



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:39 pm GMT

PDB ID : 1YPT  
Title : CRYSTAL STRUCTURE OF YERSINIA PROTEIN TYROSINE PHOSPHATASE AT 2.5 ANGSTROMS AND THE COMPLEX WITH TUNGSTATE  
Authors : Stuckey, J.A.; Schubert, H.L.; Fauman, E.B.; Zhang, Z.-Y.; Dixon, J.E.; Saper, M.A.  
Deposited on : 1994-09-16  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure 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/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) : NOT EXECUTED  
EDS : NOT EXECUTED  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

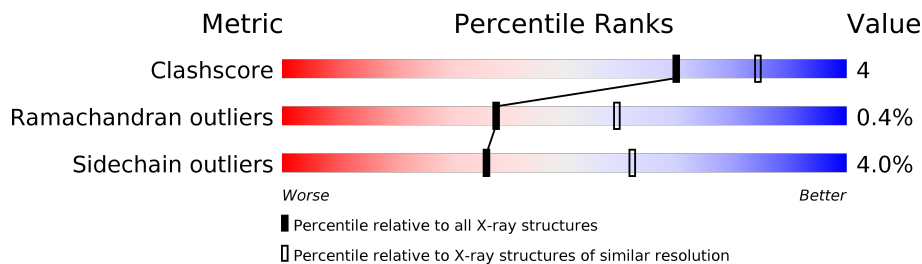
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	305	
1	B	305	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4355 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 PROTEIN-TYROSINE PHOSPHATASE YERSINIA (CATALYTIC DOMAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2137	1304	398	419	16			
1	B	280	Total	C	N	O	S	0	0	0
			2153	1315	400	422	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	ARG	CYS	CONFLICT	UNP P15273
B	235	ARG	CYS	CONFLICT	UNP P15273

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	36	Total	O	0	0
			36	36		
2	B	29	Total	O	0	0
			29	29		



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.53Å 71.53Å 107.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.50	Depositor
% Data completeness (in resolution range)	84.0 (7.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.168 , 0.222	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4355	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

## 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	0.76	0/2162	1.47	19/2918 (0.7%)
1	B	0.75	0/2179	1.52	27/2942 (0.9%)
All	All	0.76	0/4341	1.50	46/5860 (0.8%)

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	380	ARG	NE-CZ-NH1	16.54	128.57	120.30
1	A	380	ARG	NE-CZ-NH1	15.19	127.89	120.30
1	B	272	ARG	NE-CZ-NH2	13.39	126.99	120.30
1	B	380	ARG	NE-CZ-NH2	-13.16	113.72	120.30
1	A	380	ARG	NE-CZ-NH2	-12.42	114.09	120.30
1	A	272	ARG	NE-CZ-NH1	12.39	126.50	120.30
1	B	272	ARG	NH1-CZ-NH2	-9.92	108.49	119.40
1	B	354	TRP	CD1-CG-CD2	8.35	112.98	106.30
1	A	255	ARG	NE-CZ-NH2	8.29	124.45	120.30
1	B	272	ARG	NE-CZ-NH1	8.15	124.37	120.30
1	A	272	ARG	NH1-CZ-NH2	-7.55	111.10	119.40
1	A	354	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	B	241	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	B	354	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	B	216	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	205	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	A	354	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	B	303	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	432	MET	CG-SD-CE	-6.75	89.39	100.20
1	B	205	ARG	CB-CG-CD	-6.53	94.62	111.60
1	A	398	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	B	295	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	B	241	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	380	ARG	CD-NE-CZ	5.97	131.96	123.60
1	A	303	ARG	NE-CZ-NH1	5.97	123.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	366	LYS	CB-CG-CD	-5.94	96.15	111.60
1	B	216	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	278	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	354	TRP	CG-CD2-CE3	5.75	139.08	133.90
1	B	278	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	404	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	B	296	PHE	CB-CG-CD2	-5.56	116.91	120.80
1	A	334	LEU	CA-CB-CG	5.55	128.06	115.30
1	A	396	LYS	CA-CB-CG	-5.49	101.32	113.40
1	B	354	TRP	CG-CD2-CE3	5.48	138.83	133.90
1	B	228	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	A	282	LEU	CD1-CG-CD2	-5.27	94.68	110.50
1	A	366	LYS	CB-CG-CD	-5.26	97.91	111.60
1	A	402	HIS	CA-CB-CG	5.22	122.48	113.60
1	B	303	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	437	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	354	TRP	CB-CG-CD1	-5.09	120.38	127.00
1	A	236	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	205	ARG	CD-NE-CZ	-5.07	116.50	123.60
1	B	282	LEU	CD1-CG-CD2	-5.03	95.42	110.50
1	B	419	MET	CG-SD-CE	5.02	108.23	100.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-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 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	2137	0	2144	17	0
1	B	2153	0	2155	20	0
2	A	36	0	0	1	0
2	B	29	0	0	0	0
All	All	4355	0	4299	36	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 4.

