



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 08:32 AM BST

PDB ID : 6E9B  
Title : Bacteroides ovatus mixed-linkage glucan utilization locus (MLGUL) SGBP-B  
in complex with mixed-linkage heptasaccharide  
Authors : Tamura, K.; Gardill, B.R.; Brumer, H.; Van Petegem, F.  
Deposited on : 2018-07-31  
Resolution : 3.15 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

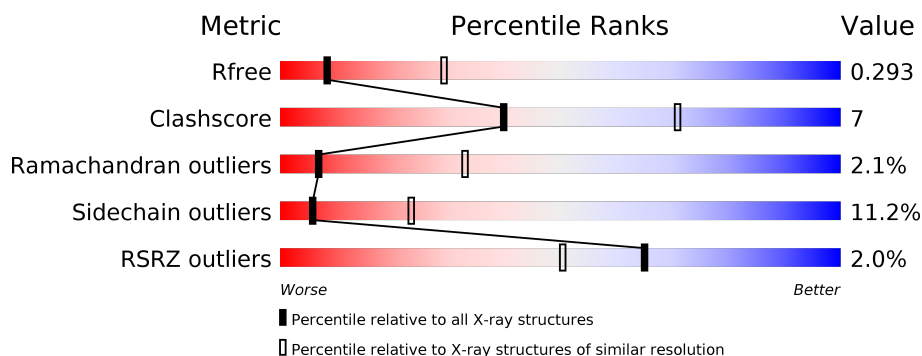
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	420	<div> <div> <div></div> <div>66%</div> <div>24%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	420	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>22%</div> <div>•</div> <div>10%</div> </div> </div>
1	C	420	<div> <div> <div></div> <div>68%</div> <div>22%</div> <div>•</div> <div>8%</div> </div> </div>
1	D	420	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>19%</div> <div>•</div> <div>12%</div> </div> </div>
2	E	7	<div> <div>14%</div> <div>57%</div> <div>29%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11363 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 Mixed-linkage glucan utilization locus (MLGUL) SGBP-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2836	1769	464	595	8			
1	B	378	Total	C	N	O	S	0	0	0
			2804	1742	462	593	7			
1	C	387	Total	C	N	O	S	0	0	0
			2877	1792	466	611	8			
1	D	368	Total	C	N	O	S	0	0	0
			2651	1641	440	562	8			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A7LY28
A	2	GLY	-	expression tag	UNP A7LY28
A	3	SER	-	expression tag	UNP A7LY28
A	4	SER	-	expression tag	UNP A7LY28
A	5	HIS	-	expression tag	UNP A7LY28
A	6	HIS	-	expression tag	UNP A7LY28
A	7	HIS	-	expression tag	UNP A7LY28
A	8	HIS	-	expression tag	UNP A7LY28
A	9	HIS	-	expression tag	UNP A7LY28
A	10	HIS	-	expression tag	UNP A7LY28
A	11	SER	-	expression tag	UNP A7LY28
A	12	SER	-	expression tag	UNP A7LY28
A	13	GLY	-	expression tag	UNP A7LY28
A	14	LEU	-	expression tag	UNP A7LY28
A	15	VAL	-	expression tag	UNP A7LY28
A	16	PRO	-	expression tag	UNP A7LY28
A	17	ARG	-	expression tag	UNP A7LY28
A	18	GLY	-	expression tag	UNP A7LY28
A	19	SER	-	expression tag	UNP A7LY28
A	20	HIS	-	expression tag	UNP A7LY28
A	21	MET	-	expression tag	UNP A7LY28

