



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 10:59 AM GMT

PDB ID : 1JM6  
Title : Pyruvate dehydrogenase kinase, isozyme 2, containing ADP  
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Deposited on : 2001-07-17  
Resolution : 2.50 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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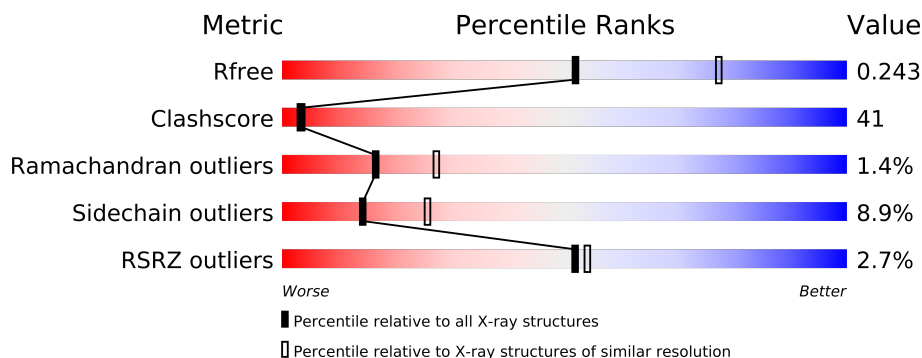
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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. 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	407	
1	B	407	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 5677 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.

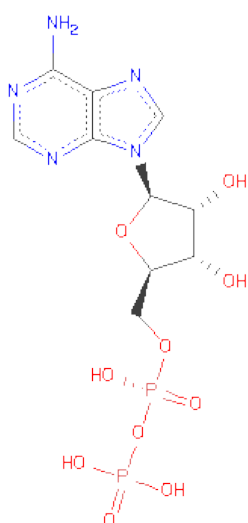
- Molecule 1 is a protein called Pyruvate dehydrogenase kinase, isozyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2709	1743	444	505	17			
1	B	336	Total	C	N	O	S	0	0	0
			2684	1728	441	498	17			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is water.

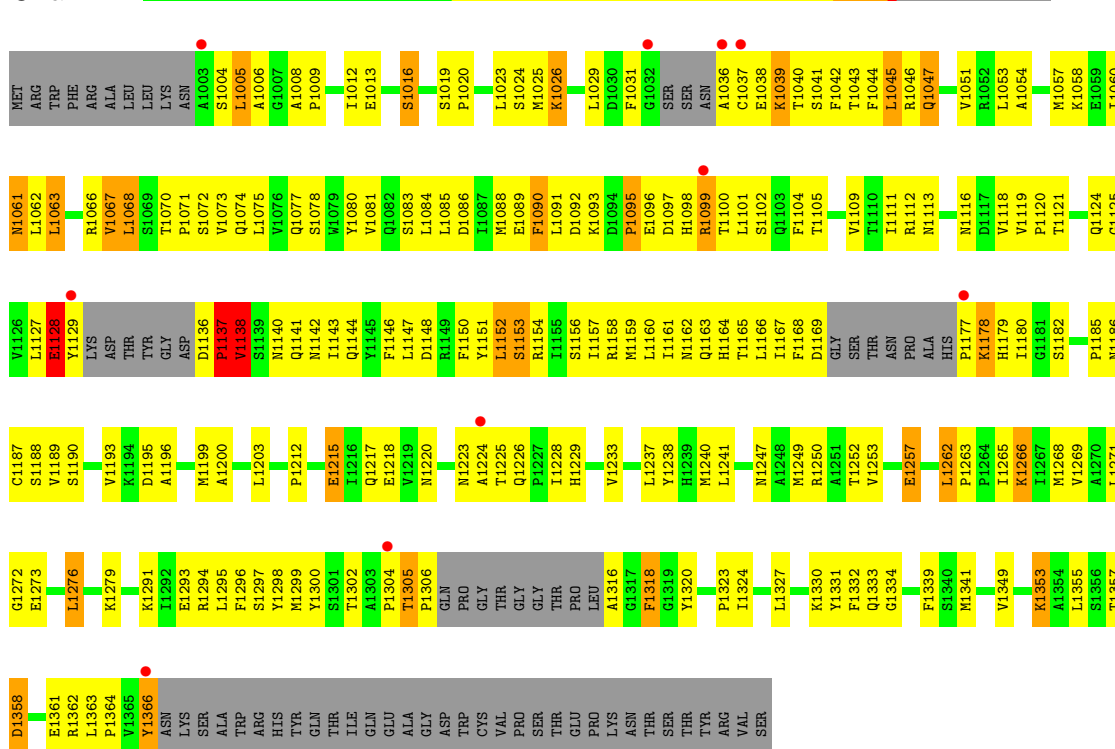
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total	O	0	0
			119	119		
4	B	109	Total	O	0	0
			109	109		

