



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 10:23 am BST

PDB ID : 1PKY  
Title : PYRUVATE KINASE FROM E. COLI IN THE T-STATE  
Authors : Mattevi, A.  
Deposited on : 1995-04-27  
Resolution : 2.50 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

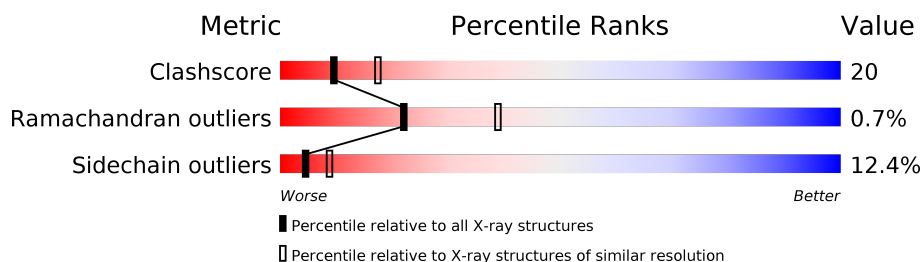
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 respectively. 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	470	
1	B	470	
1	C	470	
1	D	470	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14152 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 PYRUVATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	26	0	0
			3464	2159	600	680	25			
1	B	464	Total	C	N	O	S	16	0	0
			3464	2159	600	680	25			
1	C	433	Total	C	N	O	S	65	0	0
			3240	2022	564	630	24			
1	D	464	Total	C	N	O	S	11	0	0
			3464	2159	600	680	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	MET	GLN	CONFLICT	UNP P14178
B	279	MET	GLN	CONFLICT	UNP P14178
C	279	MET	GLN	CONFLICT	UNP P14178
D	279	MET	GLN	CONFLICT	UNP P14178

- Molecule 2 is water.

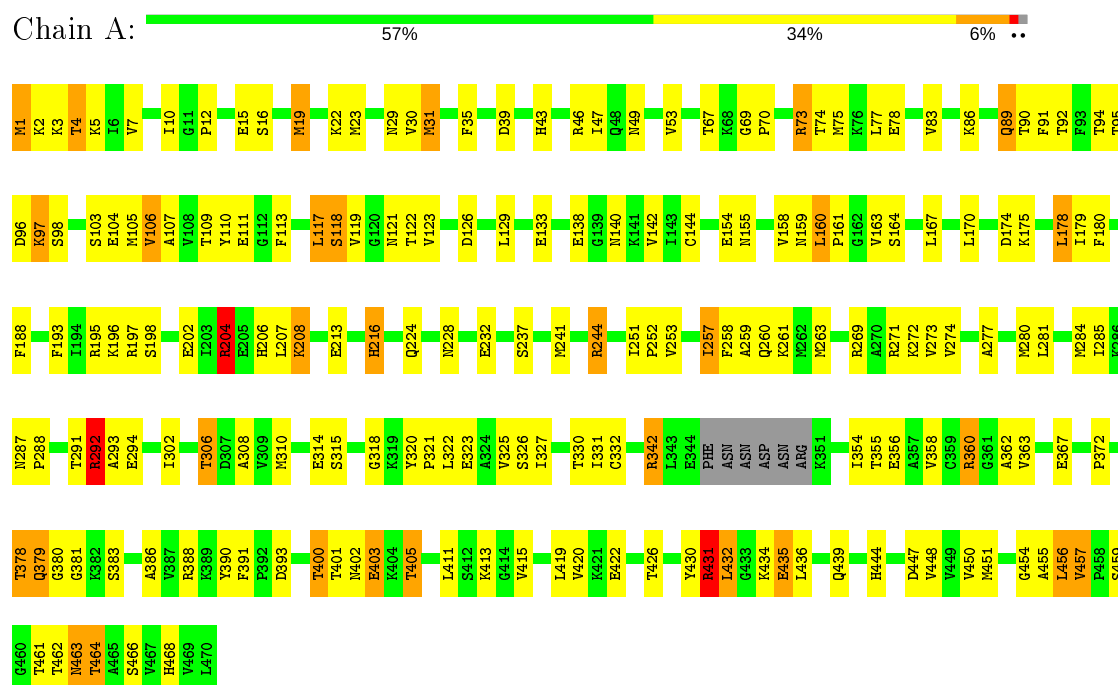
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	126	Total	O	0	0
			126	126		
2	B	137	Total	O	0	0
			137	137		
2	C	107	Total	O	0	0
			107	107		
2	D	150	Total	O	0	0
			150	150		

