



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 09:54 AM BST

PDB ID : 4FNT  
Title : Crystal structure of GH36 alpha-galactosidase AgaA A355E D548N from *Geobacillus stearothermophilus* in complex with raffinose  
Authors : Merceron, R.; Foucault, M.; Haser, R.; Mattes, R.; Watzlawick, H.; Gouet, P.  
Deposited on : 2012-06-20  
Resolution : 2.60 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](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

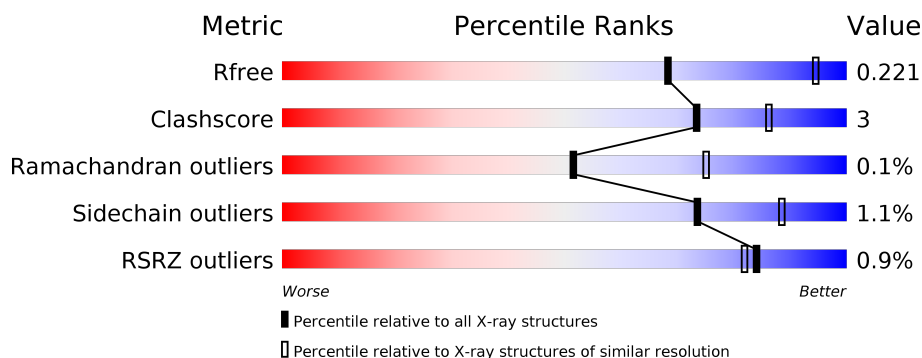
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	729	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>•</div> </div> </div>
1	B	729	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>•</div> </div> </div>
1	C	729	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>•</div> </div> </div>
1	D	729	<div> <div></div> <div> <div></div> <div>90%</div> <div>8%</div> <div>•</div> </div> </div>
2	E	3	<div> <div></div> <div> <div></div> <div>67%</div> <div>33%</div> </div> </div>
2	F	3	<div> <div></div> <div> <div></div> <div>67%</div> <div>33%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	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	FRU	E	1	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23619 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 Alpha-galactosidase AgaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	718	Total	C	N	O	S	0	0	0
			5790	3676	1021	1071	22			
1	B	718	Total	C	N	O	S	0	0	0
			5790	3676	1021	1071	22			
1	C	718	Total	C	N	O	S	0	0	0
			5790	3676	1021	1071	22			
1	D	718	Total	C	N	O	S	0	0	0
			5790	3676	1021	1071	22			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	GLU	ALA	engineered mutation	UNP Q9ALJ4
A	548	ASN	ASP	engineered mutation	UNP Q9ALJ4
A	704	VAL	MET	engineered mutation	UNP Q9ALJ4
B	355	GLU	ALA	engineered mutation	UNP Q9ALJ4
B	548	ASN	ASP	engineered mutation	UNP Q9ALJ4
B	704	VAL	MET	engineered mutation	UNP Q9ALJ4
C	355	GLU	ALA	engineered mutation	UNP Q9ALJ4
C	548	ASN	ASP	engineered mutation	UNP Q9ALJ4
C	704	VAL	MET	engineered mutation	UNP Q9ALJ4
D	355	GLU	ALA	engineered mutation	UNP Q9ALJ4
D	548	ASN	ASP	engineered mutation	UNP Q9ALJ4
D	704	VAL	MET	engineered mutation	UNP Q9ALJ4

- Molecule 2 is an oligosaccharide called alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose.



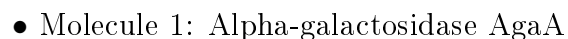
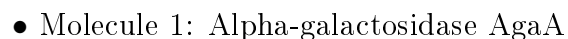
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	3	Total	C	O	0	0	0
			34	18	16			
2	F	3	Total	C	O	0	0	0
			34	18	16			
2	G	3	Total	C	O	0	0	0
			34	18	16			

