



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 03:34 PM EST

PDB ID : 4W8B  
Title : Crystal structure of XEG5B, a GH5 xyloglucan-specific beta-1,4-glucanase from ruminal metagenomic library, in complex with XXLG  
Authors : Santos, C.R.; Cordeiro, R.L.; Wong, D.W.S.; Murakami, M.T.  
Deposited on : 2014-08-22  
Resolution : 1.15 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.

The types of validation reports are described at

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

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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 : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

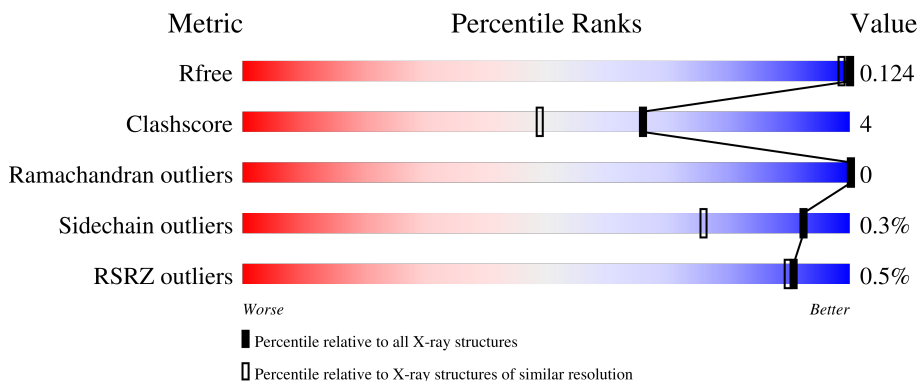
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

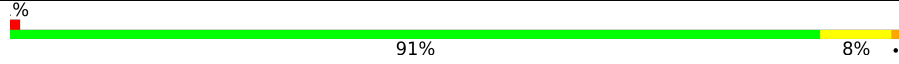
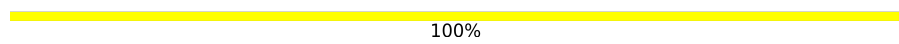

The reported resolution of this entry is 1.15 Å.

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	1492 (1.18-1.10)
Clashscore	141614	1537 (1.18-1.10)
Ramachandran outliers	138981	1483 (1.18-1.10)
Sidechain outliers	138945	1480 (1.18-1.10)
RSRZ outliers	127900	1464 (1.18-1.10)

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  $\geq 3$ , 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	386	 91% 8%
2	B	8	 100%
3	C	5	 60% 40%

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 3886 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.

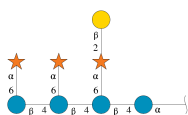
- Molecule 1 is a protein called Exo-xyloglucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	386	3044	1914	517	602	11	0	8	0

There are 8 discrepancies between the modelled and reference sequences:

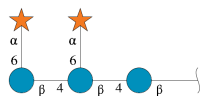
Chain	Residue	Modelled	Actual	Comment	Reference
A	517	LEU	-	expression tag	UNP D2XML9
A	518	GLU	-	expression tag	UNP D2XML9
A	519	HIS	-	expression tag	UNP D2XML9
A	520	HIS	-	expression tag	UNP D2XML9
A	521	HIS	-	expression tag	UNP D2XML9
A	522	HIS	-	expression tag	UNP D2XML9
A	523	HIS	-	expression tag	UNP D2XML9
A	524	HIS	-	expression tag	UNP D2XML9

- Molecule 2 is an oligosaccharide called alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[beta-D-galactopyranose-(1-2)-alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



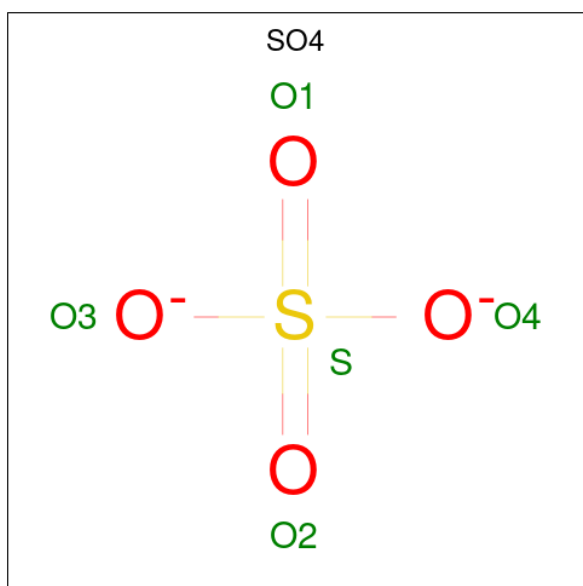
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	B	8	85	46	39	0	1	0

- Molecule 3 is an oligosaccharide called alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	5	Total	C	O	0	0	0
			52	28	24			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

