



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 02:34 PM BST

PDB ID : 5FJJ
Title : Three-dimensional structures of two heavily N-glycosylated *Aspergillus* sp. Family GH3 beta-D-glucosidases
Authors : Agirre, J.; Ariza, A.; Offen, W.A.; Turkenburg, J.P.; Roberts, S.M.; McNicholas, S.; Harris, P.V.; McBrayer, B.; Dohnalek, J.; Cowtan, K.D.; Davies, G.J.; Wilson, K.S.
Deposited on : 2015-10-09
Resolution : 1.95 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

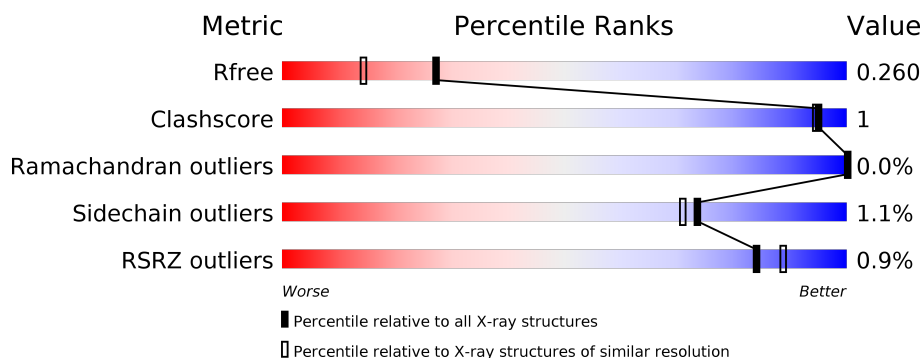
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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.










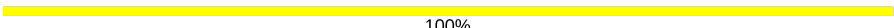
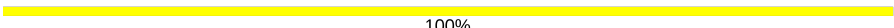


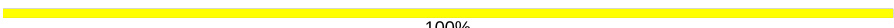
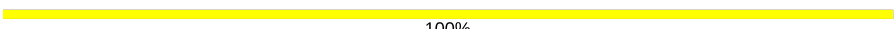
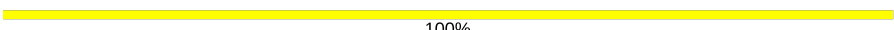

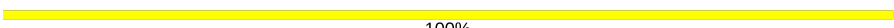


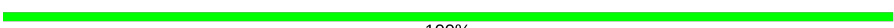






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	842	<div> <div>%</div> <div> <div></div> <div>95%</div> <div>.</div> </div> </div>
1	B	842	<div> <div>%</div> <div> <div></div> <div>96%</div> <div>.</div> </div> </div>
1	C	842	<div> <div></div> <div> <div></div> <div>96%</div> <div>.</div> </div> </div>
1	D	842	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>.</div> </div> </div>
2	E	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>
2	G	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>





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Mol	Chain	Length	Quality of chain
2	W	3	 100%
3	F	4	 50% 25% 25%
3	M	4	 100%
3	O	4	 50% 50%
3	U	4	 75% 25%
4	H	11	 91% 9%
4	P	11	 82% 18%
5	I	2	 100%
5	L	2	 100%
5	Q	2	 50% 50%
5	T	2	 50% 50%
5	Y	2	 100%
5	b	2	 100%
5	c	2	 100%
5	d	2	 50% 50%
5	g	2	 100%
6	J	6	 50% 50%
7	K	7	 86% 14%
7	i	7	 100%
8	N	6	 67% 33%
9	R	7	 71% 29%
9	Z	7	 57% 29% 14%
9	a	7	 71% 29%
9	h	7	 86% 14%
10	S	5	 60% 40%

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Mol	Chain	Length	Quality of chain
11	V	5	 80% 20%
12	X	9	 44% 56%
13	e	4	 50% 50%
14	f	8	 88% 13%

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 30056 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.

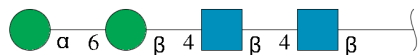
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	839	Total	C	N	O	S	0	9	0
			6506	4094	1118	1275	19			
1	B	838	Total	C	N	O	S	0	7	0
			6471	4073	1110	1269	19			
1	C	839	Total	C	N	O	S	0	8	0
			6489	4083	1114	1273	19			
1	D	838	Total	C	N	O	S	0	6	0
			6477	4079	1113	1266	19			

- Molecule 2 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.



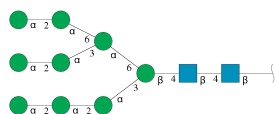
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	W	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 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
3	F	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	M	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	O	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	U	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 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
4	H	11	Total	C	N	O	0	0	0
			127	70	2	55			
4	P	11	Total	C	N	O	0	0	0
			127	70	2	55			

- Molecule 5 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
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			

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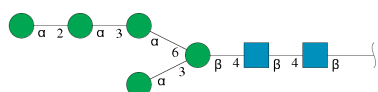
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	b	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	c	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	d	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	g	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called 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.



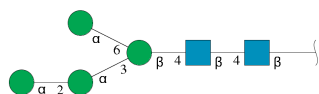
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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.



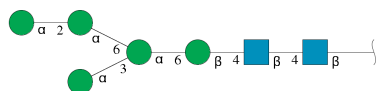
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	K	7	Total	C	N	O	0	0	0
			83	46	2	35			
7	i	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 8 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.



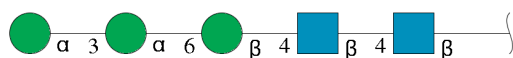
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	N	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 9 is an oligosaccharide called 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
9	R	7	Total	C	N	O	0	0	0
			83	46	2	35			
9	Z	7	Total	C	N	O	0	0	0
			83	46	2	35			
9	a	7	Total	C	N	O	0	0	0
			83	46	2	35			
9	h	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 10 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.



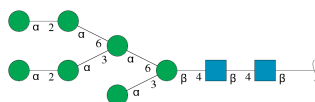
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	S	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-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
11	V	5	Total	C	N	O	0	1	0
			75	42	3	30			

- Molecule 12 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-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



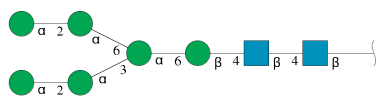
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	X	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 13 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.



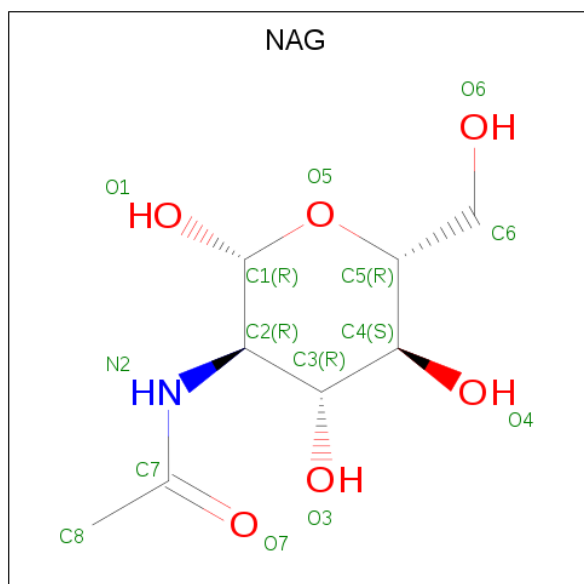
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	e	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 14 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)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



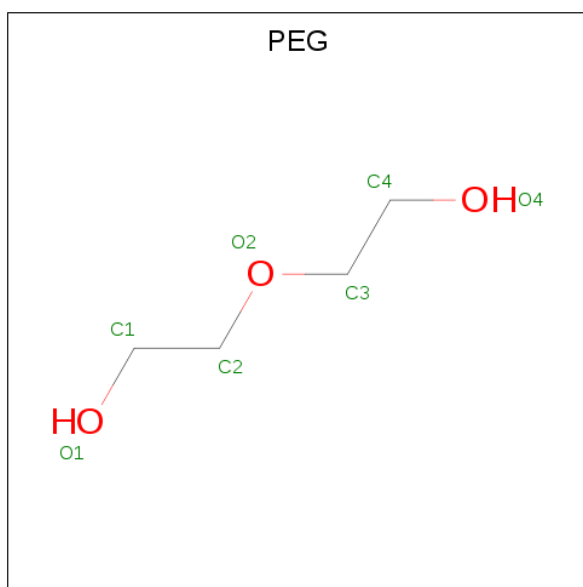
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	f	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 16 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	A	1	Total	C	O	0	0
			7	4	3		
16	A	1	Total	C	O	0	0
			7	4	3		
16	B	1	Total	C	O	0	0
			7	4	3		
16	C	1	Total	C	O	0	0
			7	4	3		
16	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	2	Total	Mg	0	0
			2	2		
17	D	1	Total	Mg	0	0
			1	1		
17	C	1	Total	Mg	0	0
			1	1		

- Molecule 18 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 19 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	B	1	Total	Cl	0	0
			1	1		
19	A	1	Total	Cl	0	0
			1	1		
19	D	1	Total	Cl	0	0
			1	1		
19	C	1	Total	Cl	0	0
			1	1		

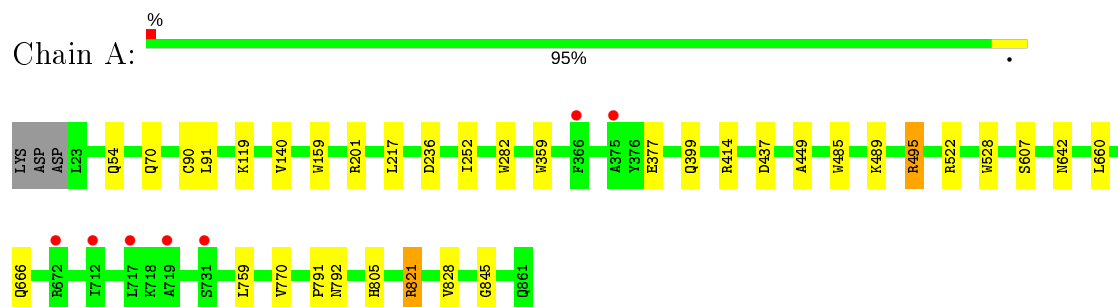
- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	533	Total	O	0	4
			535	535		
20	B	501	Total	O	0	2
			503	503		
20	C	601	Total	O	0	7
			606	606		
20	D	471	Total	O	0	2
			473	473		

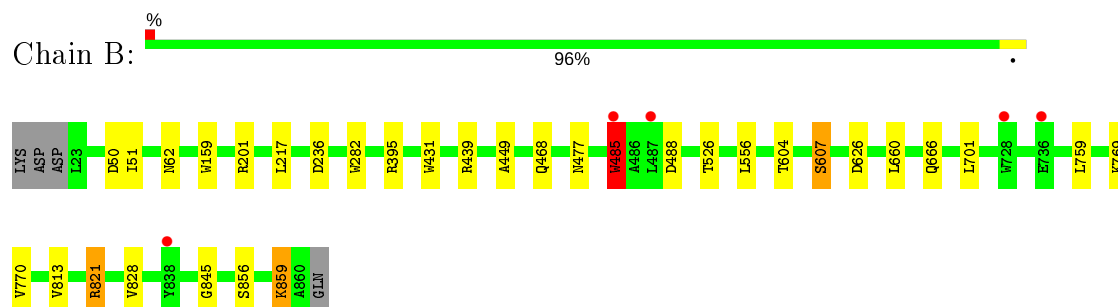
3 Residue-property plots

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

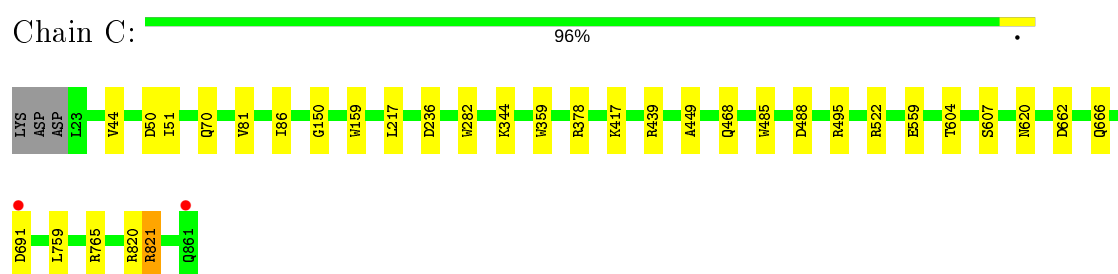
• Molecule 1: BETA-GLUCOSIDASE



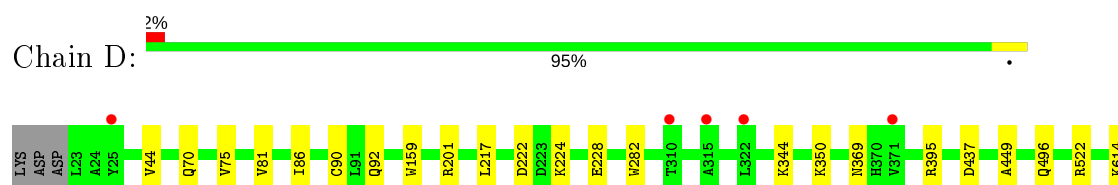
• Molecule 1: BETA-GLUCOSIDASE

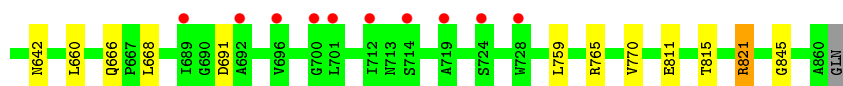


• Molecule 1: BETA-GLUCOSIDASE



• Molecule 1: BETA-GLUCOSIDASE





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



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



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

Chain U:  75% 25%

UAG1
UAG2
BMA3
MAN4

- Molecule 4: 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-(1-2)-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 H:  91% 9%

UAG1
UAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10
MAN11

- Molecule 4: 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-(1-2)-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 P:  82% 18%

UAG1
UAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10
MAN11

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

UAG1
UAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%

UAG1
UAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  50% 50%

UAG1
UAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 50%

NAG1
NAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  100%

NAG1
NAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%

NAG1
NAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  100%

NAG1
NAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  50% 50%

NAG1
NAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  100%


NAG1
NAG2

- Molecule 6: 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:  50% 50%



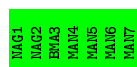
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  86% 14%



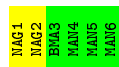
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  100%



- Molecule 8: 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 N:  67% 33%



- Molecule 9: 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 R:  71% 29%



- Molecule 9: 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 Z:  57% 29% 14%



- Molecule 9: 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 a:  71% 29%



- Molecule 9: 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 h:  86% 14%




- Molecule 10: 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:  60% 40%



- Molecule 11: 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:  80% 20%



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

Chain X:  44% 56%



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

Chain e:  50% 50%



- Molecule 14: 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 f:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	139.02Å 141.46Å 193.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	114.43 – 1.95 88.23 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.8 (114.43-1.95) 97.8 (88.23-1.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.216 , 0.255 0.223 , 0.260	Depositor DCC
R_{free} test set	13558 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.775	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30056	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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: MG, BMA, NAG, CL, PO4, PEG, 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	0.71	0/6685	0.80	9/9111 (0.1%)
1	B	0.73	0/6651	0.80	10/9067 (0.1%)
1	C	0.71	0/6667	0.81	11/9089 (0.1%)
1	D	0.68	0/6655	0.80	11/9071 (0.1%)
All	All	0.71	0/26658	0.80	41/36338 (0.1%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	821	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	D	821	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	C	821	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	A	821	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	D	201	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	C	439	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	B	701	LEU	CA-CB-CG	6.91	131.19	115.30
1	B	821	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	D	437	ASP	CB-CG-OD1	6.56	124.21	118.30
1	B	201	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	C	559	GLU	OE1-CD-OE2	-6.17	115.90	123.30
1	D	522	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	C	522	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	C	821	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	437	ASP	CB-CG-OD1	5.96	123.66	118.30
1	C	522	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	522	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	B	439	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	821	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	856	SER	N-CA-CB	5.61	118.91	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	50	ASP	CB-CG-OD1	-5.53	113.32	118.30
1	B	485	TRP	CA-CB-CG	-5.53	103.19	113.70
1	C	50	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	495[A]	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	495[B]	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	236	ASP	CB-CG-OD1	5.39	123.15	118.30
1	D	691	ASP	CB-CG-OD1	5.39	123.15	118.30
1	D	350	LYS	CB-CG-CD	5.38	125.59	111.60
1	D	201	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	522	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	236	ASP	CB-CG-OD1	5.26	123.04	118.30
1	C	236	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	222	ASP	CB-CG-OD1	5.17	122.96	118.30
1	D	811	GLU	CB-CA-C	-5.14	100.13	110.40
1	C	50	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	D	821	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	395	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	D	522	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	C	820	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	C	378	ARG	NE-CZ-NH1	5.01	122.80	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	6506	0	6166	24	0
1	B	6471	0	6137	14	0
1	C	6489	0	6151	11	0
1	D	6477	0	6151	17	0
2	E	39	0	34	0	0
2	G	39	0	34	0	0
2	W	39	0	34	0	0
3	F	50	0	43	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	50	0	43	0	0
3	O	50	0	43	0	0
3	U	50	0	43	0	0
4	H	127	0	106	0	0
4	P	127	0	106	0	0
5	I	28	0	25	0	0
5	L	28	0	25	0	0
5	Q	28	0	25	0	0
5	T	28	0	25	0	0
5	Y	28	0	25	0	0
5	b	28	0	25	0	0
5	c	28	0	25	0	0
5	d	28	0	25	0	0
5	g	28	0	25	0	0
6	J	72	0	61	3	0
7	K	83	0	70	0	0
7	i	83	0	70	0	0
8	N	72	0	61	1	0
9	R	83	0	70	2	0
9	Z	83	0	70	2	0
9	a	83	0	70	0	0
9	h	83	0	70	0	0
10	S	61	0	52	0	0
11	V	75	0	64	0	0
12	X	105	0	88	0	0
13	e	50	0	43	0	0
14	f	94	0	79	0	0
15	A	28	0	26	0	0
15	B	14	0	13	0	0
15	C	28	0	26	2	0
15	D	28	0	26	0	0
16	A	14	0	20	0	0
16	B	7	0	10	0	0
16	C	7	0	10	0	0
16	D	7	0	10	0	0
17	A	2	0	0	0	0
17	C	1	0	0	0	0
17	D	1	0	0	0	0
18	A	5	0	0	0	0
19	A	1	0	0	0	0
19	B	1	0	0	0	0
19	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	D	1	0	0	0	0
20	A	535	0	0	7	0
20	B	503	0	0	1	0
20	C	606	0	0	0	0
20	D	473	0	0	4	0
All	All	30056	0	26325	62	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 (62) 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:A:791[B]:PRO:O	1:A:792[B]:ASN:HB2	1.74	0.86
1:A:791[B]:PRO:O	1:A:792[B]:ASN:CB	2.34	0.74
1:A:414:ARG:NH1	20:A:2255:HOH:O	2.21	0.72
1:A:377:GLU:OE2	20:A:2040:HOH:O	2.08	0.69
1:C:620:ASN:ND2	15:C:1901:NAG:O6	2.26	0.69
1:D:70:GLN:OE1	20:D:2032:HOH:O	2.12	0.67
1:D:369:ASN:OD1	20:D:2032:HOH:O	2.13	0.66
1:A:666:GLN:HG3	1:C:666:GLN:HB2	1.81	0.61
1:A:399:GLN:NE2	20:A:2073:HOH:O	2.35	0.59
1:A:495[A]:ARG:NH1	20:A:2318:HOH:O	2.37	0.56
1:D:668:LEU:HD21	1:D:765[B]:ARG:HG3	1.86	0.56
1:C:604:THR:O	1:C:607[B]:SER:OG	2.25	0.55
1:D:75:VAL:HG12	1:D:92:GLN:HA	1.88	0.54
1:D:159:TRP:CE2	1:D:449:ALA:HB3	2.44	0.53
1:C:620:ASN:HD22	15:C:1901:NAG:HO6	1.58	0.52
1:B:488:ASP:OD1	9:R:6:MAN:O2	2.27	0.51
1:C:159:TRP:CE2	1:C:449:ALA:HB3	2.46	0.51
1:B:485:TRP:CE2	9:R:3:BMA:H62	2.45	0.51
1:D:642:ASN:ND2	20:D:2361:HOH:O	2.44	0.50
1:B:159:TRP:CE2	1:B:449:ALA:HB3	2.46	0.50
1:A:159:TRP:CE2	1:A:449:ALA:HB3	2.47	0.49
1:A:528:TRP:CE3	6:J:2:NAG:H81	2.48	0.49
1:D:224[A]:LYS:NZ	1:D:228:GLU:OE2	2.44	0.48
1:B:660:LEU:HD22	1:B:770:VAL:HG22	1.94	0.48
1:B:660:LEU:HD12	1:B:845:GLY:HA2	1.97	0.47
1:D:660:LEU:HD22	1:D:770:VAL:HG22	1.97	0.47
1:B:759:LEU:HB3	1:B:821:ARG:HB2	1.96	0.46
1:C:759:LEU:HB3	1:C:821:ARG:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:759:LEU:HB3	1:D:821:ARG:HB2	1.97	0.46
1:A:252:ILE:CG2	3:F:1:NAG:H82	2.46	0.46
1:D:660:LEU:HD12	1:D:845:GLY:HA2	1.98	0.46
1:A:252:ILE:HG22	3:F:1:NAG:H82	1.96	0.46
1:A:759:LEU:HB3	1:A:821:ARG:HB2	1.97	0.45
1:D:496:GLN:OE1	20:D:2285:HOH:O	2.21	0.45
1:A:414:ARG:HD3	20:A:2256:HOH:O	2.16	0.45
1:B:828:VAL:HG11	8:N:2:NAG:O3	2.16	0.45
1:A:642:ASN:ND2	20:A:2397:HOH:O	2.50	0.45
1:C:488:ASP:OD1	9:Z:6:MAN:O2	2.29	0.45
1:A:660:LEU:HD12	1:A:845:GLY:HA2	1.99	0.45
1:B:526:THR:HG22	1:B:556:LEU:HD12	1.99	0.45
1:B:626:ASP:HB3	20:B:2369:HOH:O	2.17	0.45
1:A:485:TRP:CD2	6:J:3:BMA:H62	2.52	0.44
1:A:660:LEU:HD22	1:A:770:VAL:HG22	1.98	0.44
1:B:604:THR:O	1:B:607[A]:SER:OG	2.33	0.44
1:B:813:VAL:HB	1:D:815:THR:HB	2.00	0.43
1:A:805:HIS:HB2	20:A:2467:HOH:O	2.19	0.42
1:C:70:GLN:HG2	1:C:359:TRP:CE3	2.54	0.42
1:D:81:VAL:HB	1:D:86:ILE:HB	2.02	0.42
1:B:859:LYS:HZ3	1:B:859:LYS:HG3	1.69	0.42
1:A:70:GLN:HG2	1:A:359:TRP:CE3	2.55	0.41
1:A:70:GLN:HG2	1:A:359:TRP:CD2	2.55	0.41
1:B:666:GLN:HB2	1:D:666:GLN:HG3	2.01	0.41
1:D:395[B]:ARG:HD2	1:D:395[B]:ARG:HH11	1.58	0.41
1:C:44:VAL:HG11	1:C:344:LYS:HA	2.03	0.41
1:A:91:LEU:HG	1:A:140:VAL:HB	2.03	0.41
1:D:44:VAL:HG11	1:D:344:LYS:HA	2.03	0.41
1:D:75:VAL:CG1	1:D:92:GLN:HA	2.48	0.41
1:A:489:LYS:HE3	1:B:431:TRP:CE3	2.56	0.41
1:C:485:TRP:CE2	9:Z:3:BMA:H62	2.56	0.41
1:A:828:VAL:HG11	3:F:2:NAG:O3	2.20	0.40
1:A:485:TRP:CE2	6:J:3:BMA:H62	2.56	0.40
1:C:81:VAL:HB	1:C:86:ILE:HB	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	846/842 (100%)	818 (97%)	28 (3%)	0	100	100
1	B	843/842 (100%)	819 (97%)	24 (3%)	0	100	100
1	C	845/842 (100%)	816 (97%)	28 (3%)	1 (0%)	51	43
1	D	842/842 (100%)	816 (97%)	26 (3%)	0	100	100
All	All	3376/3368 (100%)	3269 (97%)	106 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	150	GLY