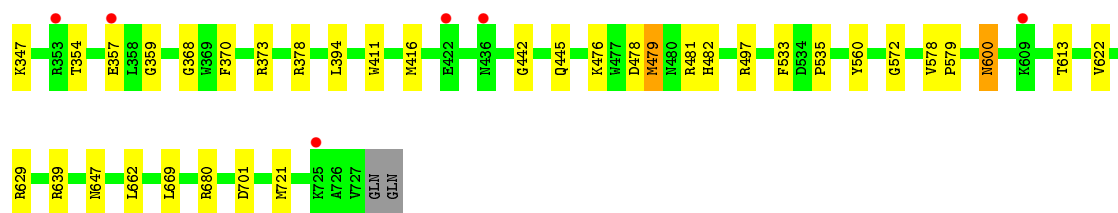
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	114	Total	O	0	0
			114	114		
3	B	86	Total	O	0	0
			86	86		
3	C	49	Total	O	0	0
			49	49		
3	D	108	Total	O	0	0
			108	108		



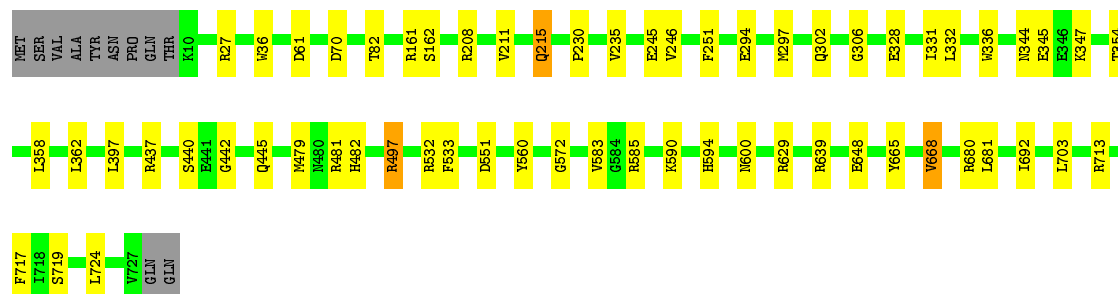
- Molecule 1: Alpha-galactosidase AgaA





• Molecule 1: Alpha-galactosidase AgaA

Chain D: 90% 8% .



• Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain E: 67% 33%



• Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain F: 67% 33%



• Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain G: 100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.68Å 149.68Å 234.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.89 – 2.60 19.89 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.89-2.60) 98.8 (19.89-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 2.59Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.170 , 0.221 0.170 , 0.221	Depositor DCC
$R_{free}$ test set	4629 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.9	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	23619	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: GLA, GLC, FRU

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	0.23	0/5937	0.41	0/8050
1	B	0.23	0/5937	0.41	0/8050
1	C	0.22	0/5937	0.41	0/8050
1	D	0.24	0/5937	0.42	0/8050
All	All	0.23	0/23748	0.41	0/32200

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	5790	0	5622	45	0
1	B	5790	0	5622	35	0
1	C	5790	0	5622	38	0
1	D	5790	0	5622	37	0
2	E	34	0	30	1	0
2	F	34	0	30	1	0
2	G	34	0	27	5	0
3	A	114	0	0	0	0
3	B	86	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	49	0	0	2	0
3	D	108	0	0	0	0
All	All	23619	0	22575	153	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.

The worst 5 of 153 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:D:328:GLU:HB3	1:D:629:ARG:HD3	1.67	0.76
1:D:481:ARG:NH1	1:D:482:HIS:O	2.21	0.72
1:C:481:ARG:NH1	1:C:482:HIS:O	2.22	0.72
1:A:440:SER:O	1:A:481:ARG:NH2	2.22	0.72
1:B:27:ARG:NH2	1:B:64:ASP:OD2	2.24	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	716/729 (98%)	691 (96%)	23 (3%)	2 (0%)	41	64
1	B	716/729 (98%)	689 (96%)	27 (4%)	0	100	100
1	C	716/729 (98%)	690 (96%)	26 (4%)	0	100	100
1	D	716/729 (98%)	686 (96%)	30 (4%)	0	100	100
All	All	2864/2916 (98%)	2756 (96%)	106 (4%)	2 (0%)	51	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	ARG
1	A	715	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	Rotameric	Outliers	Percentiles	
1	A	609/619 (98%)	601 (99%)	8 (1%)	69	86
1	B	609/619 (98%)	601 (99%)	8 (1%)	69	86
1	C	609/619 (98%)	604 (99%)	5 (1%)	81	92
1	D	609/619 (98%)	604 (99%)	5 (1%)	81	92
All	All	2436/2476 (98%)	2410 (99%)	26 (1%)	73	88

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	388	ARG
1	B	668	VAL
1	D	583	VAL
1	B	479	MET
1	B	533	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 ⓘ