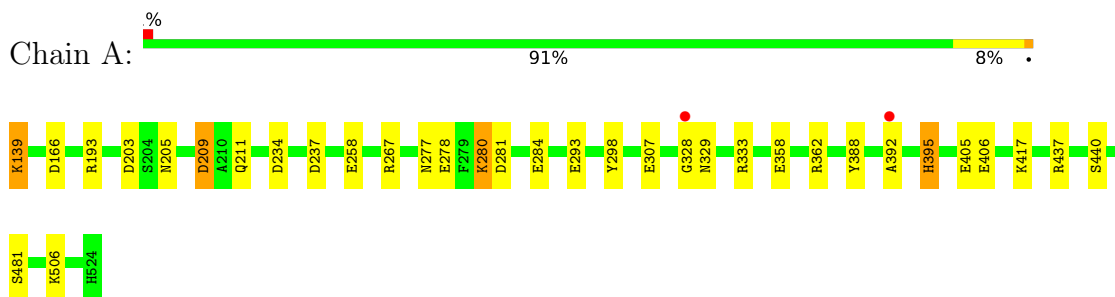
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	678	Total O 678 678	0	0

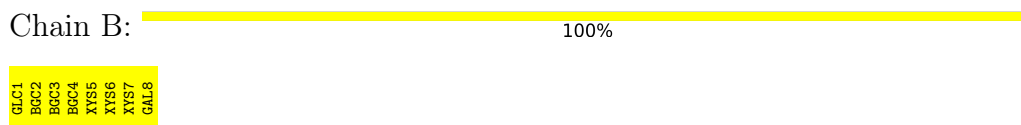
### 3 Residue-property plots [i](#)

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: Exo-xyloglucanase



- Molecule 2: alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[beta-D-galactopyranose-(1-2)-alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 3: alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.63Å 120.63Å 59.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.49 – 1.15 39.49 – 1.15	Depositor EDS
% Data completeness (in resolution range)	95.7 (39.49-1.15) 95.7 (39.49-1.15)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.74 (at 1.15Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.103 , 0.122 0.107 , 0.124	Depositor DCC
$R_{free}$ test set	8301 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	7.0	Xtrriage
Anisotropy	0.296	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	3886	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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, XYS, SO4, GOL, GAL, 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	1.17	15/3158 (0.5%)	1.07	22/4296 (0.5%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	GLU	CD-OE2	9.99	1.36	1.25
1	A	406	GLU	CB-CG	-9.85	1.33	1.52
1	A	258	GLU	CB-CG	-8.98	1.35	1.52
1	A	481	SER	CB-OG	8.44	1.53	1.42
1	A	358	GLU	CD-OE1	8.02	1.34	1.25
1	A	440	SER	CB-OG	-8.00	1.31	1.42
1	A	333	ARG	CA-CB	7.90	1.71	1.53
1	A	298	TYR	CE1-CZ	-7.85	1.28	1.38
1	A	284	GLU	CG-CD	-7.56	1.40	1.51
1	A	392	ALA	N-CA	7.00	1.60	1.46
1	A	328	GLY	N-CA	6.26	1.55	1.46
1	A	280	LYS	CD-CE	6.07	1.66	1.51
1	A	139	LYS	CA-CB	-5.71	1.41	1.53
1	A	281	ASP	CA-CB	-5.41	1.42	1.53
1	A	284	GLU	CB-CG	5.36	1.62	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ASP	CB-CG-OD1	10.65	127.89	118.30
1	A	209[A]	ASP	CB-CG-OD2	-9.07	110.14	118.30
1	A	209[B]	ASP	CB-CG-OD2	-9.07	110.14	118.30
1	A	209[A]	ASP	CB-CG-OD1	6.96	124.57	118.30
1	A	209[B]	ASP	CB-CG-OD1	6.96	124.57	118.30
1	A	281	ASP	CB-CG-OD1	6.85	124.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	LYS	CD-CE-NZ	6.58	126.83	111.70
1	A	362	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	193	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	388	TYR	CB-CG-CD1	6.20	124.72	121.00
1	A	258	GLU	CG-CD-OE2	-6.17	105.97	118.30
1	A	298	TYR	CD1-CE1-CZ	-6.16	114.25	119.80
1	A	267	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	406	GLU	CA-CB-CG	5.78	126.11	113.40
1	A	437	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	A	278	GLU	OE1-CD-OE2	-5.61	116.57	123.30
1	A	280	LYS	CG-CD-CE	5.47	128.32	111.90
1	A	203	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	298	TYR	CB-CG-CD2	5.32	124.19	121.00
1	A	193	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	234	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	A	237	ASP	CB-CG-OD2	-5.25	113.58	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3044	0	2839	19	0
2	B	85	0	65	0	0
3	C	52	0	43	5	0
4	A	15	0	0	1	0
5	A	12	0	15	0	0
6	A	678	0	0	19	0
All	All	3886	0	2962	25	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 4.

