



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:50 AM UTC

PDB ID : 1YPT / pdb_00001ypt
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,
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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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

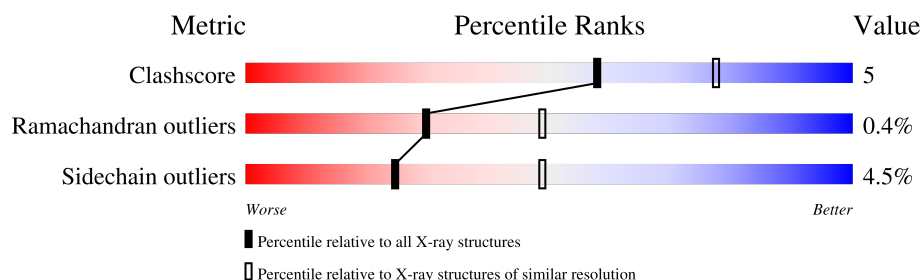
1 Overall quality at a glance

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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	305	 70% 18% • 9%
1	B	305	 71% 19% • 8%

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		

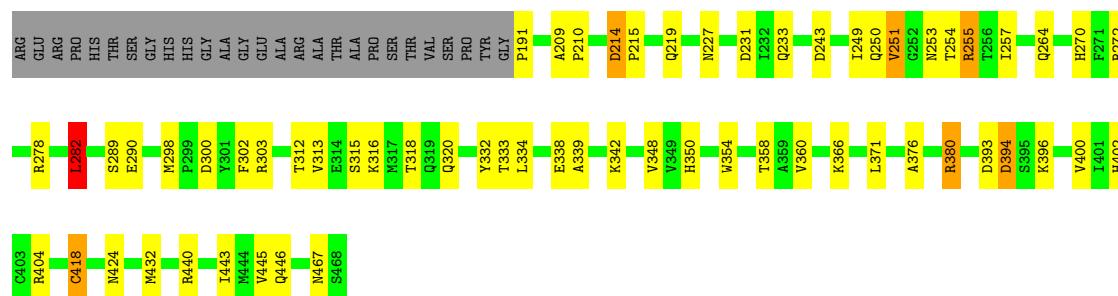
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

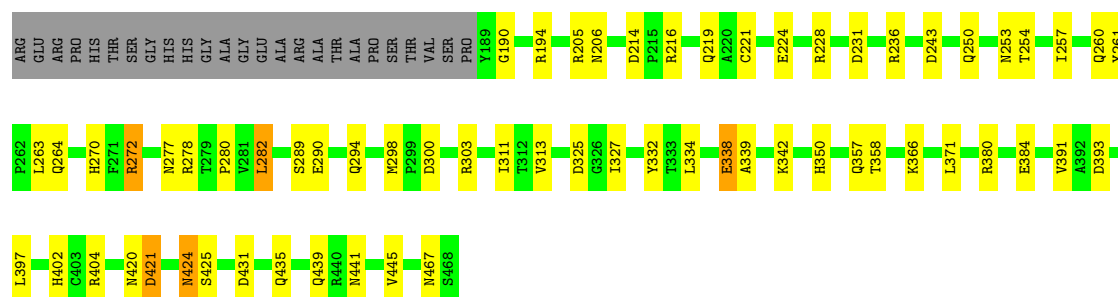
• Molecule 1: PROTEIN-TYROSINE PHOSPHATASE YERSINIA (CATALYTIC DOMAIN)

Chain A: 



• Molecule 1: PROTEIN-TYROSINE PHOSPHATASE YERSINIA (CATALYTIC DOMAIN)

Chain B: 



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, α , β , γ	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 ²)	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	0.95	4/2162 (0.2%)	1.70	31/2918 (1.1%)
1	B	0.96	3/2179 (0.1%)	1.75	38/2942 (1.3%)
All	All	0.95	7/4341 (0.2%)	1.72	69/5860 (1.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	HIS	CD2-NE2	-7.11	1.30	1.37
1	A	350	HIS	CD2-NE2	-6.88	1.30	1.37
1	B	270	HIS	CD2-NE2	-5.98	1.31	1.37
1	B	350	HIS	CD2-NE2	-5.95	1.31	1.37
1	B	402	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	350	HIS	CG-ND1	-5.62	1.32	1.38
1	A	402	HIS	CD2-NE2	-5.47	1.31	1.37

