



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2022 – 12:38 PM JST

PDB ID : 7F82  
Title : Structure of the bacterial cellulose synthase subunit Z in complex with cellobiosaccharides from *Enterobacter* sp. CJF-002  
Authors : Fujiwara, T.; Fujishima, A.; Yao, M.  
Deposited on : 2021-06-30  
Resolution : 1.30 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](mailto: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.

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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	:	2.27
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)	:	2.27

**i**

## X-RAY DIFFRACTION

A.

the following graphic. The table shows the number of entries on which the scores are based.

Metric

the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled.

Mol

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Mol	Chain	Length	Quality of chain
2	J	2	 100%
2	M	2	 50% 50%
3	F	3	 100%
3	K	3	 100%
3	N	3	 67% 33%
4	G	4	 50% 50%
4	I	4	 50% 50%
4	L	4	 75% 25%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BGC	G	1	X	-	-	-
4	BGC	I	1	X	-	-	-
4	BGC	L	1	X	-	-	-
5	SRT	C	401	X	-	-	-
5	SRT	D	401	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12518 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 Glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	6	0
			2755	1770	483	496	6			
1	B	338	Total	C	N	O	S	0	5	0
			2742	1762	477	497	6			
1	C	338	Total	C	N	O	S	0	4	0
			2741	1761	479	495	6			
1	D	338	Total	C	N	O	S	0	6	0
			2752	1768	482	496	6			

There are 20 discrepancies between the modelled and reference sequences:

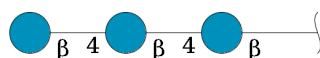
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLY	-	expression tag	UNP K0IUUV6
A	18	SER	-	expression tag	UNP K0IUUV6
A	19	HIS	-	expression tag	UNP K0IUUV6
A	20	MET	-	expression tag	UNP K0IUUV6
A	242	ALA	ASP	engineered mutation	UNP K0IUUV6
B	17	GLY	-	expression tag	UNP K0IUUV6
B	18	SER	-	expression tag	UNP K0IUUV6
B	19	HIS	-	expression tag	UNP K0IUUV6
B	20	MET	-	expression tag	UNP K0IUUV6
B	242	ALA	ASP	engineered mutation	UNP K0IUUV6
C	17	GLY	-	expression tag	UNP K0IUUV6
C	18	SER	-	expression tag	UNP K0IUUV6
C	19	HIS	-	expression tag	UNP K0IUUV6
C	20	MET	-	expression tag	UNP K0IUUV6
C	242	ALA	ASP	engineered mutation	UNP K0IUUV6
D	17	GLY	-	expression tag	UNP K0IUUV6
D	18	SER	-	expression tag	UNP K0IUUV6
D	19	HIS	-	expression tag	UNP K0IUUV6
D	20	MET	-	expression tag	UNP K0IUUV6
D	242	ALA	ASP	engineered mutation	UNP K0IUUV6

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



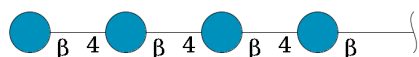
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			
2	J	2	Total	C	O	0	0	0
			23	12	11			
2	M	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	F	3	Total	C	O	0	0	0
			34	18	16			
3	K	3	Total	C	O	0	0	0
			34	18	16			
3	N	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 4 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



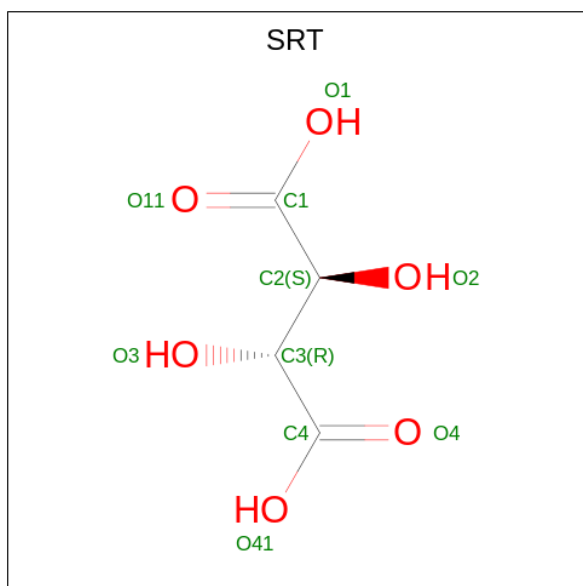
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	G	4	Total	C	O	0	0	0
			45	24	21			
4	I	4	Total	C	O	0	0	0
			45	24	21			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	L	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 5 is S,R MESO-TARTARIC ACID (three-letter code: SRT) (formula:  $C_4H_6O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			10	4	6		
5	D	1	Total	C	O	0	0
			10	4	6		

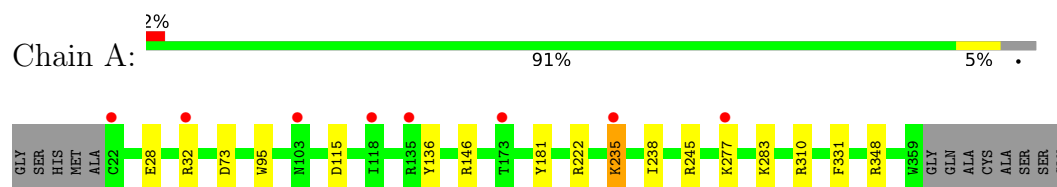
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	323	Total	O	0	0
			323	323		
6	B	313	Total	O	0	0
			313	313		
6	C	279	Total	O	0	0
			279	279		
6	D	264	Total	O	0	0
			264	264		

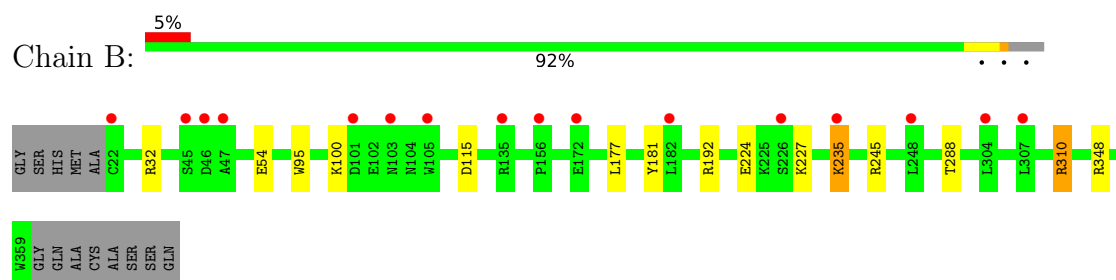
### 3 Residue-property plots [i](#)

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.

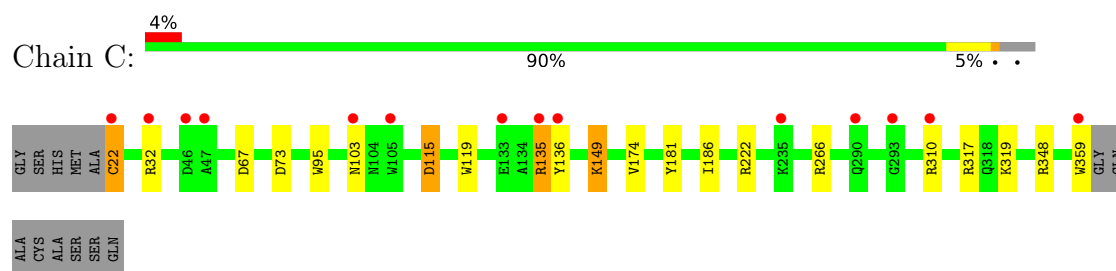
- Molecule 1: Glucanase



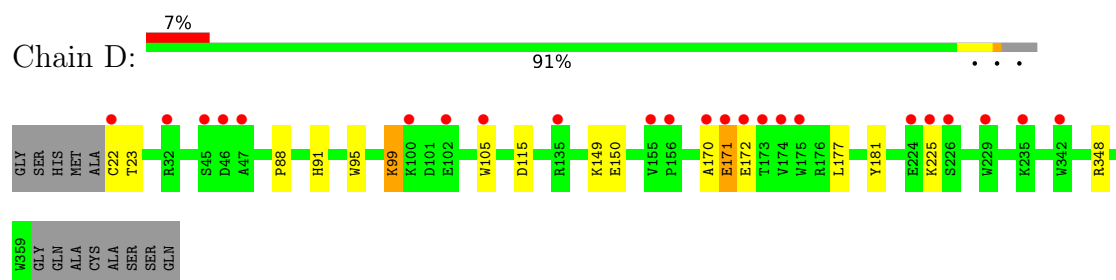
- Molecule 1: Glucanase



- Molecule 1: Glucanase



- Molecule 1: Glucanase



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain E:  100%

BGC1  
BGC2

- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain H:  100%

BGC1  
BGC2

- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain J:  100%

BGC1  
BGC2

- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain M:  50% 50%

BGC1  
BGC2

- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain F:  100%


BGC1  
BGC2  
BGC3

- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain K:  100%

BGC1  
BGC2  
BGC3

- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain N:  67% 33%

BGC1  
BGC2  
BGC3


- Molecule 4: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



Chain G:  50% 50%

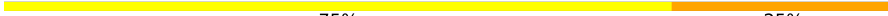
BCC1  
BCC2  
BCC3  
BCC4

- Molecule 4: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain I:  50% 50%

