

# wwPDB X-ray Structure Validation Summary Report (i)

Dec 10, 2023 – 07:46 am GMT

PDB ID : 10JJ

Title: Anatomy of glycosynthesis: Structure and kinetics of the Humicola insolens

Cel7BE197A and E197S glycosynthase mutants

Authors: Ducros, V.M.-A.; Tarling, C.A.; Zechel, D.L.; Brzozowski, A.M.; Frandsen,

T.P.; Von Ossowski, I.; Schulein, M.; Withers, S.G.; Davies, G.J.

Deposited on : 2003-07-10

Resolution : 1.40 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:

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)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

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

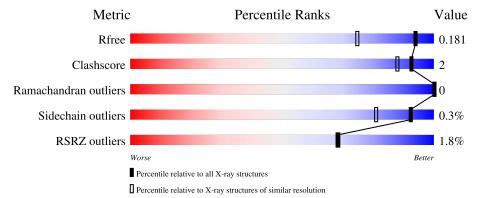
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.40 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
$R_{free}$	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	402	95%	
1	В	402	96%	ó
2	С	2	50%	50%
2	Е	2	50%	50%
3	D	2	50%	50%



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Mo	Chain	Length	Quality of chain
3	F	2	100%



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6984 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 ENDOGLUCANASE I.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	399	Total 3113	C 1953	N 535	O 595	S 30	0	6	1
1	В	399	Total 3109	C 1952	N 535	O 592	S 30	0	5	1

There are 2 discrepancies between the modelled and reference sequences:

	Chain	Residue	Modelled	Actual	Comment	Reference
	A	197	197 SER GLU engir		engineered mutation	UNP P56680
ĺ	В	197	.97 SER GLU		engineered mutation	UNP P56680

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	С	2	Total C O 23 12 11	0	0	0
2	Е	2	Total C O 23 12 11	0	0	0

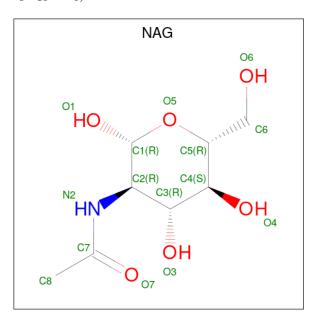
• Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-alpha-D-glucopyranos e.





$\mathbf{Mol}$	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	2	Total C O 23 12 11	0	0	0
3	F	2	Total C O 23 12 11	0	0	0

 $\bullet$  Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $\rm C_8H_{15}NO_6).$ 



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 14				0	0
4	В	1	Total 14		N 1	O 5	0	0

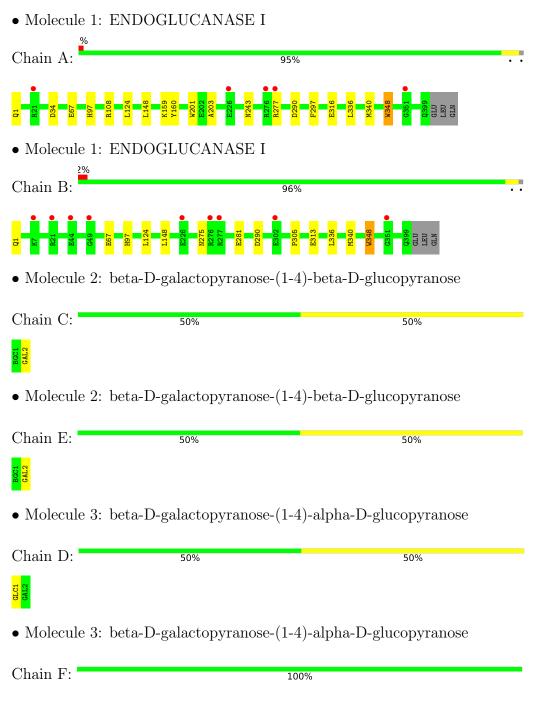
• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	333	Total O 333 333	0	0
5	В	309	Total O 309 309	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.









# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	66.36Å 74.75Å 85.82Å	Donositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 102.51° 90.00°	Depositor
Resolution (Å)	84.52 - 1.40	Depositor
Resolution (A)	14.99 - 1.40	EDS
% Data completeness	98.7 (84.52-1.40)	Depositor
(in resolution range)	98.8 (14.99-1.40)	EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.31 (at 1.41Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
P. P.	0.149 , 0.173	Depositor
$R, R_{free}$	0.158 , 0.181	DCC
$R_{free}$ test set	7944 reflections (5.04%)	wwPDB-VP
Wilson B-factor $(Å^2)$	11.7	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.45, 48.7	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6984	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 53.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2684e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: GAL, NAG, GLC, BGC, PCA

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		
IVIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.56	0/3211	0.77	3/4351 (0.1%)	
1	В	0.56	0/3203	0.76	1/4341 (0.0%)	
All	All	0.56	0/6414	0.76	4/8692 (0.0%)	

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	290	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	290	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	34	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	108	ARG	NE-CZ-NH1	5.09	122.85	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	3113	0	2946	9	1
1	В	3109	0	2948	10	0
2	С	23	0	21	0	0
2	Е	23	0	21	0	0
3	D	23	0	21	0	0



Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	23	0	21	0	0
4	A	14	0	13	0	0
4	В	14	0	13	0	0
5	A	333	0	0	2	0
5	В	309	0	0	0	0
All	All	6984	0	6004	19	1

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.

The worst 5 of 19 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:B:336:LEU:HD23	1:B:340[B]:MET:SD	2.23	0.78
1:A:67[A]:GLU:HG2	1:A:160:TYR:OH	1.85	0.76
1:A:67[A]:GLU:HG2	1:A:160:TYR:CZ	2.23	0.73
1:B:275:ASN:HB3	1:B:281:GLU:OE2	1.90	0.71
1:B:275:ASN:HB3	1:B:281:GLU:CD	2.16	0.65

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:159:LYS:NZ	1:A:316:GLU:OE2[2_555]	1.96	0.24

## 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	Perce	$\mathbf{ntiles}$
1	A	403/402 (100%)	395 (98%)	8 (2%)	0	100	100
1	В	402/402 (100%)	394 (98%)	8 (2%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
All	All	805/804 (100%)	789 (98%)	16 (2%)	0	100	100

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	Rotameric Outliers	
1	A	336/334 (101%)	335 (100%)	1 (0%)	92 81
1	В	335/334 (100%)	334 (100%)	1 (0%)	92 81
All	All	671/668 (100%)	669 (100%)	2 (0%)	92 81

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348	TRP
1	В	348	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	A	97	HIS
1	A	161	ASN
1	A	353	ASN
1	В	97	HIS
1	В	353	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)

2 non-standard protein/DNA/RNA residues 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	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain Res	Dag	T inle	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2									
1	PCA	В	1	1	7,8,9	1.23	1 (14%)	9,10,12	0.92	0									
1	PCA	A	1	1	7,8,9	1.31	1 (14%)	9,10,12	1.33	1 (11%)									

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
1	PCA	В	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

#### All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
1	В	1	PCA	CD-N	3.13	1.42	1.34
1	A	1	PCA	CD-N	2.92	1.42	1.34

#### All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	1	PCA	OE-CD-N	-2.02	120.14	124.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



### 5.5 Carbohydrates (i)

8 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	Trino	Chain	Res	Link	Во	ond leng	ths	Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BGC	С	1	2	12,12,12	0.50	0	17,17,17	0.75	0
2	GAL	С	2	2	11,11,12	0.74	0	15,15,17	1.12	2 (13%)
3	GLC	D	1	3	12,12,12	0.49	0	17,17,17	1.18	3 (17%)
3	GAL	D	2	3	11,11,12	0.41	0	15,15,17	0.83	0
2	BGC	Е	1	2	12,12,12	0.52	0	17,17,17	0.78	0
2	GAL	Е	2	2	11,11,12	0.93	0	15,15,17	1.15	1 (6%)
3	GLC	F	1	3	12,12,12	0.47	0	17,17,17	1.01	0
3	GAL	F	2	3	11,11,12	0.69	0	15,15,17	0.58	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
2	BGC	С	1	2	-	0/2/22/22	0/1/1/1
2	GAL	С	2	2	-	0/2/19/22	0/1/1/1
3	GLC	D	1	3	-	0/2/22/22	0/1/1/1
3	GAL	D	2	3	-	0/2/19/22	0/1/1/1
2	BGC	Е	1	2	-	0/2/22/22	0/1/1/1
2	GAL	Е	2	2	-	1/2/19/22	0/1/1/1
3	GLC	F	1	3	-	0/2/22/22	0/1/1/1
3	GAL	F	2	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	D	1	GLC	O2-C2-C1	-2.44	103.51	109.16
2	Е	2	GAL	O2-C2-C3	-2.41	105.31	110.14