All (25) 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:506[B]:LYS:HG2	6:A:1219:HOH:O	1.54	1.07
1:A:209[B]:ASP:OD2	6:A:701:HOH:O	1.76	1.00
6:A:1264:HOH:O	3:C:3:BGC:H6C1	1.73	0.88
1:A:506[B]:LYS:CD	6:A:1219:HOH:O	2.22	0.87
1:A:506[B]:LYS:HE2	6:A:1163:HOH:O	1.82	0.79
1:A:277:ASN:HD22	1:A:280:LYS:HE2	1.52	0.72
1:A:395:HIS:HE1	1:A:405:GLU:OE2	1.72	0.71
1:A:211:GLN:NE2	6:A:705:HOH:O	2.26	0.67
1:A:395:HIS:HD2	6:A:898:HOH:O	1.79	0.65
6:A:1264:HOH:O	3:C:3:BGC:C5	2.46	0.62
1:A:205:ASN:ND2	6:A:702:HOH:O	2.18	0.59
1:A:506[B]:LYS:CE	6:A:1163:HOH:O	2.47	0.57
1:A:506[B]:LYS:HD3	6:A:1219:HOH:O	1.93	0.57
6:A:1374:HOH:O	3:C:4:XYX:O2	1.99	0.56
6:A:1264:HOH:O	3:C:3:BGC:C6	2.39	0.56
6:A:1264:HOH:O	3:C:3:BGC:H5	2.10	0.50
1:A:506[B]:LYS:CG	6:A:1219:HOH:O	2.18	0.50
1:A:506[B]:LYS:NZ	6:A:1163:HOH:O	2.44	0.49
1:A:277:ASN:ND2	1:A:280:LYS:HE2	2.26	0.47
1:A:139:LYS:HE2	6:A:1226:HOH:O	2.15	0.47
1:A:417[B]:LYS:HE3	6:A:707:HOH:O	2.14	0.46
4:A:611:SO4:O4	6:A:703:HOH:O	2.21	0.44
1:A:280:LYS:O	1:A:329:ASN:HB2	2.18	0.44
1:A:277:ASN:HD22	1:A:280:LYS:CE	2.26	0.42

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	393/386 (102%)	380 (97%)	13 (3%)	0	<b>100</b> <b>100</b>

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	324/315 (103%)	323 (100%)	1 (0%)	<a href="#">92</a> <a href="#">76</a>

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	395	HIS

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

Mol	Chain	Res	Type
1	A	142	GLN
1	A	277	ASN
1	A	395	HIS

### 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](#)

14 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	B	1[A]	-	12,12,12	2.15	2 (16%)	17,17,17	1.60	3 (17%)
2	GLC	B	1[B]	-	12,12,12	1.12	1 (8%)	17,17,17	2.49	5 (29%)
2	BGC	B	2	2	11,11,12	2.21	4 (36%)	15,15,17	1.44	4 (26%)
2	BGC	B	3	2	11,11,12	1.84	3 (27%)	15,15,17	3.00	6 (40%)
2	BGC	B	4	2	11,11,12	1.34	1 (9%)	15,15,17	1.46	3 (20%)
2	XYS	B	5	2	9,9,10	1.52	1 (11%)	10,12,14	2.53	5 (50%)
2	XYS	B	6	2	9,9,10	1.63	2 (22%)	10,12,14	3.50	5 (50%)
2	XYS	B	7	2	9,9,10	1.30	1 (11%)	10,12,14	1.18	1 (10%)
2	GAL	B	8	2	11,11,12	1.56	2 (18%)	15,15,17	1.95	4 (26%)
3	BGC	C	1	3	12,12,12	1.38	2 (16%)	17,17,17	1.61	5 (29%)
3	BGC	C	2	3	11,11,12	1.06	1 (9%)	15,15,17	1.21	2 (13%)
3	BGC	C	3	3	11,11,12	1.24	2 (18%)	15,15,17	1.38	2 (13%)
3	XYS	C	4	3	9,9,10	2.18	5 (55%)	10,12,14	2.64	5 (50%)
3	XYS	C	5	3	9,9,10	1.70	2 (22%)	10,12,14	1.61	2 (20%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	B	1[A]	-	-	0/2/22/22	0/1/1/1
2	GLC	B	1[B]	-	-	1/2/22/22	0/1/1/1
2	BGC	B	2	2	-	1/2/19/22	0/1/1/1
2	BGC	B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	B	4	2	-	0/2/19/22	0/1/1/1
2	XYS	B	5	2	-	-	0/1/1/1
2	XYS	B	6	2	-	-	0/1/1/1
2	XYS	B	7	2	-	-	0/1/1/1
2	GAL	B	8	2	-	2/2/19/22	0/1/1/1
3	BGC	C	1	3	-	0/2/22/22	0/1/1/1
3	BGC	C	2	3	-	0/2/19/22	0/1/1/1
3	BGC	C	3	3	-	0/2/19/22	0/1/1/1
3	XYS	C	4	3	-	-	0/1/1/1
3	XYS	C	5	3	-	-	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1[A]	GLC	C6-C5	6.41	1.73	1.51
2	B	2	BGC	O2-C2	4.70	1.53	1.43
2	B	3	BGC	O5-C1	4.23	1.50	1.43
3	C	4	XYS	O3-C3	-3.63	1.34	1.43
2	B	8	GAL	O5-C1	3.55	1.49	1.43
2	B	4	BGC	O5-C1	3.47	1.49	1.43
3	C	5	XYS	C4-C3	3.25	1.57	1.52
2	B	2	BGC	C4-C5	3.14	1.59	1.53
2	B	5	XYS	C2-C3	3.06	1.57	1.52
2	B	6	XYS	C2-C3	2.88	1.56	1.52
2	B	6	XYS	C4-C3	-2.87	1.48	1.52
3	C	4	XYS	O2-C2	2.82	1.49	1.43
3	C	1	BGC	C4-C5	2.78	1.58	1.53
2	B	2	BGC	O5-C5	-2.54	1.38	1.43
2	B	1[A]	GLC	C4-C5	-2.51	1.47	1.53
2	B	1[B]	GLC	C4-C5	-2.51	1.47	1.53
2	B	3	BGC	O2-C2	-2.51	1.38	1.43
3	C	4	XYS	C4-C3	2.46	1.56	1.52
2	B	2	BGC	O4-C4	-2.33	1.37	1.43
3	C	4	XYS	O5-C5	2.32	1.47	1.42
2	B	7	XYS	C4-C3	-2.24	1.49	1.52
3	C	3	BGC	O5-C5	2.17	1.47	1.43
2	B	3	BGC	C4-C5	-2.16	1.48	1.53
2	B	8	GAL	C6-C5	2.15	1.59	1.51
3	C	4	XYS	C2-C3	-2.15	1.49	1.52
3	C	5	XYS	O4-C4	2.07	1.47	1.43
3	C	2	BGC	O5-C1	-2.06	1.40	1.43
3	C	1	BGC	C1-C2	2.04	1.57	1.52
3	C	3	BGC	C4-C5	2.02	1.57	1.53