9 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	FRU	E	1	2	11,12,12	1.67	5 (45%)	10,18,18	1.50	2 (20%)
2	GLC	E	2	2	11,11,12	1.81	3 (27%)	15,15,17	2.08	6 (40%)
2	GLA	E	3	2	11,11,12	1.82	2 (18%)	15,15,17	1.54	4 (26%)
2	FRU	F	1	2	11,12,12	1.73	4 (36%)	10,18,18	1.55	3 (30%)
2	GLC	F	2	2	11,11,12	2.01	3 (27%)	15,15,17	2.83	8 (53%)
2	GLA	F	3	2	11,11,12	1.67	2 (18%)	15,15,17	1.41	3 (20%)
2	FRU	G	1	2	11,12,12	1.67	3 (27%)	10,18,18	1.21	0
2	GLC	G	2	2	11,11,12	2.32	5 (45%)	15,15,17	2.67	10 (66%)
2	GLA	G	3	2	11,11,12	2.77	3 (27%)	15,15,17	1.58	3 (20%)

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	FRU	E	1	2	-	0/5/24/24	0/1/1/1
2	GLC	E	2	2	-	1/2/19/22	0/1/1/1
2	GLA	E	3	2	-	0/2/19/22	0/1/1/1
2	FRU	F	1	2	-	3/5/24/24	0/1/1/1
2	GLC	F	2	2	-	2/2/19/22	0/1/1/1
2	GLA	F	3	2	-	0/2/19/22	0/1/1/1
2	FRU	G	1	2	-	5/5/24/24	0/1/1/1
2	GLC	G	2	2	-	2/2/19/22	0/1/1/1
2	GLA	G	3	2	-	1/2/19/22	0/1/1/1

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	3	GLA	C2-C3	-6.43	1.43	1.52
2	G	2	GLC	C2-C3	-4.99	1.45	1.52
2	E	3	GLA	C2-C3	-4.89	1.45	1.52
2	F	2	GLC	O5-C1	4.75	1.51	1.43
2	G	3	GLA	C4-C3	-4.73	1.40	1.52

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	GLC	C1-C2-C3	5.72	116.70	109.67
2	G	2	GLC	C1-O5-C5	5.20	119.24	112.19
2	F	2	GLC	C1-O5-C5	5.06	119.04	112.19
2	E	2	GLC	C3-C4-C5	4.91	119.00	110.24
2	F	2	GLC	O5-C1-C2	3.90	116.80	110.77

