Full wwPDB X-ray Structure Validation Report (i)

Sep 27, 2023 – 01:31 AM EDT

PDB ID : 6CA3

Title : THE CRYSTAL STRUCTURE OF THE W169Y MUTANT OF ALPHA-GLUCOSIDASE (GH 31) FROM RUMINOCOCCUS OBEUM ATCC 29174 in complex with miglitol

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Deposited on : 2018-01-29

Resolution : 1.74 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

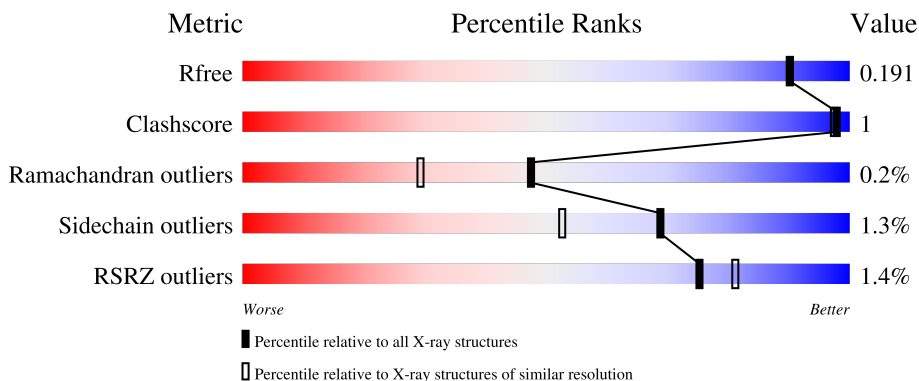|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.74 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	Percentile Ranks	Value
Rfree		0.191
Clashscore		1
Ramachandran outliers		0.2%
Sidechain outliers		1.3%
RSRZ outliers		1.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	666	% ▮ 96% ▮ ・
1	B	666	2% ▮ 97% ▮ ・

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 11920 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.
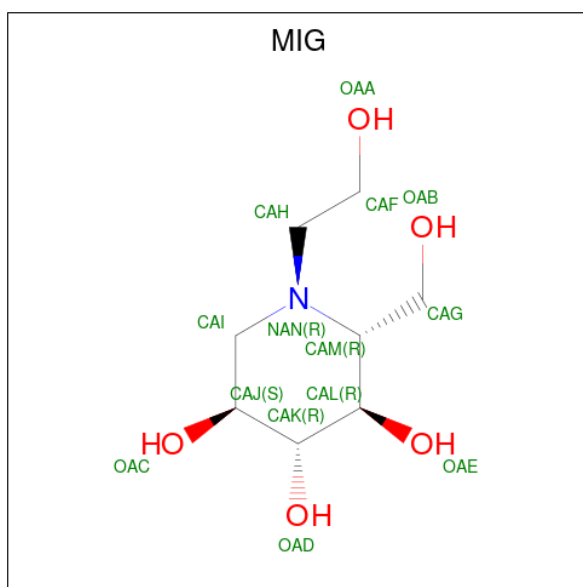
- Molecule 1 is a protein called Glycosyl hydrolase, family 31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	1	0
			5401	3472	883	1011	35			
1	B	665	Total	C	N	O	S	0	2	0
			5401	3476	884	1006	35			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A5ZY13
A	-1	ASN	-	expression tag	UNP A5ZY13
A	0	ALA	-	expression tag	UNP A5ZY13
A	169	TYR	TRP	engineered mutation	UNP A5ZY13
B	-2	SER	-	expression tag	UNP A5ZY13
B	-1	ASN	-	expression tag	UNP A5ZY13
B	0	ALA	-	expression tag	UNP A5ZY13
B	169	TYR	TRP	engineered mutation	UNP A5ZY13

- Molecule 2 is (2R,3R,4R,5S)-1-(2-hydroxyethyl)-2-(hydroxymethyl)piperidine-3,4,5-triol (three-letter code: MIG) (formula: $C_8H_{17}NO_5$).