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	BGC	O5-C1-C2	-7.71	98.87	110.77
2	B	1[B]	GLC	C6-C5-C4	7.60	130.80	113.00
2	B	3	BGC	C1-O5-C5	6.24	120.65	112.19
2	B	6	XYS	O3-C3-C4	-6.06	98.38	109.99
2	B	8	GAL	O6-C6-C5	5.43	129.93	111.29
2	B	6	XYS	C5-O5-C1	-5.17	103.57	111.52
2	B	6	XYS	C5-C4-C3	-4.86	103.69	109.67
2	B	5	XYS	C4-C3-C2	-4.73	105.30	110.92
2	B	6	XYS	C1-C2-C3	-4.64	103.96	109.67
3	C	4	XYS	C5-O5-C1	4.39	118.28	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	XYS	C5-C4-C3	4.31	114.96	109.67
2	B	5	XYS	C5-C4-C3	3.91	114.47	109.67
2	B	1[B]	GLC	O5-C5-C6	3.68	115.60	106.44
2	B	4	BGC	O5-C1-C2	-3.34	105.62	110.77
3	C	3	BGC	C1-C2-C3	3.15	113.54	109.67
2	B	3	BGC	O2-C2-C1	-3.11	102.78	109.15
3	C	4	XYS	C1-C2-C3	3.10	113.47	109.67
3	C	1	BGC	O2-C2-C1	3.05	116.23	109.16
2	B	4	BGC	O5-C5-C6	-2.96	102.57	107.20
3	C	5	XYS	C4-C3-C2	-2.92	107.46	110.92
2	B	5	XYS	O4-C4-C3	-2.85	104.42	110.14
2	B	2	BGC	C3-C4-C5	-2.77	105.31	110.24
2	B	5	XYS	O2-C2-C1	2.76	114.80	109.15
3	C	4	XYS	O3-C3-C4	2.76	115.28	109.99
2	B	6	XYS	O4-C4-C5	2.75	114.78	109.15
3	C	4	XYS	O4-C4-C3	2.74	115.62	110.14
2	B	1[A]	GLC	O6-C6-C5	2.73	120.67	111.29
2	B	3	BGC	O2-C2-C3	2.73	115.60	110.14
2	B	8	GAL	C2-C3-C4	-2.69	106.24	110.89
2	B	1[A]	GLC	O1-C1-C2	2.67	116.55	109.03
2	B	1[B]	GLC	O1-C1-C2	2.67	116.55	109.03
2	B	5	XYS	C5-O5-C1	2.66	115.61	111.52
2	B	8	GAL	O2-C2-C1	-2.65	103.73	109.15
3	C	2	BGC	C1-C2-C3	-2.53	106.55	109.67
3	C	5	XYS	O4-C4-C3	2.50	115.15	110.14
2	B	2	BGC	O3-C3-C4	-2.46	104.66	110.35
3	C	3	BGC	O4-C4-C3	-2.41	104.77	110.35
2	B	1[A]	GLC	C3-C4-C5	2.39	114.50	110.24
2	B	1[B]	GLC	C3-C4-C5	2.39	114.50	110.24
2	B	4	BGC	O2-C2-C3	-2.35	105.42	110.14
3	C	1	BGC	O5-C5-C4	2.34	113.95	109.69
2	B	2	BGC	O5-C1-C2	-2.24	107.31	110.77
3	C	1	BGC	O2-C2-C3	-2.22	105.21	110.35
3	C	1	BGC	O1-C1-O5	-2.19	103.80	110.38
2	B	1[B]	GLC	O6-C6-C5	2.18	118.78	111.29
2	B	3	BGC	C1-C2-C3	2.15	112.31	109.67
3	C	2	BGC	O6-C6-C5	-2.13	104.00	111.29
2	B	8	GAL	O5-C5-C6	-2.12	103.89	107.20
3	C	1	BGC	C3-C4-C5	2.07	113.92	110.24
2	B	2	BGC	C1-C2-C3	-2.06	107.14	109.67
2	B	3	BGC	O5-C5-C4	-2.03	105.89	110.83
2	B	7	XYS	O2-C2-C3	-2.02	106.10	110.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	8	GAL	O5-C5-C6-O6
2	B	1[B]	GLC	O5-C5-C6-O6
2	B	8	GAL	C4-C5-C6-O6
2	B	2	BGC	C4-C5-C6-O6

