

# Full wwPDB X-ray Structure Validation Report (i)

Dec 4, 2023 - 07:27 am GMT

PDB ID : 2VGF

Title: HUMAN ERYTHROCYTE PYRUVATE KINASE: T384M mutant

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Deposited on : 2007-11-12

Resolution : 2.75 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 (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 (1)) were used in the production of this report:

MolProbity : FAILED

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS: 2.36

buster-report : 1.1.7 (2018)

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)

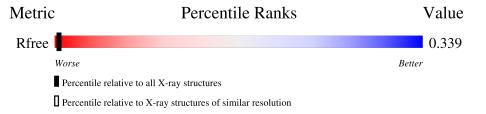
Validation Pipeline (wwPDB-VP) : 2.36

# 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 2.75 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	Similar resolution				
	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$				
$R_{free}$	130704	1235 (2.78-2.74)				

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



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15550 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 ISOZYMES R/L.

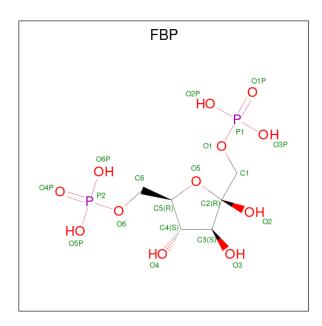
Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
1	1 A	517	Total	С	N	О	S	0	0	0
1			3913	2458	709	727	19	0	0	
1	В	491	Total	С	N	О	S	0	0	0
1	Б	491	3720	2340	673	688	19			U
1	C	517	Total	С	N	О	S	0	0	0
1		517	3913	2458	709	727	19	0		
1	D	512	Total	С	N	О	S	7	0	0
1			3880	2437	703	721	19	1	U	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	384	MET	THR	engineered mutation	UNP P30613
В	384	MET	THR	engineered mutation	UNP P30613
С	384	MET	THR	engineered mutation	UNP P30613
D	384	MET	THR	engineered mutation	UNP P30613

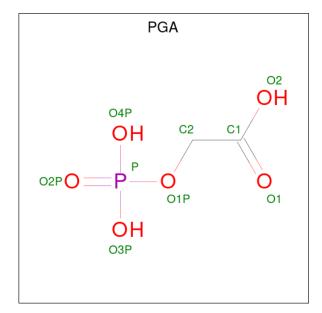
• Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FBP) (formula:  $C_6H_{14}O_{12}P_2$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	С	Ο	Р	0	0
2	2 11	1	20	6	12	2		0
2	В	1	Total	С	О	Р	0	0
2		1	20	6	12	2	U	
2	С	1	Total	С	О	Р	0	0
2			20	6	12	2	U	
2	D	D 1	Total	С	О	Р	0	0
	ש		20	6	12	2	U	U

 $\bullet \ \, \text{Molecule 3 is 2-PHOSPHOGLYCOLIC ACID (three-letter code: PGA) (formula: $C_2H_5O_6P$)}. \\$ 





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 9 2 6 1	0	0
3	В	1	Total C O P 9 2 6 1	0	0
3	C	1	Total C O P 9 2 6 1	0	0
3	D	1	Total C O P 9 2 6 1	0	0

• Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0
4	В	1	Total K 1 1	0	0
4	С	1	Total K 1 1	0	0
4	D	1	Total K 1 1	0	0

• Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mn 1 1	0	0
5	В	1	Total Mn 1 1	0	0
5	С	1	Total Mn 1 1	0	0
5	D	1	Total Mn 1 1	0	0

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



## 3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	76.30Å 172.98Å 85.78Å	Donositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 93.12° 90.00°	Depositor
Resolution (Å)	20.00 - 2.75	Depositor
Resolution (A)	19.98 - 2.75	EDS
% Data completeness	93.7 (20.00-2.75)	Depositor
(in resolution range)	93.7 (19.98-2.75)	EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.51 (at 2.75Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D.	0.268 , 0.303	Depositor
$R, R_{free}$	0.320 , $0.339$	DCC
$R_{free}$ test set	1103 reflections $(2.05\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.32 , 13.7	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	15550	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