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

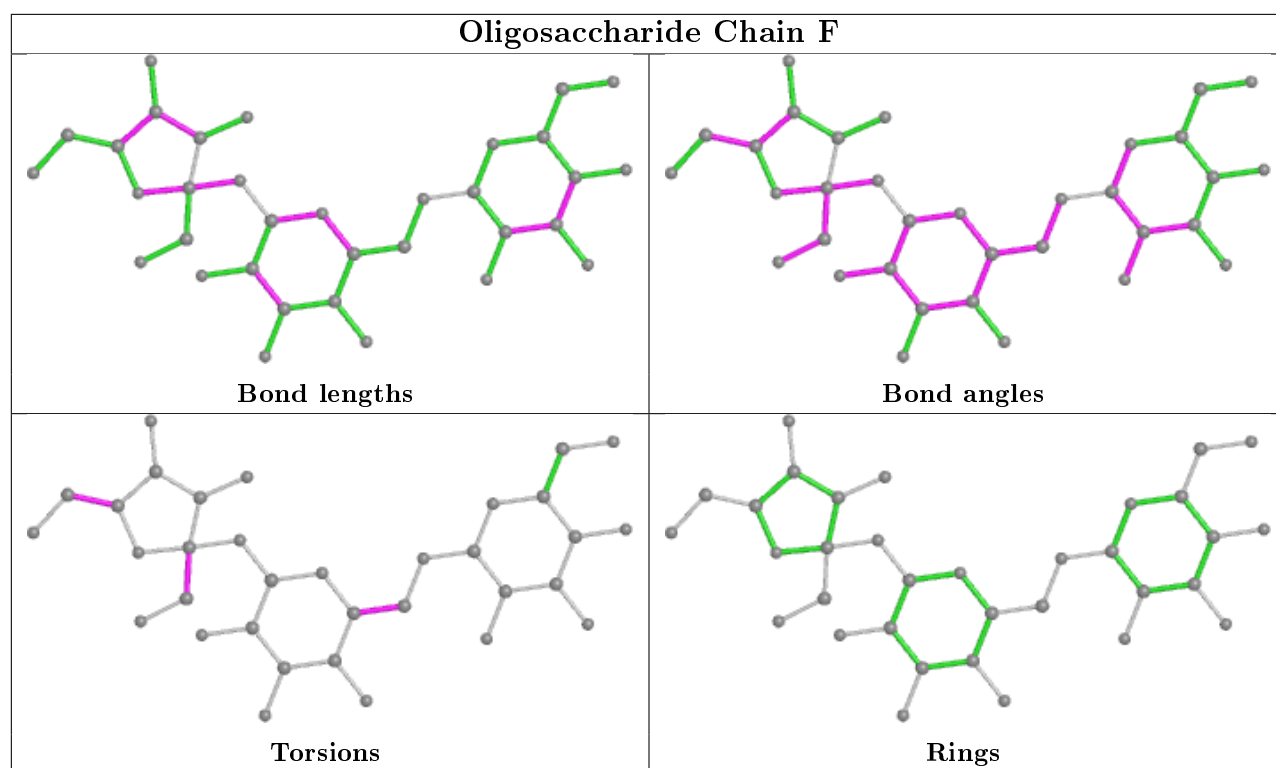
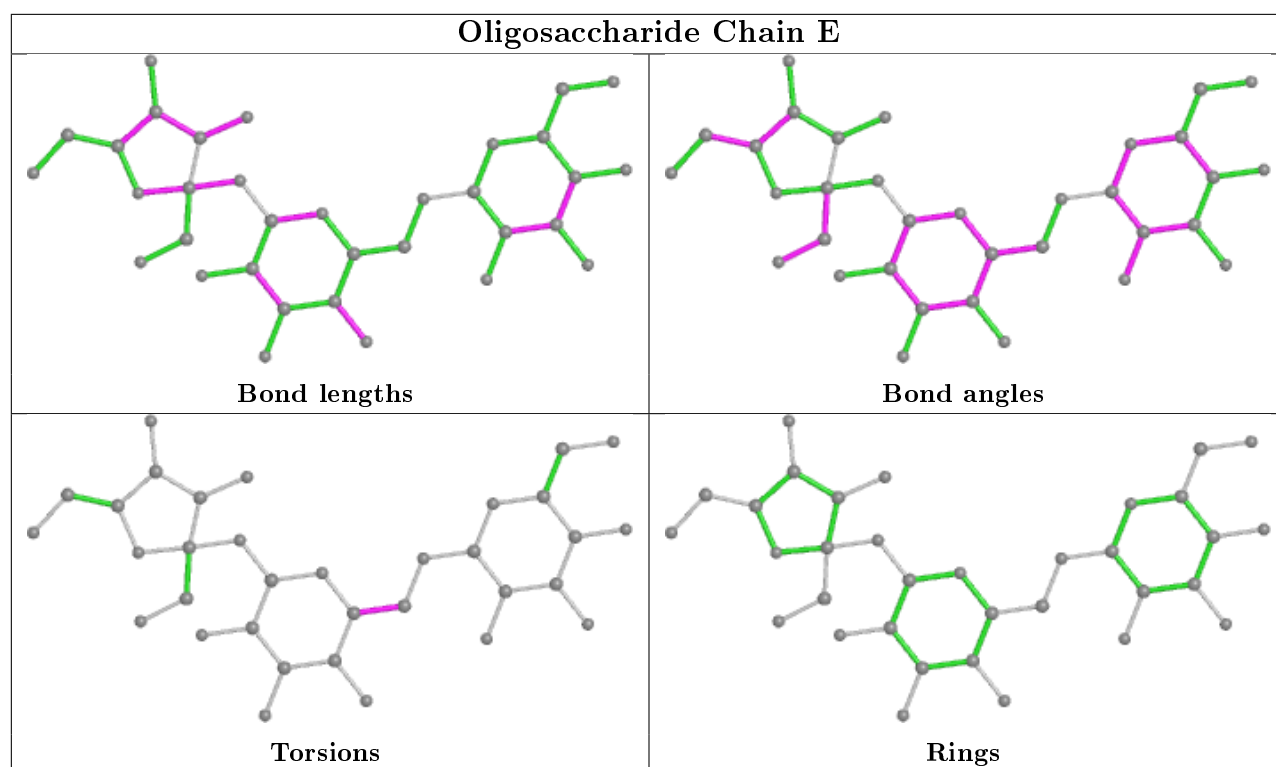
Mol	Chain	Res	Type	Atoms
2	G	1	FRU	O1-C1-C2-C3
2	G	1	FRU	O1-C1-C2-O2
2	G	1	FRU	O1-C1-C2-O5
2	G	1	FRU	C4-C5-C6-O6
2	G	1	FRU	O5-C5-C6-O6

