



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2025 – 06:09 PM JST

PDB ID : 9UNS / pdb\_00009uns  
Title : Apg mutant enzyme D448N of acarbose hydrolase from human gut flora K. grimontii TD1, complex with acarbose  
Authors : Zhou, J.H.; Huang, J.Y.  
Deposited on : 2025-04-24  
Resolution : 1.91 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 : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

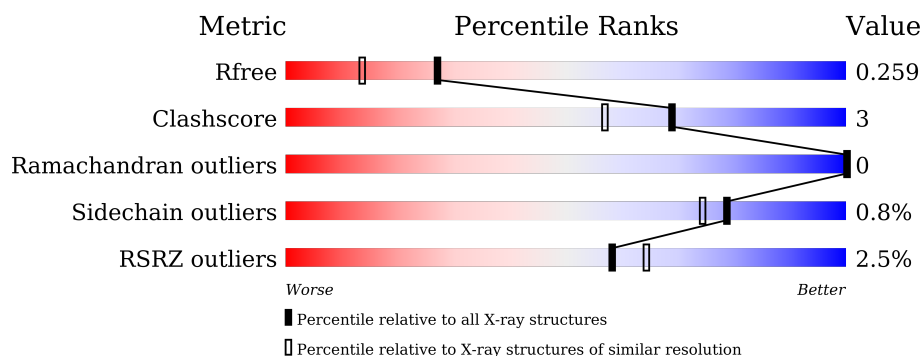
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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))
$R_{free}$	164625	1028 (1.92-1.92)
Clashscore	180529	1100 (1.92-1.92)
Ramachandran outliers	177936	1087 (1.92-1.92)
Sidechain outliers	177891	1087 (1.92-1.92)
RSRZ outliers	164620	1028 (1.92-1.92)

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	605	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>8%</div> </div> </div>
2	B	3	<div> <div>100%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5344 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 Maltodextrin glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	0	1	0
			4834	3087	863	868	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	GLU	GLY	conflict	UNP A0A7H4P971
A	448	ASN	ASP	engineered mutation	UNP A0A7H4P971

- Molecule 2 is an oligosaccharide called (2 {S},3 {R},4 {S},5 {R},6 {R})-5-[[[(1 {S},4 {R},5 {S},6 {S})-3-(hydroxymethyl)-4,5,6-tris(oxidanyl)cyclohex-2-en-1-yl]amino]-6-methyl-oxane-2,3,4-triol-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-galactopyranose.

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

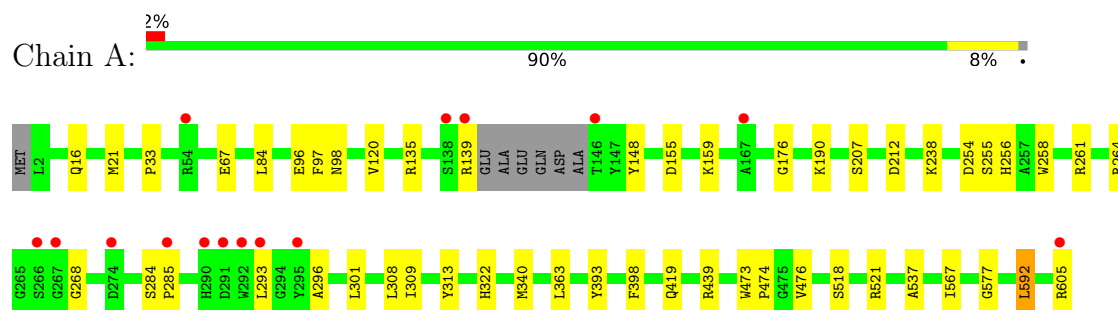
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	466	Total	O	0	0
			466	466		

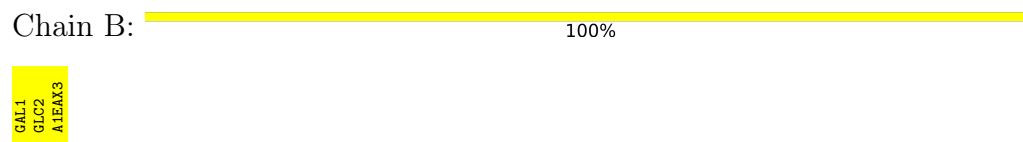
### 3 Residue-property plots [i](#)

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: Maltodextrin glucosidase



- Molecule 2: (2 {S},3 {R},4 {S},5 {R},6 {R})-5-[(1 {S},4 {R},5 {S},6 {S})-3-(hydroxymethyl)-4,5,6-tris(oxidanyl)cyclohex-2-en-1-yl]amino]-6-methyl-oxane-2,3,4-triol-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-galactopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.64Å 75.64Å 401.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.84 – 1.91 46.84 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.84-1.91) 99.7 (46.84-1.91)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.208 , 0.258 0.209 , 0.259	Depositor DCC
$R_{free}$ test set	2739 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 38.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5344	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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: GAL, GLC, A1EAX