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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(^{o})$	$\operatorname{Ideal}({}^o)$
2	С	2	GAL	O2-C2-C3	-2.29	105.56	110.14
2	С	2	GAL	O3-C3-C2	-2.18	105.83	109.99
3	D	1	GLC	O2-C2-C3	2.13	115.26	110.35

There are no chirality outliers.

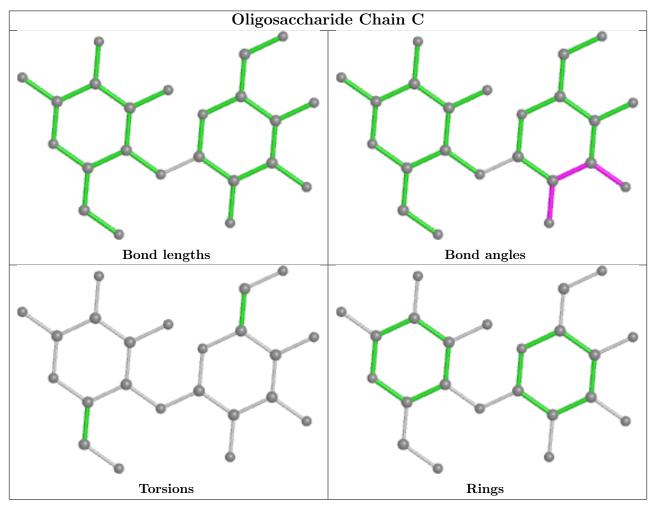
All (1) torsion outliers are listed below:

M	ol	Chain	Res	Type	Atoms
2		Е	2	GAL	O5-C5-C6-O6

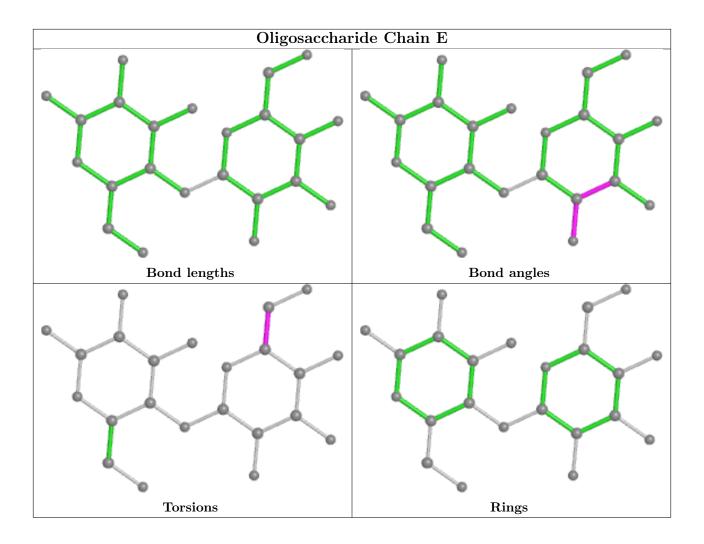
There are no ring outliers.

No monomer is involved in short contacts.

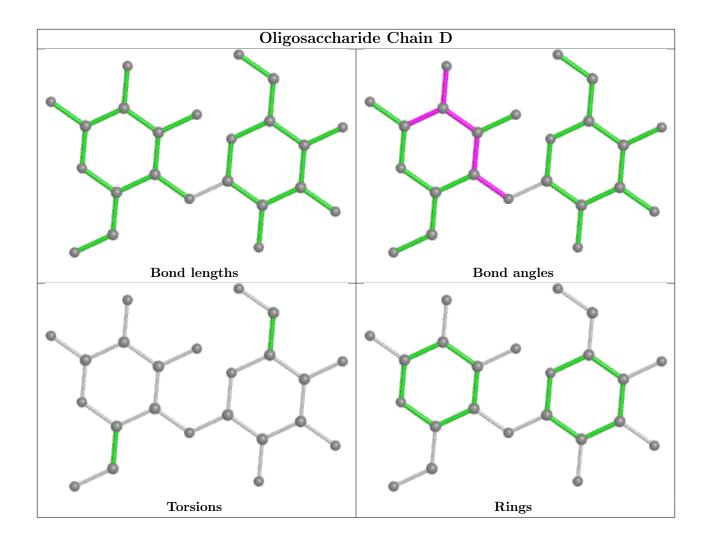
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



