

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

#### Oct 30, 2021 – 01:07 pm BST

PDB ID : 6Z2P

Title : Crystal structure of catalytic inactive OgpA from Akkermansia muciniphila in

complex with an O-glycopeptide (glycodrosocin) substrate

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Deposited on : 2020-05-18

Resolution : 2.16 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*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: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.23.2

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

Refmac : 5.8.0267

CCP4 : 7.1.010 (Gargrove) Ideal geometry (proteins) : Engh & Huber (2001)

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

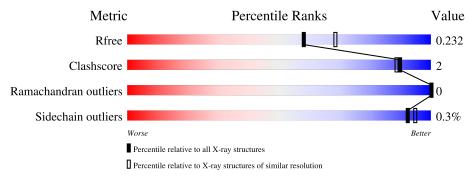
Validation Pipeline (wwPDB-VP) : 2.23.2

# 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 2.16 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
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)

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 ch	nain	
1	A	371		92%		
2	С	19	37%	16%	47%	
3	В	2	50%		50%	



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2913 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 O-glycan protease.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	356	Total	С	N	О	S	0	9	0
1	A	350	2783	1778	478	516	11	0	2	

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	=	initiating methionine	UNP B2UR60
A	205	ALA	HIS	engineered mutation	UNP B2UR60
A	206	ALA	GLU	engineered mutation	UNP B2UR60
A	386	GLY	-	expression tag	UNP B2UR60
A	387	SER	-	expression tag	UNP B2UR60
A	388	GLY	-	expression tag	UNP B2UR60
A	389	HIS	-	expression tag	UNP B2UR60
A	390	HIS	-	expression tag	UNP B2UR60
A	391	HIS	-	expression tag	UNP B2UR60
A	392	HIS	-	expression tag	UNP B2UR60
A	393	HIS	-	expression tag	UNP B2UR60
A	394	HIS	-	expression tag	UNP B2UR60

• Molecule 2 is a protein called Glycodrosocin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	С	10	Total 66	C 40	N 13	O 13	0	0	0

• Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-a lpha-D-galactopyranose.





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
3	В	2	Total 25	C 14	N 1	O 10	0	0	0

 $\bullet$  Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0

• Molecule 5 is water.

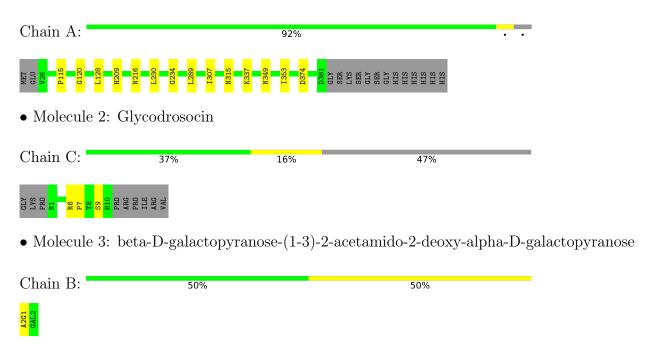
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	37	Total O 37 37	0	0
5	C	1	Total O 1 1	0	0



# 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.

• Molecule 1: O-glycan protease





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants	126.92Å 126.92Å 65.54Å	Domositon
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	44.87 - 2.16	Depositor
Resolution (A)	44.87 - 2.16	EDS
% Data completeness	96.8 (44.87-2.16)	Depositor
(in resolution range)	99.1 (44.87-2.16)	EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.15 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
D.D.	0.199 , 0.232	Depositor
$R, R_{free}$	0.199 , $0.232$	DCC
$R_{free}$ test set	1393 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.0	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2913	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	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.

<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: CA, A2G, GAL

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	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.43	0/2859	0.56	0/3877	
2	С	1.01	0/68	1.15	0/94	
All	All	0.45	0/2927	0.58	0/3971	

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	2783	0	2647	10	0
2	С	66	0	58	3	0
3	В	25	0	21	0	0
4	A	1	0	0	0	0
5	A	37	0	0	0	0
5	C	1	0	0	0	0
All	All	2913	0	2726	10	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.

