



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:39 AM GMT

PDB ID : 2I3U  
Title : Structural studies of protein tyrosine phosphatase beta catalytic domain in complex with inhibitors  
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Deposited on : 2006-08-20  
Resolution : 1.85 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  
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

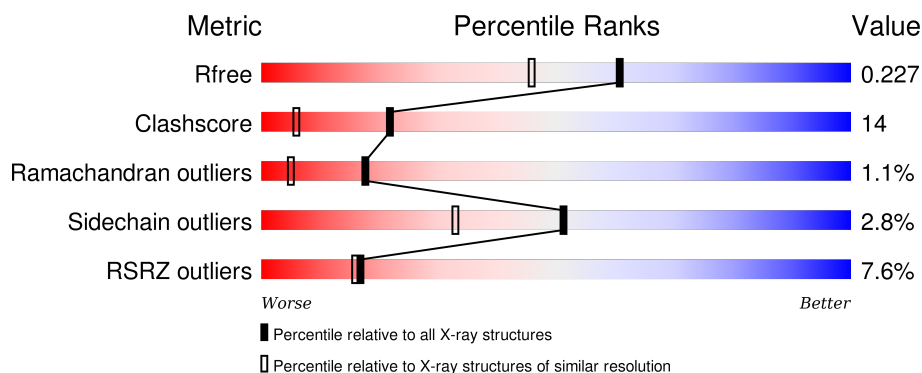
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 1.85 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	313	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2530 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 Receptor-type tyrosine-protein phosphatase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	13	0
			2326	1477	413	423	13			

There is a discrepancy between the modelled and reference sequences:

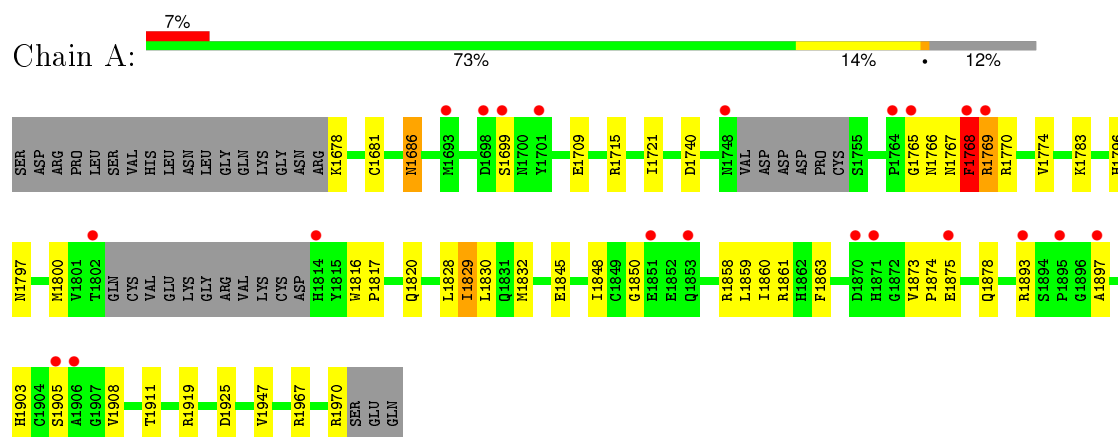
Chain	Residue	Modelled	Actual	Comment	Reference
A	1661	SER	-	CLONING ARTIFACT	UNP P23467

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	204	Total	O	0	0
			204	204		



- Molecule 1: Receptor-type tyrosine-protein phosphatase beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.78 Å 69.78 Å 118.52 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.31 – 1.85 22.31 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.3 (22.31-1.85) 98.4 (22.31-1.85)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.36 (at 1.85 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.187 , 0.226 0.186 , 0.227	Depositor DCC
$R_{free}$ test set	1402 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 55.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 27926 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2530	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% 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	0.48	0/2416	0.59	0/3275

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1768	PHE	Peptide

### 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	2326	0	2310	65	5
2	A	204	0	0	8	0
All	All	2530	0	2310	65	5

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 14.

