



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 12:58 pm GMT

PDB ID : 6HAA  
Title : Structure of a covalent complex of endo-Xyloglucanase from *Cellvibrio japonicus* after reacting with XXXG(2F)-beta-DNP  
Authors : Offen, W.; Davies, G.J.  
Deposited on : 2018-08-07  
Resolution : 1.70 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 : 1.8.4, 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

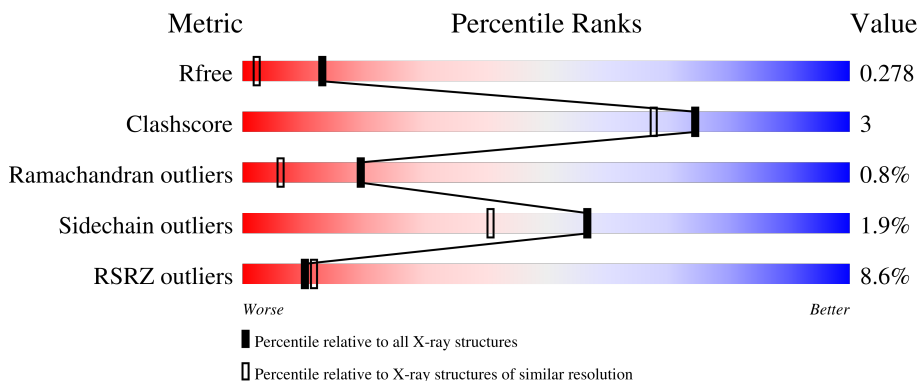
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

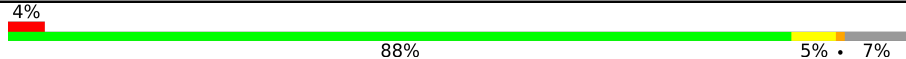

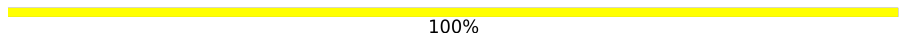
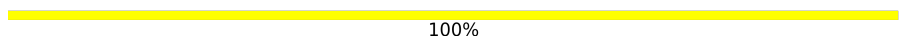
The reported resolution of this entry is 1.70 Å.

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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	396	 4% 88% 5% • 7%
1	B	396	 12% 84% 9% • 7%
2	C	6	 100%
3	D	7	 100%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6449 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 Cellulase, putative, cel5D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	370	2919	1852	498	559	10	0	1	0
1	B	370	2952	1871	505	566	10	0	6	0

There are 48 discrepancies between the modelled and reference sequences:

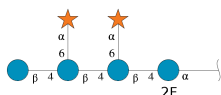
Chain	Residue	Modelled	Actual	Comment	Reference
A	73	MET	-	initiating methionine	UNP B3PD52
A	74	GLY	-	expression tag	UNP B3PD52
A	75	SER	-	expression tag	UNP B3PD52
A	76	SER	-	expression tag	UNP B3PD52
A	77	HIS	-	expression tag	UNP B3PD52
A	78	HIS	-	expression tag	UNP B3PD52
A	79	HIS	-	expression tag	UNP B3PD52
A	80	HIS	-	expression tag	UNP B3PD52
A	81	HIS	-	expression tag	UNP B3PD52
A	82	HIS	-	expression tag	UNP B3PD52
A	83	SER	-	expression tag	UNP B3PD52
A	84	SER	-	expression tag	UNP B3PD52
A	85	GLY	-	expression tag	UNP B3PD52
A	86	LEU	-	expression tag	UNP B3PD52
A	87	VAL	-	expression tag	UNP B3PD52
A	88	PRO	-	expression tag	UNP B3PD52
A	89	ARG	-	expression tag	UNP B3PD52
A	90	GLY	-	expression tag	UNP B3PD52
A	91	SER	-	expression tag	UNP B3PD52
A	92	HIS	-	expression tag	UNP B3PD52
A	93	MET	-	expression tag	UNP B3PD52
A	94	ALA	-	expression tag	UNP B3PD52
A	95	SER	-	expression tag	UNP B3PD52
A	255	ALA	GLU	engineered mutation	UNP B3PD52
B	73	MET	-	initiating methionine	UNP B3PD52

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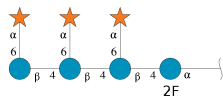
Chain	Residue	Modelled	Actual	Comment	Reference
B	74	GLY	-	expression tag	UNP B3PD52
B	75	SER	-	expression tag	UNP B3PD52
B	76	SER	-	expression tag	UNP B3PD52
B	77	HIS	-	expression tag	UNP B3PD52
B	78	HIS	-	expression tag	UNP B3PD52
B	79	HIS	-	expression tag	UNP B3PD52
B	80	HIS	-	expression tag	UNP B3PD52
B	81	HIS	-	expression tag	UNP B3PD52
B	82	HIS	-	expression tag	UNP B3PD52
B	83	SER	-	expression tag	UNP B3PD52
B	84	SER	-	expression tag	UNP B3PD52
B	85	GLY	-	expression tag	UNP B3PD52
B	86	LEU	-	expression tag	UNP B3PD52
B	87	VAL	-	expression tag	UNP B3PD52
B	88	PRO	-	expression tag	UNP B3PD52
B	89	ARG	-	expression tag	UNP B3PD52
B	90	GLY	-	expression tag	UNP B3PD52
B	91	SER	-	expression tag	UNP B3PD52
B	92	HIS	-	expression tag	UNP B3PD52
B	93	MET	-	expression tag	UNP B3PD52
B	94	ALA	-	expression tag	UNP B3PD52
B	95	SER	-	expression tag	UNP B3PD52
B	255	ALA	GLU	engineered mutation	UNP B3PD52