### 3 Residue-property plots

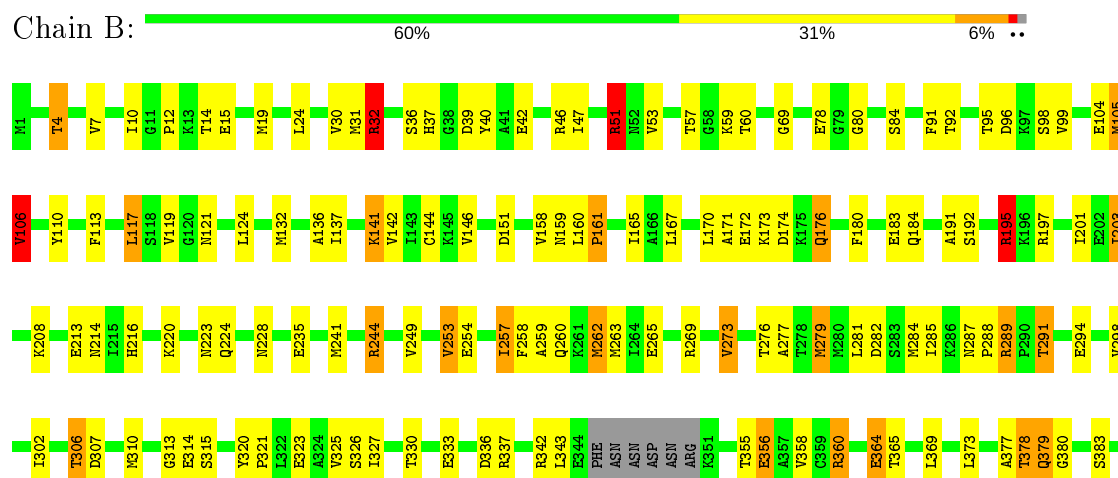
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