All (65) 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:1845:GLU:CD	1:A:1859[B]:LEU:HD11	1.58	1.21
1:A:1845:GLU:CG	1:A:1859[B]:LEU:HD11	1.75	1.17
1:A:1828[B]:LEU:HD11	1:A:1848:ILE:CD1	1.80	1.12
1:A:1845:GLU:OE2	1:A:1859[B]:LEU:HD11	1.52	1.08
1:A:1828[B]:LEU:HD11	1:A:1848:ILE:HD11	1.29	1.06
1:A:1769[B]:ARG:HD3	1:A:1769[B]:ARG:H	1.23	1.00
1:A:1828[B]:LEU:CD1	1:A:1848:ILE:HD11	1.91	1.00
1:A:1845:GLU:OE2	1:A:1859[B]:LEU:CD1	2.11	0.99
1:A:1828[B]:LEU:HD11	1:A:1848:ILE:CG1	2.00	0.91
1:A:1858:ARG:HD2	1:A:1860:ILE:HD11	1.51	0.91
1:A:1767:ASN:O	1:A:1768:PHE:CD1	2.27	0.88
1:A:1845:GLU:OE2	1:A:1859[B]:LEU:HD21	1.76	0.85
1:A:1845:GLU:OE2	1:A:1859[B]:LEU:CD2	2.27	0.82
1:A:1845:GLU:HG2	1:A:1859[B]:LEU:HD11	1.60	0.81
1:A:1828[A]:LEU:CD2	1:A:1850:GLY:HA3	2.14	0.77
1:A:1769[B]:ARG:N	1:A:1769[B]:ARG:HD3	1.99	0.77
1:A:1828[A]:LEU:CD2	1:A:1850:GLY:CA	2.64	0.76
1:A:1768:PHE:HD1	1:A:1769[B]:ARG:NH1	1.84	0.75
1:A:1845:GLU:CG	1:A:1859[B]:LEU:CD1	2.63	0.70
1:A:1820:GLN:HG2	1:A:1832:MET:O	1.92	0.69
1:A:1861[A]:ARG:NH1	2:A:374:HOH:O	2.24	0.69
1:A:1768:PHE:CE1	2:A:643:HOH:O	2.44	0.69
1:A:1769[A]:ARG:HG3	1:A:1769[A]:ARG:O	1.94	0.68
1:A:1828[B]:LEU:HD11	1:A:1848:ILE:HG12	1.73	0.68
1:A:1845:GLU:HG2	1:A:1859[B]:LEU:CD1	2.25	0.67
1:A:1828[A]:LEU:HD23	1:A:1850:GLY:HA2	1.77	0.67
1:A:1845:GLU:CD	1:A:1859[B]:LEU:CD1	2.50	0.66
1:A:1768:PHE:HE1	2:A:643:HOH:O	1.82	0.63
1:A:1828[A]:LEU:CD2	1:A:1850:GLY:HA2	2.30	0.61
1:A:1767:ASN:HB3	1:A:1768:PHE:CZ	2.36	0.61
1:A:1828[A]:LEU:HD22	1:A:1850:GLY:CA	2.33	0.59
1:A:1768:PHE:HD1	1:A:1769[B]:ARG:HH11	1.50	0.59
1:A:1828[B]:LEU:HD21	1:A:1848:ILE:HG13	1.85	0.58
1:A:1767:ASN:C	1:A:1768:PHE:CG	2.77	0.58
1:A:1686:ASN:HB2	2:A:409:HOH:O	2.04	0.57
1:A:1828[A]:LEU:HD22	1:A:1850:GLY:HA3	1.87	0.55
1:A:1765:GLY:HA2	1:A:1919:ARG:HD2	1.90	0.54
1:A:1893:ARG:HB3	2:A:632:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1767:ASN:C	1:A:1768:PHE:CD1	2.82	0.52
1:A:1769[B]:ARG:O	1:A:1770:ARG:HB2	2.09	0.52
1:A:1767:ASN:HB3	1:A:1768:PHE:CE2	2.45	0.52
1:A:1678:LYS:HD2	1:A:1681[A]:CYS:SG	2.50	0.51
1:A:1678:LYS:HE2	1:A:1709:GLU:OE1	2.11	0.51
1:A:1796:HIS:HA	1:A:1860:ILE:HD12	1.92	0.51
1:A:1678:LYS:NZ	1:A:1681[A]:CYS:SG	2.76	0.51
1:A:1769[B]:ARG:N	1:A:1769[B]:ARG:CD	2.69	0.50
1:A:1878:GLN:HG2	2:A:641:HOH:O	2.10	0.50
1:A:1897:ALA:HB3	2:A:607:HOH:O	2.12	0.50
1:A:1845:GLU:OE2	1:A:1859[B]:LEU:CG	2.61	0.48
1:A:1800:MET:HG3	1:A:1903:HIS:CE1	2.48	0.48
1:A:1925:ASP:OD1	1:A:1967:ARG:NH2	2.30	0.47
1:A:1858:ARG:CD	1:A:1860:ILE:HD11	2.33	0.46
1:A:1768:PHE:CD1	1:A:1769[B]:ARG:NH1	2.74	0.46
1:A:1905:SER:HB3	2:A:142:HOH:O	2.16	0.45
1:A:1828[B]:LEU:HD21	1:A:1848:ILE:CD1	2.47	0.45
1:A:1829:ILE:HG13	1:A:1830:LEU:N	2.31	0.45
1:A:1721[B]:ILE:HD12	1:A:1740:ASP:OD1	2.17	0.44
1:A:1774:VAL:HG13	1:A:1911:THR:HG21	2.00	0.42
1:A:1828[B]:LEU:HD21	1:A:1848:ILE:CG1	2.49	0.42
1:A:1873:VAL:HB	1:A:1874:PRO:HD2	2.01	0.42
1:A:1797:ASN:HD22	1:A:1863:PHE:HE1	1.68	0.42
1:A:1828[A]:LEU:HD21	1:A:1850:GLY:HA3	2.01	0.41
1:A:1828[B]:LEU:CD1	1:A:1848:ILE:CG1	2.86	0.41
1:A:1715:ARG:HH11	1:A:1715:ARG:HD2	1.77	0.41
1:A:1816:TRP:HD1	1:A:1817:PRO:O	2.04	0.40

