



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 30, 2024 – 12:17 PM EDT

PDB ID : 8UWA
Title : VH1-18 QxxV class antibody 09-1B12 bound to A/Perth/16/2009 H3N2 hemagglutinin
Authors : Maurer, D.P.
Deposited on : 2023-11-06
Resolution : 4.02 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

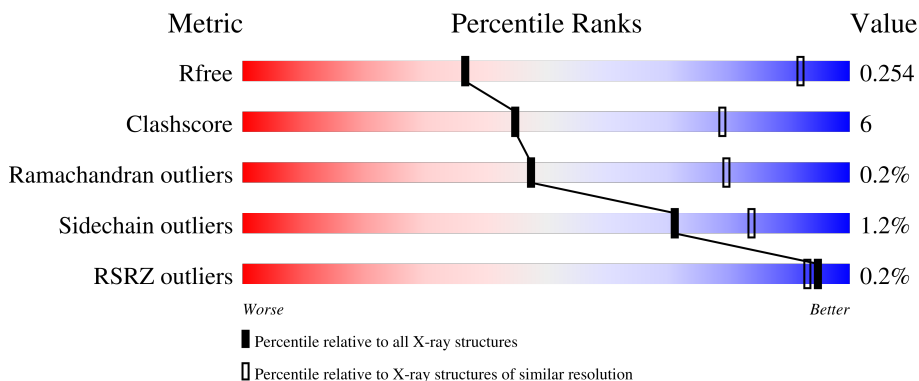
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.02 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.









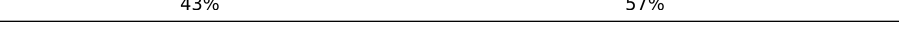
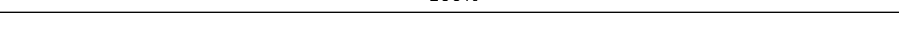
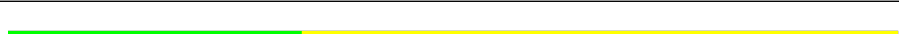

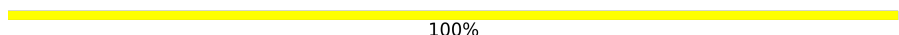






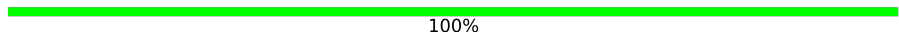


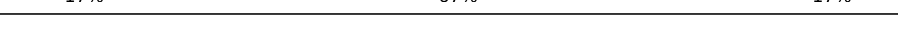
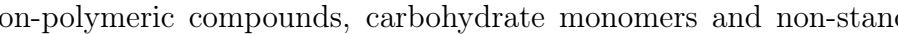

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1098 (4.34-3.70)
Clashscore	141614	1159 (4.34-3.70)
Ramachandran outliers	138981	1118 (4.34-3.70)
Sidechain outliers	138945	1108 (4.34-3.70)
RSRZ outliers	127900	1034 (4.38-3.66)

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

Mol	Chain	Length	Quality of chain
1	D	216	85% 14% .
1	E	216	81% 18% .
1	G	216	86% 14%
2	A	514	81% 13% . 5%
2	B	514	79% 15% 5%

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Mol	Chain	Length	Quality of chain
2	C	514	 82% 13% 5%
3	F	240	 88% 7% .
3	H	240	 87% 12%
3	U	240	 80% 16% .
4	I	4	 50% 50%
4	Q	4	 75% 25%
5	J	7	 43% 57%
6	K	3	 100%
6	Z	3	 100%
6	a	3	 33% 67%
7	L	5	 40% 60%
7	M	5	 100%
7	R	5	 60% 40%
7	S	5	 40% 60%
7	T	5	 20% 80%
7	V	5	 40% 60%
8	N	4	 75% 25%
8	P	4	 25% 75%
9	O	2	 50% 50%
9	W	2	 100%
9	b	2	 50% 50%
10	X	6	 17% 83%
10	Y	6	 17% 67% 17%

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
10	MAN	Y	5	-	-	-	X
11	NAG	B	603	-	-	-	X
4	MAN	Q	4	-	-	-	X
5	MAN	J	5	-	-	-	X
6	NAG	a	1	-	-	-	X
6	NAG	a	2	-	-	-	X
7	NAG	M	1	-	-	-	X
7	MAN	M	5	-	-	-	X
7	NAG	R	2	-	-	-	X
7	BMA	R	3	-	-	-	X
7	MAN	R	4	-	-	-	X
7	MAN	R	5	-	-	-	X
7	MAN	T	4	-	-	-	X
8	BMA	N	3	-	-	-	X
8	MAN	N	4	-	-	-	X
9	NAG	O	2	-	-	-	X
9	NAG	W	1	-	-	-	X
9	NAG	W	2	-	-	-	X
9	NAG	b	1	-	-	-	X
9	NAG	b	2	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 22979 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 09-1B12 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	216	1681	1050	291	335	5	0	0	0
1	E	216	1681	1050	291	335	5	0	0	0
1	G	216	1681	1050	291	335	5	0	0	0

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	489	3866	2410	690	748	18	15	0	0
2	B	486	3837	2391	685	743	18	7	0	0
2	C	490	3873	2414	691	750	18	19	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	505	ALA	-	expression tag	UNP C6KNH7
A	506	GLY	-	expression tag	UNP C6KNH7
A	507	SER	-	expression tag	UNP C6KNH7
A	508	SER	-	expression tag	UNP C6KNH7
A	509	LEU	-	expression tag	UNP C6KNH7
A	510	GLU	-	expression tag	UNP C6KNH7
A	511	VAL	-	expression tag	UNP C6KNH7
A	512	LEU	-	expression tag	UNP C6KNH7
A	513	PHE	-	expression tag	UNP C6KNH7
A	514	GLN	-	expression tag	UNP C6KNH7
B	505	ALA	-	expression tag	UNP C6KNH7
B	506	GLY	-	expression tag	UNP C6KNH7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	507	SER	-	expression tag	UNP C6KNH7
B	508	SER	-	expression tag	UNP C6KNH7
B	509	LEU	-	expression tag	UNP C6KNH7
B	510	GLU	-	expression tag	UNP C6KNH7
B	511	VAL	-	expression tag	UNP C6KNH7
B	512	LEU	-	expression tag	UNP C6KNH7
B	513	PHE	-	expression tag	UNP C6KNH7
B	514	GLN	-	expression tag	UNP C6KNH7
C	505	ALA	-	expression tag	UNP C6KNH7
C	506	GLY	-	expression tag	UNP C6KNH7
C	507	SER	-	expression tag	UNP C6KNH7
C	508	SER	-	expression tag	UNP C6KNH7
C	509	LEU	-	expression tag	UNP C6KNH7
C	510	GLU	-	expression tag	UNP C6KNH7
C	511	VAL	-	expression tag	UNP C6KNH7
C	512	LEU	-	expression tag	UNP C6KNH7
C	513	PHE	-	expression tag	UNP C6KNH7
C	514	GLN	-	expression tag	UNP C6KNH7

- Molecule 3 is a protein called 09-1B12 heavy chain.

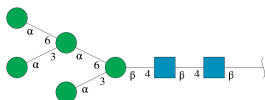
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	230	Total	C	N	O	S	0	0	0
			1725	1089	293	336	7			
3	H	239	Total	C	N	O	S	0	0	0
			1790	1129	303	351	7			
3	U	230	Total	C	N	O	S	0	0	0
			1725	1089	293	336	7			

- 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.



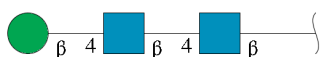
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	Q	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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.



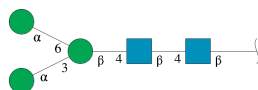
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	J	7	83	46	2	35	0	0	0

- Molecule 6 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
			Total	C	N	O			
6	K	3	39	22	2	15	0	0	0
6	Z	3	39	22	2	15	0	0	0
6	a	3	39	22	2	15	0	0	0

- Molecule 7 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
			Total	C	N	O			
7	L	5	61	34	2	25	0	0	0
7	M	5	61	34	2	25	0	0	0
7	R	5	61	34	2	25	0	0	0

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

- Molecule 8 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.



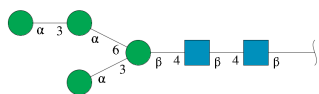
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	N	4	Total 50	C 28	N 2	O 20	0	0	0
8	P	4	Total 50	C 28	N 2	O 20	0	0	0

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



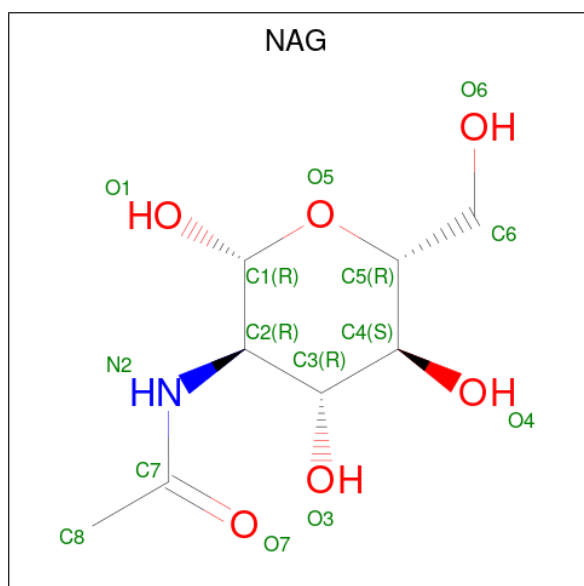
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	O	2	Total 28	C 16	N 2	O 10	0	0	0
9	W	2	Total 28	C 16	N 2	O 10	0	0	0
9	b	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 10 is an oligosaccharide called 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	
10	X	6	Total	C	N	O	0	0	0
			72	40	2	30			
10	Y	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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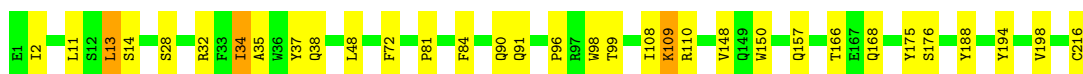
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	N	O	0	0
			14	8	1	5		
11	C	1	Total	C	N	O	0	0
			14	8	1	5		

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.

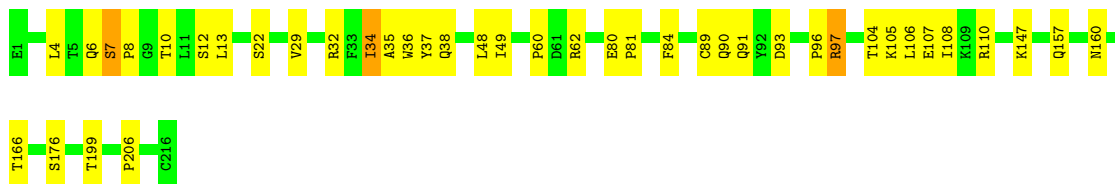
- Molecule 1: 09-1B12 light chain

Chain D: 




- Molecule 1: 09-1B12 light chain

Chain E: 




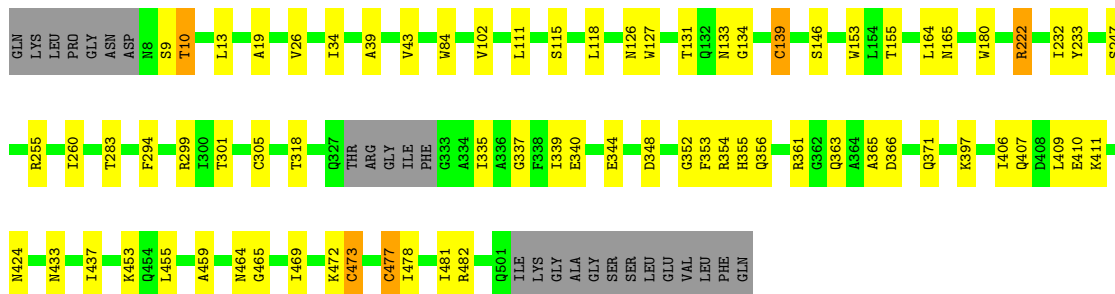
- Molecule 1: 09-1B12 light chain

Chain G: 




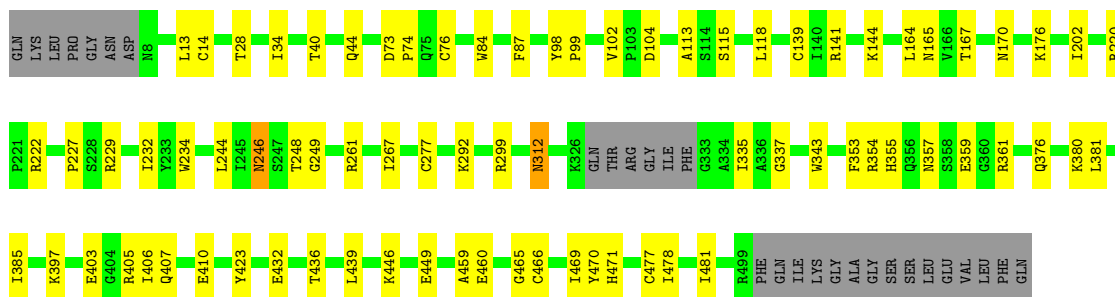
- Molecule 2: Hemagglutinin

Chain A: 




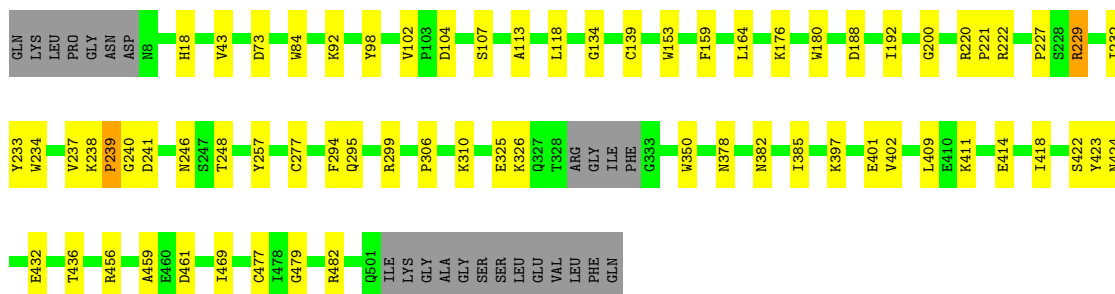
- Molecule 2: Hemagglutinin

Chain B:  79% 15% 5%




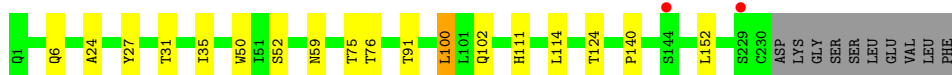
• Molecule 2: Hemagglutinin

Chain C:  82% 13% 5%




• Molecule 3: 09-1B12 heavy chain

Chain F:  88% 7% 5%




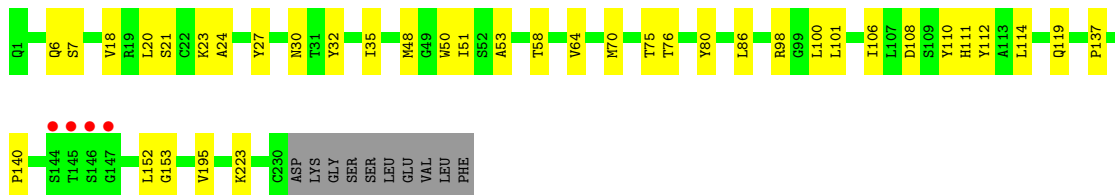
• Molecule 3: 09-1B12 heavy chain

Chain H:  87% 12%



• Molecule 3: 09-1B12 heavy chain

Chain U:  80% 16% 2%




- 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 I:  50% 50%

MAG1
MAG2
BMA3
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 Q:  75% 25%

MAG1
MAG2
BMA3
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-3)-[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 J:  43% 57%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

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

Chain K:  100%

MAG1
MAG2
BMA3

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

Chain a:  33% 67%

MAG1
MAG2
BMA3

- Molecule 7: 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 L: 

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 7: 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 M: 

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 7: 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: 

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 7: 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: 

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 7: 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: 

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 7: 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 V: 

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 8: 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:  75% 25%

MAG1
MAG2
BMA3
MAN4

- Molecule 8: 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:  25% 75%

MAG1
MAG2
BMA3
MAN4

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  50% 50%

MAG1
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%

MAG1
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  50% 50%

MAG1
MAG2

- Molecule 10: 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 X:  17% 83%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 10: 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 Y:  17% 67% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.04Å 158.04Å 417.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.21 – 4.02 50.21 – 4.02	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.21-4.02) 99.8 (50.21-4.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 4.00Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.230 , 0.254 0.231 , 0.254	Depositor DCC
R_{free} test set	2003 reflections (3.92%)	wwPDB-VP
Wilson B-factor (Å ²)	106.8	Xtrriage
Anisotropy	0.268	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	22979	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	D	0.28	0/1719	0.54	0/2332
1	E	0.27	0/1719	0.55	0/2332
1	G	0.28	0/1719	0.52	0/2332
2	A	0.27	0/3945	0.52	0/5338
2	B	0.28	0/3915	0.51	0/5298
2	C	0.29	0/3952	0.52	1/5348 (0.0%)
3	F	0.26	0/1766	0.51	0/2412
3	H	0.26	0/1831	0.51	0/2499
3	U	0.28	0/1766	0.55	0/2412
All	All	0.28	0/22332	0.52	1/30303 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	239	PRO	CA-N-CD	-5.53	103.76	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	7	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1681	0	1632	26	0
1	E	1681	0	1633	32	0
1	G	1681	0	1632	24	0
2	A	3866	0	3743	51	0
2	B	3837	0	3716	52	0
2	C	3873	0	3750	46	0
3	F	1725	0	1701	13	0
3	H	1790	0	1767	20	0
3	U	1725	0	1700	31	0
4	I	50	0	43	0	0
4	Q	50	0	43	0	0
5	J	83	0	70	0	0
6	K	39	0	34	0	0
6	Z	39	0	34	0	0
6	a	39	0	34	0	0
7	L	61	0	52	6	0
7	M	61	0	52	0	0
7	R	61	0	52	1	0
7	S	61	0	52	2	0
7	T	61	0	52	1	0
7	V	61	0	52	3	0
8	N	50	0	43	0	0
8	P	50	0	43	2	0
9	O	28	0	25	2	0
9	W	28	0	25	0	0
9	b	28	0	25	0	0
10	X	72	0	61	3	0
10	Y	72	0	61	1	0
11	A	28	0	26	0	0
11	B	42	0	39	1	0
11	C	56	0	52	0	0
All	All	22979	0	22244	289	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 6.

