

wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 09:51 PM EDT

PDB ID : 2F6D

Title : Structure of the complex of a glucoamylase from Saccharomycopsis fibuligera

with acarbose

Authors: Sevcik, J.; Hostinova, E.; Solovicova, A.; Gasperik, J.; Dauter, Z.; Wilson,

K.S.

Deposited on : 2005-11-29

Resolution : 1.60 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
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

Mol Probity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.35

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

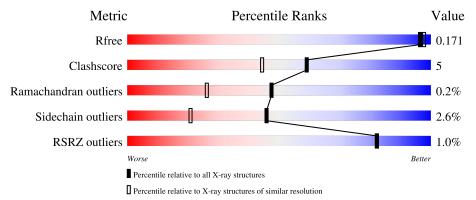
Validation Pipeline (wwPDB-VP) : 2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{\rm A})}) \end{array}$
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 >=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 <=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	492	87%	11%	-
2	В	3	100%		
2	С	3	100%		

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	В	1	X	-	-	-
2	GLC	С	1	X	-	-	=



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4775 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.

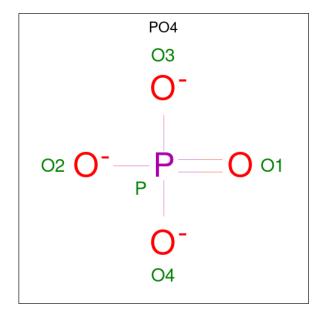
• Molecule 1 is a protein called Glucoamylase GLU1.

\mathbf{Mol}	Chain	Residues		Ator	$\mathbf{n}\mathbf{s}$		ZeroOcc	AltConf	Trace
1	A	492	Total 3870	C 2438	N 624	O 808	0	0	0

• Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose e-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	В	3	Total C N O 44 25 1 18	0	0	0
2	С	3	Total C N O 44 25 1 18	0	0	0

• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).





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

 \bullet Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

• Molecule 5 is water.

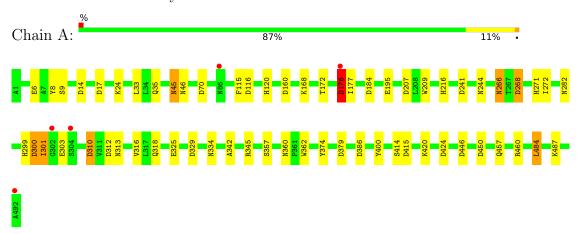
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	810	Total O 810 810	0	0



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: Glucoamylase GLU1



• Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl|amino}-alpha-D-glucopyranose-<math>(1-4)$ -alpha-D-glucopyranose

Chain B: 100%

GLC1 GLC2 AC13

• Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl|amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C: 100%

GLC1 GLC2 AC13



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	56.58Å 85.35Å 97.51Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 - 1.60	Depositor
rtesolution (A)	10.00 - 1.60	EDS
% Data completeness	94.0 (10.00-1.60)	Depositor
(in resolution range)	94.5 (10.00-1.60)	EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.87 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
D D.	0.118 , 0.160	Depositor
R, R_{free}	0.136 , 0.171	DCC
R_{free} test set	3010 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	13.2	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.43, 59.0	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4775	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.78% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: AC1, PO4, NA, 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		
MIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.55	0/3960	0.82	$19/5398 \ (0.4\%)$	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	300	ASP	CB-CG-OD2	7.58	125.12	118.30
1	A	312	ASP	CB-CG-OD2	7.21	124.79	118.30
1	A	310	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	241	ASP	CB-CG-OD2	6.98	124.59	118.30
1	A	160	ASP	CB-CG-OD2	6.81	124.43	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	ASP	Peptide



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	3870	0	3609	36	0
2	В	44	0	30	0	0
2	С	44	0	30	0	0
3	A	5	0	0	0	0
4	A	2	0	0	0	0
5	A	810	0	0	13	0
All	All	4775	0	3669	36	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 5.

