	NAG	O5-C1-C2	-2.25	107.73	111.29
18	C	935	NAG	O5-C5-C4	-2.24	105.37	110.83
19	B	945	BGC	O4-C4-C5	2.23	114.83	109.30
18	D	944	NAG	C1-C2-N2	2.21	114.27	110.49
18	D	943	NAG	C3-C4-C5	-2.20	106.31	110.24
19	A	946	BGC	O2-C2-C1	2.20	114.27	109.16
18	D	944	NAG	O4-C4-C5	2.18	114.70	109.30
18	A	940	NAG	O5-C5-C6	2.11	110.52	107.20
19	D	945	BGC	O3-C3-C4	-2.11	105.48	110.35
18	B	944	NAG	O6-C6-C5	-2.09	104.11	111.29
18	D	942	NAG	C3-C4-C5	-2.09	106.51	110.24
18	A	945	NAG	C3-C4-C5	2.09	113.97	110.24
18	C	950	NAG	C2-N2-C7	2.06	125.84	122.90
18	A	944	NAG	C3-C4-C5	-2.06	106.56	110.24
18	C	950	NAG	C1-C2-N2	-2.04	107.00	110.49
18	B	944	NAG	C3-C4-C5	-2.04	106.60	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	944	NAG	C4-C3-C2	2.03	114.00	111.02
19	A	946	BGC	O1-C1-C2	2.02	114.73	109.03
19	A	946	BGC	O4-C4-C5	2.01	114.29	109.30

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
19	B	945	BGC	1	0
19	D	945	BGC	1	0
19	A	946	BGC	1	0
19	C	951	BGC	1	0
18	A	945	NAG	1	0
20	B	905	MAN	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.48	2 (0%) 95 94	14, 25, 41, 69	7 (0%)
1	B	835/857 (97%)	-0.38	5 (0%) 89 88	16, 26, 43, 77	9 (1%)
1	C	835/857 (97%)	-0.38	4 (0%) 91 90	14, 24, 40, 75	11 (1%)
1	D	835/857 (97%)	-0.39	1 (0%) 95 95	12, 23, 39, 79	8 (0%)
All	All	3340/3428 (97%)	-0.41	12 (0%) 92 91	12, 25, 41, 79	35 (1%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	854	TYR	3.6
1	B	853	PRO	3.4
1	A	208	ASP	3.4
1	A	206	GLY	3.0
1	D	855	PRO	2.7
1	B	855	PRO	2.6
1	B	663	ASN	2.6
1	B	851	LEU	2.2
1	C	855	PRO	2.2
1	C	21	ASN	2.1
1	C	208	ASP	2.0
1	C	188	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

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
4	MAN	c	4	11/12	0.52	0.29	87,104,110,111	0
15	BMA	Z	3	11/12	0.58	0.35	82,110,119,119	0
4	MAN	N	4	11/12	0.60	0.41	81,99,110,115	0
16	MAN	f	8	11/12	0.60	0.30	70,83,92,93	0
17	MAN	a	5	11/12	0.62	0.26	74,94,99,100	0
13	MAN	T	8	11/12	0.63	0.37	82,88,94,96	0
13	MAN	b	8	11/12	0.64	0.39	88,102,108,109	0
5	MAN	V	9	11/12	0.65	0.31	84,91,100,101	0
10	BMA	P	4	11/12	0.68	0.38	78,85,94,99	0
6	MAN	I	4	11/12	0.69	0.38	89,98,103,106	0
13	GLC	b	7	11/12	0.69	0.29	66,88,96,99	0
12	MAN	S	9	11/12	0.69	0.33	73,89,92,94	0
10	MAN	P	5	11/12	0.69	0.29	92,101,109,109	0
4	BMA	N	3	11/12	0.71	0.33	73,84,91,102	0
14	MAN	U	4	11/12	0.71	0.20	91,94,99,104	0
15	BMA	e	3	11/12	0.71	0.28	72,81,84,86	0
16	MAN	X	8	11/12	0.71	0.30	55,70,76,79	0
3	MAN	F	7	11/12	0.72	0.27	56,75,83,84	0
4	MAN	G	4	11/12	0.72	0.28	69,85,86,87	0
5	MAN	H	9	11/12	0.73	0.30	70,88,92,93	0
9	MAN	d	10	11/12	0.75	0.23	77,84,86,87	0
11	MAN	Q	10	11/12	0.76	0.24	64,70,73,76	0
8	NAG	Y	2	14/15	0.77	0.39	67,82,96,100	0
6	BMA	I	3	11/12	0.77	0.21	71,77,91,102	0
2	MAN	M	4	11/12	0.77	0.17	67,75,78,81	0
7	MAN	J	6	11/12	0.77	0.26	76,85,89,90	0
2	MAN	E	5	11/12	0.78	0.26	92,94,96,97	0
11	MAN	Q	5	11/12	0.78	0.27	80,82,86,87	0
17	MAN	a	6	11/12	0.78	0.23	67,78,86,89	0
15	BMA	W	3	11/12	0.78	0.26	75,85,92,95	0
4	BMA	c	3	11/12	0.79	0.21	58,69,76,90	0
9	MAN	O	10	11/12	0.80	0.18	59,65,70,71	0
8	NAG	R	2	14/15	0.80	0.28	53,66,79,80	0
11	MAN	Q	6	11/12	0.80	0.31	75,79,86,86	0
14	MAN	U	5	11/12	0.81	0.22	77,90,95,95	0
10	BMA	P	3	11/12	0.81	0.20	77,85,90,92	0
3	MAN	F	4	11/12	0.81	0.20	73,79,86,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	GLC	T	7	11/12	0.81	0.24	58,67,73,74	0
3	MAN	F	6	11/12	0.81	0.22	77,90,96,98	0
9	MAN	d	6	11/12	0.82	0.41	56,61,64,70	0
15	NAG	Z	2	14/15	0.82	0.35	55,77,93,106	0
4	MAN	L	4	11/12	0.82	0.13	66,72,76,79	0
16	MAN	f	7	11/12	0.83	0.21	55,59,65,67	0
3	MAN	F	5	11/12	0.83	0.18	76,82,85,100	0
7	MAN	J	5	11/12	0.83	0.20	57,65,70,71	0
12	MAN	S	6	11/12	0.83	0.20	59,68,74,76	0
12	MAN	S	8	11/12	0.85	0.20	72,76,79,84	0
4	BMA	G	3	11/12	0.86	0.22	60,70,79,81	0
8	NAG	K	2	14/15	0.86	0.28	65,70,78,78	0
13	MAN	b	6	11/12	0.87	0.11	53,63,67,81	0
2	MAN	M	5	11/12	0.87	0.19	55,67,79,86	0
17	MAN	a	4	11/12	0.87	0.21	71,79,88,90	0
8	NAG	Y	1	14/15	0.87	0.29	56,66,73,77	0
5	MAN	V	8	11/12	0.88	0.17	46,48,56,72	0
12	MAN	S	7	11/12	0.88	0.26	57,63,65,71	0
2	BMA	E	3	11/12	0.88	0.23	50,59,67,73	0
16	MAN	f	4	11/12	0.88	0.13	39,42,46,47	0
2	BMA	M	3	11/12	0.88	0.13	45,54,57,67	0
12	BMA	S	3	11/12	0.89	0.17	44,54,61,62	0
14	BMA	U	3	11/12	0.89	0.12	62,70,78,83	0
2	MAN	E	4	11/12	0.89	0.15	60,70,76,77	0
3	BMA	F	3	11/12	0.89	0.10	43,48,58,64	0
5	MAN	V	7	11/12	0.89	0.19	47,52,53,60	0
17	BMA	a	3	11/12	0.89	0.21	44,65,82,84	0
15	NAG	e	2	14/15	0.90	0.14	36,43,49,60	0
10	NAG	P	2	14/15	0.90	0.14	45,48,54,67	0
11	MAN	Q	9	11/12	0.90	0.17	35,43,48,53	0
7	MAN	J	9	11/12	0.90	0.17	43,49,51,52	0
4	BMA	L	3	11/12	0.90	0.14	55,66,73,73	0
16	MAN	X	5	11/12	0.90	0.23	35,40,44,48	0
9	MAN	O	6	11/12	0.90	0.35	50,57,60,60	0
5	MAN	H	7	11/12	0.91	0.21	43,53,59,65	0
5	MAN	H	8	11/12	0.91	0.18	47,55,60,67	0
7	MAN	J	7	11/12	0.91	0.10	37,40,42,42	0
16	MAN	f	5	11/12	0.91	0.17	39,43,45,46	0
11	MAN	Q	4	11/12	0.91	0.17	45,51,55,63	0
10	NAG	P	1	14/15	0.91	0.11	32,38,42,45	0
16	MAN	f	6	11/12	0.91	0.20	39,43,46,47	0
7	BMA	J	3	11/12	0.91	0.09	33,34,37,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	N	2	14/15	0.91	0.15	36,43,50,59	0
13	MAN	b	4	11/12	0.91	0.14	40,43,45,46	0
7	NAG	J	1	14/15	0.92	0.12	26,30,32,33	0
7	MAN	J	4	11/12	0.92	0.13	43,49,57,57	0
9	MAN	O	9	11/12	0.92	0.12	42,45,47,52	0
4	NAG	c	2	14/15	0.92	0.13	29,36,43,46	0
16	MAN	X	7	11/12	0.92	0.20	46,49,52,59	0
9	MAN	d	9	11/12	0.92	0.12	38,48,53,64	0
13	MAN	T	6	11/12	0.92	0.14	45,50,55,66	0
12	MAN	S	4	11/12	0.92	0.10	52,58,63,63	0
14	NAG	U	2	14/15	0.92	0.13	39,43,46,52	0
12	MAN	S	5	11/12	0.92	0.15	48,50,53,56	0
7	MAN	J	8	11/12	0.92	0.11	40,44,47,47	0
13	NAG	b	2	14/15	0.93	0.15	29,32,38,38	0
13	BMA	T	3	11/12	0.93	0.11	33,33,44,61	0
9	MAN	d	8	11/12	0.93	0.12	29,31,33,38	0
9	MAN	O	5	11/12	0.93	0.20	39,42,45,51	0
11	NAG	Q	2	14/15	0.93	0.10	22,24,26,27	0
11	MAN	Q	8	11/12	0.93	0.18	43,49,53,57	0
13	BMA	b	3	11/12	0.93	0.12	38,39,52,70	0
13	MAN	T	5	11/12	0.94	0.12	31,36,40,43	0
5	MAN	H	6	11/12	0.94	0.12	28,30,32,37	0
16	NAG	f	2	14/15	0.94	0.12	22,25,30,33	0
17	NAG	a	2	14/15	0.94	0.13	22,28,34,41	0
8	NAG	R	1	14/15	0.94	0.19	29,38,41,53	0
11	NAG	Q	1	14/15	0.94	0.10	24,27,32,33	0
2	NAG	M	1	14/15	0.94	0.09	27,28,29,31	0
13	MAN	T	4	11/12	0.94	0.12	34,38,41,41	0
8	NAG	K	1	14/15	0.94	0.20	37,43,46,54	0
6	NAG	I	2	14/15	0.94	0.12	40,43,48,58	0
16	BMA	X	3	11/12	0.94	0.12	30,32,37,40	0
16	MAN	X	4	11/12	0.94	0.13	30,36,42,43	0
2	NAG	E	2	14/15	0.95	0.09	21,27,38,40	0
15	NAG	Z	1	14/15	0.95	0.17	31,36,42,55	0
11	MAN	Q	7	11/12	0.95	0.08	38,40,46,54	0
4	NAG	G	2	14/15	0.95	0.11	29,35,41,46	0
16	MAN	X	6	11/12	0.95	0.19	34,39,43,44	0
9	BMA	O	3	11/12	0.95	0.09	27,28,31,35	0
3	NAG	F	1	14/15	0.95	0.10	25,27,29,30	0
15	NAG	e	1	14/15	0.95	0.10	31,32,34,37	0
16	BMA	f	3	11/12	0.95	0.11	29,34,37,42	0
15	NAG	W	2	14/15	0.95	0.17	40,44,50,64	0

