



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 08:17 AM BST

PDB ID : 4AK2  
Title : Structure of BT4661, a SusE-like surface located polysaccharide binding protein from the Bacteroides thetaiotaomicron heparin utilisation locus  
Authors : Lowe, E.C.; Basle, A.; Czjzek, M.; Thomas, S.; Murray, H.; Firbank, S.J.; Bolam, D.N.  
Deposited on : 2012-02-21  
Resolution : 1.35 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.

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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

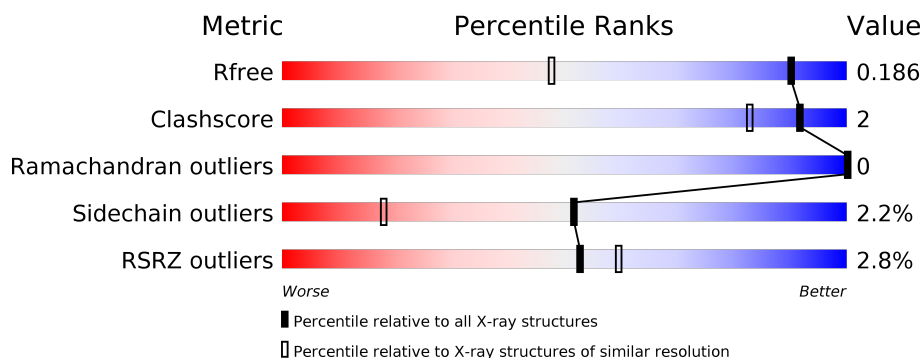
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.35 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	288	 3% 94% 5%
2	B	6	 83% 17%

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 2712 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.

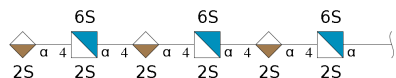
- Molecule 1 is a protein called BT\_4661.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	287	2229	1416	374	431	8	0	7	1

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	421	MET	-	expression tag	UNP Q89YS0
A	701	LEU	-	expression tag	UNP Q89YS0
A	702	GLU	-	expression tag	UNP Q89YS0
A	703	HIS	-	expression tag	UNP Q89YS0
A	704	HIS	-	expression tag	UNP Q89YS0
A	705	HIS	-	expression tag	UNP Q89YS0
A	706	HIS	-	expression tag	UNP Q89YS0
A	707	HIS	-	expression tag	UNP Q89YS0
A	708	HIS	-	expression tag	UNP Q89YS0

- Molecule 2 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	6	105	36	3	57	9	0	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Na 2 2	0	0

- Molecule 4 is water.

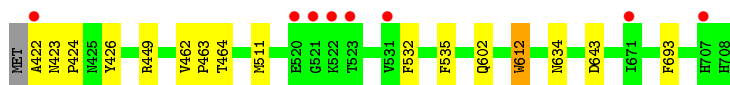
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	376	Total O 376 376	0	0

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

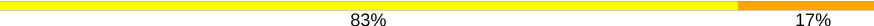
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: BT\_4661

Chain A: 



- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.60Å 68.15Å 85.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.20 – 1.35 22.37 – 1.35	Depositor EDS
% Data completeness (in resolution range)	97.7 (53.20-1.35) 97.7 (22.37-1.35)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.55 (at 1.35Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.159 , 0.191 0.155 , 0.186	Depositor DCC
$R_{free}$ test set	3363 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.8	Xtrriage
Anisotropy	0.279	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2712	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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: NA, IDS, SGN

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	0.74	1/2310 (0.0%)	0.77	2/3151 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	612	TRP	CD2-CE2	5.50	1.48	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	449	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	449	ARG	NE-CZ-NH1	5.42	123.01	120.30

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	2229	0	2088	7	0
2	B	105	0	36	1	0
3	A	2	0	0	0	0
4	A	376	0	0	1	0
All	All	2712	0	2124	7	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 2.