MIG

OAA
OH

CAH　　CAF OAB
　　　　OH

CAI
　　N
　　NAN(R)　　CAG
　　CAM(R)

CAJ(S)　CAL(R)
　CAK(R)

HO　　　　OH
OAC　　　　OAE

OH
OAD

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3
　　OH O3

C1　　C2

HO　　　OH
O1　　　O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	542	Total O 542 542	0	0
4	B	542	Total O 542 542	0	0

# 3 Residue-property plots ⓘ

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: Glycosyl hydrolase, family 31

Chain A:

• Molecule 1: Glycosyl hydrolase, family 31

Chain B:
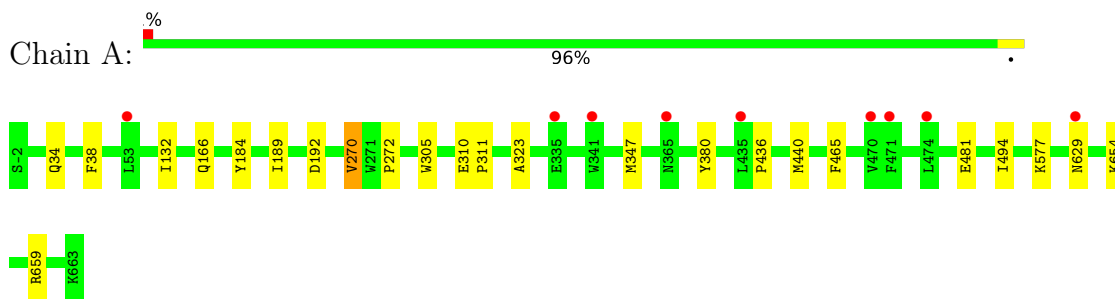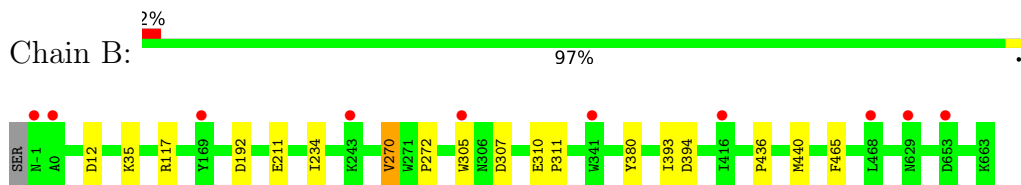
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	64.69Å　　70.83Å　　88.10Å 111.32°　　107.42°　　97.66°	Depositor
Resolution (Å)	31.74　–　1.74 31.74　–　1.74	Depositor EDS
% Data completeness (in resolution range)	96.0 (31.74-1.74) 96.0 (31.74-1.74)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 1.74Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.153　,　0.191 0.154　,　0.191	Depositor DCC
R_{free} test set	6605 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.5	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	11920	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]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.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MIG

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	0.34	0/5548	0.52	0/7492
1	B	0.34	0/5551	0.52	0/7494
All	All	0.34	0/11099	0.52	0/14986

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 ⓘ

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	5401	0	5116	9	0
1	B	5401	0	5126	6	0
2	A	14	0	16	0	0
2	B	14	0	16	0	0
3	A	6	0	8	0	0
4	A	542	0	0	2	0
4	B	542	0	0	1	0
All	All	11920	0	10282	15	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 1.

All (15) 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:B:270:VAL:HG23	1:B:272:PRO:HD2	1.78	0.64
1:B:35:LYS:NZ	4:B:805:HOH:O	2.38	0.57
1:B:393:ILE:HG22	1:B:394:ASP:HB2	1.87	0.56
1:A:270:VAL:HG23	1:A:272:PRO:HD2	1.88	0.55
1:A:577:LYS:NZ	4:A:803:HOH:O	2.39	0.54
1:A:310:GLU:N	1:A:311:PRO:HA	2.23	0.53
1:A:38:PHE:CZ	1:A:132:ILE:HD11	2.45	0.52
1:B:436:PRO:O	1:B:440:MET:HG3	2.13	0.48
1:A:481:GLU:HG2	4:A:1252:HOH:O	2.14	0.47
1:A:189:ILE:HD11	1:A:494:ILE:HD11	1.96	0.47
1:B:310:GLU:N	1:B:311:PRO:HA	2.31	0.45
1:A:436:PRO:O	1:A:440:MET:HG3	2.19	0.42
1:A:166:GLN:NE2	1:A:184:TYR:OH	2.50	0.42
1:A:323:ALA:HB1	1:A:347:MET:CE	2.50	0.42
1:B:234:ILE:HD11	1:B:307:ASP:CB	2.49	0.42

