



# wwPDB X-ray Structure Validation Summary Report

Oct 2, 2023 – 03:27 PM EDT

PDB ID : 6NN8  
Title : The structure of human liver pyruvate kinase, hLPYK-S531E  
Authors : McFarlane, J.S.; Ronnebaum, T.A.; Meneely, K.M.; Fenton, A.W.; Lamb, A.L.  
Deposited on : 2019-01-14  
Resolution : 2.42 Å(reported)

This is a wwPDB X-ray Structure 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

<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>.

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

MolProbity : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : **FAILED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
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 2.42 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 57131 atoms, of which 28756 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 PKLR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	505	7738	2410	3909	690	711	18	0	0	0
1	B	518	7937	2473	4006	710	730	18	0	0	0
1	C	499	7675	2390	3880	683	704	18	0	0	0
1	D	421	6468	2018	3259	580	592	19	0	1	0
1	E	509	7828	2438	3957	701	714	18	0	0	0
1	F	417	6429	2006	3239	577	589	18	0	0	0
1	G	395	6086	1895	3076	542	555	18	0	0	0
1	H	407	6310	1965	3184	568	575	18	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

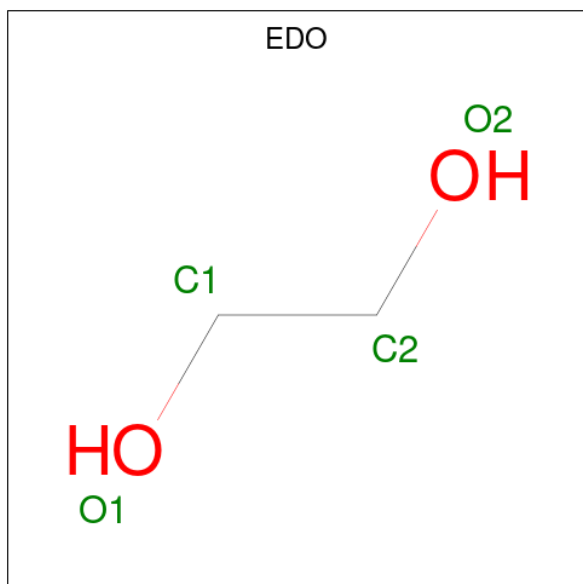
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P30613
A	2	GLU	-	expression tag	UNP P30613
A	531	GLU	SER	engineered mutation	UNP P30613
B	1	MET	-	expression tag	UNP P30613
B	2	GLU	-	expression tag	UNP P30613
B	531	GLU	SER	engineered mutation	UNP P30613
C	1	MET	-	expression tag	UNP P30613
C	2	GLU	-	expression tag	UNP P30613
C	531	GLU	SER	engineered mutation	UNP P30613
D	1	MET	-	expression tag	UNP P30613
D	2	GLU	-	expression tag	UNP P30613
D	531	GLU	SER	engineered mutation	UNP P30613
E	1	MET	-	expression tag	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2	GLU	-	expression tag	UNP P30613
E	531	GLU	SER	engineered mutation	UNP P30613
F	1	MET	-	expression tag	UNP P30613
F	2	GLU	-	expression tag	UNP P30613
F	531	GLU	SER	engineered mutation	UNP P30613
G	1	MET	-	expression tag	UNP P30613
G	2	GLU	-	expression tag	UNP P30613
G	531	GLU	SER	engineered mutation	UNP P30613
H	1	MET	-	expression tag	UNP P30613
H	2	GLU	-	expression tag	UNP P30613
H	531	GLU	SER	engineered mutation	UNP P30613

