

Full wwPDB X-ray Structure Validation Report (i)

Oct 9, 2023 – 11:49 AM EDT

PDB ID : 8EDR

Title : E. coli pyruvate kinase (PykF) P70Q

Authors: Donovan, K.A.; Coombes, D.; Dobson, R.C.J.; Cooper, T.F.

Deposited on : 2022-09-05

Resolution : 2.64 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 : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

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)

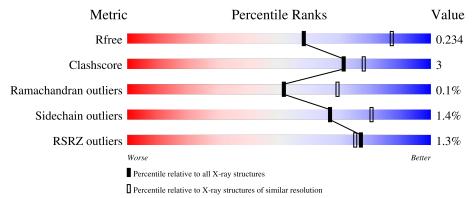
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.64 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 <=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	89%	9%	•		
1	В	470	89%	9%			



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14165 atoms, of which 7152 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.

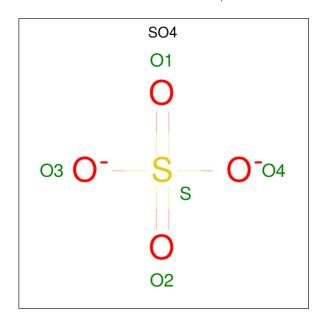
• Molecule 1 is a protein called Pyruvate kinase.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	A	462	Total 7045	C 2164	H 3571	N 604	O 682	S 24	0	1	0
1	В	463	Total 7063	C 2170	H 3581	N 605	O 683	S 24	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	GLN	PRO	engineered mutation	UNP Q2TL68
В	70	GLN	PRO	engineered mutation	UNP Q2TL68

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total O 5 4	S 1	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total O S 5 4 1	0	0

• Molecule 3 is water.

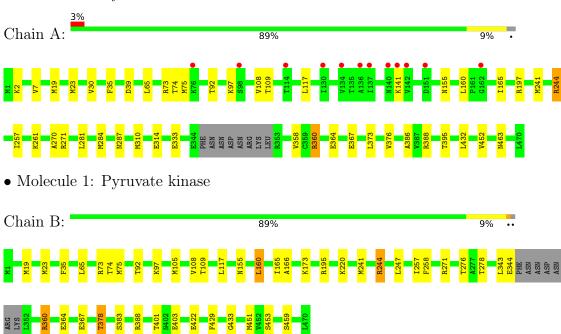
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	19	Total O 19 19	0	0
3	В	28	Total O 28 28	0	0



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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	73.54Å 241.97Å 133.75Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.83 - 2.64	Depositor
resolution (A)	44.86 - 2.64	EDS
% Data completeness	94.7 (41.83-2.64)	Depositor
(in resolution range)	94.7 (44.86-2.64)	EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.37 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.193 , 0.234	Depositor
it, it free	0.193 , 0.234	DCC
R_{free} test set	2390 reflections (7.08%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.42, 36.7	EDS
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14165	wwPDB-VP
Average B, all atoms $(Å^2)$	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	Bo	nd lengths	Bond angles		
IVIOI	Chain	RMSZ # Z >		RMSZ	# Z >5	
1	A	0.58	0/3514	0.76	1/4735 (0.0%)	
1	В	0.61	1/3515 (0.0%)	0.81	1/4736 (0.0%)	
All	All	0.59	1/7029 (0.0%)	0.78	2/9471 (0.0%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
1	В	166	ALA	C-N	-5.05	1.22	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathbf{Ideal}(^{o})$
1	A	432	LEU	CB-CG-CD2	5.22	119.88	111.00
1	В	160	LEU	CB-CG-CD1	-5.01	102.48	111.00

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	3474	3571	3563	25	1
1	В	3482	3581	3581	24	1
2	A	5	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	5	0	0	1	0
3	A	19	0	0	0	0
3	В	28	0	0	0	0
All	All	7013	7152	7144	49	1

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 3.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({ m \AA})$	overlap(Å)
1:B:378:THR:HG22	2:B:502:SO4:O3	1.80	0.81
1:A:360:ARG:NH2	1:A:364:GLU:OE1	2.18	0.77
1:B:378:THR:HG23	1:B:383:SER:OG	1.91	0.70
1:B:75:MET:HE2	1:B:108:VAL:C	2.19	0.62
1:A:117:LEU:HD21	1:A:160:LEU:HD22	1.80	0.62
1:B:73:ARG:HD3	1:B:155:ASN:OD1	2.01	0.61
1:A:75:MET:HE1	1:A:97:LYS:HG2	1.83	0.61
1:B:360:ARG:NH2	1:B:364:GLU:OE1	2.32	0.60
1:A:160:LEU:HB2	1:A:165:ILE:HD11	1.86	0.57
1:A:75:MET:HE2	1:A:108:VAL:C	2.24	0.57
1:A:373:LEU:HD12	1:A:395:THR:O	2.06	0.56
1:A:244:ARG:HD3	1:A:244:ARG:H	1.72	0.54
1:B:74:THR:O	1:B:155:ASN:HA	2.08	0.52
1:A:74:THR:O	1:A:155:ASN:HA	2.10	0.50
1:A:7:VAL:HG22	1:A:30:VAL:HB	1.94	0.50
1:B:35:PHE:O	1:B:173:LYS:NZ	2.44	0.50
1:A:271:ARG:HG2	1:A:386:ALA:HA	1.94	0.50
1:A:75:MET:CE	1:A:97:LYS:HG2	2.42	0.49
1:A:376:VAL:HG22	1:A:452:VAL:HB	1.95	0.49
1:A:92:THR:HG21	1:A:141:LYS:HD2	1.93	0.49
1:A:241:MET:HE2	1:A:310:MET:HE3	1.95	0.48
1:A:284:MET:HA	1:A:287:ASN:O	2.13	0.48
1:B:117:LEU:HD21	1:B:160:LEU:HD22	1.96	0.47
1:A:2:LYS:HB3	1:A:333:GLU:HG3	1.95	0.46
1:A:35:PHE:CE1	1:A:65:LEU:HG	2.51	0.45
1:B:244:ARG:HD2	1:B:276:THR:HG23	1.99	0.45
1:B:75:MET:CE	1:B:109:THR:HA	2.46	0.45
1:B:65:LEU:C	1:B:65:LEU:HD23	2.37	0.44
1:B:75:MET:HE1	1:B:109:THR:HA	1.99	0.44
1:A:73:ARG:O	1:A:109:THR:HG23	2.18	0.44



