



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:46 PM GMT

PDB ID : 1JY1  
Title : CRYSTAL STRUCTURE OF HUMAN TYROSYL-DNA PHOSPHODI-  
ESTERASE (TDP1)  
Authors : Davies, D.R.; Interthal, H.; Champoux, J.J.; Hol, W.G.J.  
Deposited on : 2001-09-10  
Resolution : 1.69 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

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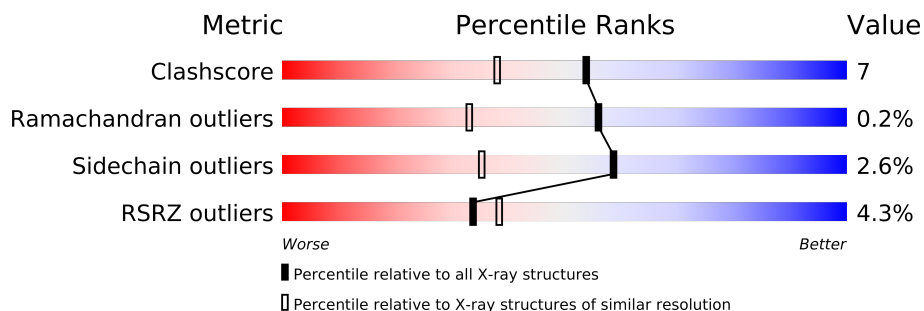
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.69 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))
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	464	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3850 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TYROSYL-DNA PHOSPHODIESTERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	439	3505	2273	590	631	3	8	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	145	LEU	-	EXPRESSION TAG	UNP Q9NUW8
A	146	GLU	-	EXPRESSION TAG	UNP Q9NUW8
A	147	ASP	-	EXPRESSION TAG	UNP Q9NUW8
A	148	PRO	-	EXPRESSION TAG	UNP Q9NUW8
A	157	MSE	MET	MODIFIED RESIDUE	UNP Q9NUW8
A	266	MSE	MET	MODIFIED RESIDUE	UNP Q9NUW8
A	267	MSE	MET	MODIFIED RESIDUE	UNP Q9NUW8
A	322	ASN	ASP	ENGINEERED	UNP Q9NUW8
A	328	THR	MET	ENGINEERED	UNP Q9NUW8
A	386	MSE	MET	MODIFIED RESIDUE	UNP Q9NUW8
A	420	MSE	MET	MODIFIED RESIDUE	UNP Q9NUW8
A	491	MSE	MET	MODIFIED RESIDUE	UNP Q9NUW8
A	498	MSE	MET	MODIFIED RESIDUE	UNP Q9NUW8
A	533	MSE	MET	MODIFIED RESIDUE	UNP Q9NUW8
A	548	LEU	PHE	ENGINEERED	UNP Q9NUW8
A	567	MSE	MET	MODIFIED RESIDUE	UNP Q9NUW8
A	604	MSE	MET	MODIFIED RESIDUE	UNP Q9NUW8

- Molecule 2 is water.

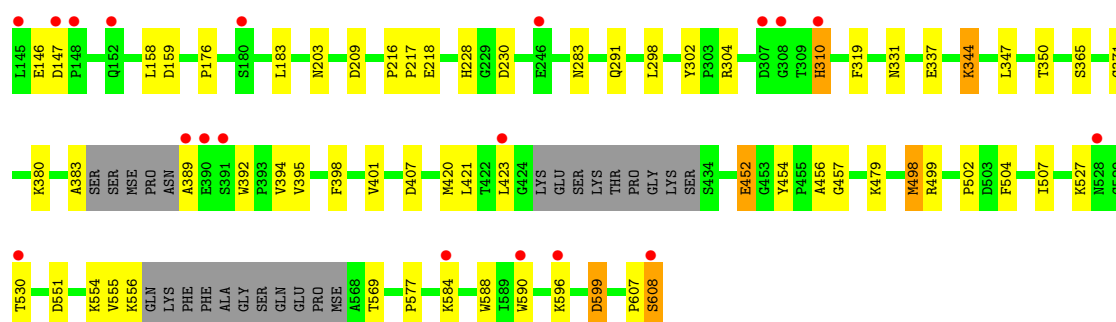
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	345	Total	O	0	0
			345	345		

### 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 ( $RSRZ > 2$ ). 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: TYROSYL-DNA PHOSPHODIESTERASE

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.44Å 52.03Å 56.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.69 19.95 – 1.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.69) 92.8 (19.95-1.65)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.29 (at 1.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.198 , 0.229 0.198 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 35.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 62342 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3850	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.79	1/3610 (0.0%)	0.95	7/4896 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	498	MSE	SE-CE	-5.48	1.63	1.95

