



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 01:18 PM BST

PDB ID : 5D0F  
Title : Crystal Structure of the Candida Glabrata Glycogen Debranching Enzyme (E564Q) in complex with maltopentaose  
Authors : Zhai, L.; Xiang, S.  
Deposited on : 2015-08-03  
Resolution : 3.30 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 : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

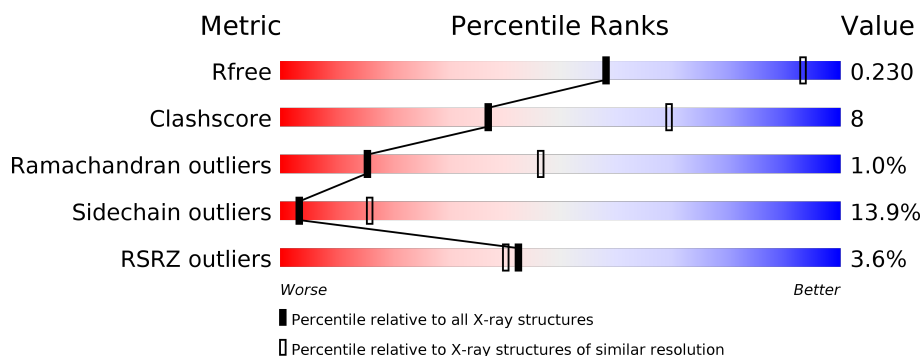
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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.



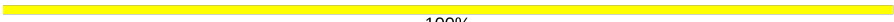
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1528	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>.</div> </div> </div>
1	B	1528	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>.</div> </div> </div>
2	C	4	<div> <div></div> <div>100%</div> </div>
2	E	4	<div> <div></div> <div>100%</div> </div>
2	H	4	<div> <div></div> <div>100%</div> </div>
2	I	4	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	K	4	 100%
3	D	5	 100%
3	G	5	 100%
3	J	5	 100%
3	M	5	 20% 60% 20%
4	F	3	 100%
4	L	3	 67% 33%

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	GLC	G	1	-	-	-	X
3	GLC	M	5	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25070 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1526	Total	C	N	O	S	0	0	0
			12278	7830	2066	2330	52			
1	B	1526	Total	C	N	O	S	0	0	0
			12278	7830	2066	2330	52			

There are 2 discrepancies between the modelled and reference sequences:

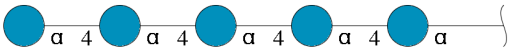
Chain	Residue	Modelled	Actual	Comment	Reference
A	564	GLN	GLU	engineered mutation	UNP Q6FSK0
B	564	GLN	GLU	engineered mutation	UNP Q6FSK0

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



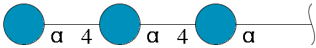
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	4	Total	C	O	0	0	0
			45	24	21			
2	E	4	Total	C	O	0	0	0
			44	24	20			
2	H	4	Total	C	O	0	0	0
			44	24	20			
2	I	4	Total	C	O	0	0	0
			45	24	21			
2	K	4	Total	C	O	0	0	0
			44	24	20			

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



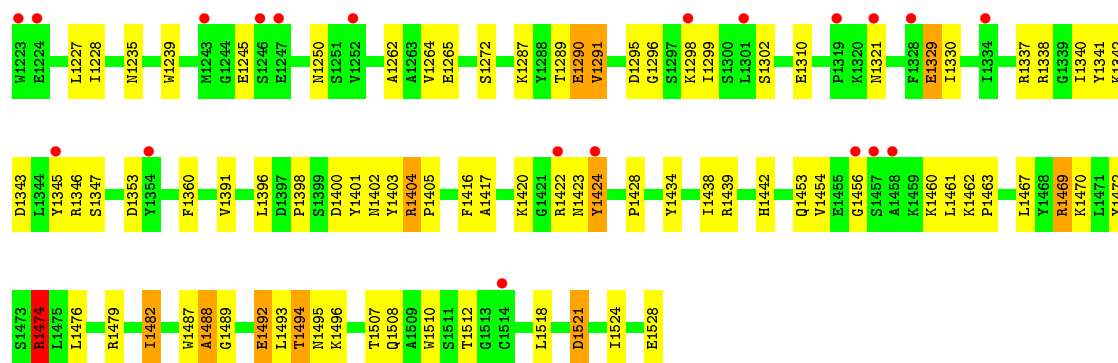
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	5	Total	C	O	0	0	0
			56	30	26			
3	G	5	Total	C	O	0	0	0
			56	30	26			
3	J	5	Total	C	O	0	0	0
			56	30	26			
3	M	5	Total	C	O	0	0	0
			56	30	26			

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

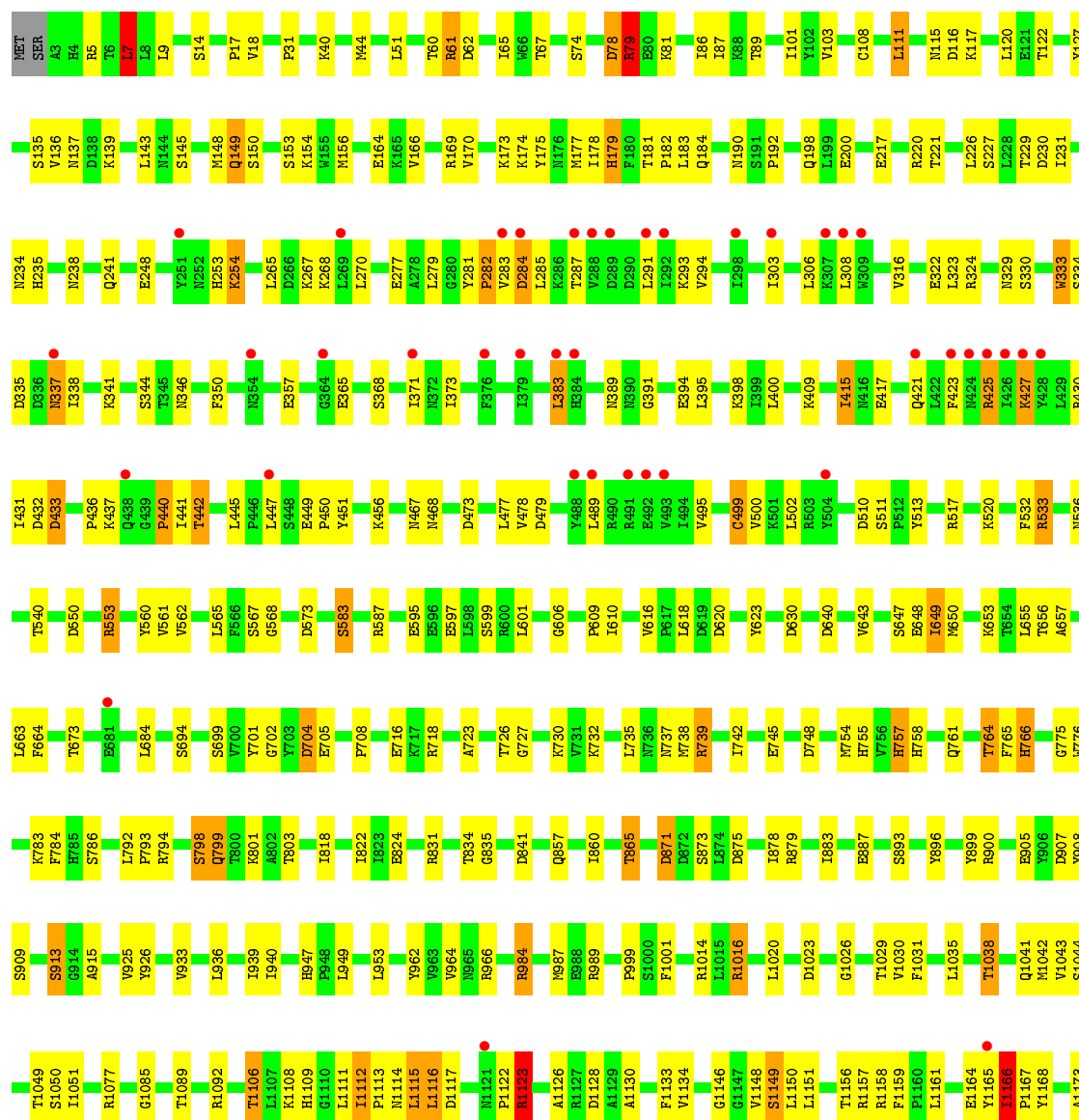
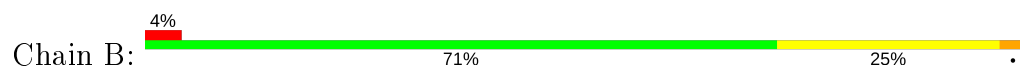


