



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:35 PM UTC

PDB ID : 3E0W / pdb_00003e0w
Title : Crystal structure of pyruvate kinase from Leishmania mexicana
Authors : Tulloch, L.B.; Gillmore, L.A.; Walkinshaw, M.D.
Deposited on : 2008-08-01
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

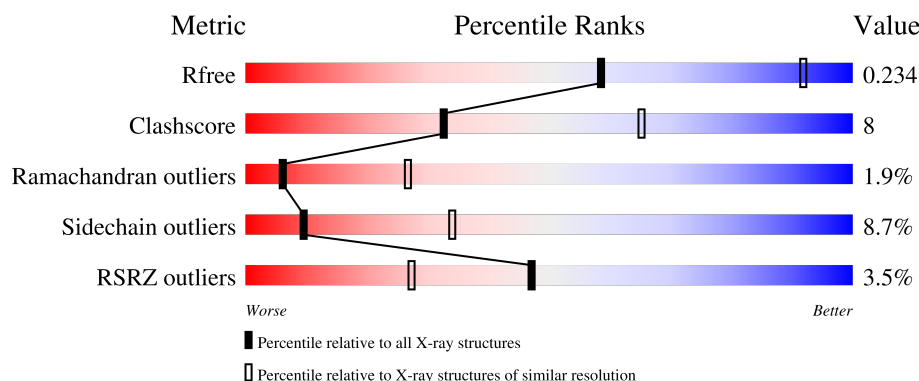
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$. 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	539	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3773 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	485	Total	C	N	O	S	0	0	0
			3698	2306	650	716	26			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MET	-	expression tag	UNP Q27686
A	-39	GLY	-	expression tag	UNP Q27686
A	-38	SER	-	expression tag	UNP Q27686
A	-37	SER	-	expression tag	UNP Q27686
A	-36	HIS	-	expression tag	UNP Q27686
A	-35	HIS	-	expression tag	UNP Q27686
A	-34	HIS	-	expression tag	UNP Q27686
A	-33	HIS	-	expression tag	UNP Q27686
A	-32	HIS	-	expression tag	UNP Q27686
A	-31	HIS	-	expression tag	UNP Q27686
A	-30	SER	-	expression tag	UNP Q27686
A	-29	SER	-	expression tag	UNP Q27686
A	-28	GLY	-	expression tag	UNP Q27686
A	-27	LEU	-	expression tag	UNP Q27686
A	-26	VAL	-	expression tag	UNP Q27686
A	-25	PRO	-	expression tag	UNP Q27686
A	-24	ARG	-	expression tag	UNP Q27686
A	-23	GLY	-	expression tag	UNP Q27686
A	-22	SER	-	expression tag	UNP Q27686
A	-21	HIS	-	expression tag	UNP Q27686
A	-20	MET	-	expression tag	UNP Q27686
A	-19	GLY	-	expression tag	UNP Q27686
A	-18	SER	-	expression tag	UNP Q27686
A	-17	SER	-	expression tag	UNP Q27686
A	-16	HIS	-	expression tag	UNP Q27686
A	-15	HIS	-	expression tag	UNP Q27686
A	-14	HIS	-	expression tag	UNP Q27686

Continued on next page...

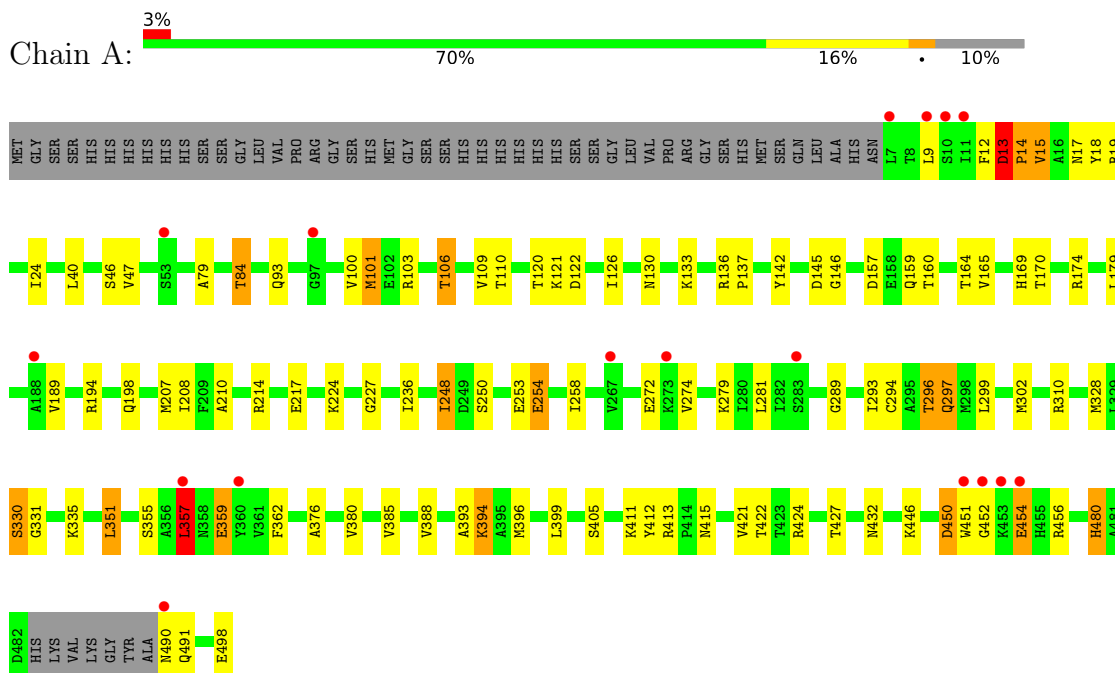
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	HIS	-	expression tag	UNP Q27686
A	-12	HIS	-	expression tag	UNP Q27686
A	-11	HIS	-	expression tag	UNP Q27686
A	-10	SER	-	expression tag	UNP Q27686
A	-9	SER	-	expression tag	UNP Q27686
A	-8	GLY	-	expression tag	UNP Q27686
A	-7	LEU	-	expression tag	UNP Q27686
A	-6	VAL	-	expression tag	UNP Q27686
A	-5	PRO	-	expression tag	UNP Q27686
A	-4	ARG	-	expression tag	UNP Q27686
A	-3	GLY	-	expression tag	UNP Q27686
A	-2	SER	-	expression tag	UNP Q27686
A	-1	HIS	-	expression tag	UNP Q27686
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
A	451	TRP	GLU	engineered mutation	UNP Q27686

