



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:06 AM UTC

PDB ID : 8EDT / pdb_00008edt
Title : E. coli Pyruvate kinase (PykF) T462I
Authors : Donovan, K.A.; Coombes, D.; Dobson, R.C.J.; Cooper, T.F.
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	:	4-5-2 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

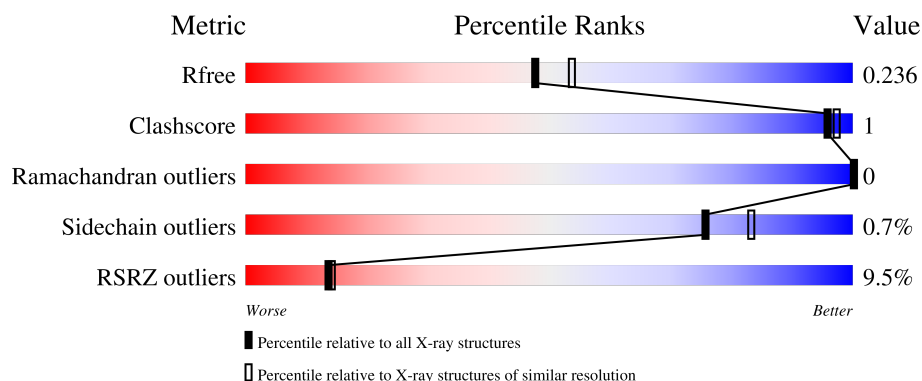
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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	16% 95% ..
1	B	470	3% 95% ..

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
1	A	463	Total	C	H	N	O	S	0	1	0
			6978	2155	3514	604	681	24			
1	B	463	Total	C	H	N	O	S	0	0	0
			7067	2172	3586	605	680	24			

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

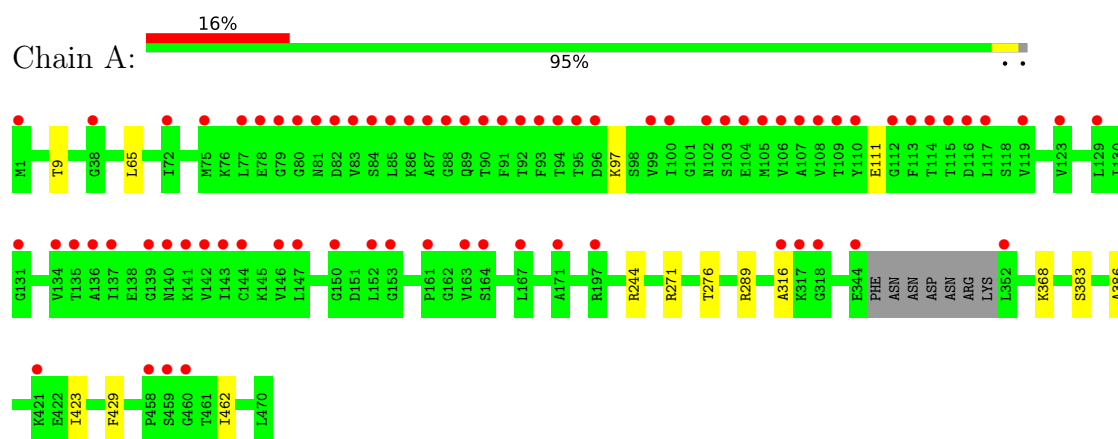
- Molecule 2 is water.

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

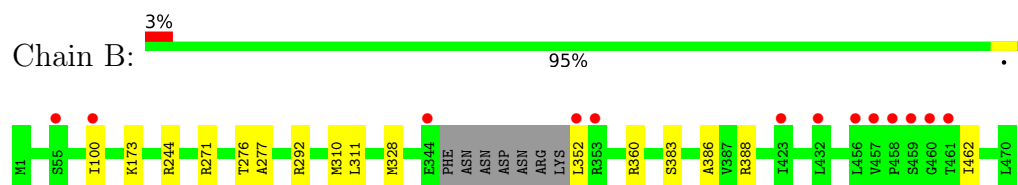
3 Residue-property plots [i](#)

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 40.89 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.89-2.09) 100.0 (40.89-2.09)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.08Å)	Xtriage
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	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14110	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage'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

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	0.13	0/3499	0.32	0/4722
1	B	0.15	0/3515	0.35	0/4738
All	All	0.14	0/7014	0.34	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