The worst 5 of 36 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:301:ILE:HB	5:A:1803:HOH:O	1.71	0.89
1:A:334:ASN:HD21	1:A:342:ALA:H	1.37	0.69
1:A:487:LYS:HD3	5:A:1805:HOH:O	1.94	0.67
1:A:120:HIS:HE1	1:A:195:GLU:OE2	1.78	0.67
1:A:266:ASN:HD21	1:A:268:ASP:HB2	1.61	0.65

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	490/492 (100%)	480 (98%)	9 (2%)	1 (0%)	47 26



All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	SER

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	Analysed Rotameric		Percentiles	
1	A	422/422 (100%)	411 (97%)	11 (3%)	46 21	

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	301	ILE
1	A	414	SER
1	A	484	LEU
1	A	420	LYS
1	A	70	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	ASN
1	A	432	ASN
1	A	457	GLN
1	A	449	ASN
1	A	159	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)

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	Во	ond leng	ths	В	ond ang	gles
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	GLC	В	1	2	12,12,12	0.50	0	17,17,17	2.61	8 (47%)
2	GLC	В	2	2	11,11,12	0.94	1 (9%)	15,15,17	3.02	9 (60%)
2	AC1	В	3	2	21,22,23	1.21	2 (9%)	22,32,34	3.15	13 (59%)
2	GLC	С	1	2	12,12,12	0.45	0	17,17,17	3.11	7 (41%)
2	GLC	С	2	2	11,11,12	0.52	0	15,15,17	3.54	8 (53%)
2	AC1	С	3	2	21,22,23	0.74	1 (4%)	22,32,34	3.09	12 (54%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	В	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	GLC	В	2	2	-	0/2/19/22	0/1/1/1
2	AC1	В	3	2	-	1/6/43/46	0/2/2/2
2	GLC	С	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	GLC	С	2	2	-	1/2/19/22	0/1/1/1
2	AC1	С	3	2	-	0/6/43/46	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\operatorname{Ideal}(ext{\AA})$
2	В	3	AC1	C2B-C1B	-2.80	1.49	1.52
2	В	3	AC1	O5-C1	-2.47	1.39	1.43
2	В	2	GLC	O5-C1	-2.06	1.40	1.43
2	С	3	AC1	C7B-C5B	2.04	1.35	1.32

The worst 5 of 57 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	С	3	AC1	C2-C3-C4	6.82	116.64	110.63
2	В	3	AC1	C2-C3-C4	6.74	116.57	110.63
2	С	3	AC1	O5-C1-C2	6.61	120.98	110.77
2	С	2	GLC	O5-C1-C2	6.31	120.51	110.77
2	С	1	GLC	C1-O5-C5	6.25	125.46	113.66

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	В	1	GLC	C1
2	С	1	GLC	C1

All (2) torsion outliers are listed below:

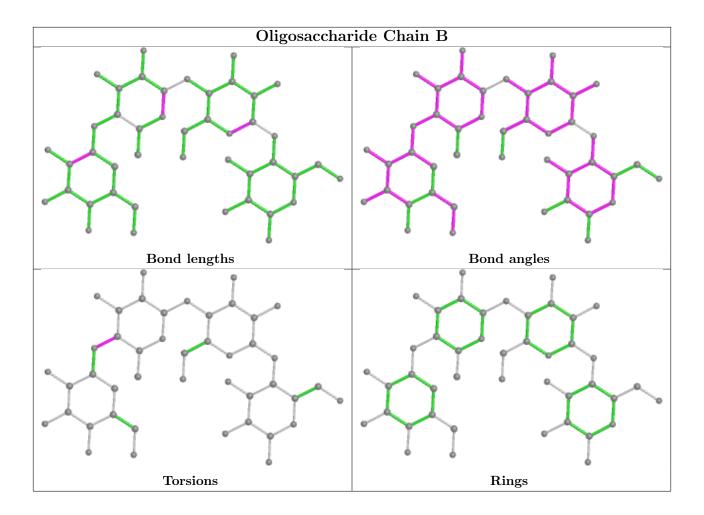
Mol	Chain	Res	Type	Atoms
2	С	2	GLC	C4-C5-C6-O6
2	В	3	AC1	C3-C4-N4A-C1B

There are no ring outliers.