### 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.

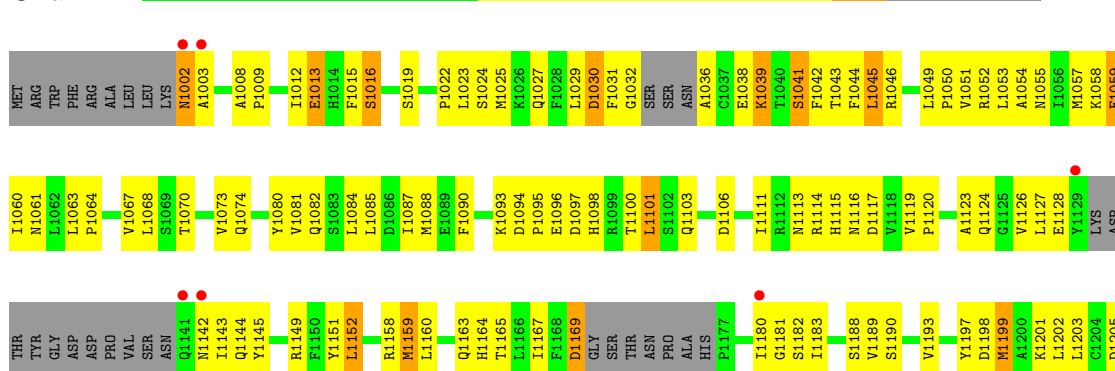
- Molecule 1: Pyruvate dehydrogenase kinase, isozyme 2

Chain A:



- Molecule 1: Pyruvate dehydrogenase kinase, isozyme 2

Chain B:



K1206	E1293	V1365
Y1207	R1294	TYR
M1208	L1295	ASN
M1209	F1296	LYS
	S1297	SER
P1212	Y1298	ALA
		TRP
E1215	T1302	ARG
I1216	A1303	HIS
Q1217	P1304	TYR
E1218	T1305	GLN
V1219	P1306	THR
N1220	GLN	ILE
	PRO	GLN
N1223	GLY	GLU
	THR	ALA
I1228	GLY	ALA
	GLY	GLY
	ASP	GLY
Y1232	THR	TRP
V1233	P1314	CYS
P1234	L1315	VAL
S1235	A1316	PRO
H1236	G1317	SER
L1237	F1318	THR
Y1238	G1319	GLU
	Y1320	PRO
F1245	G1321	LYS
K1246	L1322	ASN
N1247	P1323	THR
A1248	I1324	SER
M1249		THR
R1250	S1325	TYR
	R1326	ARG
	L1327	VAL
V1253		SER
S1258	K1330	
	Y1331	
	F1332	
T1261	Q1333	
L1262	G1334	
P1263	D1335	
P1264		
I1265	L1338	
K1266	F1339	
I1267	S1340	
M1268	M1341	
V1269	E1342	
A1270	G1343	
L1271	F1344	
	G1345	
L1276	T1346	
	D1347	
K1279		
	T1357	
R1283	D1358	
	S1359	
V1287	V1360	
	E1361	
R1290	R1362	
K1291	L1363	
I1292	P1364	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.42Å 109.87Å 71.41Å 90.00° 104.52° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50 29.26 – 2.40	Depositor EDS
% Data completeness (in resolution range)	84.2 (6.00-2.50) 85.4 (29.26-2.40)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 2.39Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.202 , 0.262 0.191 , 0.243	Depositor DCC
$R_{free}$ test set	1626 reflections (4.78%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.0	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.5	EDS
Estimated twinning fraction	0.478 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 35644 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5677	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.78	6/2771 (0.2%)	1.14	16/3752 (0.4%)
1	B	0.65	5/2745 (0.2%)	0.94	6/3715 (0.2%)
All	All	0.72	11/5516 (0.2%)	1.05	22/7467 (0.3%)