The worst 5 of 289 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)
3:U:35:ILE:HD11	3:U:114:LEU:HD21	1.51	0.89
1:E:7:SER:HB3	1:E:22:SER:HB3	1.57	0.86
1:D:34:ILE:HA	1:D:90:GLN:O	1.76	0.85
1:E:34:ILE:HA	1:E:90:GLN:O	1.81	0.81
2:A:115:SER:HB2	2:A:260:ILE:HD12	1.63	0.81

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	D	214/216 (99%)	201 (94%)	11 (5%)	2 (1%)	17	55
1	E	214/216 (99%)	202 (94%)	10 (5%)	2 (1%)	17	55
1	G	214/216 (99%)	204 (95%)	9 (4%)	1 (0%)	29	67
2	A	485/514 (94%)	457 (94%)	27 (6%)	1 (0%)	47	80
2	B	482/514 (94%)	462 (96%)	20 (4%)	0	100	100
2	C	486/514 (95%)	467 (96%)	19 (4%)	0	100	100
3	F	228/240 (95%)	219 (96%)	9 (4%)	0	100	100
3	H	237/240 (99%)	229 (97%)	8 (3%)	0	100	100
3	U	228/240 (95%)	220 (96%)	8 (4%)	0	100	100
All	All	2788/2910 (96%)	2661 (95%)	121 (4%)	6 (0%)	47	80

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	8	PRO
1	D	34	ILE
1	G	34	ILE
2	A	10	THR
1	D	109	LYS

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	D	189/189 (100%)	187 (99%)	2 (1%)	73	85
1	E	189/189 (100%)	185 (98%)	4 (2%)	53	72
1	G	189/189 (100%)	189 (100%)	0	100	100
2	A	427/447 (96%)	421 (99%)	6 (1%)	67	81
2	B	424/447 (95%)	416 (98%)	8 (2%)	57	75
2	C	428/447 (96%)	421 (98%)	7 (2%)	62	79
3	F	191/200 (96%)	190 (100%)	1 (0%)	88	93
3	H	199/200 (100%)	199 (100%)	0	100	100
3	U	191/200 (96%)	191 (100%)	0	100	100
All	All	2427/2508 (97%)	2399 (99%)	28 (1%)	71	84

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	139	CYS
3	F	100	LEU
2	B	277	CYS
2	C	229	ARG
2	B	246	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	90	GLN
2	C	407	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

80 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
4	NAG	I	1	4,2	14,14,15	1.17	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	I	2	4	14,14,15	0.29	0	17,19,21	0.52	0
4	BMA	I	3	4	11,11,12	0.69	0	15,15,17	0.86	0
4	MAN	I	4	4	11,11,12	0.86	1 (9%)	15,15,17	1.18	2 (13%)
5	NAG	J	1	5,2	14,14,15	0.46	0	17,19,21	0.65	0
5	NAG	J	2	5	14,14,15	0.39	0	17,19,21	0.51	0
5	BMA	J	3	5	11,11,12	0.91	0	15,15,17	1.02	0
5	MAN	J	4	5	11,11,12	0.78	0	15,15,17	0.93	1 (6%)
5	MAN	J	5	5	11,11,12	0.93	0	15,15,17	1.23	2 (13%)
5	MAN	J	6	5	11,11,12	0.61	0	15,15,17	1.02	2 (13%)
5	MAN	J	7	5	11,11,12	0.93	0	15,15,17	1.03	2 (13%)
6	NAG	K	1	6,2	14,14,15	0.67	0	17,19,21	0.85	1 (5%)
6	NAG	K	2	6	14,14,15	0.64	0	17,19,21	0.99	1 (5%)
6	BMA	K	3	6	11,11,12	1.26	2 (18%)	15,15,17	1.24	3 (20%)
7	NAG	L	1	7,2	14,14,15	0.36	0	17,19,21	0.82	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	L	2	7	14,14,15	0.32	0	17,19,21	1.06	1 (5%)
7	BMA	L	3	7	11,11,12	1.03	0	15,15,17	0.87	0
7	MAN	L	4	7	11,11,12	1.22	1 (9%)	15,15,17	1.21	2 (13%)
7	MAN	L	5	7	11,11,12	1.33	2 (18%)	15,15,17	1.31	2 (13%)
7	NAG	M	1	7,2	14,14,15	1.03	1 (7%)	17,19,21	1.00	1 (5%)
7	NAG	M	2	7	14,14,15	0.97	1 (7%)	17,19,21	1.02	2 (11%)
7	BMA	M	3	7	11,11,12	1.89	3 (27%)	15,15,17	2.52	4 (26%)
7	MAN	M	4	7	11,11,12	1.33	2 (18%)	15,15,17	1.62	3 (20%)
7	MAN	M	5	7	11,11,12	0.96	1 (9%)	15,15,17	1.13	2 (13%)
8	NAG	N	1	8,2	14,14,15	0.33	0	17,19,21	0.59	0
8	NAG	N	2	8	14,14,15	0.21	0	17,19,21	0.61	0
8	BMA	N	3	8	11,11,12	0.94	0	15,15,17	0.86	0
8	MAN	N	4	8	11,11,12	0.85	1 (9%)	15,15,17	1.18	2 (13%)
9	NAG	O	1	9,2	14,14,15	0.34	0	17,19,21	1.17	2 (11%)
9	NAG	O	2	9	14,14,15	0.23	0	17,19,21	0.91	0
8	NAG	P	1	8,2	14,14,15	0.50	0	17,19,21	1.84	5 (29%)
8	NAG	P	2	8	14,14,15	0.56	0	17,19,21	0.45	0
8	BMA	P	3	8	11,11,12	1.02	1 (9%)	15,15,17	1.04	2 (13%)
8	MAN	P	4	8	11,11,12	1.30	2 (18%)	15,15,17	1.18	2 (13%)
4	NAG	Q	1	4,2	14,14,15	0.21	0	17,19,21	0.57	0
4	NAG	Q	2	4	14,14,15	0.36	0	17,19,21	0.64	0
4	BMA	Q	3	4	11,11,12	0.81	0	15,15,17	0.76	0
4	MAN	Q	4	4	11,11,12	0.92	1 (9%)	15,15,17	1.13	2 (13%)
7	NAG	R	1	7,2	14,14,15	1.37	1 (7%)	17,19,21	1.40	2 (11%)
7	NAG	R	2	7	14,14,15	0.77	1 (7%)	17,19,21	1.06	2 (11%)
7	BMA	R	3	7	11,11,12	1.92	3 (27%)	15,15,17	2.26	3 (20%)
7	MAN	R	4	7	11,11,12	1.46	2 (18%)	15,15,17	1.65	3 (20%)
7	MAN	R	5	7	11,11,12	1.32	2 (18%)	15,15,17	1.37	2 (13%)
7	NAG	S	1	7,2	14,14,15	0.66	1 (7%)	17,19,21	0.81	1 (5%)
7	NAG	S	2	7	14,14,15	0.55	0	17,19,21	1.61	2 (11%)
7	BMA	S	3	7	11,11,12	1.01	1 (9%)	15,15,17	0.90	1 (6%)
7	MAN	S	4	7	11,11,12	1.39	2 (18%)	15,15,17	1.31	1 (6%)
7	MAN	S	5	7	11,11,12	0.76	0	15,15,17	1.17	2 (13%)
7	NAG	T	1	7,2	14,14,15	0.26	0	17,19,21	0.69	0
7	NAG	T	2	7	14,14,15	0.43	0	17,19,21	0.57	0
7	BMA	T	3	7	11,11,12	0.76	0	15,15,17	0.80	0
7	MAN	T	4	7	11,11,12	0.81	0	15,15,17	1.01	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	T	5	7	11,11,12	0.92	1 (9%)	15,15,17	1.05	2 (13%)
7	NAG	V	1	7,2	14,14,15	0.59	0	17,19,21	0.65	0
7	NAG	V	2	7	14,14,15	0.63	1 (7%)	17,19,21	1.08	1 (5%)
7	BMA	V	3	7	11,11,12	1.16	1 (9%)	15,15,17	1.54	2 (13%)
7	MAN	V	4	7	11,11,12	0.89	0	15,15,17	1.15	1 (6%)
7	MAN	V	5	7	11,11,12	1.13	1 (9%)	15,15,17	1.06	2 (13%)
9	NAG	W	1	9,2	14,14,15	0.36	0	17,19,21	0.62	0
9	NAG	W	2	9	14,14,15	0.38	0	17,19,21	0.46	0
10	NAG	X	1	10,2	14,14,15	0.68	1 (7%)	17,19,21	0.87	0
10	NAG	X	2	10	14,14,15	1.08	1 (7%)	17,19,21	1.34	1 (5%)
10	BMA	X	3	10	11,11,12	1.21	1 (9%)	15,15,17	1.63	2 (13%)
10	MAN	X	4	10	11,11,12	0.92	0	15,15,17	1.04	1 (6%)
10	MAN	X	5	10	11,11,12	1.00	1 (9%)	15,15,17	1.08	1 (6%)
10	MAN	X	6	10	11,11,12	0.86	1 (9%)	15,15,17	1.09	1 (6%)
10	NAG	Y	1	10,2	14,14,15	0.41	0	17,19,21	0.63	0
10	NAG	Y	2	10	14,14,15	0.35	0	17,19,21	0.75	1 (5%)
10	BMA	Y	3	10	11,11,12	0.76	0	15,15,17	1.13	1 (6%)
10	MAN	Y	4	10	11,11,12	1.37	2 (18%)	15,15,17	1.81	3 (20%)
10	MAN	Y	5	10	11,11,12	0.90	0	15,15,17	0.92	1 (6%)
10	MAN	Y	6	10	11,11,12	0.85	0	15,15,17	1.05	2 (13%)
6	NAG	Z	1	6,2	14,14,15	0.22	0	17,19,21	0.47	0
6	NAG	Z	2	6	14,14,15	0.19	0	17,19,21	0.56	0
6	BMA	Z	3	6	11,11,12	0.68	0	15,15,17	0.74	0
6	NAG	a	1	6,2	14,14,15	0.32	0	17,19,21	0.43	0
6	NAG	a	2	6	14,14,15	0.44	0	17,19,21	1.05	1 (5%)
6	BMA	a	3	6	11,11,12	1.83	4 (36%)	15,15,17	2.25	5 (33%)
9	NAG	b	1	9,2	14,14,15	0.92	1 (7%)	17,19,21	1.25	2 (11%)
9	NAG	b	2	9	14,14,15	0.29	0	17,19,21	0.69	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
4	NAG	I	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	1/6/23/26	0/1/1/1
4	BMA	I	3	4	-	1/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	R	5	7	-	2/2/19/22	1/1/1/1
7	NAG	S	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	S	2	7	-	2/6/23/26	0/1/1/1
7	BMA	S	3	7	-	2/2/19/22	0/1/1/1
7	MAN	S	4	7	-	1/2/19/22	1/1/1/1
7	MAN	S	5	7	-	0/2/19/22	0/1/1/1
7	NAG	T	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	T	2	7	-	0/6/23/26	0/1/1/1
7	BMA	T	3	7	-	0/2/19/22	0/1/1/1
7	MAN	T	4	7	-	1/2/19/22	0/1/1/1
7	MAN	T	5	7	-	0/2/19/22	0/1/1/1
7	NAG	V	1	7,2	-	4/6/23/26	0/1/1/1
7	NAG	V	2	7	-	2/6/23/26	0/1/1/1
7	BMA	V	3	7	-	1/2/19/22	0/1/1/1
7	MAN	V	4	7	-	1/2/19/22	0/1/1/1
7	MAN	V	5	7	-	0/2/19/22	0/1/1/1
9	NAG	W	1	9,2	-	1/6/23/26	0/1/1/1
9	NAG	W	2	9	-	1/6/23/26	0/1/1/1
10	NAG	X	1	10,2	-	3/6/23/26	0/1/1/1
10	NAG	X	2	10	-	2/6/23/26	0/1/1/1
10	BMA	X	3	10	-	1/2/19/22	0/1/1/1
10	MAN	X	4	10	-	1/2/19/22	0/1/1/1
10	MAN	X	5	10	-	0/2/19/22	0/1/1/1
10	MAN	X	6	10	-	1/2/19/22	0/1/1/1
10	NAG	Y	1	10,2	-	3/6/23/26	0/1/1/1
10	NAG	Y	2	10	-	1/6/23/26	0/1/1/1
10	BMA	Y	3	10	-	2/2/19/22	0/1/1/1
10	MAN	Y	4	10	-	0/2/19/22	0/1/1/1
10	MAN	Y	5	10	-	1/2/19/22	0/1/1/1
10	MAN	Y	6	10	-	0/2/19/22	0/1/1/1
6	NAG	Z	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	2/6/23/26	0/1/1/1
6	BMA	Z	3	6	-	0/2/19/22	0/1/1/1
6	NAG	a	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	a	2	6	-	4/6/23/26	0/1/1/1
6	BMA	a	3	6	-	1/2/19/22	0/1/1/1
9	NAG	b	1	9,2	-	2/6/23/26	0/1/1/1
9	NAG	b	2	9	-	0/6/23/26	0/1/1/1

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	1	NAG	O5-C1	-4.76	1.36	1.43
7	M	3	BMA	C4-C5	3.99	1.61	1.53
4	I	1	NAG	O5-C1	-3.97	1.37	1.43
7	S	4	MAN	C1-C2	3.79	1.60	1.52
7	R	3	BMA	C4-C5	3.74	1.60	1.53

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	3	BMA	C1-C2-C3	-5.99	102.30	109.67
8	P	1	NAG	C1-O5-C5	5.49	119.64	112.19
7	S	2	NAG	C3-C4-C5	5.16	119.44	110.24
6	a	3	BMA	C1-C2-C3	-4.97	103.56	109.67
10	X	2	NAG	C1-O5-C5	4.96	118.92	112.19

There are no chirality outliers.

5 of 90 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	b	1	NAG	C1-C2-N2-C7
7	M	3	BMA	C4-C5-C6-O6
7	M	3	BMA	O5-C5-C6-O6
7	V	1	NAG	C4-C5-C6-O6
7	M	4	MAN	C4-C5-C6-O6

5 of 7 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	R	4	MAN	C1-C2-C3-C4-C5-O5
7	R	5	MAN	C1-C2-C3-C4-C5-O5
7	S	4	MAN	C1-C2-C3-C4-C5-O5
7	M	5	MAN	C1-C2-C3-C4-C5-O5
7	L	4	MAN	C1-C2-C3-C4-C5-O5

26 monomers are involved in 21 short contacts:

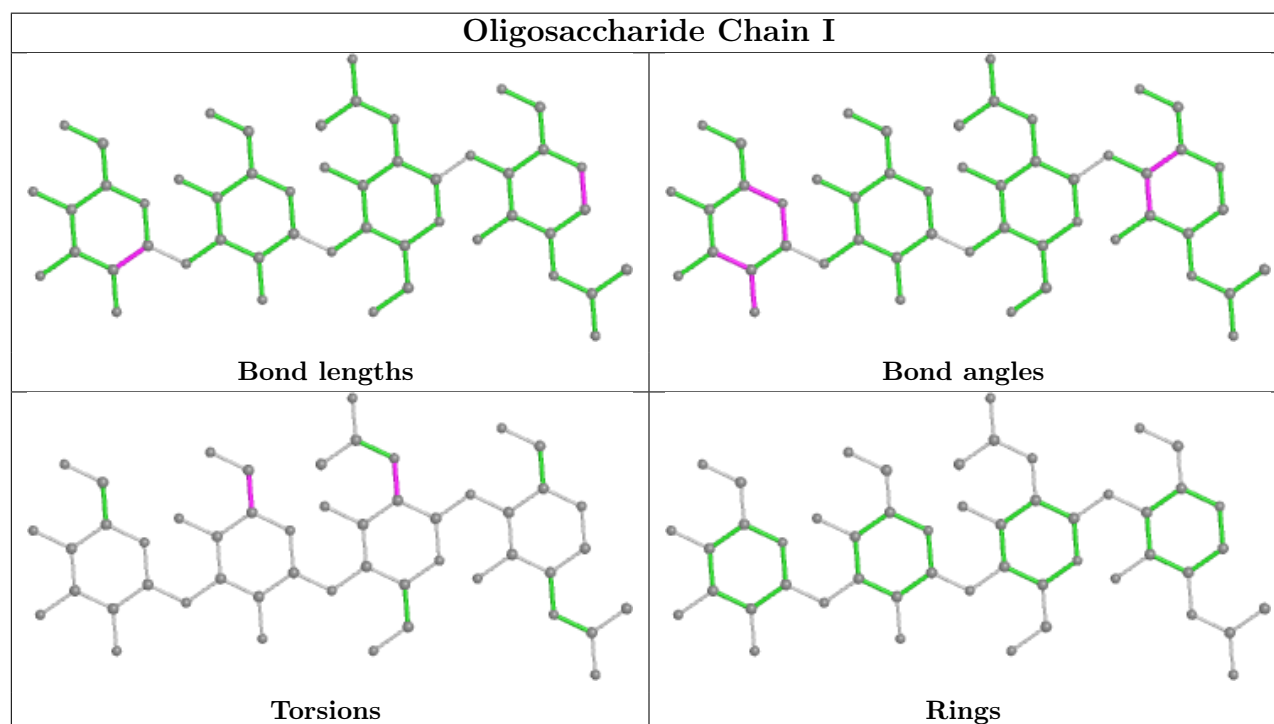
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	2	NAG	4	0
10	X	6	MAN	1	0
8	P	3	BMA	1	0
7	S	1	NAG	1	0
10	X	3	BMA	1	0