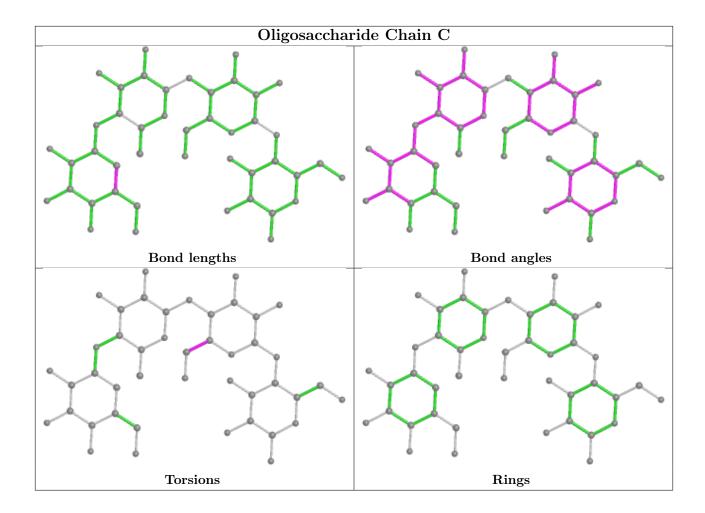
No monomer is involved in short contacts.

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)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	Pog	Res	Res Link	Bond lengths			Bond angles		
Moi Type	Type	Chain	Lilik		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	PO4	A	900	-	4,4,4	0.73	0	6,6,6	0.88	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.

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^{th} 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>	$\#\mathrm{RSRZ}{>}2$		$OWAB(A^2)$	Q<0.9
1	A	492/492 (100%)	-0.56	5 (1%) 8	82 82	7, 12, 23, 30	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	304	SER	3.4
1	A	302	GLY	2.9
1	A	176	ASP	2.8
1	A	86	ASN	2.4
1	A	492	ALA	2.2

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

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

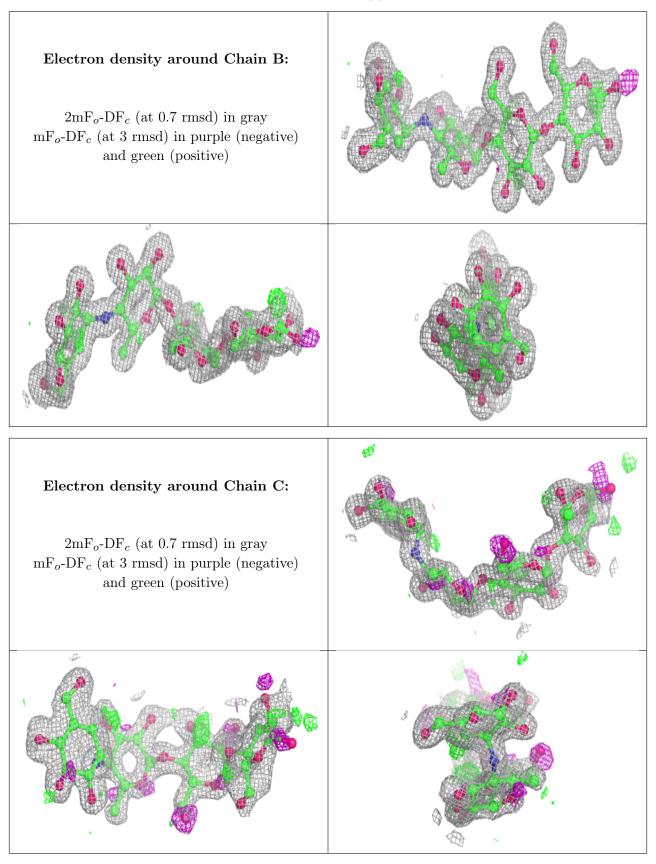
6.3 Carbohydrates (i)

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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	GLC	С	1	12/12	0.64	0.23	35,45,46,48	0
2	GLC	С	2	11/12	0.76	0.18	26,28,31,34	0
2	AC1	С	3	21/22	0.84	0.13	23,26,31,31	0
2	GLC	В	1	12/12	0.91	0.10	13,19,24,29	0
2	GLC	В	2	11/12	0.97	0.05	8,10,14,14	0
2	AC1	В	3	21/22	0.98	0.06	7,8,9,10	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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	PO4	A	900	5/5	0.81	0.27	28,32,32,33	0
4	NA	A	997	1/1	0.97	0.33	17,17,17,17	0
4	NA	A	998	1/1	0.98	0.25	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.