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	0.33	0/4982	0.53	1/6779 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	GLU	CB-CA-C	-5.10	109.20	116.34

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	4834	0	4624	32	0
2	B	44	0	19	0	0
3	A	466	0	0	5	0
All	All	5344	0	4643	32	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 (32) 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:120:VAL:HG12	1:A:476[A]:VAL:HG21	1.59	0.84
1:A:16:GLN:HB2	1:A:21:MET:HE1	1.71	0.71
1:A:120:VAL:HG12	1:A:476[B]:VAL:HG11	1.72	0.70
1:A:135:ARG:HH21	1:A:139:ARG:HG2	1.67	0.58
1:A:135:ARG:NH2	1:A:139:ARG:HG2	2.19	0.58
1:A:293:LEU:HD11	1:A:340:MET:HE1	1.86	0.57
1:A:577:GLY:O	1:A:605:ARG:N	2.39	0.55
1:A:322:HIS:NE2	3:A:706:HOH:O	2.33	0.55
1:A:255:SER:O	1:A:264:ARG:NH2	2.27	0.53
1:A:521:ARG:NH1	3:A:716:HOH:O	2.42	0.52
1:A:135:ARG:HG2	1:A:176:GLY:O	2.13	0.49
1:A:284:SER:HB2	1:A:285:PRO:HD2	1.95	0.48
1:A:256:HIS:CE1	1:A:258:TRP:CD2	3.01	0.48
1:A:309:ILE:HG23	1:A:313:TYR:CZ	2.49	0.47
1:A:301:LEU:HB3	1:A:308:LEU:HD21	1.97	0.47
1:A:207:SER:OG	1:A:212:ASP:OD1	2.34	0.46
1:A:567:ILE:HD11	1:A:592:LEU:HD22	1.96	0.46
1:A:261:ARG:NH1	1:A:296:ALA:HB1	2.30	0.46
1:A:419:GLN:HG3	1:A:537:ALA:O	2.17	0.45
1:A:261:ARG:HH12	1:A:296:ALA:HB1	1.82	0.45
1:A:254:ASP:OD2	1:A:261:ARG:HD2	2.17	0.45
1:A:97:PHE:C	1:A:98:ASN:HD22	2.25	0.44
1:A:148:TYR:HA	1:A:155:ASP:HA	2.00	0.44
1:A:439:ARG:HA	1:A:476[A]:VAL:HG23	2.00	0.43
1:A:473:TRP:CD2	1:A:474:PRO:HD2	2.53	0.43
1:A:393:TYR:HB3	1:A:398:PHE:CE2	2.54	0.43
1:A:33:PRO:HD2	1:A:84:LEU:O	2.19	0.43
1:A:120:VAL:CG1	1:A:476[A]:VAL:HG21	2.41	0.43
1:A:268:GLY:N	3:A:704:HOH:O	2.32	0.42
1:A:518:SER:HB3	3:A:855:HOH:O	2.21	0.41
1:A:190:LYS:HG2	3:A:1019:HOH:O	2.20	0.41
1:A:21:MET:SD	1:A:67:GLU:HG2	2.62	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	595/605 (98%)	576 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	500/505 (99%)	496 (99%)	4 (1%)	79	74

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	LYS
1	A	238	LYS
1	A	363	LEU
1	A	592	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	95	GLN
1	A	98	ASN
1	A	127	GLN
1	A	200	ASN
1	A	262	HIS
1	A	290	HIS
1	A	414	GLN
1	A	427	ASN
1	A	443	GLN
1	A	533	GLN



### 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 ⓘ

3 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	GAL	B	1	2	12,12,12	1.39	2 (16%)	17,17,17	2.51	6 (35%)
2	GLC	B	2	2	11,11,12	1.88	4 (36%)	15,15,17	2.26	3 (20%)
2	A1EAX	B	3	2	21,22,23	7.04	10 (47%)	22,32,34	1.87	4 (18%)