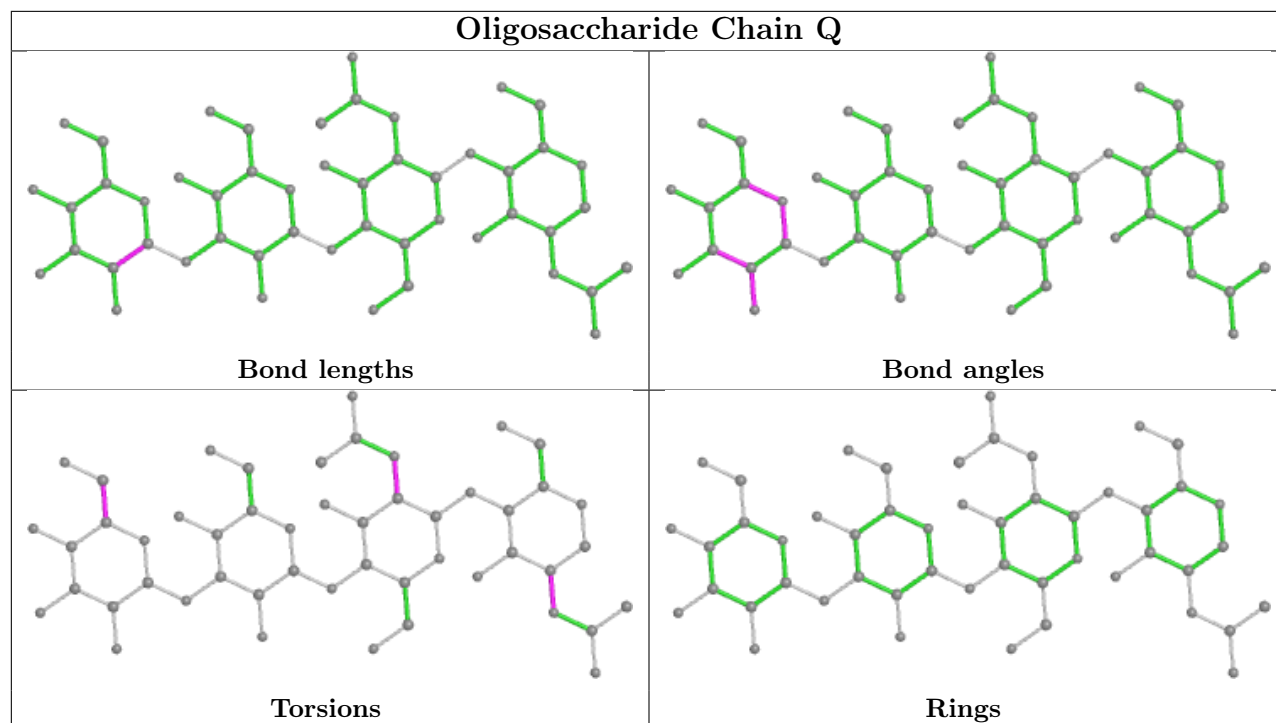
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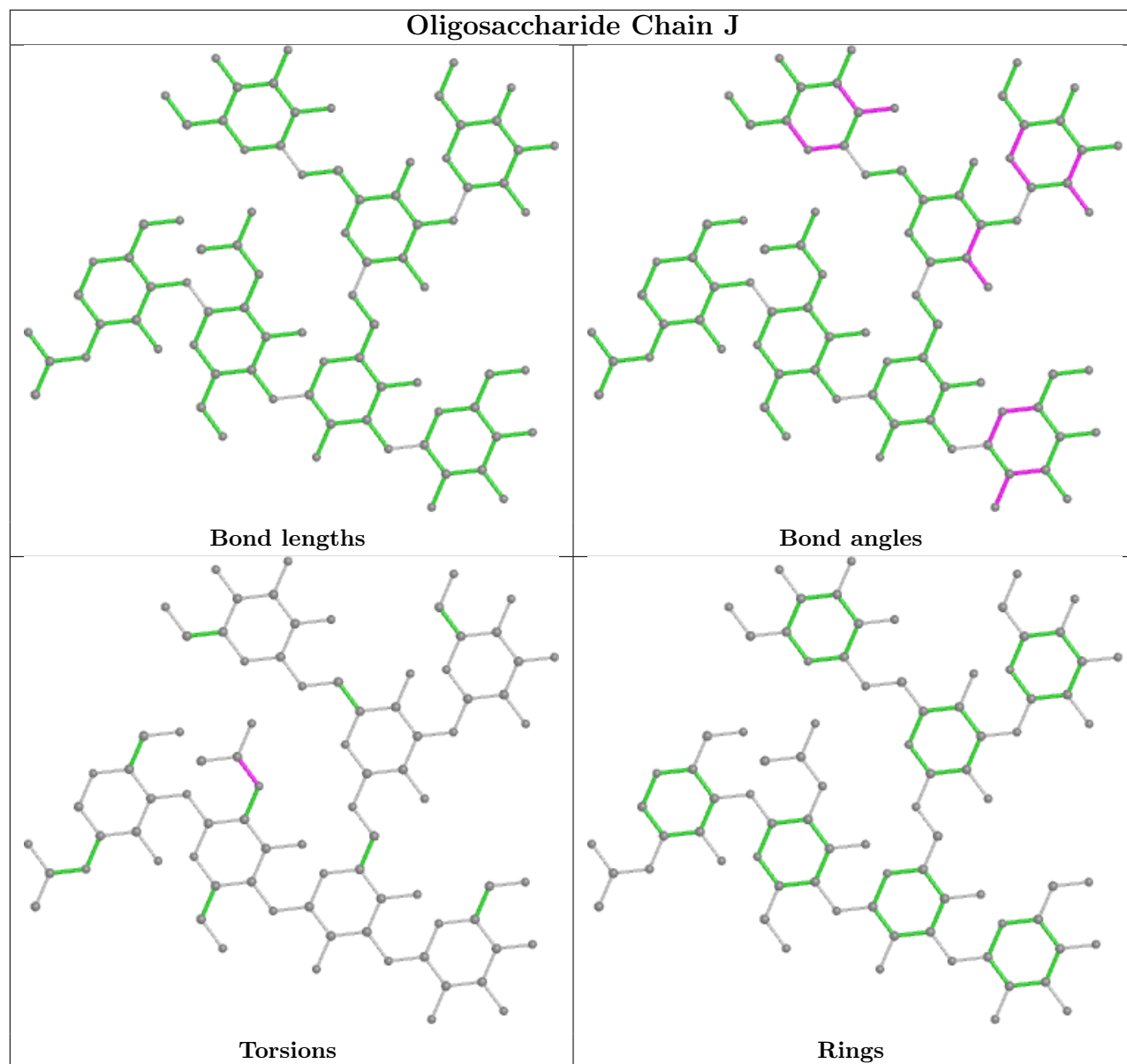
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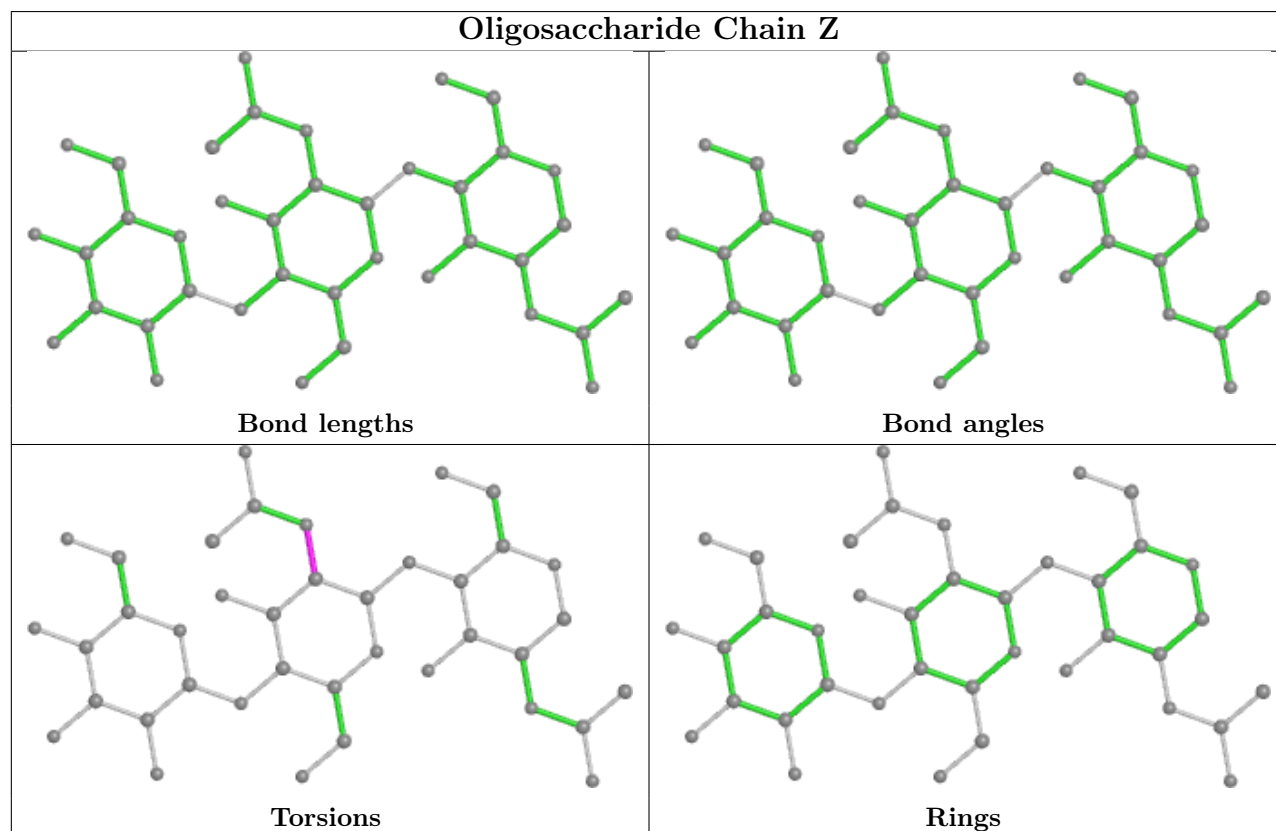
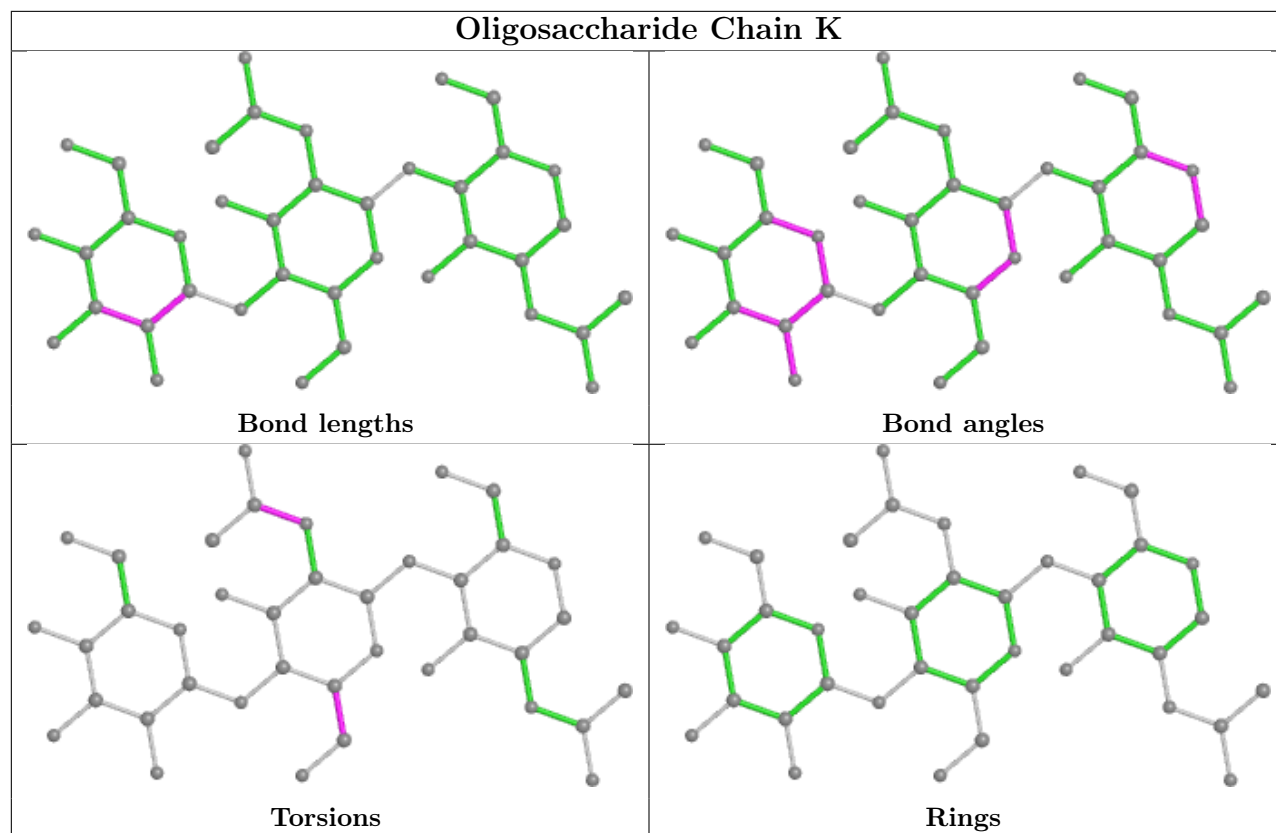
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	X	4	MAN	1	0
7	L	3	BMA	2	0
7	V	1	NAG	1	0
7	V	5	MAN	1	0
7	V	3	BMA	1	0
10	X	5	MAN	1	0
7	S	4	MAN	1	0
10	X	2	NAG	1	0
7	R	5	MAN	1	0
7	R	3	BMA	1	0
9	O	2	NAG	1	0
8	P	1	NAG	1	0
9	O	1	NAG	2	0
10	Y	2	NAG	1	0
7	L	5	MAN	1	0
7	S	3	BMA	1	0
7	T	1	NAG	1	0
7	V	2	NAG	1	0
7	L	4	MAN	1	0
8	P	4	MAN	1	0
7	T	2	NAG	1	0

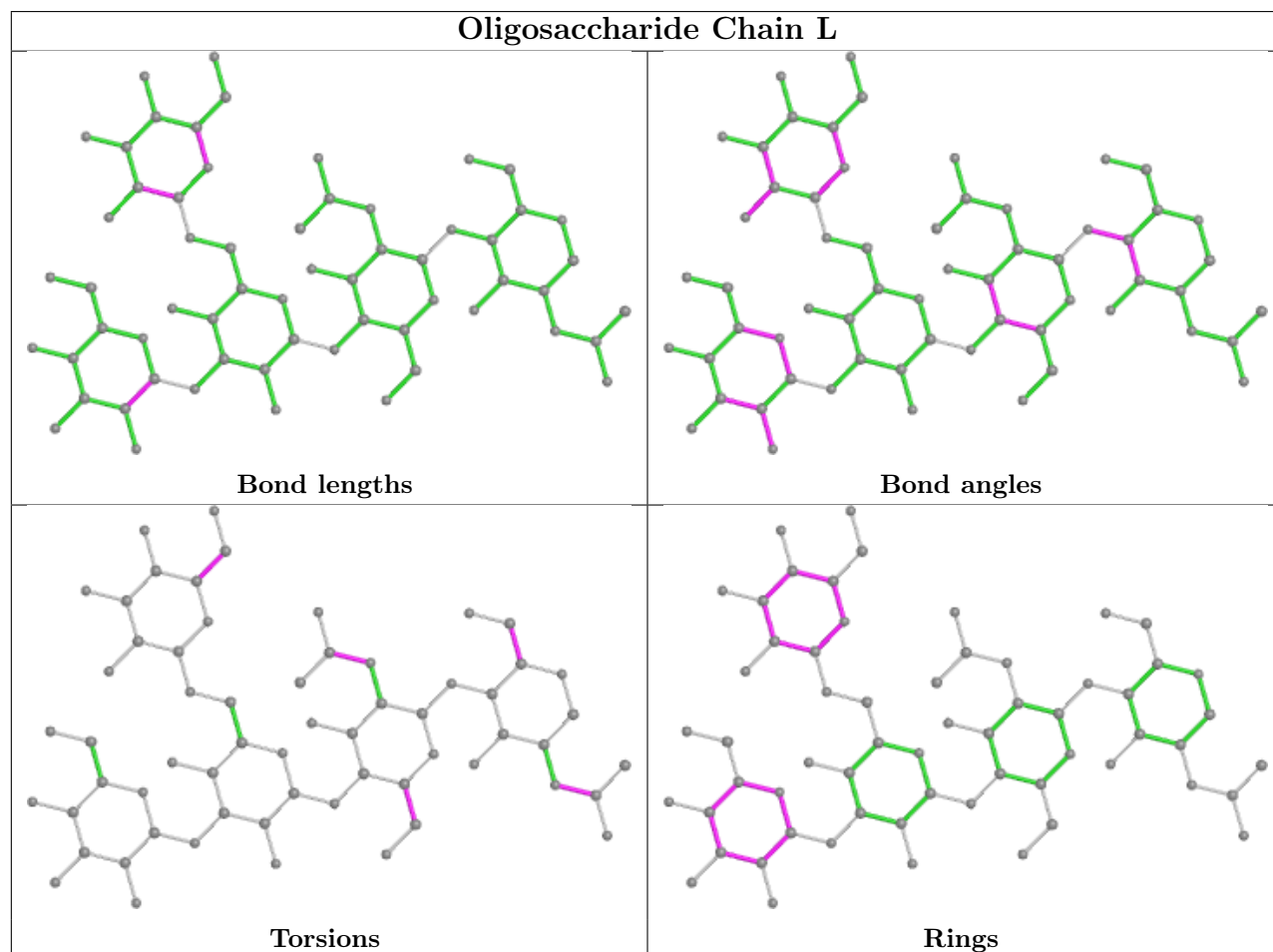
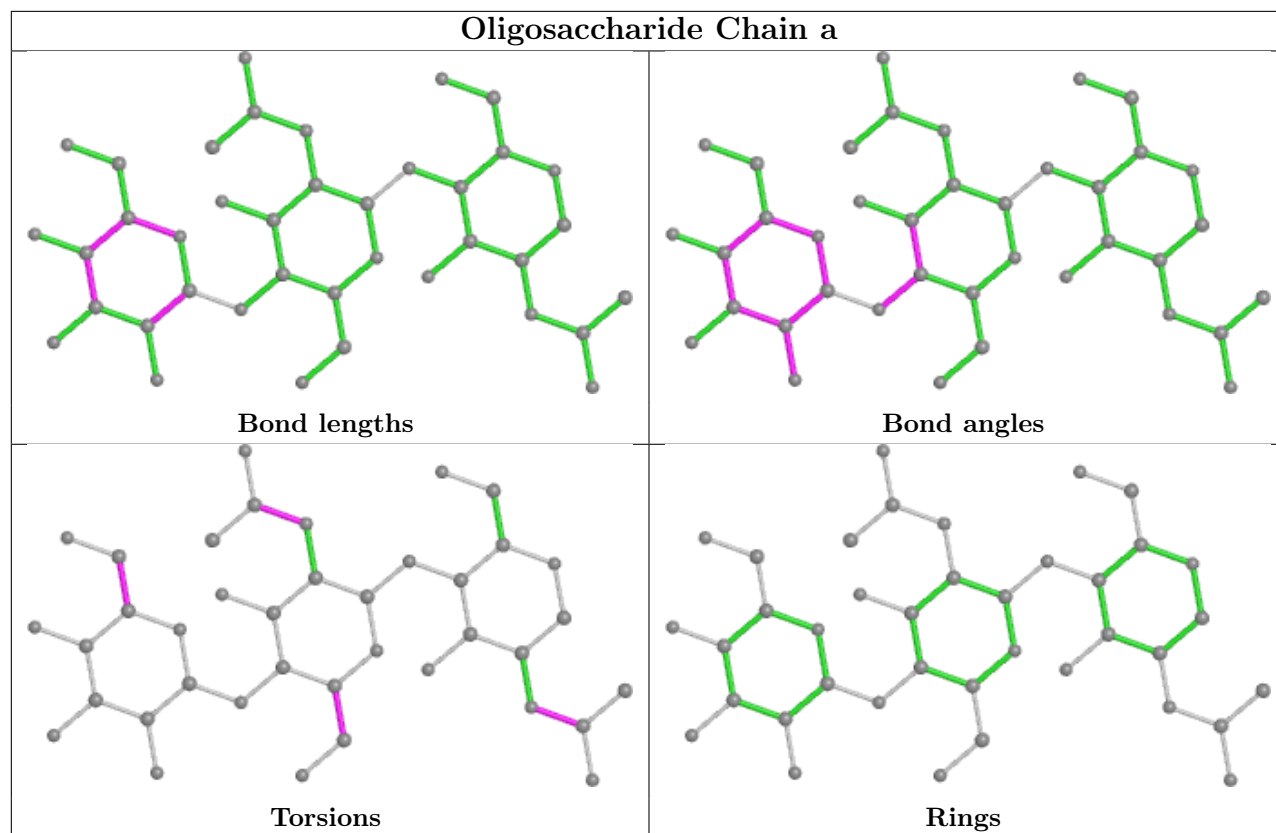
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