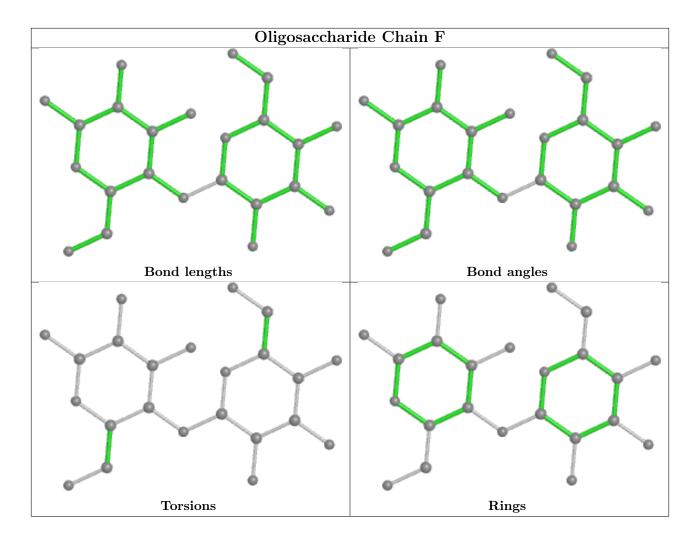












## 5.6 Ligand geometry (i)

#### 2 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	Type Chain		Link	Bo	ond leng	$ ag{ths}$	В	ond angles	
WIOI	Туре	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	В	1399	1	14,14,15	0.63	0	17,19,21	0.72	0
4	NAG	A	1404	1	14,14,15	0.61	0	17,19,21	1.01	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	NAG	В	1399	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	0/6/23/26	0/1/1/1

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	$\langle { m RSRZ} \rangle$	# RSRZ > 2	$OWAB(A^2)$	Q < 0.9
1	A	398/402 (99%)	-0.24	5 (1%) 77 75	8, 11, 19, 35	0
1	В	398/402 (99%)	-0.12	9 (2%) 60 60	8, 12, 21, 37	0
All	All	796/804 (99%)	-0.18	14 (1%) 68 68	8, 12, 20, 37	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	RSRZ
1	В	276	ARG	8.4
1	A	276	ARG	6.8
1	A	277	ARG	6.2
1	В	277	ARG	5.4
1	A	21	ARG	4.2

## 6.2 Non-standard residues in protein, DNA, RNA chains (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
1	PCA	В	1	8/9	0.97	0.05	11,13,13,14	0
1	PCA	A	1	8/9	0.98	0.06	10,10,11,12	0

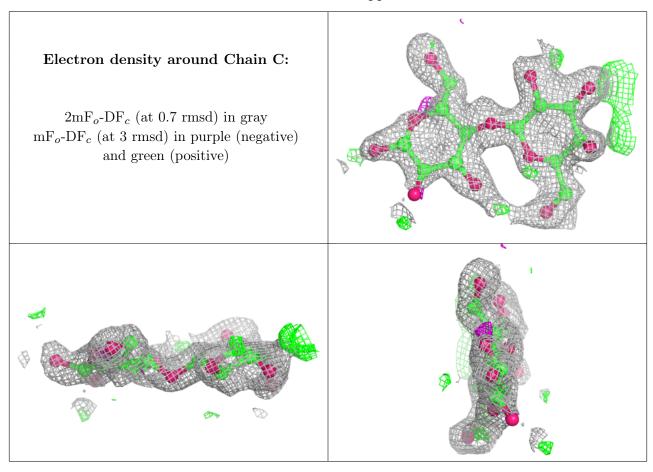
### 6.3 Carbohydrates (i)

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.

