



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 11, 2023 – 08:32 AM EDT

PDB ID : 6X3M
Title : Crystal structure of full-length Streptococcal bacteriophage hyaluronidase in complex with unsaturated hyaluronan octa-saccharides
Authors : Deivanayagam, C.; Schormann, N.
Deposited on : 2020-05-21
Resolution : 3.58 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 : 2.35.1
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) : 2.35.1

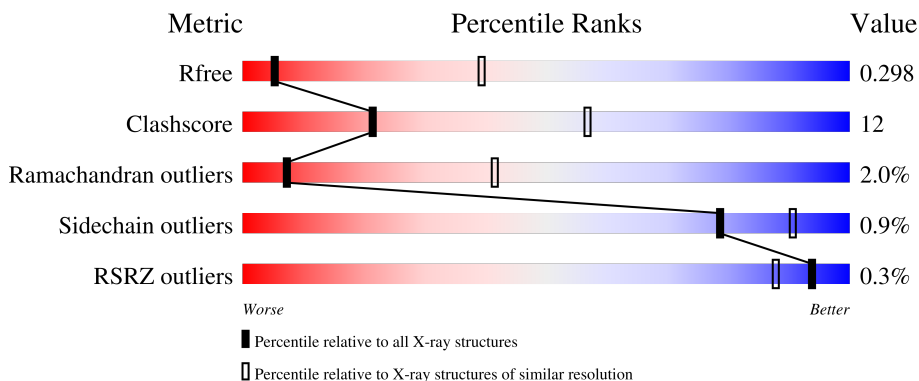
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.58 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	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	379	
1	B	379	
1	C	379	
1	D	379	
1	E	379	

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Mol	Chain	Length	Quality of chain
1	F	379	66% 29% ..
1	G	379	72% 24% ..
1	H	379	72% 22% • 5%
1	I	379	69% 25% ..
2	J	4	75% 25%
2	N	4	25% 25% 50%
2	O	4	25% 25% 50%
2	Q	4	75% 25%
2	T	4	100%
2	U	4	50% 50%
2	V	4	25% 75%
2	Z	4	25% 25% 50%
2	a	4	100%
3	K	8	38% 38% 25%
3	L	8	38% 50% 12%
3	M	8	25% 50% 25%
3	P	8	25% 75%
3	R	8	12% 50% 38%
3	S	8	12% 38% 50%
3	W	8	12% 62% 25%
3	X	8	12% 50% 38%
3	Y	8	62% 38%

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
3	NAG	M	1	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25574 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 Hyaluronoglucosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	361	2693	1671	469	545	8	0	0	0
1	B	361	2692	1670	469	545	8	0	0	0
1	C	361	2692	1670	469	545	8	0	0	0
1	D	349	2599	1610	454	527	8	0	0	0
1	E	357	2662	1650	464	540	8	0	0	0
1	F	366	2733	1697	475	553	8	0	0	0
1	G	363	2708	1682	471	547	8	0	0	0
1	H	361	2693	1673	468	544	8	0	0	0
1	I	362	2700	1676	470	546	8	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	372	LEU	-	expression tag	UNP P15316
A	373	GLU	-	expression tag	UNP P15316
A	374	HIS	-	expression tag	UNP P15316
A	375	HIS	-	expression tag	UNP P15316
A	376	HIS	-	expression tag	UNP P15316
A	377	HIS	-	expression tag	UNP P15316
A	378	HIS	-	expression tag	UNP P15316
A	379	HIS	-	expression tag	UNP P15316
B	372	LEU	-	expression tag	UNP P15316
B	373	GLU	-	expression tag	UNP P15316
B	374	HIS	-	expression tag	UNP P15316

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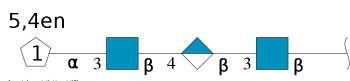
Chain	Residue	Modelled	Actual	Comment	Reference
B	375	HIS	-	expression tag	UNP P15316
B	376	HIS	-	expression tag	UNP P15316
B	377	HIS	-	expression tag	UNP P15316
B	378	HIS	-	expression tag	UNP P15316
B	379	HIS	-	expression tag	UNP P15316
C	372	LEU	-	expression tag	UNP P15316
C	373	GLU	-	expression tag	UNP P15316
C	374	HIS	-	expression tag	UNP P15316
C	375	HIS	-	expression tag	UNP P15316
C	376	HIS	-	expression tag	UNP P15316
C	377	HIS	-	expression tag	UNP P15316
C	378	HIS	-	expression tag	UNP P15316
C	379	HIS	-	expression tag	UNP P15316
D	372	LEU	-	expression tag	UNP P15316
D	373	GLU	-	expression tag	UNP P15316
D	374	HIS	-	expression tag	UNP P15316
D	375	HIS	-	expression tag	UNP P15316
D	376	HIS	-	expression tag	UNP P15316
D	377	HIS	-	expression tag	UNP P15316
D	378	HIS	-	expression tag	UNP P15316
D	379	HIS	-	expression tag	UNP P15316
E	372	LEU	-	expression tag	UNP P15316
E	373	GLU	-	expression tag	UNP P15316
E	374	HIS	-	expression tag	UNP P15316
E	375	HIS	-	expression tag	UNP P15316
E	376	HIS	-	expression tag	UNP P15316
E	377	HIS	-	expression tag	UNP P15316
E	378	HIS	-	expression tag	UNP P15316
E	379	HIS	-	expression tag	UNP P15316
F	372	LEU	-	expression tag	UNP P15316
F	373	GLU	-	expression tag	UNP P15316
F	374	HIS	-	expression tag	UNP P15316
F	375	HIS	-	expression tag	UNP P15316
F	376	HIS	-	expression tag	UNP P15316
F	377	HIS	-	expression tag	UNP P15316
F	378	HIS	-	expression tag	UNP P15316
F	379	HIS	-	expression tag	UNP P15316
G	372	LEU	-	expression tag	UNP P15316
G	373	GLU	-	expression tag	UNP P15316
G	374	HIS	-	expression tag	UNP P15316
G	375	HIS	-	expression tag	UNP P15316
G	376	HIS	-	expression tag	UNP P15316

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Chain	Residue	Modelled	Actual	Comment	Reference
G	377	HIS	-	expression tag	UNP P15316
G	378	HIS	-	expression tag	UNP P15316
G	379	HIS	-	expression tag	UNP P15316
H	372	LEU	-	expression tag	UNP P15316
H	373	GLU	-	expression tag	UNP P15316
H	374	HIS	-	expression tag	UNP P15316
H	375	HIS	-	expression tag	UNP P15316
H	376	HIS	-	expression tag	UNP P15316
H	377	HIS	-	expression tag	UNP P15316
H	378	HIS	-	expression tag	UNP P15316
H	379	HIS	-	expression tag	UNP P15316
I	372	LEU	-	expression tag	UNP P15316
I	373	GLU	-	expression tag	UNP P15316
I	374	HIS	-	expression tag	UNP P15316
I	375	HIS	-	expression tag	UNP P15316
I	376	HIS	-	expression tag	UNP P15316
I	377	HIS	-	expression tag	UNP P15316
I	378	HIS	-	expression tag	UNP P15316
I	379	HIS	-	expression tag	UNP P15316

- Molecule 2 is an oligosaccharide called 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



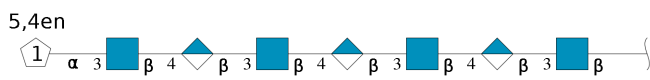
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	4	Total	C	N	O	0	0	0
			51	28	2	21			
2	N	4	Total	C	N	O	0	0	0
			52	28	2	22			
2	O	4	Total	C	N	O	0	0	0
			52	28	2	22			
2	Q	4	Total	C	N	O	0	0	0
			52	28	2	22			
2	T	4	Total	C	N	O	0	0	0
			52	28	2	22			
2	U	4	Total	C	N	O	0	0	0
			52	28	2	22			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	V	4	Total	C	N	O	0	0	0
			51	28	2	21			
2	Z	4	Total	C	N	O	0	0	0
			52	28	2	22			
2	a	4	Total	C	N	O	0	0	0
			52	28	2	22			

- Molecule 3 is an oligosaccharide called 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



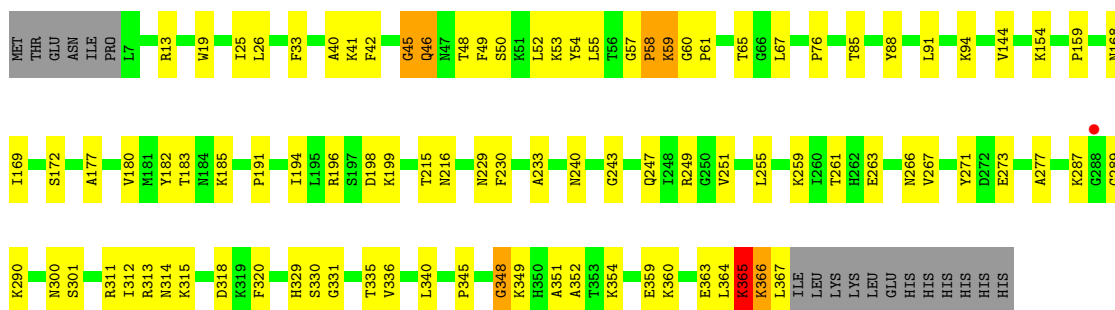
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	8	Total	C	N	O	0	0	0
			104	56	4	44			
3	L	8	Total	C	N	O	0	0	0
			104	56	4	44			
3	M	8	Total	C	N	O	0	0	0
			104	56	4	44			
3	P	8	Total	C	N	O	0	0	0
			104	56	4	44			
3	R	8	Total	C	N	O	0	0	0
			104	56	4	44			
3	S	8	Total	C	N	O	0	0	0
			104	56	4	44			
3	W	8	Total	C	N	O	0	0	0
			104	56	4	44			
3	X	8	Total	C	N	O	0	0	0
			104	56	4	44			
3	Y	8	Total	C	N	O	0	0	0
			104	56	4	44			

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.

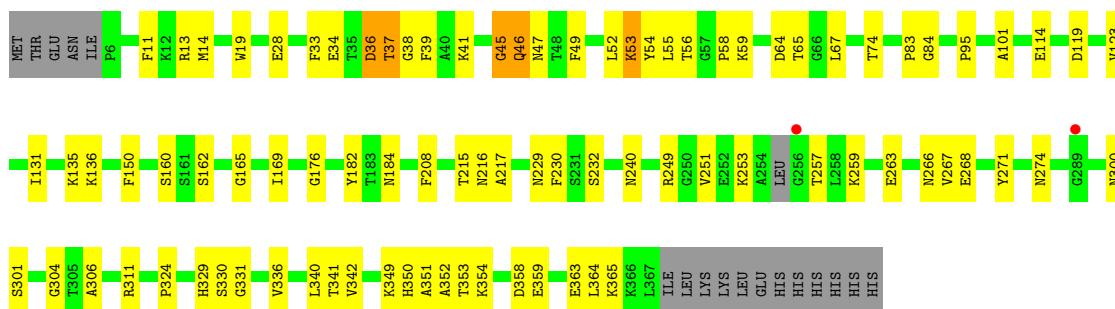
- Molecule 1: Hyaluronoglucosaminidase

Chain A: 



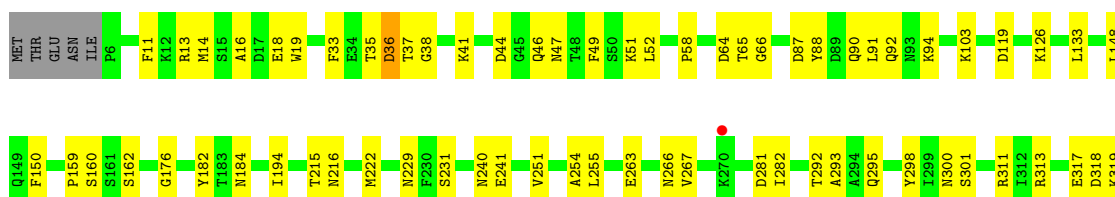
- Molecule 1: Hyaluronoglucosaminidase

Chain B: 



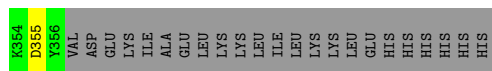
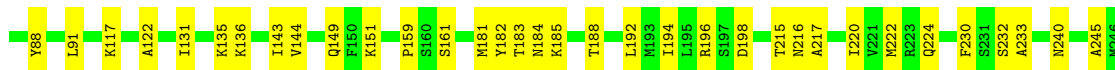
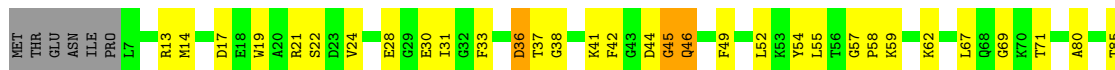
- Molecule 1: Hyaluronoglucosaminidase

Chain C: 

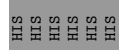
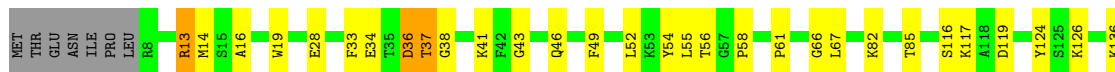




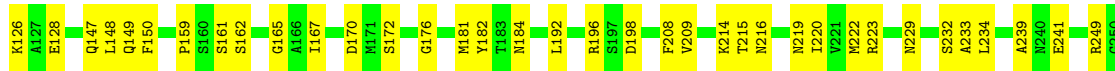
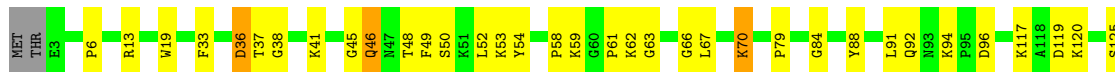
• Molecule 1: Hyaluronoglucosaminidase