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	686/681 (101%)	679 (99%)	7 (1%)	76	74
1	B	683/681 (100%)	672 (98%)	11 (2%)	62	58
1	C	684/681 (100%)	675 (99%)	9 (1%)	69	65
1	D	683/681 (100%)	679 (99%)	4 (1%)	86	85
All	All	2736/2724 (100%)	2705 (99%)	31 (1%)	73	71

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54[A]	GLN
1	A	54[B]	GLN
1	A	90	CYS
1	A	119	LYS
1	A	217	LEU
1	A	282	TRP
1	A	607	SER
1	B	51	ILE
1	B	62	ASN
1	B	217	LEU
1	B	282	TRP
1	B	468	GLN
1	B	477	ASN
1	B	485	TRP
1	B	607[A]	SER
1	B	607[B]	SER
1	B	769	LYS
1	B	859	LYS
1	C	51	ILE
1	C	217	LEU
1	C	282	TRP
1	C	417	LYS
1	C	468	GLN
1	C	495	ARG
1	C	662	ASP
1	C	691	ASP
1	C	765	ARG
1	D	90	CYS
1	D	217	LEU
1	D	282	TRP
1	D	614	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	473	GLN
1	A	620	ASN
1	A	669	ASN
1	A	861	GLN
1	B	473	GLN
1	C	195	ASN
1	C	473	GLN
1	C	620	ASN

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Mol	Chain	Res	Type
1	C	825	ASN
1	D	369	ASN
1	D	473	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 ⓘ

151 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	0.80	1 (7%)	17,19,21	0.71	0
2	NAG	E	2	2	14,14,15	0.39	0	17,19,21	0.50	0
2	BMA	E	3	2	11,11,12	0.28	0	15,15,17	0.45	0
3	NAG	F	1	1,3	14,14,15	0.90	1 (7%)	17,19,21	0.98	2 (11%)
3	NAG	F	2	3	14,14,15	0.48	0	17,19,21	0.65	0
3	BMA	F	3	3	11,11,12	0.33	0	15,15,17	0.49	0
3	MAN	F	4	3	11,11,12	0.27	0	15,15,17	0.49	0
2	NAG	G	1	1,2	14,14,15	0.57	0	17,19,21	0.73	1 (5%)
2	NAG	G	2	2	14,14,15	0.44	0	17,19,21	0.66	0
2	BMA	G	3	2	11,11,12	0.40	0	15,15,17	0.62	0
4	NAG	H	1	1,4	14,14,15	0.38	0	17,19,21	0.66	0
4	MAN	H	10	4	11,11,12	0.41	0	15,15,17	0.69	0
4	MAN	H	11	4	11,11,12	0.33	0	15,15,17	0.74	0
4	NAG	H	2	4	14,14,15	0.62	0	17,19,21	0.76	1 (5%)
4	BMA	H	3	4	11,11,12	0.26	0	15,15,17	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	H	4	4	11,11,12	0.32	0	15,15,17	0.56	0
4	MAN	H	5	4	11,11,12	0.34	0	15,15,17	0.58	0
4	MAN	H	6	4	11,11,12	0.25	0	15,15,17	0.63	0
4	MAN	H	7	4	11,11,12	0.19	0	15,15,17	0.45	0
4	MAN	H	8	4	11,11,12	0.28	0	15,15,17	0.63	0
4	MAN	H	9	4	11,11,12	0.28	0	15,15,17	0.45	0
5	NAG	I	1	1,5	14,14,15	0.65	0	17,19,21	1.11	1 (5%)
5	NAG	I	2	5	14,14,15	0.85	1 (7%)	17,19,21	1.30	2 (11%)
6	NAG	J	1	1,6	14,14,15	0.50	0	17,19,21	0.43	0
6	NAG	J	2	6	14,14,15	0.60	0	17,19,21	0.55	0
6	BMA	J	3	6	11,11,12	0.25	0	15,15,17	0.40	0
6	MAN	J	4	6	11,11,12	0.30	0	15,15,17	0.48	0
6	MAN	J	5	6	11,11,12	0.33	0	15,15,17	0.67	0
6	MAN	J	6	6	11,11,12	0.38	0	15,15,17	0.66	1 (6%)
7	NAG	K	1	1,7	14,14,15	0.72	1 (7%)	17,19,21	0.34	0
7	NAG	K	2	7	14,14,15	0.45	0	17,19,21	0.67	0
7	BMA	K	3	7	11,11,12	0.33	0	15,15,17	0.79	0
7	MAN	K	4	7	11,11,12	0.31	0	15,15,17	0.66	0
7	MAN	K	5	7	11,11,12	0.34	0	15,15,17	0.63	0
7	MAN	K	6	7	11,11,12	0.21	0	15,15,17	0.59	0
7	MAN	K	7	7	11,11,12	0.27	0	15,15,17	0.54	0
5	NAG	L	1	1,5	14,14,15	0.48	0	17,19,21	0.68	1 (5%)
5	NAG	L	2	5	14,14,15	0.44	0	17,19,21	0.68	1 (5%)
3	NAG	M	1	1,3	14,14,15	0.66	0	17,19,21	0.57	0
3	NAG	M	2	3	14,14,15	0.50	0	17,19,21	0.47	0
3	BMA	M	3	3	11,11,12	0.26	0	15,15,17	0.51	0
3	MAN	M	4	3	11,11,12	0.36	0	15,15,17	0.59	0
8	NAG	N	1	1,8	14,14,15	0.82	1 (7%)	17,19,21	1.00	1 (5%)
8	NAG	N	2	8	14,14,15	0.53	0	17,19,21	0.59	0
8	BMA	N	3	8	11,11,12	0.35	0	15,15,17	0.52	0
8	MAN	N	4	8	11,11,12	0.31	0	15,15,17	0.69	0
8	MAN	N	5	8	11,11,12	0.33	0	15,15,17	0.56	0
8	MAN	N	6	8	11,11,12	0.28	0	15,15,17	0.57	0
3	NAG	O	1	1,3	14,14,15	0.99	1 (7%)	17,19,21	0.73	0
3	NAG	O	2	3	14,14,15	0.68	1 (7%)	17,19,21	0.65	0
3	BMA	O	3	3	11,11,12	0.24	0	15,15,17	0.30	0
3	MAN	O	4	3	11,11,12	0.27	0	15,15,17	0.57	0
4	NAG	P	1	1,4	14,14,15	0.50	0	17,19,21	0.53	0
4	MAN	P	10	4	11,11,12	0.33	0	15,15,17	0.71	0
4	MAN	P	11	4	11,11,12	0.34	0	15,15,17	0.69	0
4	NAG	P	2	4	14,14,15	0.54	0	17,19,21	0.92	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	P	3	4	11,11,12	0.22	0	15,15,17	0.52	0
4	MAN	P	4	4	11,11,12	0.26	0	15,15,17	0.54	0
4	MAN	P	5	4	11,11,12	0.29	0	15,15,17	0.75	1 (6%)
4	MAN	P	6	4	11,11,12	0.30	0	15,15,17	0.56	0
4	MAN	P	7	4	11,11,12	0.28	0	15,15,17	0.55	0
4	MAN	P	8	4	11,11,12	0.31	0	15,15,17	0.60	0
4	MAN	P	9	4	11,11,12	0.25	0	15,15,17	0.42	0
5	NAG	Q	1	1,5	14,14,15	0.50	0	17,19,21	0.84	0
5	NAG	Q	2	5	14,14,15	0.47	0	17,19,21	0.88	1 (5%)
9	NAG	R	1	1,9	14,14,15	0.64	0	17,19,21	0.71	0
9	NAG	R	2	9	14,14,15	0.40	0	17,19,21	0.63	0
9	BMA	R	3	9	11,11,12	0.29	0	15,15,17	0.47	0
9	MAN	R	4	9	11,11,12	0.36	0	15,15,17	0.48	0
9	MAN	R	5	9	11,11,12	0.27	0	15,15,17	0.47	0
9	MAN	R	6	9	11,11,12	0.30	0	15,15,17	0.67	0
9	MAN	R	7	9	11,11,12	0.24	0	15,15,17	0.38	0
10	NAG	S	1	1,10	14,14,15	0.51	0	17,19,21	0.60	0
10	NAG	S	2	10	14,14,15	0.44	0	17,19,21	0.88	2 (11%)
10	BMA	S	3	10	11,11,12	0.20	0	15,15,17	0.44	0
10	MAN	S	4	10	11,11,12	0.28	0	15,15,17	0.64	1 (6%)
10	MAN	S	5	10	11,11,12	0.29	0	15,15,17	0.48	0
5	NAG	T	1	1,5	14,14,15	0.47	0	17,19,21	0.58	0
5	NAG	T	2	5	14,14,15	0.59	0	17,19,21	0.84	1 (5%)
3	NAG	U	1	1,3	14,14,15	0.73	1 (7%)	17,19,21	0.56	0
3	NAG	U	2	3	14,14,15	0.45	0	17,19,21	0.54	0
3	BMA	U	3	3	11,11,12	0.42	0	15,15,17	0.65	0
3	MAN	U	4	3	11,11,12	0.28	0	15,15,17	0.56	0
11	NAG	V	1	1,11	14,14,15	0.40	0	17,19,21	0.59	0
11	NAG	V	2[A]	11	14,14,15	0.46	0	17,19,21	0.77	1 (5%)
11	NAG	V	2[B]	11	14,14,15	0.44	0	17,19,21	0.55	0
11	BMA	V	3	11	11,11,12	0.28	0	15,15,17	0.41	0
11	MAN	V	4	11	11,11,12	0.44	0	15,15,17	0.75	0
11	MAN	V	5	11	11,11,12	0.28	0	15,15,17	0.63	0
2	NAG	W	1	1,2	14,14,15	0.50	0	17,19,21	0.55	0
2	NAG	W	2	2	14,14,15	0.51	0	17,19,21	0.61	0
2	BMA	W	3	2	11,11,12	0.33	0	15,15,17	0.57	0
12	NAG	X	1	1,12	14,14,15	0.78	1 (7%)	17,19,21	0.48	0
12	NAG	X	2	12	14,14,15	0.97	1 (7%)	17,19,21	0.82	0
12	BMA	X	3	12	11,11,12	0.23	0	15,15,17	0.52	0
12	MAN	X	4	12	11,11,12	0.23	0	15,15,17	0.50	0
12	MAN	X	5	12	11,11,12	0.25	0	15,15,17	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MAN	X	6	12	11,11,12	0.26	0	15,15,17	0.44	0
12	MAN	X	7	12	11,11,12	0.55	0	15,15,17	0.68	1 (6%)
12	MAN	X	8	12	11,11,12	0.38	0	15,15,17	0.74	1 (6%)
12	MAN	X	9	12	11,11,12	0.35	0	15,15,17	0.68	1 (6%)
5	NAG	Y	1	1,5	14,14,15	0.63	0	17,19,21	1.06	1 (5%)
5	NAG	Y	2	5	14,14,15	0.50	0	17,19,21	0.80	1 (5%)
9	NAG	Z	1	1,9	14,14,15	0.53	0	17,19,21	0.56	0
9	NAG	Z	2	9	14,14,15	0.46	0	17,19,21	0.54	0
9	BMA	Z	3	9	11,11,12	0.22	0	15,15,17	0.47	0
9	MAN	Z	4	9	11,11,12	0.25	0	15,15,17	0.51	0
9	MAN	Z	5	9	11,11,12	0.39	0	15,15,17	0.73	1 (6%)
9	MAN	Z	6	9	11,11,12	0.42	0	15,15,17	0.94	2 (13%)
9	MAN	Z	7	9	11,11,12	0.24	0	15,15,17	0.59	0
9	NAG	a	1	1,9	14,14,15	0.57	0	17,19,21	0.75	1 (5%)
9	NAG	a	2	9	14,14,15	0.55	0	17,19,21	0.71	0
9	BMA	a	3	9	11,11,12	0.19	0	15,15,17	0.56	0
9	MAN	a	4	9	11,11,12	0.31	0	15,15,17	0.62	0
9	MAN	a	5	9	11,11,12	0.21	0	15,15,17	0.52	0
9	MAN	a	6	9	11,11,12	0.29	0	15,15,17	0.70	1 (6%)
9	MAN	a	7	9	11,11,12	0.34	0	15,15,17	0.42	0
5	NAG	b	1	1,5	14,14,15	0.45	0	17,19,21	0.89	1 (5%)
5	NAG	b	2	5	14,14,15	0.50	0	17,19,21	0.81	1 (5%)
5	NAG	c	1	1,5	14,14,15	0.54	0	17,19,21	0.88	1 (5%)
5	NAG	c	2	5	14,14,15	0.77	1 (7%)	17,19,21	0.72	1 (5%)
5	NAG	d	1	1,5	14,14,15	0.81	1 (7%)	17,19,21	0.63	0
5	NAG	d	2	5	14,14,15	0.48	0	17,19,21	0.57	0
13	NAG	e	1	1,13	14,14,15	0.50	0	17,19,21	0.73	1 (5%)
13	NAG	e	2	13	14,14,15	0.65	0	17,19,21	0.95	1 (5%)
13	BMA	e	3	13	11,11,12	0.22	0	15,15,17	0.39	0
13	MAN	e	4	13	11,11,12	0.33	0	15,15,17	0.69	0
14	NAG	f	1	1,14	14,14,15	0.44	0	17,19,21	0.73	0
14	NAG	f	2	14	14,14,15	0.93	1 (7%)	17,19,21	0.71	0
14	BMA	f	3	14	11,11,12	0.35	0	15,15,17	0.51	0
14	MAN	f	4	14	11,11,12	0.35	0	15,15,17	0.45	0
14	MAN	f	5	14	11,11,12	0.32	0	15,15,17	0.58	0
14	MAN	f	6	14	11,11,12	0.26	0	15,15,17	0.38	0
14	MAN	f	7	14	11,11,12	0.29	0	15,15,17	0.46	0
14	MAN	f	8	14	11,11,12	0.39	0	15,15,17	0.75	0
5	NAG	g	1	1,5	14,14,15	0.48	0	17,19,21	0.84	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	g	2	5	14,14,15	0.50	0	17,19,21	0.70	1 (5%)
9	NAG	h	1	1,9	14,14,15	0.50	0	17,19,21	0.48	0
9	NAG	h	2	9	14,14,15	0.43	0	17,19,21	0.64	0
9	BMA	h	3	9	11,11,12	0.30	0	15,15,17	0.46	0
9	MAN	h	4	9	11,11,12	0.29	0	15,15,17	0.48	0
9	MAN	h	5	9	11,11,12	0.34	0	15,15,17	0.69	1 (6%)
9	MAN	h	6	9	11,11,12	0.25	0	15,15,17	0.59	0
9	MAN	h	7	9	11,11,12	0.22	0	15,15,17	0.45	0
7	NAG	i	1	1,7	14,14,15	0.44	0	17,19,21	0.45	0
7	NAG	i	2	7	14,14,15	0.65	0	17,19,21	0.52	0
7	BMA	i	3	7	11,11,12	0.24	0	15,15,17	0.56	0
7	MAN	i	4	7	11,11,12	0.30	0	15,15,17	0.51	0
7	MAN	i	5	7	11,11,12	0.33	0	15,15,17	0.59	0
7	MAN	i	6	7	11,11,12	0.27	0	15,15,17	0.52	0
7	MAN	i	7	7	11,11,12	0.21	0	15,15,17	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	2/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	BMA	G	3	2	-	2/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	MAN	H	10	4	-	0/2/19/22	0/1/1/1
4	MAN	H	11	4	-	0/2/19/22	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
4	MAN	H	4	4	-	1/2/19/22	0/1/1/1
4	MAN	H	5	4	-	1/2/19/22	0/1/1/1
4	MAN	H	6	4	-	0/2/19/22	0/1/1/1
4	MAN	H	7	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	H	8	4	-	0/2/19/22	0/1/1/1
4	MAN	H	9	4	-	2/2/19/22	0/1/1/1
5	NAG	I	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
6	NAG	J	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1
6	MAN	J	4	6	-	2/2/19/22	0/1/1/1
6	MAN	J	5	6	-	2/2/19/22	0/1/1/1
6	MAN	J	6	6	-	0/2/19/22	0/1/1/1
7	NAG	K	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	0/6/23/26	0/1/1/1
7	BMA	K	3	7	-	0/2/19/22	0/1/1/1
7	MAN	K	4	7	-	2/2/19/22	0/1/1/1
7	MAN	K	5	7	-	0/2/19/22	0/1/1/1
7	MAN	K	6	7	-	2/2/19/22	0/1/1/1
7	MAN	K	7	7	-	0/2/19/22	0/1/1/1
5	NAG	L	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	0/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	BMA	M	3	3	-	0/2/19/22	0/1/1/1
3	MAN	M	4	3	-	2/2/19/22	0/1/1/1
8	NAG	N	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	N	2	8	-	2/6/23/26	0/1/1/1
8	BMA	N	3	8	-	0/2/19/22	0/1/1/1
8	MAN	N	4	8	-	0/2/19/22	0/1/1/1
8	MAN	N	5	8	-	0/2/19/22	0/1/1/1
8	MAN	N	6	8	-	0/2/19/22	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	BMA	O	3	3	-	0/2/19/22	0/1/1/1
3	MAN	O	4	3	-	1/2/19/22	0/1/1/1
4	NAG	P	1	1,4	-	2/6/23/26	0/1/1/1
4	MAN	P	10	4	-	0/2/19/22	0/1/1/1
4	MAN	P	11	4	-	0/2/19/22	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	BMA	P	3	4	-	0/2/19/22	0/1/1/1
4	MAN	P	4	4	-	2/2/19/22	0/1/1/1
4	MAN	P	5	4	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	P	6	4	-	2/2/19/22	0/1/1/1
4	MAN	P	7	4	-	0/2/19/22	0/1/1/1
4	MAN	P	8	4	-	0/2/19/22	0/1/1/1
4	MAN	P	9	4	-	2/2/19/22	0/1/1/1
5	NAG	Q	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1
9	NAG	R	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	R	2	9	-	2/6/23/26	0/1/1/1
9	BMA	R	3	9	-	0/2/19/22	0/1/1/1
9	MAN	R	4	9	-	0/2/19/22	0/1/1/1
9	MAN	R	5	9	-	2/2/19/22	0/1/1/1
9	MAN	R	6	9	-	0/2/19/22	0/1/1/1
9	MAN	R	7	9	-	1/2/19/22	0/1/1/1
10	NAG	S	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	S	2	10	-	2/6/23/26	0/1/1/1
10	BMA	S	3	10	-	2/2/19/22	0/1/1/1
10	MAN	S	4	10	-	0/2/19/22	0/1/1/1
10	MAN	S	5	10	-	0/2/19/22	0/1/1/1
5	NAG	T	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	1/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	BMA	U	3	3	-	0/2/19/22	0/1/1/1
3	MAN	U	4	3	-	1/2/19/22	0/1/1/1
11	NAG	V	1	1,11	-	0/6/23/26	0/1/1/1
11	NAG	V	2[A]	11	-	2/6/23/26	0/1/1/1
11	NAG	V	2[B]	11	-	2/6/23/26	0/1/1/1
11	BMA	V	3	11	-	0/2/19/22	0/1/1/1
11	MAN	V	4	11	-	0/2/19/22	0/1/1/1
11	MAN	V	5	11	-	1/2/19/22	0/1/1/1
2	NAG	W	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	2/6/23/26	0/1/1/1
2	BMA	W	3	2	-	0/2/19/22	0/1/1/1
12	NAG	X	1	1,12	-	0/6/23/26	0/1/1/1
12	NAG	X	2	12	-	0/6/23/26	0/1/1/1
12	BMA	X	3	12	-	0/2/19/22	0/1/1/1
12	MAN	X	4	12	-	0/2/19/22	0/1/1/1
12	MAN	X	5	12	-	0/2/19/22	0/1/1/1
12	MAN	X	6	12	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	X	7	12	-	0/2/19/22	0/1/1/1
12	MAN	X	8	12	-	1/2/19/22	0/1/1/1
12	MAN	X	9	12	-	0/2/19/22	0/1/1/1
5	NAG	Y	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	2/6/23/26	0/1/1/1
9	NAG	Z	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	0/6/23/26	0/1/1/1
9	BMA	Z	3	9	-	0/2/19/22	0/1/1/1
9	MAN	Z	4	9	-	0/2/19/22	0/1/1/1
9	MAN	Z	5	9	-	2/2/19/22	0/1/1/1
9	MAN	Z	6	9	-	0/2/19/22	0/1/1/1
9	MAN	Z	7	9	-	1/2/19/22	0/1/1/1
9	NAG	a	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	a	2	9	-	0/6/23/26	0/1/1/1
9	BMA	a	3	9	-	0/2/19/22	0/1/1/1
9	MAN	a	4	9	-	0/2/19/22	0/1/1/1
9	MAN	a	5	9	-	0/2/19/22	0/1/1/1
9	MAN	a	6	9	-	2/2/19/22	0/1/1/1
9	MAN	a	7	9	-	2/2/19/22	0/1/1/1
5	NAG	b	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	0/6/23/26	0/1/1/1
5	NAG	c	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	c	2	5	-	2/6/23/26	0/1/1/1
5	NAG	d	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	d	2	5	-	0/6/23/26	0/1/1/1
13	NAG	e	1	1,13	-	0/6/23/26	0/1/1/1
13	NAG	e	2	13	-	0/6/23/26	0/1/1/1
13	BMA	e	3	13	-	0/2/19/22	0/1/1/1
13	MAN	e	4	13	-	1/2/19/22	0/1/1/1
14	NAG	f	1	1,14	-	0/6/23/26	0/1/1/1
14	NAG	f	2	14	-	0/6/23/26	0/1/1/1
14	BMA	f	3	14	-	0/2/19/22	0/1/1/1
14	MAN	f	4	14	-	0/2/19/22	0/1/1/1
14	MAN	f	5	14	-	2/2/19/22	0/1/1/1
14	MAN	f	6	14	-	2/2/19/22	0/1/1/1
14	MAN	f	7	14	-	0/2/19/22	0/1/1/1
14	MAN	f	8	14	-	0/2/19/22	0/1/1/1
5	NAG	g	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	g	2	5	-	2/6/23/26	0/1/1/1
9	NAG	h	1	1,9	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	h	2	9	-	0/6/23/26	0/1/1/1
9	BMA	h	3	9	-	0/2/19/22	0/1/1/1
9	MAN	h	4	9	-	0/2/19/22	0/1/1/1
9	MAN	h	5	9	-	0/2/19/22	0/1/1/1
9	MAN	h	6	9	-	1/2/19/22	0/1/1/1
9	MAN	h	7	9	-	2/2/19/22	0/1/1/1
7	NAG	i	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	i	2	7	-	0/6/23/26	0/1/1/1
7	BMA	i	3	7	-	0/2/19/22	0/1/1/1
7	MAN	i	4	7	-	2/2/19/22	0/1/1/1
7	MAN	i	5	7	-	0/2/19/22	0/1/1/1
7	MAN	i	6	7	-	2/2/19/22	0/1/1/1
7	MAN	i	7	7	-	2/2/19/22	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	1	NAG	C1-C2	-3.25	1.47	1.52
3	F	1	NAG	C1-C2	3.12	1.57	1.52
14	f	2	NAG	C1-C2	2.81	1.56	1.52
8	N	1	NAG	C1-C2	2.77	1.56	1.52
12	X	2	NAG	C1-C2	2.71	1.56	1.52
2	E	1	NAG	C1-C2	2.67	1.56	1.52
5	I	2	NAG	C1-C2	2.66	1.56	1.52
5	d	1	NAG	C1-C2	2.49	1.56	1.52
5	c	2	NAG	C1-C2	2.45	1.56	1.52
12	X	1	NAG	C1-C2	2.43	1.56	1.52
3	U	1	NAG	C1-C2	2.22	1.55	1.52
7	K	1	NAG	C1-C2	2.16	1.55	1.52
3	O	2	NAG	C1-C2	2.04	1.55	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	2	NAG	O5-C1-C2	4.59	118.53	111.29
8	N	1	NAG	C1-C2-N2	3.17	115.90	110.49
13	e	2	NAG	O5-C1-C2	3.16	116.27	111.29
5	Y	1	NAG	C1-C2-N2	-3.01	105.34	110.49
5	T	2	NAG	O5-C1-C2	2.97	115.98	111.29
5	Q	2	NAG	C1-C2-N2	2.89	115.42	110.49
5	b	2	NAG	O5-C1-C2	2.83	115.76	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	b	1	NAG	O5-C1-C2	2.83	115.75	111.29
5	Y	2	NAG	C1-C2-N2	2.81	115.29	110.49
5	I	1	NAG	C2-N2-C7	2.75	126.82	122.90
5	c	1	NAG	O5-C1-C2	2.75	115.63	111.29
3	F	1	NAG	C1-C2-N2	2.65	115.01	110.49
4	P	2	NAG	O5-C1-C2	2.60	115.39	111.29
9	Z	6	MAN	C1-O5-C5	2.57	115.68	112.19
11	V	2[A]	NAG	O5-C1-C2	-2.50	107.34	111.29
10	S	2	NAG	C1-C2-N2	2.44	114.66	110.49
12	X	8	MAN	C1-O5-C5	2.43	115.48	112.19
5	I	2	NAG	C2-N2-C7	2.38	126.28	122.90
12	X	9	MAN	C1-O5-C5	2.35	115.37	112.19
5	c	2	NAG	C1-C2-N2	2.31	114.43	110.49
4	P	5	MAN	C1-O5-C5	2.26	115.25	112.19
3	F	1	NAG	O5-C1-C2	2.25	114.83	111.29
9	h	5	MAN	C1-O5-C5	2.23	115.22	112.19
4	H	2	NAG	O5-C1-C2	2.22	114.80	111.29
6	J	6	MAN	C1-O5-C5	2.22	115.20	112.19
10	S	2	NAG	O5-C1-C2	-2.20	107.81	111.29
9	a	6	MAN	C1-O5-C5	2.17	115.13	112.19
9	a	1	NAG	O5-C1-C2	2.15	114.69	111.29
5	g	2	NAG	C2-N2-C7	2.15	125.96	122.90
5	L	2	NAG	O5-C1-C2	2.15	114.68	111.29
5	L	1	NAG	O5-C1-C2	2.13	114.64	111.29
10	S	4	MAN	C1-O5-C5	2.11	115.05	112.19
5	g	1	NAG	O5-C1-C2	2.09	114.58	111.29
2	G	1	NAG	O5-C1-C2	-2.08	108.00	111.29
9	Z	6	MAN	O5-C1-C2	-2.07	107.57	110.77
13	e	1	NAG	C1-C2-N2	2.07	114.02	110.49
12	X	7	MAN	C1-O5-C5	2.05	114.97	112.19
9	Z	5	MAN	C1-O5-C5	2.00	114.91	112.19