BCC1  
BCC2  
BCC3  
BCC4

- Molecule 4: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain L:  75% 25%

BCC1  
BCC2  
BCC3  
BCC4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.28Å 92.86Å 90.50Å 90.00° 98.41° 90.00°	Depositor
Resolution (Å)	42.51 – 1.30 42.51 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.51-1.30) 99.5 (42.51-1.30)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 1.30Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.169 , 0.187 0.169 , 0.170	Depositor DCC
$R_{free}$ test set	17808 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.7	Xtriage
Anisotropy	0.649	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	12518	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BGC, SRT

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	0.72	3/2851 (0.1%)	0.94	9/3885 (0.2%)
1	B	0.68	1/2835 (0.0%)	0.88	8/3865 (0.2%)
1	C	0.67	2/2831 (0.1%)	0.97	16/3858 (0.4%)
1	D	0.66	2/2848 (0.1%)	0.85	11/3880 (0.3%)
All	All	0.69	8/11365 (0.1%)	0.91	44/15488 (0.3%)

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	C	1	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	171	GLU	CB-CG	-8.60	1.35	1.52
1	C	149	LYS	CE-NZ	7.54	1.68	1.49
1	B	54	GLU	CD-OE1	6.07	1.32	1.25
1	D	171	GLU	CD-OE2	6.00	1.32	1.25
1	A	277	LYS	CG-CD	5.56	1.71	1.52

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	135	ARG	NE-CZ-NH1	-12.70	113.95	120.30
1	A	310[A]	ARG	NE-CZ-NH2	11.62	126.11	120.30
1	A	310[B]	ARG	NE-CZ-NH2	11.62	126.11	120.30
1	A	310[A]	ARG	NE-CZ-NH1	-10.90	114.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310[B]	ARG	NE-CZ-NH1	-10.90	114.85	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	22	CYS	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	22	CYS	Mainchain

## 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	A	2755	0	2690	14	0
1	B	2742	0	2670	7	1
1	C	2741	0	2669	15	0
1	D	2752	0	2687	9	0
2	E	23	0	20	4	1
2	H	23	0	20	0	0
2	J	23	0	20	0	0
2	M	23	0	20	1	0
3	F	34	0	29	0	0
3	K	34	0	30	0	0
3	N	34	0	30	1	0
4	G	45	0	39	3	0
4	I	45	0	39	2	0
4	L	45	0	39	4	0
5	C	10	0	3	0	0
5	D	10	0	3	0	0
6	A	323	0	0	2	0
6	B	313	0	0	1	0
6	C	279	0	0	4	2
6	D	264	0	0	4	2
All	All	12518	0	11008	49	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 49 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LYS:CE	1:C:149:LYS:NZ	1.67	1.53
1:C:149:LYS:NZ	1:C:149:LYS:CD	2.22	1.01
1:C:222:ARG:NH1	6:C:501:HOH:O	2.13	0.81
1:C:149:LYS:NZ	1:C:149:LYS:HD3	1.97	0.78
1:C:32:ARG:NH2	6:C:502:HOH:O	2.19	0.76

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:511:HOH:O	6:D:504:HOH:O[1_556]	1.82	0.38
6:C:679:HOH:O	6:D:534:HOH:O[2_445]	2.11	0.09
1:B:288:THR:O	2:E:1:BGC:O2[2_555]	2.18	0.02

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	342/351 (97%)	338 (99%)	4 (1%)	0	100	100
1	B	341/351 (97%)	336 (98%)	5 (2%)	0	100	100
1	C	340/351 (97%)	336 (99%)	4 (1%)	0	100	100
1	D	342/351 (97%)	336 (98%)	6 (2%)	0	100	100
All	All	1365/1404 (97%)	1346 (99%)	19 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	283/285 (99%)	282 (100%)	1 (0%)	91	76
1	B	282/285 (99%)	281 (100%)	1 (0%)	91	76
1	C	281/285 (99%)	280 (100%)	1 (0%)	91	76
1	D	283/285 (99%)	282 (100%)	1 (0%)	91	76
All	All	1129/1140 (99%)	1125 (100%)	4 (0%)	91	76

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	LYS
1	B	235	LYS
1	C	135	ARG
1	D	177	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

29 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	BGC	E	1	2	12,12,12	1.36	1 (8%)	17,17,17	1.77	4 (23%)
2	BGC	E	2	2	11,11,12	1.98	2 (18%)	15,15,17	1.70	6 (40%)
3	BGC	F	1	3	12,12,12	1.39	2 (16%)	17,17,17	1.25	2 (11%)
3	BGC	F	2	3	11,11,12	1.44	2 (18%)	15,15,17	1.44	3 (20%)
3	BGC	F	3	3	11,11,12	2.22	2 (18%)	15,15,17	0.94	0
4	BGC	G	1	4	12,12,12	1.40	1 (8%)	17,17,17	3.15	8 (47%)
4	BGC	G	2	4	11,11,12	1.22	1 (9%)	15,15,17	1.34	1 (6%)
4	BGC	G	3	4	11,11,12	1.58	2 (18%)	15,15,17	1.08	1 (6%)
4	BGC	G	4	4	11,11,12	2.65	6 (54%)	15,15,17	1.28	1 (6%)
2	BGC	H	1	2	12,12,12	1.30	1 (8%)	17,17,17	0.98	0
2	BGC	H	2	2	11,11,12	1.83	3 (27%)	15,15,17	1.61	4 (26%)
4	BGC	I	1	4	12,12,12	1.47	3 (25%)	17,17,17	1.65	4 (23%)
4	BGC	I	2	4	11,11,12	1.32	2 (18%)	15,15,17	1.55	4 (26%)
4	BGC	I	3	4	11,11,12	1.75	3 (27%)	15,15,17	1.21	1 (6%)
4	BGC	I	4	4	11,11,12	2.38	5 (45%)	15,15,17	1.07	1 (6%)
2	BGC	J	1	2	12,12,12	1.32	1 (8%)	17,17,17	0.87	0
2	BGC	J	2	2	11,11,12	1.92	3 (27%)	15,15,17	1.46	2 (13%)
3	BGC	K	1	3	12,12,12	1.20	1 (8%)	17,17,17	0.98	0
3	BGC	K	2	3	11,11,12	1.41	1 (9%)	15,15,17	1.30	2 (13%)
3	BGC	K	3	3	11,11,12	1.58	2 (18%)	15,15,17	1.04	1 (6%)
4	BGC	L	1	4	12,12,12	1.50	2 (16%)	17,17,17	2.92	8 (47%)
4	BGC	L	2	4	11,11,12	1.09	0	15,15,17	0.91	0
4	BGC	L	3	4	11,11,12	1.46	3 (27%)	15,15,17	1.25	2 (13%)
4	BGC	L	4	4	11,11,12	2.83	6 (54%)	15,15,17	1.68	3 (20%)
2	BGC	M	1	2	12,12,12	1.35	1 (8%)	17,17,17	1.17	2 (11%)
2	BGC	M	2	2	11,11,12	1.82	2 (18%)	15,15,17	1.11	2 (13%)
3	BGC	N	1	3	12,12,12	1.23	1 (8%)	17,17,17	0.99	0
3	BGC	N	2	3	11,11,12	1.58	3 (27%)	15,15,17	0.96	0
3	BGC	N	3	3	11,11,12	2.04	2 (18%)	15,15,17	1.14	1 (6%)

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	BGC	E	1	2	-	1/2/22/22	0/1/1/1
2	BGC	E	2	2	-	0/2/19/22	0/1/1/1
3	BGC	F	1	3	-	0/2/22/22	0/1/1/1
3	BGC	F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	F	3	3	-	0/2/19/22	0/1/1/1
4	BGC	G	1	4	1/1/5/5	0/2/22/22	0/1/1/1
4	BGC	G	2	4	-	0/2/19/22	0/1/1/1
4	BGC	G	3	4	-	0/2/19/22	0/1/1/1
4	BGC	G	4	4	-	2/2/19/22	0/1/1/1
2	BGC	H	1	2	-	0/2/22/22	0/1/1/1
2	BGC	H	2	2	-	0/2/19/22	0/1/1/1
4	BGC	I	1	4	1/1/5/5	1/2/22/22	0/1/1/1
4	BGC	I	2	4	-	0/2/19/22	0/1/1/1
4	BGC	I	3	4	-	0/2/19/22	0/1/1/1
4	BGC	I	4	4	-	0/2/19/22	0/1/1/1
2	BGC	J	1	2	-	0/2/22/22	0/1/1/1
2	BGC	J	2	2	-	0/2/19/22	0/1/1/1
3	BGC	K	1	3	-	0/2/22/22	0/1/1/1
3	BGC	K	2	3	-	0/2/19/22	0/1/1/1
3	BGC	K	3	3	-	0/2/19/22	0/1/1/1
4	BGC	L	1	4	1/1/5/5	0/2/22/22	0/1/1/1
4	BGC	L	2	4	-	0/2/19/22	0/1/1/1
4	BGC	L	3	4	-	0/2/19/22	0/1/1/1
4	BGC	L	4	4	-	2/2/19/22	0/1/1/1
2	BGC	M	1	2	-	0/2/22/22	0/1/1/1
2	BGC	M	2	2	-	0/2/19/22	0/1/1/1
3	BGC	N	1	3	-	0/2/22/22	0/1/1/1
3	BGC	N	2	3	-	0/2/19/22	0/1/1/1
3	BGC	N	3	3	-	2/2/19/22	0/1/1/1