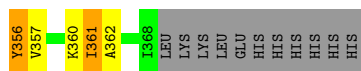


• Molecule 1: Hyaluronoglucosaminidase



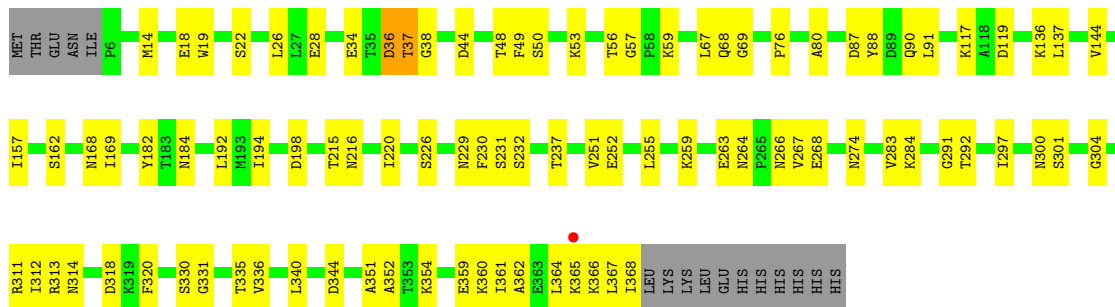
• Molecule 1: Hyaluronoglucosaminidase





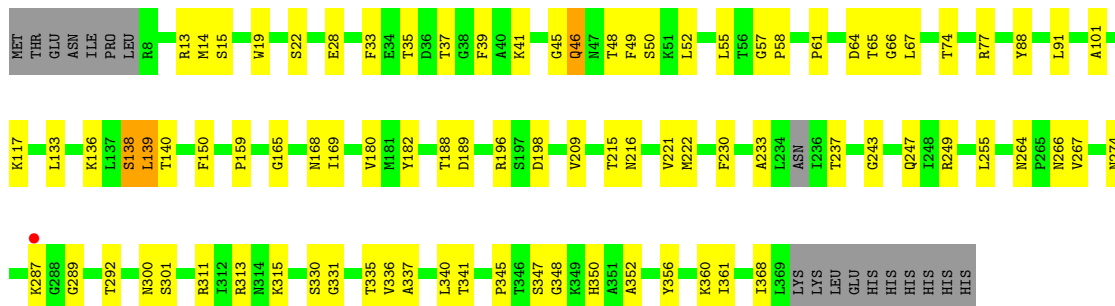
- Molecule 1: Hyaluronoglucosaminidase

Chain G: 72% 24%



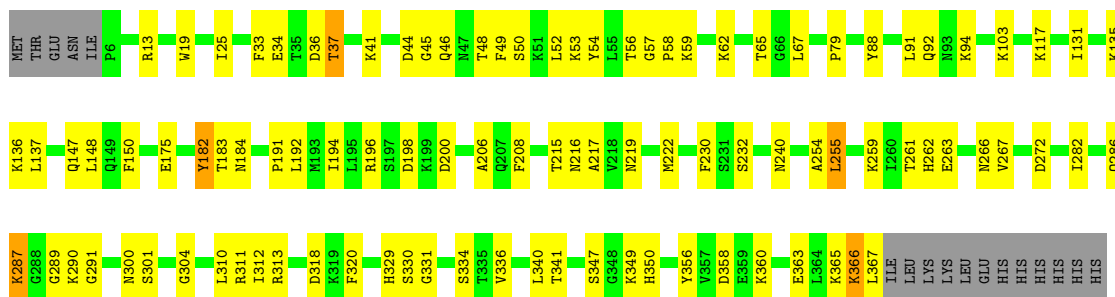
- Molecule 1: Hyaluronoglucosaminidase

Chain H: 72% 22% 5%



- Molecule 1: Hyaluronoglucosaminidase

Chain I: 69% 25%



- Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 75% 25%



- Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 25% 25% 50%



- Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 25% 25% 50%



- Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 75% 25%



- Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 100%



- Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U: 50% 50%




- Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  25% 75%

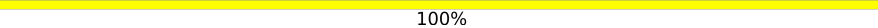
MAG1
BDP2
MAG3
CCD4

- Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  25% 25% 50%

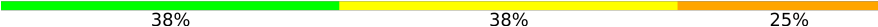
MAG1
BDP2
MAG3
CCD4

- Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  100%

MAG1
BDP2
MAG3
CCD4

- Molecule 3: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  38% 38% 25%

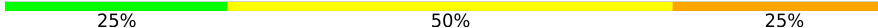
MAG1
BDP2
MAG3
BDP4
MAG5
BDP6
MAG7
CCD8

- Molecule 3: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  38% 50% 12%

MAG1
BDP2
MAG3
BDP4
MAG5
BDP6
MAG7
CCD8

- Molecule 3: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  25% 50% 25%



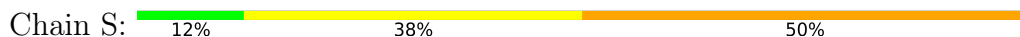
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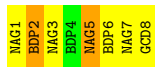
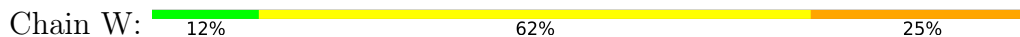
- Molecule 3: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



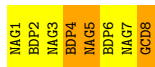
- Molecule 3: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 3: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 62% 38%



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	338.17Å 56.80Å 276.95Å 90.00° 126.68° 90.00°	Depositor
Resolution (Å)	29.87 – 3.58 29.87 – 3.58	Depositor EDS
% Data completeness (in resolution range)	95.8 (29.87-3.58) 95.8 (29.87-3.58)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 3.56Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.247 , 0.299 0.247 , 0.298	Depositor DCC
R_{free} test set	2519 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	91.9	Xtrriage
Anisotropy	0.126	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	25574	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.32% 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: BDP, NAG, GCD

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	0.26	0/2732	0.51	0/3670
1	B	0.26	0/2731	0.51	0/3667
1	C	0.28	0/2732	0.50	0/3670
1	D	0.27	0/2637	0.51	0/3542
1	E	0.26	0/2700	0.51	0/3626
1	F	0.26	0/2773	0.52	0/3727
1	G	0.27	0/2748	0.51	0/3692
1	H	0.26	0/2731	0.51	0/3667
1	I	0.28	0/2740	0.53	0/3681
All	All	0.27	0/24524	0.51	0/32942

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2693	0	2702	91	0
1	B	2692	0	2698	83	0
1	C	2692	0	2699	73	0
1	D	2599	0	2594	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2662	0	2661	98	0
1	F	2733	0	2743	100	0
1	G	2708	0	2721	94	0
1	H	2693	0	2706	82	0
1	I	2700	0	2710	89	0
2	J	51	0	35	0	0
2	N	52	0	37	3	0
2	O	52	0	37	6	0
2	Q	52	0	37	0	0
2	T	52	0	37	4	0
2	U	52	0	37	6	0
2	V	51	0	35	5	0
2	Z	52	0	37	2	0
2	a	52	0	38	0	0
3	K	104	0	73	5	0
3	L	104	0	73	1	0
3	M	104	0	73	8	0
3	P	104	0	73	11	0
3	R	104	0	73	6	0
3	S	104	0	73	7	0
3	W	104	0	73	6	0
3	X	104	0	73	6	0
3	Y	104	0	73	10	0
All	All	25574	0	25221	606	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 12.

The worst 5 of 606 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:55:LEU:HD12	1:A:55:LEU:O	1.30	1.30
1:G:364:LEU:HD22	1:H:361:ILE:HG23	1.36	1.01
1:A:55:LEU:O	1:A:55:LEU:CD1	2.13	0.96
1:A:364:LEU:HD12	1:A:364:LEU:O	1.72	0.87
1:H:237:THR:HG21	3:Y:3:NAG:H62	1.56	0.85

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	359/379 (95%)	323 (90%)	26 (7%)	10 (3%)	5	34
1	B	357/379 (94%)	321 (90%)	26 (7%)	10 (3%)	5	34
1	C	359/379 (95%)	322 (90%)	32 (9%)	5 (1%)	11	48
1	D	345/379 (91%)	311 (90%)	26 (8%)	8 (2%)	6	38
1	E	353/379 (93%)	317 (90%)	29 (8%)	7 (2%)	7	41
1	F	364/379 (96%)	325 (89%)	30 (8%)	9 (2%)	5	36
1	G	361/379 (95%)	331 (92%)	25 (7%)	5 (1%)	11	48
1	H	357/379 (94%)	322 (90%)	29 (8%)	6 (2%)	9	44
1	I	360/379 (95%)	324 (90%)	31 (9%)	5 (1%)	11	48
All	All	3215/3411 (94%)	2896 (90%)	254 (8%)	65 (2%)	7	41

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	GLY
1	A	46	GLN
1	A	287	LYS
1	A	366	LYS
1	B	37	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	288/306 (94%)	287 (100%)	1 (0%)	92	98
1	B	288/306 (94%)	285 (99%)	3 (1%)	76	89
1	C	288/306 (94%)	286 (99%)	2 (1%)	84	93
1	D	278/306 (91%)	275 (99%)	3 (1%)	73	88
1	E	284/306 (93%)	282 (99%)	2 (1%)	84	93
1	F	293/306 (96%)	289 (99%)	4 (1%)	67	85
1	G	290/306 (95%)	289 (100%)	1 (0%)	92	98
1	H	288/306 (94%)	286 (99%)	2 (1%)	84	93
1	I	289/306 (94%)	285 (99%)	4 (1%)	67	85
All	All	2586/2754 (94%)	2564 (99%)	22 (1%)	78	90

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	356	TYR
1	H	222	MET
1	H	182	TYR
1	I	182	TYR
1	D	222	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	295	GLN
1	D	240	ASN
1	I	247	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