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	6	MAN	C4-C5-C6-O6
5	Q	2	NAG	O5-C5-C6-O6
6	J	5	MAN	O5-C5-C6-O6
4	P	6	MAN	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
8	N	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	Y	2	NAG	C4-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6
9	R	5	MAN	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
2	G	3	BMA	C4-C5-C6-O6
7	i	7	MAN	O5-C5-C6-O6
3	M	4	MAN	O5-C5-C6-O6
7	i	7	MAN	C4-C5-C6-O6
5	Q	2	NAG	C4-C5-C6-O6
9	a	7	MAN	O5-C5-C6-O6
7	K	4	MAN	O5-C5-C6-O6
5	c	2	NAG	C4-C5-C6-O6
2	G	3	BMA	O5-C5-C6-O6
9	h	7	MAN	O5-C5-C6-O6
9	a	6	MAN	O5-C5-C6-O6
10	S	2	NAG	O5-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6
6	J	5	MAN	C4-C5-C6-O6
8	N	2	NAG	O5-C5-C6-O6
10	S	1	NAG	C4-C5-C6-O6
14	f	5	MAN	C4-C5-C6-O6
9	a	6	MAN	C4-C5-C6-O6
3	M	4	MAN	C4-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	F	4	MAN	C4-C5-C6-O6
7	K	4	MAN	C4-C5-C6-O6
9	R	5	MAN	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
10	S	2	NAG	C4-C5-C6-O6
14	f	6	MAN	C4-C5-C6-O6
14	f	5	MAN	O5-C5-C6-O6
11	V	2[A]	NAG	O5-C5-C6-O6
9	h	7	MAN	C4-C5-C6-O6
10	S	1	NAG	O5-C5-C6-O6
7	K	6	MAN	O5-C5-C6-O6
2	W	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
11	V	2[A]	NAG	C4-C5-C6-O6
9	Z	5	MAN	O5-C5-C6-O6
9	R	2	NAG	O5-C5-C6-O6
7	K	6	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	J	4	MAN	O5-C5-C6-O6
7	i	4	MAN	O5-C5-C6-O6
11	V	2[B]	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
6	J	4	MAN	C4-C5-C6-O6
7	i	6	MAN	C4-C5-C6-O6
14	f	6	MAN	O5-C5-C6-O6
9	a	7	MAN	C4-C5-C6-O6
10	S	3	BMA	C4-C5-C6-O6
2	W	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	O	4	MAN	O5-C5-C6-O6
9	Z	7	MAN	O5-C5-C6-O6
3	U	4	MAN	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
11	V	2[B]	NAG	O5-C5-C6-O6
7	i	6	MAN	O5-C5-C6-O6
4	H	9	MAN	C4-C5-C6-O6
4	P	4	MAN	C4-C5-C6-O6
4	H	5	MAN	O5-C5-C6-O6
4	P	4	MAN	O5-C5-C6-O6
13	e	4	MAN	O5-C5-C6-O6
4	P	9	MAN	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
9	R	7	MAN	O5-C5-C6-O6
9	R	2	NAG	C4-C5-C6-O6
10	S	3	BMA	O5-C5-C6-O6
9	Z	5	MAN	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	P	5	MAN	O5-C5-C6-O6
4	H	9	MAN	O5-C5-C6-O6
4	P	9	MAN	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
7	i	4	MAN	C4-C5-C6-O6
4	H	4	MAN	C4-C5-C6-O6
11	V	5	MAN	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
5	g	2	NAG	O5-C5-C6-O6
12	X	8	MAN	O5-C5-C6-O6
5	g	2	NAG	C4-C5-C6-O6

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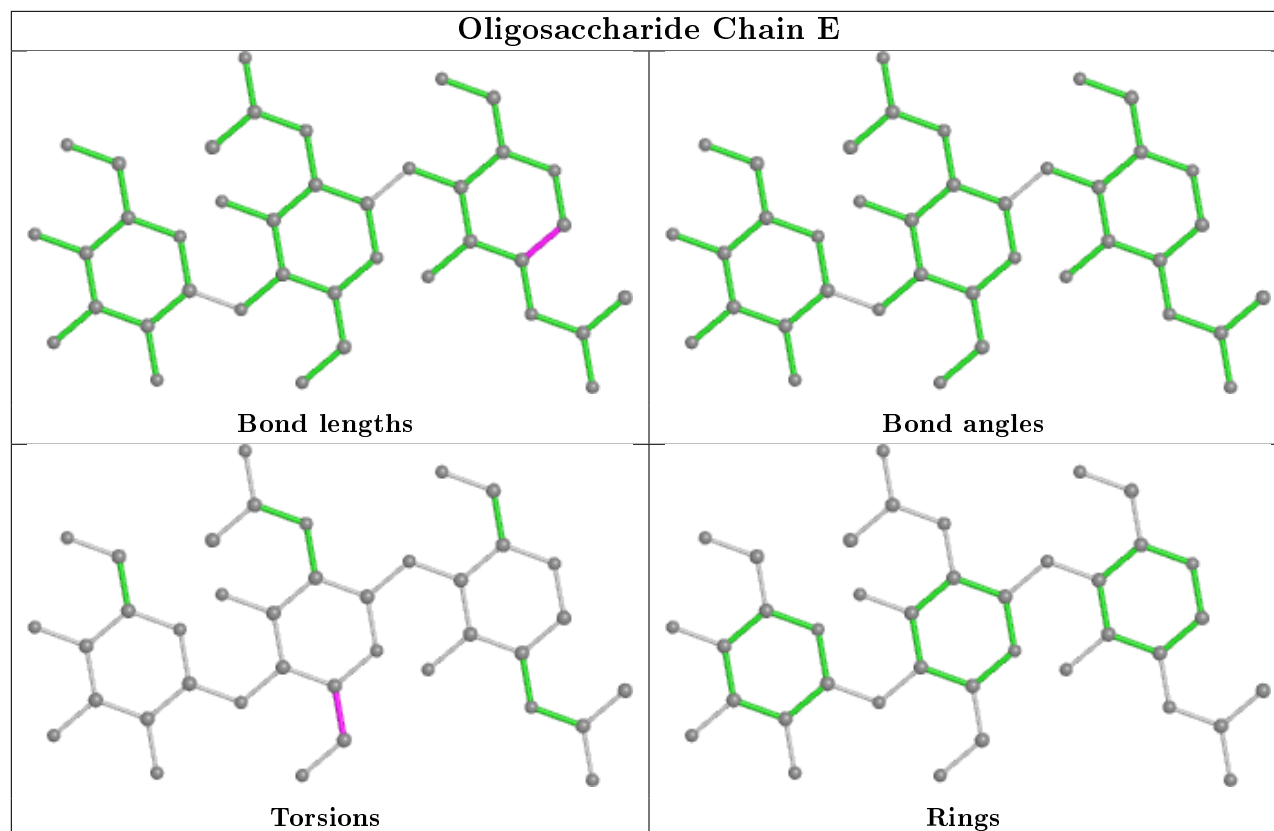
Mol	Chain	Res	Type	Atoms
5	T	2	NAG	C4-C5-C6-O6
9	h	6	MAN	C4-C5-C6-O6

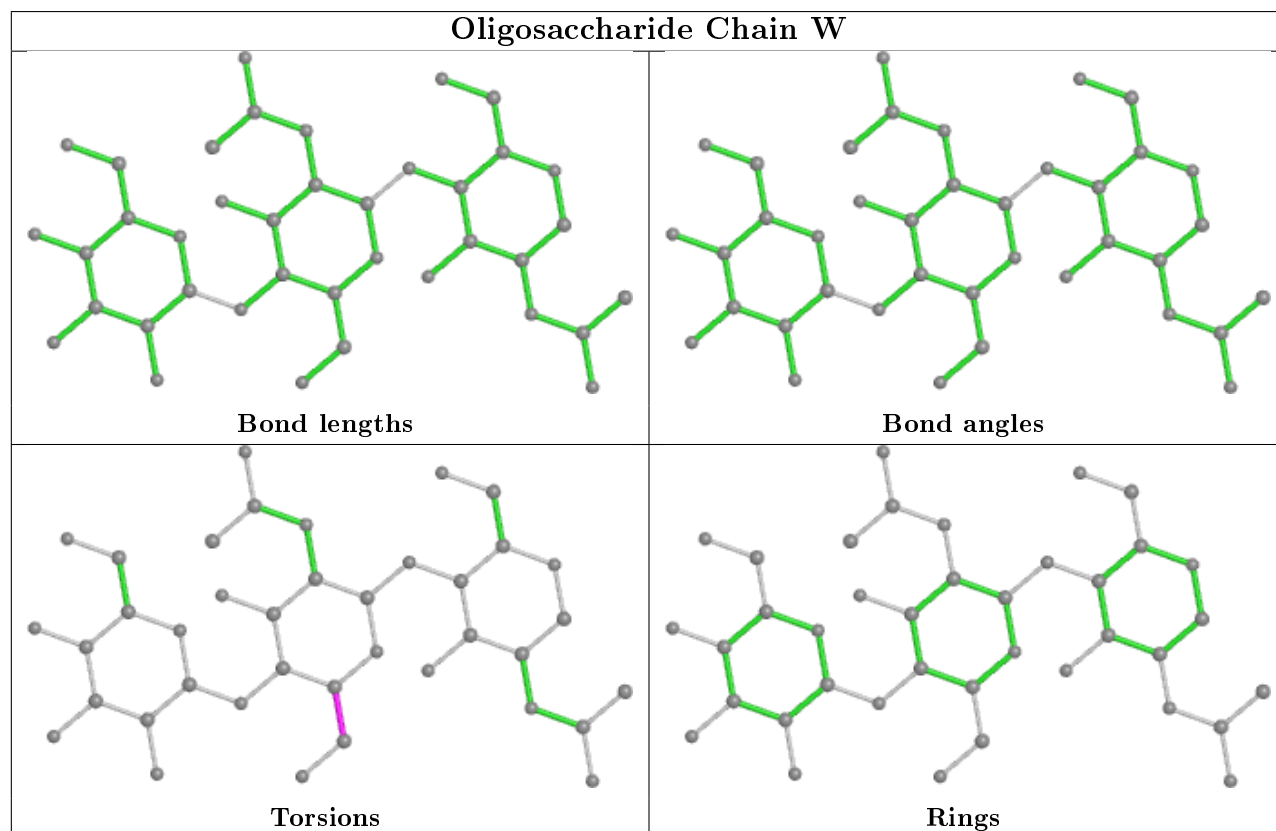
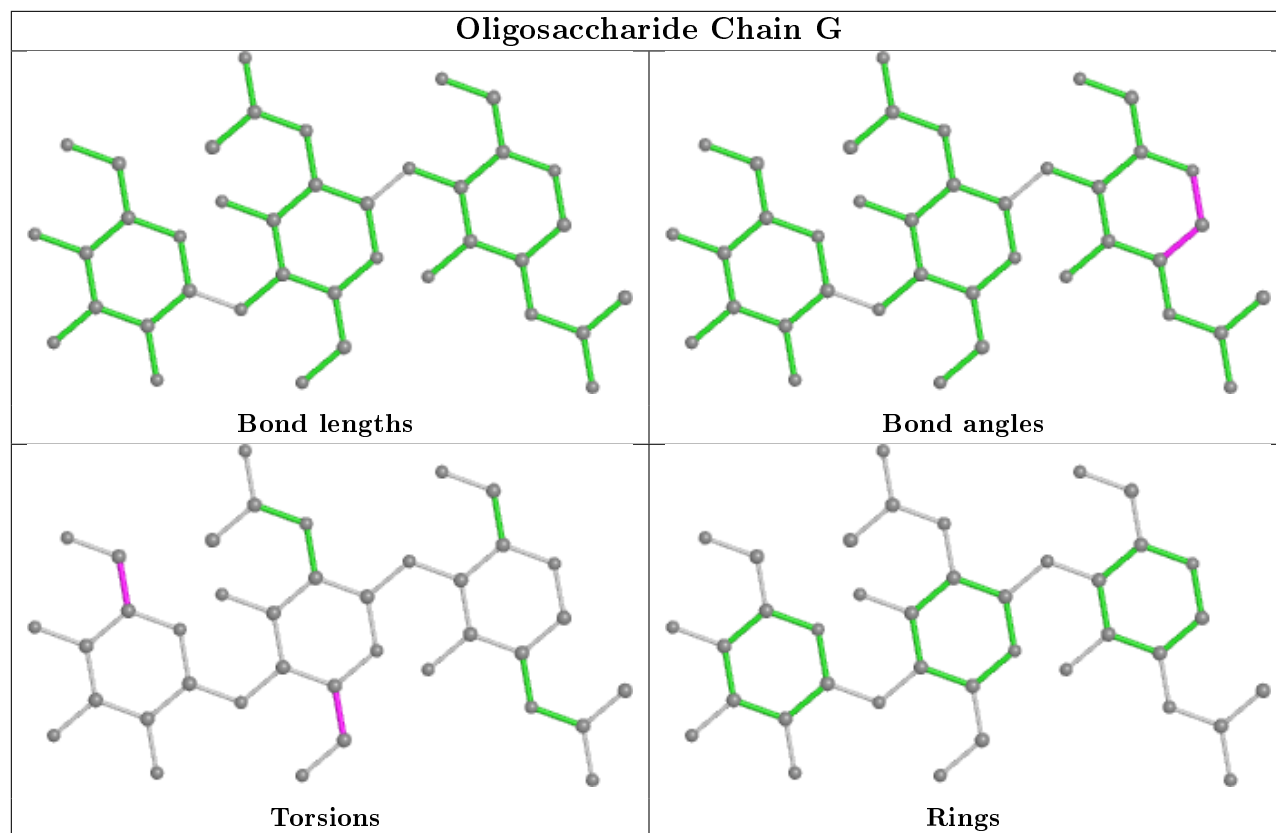
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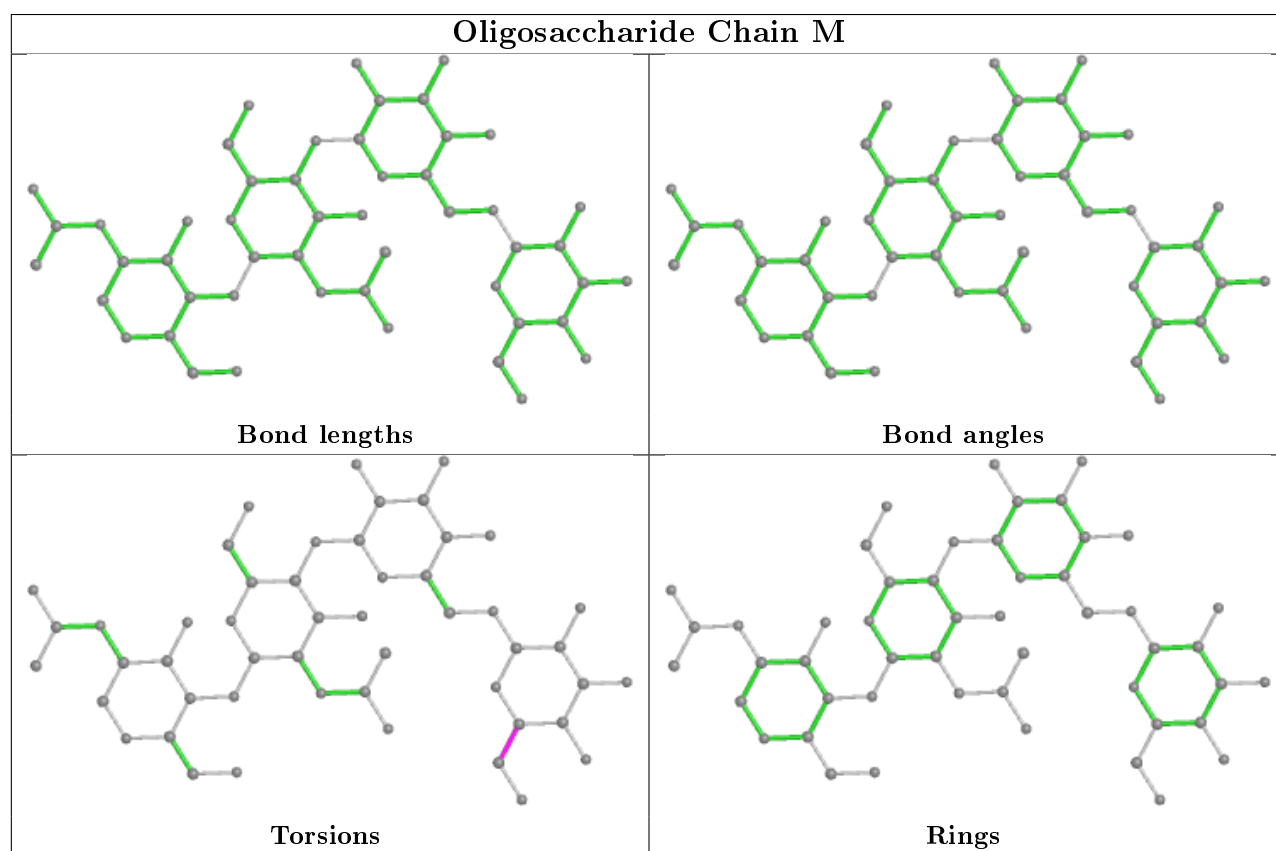
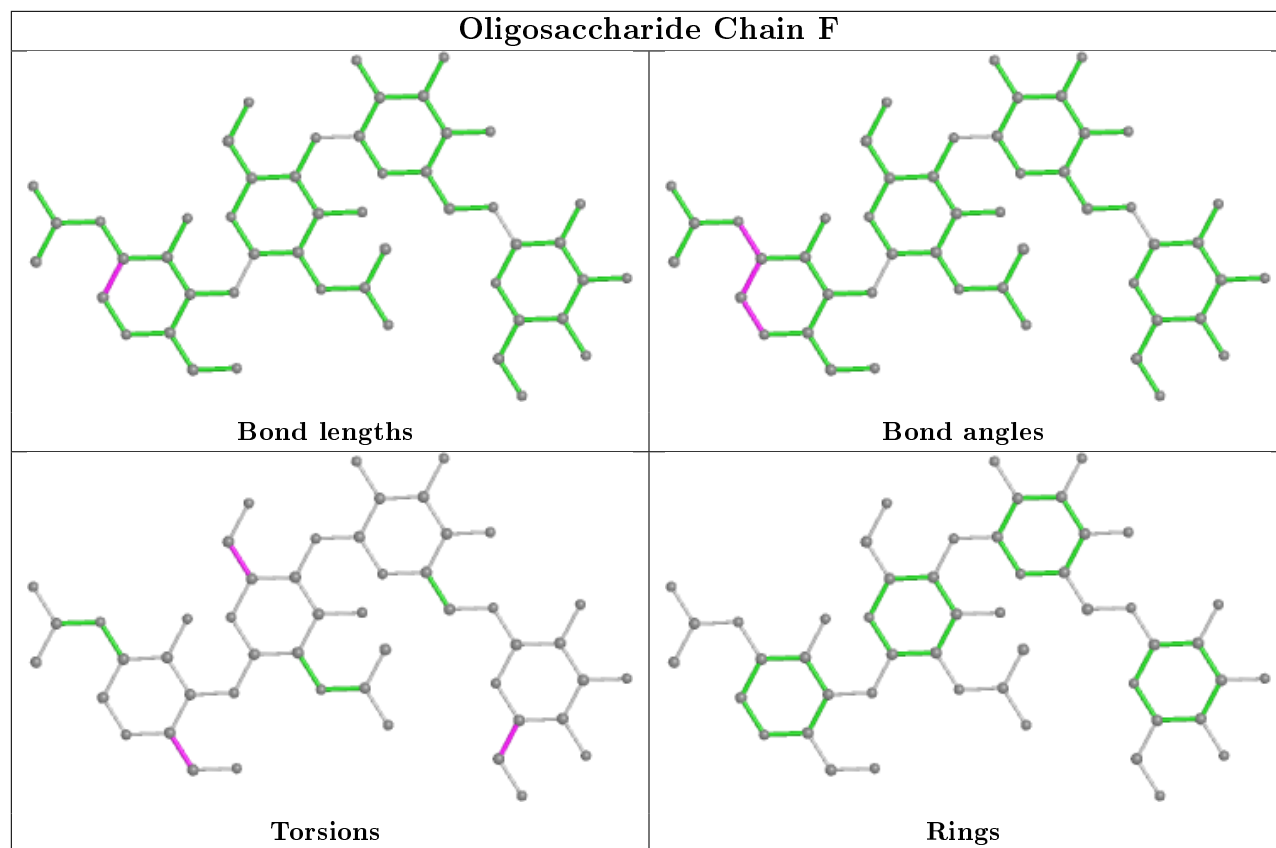
9 monomers are involved in 11 short contacts:

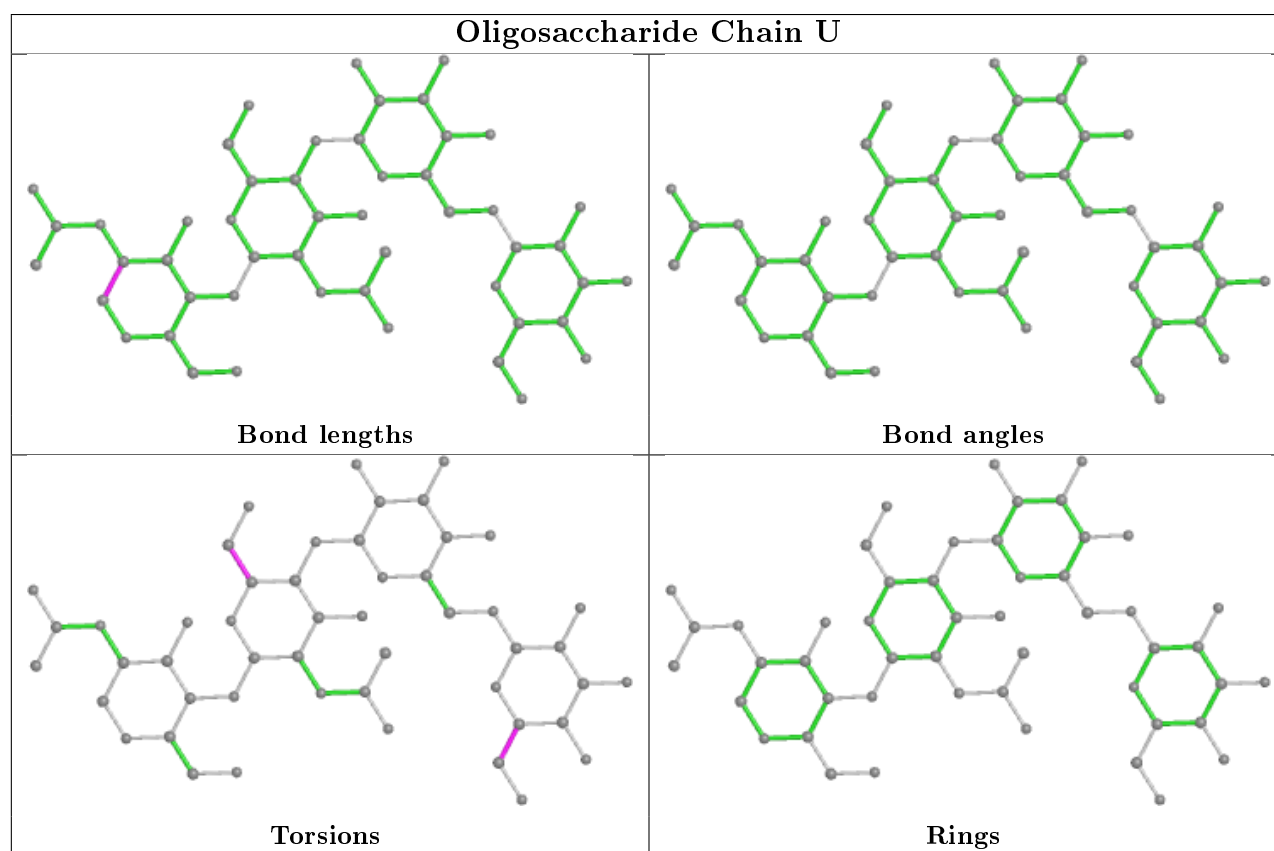
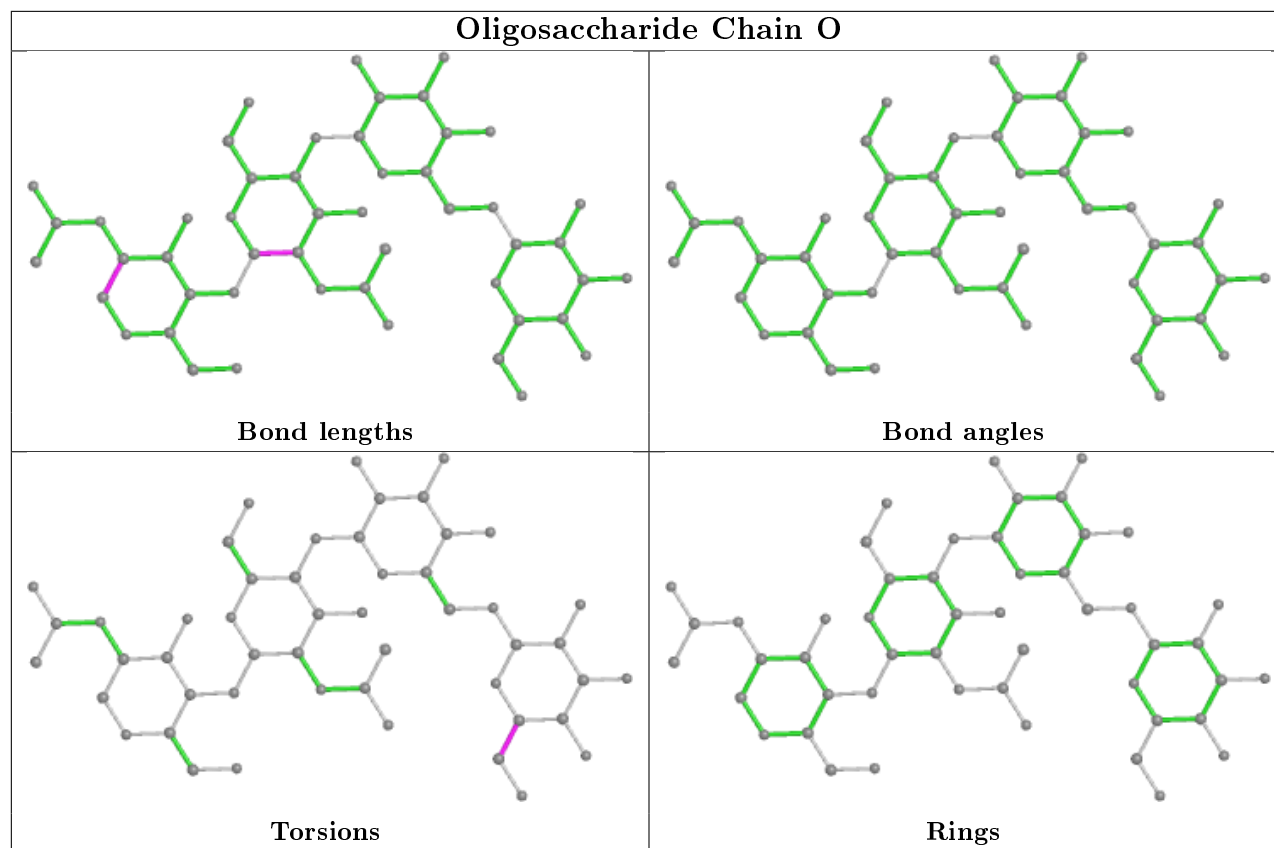
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Z	3	BMA	1	0
6	J	3	BMA	2	0
3	F	1	NAG	2	0
3	F	2	NAG	1	0
9	R	6	MAN	1	0
8	N	2	NAG	1	0
9	Z	6	MAN	1	0
6	J	2	NAG	1	0
9	R	3	BMA	1	0

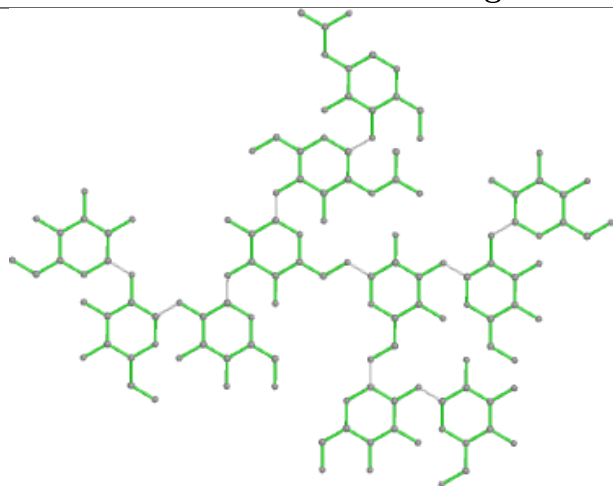
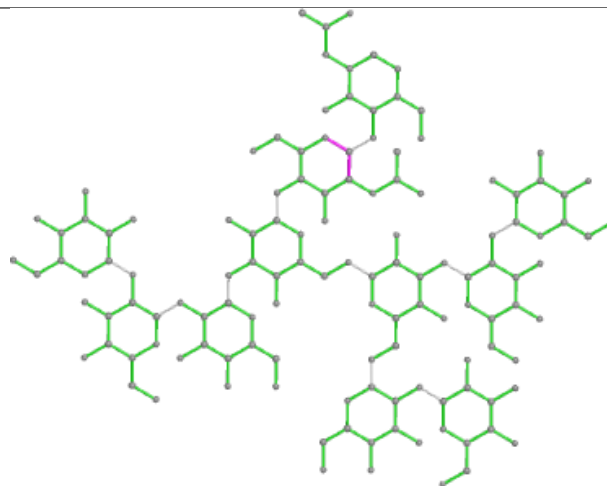
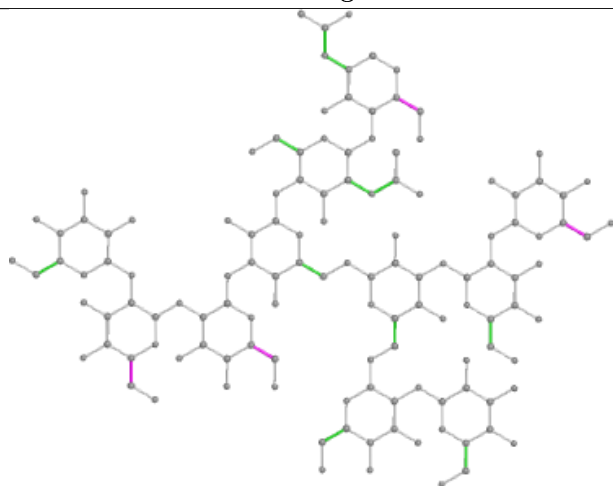
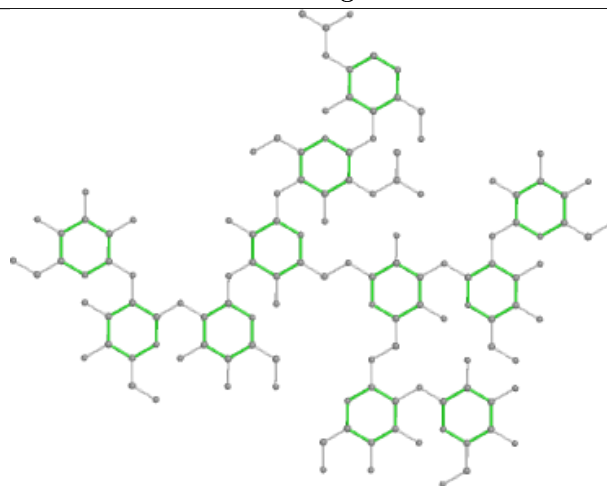
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

