



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:48 PM GMT

PDB ID : 4AK6  
Title : BpGH117\_H302E mutant glycoside hydrolase  
Authors : Hehemann, J.H.; Smyth, L.; Yadav, A.; Vocadlo, D.J.; Boraston, A.B.  
Deposited on : 2012-02-21  
Resolution : 1.90 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

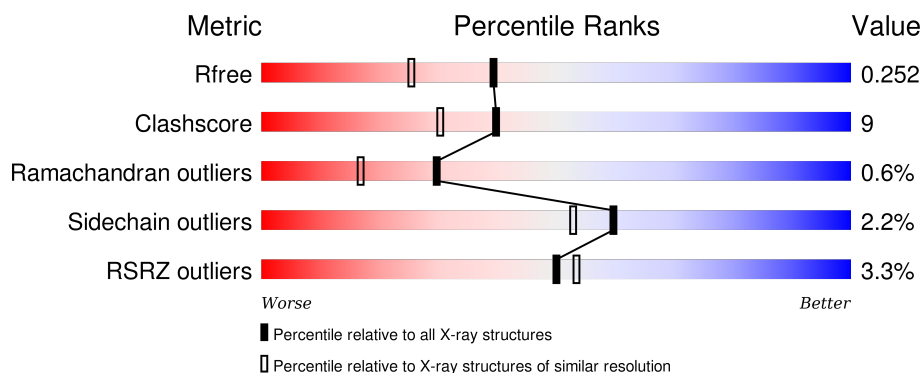
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 1.90 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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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. 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	404	 4% 76% 14% 9%
1	B	404	 2% 73% 15% 10%

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	MG	A	1402	-	-	-	X
2	MG	B	1398	-	-	-	X
2	MG	B	1399	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6199 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 ANHYDRO-ALPHA-L-GALACTOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	13	3	0
			2925	1862	489	557	17			
1	B	362	Total	C	N	O	S	13	1	0
			2861	1821	474	550	16			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP B5CY74
A	0	GLY	-	EXPRESSION TAG	UNP B5CY74
A	1	SER	-	EXPRESSION TAG	UNP B5CY74
A	2	SER	-	EXPRESSION TAG	UNP B5CY74
A	3	HIS	-	EXPRESSION TAG	UNP B5CY74
A	4	HIS	-	EXPRESSION TAG	UNP B5CY74
A	5	HIS	-	EXPRESSION TAG	UNP B5CY74
A	6	HIS	-	EXPRESSION TAG	UNP B5CY74
A	7	HIS	-	EXPRESSION TAG	UNP B5CY74
A	8	HIS	-	EXPRESSION TAG	UNP B5CY74
A	9	SER	-	EXPRESSION TAG	UNP B5CY74
A	10	SER	-	EXPRESSION TAG	UNP B5CY74
A	11	GLY	-	EXPRESSION TAG	UNP B5CY74
A	12	LEU	-	EXPRESSION TAG	UNP B5CY74
A	13	VAL	-	EXPRESSION TAG	UNP B5CY74
A	14	PRO	-	EXPRESSION TAG	UNP B5CY74
A	15	ARG	-	EXPRESSION TAG	UNP B5CY74
A	16	GLY	-	EXPRESSION TAG	UNP B5CY74
A	17	SER	-	EXPRESSION TAG	UNP B5CY74
A	18	HIS	-	EXPRESSION TAG	UNP B5CY74
A	19	MET	-	EXPRESSION TAG	UNP B5CY74
A	20	ALA	-	EXPRESSION TAG	UNP B5CY74
A	21	SER	-	EXPRESSION TAG	UNP B5CY74
A	302	GLU	HIS	ENGINEERED MUTATION	UNP B5CY74
B	-1	MET	-	EXPRESSION TAG	UNP B5CY74

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	EXPRESSION TAG	UNP B5CY74
B	1	SER	-	EXPRESSION TAG	UNP B5CY74
B	2	SER	-	EXPRESSION TAG	UNP B5CY74
B	3	HIS	-	EXPRESSION TAG	UNP B5CY74
B	4	HIS	-	EXPRESSION TAG	UNP B5CY74
B	5	HIS	-	EXPRESSION TAG	UNP B5CY74
B	6	HIS	-	EXPRESSION TAG	UNP B5CY74
B	7	HIS	-	EXPRESSION TAG	UNP B5CY74
B	8	HIS	-	EXPRESSION TAG	UNP B5CY74
B	9	SER	-	EXPRESSION TAG	UNP B5CY74
B	10	SER	-	EXPRESSION TAG	UNP B5CY74
B	11	GLY	-	EXPRESSION TAG	UNP B5CY74
B	12	LEU	-	EXPRESSION TAG	UNP B5CY74
B	13	VAL	-	EXPRESSION TAG	UNP B5CY74
B	14	PRO	-	EXPRESSION TAG	UNP B5CY74
B	15	ARG	-	EXPRESSION TAG	UNP B5CY74
B	16	GLY	-	EXPRESSION TAG	UNP B5CY74
B	17	SER	-	EXPRESSION TAG	UNP B5CY74
B	18	HIS	-	EXPRESSION TAG	UNP B5CY74
B	19	MET	-	EXPRESSION TAG	UNP B5CY74
B	20	ALA	-	EXPRESSION TAG	UNP B5CY74
B	21	SER	-	EXPRESSION TAG	UNP B5CY74
B	302	GLU	HIS	ENGINEERED MUTATION	UNP B5CY74