108 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	J	1	2	14,14,15	0.26	0	17,19,21	0.43	0
2	BDP	J	2	2	12,12,13	1.18	2 (16%)	14,17,19	1.01	1 (7%)
2	NAG	J	3	2	14,14,15	0.25	0	17,19,21	0.75	0
2	GCD	J	4	2	10,11,12	0.30	0	13,15,17	0.60	0
3	NAG	K	1	3	15,15,15	0.12	0	21,21,21	0.51	0
3	BDP	K	2	3	12,12,13	0.15	0	14,17,19	0.44	0
3	NAG	K	3	3	14,14,15	0.34	0	17,19,21	0.57	0
3	BDP	K	4	3	12,12,13	1.19	2 (16%)	14,17,19	0.97	1 (7%)
3	NAG	K	5	3	14,14,15	0.25	0	17,19,21	0.73	0
3	BDP	K	6	3	12,12,13	1.17	2 (16%)	14,17,19	1.35	3 (21%)
3	NAG	K	7	3	14,14,15	0.30	0	17,19,21	0.94	1 (5%)
3	GCD	K	8	3	10,11,12	0.57	0	13,15,17	1.55	4 (30%)
3	NAG	L	1	3	15,15,15	0.11	0	21,21,21	0.47	0
3	BDP	L	2	3	12,12,13	0.42	0	14,17,19	1.83	4 (28%)
3	NAG	L	3	3	14,14,15	0.33	0	17,19,21	0.98	1 (5%)
3	BDP	L	4	3	12,12,13	0.57	0	14,17,19	0.67	1 (7%)
3	NAG	L	5	3	14,14,15	0.26	0	17,19,21	0.82	1 (5%)
3	BDP	L	6	3	12,12,13	1.20	2 (16%)	14,17,19	0.94	0
3	NAG	L	7	3	14,14,15	0.26	0	17,19,21	0.63	0
3	GCD	L	8	3	10,11,12	0.38	0	13,15,17	0.50	0
3	NAG	M	1	3	15,15,15	0.21	0	21,21,21	1.00	2 (9%)
3	BDP	M	2	3	12,12,13	1.23	2 (16%)	14,17,19	1.13	0
3	NAG	M	3	3	14,14,15	0.27	0	17,19,21	0.72	0
3	BDP	M	4	3	12,12,13	1.20	2 (16%)	14,17,19	1.30	2 (14%)
3	NAG	M	5	3	14,14,15	0.29	0	17,19,21	1.68	4 (23%)
3	BDP	M	6	3	12,12,13	0.23	0	14,17,19	0.42	0
3	NAG	M	7	3	14,14,15	0.29	0	17,19,21	1.49	2 (11%)
3	GCD	M	8	3	10,11,12	1.45	3 (30%)	13,15,17	1.54	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	N	1	2	15,15,15	0.17	0	21,21,21	0.63	0
2	BDP	N	2	2	12,12,13	1.16	2 (16%)	14,17,19	1.63	2 (14%)
2	NAG	N	3	2	14,14,15	0.32	0	17,19,21	2.05	4 (23%)
2	GCD	N	4	2	10,11,12	0.49	0	13,15,17	1.34	2 (15%)
2	NAG	O	1	2	15,15,15	0.14	0	21,21,21	0.43	0
2	BDP	O	2	2	12,12,13	1.17	2 (16%)	14,17,19	1.16	2 (14%)
2	NAG	O	3	2	14,14,15	0.62	0	17,19,21	2.20	6 (35%)
2	GCD	O	4	2	10,11,12	1.34	2 (20%)	13,15,17	1.81	5 (38%)
3	NAG	P	1	3	15,15,15	0.13	0	21,21,21	0.22	0
3	BDP	P	2	3	12,12,13	0.20	0	14,17,19	0.56	0
3	NAG	P	3	3	14,14,15	0.45	0	17,19,21	1.41	3 (17%)
3	BDP	P	4	3	12,12,13	1.23	2 (16%)	14,17,19	1.05	1 (7%)
3	NAG	P	5	3	14,14,15	0.33	0	17,19,21	1.74	3 (17%)
3	BDP	P	6	3	12,12,13	0.34	0	14,17,19	1.14	2 (14%)
3	NAG	P	7	3	14,14,15	0.50	0	17,19,21	1.18	2 (11%)
3	GCD	P	8	3	10,11,12	0.46	0	13,15,17	1.12	1 (7%)
2	NAG	Q	1	2	15,15,15	0.16	0	21,21,21	0.56	0
2	BDP	Q	2	2	12,12,13	1.35	2 (16%)	14,17,19	2.09	3 (21%)
2	NAG	Q	3	2	14,14,15	0.28	0	17,19,21	0.77	0
2	GCD	Q	4	2	10,11,12	0.41	0	13,15,17	0.49	0
3	NAG	R	1	3	15,15,15	0.28	0	21,21,21	0.86	0
3	BDP	R	2	3	12,12,13	1.32	2 (16%)	14,17,19	1.46	2 (14%)
3	NAG	R	3	3	14,14,15	0.43	0	17,19,21	0.76	0
3	BDP	R	4	3	12,12,13	1.25	2 (16%)	14,17,19	1.62	2 (14%)
3	NAG	R	5	3	14,14,15	0.31	0	17,19,21	0.90	1 (5%)
3	BDP	R	6	3	12,12,13	0.25	0	14,17,19	0.61	0
3	NAG	R	7	3	14,14,15	0.23	0	17,19,21	0.41	0
3	GCD	R	8	3	10,11,12	0.60	0	13,15,17	1.61	3 (23%)
3	NAG	S	1	3	15,15,15	0.20	0	21,21,21	0.83	2 (9%)
3	BDP	S	2	3	12,12,13	0.41	0	14,17,19	1.18	2 (14%)
3	NAG	S	3	3	14,14,15	0.48	0	17,19,21	1.80	2 (11%)
3	BDP	S	4	3	12,12,13	1.24	2 (16%)	14,17,19	1.89	4 (28%)
3	NAG	S	5	3	14,14,15	1.06	1 (7%)	17,19,21	2.19	5 (29%)
3	BDP	S	6	3	12,12,13	0.46	0	14,17,19	0.74	1 (7%)
3	NAG	S	7	3	14,14,15	0.28	0	17,19,21	0.77	0
3	GCD	S	8	3	10,11,12	1.35	2 (20%)	13,15,17	1.12	2 (15%)
2	NAG	T	1	2	15,15,15	0.23	0	21,21,21	1.36	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BDP	T	2	2	12,12,13	0.50	0	14,17,19	1.58	3 (21%)
2	NAG	T	3	2	14,14,15	0.61	0	17,19,21	1.72	3 (17%)
2	GCD	T	4	2	10,11,12	1.47	2 (20%)	13,15,17	1.69	3 (23%)
2	NAG	U	1	2	15,15,15	0.22	0	21,21,21	0.70	1 (4%)
2	BDP	U	2	2	12,12,13	0.19	0	14,17,19	1.06	1 (7%)
2	NAG	U	3	2	14,14,15	0.26	0	17,19,21	0.84	0
2	GCD	U	4	2	10,11,12	1.46	2 (20%)	13,15,17	1.97	3 (23%)
2	NAG	V	1	2	14,14,15	0.30	0	17,19,21	0.88	1 (5%)
2	BDP	V	2	2	12,12,13	1.19	2 (16%)	14,17,19	1.46	4 (28%)
2	NAG	V	3	2	14,14,15	0.60	0	17,19,21	1.69	3 (17%)
2	GCD	V	4	2	10,11,12	0.48	0	13,15,17	1.50	2 (15%)
3	NAG	W	1	3	15,15,15	0.29	0	21,21,21	0.63	0
3	BDP	W	2	3	12,12,13	0.54	0	14,17,19	2.18	3 (21%)
3	NAG	W	3	3	14,14,15	0.42	0	17,19,21	0.93	1 (5%)
3	BDP	W	4	3	12,12,13	0.33	0	14,17,19	0.66	0
3	NAG	W	5	3	14,14,15	0.39	0	17,19,21	1.27	2 (11%)
3	BDP	W	6	3	12,12,13	1.45	3 (25%)	14,17,19	1.34	3 (21%)
3	NAG	W	7	3	14,14,15	0.26	0	17,19,21	0.93	1 (5%)
3	GCD	W	8	3	10,11,12	0.60	0	13,15,17	1.46	2 (15%)
3	NAG	X	1	3	15,15,15	0.13	0	21,21,21	0.49	0
3	BDP	X	2	3	12,12,13	0.31	0	14,17,19	0.88	1 (7%)
3	NAG	X	3	3	14,14,15	0.35	0	17,19,21	0.70	0
3	BDP	X	4	3	12,12,13	0.25	0	14,17,19	0.70	1 (7%)
3	NAG	X	5	3	14,14,15	0.37	0	17,19,21	0.91	1 (5%)
3	BDP	X	6	3	12,12,13	0.30	0	14,17,19	0.96	1 (7%)
3	NAG	X	7	3	14,14,15	0.45	0	17,19,21	1.04	1 (5%)
3	GCD	X	8	3	10,11,12	0.52	0	13,15,17	0.65	0
3	NAG	Y	1	3	15,15,15	0.21	0	21,21,21	0.59	0
3	BDP	Y	2	3	12,12,13	1.18	2 (16%)	14,17,19	1.02	1 (7%)
3	NAG	Y	3	3	14,14,15	0.40	0	17,19,21	0.83	0
3	BDP	Y	4	3	12,12,13	1.18	2 (16%)	14,17,19	1.03	2 (14%)
3	NAG	Y	5	3	14,14,15	0.37	0	17,19,21	2.11	3 (17%)
3	BDP	Y	6	3	12,12,13	0.71	0	14,17,19	1.38	3 (21%)
3	NAG	Y	7	3	14,14,15	0.26	0	17,19,21	0.86	0
3	GCD	Y	8	3	10,11,12	1.80	3 (30%)	13,15,17	1.11	1 (7%)
2	NAG	Z	1	2	15,15,15	0.13	0	21,21,21	0.42	0
2	BDP	Z	2	2	12,12,13	0.55	0	14,17,19	1.28	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	Z	3	2	14,14,15	0.62	0	17,19,21	2.18	4 (23%)
2	GCD	Z	4	2	10,11,12	0.44	0	13,15,17	1.69	4 (30%)
2	NAG	a	1	2	15,15,15	0.22	0	21,21,21	0.84	1 (4%)
2	BDP	a	2	2	12,12,13	0.27	0	14,17,19	0.85	1 (7%)
2	NAG	a	3	2	14,14,15	0.39	0	17,19,21	0.97	1 (5%)
2	GCD	a	4	2	10,11,12	1.03	1 (10%)	13,15,17	1.52	3 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	1	2	-	4/6/23/26	0/1/1/1
2	BDP	J	2	2	-	0/4/21/24	0/1/1/1
2	NAG	J	3	2	-	0/6/23/26	0/1/1/1
2	GCD	J	4	2	-	0/4/17/20	0/1/1/1
3	NAG	K	1	3	-	3/6/26/26	0/1/1/1
3	BDP	K	2	3	-	2/4/21/24	0/1/1/1
3	NAG	K	3	3	-	2/6/23/26	0/1/1/1
3	BDP	K	4	3	-	0/4/21/24	0/1/1/1
3	NAG	K	5	3	-	3/6/23/26	0/1/1/1
3	BDP	K	6	3	-	0/4/21/24	0/1/1/1
3	NAG	K	7	3	-	5/6/23/26	0/1/1/1
3	GCD	K	8	3	-	0/4/17/20	0/1/1/1
3	NAG	L	1	3	-	0/6/26/26	0/1/1/1
3	BDP	L	2	3	-	2/4/21/24	0/1/1/1
3	NAG	L	3	3	-	3/6/23/26	0/1/1/1
3	BDP	L	4	3	-	0/4/21/24	1/1/1/1
3	NAG	L	5	3	-	0/6/23/26	0/1/1/1
3	BDP	L	6	3	-	0/4/21/24	0/1/1/1
3	NAG	L	7	3	-	4/6/23/26	0/1/1/1
3	GCD	L	8	3	-	0/4/17/20	0/1/1/1
3	NAG	M	1	3	-	4/6/26/26	0/1/1/1
3	BDP	M	2	3	-	0/4/21/24	0/1/1/1
3	NAG	M	3	3	-	1/6/23/26	0/1/1/1
3	BDP	M	4	3	-	3/4/21/24	0/1/1/1
3	NAG	M	5	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BDP	M	6	3	-	0/4/21/24	1/1/1/1
3	NAG	M	7	3	-	3/6/23/26	0/1/1/1
3	GCD	M	8	3	-	0/4/17/20	0/1/1/1
2	NAG	N	1	2	-	6/6/26/26	0/1/1/1
2	BDP	N	2	2	-	1/4/21/24	1/1/1/1
2	NAG	N	3	2	-	4/6/23/26	0/1/1/1
2	GCD	N	4	2	-	0/4/17/20	0/1/1/1
2	NAG	O	1	2	-	3/6/26/26	0/1/1/1
2	BDP	O	2	2	-	1/4/21/24	0/1/1/1
2	NAG	O	3	2	-	3/6/23/26	0/1/1/1
2	GCD	O	4	2	-	0/4/17/20	0/1/1/1
3	NAG	P	1	3	-	2/6/26/26	0/1/1/1
3	BDP	P	2	3	-	2/4/21/24	0/1/1/1
3	NAG	P	3	3	-	1/6/23/26	0/1/1/1
3	BDP	P	4	3	-	0/4/21/24	0/1/1/1
3	NAG	P	5	3	-	1/6/23/26	0/1/1/1
3	BDP	P	6	3	-	0/4/21/24	0/1/1/1
3	NAG	P	7	3	-	6/6/23/26	0/1/1/1
3	GCD	P	8	3	-	0/4/17/20	0/1/1/1
2	NAG	Q	1	2	-	4/6/26/26	0/1/1/1
2	BDP	Q	2	2	-	0/4/21/24	0/1/1/1
2	NAG	Q	3	2	-	2/6/23/26	0/1/1/1
2	GCD	Q	4	2	-	0/4/17/20	0/1/1/1
3	NAG	R	1	3	-	2/6/26/26	0/1/1/1
3	BDP	R	2	3	-	0/4/21/24	0/1/1/1
3	NAG	R	3	3	-	2/6/23/26	0/1/1/1
3	BDP	R	4	3	-	0/4/21/24	0/1/1/1
3	NAG	R	5	3	-	4/6/23/26	0/1/1/1
3	BDP	R	6	3	-	0/4/21/24	1/1/1/1
3	NAG	R	7	3	-	1/6/23/26	0/1/1/1
3	GCD	R	8	3	-	0/4/17/20	0/1/1/1
3	NAG	S	1	3	-	5/6/26/26	0/1/1/1
3	BDP	S	2	3	-	2/4/21/24	0/1/1/1
3	NAG	S	3	3	-	2/6/23/26	0/1/1/1
3	BDP	S	4	3	-	2/4/21/24	0/1/1/1
3	NAG	S	5	3	-	2/6/23/26	0/1/1/1
3	BDP	S	6	3	-	0/4/21/24	0/1/1/1
3	NAG	S	7	3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GCD	S	8	3	-	0/4/17/20	0/1/1/1
2	NAG	T	1	2	-	3/6/26/26	0/1/1/1
2	BDP	T	2	2	-	0/4/21/24	0/1/1/1
2	NAG	T	3	2	-	2/6/23/26	0/1/1/1
2	GCD	T	4	2	-	0/4/17/20	0/1/1/1
2	NAG	U	1	2	-	3/6/26/26	0/1/1/1
2	BDP	U	2	2	-	0/4/21/24	1/1/1/1
2	NAG	U	3	2	-	4/6/23/26	0/1/1/1
2	GCD	U	4	2	-	0/4/17/20	0/1/1/1
2	NAG	V	1	2	-	5/6/23/26	0/1/1/1
2	BDP	V	2	2	-	2/4/21/24	1/1/1/1
2	NAG	V	3	2	-	2/6/23/26	0/1/1/1
2	GCD	V	4	2	-	0/4/17/20	0/1/1/1
3	NAG	W	1	3	-	6/6/26/26	0/1/1/1
3	BDP	W	2	3	-	0/4/21/24	0/1/1/1
3	NAG	W	3	3	-	4/6/23/26	0/1/1/1
3	BDP	W	4	3	-	2/4/21/24	0/1/1/1
3	NAG	W	5	3	-	6/6/23/26	0/1/1/1
3	BDP	W	6	3	-	2/4/21/24	0/1/1/1
3	NAG	W	7	3	-	4/6/23/26	0/1/1/1
3	GCD	W	8	3	-	0/4/17/20	0/1/1/1
3	NAG	X	1	3	-	1/6/26/26	0/1/1/1
3	BDP	X	2	3	-	2/4/21/24	0/1/1/1
3	NAG	X	3	3	-	4/6/23/26	0/1/1/1
3	BDP	X	4	3	-	0/4/21/24	0/1/1/1
3	NAG	X	5	3	-	2/6/23/26	0/1/1/1
3	BDP	X	6	3	-	2/4/21/24	1/1/1/1
3	NAG	X	7	3	-	4/6/23/26	0/1/1/1
3	GCD	X	8	3	-	0/4/17/20	0/1/1/1
3	NAG	Y	1	3	-	5/6/26/26	0/1/1/1
3	BDP	Y	2	3	-	0/4/21/24	0/1/1/1
3	NAG	Y	3	3	-	1/6/23/26	0/1/1/1
3	BDP	Y	4	3	-	2/4/21/24	1/1/1/1
3	NAG	Y	5	3	-	4/6/23/26	0/1/1/1
3	BDP	Y	6	3	-	0/4/21/24	1/1/1/1
3	NAG	Y	7	3	-	0/6/23/26	0/1/1/1
3	GCD	Y	8	3	-	0/4/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	Z	1	2	-	3/6/26/26	0/1/1/1
2	BDP	Z	2	2	-	0/4/21/24	0/1/1/1
2	NAG	Z	3	2	-	5/6/23/26	0/1/1/1
2	GCD	Z	4	2	-	0/4/17/20	0/1/1/1
2	NAG	a	1	2	-	6/6/26/26	0/1/1/1
2	BDP	a	2	2	-	2/4/21/24	0/1/1/1
2	NAG	a	3	2	-	3/6/23/26	0/1/1/1
2	GCD	a	4	2	-	1/4/17/20	0/1/1/1

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	8	GCD	O6A-C6	3.76	1.32	1.22
2	T	4	GCD	O6A-C6	3.71	1.32	1.22
2	U	4	GCD	O6A-C6	3.36	1.31	1.22
3	S	8	GCD	O6A-C6	3.30	1.31	1.22
2	O	4	GCD	O6A-C6	3.28	1.31	1.22

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	5	NAG	C1-O5-C5	7.29	122.07	112.19
3	S	5	NAG	C1-O5-C5	6.82	121.44	112.19
3	S	3	NAG	C1-O5-C5	6.55	121.06	112.19
3	W	2	BDP	O4-C4-C5	6.49	124.30	109.74
2	Z	3	NAG	C1-O5-C5	6.25	120.66	112.19

There are no chirality outliers.

5 of 196 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	1	NAG	C8-C7-N2-C2
2	N	1	NAG	O7-C7-N2-C2
2	O	3	NAG	C3-C2-N2-C7
2	Q	1	NAG	C1-C2-N2-C7
2	Q	1	NAG	C8-C7-N2-C2

5 of 9 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	6	BDP	C1-C2-C3-C4-C5-O5
3	Y	6	BDP	C1-C2-C3-C4-C5-O5
2	U	2	BDP	C1-C2-C3-C4-C5-O5
2	V	2	BDP	C1-C2-C3-C4-C5-O5
3	R	6	BDP	C1-C2-C3-C4-C5-O5

54 monomers are involved in 86 short contacts:

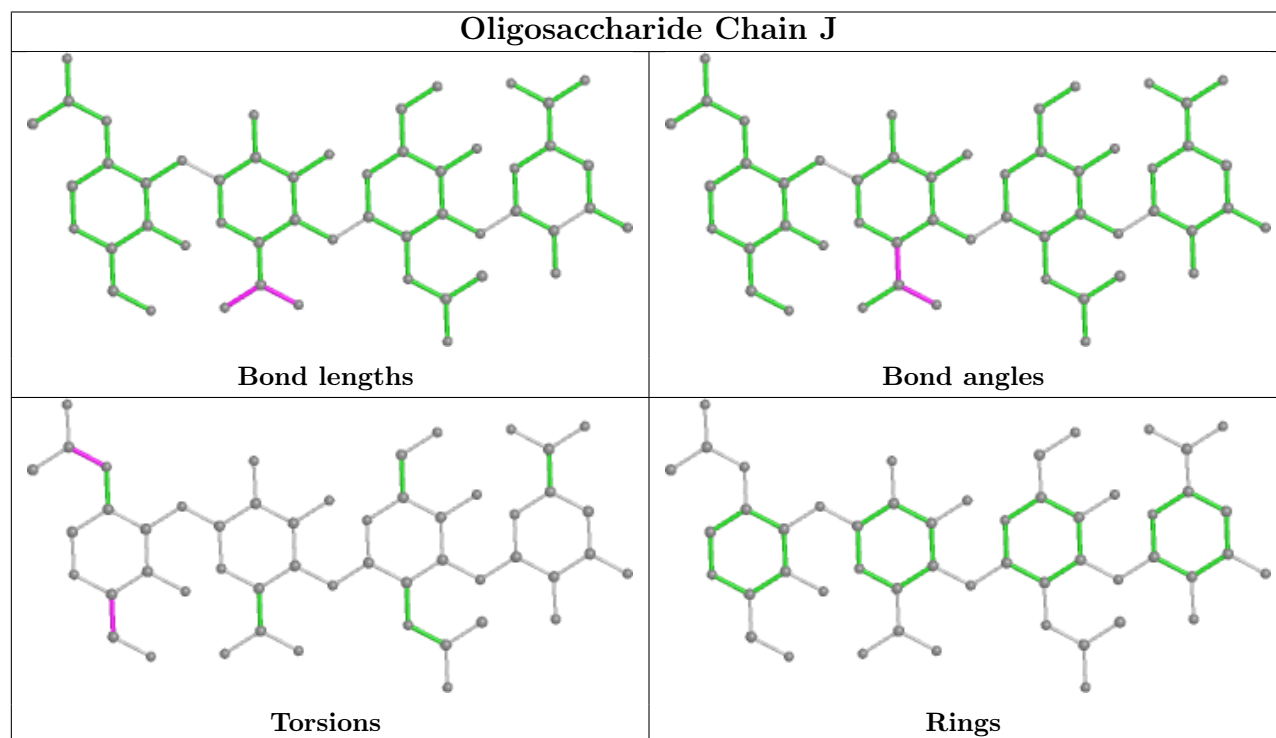
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	7	NAG	1	0
3	M	7	NAG	1	0
3	W	1	NAG	4	0
2	U	1	NAG	3	0
2	T	2	BDP	1	0
3	P	5	NAG	2	0
3	R	6	BDP	1	0
3	R	8	GCD	1	0
2	V	3	NAG	1	0
3	W	2	BDP	2	0
3	P	7	NAG	2	0
3	R	4	BDP	1	0
3	K	1	NAG	3	0
2	U	2	BDP	3	0
3	X	3	NAG	1	0
3	Y	3	NAG	3	0
2	U	3	NAG	2	0
3	W	5	NAG	1	0
2	N	3	NAG	2	0
3	P	1	NAG	3	0
3	S	1	NAG	2	0
3	K	8	GCD	1	0
2	V	1	NAG	2	0
3	L	6	BDP	1	0
3	M	1	NAG	7	0
3	X	6	BDP	1	0
3	S	6	BDP	1	0
3	Y	5	NAG	1	0
3	P	4	BDP	2	0
2	O	2	BDP	2	0
3	S	5	NAG	4	0
3	Y	1	NAG	5	0
3	P	8	GCD	1	0
2	T	4	GCD	2	0
3	S	4	BDP	3	0

