



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:34 pm GMT

PDB ID : 4L00  
Title : Crystal structure of the apo Jak1 pseudokinase domain  
Authors : Toms, A.V.; Eck, M.J.  
Deposited on : 2013-05-30  
Resolution : 1.80 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) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

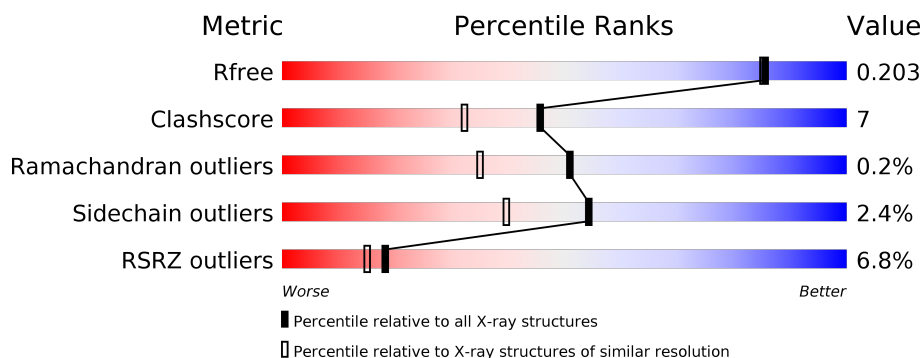
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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	304	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	304	<div> <div>8%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>•</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4931 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 Tyrosine-protein kinase JAK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	7	0
			2268	1453	383	412	20			
1	B	278	Total	C	N	O	S	0	9	0
			2287	1467	384	416	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	557	GLY	-	EXPRESSION TAG	UNP P23458
A	558	SER	-	EXPRESSION TAG	UNP P23458
A	559	THR	-	EXPRESSION TAG	UNP P23458
A	560	SER	-	EXPRESSION TAG	UNP P23458
B	557	GLY	-	EXPRESSION TAG	UNP P23458
B	558	SER	-	EXPRESSION TAG	UNP P23458
B	559	THR	-	EXPRESSION TAG	UNP P23458
B	560	SER	-	EXPRESSION TAG	UNP P23458

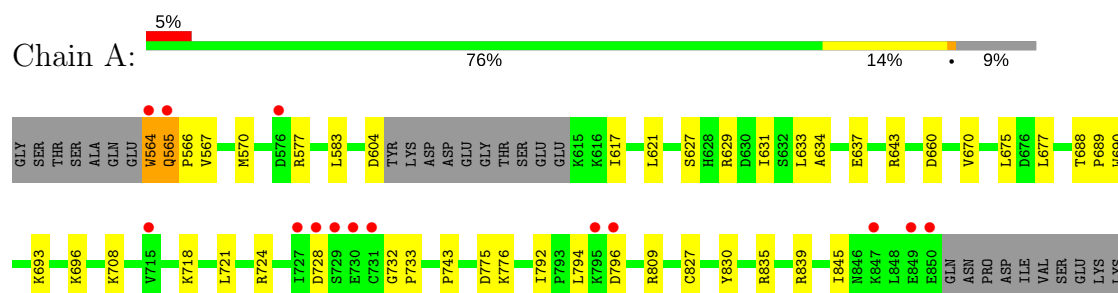
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	217	Total	O	0	0
			217	217		
2	B	159	Total	O	0	0
			159	159		

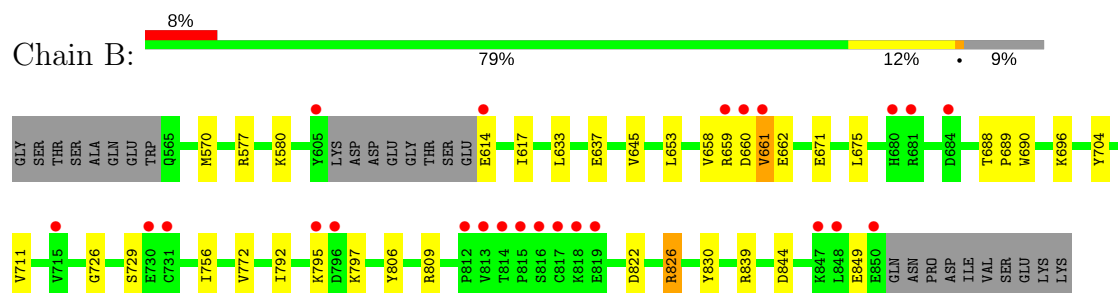
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 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 JAK1