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	4	BGC	C2-C3	-6.56	1.42	1.52
3	F	3	BGC	O5-C1	6.38	1.53	1.43
3	N	3	BGC	O5-C1	6.05	1.53	1.43
4	G	4	BGC	C2-C3	-5.64	1.44	1.52
3	K	3	BGC	O5-C1	4.48	1.50	1.43

The worst 5 of 63 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	BGC	O5-C1-C2	-7.75	96.45	110.28
4	L	1	BGC	O2-C2-C1	7.30	126.08	109.16
4	G	1	BGC	O2-C2-C1	6.62	124.51	109.16
4	L	1	BGC	O5-C1-C2	-6.43	98.81	110.28
4	G	1	BGC	O3-C3-C2	-4.47	100.01	110.35

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	G	1	BGC	C1
4	I	1	BGC	C1
4	L	1	BGC	C1

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	4	BGC	O5-C5-C6-O6
4	L	4	BGC	C4-C5-C6-O6
4	G	4	BGC	O5-C5-C6-O6
4	G	4	BGC	C4-C5-C6-O6
2	E	1	BGC	O5-C5-C6-O6

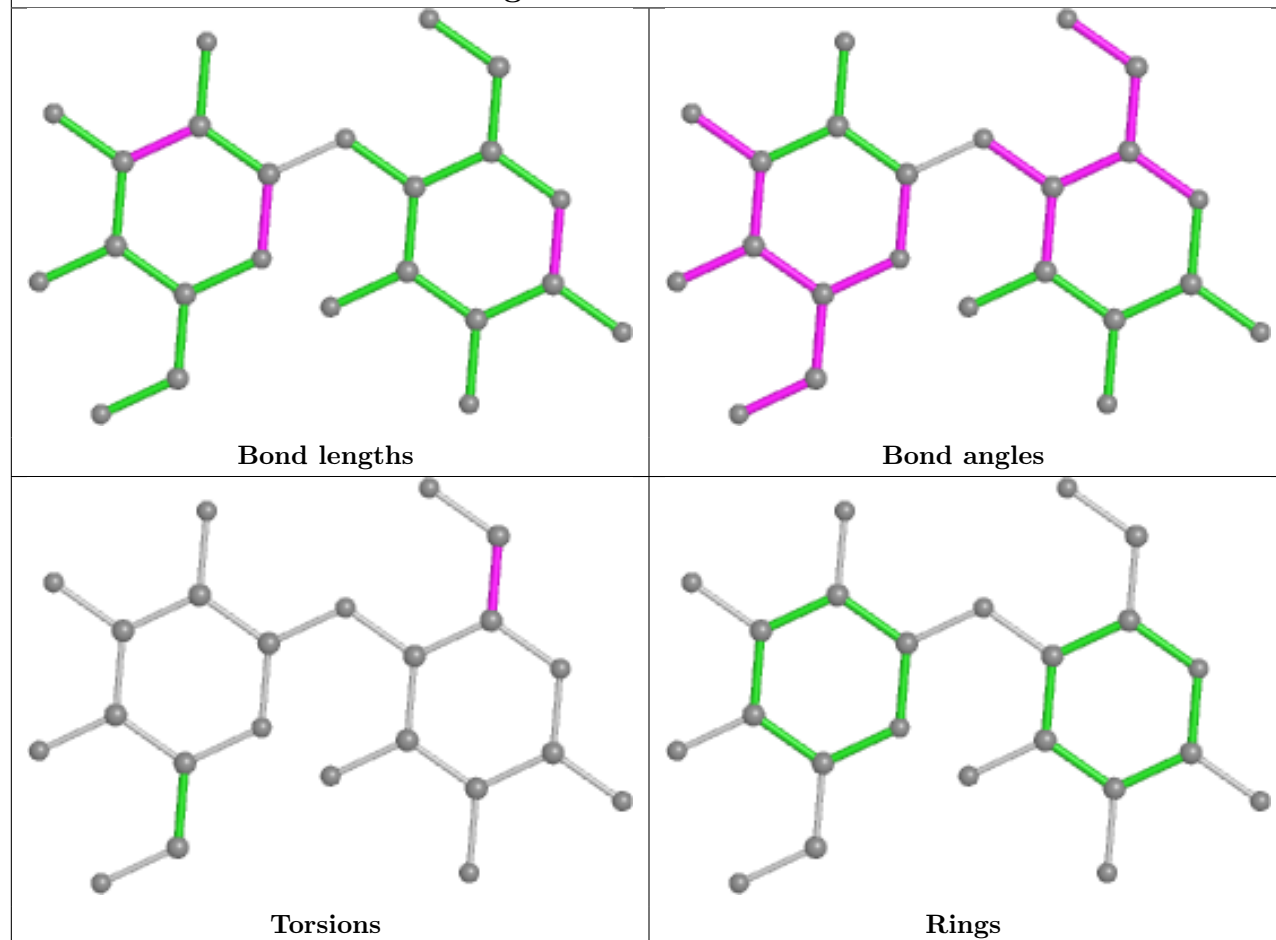
There are no ring outliers.

10 monomers are involved in 16 short contacts:

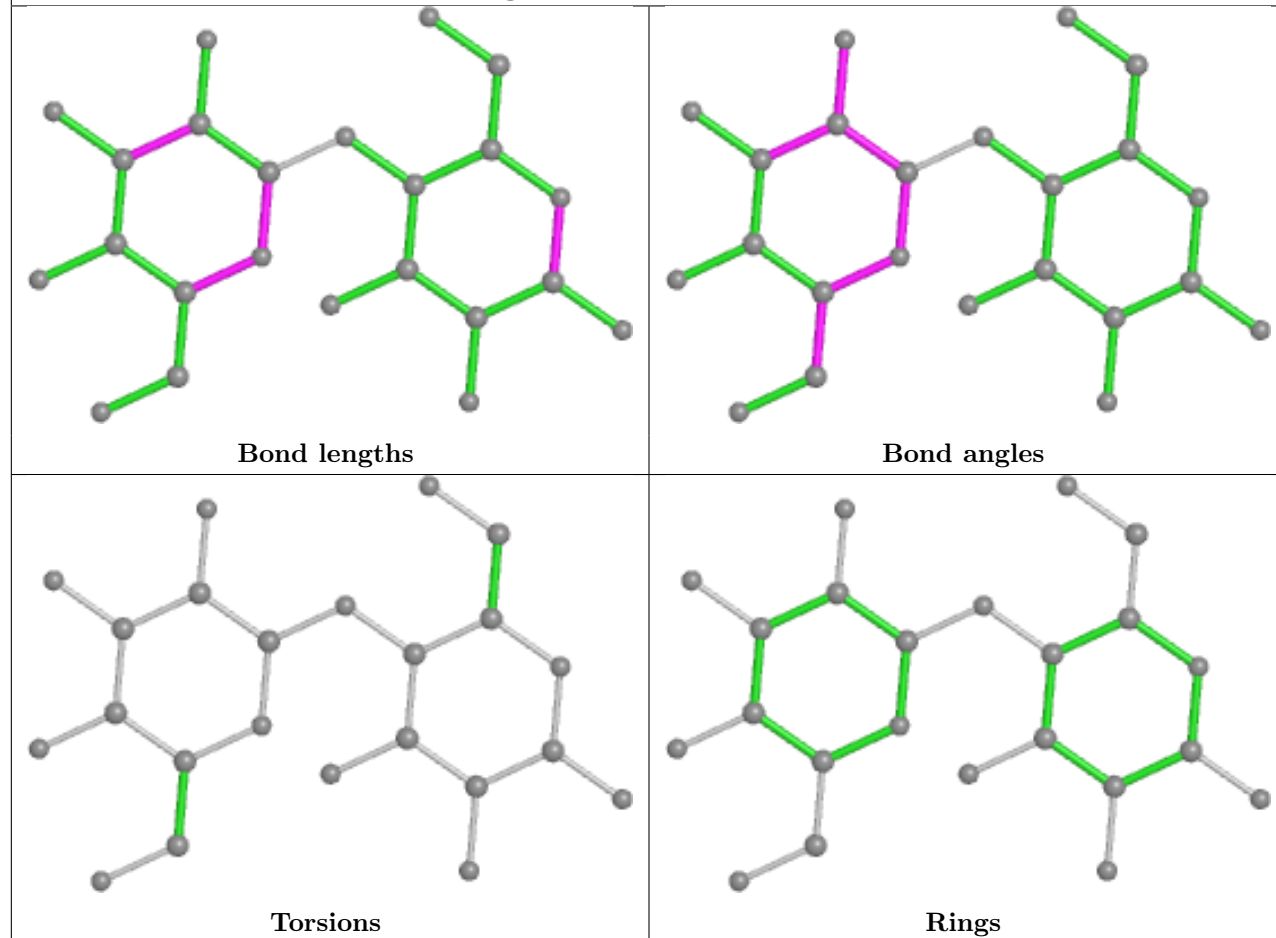
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	2	BGC	1	0
4	L	2	BGC	1	0
4	G	1	BGC	2	0
2	E	2	BGC	2	0
2	E	1	BGC	2	1
4	I	1	BGC	1	0
4	G	2	BGC	1	0
3	N	1	BGC	1	0
2	M	1	BGC	1	0
4	L	1	BGC	3	0