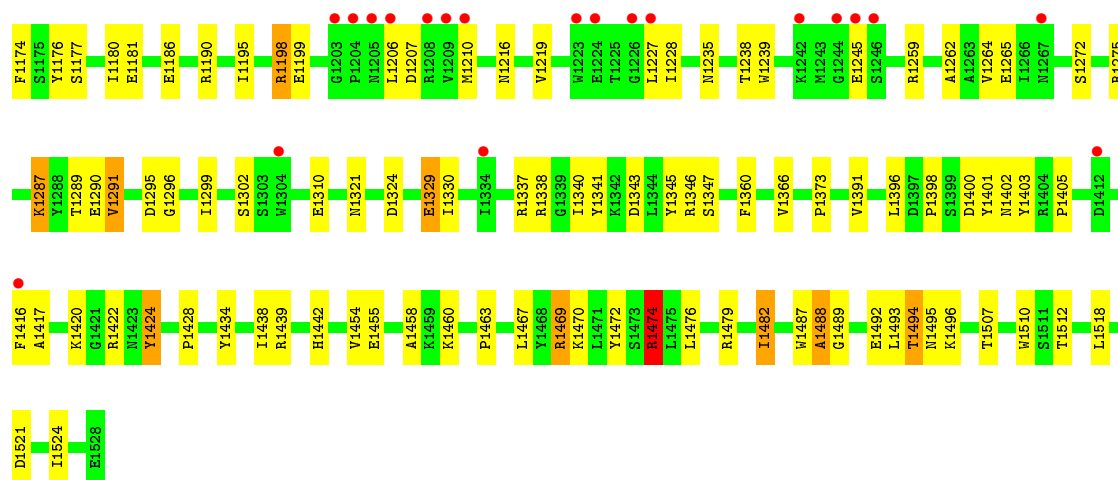
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	F	3	Total	C	O	0	0	0
			34	18	16			
4	L	3	Total	C	O	0	0	0
			34	18	16			





• Molecule 1: Uncharacterized protein





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

Chain C: 100%



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

Chain E: 100%



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

Chain H: 100%



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

Chain I: 100%



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

Chain K: 100%



GLC1  
GLC2  
GLC3  
GLC4

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

Chain D:  100%

GLC1  
GLC2  
GLC3  
GLC4  
GLC5

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

Chain G:  100%

GLC1  
GLC2  
GLC3  
GLC4  
GLC5

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

Chain J:  100%

GLC1  
GLC2  
GLC3  
GLC4  
GLC5

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

Chain M:  20% 60% 20%

GLC1  
GLC2  
GLC3  
GLC4  
GLC5

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

Chain F:  100%

GLC1  
GLC2  
GLC3

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

Chain L:  67% 33%

GLC1  
GLC2  
GLC3

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.07Å 202.01Å 135.24Å 90.00° 101.32° 90.00°	Depositor
Resolution (Å)	49.05 – 3.30 49.05 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.8 (49.05-3.30) 95.9 (49.05-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.192 , 0.228 0.197 , 0.230	Depositor DCC
$R_{free}$ test set	3072 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.3	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 32.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	25070	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: GLC

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	0.81	2/12589 (0.0%)	1.00	20/17071 (0.1%)
1	B	0.81	0/12589	1.00	26/17071 (0.2%)
All	All	0.81	2/25178 (0.0%)	1.00	46/34142 (0.1%)

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	A	0	3
1	B	0	4
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1071	TYR	CB-CG	5.10	1.59	1.51
1	A	832	GLU	CD-OE2	5.09	1.31	1.25

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1474	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	B	1469	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	B	61	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	B	1014	ARG	NE-CZ-NH2	-7.81	116.40	120.30
1	A	1469	ARG	NE-CZ-NH1	7.79	124.19	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1492	GLU	Peptide
1	A	306	LEU	Peptide
1	A	442	THR	Peptide
1	B	241	GLN	Peptide
1	B	306	LEU	Peptide

## 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	12278	0	11962	192	0
1	B	12278	0	11962	192	0
2	C	45	0	39	0	0
2	E	44	0	37	0	0
2	H	44	0	37	0	0
2	I	45	0	39	0	0
2	K	44	0	37	0	0
3	D	56	0	48	0	0
3	G	56	0	48	0	0
3	J	56	0	48	0	0
3	M	56	0	48	1	0
4	F	34	0	30	0	0
4	L	34	0	30	1	0
All	All	25070	0	24365	383	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 8.

The worst 5 of 383 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:B:1158:ARG:O	1:B:1159:PHE:HD2	1.38	1.04
1:B:1158:ARG:O	1:B:1159:PHE:CD2	2.17	0.97
1:A:1062:ALA:O	1:A:1508:GLN:OE1	1.92	0.86
1:A:230:ASP:OD1	1:A:533:ARG:HD3	1.77	0.84
1:B:230:ASP:OD1	1:B:533:ARG:HD3	1.79	0.83

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1524/1528 (100%)	1314 (86%)	195 (13%)	15 (1%)	15	46
1	B	1524/1528 (100%)	1321 (87%)	188 (12%)	15 (1%)	15	46
All	All	3048/3056 (100%)	2635 (86%)	383 (13%)	30 (1%)	15	46

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	887	GLU
1	B	887	GLU
1	A	440	PRO
1	A	723	ALA
1	A	1424	TYR

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1344/1346 (100%)	1157 (86%)	187 (14%)	3	16
1	B	1344/1346 (100%)	1157 (86%)	187 (14%)	3	16
All	All	2688/2692 (100%)	2314 (86%)	374 (14%)	3	16

5 of 374 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1347	SER
1	B	149	GLN
1	B	1287	LYS
1	A	1420	LYS
1	B	18	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1442	HIS
1	B	179	HIS
1	B	1355	GLN
1	A	1453	GLN
1	B	238	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

46 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	GLC	C	1	2	12,12,12	0.88	0	17,17,17	1.39	2 (11%)
2	GLC	C	2	2	11,11,12	0.98	1 (9%)	15,15,17	1.24	2 (13%)
2	GLC	C	3	2	11,11,12	1.24	3 (27%)	15,15,17	1.36	2 (13%)
2	GLC	C	4	2	11,11,12	1.86	3 (27%)	15,15,17	1.60	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GLC	D	1	3	12,12,12	0.99	0	17,17,17	1.20	3 (17%)
3	GLC	D	2	3	11,11,12	1.59	2 (18%)	15,15,17	1.61	2 (13%)
3	GLC	D	3	3	11,11,12	0.85	0	15,15,17	1.29	2 (13%)
3	GLC	D	4	3	11,11,12	0.68	0	15,15,17	1.47	3 (20%)
3	GLC	D	5	3	11,11,12	0.76	0	15,15,17	0.96	1 (6%)
2	GLC	E	1	2	11,11,12	1.18	1 (9%)	15,15,17	2.04	5 (33%)
2	GLC	E	2	2	11,11,12	0.89	0	15,15,17	1.24	2 (13%)
2	GLC	E	3	2	11,11,12	1.00	1 (9%)	15,15,17	1.41	2 (13%)
2	GLC	E	4	2	11,11,12	1.10	1 (9%)	15,15,17	2.10	1 (6%)
4	GLC	F	1	4	12,12,12	0.98	0	17,17,17	1.00	1 (5%)
4	GLC	F	2	4	11,11,12	1.57	2 (18%)	15,15,17	2.74	3 (20%)
4	GLC	F	3	4	11,11,12	0.89	1 (9%)	15,15,17	1.53	1 (6%)
3	GLC	G	1	3	12,12,12	0.96	0	17,17,17	1.02	1 (5%)
3	GLC	G	2	3	11,11,12	1.10	1 (9%)	15,15,17	1.18	3 (20%)
3	GLC	G	3	3	11,11,12	0.86	0	15,15,17	1.26	1 (6%)
3	GLC	G	4	3	11,11,12	0.86	0	15,15,17	1.39	2 (13%)
3	GLC	G	5	3	11,11,12	1.29	2 (18%)	15,15,17	1.66	5 (33%)
2	GLC	H	1	2	11,11,12	1.27	1 (9%)	15,15,17	1.04	1 (6%)
2	GLC	H	2	2	11,11,12	1.62	3 (27%)	15,15,17	1.90	4 (26%)
2	GLC	H	3	2	11,11,12	1.22	2 (18%)	15,15,17	1.92	2 (13%)
2	GLC	H	4	2	11,11,12	0.97	1 (9%)	15,15,17	1.66	2 (13%)
2	GLC	I	1	2	12,12,12	1.10	0	17,17,17	1.32	2 (11%)
2	GLC	I	2	2	11,11,12	0.92	0	15,15,17	1.80	4 (26%)
2	GLC	I	3	2	11,11,12	1.25	1 (9%)	15,15,17	2.47	3 (20%)
2	GLC	I	4	2	11,11,12	1.65	2 (18%)	15,15,17	1.74	3 (20%)
3	GLC	J	1	3	12,12,12	1.26	2 (16%)	17,17,17	1.05	1 (5%)
3	GLC	J	2	3	11,11,12	2.06	3 (27%)	15,15,17	2.72	2 (13%)
3	GLC	J	3	3	11,11,12	0.83	0	15,15,17	1.69	3 (20%)
3	GLC	J	4	3	11,11,12	0.94	1 (9%)	15,15,17	1.23	2 (13%)
3	GLC	J	5	3	11,11,12	0.96	1 (9%)	15,15,17	1.37	2 (13%)
2	GLC	K	1	2	11,11,12	1.35	3 (27%)	15,15,17	3.24	7 (46%)
2	GLC	K	2	2	11,11,12	0.84	1 (9%)	15,15,17	1.23	2 (13%)
2	GLC	K	3	2	11,11,12	1.10	1 (9%)	15,15,17	1.92	3 (20%)
2	GLC	K	4	2	11,11,12	1.21	2 (18%)	15,15,17	1.75	1 (6%)
4	GLC	L	1	4	12,12,12	0.78	0	17,17,17	0.88	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GLC	L	2	4	11,11,12	0.90	0	15,15,17	1.92	2 (13%)
4	GLC	L	3	4	11,11,12	0.71	0	15,15,17	1.75	1 (6%)
3	GLC	M	1	3	12,12,12	0.71	0	17,17,17	0.89	1 (5%)
3	GLC	M	2	3	11,11,12	0.90	0	15,15,17	1.02	0
3	GLC	M	3	3	11,11,12	0.85	0	15,15,17	1.03	2 (13%)
3	GLC	M	4	3	11,11,12	0.86	0	15,15,17	1.67	1 (6%)
3	GLC	M	5	3	11,11,12	1.04	1 (9%)	15,15,17	1.32	2 (13%)