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	H	O	0	0
			10	2	6	2		
2	E	1	Total	C	H	O	0	0
			10	2	6	2		
2	E	1	Total	C	H	O	0	0
			10	2	6	2		
2	E	1	Total	C	H	O	0	0
			10	2	6	2		
2	E	1	Total	C	H	O	0	0
			10	2	6	2		
2	F	1	Total	C	H	O	0	0
			10	2	6	2		
2	F	1	Total	C	H	O	0	0
			10	2	6	2		
2	G	1	Total	C	H	O	0	0
			10	2	6	2		
2	G	1	Total	C	H	O	0	0
			10	2	6	2		
2	H	1	Total	C	H	O	0	0
			10	2	6	2		
2	H	1	Total	C	H	O	0	0
			10	2	6	2		
2	H	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	71	Total	O	0	0
			71	71		
3	B	58	Total	O	0	0
			58	58		
3	C	54	Total	O	0	0
			54	54		
3	D	16	Total	O	0	0
			16	16		
3	E	34	Total	O	0	0
			34	34		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
3	F	6	Total O 6 6	0	0
3	G	10	Total O 10 10	0	0
3	H	1	Total O 1 1	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

### 3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.91Å 139.41Å 181.29Å 90.00° 103.35° 90.00°	Depositor
Resolution (Å)	39.54 – 2.42	Depositor
% Data completeness (in resolution range)	98.7 (39.54-2.42)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 2.42Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.208 , 0.260	Depositor
Wilson B-factor (Å <sup>2</sup> )	45.7	Xtrriage
Anisotropy	0.139	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtrriage
Total number of atoms	57131	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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.



## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

41 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	EDO	A	608	-	3,3,3	0.95	0	2,2,2	0.62	0
2	EDO	E	601	-	3,3,3	0.60	0	2,2,2	1.06	0
2	EDO	A	607	-	3,3,3	0.57	0	2,2,2	0.14	0
2	EDO	E	604	-	3,3,3	0.62	0	2,2,2	0.84	0
2	EDO	B	604	-	3,3,3	0.64	0	2,2,2	1.30	0
2	EDO	H	603	-	3,3,3	0.45	0	2,2,2	0.51	0
2	EDO	B	607	-	3,3,3	0.44	0	2,2,2	0.63	0
2	EDO	F	601	-	3,3,3	0.53	0	2,2,2	0.20	0
2	EDO	D	602	-	3,3,3	0.59	0	2,2,2	0.50	0
2	EDO	C	604	-	3,3,3	0.44	0	2,2,2	0.75	0
2	EDO	A	601	-	3,3,3	0.59	0	2,2,2	1.57	1 (50%)
2	EDO	C	605	-	3,3,3	0.44	0	2,2,2	0.40	0
2	EDO	B	605	-	3,3,3	0.52	0	2,2,2	0.21	0
2	EDO	A	605	-	3,3,3	0.81	0	2,2,2	0.49	0
2	EDO	G	601	-	3,3,3	0.43	0	2,2,2	0.63	0
2	EDO	D	603	-	3,3,3	0.46	0	2,2,2	0.48	0
2	EDO	H	601	-	3,3,3	0.68	0	2,2,2	0.55	0
2	EDO	A	602	-	3,3,3	0.45	0	2,2,2	0.39	0
2	EDO	E	603	-	3,3,3	0.61	0	2,2,2	0.36	0
2	EDO	B	603	-	3,3,3	1.05	0	2,2,2	1.13	0
2	EDO	A	610	-	3,3,3	0.49	0	2,2,2	0.42	0
2	EDO	A	606	-	3,3,3	0.52	0	2,2,2	0.15	0
2	EDO	B	602	-	3,3,3	0.43	0	2,2,2	0.51	0
2	EDO	E	607	-	3,3,3	0.57	0	2,2,2	0.69	0
2	EDO	D	604	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	G	602	-	3,3,3	0.52	0	2,2,2	0.12	0
2	EDO	H	602	-	3,3,3	0.47	0	2,2,2	0.58	0
2	EDO	C	603	-	3,3,3	0.36	0	2,2,2	1.01	0
2	EDO	A	609	-	3,3,3	0.46	0	2,2,2	0.55	0
2	EDO	B	606	-	3,3,3	0.41	0	2,2,2	0.39	0
2	EDO	E	605	-	3,3,3	0.46	0	2,2,2	0.03	0
2	EDO	E	602	-	3,3,3	0.68	0	2,2,2	0.36	0
2	EDO	D	601	-	3,3,3	0.52	0	2,2,2	0.05	0
2	EDO	A	604	-	3,3,3	0.48	0	2,2,2	0.31	0
2	EDO	C	601	-	3,3,3	0.79	0	2,2,2	0.54	0
2	EDO	E	606	-	3,3,3	0.43	0	2,2,2	0.70	0
2	EDO	C	606	-	3,3,3	0.57	0	2,2,2	0.14	0
2	EDO	F	602	-	3,3,3	0.49	0	2,2,2	0.20	0
2	EDO	A	603	-	3,3,3	0.55	0	2,2,2	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	B	601	-	3,3,3	0.57	0	2,2,2	0.45	0
2	EDO	C	602	-	3,3,3	0.73	0	2,2,2	0.32	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	608	-	-	1/1/1/1	-
2	EDO	E	601	-	-	0/1/1/1	-
2	EDO	A	607	-	-	1/1/1/1	-
2	EDO	E	604	-	-	0/1/1/1	-
2	EDO	B	604	-	-	0/1/1/1	-
2	EDO	H	603	-	-	1/1/1/1	-
2	EDO	B	607	-	-	1/1/1/1	-
2	EDO	F	601	-	-	1/1/1/1	-
2	EDO	D	602	-	-	0/1/1/1	-
2	EDO	C	604	-	-	1/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
2	EDO	C	605	-	-	0/1/1/1	-
2	EDO	B	605	-	-	0/1/1/1	-
2	EDO	A	605	-	-	1/1/1/1	-
2	EDO	G	601	-	-	0/1/1/1	-
2	EDO	D	603	-	-	1/1/1/1	-
2	EDO	H	601	-	-	0/1/1/1	-
2	EDO	A	602	-	-	1/1/1/1	-
2	EDO	E	603	-	-	1/1/1/1	-
2	EDO	B	603	-	-	0/1/1/1	-
2	EDO	A	610	-	-	0/1/1/1	-
2	EDO	A	606	-	-	1/1/1/1	-
2	EDO	B	602	-	-	1/1/1/1	-
2	EDO	E	607	-	-	0/1/1/1	-
2	EDO	D	604	-	-	1/1/1/1	-
2	EDO	G	602	-	-	0/1/1/1	-
2	EDO	H	602	-	-	1/1/1/1	-
2	EDO	C	603	-	-	1/1/1/1	-
2	EDO	A	609	-	-	1/1/1/1	-
2	EDO	B	606	-	-	1/1/1/1	-
2	EDO	E	605	-	-	1/1/1/1	-
2	EDO	E	602	-	-	1/1/1/1	-
2	EDO	D	601	-	-	1/1/1/1	-
2	EDO	A	604	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	C	601	-	-	0/1/1/1	-
2	EDO	E	606	-	-	0/1/1/1	-
2	EDO	C	606	-	-	1/1/1/1	-
2	EDO	F	602	-	-	1/1/1/1	-
2	EDO	A	603	-	-	0/1/1/1	-
2	EDO	B	601	-	-	0/1/1/1	-
2	EDO	C	602	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	EDO	O1-C1-C2	-2.22	95.90	111.91

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	EDO	O1-C1-C2-O2
2	A	605	EDO	O1-C1-C2-O2
2	B	606	EDO	O1-C1-C2-O2
2	E	602	EDO	O1-C1-C2-O2
2	F	602	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 4.7 Other polymers [i](#)

There are no such residues in this entry.

## 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 5 Fit of model and data

### 5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

### 5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers

EDS failed to run properly - this section is therefore empty.