All (7) 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:423:ASN:HB2	1:A:424:PRO:HD2	1.75	0.67
1:A:422:ALA:HB3	1:A:426:TYR:CG	2.32	0.64
1:A:602:GLN:NE2	2:B:2:IDS:O2S	2.35	0.57
1:A:462[B]:VAL:CG1	1:A:463:PRO:HD2	2.39	0.52
1:A:464[B]:THR:HG22	4:A:2075:HOH:O	2.11	0.50
1:A:462[B]:VAL:HG12	1:A:463:PRO:HD2	2.02	0.42
1:A:511[B]:MET:HG3	1:A:532:PHE:CE2	2.55	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	292/288 (101%)	285 (98%)	7 (2%)	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	234/241 (97%)	229 (98%)	5 (2%)	53 19

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	535	PHE
1	A	612	TRP
1	A	634	ASN
1	A	643	ASP
1	A	693	PHE

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

6 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	SGN	B	1	2	19,20,20	1.38	3 (15%)	24,31,31	1.35	4 (16%)
2	IDS	B	2	2	13,16,17	0.88	1 (7%)	15,24,26	1.41	2 (13%)
2	SGN	B	3	2	18,19,20	1.39	2 (11%)	22,29,31	1.56	6 (27%)
2	IDS	B	4	2	13,16,17	0.84	1 (7%)	15,24,26	1.86	3 (20%)
2	SGN	B	5	2	18,19,20	1.24	1 (5%)	22,29,31	1.45	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	IDS	B	6	2	12,15,17	0.79	1 (8%)	12,22,26	2.38	4 (33%)

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	SGN	B	1	2	-	1/11/31/31	0/1/1/1
2	IDS	B	2	2	-	0/5/26/29	0/1/1/1
2	SGN	B	3	2	-	1/11/28/31	0/1/1/1
2	IDS	B	4	2	-	3/5/26/29	0/1/1/1
2	SGN	B	5	2	-	1/11/28/31	0/1/1/1
2	IDS	B	6	2	-	0/5/22/29	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	SGN	O5S-S2	4.53	1.64	1.45
2	B	5	SGN	O5S-S2	3.56	1.60	1.45
2	B	3	SGN	O5S-S2	3.40	1.59	1.45
2	B	3	SGN	O1S-S1	2.88	1.45	1.42
2	B	1	SGN	O1S-S1	2.56	1.45	1.42
2	B	4	IDS	O2-C2	-2.21	1.44	1.47
2	B	2	IDS	O2-C2	-2.20	1.44	1.47
2	B	6	IDS	O2-C2	-2.09	1.44	1.47
2	B	1	SGN	O2S-S1	2.01	1.44	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	IDS	C2-O2-S	5.20	124.69	117.91
2	B	4	IDS	O2-C2-C3	4.51	113.25	106.95
2	B	3	SGN	O4-C4-C5	-3.66	100.21	109.30
2	B	1	SGN	O2S-S1-O1S	-3.62	111.60	120.16
2	B	6	IDS	C4-C3-C2	3.48	115.28	110.77
2	B	4	IDS	C1-C2-C3	3.47	114.59	109.40
2	B	6	IDS	O5-C5-C4	3.32	113.64	109.49
2	B	4	IDS	C2-O2-S	3.10	121.96	117.91
2	B	2	IDS	C2-O2-S	3.09	121.94	117.91
2	B	6	IDS	C1-C2-C3	2.89	114.03	109.94
2	B	5	SGN	O2S-S1-O1S	-2.77	113.61	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	IDS	C1-C2-C3	2.68	113.41	109.40
2	B	5	SGN	O4-C4-C5	-2.57	102.92	109.30
2	B	5	SGN	O2S-S1-N2	-2.47	104.35	108.87
2	B	3	SGN	C3-C2-N2	2.32	113.38	110.32
2	B	3	SGN	O6S-S2-O5S	2.29	116.47	108.49
2	B	3	SGN	O2S-S1-O1S	-2.29	114.75	120.16
2	B	1	SGN	O2S-S1-N2	2.26	112.99	108.87
2	B	1	SGN	O4-C4-C5	-2.25	103.72	109.30
2	B	3	SGN	C6-C5-C4	2.14	116.57	112.09
2	B	1	SGN	O6S-S2-O4S	2.09	115.77	108.49
2	B	3	SGN	C4-C3-C2	-2.01	108.07	111.02
2	B	5	SGN	O6-S2-O4S	2.00	112.94	106.88

There are no chirality outliers.