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



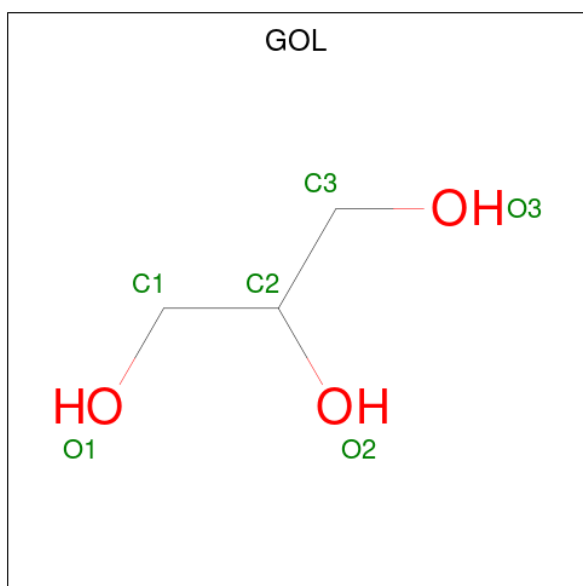
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	F	O			
2	C	6	62	34	1	27	0	0	0

- 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)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-2-deoxy-2-fluoro-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	F				O
3	D	7	71	39	1	31	0	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



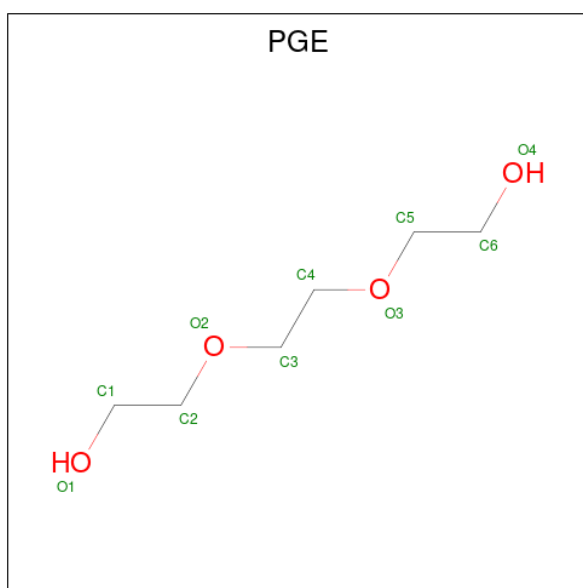
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
4	A	1	6	3	3	0	0
4	B	1	6	3	3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



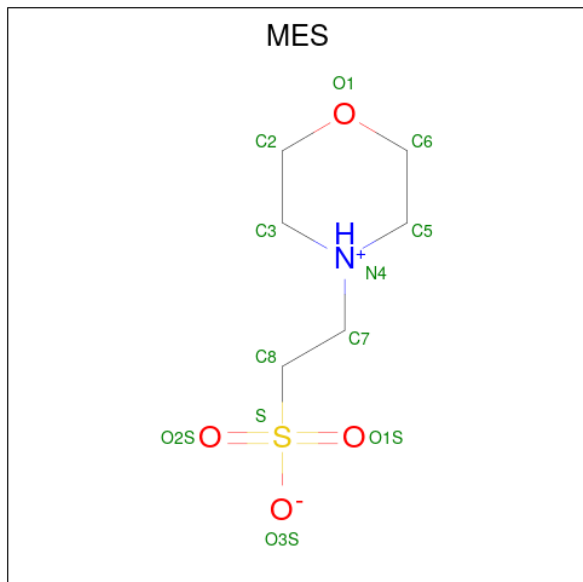
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



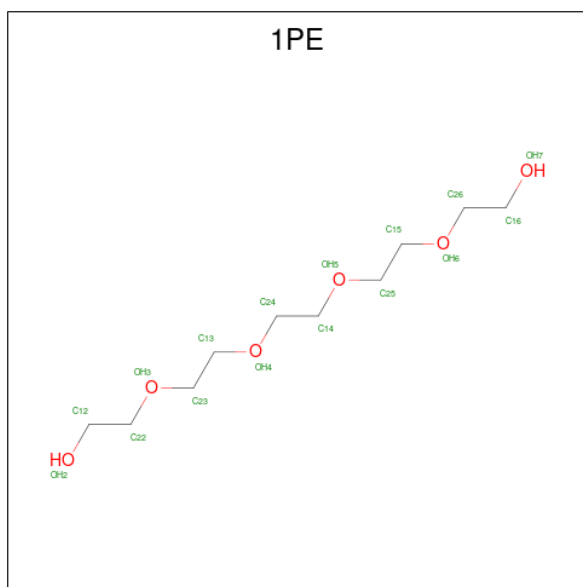
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 10 6 4	0	0
6	A	1	Total C O 10 6 4	0	0

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	S			
7	A	1	Total	12	6	1	4	1	0	0
7	B	1	Total	12	6	1	4	1	0	0

- Molecule 8 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 9 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	203	Total	O	0	0
			203	203		
9	B	154	Total	O	0	0
			154	154		

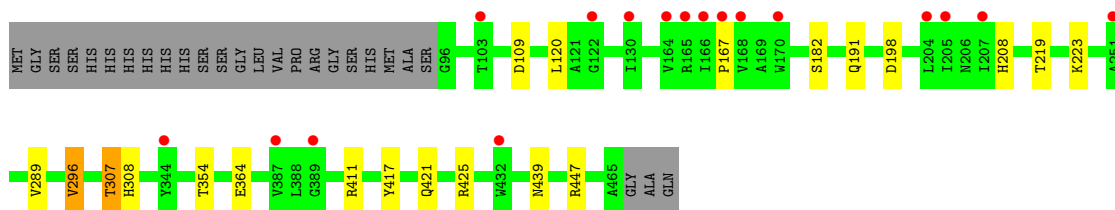


### 3 Residue-property plots [i](#)


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.