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	75	Total O 75 75	0	0

- Molecule 1: Pyruvate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 3 2	Depositor
Cell constants a, b, c, α , β , γ	184.55Å 184.55Å 184.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.26 – 3.10 40.26 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.26-3.10) 99.3 (40.26-3.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.215 , 0.246 0.207 , 0.234	Depositor DCC
R_{free} test set	995 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	99.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 126.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3773	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.45	0/3753	0.86	4/5082 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	ASN	N-CA-C	6.56	118.43	111.28
1	A	451	TRP	N-CA-C	-5.91	105.84	113.16
1	A	227	GLY	CA-C-N	5.16	125.20	119.32
1	A	227	GLY	C-N-CA	5.16	125.20	119.32

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	3698	0	3687	58	0
2	A	75	0	0	7	0
All	All	3773	0	3687	58	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 8.

All (58) 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:388:VAL:HG21	1:A:396:MET:HE2	1.42	1.01
1:A:422:THR:HG22	1:A:424:ARG:H	1.38	0.88
1:A:388:VAL:CG2	1:A:396:MET:HE2	2.14	0.78
1:A:328:MET:SD	2:A:564:HOH:O	2.44	0.75
1:A:393:ALA:HB1	1:A:394:LYS:HB2	1.70	0.73
1:A:136:ARG:HG3	1:A:137:PRO:HD2	1.76	0.68
1:A:15:VAL:HG11	1:A:351:LEU:O	1.97	0.65
1:A:450:ASP:OD2	1:A:456:ARG:HG2	1.96	0.65
1:A:13:ASP:OD2	1:A:14:PRO:HD3	1.98	0.62
1:A:299:LEU:HD22	1:A:302:MET:HE2	1.82	0.61
1:A:130:ASN:HD21	1:A:133:LYS:HD2	1.64	0.60
1:A:359:GLU:HA	1:A:362:PHE:HB3	1.84	0.58
1:A:47:VAL:HG22	1:A:79:ALA:HB3	1.87	0.55
1:A:422:THR:HG21	1:A:427:THR:HB	1.89	0.55
1:A:248:ILE:HD13	1:A:281:LEU:HG	1.89	0.55
1:A:289:GLY:HA3	1:A:411:LYS:HD2	1.88	0.54
1:A:422:THR:HG22	1:A:424:ARG:N	2.17	0.54
1:A:145:ASP:HB2	2:A:532:HOH:O	2.07	0.54
1:A:393:ALA:CB	1:A:394:LYS:HB2	2.38	0.54
1:A:498:GLU:H	1:A:498:GLU:CD	2.16	0.53
1:A:46:SER:HB3	1:A:432:ASN:HB3	1.91	0.53
1:A:380:VAL:HG21	1:A:490:ASN:HB3	1.91	0.52
1:A:100:VAL:HG13	1:A:170:THR:HG22	1.91	0.52
1:A:103:ARG:O	1:A:165:VAL:O	2.28	0.52
1:A:120:THR:HG23	1:A:122:ASP:H	1.75	0.51
1:A:385:VAL:HG22	1:A:396:MET:HE1	1.92	0.51
1:A:19:ARG:HH12	1:A:357:LEU:HB3	1.77	0.50
1:A:480:HIS:CE1	1:A:491:GLN:HE21	2.29	0.50
1:A:294:CYS:SG	1:A:296:THR:HG23	2.52	0.50
1:A:174:ARG:NH2	2:A:557:HOH:O	2.43	0.49
1:A:297:GLN:NE2	2:A:564:HOH:O	2.42	0.49
1:A:296:THR:HG21	2:A:565:HOH:O	2.11	0.49
1:A:421:VAL:HG11	1:A:456:ARG:HB2	1.93	0.49
1:A:24:ILE:HG12	1:A:47:VAL:HB	1.95	0.49
1:A:106:THR:HG22	2:A:540:HOH:O	2.13	0.49
1:A:385:VAL:HG11	1:A:412:TYR:O	2.14	0.48
1:A:388:VAL:HG21	1:A:396:MET:CE	2.29	0.48
