



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 4, 2017 – 03:24 PM EST

PDB ID : 5GL5  
Title : Sterol 3-beta-glucosyltransferase (ugt51) from *Saccharomyces cerevisiae*  
(strain ATCC 204508 / S288c): UDPG complex  
Authors : Feng, Y.; Chen, L.-Q.  
Deposited on : 2016-07-08  
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.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

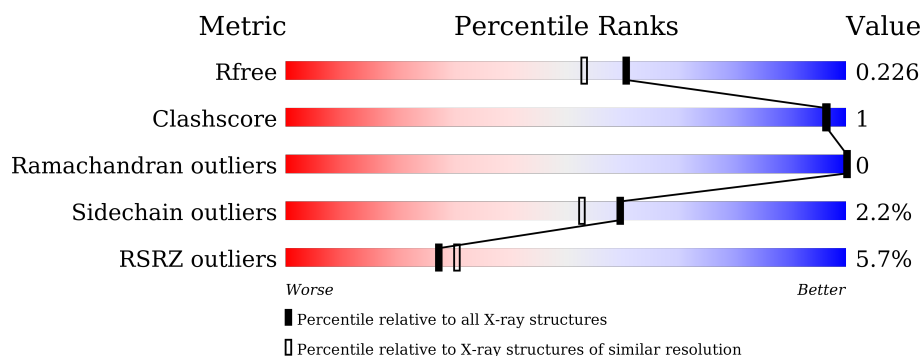
# 1 Overall quality at a glance ⓘ

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	498	<div> <div>7%</div> <div> <div></div> <div>81%</div> <div>6%</div> <div>13%</div> </div> </div>
1	B	498	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>6%</div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7204 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 Sterol 3-beta-glucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	1	0
			3427	2211	585	620	11			
1	B	431	Total	C	N	O	S	0	1	0
			3419	2206	583	619	11			

There are 42 discrepancies between the modelled and reference sequences:

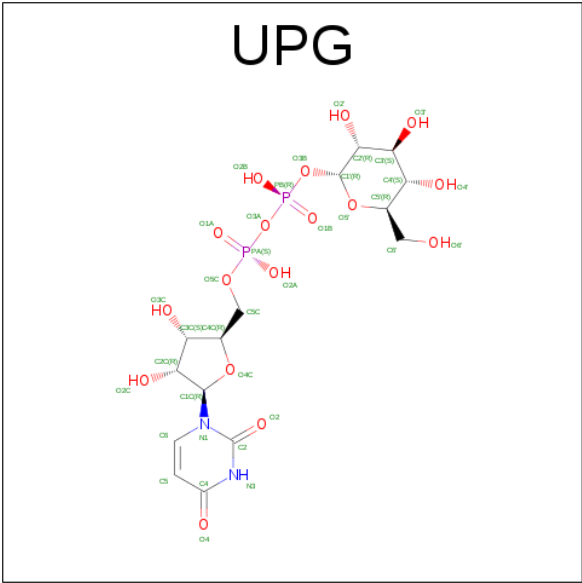
Chain	Residue	Modelled	Actual	Comment	Reference
A	701	MET	-	expression tag	UNP Q06321
A	702	GLY	-	expression tag	UNP Q06321
A	703	SER	-	expression tag	UNP Q06321
A	704	SER	-	expression tag	UNP Q06321
A	705	HIS	-	expression tag	UNP Q06321
A	706	HIS	-	expression tag	UNP Q06321
A	707	HIS	-	expression tag	UNP Q06321
A	708	HIS	-	expression tag	UNP Q06321
A	709	HIS	-	expression tag	UNP Q06321
A	710	HIS	-	expression tag	UNP Q06321
A	711	SER	-	expression tag	UNP Q06321
A	712	SER	-	expression tag	UNP Q06321
A	713	GLY	-	expression tag	UNP Q06321
A	714	LEU	-	expression tag	UNP Q06321
A	715	VAL	-	expression tag	UNP Q06321
A	716	PRO	-	expression tag	UNP Q06321
A	717	ARG	-	expression tag	UNP Q06321
A	718	GLY	-	expression tag	UNP Q06321
A	719	SER	-	expression tag	UNP Q06321
A	720	HIS	-	expression tag	UNP Q06321
A	721	MET	-	expression tag	UNP Q06321
B	701	MET	-	expression tag	UNP Q06321
B	702	GLY	-	expression tag	UNP Q06321
B	703	SER	-	expression tag	UNP Q06321
B	704	SER	-	expression tag	UNP Q06321