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ASP	CB-CG-OD2	8.28	125.75	118.30
1	A	407	ASP	CB-CG-OD2	7.91	125.42	118.30
1	A	159	ASP	CB-CG-OD2	7.64	125.17	118.30
1	A	551	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	147	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	479	LYS	CD-CE-NZ	-5.09	99.99	111.70
1	A	599	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3505	0	3424	48	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	345	0	0	2	1
All	All	3850	0	3424	48	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (48) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:394:VAL:HG11	1:A:420:MSE:CE	1.72	1.18
1:A:394:VAL:HG11	1:A:420:MSE:HE3	1.11	1.10
1:A:607:PRO:O	1:A:608:SER:HB2	1.52	1.10
1:A:394:VAL:CG1	1:A:420:MSE:HE3	1.92	0.97
1:A:394:VAL:CG1	1:A:420:MSE:CE	2.44	0.96
1:A:389:ALA:CB	1:A:423:LEU:CD1	2.53	0.86
1:A:291:GLN:HB2	1:A:452:GLU:OE2	1.77	0.85
1:A:228:HIS:HD2	1:A:230:ASP:H	1.30	0.79
1:A:498:MSE:HE1	1:A:507:ILE:HG21	1.68	0.76
1:A:389:ALA:CB	1:A:423:LEU:HD12	2.16	0.75
1:A:394:VAL:CG1	1:A:420:MSE:HE1	2.17	0.74
1:A:389:ALA:HB3	1:A:423:LEU:CD1	2.23	0.68
1:A:607:PRO:O	1:A:608:SER:CB	2.39	0.66
1:A:421:LEU:HD12	1:A:421:LEU:C	2.16	0.66
1:A:389:ALA:HB1	1:A:423:LEU:HD12	1.80	0.64
1:A:498:MSE:CE	1:A:507:ILE:HG21	2.28	0.63
1:A:389:ALA:HB1	1:A:423:LEU:CD1	2.29	0.62
1:A:389:ALA:HB3	1:A:423:LEU:HD12	1.82	0.61
1:A:389:ALA:CB	1:A:423:LEU:HD13	2.33	0.56
1:A:218:GLU:OE1	1:A:218:GLU:N	2.29	0.55
1:A:228:HIS:HD2	1:A:230:ASP:N	2.01	0.54
1:A:389:ALA:HB3	1:A:423:LEU:HD13	1.92	0.52
1:A:498:MSE:HE1	1:A:507:ILE:CG2	2.39	0.51
1:A:310:HIS:ND1	1:A:310:HIS:O	2.37	0.50
1:A:555:VAL:O	1:A:556:LYS:CB	2.59	0.50
1:A:319:PHE:CG	1:A:350:THR:HG21	2.48	0.48
1:A:457:GLY:HA3	1:A:588:TRP:CZ2	2.49	0.48
1:A:344:LYS:HD3	1:A:344:LYS:HA	1.61	0.48
1:A:304:ARG:NH2	2:A:1047:HOH:O	2.48	0.47
1:A:183:LEU:CD1	1:A:298:LEU:HD11	2.45	0.46
1:A:383:ALA:HB1	1:A:423:LEU:HD22	1.98	0.46
1:A:395:VAL:HB	1:A:498:MSE:HG3	1.99	0.45
1:A:452:GLU:HB2	1:A:456:ALA:HB2	1.97	0.45
1:A:498:MSE:CE	1:A:507:ILE:CG2	2.95	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:176:PRO:HG2	2:A:994:HOH:O	2.17	0.45
1:A:421:LEU:CD1	1:A:421:LEU:C	2.85	0.44
1:A:302:TYR:CD1	1:A:347:LEU:HA	2.52	0.44
1:A:228:HIS:CD2	1:A:230:ASP:H	2.20	0.44
1:A:554:LYS:HB2	1:A:569:THR:HG22	2.01	0.43
1:A:454:TYR:CD2	1:A:599:ASP:HB3	2.54	0.42
1:A:392:TRP:CD1	1:A:502:PRO:HD3	2.55	0.42
1:A:398:PHE:CE2	1:A:401:VAL:HG22	2.54	0.41
1:A:203:ASN:OD1	1:A:283:ASN:HA	2.20	0.41
1:A:504:PHE:CE1	1:A:577:PRO:HB3	2.56	0.41
1:A:394:VAL:HG22	1:A:499:ARG:HD2	2.01	0.41
1:A:158:LEU:HD21	1:A:298:LEU:CD1	2.51	0.41
1:A:527:LYS:O	1:A:530:THR:HG23	2.21	0.40
1:A:216:PRO:O	1:A:217:PRO:C	2.59	0.40

All (2) 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	Distance(Å)	Clash(Å)
2:A:845:HOH:O	2:A:845:HOH:O[2_655]	1.85	0.35
1:A:365:SER:OG	1:A:380:LYS:NZ[2_655]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	431/464 (93%)	422 (98%)	8 (2%)	1 (0%)	56 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	371	GLY



### 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	378/393 (96%)	368 (97%)	10 (3%)	59 35

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	310	HIS
1	A	331	ASN
1	A	337	GLU
1	A	344	LYS
1	A	452	GLU
1	A	584	LYS
1	A	590	TRP
1	A	596	LYS
1	A	608	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	228	HIS
1	A	331	ASN
1	A	363	GLN
1	A	397	GLN
1	A	531	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 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	439/464 (94%)	0.09	19 (4%) 34 38	10, 20, 37, 47	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	389	ALA	7.0
1	A	608	SER	5.0
1	A	590	TRP	4.1
1	A	308	GLY	3.9
1	A	423	LEU	3.8
1	A	307	ASP	3.5
1	A	180	SER	2.9
1	A	528	ASN	2.9
1	A	310	HIS	2.9
1	A	391	SER	2.8
1	A	530	THR	2.7
1	A	390	GLU	2.6
1	A	148	PRO	2.4
1	A	145	LEU	2.3
1	A	246	GLU	2.3
1	A	596	LYS	2.2
1	A	147	ASP	2.1
1	A	152	GLN	2.1
1	A	584	LYS	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.