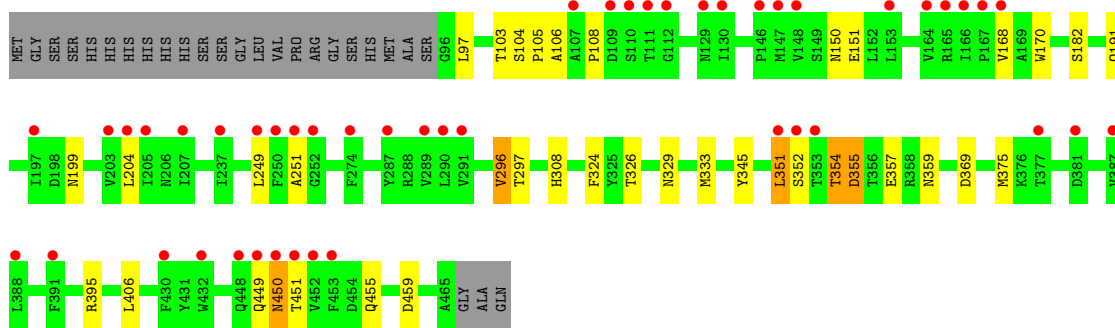
- Molecule 1: Cellulase, putative, cel5D

Chain A: 



- Molecule 1: Cellulase, putative, cel5D

Chain B: 



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

Chain C: 



- Molecule 3: alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-2-deoxy-2-fluoro-alpha-D-glucopyranose

Chain D:

100%

G2F1  
B6C2  
B6C3  
B6C4  
XY85  
XY86  
XY87

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.06Å 97.21Å 156.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.25 – 1.70 33.25 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (33.25-1.70) 98.2 (33.25-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.218 , 0.271 0.225 , 0.278	Depositor DCC
$R_{free}$ test set	4564 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.9	Xtrriage
Anisotropy	0.504	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 36.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6449	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES, BGC, PGE, 1PE, GOL, G2F, SO4, XYS

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	1.01	0/2992	0.97	6/4078 (0.1%)
1	B	0.94	0/3028	0.96	5/4128 (0.1%)
All	All	0.98	0/6020	0.97	11/8206 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	355[A]	ASP	CB-CG-OD1	7.96	125.46	118.30
1	B	355[B]	ASP	CB-CG-OD1	7.96	125.46	118.30
1	A	425	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	A	447	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	425	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	109	ASP	CB-CG-OD1	5.95	123.66	118.30
1	A	411	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	375	MET	CG-SD-CE	5.61	109.18	100.20
1	B	369	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	447	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	395	ARG	NE-CZ-NH2	5.01	122.81	120.30

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	2919	0	2757	11	0
1	B	2952	0	2781	26	0
2	C	62	0	50	0	0
3	D	71	0	57	0	0
4	A	12	0	16	1	0
4	B	6	0	8	0	0
5	A	5	0	0	1	0
5	B	5	0	0	1	0
6	A	20	0	28	0	0
7	A	12	0	13	0	0
7	B	12	0	13	0	0
8	B	16	0	22	2	0
9	A	203	0	0	3	0
9	B	154	0	0	11	0
All	All	6449	0	5745	38	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 3.