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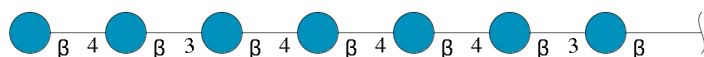
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP A7LY28
B	2	GLY	-	expression tag	UNP A7LY28
B	3	SER	-	expression tag	UNP A7LY28
B	4	SER	-	expression tag	UNP A7LY28
B	5	HIS	-	expression tag	UNP A7LY28
B	6	HIS	-	expression tag	UNP A7LY28
B	7	HIS	-	expression tag	UNP A7LY28
B	8	HIS	-	expression tag	UNP A7LY28
B	9	HIS	-	expression tag	UNP A7LY28
B	10	HIS	-	expression tag	UNP A7LY28
B	11	SER	-	expression tag	UNP A7LY28
B	12	SER	-	expression tag	UNP A7LY28
B	13	GLY	-	expression tag	UNP A7LY28
B	14	LEU	-	expression tag	UNP A7LY28
B	15	VAL	-	expression tag	UNP A7LY28
B	16	PRO	-	expression tag	UNP A7LY28
B	17	ARG	-	expression tag	UNP A7LY28
B	18	GLY	-	expression tag	UNP A7LY28
B	19	SER	-	expression tag	UNP A7LY28
B	20	HIS	-	expression tag	UNP A7LY28
B	21	MET	-	expression tag	UNP A7LY28
C	1	MET	-	initiating methionine	UNP A7LY28
C	2	GLY	-	expression tag	UNP A7LY28
C	3	SER	-	expression tag	UNP A7LY28
C	4	SER	-	expression tag	UNP A7LY28
C	5	HIS	-	expression tag	UNP A7LY28
C	6	HIS	-	expression tag	UNP A7LY28
C	7	HIS	-	expression tag	UNP A7LY28
C	8	HIS	-	expression tag	UNP A7LY28
C	9	HIS	-	expression tag	UNP A7LY28
C	10	HIS	-	expression tag	UNP A7LY28
C	11	SER	-	expression tag	UNP A7LY28
C	12	SER	-	expression tag	UNP A7LY28
C	13	GLY	-	expression tag	UNP A7LY28
C	14	LEU	-	expression tag	UNP A7LY28
C	15	VAL	-	expression tag	UNP A7LY28
C	16	PRO	-	expression tag	UNP A7LY28
C	17	ARG	-	expression tag	UNP A7LY28
C	18	GLY	-	expression tag	UNP A7LY28
C	19	SER	-	expression tag	UNP A7LY28
C	20	HIS	-	expression tag	UNP A7LY28
C	21	MET	-	expression tag	UNP A7LY28

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP A7LY28
D	2	GLY	-	expression tag	UNP A7LY28
D	3	SER	-	expression tag	UNP A7LY28
D	4	SER	-	expression tag	UNP A7LY28
D	5	HIS	-	expression tag	UNP A7LY28
D	6	HIS	-	expression tag	UNP A7LY28
D	7	HIS	-	expression tag	UNP A7LY28
D	8	HIS	-	expression tag	UNP A7LY28
D	9	HIS	-	expression tag	UNP A7LY28
D	10	HIS	-	expression tag	UNP A7LY28
D	11	SER	-	expression tag	UNP A7LY28
D	12	SER	-	expression tag	UNP A7LY28
D	13	GLY	-	expression tag	UNP A7LY28
D	14	LEU	-	expression tag	UNP A7LY28
D	15	VAL	-	expression tag	UNP A7LY28
D	16	PRO	-	expression tag	UNP A7LY28
D	17	ARG	-	expression tag	UNP A7LY28
D	18	GLY	-	expression tag	UNP A7LY28
D	19	SER	-	expression tag	UNP A7LY28
D	20	HIS	-	expression tag	UNP A7LY28
D	21	MET	-	expression tag	UNP A7LY28

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	7	Total	C	O	0	0	0
			78	42	36			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	13	Total	O	0	0
			13	13		

