



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:48 PM GMT

PDB ID : 1FVR  
Title : TIE2 KINASE DOMAIN  
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Deposited on : 2000-09-20  
Resolution : 2.20 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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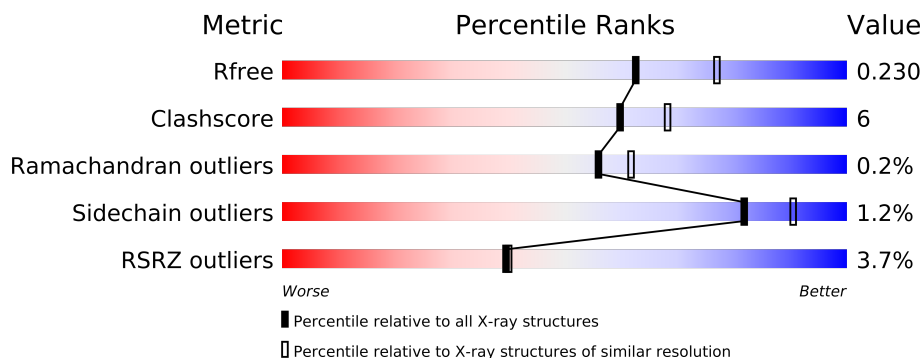
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.20 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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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	327	
1	B	327	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5201 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 TYROSINE-PROTEIN KINASE TIE-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2382	1524	402	442	14			
1	B	300	Total	C	N	O	S	0	0	0
			2378	1521	399	444	14			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	798	MET	-	EXPRESSION TAG	UNP Q02763
A	799	LYS	-	EXPRESSION TAG	UNP Q02763
A	800	LYS	-	EXPRESSION TAG	UNP Q02763
A	801	HIS	-	EXPRESSION TAG	UNP Q02763
A	802	HIS	-	EXPRESSION TAG	UNP Q02763
A	803	HIS	-	EXPRESSION TAG	UNP Q02763
A	804	HIS	-	EXPRESSION TAG	UNP Q02763
A	805	HIS	-	EXPRESSION TAG	UNP Q02763
A	806	HIS	-	EXPRESSION TAG	UNP Q02763
A	807	GLY	-	EXPRESSION TAG	UNP Q02763
B	798	MET	-	EXPRESSION TAG	UNP Q02763
B	799	LYS	-	EXPRESSION TAG	UNP Q02763
B	800	LYS	-	EXPRESSION TAG	UNP Q02763
B	801	HIS	-	EXPRESSION TAG	UNP Q02763
B	802	HIS	-	EXPRESSION TAG	UNP Q02763
B	803	HIS	-	EXPRESSION TAG	UNP Q02763
B	804	HIS	-	EXPRESSION TAG	UNP Q02763
B	805	HIS	-	EXPRESSION TAG	UNP Q02763
B	806	HIS	-	EXPRESSION TAG	UNP Q02763
B	807	GLY	-	EXPRESSION TAG	UNP Q02763

- Molecule 2 is water.

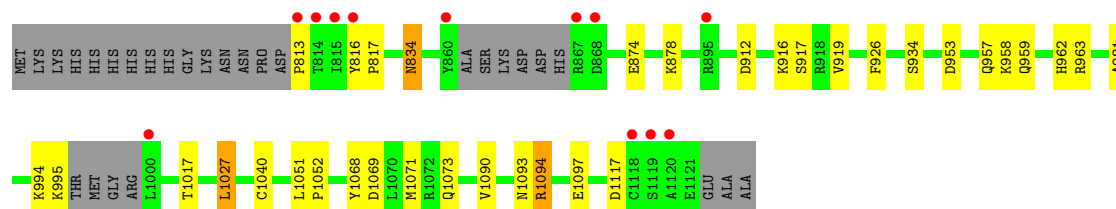
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	225	Total 225	O 225	0	0
2	B	216	Total 216	O 216	0	0