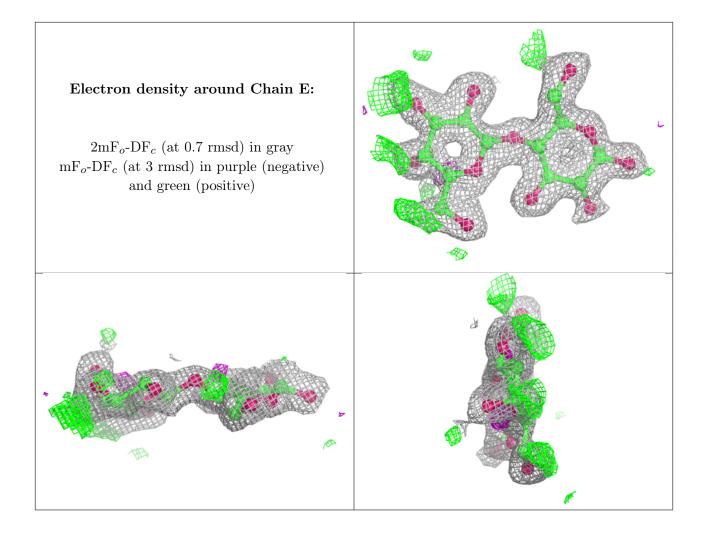


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	BGC	С	1	12/12	0.62	0.28	30,36,38,40	0
2	GAL	С	2	11/12	0.73	0.20	26,28,30,32	0
2	BGC	Е	1	12/12	0.78	0.22	25,32,36,36	0
2	$\operatorname{GAL}$	Е	2	11/12	0.81	0.20	20,23,26,29	0
3	GLC	D	1	12/12	0.96	0.07	8,9,12,14	0
3	GAL	D	2	11/12	0.97	0.06	8,9,10,13	0
3	GLC	F	1	12/12	0.97	0.07	9,10,14,15	0
3	GAL	F	2	11/12	0.98	0.06	8,9,11,13	0

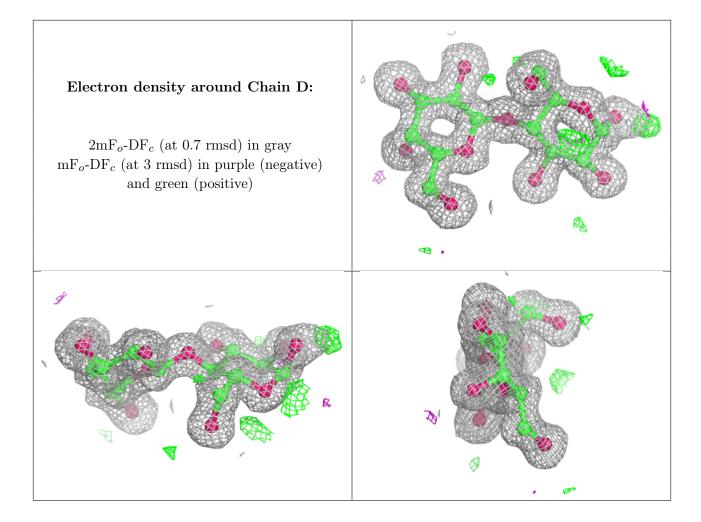
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



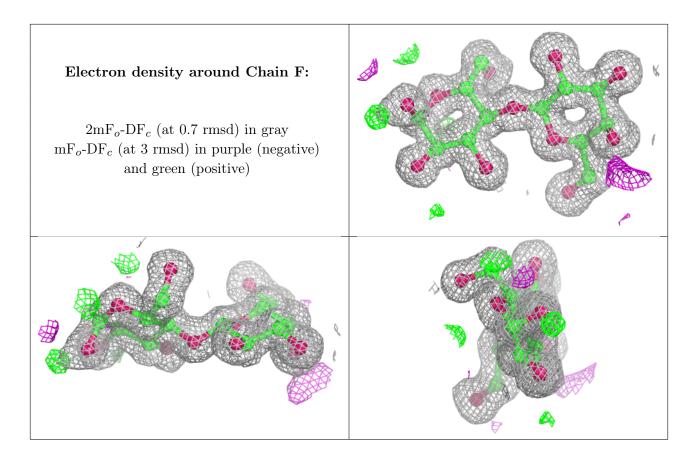












# 6.4 Ligands (i)

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	$ig   ext{B-factors}( ext{Å}^2)$	Q<0.9
4	NAG	A	1404	14/15	0.88	0.15	18,22,26,27	0
4	NAG	В	1399	14/15	0.89	0.15	14,16,23,27	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