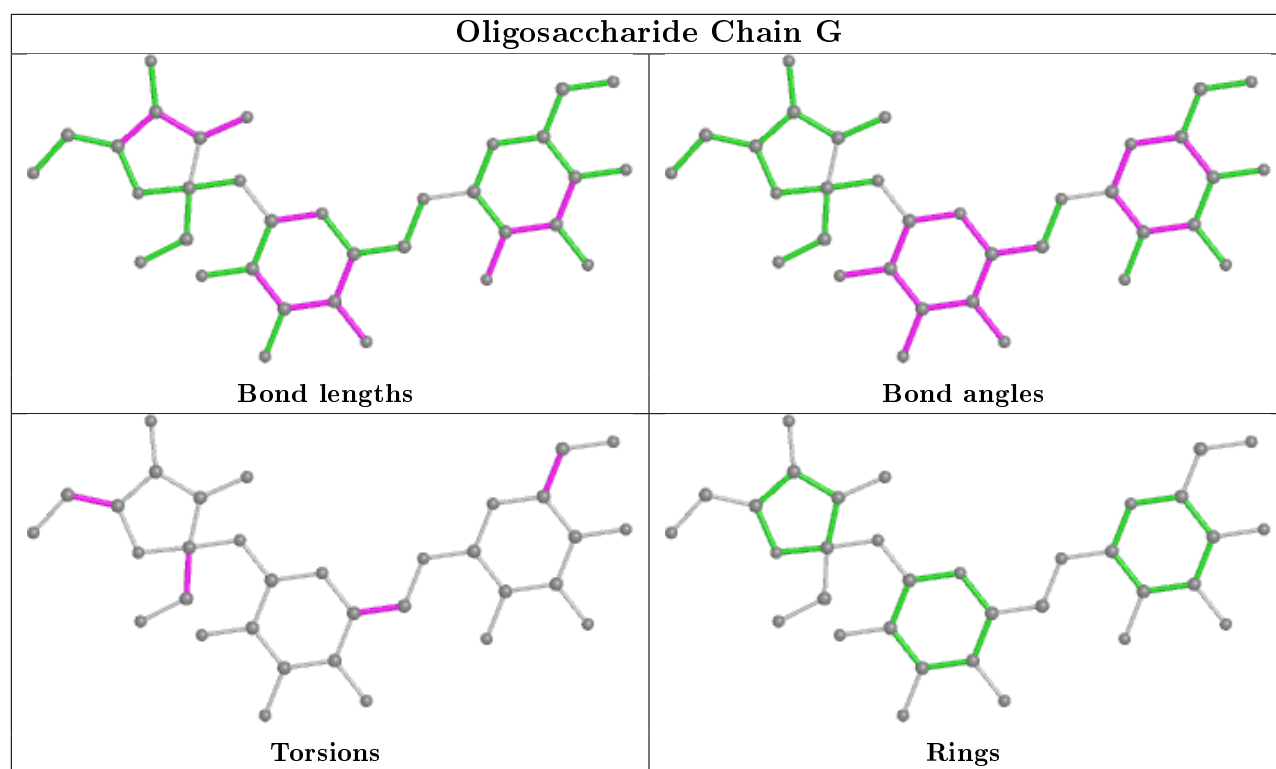
There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	FRU	4	0
2	G	3	GLA	1	0
2	G	2	GLC	3	0
2	F	3	GLA	1	0
2	E	3	GLA	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](#)