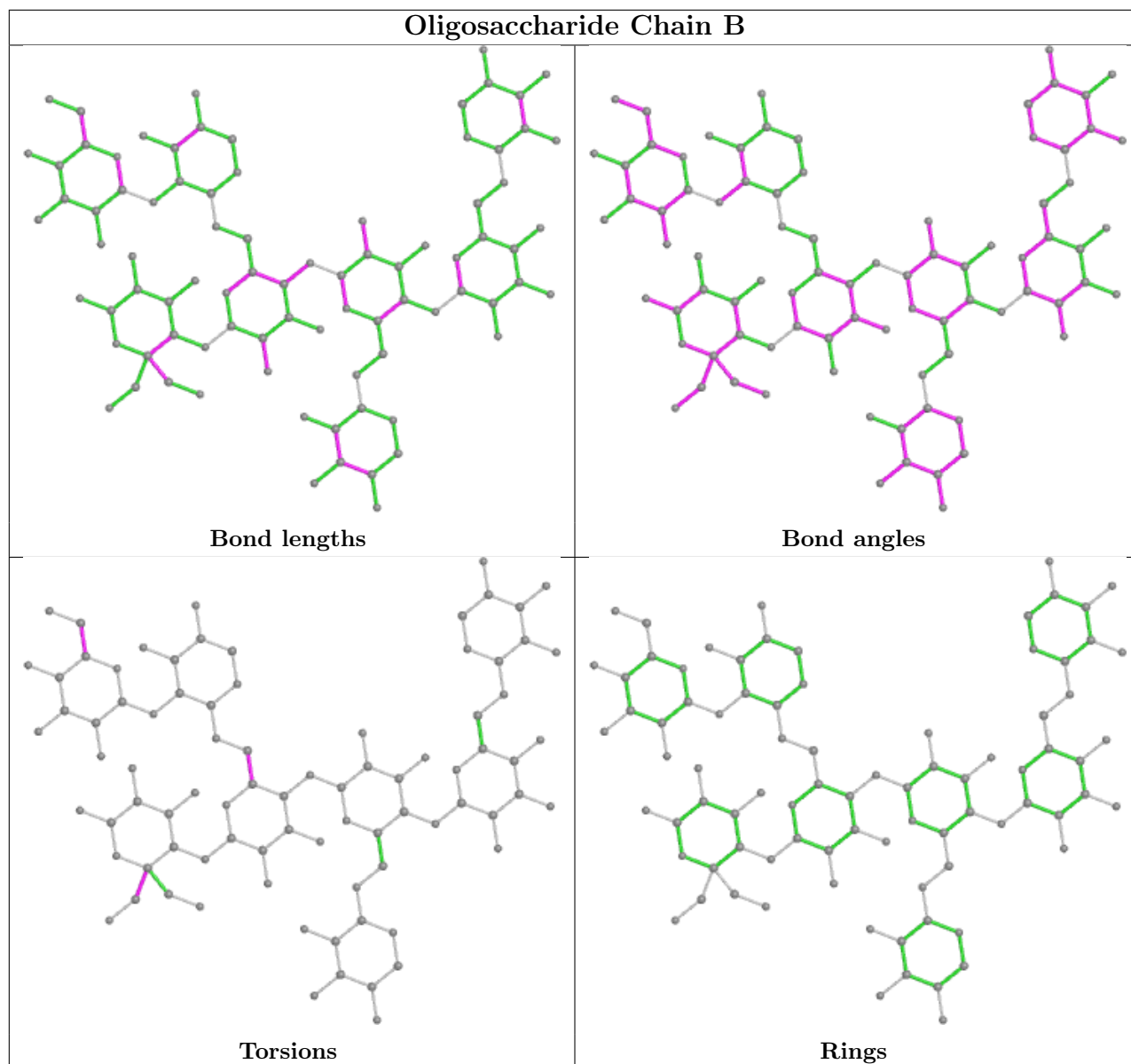
There are no ring outliers.