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

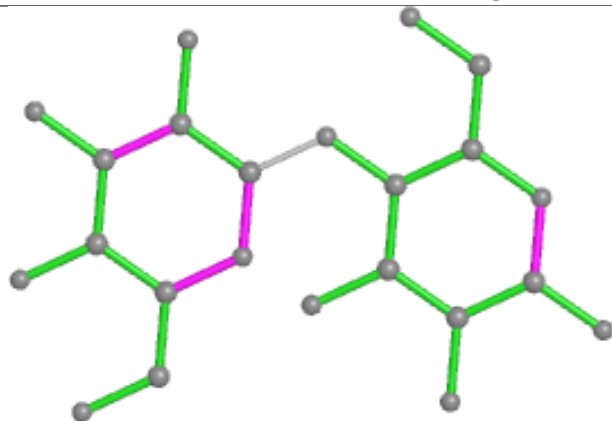
## Oligosaccharide Chain E



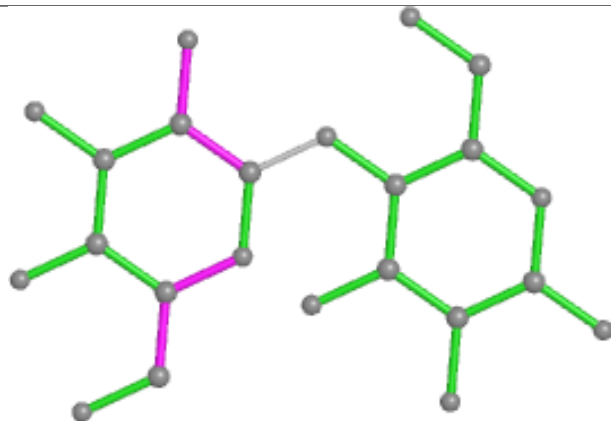
## Oligosaccharide Chain H



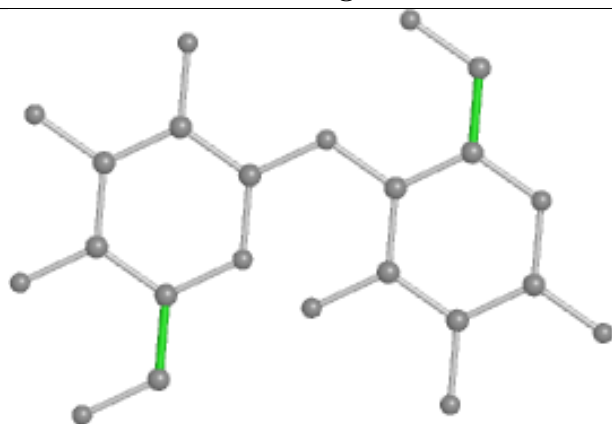
## Oligosaccharide Chain J



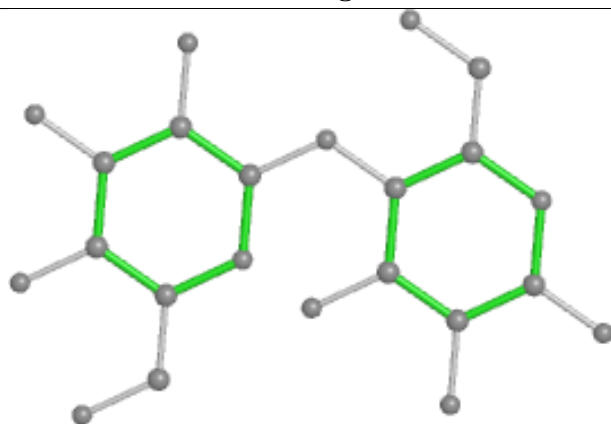
Bond lengths



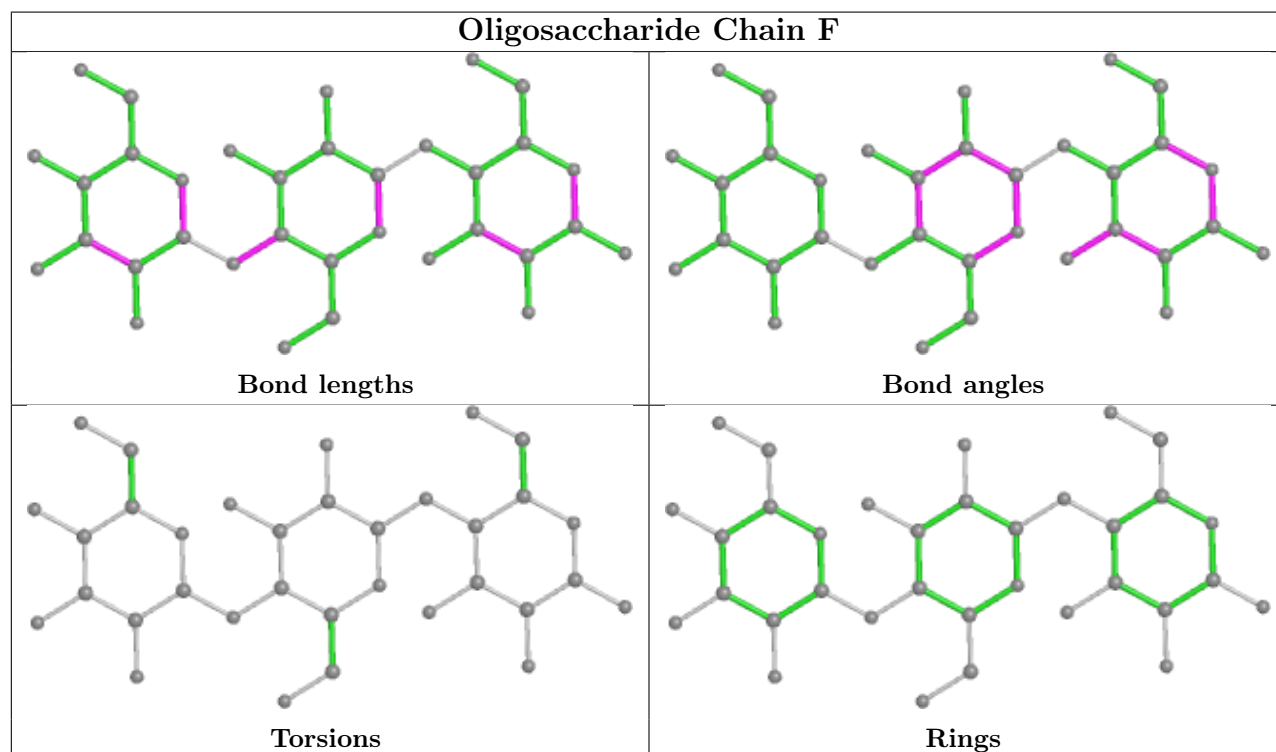
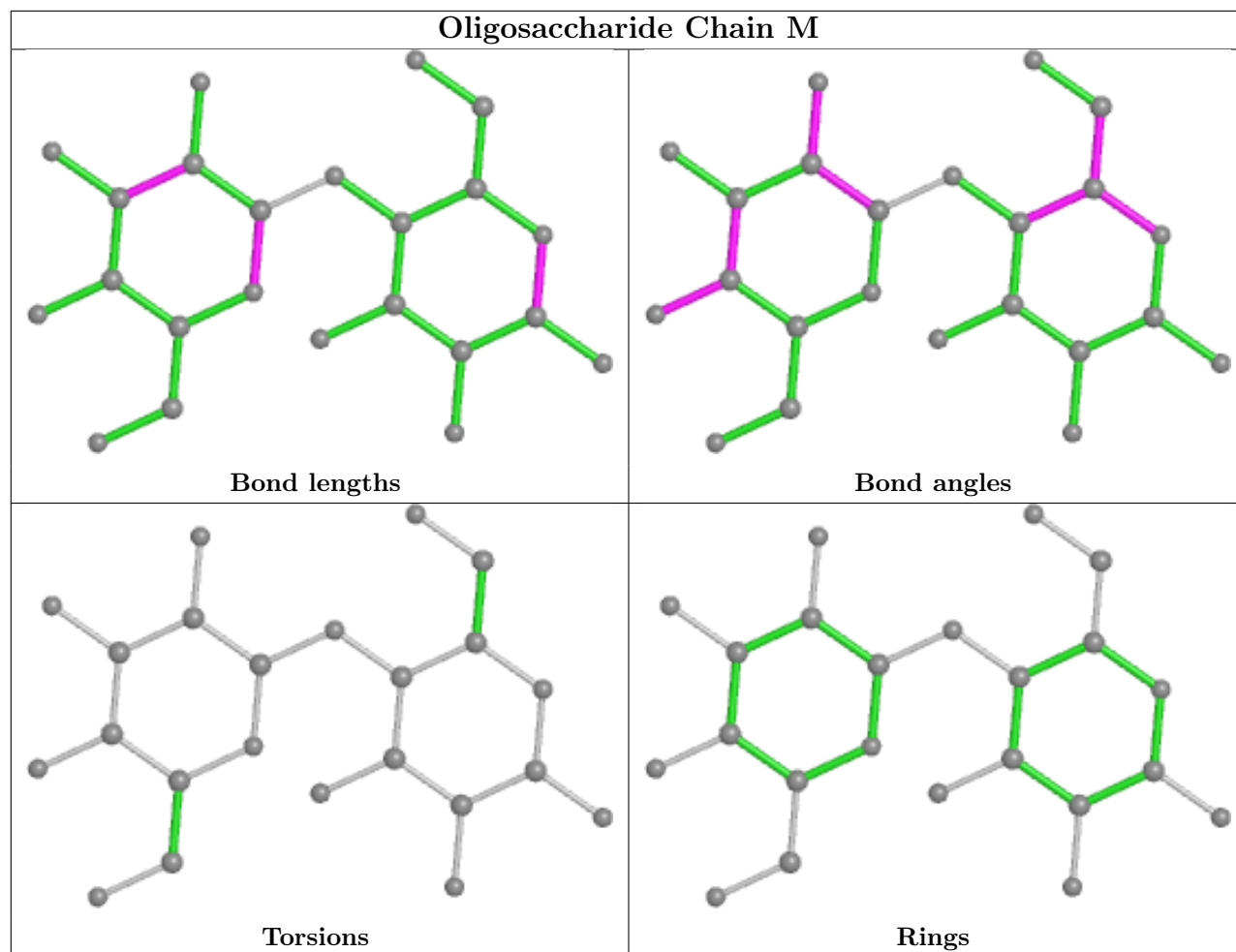
Bond angles