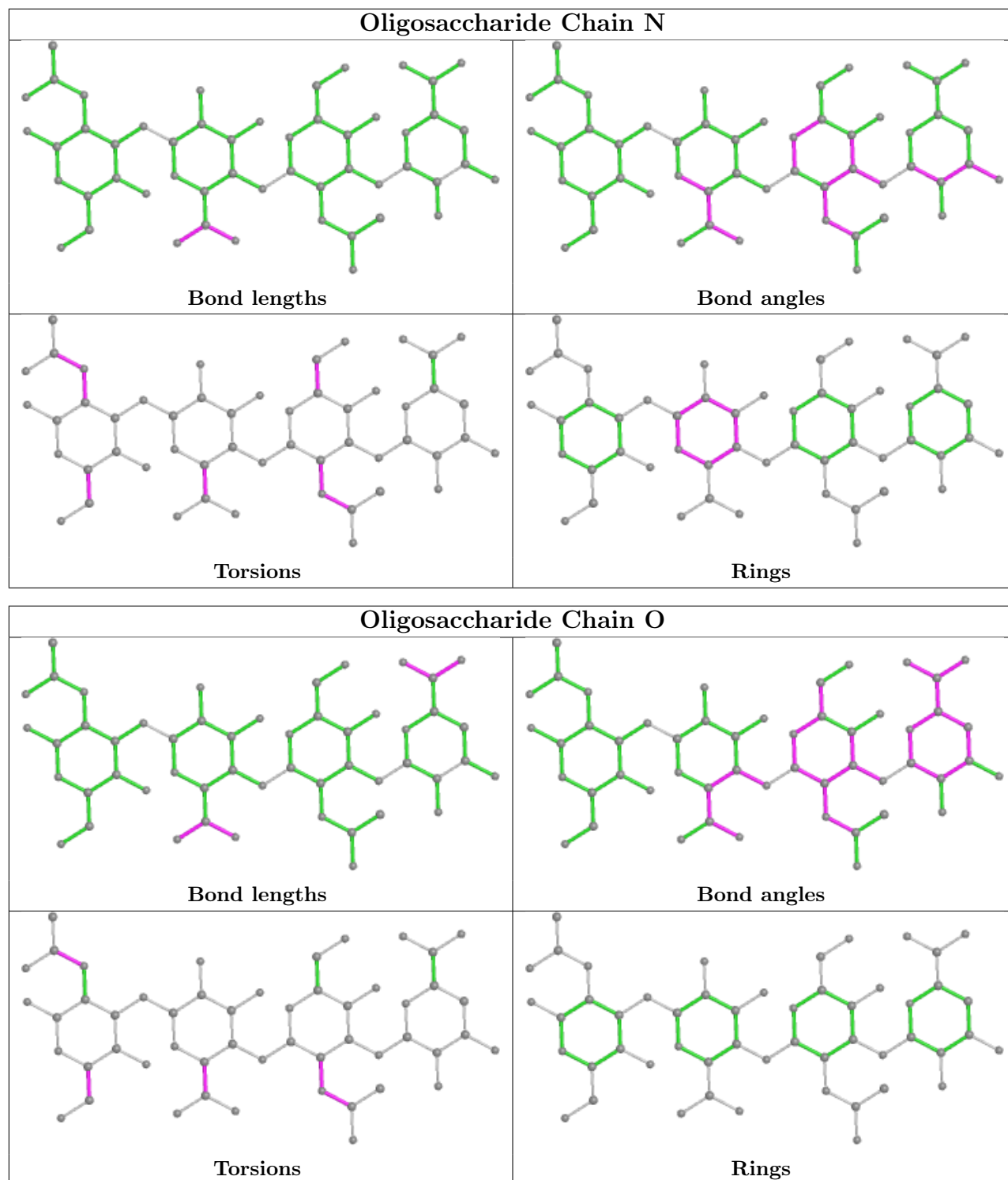
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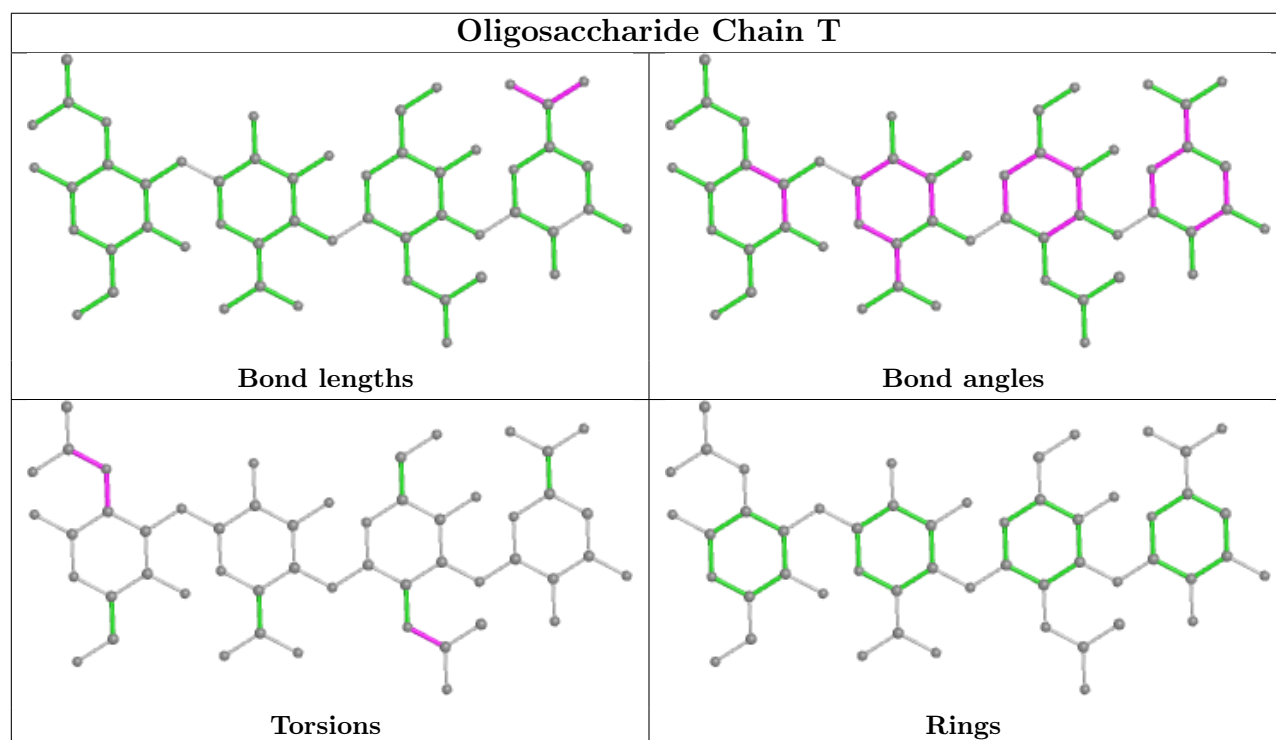
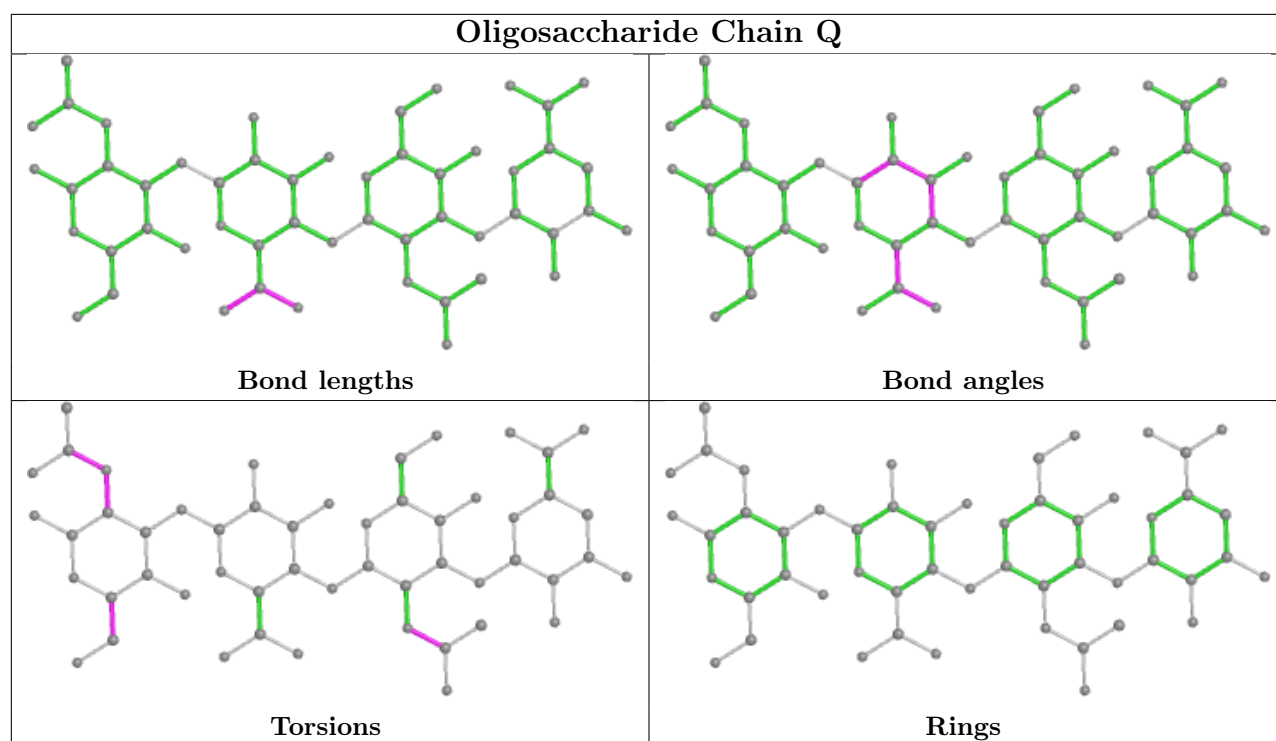
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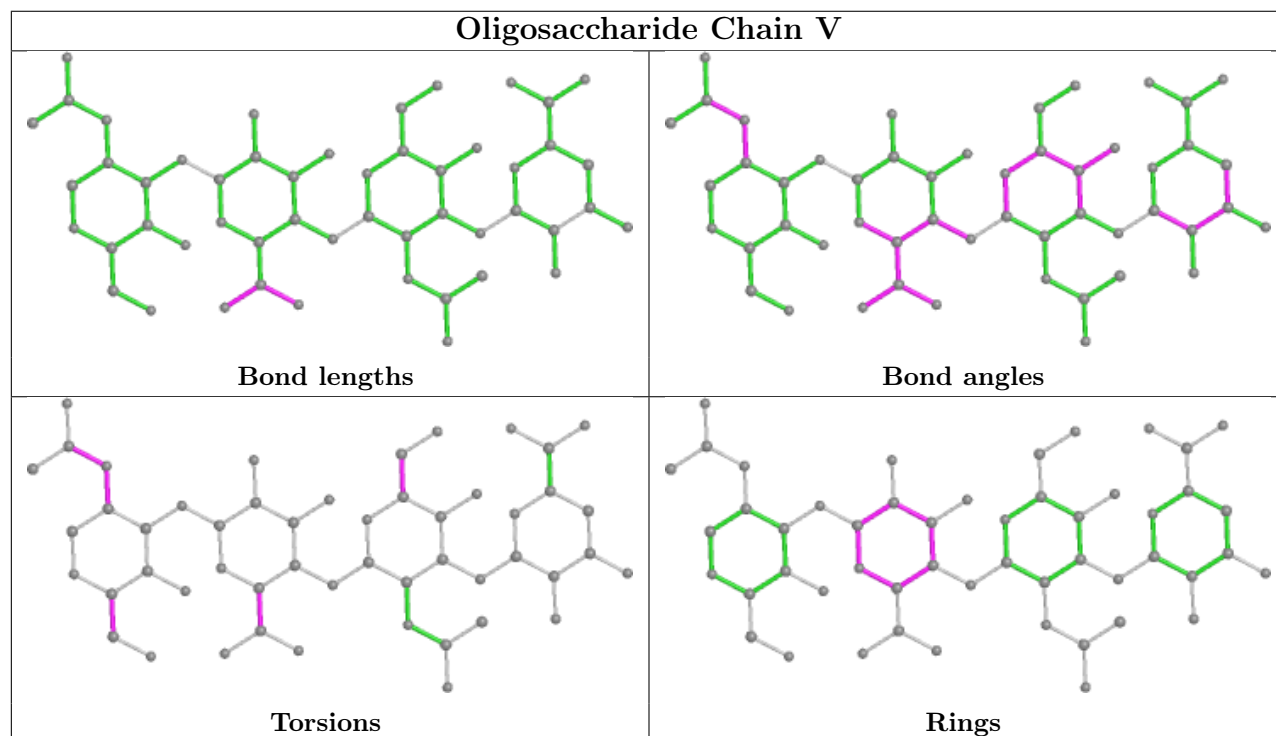
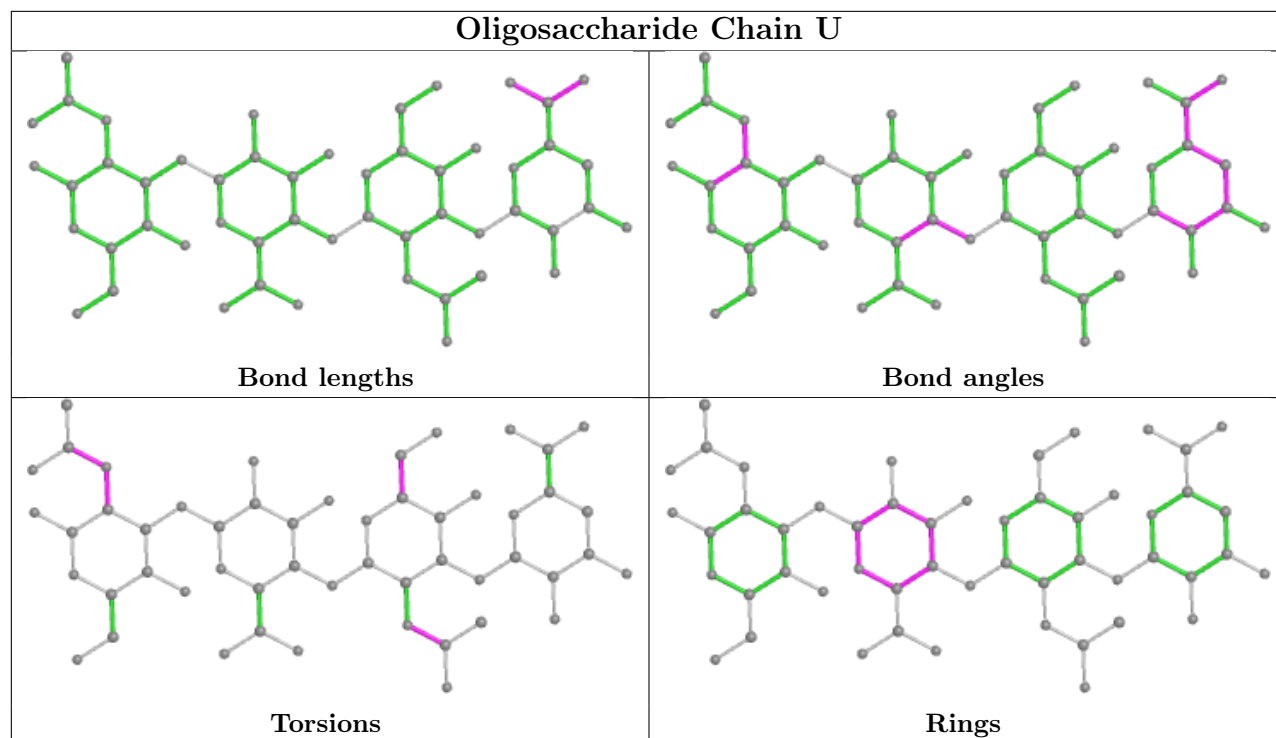
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	2	BDP	1	0
3	K	7	NAG	2	0
3	X	1	NAG	2	0
2	N	2	BDP	1	0
3	P	6	BDP	1	0
3	X	4	BDP	2	0
3	X	5	NAG	1	0
3	Y	4	BDP	1	0
2	O	3	NAG	5	0
3	R	2	BDP	1	0
3	P	3	NAG	2	0
2	V	2	BDP	3	0
2	Z	2	BDP	1	0
2	T	1	NAG	1	0
3	Y	7	NAG	1	0
3	Y	8	GCD	1	0
2	Z	3	NAG	1	0
3	R	1	NAG	3	0
2	T	3	NAG	1	0