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	GAL	B	1	2	-	2/2/22/22	0/1/1/1
2	GLC	B	2	2	-	0/2/19/22	0/1/1/1
2	A1EAX	B	3	2	-	4/6/43/46	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	A1EAX	C6H-C5H	20.64	1.61	1.32
2	B	3	A1EAX	C2H-C1H	15.06	1.72	1.52
2	B	3	A1EAX	C3H-C4H	13.40	1.72	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	A1EAX	C4H-C5H	-8.89	1.44	1.51
2	B	3	A1EAX	C3H-C2H	-8.27	1.31	1.52
2	B	3	A1EAX	C1H-C6H	-3.81	1.45	1.50
2	B	3	A1EAX	O5-C5	3.43	1.50	1.43
2	B	2	GLC	O5-C1	3.42	1.49	1.43
2	B	2	GLC	O4-C4	3.35	1.50	1.43
2	B	3	A1EAX	C4-N4	2.72	1.52	1.47
2	B	1	GAL	O5-C5	2.63	1.50	1.44
2	B	1	GAL	O4-C4	2.56	1.49	1.43
2	B	3	A1EAX	O5-C1	2.52	1.47	1.43
2	B	2	GLC	C2-C3	-2.08	1.49	1.52
2	B	3	A1EAX	O4H-C4H	-2.03	1.38	1.42
2	B	2	GLC	O5-C5	2.01	1.47	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	GLC	C1-C2-C3	6.96	118.22	109.67
2	B	1	GAL	O4-C4-C3	6.63	125.69	110.35
2	B	3	A1EAX	C2-C3-C4	5.82	115.76	110.63
2	B	1	GAL	C4-C3-C2	4.03	117.86	110.82
2	B	1	GAL	O5-C5-C4	4.01	116.97	109.69
2	B	3	A1EAX	C4H-C5H-C6H	-3.48	116.52	122.23
2	B	1	GAL	C3-C4-C5	3.43	116.36	110.24
2	B	2	GLC	O2-C2-C3	-3.12	103.89	110.14
2	B	1	GAL	O3-C3-C4	2.78	116.78	110.35
2	B	3	A1EAX	O5-C5-C4	2.73	115.08	110.05
2	B	1	GAL	C1-C2-C3	2.13	114.72	110.31
2	B	3	A1EAX	C1-C2-C3	2.08	112.23	109.67
2	B	2	GLC	C3-C4-C5	2.01	113.82	110.24

There are no chirality outliers.

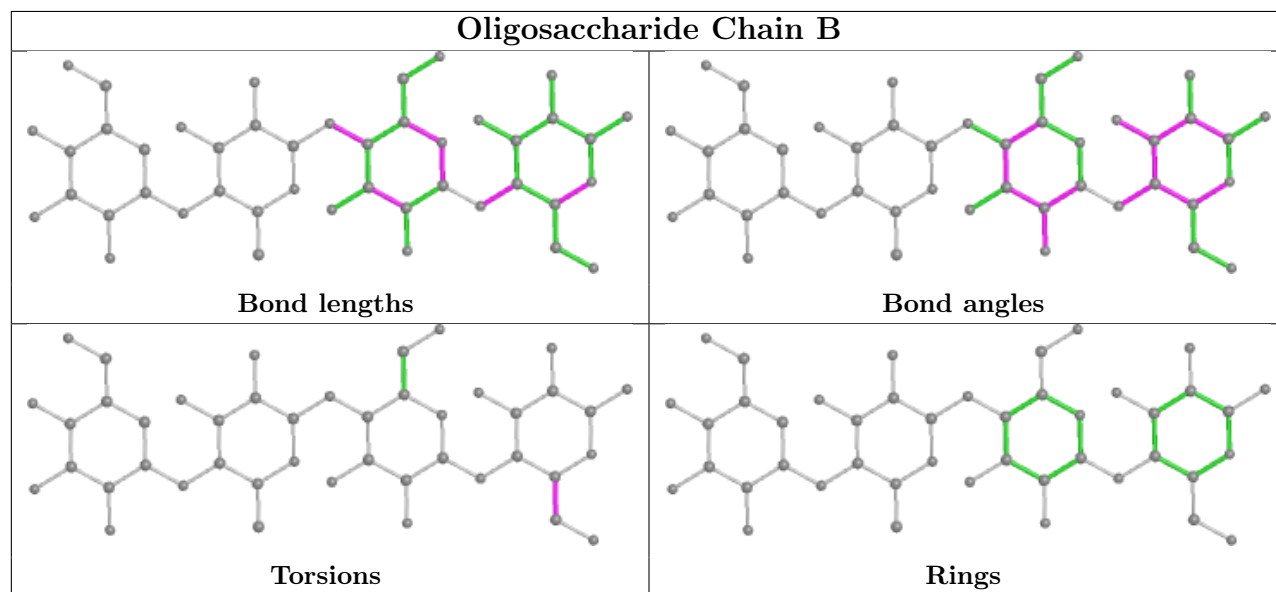
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	A1EAX	C2H-C1H-N4-C4
2	B	3	A1EAX	C6H-C1H-N4-C4
2	B	3	A1EAX	C5-C4-N4-C1H
2	B	1	GAL	C4-C5-C6-O6
2	B	1	GAL	O5-C5-C6-O6
2	B	3	A1EAX	C3-C4-N4-C1H

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](#)

There are no ligands in this entry.