All (6) torsion outliers are listed below:

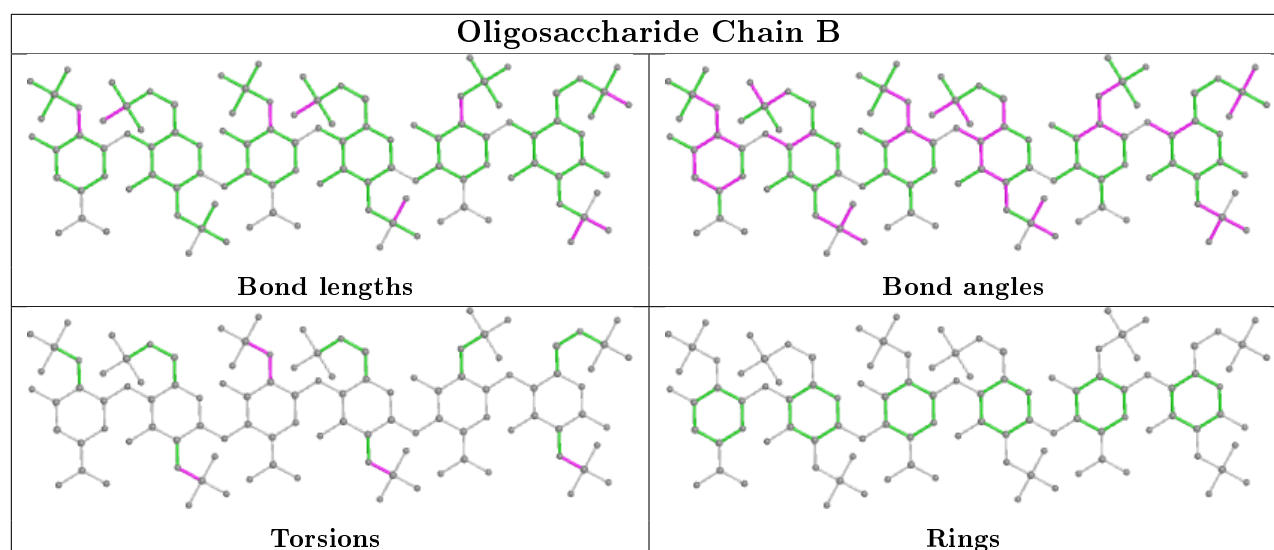
Mol	Chain	Res	Type	Atoms
2	B	5	SGN	C2-N2-S1-O1S
2	B	1	SGN	C2-N2-S1-O2S
2	B	4	IDS	C3-C2-O2-S
2	B	4	IDS	C2-O2-S-O3S
2	B	4	IDS	C1-C2-O2-S
2	B	3	SGN	C2-N2-S1-O2S

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	IDS	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	287/288 (99%)	0.14	8 (2%) 53 59	10, 16, 29, 50	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	422	ALA	4.7
1	A	523	THR	4.3
1	A	521	GLY	3.1
1	A	531	VAL	2.7
1	A	671	ILE	2.7
1	A	522	LYS	2.4
1	A	707	HIS	2.3
1	A	520	GLU	2.3

