



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 26, 2017 – 04:04 PM EDT

PDB ID : 3LPG  
Title : Structure of E. coli beta-Glucuronidase bound with a novel, potent inhibitor 3-(2-fluorophenyl)-1-(2-hydroxyethyl)-1-((6-methyl-2-oxo-1,2-dihydroquinolin-3-yl)methyl)urea  
Authors : Wallace, B.D.; Redinbo, M.R.  
Deposited on : unknown  
Resolution : 2.42 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.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

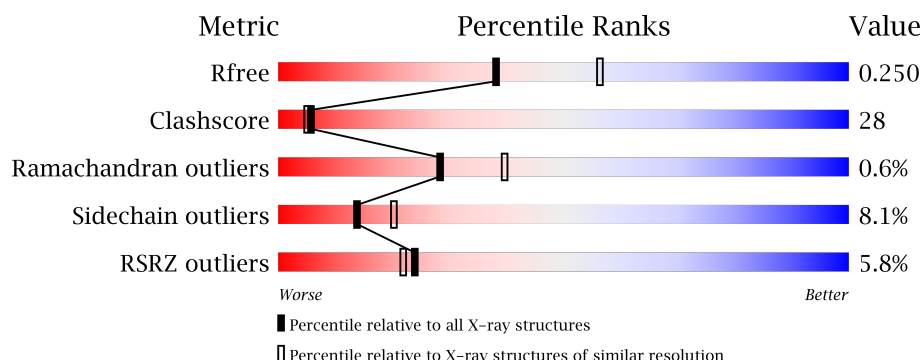
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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))
$R_{free}$	100719	3709 (2.44-2.40)
Clashscore	112137	4241 (2.44-2.40)
Ramachandran outliers	110173	4178 (2.44-2.40)
Sidechain outliers	110143	4179 (2.44-2.40)
RSRZ outliers	101464	3740 (2.44-2.40)

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	605	<div> <div>3%</div> <div>55%</div> <div>37%</div> <div>7%</div> </div>
1	B	605	<div> <div>9%</div> <div>54%</div> <div>36%</div> <div>8%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10067 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.

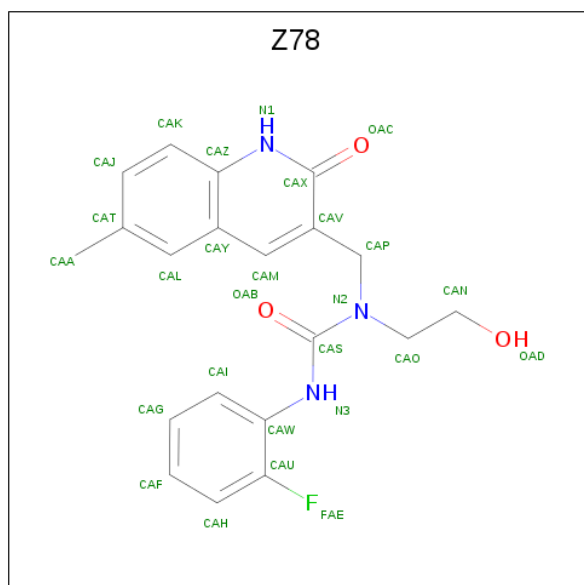
- Molecule 1 is a protein called Beta-glucuronidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	603	Total	C	N	O	S	Se	0	0	0
			4826	3063	834	907	9	13			
1	B	603	Total	C	N	O	S	Se	0	0	0
			4829	3066	834	907	9	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP P05804
A	0	HIS	-	EXPRESSION TAG	UNP P05804
B	-1	SER	-	EXPRESSION TAG	UNP P05804
B	0	HIS	-	EXPRESSION TAG	UNP P05804

- Molecule 2 is 3-(2-fluorophenyl)-1-(2-hydroxyethyl)-1-[(6-methyl-2-oxo-1,2-dihydroquinolin-3-yl)methyl]urea (three-letter code: Z78) (formula: C<sub>20</sub>H<sub>20</sub>FN<sub>3</sub>O<sub>3</sub>).