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Chain	Residue	Modelled	Actual	Comment	Reference
B	705	HIS	-	expression tag	UNP Q06321
B	706	HIS	-	expression tag	UNP Q06321
B	707	HIS	-	expression tag	UNP Q06321
B	708	HIS	-	expression tag	UNP Q06321
B	709	HIS	-	expression tag	UNP Q06321
B	710	HIS	-	expression tag	UNP Q06321
B	711	SER	-	expression tag	UNP Q06321
B	712	SER	-	expression tag	UNP Q06321
B	713	GLY	-	expression tag	UNP Q06321
B	714	LEU	-	expression tag	UNP Q06321
B	715	VAL	-	expression tag	UNP Q06321
B	716	PRO	-	expression tag	UNP Q06321
B	717	ARG	-	expression tag	UNP Q06321
B	718	GLY	-	expression tag	UNP Q06321
B	719	SER	-	expression tag	UNP Q06321
B	720	HIS	-	expression tag	UNP Q06321
B	721	MET	-	expression tag	UNP Q06321

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: C<sub>15</sub>H<sub>24</sub>N<sub>2</sub>O<sub>17</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	133	Total 133	O 133	0	0
3	B	153	Total 153	O 153	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.66 Å 80.56 Å 154.59 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.29 – 1.90 41.43 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.5 (77.29-1.90) 89.5 (41.43-1.90)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.16 (at 1.91 Å)	Xtriage
Refinement program	REFMAC 5.8.0157	Depositor
R, $R_{free}$	0.185 , 0.219 0.197 , 0.226	Depositor DCC
$R_{free}$ test set	3095 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7204	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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

### 5.1 Standard geometry

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

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	0.76	2/3507 (0.1%)	0.83	4/4744 (0.1%)
1	B	0.77	0/3500	0.86	4/4737 (0.1%)
All	All	0.76	2/7007 (0.0%)	0.84	8/9481 (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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1041	GLU	CD-OE1	5.41	1.31	1.25
1	A	739	SER	CB-OG	5.30	1.49	1.42

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	839	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	B	935	ASN	CB-CA-C	-7.67	95.06	110.40
1	B	839	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	1146	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	839	ARG	NE-CZ-NH1	6.03	123.31	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	B	1033	GLY	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	3427	0	3455	11	0
1	B	3419	0	3442	10	0
2	A	36	0	22	0	0
2	B	36	0	22	0	0
3	A	133	0	0	0	0
3	B	153	0	0	0	0
All	All	7204	0	6941	19	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.

The worst 5 of 19 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:802:LEU:HD21	1:A:806:ASN:HD22	1.60	0.66
1:A:1083:LEU:O	1:A:1085:THR:HG23	1.97	0.64
1:A:941:ASN:HB3	1:A:963:TRP:CE2	2.43	0.54
1:B:826:ASP:OD1	1:B:912:GLN:NE2	2.41	0.53
1:A:1015:VAL:O	1:A:1018:ALA:O	2.26	0.53

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	Percentiles	
1	A	428/498 (86%)	415 (97%)	13 (3%)	0	100	100
1	B	428/498 (86%)	418 (98%)	10 (2%)	0	100	100
All	All	856/996 (86%)	833 (97%)	23 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	369/427 (86%)	361 (98%)	8 (2%)	60	53
1	B	367/427 (86%)	359 (98%)	8 (2%)	60	53
All	All	736/854 (86%)	720 (98%)	16 (2%)	60	53

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1134	ARG
1	B	801	SER
1	B	967	ASP
1	A	1039	LYS
1	B	1005	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

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](#)

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	UPG	A	1201	-	32,38,38	0.67	1 (3%)	43,58,58	1.50	2 (4%)
2	UPG	B	1201	-	32,38,38	0.75	0	43,58,58	1.83	4 (9%)

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	UPG	A	1201	-	-	0/19/59/59	0/3/3/3
2	UPG	B	1201	-	-	0/19/59/59	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	UPG	O4C-C1C	2.05	1.44	1.41

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	UPG	C4C-O4C-C1C	-2.36	107.15	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	UPG	O2B-PB-O3A	-2.34	95.25	105.27
2	B	1201	UPG	O2A-PA-O1A	2.14	123.68	112.56
2	B	1201	UPG	O2B-PB-O1B	2.59	126.02	112.56
2	A	1201	UPG	C4-N3-C2	7.35	121.95	114.21

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](#)

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	431/498 (86%)	0.30	37 (8%)	13 14	10, 24, 75, 123	0
1	B	431/498 (86%)	-0.03	12 (2%)	56 60	10, 23, 57, 100	0
All	All	862/996 (86%)	0.14	49 (5%)	27 30	10, 24, 69, 123	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1032	LEU	6.1
1	B	1033	GLY	5.6
1	A	802	LEU	4.7
1	A	805	GLU	4.5
1	A	1031	ARG	4.1

### 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	UPG	A	1201	36/36	0.97	0.08	-0.83	17,24,32,37	0
2	UPG	B	1201	36/36	0.96	0.08	-1.22	13,24,44,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.