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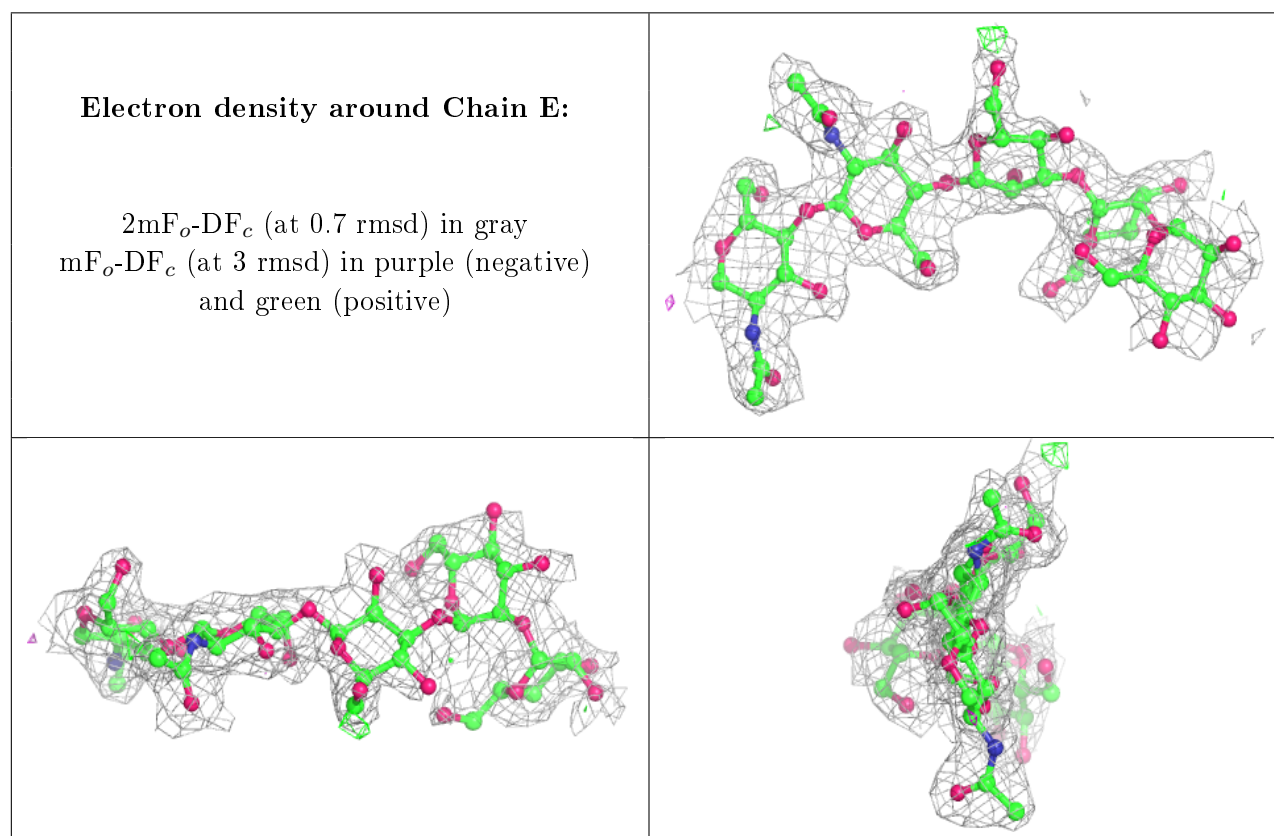
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	BMA	V	3	11/12	0.95	0.10	26,30,33,37	0
12	NAG	S	2	14/15	0.95	0.15	31,35,39,46	0
15	NAG	W	1	14/15	0.95	0.10	30,33,35,35	0
11	BMA	Q	3	11/12	0.95	0.09	29,32,36,44	0
13	MAN	b	5	11/12	0.95	0.10	40,43,46,54	0
6	NAG	I	1	14/15	0.95	0.10	26,31,34,34	0
13	NAG	b	1	14/15	0.95	0.11	22,24,27,28	0
4	NAG	L	1	14/15	0.95	0.10	22,28,29,30	0
13	NAG	T	2	14/15	0.96	0.08	25,27,30,31	0
7	NAG	J	2	14/15	0.96	0.08	24,28,31,32	0
5	NAG	H	1	14/15	0.96	0.09	24,25,28,29	0
16	NAG	f	1	14/15	0.96	0.10	23,25,30,30	0
5	MAN	V	6	11/12	0.96	0.08	25,27,29,33	0
9	MAN	O	7	11/12	0.96	0.09	24,25,29,29	0
9	NAG	d	1	14/15	0.96	0.10	20,24,27,28	0
5	MAN	V	4	11/12	0.96	0.09	25,31,35,40	0
9	MAN	d	5	11/12	0.96	0.19	35,39,42,45	0
16	NAG	X	2	14/15	0.96	0.09	22,24,28,28	0
2	NAG	M	2	14/15	0.96	0.09	34,37,41,45	0
4	NAG	L	2	14/15	0.96	0.09	30,33,38,45	0
9	NAG	O	1	14/15	0.96	0.09	25,26,27,28	0
9	MAN	d	7	11/12	0.96	0.09	20,24,26,27	0
14	NAG	U	1	14/15	0.96	0.10	24,29,32,34	0
5	NAG	V	2	14/15	0.96	0.09	21,26,29,29	0
5	NAG	V	1	14/15	0.96	0.11	25,27,32,34	0
16	NAG	X	1	14/15	0.96	0.09	23,25,28,30	0
9	MAN	O	4	11/12	0.96	0.10	27,28,34,36	0
9	NAG	O	2	14/15	0.96	0.10	23,26,27,27	0
3	NAG	F	2	14/15	0.96	0.12	29,32,37,40	0
4	NAG	G	1	14/15	0.96	0.10	20,22,27,27	0
13	NAG	T	1	14/15	0.96	0.10	18,21,23,24	0
9	MAN	d	4	11/12	0.96	0.11	22,25,27,29	0
5	NAG	H	2	14/15	0.97	0.08	21,24,30,31	0
4	NAG	N	1	14/15	0.97	0.08	22,25,27,30	0
5	MAN	V	5	11/12	0.97	0.10	22,24,26,29	0
17	NAG	a	1	14/15	0.97	0.07	21,23,25,26	0
4	NAG	c	1	14/15	0.97	0.08	19,20,22,27	0
9	BMA	d	3	11/12	0.97	0.09	22,24,29,35	0
12	NAG	S	1	14/15	0.97	0.10	24,25,28,28	0
5	MAN	H	4	11/12	0.97	0.10	27,29,33,40	0
9	MAN	O	8	11/12	0.97	0.09	26,27,31,36	0
9	NAG	d	2	14/15	0.97	0.08	20,21,24,24	0

