W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 28, 2014 – 09:39 AM GMT

PDB ID : 3KTX
Title : Crystal structure of Leishmania mexicana pyruvate kinase (LmPYK)in complex with 1,3,6,8-pyrenetetrasulfonicacid
Authors : Morgan, H.P.; Walkinshaw, M.D.
Deposited on : 2009-11-26
Resolution : 2.10 Å(reported)

1 Overall quality at a glance (i)

The reported resolution of this entry is 2.10 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	Percentile Ranks	Value
Rfree		0.237
Clashscore		10
Ramachandran outliers		0.2%
Sidechain outliers		4.3%
RSRZ outliers		13.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
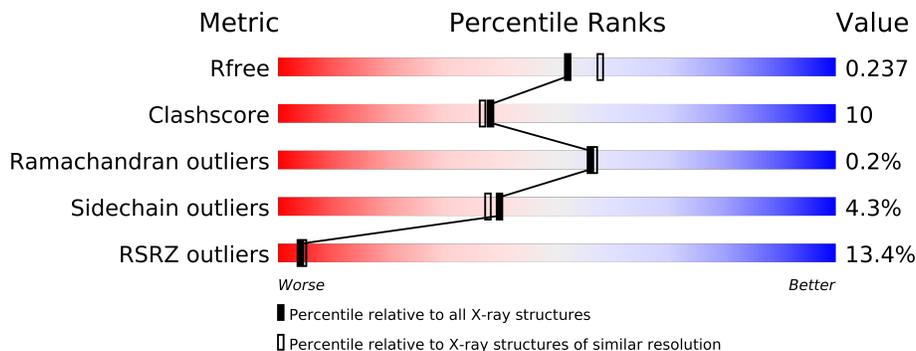
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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 >=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	499	
1	B	499	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	A	500	-	X
2	GOL	A	502	-	X
3	PTK	A	501	-	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 8214 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 kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total 3753	C 2339	N 660	O 728	S 26	0	0	0
1	B	492	Total 3753	C 2339	N 660	O 728	S 26	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	SER	GLY	CONFLICT	UNP Q27686
A	389	TYR	SER	CONFLICT	UNP Q27686
A	404	ARG	ALA	CONFLICT	UNP Q27686
A	405	SER	GLY	CONFLICT	UNP Q27686
B	382	SER	GLY	CONFLICT	UNP Q27686
B	389	TYR	SER	CONFLICT	UNP Q27686
B	404	ARG	ALA	CONFLICT	UNP Q27686
B	405	SER	GLY	CONFLICT	UNP Q27686

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
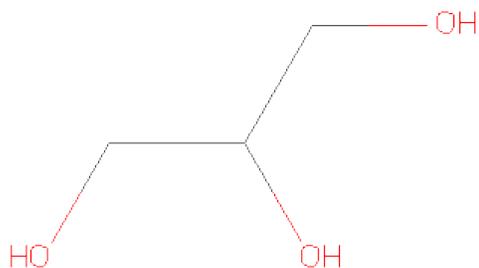
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0

- Molecule 3 is PYRENE-1,3,6,8-TETRASULFONICACID (three-letter code: PTK) (formula: $C_{16}H_{10}O_{12}S_4$).
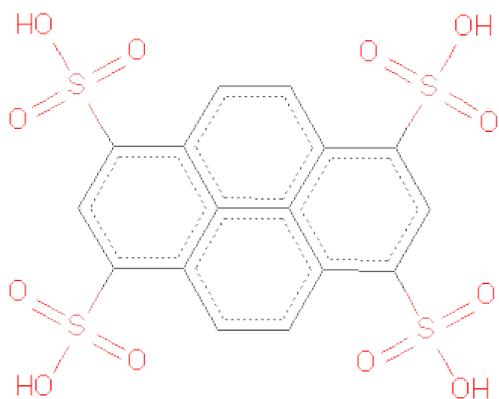
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
3	A	1	32	16	12	4	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	344	344	344	0	0
4	B	296	296	296	0	0