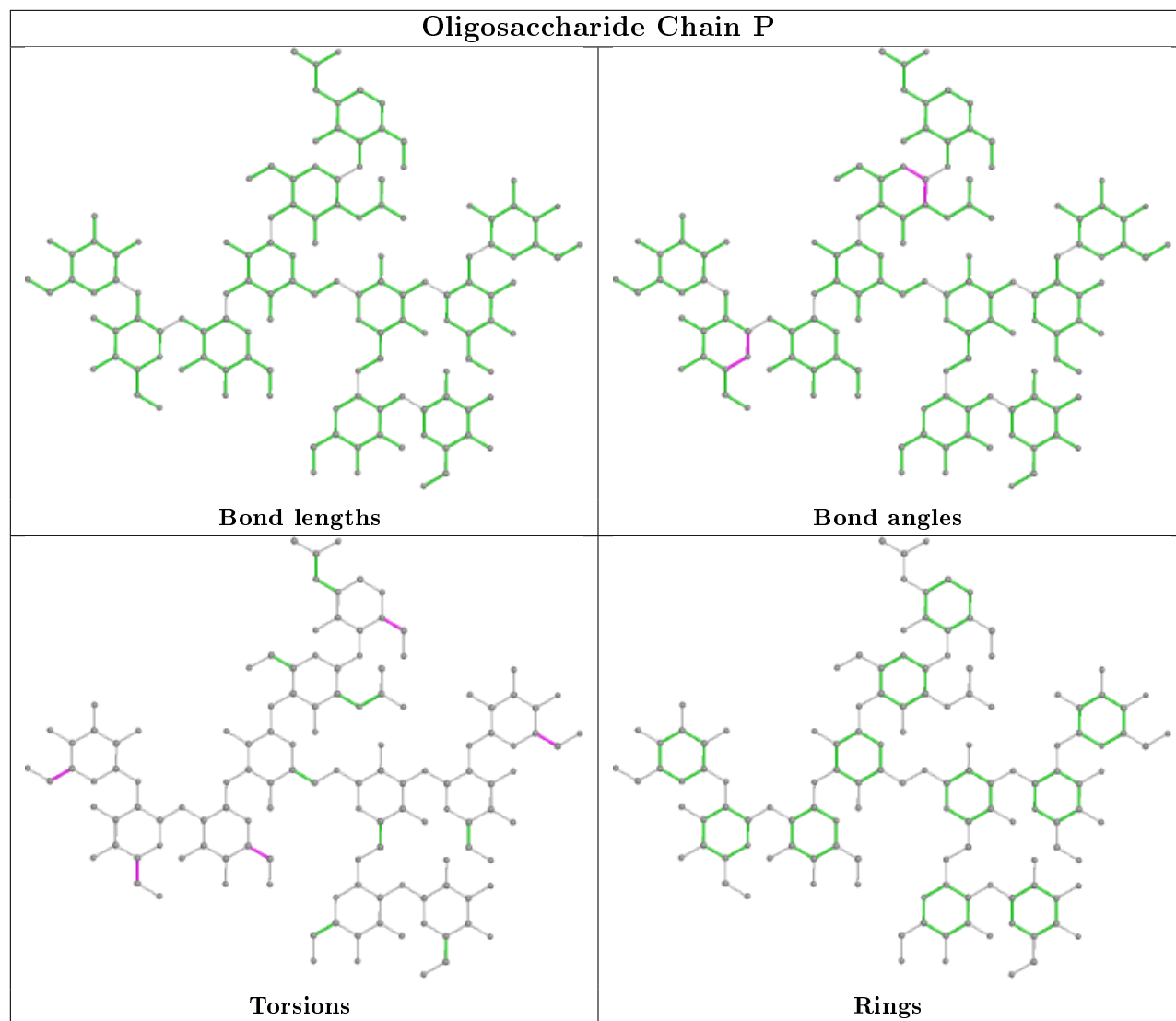


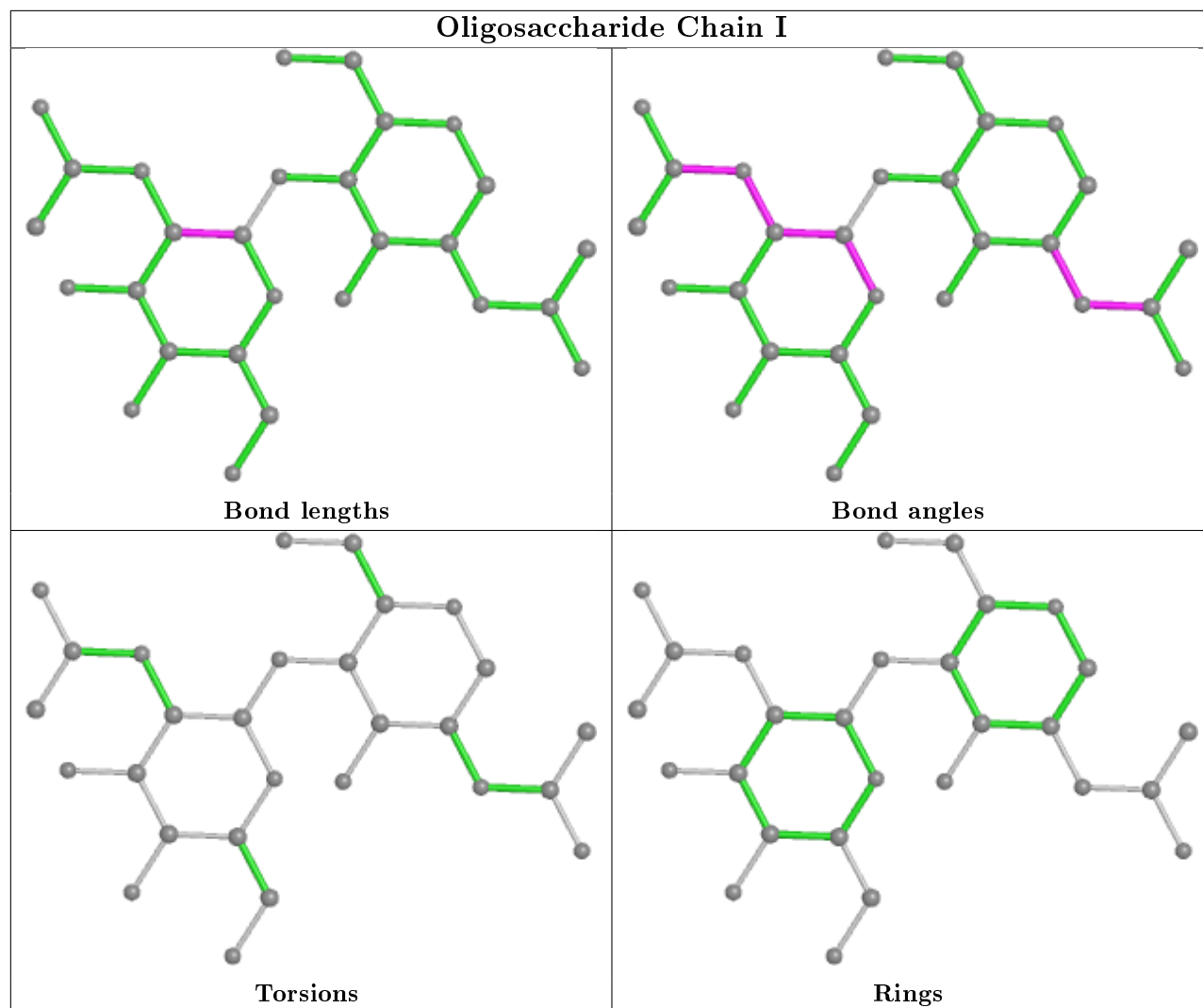


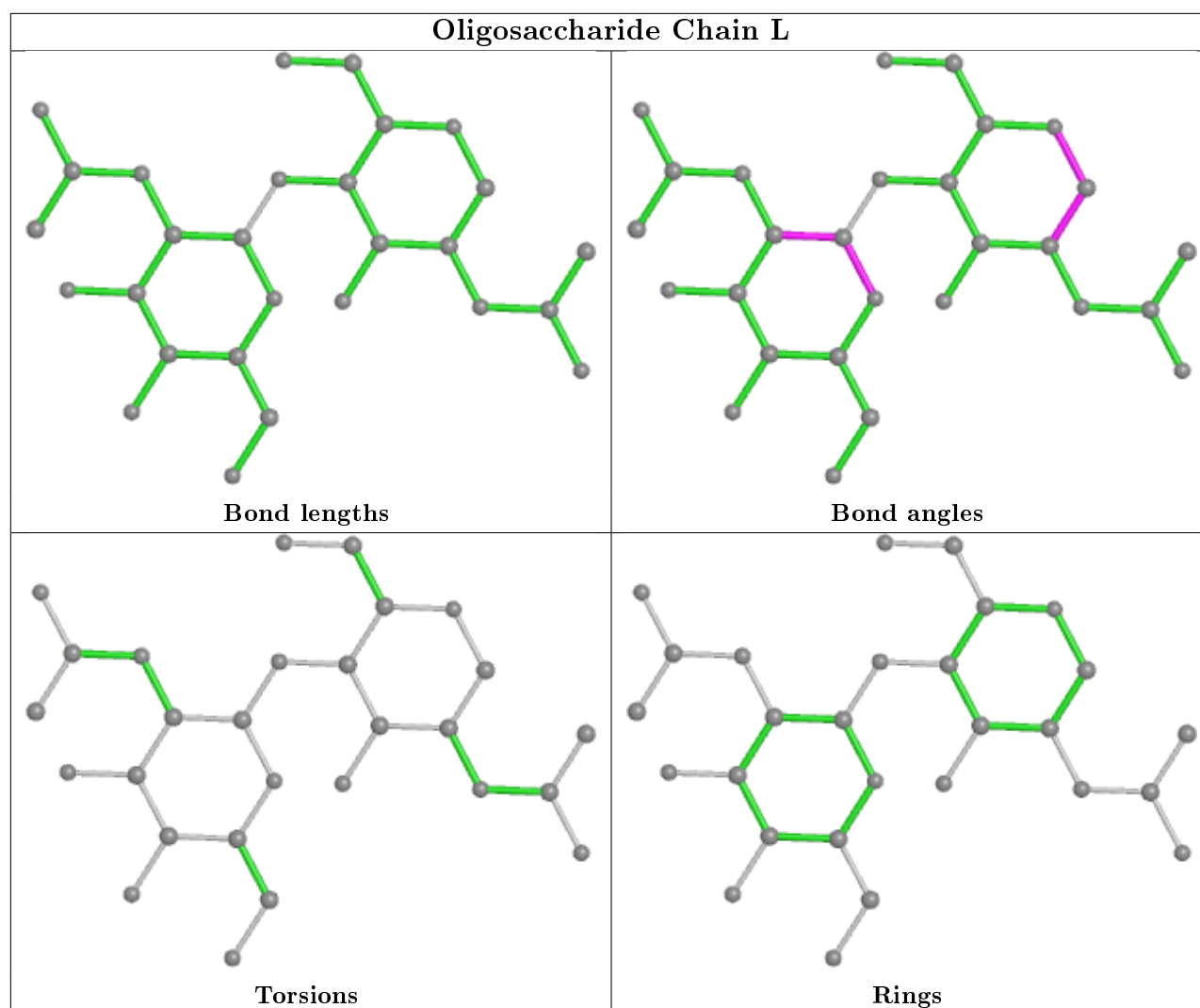


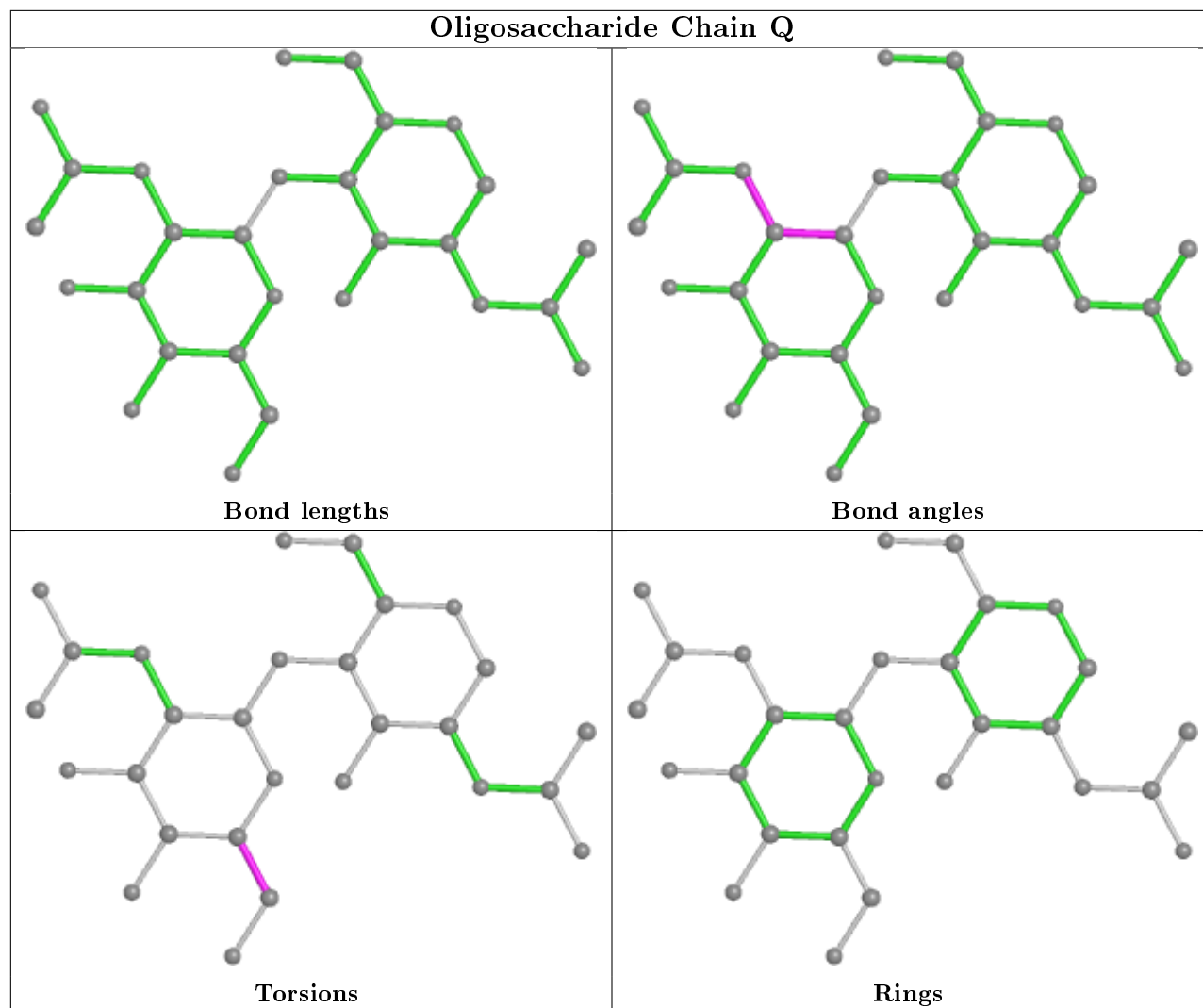


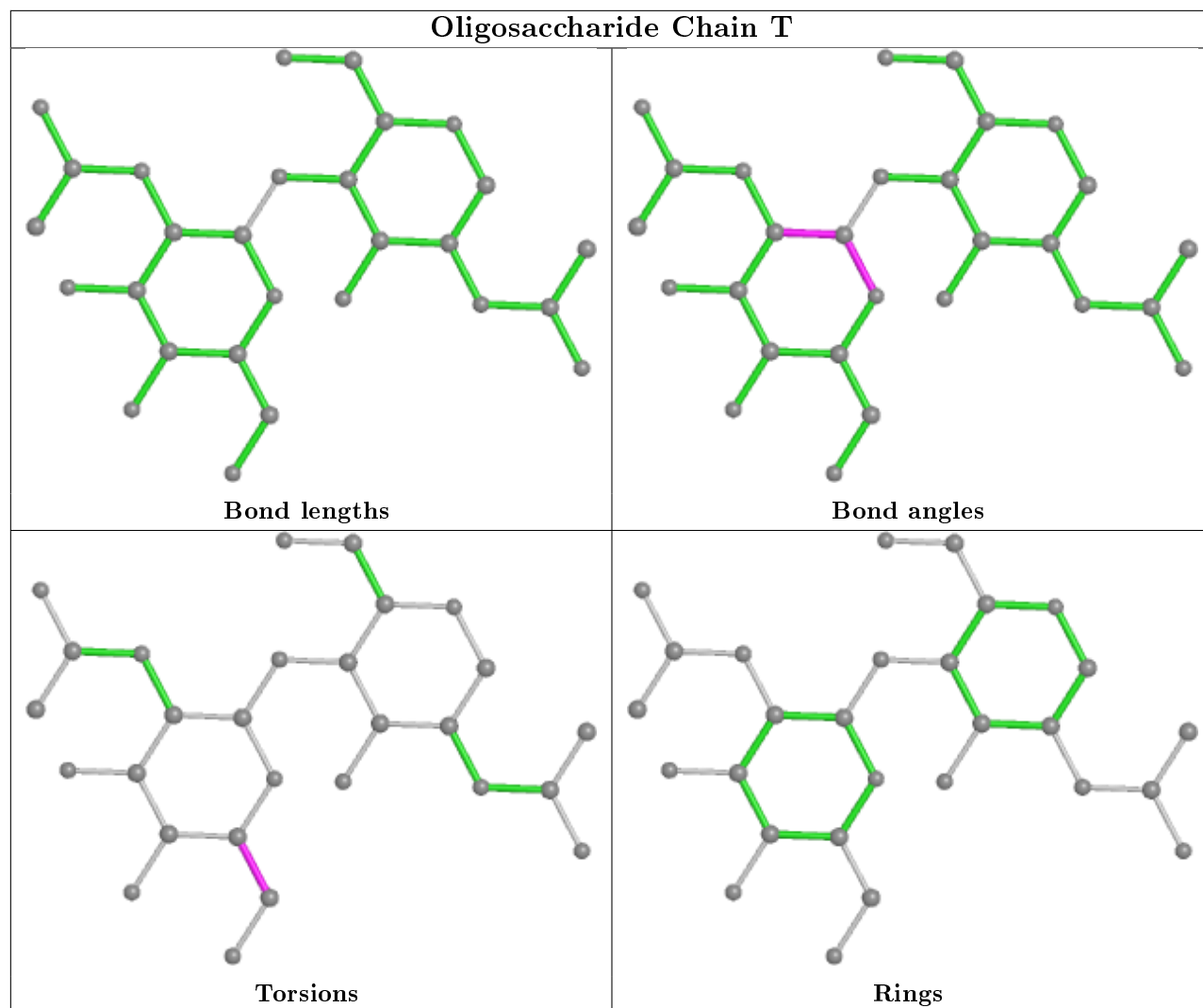
Oligosaccharide Chain H**Bond lengths****Bond angles****Torsions****Rings**

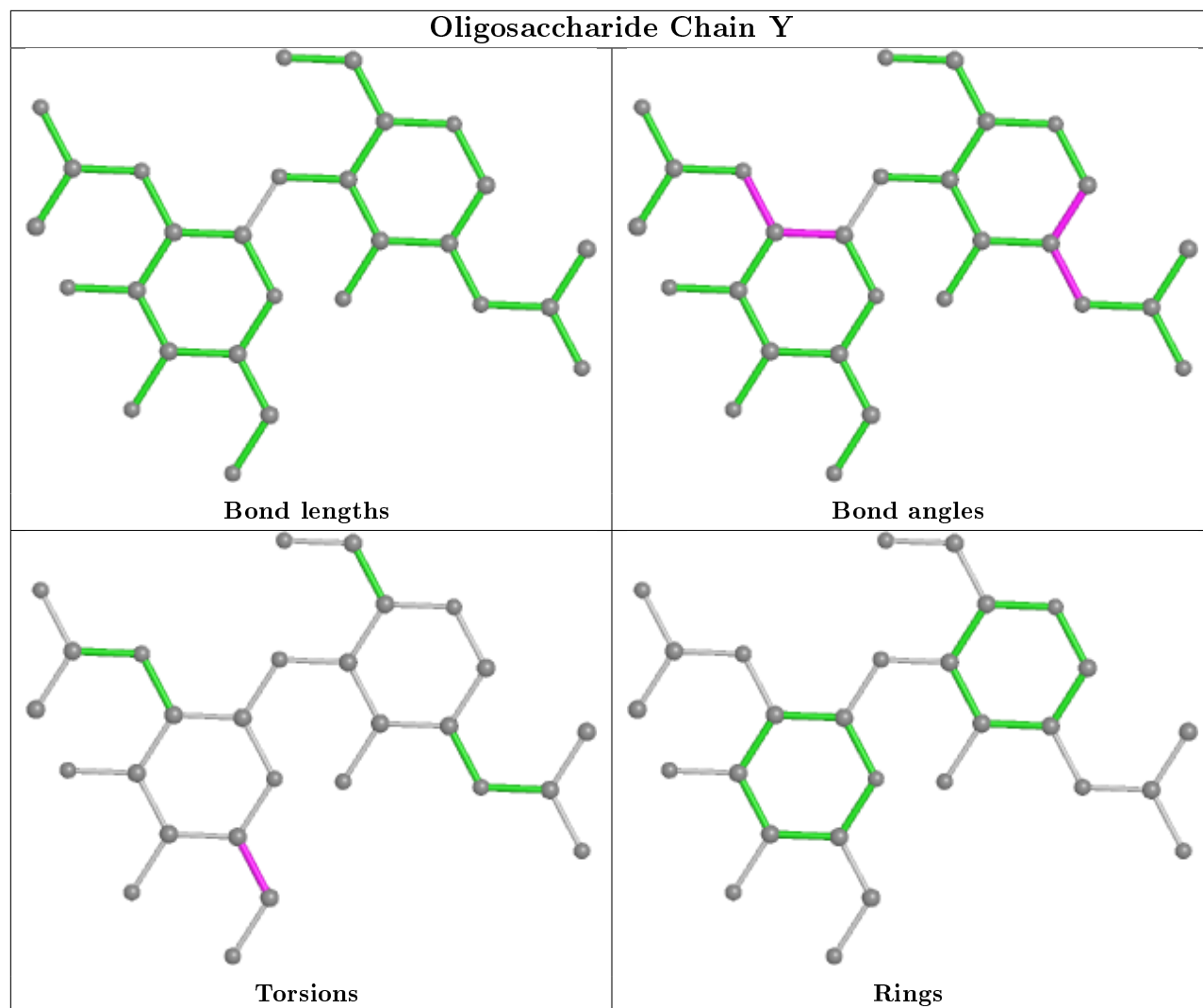


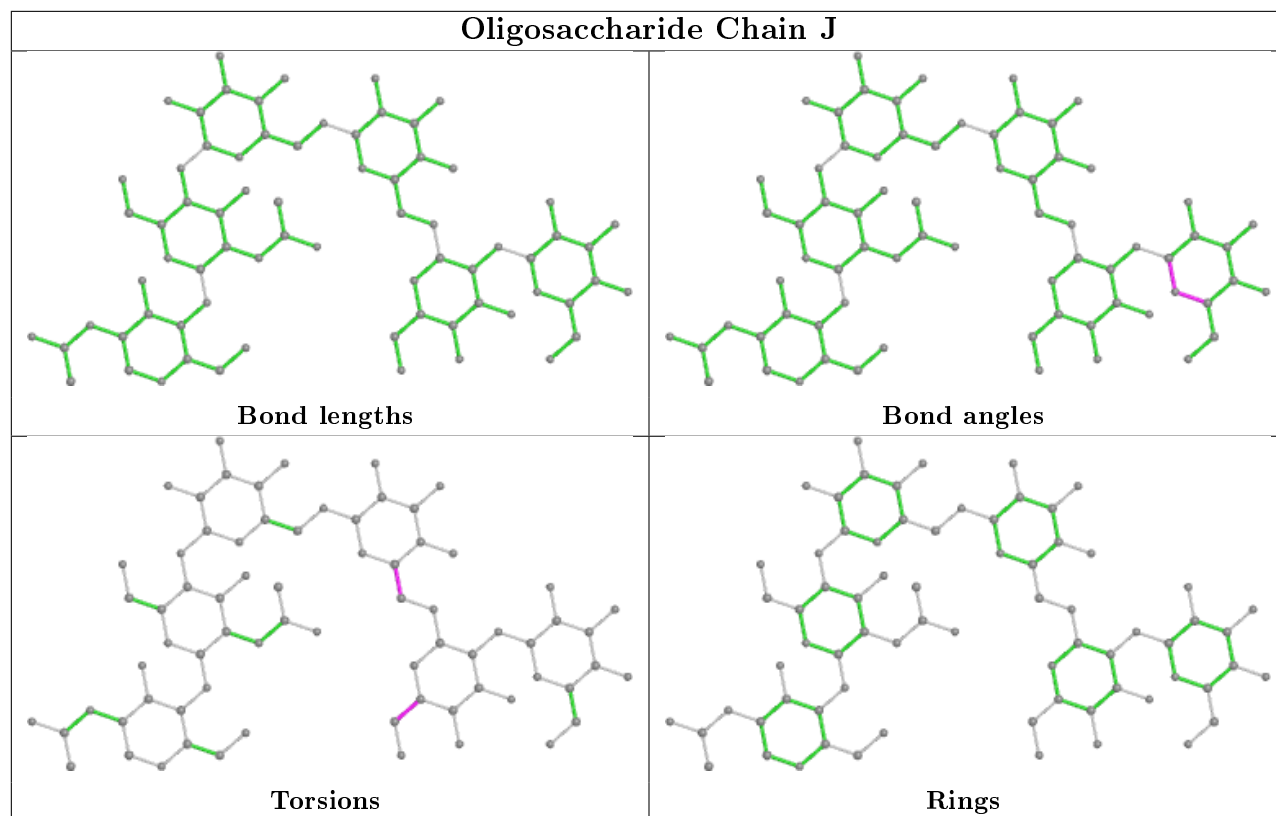
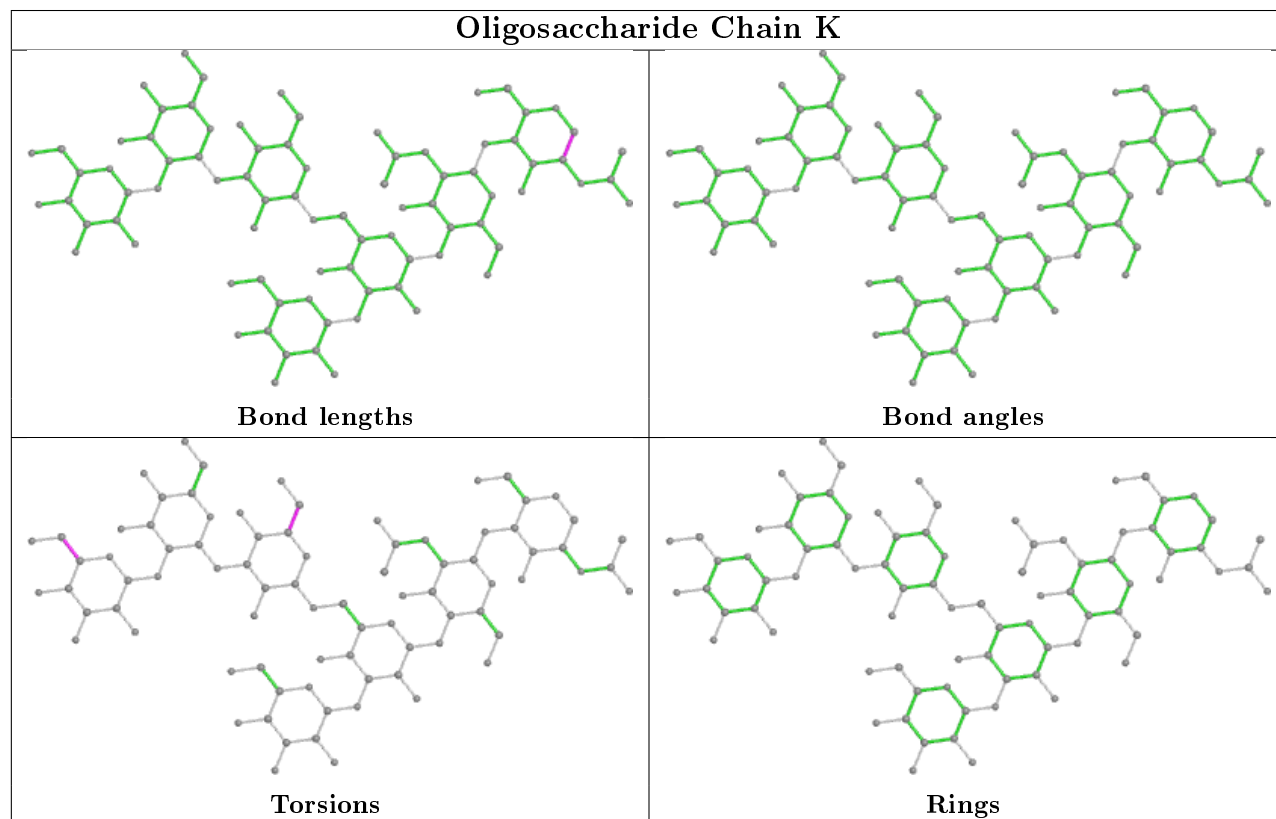