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	GLC	C	1	2	-	2/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	1/2/19/22	0/1/1/1
3	GLC	D	1	3	-	0/2/22/22	0/1/1/1
3	GLC	D	2	3	-	2/2/19/22	0/1/1/1
3	GLC	D	3	3	-	2/2/19/22	0/1/1/1
3	GLC	D	4	3	-	1/2/19/22	0/1/1/1
3	GLC	D	5	3	-	2/2/19/22	0/1/1/1
2	GLC	E	1	2	-	2/2/19/22	0/1/1/1
2	GLC	E	2	2	-	1/2/19/22	0/1/1/1
2	GLC	E	3	2	-	2/2/19/22	0/1/1/1
2	GLC	E	4	2	-	1/2/19/22	0/1/1/1
4	GLC	F	1	4	-	1/2/22/22	0/1/1/1
4	GLC	F	2	4	-	0/2/19/22	0/1/1/1
4	GLC	F	3	4	-	1/2/19/22	0/1/1/1
3	GLC	G	1	3	-	0/2/22/22	0/1/1/1
3	GLC	G	2	3	-	0/2/19/22	0/1/1/1
3	GLC	G	3	3	-	0/2/19/22	0/1/1/1
3	GLC	G	4	3	-	0/2/19/22	0/1/1/1
3	GLC	G	5	3	-	0/2/19/22	0/1/1/1
2	GLC	H	1	2	-	2/2/19/22	0/1/1/1
2	GLC	H	2	2	-	2/2/19/22	0/1/1/1
2	GLC	H	3	2	-	0/2/19/22	0/1/1/1
2	GLC	H	4	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	I	1	2	-	2/2/22/22	0/1/1/1
2	GLC	I	2	2	-	0/2/19/22	0/1/1/1
2	GLC	I	3	2	-	2/2/19/22	0/1/1/1
2	GLC	I	4	2	-	1/2/19/22	0/1/1/1
3	GLC	J	1	3	-	2/2/22/22	0/1/1/1
3	GLC	J	2	3	-	1/2/19/22	0/1/1/1
3	GLC	J	3	3	-	2/2/19/22	0/1/1/1
3	GLC	J	4	3	-	2/2/19/22	0/1/1/1
3	GLC	J	5	3	-	2/2/19/22	0/1/1/1
2	GLC	K	1	2	-	0/2/19/22	0/1/1/1
2	GLC	K	2	2	-	2/2/19/22	0/1/1/1
2	GLC	K	3	2	-	0/2/19/22	0/1/1/1
2	GLC	K	4	2	-	1/2/19/22	0/1/1/1
4	GLC	L	1	4	-	0/2/22/22	0/1/1/1
4	GLC	L	2	4	-	1/2/19/22	0/1/1/1
4	GLC	L	3	4	-	2/2/19/22	0/1/1/1
3	GLC	M	1	3	-	2/2/22/22	0/1/1/1
3	GLC	M	2	3	-	0/2/19/22	0/1/1/1
3	GLC	M	3	3	-	2/2/19/22	0/1/1/1
3	GLC	M	4	3	-	1/2/19/22	0/1/1/1
3	GLC	M	5	3	-	0/2/19/22	0/1/1/1

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	2	GLC	O5-C1	4.25	1.50	1.43
2	I	4	GLC	O5-C1	4.05	1.50	1.43
3	J	2	GLC	O5-C5	3.87	1.51	1.43
3	D	2	GLC	O5-C1	3.69	1.49	1.43
2	C	4	GLC	O5-C1	3.58	1.49	1.43

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	2	GLC	C1-O5-C5	9.60	125.20	112.19
4	F	2	GLC	C1-O5-C5	8.92	124.28	112.19
2	I	3	GLC	C1-O5-C5	8.55	123.77	112.19
2	K	1	GLC	O5-C5-C6	7.07	118.29	107.20
2	E	4	GLC	C1-O5-C5	7.00	121.67	112.19

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

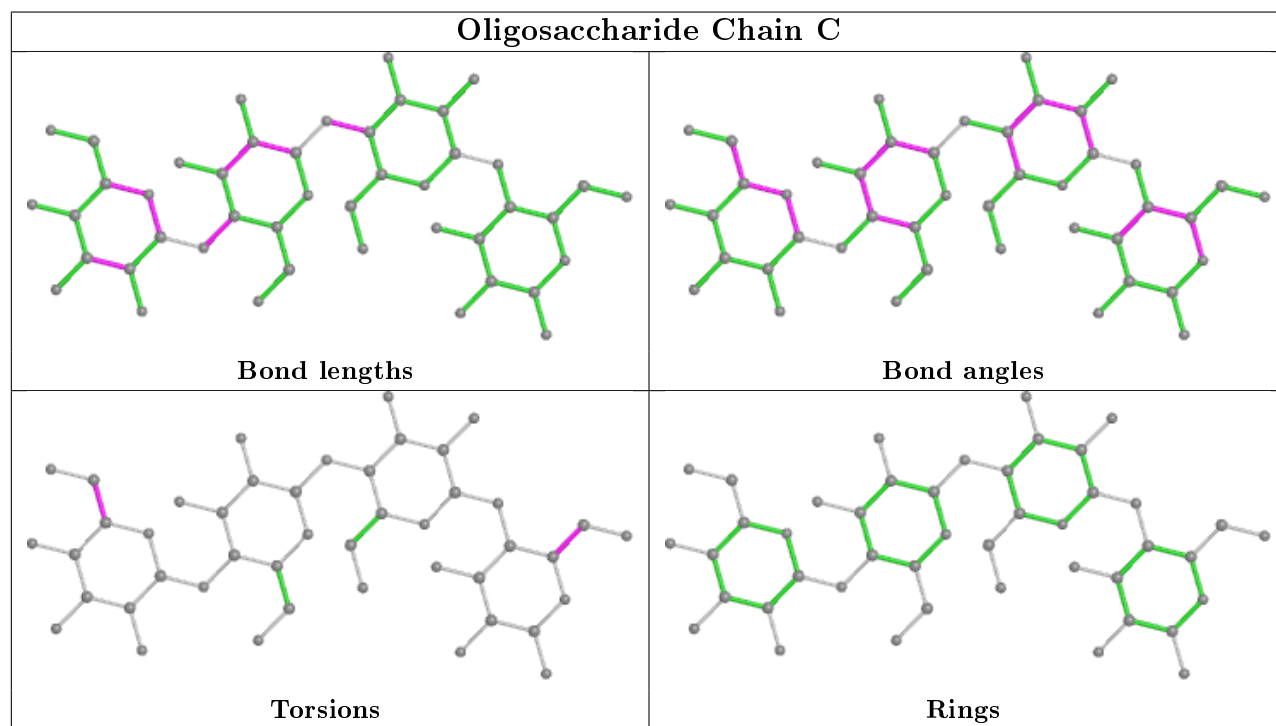
Mol	Chain	Res	Type	Atoms
2	H	4	GLC	O5-C5-C6-O6
3	J	3	GLC	O5-C5-C6-O6
2	H	2	GLC	C4-C5-C6-O6
3	D	3	GLC	O5-C5-C6-O6
2	I	3	GLC	O5-C5-C6-O6

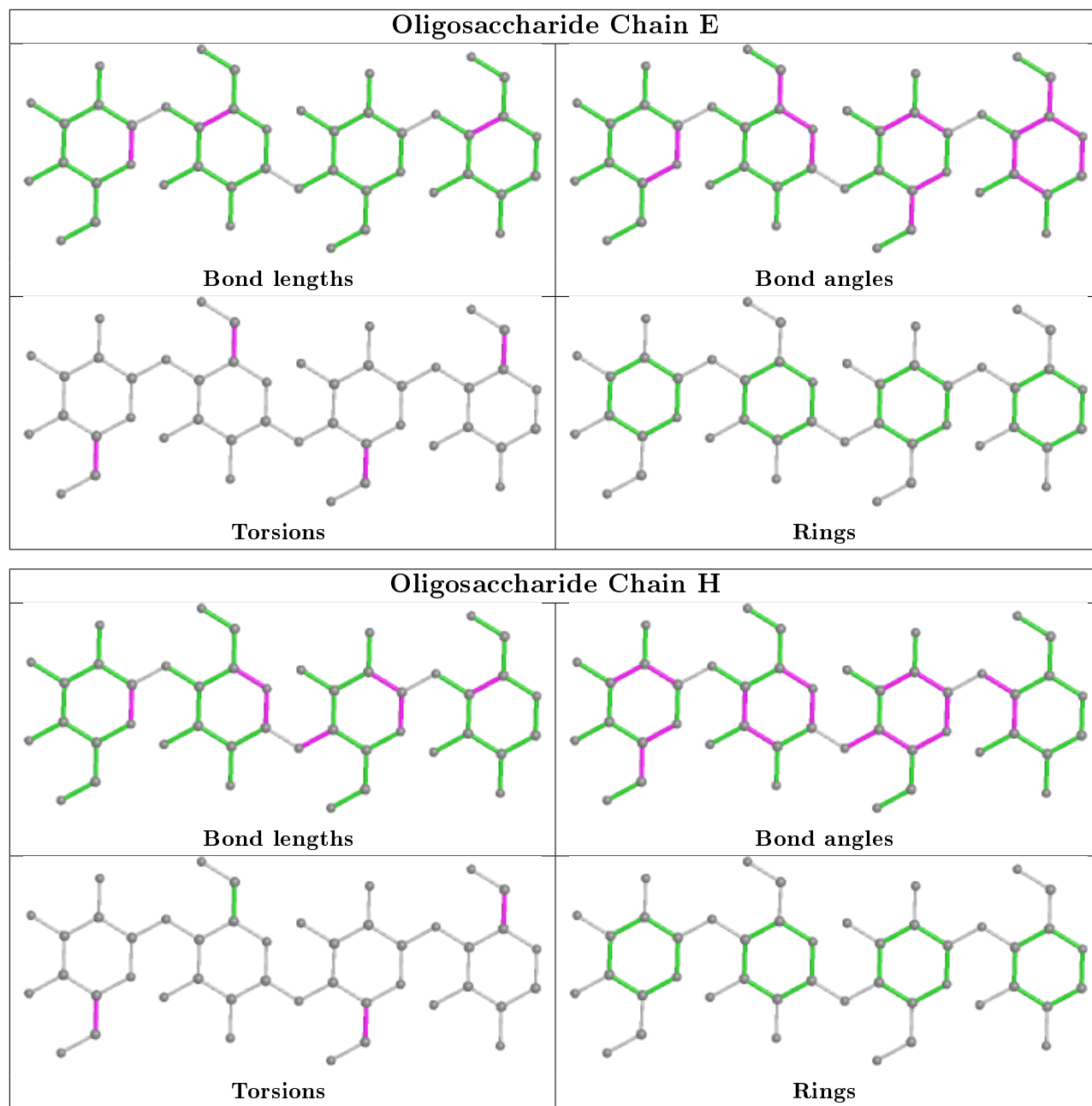
There are no ring outliers.