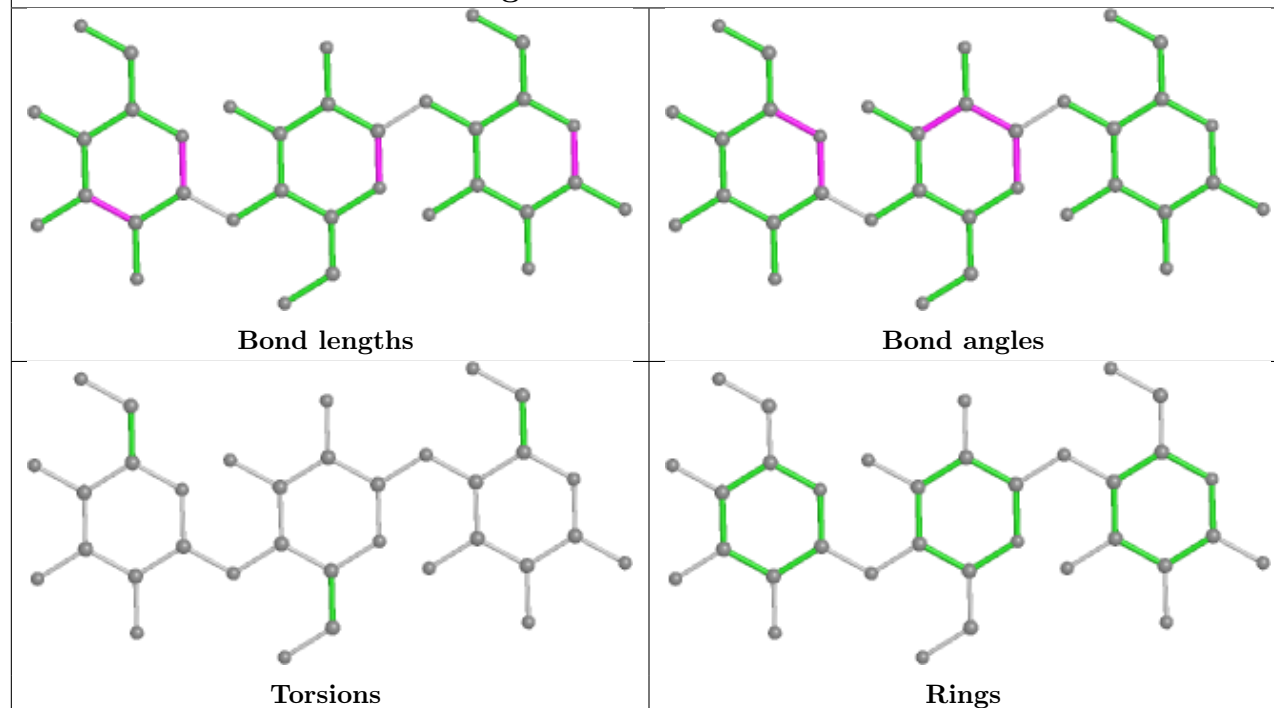
Torsions



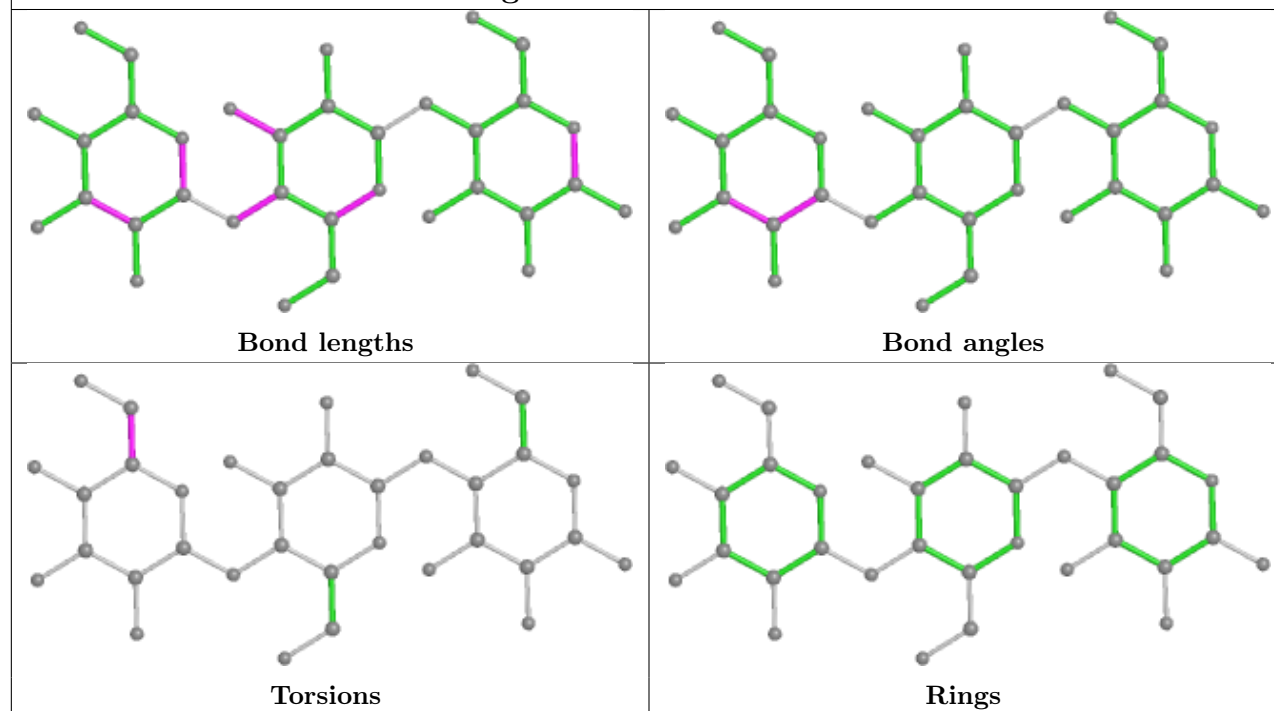
Rings

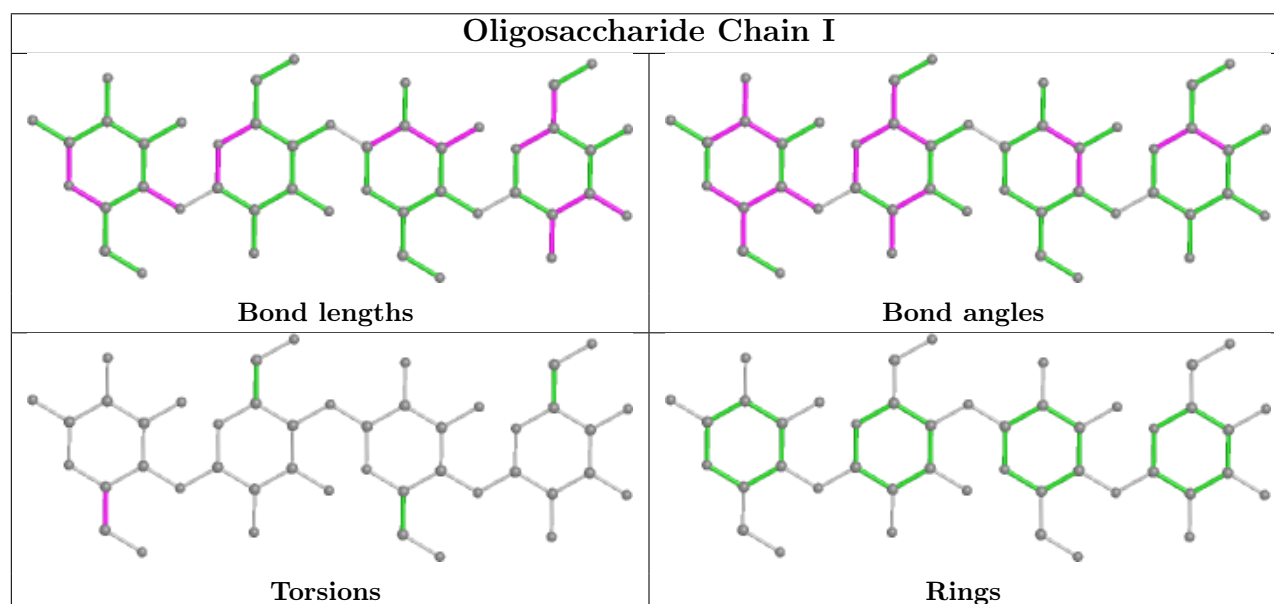
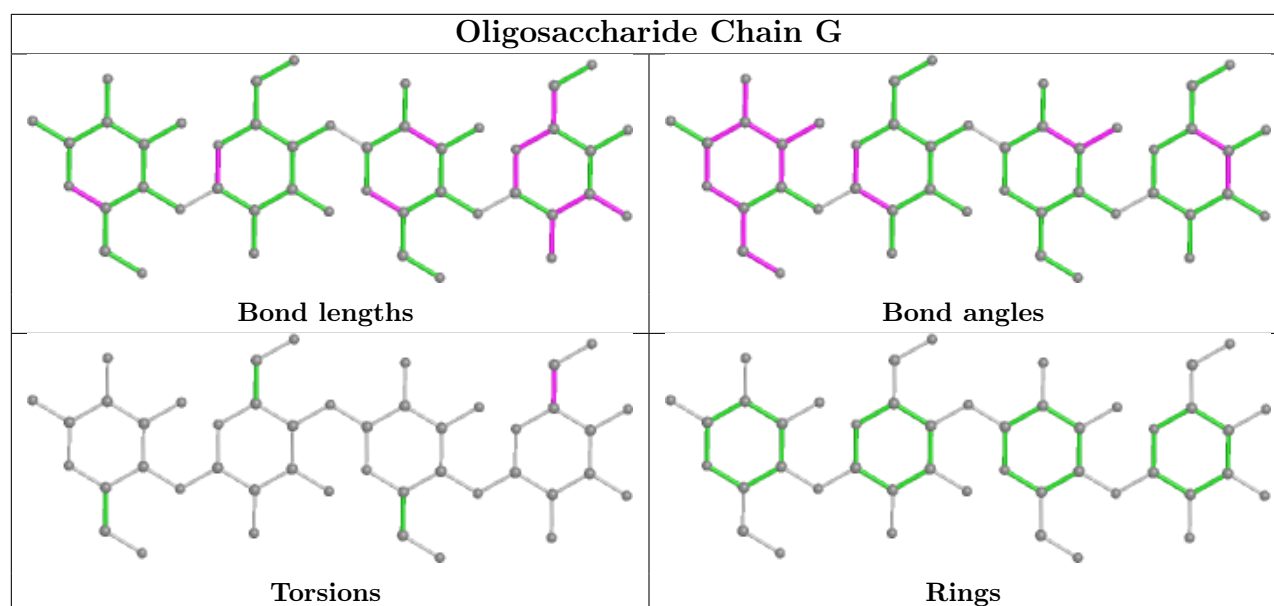


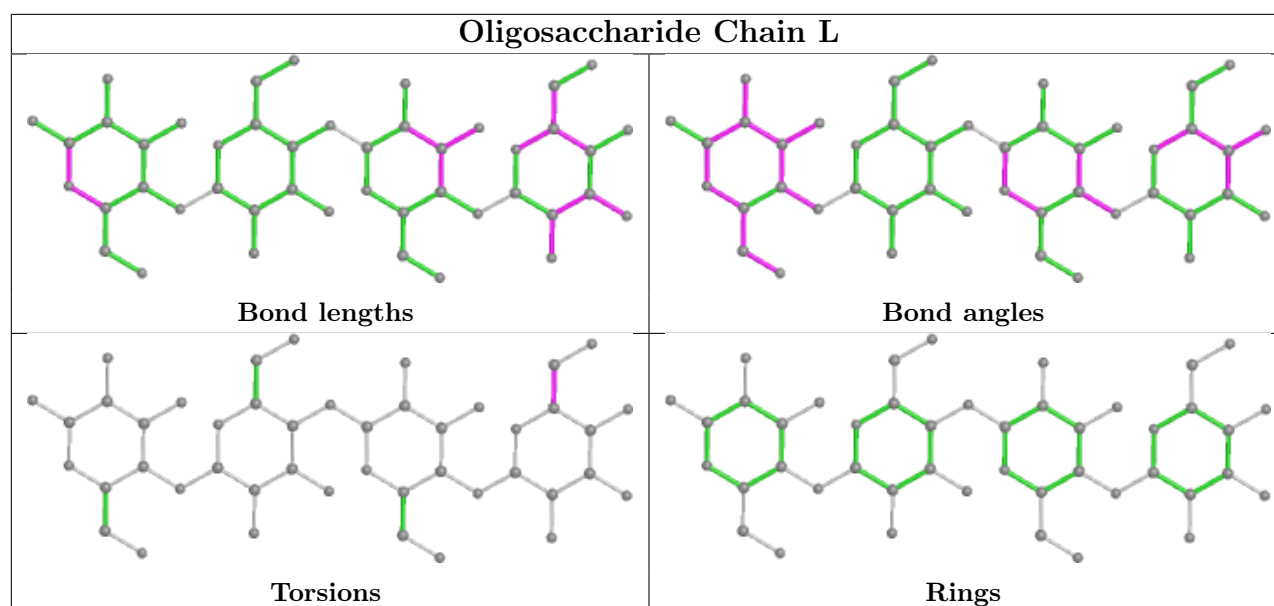
## Oligosaccharide Chain K



## Oligosaccharide Chain N







## 5.6 Ligand geometry [i](#)

2 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	$\# Z  > 2$
5	SRT	C	401	-	3,9,9	1.18	0	6,12,12	2.93	4 (66%)
5	SRT	D	401	-	3,9,9	1.29	0	6,12,12	2.44	4 (66%)

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
5	SRT	C	401	-	1/1/4/4	4/4/12/12	-
5	SRT	D	401	-	1/1/4/4	4/4/12/12	-

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	401	SRT	C1-C2-C3	4.56	122.92	113.11
5	C	401	SRT	O2-C2-C1	3.56	119.66	111.10
5	C	401	SRT	O3-C3-C2	-3.33	97.78	108.90
5	D	401	SRT	O2-C2-C3	3.24	119.72	108.90
5	D	401	SRT	O3-C3-C2	-2.95	99.04	108.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	401	SRT	C2
5	D	401	SRT	C2

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	401	SRT	C1-C2-C3-C4
5	C	401	SRT	O2-C2-C3-O3
5	D	401	SRT	C1-C2-C3-C4
5	D	401	SRT	O2-C2-C3-O3
5	C	401	SRT	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	338/351 (96%)	0.18	8 (2%) 59 58	13, 20, 34, 66	0
1	B	338/351 (96%)	0.24	16 (4%) 31 29	14, 22, 36, 57	0
1	C	338/351 (96%)	0.34	14 (4%) 37 34	16, 24, 39, 74	0
1	D	338/351 (96%)	0.32	23 (6%) 17 14	17, 25, 44, 77	0
All	All	1352/1404 (96%)	0.27	61 (4%) 33 31	13, 23, 40, 77	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	CYS	9.9
1	C	22	CYS	6.5
1	B	22	CYS	5.8
1	D	22	CYS	5.3
1	D	171	GLU	5.0

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

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

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	BGC	E	1	12/12	0.44	0.31	33,43,44,46	12
2	BGC	J	1	12/12	0.61	0.17	50,57,59,59	12

