



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 04:39 pm GMT

PDB ID : 3JUU  
Title : The crystal structure of apo- UDP-glucose pyrophosphorylase  
Authors : Kim, H.; Kim, K.K.  
Deposited on : 2009-09-15  
Resolution : 2.90 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

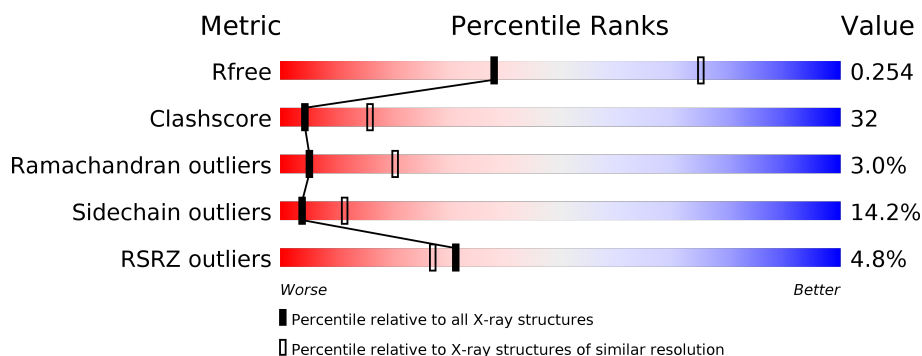
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	281	<div> <div>2%</div> <div> <div></div> <div>49%</div> <div>37%</div> <div>10%</div> <div>••</div> </div> </div>
1	B	281	<div> <div>5%</div> <div> <div></div> <div>46%</div> <div>39%</div> <div>11%</div> <div>••</div> </div> </div>
1	C	281	<div> <div>6%</div> <div> <div></div> <div>48%</div> <div>39%</div> <div>10%</div> <div>•</div> </div> </div>
1	D	281	<div> <div>5%</div> <div> <div></div> <div>48%</div> <div>40%</div> <div>7%</div> <div>••</div> </div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8783 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 UDP-glucose pyrophosphorylase (GalU).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2172	1383	364	411	14			
1	B	273	Total	C	N	O	S	0	0	0
			2172	1383	364	411	14			
1	C	273	Total	C	N	O	S	0	0	0
			2172	1383	364	411	14			
1	D	273	Total	C	N	O	S	0	0	0
			2172	1383	364	411	14			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	LEU	-	EXPRESSION TAG	UNP O25363
A	275	GLU	-	EXPRESSION TAG	UNP O25363
A	276	HIS	-	EXPRESSION TAG	UNP O25363
A	277	HIS	-	EXPRESSION TAG	UNP O25363
A	278	HIS	-	EXPRESSION TAG	UNP O25363
A	279	HIS	-	EXPRESSION TAG	UNP O25363
A	280	HIS	-	EXPRESSION TAG	UNP O25363
A	281	HIS	-	EXPRESSION TAG	UNP O25363
B	274	LEU	-	EXPRESSION TAG	UNP O25363
B	275	GLU	-	EXPRESSION TAG	UNP O25363
B	276	HIS	-	EXPRESSION TAG	UNP O25363
B	277	HIS	-	EXPRESSION TAG	UNP O25363
B	278	HIS	-	EXPRESSION TAG	UNP O25363
B	279	HIS	-	EXPRESSION TAG	UNP O25363
B	280	HIS	-	EXPRESSION TAG	UNP O25363
B	281	HIS	-	EXPRESSION TAG	UNP O25363
C	274	LEU	-	EXPRESSION TAG	UNP O25363
C	275	GLU	-	EXPRESSION TAG	UNP O25363
C	276	HIS	-	EXPRESSION TAG	UNP O25363
C	277	HIS	-	EXPRESSION TAG	UNP O25363
C	278	HIS	-	EXPRESSION TAG	UNP O25363

