



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 12:38 pm GMT

PDB ID : 2F7K  
Title : Crystal Structure of Human Pyridoxal Kinase  
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Deposited on : 2005-12-01  
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/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)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

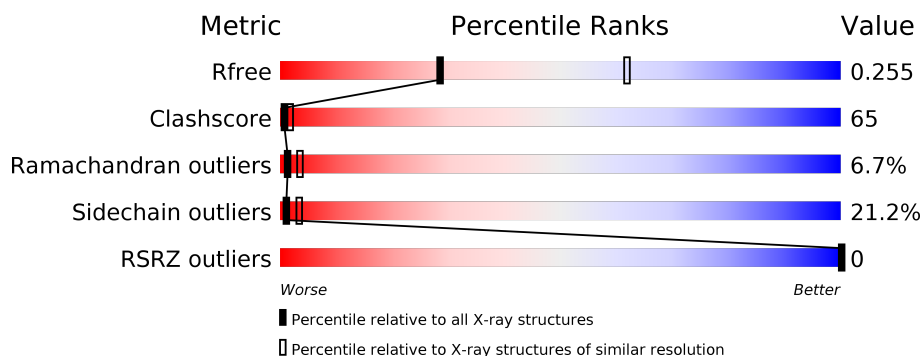
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

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	327	
1	B	327	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5327 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 Pyridoxal kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2560	1608	458	478	16			
1	B	323	Total	C	N	O	S	0	0	0
			2560	1608	458	478	16			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	SER	-	CLONING ARTIFACT	UNP O00764
A	-13	TYR	-	CLONING ARTIFACT	UNP O00764
A	-12	TYR	-	CLONING ARTIFACT	UNP O00764
A	-11	HIS	-	EXPRESSION TAG	UNP O00764
A	-10	HIS	-	EXPRESSION TAG	UNP O00764
A	-9	HIS	-	EXPRESSION TAG	UNP O00764
A	-8	HIS	-	EXPRESSION TAG	UNP O00764
A	-7	HIS	-	EXPRESSION TAG	UNP O00764
A	-6	HIS	-	EXPRESSION TAG	UNP O00764
A	-5	HIS	-	EXPRESSION TAG	UNP O00764
A	-4	GLU	-	CLONING ARTIFACT	UNP O00764
A	-3	GLY	-	CLONING ARTIFACT	UNP O00764
A	-2	VAL	-	CLONING ARTIFACT	UNP O00764
A	-1	ARG	-	CLONING ARTIFACT	UNP O00764
A	0	THR	-	CLONING ARTIFACT	UNP O00764
B	-14	SER	-	CLONING ARTIFACT	UNP O00764
B	-13	TYR	-	CLONING ARTIFACT	UNP O00764
B	-12	TYR	-	CLONING ARTIFACT	UNP O00764
B	-11	HIS	-	EXPRESSION TAG	UNP O00764
B	-10	HIS	-	EXPRESSION TAG	UNP O00764
B	-9	HIS	-	EXPRESSION TAG	UNP O00764
B	-8	HIS	-	EXPRESSION TAG	UNP O00764
B	-7	HIS	-	EXPRESSION TAG	UNP O00764
B	-6	HIS	-	EXPRESSION TAG	UNP O00764
B	-5	HIS	-	EXPRESSION TAG	UNP O00764

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLU	-	CLONING ARTIFACT	UNP O00764
B	-3	GLY	-	CLONING ARTIFACT	UNP O00764
B	-2	VAL	-	CLONING ARTIFACT	UNP O00764
B	-1	ARG	-	CLONING ARTIFACT	UNP O00764
B	0	THR	-	CLONING ARTIFACT	UNP O00764

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	96	Total O 96 96	0	0
2	B	111	Total O 111 111	0	0



- Molecule 1: Pyridoxal kinase



P249	N250	N251	L252	K253	C256	E257	T259	V260	S261	T262	L263	H264	H265	V266	L267	Q268	R269	T270	L271	Q272	C273	A274	A278	G279	E280	Q281	V282	R283	P284	S285	P286	M287	Q288	L289	R292	M293	V294	Q295	S296	K297	R298	D299	I300	E301	D302	F303	E304	I305	V306	V307	O308	A309	T310	V311	L312
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.50Å 52.50Å 301.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 7.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	81.0 (8.00-2.80) 81.0 (7.99-2.80)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.94 (at 2.78Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.228 , 0.271 0.213 , 0.255	Depositor DCC
$R_{free}$ test set	709 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.3	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 71.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.190 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5327	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% 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	0.46	0/2612	0.87	10/3540 (0.3%)
1	B	0.45	0/2612	0.83	3/3540 (0.1%)
All	All	0.45	0/5224	0.85	13/7080 (0.2%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	PRO	CA-N-CD	-7.94	100.39	111.50
1	A	149	PRO	CA-N-CD	-7.75	100.66	111.50
1	B	120	TRP	CA-CB-CG	6.54	126.12	113.70
1	A	-3	GLY	N-CA-C	-6.51	96.83	113.10
1	A	192	SER	N-CA-C	-5.85	95.22	111.00

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	2560	0	2551	354	0
1	B	2560	0	2551	334	0
2	A	96	0	0	0	0
2	B	111	0	0	3	0
All	All	5327	0	5102	660	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 65.

The worst 5 of 660 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:199:LEU:HB2	1:A:223:ILE:HB	1.38	1.05
1:A:72:ASN:HD21	1:A:74:MET:HG3	1.22	1.04
1:A:221:MET:HG2	1:A:309:ALA:HA	1.39	1.02
1:A:147:ILE:H	1:A:147:ILE:CD1	1.74	1.00
1:A:147:ILE:H	1:A:147:ILE:HD13	1.24	1.00

There are no symmetry-related clashes.

## 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	321/327 (98%)	229 (71%)	65 (20%)	27 (8%)	1	2
1	B	321/327 (98%)	240 (75%)	65 (20%)	16 (5%)	2	7
All	All	642/654 (98%)	469 (73%)	130 (20%)	43 (7%)	1	3

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-9	HIS
1	A	59	SER
1	A	109	VAL
1	A	195	GLY
1	A	210	PRO

### 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	285/289 (99%)	226 (79%)	59 (21%)	1	3
1	B	285/289 (99%)	223 (78%)	62 (22%)	1	3
All	All	570/578 (99%)	449 (79%)	121 (21%)	1	3

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	292	ARG
1	B	5	CYS
1	B	273	CYS
1	A	305	ILE
1	B	-8	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	GLN
1	B	-10	HIS
1	B	209	ASN
1	A	288	GLN
1	A	308	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 [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	323/327 (98%)	-0.28	0 100 100	36, 44, 50, 56	0
1	B	323/327 (98%)	-0.28	0 100 100	35, 44, 50, 55	0
All	All	646/654 (98%)	-0.28	0 100 100	35, 44, 50, 56	0

There are no RSRZ outliers to report.

### 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.