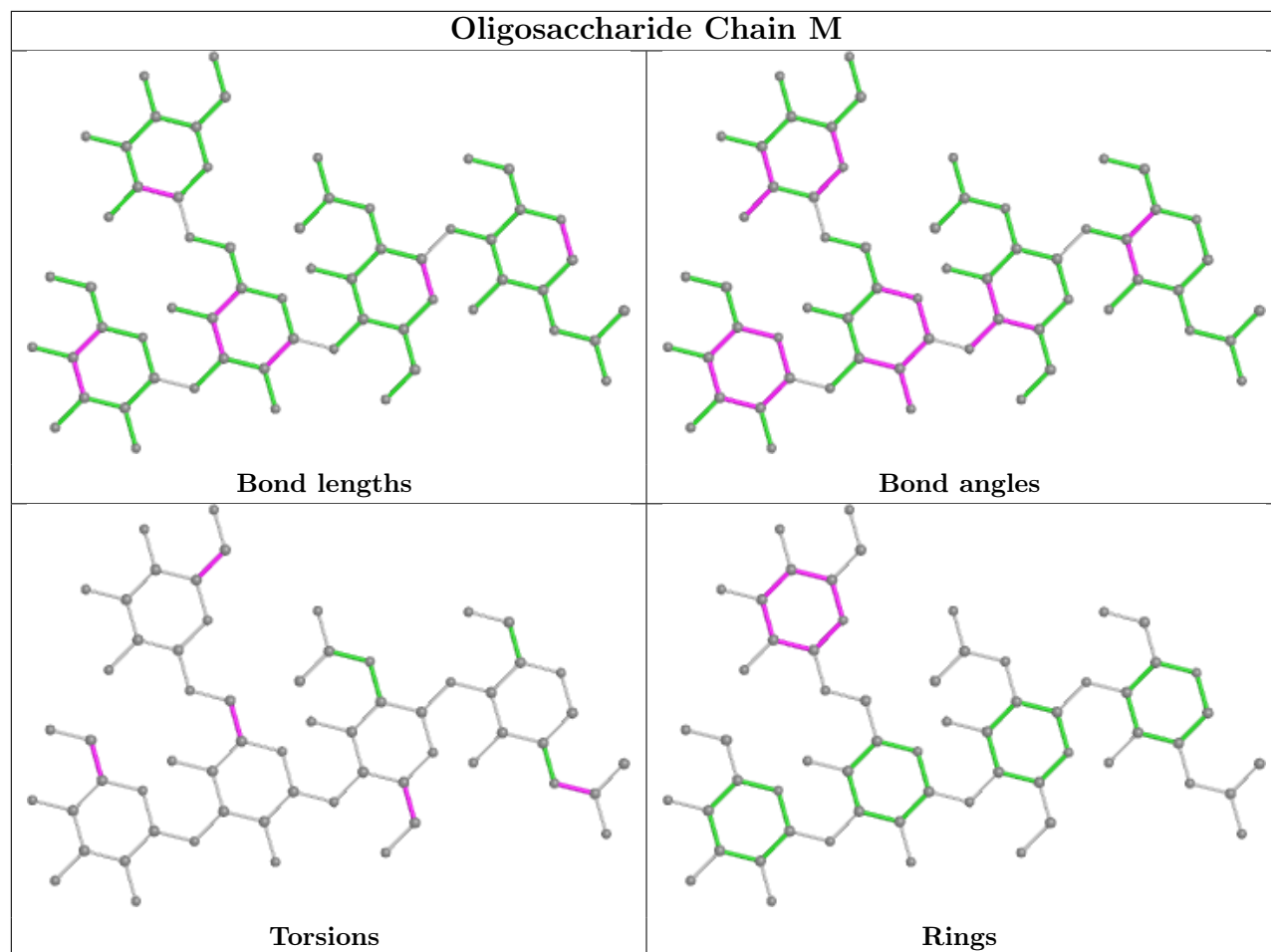


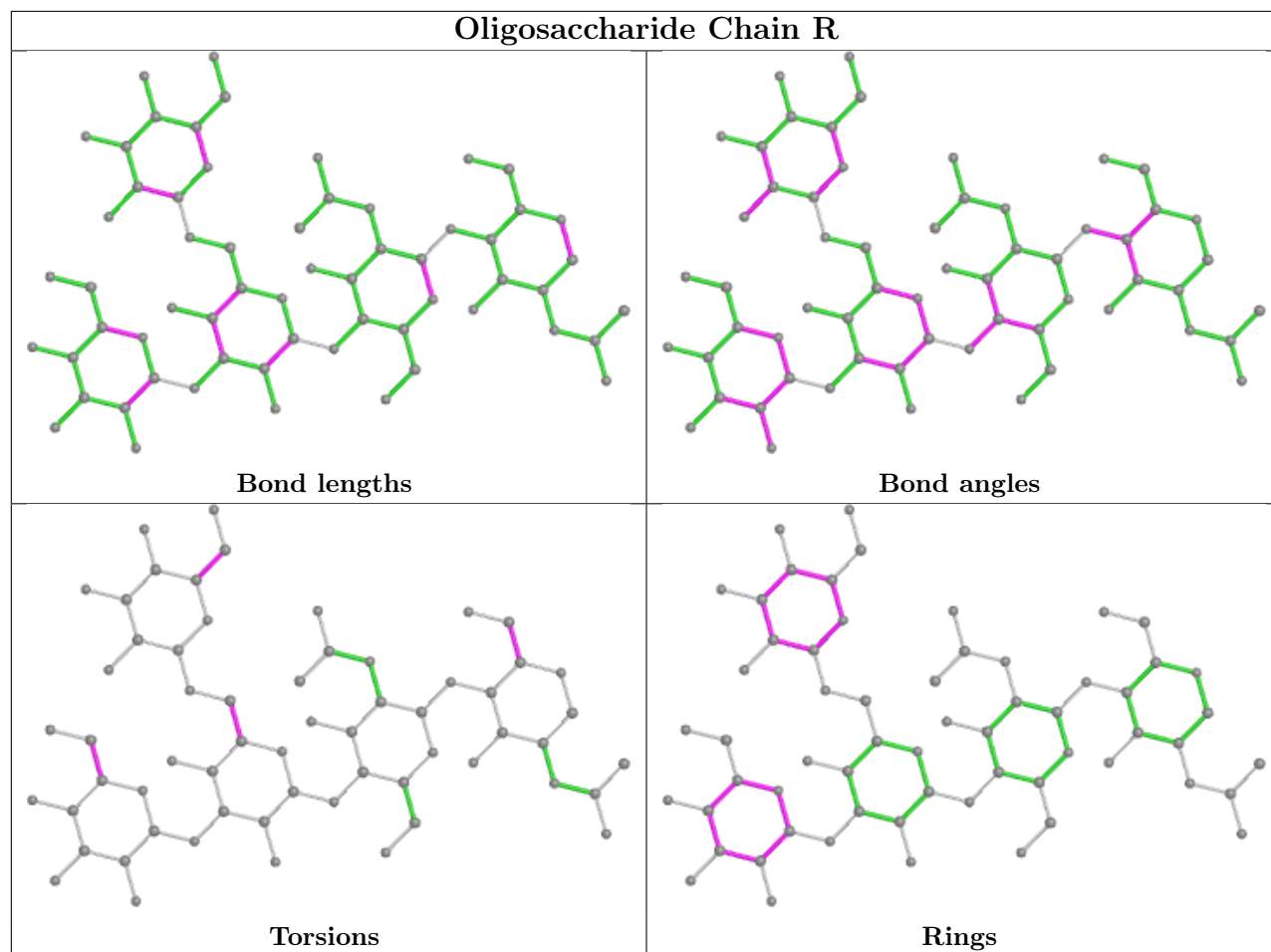


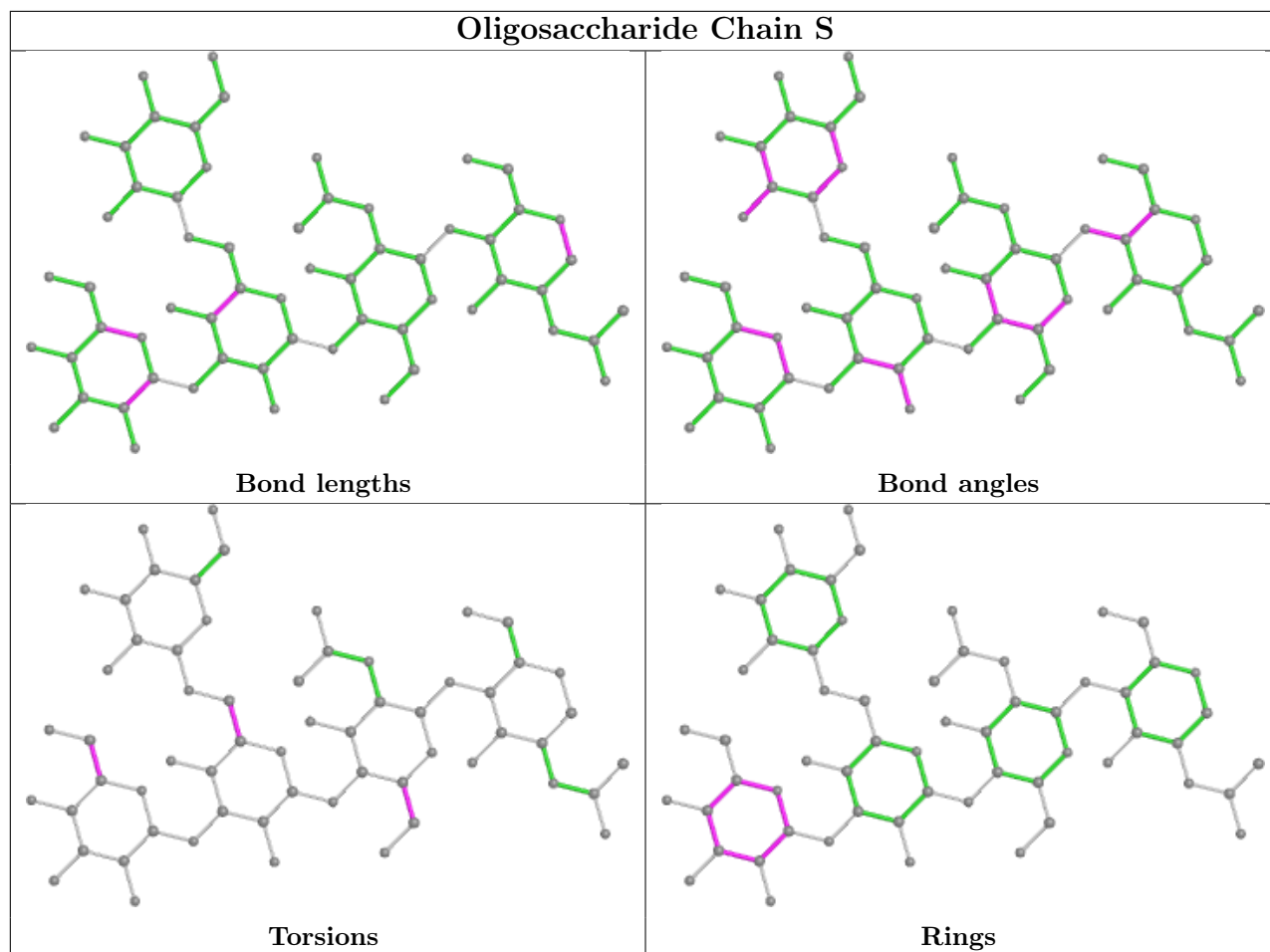


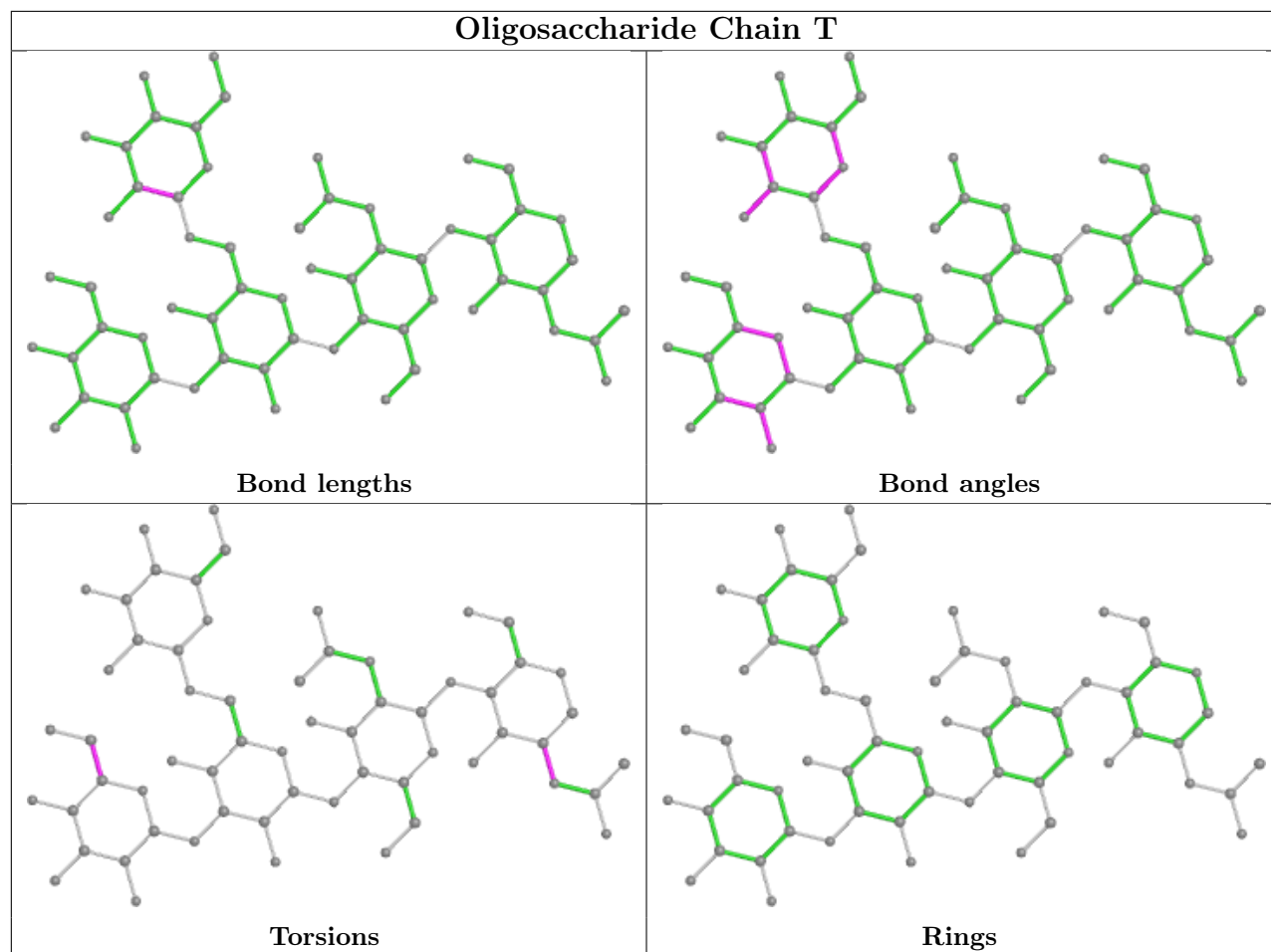


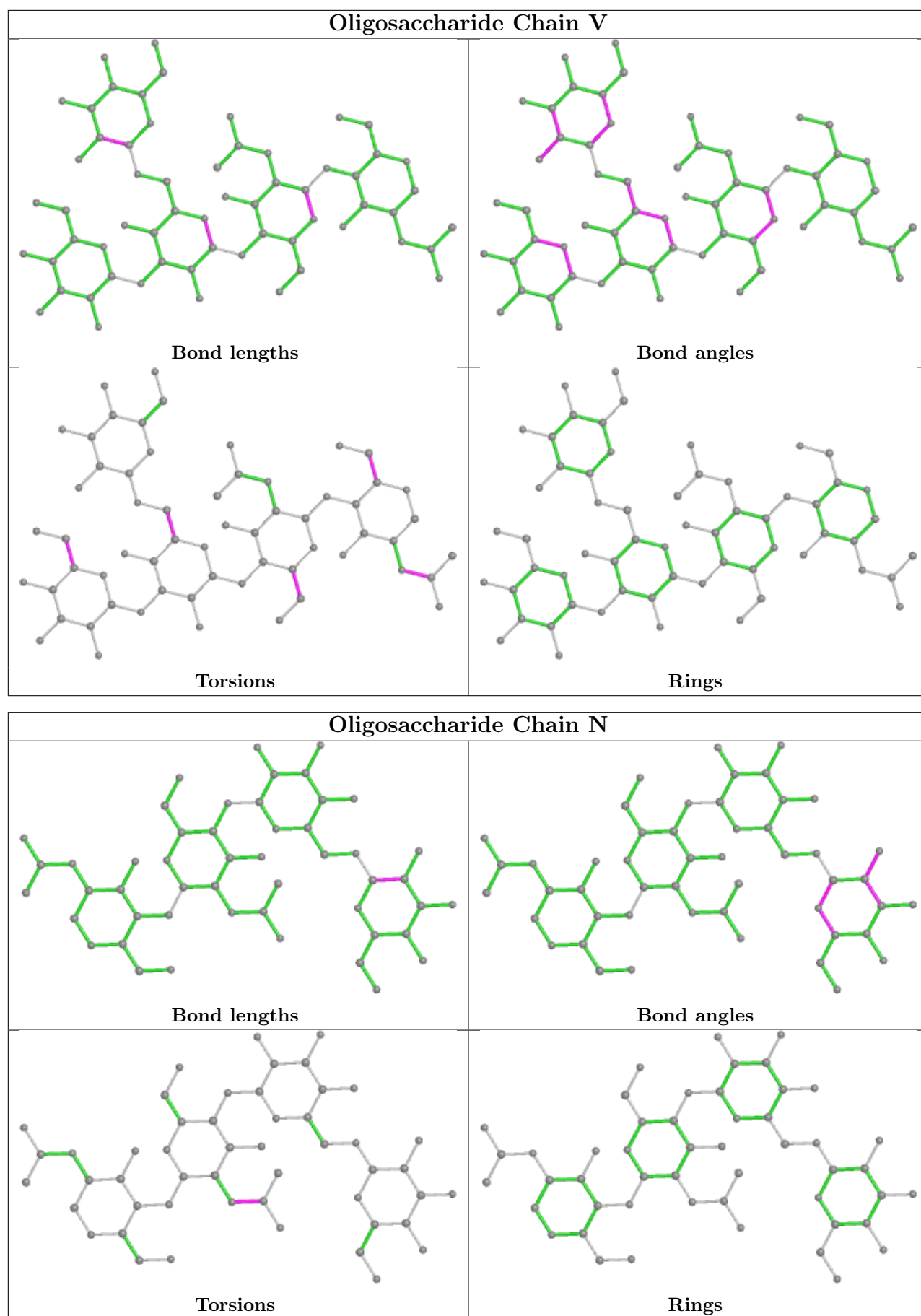


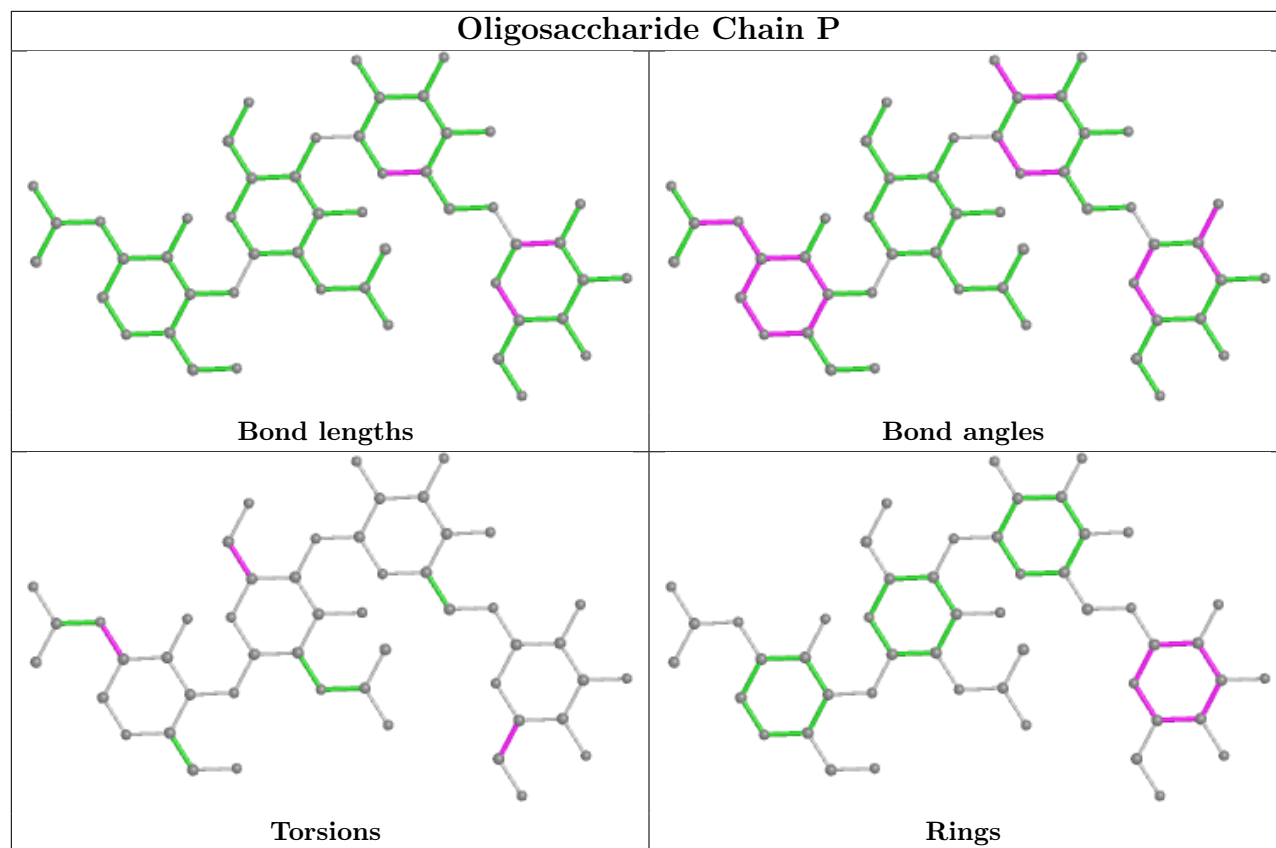


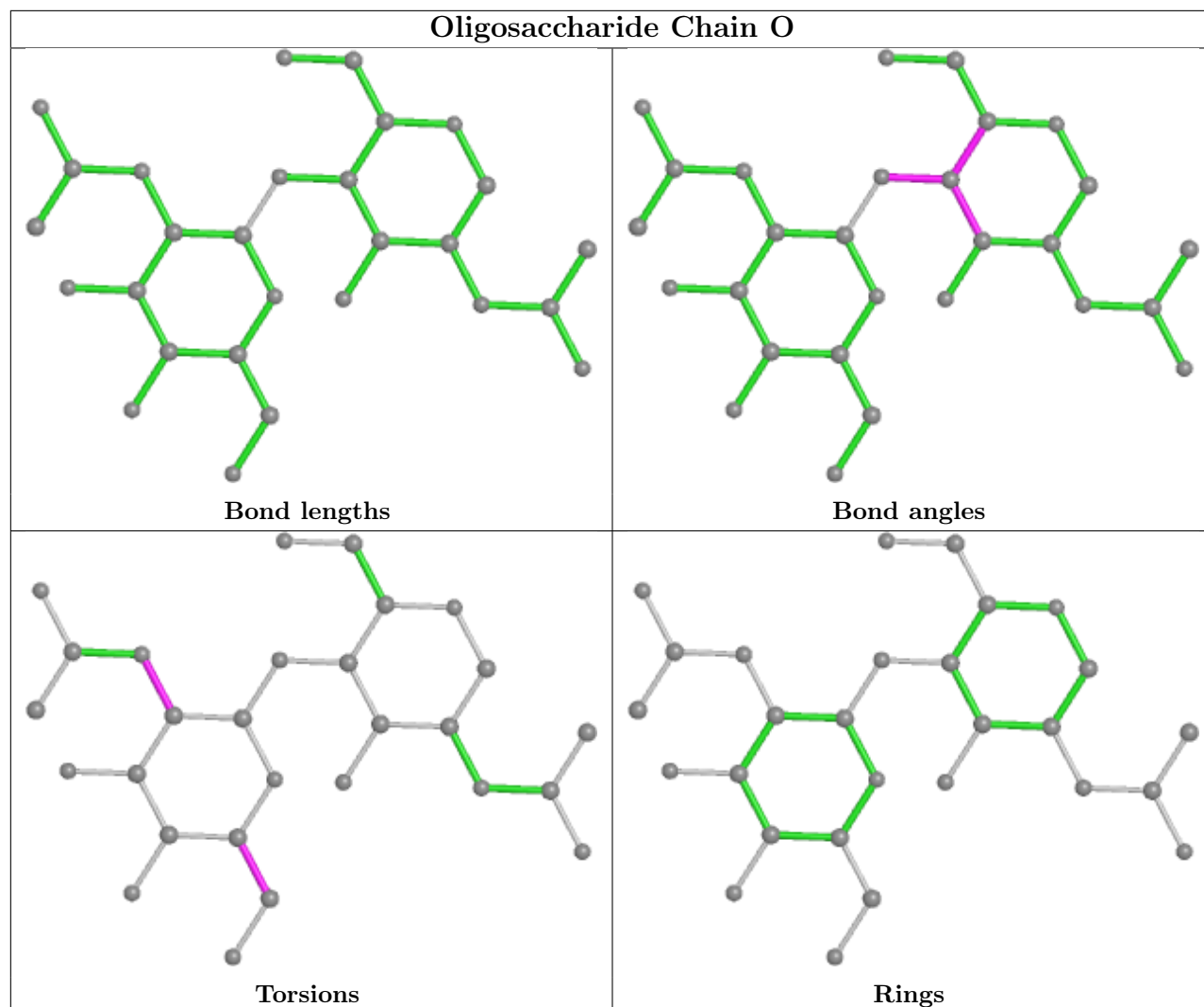


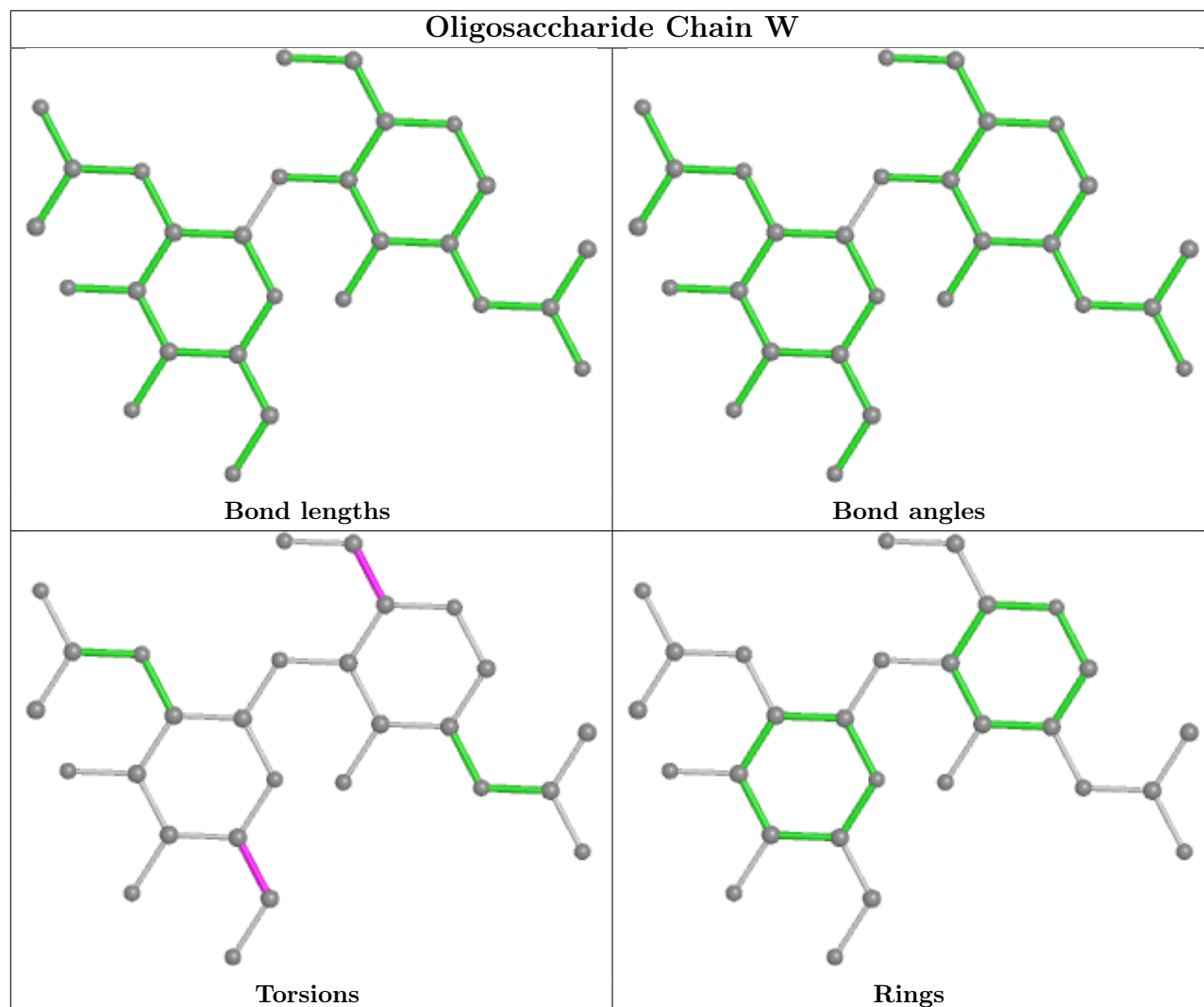


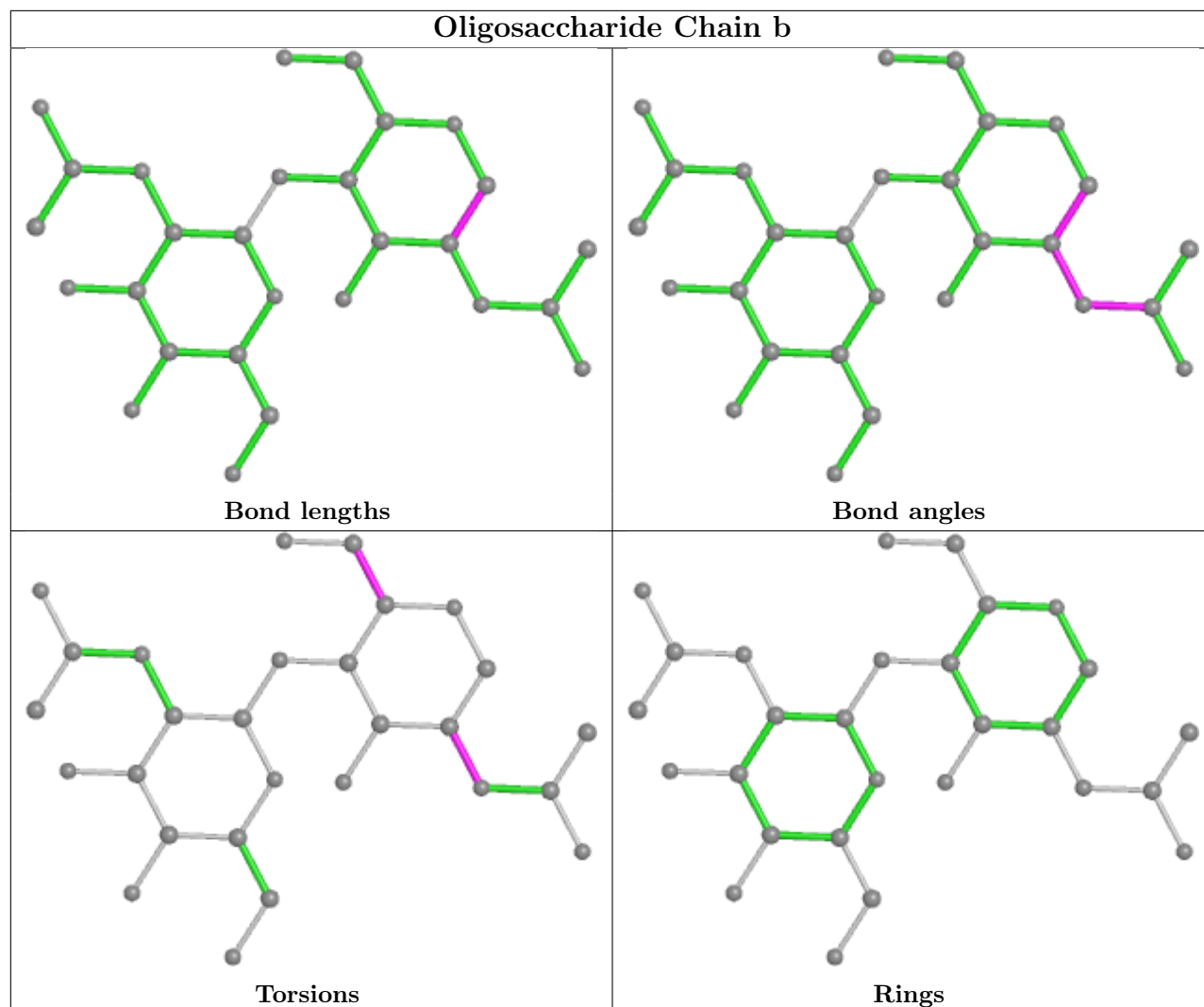


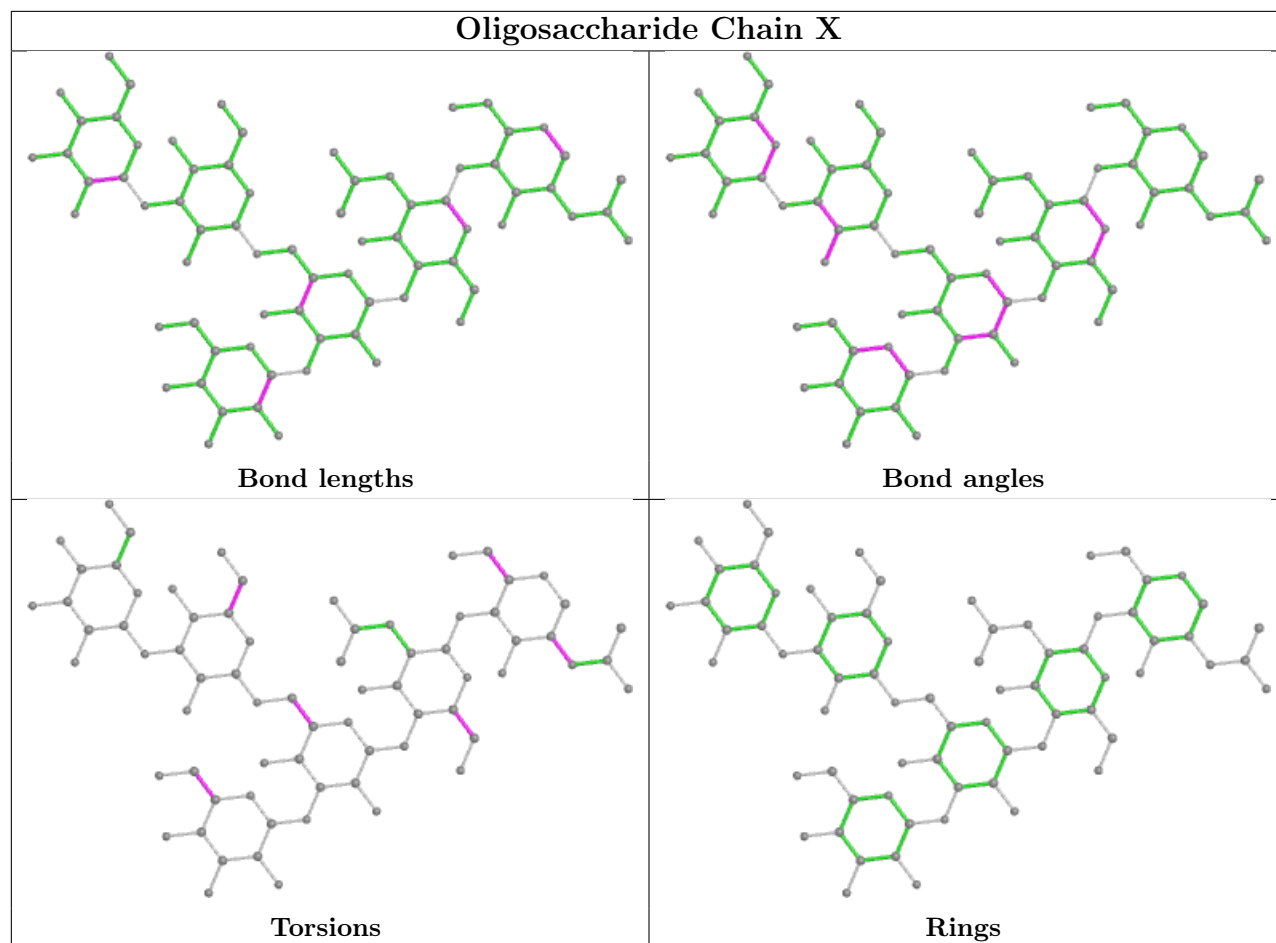


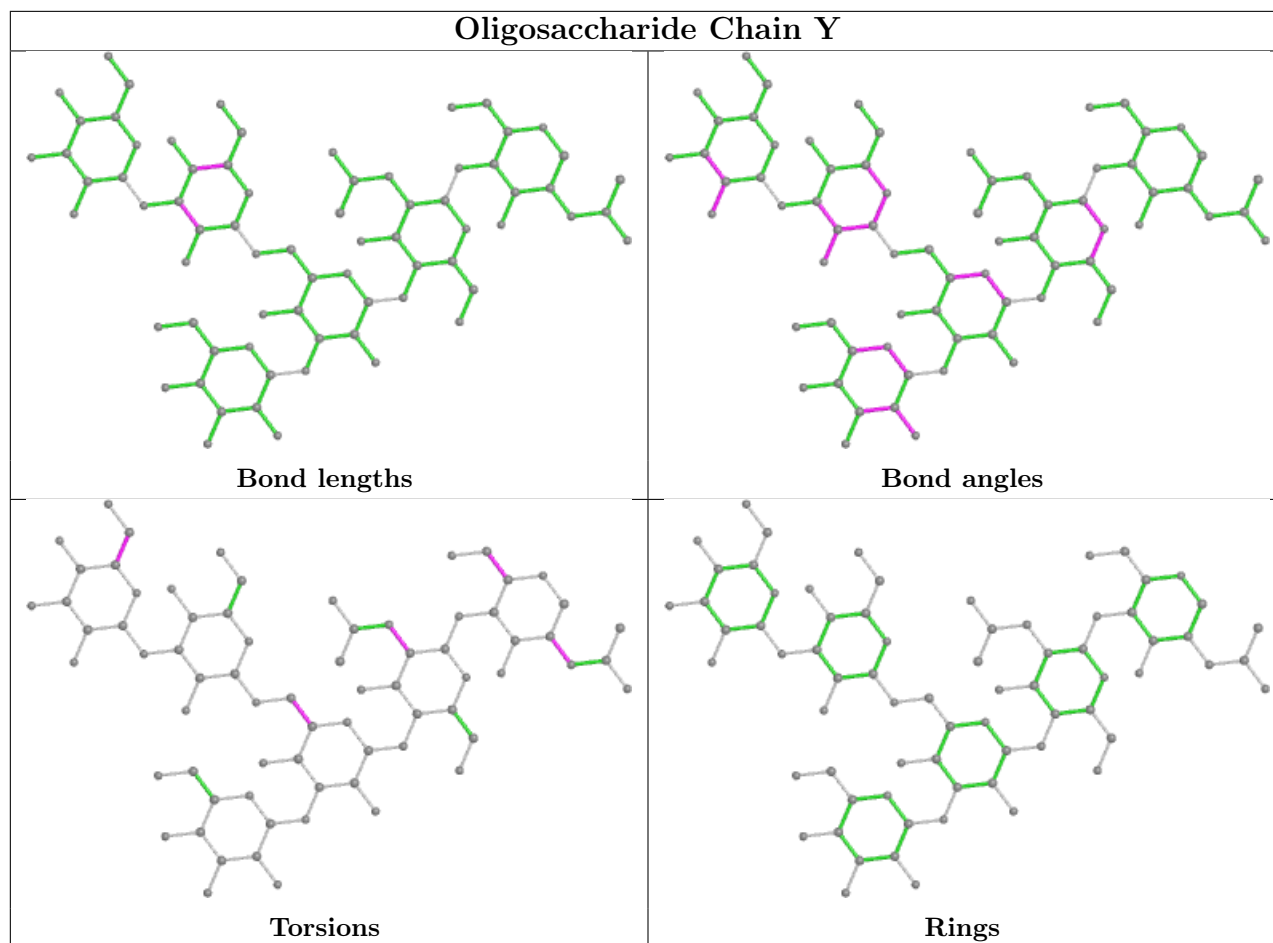












5.6 Ligand geometry [i](#)

9 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
11	NAG	B	603	2	14,14,15	0.95	1 (7%)	17,19,21	0.93	1 (5%)
11	NAG	C	604	2	14,14,15	1.55	1 (7%)	17,19,21	1.72	1 (5%)
11	NAG	A	601	2	14,14,15	0.48	0	17,19,21	1.31	1 (5%)
11	NAG	C	602	2	14,14,15	0.39	0	17,19,21	1.13	2 (11%)
11	NAG	B	602	2	14,14,15	0.48	0	17,19,21	0.40	0
11	NAG	B	601	2	14,14,15	0.36	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	C	601	2	14,14,15	0.27	0	17,19,21	0.42	0
11	NAG	A	602	2	14,14,15	0.51	0	17,19,21	0.73	1 (5%)
11	NAG	C	603	2	14,14,15	0.45	0	17,19,21	0.48	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
11	NAG	B	603	2	-	2/6/23/26	0/1/1/1
11	NAG	C	604	2	-	2/6/23/26	0/1/1/1
11	NAG	A	601	2	-	1/6/23/26	0/1/1/1
11	NAG	C	602	2	-	2/6/23/26	0/1/1/1
11	NAG	B	602	2	-	3/6/23/26	0/1/1/1
11	NAG	B	601	2	-	0/6/23/26	0/1/1/1
11	NAG	C	601	2	-	1/6/23/26	0/1/1/1
11	NAG	A	602	2	-	2/6/23/26	0/1/1/1
11	NAG	C	603	2	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	604	NAG	O5-C1	5.45	1.52	1.43
11	B	603	NAG	O5-C1	-3.21	1.38	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	604	NAG	C1-O5-C5	6.54	121.05	112.19
11	A	601	NAG	C1-O5-C5	4.23	117.92	112.19
11	C	602	NAG	C2-N2-C7	3.18	127.43	122.90
11	B	603	NAG	C3-C4-C5	2.32	114.38	110.24
11	A	602	NAG	C1-O5-C5	2.25	115.23	112.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	602	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
11	B	602	NAG	C8-C7-N2-C2
11	B	602	NAG	O7-C7-N2-C2
11	B	603	NAG	C8-C7-N2-C2
11	B	603	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	603	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	D	216/216 (100%)	-0.40	0 100 100	76, 104, 131, 164	0
1	E	216/216 (100%)	-0.26	0 100 100	85, 119, 145, 201	0