### 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.

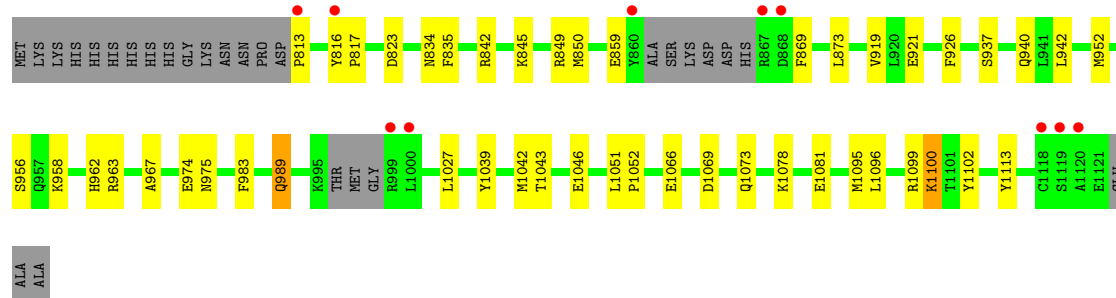
#### • Molecule 1: TYROSINE-PROTEIN KINASE TIE-2

Chain A: 



#### • Molecule 1: TYROSINE-PROTEIN KINASE TIE-2

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.49Å 92.89Å 70.80Å 90.00° 108.93° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.77 – 1.92	Depositor EDS
% Data completeness (in resolution range)	96.3 (20.00-2.20) 91.8 (19.77-1.92)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 1.92Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.225 , 0.225 0.205 , 0.230	Depositor DCC
$R_{free}$ test set	4089 reflections (10.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.2	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 58904 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5201	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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	0.34	0/2433	0.58	1/3295 (0.0%)
1	B	0.34	0/2429	0.58	1/3292 (0.0%)
All	All	0.34	0/4862	0.58	2/6587 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	813	PRO	N-CA-CB	5.49	109.89	103.30
1	A	813	PRO	N-CA-CB	5.41	109.79	103.30

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	2382	0	2327	21	0
1	B	2378	0	2310	35	0
2	A	225	0	0	3	0
2	B	216	0	0	2	0
All	All	5201	0	4637	56	0

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 6.

All (56) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:937:SER:H	1:B:940:GLN:HE21	1.15	0.87
1:A:1017:THR:HG22	2:A:51:HOH:O	1.78	0.81
1:B:919:VAL:HG21	1:B:926:PHE:HD2	1.55	0.72
1:B:1039:TYR:HD1	1:B:1042:MET:HE1	1.54	0.71
1:B:937:SER:H	1:B:940:GLN:NE2	1.88	0.71
1:B:1069:ASP:O	1:B:1073:GLN:HG3	1.93	0.69
1:B:1078:LYS:HB2	1:B:1081:GLU:CG	2.25	0.66
1:B:1051:LEU:HB2	1:B:1052:PRO:HD3	1.78	0.65
1:B:1078:LYS:HB2	1:B:1081:GLU:HG3	1.80	0.63
1:B:842:ARG:HH21	1:B:850:MET:HA	1.63	0.63
1:B:1066:GLU:HB3	1:B:1095:MET:CE	2.29	0.62
1:A:919:VAL:HG21	1:A:926:PHE:HD2	1.65	0.62
1:B:1042:MET:HE2	2:B:108:HOH:O	1.99	0.61
1:B:1043:THR:OG1	1:B:1046:GLU:HG3	2.01	0.61
1:A:1093:ASN:O	1:A:1097:GLU:HG2	2.01	0.60
1:B:1039:TYR:CD1	1:B:1042:MET:HE1	2.36	0.60
1:A:919:VAL:HG21	1:A:926:PHE:CD2	2.38	0.59
1:A:994:LYS:O	1:A:995:LYS:CB	2.51	0.58
1:A:1069:ASP:O	1:A:1073:GLN:HG3	2.04	0.57
1:B:919:VAL:HG21	1:B:926:PHE:CD2	2.39	0.57
1:B:823:ASP:O	1:B:849:ARG:NH2	2.38	0.57
1:A:816:TYR:HB3	1:A:817:PRO:HA	1.85	0.56
1:A:1051:LEU:HB2	1:A:1052:PRO:HD3	1.87	0.55
1:B:1078:LYS:HB2	1:B:1081:GLU:HG2	1.89	0.55
1:B:859:GLU:HG2	1:B:869:PHE:CZ	2.42	0.55
1:B:989:GLN:NE2	2:B:121:HOH:O	2.42	0.52
1:B:1066:GLU:HB3	1:B:1095:MET:HE3	1.91	0.51
1:B:845:LYS:HB3	1:B:850:MET:CE	2.41	0.51
1:B:1099:ARG:O	1:B:1100:LYS:O	2.28	0.51
1:A:953:ASP:O	1:A:957:GLN:HG2	2.11	0.50
1:B:816:TYR:HB3	1:B:817:PRO:HA	1.93	0.50
1:A:1027:LEU:O	1:A:1027:LEU:HD12	2.11	0.49
1:A:1040:CYS:SG	1:A:1117:ASP:HB2	2.52	0.49
1:A:1017:THR:HG21	2:A:62:HOH:O	2.12	0.48
1:B:942:LEU:HB2	1:B:1096:LEU:HD21	1.96	0.47
1:A:962:HIS:O	1:A:963:ARG:HB2	2.14	0.47
1:B:842:ARG:HH21	1:B:850:MET:CA	2.28	0.47
1:B:967:ALA:N	1:B:1027:LEU:HD23	2.29	0.47
1:B:873:LEU:O	1:B:873:LEU:HD23	2.15	0.46
1:A:874:GLU:O	1:A:878:LYS:HG2	2.16	0.46
1:A:1017:THR:CG2	2:A:62:HOH:O	2.65	0.45
1:B:845:LYS:HB3	1:B:850:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:834:ASN:ND2	1:A:981:ALA:HB1	2.33	0.43
1:B:1027:LEU:C	1:B:1027:LEU:HD13	2.38	0.43
1:B:962:HIS:O	1:B:963:ARG:HB2	2.17	0.43
1:A:1068:TYR:O	1:A:1071:MET:HB2	2.18	0.43
1:A:1090:VAL:O	1:A:1094:ARG:HG2	2.18	0.43
1:B:921:GLU:HG3	1:B:1113:TYR:HE2	1.83	0.43
1:A:912:ASP:OD1	1:A:916:LYS:HE2	2.19	0.42
1:A:917:SER:O	1:A:934:SER:HA	2.19	0.42
1:B:974:GLU:O	1:B:975:ASN:HB2	2.20	0.41
1:B:835:PHE:CD2	1:B:983:PHE:HB2	2.55	0.41
1:A:958:LYS:O	1:A:959:GLN:HB2	2.20	0.41
1:B:952:MET:O	1:B:956:SER:HB2	2.21	0.41
1:B:1100:LYS:HD3	1:B:1102:TYR:CZ	2.56	0.40
1:B:1095:MET:HE2	1:B:1102:TYR:CD2	2.56	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	293/327 (90%)	285 (97%)	8 (3%)	0	100	100
1	B	294/327 (90%)	284 (97%)	9 (3%)	1 (0%)	50	53
All	All	587/654 (90%)	569 (97%)	17 (3%)	1 (0%)	56	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1100	LYS