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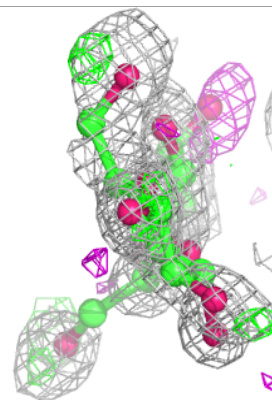
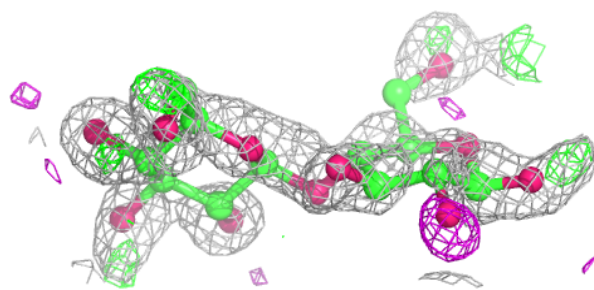
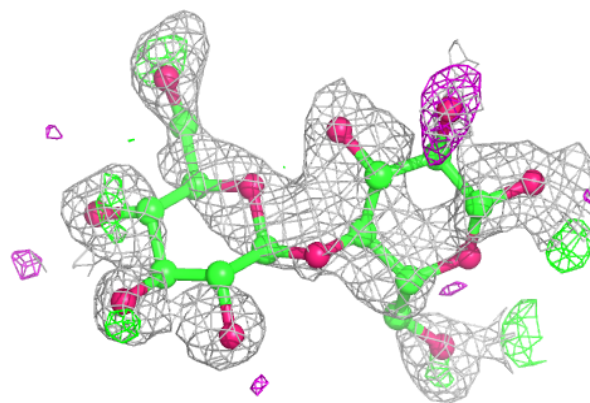
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BGC	E	2	11/12	0.64	0.28	25,33,38,39	11
4	BGC	L	4	11/12	0.65	0.21	36,41,47,49	11
4	BGC	G	4	11/12	0.68	0.21	33,40,44,45	11
4	BGC	G	1	12/12	0.68	0.23	22,27,31,33	12
2	BGC	H	1	12/12	0.69	0.16	30,35,38,38	12
4	BGC	I	1	12/12	0.72	0.25	21,37,43,43	12
4	BGC	I	4	11/12	0.72	0.20	29,34,38,40	11
2	BGC	J	2	11/12	0.72	0.17	30,36,45,47	11
3	BGC	N	3	11/12	0.75	0.27	34,40,46,50	11
2	BGC	M	1	12/12	0.76	0.20	37,41,45,46	12
2	BGC	H	2	11/12	0.78	0.16	21,28,36,39	11
3	BGC	F	3	11/12	0.78	0.19	34,37,41,42	11
4	BGC	L	1	12/12	0.81	0.19	21,26,31,34	12
2	BGC	M	2	11/12	0.82	0.14	25,31,36,37	11
3	BGC	F	1	12/12	0.82	0.19	27,30,34,36	12
3	BGC	N	2	11/12	0.83	0.17	23,26,30,33	11
3	BGC	F	2	11/12	0.84	0.13	28,31,33,34	11
3	BGC	K	1	12/12	0.84	0.12	21,24,27,27	12
3	BGC	N	1	12/12	0.85	0.11	20,23,28,31	12
4	BGC	L	3	11/12	0.86	0.12	20,25,30,33	11
4	BGC	I	3	11/12	0.88	0.10	19,22,25,29	11
4	BGC	L	2	11/12	0.89	0.19	19,21,26,27	11
4	BGC	I	2	11/12	0.89	0.09	18,20,25,27	11
3	BGC	K	3	11/12	0.89	0.10	22,25,30,31	11
4	BGC	G	3	11/12	0.90	0.09	23,26,30,31	11
4	BGC	G	2	11/12	0.91	0.12	21,24,27,28	11
3	BGC	K	2	11/12	0.92	0.08	20,21,24,24	11

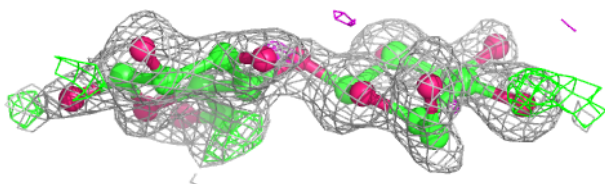
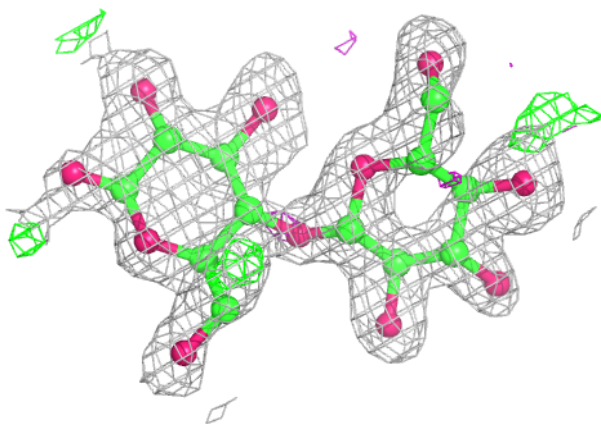
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain E:**

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

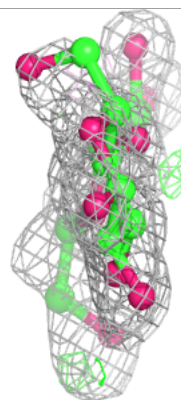
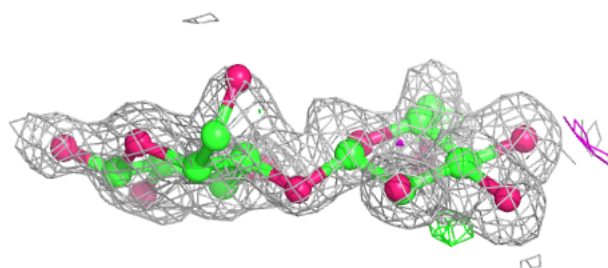
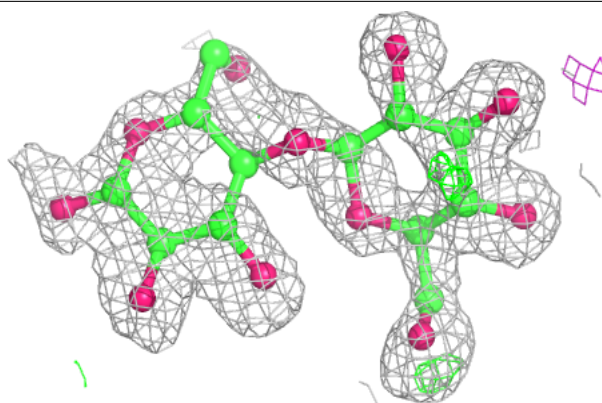
**Electron density around Chain H:**

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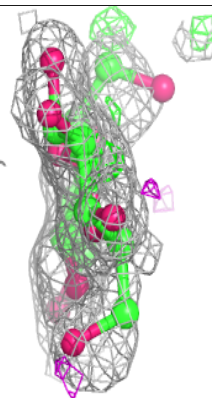
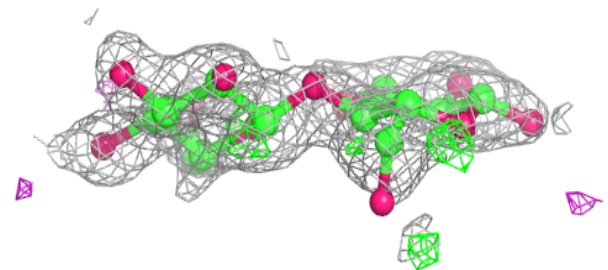
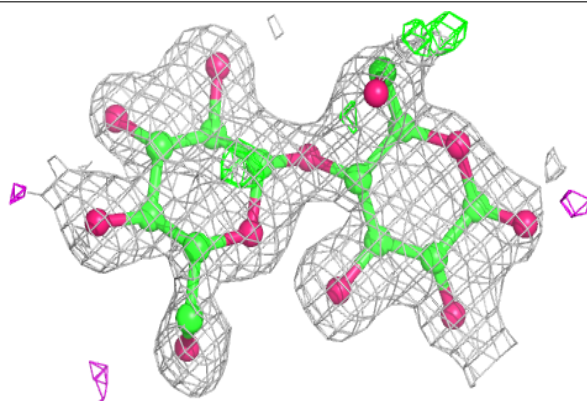


**Electron density around Chain J:**

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and green (positive)

**Electron density around Chain M:**

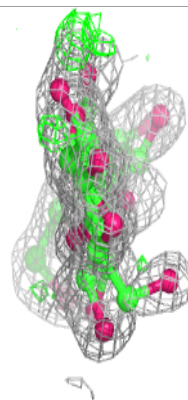
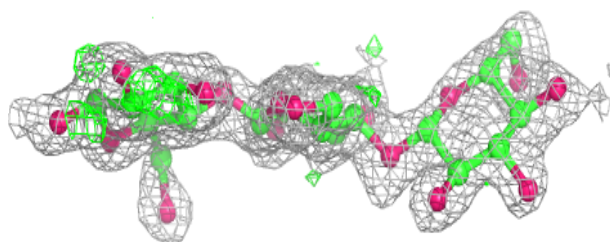
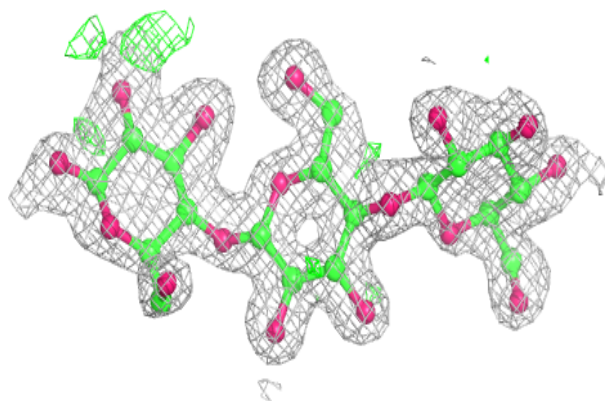
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