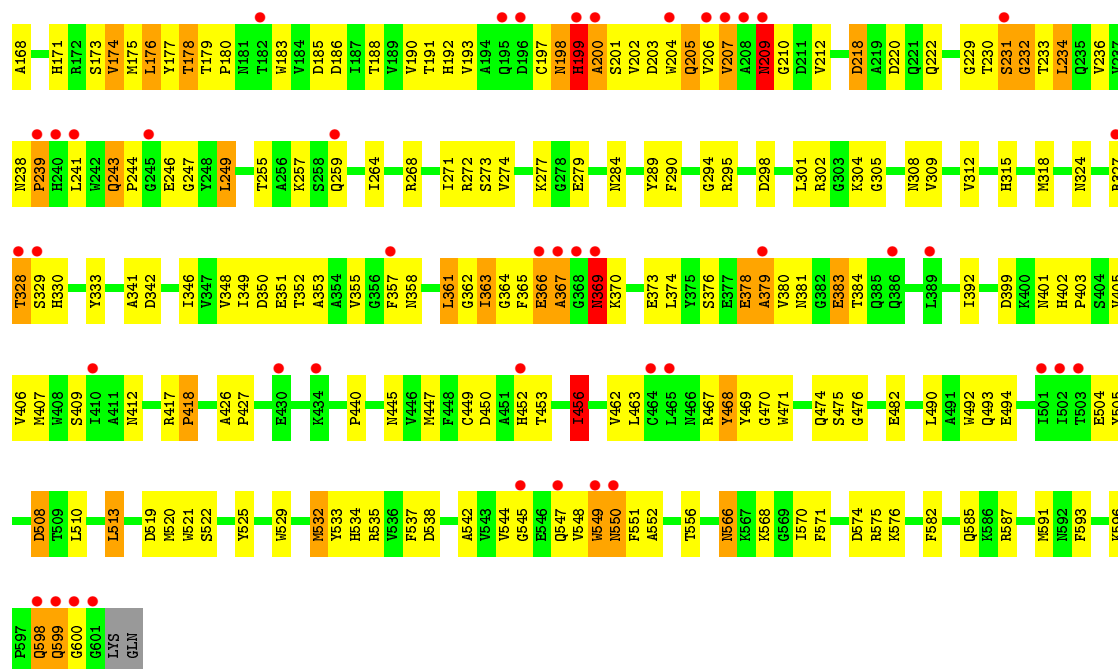


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			27	20	1	3	3		
2	B	1	Total	C	F	N	O	0	0
			27	20	1	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	240	Total	O	0	0
			240	240		
3	B	118	Total	O	0	0
			118	118		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.81Å 76.93Å 125.81Å 90.00° 124.75° 90.00°	Depositor
Resolution (Å)	30.86 – 2.42 30.86 – 2.42	Depositor EDS
% Data completeness (in resolution range)	89.5 (30.86-2.42) 98.0 (30.86-2.42)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.42Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.204 , 0.246 0.214 , 0.250	Depositor DCC
$R_{free}$ test set	2487 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.0	Xtriage
Anisotropy	0.736	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10067	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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: Z78

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	0.36	1/4943 (0.0%)	0.95	44/6704 (0.7%)
1	B	0.28	0/4946	1.12	59/6708 (0.9%)
All	All	0.32	1/9889 (0.0%)	1.04	103/13412 (0.8%)

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	1	2
1	B	1	2
All	All	2	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	PRO	N-CD	5.21	1.55	1.47

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	ALA	CB-CA-C	-22.81	75.89	110.10
1	B	6	GLU	N-CA-C	17.13	157.26	111.00
1	B	15	LEU	CB-CA-C	-16.52	78.81	110.20
1	B	367	ALA	CB-CA-C	-16.27	85.69	110.10
1	A	551	PHE	N-CA-CB	-16.19	81.46	110.60

All (2) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
1	A	231	SER	CA
1	B	18	LEU	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	ILE	Peptide
1	A	47	VAL	Peptide
1	B	369	ASN	Peptide
1	B	47	VAL	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	4826	0	4604	291	0
1	B	4829	0	4613	250	1
2	A	27	0	19	2	0
2	B	27	0	18	3	0
3	A	240	0	0	21	1
3	B	118	0	0	6	0
All	All	10067	0	9254	532	1

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 28.