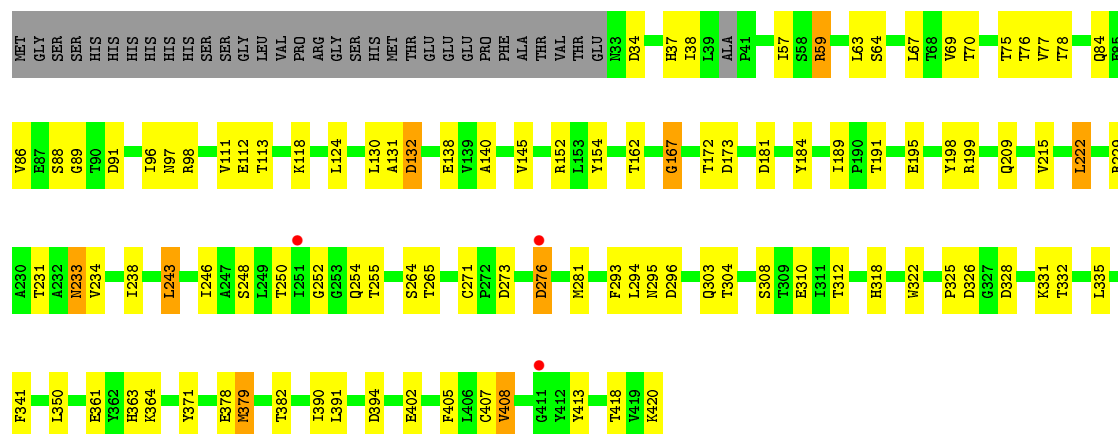
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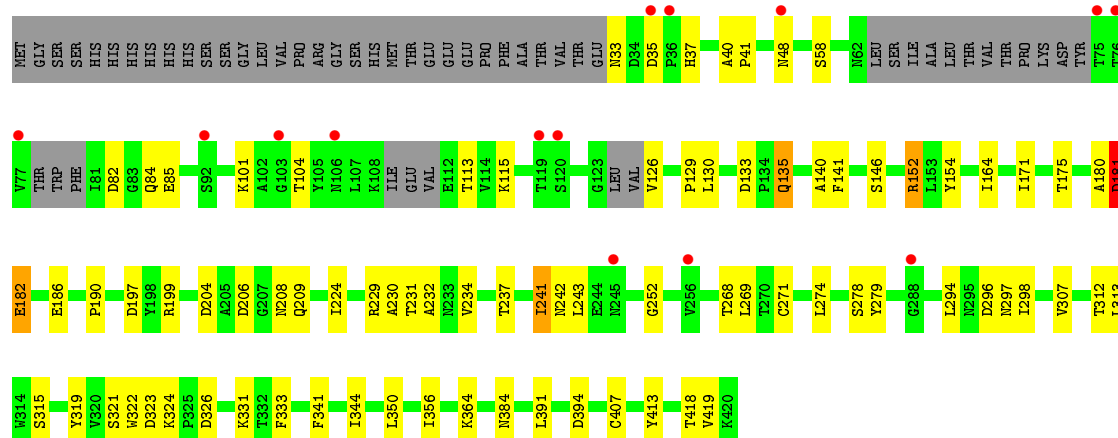
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	23	Total 23	O 23	0	0
4	D	18	Total 18	O 18	0	0



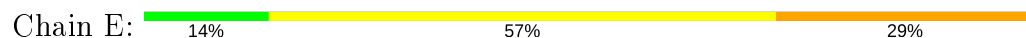




• Molecule 1: Mixed-linkage glucan utilization locus (MLGUL) SGBP-B



• Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.29Å 242.21Å 75.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.33 – 3.15 34.32 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.33-3.15) 99.9 (34.32-3.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 3.18Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.221 , 0.272 0.240 , 0.293	Depositor DCC
$R_{free}$ test set	2505 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	90.3	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 87.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11363	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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, SO4

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	0.52	0/2887	0.78	0/3947
1	B	0.51	0/2852	0.75	0/3898
1	C	0.52	0/2929	0.78	0/4011
1	D	0.54	0/2694	0.76	0/3685
All	All	0.52	0/11362	0.77	0/15541

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2836	0	2651	42	0
1	B	2804	0	2592	48	0
1	C	2877	0	2678	36	0
1	D	2651	0	2405	36	0
2	E	78	0	66	2	0
3	A	20	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	13	0	0	0	0
4	B	13	0	0	0	0
4	C	23	0	0	1	0
4	D	18	0	0	0	0
All	All	11363	0	10392	158	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 7.