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Mg 3 3	0	0
2	A	2	Total Mg 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	222	Total O 222 222	0	0
3	B	186	Total O 186 186	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.26Å 96.55Å 103.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.28 – 1.90 35.29 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.28-1.90) 99.8 (35.29-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.81 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.216 , 0.252 0.215 , 0.252	Depositor DCC
$R_{free}$ test set	3436 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 67773 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6199	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG

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	0.56	5/3014 (0.2%)	0.56	3/4090 (0.1%)
1	B	1.38	5/2946 (0.2%)	0.64	6/4002 (0.1%)
All	All	1.05	10/5960 (0.2%)	0.60	9/8092 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	223	GLU	CD-OE2	-48.78	0.71	1.25
1	B	223	GLU	CD-OE1	47.82	1.78	1.25
1	B	226	GLU	CD-OE1	-13.65	1.10	1.25
1	A	129	ARG	CD-NE	13.21	1.69	1.46
1	B	211	LYS	CD-CE	-11.88	1.21	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	GLU	CG-CD-OE2	15.99	150.29	118.30
1	B	223	GLU	CG-CD-OE1	-11.57	95.17	118.30
1	A	77	LYS	CD-CE-NZ	-11.12	86.13	111.70
1	B	226	GLU	OE1-CD-OE2	11.05	136.56	123.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ARG	CG-CD-NE	-10.87	88.97	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	265	GLY	Peptide
1	B	37	ARG	Peptide
1	B	40	ASP	Peptide

## 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	2925	0	2741	54	0
1	B	2861	0	2669	52	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
3	A	222	0	0	4	0
3	B	186	0	0	1	0
All	All	6199	0	5410	98	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 9.

The worst 5 of 98 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:A:294:TYR:CZ	1:B:49:LYS:HD2	2.01	0.96
1:A:294:TYR:CE1	1:B:49:LYS:HD2	2.07	0.89
1:A:235:LYS:HG2	1:A:263:ARG:CZ	2.07	0.85
1:A:246:PRO:HB3	1:A:257:MET:HE3	1.61	0.81
1:A:222:TRP:CZ3	1:A:229:ARG:HA	2.16	0.80

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	369/404 (91%)	352 (95%)	16 (4%)	1 (0%)	46	35
1	B	361/404 (89%)	347 (96%)	11 (3%)	3 (1%)	24	11
All	All	730/808 (90%)	699 (96%)	27 (4%)	4 (0%)	30	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	PRO
1	B	40	ASP
1	B	38	LYS
1	B	302	GLU

### 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	301/344 (88%)	295 (98%)	6 (2%)	63	57
1	B	295/344 (86%)	288 (98%)	7 (2%)	57	49
All	All	596/688 (87%)	583 (98%)	13 (2%)	60	53

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	ASN
1	B	59	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	205	LEU
1	A	241	HIS
1	B	186	TYR

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

Mol	Chain	Res	Type
1	B	146	GLN

### 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](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are 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 ⓘ

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<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	368/404 (91%)	0.31	15 (4%) 41 45	17, 31, 48, 61	8 (2%)
1	B	362/404 (89%)	0.19	9 (2%) 61 64	17, 28, 49, 62	8 (2%)
All	All	730/808 (90%)	0.25	24 (3%) 50 53	17, 29, 48, 62	16 (2%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	396	GLY	5.1
1	B	50	LEU	4.4
1	A	398	SER	4.3
1	A	217	SER	4.1
1	A	304	VAL	3.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	B	1398	1/1	0.99	0.39	10.11	40,40,40,40	0
2	MG	A	1402	1/1	0.94	0.34	5.77	35,35,35,35	0
2	MG	B	1399	1/1	0.98	0.23	2.75	17,17,17,17	0
2	MG	A	1399	1/1	0.99	0.17	0.06	17,17,17,17	0
2	MG	B	1400	1/1	0.87	0.25	-	50,50,50,50	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.