### 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.

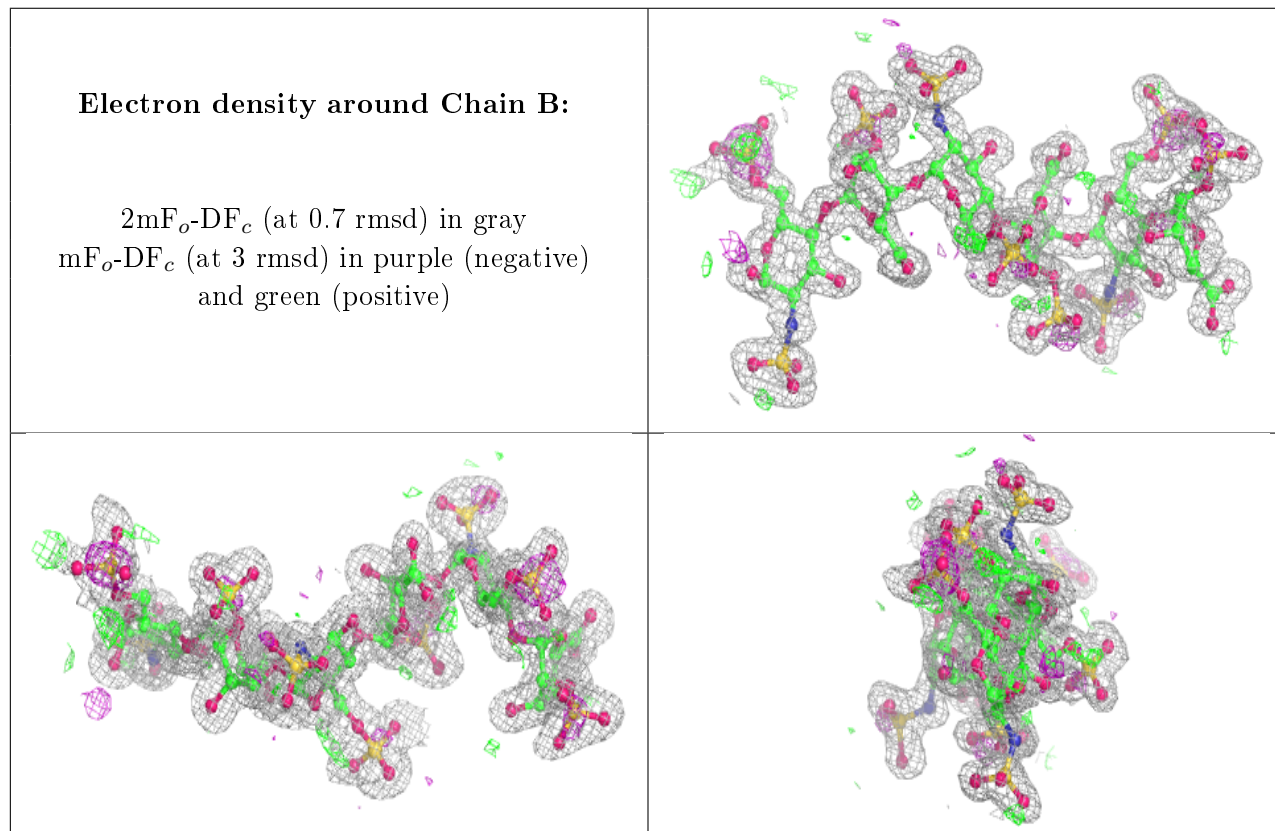
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	IDS	B	6	15/17	0.94	0.16	22,29,40,42	0
2	SGN	B	5	19/20	0.96	0.15	18,21,34,41	0
2	SGN	B	1	20/20	0.96	0.13	17,19,51,68	0
2	IDS	B	4	16/17	0.97	0.09	17,19,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	IDS	B	2	16/17	0.97	0.11	16,19,27,28	0
2	SGN	B	3	19/20	0.98	0.09	16,17,24,27	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	NA	A	1716	1/1	0.97	0.05	35,35,35,35	0
3	NA	A	1715	1/1	0.98	0.09	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.