



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:34 AM GMT

PDB ID : 3PAW  
Title : Low resolution X-ray crystal structure of Yeast Rnr1p with dATP bound in the A-site  
Authors : Fairman, J.W.; Wijerathna, S.R.; Dealwis, C.G.  
Deposited on : 2010-10-19  
Resolution : 6.61 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 (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

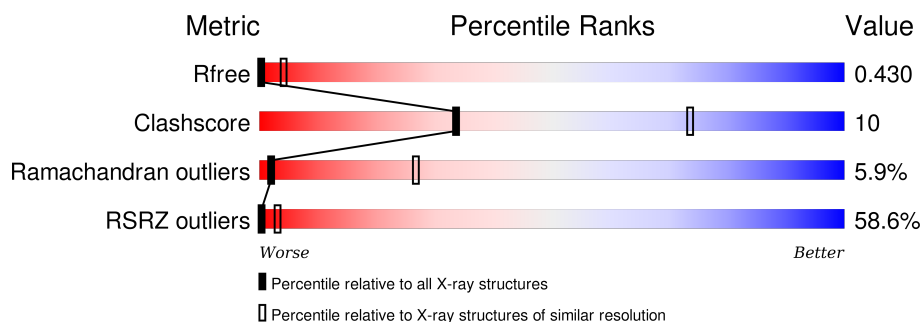
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 6.61 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	1014 (9.50-3.66)
Clashscore	102246	1062 (9.50-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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	888	
1	B	888	
1	C	888	
1	D	888	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14596 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.

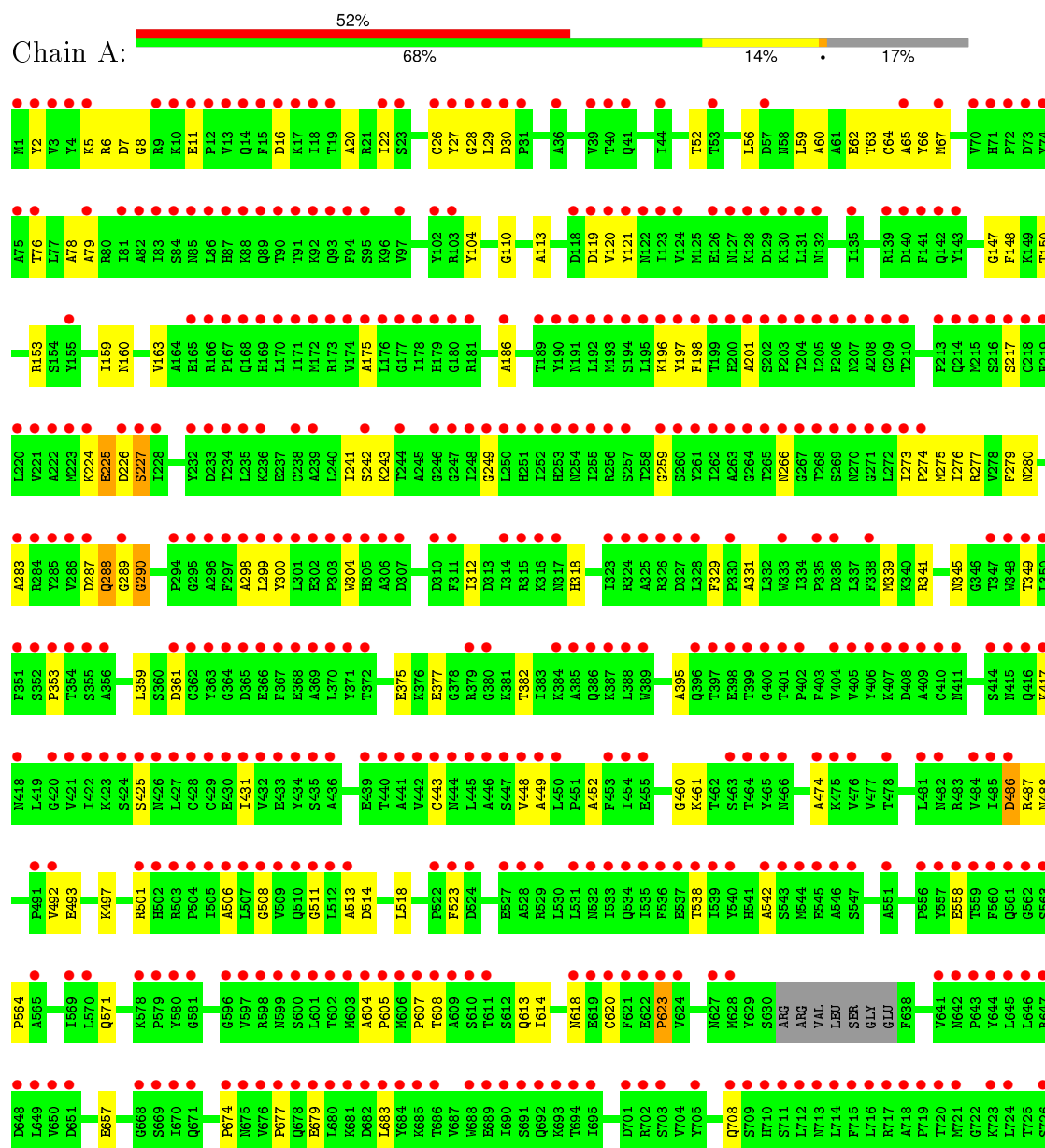
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large chain 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	739	Total	C	N	O	0	0	0
			3649	2171	739	739			
1	B	739	Total	C	N	O	0	0	0
			3649	2171	739	739			
1	C	739	Total	C	N	O	0	0	0
			3649	2171	739	739			
1	D	739	Total	C	N	O	0	0	0
			3649	2171	739	739			