### 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)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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	Tuno	Chain	Res	Link	Bo	ond leng	ths	Bond angles			
WIOI	Type	Chain	rtes	ries	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FBP	С	580	-	18,20,20	1.08	1 (5%)	23,32,32	0.97	2 (8%)	
3	PGA	В	581	5,4	8,8,8	1.40	1 (12%)	10,11,11	1.19	2 (20%)	
2	FBP	В	580	-	18,20,20	1.06	0	23,32,32	0.97	2 (8%)	
3	PGA	A	581	5,4	8,8,8	1.59	1 (12%)	10,11,11	1.06	0	
2	FBP	D	580	-	18,20,20	1.06	1 (5%)	23,32,32	1.04	1 (4%)	
3	PGA	С	581	5,4	8,8,8	1.74	1 (12%)	10,11,11	1.06	0	
2	FBP	A	580	-	18,20,20	0.89	1 (5%)	23,32,32	0.88	0	
3	PGA	D	581	5,4	8,8,8	1.44	1 (12%)	10,11,11	1.01	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	FBP	С	580	-	-	5/13/32/32	0/1/1/1
3	PGA	В	581	5,4	-	3/6/6/6	-
2	FBP	В	580	-	-	5/13/32/32	0/1/1/1
3	PGA	A	581	5,4	-	3/6/6/6	-
2	FBP	D	580	_	-	5/13/32/32	0/1/1/1
3	PGA	С	581	5,4	-	3/6/6/6	-
2	FBP	A	580	-	-	5/13/32/32	0/1/1/1
3	PGA	D	581	5,4	-	3/6/6/6	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(A)
3	С	581	PGA	O1P-C2	-4.11	1.40	1.43
3	A	581	PGA	O1P-C2	-3.79	1.40	1.43
3	D	581	PGA	O1P-C2	-3.20	1.40	1.43
3	В	581	PGA	O1P-C2	-3.05	1.41	1.43
2	С	580	FBP	O2-C2	2.25	1.44	1.40
2	A	580	FBP	O2-C2	2.04	1.44	1.40
2	D	580	FBP	O2-C2	2.02	1.44	1.40



All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
2	D	580	FBP	P2-O6-C6	2.51	125.22	118.30
2	В	580	FBP	O2P-P1-O1	2.28	112.81	106.73
2	С	580	FBP	O2P-P1-O1	2.28	112.80	106.73
3	В	581	PGA	O2-C1-O1	-2.24	117.72	123.30
3	В	581	PGA	O3P-P-O1P	2.20	112.60	106.73
2	В	580	FBP	P2-O6-C6	2.02	123.86	118.30
2	С	580	FBP	P2-O6-C6	2.01	123.84	118.30

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	580	FBP	O5-C5-C6-O6
2	A	580	FBP	C6-O6-P2-O5P
2	A	580	FBP	C6-O6-P2-O6P
2	В	580	FBP	O5-C5-C6-O6
2	В	580	FBP	C6-O6-P2-O4P
2	В	580	FBP	C6-O6-P2-O5P
2	С	580	FBP	C6-O6-P2-O4P
2	С	580	FBP	C6-O6-P2-O5P
2	D	580	FBP	O5-C5-C6-O6
2	D	580	FBP	C6-O6-P2-O5P
2	D	580	FBP	C6-O6-P2-O6P
3	A	581	PGA	C2-O1P-P-O3P
3	A	581	PGA	C2-O1P-P-O4P
3	В	581	PGA	C2-O1P-P-O3P
3	В	581	PGA	C2-O1P-P-O4P
3	С	581	PGA	C2-O1P-P-O3P
3	С	581	PGA	C2-O1P-P-O4P
3	D	581	PGA	C2-O1P-P-O3P
3	D	581	PGA	C2-O1P-P-O4P
2	В	580	FBP	C4-C5-C6-O6
2	С	580	FBP	C4-C5-C6-O6
2	С	580	FBP	O5-C5-C6-O6
2	A	580	FBP	C4-C5-C6-O6
2	D	580	FBP	C4-C5-C6-O6
2	A	580	FBP	C6-O6-P2-O4P
2	D	580	FBP	C6-O6-P2-O4P
3	A	581	PGA	C2-O1P-P-O2P
3	В	581	PGA	C2-O1P-P-O2P
3	С	581	PGA	C2-O1P-P-O2P

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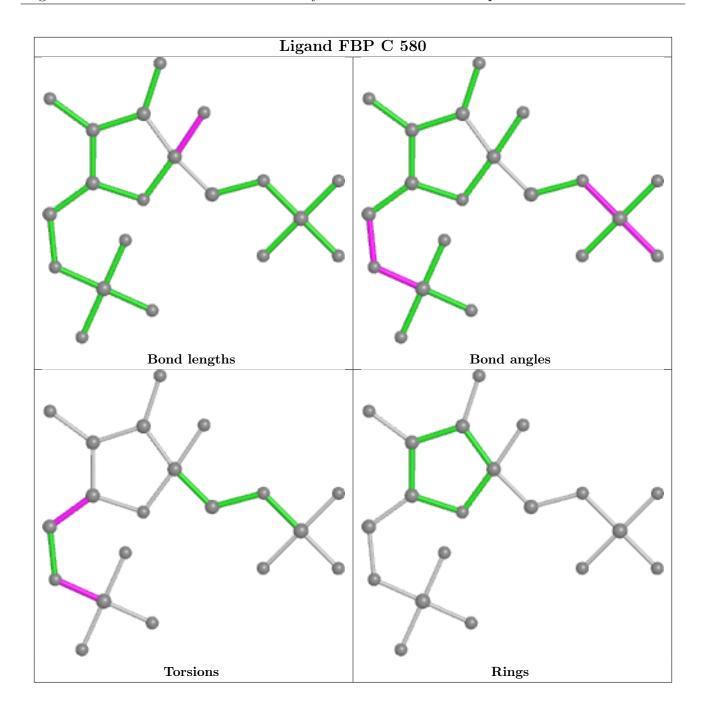
Mol	Chain	Res	Type	Atoms
3	D	581	PGA	C2-O1P-P-O2P
2	В	580	FBP	C6-O6-P2-O6P
2	С	580	FBP	C6-O6-P2-O6P

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





### 4.7 Other polymers (i)

There are no such residues in this entry.