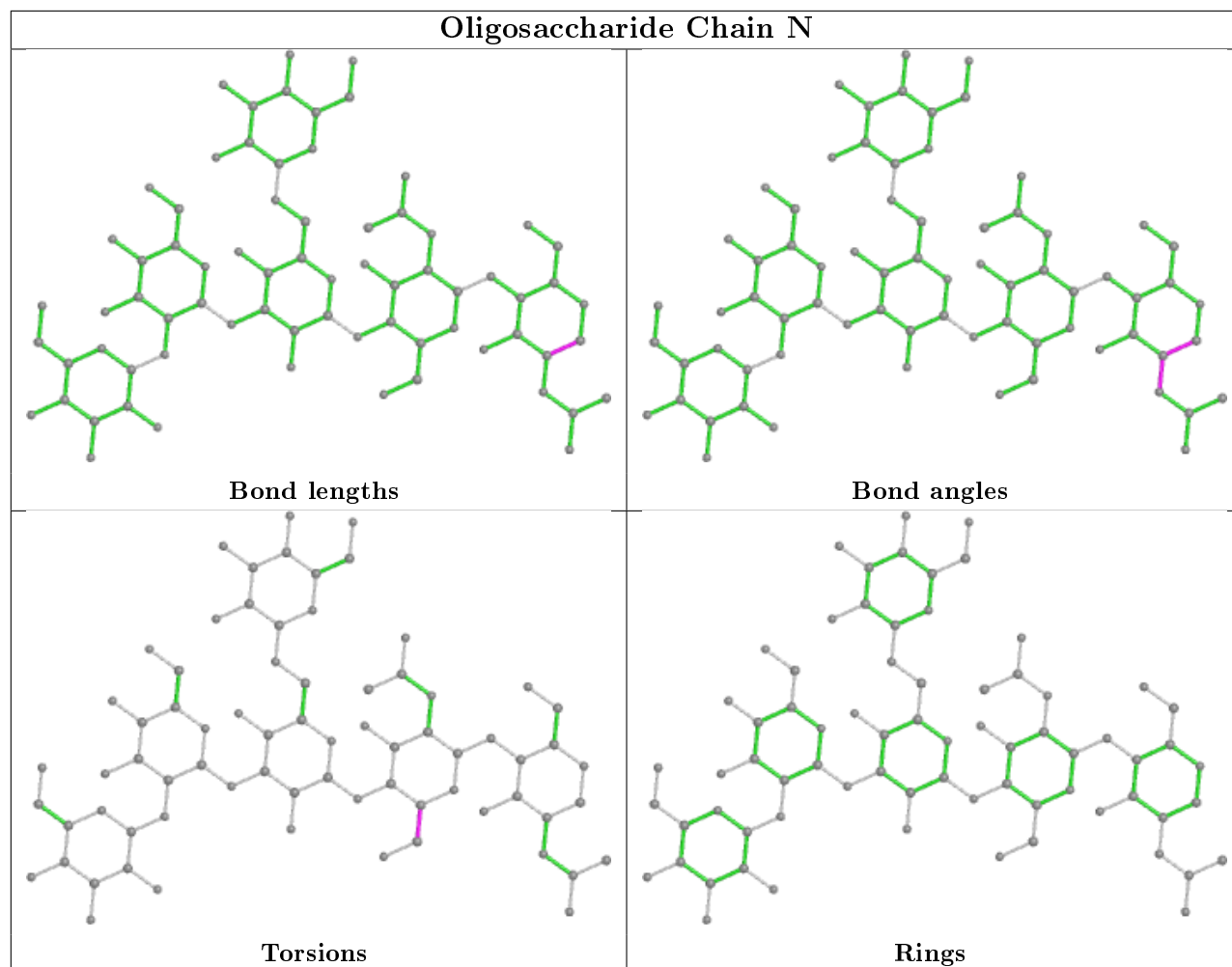


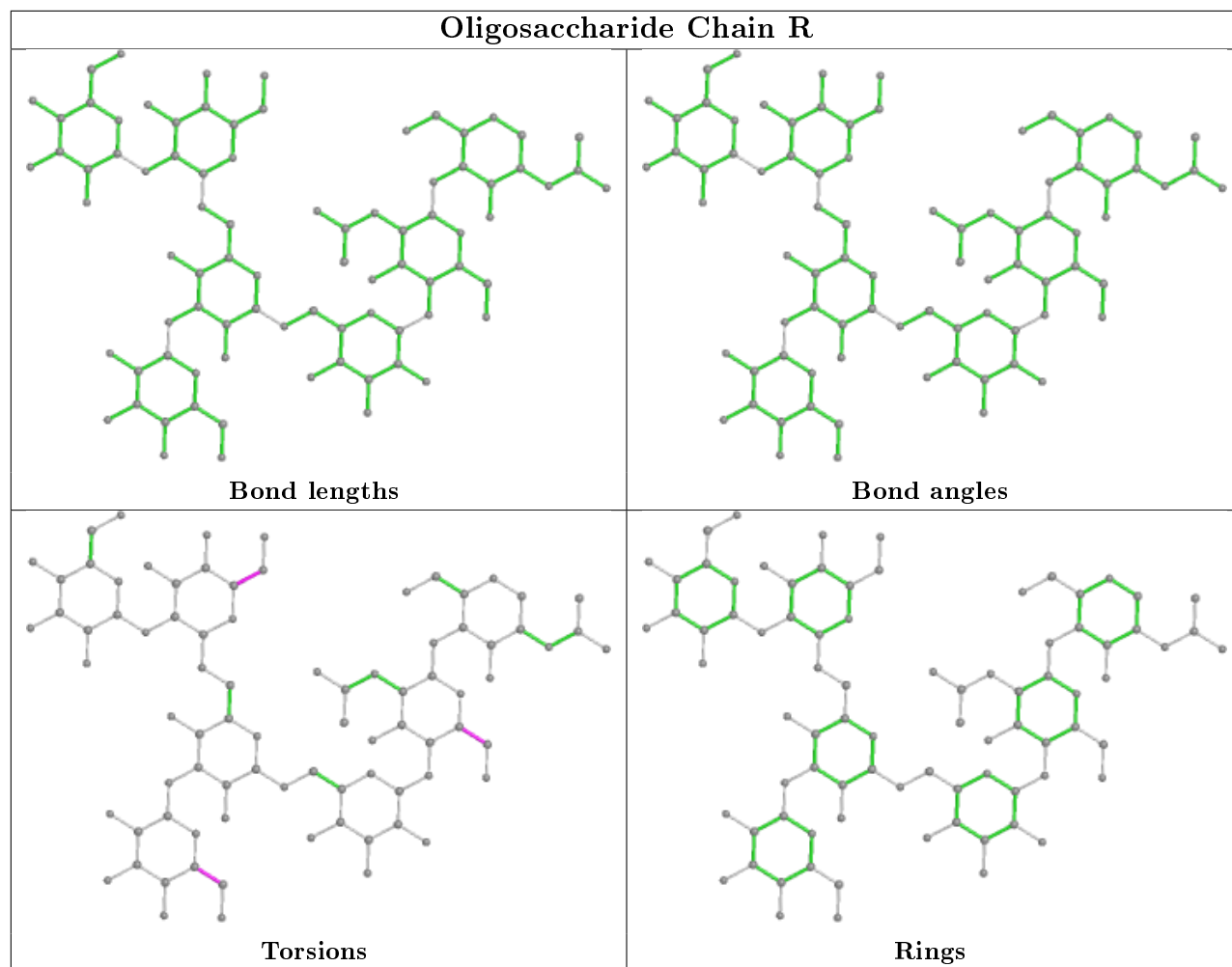


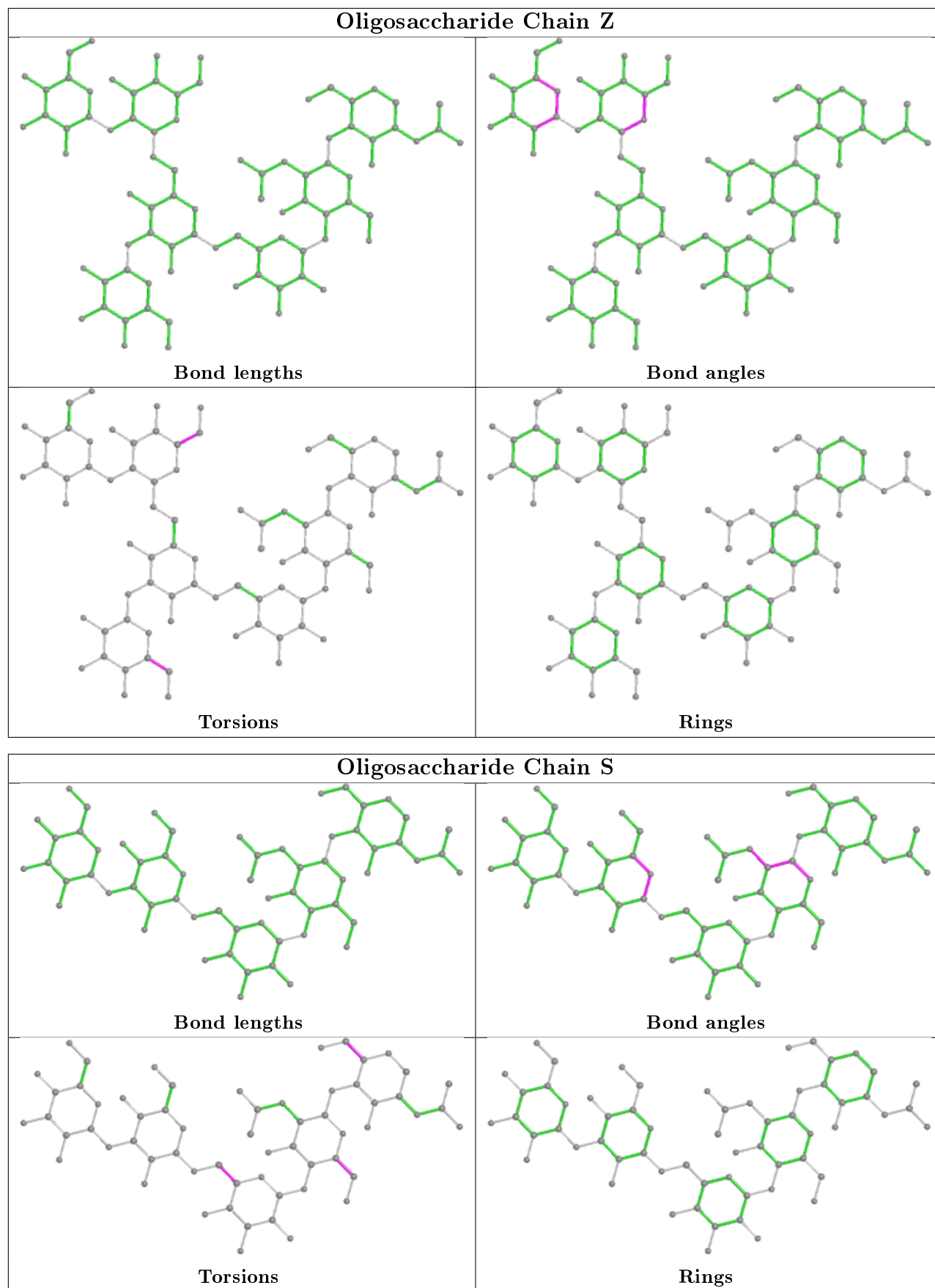


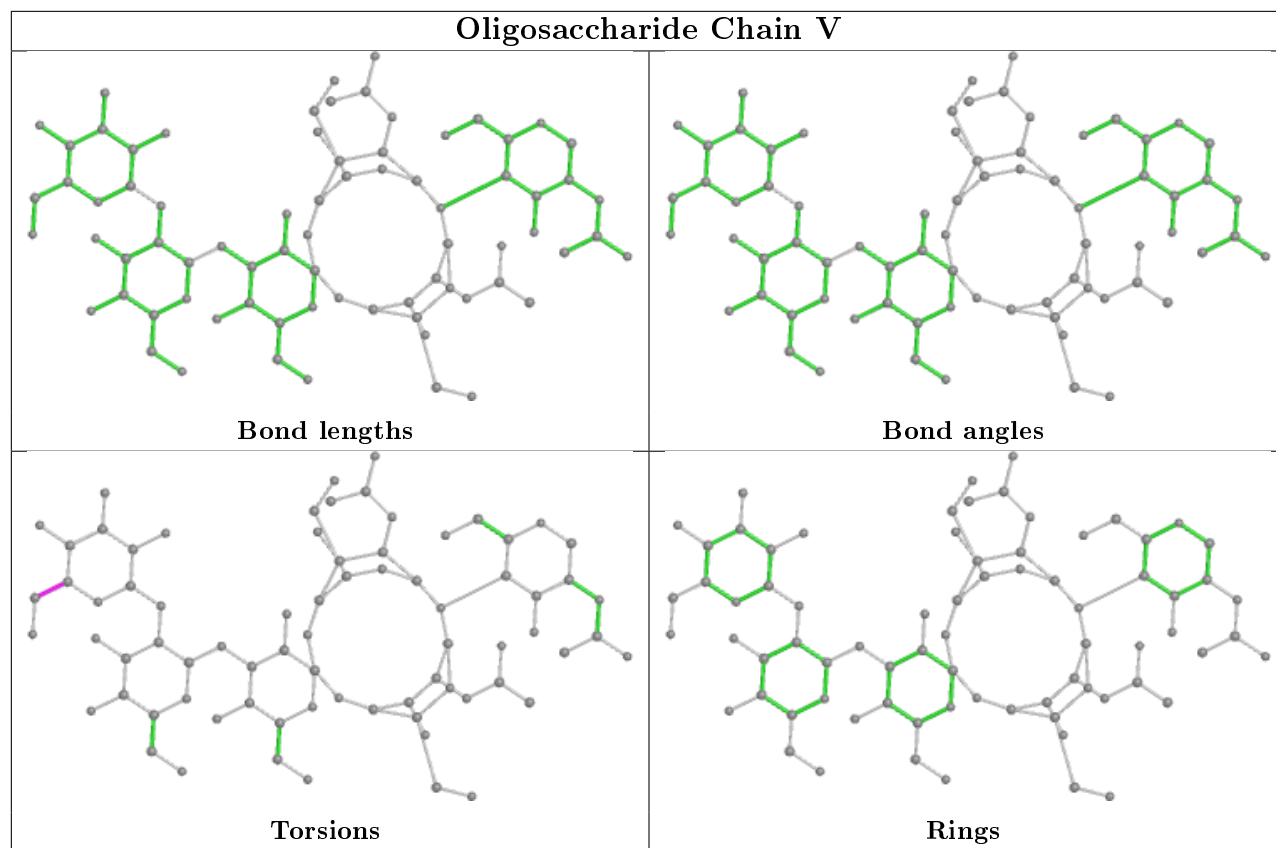


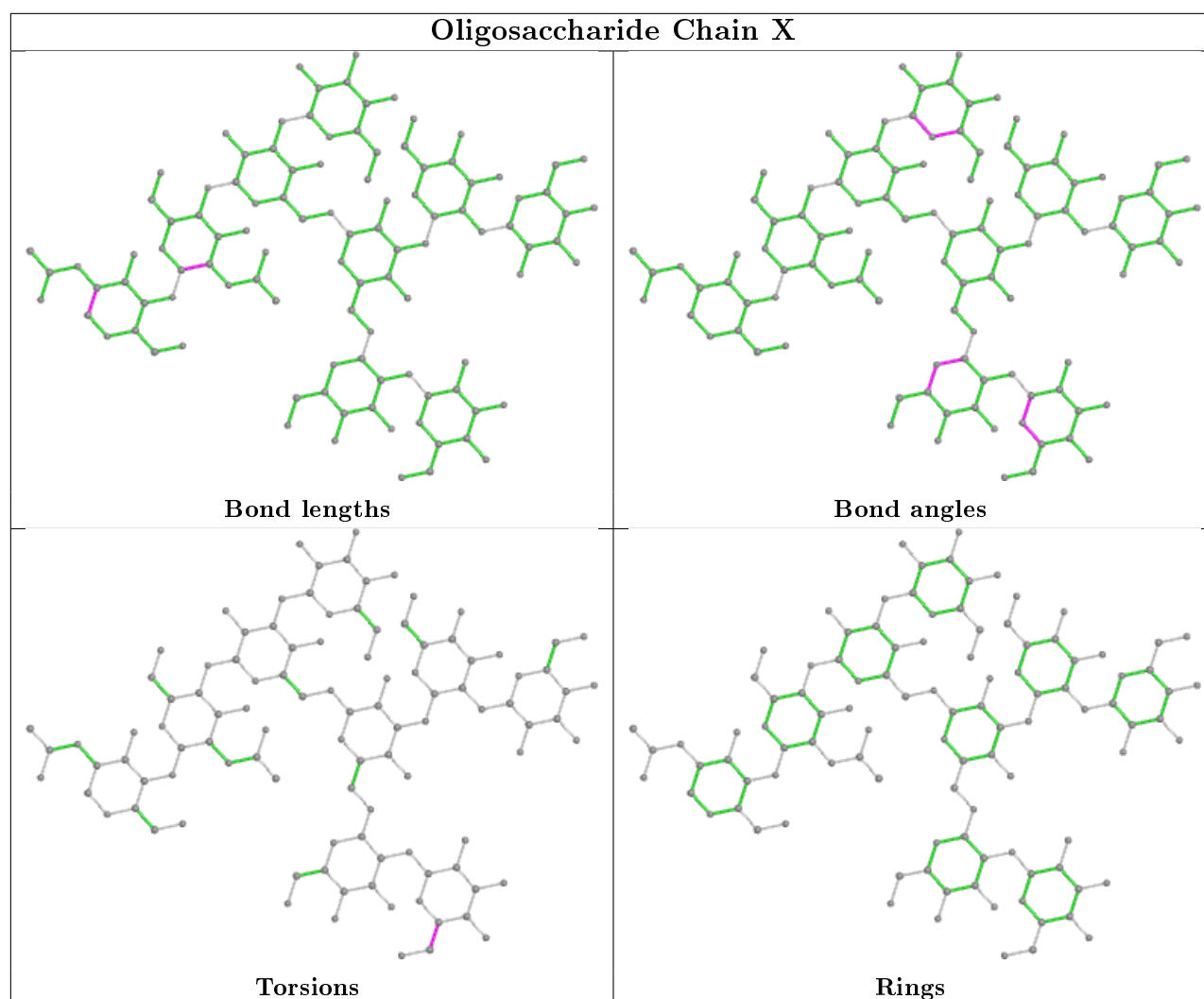
Oligosaccharide Chain J**Oligosaccharide Chain K**











5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 for Mogul analysis.

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	$\# Z > 2$
16	PEG	C	6001	-	6,6,6	0.82	0	5,5,5	1.16	1 (20%)
16	PEG	B	6001	-	6,6,6	0.32	0	5,5,5	0.71	0
16	PEG	A	6002	-	6,6,6	0.51	0	5,5,5	0.90	0
15	NAG	A	1601	1	14,14,15	0.59	0	17,19,21	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	NAG	C	1601	1	14,14,15	0.35	0	17,19,21	0.83	1 (5%)
18	PO4	A	5001	-	4,4,4	1.28	0	6,6,6	0.94	0
15	NAG	C	1901	1	14,14,15	0.87	1 (7%)	17,19,21	1.28	1 (5%)
16	PEG	D	6001	-	6,6,6	0.64	0	5,5,5	0.51	0
15	NAG	B	1601	1	14,14,15	1.11	1 (7%)	17,19,21	1.62	3 (17%)
15	NAG	D	1601	1	14,14,15	0.47	0	17,19,21	0.77	1 (5%)
15	NAG	A	1901	1	14,14,15	0.48	0	17,19,21	0.43	0
16	PEG	A	3001	-	6,6,6	0.49	0	5,5,5	0.78	0
15	NAG	D	1801	1	14,14,15	0.59	0	17,19,21	0.85	1 (5%)

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
16	PEG	C	6001	-	-	2/4/4/4	-
16	PEG	B	6001	-	-	3/4/4/4	-
16	PEG	A	6002	-	-	3/4/4/4	-
15	NAG	A	1601	1	-	2/6/23/26	0/1/1/1
15	NAG	C	1601	1	-	0/6/23/26	0/1/1/1
15	NAG	D	1801	1	-	0/6/23/26	0/1/1/1
15	NAG	C	1901	1	-	2/6/23/26	0/1/1/1
15	NAG	B	1601	1	-	1/6/23/26	0/1/1/1
15	NAG	D	1601	1	-	0/6/23/26	0/1/1/1
15	NAG	A	1901	1	-	1/6/23/26	0/1/1/1
16	PEG	A	3001	-	-	2/4/4/4	-
16	PEG	D	6001	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1601	NAG	C1-C2	3.97	1.58	1.52
15	C	1901	NAG	C1-C2	2.95	1.56	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	1901	NAG	O5-C1-C2	4.87	118.97	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1601	NAG	C1-C2-N2	4.58	118.32	110.49
15	B	1601	NAG	O5-C1-C2	3.32	116.53	111.29
15	A	1601	NAG	C1-C2-N2	3.20	115.95	110.49
15	D	1801	NAG	O5-C1-C2	3.14	116.25	111.29
15	B	1601	NAG	C2-N2-C7	2.94	127.09	122.90
15	C	1601	NAG	O5-C1-C2	2.75	115.63	111.29
15	D	1601	NAG	C1-C2-N2	2.66	115.03	110.49
16	C	6001	PEG	C3-O2-C2	2.37	123.57	113.29

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	C	1901	NAG	O5-C5-C6-O6
16	C	6001	PEG	O2-C3-C4-O4
16	A	6002	PEG	O2-C3-C4-O4
15	A	1601	NAG	O5-C5-C6-O6
15	A	1601	NAG	C4-C5-C6-O6
15	C	1901	NAG	C4-C5-C6-O6
15	B	1601	NAG	C1-C2-N2-C7
16	B	6001	PEG	O1-C1-C2-O2
16	D	6001	PEG	O1-C1-C2-O2
16	C	6001	PEG	O1-C1-C2-O2
16	D	6001	PEG	O2-C3-C4-O4
16	B	6001	PEG	C4-C3-O2-C2
16	A	6002	PEG	C1-C2-O2-C3
16	B	6001	PEG	O2-C3-C4-O4
15	A	1901	NAG	O7-C7-N2-C2
16	A	6002	PEG	O1-C1-C2-O2
16	A	3001	PEG	O2-C3-C4-O4
16	A	3001	PEG	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	1901	NAG	2	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	839/842 (99%)	0.23	7 (0%) 86 90	17, 30, 46, 61	12 (1%)
1	B	838/842 (99%)	0.10	5 (0%) 89 93	17, 28, 43, 58	17 (2%)
1	C	839/842 (99%)	-0.05	2 (0%) 95 97	17, 25, 39, 54	12 (1%)
1	D	838/842 (99%)	0.23	15 (1%) 68 76	18, 30, 50, 61	28 (3%)
All	All	3354/3368 (99%)	0.13	29 (0%) 84 89	17, 28, 46, 61	69 (2%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	689	ILE	3.9
1	D	719	ALA	3.6
1	A	375	ALA	3.2
1	B	728	TRP	3.1
1	D	701	LEU	2.9
1	A	712	ILE	2.8
1	D	371	VAL	2.7
1	D	728	TRP	2.7
1	B	838	TYR	2.6
1	D	25	TYR	2.6
1	D	696	VAL	2.6
1	D	712	ILE	2.5
1	B	736	GLU	2.5
1	D	714	SER	2.5
1	A	731	SER	2.4
1	B	485	TRP	2.4
1	A	366	PHE	2.4
1	A	672	ARG	2.2
1	C	691	ASP	2.2
1	D	724	SER	2.2
1	D	700	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	717	LEU	2.2
1	C	861	GLN	2.2
1	B	487	LEU	2.1
1	D	322	LEU	2.1
1	A	719	ALA	2.1
1	D	315	ALA	2.1
1	D	310	THR	2.0
1	D	692	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MAN	O	4	11/12	0.46	0.31	40,43,45,48	11
3	MAN	U	4	11/12	0.67	0.29	31,37,43,47	11
9	MAN	h	5	11/12	0.68	0.26	40,41,44,45	11
3	MAN	F	4	11/12	0.70	0.26	42,42,46,46	11
8	MAN	N	6	11/12	0.71	0.18	40,47,52,54	11
5	NAG	L	2	14/15	0.71	0.27	27,30,34,35	14
3	MAN	M	4	11/12	0.71	0.21	33,36,39,41	11
9	MAN	h	7	11/12	0.72	0.30	39,44,50,51	11
10	MAN	S	5	11/12	0.73	0.20	34,37,40,48	11
9	MAN	R	7	11/12	0.73	0.28	45,48,51,56	11
9	MAN	Z	7	11/12	0.73	0.22	47,49,52,53	11
7	MAN	i	7	11/12	0.74	0.28	42,44,48,50	11
5	NAG	I	2	14/15	0.74	0.24	39,48,51,54	14
13	BMA	e	3	11/12	0.75	0.21	41,45,47,48	11
8	MAN	N	5	11/12	0.75	0.15	47,51,55,56	11
7	MAN	K	7	11/12	0.76	0.23	54,57,59,65	0
13	MAN	e	4	11/12	0.76	0.16	43,49,53,58	11
3	BMA	O	3	11/12	0.76	0.17	33,36,41,46	11
11	MAN	V	5	11/12	0.78	0.17	38,47,51,52	11
4	MAN	H	5	11/12	0.78	0.24	57,61,71,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	BMA	S	3	11/12	0.79	0.18	37,42,44,47	11
2	BMA	W	3	11/12	0.79	0.17	40,45,51,55	0
4	MAN	P	6	11/12	0.80	0.22	32,35,37,38	11
3	BMA	F	3	11/12	0.80	0.16	50,53,56,56	0
2	BMA	G	3	11/12	0.81	0.14	27,33,36,41	11
4	MAN	P	5	11/12	0.81	0.26	35,39,40,44	11
14	BMA	f	3	11/12	0.81	0.14	37,44,46,49	0
5	NAG	g	2	14/15	0.81	0.26	22,33,38,43	14
9	MAN	Z	5	11/12	0.81	0.16	55,61,64,68	0
9	MAN	h	6	11/12	0.82	0.24	33,37,39,40	11
14	MAN	f	6	11/12	0.82	0.17	30,37,41,44	11
11	MAN	V	4	11/12	0.82	0.13	45,54,59,60	0
5	NAG	Y	2	14/15	0.83	0.19	45,52,58,71	0
6	MAN	J	6	11/12	0.83	0.14	41,48,50,55	11
10	MAN	S	4	11/12	0.83	0.23	35,36,40,41	11
9	MAN	h	4	11/12	0.84	0.15	48,53,55,60	0
2	BMA	E	3	11/12	0.84	0.17	56,59,61,69	0
6	MAN	J	5	11/12	0.84	0.16	45,50,56,60	11
12	MAN	X	9	11/12	0.84	0.13	40,41,45,47	0
5	NAG	T	2	14/15	0.84	0.16	46,53,60,63	0
5	NAG	I	1	14/15	0.84	0.13	43,50,54,58	0
6	MAN	J	4	11/12	0.85	0.14	51,55,58,65	0
4	MAN	H	9	11/12	0.85	0.16	46,49,55,58	0
9	MAN	R	6	11/12	0.85	0.25	52,58,63,68	0
4	MAN	H	6	11/12	0.85	0.14	50,51,53,55	11
14	MAN	f	5	11/12	0.86	0.16	36,41,43,44	0
9	MAN	a	6	11/12	0.86	0.28	34,38,40,41	11
3	BMA	U	3	11/12	0.86	0.11	39,45,50,54	0
5	NAG	c	2	14/15	0.86	0.17	48,56,58,58	0
9	MAN	Z	4	11/12	0.86	0.14	45,49,57,58	0
6	BMA	J	3	11/12	0.87	0.12	40,45,49,54	0
5	NAG	g	1	14/15	0.87	0.13	34,44,55,56	0
5	NAG	d	2	14/15	0.87	0.20	27,34,41,42	14
4	MAN	H	10	11/12	0.87	0.17	29,40,47,53	0
3	BMA	M	3	11/12	0.87	0.12	35,36,38,39	11
7	MAN	K	6	11/12	0.87	0.20	43,44,48,56	11
7	NAG	K	2	14/15	0.87	0.13	34,39,52,53	0
9	MAN	Z	6	11/12	0.87	0.20	48,56,63,64	0
8	BMA	N	3	11/12	0.88	0.13	46,50,54,59	0
5	NAG	b	2	14/15	0.88	0.21	22,28,30,30	14
9	MAN	R	5	11/12	0.88	0.22	50,58,67,72	0
11	BMA	V	3	11/12	0.88	0.11	36,43,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MAN	i	6	11/12	0.88	0.17	41,44,45,48	11
7	MAN	K	4	11/12	0.88	0.13	44,48,54,60	0
14	MAN	f	8	11/12	0.88	0.14	37,39,45,45	0
5	NAG	Q	1	14/15	0.88	0.15	40,48,59,65	0
4	BMA	H	3	11/12	0.88	0.16	27,36,39,39	0
10	NAG	S	2	14/15	0.88	0.14	40,43,56,70	0
9	MAN	a	7	11/12	0.89	0.16	48,51,66,68	0
5	NAG	Q	2	14/15	0.89	0.13	44,52,57,66	0
9	MAN	a	5	11/12	0.89	0.15	46,47,49,51	11
7	BMA	K	3	11/12	0.89	0.15	42,49,52,54	0
5	NAG	Y	1	14/15	0.89	0.13	37,44,50,58	0
8	MAN	N	4	11/12	0.89	0.15	47,51,52,54	11
4	MAN	H	4	11/12	0.89	0.17	40,45,52,59	0
13	NAG	e	2	14/15	0.89	0.19	42,45,54,60	0
9	BMA	a	3	11/12	0.90	0.15	44,56,68,71	0
4	MAN	H	8	11/12	0.90	0.11	33,34,41,43	0
14	NAG	f	1	14/15	0.90	0.17	37,48,60,60	0
4	MAN	P	4	11/12	0.90	0.14	43,48,52,58	0
4	MAN	P	9	11/12	0.90	0.16	42,51,54,67	0
9	MAN	R	4	11/12	0.90	0.11	51,53,57,62	0
7	MAN	i	4	11/12	0.90	0.12	36,41,43,46	0
9	BMA	Z	3	11/12	0.91	0.12	33,37,44,45	0
4	MAN	H	7	11/12	0.91	0.13	30,32,36,37	0
3	NAG	M	1	14/15	0.91	0.11	27,30,31,33	0
7	MAN	K	5	11/12	0.91	0.15	38,45,55,62	0
4	NAG	H	2	14/15	0.91	0.15	34,40,42,46	0
9	BMA	h	3	11/12	0.91	0.12	39,41,45,49	0
12	MAN	X	6	11/12	0.91	0.14	37,43,47,49	0
5	NAG	c	1	14/15	0.91	0.11	32,43,49,52	0
7	MAN	i	5	11/12	0.91	0.15	39,43,50,55	0
14	NAG	f	2	14/15	0.91	0.15	37,41,48,48	0
14	MAN	f	4	11/12	0.91	0.12	34,39,43,43	0
14	MAN	f	7	11/12	0.91	0.15	35,38,40,40	0
9	NAG	a	2	14/15	0.92	0.12	38,42,52,55	0
5	NAG	L	1	14/15	0.92	0.17	36,44,57,65	0
4	NAG	H	1	14/15	0.92	0.15	35,42,46,47	0
4	MAN	P	8	11/12	0.92	0.10	27,33,37,42	0
6	NAG	J	2	14/15	0.92	0.11	36,39,44,47	0
2	NAG	E	1	14/15	0.92	0.11	32,35,38,39	0
7	NAG	i	2	14/15	0.92	0.11	33,37,42,43	0
3	NAG	M	2	14/15	0.92	0.10	28,32,39,45	0
4	NAG	P	1	14/15	0.92	0.14	28,31,36,40	0