All (38) 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:355[B]:ASP:OD1	9:B:1101:HOH:O	1.57	1.19
1:B:150:ASN:OD1	1:B:199:ASN:ND2	2.09	0.86
1:A:307:THR:HG1	1:A:308:HIS:HD1	0.85	0.85
1:B:359:ASN:ND2	9:B:1102:HOH:O	2.05	0.78
1:B:355[B]:ASP:CG	9:B:1101:HOH:O	2.14	0.76
1:B:151:GLU:CB	1:B:450:ASN:OD1	2.35	0.74
1:B:352:SER:N	9:B:1104:HOH:O	2.22	0.72
1:B:351:LEU:C	9:B:1104:HOH:O	2.27	0.70
1:B:352:SER:HB2	9:B:1104:HOH:O	1.95	0.67
1:B:204:LEU:HD11	1:B:251:ALA:HB2	1.82	0.61
1:B:97:LEU:HD21	8:B:1011:1PE:H241	1.83	0.60
1:B:455:GLN:NE2	1:B:459:ASP:OD1	2.33	0.60
1:B:449:GLN:O	1:B:451:THR:HG23	2.05	0.57
1:B:352:SER:CB	9:B:1104:HOH:O	2.53	0.57
1:B:352:SER:CA	9:B:1104:HOH:O	2.53	0.56
1:A:417:TYR:CZ	1:A:421:GLN:HG3	2.44	0.52
1:B:352:SER:OG	1:B:354[B]:THR:HG23	2.10	0.52
1:B:104:SER:O	1:B:106:ALA:N	2.44	0.51
1:A:417:TYR:CE2	1:A:421:GLN:HG3	2.47	0.50
1:B:355[B]:ASP:OD2	9:B:1101:HOH:O	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLN:OE1	9:A:1101:HOH:O	2.20	0.50
8:B:1011:1PE:H252	9:B:1204:HOH:O	2.13	0.49
1:B:324:PHE:CZ	1:B:326:THR:HB	2.49	0.48
1:A:198:ASP:OD2	9:A:1102:HOH:O	2.21	0.46
1:B:249:LEU:N	1:B:249:LEU:HD12	2.31	0.45
1:B:168:VAL:HG11	1:B:170:TRP:CZ2	2.52	0.45
1:A:223:LYS:NZ	5:A:1009:SO4:O2	2.45	0.45
1:A:120:LEU:HD22	1:A:289:VAL:HG21	2.00	0.43
1:A:219:THR:HB	9:B:1213:HOH:O	2.18	0.43
1:B:450:ASN:HD22	1:B:450:ASN:HA	1.63	0.43
1:B:345:TYR:CE1	1:B:406:LEU:HD23	2.54	0.42
1:B:308:HIS:HA	5:B:1009:SO4:O2	2.19	0.42
1:B:354[A]:THR:HB	1:B:355[A]:ASP:H	1.51	0.42
1:B:352:SER:OG	1:B:354[B]:THR:N	2.49	0.41
1:B:329:ASN:HA	1:B:333:MET:HB2	2.02	0.41
1:A:439:ASN:H	4:A:1008:GOL:H32	1.85	0.41
1:A:364:GLU:HB2	9:A:1240:HOH:O	2.20	0.41
1:A:167:PRO:HB3	1:A:208:HIS:ND1	2.36	0.40

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	369/396 (93%)	352 (95%)	16 (4%)	1 (0%)	41 24
1	B	374/396 (94%)	344 (92%)	25 (7%)	5 (1%)	12 2
All	All	743/792 (94%)	696 (94%)	41 (6%)	6 (1%)	19 6

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	357	GLU
1	B	108	PRO
1	B	297	THR
1	B	296	VAL
1	A	296	VAL
1	B	105	PRO

### 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	299/326 (92%)	295 (99%)	4 (1%)	69	56
1	B	301/326 (92%)	293 (97%)	8 (3%)	44	26
All	All	600/652 (92%)	588 (98%)	12 (2%)	57	38

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	SER
1	A	296	VAL
1	A	307	THR
1	A	354	THR
1	B	103	THR
1	B	182	SER
1	B	191	GLN
1	B	296	VAL
1	B	351	LEU
1	B	354[A]	THR
1	B	354[B]	THR
1	B	450	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	359	ASN

### 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](#)

13 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	G2F	C	1	1,2	11,11,12	1.39	1 (9%)	10,15,17	0.92	0
2	BGC	C	2	2	11,11,12	1.33	1 (9%)	15,15,17	1.67	2 (13%)
2	BGC	C	3	2	11,11,12	0.88	0	15,15,17	1.71	4 (26%)
2	BGC	C	4	2	11,11,12	1.01	0	15,15,17	1.34	3 (20%)
2	XYS	C	5	2	9,9,10	1.20	1 (11%)	10,12,14	1.64	2 (20%)
2	XYS	C	6	2	9,9,10	1.06	1 (11%)	10,12,14	1.15	1 (10%)
3	G2F	D	1	3,1	11,11,12	1.68	2 (18%)	10,15,17	1.43	1 (10%)
3	BGC	D	2	3	11,11,12	1.02	0	15,15,17	1.59	5 (33%)
3	BGC	D	3	3	11,11,12	0.69	0	15,15,17	1.51	3 (20%)
3	BGC	D	4	3	11,11,12	0.42	0	15,15,17	1.57	3 (20%)
3	XYS	D	5	3	9,9,10	0.33	0	10,12,14	1.37	2 (20%)
3	XYS	D	6	3	9,9,10	0.72	0	10,12,14	1.64	2 (20%)
3	XYS	D	7	3	9,9,10	0.98	1 (11%)	10,12,14	0.84	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G2F	C	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	C	4	2	-	0/2/19/22	0/1/1/1
2	XYS	C	5	2	-	-	0/1/1/1
2	XYS	C	6	2	-	-	0/1/1/1
3	G2F	D	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	D	2	3	-	2/2/19/22	0/1/1/1
3	BGC	D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	D	4	3	-	0/2/19/22	0/1/1/1
3	XYS	D	5	3	-	-	0/1/1/1
3	XYS	D	6	3	-	-	0/1/1/1
3	XYS	D	7	3	-	-	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	G2F	C2-C3	3.64	1.56	1.51
3	D	1	G2F	C2-C3	3.19	1.55	1.51
2	C	2	BGC	O5-C1	-2.63	1.39	1.43
2	C	5	XYS	O3-C3	2.31	1.48	1.43
3	D	1	G2F	O5-C5	2.28	1.48	1.43
2	C	6	XYS	C2-C3	2.09	1.55	1.52
3	D	7	XYS	C4-C3	2.08	1.55	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	BGC	C1-O5-C5	4.40	118.15	112.19
2	C	2	BGC	C1-O5-C5	4.12	117.78	112.19
3	D	1	G2F	O5-C5-C6	-3.82	101.21	107.20
2	C	2	BGC	O5-C1-C2	-3.60	105.22	110.77
2	C	3	BGC	C1-O5-C5	3.31	116.68	112.19
2	C	5	XYS	O2-C2-C3	-3.29	103.54	110.14
3	D	6	XYS	O2-C2-C3	-3.28	103.57	110.14
2	C	4	BGC	O4-C4-C3	-3.14	103.09	110.35
2	C	5	XYS	C5-O5-C1	3.04	116.20	111.52
2	C	3	BGC	O4-C4-C5	-2.99	101.88	109.30
3	D	3	BGC	O5-C1-C2	-2.81	106.44	110.77
3	D	6	XYS	C1-C2-C3	2.70	112.98	109.67
3	D	2	BGC	C2-C3-C4	-2.64	106.33	110.89
3	D	2	BGC	O5-C1-C2	-2.53	106.86	110.77
3	D	3	BGC	C1-O5-C5	2.43	115.48	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	BGC	O2-C2-C3	-2.42	105.30	110.14
2	C	3	BGC	O5-C1-C2	-2.39	107.09	110.77
3	D	2	BGC	C1-C2-C3	2.36	112.56	109.67
2	C	3	BGC	O3-C3-C2	2.34	114.47	109.99
2	C	6	XYS	O2-C2-C3	-2.31	105.52	110.14
3	D	5	XYS	O4-C4-C3	-2.27	105.58	110.14
3	D	2	BGC	O4-C4-C5	-2.20	103.84	109.30
3	D	3	BGC	O6-C6-C5	2.19	118.80	111.29
3	D	5	XYS	C5-O5-C1	2.17	114.86	111.52
3	D	2	BGC	O2-C2-C3	2.16	114.45	110.14
3	D	4	BGC	O5-C1-C2	2.12	114.04	110.77
2	C	4	BGC	O3-C3-C4	2.10	115.20	110.35
3	D	4	BGC	O3-C3-C2	-2.01	106.14	109.99