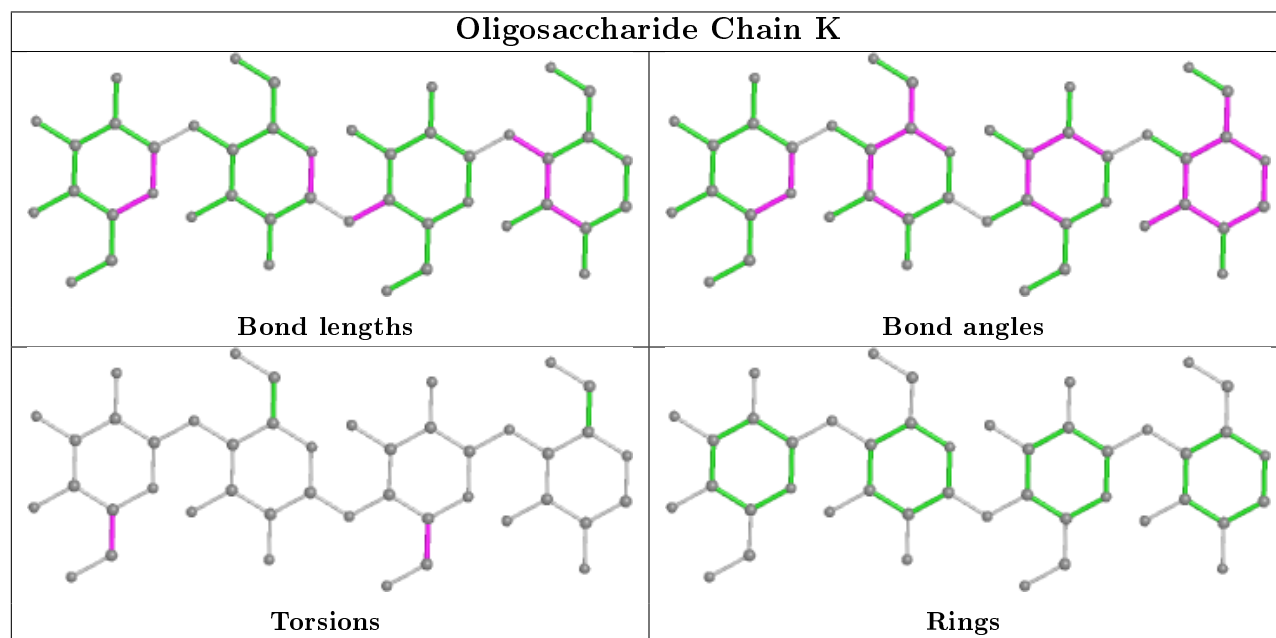
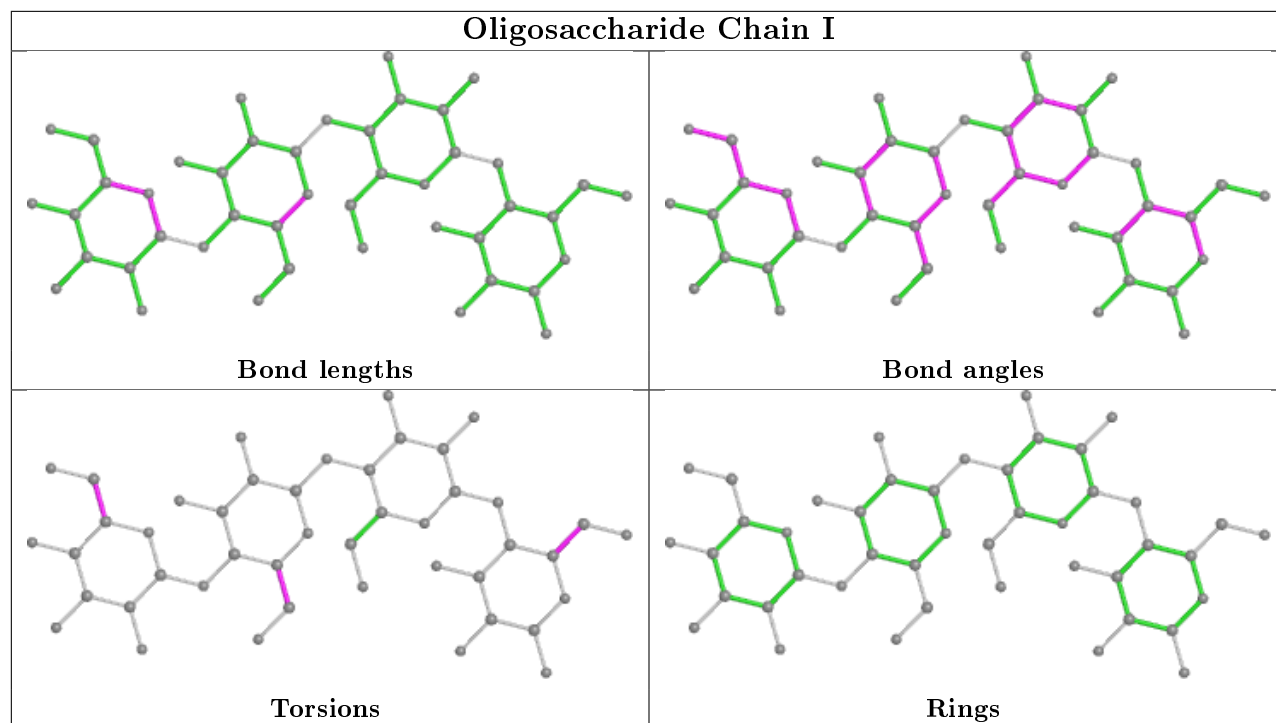
2 monomers are involved in 2 short contacts:

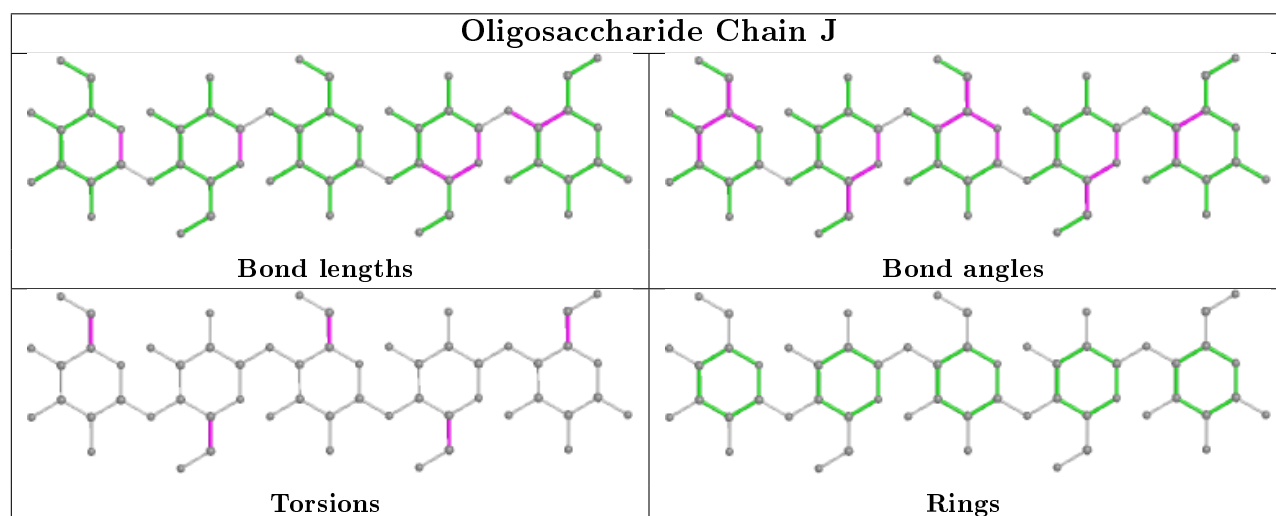
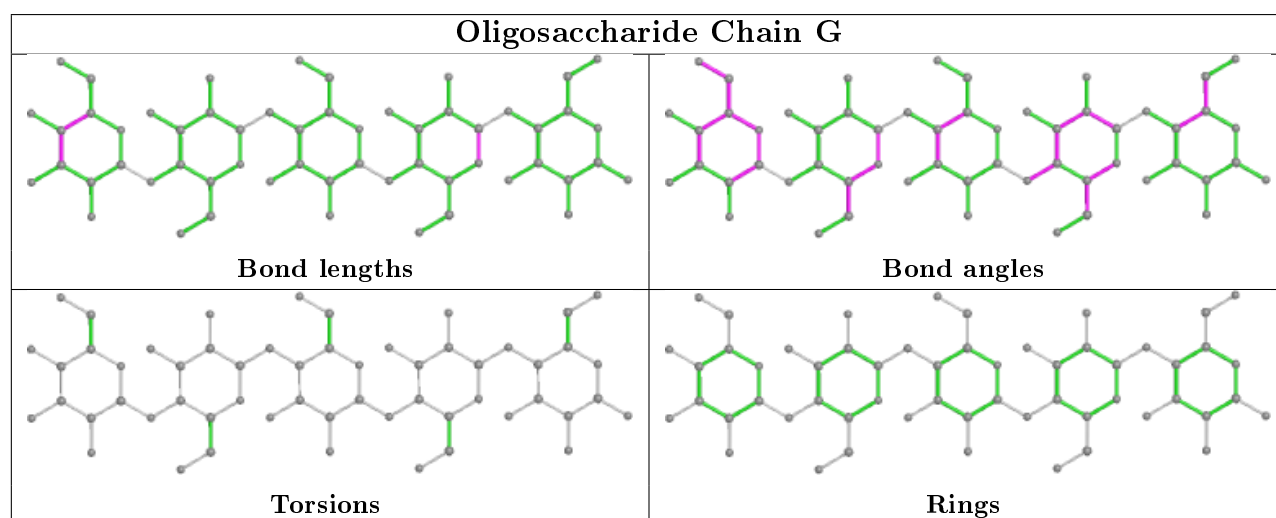
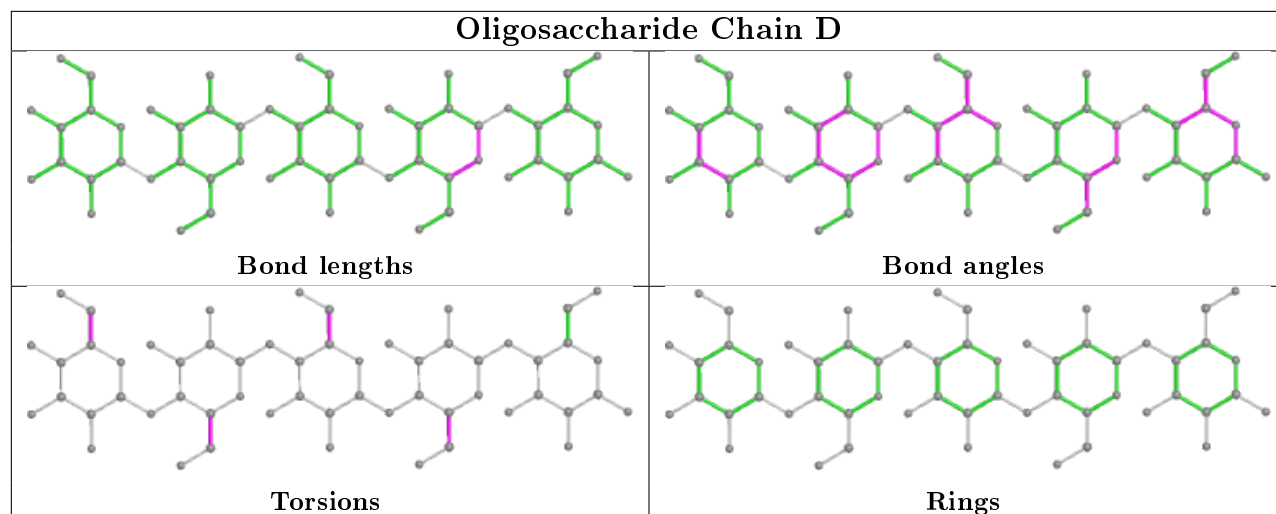
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	4	GLC	1	0
4	L	1	GLC	1	0

