wwPDB X-ray Structure Validation Summary Report (i)

Oct 2, 2023 – 04:07 PM EDT

PDB ID	:	6NN7
Title	:	The structure of human liver pyruvate kinase, hLPYK-GGG
Authors	:	McFarlane, J.S.; Ronnebaum, T.A.; Meneely, K.M.; Fenton, A.W.; Lamb, A.L.
Deposited on	:	2019-01-14
Resolution	:	2.32 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FLC	C	601	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 58243 atoms, of which 29236 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
1	A	516	Total	C	H	N	O	S	0	0	0
			7927	2469	4006	706	728	18			
1	B	414	Total	C	H	N	O	S	0	0	0
			6369	1980	3212	574	585	18			
1	C	514	Total	C	H	N	O	S	0	0	0
			7851	2440	3964	705	724	18			
1	E	518	Total	C	H	N	O	S	0	0	0
			7919	2463	3998	710	730	18			
1	D	479	Total	C	H	N	O	S	0	0	0
			7361	2295	3715	658	675	18			
1	F	406	Total	C	H	N	O	S	0	0	0
			6256	1943	3158	562	575	18			
1	G	496	Total	C	H	N	O	S	0	0	0
			7660	2388	3869	685	700	18			
1	H	398	Total	C	H	N	O	S	0	0	0
			6118	1895	3092	552	561	18			

There are 32 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	?	-	PRO	deletion	UNP P30613
A	531	GLY	SER	engineered mutation	UNP P30613
B	1	MET	-	expression tag	UNP P30613
B	2	GLU	-	expression tag	UNP P30613
B	?	-	PRO	deletion	UNP P30613
B	531	GLY	SER	engineered mutation	UNP P30613
C	1	MET	-	expression tag	UNP P30613
C	2	GLU	-	expression tag	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	531	GLY	SER	engineered mutation	UNP P30613
E	1	MET	-	expression tag	UNP P30613

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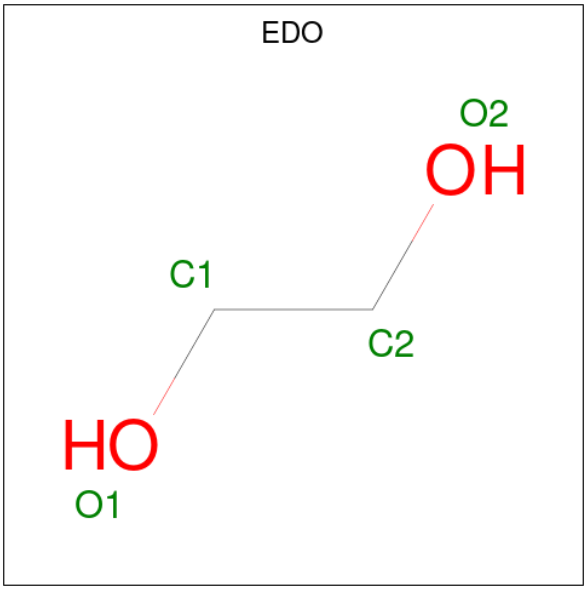
Chain	Residue	Modelled	Actual	Comment	Reference
E	2	GLU	-	expression tag	UNP P30613
E	?	-	PRO	deletion	UNP P30613
E	531	GLY	SER	engineered mutation	UNP P30613
D	1	MET	-	expression tag	UNP P30613
D	2	GLU	-	expression tag	UNP P30613
D	?	-	PRO	deletion	UNP P30613
D	531	GLY	SER	engineered mutation	UNP P30613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

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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		