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 ⓘ

### 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	718/729 (98%)	-0.50	9 (1%) 77 73	26, 37, 59, 88	0
1	B	718/729 (98%)	-0.48	7 (0%) 82 80	27, 41, 64, 84	0
1	C	718/729 (98%)	-0.34	10 (1%) 75 71	29, 48, 68, 86	0
1	D	718/729 (98%)	-0.57	0 100 100	26, 36, 53, 66	0
All	All	2872/2916 (98%)	-0.47	26 (0%) 84 82	26, 40, 62, 88	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	353	ARG	4.1
1	B	47	ARG	3.9
1	B	48	ALA	3.5
1	B	46	ALA	3.4
1	B	50	PRO	3.3

### 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	FRU	E	1	12/12	0.65	0.48	95,117,128,131	0
2	FRU	F	1	12/12	0.68	0.34	80,111,122,129	0

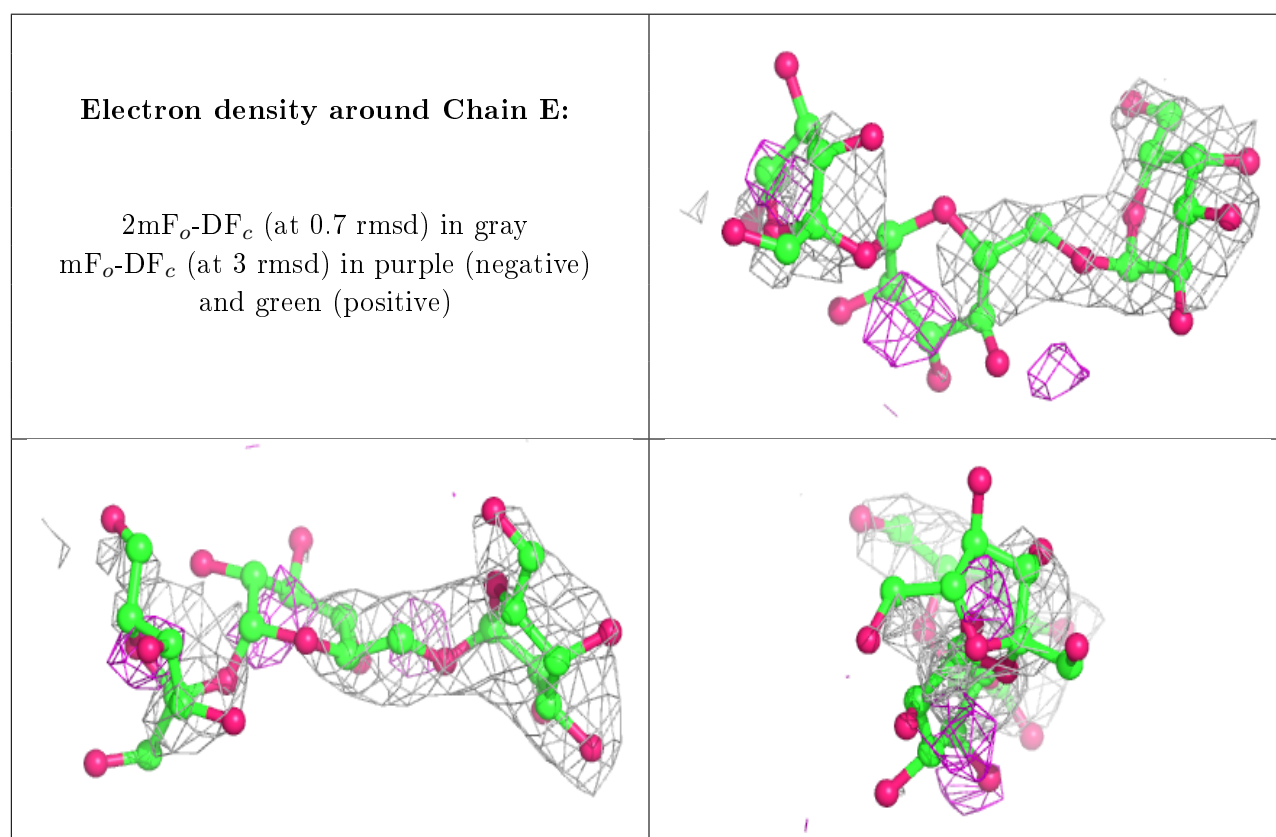
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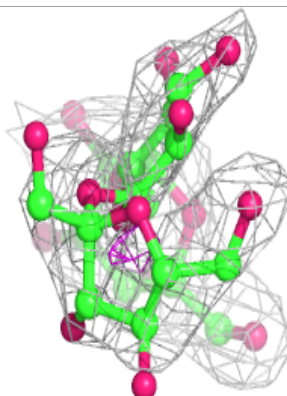
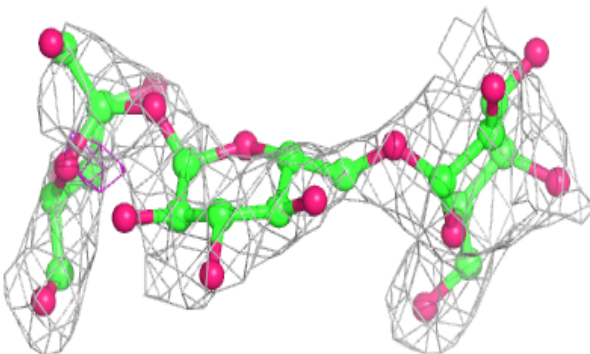
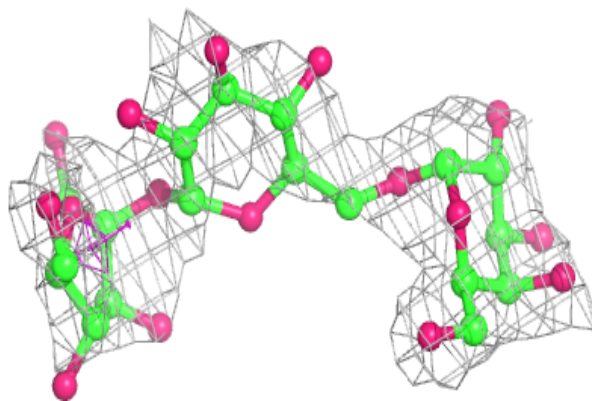
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FRU	G	1	12/12	0.73	0.30	80,101,108,120	0
2	GLC	F	2	11/12	0.81	0.26	75,87,98,105	0
2	GLC	E	2	11/12	0.81	0.38	71,98,109,118	0
2	GLC	G	2	11/12	0.84	0.25	56,79,95,100	0
2	GLA	E	3	11/12	0.93	0.19	54,66,69,77	0
2	GLA	F	3	11/12	0.94	0.14	46,61,71,73	0
2	GLA	G	3	11/12	0.95	0.12	44,46,54,55	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.