## 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	598/605 (98%)	-0.05	15 (2%) 58 64	9, 23, 41, 65	1 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	SER	2.9
1	A	139	ARG	2.8
1	A	138	SER	2.7
1	A	291	ASP	2.6
1	A	146	THR	2.5
1	A	605	ARG	2.5
1	A	285	PRO	2.4
1	A	293	LEU	2.4
1	A	295	TYR	2.2
1	A	292	TRP	2.2
1	A	267	GLY	2.1
1	A	290	HIS	2.0
1	A	274	ASP	2.0
1	A	167	ALA	2.0
1	A	54	ARG	2.0

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

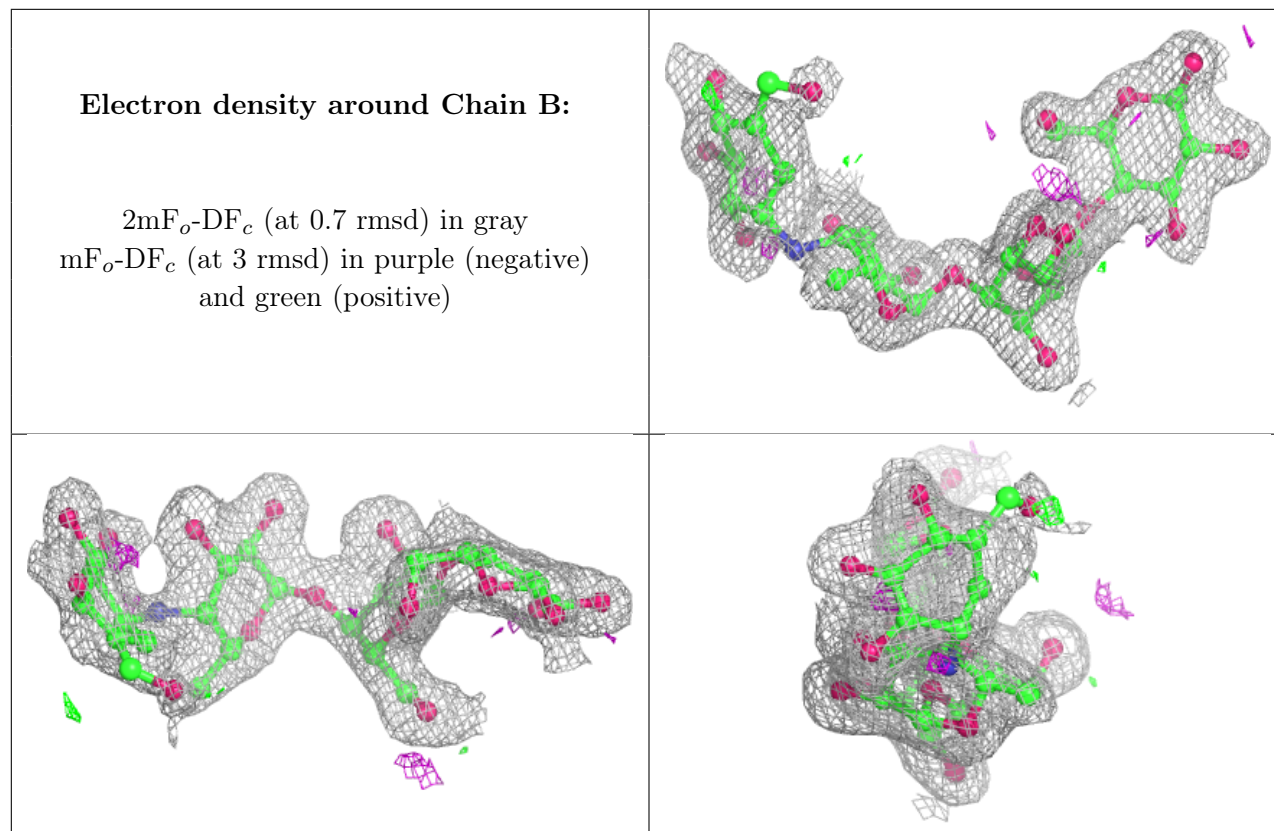
There are no non-standard protein/DNA/RNA residues in this entry.

### 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( $\text{\AA}^2$ )	Q<0.9
2	A1EAX	B	3	21/22	0.87	0.12	26,33,44,55	0
2	GAL	B	1	12/12	0.92	0.09	26,28,33,34	0
2	GLC	B	2	11/12	0.94	0.07	22,27,30,37	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.