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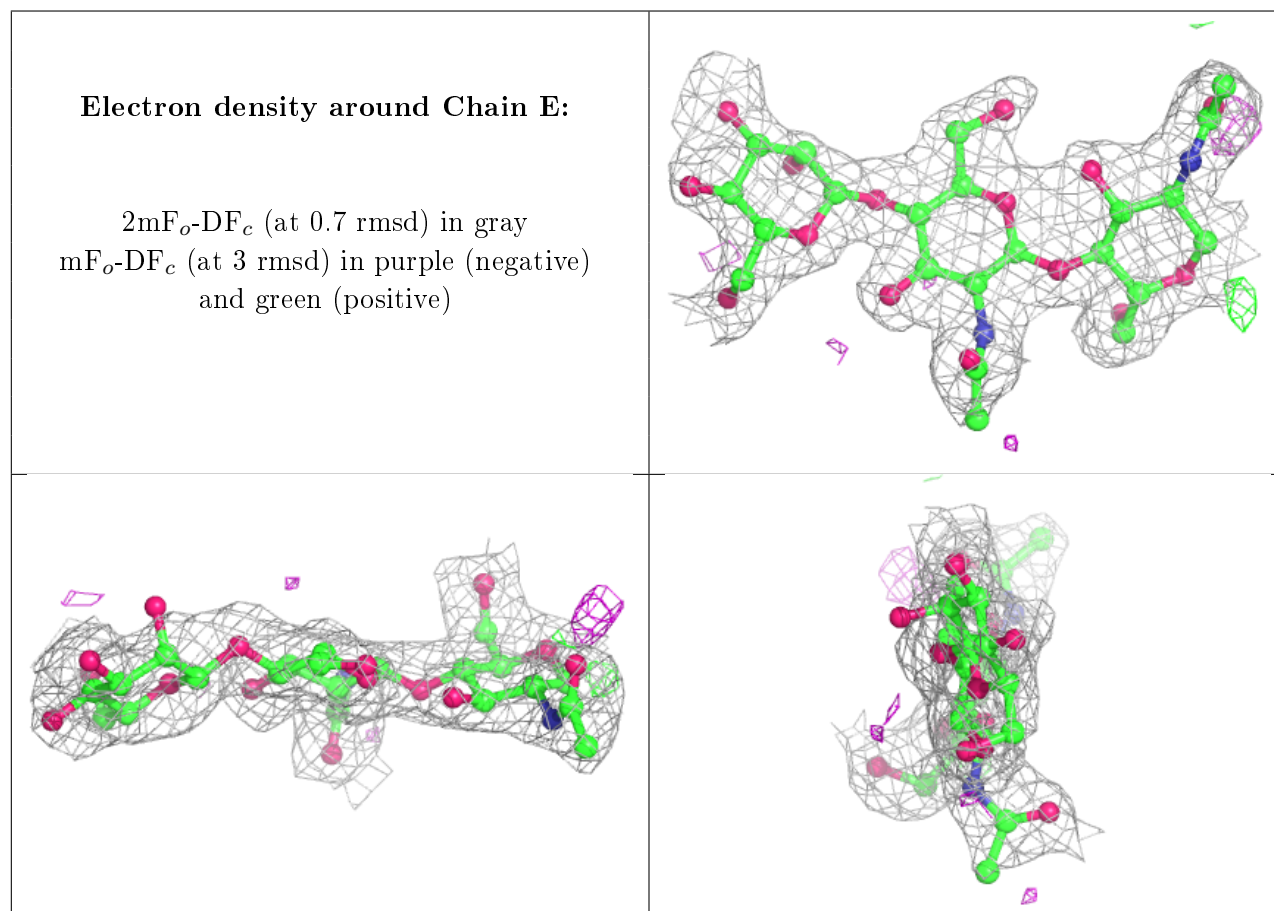
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	NAG	N	2	14/15	0.92	0.12	33,38,45,51	0
5	NAG	b	1	14/15	0.92	0.14	33,37,46,54	0
4	BMA	P	3	11/12	0.92	0.10	29,34,41,42	0
13	NAG	e	1	14/15	0.92	0.14	32,37,42,46	0
9	BMA	R	3	11/12	0.92	0.17	39,42,45,52	0
7	BMA	i	3	11/12	0.93	0.08	34,38,44,45	0
9	NAG	R	1	14/15	0.93	0.15	33,37,57,59	0
3	NAG	F	2	14/15	0.93	0.12	41,45,55,62	0
5	NAG	T	1	14/15	0.93	0.13	36,40,43,43	0
12	MAN	X	7	11/12	0.93	0.09	25,26,28,29	0
4	MAN	H	11	11/12	0.93	0.11	31,38,41,43	0
5	NAG	d	1	14/15	0.93	0.12	33,39,44,44	0
2	NAG	G	1	14/15	0.93	0.12	26,33,39,41	0
2	NAG	E	2	14/15	0.93	0.10	40,44,48,48	0
9	NAG	R	2	14/15	0.93	0.15	31,37,40,46	0
4	MAN	P	7	11/12	0.93	0.10	28,29,32,32	0
2	NAG	G	2	14/15	0.93	0.11	30,32,36,38	0
12	MAN	X	4	11/12	0.94	0.10	24,25,27,27	0
9	NAG	a	1	14/15	0.94	0.09	28,31,34,38	0
10	NAG	S	1	14/15	0.94	0.11	34,36,39,42	0
11	NAG	V	2[A]	14/15	0.94	0.14	31,35,37,41	14
7	NAG	i	1	14/15	0.94	0.11	25,29,33,33	0
4	MAN	P	11	11/12	0.94	0.12	32,34,35,36	0
8	NAG	N	1	14/15	0.94	0.12	23,30,34,34	0
9	NAG	h	1	14/15	0.94	0.11	27,32,42,42	0
9	MAN	a	4	11/12	0.94	0.13	48,54,60,63	0
9	NAG	h	2	14/15	0.94	0.09	28,31,35,38	0
11	NAG	V	2[B]	14/15	0.94	0.14	29,32,36,40	14
4	MAN	P	10	11/12	0.94	0.13	28,31,33,36	0
3	NAG	F	1	14/15	0.94	0.14	33,36,39,41	0
2	NAG	W	1	14/15	0.94	0.12	22,26,30,34	0
12	NAG	X	2	14/15	0.94	0.12	23,26,29,30	0
3	NAG	U	2	14/15	0.94	0.10	26,31,39,39	0
3	NAG	U	1	14/15	0.94	0.10	25,27,30,31	0
6	NAG	J	1	14/15	0.94	0.11	31,34,49,53	0
9	NAG	Z	1	14/15	0.95	0.11	26,29,41,46	0
12	BMA	X	3	11/12	0.95	0.09	24,27,31,34	0
3	NAG	O	2	14/15	0.95	0.10	29,31,33,35	0
7	NAG	K	1	14/15	0.95	0.13	26,30,33,34	0
4	NAG	P	2	14/15	0.95	0.12	29,32,37,38	0
12	MAN	X	8	11/12	0.95	0.09	28,29,31,32	0
12	NAG	X	1	14/15	0.95	0.17	25,29,32,32	0

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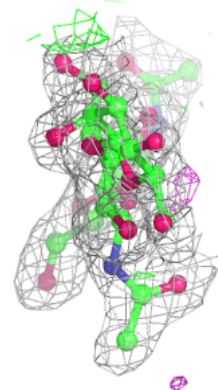
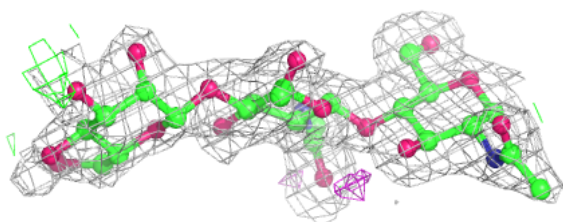
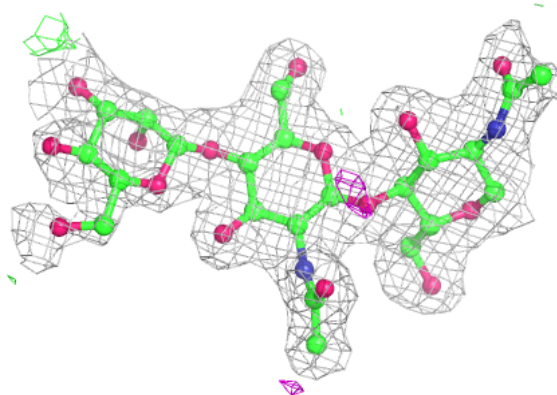
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	NAG	V	1	14/15	0.95	0.10	27,29,31,33	0
12	MAN	X	5	11/12	0.96	0.09	24,25,28,31	0
3	NAG	O	1	14/15	0.96	0.09	24,27,29,29	0
9	NAG	Z	2	14/15	0.96	0.12	25,29,31,32	0
2	NAG	W	2	14/15	0.96	0.09	27,29,34,35	0

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.

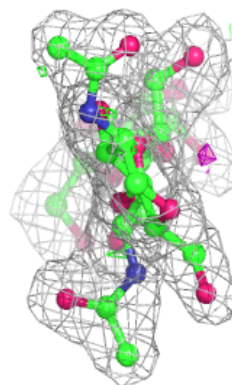
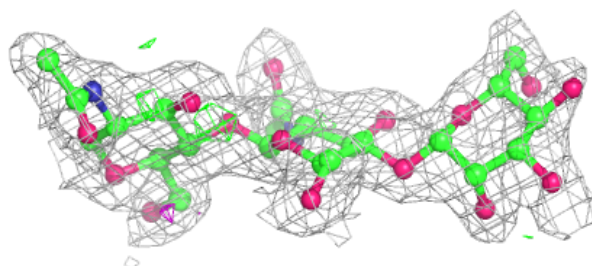
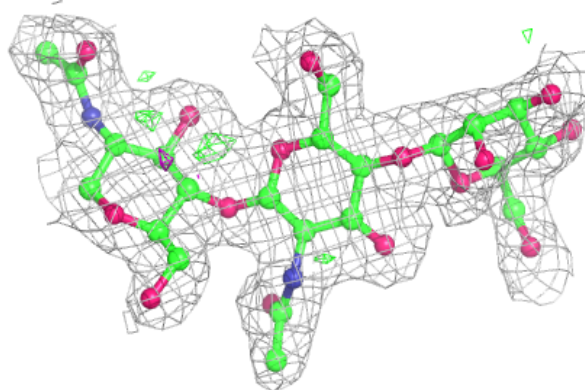


Electron density around Chain G:

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

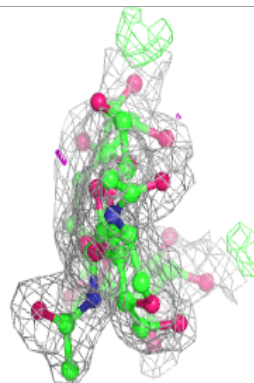
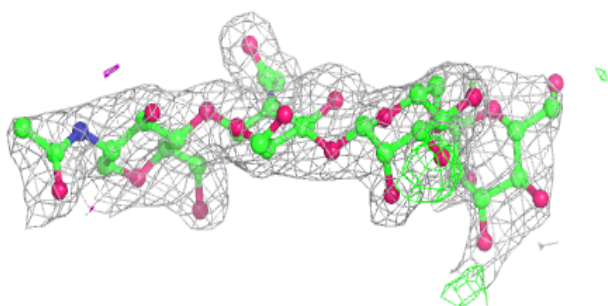
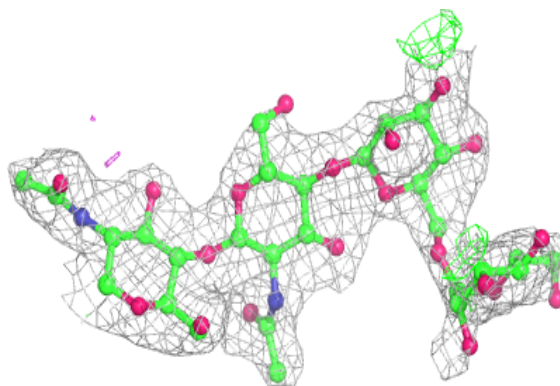
**Electron density around Chain W:**

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

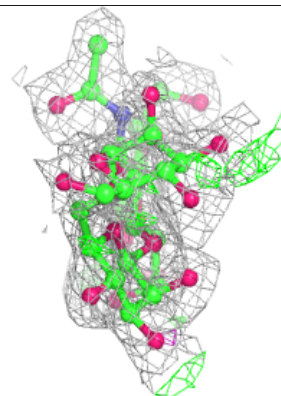
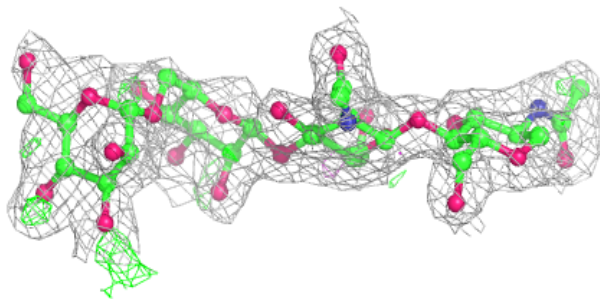
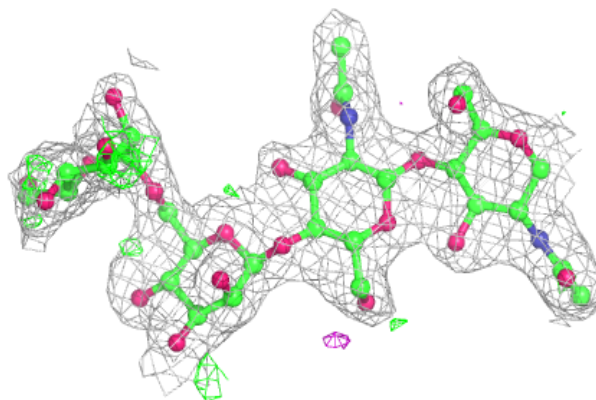


Electron density around Chain F:

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

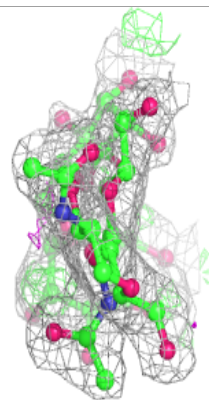
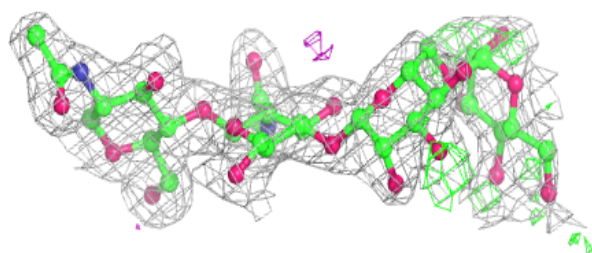
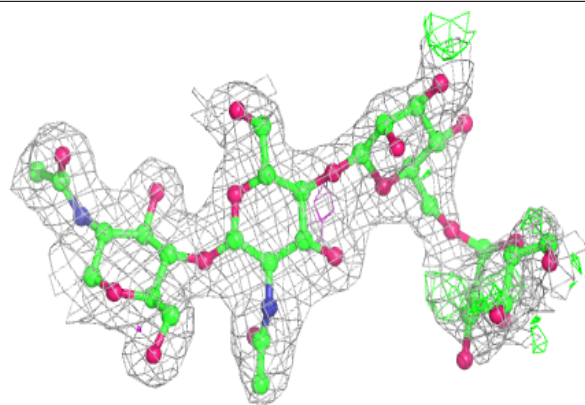
**Electron density around Chain M:**

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

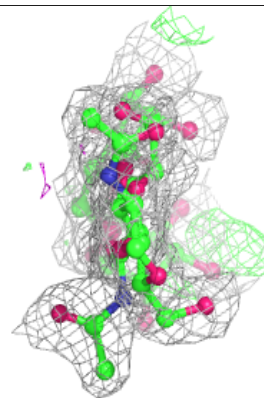
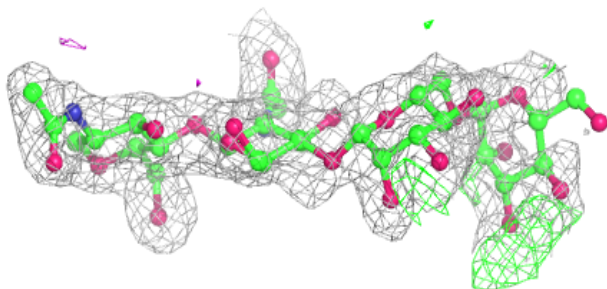
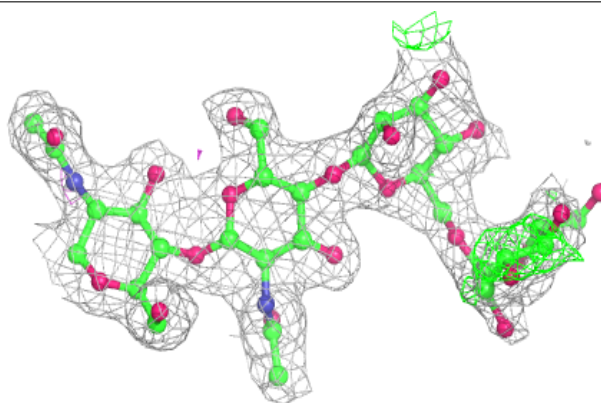


Electron density around Chain O:

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

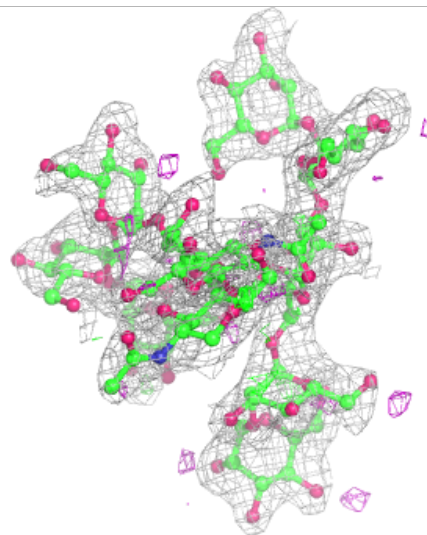
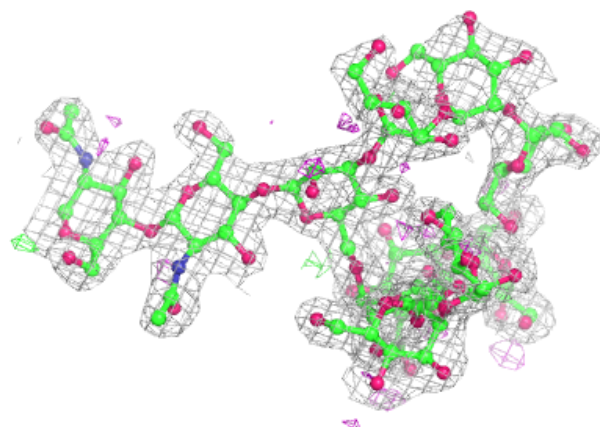
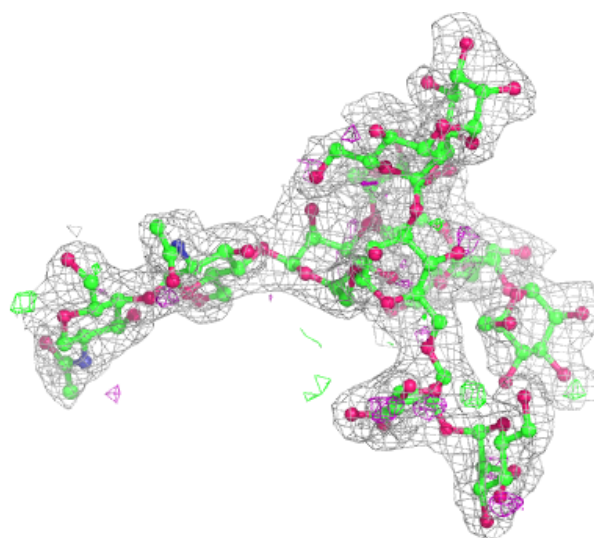
**Electron density around Chain U:**

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



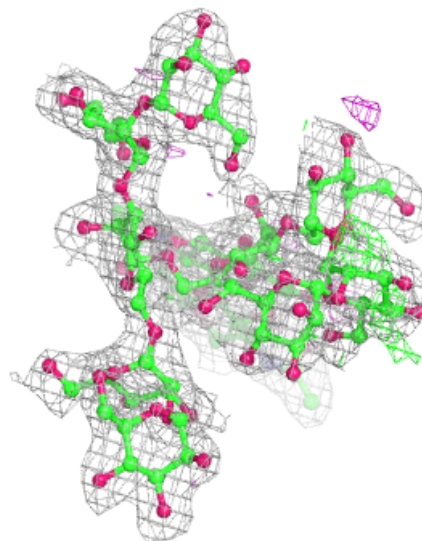
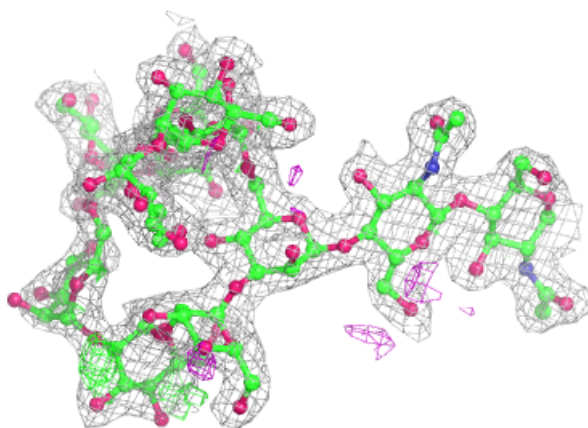
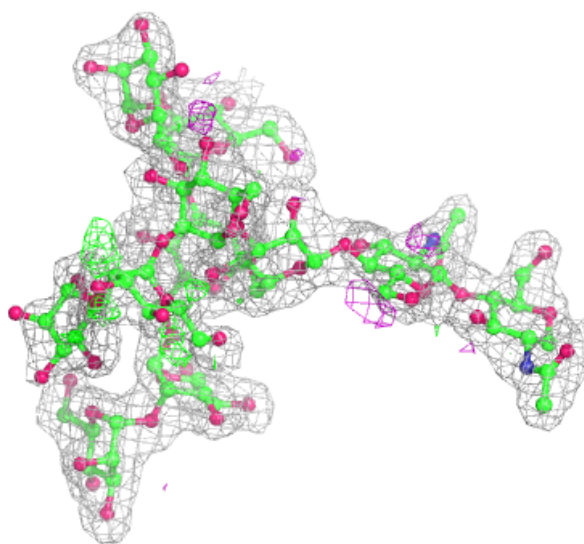
Electron density around Chain H:

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



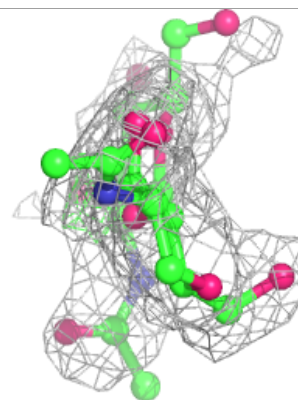
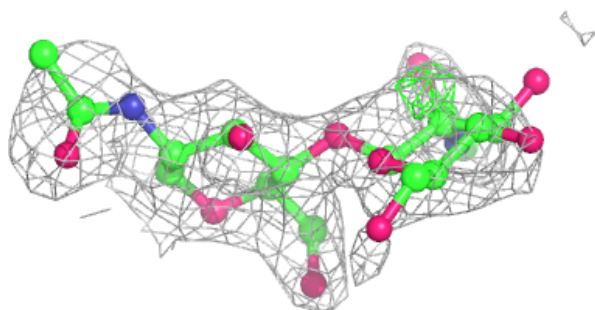
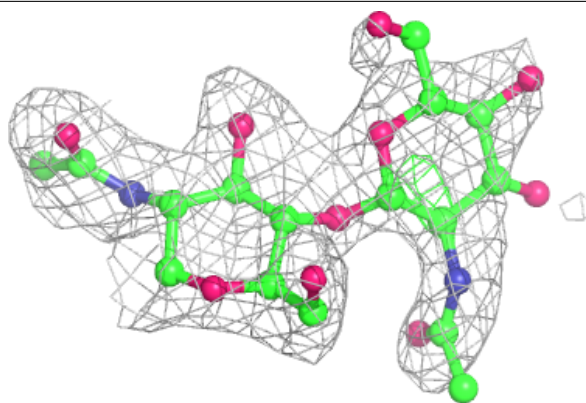
Electron density around Chain P:

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

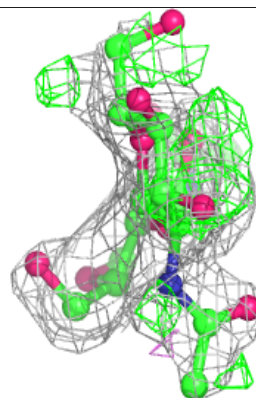
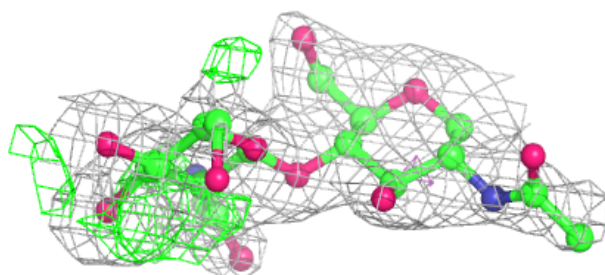
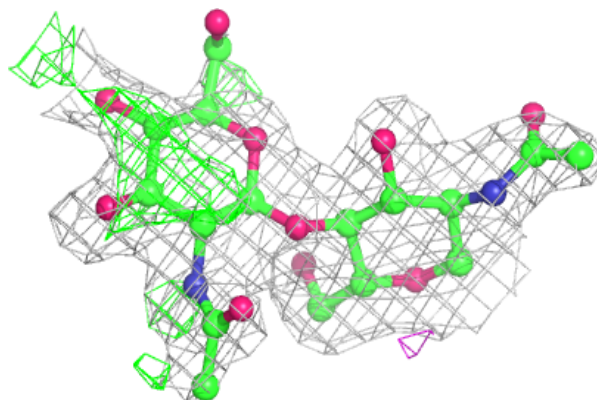