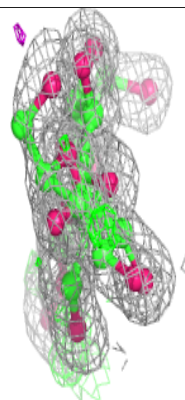
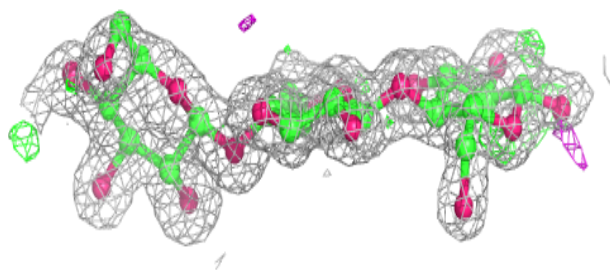
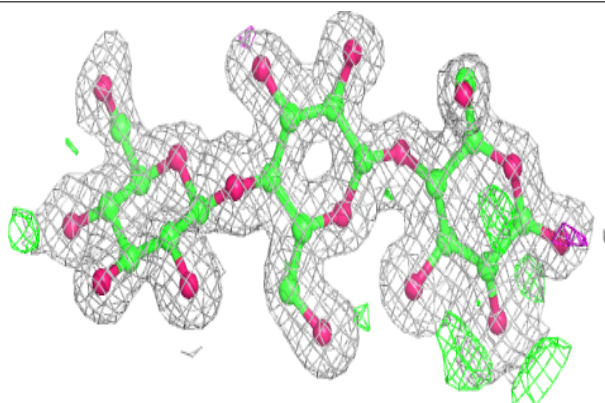


**Electron density around Chain F:**

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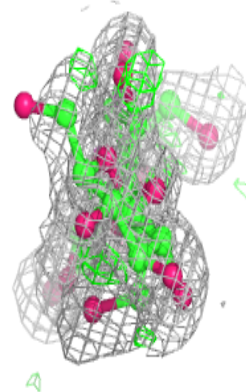
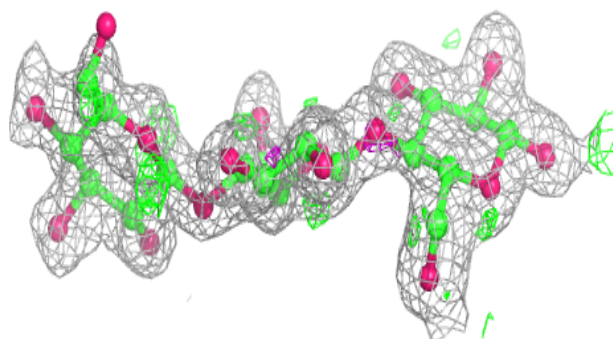
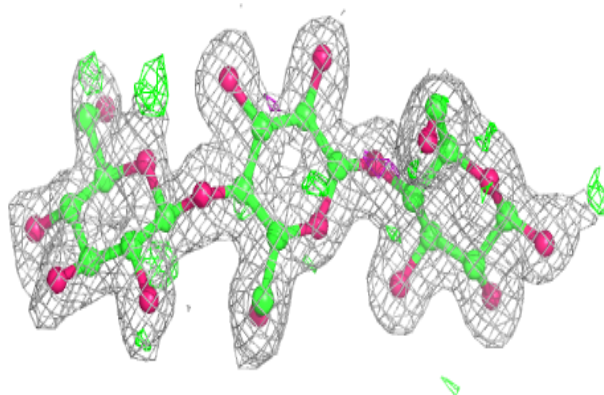
**Electron density around Chain K:**

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and green (positive)

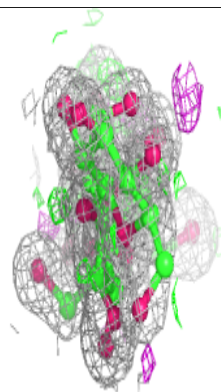
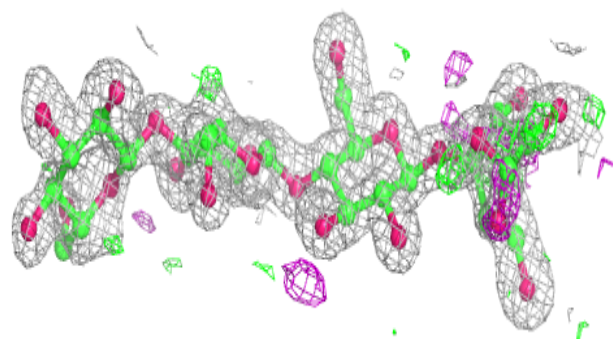
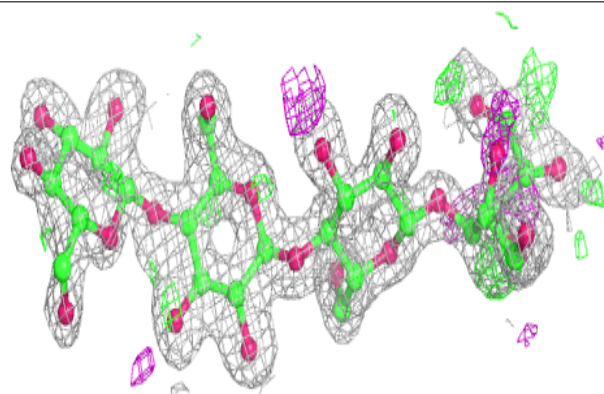


**Electron density around Chain N:**

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and green (positive)

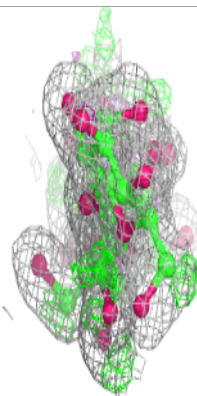
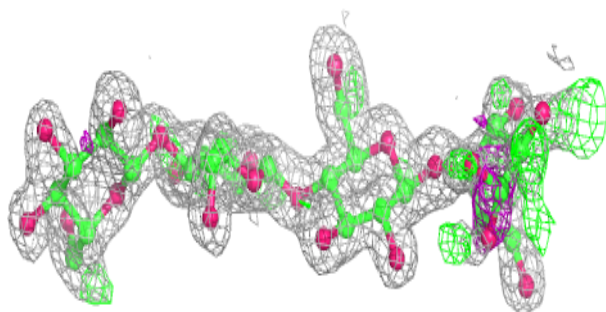
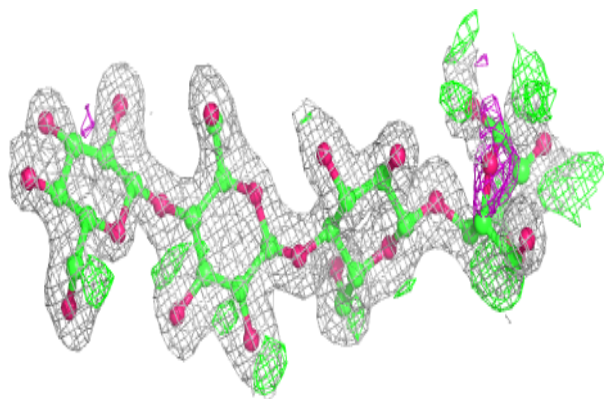
**Electron density around Chain G:**

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

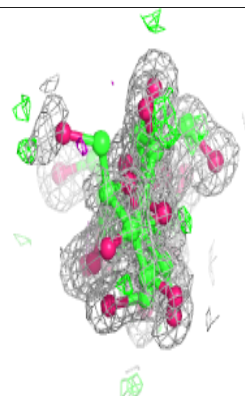
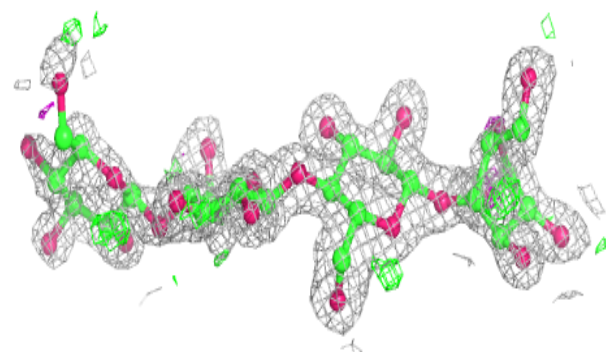
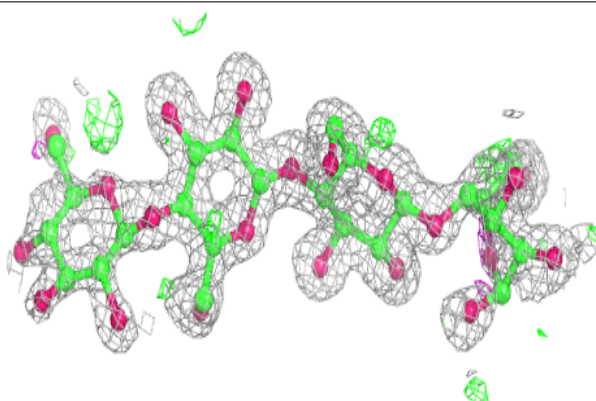


**Electron density around Chain I:**

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

**Electron density around Chain L:**

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





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	SRT	D	401	10/10	0.92	0.07	20,22,24,25	0
5	SRT	C	401	10/10	0.93	0.09	19,20,23,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.