The worst 5 of 158 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ALA:O	1:C:132:ASP:HB2	1.68	0.91
1:D:152:ARG:HG3	1:D:152:ARG:HH11	1.40	0.83
1:C:181:ASP:HA	1:D:181:ASP:HA	1.67	0.76
1:A:153:LEU:HG	1:A:187:TYR:HE1	1.57	0.70
1:A:202:LEU:HG	1:A:212:ALA:HB2	1.74	0.70

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	375/420 (89%)	335 (89%)	31 (8%)	9 (2%)	6	30
1	B	368/420 (88%)	314 (85%)	47 (13%)	7 (2%)	8	36
1	C	383/420 (91%)	339 (88%)	36 (9%)	8 (2%)	7	33
1	D	358/420 (85%)	299 (84%)	52 (14%)	7 (2%)	7	34
All	All	1484/1680 (88%)	1287 (87%)	166 (11%)	31 (2%)	7	33

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	GLN
1	A	213	ASP
1	B	232	ALA
1	B	335	LEU
1	B	403	ALA

### 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	304/358 (85%)	275 (90%)	29 (10%)	8	30
1	B	298/358 (83%)	266 (89%)	32 (11%)	6	25
1	C	310/358 (87%)	267 (86%)	43 (14%)	3	15
1	D	271/358 (76%)	242 (89%)	29 (11%)	6	25
All	All	1183/1432 (83%)	1050 (89%)	133 (11%)	6	23

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	407	CYS
1	C	124	LEU
1	D	237	THR
1	C	34	ASP
1	C	70	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	292	GLN
1	C	303	GLN
1	C	50	GLN
1	B	62	ASN
1	C	233	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 ⓘ

7 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	BGC	E	1	2	12,12,12	0.35	0	17,17,17	0.53	0
2	BGC	E	2	2	11,11,12	0.31	0	15,15,17	1.20	2 (13%)
2	BGC	E	3	2	11,11,12	0.46	0	15,15,17	1.25	2 (13%)
2	BGC	E	4	2	11,11,12	0.42	0	15,15,17	1.29	2 (13%)
2	BGC	E	5	2	11,11,12	0.58	0	15,15,17	1.42	1 (6%)
2	BGC	E	6	2	11,11,12	0.52	0	15,15,17	1.20	2 (13%)
2	BGC	E	7	2	11,11,12	0.57	0	15,15,17	0.83	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	E	2	2	-	1/2/19/22	0/1/1/1
2	BGC	E	3	2	-	1/2/19/22	0/1/1/1
2	BGC	E	4	2	-	2/2/19/22	0/1/1/1
2	BGC	E	5	2	-	1/2/19/22	0/1/1/1
2	BGC	E	6	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	E	7	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5	BGC	C1-O5-C5	4.34	118.08	112.19
2	E	4	BGC	C1-O5-C5	2.94	116.17	112.19
2	E	6	BGC	C1-C2-C3	2.53	112.78	109.67
2	E	6	BGC	C2-C3-C4	2.50	115.22	110.89
2	E	3	BGC	O2-C2-C3	-2.50	105.14	110.14