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 kinase

Chain A:
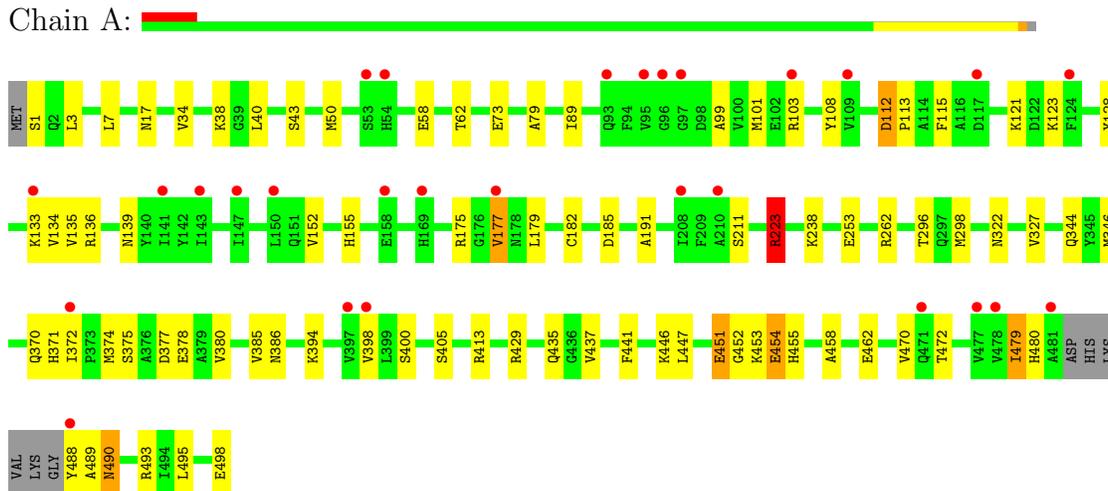
• Molecule 1: Pyruvate kinase

Chain B:
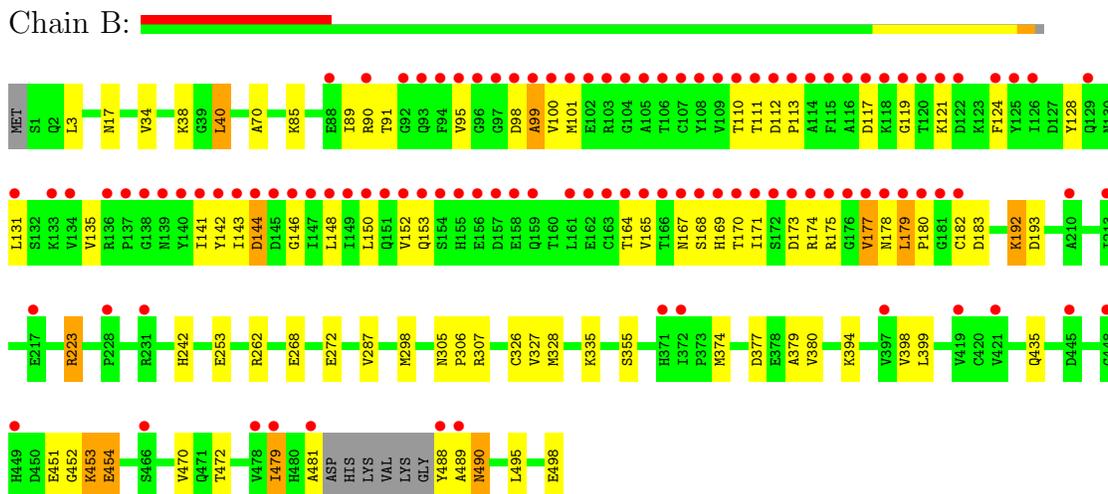
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	122.86Å 129.86Å 165.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.69 – 2.10 20.69 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.69-2.10) 100.0 (20.69-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.186 , 0.239 0.186 , 0.237	Depositor DCC
R_{free} test set	3865 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	32.6	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 53.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 76957 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8214	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]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: GOL, PTK

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	1.13	7/3808 (0.2%)	0.92	5/5154 (0.1%)
1	B	1.05	4/3808 (0.1%)	0.93	5/5154 (0.1%)
All	All	1.09	11/7616 (0.1%)	0.93	10/10308 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	451	GLU	CG-CD	6.53	1.61	1.51
1	A	458	ALA	CA-CB	6.21	1.65	1.52
1	A	191	ALA	CA-CB	6.09	1.65	1.52
1	A	437	VAL	CB-CG2	5.83	1.65	1.52
1	A	441	PHE	CE2-CZ	5.68	1.48	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	99	ALA	CB-CA-C	21.84	142.85	110.10
1	B	99	ALA	N-CA-C	-7.84	89.83	111.00
1	A	223	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	112	ASP	CB-CG-OD1	6.26	123.94	118.30
1	B	495	LEU	CA-CB-CG	6.16	129.46	115.30

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	3753	0	3752	67	0
1	B	3753	0	3752	72	0
2	A	30	0	40	2	0
2	B	6	0	8	3	0
3	A	32	0	10	10	0
4	A	344	0	0	12	0
4	B	296	0	0	6	0
All	All	8214	0	7562	150	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 10.

