

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

Mar 7, 2022 – 12:06 pm GMT

PDB ID : 7PUK

Title : Crystal structure of Endoglycosidase E GH18 domain from Enterococcus fae-

calis in complex with Man5 product

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Deposited on : 2021-09-30

Resolution : 2.69 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 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 : 2.27

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

Refmac : 5.8.0267

CCP4 : 7.1.010 (Gargrove) roteins) : Engh & Huber (2001)

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

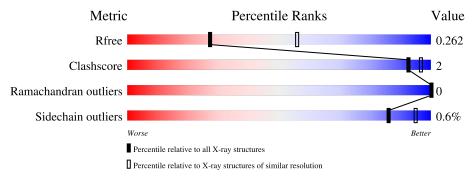
Validation Pipeline (wwPDB-VP) : 2.27

## 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 2.69 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	Similar resolution
TVIOUTE	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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%

Mol	Chain	Length	Quality of chain	
1	A	435	95%	
1	С	435	92%	5% •
2	В	6	83%	17%
2	D	6	67%	33%



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6787 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 Beta-N-acetylhexosaminidase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	425	Total 3334	C 2110	N 552	O 663	S 9	0	0	0
1	С	422	Total 3313	C 2095	N 550	O 659	S 9	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	GLY	-	expression tag	UNP Q6U890
A	53	GLY	-	expression tag	UNP Q6U890
A	54	SER	-	expression tag	UNP Q6U890
A	55	GLY	ALA	conflict	UNP Q6U890
A	250	LYS	GLN	conflict	UNP Q6U890
A	380	THR	ALA	conflict	UNP Q6U890
С	52	GLY	-	expression tag	UNP Q6U890
С	53	GLY	-	expression tag	UNP Q6U890
С	54	SER	-	expression tag	UNP Q6U890
С	55	GLY	ALA	conflict	UNP Q6U890
С	250	LYS	GLN	conflict	UNP Q6U890
С	380	THR	ALA	conflict	UNP Q6U890

• Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	В	6	Total 70	C 38	N 1	O 31	0	0	0

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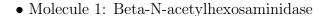
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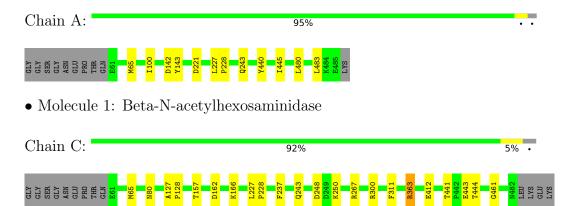
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	D	6	Total 70	C 38	N 1	O 31	0	0	0



## 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. 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. 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.





Chain B: 83% 17%

 $\bullet$  Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 67% 33%



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	222.03Å 54.55Å 83.92Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $110.36^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	45.73 - 2.69	Depositor
Resolution (A)	45.73 - 2.69	EDS
% Data completeness	97.6 (45.73-2.69)	Depositor
(in resolution range)	98.8 (45.73-2.69)	EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.47 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
D.D.	0.226 , $0.262$	Depositor
$R, R_{free}$	0.228 , $0.262$	DCC
$R_{free}$ test set	1313 reflections $(5.00\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.8	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$< L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.000 for -h-2*l,-k,l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6787	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.

<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: MAN, NAG, BMA

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		
Chain		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.25	0/3405	0.43	0/4641	
1	С	0.25	0/3387	0.42	0/4614	
All	All	0.25	0/6792	0.42	0/9255	

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	3334	0	3196	7	0
1	С	3313	0	3172	13	0
2	В	70	0	60	2	0
2	D	70	0	60	3	0
All	All	6787	0	6488	20	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.

The worst 5 of 20 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:243:GLN:OE1	2:B:1:NAG:O1	2.00	0.79
1:C:243:GLN:OE1	2:D:1:NAG:O1	2.05	0.75
1:C:162:ASP:OD2	1:C:166:LYS:NZ	2.31	0.58
1:C:363:ARG:NH2	1:C:461:GLY:O	2.37	0.58
1:C:243:GLN:NE2	2:D:1:NAG:H83	2.22	0.54

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	Percentile	S
1	A	423/435 (97%)	411 (97%)	12 (3%)	0	100 100	)
1	С	421/435 (97%)	410 (97%)	11 (3%)	0	100 100	)
All	All	844/870 (97%)	821 (97%)	23 (3%)	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	Outliers	Percentiles		
1	A	348/367 (95%)	347 (100%)	1 (0%)	92	98	
1	$\mathbf{C}$	345/367~(94%)	342 (99%)	3 (1%)	78	92	
All	All	693/734 (94%)	689 (99%)	4 (1%)	86	95	



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

Mol	Chain	Res	Type
1	A	221	ASP
1	С	157	THR
1	С	300	ARG
1	С	363	ARG

Sometimes 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)

12 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).

