



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 16, 2018 – 10:09 AM EST

PDB ID : 1M26  
Title : Crystal structure of jacalin-T-antigen complex  
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Deposited on : 2002-06-21  
Resolution : 1.62 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 : **FAILED**  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
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-20030736

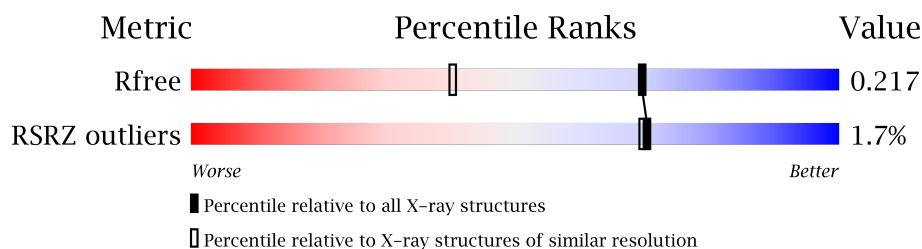
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.62 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	3539 (1.64-1.60)
RSRZ outliers	101464	3562 (1.64-1.60)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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
3	GAL	A	134	-	-	-	X
3	GAL	G	134	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5187 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 Jacalin, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1036	676	159	199	2			
1	C	133	Total	C	N	O	S	0	0	0
			1040	679	160	199	2			
1	E	133	Total	C	N	O	S	0	0	0
			1040	679	160	199	2			
1	G	133	Total	C	N	O	S	0	0	0
			1036	676	159	199	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	VAL	ILE	CONFLICT	GB 289162
C	98	VAL	ILE	CONFLICT	GB 289162
E	98	VAL	ILE	CONFLICT	GB 289162
G	98	VAL	ILE	CONFLICT	GB 289162

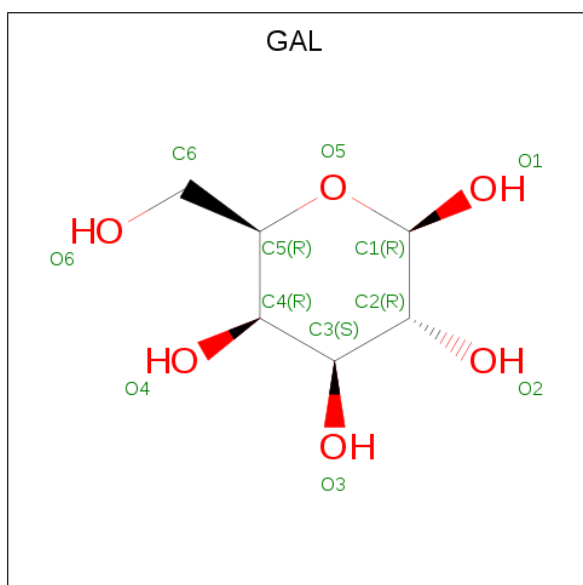
- Molecule 2 is a protein called Jacalin, beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	0	0	0
			105	68	18	19			
2	D	17	Total	C	N	O	0	0	0
			117	74	20	23			
2	F	15	Total	C	N	O	0	0	0
			105	68	18	19			
2	H	15	Total	C	N	O	0	0	0
			105	68	18	19			

There are 8 discrepancies between the modelled and reference sequences:

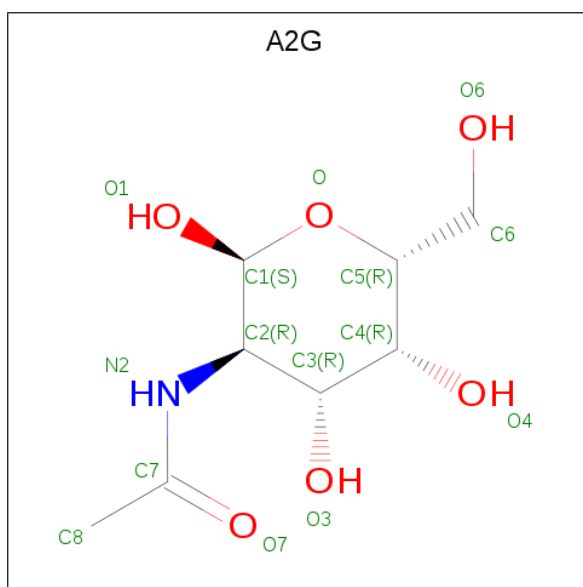
Chain	Residue	Modelled	Actual	Comment	Reference
B	19	SER	VAL	CONFLICT	GB 289162
B	20	ALA	SER	CONFLICT	GB 289162
D	19	SER	VAL	CONFLICT	GB 289162
D	20	ALA	SER	CONFLICT	GB 289162
F	19	SER	VAL	CONFLICT	GB 289162
F	20	ALA	SER	CONFLICT	GB 289162
H	19	SER	VAL	CONFLICT	GB 289162
H	20	ALA	SER	CONFLICT	GB 289162