1	G	216/216 (100%)	-0.37	0 100 100	83, 122, 157, 177	0
2	A	489/514 (95%)	-0.39	0 100 100	73, 106, 137, 169	3 (0%)
2	B	486/514 (94%)	-0.39	0 100 100	72, 110, 140, 154	1 (0%)
2	C	490/514 (95%)	-0.30	0 100 100	76, 112, 139, 171	4 (0%)
3	F	230/240 (95%)	-0.41	2 (0%) 84 77	82, 102, 152, 192	0
3	H	239/240 (99%)	-0.38	0 100 100	79, 105, 151, 197	0
3	U	230/240 (95%)	-0.31	4 (1%) 70 60	77, 100, 136, 212	0
All	All	2812/2910 (96%)	-0.36	6 (0%) 95 93	72, 109, 143, 212	8 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	U	146	SER	4.9
3	U	145	THR	4.2
3	U	147	GLY	3.6
3	F	144	SER	2.8
3	U	144	SER	2.6

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MAN	M	5	11/12	0.30	0.49	152,181,188,196	0
7	BMA	T	3	11/12	0.42	0.33	211,219,226,228	0
9	NAG	W	2	14/15	0.42	0.86	144,177,189,194	0
7	MAN	T	4	11/12	0.45	0.62	218,230,236,238	0
7	MAN	T	5	11/12	0.47	0.31	168,200,210,212	0
10	MAN	X	5	11/12	0.55	0.39	143,174,183,184	0
7	BMA	R	3	11/12	0.56	0.62	157,179,198,200	0
7	MAN	R	5	11/12	0.57	0.57	172,186,199,202	0
10	MAN	Y	5	11/12	0.58	0.41	192,201,209,214	0
10	MAN	Y	6	11/12	0.59	0.31	173,191,197,198	0
6	NAG	a	1	14/15	0.60	0.56	157,183,203,206	0
7	MAN	V	4	11/12	0.60	0.31	120,145,157,159	0
7	BMA	S	3	11/12	0.61	0.26	169,181,185,187	0
7	MAN	S	4	11/12	0.61	0.30	143,180,186,188	0
9	NAG	b	2	14/15	0.64	0.57	199,213,218,219	0
9	NAG	W	1	14/15	0.64	0.56	139,157,179,188	0
7	MAN	R	4	11/12	0.65	0.50	137,161,177,181	0
7	NAG	M	1	14/15	0.65	0.44	131,147,165,179	0
6	BMA	a	3	11/12	0.66	0.29	154,195,205,206	0
4	MAN	I	4	11/12	0.66	0.24	149,178,192,196	0
10	MAN	X	4	11/12	0.67	0.30	166,179,187,189	0
7	MAN	V	5	11/12	0.67	0.28	144,164,175,182	0
8	BMA	P	3	11/12	0.69	0.25	166,176,184,193	0
9	NAG	O	2	14/15	0.69	0.45	154,182,192,194	0
7	NAG	R	2	14/15	0.69	0.58	183,198,202,202	0
8	MAN	P	4	11/12	0.70	0.31	150,180,191,193	0
10	MAN	Y	4	11/12	0.70	0.25	180,201,209,211	0
6	NAG	a	2	14/15	0.72	0.53	199,204,209,214	0
8	MAN	N	4	11/12	0.73	0.58	171,191,195,195	0
4	MAN	Q	4	11/12	0.73	0.48	170,187,192,192	0
8	BMA	N	3	11/12	0.73	0.48	168,178,187,187	0
4	BMA	Q	3	11/12	0.75	0.34	168,174,185,194	0
7	NAG	R	1	14/15	0.75	0.30	161,181,187,194	0
9	NAG	O	1	14/15	0.75	0.40	149,172,182,192	0
7	NAG	M	2	14/15	0.75	0.33	152,181,195,200	0