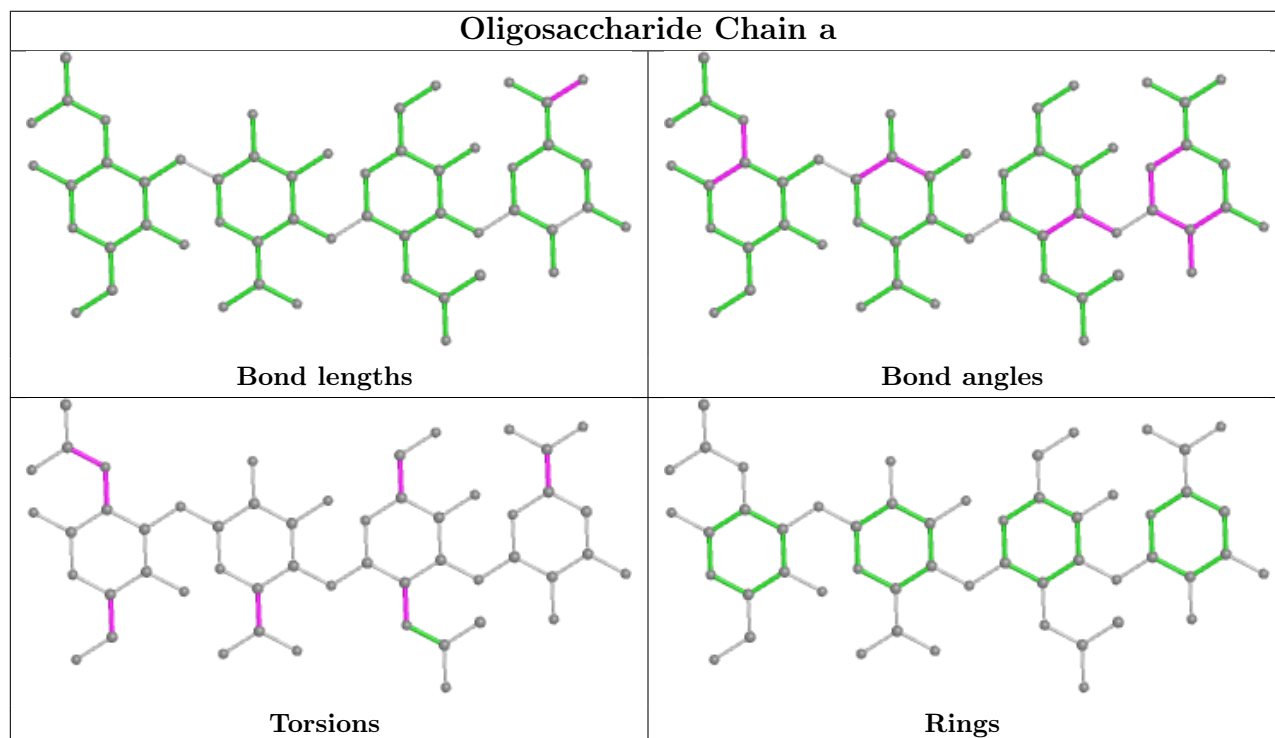
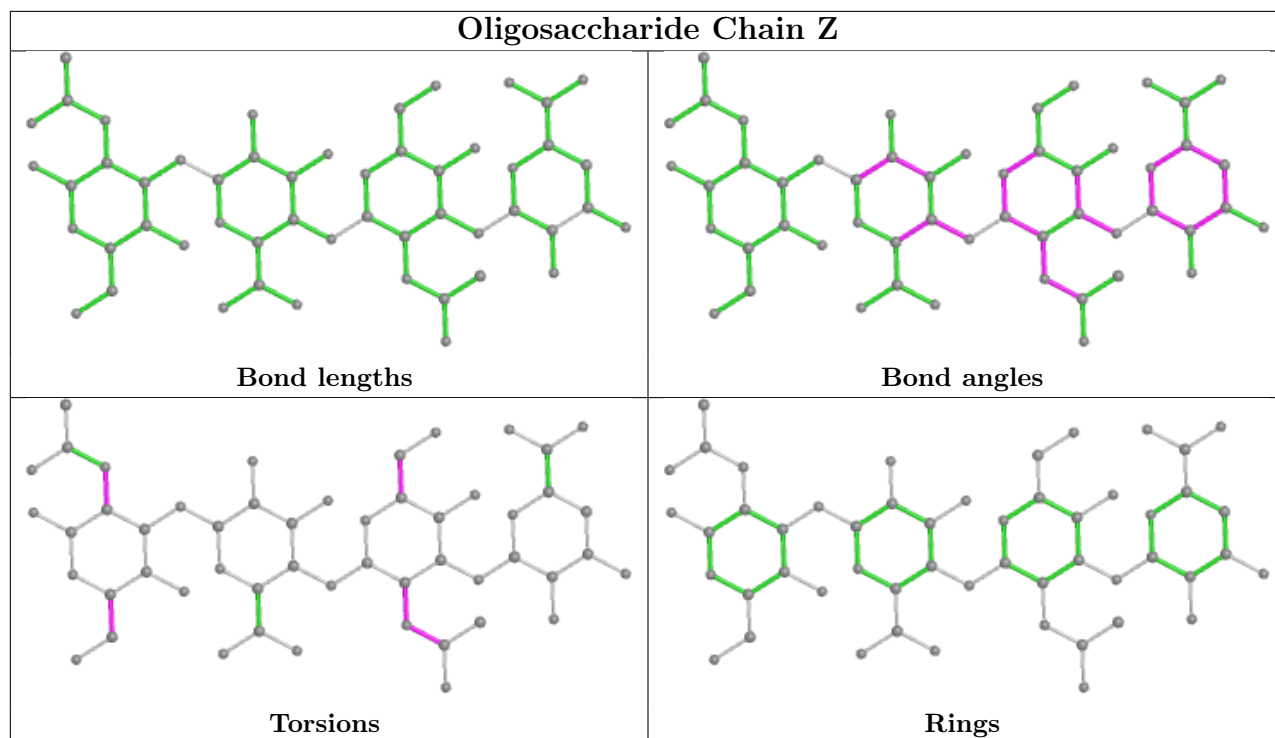
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