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

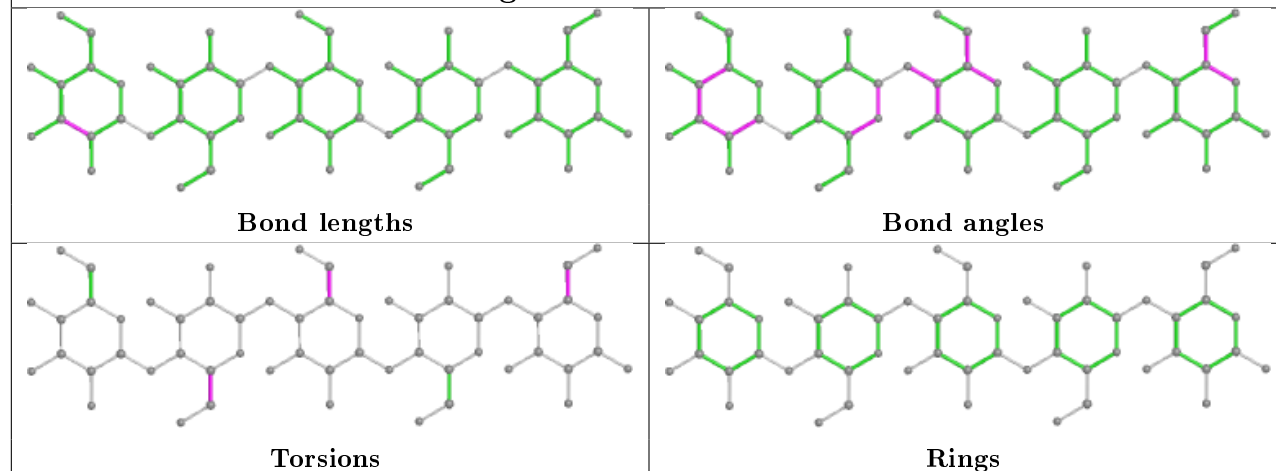




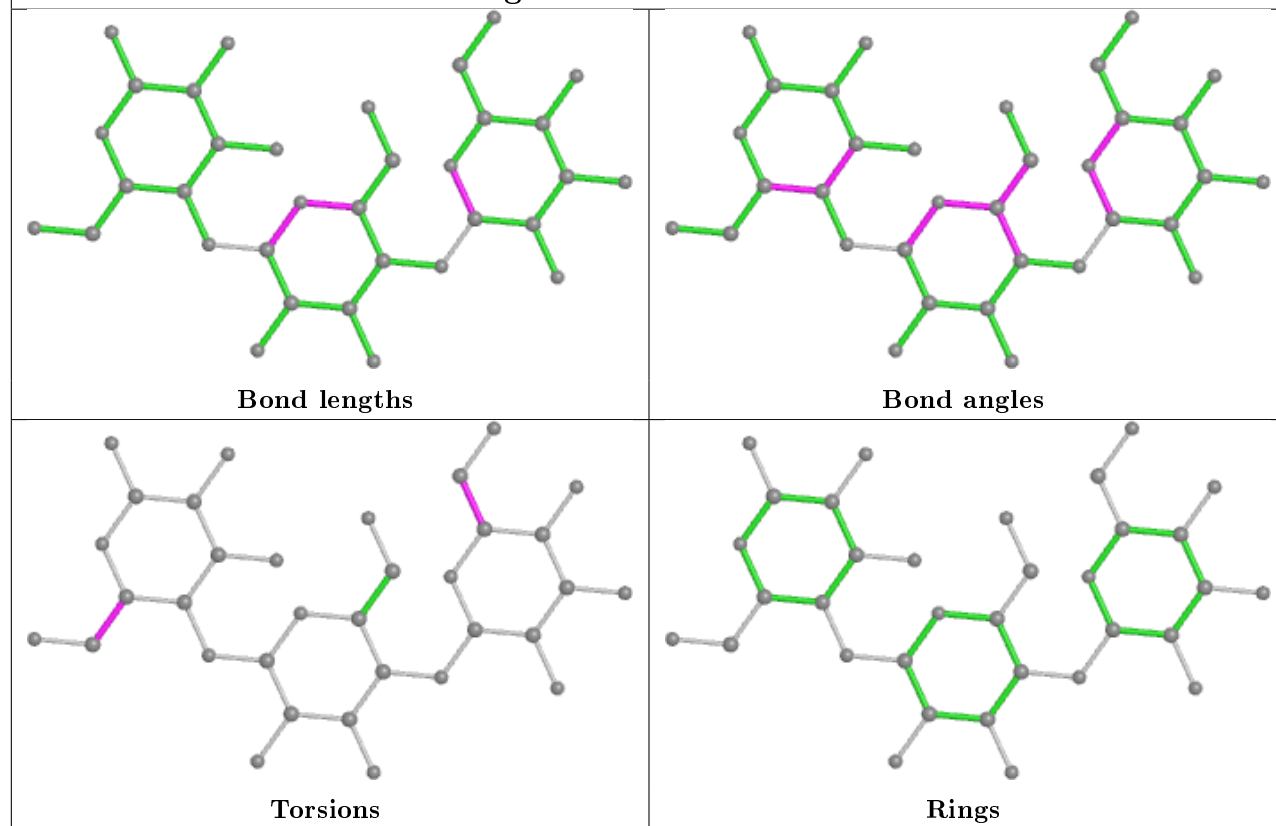


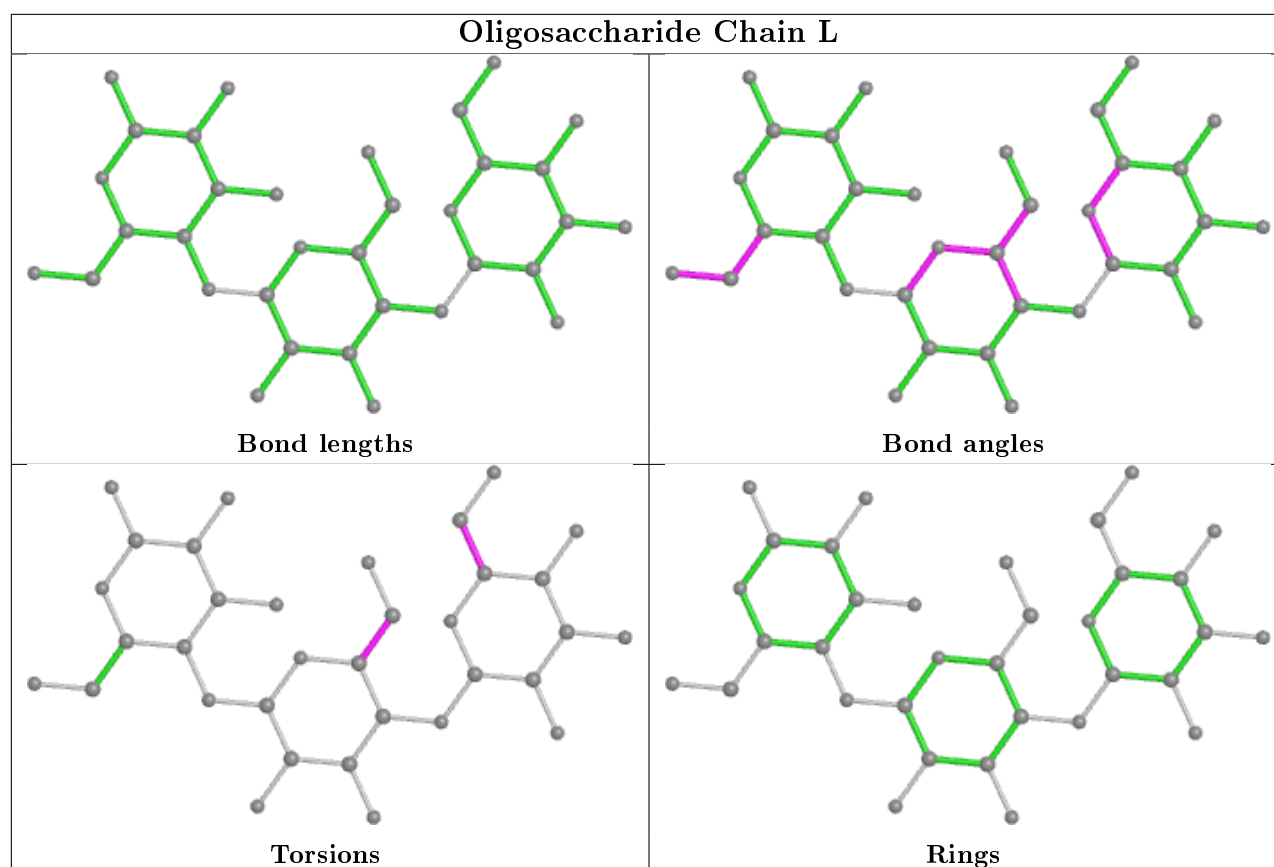


## Oligosaccharide Chain M



## Oligosaccharide Chain F





## 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 [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	1526/1528 (99%)	0.06	50 (3%) 46 44	50, 86, 144, 176	0
1	B	1526/1528 (99%)	0.07	60 (3%) 39 37	50, 83, 146, 191	0
All	All	3052/3056 (99%)	0.07	110 (3%) 42 40	50, 85, 145, 191	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	TYR	5.7
1	B	1245	GLU	5.7
1	A	1457	SER	5.5
1	A	1458	ALA	4.6
1	B	1244	GLY	4.1

### 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	GLC	H	3	11/12	0.48	0.24	147,167,186,188	0
3	GLC	M	5	11/12	0.58	0.62	186,201,208,211	0
2	GLC	H	4	11/12	0.60	0.31	154,180,189,196	0
3	GLC	G	1	12/12	0.62	0.67	131,183,190,194	0
3	GLC	M	2	11/12	0.65	0.33	150,177,181,188	0

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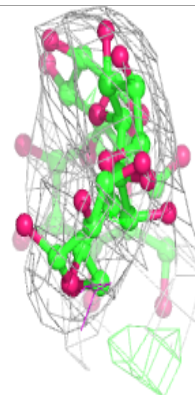
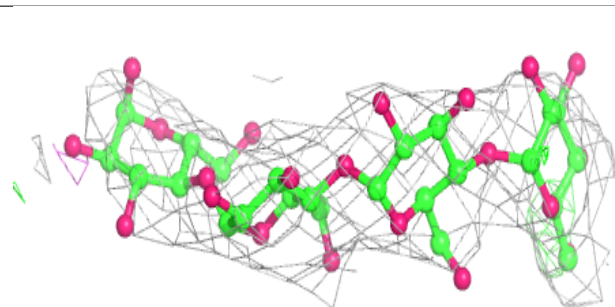
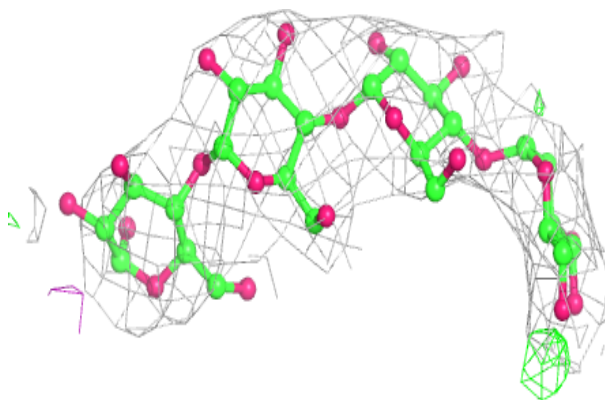
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLC	H	1	11/12	0.65	0.25	113,137,147,147	0
3	GLC	M	3	11/12	0.69	0.31	146,173,184,185	0
2	GLC	I	4	11/12	0.71	0.28	110,127,136,153	0
2	GLC	K	4	11/12	0.72	0.33	108,120,135,136	0
3	GLC	G	5	11/12	0.73	0.25	174,185,191,192	0
2	GLC	C	4	11/12	0.75	0.35	98,128,136,141	0
2	GLC	H	2	11/12	0.76	0.32	135,152,165,172	0
4	GLC	L	3	11/12	0.80	0.22	130,145,159,162	0
3	GLC	M	4	11/12	0.82	0.44	159,174,189,199	0
3	GLC	M	1	12/12	0.82	0.38	137,168,174,178	0
2	GLC	K	1	11/12	0.82	0.21	104,121,127,130	0
3	GLC	D	5	11/12	0.82	0.34	144,152,172,173	0
3	GLC	D	1	12/12	0.83	0.59	117,135,142,144	0
2	GLC	I	1	12/12	0.84	0.29	138,144,158,162	0
3	GLC	D	2	11/12	0.84	0.37	126,132,138,142	0
3	GLC	G	2	11/12	0.84	0.38	138,157,166,171	0
3	GLC	G	4	11/12	0.84	0.24	147,197,208,208	0
3	GLC	G	3	11/12	0.85	0.33	151,166,173,187	0
4	GLC	F	2	11/12	0.85	0.21	129,167,181,185	0
2	GLC	C	3	11/12	0.85	0.28	107,113,133,135	0
2	GLC	C	1	12/12	0.86	0.42	124,143,157,171	0
3	GLC	J	1	12/12	0.86	0.38	129,138,144,145	0
2	GLC	E	4	11/12	0.86	0.20	105,119,126,132	0
2	GLC	E	1	11/12	0.86	0.17	120,125,132,135	0
4	GLC	F	3	11/12	0.87	0.30	152,169,173,179	0
4	GLC	F	1	12/12	0.87	0.22	157,161,164,164	0
2	GLC	C	2	11/12	0.88	0.39	102,114,121,128	0
2	GLC	I	3	11/12	0.88	0.24	105,118,134,142	0
4	GLC	L	1	12/12	0.90	0.13	114,131,133,141	0
3	GLC	J	5	11/12	0.90	0.44	121,129,135,137	0
3	GLC	J	2	11/12	0.91	0.50	123,129,144,145	0
2	GLC	I	2	11/12	0.91	0.21	102,109,115,120	0
4	GLC	L	2	11/12	0.92	0.18	124,134,166,190	0
3	GLC	D	4	11/12	0.92	0.24	123,133,142,148	0
3	GLC	J	4	11/12	0.92	0.49	108,120,128,128	0
2	GLC	E	2	11/12	0.92	0.17	92,108,117,118	0
2	GLC	K	2	11/12	0.92	0.19	112,113,119,119	0
3	GLC	J	3	11/12	0.95	0.42	105,117,120,125	0
2	GLC	K	3	11/12	0.95	0.19	91,93,100,105	0
3	GLC	D	3	11/12	0.95	0.30	112,129,140,143	0
2	GLC	E	3	11/12	0.96	0.14	71,78,90,91	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