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ribonucleoside-diphosphate reductase large chain 1





Chain C:



Chain D:



VAL	TTR	HT10	R647	M800	C429	P361	A298	E237	H169	D73	M1
GLU	MET	S711	D648	R501	E430	C362	L299	C238	L170	T74	T2
VAL	PRO	L712	L649	H502	V432	Y363	Y300	A239	V174	A75	V3
PRO	SER	N713	V650	R503	V432	G364	L301	L240	V174	T76	Y4
GLU	SER	N714	D651	P504	E433	D365	E302	I241	L175	L77	K5
VAL	ALA	L715	L652	I505	S434	F366	E303	S242	L176	A78	R6
SER	SER	L716	G653	L506	S435	F367	R304	K243	G177	A79	D7
ALA	TTR		D654	L507	A436	E368	R305	T244	H178		G8
PRO	ALA	P719	D655	G508	P437	A369	A306	G246	H179		R9
PRO	ALA		D656	V509	D438	L370	D307	G247	G180		K10
TTR	ALA			Q510	E439	Y371	L308	G247	G181		E11
LYS	SER	T725		G511	T440	T372	D310	I248	D182		P12
ASN	ASP	S726		L512	A441	R373	R310	G249	T90		V13
GLU	PHE	M727		A513	V442	Y374	F311	L250	T91		Q14
GLU	VAL	H728		D514	C443	E375	L312	H251	K92		F15
LYS	PRO			T515	N444		D313	R252	D100		D16
ALA	ALA			L518	L445	R379	R314	E253			H18
ALA	ALA			L519	L446	K381	K315	N254	Y104		R21
PRO	VAL	L736		L520	A447	T382	K316	I255	Y104		
ILE	TTR	K737		P222	V448	T383	R317	R256	P112		L29
VAL	ASN	T738		P523	A449	L384	R318	S257	P112		D30
ASP	ASP	L670		D524	A450	A385	G319	T258	A113		P31
GLU	ALA	G671		L531	P451	A386		G259	P114		K32
ASP	TTR	G672		L532	A452	Q386	E322	S260	S117		R33
ILE	PRO	L673		N532	A453	K387	I323	Y261	D18		I34
TTR	GLU	R674		I533	I454	L388	R324	I262	D19		D35
GLU	SER	N675		T534	E455	F389	A325	A263			A36
PHE	LEU	G676		I535	S457	S391	R326	G264	T203		V37
ASP	ASP	P677		L536	S458	L392	L328	T265	T204		K38
ILE	ILE	G678		T538	D459	L393	F329	N266	L205		V39
LYS	SER	E679		A542	T462	E394	P330	G267	N127		T40
ASN	SER	G613		S543	S463	G400	A331	T268	A208		Q41
ASN	SER	L614		M544	T464	T401	L332	S269	G209		R42
SER	GLU			E545	Y465	P402	N333	N270	T210		I43
ALA	VAL			A546	N466	F403	I334	G271	P211		I44
ALA	GLU			S547		F404	P335	L272	K212		S45
CYS	ALA			C548	H471	V404	D336	I273	P213		G46
ALA	SER			E549		Y406	L337	P274	Q142		V47
ILE	PRO			L550	A474	Y406	F338	T275	Y143		Y48
ASN	ALA			A551	K474	K407	K339	F278	Y145		E49
PRO	PRO			S556	K475	D408	R341	N280	F146		G50
GLU	GLY			P557	N480	A409	V242	N281	C218		V51
ALA	SER			E558	L481	C410	R342	N282	F147		T52
CYS	HIS			T559	N482	N411	E343	T283	G147		T53
GLU	SER			F560	R483	R412	E344	A283	L151		L56
MET	LEU			Q561	V484	R413	N345	Y285	R153		A60
CYS	TTR			S562	I485	S414	T349	V286	S154		A61
LYS	LYS			S563	Y489	N415	L350	D287	Y155		E62
GLY	GLY			P564	Y489	Q416	F351	Q288	L156		T63
MET	GLY			A565	Y490	G420	S352	G289	L157		T64
ALA	ALA				P491	V421	P353	G290	R158		C64
ASP	GLU				Y492	I422	T354	N291	I159		A65
LEU	LEU				E493	K423	S355	K292	G230		Y66
ASN	ASN				E494	S424	A356	I231	I231		T67
VAL	ASN				A495	S425	F357	K293	Y67		T68
LEU	VAL				S498	N426	G358	P294	A162		T69
GLN	GLN				S498	L427	L359	G295	E165		T69
GLU	GLU				S498	L427	L359	G295	R166		V70
PRO	SER				S498	L427	L359	G295	P167		H71
LYS	LYS				S498	L427	L359	G295	Q168		P72