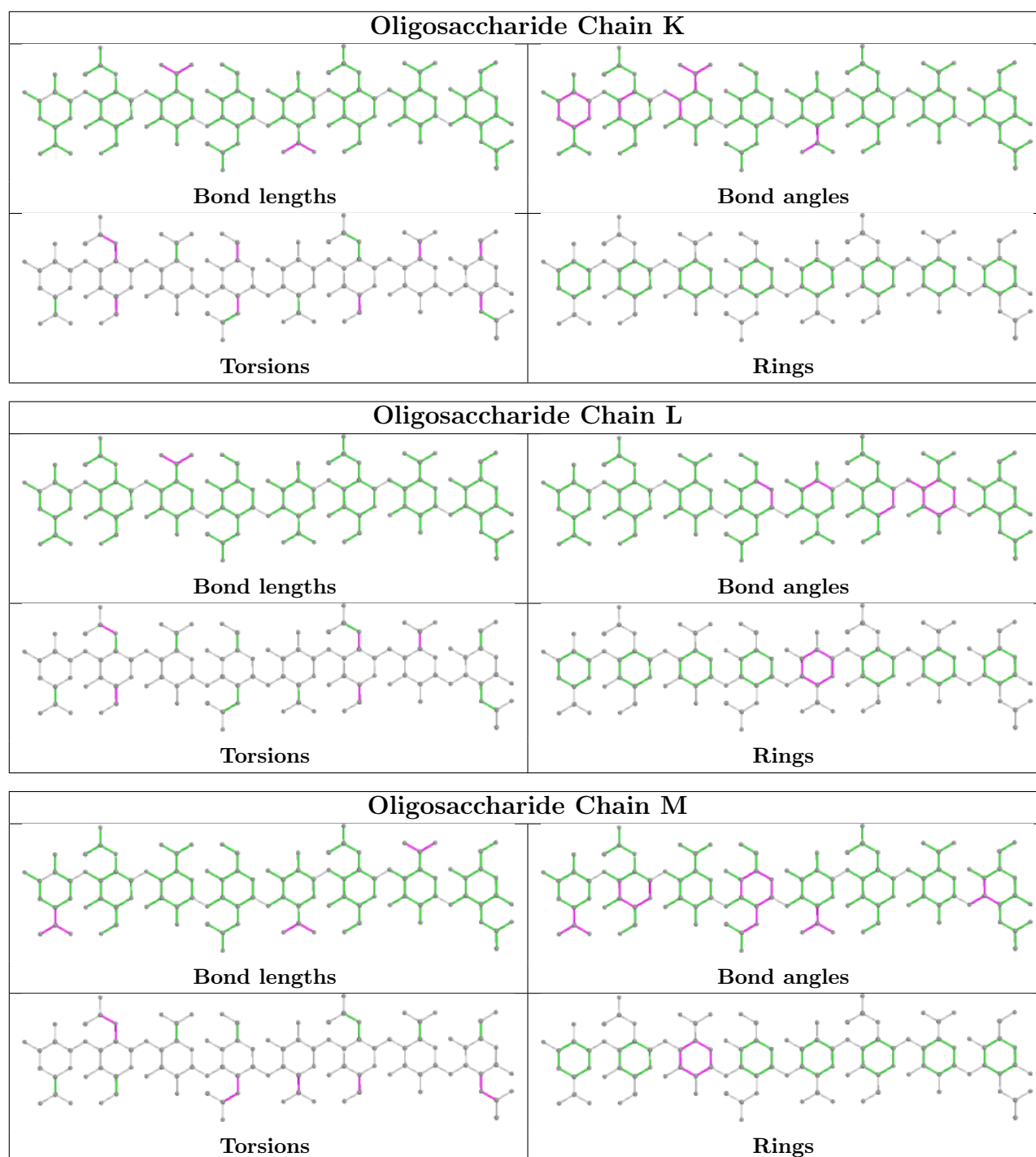


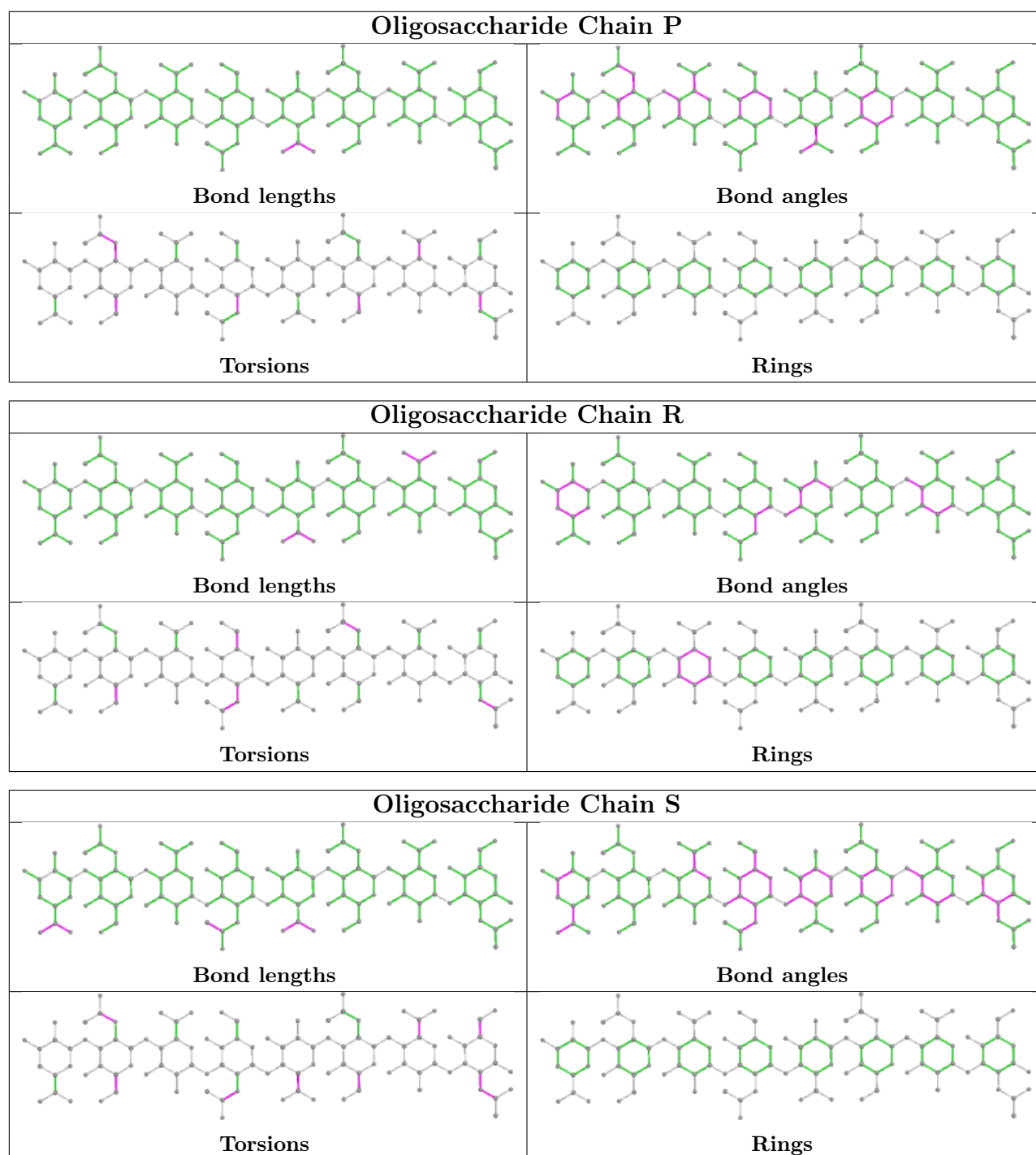


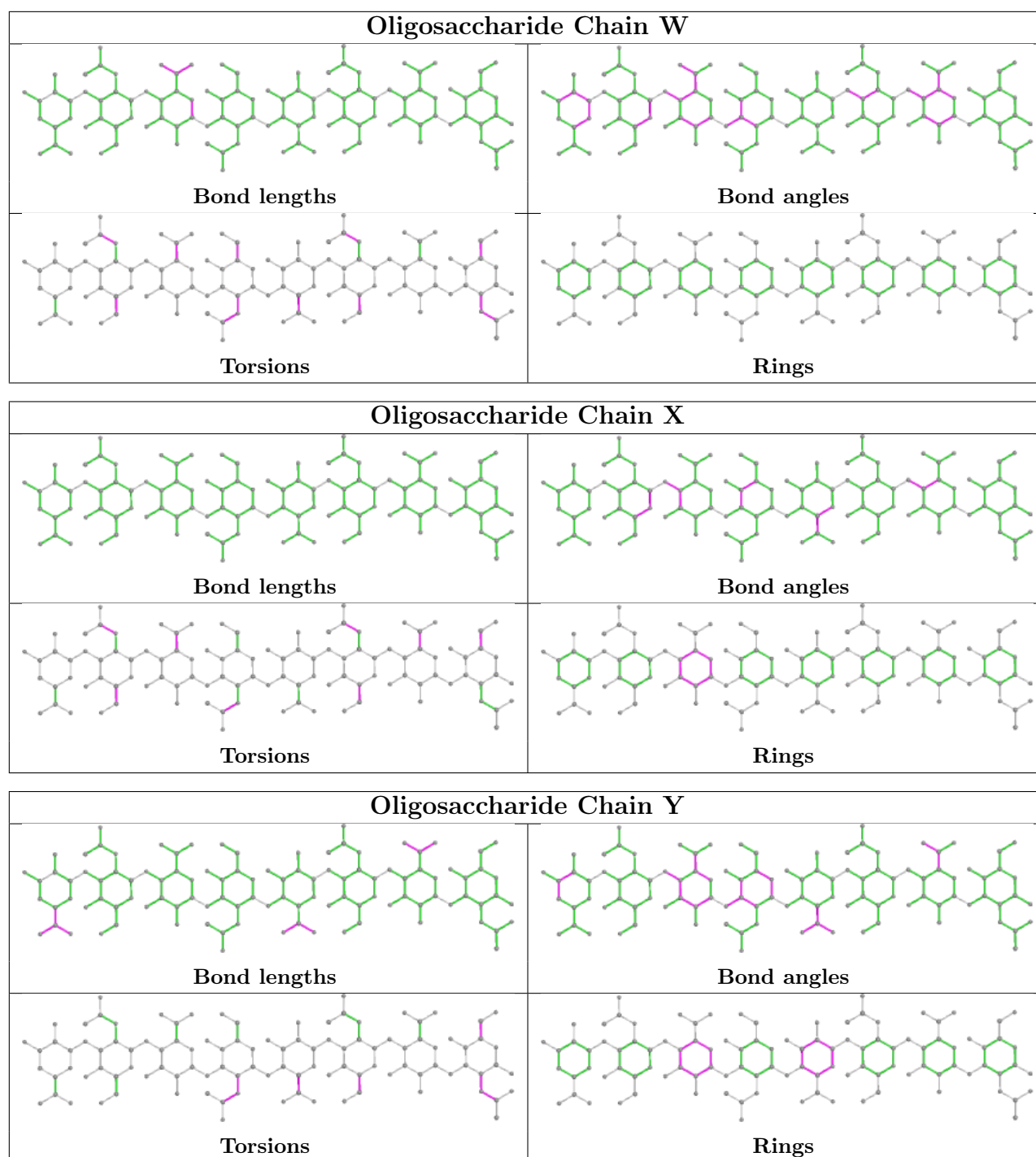












5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	361/379 (95%)	-0.35	1 (0%) 94 88	58, 100, 156, 180	0
1	B	361/379 (95%)	-0.35	2 (0%) 89 80	44, 98, 154, 201	0
1	C	361/379 (95%)	-0.39	1 (0%) 94 88	50, 98, 157, 223	0
1	D	349/379 (92%)	-0.32	1 (0%) 94 88	57, 110, 164, 216	0
1	E	357/379 (94%)	-0.27	2 (0%) 89 80	40, 113, 165, 216	0
1	F	366/379 (96%)	-0.23	1 (0%) 94 88	41, 113, 175, 229	0
1	G	363/379 (95%)	-0.39	1 (0%) 94 88	53, 103, 152, 205	0
1	H	361/379 (95%)	-0.37	1 (0%) 94 88	31, 100, 155, 199	0
1	I	362/379 (95%)	-0.43	0 100 100	33, 101, 150, 207	0
All	All	3241/3411 (95%)	-0.34	10 (0%) 94 88	31, 104, 161, 229	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	287	LYS	4.0
1	A	288	GLY	2.7
1	C	270	LYS	2.6
1	F	253	LYS	2.5
1	B	289	GLY	2.5

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
2	NAG	V	3	14/15	0.73	0.23	96,103,105,105	0
3	BDP	R	4	12/13	0.74	0.32	99,102,105,105	0
2	BDP	N	2	12/13	0.75	0.22	120,124,124,125	0
2	NAG	T	3	14/15	0.75	0.38	92,96,97,97	0
2	NAG	a	1	15/15	0.77	0.20	94,96,96,97	0
2	GCD	V	4	11/12	0.77	0.23	103,103,104,105	0
3	GCD	X	8	11/12	0.77	0.28	105,107,107,107	0
3	NAG	R	5	14/15	0.78	0.33	103,106,108,109	0
3	BDP	R	6	12/13	0.78	0.24	108,110,110,110	0
2	GCD	O	4	11/12	0.78	0.30	110,110,111,112	0
2	GCD	a	4	11/12	0.79	0.29	91,93,95,95	0
3	BDP	P	4	12/13	0.79	0.22	91,92,92,93	0
2	NAG	T	1	15/15	0.79	0.26	91,94,96,96	0
2	NAG	Z	3	14/15	0.80	0.25	102,106,107,108	0
2	BDP	V	2	12/13	0.80	0.22	104,105,106,106	0
3	BDP	K	4	12/13	0.81	0.22	91,93,93,93	0
2	NAG	U	1	15/15	0.81	0.29	107,113,113,114	0
3	BDP	K	6	12/13	0.82	0.25	95,97,97,98	0
2	GCD	U	4	11/12	0.82	0.36	106,106,107,107	0
3	NAG	X	7	14/15	0.82	0.24	102,105,106,107	0
2	NAG	a	3	14/15	0.82	0.24	93,94,95,95	0
2	NAG	U	3	14/15	0.83	0.29	107,108,109,110	0
3	BDP	X	6	12/13	0.83	0.29	104,105,106,107	0
3	NAG	Y	5	14/15	0.83	0.22	83,91,94,97	0
3	NAG	S	5	14/15	0.84	0.25	84,87,90,90	0
3	GCD	W	8	11/12	0.84	0.29	97,98,100,101	0
2	NAG	N	3	14/15	0.84	0.19	109,117,119,120	0
2	BDP	T	2	12/13	0.84	0.21	96,96,97,97	0
3	NAG	R	1	15/15	0.84	0.22	97,98,100,101	0
3	GCD	R	8	11/12	0.84	0.23	108,110,111,111	0
2	GCD	Q	4	11/12	0.85	0.23	86,86,87,87	0
3	NAG	X	5	14/15	0.85	0.19	96,100,101,102	0
3	NAG	L	5	14/15	0.85	0.23	85,88,91,92	0
2	GCD	N	4	11/12	0.85	0.24	92,100,102,103	0
3	NAG	P	7	14/15	0.85	0.20	95,96,97,97	0
2	BDP	a	2	12/13	0.85	0.14	94,96,97,97	0
2	NAG	Q	3	14/15	0.86	0.21	83,86,87,88	0
3	NAG	R	3	14/15	0.86	0.19	93,95,96,98	0
2	GCD	Z	4	11/12	0.86	0.18	103,103,105,105	0
3	GCD	S	8	11/12	0.86	0.33	99,100,102,102	0
3	BDP	L	2	12/13	0.86	0.20	85,86,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BDP	R	2	12/13	0.87	0.19	96,97,98,99	0
2	NAG	N	1	15/15	0.87	0.25	116,119,120,122	0
3	BDP	X	4	12/13	0.87	0.16	96,99,101,101	0
3	NAG	M	5	14/15	0.87	0.17	91,94,96,98	0
3	NAG	M	7	14/15	0.87	0.27	100,101,102,104	0
3	NAG	K	7	14/15	0.87	0.17	97,98,99,99	0
3	GCD	K	8	11/12	0.87	0.19	95,97,98,98	0
2	BDP	Q	2	12/13	0.87	0.17	85,86,87,87	0
3	BDP	M	2	12/13	0.88	0.19	90,92,94,94	0
3	BDP	W	4	12/13	0.88	0.18	82,86,88,88	0
3	BDP	W	6	12/13	0.88	0.30	92,94,95,95	0
2	NAG	O	1	15/15	0.88	0.16	104,105,107,109	0
2	NAG	J	1	14/15	0.88	0.20	84,85,87,87	0
2	NAG	Z	1	15/15	0.88	0.23	107,108,108,109	0
3	BDP	P	6	12/13	0.88	0.20	95,96,97,97	0
3	NAG	R	7	14/15	0.88	0.28	110,111,112,112	0
2	NAG	Q	1	15/15	0.88	0.16	86,86,90,91	0
2	GCD	T	4	11/12	0.88	0.26	95,97,98,99	0
3	BDP	Y	6	12/13	0.88	0.26	100,102,103,103	0
3	NAG	P	5	14/15	0.89	0.23	93,94,95,95	0
3	NAG	M	3	14/15	0.89	0.19	90,92,93,93	0
3	BDP	X	2	12/13	0.89	0.17	97,98,98,98	0
3	BDP	M	4	12/13	0.89	0.17	93,95,95,95	0
2	BDP	U	2	12/13	0.89	0.17	112,113,113,114	0
3	BDP	S	2	12/13	0.89	0.16	75,78,82,82	0
3	BDP	S	4	12/13	0.89	0.17	77,79,82,83	0
2	BDP	Z	2	12/13	0.89	0.20	108,109,109,110	0
3	BDP	Y	2	12/13	0.89	0.19	81,82,86,87	0
3	GCD	M	8	11/12	0.89	0.28	105,105,106,106	0
2	NAG	O	3	14/15	0.89	0.19	112,114,115,115	0
3	BDP	L	4	12/13	0.90	0.19	87,88,89,90	0
3	NAG	W	3	14/15	0.90	0.17	77,85,86,87	0
3	NAG	K	1	15/15	0.90	0.24	93,94,97,97	0
3	NAG	M	1	15/15	0.90	0.21	76,89,91,91	0
2	BDP	O	2	12/13	0.90	0.27	111,113,113,114	0
2	NAG	J	3	14/15	0.90	0.17	68,74,76,76	0
3	NAG	L	3	14/15	0.90	0.18	85,87,88,89	0
3	BDP	M	6	12/13	0.91	0.23	100,101,101,102	0
3	BDP	P	2	12/13	0.91	0.15	83,87,91,91	0
3	NAG	W	5	14/15	0.91	0.19	87,89,90,91	0
3	BDP	Y	4	12/13	0.91	0.18	86,89,92,92	0
3	BDP	W	2	12/13	0.91	0.21	85,86,91,91	0

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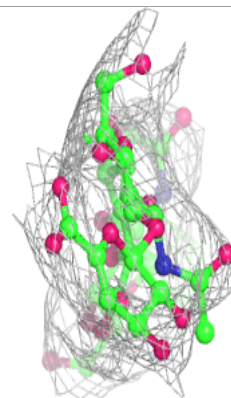
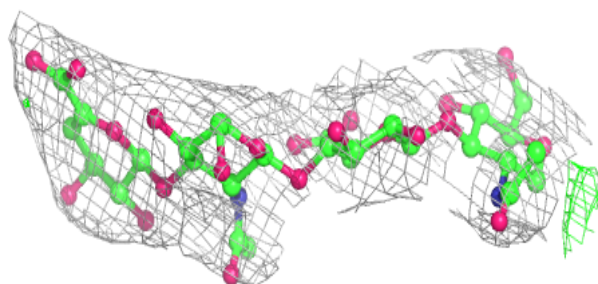
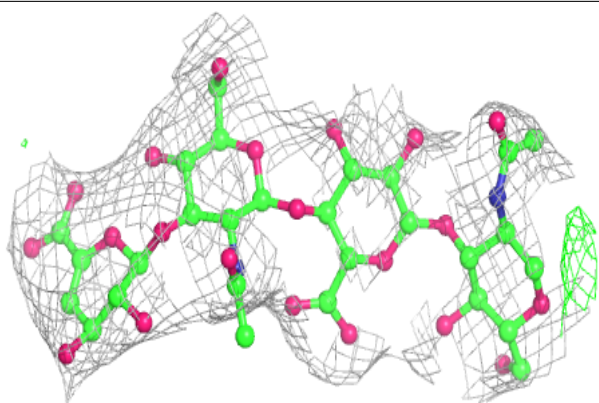
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	W	7	14/15	0.91	0.28	95,96,97,98	0
3	GCD	Y	8	11/12	0.91	0.21	104,104,105,105	0
3	NAG	P	1	15/15	0.92	0.18	90,90,94,95	0
3	NAG	X	3	14/15	0.92	0.15	96,97,98,98	0
3	NAG	S	7	14/15	0.92	0.25	94,95,96,98	0
2	NAG	V	1	14/15	0.92	0.17	101,103,104,105	0
3	NAG	K	3	14/15	0.92	0.16	86,90,91,91	0
2	GCD	J	4	11/12	0.92	0.15	76,78,80,81	0
3	GCD	P	8	11/12	0.93	0.17	92,93,94,94	0
3	BDP	L	6	12/13	0.93	0.19	88,90,91,92	0
3	NAG	Y	3	14/15	0.93	0.18	79,80,82,85	0
3	GCD	L	8	11/12	0.93	0.33	95,96,97,97	0
3	BDP	K	2	12/13	0.93	0.11	92,93,93,93	0
3	NAG	W	1	15/15	0.93	0.17	80,83,85,85	0
3	NAG	Y	7	14/15	0.93	0.28	102,104,105,106	0
3	NAG	P	3	14/15	0.93	0.15	85,87,88,90	0
3	BDP	S	6	12/13	0.94	0.19	91,92,93,94	0
3	NAG	L	1	15/15	0.94	0.15	80,81,83,84	0
3	NAG	Y	1	15/15	0.94	0.16	83,84,86,86	0
3	NAG	X	1	15/15	0.94	0.18	97,98,98,99	0
3	NAG	L	7	14/15	0.94	0.22	91,94,95,95	0
3	NAG	S	3	14/15	0.95	0.14	77,77,78,79	0
3	NAG	S	1	15/15	0.95	0.16	79,80,82,83	0
2	BDP	J	2	12/13	0.95	0.12	77,82,83,83	0
3	NAG	K	5	14/15	0.96	0.16	92,93,94,95	0

