



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 12:02 PM EDT

PDB ID : 8EDT
Title : E. coli Pyruvate kinase (PykF) T462I
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Deposited on : 2022-09-05
Resolution : 2.09 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

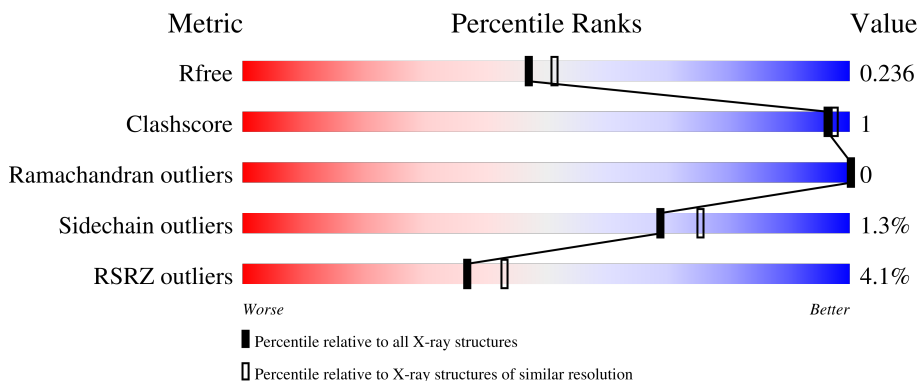
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

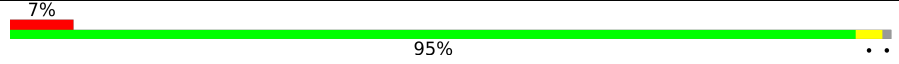
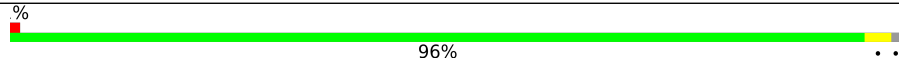
The reported resolution of this entry is 2.09 Å.

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 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	470	
1	B	470	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14110 atoms, of which 7100 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
			Total	C	H	N	O	S			
1	A	463	6978	2155	3514	604	681	24	0	1	0
1	B	463	7067	2172	3586	605	680	24	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	462	ILE	THR	engineered mutation	UNP Q2TL68
B	462	ILE	THR	engineered mutation	UNP Q2TL68

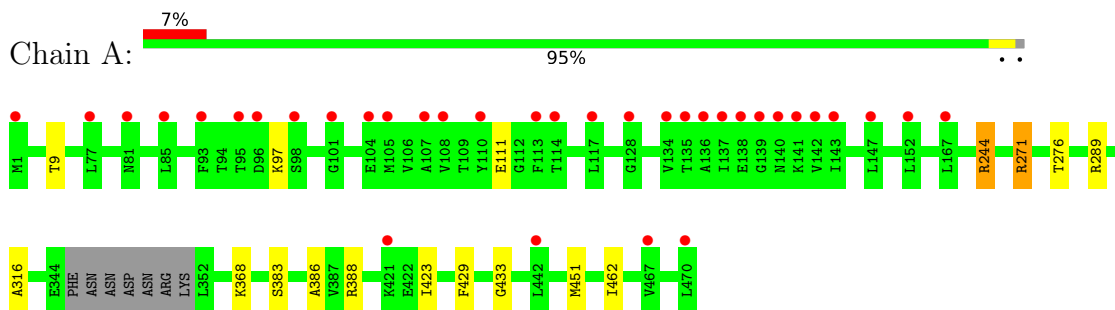
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	18	Total	O	0	0
			18	18		
2	B	47	Total	O	0	0
			47	47		

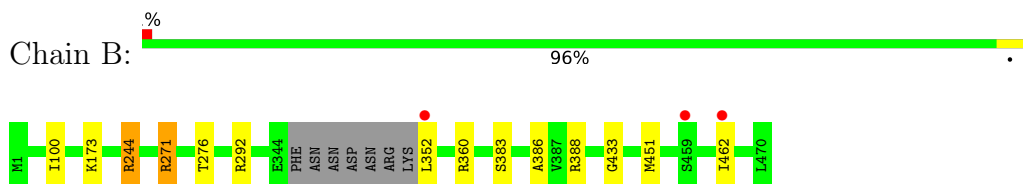
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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



- Molecule 1: Pyruvate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	74.68Å 247.41Å 129.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.89 – 2.09 48.09 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.89-2.09) 99.9 (48.09-2.09)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.08Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.218 , 0.236 0.218 , 0.236	Depositor DCC
R_{free} test set	3091 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtrriage
Anisotropy	0.010	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14110	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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	0.27	0/3499	0.51	0/4722
1	B	0.28	0/3515	0.53	0/4738
All	All	0.27	0/7014	0.52	0/9460

There are no bond length outliers.