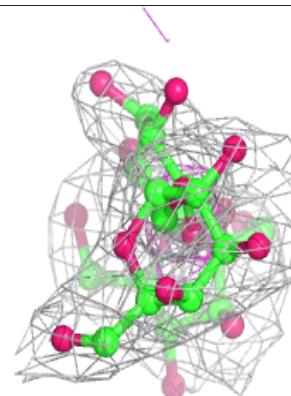
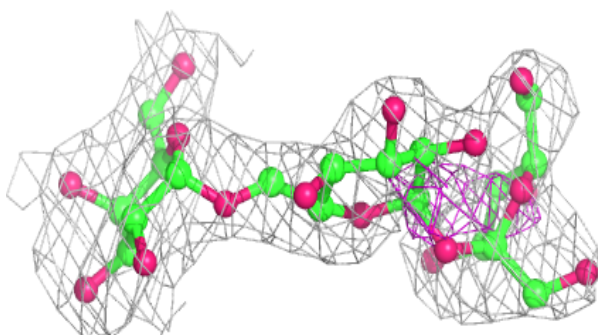
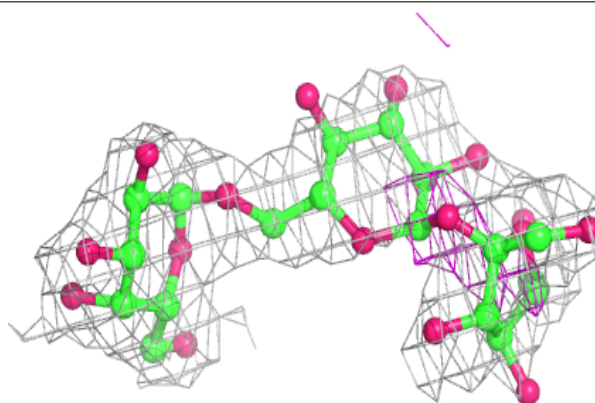


**Electron density around Chain F:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain G:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.