### 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	250/280 (89%)	247 (99%)	3 (1%)	82	90
1	B	249/280 (89%)	246 (99%)	3 (1%)	82	90
All	All	499/560 (89%)	493 (99%)	6 (1%)	82	90

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	834	ASN
1	A	1027	LEU
1	A	1094	ARG
1	B	834	ASN
1	B	958	LYS
1	B	989	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	834	ASN
1	A	930	ASN
1	A	989	GLN
1	A	1053	GLN
1	A	1073	GLN
1	B	834	ASN
1	B	940	GLN
1	B	975	ASN
1	B	989	GLN
1	B	1053	GLN
1	B	1073	GLN
1	B	1093	ASN

### 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	299/327 (91%)	-0.20	12 (4%) 36 37	19, 31, 52, 66	0
1	B	300/327 (91%)	-0.20	10 (3%) 44 45	20, 31, 53, 68	0
All	All	599/654 (91%)	-0.20	22 (3%) 39 40	19, 31, 53, 68	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1118	CYS	5.6
1	A	860	TYR	5.0
1	B	1118	CYS	4.8
1	A	867	ARG	4.8
1	B	867	ARG	3.7
1	B	1119	SER	3.6
1	A	813	PRO	3.3
1	B	999	ARG	3.2
1	B	1120	ALA	3.1
1	A	1000	LEU	3.1
1	B	1000	LEU	3.1
1	A	814	THR	2.9
1	A	868	ASP	2.8
1	A	1119	SER	2.8
1	B	813	PRO	2.7
1	B	868	ASP	2.7
1	A	1120	ALA	2.6
1	A	816	TYR	2.6
1	B	816	TYR	2.5
1	B	860	TYR	2.5
1	A	895	ARG	2.2
1	A	815	ILE	2.0

## 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.