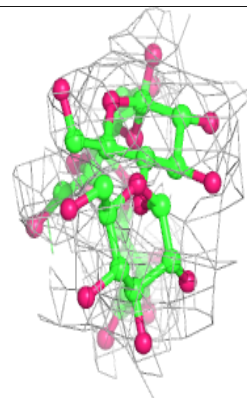
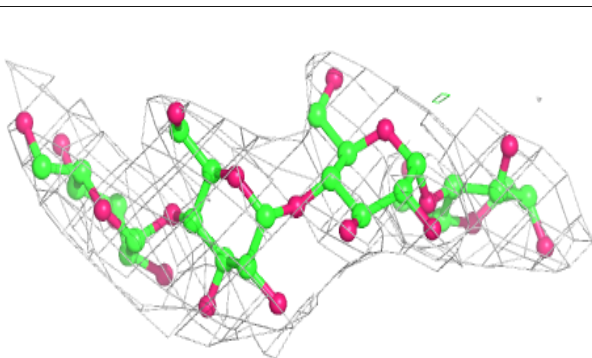
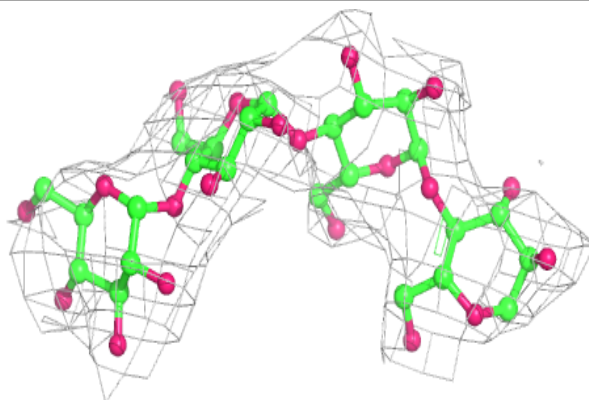
**Electron density around Chain C:**

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



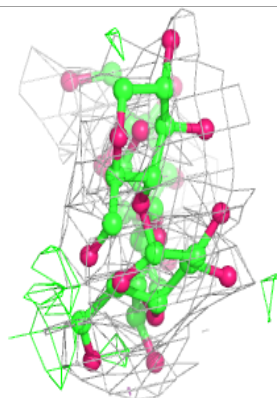
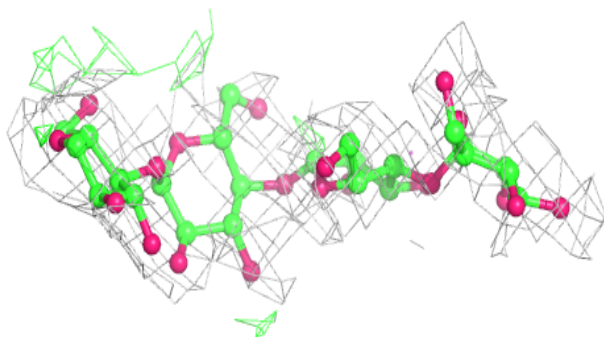
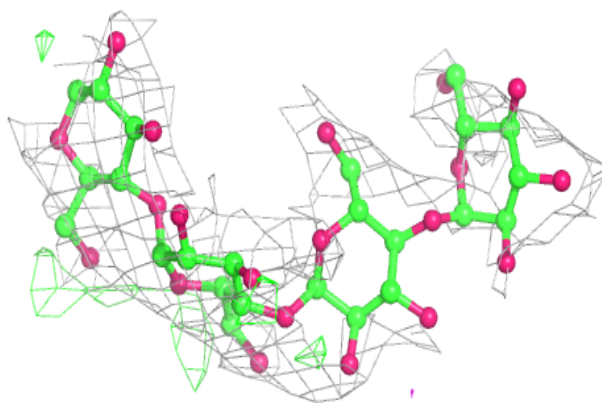
**Electron density around Chain E:**

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

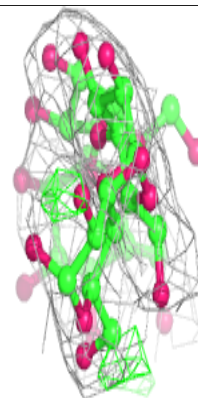
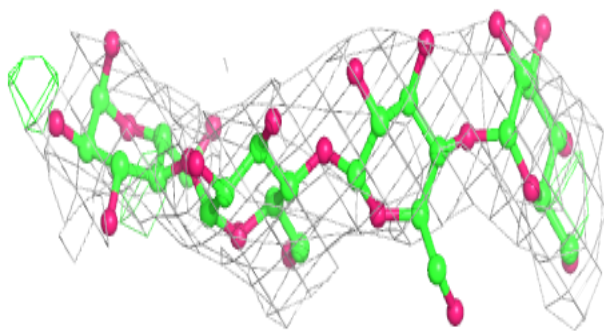
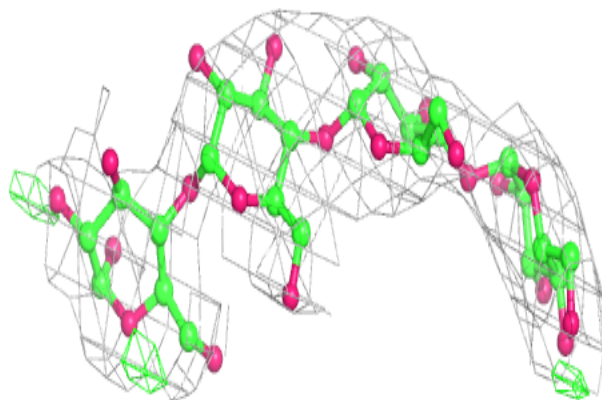


**Electron density around Chain H:**

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

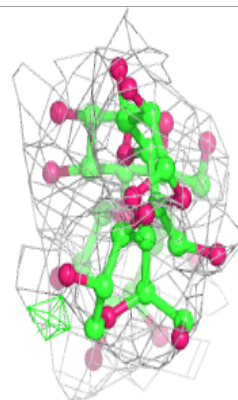
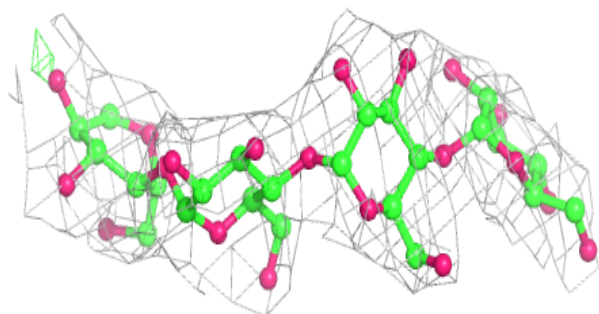
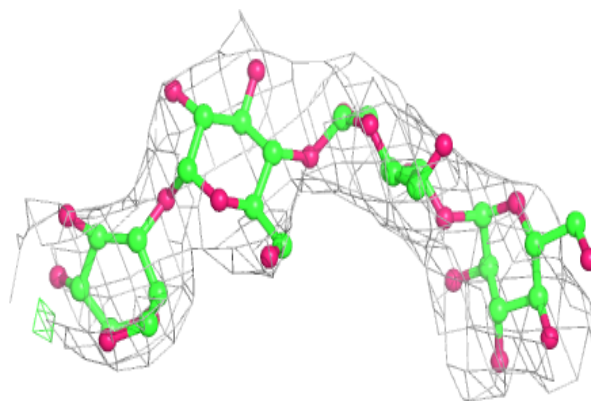
**Electron density around Chain I:**

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

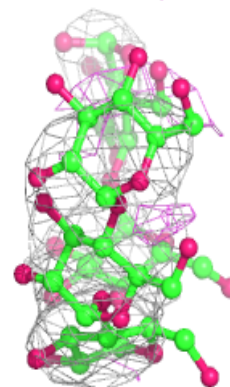
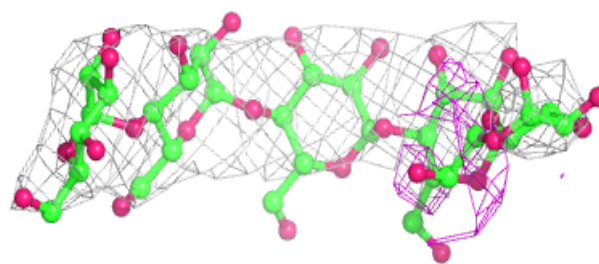
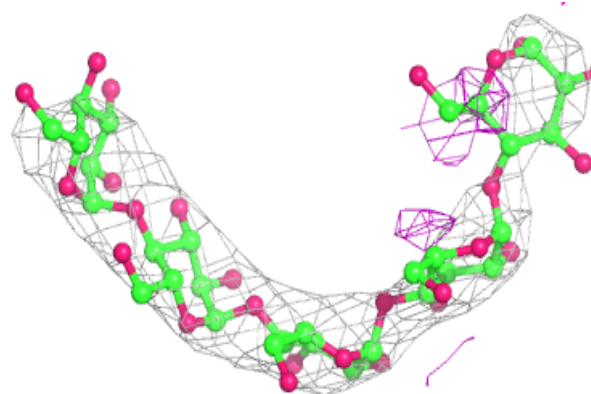