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1090	PHE	C-N	-8.56	1.14	1.34
1	A	1178	LYS	C-N	-7.66	1.16	1.34
1	B	1306	PRO	CA-C	7.37	1.67	1.52
1	A	1215	GLU	CB-CG	7.13	1.65	1.52
1	B	1215	GLU	CD-OE2	6.47	1.32	1.25

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1090	PHE	O-C-N	-12.48	102.73	122.70
1	A	1137	PRO	C-N-CA	10.68	148.39	121.70
1	A	1138	VAL	N-CA-C	10.08	138.22	111.00
1	A	1006	ALA	C-N-CA	-9.54	102.27	122.30
1	A	1090	PHE	CA-C-N	9.25	137.55	117.20

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 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	2709	0	2692	254	0
1	B	2684	0	2679	192	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	1	0
3	B	27	0	12	9	0
4	A	119	0	0	17	0
4	B	109	0	0	16	0
All	All	5677	0	5395	442	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 41.

The worst 5 of 442 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1042:PHE:CE2	1:A:1095:PRO:HG3	1.64	1.33
1:A:1138:VAL:CG1	1:A:1138:VAL:O	1.75	1.29
1:A:1223:ASN:HD22	1:A:1226:GLN:CB	1.58	1.16
1:A:1031:PHE:HA	1:A:1036:ALA:N	1.60	1.15
1:A:1177:PRO:HD2	1:A:1179:HIS:NE2	1.62	1.14

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	329/407 (81%)	290 (88%)	32 (10%)	7 (2%)	11	16
1	B	326/407 (80%)	306 (94%)	18 (6%)	2 (1%)	33	55
All	All	655/814 (80%)	596 (91%)	50 (8%)	9 (1%)	16	27

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1138	VAL
1	A	1224	ALA
1	A	1295	LEU
1	A	1039	LYS
1	B	1199	MET

### 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	305/363 (84%)	277 (91%)	28 (9%)	13	24
1	B	302/363 (83%)	276 (91%)	26 (9%)	15	27
All	All	607/726 (84%)	553 (91%)	54 (9%)	14	26

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1353	LYS
1	B	1016	SER
1	B	1340	SER
1	A	1357	THR
1	A	1362	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1236	HIS
1	A	1239	HIS
1	B	1082	GLN
1	A	1217	GLN
1	A	1223	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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
3	ADP	A	3500	2	29,29,29	1.50	5 (17%)	45,45,45	2.46	7 (15%)
3	ADP	B	3510	2	29,29,29	1.49	5 (17%)	45,45,45	2.46	7 (15%)

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
3	ADP	A	3500	2	-	0/16/32/32	0/1/3/3
3	ADP	B	3510	2	-	0/16/32/32	0/1/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3500	ADP	C4-N9	-3.98	1.31	1.37
3	B	3510	ADP	C4-N9	-3.96	1.32	1.37
3	A	3500	ADP	PB-O3A	-2.85	1.55	1.60
3	B	3510	ADP	PB-O2B	2.84	1.65	1.54
3	A	3500	ADP	PB-O2B	2.84	1.65	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3500	ADP	N3-C2-N1	-11.30	119.27	128.71
3	B	3510	ADP	N3-C2-N1	-11.29	119.27	128.71
3	B	3510	ADP	O4'-C1'-N9	6.12	114.14	108.44
3	A	3500	ADP	O4'-C1'-N9	6.11	114.12	108.44
3	A	3500	ADP	C4-C5-N7	-5.59	104.73	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	339/407 (83%)	0.21	10 (2%) 49 51	19, 41, 80, 117	0
1	B	336/407 (82%)	0.19	8 (2%) 56 58	20, 40, 70, 107	0
All	All	675/814 (82%)	0.20	18 (2%) 52 54	19, 41, 74, 117	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1366	TYR	7.1
1	A	1177	PRO	6.1
1	A	1036	ALA	5.6
1	B	1002	ASN	5.5
1	A	1003	ALA	4.5

### 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

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( $\text{\AA}^2$ )	Q<0.9
3	ADP	A	3500	27/27	0.15	-0.31	16,26,35,38	0
3	ADP	B	3510	27/27	0.15	-0.44	16,26,35,38	0
2	MG	B	4611	1/1	0.12	-1.60	47,47,47,47	0
2	MG	A	4601	1/1	0.09	-8.24	44,44,44,44	0

## 6.5 Other polymers

There are no such residues in this entry.