1:A:157:ASP:C	1:A:159:GLN:H	2.23	0.46
1:A:84:THR:CG2	1:A:210:ALA:HA	2.47	0.45
1:A:101:MET:HB2	1:A:169:HIS:O	2.17	0.45
1:A:109:VAL:HG11	1:A:126:ILE:HD12	1.99	0.45
1:A:359:GLU:HG3	1:A:415:ASN:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:GLY:HA3	1:A:454:GLU:H	1.83	0.44
1:A:279:LYS:HE2	1:A:279:LYS:HA	1.99	0.44
1:A:18:TYR:O	1:A:19:ARG:HG2	2.17	0.44
1:A:399:LEU:HD13	1:A:456:ARG:HD2	1.99	0.43
1:A:330:SER:HB3	1:A:331:GLY:H	1.50	0.43
1:A:236:ILE:HG21	1:A:293:ILE:HD12	2.00	0.42
1:A:250:SER:O	1:A:254:GLU:HB2	2.18	0.42
1:A:393:ALA:CA	1:A:394:LYS:HB2	2.50	0.42
1:A:142:TYR:HB3	1:A:146:GLY:HA2	2.01	0.41
1:A:194:ARG:O	1:A:198:GLN:HG2	2.20	0.41
1:A:100:VAL:HG13	1:A:170:THR:CG2	2.50	0.41
1:A:446:LYS:HE2	1:A:446:LYS:HA	2.01	0.41
1:A:359:GLU:HB3	2:A:550:HOH:O	2.21	0.41
1:A:376:ALA:O	1:A:380:VAL:HG23	2.21	0.41
1:A:19:ARG:NH1	1:A:357:LEU:HB3	2.35	0.40
1:A:130:ASN:ND2	1:A:133:LYS:HD2	2.35	0.40

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	481/539 (89%)	444 (92%)	28 (6%)	9 (2%)	6 27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	PRO
1	A	355	SER
1	A	357	LEU
1	A	394	LYS
1	A	13	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	450	ASP
1	A	15	VAL
1	A	454	GLU
1	A	413	ARG

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	404/451 (90%)	369 (91%)	35 (9%)	9 34

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	12	PHE
1	A	13	ASP
1	A	40	LEU
1	A	84	THR
1	A	93	GLN
1	A	101	MET
1	A	106	THR
1	A	110	THR
1	A	121	LYS
1	A	160	THR
1	A	164	THR
1	A	179	LEU
1	A	189	VAL
1	A	207	MET
1	A	208	ILE
1	A	214	ARG
1	A	217	GLU
1	A	224	LYS
1	A	248	ILE
1	A	253	GLU
1	A	254	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	258	ILE
1	A	272	GLU
1	A	274	VAL
1	A	296	THR
1	A	297	GLN
1	A	310	ARG
1	A	330	SER
1	A	335	LYS
1	A	351	LEU
1	A	357	LEU
1	A	359	GLU
1	A	405	SER
1	A	480	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	93	GLN
1	A	129	GLN
1	A	130	ASN
1	A	151	GLN
1	A	153	GLN
1	A	155	HIS
1	A	286	ASN
1	A	322	ASN
1	A	401	ASN
1	A	430	GLN
1	A	471	GLN
1	A	480	HIS
1	A	491	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 oligosaccharides 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, 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(Å ²)	Q<0.9
1	A	485/539 (89%)	0.38	17 (3%)	47 27	59, 101, 113, 126	5 (1%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	451	TRP	15.6
1	A	453	LYS	5.5
1	A	452	GLY	4.6
1	A	7	LEU	3.7
1	A	11	ILE	3.4
1	A	360	TYR	3.1
1	A	490	ASN	3.0
1	A	283	SER	2.9
1	A	9	LEU	2.9
1	A	454	GLU	2.9
1	A	273	LYS	2.7
1	A	53	SER	2.5
1	A	267	VAL	2.4
1	A	10	SER	2.4
1	A	97	GLY	2.2
1	A	357	LEU	2.2
1	A	188	ALA	2.0

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 oligosaccharides 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.