7	NAG	S	2	14/15	0.76	0.31	134,152,159,162	0
5	MAN	J	7	11/12	0.76	0.38	139,160,169,169	0
9	NAG	b	1	14/15	0.76	0.54	177,191,209,214	0
7	NAG	S	1	14/15	0.77	0.37	102,131,146,152	0
7	MAN	L	5	11/12	0.77	0.21	138,165,171,171	0

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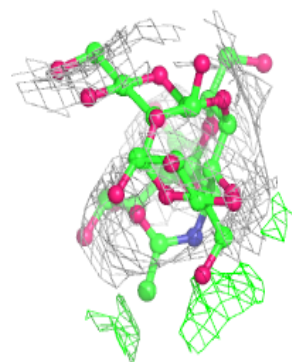
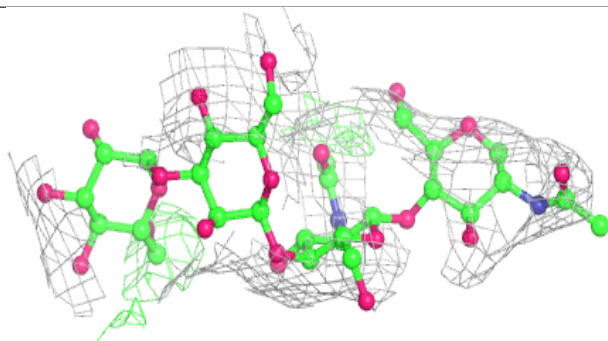
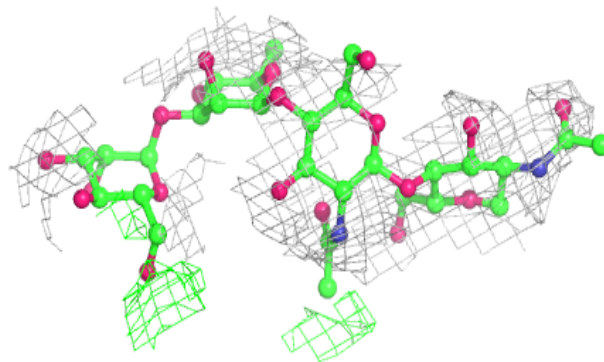
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	NAG	P	2	14/15	0.77	0.29	124,140,155,170	0
7	BMA	M	3	11/12	0.77	0.20	177,182,189,191	0
8	NAG	P	1	14/15	0.78	0.38	108,133,141,142	0
7	MAN	L	4	11/12	0.78	0.26	164,174,181,182	0
7	BMA	L	3	11/12	0.78	0.17	155,165,173,176	0
6	NAG	K	2	14/15	0.79	0.37	111,155,163,167	0
7	MAN	M	4	11/12	0.79	0.31	162,186,190,192	0
10	BMA	Y	3	11/12	0.80	0.16	174,182,191,194	0
10	BMA	X	3	11/12	0.80	0.19	171,176,181,183	0
5	MAN	J	5	11/12	0.80	0.42	162,171,182,186	0
4	BMA	I	3	11/12	0.80	0.29	187,196,202,203	0
7	NAG	V	2	14/15	0.81	0.27	138,152,160,172	0
8	NAG	N	2	14/15	0.81	0.34	149,164,177,177	0
7	MAN	S	5	11/12	0.81	0.29	151,166,173,177	0
6	NAG	K	1	14/15	0.82	0.26	120,137,160,171	0
7	NAG	T	2	14/15	0.82	0.31	170,186,201,211	0
4	NAG	I	1	14/15	0.83	0.33	126,148,165,170	0
6	BMA	K	3	11/12	0.83	0.25	131,154,164,170	0
6	BMA	Z	3	11/12	0.84	0.41	156,168,174,177	0
10	MAN	X	6	11/12	0.84	0.26	166,177,181,182	0
7	NAG	V	1	14/15	0.84	0.20	125,143,159,160	0
5	NAG	J	1	14/15	0.85	0.28	132,140,158,161	0
10	NAG	X	2	14/15	0.85	0.21	119,160,176,177	0
10	NAG	X	1	14/15	0.86	0.22	105,131,155,168	0
4	NAG	Q	1	14/15	0.86	0.22	110,114,122,135	0
8	NAG	N	1	14/15	0.87	0.20	102,117,133,143	0
5	NAG	J	2	14/15	0.87	0.36	147,156,160,163	0
7	NAG	L	1	14/15	0.87	0.28	107,121,132,149	0
7	BMA	V	3	11/12	0.88	0.25	147,158,163,167	0
7	NAG	L	2	14/15	0.88	0.29	140,150,173,178	0
7	NAG	T	1	14/15	0.88	0.31	122,162,176,180	0
10	NAG	Y	2	14/15	0.89	0.22	146,158,169,175	0
4	NAG	I	2	14/15	0.89	0.26	164,179,190,196	0
5	MAN	J	6	11/12	0.89	0.18	111,143,149,157	0
5	MAN	J	4	11/12	0.89	0.27	142,155,168,175	0
10	NAG	Y	1	14/15	0.89	0.23	114,125,140,159	0
4	NAG	Q	2	14/15	0.90	0.18	135,154,166,169	0
6	NAG	Z	2	14/15	0.90	0.27	127,136,155,162	0
6	NAG	Z	1	14/15	0.92	0.19	93,113,125,132	0
5	BMA	J	3	11/12	0.92	0.22	146,151,155,157	0