## 4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1



All chain breaks are listed below:

Mod	el Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	171:PRO	С	172:GLU	N	1.95



### 5 Fit of model and data (i)

#### 5.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

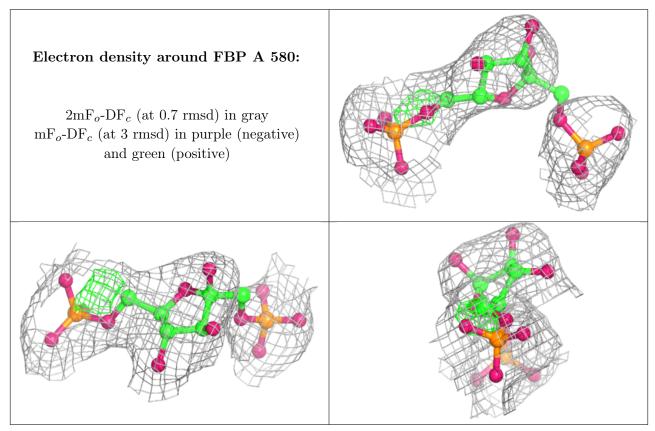
### 5.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

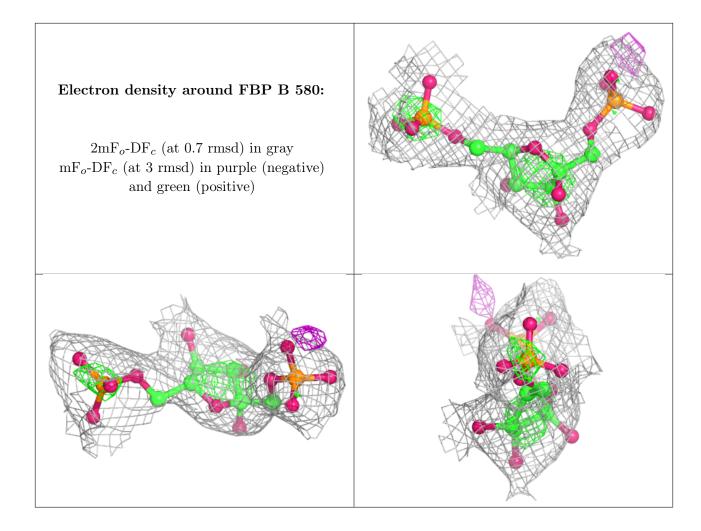
### 5.4 Ligands (i)

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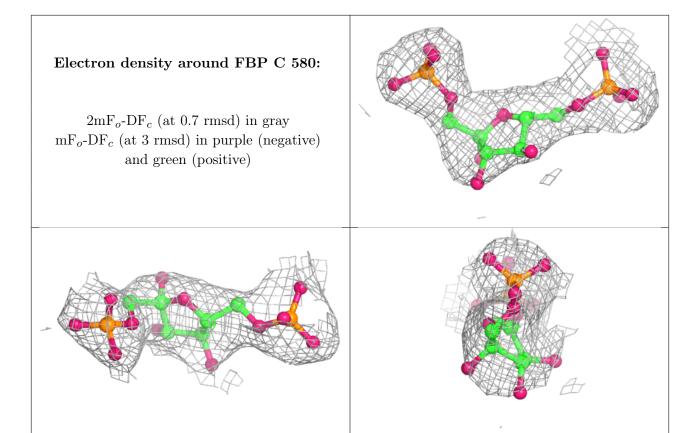
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





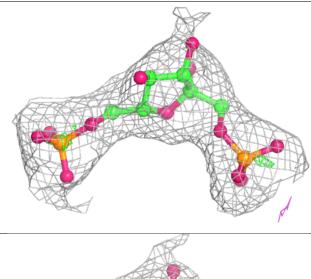


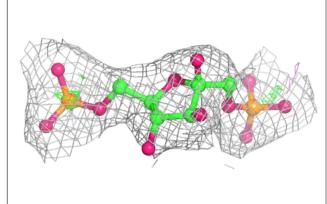


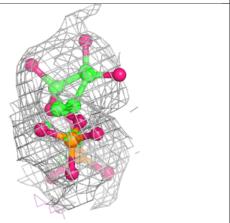


# Electron density around FBP D 580:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$  (at 0.7 rmsd) in gray  ${\rm mF}_o\text{-}{\rm DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)









## 5.5 Other polymers (i)

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