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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	$overlap(ext{Å})$
1:B:433:GLY:HA3	1:B:451:MET:CE	2.48	0.44
1:B:92:THR:O	1:B:105:MET:HA	2.19	0.43
1:A:358:VAL:HG21	1:A:463:ASN:HA	2.00	0.43
1:A:75:MET:HE3	1:A:97:LYS:HA	2.01	0.43
1:B:429:PHE:CE2	1:B:453:SER:HB3	2.53	0.43
1:A:270:ALA:O	1:A:271:ARG:HB2	2.19	0.43
1:B:247:LEU:HD12	1:B:247:LEU:HA	1.90	0.43
1:B:401:THR:HG21	1:B:422:GLU:HA	1.99	0.43
1:B:257:ILE:HG23	1:B:258:PHE:N	2.34	0.43
1:B:343:LEU:O	1:B:344:GLU:HG2	2.19	0.43
1:B:75:MET:HE1	1:B:97:LYS:HG2	2.01	0.42
1:A:281:LEU:O	1:A:314:GLU:HG2	2.19	0.42
1:A:257:ILE:HG12	1:A:261:LYS:HE2	2.01	0.42
1:A:19:MET:O	1:A:23:MET:HG2	2.19	0.42
1:B:19:MET:O	1:B:23:MET:HG2	2.20	0.41
1:B:35:PHE:CE1	1:B:65:LEU:HG	2.55	0.41
1:B:220:LYS:HG2	1:B:241:MET:HB3	2.03	0.41
1:A:39:ASP:C	1:A:39:ASP:OD1	2.58	0.40
1:B:165:ILE:O	1:B:195:ARG:NH1	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:197:ARG:NH2	1:B:403:GLU:OE2[8_545]	2.15	0.05

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	459/470 (98%)	450 (98%)	9 (2%)	0	100 100



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Mol	Chain	Analysed	Analysed Favoured Allo		Outliers	Percentile	s
1	В	459/470 (98%)	449 (98%)	9 (2%)	1 (0%)	47 64	
All	All	918/940 (98%)	899 (98%)	18 (2%)	1 (0%)	51 69	

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	278	THR

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	sed Rotameric Outlier		Percentiles
1	A	381/389 (98%)	377 (99%)	4 (1%)	76 86
1	В	381/389 (98%)	374 (98%)	7 (2%)	59 75
All	All	762/778 (98%)	751 (99%)	11 (1%)	67 80

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	ARG
1	A	360	ARG
1	A	367	GLU
1	A	388	ARG
1	В	244	ARG
1	В	271	ARG
1	В	360	ARG
1	В	367	GLU
1	В	378	THR
1	В	388	ARG
1	В	459	SER

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)

2 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	Pag	Link	B	ond leng	${ m gths}$	В	ond ang	gles
MIOI	туре	Chain	Res	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	SO4	В	502	-	4,4,4	0.62	0	6,6,6	0.08	0
2	SO4	A	502	-	4,4,4	0.65	0	6,6,6	0.14	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	502	SO4	1	0



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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95^{th} 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	$OWAB(A^2)$	Q<0.9
1	A	462/470 (98%)	0.05	12 (2%) 56 52	17, 33, 62, 93	0
1	В	463/470 (98%)	-0.13	0 100 100	16, 27, 40, 88	0
All	All	925/940 (98%)	-0.04	12 (1%) 77 75	16, 29, 55, 93	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	ASN	3.3
1	A	136	ALA	3.3
1	A	141	LYS	3.2
1	A	142	VAL	2.9
1	A	130	ILE	2.8
1	A	137	ILE	2.7
1	A	134	VAL	2.7
1	A	151	ASP	2.4
1	A	98	SER	2.2
1	A	162	GLY	2.1
1	A	76	LYS	2.1
1	A	114	THR	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	SO4	A	502	5/5	0.97	0.17	30,30,30,30	0
2	SO4	В	502	5/5	0.97	0.20	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.

