



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:06 AM GMT

PDB ID : 4JDH  
Title : Crystal structure of Serine/threonine-proteinkinase PAK 4 in complex with  
Paktide T peptide substrate  
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Deposited on : 2013-02-25  
Resolution : 2.00 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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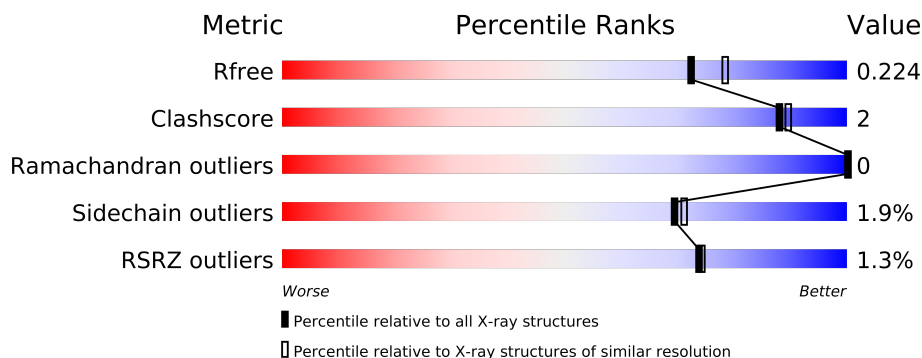
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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	346	
2	B	15	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2455 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 Serine/threonine-proteinkinase PAK 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	290	2300	1467	405	413	1	14	0	1	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	MET	-	EXPRESSION TAG	UNP O96013
A	247	GLY	-	EXPRESSION TAG	UNP O96013
A	248	SER	-	EXPRESSION TAG	UNP O96013
A	249	SER	-	EXPRESSION TAG	UNP O96013
A	250	HIS	-	EXPRESSION TAG	UNP O96013
A	251	HIS	-	EXPRESSION TAG	UNP O96013
A	252	HIS	-	EXPRESSION TAG	UNP O96013
A	253	HIS	-	EXPRESSION TAG	UNP O96013
A	254	HIS	-	EXPRESSION TAG	UNP O96013
A	255	HIS	-	EXPRESSION TAG	UNP O96013
A	256	SER	-	EXPRESSION TAG	UNP O96013
A	257	SER	-	EXPRESSION TAG	UNP O96013
A	258	GLY	-	EXPRESSION TAG	UNP O96013
A	259	LEU	-	EXPRESSION TAG	UNP O96013
A	260	VAL	-	EXPRESSION TAG	UNP O96013
A	261	PRO	-	EXPRESSION TAG	UNP O96013
A	262	ARG	-	EXPRESSION TAG	UNP O96013
A	263	GLY	-	EXPRESSION TAG	UNP O96013
A	264	SER	-	EXPRESSION TAG	UNP O96013
A	265	HIS	-	EXPRESSION TAG	UNP O96013
A	266	MET	-	EXPRESSION TAG	UNP O96013
A	267	GLU	-	EXPRESSION TAG	UNP O96013
A	268	ASN	-	EXPRESSION TAG	UNP O96013
A	269	LEU	-	EXPRESSION TAG	UNP O96013
A	270	TYR	-	EXPRESSION TAG	UNP O96013
A	271	PHE	-	EXPRESSION TAG	UNP O96013
A	272	GLN	-	EXPRESSION TAG	UNP O96013

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Chain	Residue	Modelled	Actual	Comment	Reference
A	273	GLY	-	EXPRESSION TAG	UNP O96013
A	274	ALA	-	EXPRESSION TAG	UNP O96013
A	275	ARG	-	EXPRESSION TAG	UNP O96013
A	276	ALA	-	EXPRESSION TAG	UNP O96013
A	277	ARG	-	EXPRESSION TAG	UNP O96013
A	278	GLN	-	EXPRESSION TAG	UNP O96013
A	279	GLU	-	EXPRESSION TAG	UNP O96013
A	280	ASN	-	EXPRESSION TAG	UNP O96013
A	281	GLY	-	EXPRESSION TAG	UNP O96013
A	282	MET	-	EXPRESSION TAG	UNP O96013
A	283	PRO	-	EXPRESSION TAG	UNP O96013
A	284	GLU	-	EXPRESSION TAG	UNP O96013
A	285	LYS	-	EXPRESSION TAG	UNP O96013

- Molecule 2 is a protein called Paktide T.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	0	0	0
			85	55	19	11			

- Molecule 3 is water.