**Electron density around Chain K:**

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

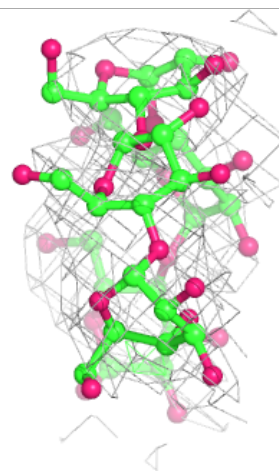
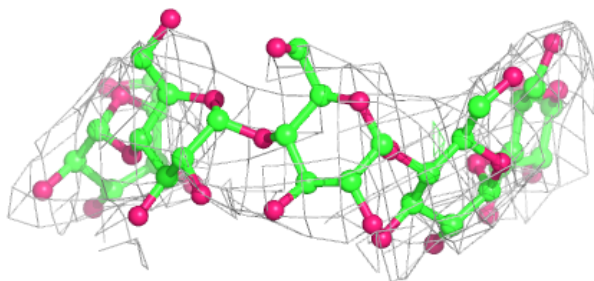
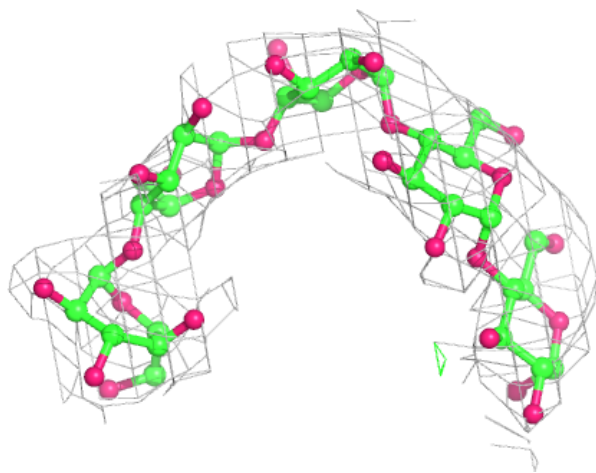
**Electron density around Chain D:**

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



**Electron density around Chain G:**

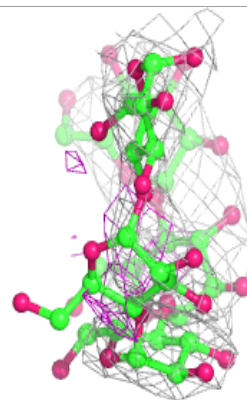
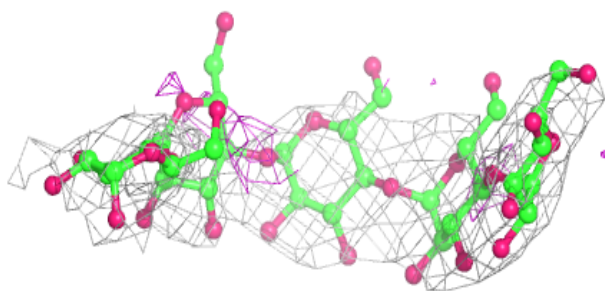
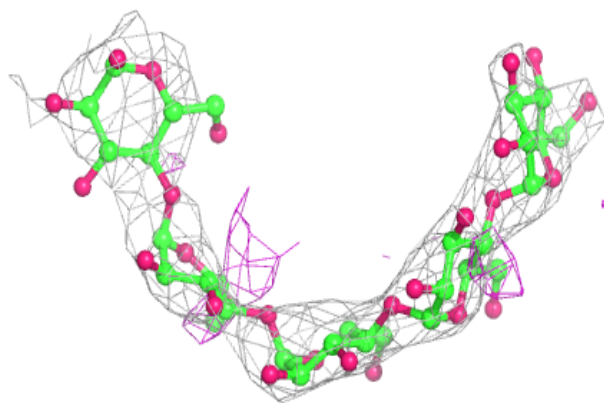
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



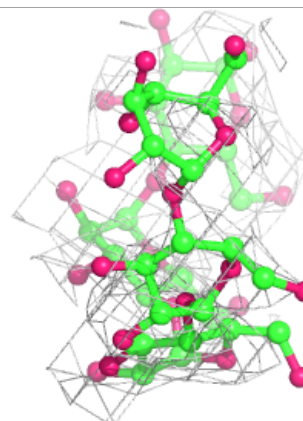
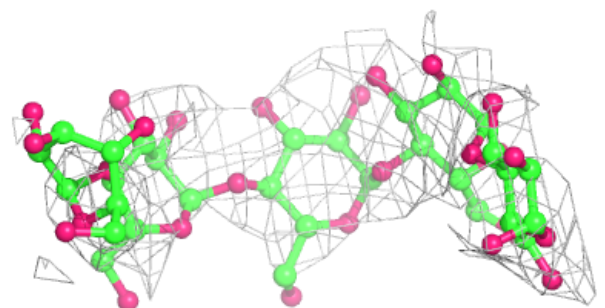
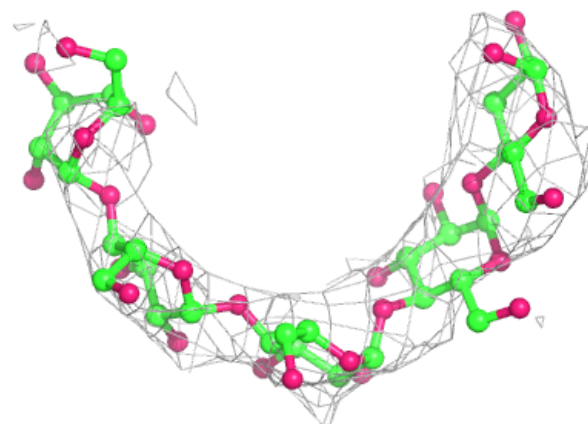


**Electron density around Chain J:**

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

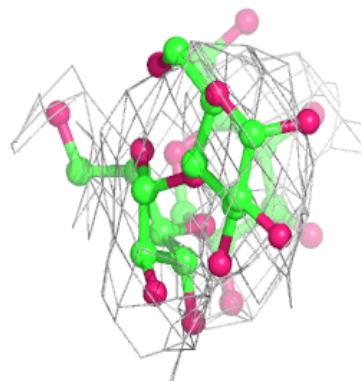
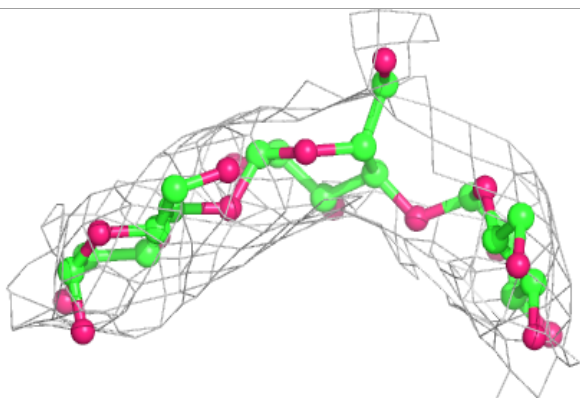
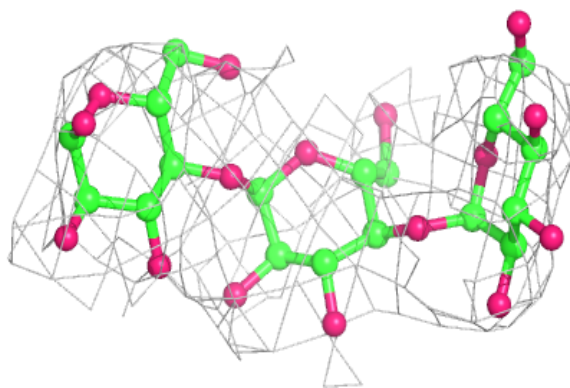
**Electron density around Chain M:**

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

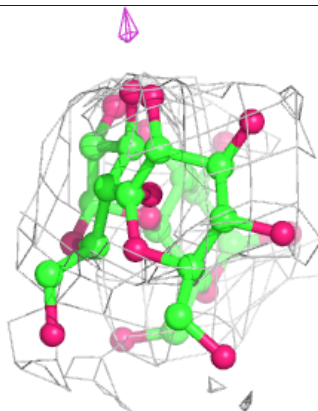
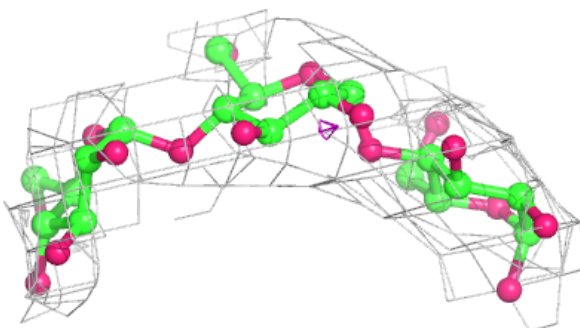
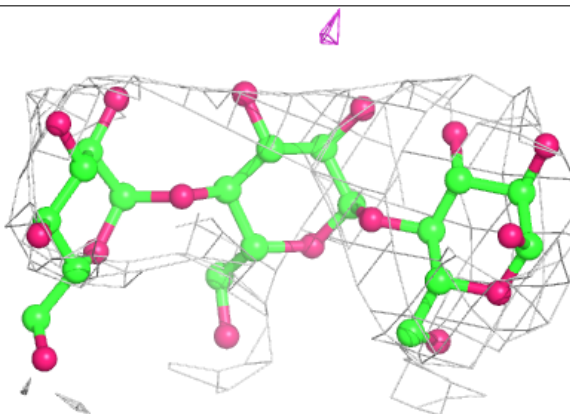


**Electron density around Chain F:**

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

**Electron density around Chain 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

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.