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	665/666 (100%)	637 (96%)	26 (4%)	2 (0%)	41	23
1	B	665/666 (100%)	637 (96%)	27 (4%)	1 (0%)	47	29
All	All	1330/1332 (100%)	1274 (96%)	53 (4%)	3 (0%)	47	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	629	ASN

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Mol	Chain	Res	Type
1	A	270	VAL
1	B	270	VAL

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	558/575 (97%)	551 (99%)	7 (1%)	69	52
1	B	556/575 (97%)	549 (99%)	7 (1%)	69	52
All	All	1114/1150 (97%)	1100 (99%)	14 (1%)	69	52

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	192	ASP
1	A	305	TRP
1	A	380	TYR
1	A	465	PHE
1	A	654	LYS
1	A	659	ARG
1	B	12	ASP
1	B	117	ARG
1	B	192	ASP
1	B	211	GLU
1	B	305	TRP
1	B	380	TYR
1	B	465	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	B	550	ASN

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	MIG	A	701	-	14,14,14	1.40	1 (7%)	17,19,19	1.47	3 (17%)
3	GOL	A	702	-	5,5,5	0.36	0	5,5,5	0.24	0
2	MIG	B	701	-	14,14,14	1.35	1 (7%)	17,19,19	1.40	3 (17%)

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	MIG	A	701	-	-	1/5/25/25	0/1/1/1
3	GOL	A	702	-	-	2/4/4/4	-
2	MIG	B	701	-	-	1/5/25/25	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	MIG	CAJ-CAK	-3.87	1.46	1.52
2	B	701	MIG	CAJ-CAK	-3.46	1.47	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	MIG	CAH-NAN-CAM	3.30	122.13	113.29
2	B	701	MIG	CAH-NAN-CAM	2.90	121.06	113.29
2	A	701	MIG	CAI-CAJ-CAK	2.49	113.08	110.24
2	B	701	MIG	CAI-NAN-CAM	2.27	114.95	109.69
2	B	701	MIG	OAB-CAG-CAM	2.04	115.79	111.42
2	A	701	MIG	OAA-CAF-CAH	2.00	119.48	111.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	GOL	C1-C2-C3-O3
3	A	702	GOL	O2-C2-C3-O3
2	B	701	MIG	OAA-CAF-CAH-NAN
2	A	701	MIG	OAA-CAF-CAH-NAN

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 ⓘ

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, 95th 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(Å²)	Q<0.9
1	A	666/666 (100%)	-0.30	9 (1%)	75	81	18, 27, 43, 79	0
1	B	665/666 (99%)	-0.17	10 (1%)	73	80	16, 27, 44, 81	0
All	All	1331/1332 (99%)	-0.24	19 (1%)	75	81	16, 27, 44, 81	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	629	ASN	4.6
1	B	0	ALA	3.8
1	B	341[A]	TRP	3.3
1	A	341[A]	TRP	3.2
1	B	-1	ASN	3.2
1	B	653	ASP	2.7
1	A	365	ASN	2.7
1	B	416	ILE	2.6
1	A	53	LEU	2.6
1	A	435	LEU	2.6
1	B	243	LYS	2.5
1	A	335	GLU	2.5
1	B	629	ASN	2.3
1	A	471	PHE	2.3
1	A	470	VAL	2.2
1	B	169	TYR	2.1
1	B	468	LEU	2.1
1	A	474	LEU	2.1
1	B	305	TRP	2.1

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th 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^2)	Q<0.9
3	GOL	A	702	6/6	0.91	0.15	35,46,50,51	0
2	MIG	B	701	14/14	0.95	0.08	23,25,35,44	0
2	MIG	A	701	14/14	0.95	0.07	20,24,34,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.