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

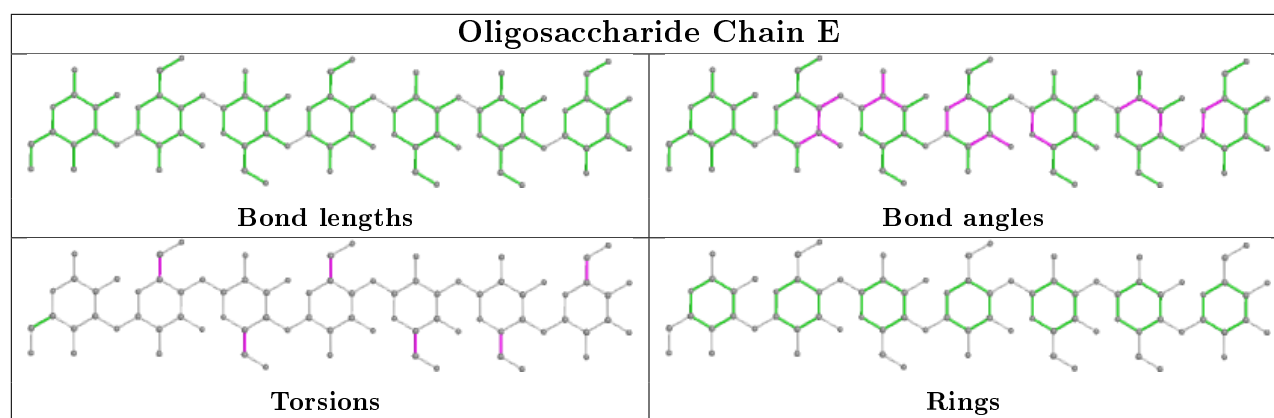
Mol	Chain	Res	Type	Atoms
2	E	4	BGC	O5-C5-C6-O6
2	E	7	BGC	O5-C5-C6-O6
2	E	5	BGC	O5-C5-C6-O6
2	E	3	BGC	O5-C5-C6-O6
2	E	2	BGC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	5	BGC	1	0
2	E	7	BGC	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](#)

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	$\# Z  > 2$
3	SO4	B	501	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	A	504	-	4,4,4	0.27	0	6,6,6	0.36	0
3	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	C	502	-	4,4,4	0.16	0	6,6,6	0.23	0
3	SO4	A	501	-	4,4,4	0.21	0	6,6,6	0.09	0
3	SO4	C	501	-	4,4,4	0.23	0	6,6,6	0.20	0
3	SO4	D	508	-	4,4,4	0.21	0	6,6,6	0.33	0
3	SO4	A	502	-	4,4,4	0.12	0	6,6,6	0.12	0
3	SO4	B	502	-	4,4,4	0.18	0	6,6,6	0.08	0
3	SO4	D	509	-	4,4,4	0.19	0	6,6,6	0.23	0

There are no bond length outliers.

There are no bond angle outliers.

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
3	D	509	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	381/420 (90%)	-0.07	4 (1%) 82 73	41, 84, 154, 174	0
1	B	378/420 (90%)	0.09	10 (2%) 56 40	63, 111, 156, 188	0
1	C	387/420 (92%)	-0.14	3 (0%) 86 78	48, 93, 125, 140	0
1	D	368/420 (87%)	0.11	14 (3%) 40 25	41, 114, 171, 189	0
All	All	1514/1680 (90%)	-0.01	31 (2%) 65 50	41, 100, 158, 189	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	ASP	4.2
1	D	288	GLY	3.6
1	D	119	THR	3.3
1	A	203	GLN	3.3
1	D	36	PRO	3.2