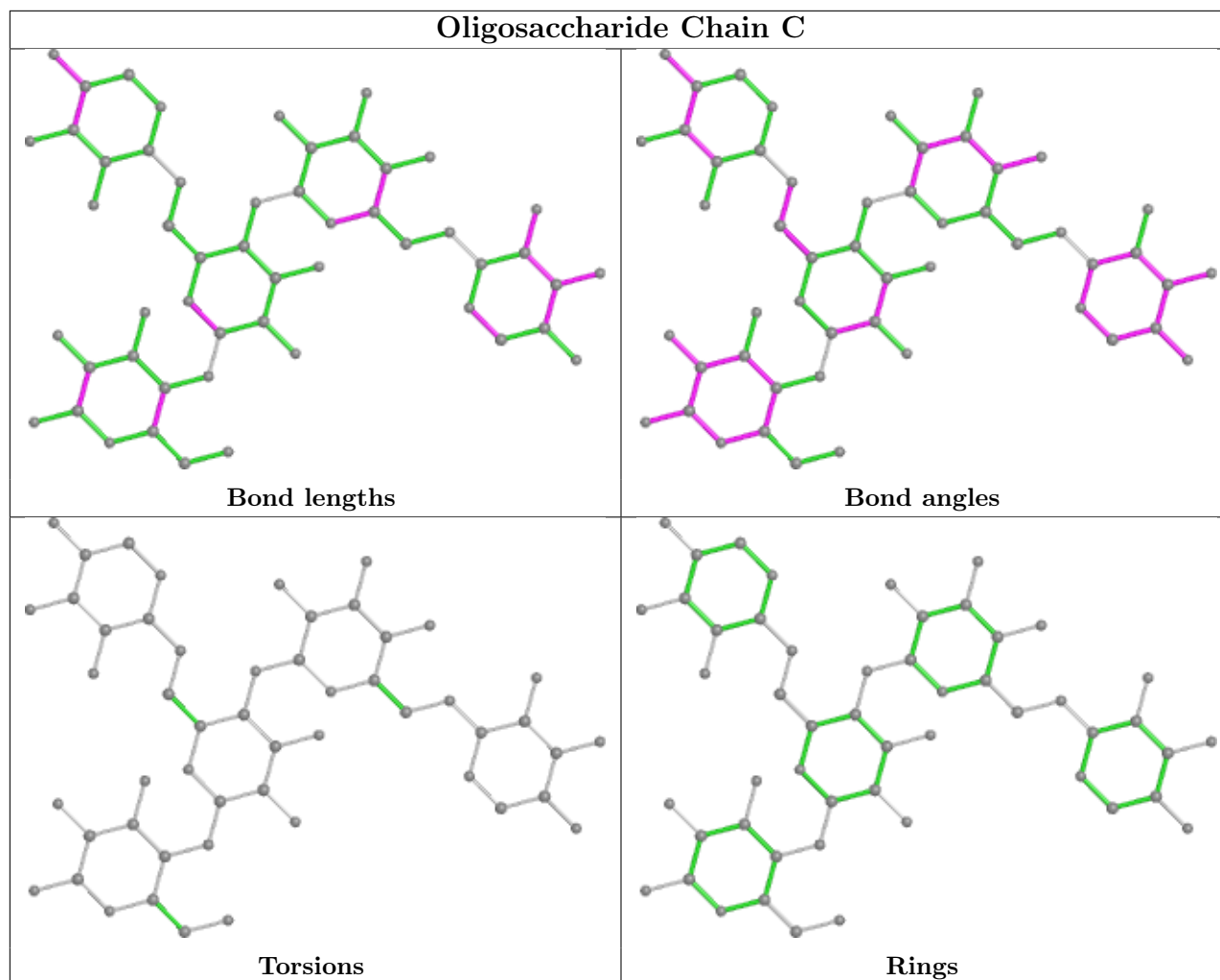
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3	BGC	4	0
3	C	4	XYS	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](#)

5 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	$\# Z  > 2$
4	SO4	A	609	-	4,4,4	0.67	0	6,6,6	1.85	1 (16%)
4	SO4	A	611	-	4,4,4	2.17	1 (25%)	6,6,6	1.62	1 (16%)
4	SO4	A	610	-	4,4,4	0.56	0	6,6,6	0.22	0
5	GOL	A	613	-	5,5,5	1.38	1 (20%)	5,5,5	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	A	612	-	5,5,5	1.22	0	5,5,5	1.78	2 (40%)