There are no bond angle outliers.

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	3464	3514	3513	9	0
1	B	3481	3586	3585	7	0
2	A	18	0	0	0	0
2	B	47	0	0	0	0
All	All	7010	7100	7098	14	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 1.

All (14) 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:368:LYS:O	1:B:352:LEU:HD23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LYS:HB3	1:B:352:LEU:HD21	1.94	0.48
1:B:244:ARG:HD2	1:B:276:THR:HG23	1.96	0.47
1:B:100:ILE:N	1:B:100:ILE:HD12	2.29	0.47
1:A:383:SER:OG	1:A:462:ILE:HD11	2.17	0.44
1:B:383:SER:OG	1:B:462:ILE:HD11	2.18	0.43
1:A:97:LYS:NZ	1:A:111:GLU:OE1	2.51	0.43
1:A:271:ARG:HG2	1:A:386:ALA:HA	2.01	0.42
1:A:433:GLY:HA3	1:A:451:MET:HE1	2.02	0.42
1:A:9:THR:HG22	1:A:316:ALA:HB2	2.02	0.41
1:A:423:ILE:HG21	1:A:429:PHE:CA	2.51	0.41
1:B:433:GLY:HA3	1:B:451:MET:HE1	2.02	0.40
1:A:244:ARG:HD2	1:A:276:THR:HG23	2.03	0.40
1:B:271:ARG:HG2	1:B:386:ALA:HA	2.03	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	460/470 (98%)	452 (98%)	8 (2%)	0	100	100
1	B	459/470 (98%)	452 (98%)	7 (2%)	0	100	100
All	All	919/940 (98%)	904 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	374/389 (96%)	370 (99%)	4 (1%)	73	79
1	B	381/389 (98%)	375 (98%)	6 (2%)	62	69
All	All	755/778 (97%)	745 (99%)	10 (1%)	69	75

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	ARG
1	A	271	ARG
1	A	289	ARG
1	A	388	ARG
1	B	173	LYS
1	B	244	ARG
1	B	271	ARG
1	B	292	ARG
1	B	360	ARG
1	B	388	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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

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(Å ²)	Q<0.9
1	A	463/470 (98%)	0.39	35 (7%) 13 18	20, 39, 93, 112	0
1	B	463/470 (98%)	-0.12	3 (0%) 89 91	16, 30, 59, 106	0
All	All	926/940 (98%)	0.14	38 (4%) 37 43	16, 35, 84, 112	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	VAL	6.4
1	A	139	GLY	4.9
1	A	137	ILE	4.2
1	A	143	ILE	4.0
1	B	352	LEU	3.9
1	A	96	ASP	3.7
1	A	93	PHE	3.5
1	A	105	MET	3.4
1	A	135	THR	3.1
1	A	107	ALA	3.0
1	A	147	LEU	3.0
1	A	134	VAL	2.9
1	B	462	ILE	2.9
1	B	459	SER	2.8
1	A	117	LEU	2.8
1	A	140	ASN	2.7
1	A	113	PHE	2.6
1	A	104	GLU	2.6
1	A	85	LEU	2.6
1	A	114	THR	2.4
1	A	81	ASN	2.4
1	A	1	MET	2.4
1	A	152	LEU	2.3
1	A	108	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	421	LYS	2.3
1	A	442	LEU	2.2
1	A	141	LYS	2.2
1	A	136	ALA	2.2
1	A	95	THR	2.2
1	A	138	GLU	2.2
1	A	470	LEU	2.2
1	A	101	GLY	2.1
1	A	467	VAL	2.1
1	A	77	LEU	2.1
1	A	110	TYR	2.1
1	A	98	SER	2.0
1	A	167	LEU	2.0
1	A	128	GLY	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 monosaccharides 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.