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

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

### 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

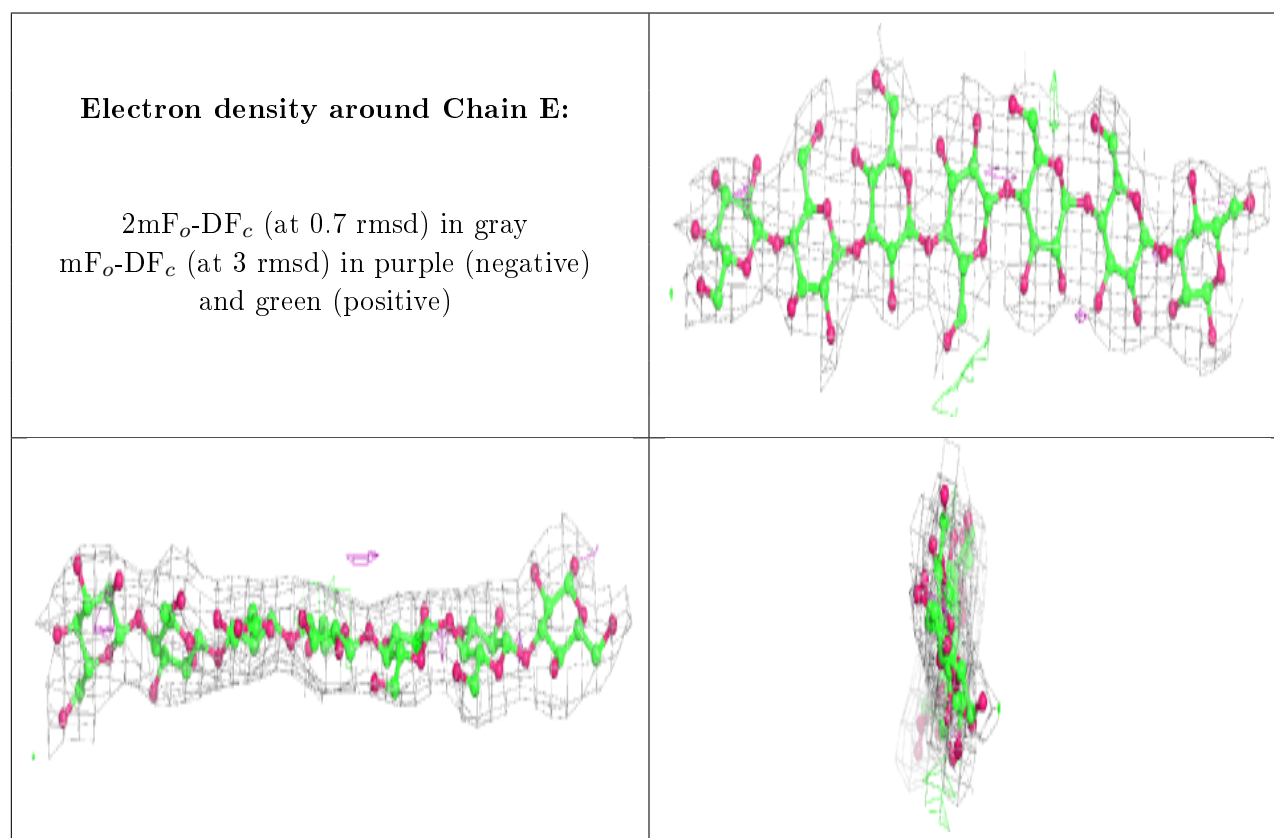
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BGC	E	1	12/12	0.87	0.17	92,104,111,112	0
2	BGC	E	7	11/12	0.88	0.29	85,91,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BGC	E	6	11/12	0.91	0.18	60,71,79,82	0
2	BGC	E	4	11/12	0.94	0.28	55,58,74,79	0
2	BGC	E	2	11/12	0.95	0.19	57,60,73,77	0
2	BGC	E	3	11/12	0.97	0.23	44,57,65,66	0
2	BGC	E	5	11/12	0.97	0.18	50,61,68,70	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( $\text{\AA}^2$ )	Q<0.9
3	SO4	C	502	5/5	0.75	0.33	152,152,153,154	0
3	SO4	A	503	5/5	0.76	0.38	189,189,189,190	0
3	SO4	A	502	5/5	0.78	0.28	179,179,179,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	D	509	5/5	0.82	0.24	137,138,139,139	0
3	SO4	B	502	5/5	0.83	0.13	172,172,173,173	0
3	SO4	B	501	5/5	0.85	0.21	153,154,154,155	0
3	SO4	C	501	5/5	0.90	0.21	127,129,129,131	0
3	SO4	A	501	5/5	0.91	0.21	139,139,139,141	0
3	SO4	A	504	5/5	0.93	0.14	122,122,124,124	0
3	SO4	D	508	5/5	0.95	0.20	115,116,117,120	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.