All (10) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom-1	Atom-2	Interatomic	Clash
1100111 1	1100111 2	$\operatorname{distance}\left(\mathrm{\AA}\right)$	overlap (Å)
1:A:315:ASN:OD1	2:C:7:PRO:HD2	1.90	0.71
1:A:115:PRO:O	1:A:120:GLY:HA3	2.05	0.57
1:A:289[B]:LEU:HD13	1:A:337:LYS:HD3	1.89	0.54
1:A:209:HIS:ND1	2:C:6:ARG:HD3	2.29	0.48
1:A:216[B]:ASN:C	1:A:216[B]:ASN:HD22	2.19	0.46
1:A:230:LEU:HA	1:A:234:GLY:HA3	2.00	0.44
1:A:349:ASN:HB3	1:A:374:ASP:OD1	2.17	0.44
1:A:315:ASN:OD1	2:C:7:PRO:CD	2.65	0.42
1:A:128:LEU:HD23	1:A:128:LEU:HA	1.90	0.41
1:A:307:ILE:HG12	1:A:353:ILE:HG12	2.03	0.41

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	Perce	ntiles
1	A	356/371~(96%)	346 (97%)	10 (3%)	0	100	100
2	$\mathbf{C}$	8/19 (42%)	8 (100%)	0	0	100	100
All	All	364/390 (93%)	354 (97%)	10 (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	Perce	ntiles
1	A	284/309 (92%)	284 (100%)	0	100	100
2	C	7/18 (39%)	6 (86%)	1 (14%)	3	1
All	All	291/327 (89%)	290 (100%)	1 (0%)	92	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type	
2	С	9	SER	

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type	
1	A	160	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)

2 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	Tuno	Chain	Res	Link	Во	ond leng	$ ag{ths}$	В	ond ang	les
MOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
3	A2G	В	1	2,3	14,14,15	0.16	0	17,19,21	0.80	1 (5%)
3	GAL	В	2	3	11,11,12	0.36	0	15,15,17	0.29	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
3	A2G	В	1	2,3	-	0/6/23/26	0/1/1/1
3	GAL	В	2	3	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	В	1	A2G	O3-C3-C2	-2.59	104.10	109.47

There are no chirality outliers.

All (1) torsion outliers are listed below:

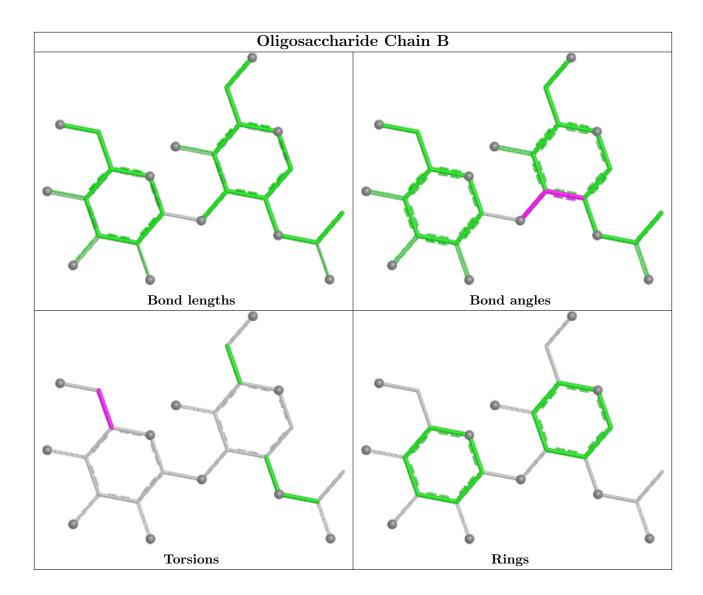
Mol	Chain	Res	Type	Atoms
3	В	2	GAL	O5-C5-C6-O6

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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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)

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

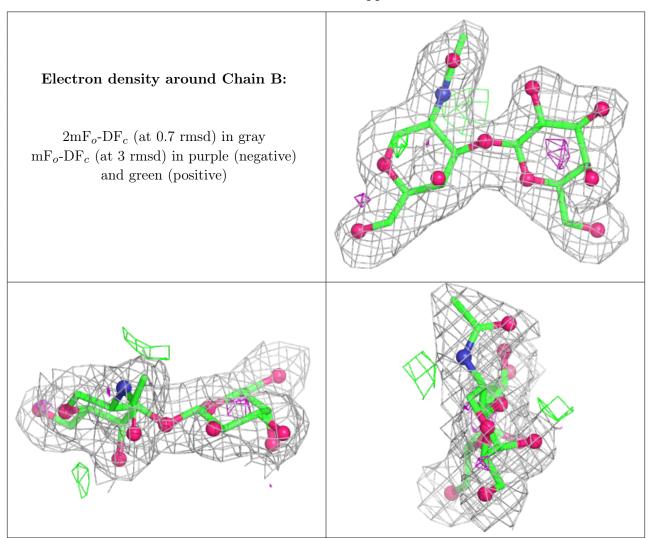
### 6.2 Non-standard residues in protein, DNA, RNA chains (i)

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.