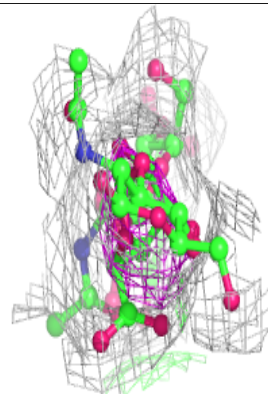
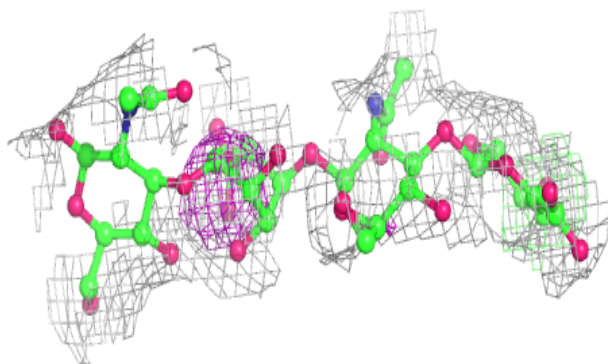
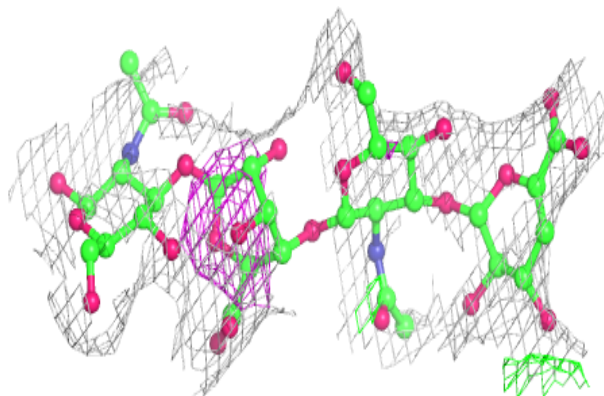
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain J:

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

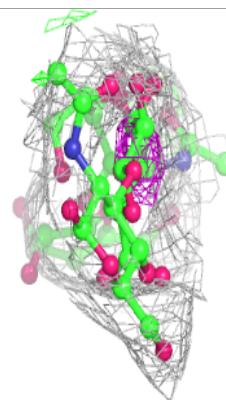
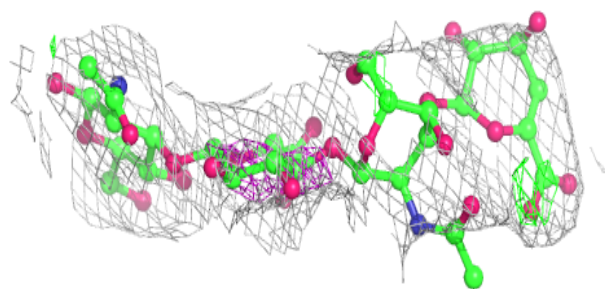
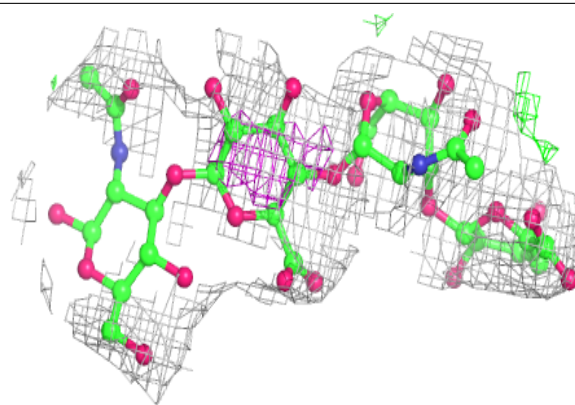
**Electron density around Chain N:**

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

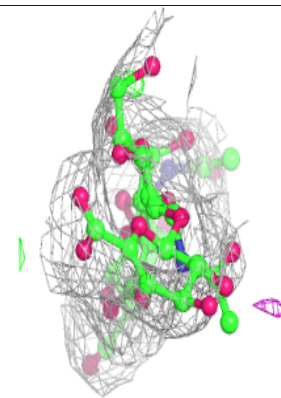
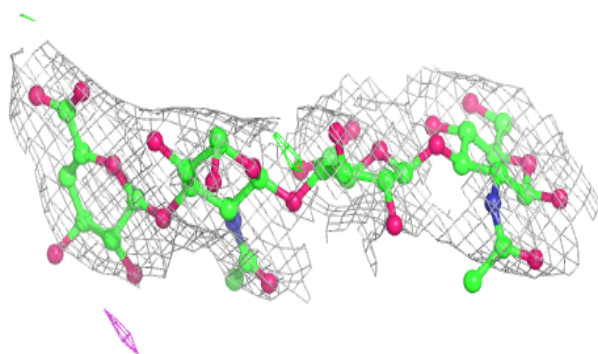
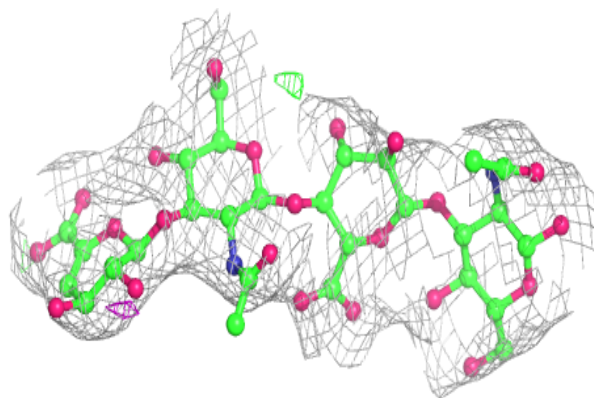


Electron density around Chain O:

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

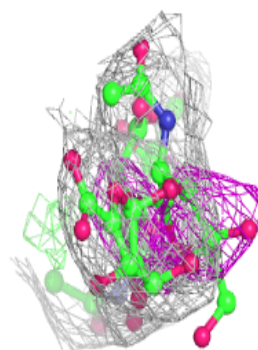
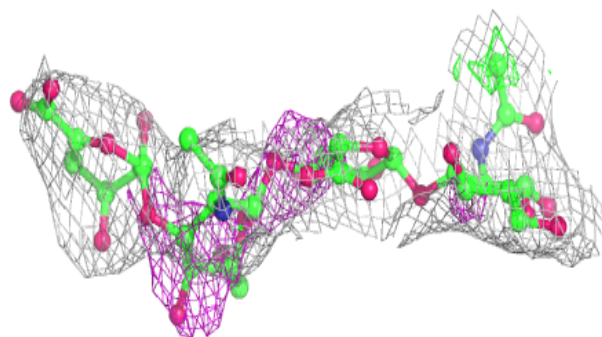
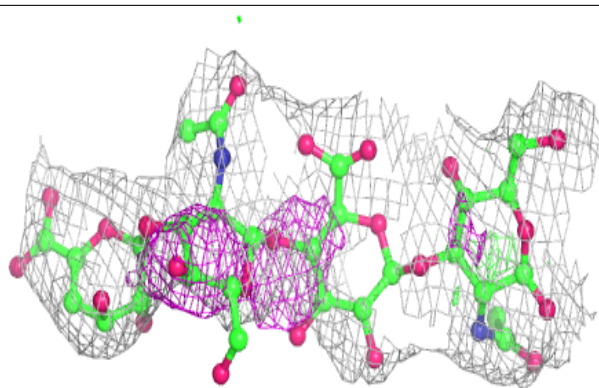
**Electron density around Chain Q:**

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

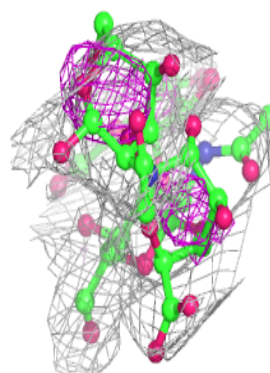
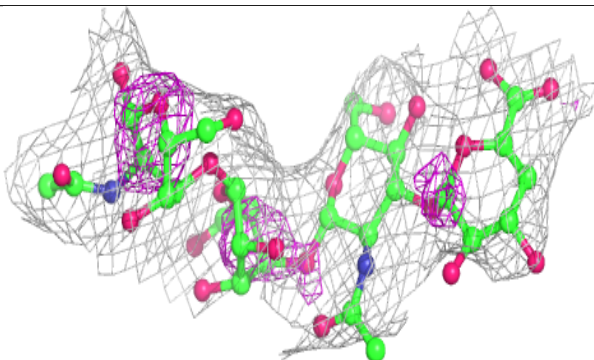
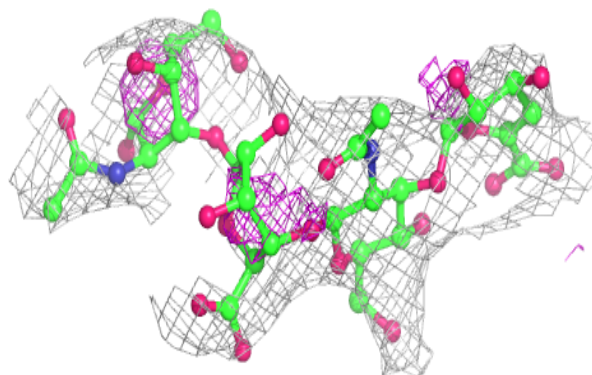


Electron density around Chain T:

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

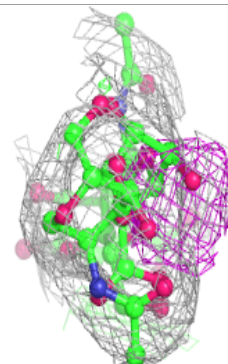
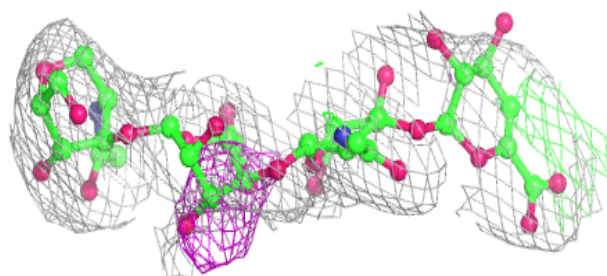
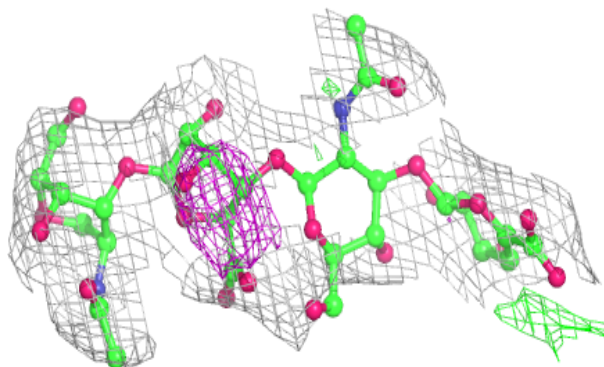
**Electron density around Chain U:**

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

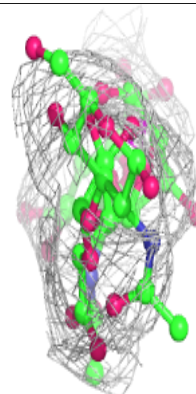
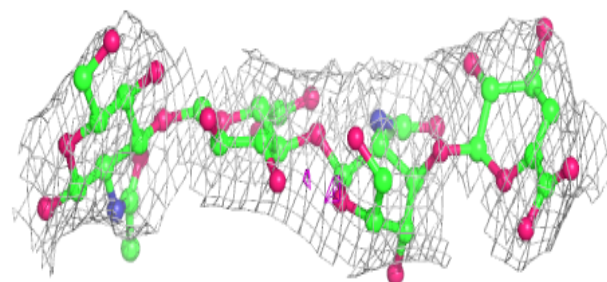
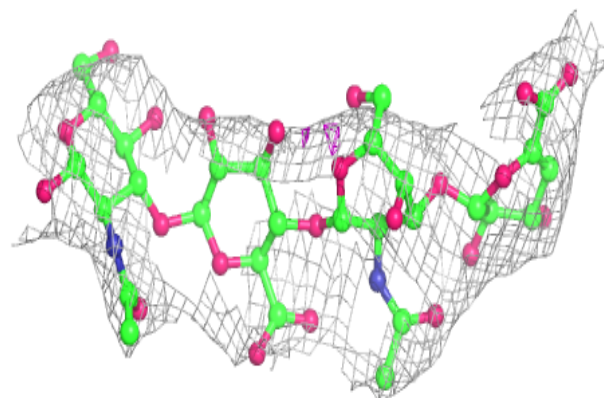


Electron density around Chain V:

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

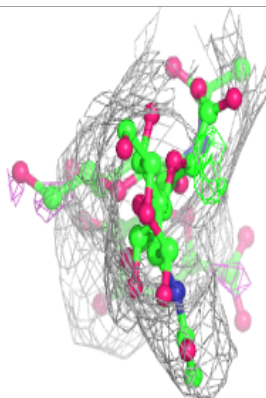
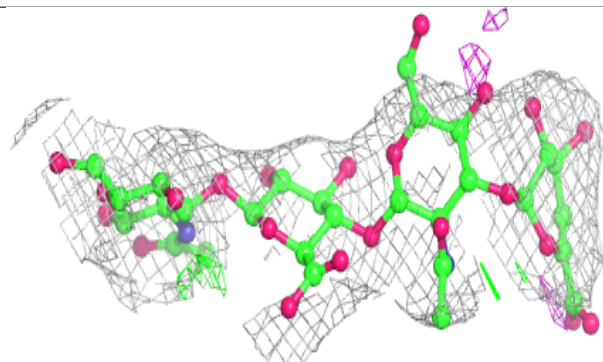
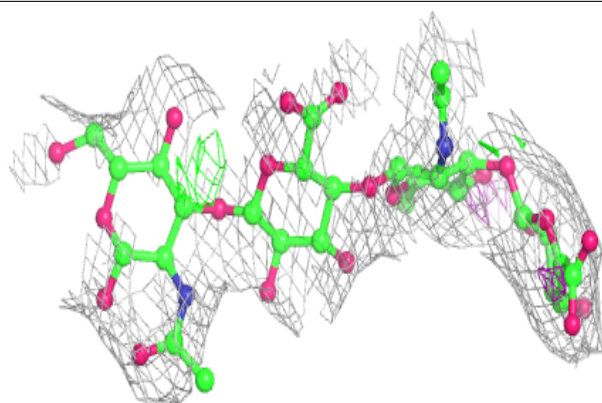
**Electron density around Chain Z:**

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

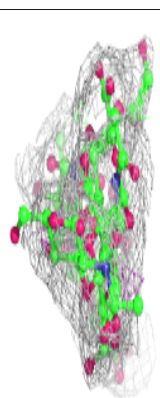
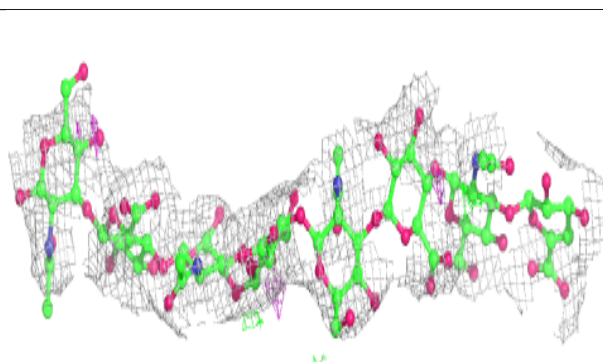
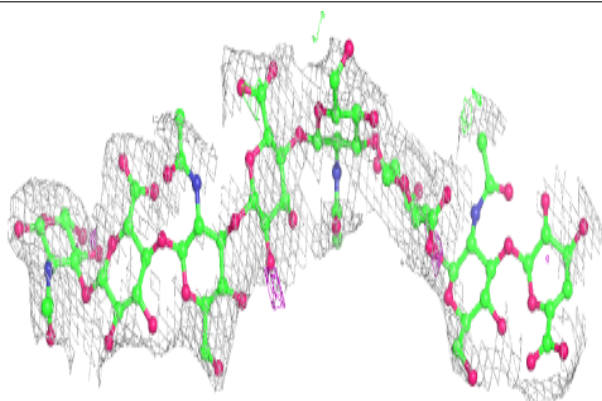