The worst 5 of 532 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:15:LEU:HD12	1:A:173:SER:CB	1.77	1.13
1:B:482:GLU:HB2	1:B:532:MSE:HE1	1.20	1.10
1:A:108:GLN:HG3	1:A:108:GLN:O	1.31	1.06
1:B:209:ASN:O	1:B:209:ASN:ND2	1.91	1.03
1:B:361:LEU:O	2:B:604:Z78:OAC	1.77	1.03

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:GLU:OE1	3:A:839:HOH:O[2_555]	1.87	0.33

## 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	601/605 (99%)	575 (96%)	23 (4%)	3 (0%)	32	45
1	B	601/605 (99%)	566 (94%)	31 (5%)	4 (1%)	25	35
All	All	1202/1210 (99%)	1141 (95%)	54 (4%)	7 (1%)	28	40

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	PRO
1	A	144	PRO
1	B	48	PRO
1	A	8	PRO
1	B	144	PRO

### 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	510/500 (102%)	468 (92%)	42 (8%)	13	20
1	B	511/500 (102%)	470 (92%)	41 (8%)	14	21
All	All	1021/1000 (102%)	938 (92%)	83 (8%)	14	20

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	544	VAL
1	B	47	VAL
1	B	532	MSE
1	A	550	ASN
1	B	16	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	585	GLN
1	B	93	HIS
1	B	419	GLN
1	A	599	GLN
1	B	52	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 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	Z78	A	604	-	28,29,29	3.72	14 (50%)	36,40,40	3.10	11 (30%)
2	Z78	B	604	-	28,29,29	3.72	14 (50%)	36,40,40	3.10	11 (30%)

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	Z78	A	604	-	-	0/15/15/15	0/3/3/3
2	Z78	B	604	-	-	0/15/15/15	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	604	Z78	OAD-CAN	-4.34	1.19	1.42
2	A	604	Z78	OAD-CAN	-4.33	1.19	1.42
2	B	604	Z78	OAB-CAS	-2.04	1.19	1.23
2	A	604	Z78	CAP-CAV	2.06	1.55	1.51
2	A	604	Z78	CAL-CAT	2.11	1.41	1.37

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	604	Z78	CAV-CAX-N1	-4.65	119.92	125.16
2	B	604	Z78	CAV-CAX-N1	-3.69	121.00	125.16
2	A	604	Z78	OAB-CAS-N3	-3.28	117.63	124.24
2	A	604	Z78	CAP-N2-CAO	-3.21	108.80	116.57
2	B	604	Z78	OAB-CAS-N3	-3.12	117.95	124.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	Z78	2	0
2	B	604	Z78	3	0

## 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](#)

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	590/605 (97%)	-0.14	16 (2%) 55 52	21, 49, 100, 132	0
1	B	590/605 (97%)	0.34	52 (8%) 11 9	34, 83, 157, 189	0
All	All	1180/1210 (97%)	0.10	68 (5%) 24 22	21, 66, 138, 189	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	209	ASN	8.1
1	B	601	GLY	6.5
1	A	368	GLY	6.2
1	A	231	SER	5.5
1	A	207	VAL	5.2

### 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	Z78	A	604	27/27	0.78	0.25	1.54	52,64,100,101	0
2	Z78	B	604	27/27	0.79	0.26	0.96	86,94,111,112	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.