The worst 5 of 150 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:501:PTK:OAB	3:A:501:PTK:HAO	1.39	1.19
3:A:501:PTK:OAJ	3:A:501:PTK:HAQ	1.44	1.15
3:A:501:PTK:HAP	3:A:501:PTK:OAK	1.43	1.09
3:A:501:PTK:HAR	3:A:501:PTK:OAG	1.43	1.06
1:A:223:ARG:HD2	4:A:553:HOH:O	1.58	1.01

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	488/499 (98%)	477 (98%)	10 (2%)	1 (0%)	56	57
1	B	488/499 (98%)	462 (95%)	25 (5%)	1 (0%)	56	57
All	All	976/998 (98%)	939 (96%)	35 (4%)	2 (0%)	56	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	144	ASP
1	A	296	THR

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	411/417 (99%)	395 (96%)	16 (4%)	43	43
1	B	411/417 (99%)	392 (95%)	19 (5%)	37	34
All	All	822/834 (99%)	787 (96%)	35 (4%)	40	37

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	490	ASN
1	B	112	ASP
1	B	454	GLU
1	B	17	ASN
1	B	40	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	471	GLN
1	A	490	ASN
1	B	153	GLN
1	A	435	GLN
1	B	69	GLN

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 ⓘ

7 ligands are 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	$\#|Z| > 2$
2	GOL	A	499	-	5,5,5	0.77	0	5,5,5	1.39	1 (20%)
2	GOL	A	500	-	5,5,5	0.65	0	5,5,5	1.05	0
3	PTK	A	501	-	35,35,35	1.78	6 (17%)	60,60,60	2.54	27 (45%)
2	GOL	A	502	-	5,5,5	0.72	0	5,5,5	1.62	2 (40%)
2	GOL	A	503	-	5,5,5	0.40	0	5,5,5	0.75	0
2	GOL	A	504	-	5,5,5	0.30	0	5,5,5	0.43	0
2	GOL	B	499	-	5,5,5	0.57	0	5,5,5	0.77	0

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
2	GOL	A	499	-	-	0/4/4/4	0/0/0/0
2	GOL	A	500	-	-	0/4/4/4	0/0/0/0
3	PTK	A	501	-	-	0/24/24/24	0/0/4/4
2	GOL	A	502	-	-	0/4/4/4	0/0/0/0
2	GOL	A	503	-	-	0/4/4/4	0/0/0/0
2	GOL	A	504	-	-	0/4/4/4	0/0/0/0
2	GOL	B	499	-	-	0/4/4/4	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	PTK	CAV-CAZ	-3.40	1.38	1.43
3	A	501	PTK	CAU-CAY	-3.33	1.38	1.43
3	A	501	PTK	CAS-CAW	-3.12	1.38	1.43
3	A	501	PTK	CAT-CAX	-3.01	1.38	1.43
3	A	501	PTK	CAM-CAT	2.30	1.40	1.37

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	PTK	CAM-CAS-SBC	6.47	124.69	117.67
3	A	501	PTK	CAM-CAT-SBD	5.76	123.93	117.67
3	A	501	PTK	CAN-CAU-SBE	5.05	123.16	117.67
3	A	501	PTK	CAN-CAV-SBF	4.80	122.89	117.67
3	A	501	PTK	CAW-CAS-SBC	-4.74	115.47	121.05

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, 95th 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(Å²)	Q<0.9
1	A	492/499 (98%)	0.14	28 (5%)	23	25	20, 34, 55, 70	0
1	B	492/499 (98%)	1.26	105 (21%)	1	1	22, 36, 124, 135	0
All	All	984/998 (98%)	0.70	133 (13%)	4	4	20, 35, 121, 135	0

The worst 5 of 133 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	172	SER	20.0
1	B	171	ILE	18.7
1	B	104	GLY	16.0
1	B	166	THR	15.0
1	B	95	VAL	13.5

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, 95th 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.

wwPDB X-ray Structure Validation Summary Report

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	PTK	A	501	32/32	0.25	3.45	96,98,100,100	32
2	GOL	A	500	6/6	0.25	2.80	53,61,62,62	0
2	GOL	A	502	6/6	0.19	2.59	28,46,48,51	0
2	GOL	A	504	6/6	0.23	1.26	67,69,71,71	0
2	GOL	B	499	6/6	0.18	1.19	48,59,63,65	0
2	GOL	A	503	6/6	0.17	0.69	51,63,65,66	0
2	GOL	A	499	6/6	0.22	0.36	33,48,49,52	0

6.5 Other polymers ⓘ

There are no such residues in this entry.