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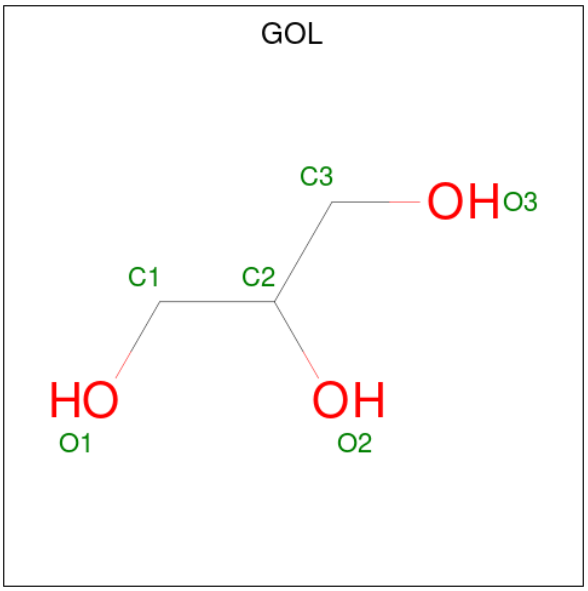
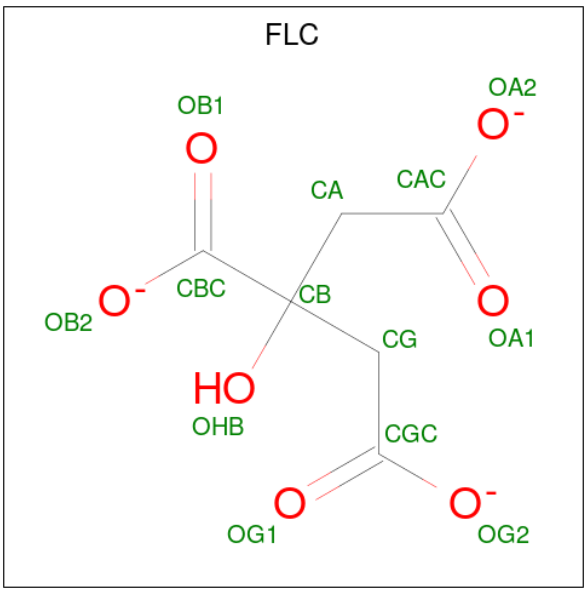
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C H O 10 2 6 2	0	0
2	B	1	Total C H O 10 2 6 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	C	1	Total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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			13	3	7	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			13	3	7	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	F	1	Total	C	H	O	0	0
			14	3	8	3		
3	F	1	Total	C	H	O	0	0
			14	3	8	3		
3	G	1	Total	C	H	O	0	0
			14	3	8	3		
3	H	1	Total	C	H	O	0	0
			14	3	8	3		
3	H	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C H O 18 6 5 7	0	0
4	D	1	Total C H O 18 6 5 7	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	87	Total O 87 87	0	0
5	B	63	Total O 63 63	0	0
5	C	67	Total O 67 67	0	0
5	E	64	Total O 64 64	0	0
5	D	73	Total O 73 73	0	0
5	F	15	Total O 15 15	0	0
5	G	11	Total O 11 11	0	0
5	H	2	Total O 2 2	0	0

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

3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	79.36Å 106.20Å 151.71Å 76.44° 80.06° 71.37°	Depositor
Resolution (Å)	39.06 – 2.32	Depositor
% Data completeness (in resolution range)	89.4 (39.06-2.32)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.31Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.191 , 0.251	Depositor
Wilson B-factor (Å^2)	38.5	Xtriage
Anisotropy	0.438	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	58243	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