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	GOL	A	613	-	-	0/4/4/4	-
5	GOL	A	612	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	611	SO4	O2-S	-3.55	1.26	1.46
5	A	613	GOL	O3-C3	2.16	1.51	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	609	SO4	O4-S-O3	-4.20	91.15	109.06
5	A	612	GOL	C3-C2-C1	-3.07	99.75	111.70
4	A	611	SO4	O4-S-O2	2.97	124.83	109.31
5	A	612	GOL	O2-C2-C3	2.17	118.66	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	611	SO4	1	0

## 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, 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	386/386 (100%)	0.01	2 (0%) 91 90	4, 7, 15, 39	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	GLY	2.9
1	A	392	ALA	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, 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.

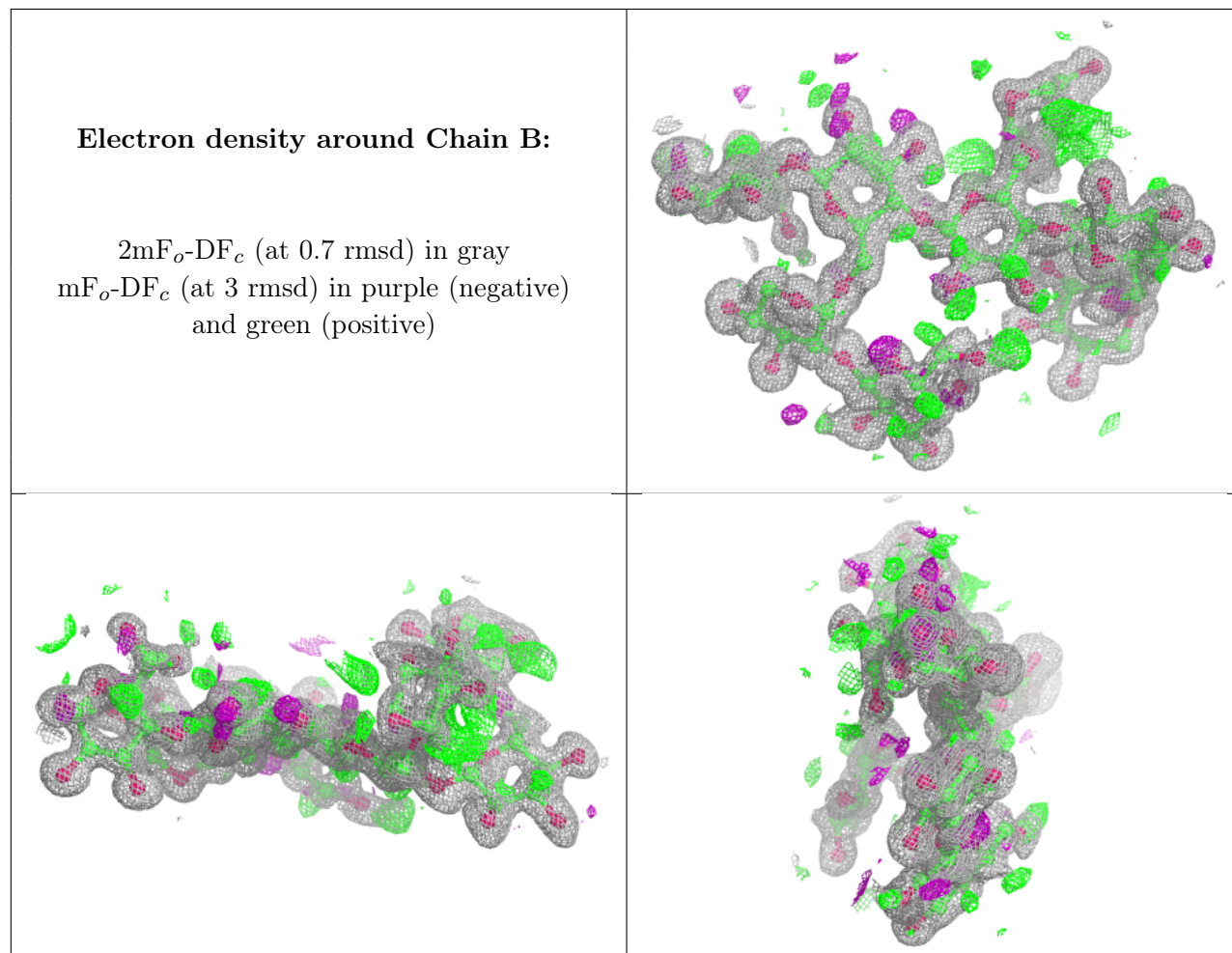
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	BGC	C	1	12/12	0.78	0.30	21,27,36,37	12
3	XYS	C	5	9/10	0.81	0.38	24,30,37,37	9
2	XYS	B	6	9/10	0.87	0.14	15,19,32,34	9
3	BGC	C	3	11/12	0.89	0.33	18,19,23,26	11
3	BGC	C	2	11/12	0.90	0.29	18,19,25,27	11
2	GAL	B	8	11/12	0.92	0.13	15,16,27,36	0
3	XYS	C	4	9/10	0.95	0.16	12,15,16,18	9
2	XYS	B	5	9/10	0.95	0.09	13,13,16,19	9
2	BGC	B	4	11/12	0.97	0.08	11,13,16,16	0
2	BGC	B	2	11/12	0.97	0.07	9,11,12,14	0