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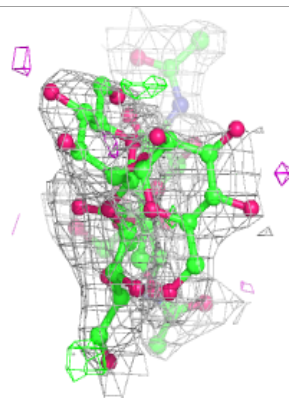
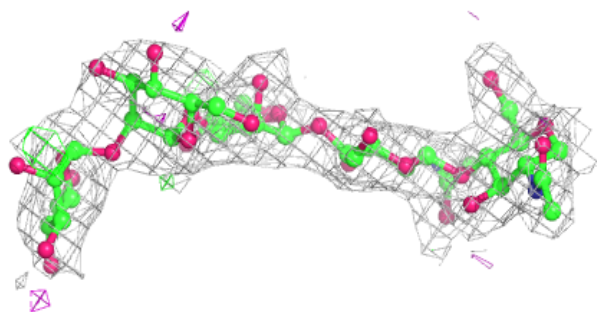
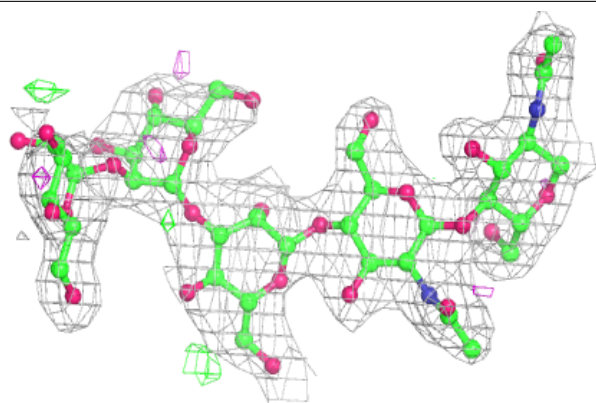
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	BMA	H	3	11/12	0.97	0.10	26,28,31,40	0
5	MAN	H	5	11/12	0.98	0.08	18,21,23,24	0
2	NAG	E	1	14/15	0.98	0.08	22,24,27,30	0

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.

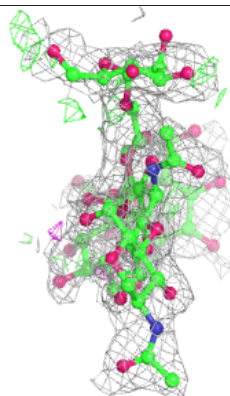
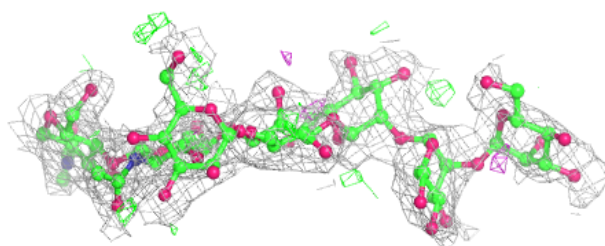
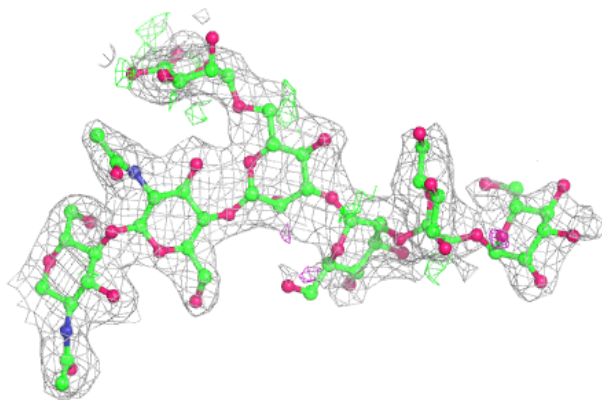


Electron density around Chain M:

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

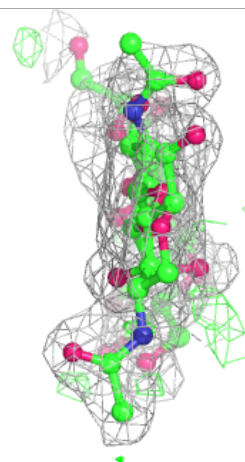
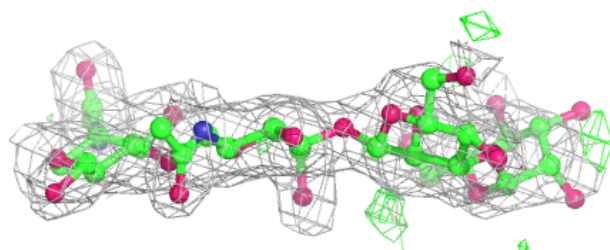
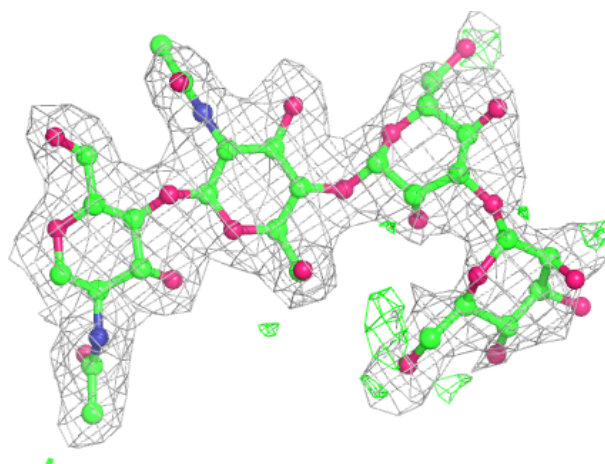
**Electron density around Chain F:**