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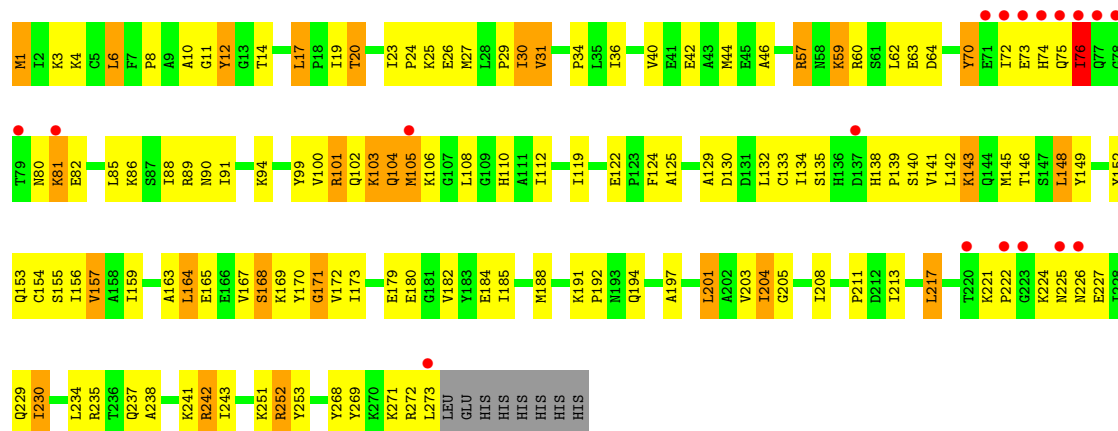
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Chain	Residue	Modelled	Actual	Comment	Reference
C	279	HIS	-	EXPRESSION TAG	UNP O25363
C	280	HIS	-	EXPRESSION TAG	UNP O25363
C	281	HIS	-	EXPRESSION TAG	UNP O25363
D	274	LEU	-	EXPRESSION TAG	UNP O25363
D	275	GLU	-	EXPRESSION TAG	UNP O25363
D	276	HIS	-	EXPRESSION TAG	UNP O25363
D	277	HIS	-	EXPRESSION TAG	UNP O25363
D	278	HIS	-	EXPRESSION TAG	UNP O25363
D	279	HIS	-	EXPRESSION TAG	UNP O25363
D	280	HIS	-	EXPRESSION TAG	UNP O25363
D	281	HIS	-	EXPRESSION TAG	UNP O25363

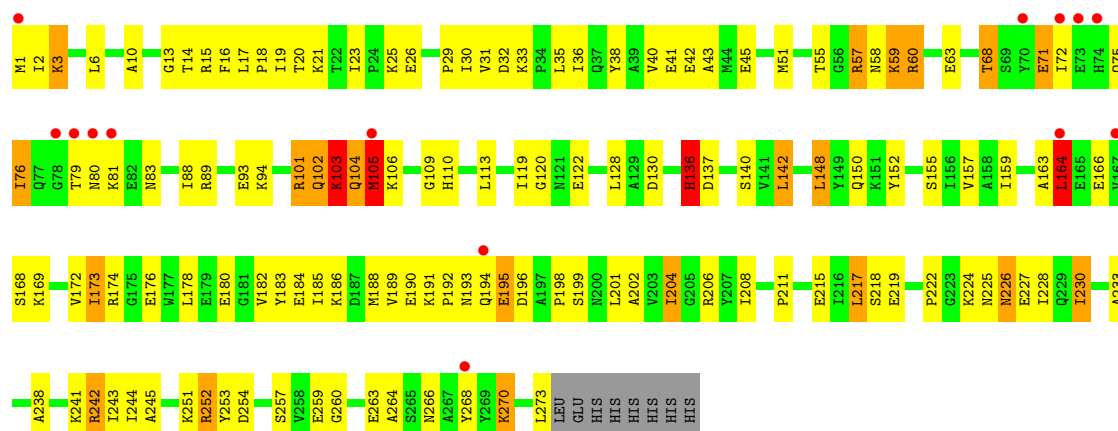
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	20	Total O 20 20	0	0
2	B	24	Total O 24 24	0	0
2	C	30	Total O 30 30	0	0
2	D	21	Total O 21 21	0	0