33 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	C	608	-	3,3,3	0.42	0	2,2,2	0.40	0
2	EDO	C	605	-	3,3,3	0.58	0	2,2,2	0.29	0
3	GOL	F	602	-	5,5,5	0.50	0	5,5,5	0.66	0
3	GOL	D	603	-	5,5,5	0.48	0	5,5,5	1.04	0
4	FLC	C	601	-	12,12,12	2.11	1 (8%)	17,17,17	3.25	10 (58%)
2	EDO	C	607	-	3,3,3	0.49	0	2,2,2	0.33	0
2	EDO	C	604	-	3,3,3	0.49	0	2,2,2	0.30	0
3	GOL	E	603	-	5,5,5	0.45	0	5,5,5	0.55	0
2	EDO	A	602	-	3,3,3	0.45	0	2,2,2	0.71	0
2	EDO	B	601	-	3,3,3	0.54	0	2,2,2	0.72	0
2	EDO	G	602	-	3,3,3	0.54	0	2,2,2	0.58	0
3	GOL	B	603	-	5,5,5	0.69	0	5,5,5	0.76	0
2	EDO	E	601	-	3,3,3	0.51	0	2,2,2	0.40	0
2	EDO	A	601	-	3,3,3	0.44	0	2,2,2	0.66	0
2	EDO	E	602	-	3,3,3	0.44	0	2,2,2	0.58	0
3	GOL	H	602	-	5,5,5	0.52	0	5,5,5	0.52	0
3	GOL	E	605	-	5,5,5	0.57	0	5,5,5	1.05	0
2	EDO	C	606	-	3,3,3	0.65	0	2,2,2	0.31	0
3	GOL	G	603	-	5,5,5	0.66	0	5,5,5	1.41	1 (20%)
3	GOL	F	603	-	5,5,5	0.65	0	5,5,5	0.80	0
3	GOL	A	603	-	5,5,5	0.63	0	5,5,5	1.03	0
3	GOL	H	601	-	5,5,5	0.38	0	5,5,5	0.34	0
2	EDO	G	601	-	3,3,3	0.48	0	2,2,2	0.40	0
3	GOL	A	604	-	5,5,5	0.50	0	5,5,5	1.39	1 (20%)
2	EDO	F	601	-	3,3,3	0.49	0	2,2,2	0.86	0
2	EDO	C	602	-	3,3,3	0.50	0	2,2,2	0.32	0
4	FLC	D	601	-	12,12,12	1.47	1 (8%)	17,17,17	1.59	2 (11%)
3	GOL	B	604	-	5,5,5	0.60	0	5,5,5	0.78	0
2	EDO	D	602	-	3,3,3	0.58	0	2,2,2	0.56	0
3	GOL	C	609	-	5,5,5	0.91	0	5,5,5	1.22	0
3	GOL	E	604	-	5,5,5	0.88	0	5,5,5	1.45	1 (20%)
2	EDO	C	603	-	3,3,3	0.53	0	2,2,2	0.30	0
2	EDO	B	602	-	3,3,3	0.62	0	2,2,2	0.18	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	EDO	C	608	-	-	0/1/1/1	-
2	EDO	C	605	-	-	1/1/1/1	-
3	GOL	F	602	-	-	2/4/4/4	-
3	GOL	D	603	-	-	3/4/4/4	-
4	FLC	C	601	-	-	8/16/16/16	-
2	EDO	C	607	-	-	0/1/1/1	-
2	EDO	C	604	-	-	0/1/1/1	-
3	GOL	E	603	-	-	4/4/4/4	-
2	EDO	A	602	-	-	1/1/1/1	-
2	EDO	B	601	-	-	1/1/1/1	-
2	EDO	G	602	-	-	1/1/1/1	-
3	GOL	B	603	-	-	2/4/4/4	-
2	EDO	E	601	-	-	1/1/1/1	-
2	EDO	A	601	-	-	1/1/1/1	-
2	EDO	E	602	-	-	0/1/1/1	-
3	GOL	H	602	-	-	4/4/4/4	-
3	GOL	E	605	-	-	2/4/4/4	-
2	EDO	C	606	-	-	0/1/1/1	-
3	GOL	G	603	-	-	3/4/4/4	-
3	GOL	F	603	-	-	2/4/4/4	-
3	GOL	A	603	-	-	0/4/4/4	-
3	GOL	H	601	-	-	2/4/4/4	-
2	EDO	G	601	-	-	1/1/1/1	-
3	GOL	A	604	-	-	4/4/4/4	-
2	EDO	F	601	-	-	1/1/1/1	-
2	EDO	C	602	-	-	1/1/1/1	-
4	FLC	D	601	-	-	9/16/16/16	-
3	GOL	B	604	-	-	4/4/4/4	-
2	EDO	D	602	-	-	1/1/1/1	-
3	GOL	C	609	-	-	2/4/4/4	-
3	GOL	E	604	-	-	2/4/4/4	-
2	EDO	C	603	-	-	0/1/1/1	-
2	EDO	B	602	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	FLC	CB-CBC	5.90	1.59	1.53
4	D	601	FLC	CB-CBC	2.67	1.56	1.53

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	601	FLC	OB2-CBC-CB	5.98	123.44	113.05
4	C	601	FLC	CA-CB-CBC	5.43	121.76	110.11
4	C	601	FLC	OB2-CBC-OB1	-5.17	107.38	123.82
4	C	601	FLC	OB1-CBC-CB	4.78	129.02	122.25
4	D	601	FLC	OB2-CBC-CB	4.26	120.46	113.05

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	GOL	O1-C1-C2-C3
3	A	604	GOL	C1-C2-C3-O3
3	B	603	GOL	O1-C1-C2-C3
3	C	609	GOL	C1-C2-C3-O3
3	C	609	GOL	O2-C2-C3-O3

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.