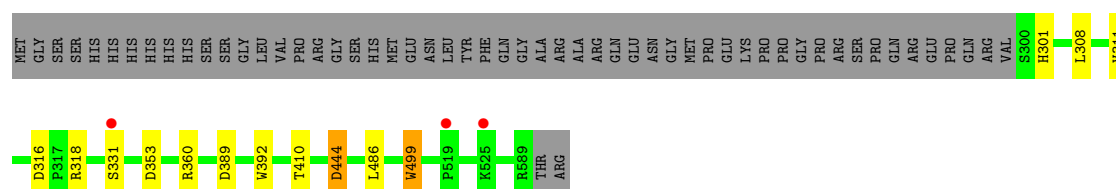
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total	O	0	0
			70	70		

### 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: Serine/threonine-proteinkinase PAK 4

Chain A: 



- Molecule 2: Paktide T

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.93Å 61.93Å 179.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 43.79 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.00) 100.0 (43.79-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.183 , 0.224 0.181 , 0.224	Depositor DCC
$R_{free}$ test set	1250 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.9	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 44.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 24506 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2455	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SEP

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	2/2340 (0.1%)	0.98	3/3168 (0.1%)
2	B	1.30	1/88 (1.1%)	1.00	0/116
All	All	0.97	3/2428 (0.1%)	0.98	3/3284 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	TRP	CD2-CE2	5.95	1.48	1.41
1	A	499	TRP	CD2-CE2	5.43	1.47	1.41
1	A	392	TRP	CD2-CE2	5.05	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	444	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	486	LEU	CB-CG-CD2	-5.31	101.97	111.00
1	A	353	ASP	CB-CG-OD2	-5.13	113.68	118.30

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	2300	0	0	4	0
2	B	85	0	82	2	0
3	A	70	0	0	1	0
All	All	2455	0	82	6	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 2.

All (6) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:316:ASP:OD2	1:A:318:ARG:NH2	2.47	0.46
2:B:-3:ARG:HG3	2:B:-1:ARG:H	1.81	0.45
2:B:-3:ARG:HH11	2:B:-1:ARG:HG2	1.83	0.43
1:A:301:HIS:NE2	1:A:389:ASP:OD1	2.52	0.43
1:A:499:TRP:C	1:A:499:TRP:CD1	2.94	0.41
1:A:331:SER:N	3:A:640:HOH:O	2.53	0.41

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	288/346 (83%)	282 (98%)	6 (2%)	0	100	100
2	B	7/15 (47%)	6 (86%)	1 (14%)	0	100	100
All	All	295/361 (82%)	288 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	253/300 (84%)	248 (98%)	5 (2%)	68	69
2	B	7/10 (70%)	7 (100%)	0	100	100
All	All	260/310 (84%)	255 (98%)	5 (2%)	69	71

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	308	LEU
1	A	311	VAL
1	A	360	ARG
1	A	410	THR
1	A	444	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	SEP	A	474	1	9,9,10	6.63	2 (22%)	10,12,14	1.79	3 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	474	1	-	0/6/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	474	SEP	O-C	19.70	1.25	1.11
1	A	474	SEP	CA-C	2.08	1.52	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	474	SEP	O3P-P-O1P	3.23	121.01	110.44
1	A	474	SEP	C-CA-N	-3.04	110.80	113.83
1	A	474	SEP	O2P-P-OG	-2.61	99.45	106.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	290/346 (83%)	-0.01	3 (1%) 79 80	30, 43, 63, 76	0
2	B	9/15 (60%)	1.33	1 (11%) 6 6	45, 60, 77, 92	0
All	All	299/361 (82%)	0.03	4 (1%) 74 74	30, 43, 64, 92	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	3	PHE	4.3
1	A	331	SER	2.9
1	A	525	LYS	2.4
1	A	519	PRO	2.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	A	474	10/11	0.09	-0.74	37,39,40,44	0

### 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.