There are no chirality outliers.

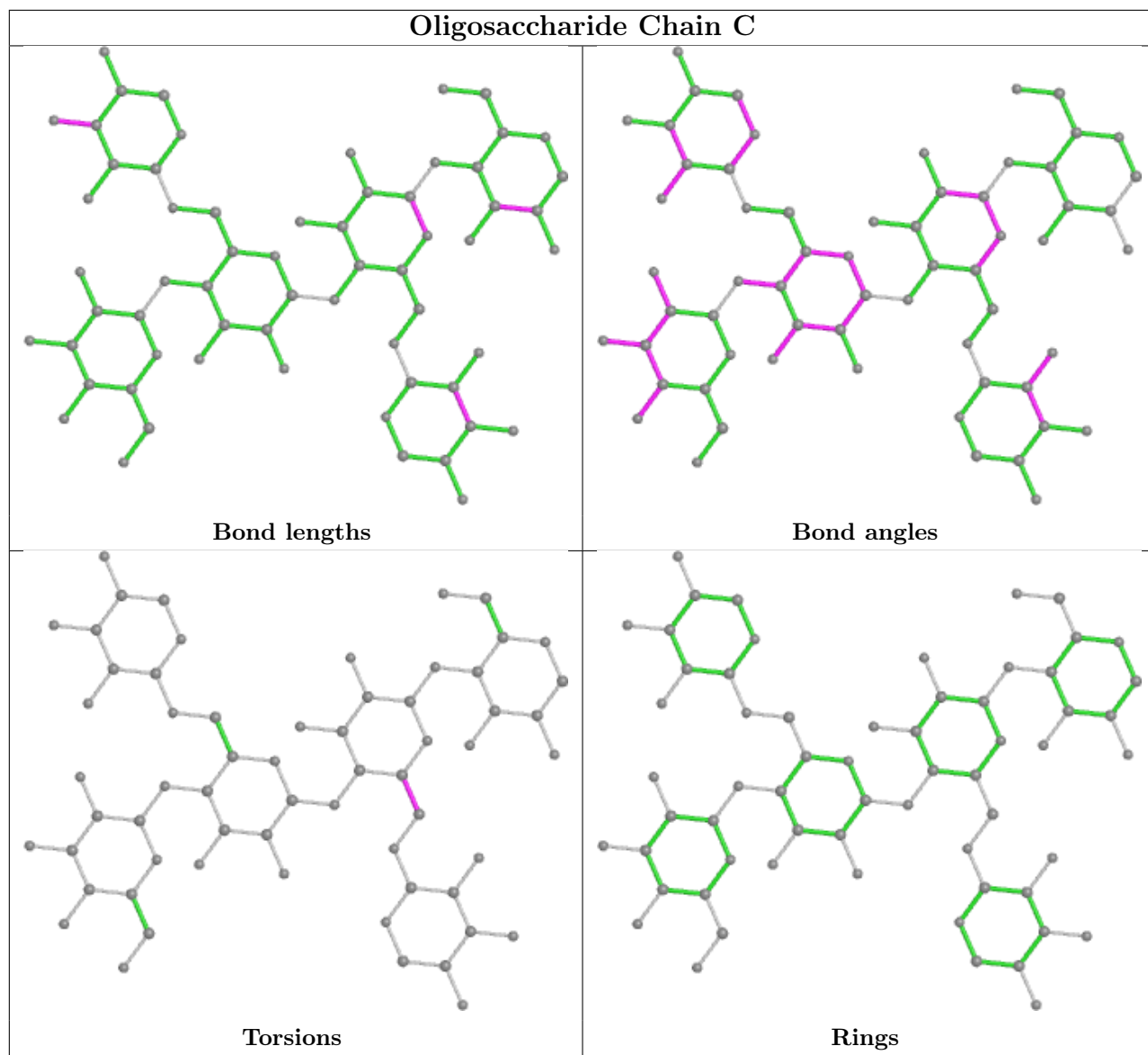
All (4) torsion outliers are listed below:

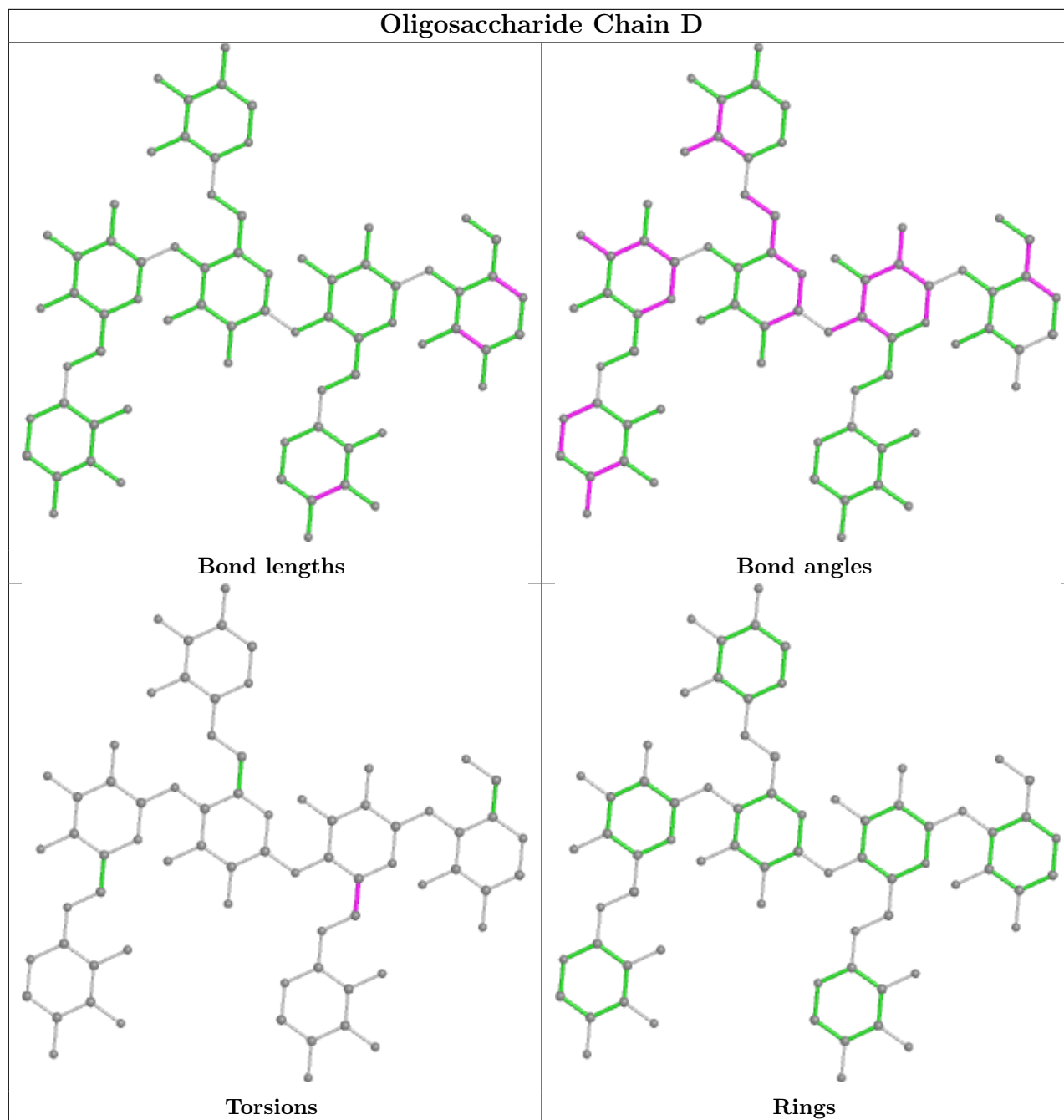
Mol	Chain	Res	Type	Atoms
2	C	2	BGC	O5-C5-C6-O6
2	C	2	BGC	C4-C5-C6-O6
3	D	2	BGC	C4-C5-C6-O6
3	D	2	BGC	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

10 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	GOL	B	1008	-	5,5,5	0.26	0	5,5,5	0.45	0
6	PGE	A	1011	-	9,9,9	0.74	0	8,8,8	0.68	0
5	SO4	A	1009	-	4,4,4	0.39	0	6,6,6	0.36	0
7	MES	A	1012	-	12,12,12	2.33	1 (8%)	14,16,16	1.86	5 (35%)
8	1PE	B	1011	-	15,15,15	0.51	0	14,14,14	0.64	0
6	PGE	A	1010	-	9,9,9	0.69	0	8,8,8	0.62	0
7	MES	B	1010	-	12,12,12	2.08	1 (8%)	14,16,16	3.65	3 (21%)
4	GOL	A	1008	-	5,5,5	0.37	0	5,5,5	1.07	0
5	SO4	B	1009	-	4,4,4	0.35	0	6,6,6	0.60	0
4	GOL	A	1007	-	5,5,5	0.47	0	5,5,5	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	1008	-	-	2/4/4/4	-
6	PGE	A	1011	-	-	3/7/7/7	-
7	MES	A	1012	-	-	5/6/14/14	0/1/1/1
8	1PE	B	1011	-	-	4/13/13/13	-
6	PGE	A	1010	-	-	5/7/7/7	-
7	MES	B	1010	-	-	5/6/14/14	0/1/1/1
4	GOL	A	1008	-	-	3/4/4/4	-
4	GOL	A	1007	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1012	MES	C8-S	-7.71	1.66	1.77
7	B	1010	MES	C8-S	-6.95	1.67	1.77