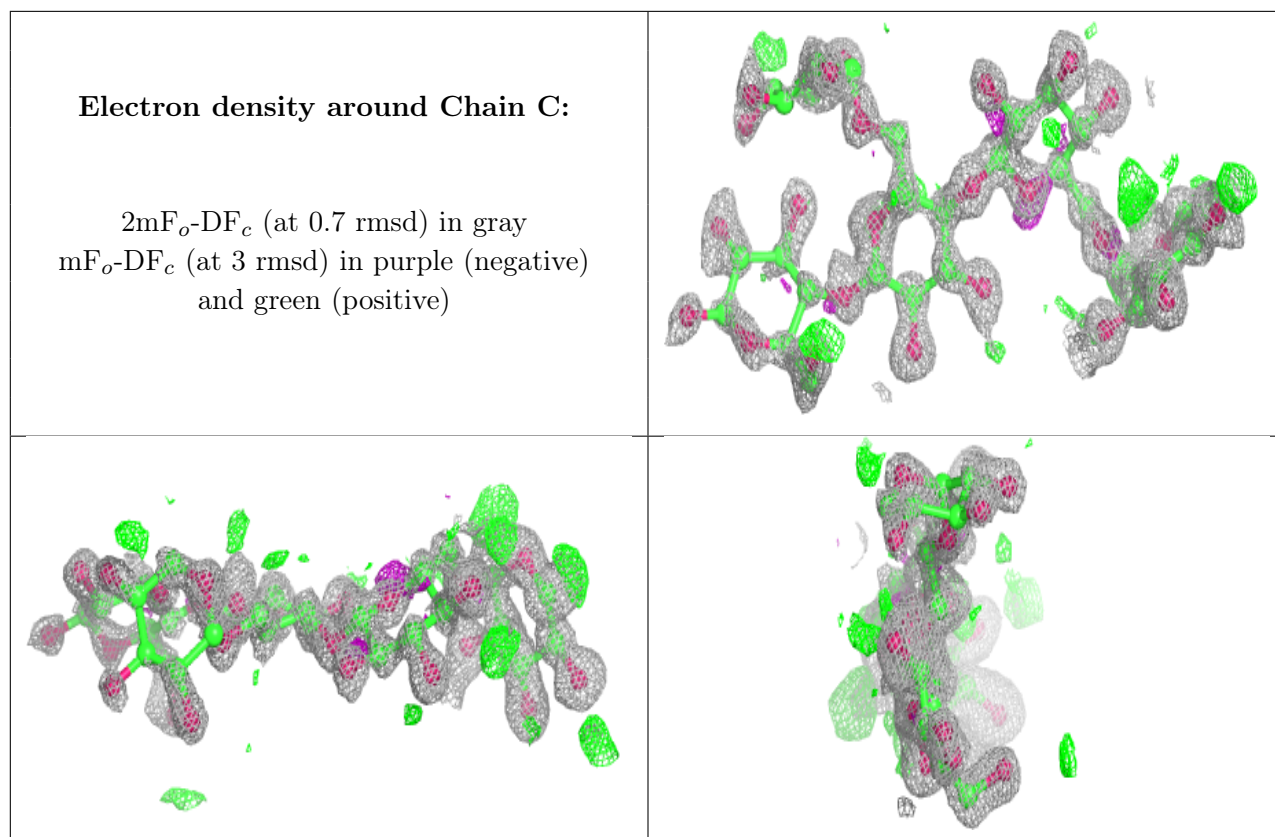
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BGC	B	3	11/12	0.97	0.07	10,12,18,22	0
2	GLC	B	1[B]	12/12	0.98	0.09	6,8,10,13	2
2	GLC	B	1[A]	12/12	0.98	0.09	6,8,12,13	2
2	XYS	B	7	9/10	0.99	0.06	6,8,9,10	0

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.





## 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	GOL	A	612	6/6	0.97	0.12	10,21,31,44	0
5	GOL	A	613	6/6	0.97	0.14	12,20,25,30	0
4	SO4	A	611	5/5	0.98	0.14	9,11,17,18	5
4	SO4	A	610	5/5	0.99	0.07	9,9,10,12	0
4	SO4	A	609	5/5	0.99	0.05	8,9,12,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.