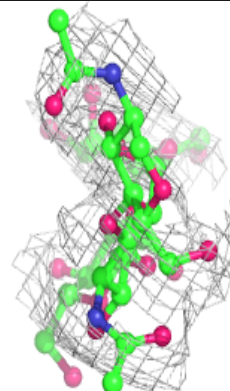
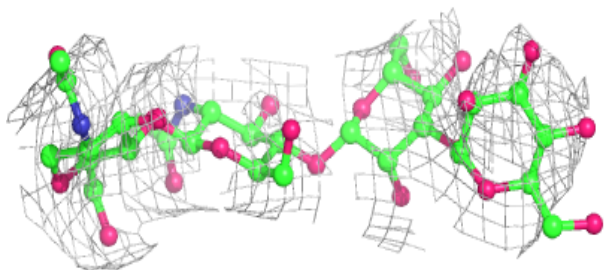
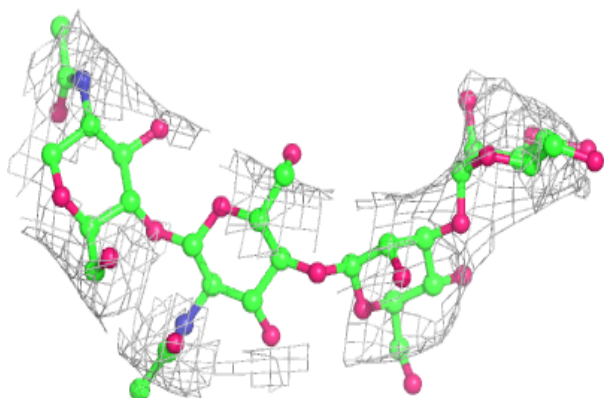
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

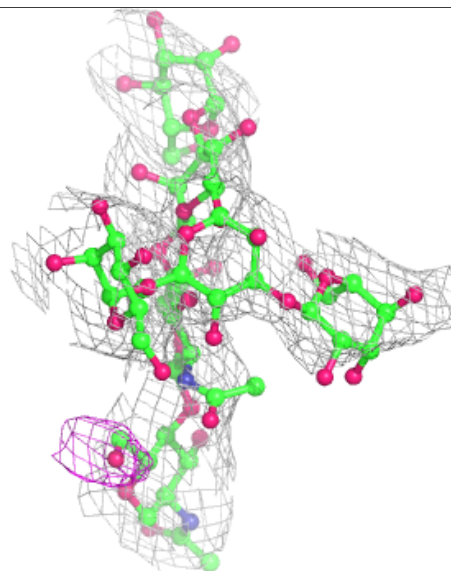
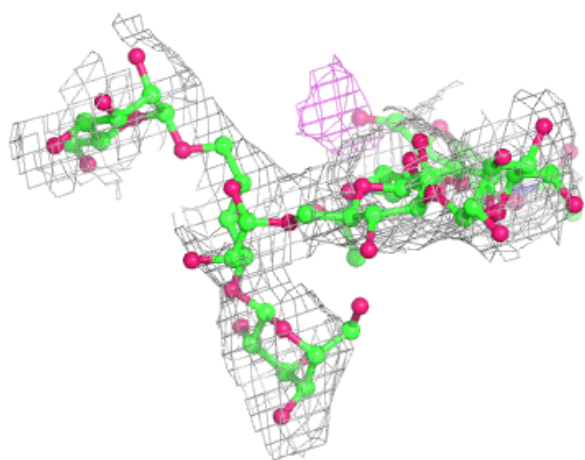
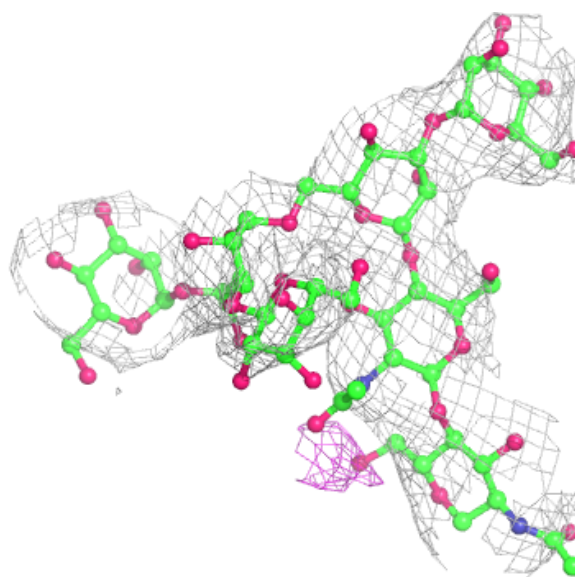
**Electron density around Chain Q:**

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



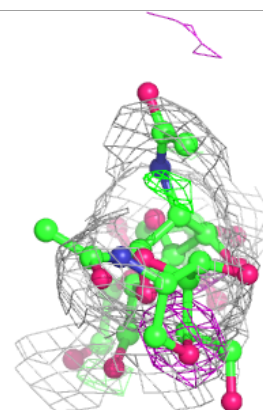
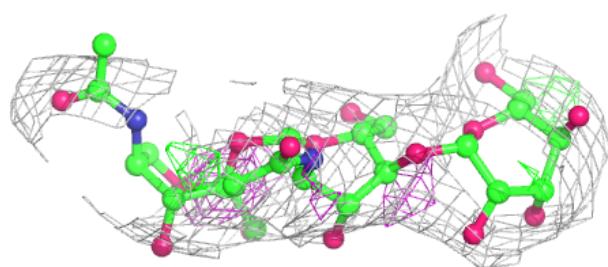
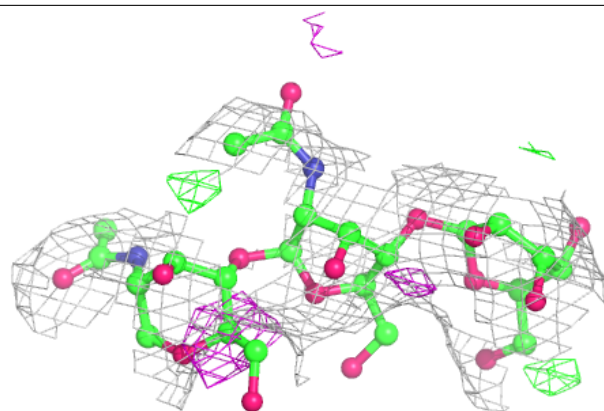
Electron density around Chain J:

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

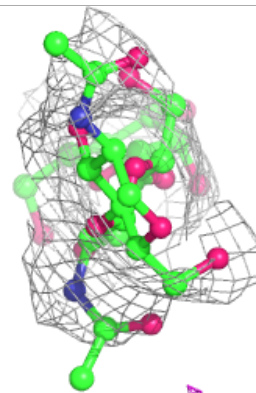
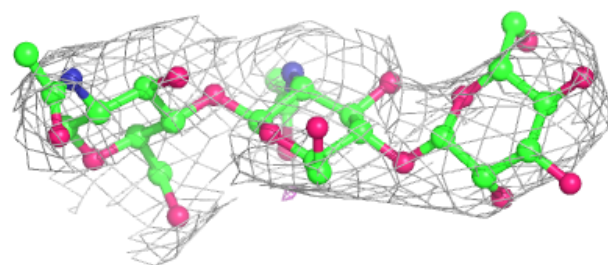
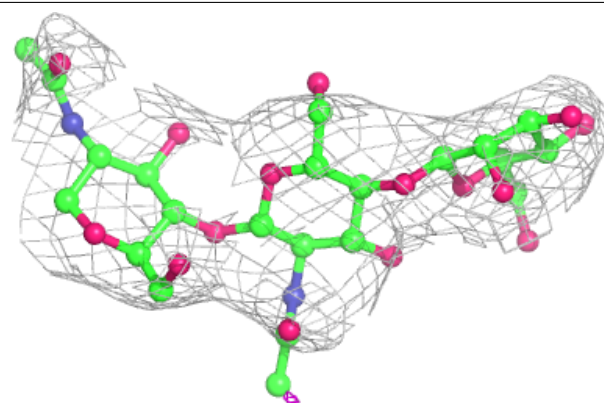


Electron density around Chain K:

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

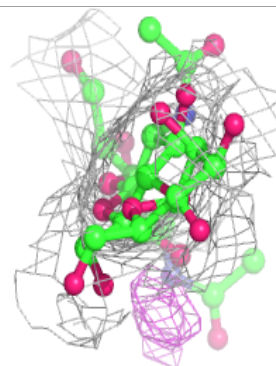
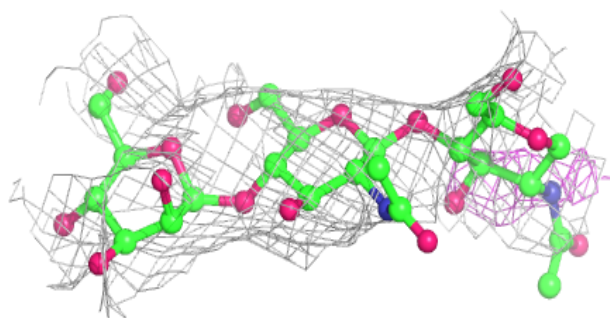
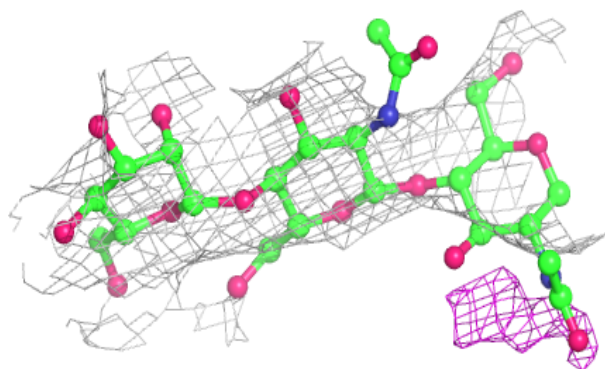
**Electron density around Chain Z:**

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

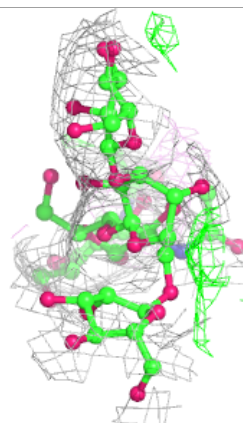
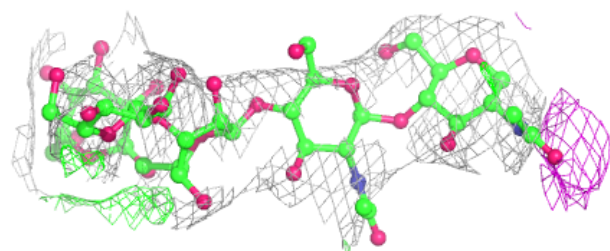
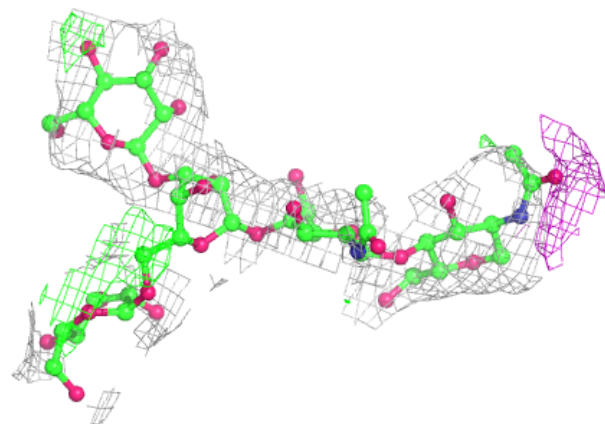


Electron density around Chain a:

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

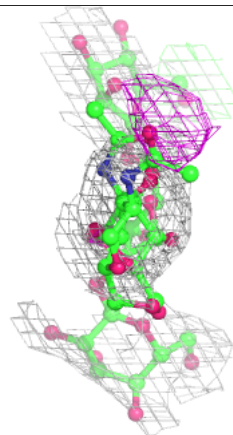
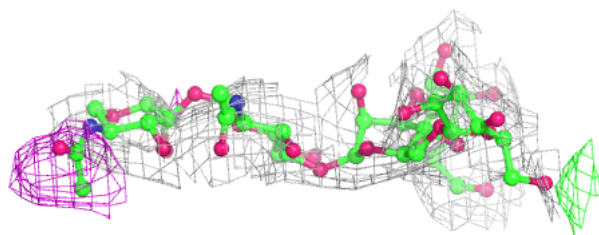
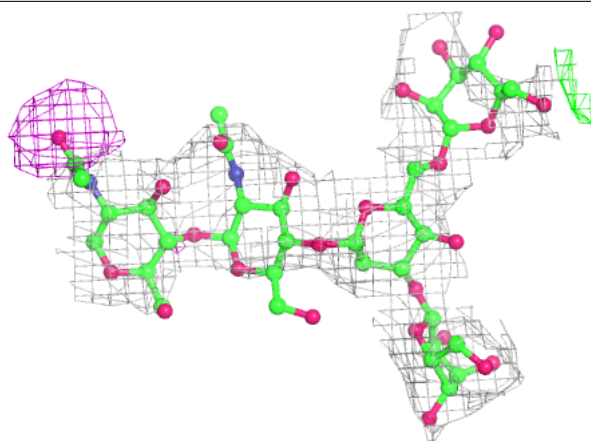
**Electron density around Chain L:**

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



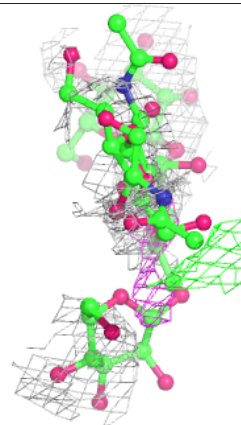
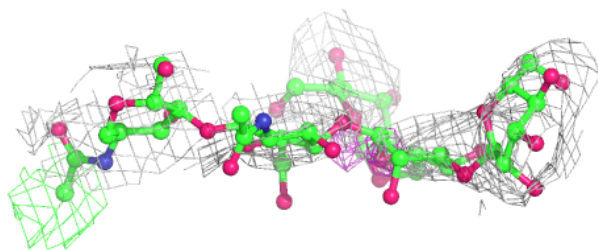
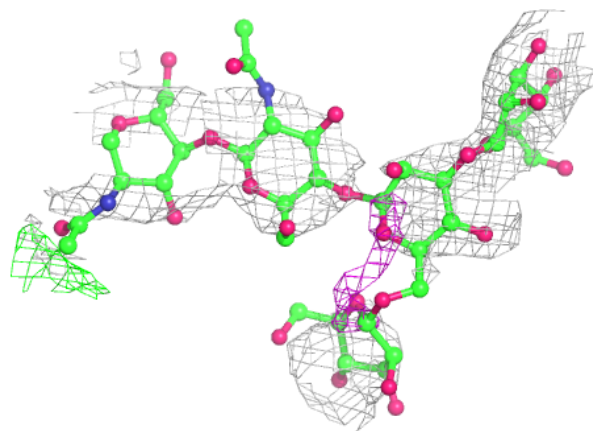
Electron density around Chain M:

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



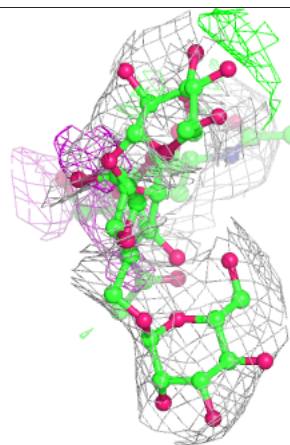
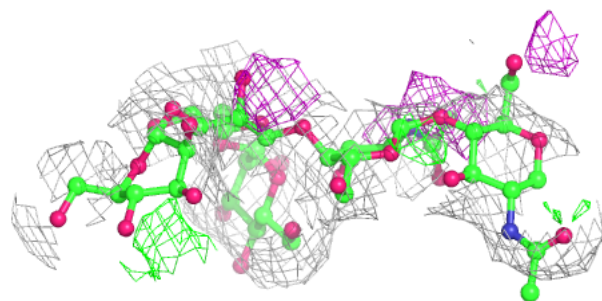
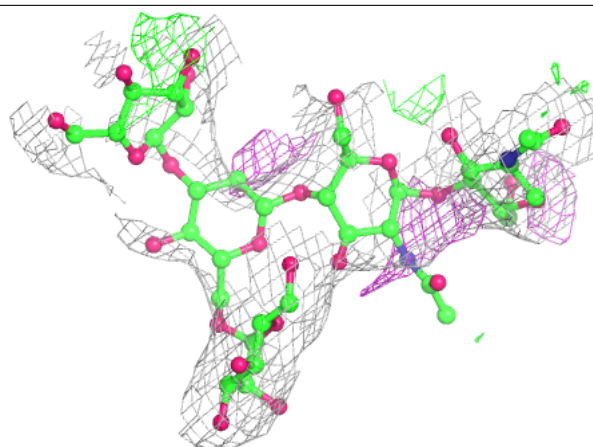
Electron density around Chain R:

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



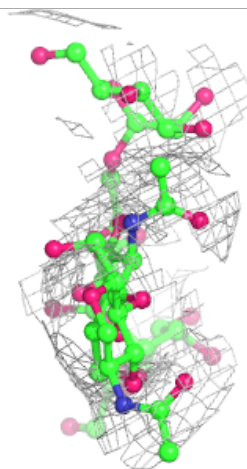
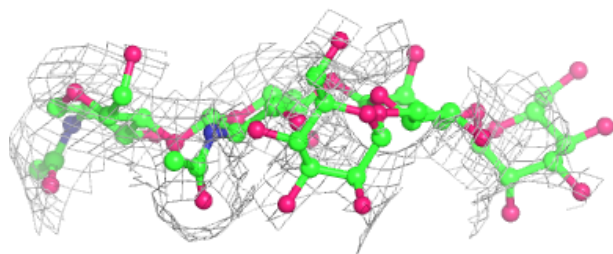
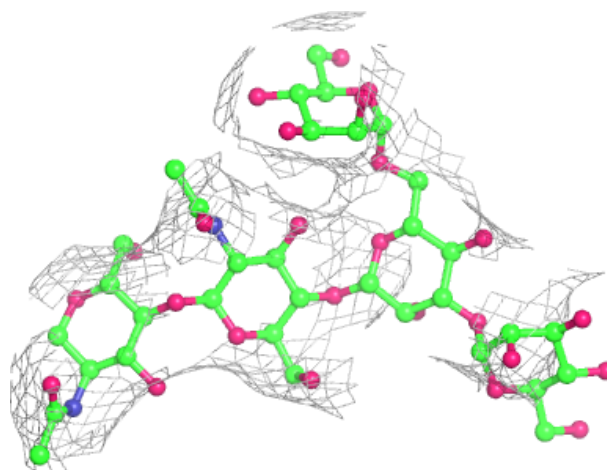
Electron density around Chain S:

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



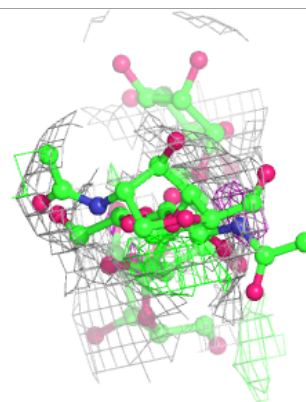
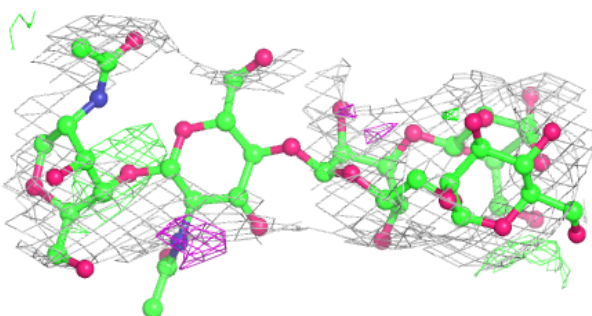
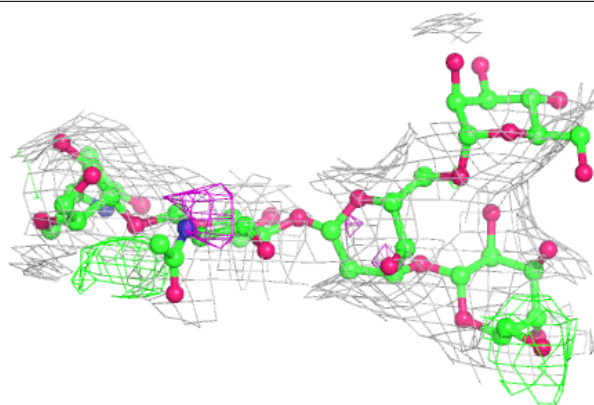
Electron density around Chain T:

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

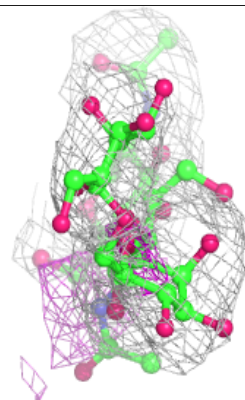
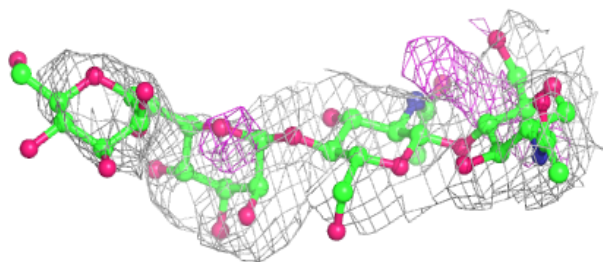
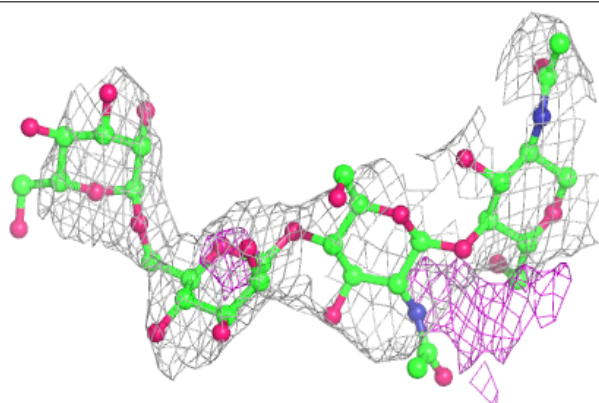


Electron density around Chain V:

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

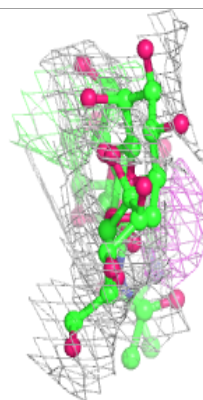
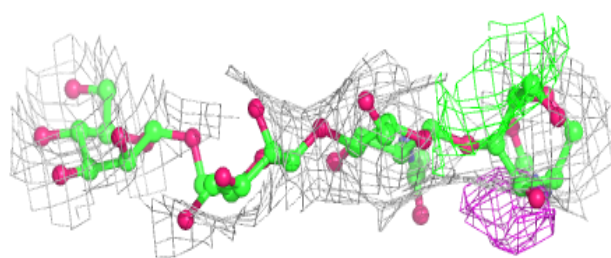
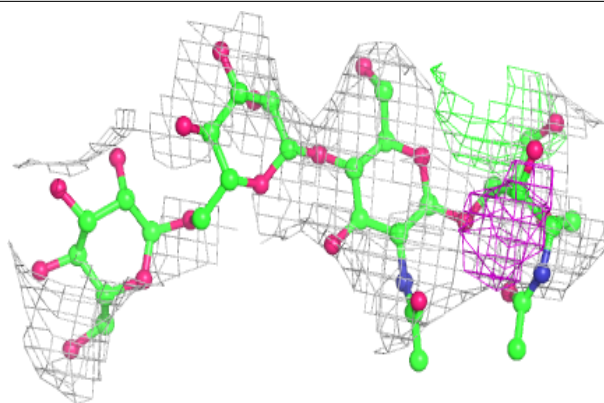
**Electron density around Chain N:**

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

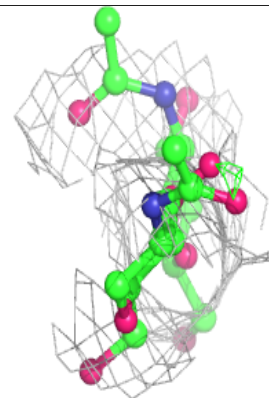
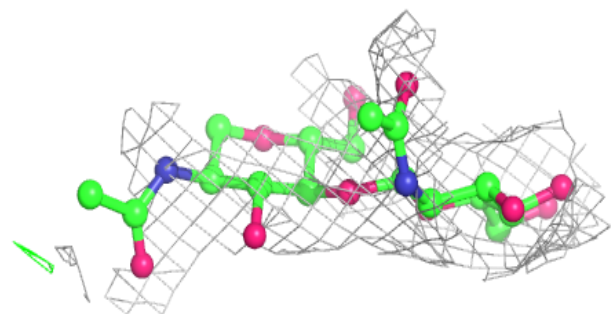
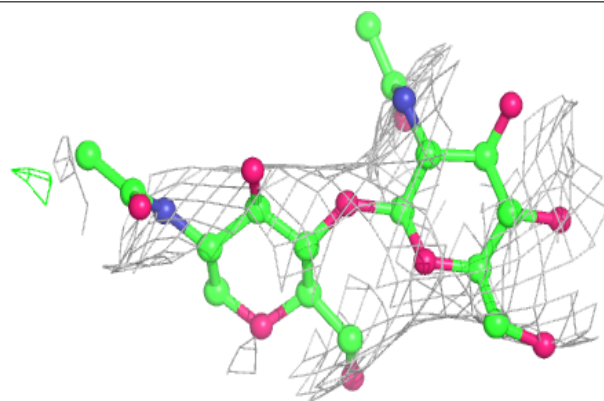


Electron density around Chain P:

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

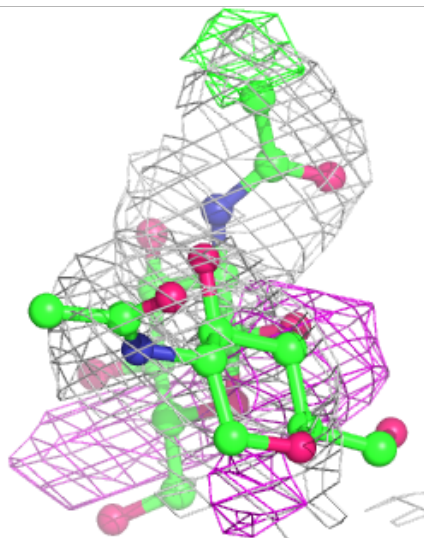
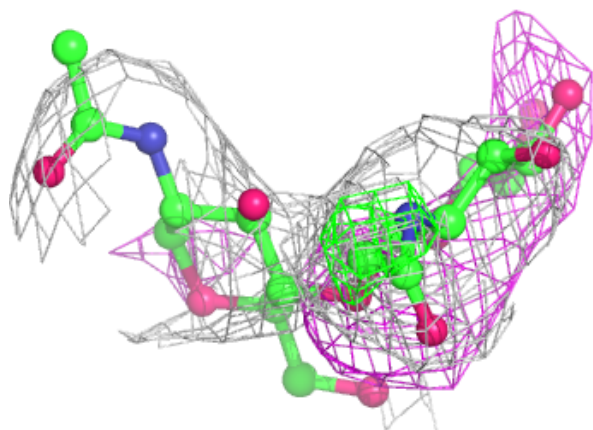
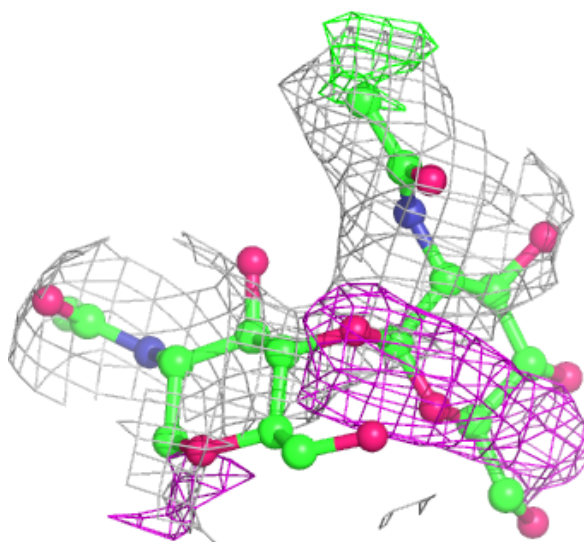
**Electron density around Chain O:**

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



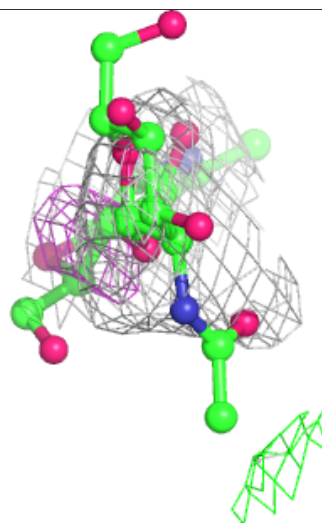
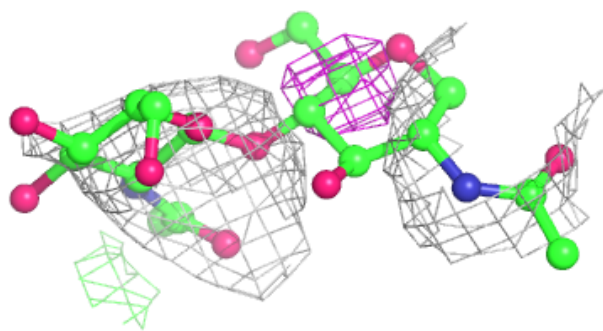
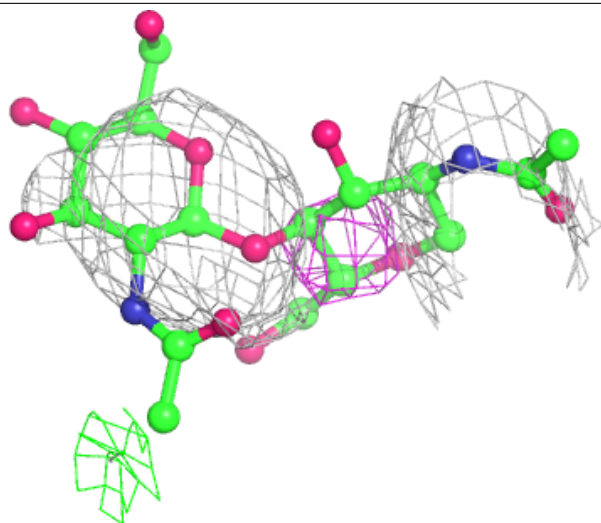
Electron density around Chain W:

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



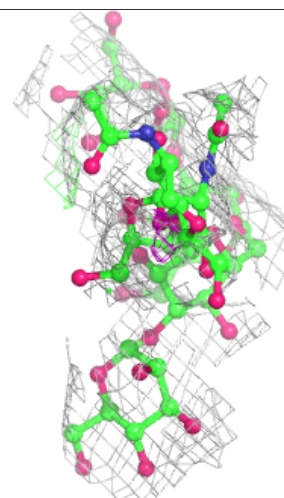
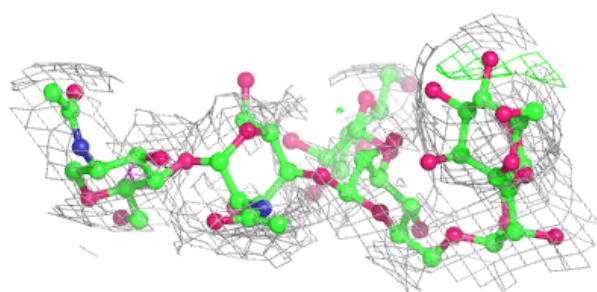
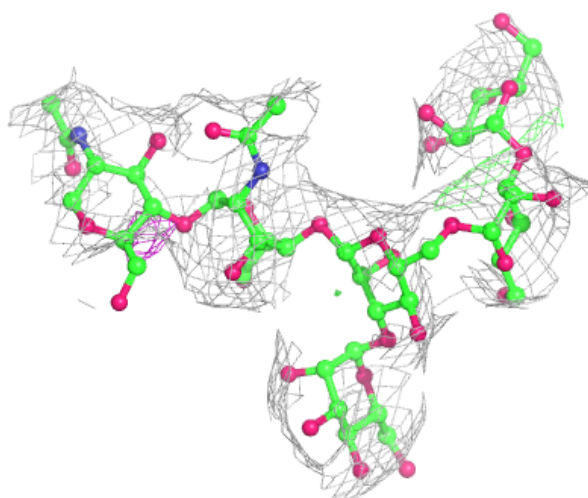
Electron density around Chain b:

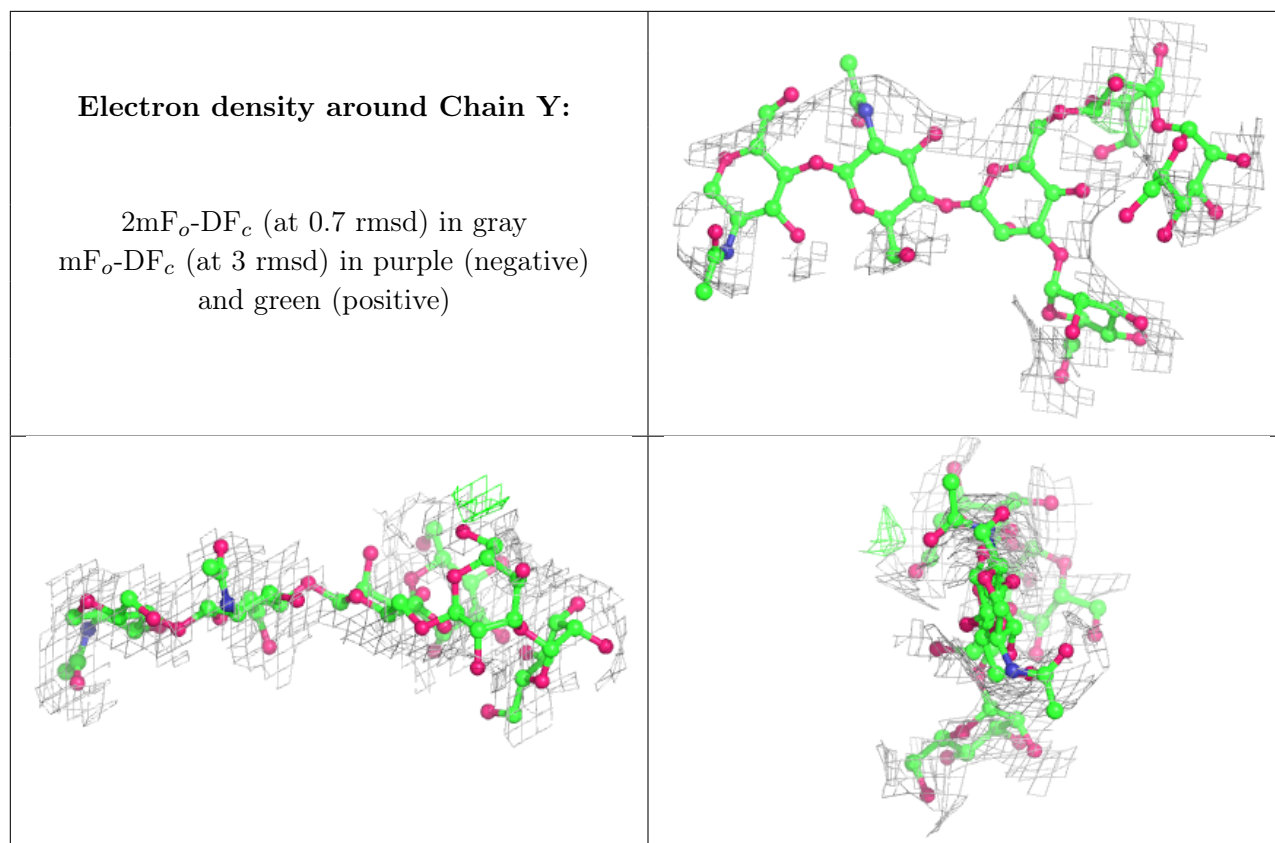
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain X:

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
11	NAG	B	603	14/15	0.62	0.72	139,166,172,175	0
11	NAG	B	601	14/15	0.64	0.34	147,156,165,168	0
11	NAG	C	604	14/15	0.64	0.35	156,164,179,180	0
11	NAG	C	602	14/15	0.68	0.32	134,147,165,173	0
11	NAG	C	601	14/15	0.78	0.19	135,153,166,176	0
11	NAG	A	602	14/15	0.79	0.34	136,165,171,175	0
11	NAG	A	601	14/15	0.80	0.21	122,147,157,165	0
11	NAG	B	602	14/15	0.80	0.20	127,137,144,149	0
11	NAG	C	603	14/15	0.83	0.21	124,149,158,160	0

6.5 Other polymers [i](#)

There are no such residues in this entry.