#### • Molecule 1: Tyrosine-protein kinase JAK1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.03Å 80.66Å 76.23Å 90.00° 95.44° 90.00°	Depositor
Resolution (Å)	28.89 – 1.80 28.89 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (28.89-1.80) 97.4 (28.89-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.169 , 0.203 0.168 , 0.203	Depositor DCC
$R_{free}$ test set	2527 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 56.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4931	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 5.46% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.62	0/2338	0.77	2/3156 (0.1%)
1	B	0.57	0/2362	0.74	0/3188
All	All	0.60	0/4700	0.76	2/6344 (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	A	835	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	775	ASP	CB-CG-OD1	5.08	122.87	118.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2268	0	2310	39	0
1	B	2287	0	2338	37	0
2	A	217	0	0	12	0
2	B	159	0	0	6	0
All	All	4931	0	4648	67	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 7.

All (67) 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:B:645[B]:VAL:HG23	1:B:704:TYR:CE1	1.77	1.19
1:B:645[B]:VAL:HG23	1:B:704:TYR:HE1	1.05	1.13
1:B:822:ASP:OD2	1:B:826:ARG:NH1	1.95	1.00
1:B:662:GLU:HG2	2:B:961:HOH:O	1.62	0.99
1:A:796:ASP:HB2	2:A:1116:HOH:O	1.72	0.89
1:A:633:LEU:HD11	1:B:570[B]:MET:HG2	1.54	0.88
1:B:617:ILE:HD11	2:B:1008:HOH:O	1.73	0.88
1:A:670:VAL:HB	1:A:721[A]:LEU:HD23	1.63	0.80
1:B:839:ARG:HG2	2:B:904:HOH:O	1.85	0.76
1:B:826:ARG:NH2	1:B:844:ASP:OD2	2.23	0.72
1:A:565:GLN:H	1:A:566:PRO:HD3	1.53	0.72
1:A:570[B]:MET:HG3	1:B:570[B]:MET:CE	2.22	0.69
1:B:645[B]:VAL:CG2	1:B:704:TYR:HE1	1.96	0.67
1:B:645[B]:VAL:CG2	1:B:704:TYR:CE1	2.68	0.67
1:B:662:GLU:HA	2:B:943:HOH:O	1.95	0.66
1:B:580:LYS:HE3	2:B:972:HOH:O	1.95	0.65
1:A:570[B]:MET:HG3	1:B:570[B]:MET:HE2	1.80	0.64
1:A:564:TRP:HA	2:A:1108:HOH:O	1.96	0.64
1:B:580:LYS:HB3	1:B:659:ARG:HH11	1.63	0.62
1:A:583:LEU:HD11	1:A:621:LEU:HD21	1.82	0.61
1:B:660:ASP:O	1:B:661:VAL:HG12	2.01	0.60
1:A:565:GLN:N	1:A:566:PRO:HD3	2.18	0.58
1:A:566:PRO:HG2	2:A:1112:HOH:O	2.05	0.57
1:A:724:ARG:HD2	1:A:732:GLY:O	2.06	0.56
1:A:633:LEU:CD1	1:B:570[B]:MET:HG2	2.31	0.56
1:A:629:ARG:HH21	1:B:577:ARG:HH22	1.56	0.53
1:A:564:TRP:N	1:A:564:TRP:CD1	2.77	0.52
1:A:633:LEU:HD11	1:B:570[B]:MET:CG	2.34	0.52
1:B:580:LYS:HB3	1:B:659:ARG:NH1	2.23	0.52
1:A:565:GLN:N	1:A:566:PRO:CD	2.73	0.51
1:A:570[A]:MET:HE2	1:B:633:LEU:HD11	1.93	0.50
1:A:564:TRP:N	2:A:1087:HOH:O	2.44	0.50
1:B:696:LYS:NZ	1:B:849:GLU:OE1	2.42	0.50
1:A:564:TRP:CE3	1:A:708:LYS:HD2	2.47	0.49
1:A:792:ILE:HD13	2:A:924:HOH:O	2.13	0.48
1:B:726:GLY:HA2	1:B:729[B]:SER:OG	2.12	0.48
1:A:721[A]:LEU:HD21	2:A:1025:HOH:O	2.13	0.48
1:A:696:LYS:HG3	1:A:845:ILE:HG21	1.96	0.47
1:A:577:ARG:NH2	2:A:1115:HOH:O	2.48	0.47
1:A:570[B]:MET:SD	1:A:637:GLU:HA	2.55	0.46
1:A:693:LYS:HD2	1:A:733:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:LYS:HB3	1:A:718:LYS:HE2	1.62	0.46
1:B:661:VAL:HG22	2:B:999:HOH:O	2.15	0.46
1:A:634:ALA:HB1	1:A:743:PRO:HD2	1.98	0.45
1:A:839:ARG:HG2	2:A:1072:HOH:O	2.16	0.44
1:A:675:LEU:HD11	1:A:690:TRP:HH2	1.82	0.44
1:A:617[A]:ILE:HD11	2:A:961:HOH:O	2.18	0.44
1:B:658:VAL:HG12	1:B:659:ARG:N	2.32	0.44
1:B:711[B]:VAL:HG12	1:B:772:VAL:HG22	1.99	0.43
1:B:711[B]:VAL:HG12	1:B:772:VAL:CG2	2.48	0.43
1:B:792:ILE:HB	1:B:795:LYS:HB2	2.01	0.43
1:A:570[B]:MET:HG3	1:B:570[B]:MET:HE3	2.00	0.43
1:A:688:THR:HB	1:A:689:PRO:HD3	2.01	0.43
1:B:570[A]:MET:SD	1:B:637:GLU:HA	2.58	0.43
1:B:797:LYS:HD3	1:B:797:LYS:HA	1.72	0.43
1:B:809:ARG:HA	1:B:830:TYR:CZ	2.54	0.42
1:A:809:ARG:HA	1:A:830:TYR:CZ	2.55	0.42
1:B:675:LEU:HD11	1:B:690:TRP:HH2	1.84	0.42
1:A:570[A]:MET:SD	1:B:570[A]:MET:HE3	2.60	0.41
1:B:756:ILE:HG12	1:B:806:TYR:CE2	2.55	0.41
1:A:721[A]:LEU:CD2	2:A:1025:HOH:O	2.68	0.41
1:A:792:ILE:CD1	2:A:943:HOH:O	2.68	0.41
1:A:627:SER:HB3	1:A:631:ILE:HB	2.01	0.41
1:A:643:ARG:HG2	2:A:935:HOH:O	2.20	0.41
1:B:658:VAL:HG12	1:B:659:ARG:H	1.86	0.41
1:B:688:THR:HB	1:B:689:PRO:HD3	2.03	0.40
1:A:776:LYS:O	1:A:827:CYS:HB3	2.22	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	280/304 (92%)	275 (98%)	4 (1%)	1 (0%)	38	23
1	B	283/304 (93%)	279 (99%)	4 (1%)	0	100	100
All	All	563/608 (93%)	554 (98%)	8 (1%)	1 (0%)	51	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	565	GLN