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	8	0
2	A	18	0	0	0	0
2	B	47	0	0	0	0
All	All	7010	7100	7098	15	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 (15) 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:B:311:LEU:HD21	1:B:328:MET:HE2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LYS:O	1:B:352:LEU:HD23	2.11	0.51
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:65:LEU:HD23	1:A:65:LEU:C	2.44	0.43
1:A:271:ARG:HG2	1:A:386:ALA:HA	2.01	0.42
1:B:277:ALA:HB1	1:B:310:MET:HE2	2.02	0.41
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: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%)	373 (100%)	1 (0%)	86	91
1	B	381/389 (98%)	377 (99%)	4 (1%)	68	76
All	All	755/778 (97%)	750 (99%)	5 (1%)	76	83

All (5) residues with a non-rotameric sidechain are listed below:

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	GLN
1	B	159	ASN
1	B	176	GLN
1	B	224	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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(Å ²)	Q<0.9
1	A	463/470 (98%)	0.66	75 (16%) 4 4	16, 45, 102, 122	1 (0%)
1	B	463/470 (98%)	0.02	13 (2%) 55 57	19, 34, 65, 115	0
All	All	926/940 (98%)	0.34	88 (9%) 14 14	16, 39, 93, 122	1 (0%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	ILE	7.0
1	B	460	GLY	5.5
1	A	142	VAL	5.5
1	A	113	PHE	5.3
1	A	352	LEU	5.1
1	A	93	PHE	4.6
1	A	108	VAL	4.6
1	A	460	GLY	4.0
1	B	352	LEU	3.9
1	A	87	ALA	3.8
1	A	139	GLY	3.8
1	B	458	PRO	3.7
1	A	99	VAL	3.7
1	A	344	GLU	3.6
1	A	167	LEU	3.6
1	A	110	TYR	3.5
1	A	95	THR	3.5
1	A	137	ILE	3.4
1	B	461	THR	3.4
1	A	114	THR	3.4
1	A	143	ILE	3.4
1	B	344	GLU	3.3
1	A	147	LEU	3.3
1	A	150	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	119	VAL	3.2
1	A	152	LEU	3.2
1	A	112	GLY	3.2
1	A	85	LEU	3.1
1	A	153	GLY	3.1
1	A	107	ALA	3.1
1	A	83	VAL	3.0
1	A	117	LEU	3.0
1	A	88	GLY	3.0
1	A	144	CYS	2.9
1	A	103	SER	2.9
1	A	89	GLN	2.8
1	A	134	VAL	2.8
1	A	146	VAL	2.8
1	A	459	SER	2.8
1	A	94	THR	2.8
1	A	72	ILE	2.8
1	B	457	VAL	2.8
1	B	456	LEU	2.7
1	B	423	ILE	2.7
1	A	116	ASP	2.7
1	A	163	VAL	2.7
1	A	458	PRO	2.6
1	A	84	SER	2.6
1	B	459	SER	2.6
1	A	104	GLU	2.5
1	A	90	THR	2.5
1	A	109	THR	2.5
1	A	161	PRO	2.5
1	A	105	MET	2.5
1	B	100	ILE	2.5
1	A	136	ALA	2.4
1	A	141	LYS	2.4
1	A	82	ASP	2.4
1	A	75	MET	2.4
1	A	79	GLY	2.4
1	A	106	VAL	2.4
1	A	123	VAL	2.4
1	A	92	THR	2.4
1	A	140	ASN	2.4
1	A	96	ASP	2.4
1	A	317	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	129	LEU	2.3
1	A	91	PHE	2.3
1	A	115	THR	2.3
1	A	316	ALA	2.3
1	A	135	THR	2.3
1	A	171	ALA	2.3
1	A	131	GLY	2.3
1	A	78	GLU	2.3
1	A	421	LYS	2.2
1	A	318	GLY	2.2
1	B	353	ARG	2.2
1	A	80	GLY	2.1
1	A	102	ASN	2.1
1	A	77	LEU	2.1
1	B	55	SER	2.1
1	A	86	LYS	2.1
1	A	197	ARG	2.0
1	A	1	MET	2.0
1	A	164	SER	2.0
1	A	81	ASN	2.0
1	B	432	LEU	2.0
1	A	38	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 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.