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1010	MES	O2S-S-C8	12.22	121.63	106.92
7	B	1010	MES	O2S-S-O1S	-3.92	100.40	113.95
7	A	1012	MES	O1S-S-C8	3.62	111.27	106.92
7	A	1012	MES	O3S-S-C8	3.40	111.27	105.77
7	B	1010	MES	O1S-S-C8	3.15	110.71	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1012	MES	O2S-S-C8	-3.12	103.16	106.92
7	A	1012	MES	C7-N4-C3	-2.38	105.14	111.23
7	A	1012	MES	C2-C3-N4	2.04	113.19	110.10

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1007	GOL	O1-C1-C2-O2
4	A	1008	GOL	C1-C2-C3-O3
4	B	1008	GOL	C1-C2-C3-O3
7	A	1012	MES	C7-C8-S-O2S
7	A	1012	MES	C7-C8-S-O3S
7	B	1010	MES	C8-C7-N4-C5
7	B	1010	MES	C7-C8-S-O1S
7	B	1010	MES	C7-C8-S-O3S
6	A	1010	PGE	O2-C3-C4-O3
8	B	1011	1PE	OH5-C14-C24-OH4
6	A	1010	PGE	O1-C1-C2-O2
6	A	1011	PGE	O1-C1-C2-O2
4	A	1007	GOL	O1-C1-C2-C3
4	A	1008	GOL	O1-C1-C2-C3
6	A	1010	PGE	O3-C5-C6-O4
4	A	1008	GOL	O2-C2-C3-O3
4	B	1008	GOL	O2-C2-C3-O3
7	A	1012	MES	C8-C7-N4-C3
7	A	1012	MES	C8-C7-N4-C5
6	A	1011	PGE	O2-C3-C4-O3
6	A	1010	PGE	C3-C4-O3-C5
7	A	1012	MES	C7-C8-S-O1S
7	B	1010	MES	C7-C8-S-O2S
6	A	1010	PGE	C4-C3-O2-C2
6	A	1011	PGE	C4-C3-O2-C2
8	B	1011	1PE	OH6-C15-C25-OH5
8	B	1011	1PE	OH4-C13-C23-OH3
8	B	1011	1PE	C23-C13-OH4-C24
7	B	1010	MES	C8-C7-N4-C3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1009	SO4	1	0
8	B	1011	1PE	2	0
4	A	1008	GOL	1	0
5	B	1009	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	370/396 (93%)	0.28	17 (4%) 32 36	24, 36, 51, 64	14 (3%)
1	B	370/396 (93%)	0.75	47 (12%) 3 4	25, 42, 59, 70	45 (12%)
All	All	740/792 (93%)	0.51	64 (8%) 10 12	24, 39, 57, 70	59 (7%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	ILE	6.0
1	B	166	ILE	5.8
1	B	204	LEU	5.1
1	B	353	THR	4.7
1	B	430	PHE	4.7
1	B	250	PHE	4.6
1	B	203	VAL	4.5
1	B	197	ILE	4.5
1	B	352	SER	4.4
1	B	351	LEU	4.4
1	B	291	VAL	4.4
1	B	249	LEU	4.4
1	B	287	TYR	3.8
1	B	164	VAL	3.8
1	B	251	ALA	3.8
1	A	205	ILE	3.6
1	B	107	ALA	3.5
1	A	130	ILE	3.5
1	B	207	ILE	3.4
1	A	103	THR	3.4
1	B	387	VAL	3.3
1	A	166	ILE	3.3
1	B	168	VAL	3.3
1	B	432	TRP	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	388	LEU	3.2
1	A	164	VAL	3.1
1	A	207	ILE	3.0
1	B	165	ARG	3.0
1	B	148	VAL	3.0
1	B	110	SER	2.9
1	B	391	PHE	2.9
1	B	111	THR	2.8
1	A	204	LEU	2.8
1	B	450	ASN	2.8
1	B	112	GLY	2.8
1	B	449	GLN	2.8
1	B	451	THR	2.7
1	B	377	THR	2.6
1	B	381	ASP	2.6
1	A	167	PRO	2.6
1	B	252	GLY	2.6
1	B	129	ASN	2.5
1	A	432	TRP	2.5
1	B	147	MET	2.5
1	B	274	PHE	2.5
1	B	290	LEU	2.5
1	B	167	PRO	2.4
1	A	344	TYR	2.4
1	B	453	PHE	2.3
1	B	130	ILE	2.3
1	B	452	VAL	2.3
1	B	109	ASP	2.3
1	A	165	ARG	2.3
1	B	237	ILE	2.3
1	B	289	VAL	2.2
1	B	153	LEU	2.2
1	A	387	VAL	2.1
1	B	146	PRO	2.1
1	A	170	TRP	2.1
1	A	122	GLY	2.1
1	A	251	ALA	2.1
1	B	448	GLN	2.0
1	A	168	VAL	2.0
1	A	389	GLY	2.0