#### • Molecule 1: PYRUVATE KINASE



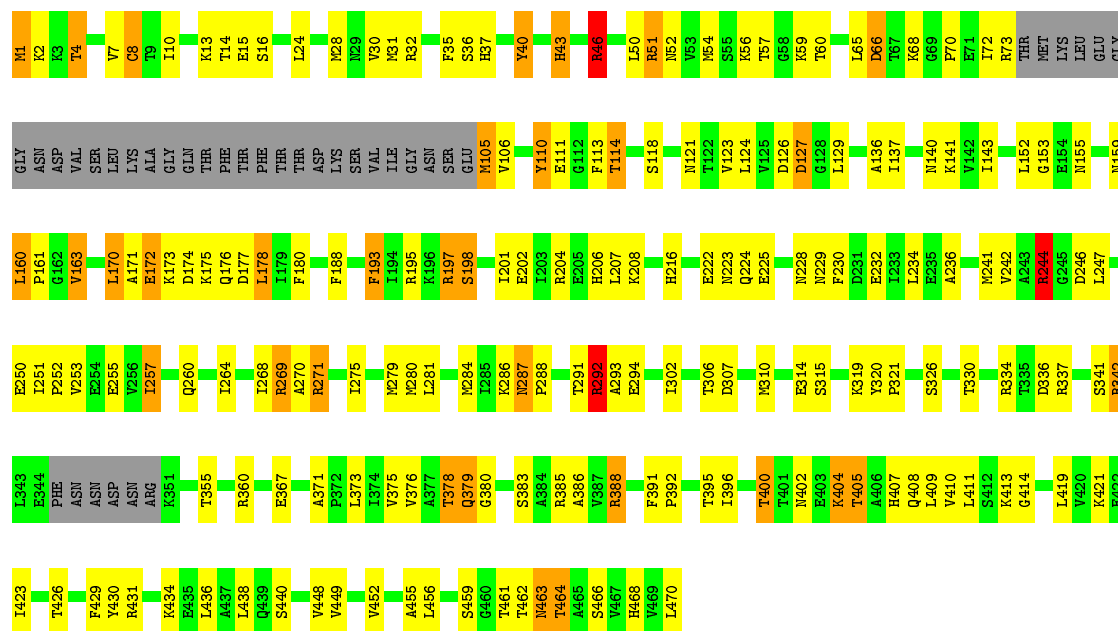
#### • Molecule 1: PYRUVATE KINASE





• Molecule 1: PYRUVATE KINASE

Chain C: 52% 33% 7% 8%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.91Å 129.58Å 241.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	99.9 (6.00-2.50)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.203 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14152	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

## 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	0.74	1/3498 (0.0%)	0.82	6/4719 (0.1%)
1	B	0.74	1/3498 (0.0%)	0.82	4/4719 (0.1%)
1	C	0.73	1/3271 (0.0%)	0.80	1/4411 (0.0%)
1	D	0.76	0/3498	0.81	3/4719 (0.1%)
All	All	0.74	3/13765 (0.0%)	0.81	14/18568 (0.1%)

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	7
1	B	0	8
1	C	0	8
1	D	0	5
All	All	0	28

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	8	CYS	CB-SG	-6.36	1.71	1.82
1	A	332	CYS	CB-SG	-5.89	1.72	1.81
1	B	144	CYS	CB-SG	-5.13	1.73	1.81

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	ALA	N-CA-C	8.30	133.42	111.00
1	A	277	ALA	CB-CA-C	-8.26	97.72	110.10
1	B	51	ARG	NE-CZ-NH1	-7.92	116.34	120.30
1	A	204	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	A	292	ARG	NE-CZ-NH2	-7.22	116.69	120.30

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	TYR	Sidechain
1	A	204	ARG	Sidechain
1	A	269	ARG	Sidechain
1	A	292	ARG	Sidechain
1	A	342	ARG	Sidechain

## 5.2 Too-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 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	3464	0	3541	152	0
1	B	3464	0	3541	130	0
1	C	3240	0	3327	149	0
1	D	3464	0	3541	110	0
2	A	126	0	0	8	0
2	B	137	0	0	10	0
2	C	107	0	0	12	0
2	D	150	0	0	9	0
All	All	14152	0	13950	532	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 20.

The worst 5 of 532 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:291:THR:HG22	1:A:293:ALA:H	1.18	1.07
1:A:4:THR:HG22	1:A:413:LYS:HE3	1.39	1.04
1:C:172:GLU:HA	1:C:175:LYS:HD2	1.43	0.96
1:A:291:THR:HG22	1:A:293:ALA:N	1.85	0.91
1:D:291:THR:HG22	1:D:293:ALA:H	1.35	0.90

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	460/470 (98%)	430 (94%)	27 (6%)	3 (1%)	22	39
1	B	460/470 (98%)	434 (94%)	24 (5%)	2 (0%)	34	54
1	C	427/470 (91%)	403 (94%)	17 (4%)	7 (2%)	9	17
1	D	460/470 (98%)	441 (96%)	18 (4%)	1 (0%)	47	68
All	All	1807/1880 (96%)	1708 (94%)	86 (5%)	13 (1%)	22	39

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	459	SER
1	C	459	SER
1	D	459	SER
1	A	97	LYS
1	A	164	SER

### 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	377/389 (97%)	329 (87%)	48 (13%)	4	8
1	B	377/389 (97%)	328 (87%)	49 (13%)	4	7
1	C	352/389 (90%)	307 (87%)	45 (13%)	4	8
1	D	377/389 (97%)	335 (89%)	42 (11%)	6	11
All	All	1483/1556 (95%)	1299 (88%)	184 (12%)	4	9

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	373	LEU
1	C	51	ARG
1	D	378	THR
1	B	379	GLN
1	B	449	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	149	ASN
1	C	224	GLN
1	D	407	HIS
1	C	155	ASN
1	C	206	HIS

### 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 ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.