All (36) 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:298:MET:SD	1:A:404:ARG:HG3	2.29	0.73
1:B:250:GLN:H	1:B:439:GLN:NE2	1.91	0.68
1:B:250:GLN:H	1:B:439:GLN:HE22	1.42	0.67
1:B:300:ASP:OD1	1:B:303:ARG:HD3	2.05	0.56
1:B:298:MET:SD	1:B:404:ARG:HG3	2.46	0.55
1:B:311:ILE:HG12	1:B:338:GLU:HG3	1.90	0.54
1:B:303:ARG:HG2	1:B:332:TYR:CZ	2.43	0.53
1:B:190:GLY:O	1:B:194:ARG:HG3	2.09	0.52
1:A:300:ASP:OD1	1:A:303:ARG:HD3	2.10	0.52
1:A:303:ARG:HG2	1:A:332:TYR:CZ	2.45	0.51
1:A:302:PHE:CE2	1:A:303:ARG:HD2	2.45	0.51
1:A:316:LYS:HE2	1:A:318:THR:HG22	1.92	0.51
1:B:391:VAL:HA	1:B:397:LEU:HD12	1.95	0.47
1:A:249:ILE:HD11	1:A:440:ARG:HB2	1.96	0.46
1:B:228:ARG:HA	1:B:263:LEU:HD21	1.97	0.46
1:B:219:GLN:HG2	1:B:236:ARG:NH2	2.32	0.45
1:A:227:ASN:ND2	1:A:233:GLN:HG2	2.31	0.45
1:B:250:GLN:HA	1:B:254:THR:O	2.17	0.44
1:B:338:GLU:HG2	1:B:339:ALA:N	2.33	0.43
1:B:219:GLN:HG2	1:B:236:ARG:HH21	1.83	0.43
1:A:255:ARG:NH1	1:A:394:ASP:HB3	2.34	0.42
1:B:228:ARG:NH1	1:B:261:TYR:O	2.53	0.42
1:A:251:VAL:HB	1:A:418:CYS:SG	2.59	0.42
1:B:431:ASP:O	1:B:435:GLN:HG3	2.20	0.42
1:B:421:ASP:HB3	1:B:424:ASN:ND2	2.35	0.42
1:A:282:LEU:HD23	1:A:348:VAL:HG13	2.01	0.41
1:B:384:GLU:HG3	1:B:391:VAL:HG11	2.01	0.41
1:A:360:VAL:HA	1:B:325:ASP:OD1	2.21	0.41
1:A:209:ALA:HA	1:A:210:PRO:HD3	1.86	0.41
1:A:250:GLN:HA	1:A:254:THR:O	2.21	0.41
1:A:338:GLU:HG2	1:A:339:ALA:N	2.36	0.41
1:A:250:GLN:HB2	2:A:565:HOH:O	2.20	0.40
1:A:214:ASP:HA	1:A:215:PRO:HD2	1.94	0.40
1:A:376:ALA:O	1:A:380:ARG:HB2	2.22	0.40
1:B:280:PRO:HD3	1:B:397:LEU:HA	2.02	0.40
1:B:250:GLN:N	1:B:439:GLN:HE22	2.16	0.40

There are no symmetry-related clashes.



## 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	276/305 (90%)	263 (95%)	12 (4%)	1 (0%)	38	59
1	B	278/305 (91%)	270 (97%)	7 (2%)	1 (0%)	38	59
All	All	554/610 (91%)	533 (96%)	19 (3%)	2 (0%)	38	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	VAL
1	B	445	VAL

### 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	235/254 (92%)	226 (96%)	9 (4%)	38	64
1	B	236/254 (93%)	226 (96%)	10 (4%)	34	59
All	All	471/508 (93%)	452 (96%)	19 (4%)	36	62

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	ARG
1	A	253	ASN
1	A	282	LEU
1	A	289	SER

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Mol	Chain	Res	Type
1	A	313	VAL
1	A	334	LEU
1	A	358	THR
1	A	371	LEU
1	A	443	ILE
1	B	221	CYS
1	B	253	ASN
1	B	282	LEU
1	B	289	SER
1	B	327	ILE
1	B	334	LEU
1	B	358	THR
1	B	371	LEU
1	B	420	ASN
1	B	423	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	439	GLN

### 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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.