- Molecule 3 is BETA-D-GALACTOSE (three-letter code: GAL) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	E	1	Total	C	O	0	0
			11	6	5		
3	G	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is N-ACETYL-2-DEOXY-2-AMINO-GALACTOSE (three-letter code: A2G) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	8	1	6		
4	C	1	Total	C	N	O	0	1
			16	8	1	7		
4	E	1	Total	C	N	O	0	1
			16	8	1	7		
4	G	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	141	Total	O	0	0
			141	141		
5	B	15	Total	O	0	0
			15	15		
5	C	105	Total	O	0	0
			105	105		
5	D	19	Total	O	0	0
			19	19		
5	E	97	Total	O	0	0
			97	97		
5	F	16	Total	O	0	0
			16	16		
5	G	92	Total	O	0	0
			92	92		
5	H	12	Total	O	0	0
			12	12		

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### 3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.92Å 78.00Å 67.91Å 90.00° 100.73° 90.00°	Depositor
Resolution (Å)	19.58 – 1.62 19.58 – 1.62	Depositor EDS
% Data completeness (in resolution range)	96.7 (19.58-1.62) 96.8 (19.58-1.62)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 1.62Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.189 , 0.206 0.203 , 0.217	Depositor DCC
$R_{free}$ test set	3787 reflections (5.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.4	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5187	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.76% 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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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### 4.2 Too-close contacts [i](#)

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### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

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#### 4.3.2 Protein sidechains [i](#)

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#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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### 4.5 Carbohydrates [i](#)

validation-pack failed to run properly - this section is therefore empty.

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

validation-pack failed to run properly - this section is therefore empty.

### 4.7 Other polymers [i](#)

validation-pack failed to run properly - this section is therefore empty.



## 4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 5 Fit of model and data ⓘ

### 5.1 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, 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	133/133 (100%)	-0.14	1 (0%) 86 86	14, 20, 30, 33	0
1	C	133/133 (100%)	-0.11	2 (1%) 74 74	14, 21, 32, 36	0
1	E	133/133 (100%)	-0.19	1 (0%) 86 86	14, 20, 27, 35	0
1	G	133/133 (100%)	-0.09	1 (0%) 86 86	16, 22, 30, 37	0
2	B	15/17 (88%)	0.15	1 (6%) 19 17	16, 20, 32, 43	0
2	D	17/17 (100%)	0.05	2 (11%) 5 4	16, 20, 37, 42	0
2	F	15/17 (88%)	0.06	1 (6%) 19 17	15, 21, 31, 40	0
2	H	15/17 (88%)	0.30	1 (6%) 19 17	18, 22, 38, 47	0
All	All	594/600 (99%)	-0.11	10 (1%) 70 70	14, 21, 32, 47	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	18	LYS	5.3
2	D	20	ALA	3.8
2	F	18	LYS	3.6
2	B	18	LYS	3.5
1	C	21	LYS	2.4

### 5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.4 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(Å <sup>2</sup> )	Q<0.9
3	GAL	A	134	11/12	0.75	0.17	4.00	30,33,33,35	0
3	GAL	G	134	11/12	0.80	0.13	2.60	33,36,38,38	0
3	GAL	E	134	11/12	0.86	0.12	0.82	26,29,31,32	0
4	A2G	E	135[A]	15/15	0.93	0.10	0.51	18,23,29,29	1
4	A2G	E	135[B]	15/15	0.93	0.10	0.51	18,22,29,29	1
4	A2G	A	135	15/15	0.92	0.10	0.27	17,21,26,27	0
3	GAL	C	134	11/12	0.93	0.08	0.20	23,24,26,27	0
4	A2G	G	135	15/15	0.89	0.11	0.08	24,28,32,33	0
4	A2G	C	135[A]	15/15	0.95	0.08	-0.06	19,20,26,27	1
4	A2G	C	135[B]	15/15	0.95	0.08	-0.06	19,21,26,27	1

## 5.5 Other polymers [i](#)

There are no such residues in this entry.