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



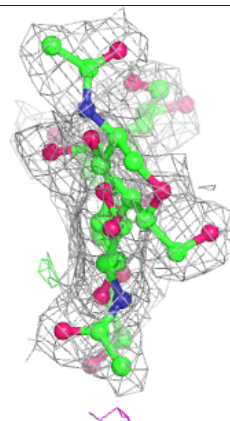
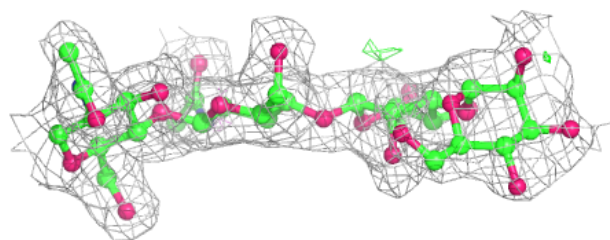
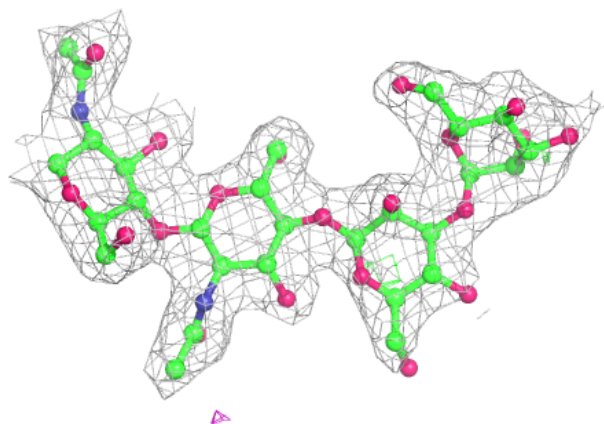
Electron density around Chain G:

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



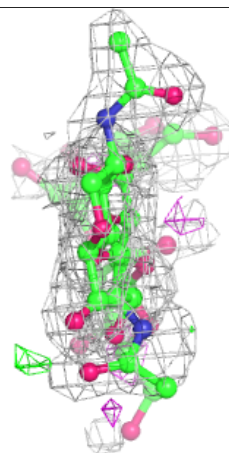
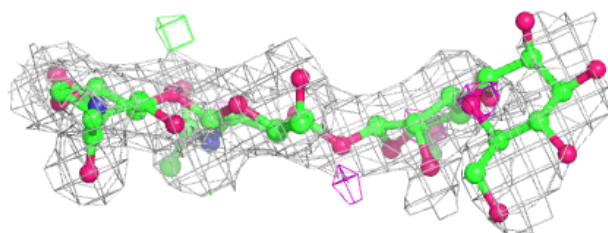
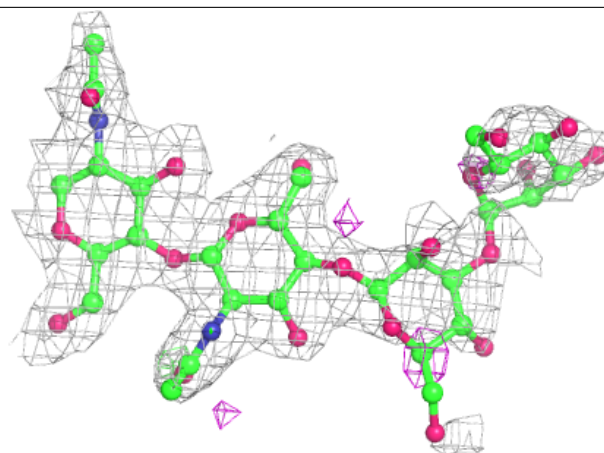
Electron density around Chain L:

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



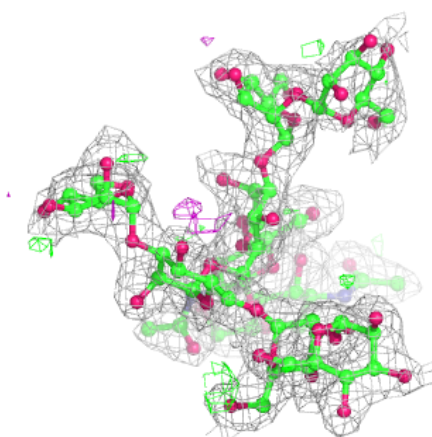
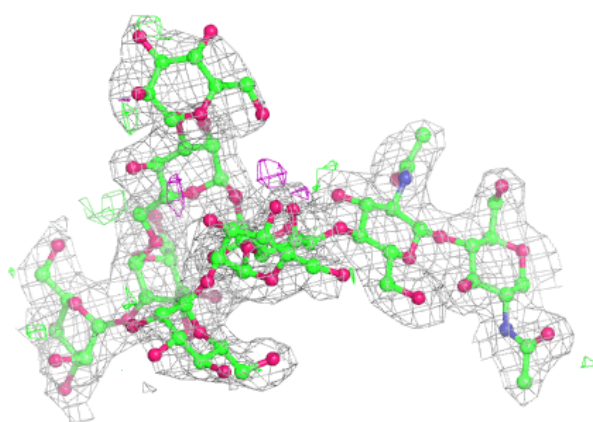
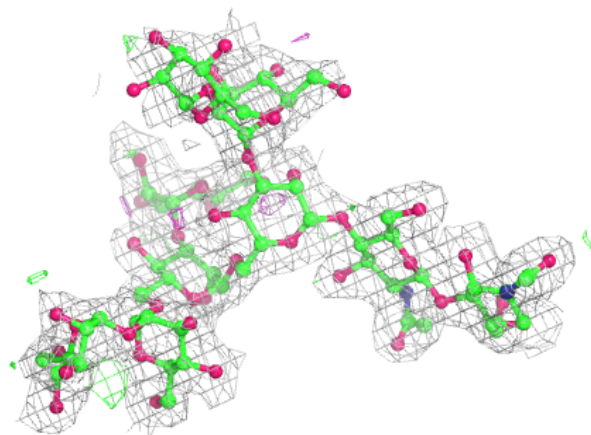
Electron density around Chain N:

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



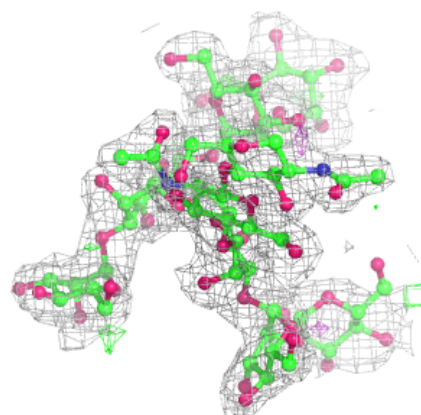
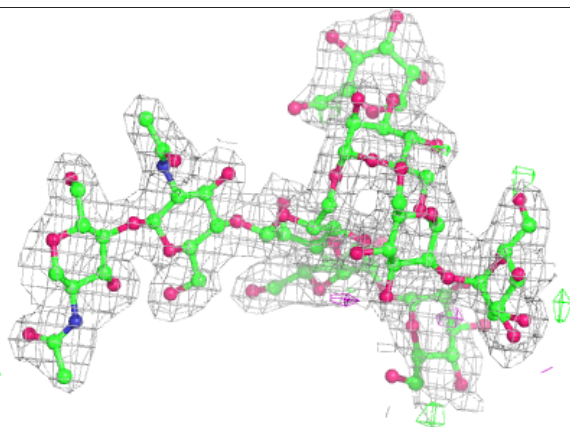
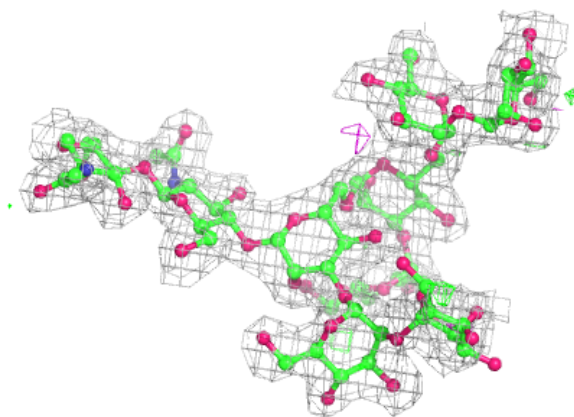
Electron density around Chain H:

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



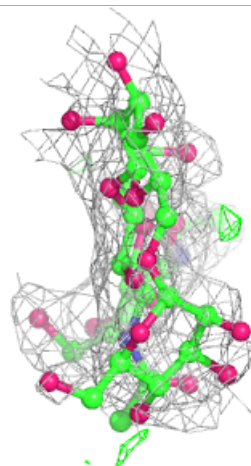
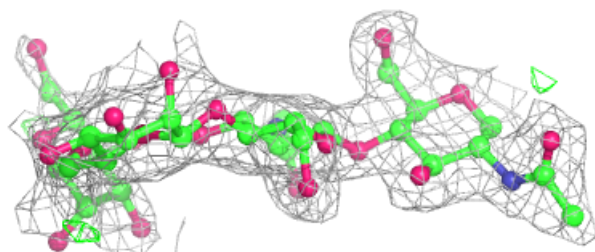
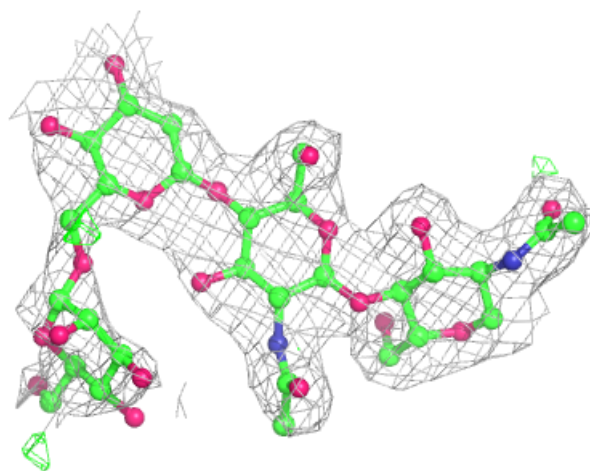
Electron density around Chain V:

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



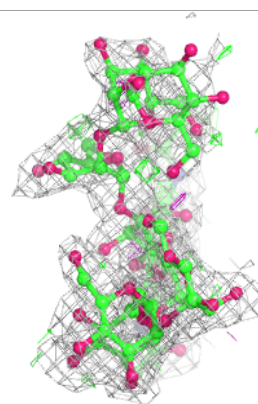
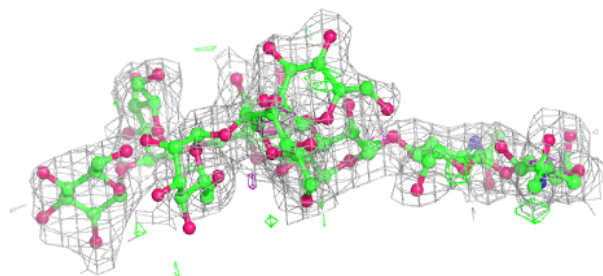
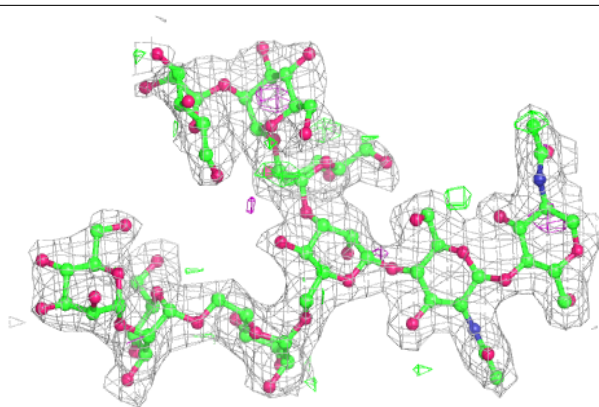
Electron density around Chain I:

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



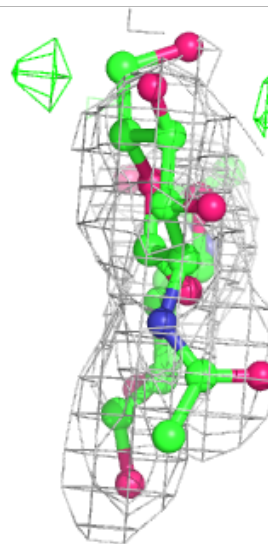
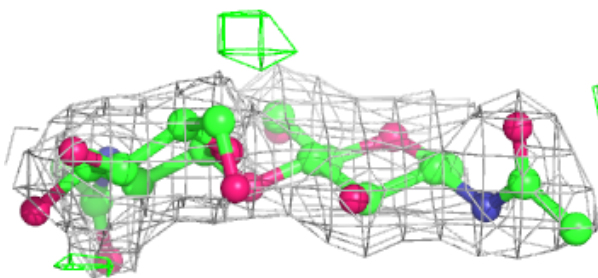
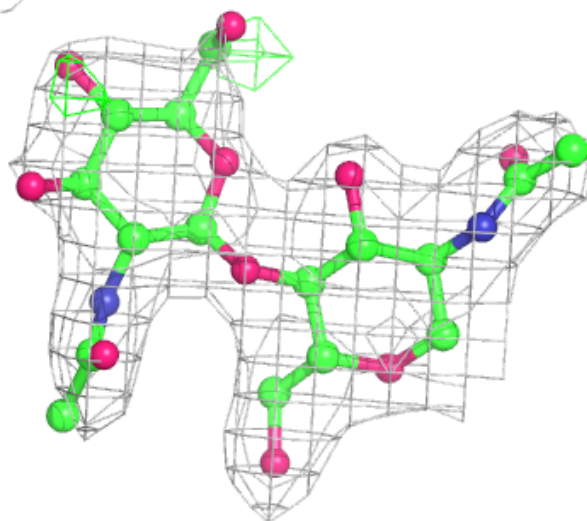
Electron density around Chain J:

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



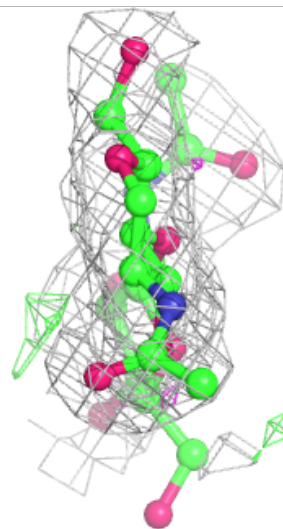
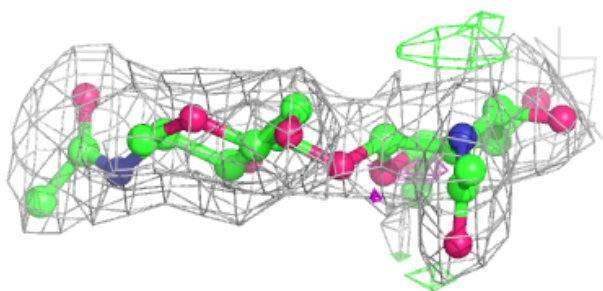
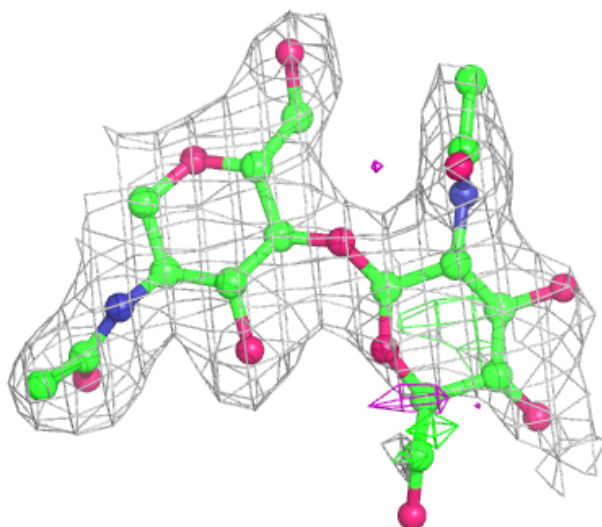
Electron density around Chain K:

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



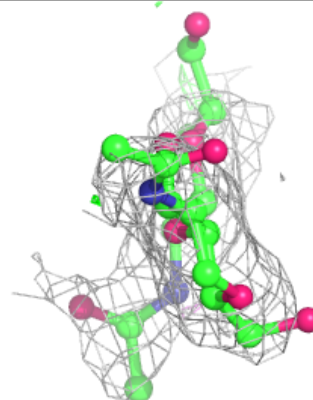
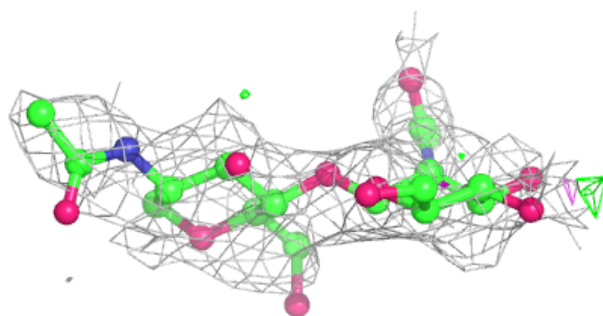
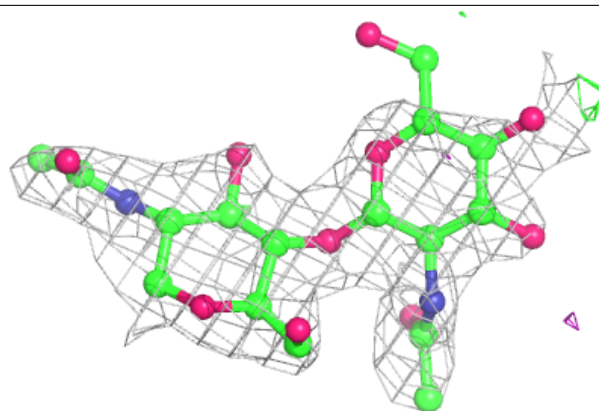
Electron density around Chain R:

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



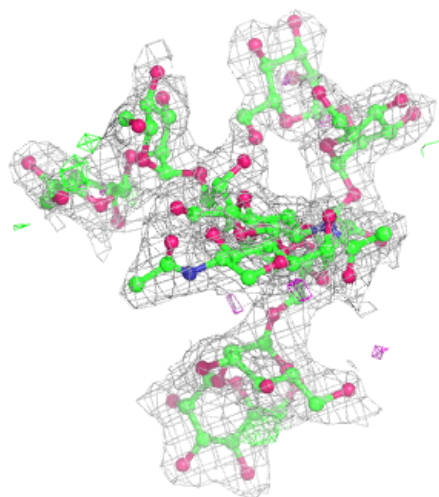
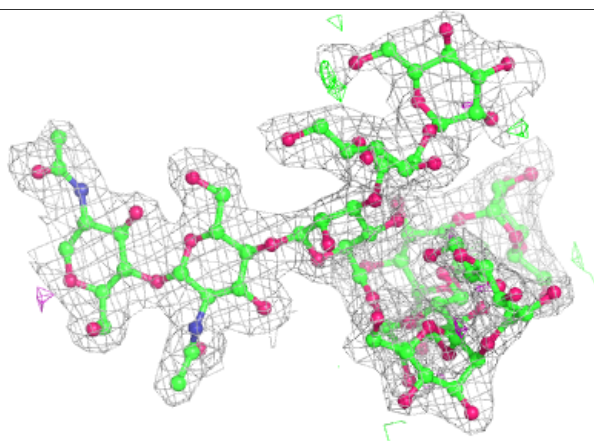
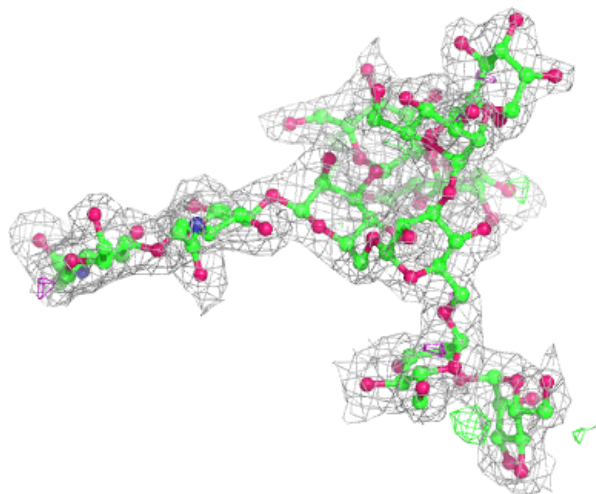
Electron density around Chain Y:

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



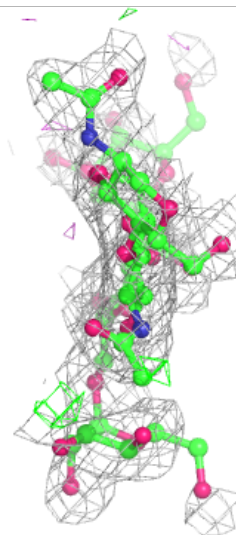
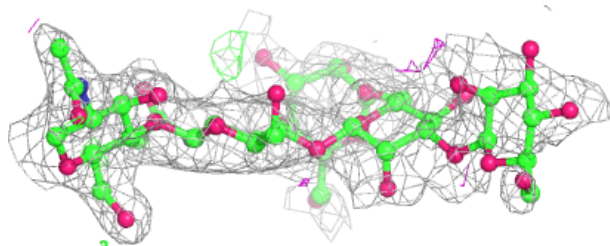
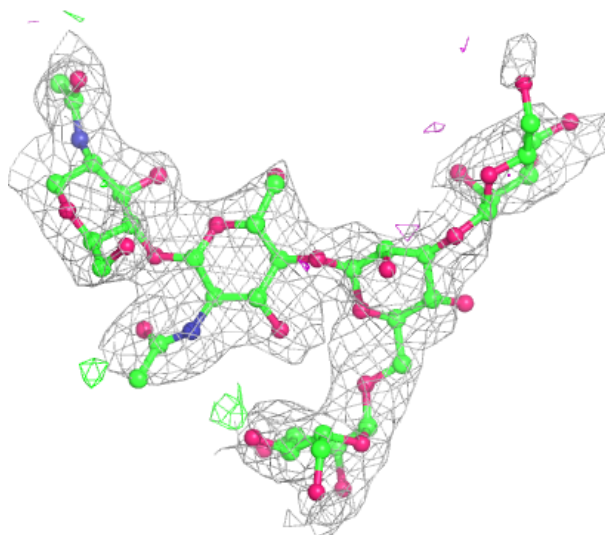
Electron density around Chain O:

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



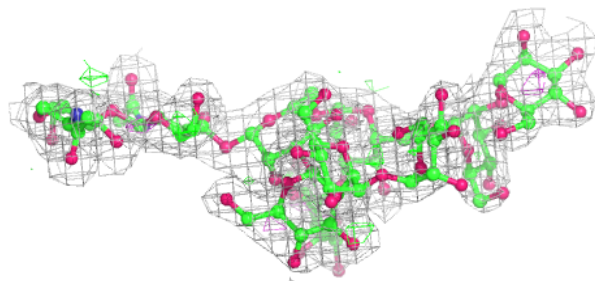
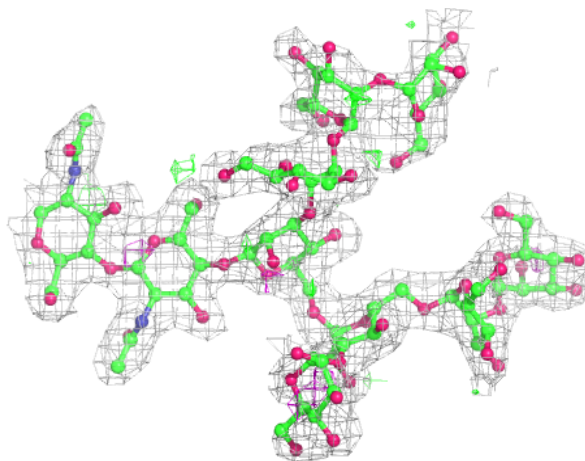
Electron density around Chain P:

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



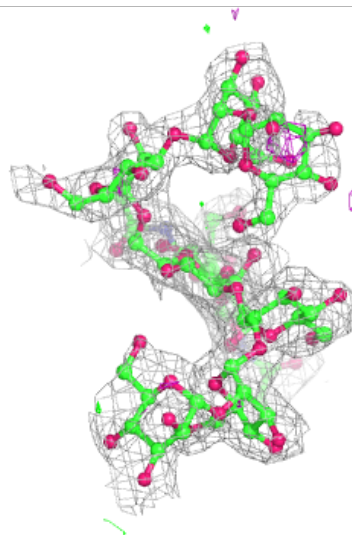
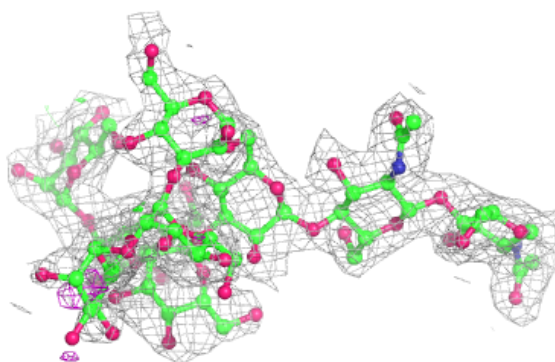
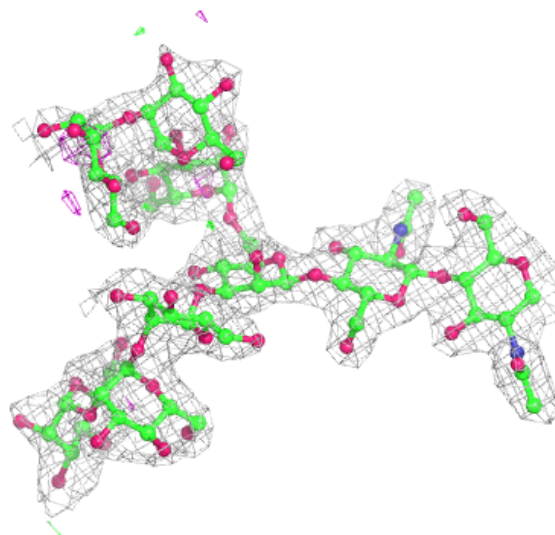
Electron density around Chain Q:

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



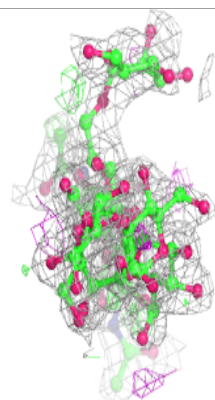
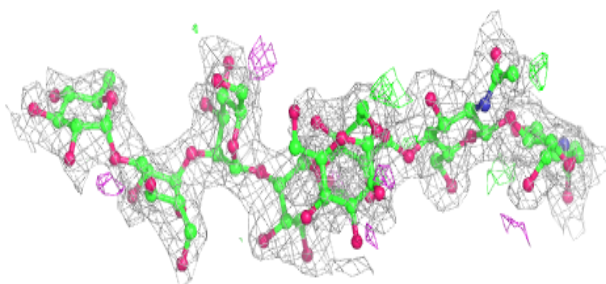
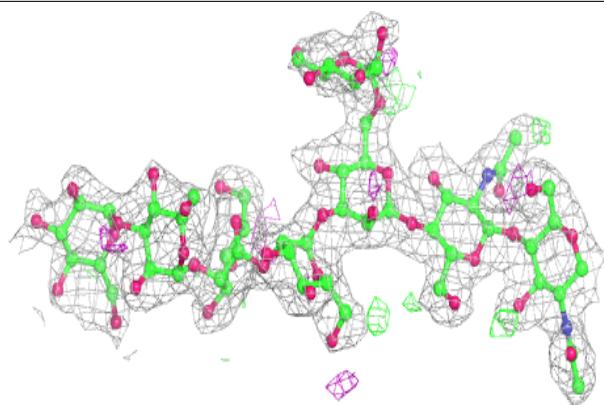
Electron density around Chain S:

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

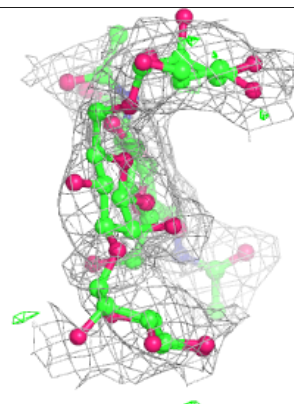
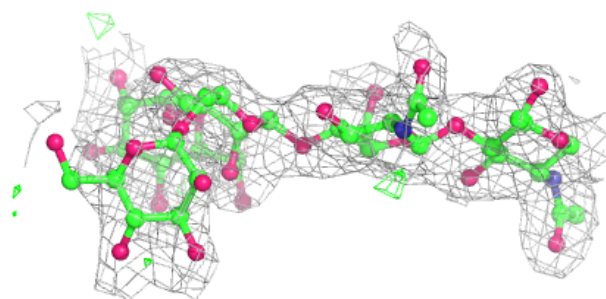
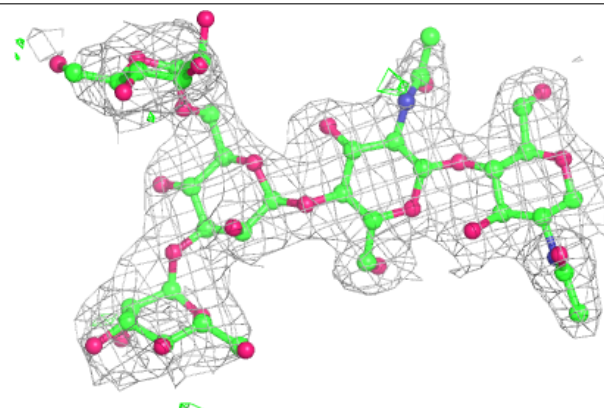


Electron density around Chain T:

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

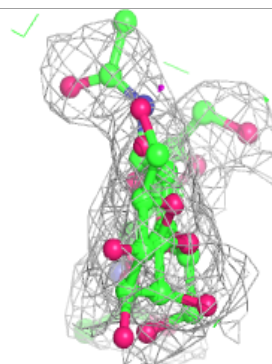
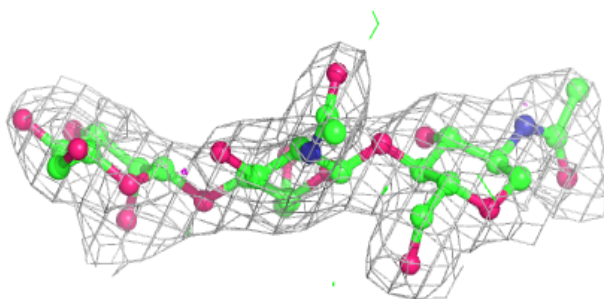
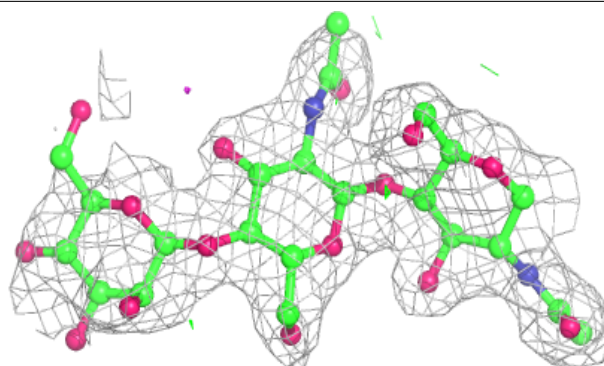
**Electron density around Chain U:**

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

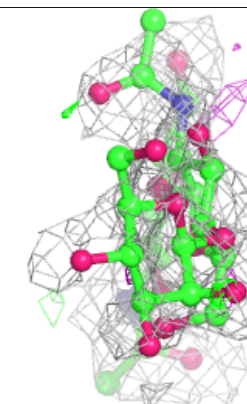
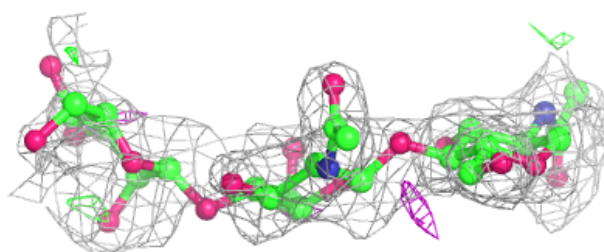
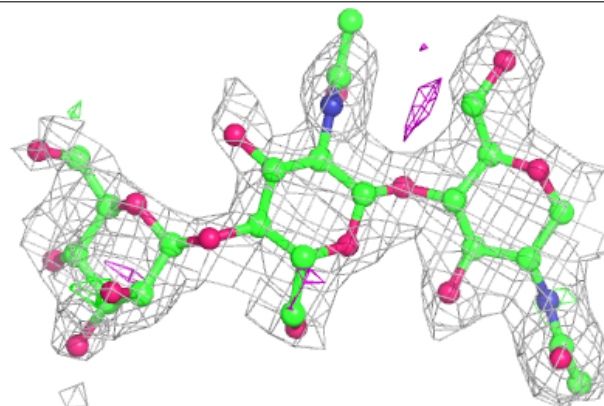


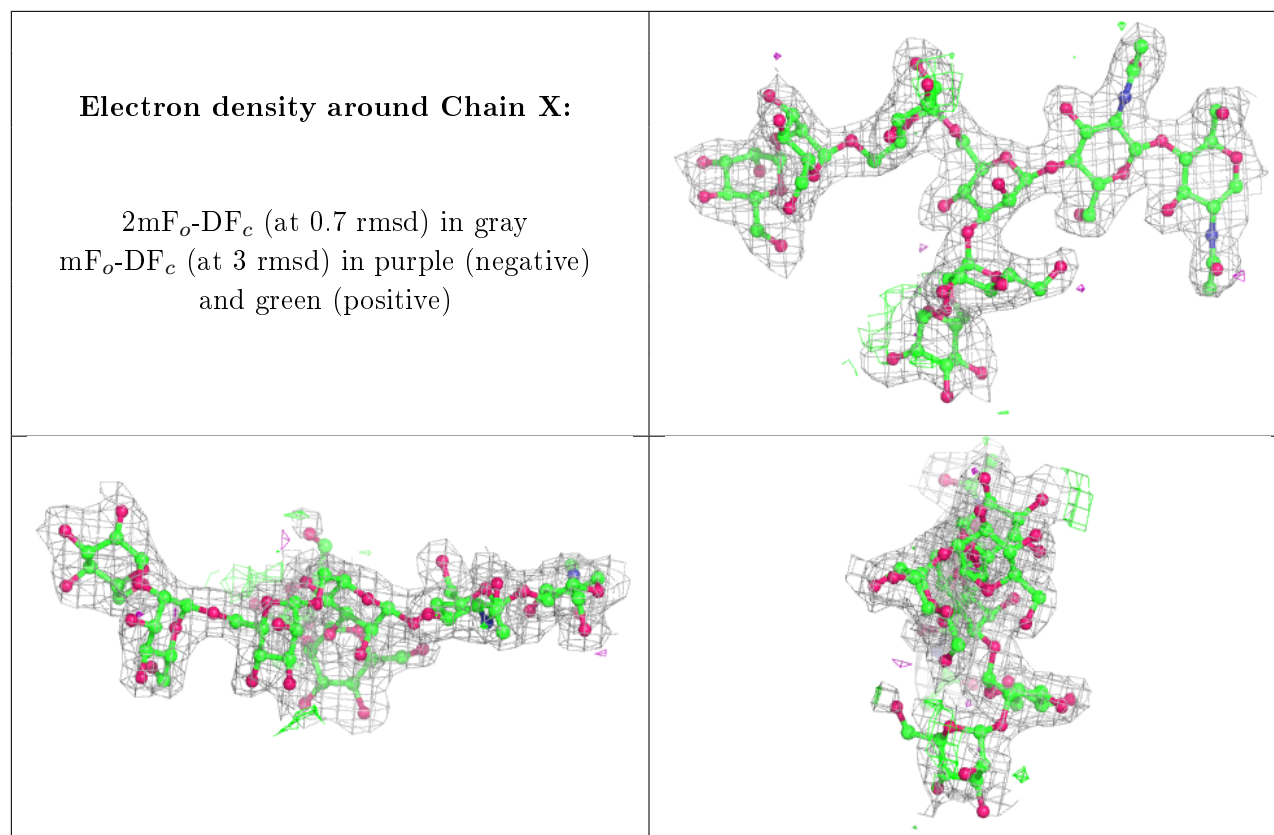
Electron density around Chain W:

$2mF_o-DF_c$ (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)





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(\AA^2)	Q<0.9
20	MAN	B	905	11/12	0.68	0.20	63,88,99,102	0
19	BGC	C	951	12/12	0.69	0.27	44,58,64,67	0
18	NAG	D	944	14/15	0.72	0.23	62,80,88,88	0
18	NAG	D	940	14/15	0.74	0.21	58,63,68,73	0
19	BGC	B	945	12/12	0.77	0.28	39,47,55,63	0
18	NAG	C	950	14/15	0.80	0.31	62,72,82,88	0
18	NAG	B	944	14/15	0.80	0.19	54,65,70,76	0
18	NAG	C	935	14/15	0.81	0.21	61,72,85,87	0
18	NAG	B	943	14/15	0.82	0.22	64,74,84,84	0
18	NAG	A	930	14/15	0.83	0.17	57,62,65,72	0
18	NAG	A	941	14/15	0.84	0.25	59,66,69,70	0
19	BGC	A	946	12/12	0.87	0.20	36,46,49,53	0
19	BGC	D	945	12/12	0.88	0.21	46,52,57,61	0
18	NAG	C	944	14/15	0.89	0.16	41,47,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	NAG	B	940	14/15	0.89	0.17	42,58,66,71	0
18	NAG	D	941	14/15	0.90	0.34	64,79,84,85	0
18	NAG	A	945	14/15	0.90	0.13	46,52,54,62	0
18	NAG	A	944	14/15	0.92	0.13	29,32,37,40	0
18	NAG	D	942	14/15	0.92	0.18	32,34,35,38	0
18	NAG	A	940	14/15	0.93	0.19	41,51,56,57	0
18	NAG	D	943	14/15	0.95	0.11	25,28,36,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.