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.51Å 166.51Å 381.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	192.45 – 6.61 36.56 – 6.61	Depositor EDS
% Data completeness (in resolution range)	87.8 (192.45-6.61) 88.3 (36.56-6.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 6.63Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.391 , 0.442 0.370 , 0.430	Depositor DCC
$R_{free}$ test set	469 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	225.0	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 170.6	EDS
Estimated twinning fraction	0.437 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 9847 reflections	Xtriage
$F_o, F_c$ correlation	0.64	EDS
Total number of atoms	14596	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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](#)

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	0.52	0/3647	0.65	0/5075
1	B	0.52	0/3647	0.65	0/5075
1	C	0.53	0/3647	0.66	0/5075
1	D	0.53	0/3647	0.63	0/5075
All	All	0.52	0/14588	0.65	0/20300

There are no bond length outliers.

There are no bond angle outliers.

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	3649	0	1652	61	0
1	B	3649	0	1652	55	0
1	C	3649	0	1652	58	0
1	D	3649	0	1652	44	0
All	All	14596	0	6608	217	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 10.

The worst 5 of 217 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:147:GLY:HA3	1:A:614:ILE:HA	1.42	0.99
1:D:147:GLY:HA2	1:D:614:ILE:HA	1.48	0.95
1:C:603:MET:CB	1:C:706:ILE:HA	1.99	0.92
1:A:147:GLY:CA	1:A:614:ILE:HA	2.02	0.90
1:D:147:GLY:CA	1:D:614:ILE:HA	2.07	0.85

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	735/888 (83%)	533 (72%)	157 (21%)	45 (6%)	2	26
1	B	735/888 (83%)	518 (70%)	180 (24%)	37 (5%)	3	31
1	C	735/888 (83%)	536 (73%)	154 (21%)	45 (6%)	2	26
1	D	735/888 (83%)	542 (74%)	148 (20%)	45 (6%)	2	26
All	All	2940/3552 (83%)	2129 (72%)	639 (22%)	172 (6%)	2	27

5 of 172 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	GLU
1	A	227	SER
1	A	288	GLN
1	A	461	LYS
1	A	486	ASP

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

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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	739/888 (83%)	3.34	458 (61%) 0 3	39, 81, 170, 183	0
1	B	739/888 (83%)	2.85	388 (52%) 0 4	52, 74, 175, 188	0
1	C	739/888 (83%)	3.11	403 (54%) 0 3	51, 73, 173, 194	0
1	D	739/888 (83%)	3.55	483 (65%) 0 3	58, 80, 175, 186	0
All	All	2956/3552 (83%)	3.21	1732 (58%) 0 3	39, 78, 173, 194	0

The worst 5 of 1732 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	711	SER	18.8
1	C	433	GLU	18.8
1	B	415	ASN	18.6
1	B	414	SER	17.5
1	D	218	CYS	17.2

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.