Electron density around Chain a:

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

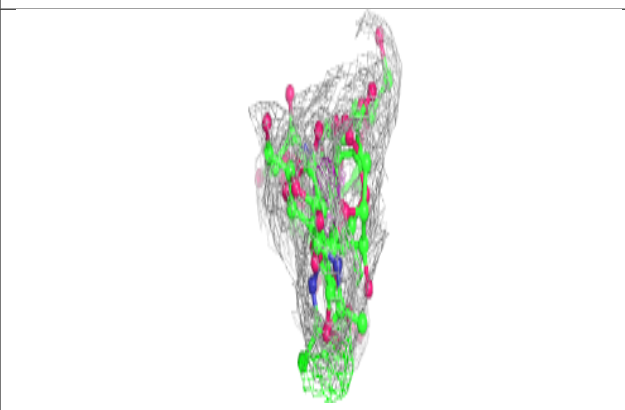
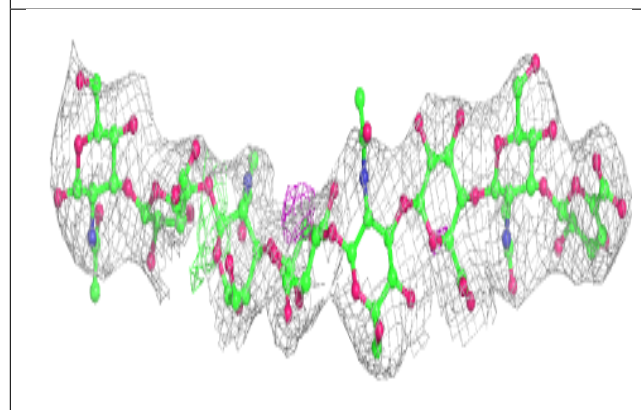
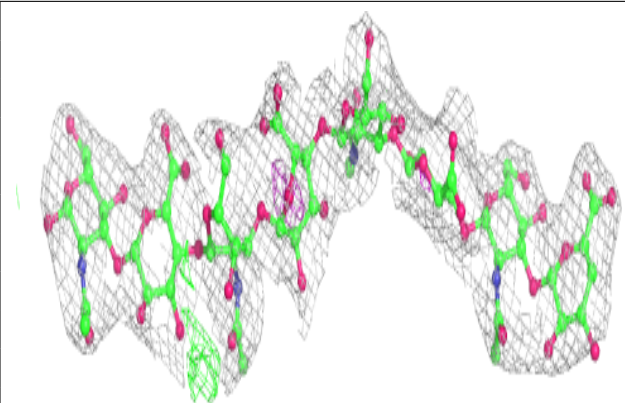
**Electron density around Chain K:**

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

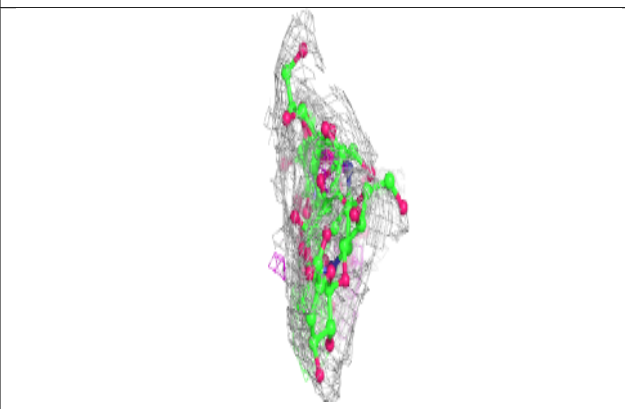
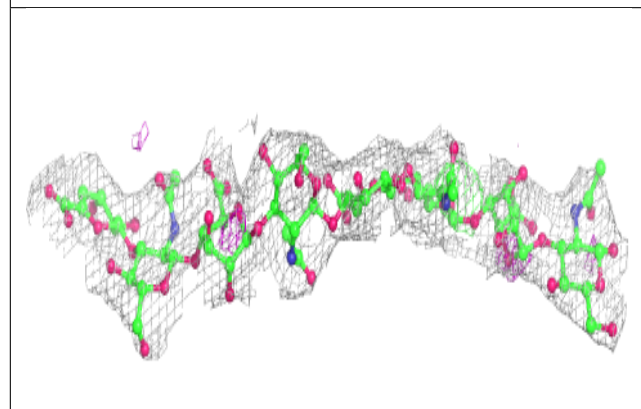
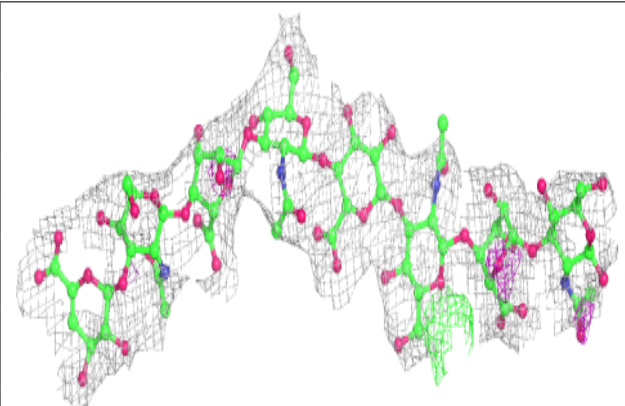


Electron density around Chain L:

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

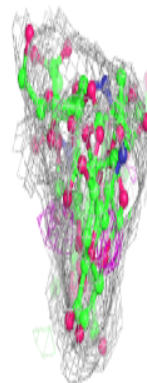
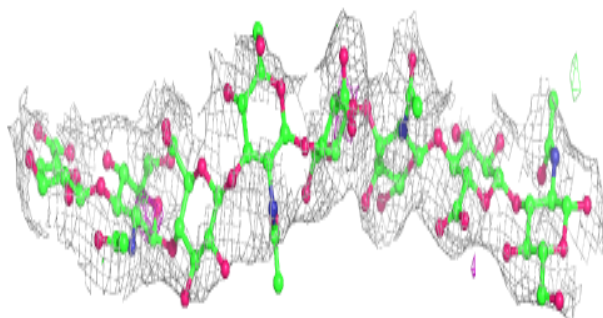
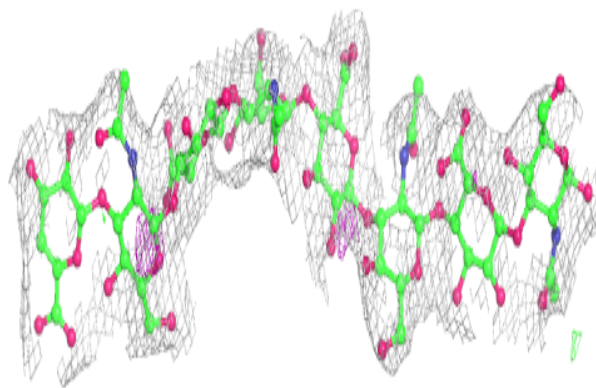
**Electron density around Chain M:**

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

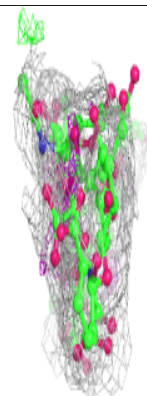
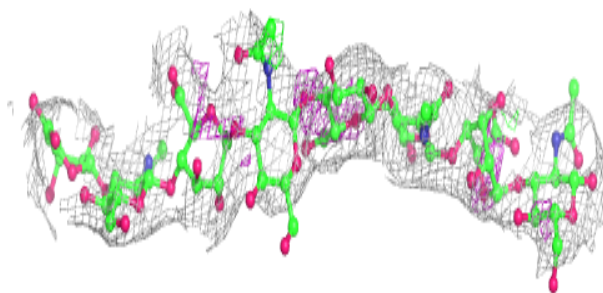
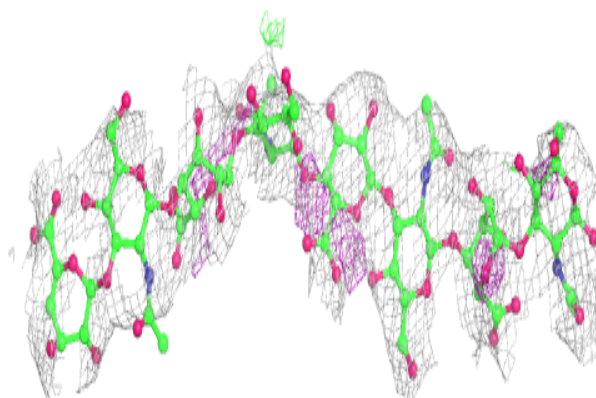


Electron density around Chain P:

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

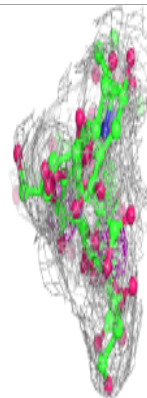
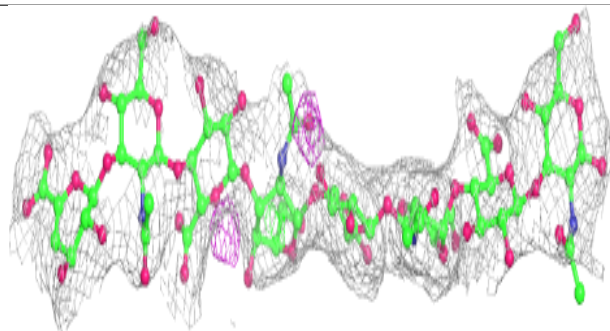
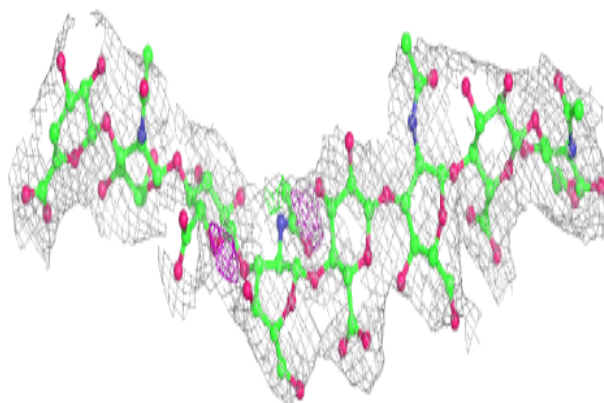
**Electron density around Chain R:**

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

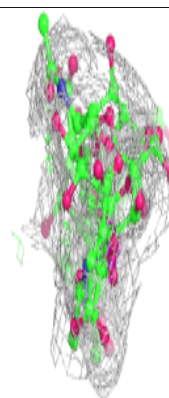
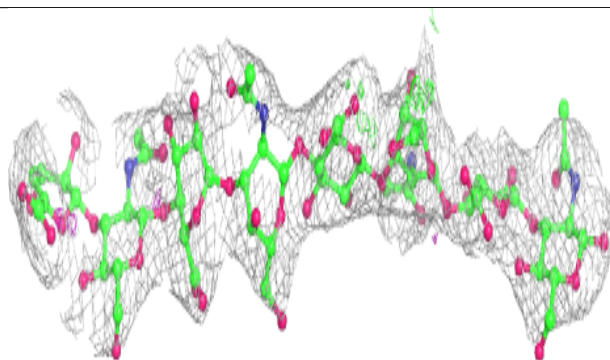
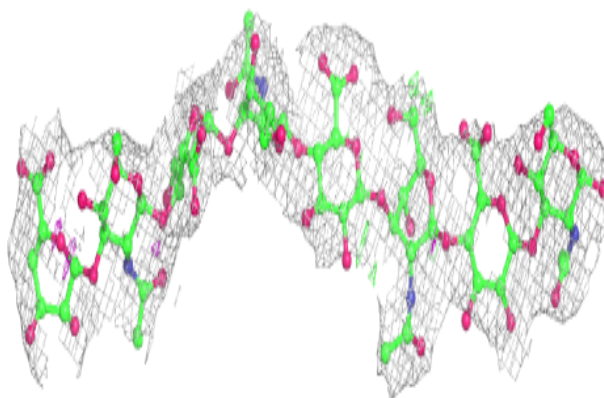


Electron density around Chain S:

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

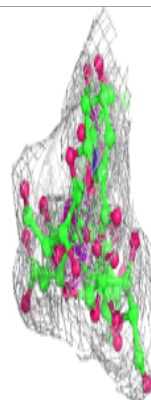
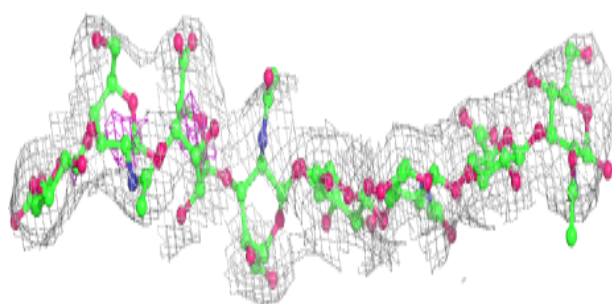
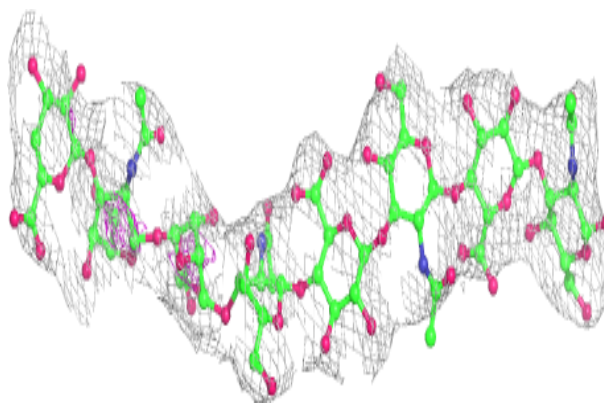
**Electron density around Chain W:**

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

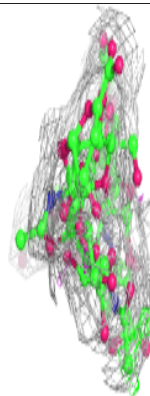
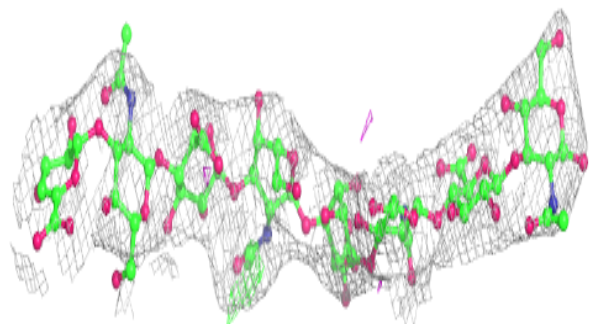
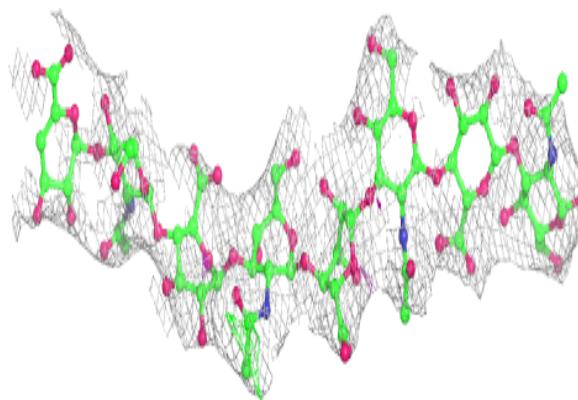


Electron density around Chain X:

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

**Electron density around Chain Y:**

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.