All (5) 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:1768:PHE:CB	1:A:1970:ARG:NH2[4_455]	1.40	0.80
1:A:1768:PHE:CD2	1:A:1970:ARG:NH1[4_455]	1.44	0.76
1:A:1768:PHE:CG	1:A:1970:ARG:NH2[4_455]	2.15	0.05
1:A:1768:PHE:CE2	1:A:1970:ARG:NH1[4_455]	2.17	0.03
1:A:1768:PHE:CD2	1:A:1970:ARG:CZ[4_455]	2.19	0.01



## 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	282/313 (90%)	269 (95%)	9 (3%)	4 (1%)	14 3

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1908	VAL
1	A	1769[A]	ARG
1	A	1769[B]	ARG
1	A	1947	VAL

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

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	263/284 (93%)	256 (97%)	7 (3%)	52 34

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1686	ASN
1	A	1699	SER
1	A	1766	ASN
1	A	1768	PHE
1	A	1783	LYS
1	A	1829	ILE
1	A	1875	GLU

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

Mol	Chain	Res	Type
1	A	1687	GLN
1	A	1797	ASN

### 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	276/313 (88%)	0.41	21 (7%) 17 16	18, 28, 45, 57	3 (1%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1768	PHE	7.1
1	A	1699	SER	4.6
1	A	1748	ASN	4.6
1	A	1853	GLN	4.2
1	A	1871	HIS	4.0
1	A	1895	PRO	3.9
1	A	1814	HIS	3.6
1	A	1769[A]	ARG	3.5
1	A	1893	ARG	3.2
1	A	1701	TYR	2.8
1	A	1897	ALA	2.6
1	A	1802	THR	2.6
1	A	1765	GLY	2.5
1	A	1875	GLU	2.4
1	A	1698	ASP	2.4
1	A	1851	GLU	2.2
1	A	1870	ASP	2.2
1	A	1905	SER	2.2
1	A	1764	PRO	2.1
1	A	1693[A]	MET	2.1
1	A	1906	ALA	2.0

### 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

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.