Mal	Mol Type Chain Re		Res	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	В	1	2	15,15,15	0.18	0	21,21,21	0.48	0
2	BMA	В	2	2	11,11,12	0.37	0	15,15,17	0.49	0
2	MAN	В	3	2	11,11,12	0.40	0	15,15,17	0.44	0
2	MAN	В	4	2	11,11,12	0.36	0	15,15,17	0.38	0
2	MAN	В	5	2	11,11,12	0.39	0	15,15,17	0.25	0
2	MAN	В	6	2	11,11,12	0.37	0	15,15,17	0.35	0
2	NAG	D	1	2	15,15,15	0.22	0	21,21,21	0.49	0
2	BMA	D	2	2	11,11,12	0.36	0	15,15,17	0.53	0
2	MAN	D	3	2	11,11,12	0.37	0	15,15,17	0.41	0
2	MAN	D	4	2	11,11,12	0.33	0	15,15,17	0.46	0
2	MAN	D	5	2	11,11,12	0.38	0	15,15,17	0.27	0



1/1/	Mol Type Chain		Res	Res Link Bond le		ond leng	gths Bond angles		les		
1010	wioi Type Chair	Chain		) LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
2		MAN	D	6	2	11,11,12	0.39	0	15,15,17	0.30	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	NAG	В	1	2	-	3/6/26/26	0/1/1/1
2	BMA	В	2	2	-	0/2/19/22	0/1/1/1
2	MAN	В	3	2	-	0/2/19/22	0/1/1/1
2	MAN	В	4	2	-	0/2/19/22	0/1/1/1
2	MAN	В	5	2	-	0/2/19/22	0/1/1/1
2	MAN	В	6	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	2	-	2/6/26/26	0/1/1/1
2	BMA	D	2	2	-	0/2/19/22	0/1/1/1
2	MAN	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	MAN	D	5	2	-	0/2/19/22	0/1/1/1
2	MAN	D	6	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	1	NAG	O5-C5-C6-O6
2	D	6	MAN	O5-C5-C6-O6
2	D	1	NAG	C3-C2-N2-C7
2	В	1	NAG	C1-C2-N2-C7
2	D	1	NAG	C1-C2-N2-C7

There are no ring outliers.

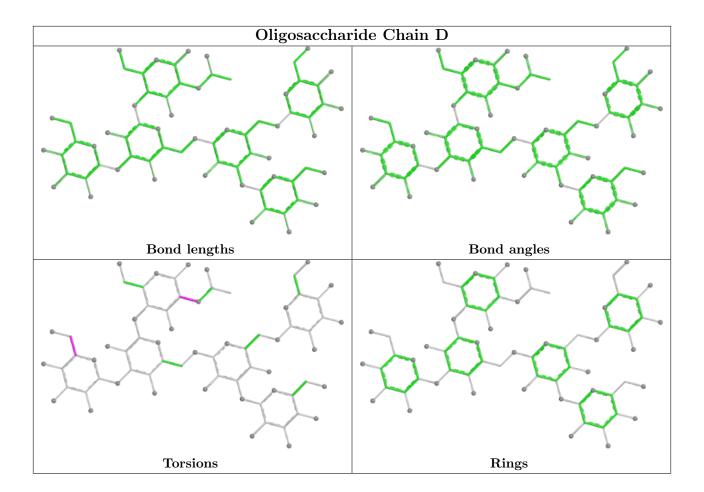
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	2	0
2	D	6	MAN	1	0
2	В	1	NAG	2	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 (i)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

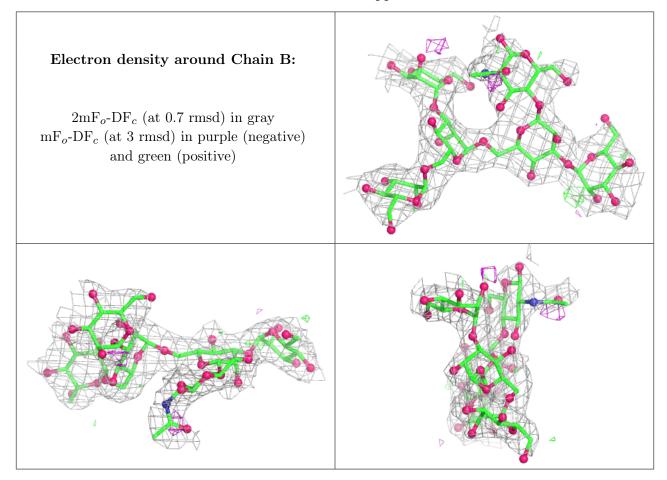
#### 6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

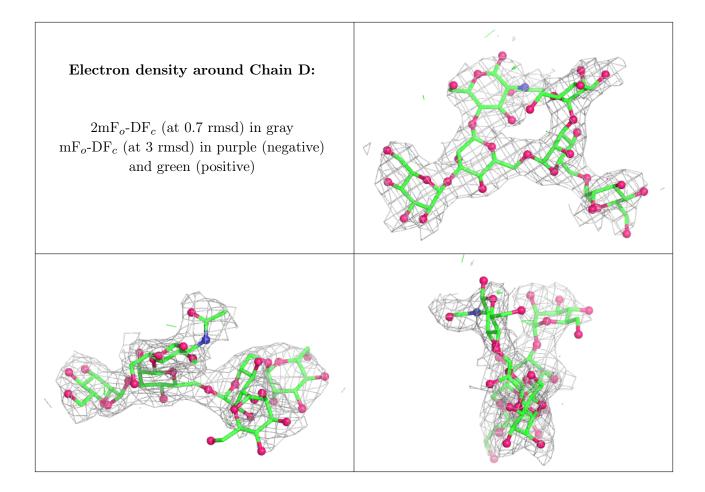
### 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

