



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 10:02 pm GMT

PDB ID : 2PFK
Title : THE CRYSTAL STRUCTURE OF UNLIGANDED PHOSPHOFRUCTOKINASE FROM ESCHERICHIA COLI
Authors : Rypniewski, W.R.; Evans, P.R.
Deposited on : 1988-01-25
Resolution : 2.40 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

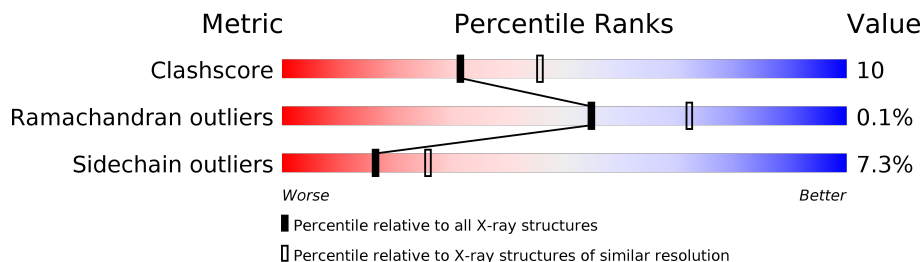
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	320	
1	B	320	
1	C	320	
1	D	320	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9371 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 6-PHOSPHOFRUCTOKINASE ISOZYME I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2255	1413	395	431	16			
1	B	301	Total	C	N	O	S	0	0	0
			2233	1401	390	426	16			
1	C	302	Total	C	N	O	S	0	0	1
			2251	1409	394	433	15			
1	D	305	Total	C	N	O	S	0	0	0
			2285	1432	396	441	16			

- Molecule 2 is water.

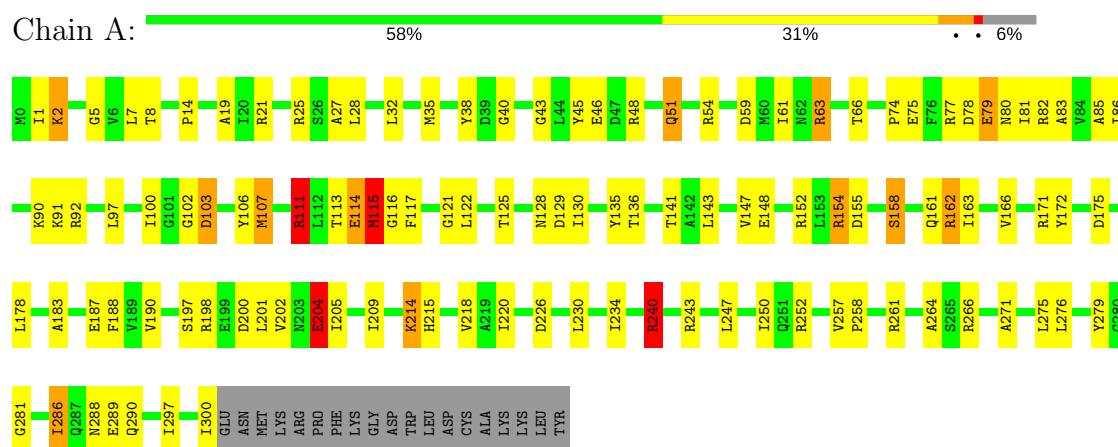
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	81	Total	O	0	0
			81	81		
2	B	76	Total	O	0	0
			76	76		
2	C	94	Total	O	0	0
			94	94		
2	D	96	Total	O	0	0
			96	96		

3 Residue-property plots

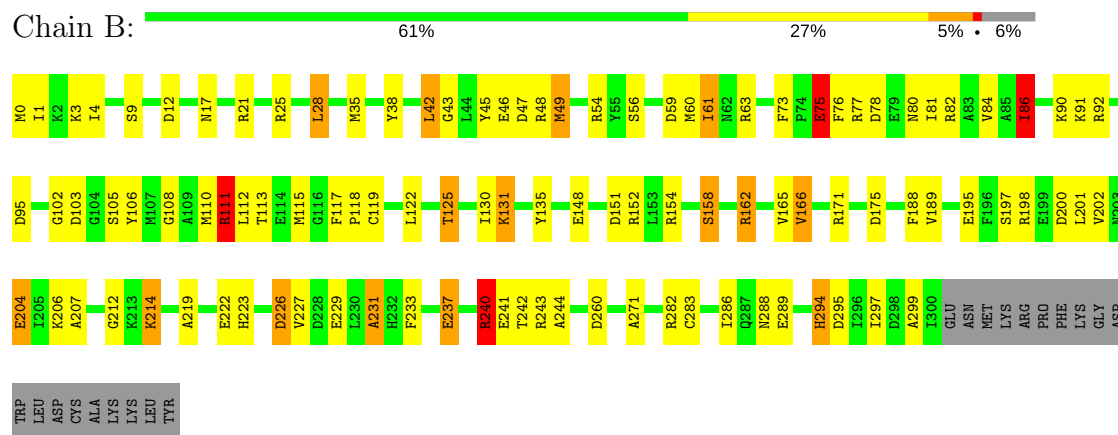
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