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	HIS	CA-CB-CG	8.68	122.48	113.80
1	B	272	ARG	NE-CZ-NH2	8.66	126.99	119.20
1	B	272	ARG	NH1-CZ-NH2	-8.31	108.49	119.30
1	B	421	ASP	CA-CB-CG	7.41	120.01	112.60
1	B	243	ASP	CA-CB-CG	7.40	120.00	112.60
1	A	282	LEU	CD1-CG-CD2	-7.33	94.68	110.80
1	B	205	ARG	CB-CG-CD	-7.25	94.62	111.30
1	B	380	ARG	NE-CZ-NH1	7.07	128.57	121.50
1	B	282	LEU	CD1-CG-CD2	-6.99	95.42	110.80
1	B	277	ASN	CA-CB-CG	6.76	119.36	112.60
1	A	393	ASP	CA-CB-CG	6.75	119.34	112.60
1	B	231	ASP	CA-CB-CG	6.72	119.33	112.60
1	B	366	LYS	CB-CG-CD	-6.59	96.15	111.30
1	A	243	ASP	CA-CB-CG	6.48	119.08	112.60
1	A	380	ARG	NE-CZ-NH1	6.39	127.89	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	LYS	CA-CB-CG	-6.39	101.32	114.10
1	B	260	GLN	OE1-CD-NE2	-6.33	116.27	122.60
1	A	272	ARG	NH1-CZ-NH2	-6.31	111.10	119.30
1	B	467	ASN	O-C-N	6.23	130.26	123.10
1	B	467	ASN	CA-C-N	6.14	132.75	121.70
1	B	467	ASN	C-N-CA	6.14	132.75	121.70
1	B	380	ARG	NE-CZ-NH2	-6.09	113.72	119.20
1	A	270	HIS	CB-CG-CD2	-6.07	123.31	131.20
1	A	251	VAL	N-CA-C	-5.91	97.88	107.28
1	B	425	SER	N-CA-C	5.87	118.43	111.33
1	B	402	HIS	CA-CB-CG	5.85	119.65	113.80
1	B	393	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	255	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	A	366	LYS	CB-CG-CD	-5.82	97.91	111.30
1	B	257	ILE	N-CA-C	-5.80	99.76	108.12
1	B	402	HIS	CB-CG-CD2	-5.78	123.68	131.20
1	A	467	ASN	O-C-N	5.76	129.72	123.10
1	A	400	VAL	N-CA-C	-5.72	100.16	108.17
1	A	380	ARG	NE-CZ-NH2	-5.68	114.09	119.20
1	A	214	ASP	CA-C-N	5.65	125.35	119.82
1	A	214	ASP	C-N-CA	5.65	125.35	119.82
1	B	205	ARG	CD-NE-CZ	-5.64	116.50	124.40
1	A	394	ASP	N-CA-C	5.62	119.88	113.19
1	B	294	GLN	OE1-CD-NE2	-5.62	116.98	122.60
1	A	264	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	B	424	ASN	OD1-CG-ND2	-5.58	117.02	122.60
1	A	446	GLN	N-CA-C	5.54	118.50	111.69
1	B	214	ASP	CA-C-N	5.52	125.19	119.56
1	B	214	ASP	C-N-CA	5.52	125.19	119.56
1	A	402	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	B	420	ASN	CA-CB-CG	5.41	118.01	112.60
1	B	420	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	B	380	ARG	CD-NE-CZ	5.40	131.96	124.40
1	B	216	ARG	N-CA-C	-5.35	106.26	112.89
1	B	441	ASN	O-C-N	-5.33	117.66	123.26
1	A	342	LYS	CB-CG-CD	-5.31	99.09	111.30
1	B	270	HIS	CB-CG-CD2	-5.29	124.32	131.20
1	B	357	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	A	231	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	264	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	A	432	MET	CG-SD-CE	-5.23	89.39	100.90
1	B	224	GLU	N-CA-C	-5.23	100.38	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	B	260	GLN	CG-CD-NE2	5.18	124.17	116.40
1	A	354	TRP	CG-CD2-CE3	5.18	139.08	133.90
1	B	338	GLU	CA-CB-CG	-5.11	103.89	114.10
1	A	219	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	A	312	THR	CA-CB-OG1	-5.10	101.95	109.60
1	A	320	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	A	257	ILE	N-CA-C	-5.06	101.02	108.11
1	A	333	THR	N-CA-C	-5.05	100.67	108.90
1	B	342	LYS	CB-CG-CD	-5.04	99.70	111.30
1	A	424	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	A	418	CYS	CB-CA-C	-5.03	102.98	110.88

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	18	0
1	B	2153	0	2155	22	0
2	A	36	0	0	1	0
2	B	29	0	0	0	0
All	All	4355	0	4299	39	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 5.

All (39) 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:A:290:GLU:HB3	1:A:298:MET:HE1	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:290:GLU:HB3	1:B:298:MET:HE1	1.91	0.53
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:B:272:ARG:HH12	1:B:338:GLU:CD	2.28	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%)	30	49
1	B	278/305 (91%)	270 (97%)	7 (2%)	1 (0%)	30	49
All	All	554/610 (91%)	533 (96%)	19 (3%)	2 (0%)	30	49

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%)	224 (95%)	11 (5%)	23	47
1	B	236/254 (93%)	226 (96%)	10 (4%)	26	52
All	All	471/508 (93%)	450 (96%)	21 (4%)	24	49

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	PRO
1	A	253	ASN
1	A	278	ARG
1	A	282	LEU

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Mol	Chain	Res	Type
1	A	289	SER
1	A	313	VAL
1	A	315	SER
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	278	ARG
1	B	282	LEU
1	B	289	SER
1	B	313	VAL
1	B	327	ILE
1	B	334	LEU
1	B	358	THR
1	B	371	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
1	B	439	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides 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

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.