### 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	259/276 (94%)	252 (97%)	7 (3%)	50	35
1	B	262/276 (95%)	257 (98%)	5 (2%)	62	50
All	All	521/552 (94%)	509 (98%)	12 (2%)	54	41

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	564	TRP
1	A	567	VAL
1	A	604	ASP
1	A	660	ASP
1	A	677	LEU
1	A	728	ASP
1	A	794	LEU
1	B	614	GLU
1	B	653	LEU
1	B	661	VAL
1	B	671	GLU
1	B	826	ARG

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	663	ASN
1	B	663	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 ⓘ

### 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	277/304 (91%)	0.13	14 (5%) 29 24	12, 24, 48, 85	0
1	B	278/304 (91%)	0.25	24 (8%) 11 9	15, 27, 58, 81	0
All	All	555/608 (91%)	0.19	38 (6%) 18 15	12, 26, 54, 85	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	564	TRP	8.7
1	A	731	CYS	7.7
1	A	730	GLU	7.2
1	A	729	SER	6.4
1	B	816	SER	5.7
1	A	728	ASP	5.3
1	B	661	VAL	4.6
1	B	614	GLU	4.6
1	B	814	THR	4.5
1	B	660	ASP	4.5
1	B	818	LYS	4.3
1	B	813	VAL	4.0
1	B	659	ARG	4.0
1	A	850	GLU	4.0
1	A	727	ILE	3.6
1	B	847	LYS	3.4
1	B	605	TYR	3.4
1	A	796	ASP	3.3
1	B	796	ASP	3.2
1	A	576	ASP	3.1
1	B	684	ASP	3.1
1	B	730	GLU	3.0
1	B	819	GLU	2.7
1	B	815	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	681	ARG	2.6
1	B	850	GLU	2.5
1	A	565	GLN	2.4
1	B	715	VAL	2.4
1	B	731	CYS	2.4
1	B	795	LYS	2.4
1	A	795	LYS	2.4
1	A	847	LYS	2.3
1	B	848	LEU	2.3
1	B	680	HIS	2.2
1	A	715	VAL	2.2
1	A	849	GLU	2.1
1	B	812	PRO	2.1
1	B	817	CYS	2.1

## 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 [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.