• Molecule 1: UDP-glucose pyrophosphorylase (GalU)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.47Å 98.61Å 245.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 48.34 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.2 (50.00-2.90) 90.2 (48.34-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.15 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.225 , 0.254 0.225 , 0.254	Depositor DCC
$R_{free}$ test set	2263 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.4	Xtriage
Anisotropy	0.993	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 66.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8783	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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](#)

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	0.38	0/2210	0.68	1/2978 (0.0%)
1	B	0.40	0/2210	0.69	0/2978
1	C	0.40	0/2210	0.68	2/2978 (0.1%)
1	D	0.39	0/2210	0.68	0/2978
All	All	0.39	0/8840	0.68	3/11912 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	GLY	N-CA-C	-5.47	99.43	113.10
1	C	171	GLY	N-CA-C	-5.03	100.53	113.10
1	C	30	ILE	N-CA-C	-5.01	97.46	111.00

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	2172	0	2206	157	0
1	B	2172	0	2206	160	0
1	C	2172	0	2206	144	0
1	D	2172	0	2206	131	0
2	A	20	0	0	1	0
2	B	24	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	30	0	0	2	0
2	D	21	0	0	2	0
All	All	8783	0	8824	555	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 32.

The worst 5 of 555 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:76:ILE:HG23	1:A:82:GLU:HA	1.22	1.10
1:D:76:ILE:HD11	1:D:81:LYS:HB2	1.29	1.10
1:A:79:THR:HG23	1:A:81:LYS:H	1.22	1.04
1:A:179:GLU:HG2	1:A:180:GLU:H	1.23	1.01
1:D:230:ILE:H	1:D:230:ILE:HD12	1.26	1.00

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	271/281 (96%)	233 (86%)	31 (11%)	7 (3%)	6	24
1	B	271/281 (96%)	233 (86%)	30 (11%)	8 (3%)	5	20
1	C	271/281 (96%)	235 (87%)	27 (10%)	9 (3%)	4	18
1	D	271/281 (96%)	235 (87%)	27 (10%)	9 (3%)	4	18
All	All	1084/1124 (96%)	936 (86%)	115 (11%)	33 (3%)	5	20

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	B	12	TYR
1	B	57	ARG
1	B	76	ILE
1	C	75	GLN

### 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	236/244 (97%)	200 (85%)	36 (15%)	3	10
1	B	236/244 (97%)	199 (84%)	37 (16%)	3	9
1	C	236/244 (97%)	209 (89%)	27 (11%)	7	20
1	D	236/244 (97%)	202 (86%)	34 (14%)	4	11
All	All	944/976 (97%)	810 (86%)	134 (14%)	4	11

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	193	ASN
1	C	12	TYR
1	D	173	ILE
1	B	207	TYR
1	B	242	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	229	GLN
1	C	153	GLN
1	D	136	HIS
1	C	77	GLN
1	C	80	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](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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	273/281 (97%)	0.01	6 (2%) 62 59	34, 55, 83, 101	0
1	B	273/281 (97%)	0.11	14 (5%) 29 24	31, 54, 99, 113	0
1	C	273/281 (97%)	0.19	18 (6%) 19 14	34, 51, 99, 132	0
1	D	273/281 (97%)	0.19	14 (5%) 29 24	35, 55, 93, 107	0
All	All	1092/1124 (97%)	0.13	52 (4%) 31 27	31, 54, 94, 132	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	225	ASN	5.0
1	A	226	ASN	4.7
1	C	226	ASN	4.6
1	C	72	ILE	4.5
1	B	226	ASN	4.5

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.