## 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](#)

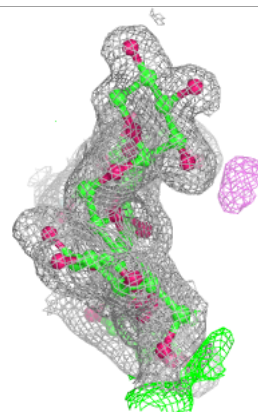
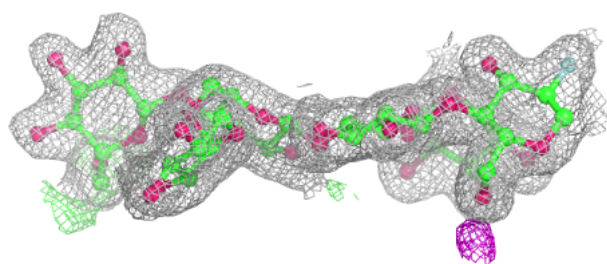
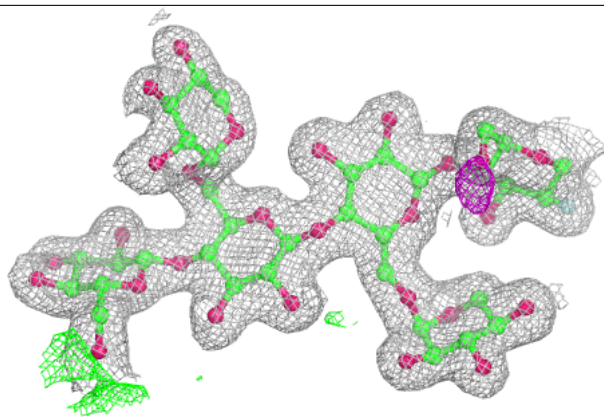
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	XYS	D	5	9/10	0.83	0.18	51,54,59,64	9
3	XYS	D	6	9/10	0.87	0.12	40,42,45,45	9
2	BGC	C	4	11/12	0.88	0.18	33,42,46,46	0
3	BGC	D	4	11/12	0.90	0.18	46,54,58,67	0
3	BGC	D	3	11/12	0.91	0.12	35,38,42,44	0
2	XYS	C	5	9/10	0.92	0.18	33,36,40,41	0
3	BGC	D	2	11/12	0.94	0.07	29,30,33,35	0
3	G2F	D	1	11/12	0.95	0.12	26,29,31,31	0
2	BGC	C	3	11/12	0.95	0.08	26,29,34,36	0
2	XYS	C	6	9/10	0.95	0.09	25,26,29,30	0
3	XYS	D	7	9/10	0.96	0.07	27,30,32,32	0
2	BGC	C	2	11/12	0.97	0.07	24,26,27,29	0
2	G2F	C	1	11/12	0.98	0.08	23,26,29,30	0

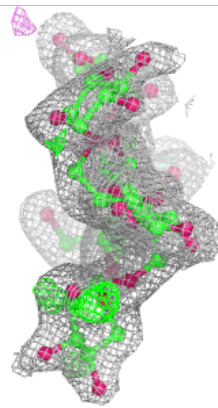
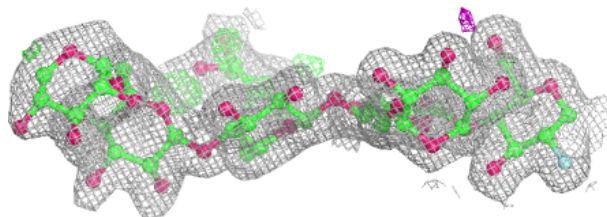
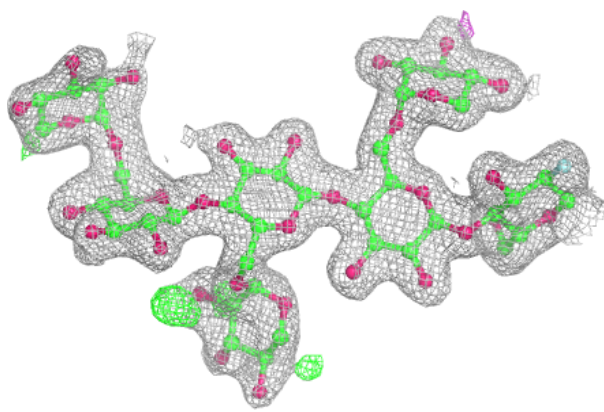
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain 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 D:**

$2mF_o-DF_c$  (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
6	PGE	A	1011	10/10	0.80	0.13	63,76,78,80	0
4	GOL	A	1008	6/6	0.83	0.18	51,56,58,67	0
6	PGE	A	1010	10/10	0.86	0.10	51,61,70,70	0
4	GOL	A	1007	6/6	0.88	0.16	35,43,45,46	6
5	SO4	A	1009	5/5	0.89	0.22	48,58,64,67	5
7	MES	B	1010	12/12	0.89	0.15	27,29,34,39	12
5	SO4	B	1009	5/5	0.91	0.23	43,49,50,50	5
8	1PE	B	1011	16/16	0.91	0.12	48,55,65,67	0
4	GOL	B	1008	6/6	0.94	0.11	36,41,43,44	6
7	MES	A	1012	12/12	0.94	0.14	26,29,34,39	12

## 6.5 Other polymers [i](#)

There are no such residues in this entry.