Electron density around Chain I:

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

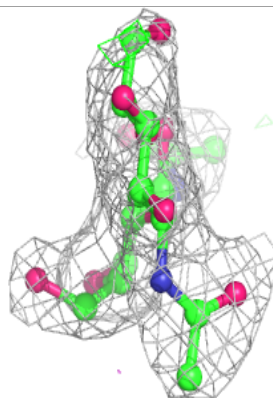
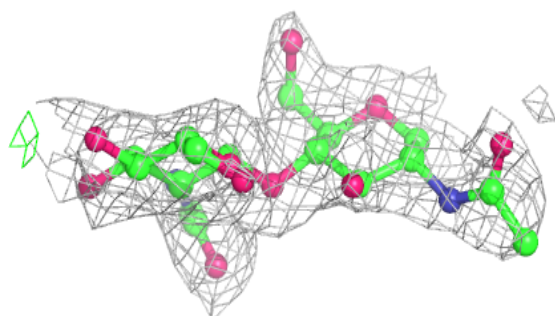
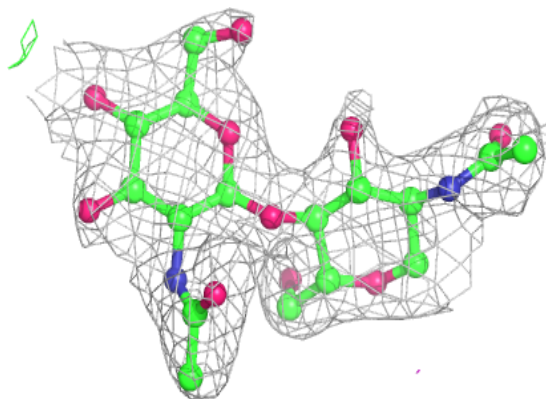
**Electron density around Chain L:**

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

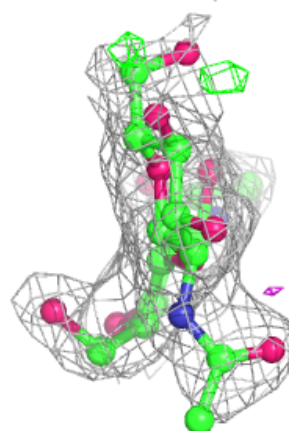
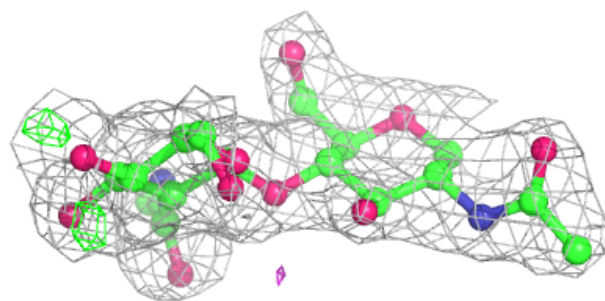
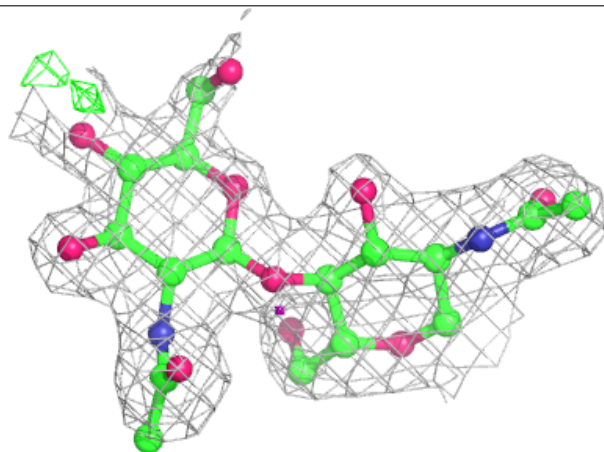


Electron density around Chain Q:

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

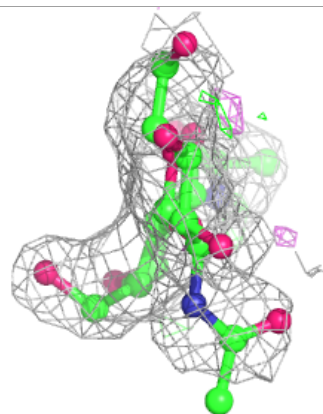
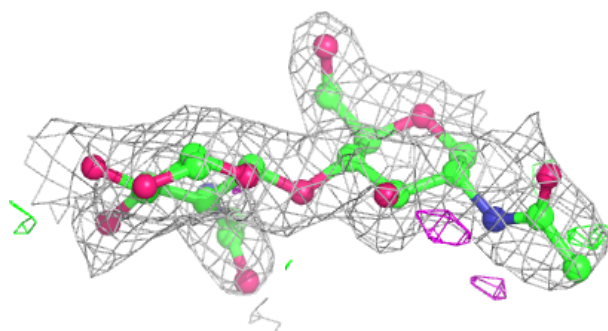
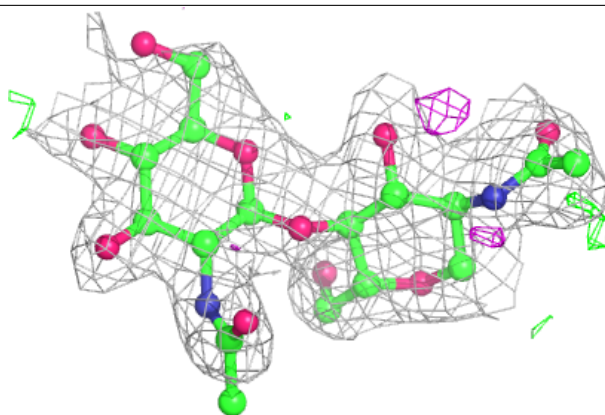
**Electron density around Chain T:**

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

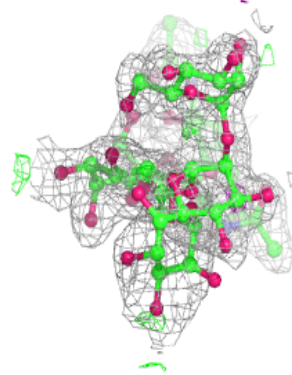
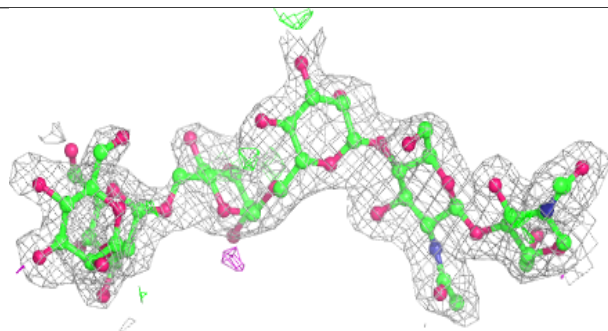
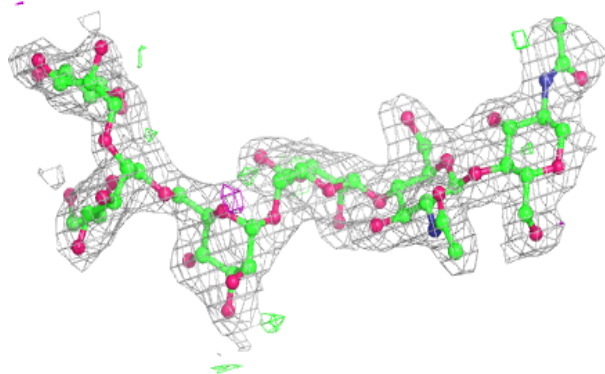


Electron density around Chain Y:

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

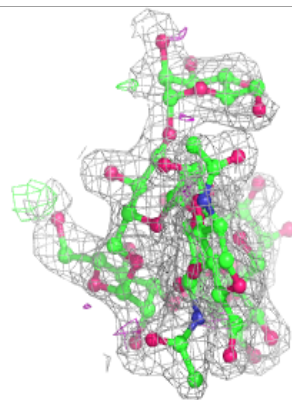
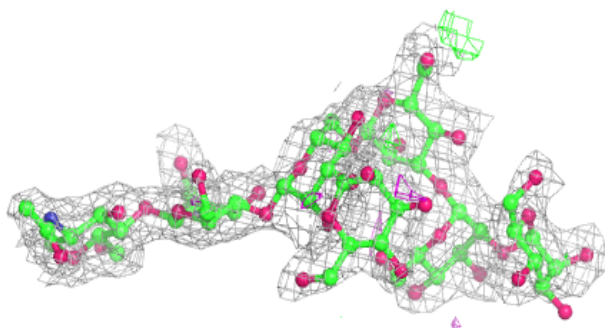
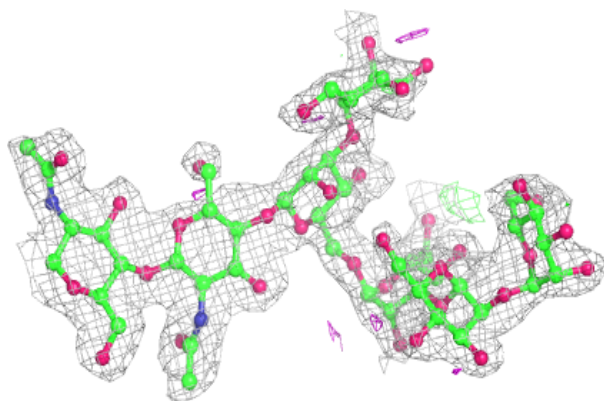
**Electron density around Chain J:**

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

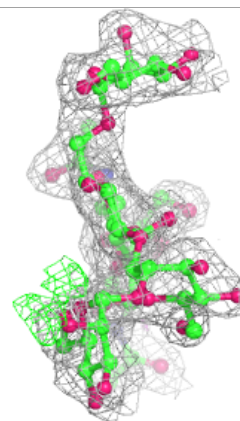
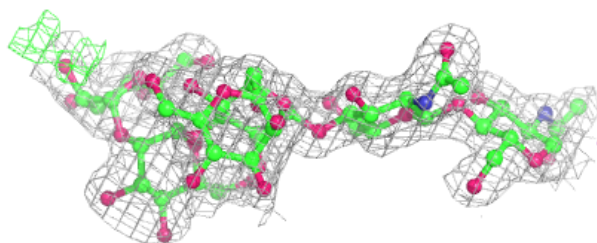
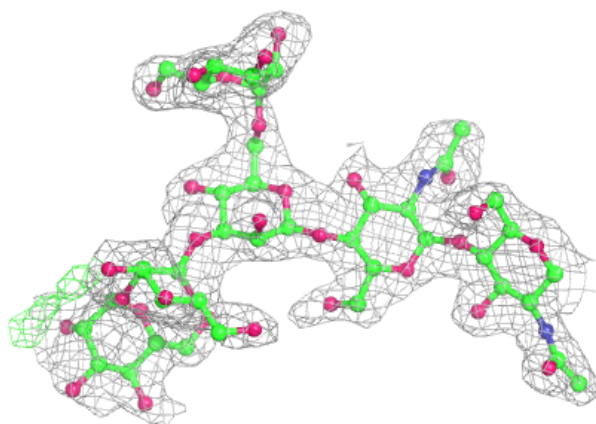


Electron density around Chain K:

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

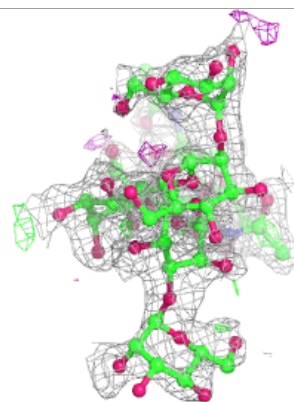
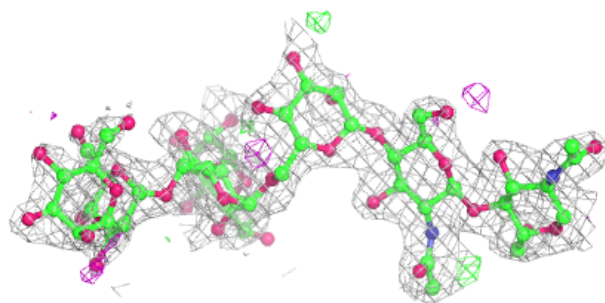
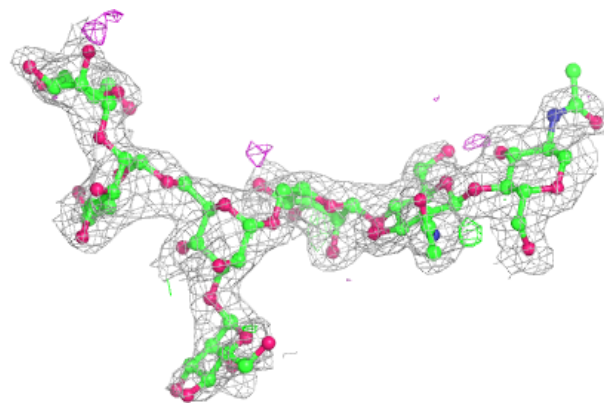
**Electron density around Chain N:**

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

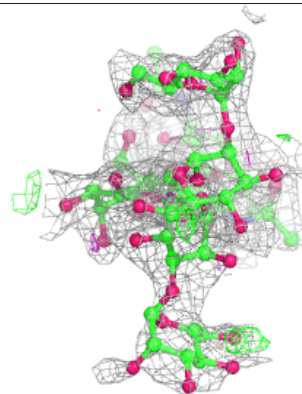
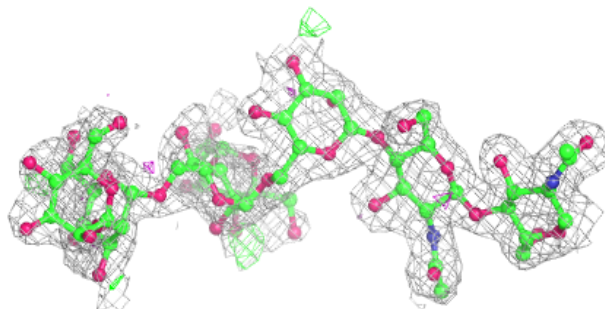
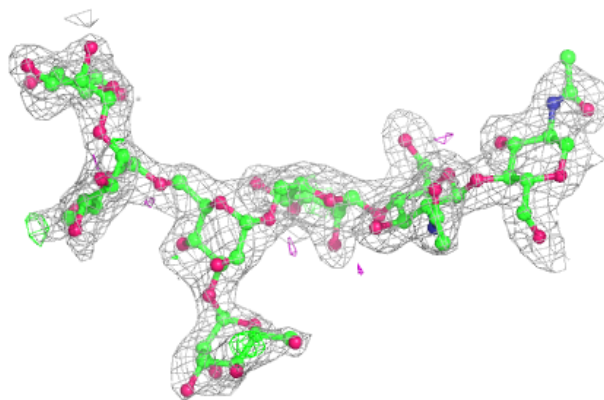


Electron density around Chain R:

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

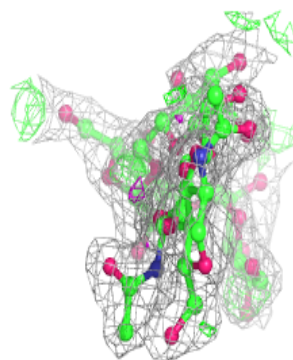
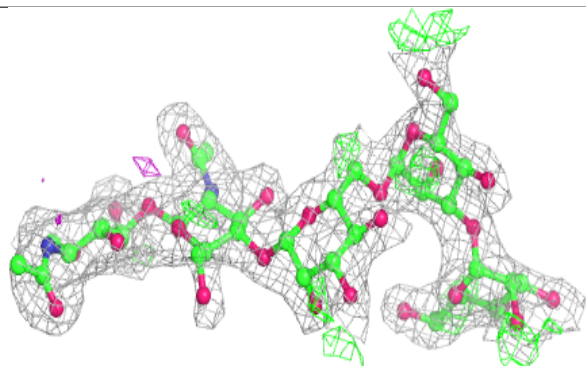
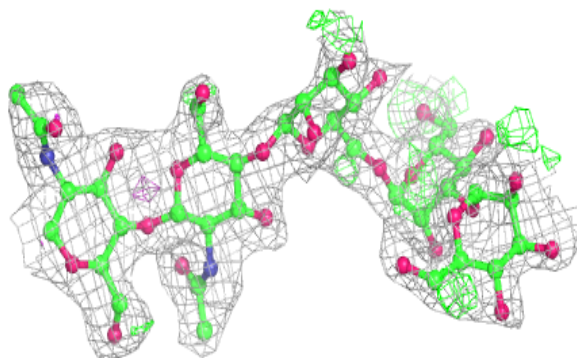
**Electron density around Chain Z:**

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

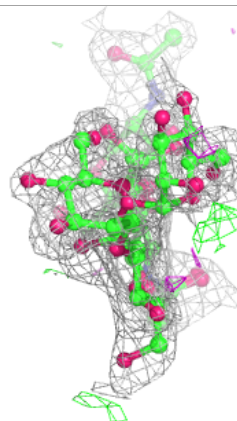
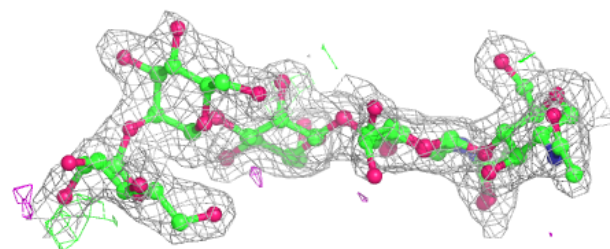
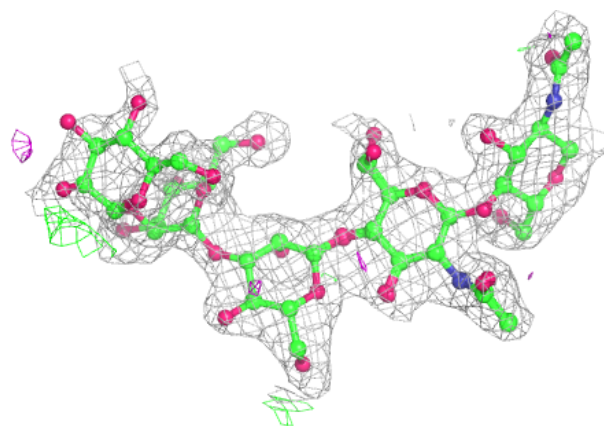


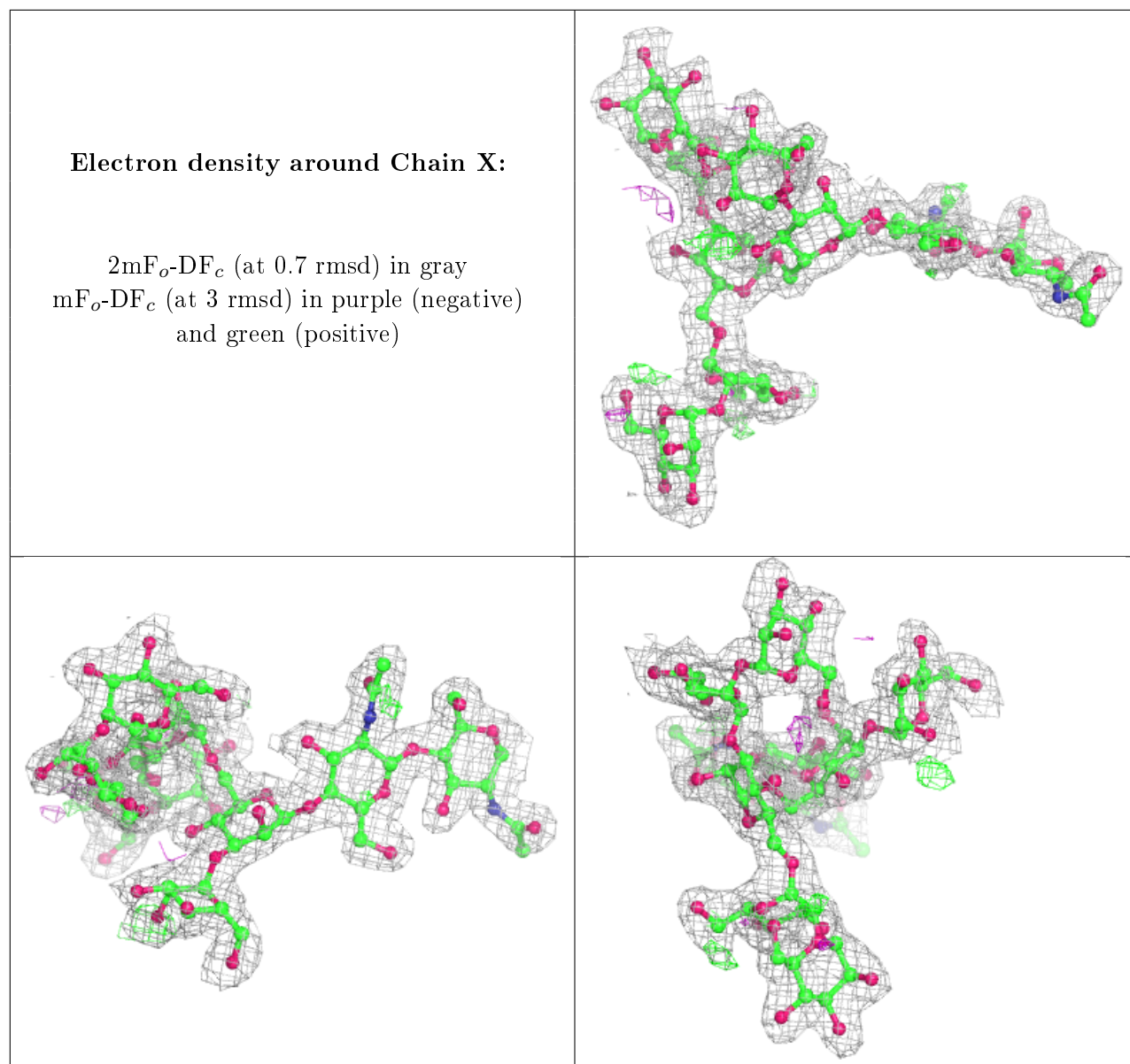
Electron density around Chain S:

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

**Electron density around Chain V:**

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	NAG	B	1601	14/15	0.69	0.35	36,39,45,46	14
15	NAG	A	1901	14/15	0.69	0.24	44,47,49,49	14
15	NAG	C	1901	14/15	0.74	0.27	66,72,81,84	0
15	NAG	C	1601	14/15	0.77	0.28	43,48,54,57	14
15	NAG	D	1601	14/15	0.80	0.17	47,60,67,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	NAG	D	1801	14/15	0.83	0.17	54,58,62,63	0
16	PEG	A	3001	7/7	0.83	0.20	46,52,53,57	0
16	PEG	D	6001	7/7	0.83	0.12	37,40,48,48	0
16	PEG	C	6001	7/7	0.85	0.17	29,30,37,39	0
16	PEG	A	6002	7/7	0.86	0.14	37,40,46,47	0
17	MG	C	3001	1/1	0.87	0.10	42,42,42,42	0
15	NAG	A	1601	14/15	0.89	0.13	38,45,51,55	0
16	PEG	B	6001	7/7	0.92	0.14	32,33,38,47	0
17	MG	A	3002	1/1	0.92	0.13	46,46,46,46	0
18	PO4	A	5001	5/5	0.94	0.19	58,59,67,69	0
19	CL	A	6001	1/1	0.94	0.10	36,36,36,36	0
19	CL	B	5001	1/1	0.95	0.13	35,35,35,35	0
19	CL	D	5001	1/1	0.96	0.07	39,39,39,39	0
19	CL	C	5001	1/1	0.97	0.11	33,33,33,33	0
17	MG	D	4001	1/1	0.98	0.03	27,27,27,27	0
17	MG	A	4001	1/1	0.98	0.06	31,31,31,31	0

6.5 Other polymers

There are no such residues in this entry.