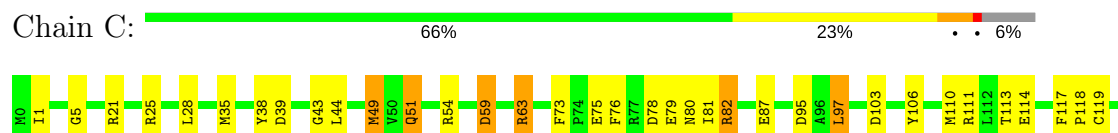
• Molecule 1: 6-PHOSPHOFRUCTOKINASE ISOZYME I

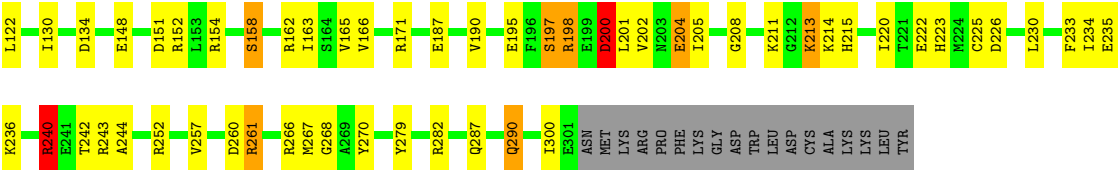


• Molecule 1: 6-PHOSPHOFRUCTOKINASE ISOZYME I

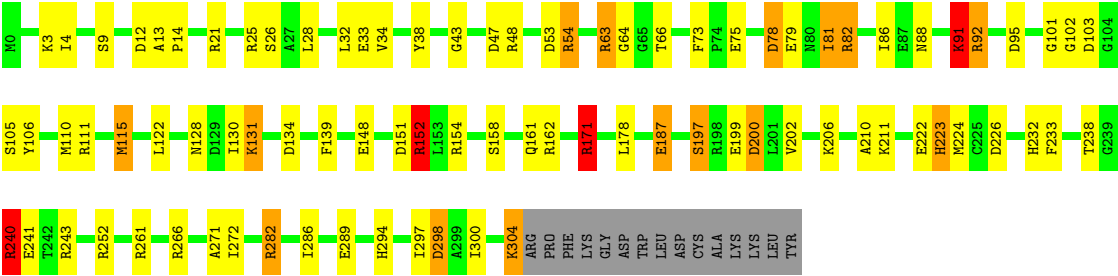


• Molecule 1: 6-PHOSPHOFRUCTOKINASE ISOZYME I





• Molecule 1: 6-PHOSPHOFRUCTOKINASE ISOZYME I



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	177.00Å 66.40Å 154.00Å 90.00° 118.80° 90.00°	Depositor
Resolution (Å)	100.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (100.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9371	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

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	0.84	0/2286	1.95	48/3085 (1.6%)
1	B	0.83	0/2264	1.92	49/3057 (1.6%)
1	C	0.86	0/2282	1.89	55/3081 (1.8%)
1	D	0.84	0/2317	1.92	69/3128 (2.2%)
All	All	0.84	0/9149	1.92	221/12351 (1.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 221 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ARG	CD-NE-CZ	22.66	155.32	123.60
1	D	243	ARG	NE-CZ-NH1	20.52	130.56	120.30
1	B	152	ARG	CD-NE-CZ	20.30	152.02	123.60
1	A	152	ARG	NE-CZ-NH2	-19.54	110.53	120.30
1	B	152	ARG	NE-CZ-NH2	-18.16	111.22	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	300	ILE	Mainchain
1	D	152	ARG	Sidechain

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	2255	0	2250	57	1
1	B	2233	0	2212	66	0
1	C	2251	0	2239	35	2
1	D	2285	0	2262	32	1
2	A	81	0	0	1	0
2	B	76	0	0	4	0
2	C	94	0	0	4	0
2	D	96	0	0	2	1
All	All	9371	0	8963	183	3

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 10.

The worst 5 of 183 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:131:LYS:HD2	1:B:131:LYS:H	1.09	1.09
1:A:240:ARG:HG2	1:A:240:ARG:HH11	1.17	1.08
1:C:240:ARG:HH11	1:C:240:ARG:HG2	1.28	0.95
1:B:75:GLU:HB3	1:B:81:ILE:HD13	1.58	0.84
1:B:131:LYS:N	1:B:131:LYS:HD2	1.93	0.81

All (3) 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	Interatomic distance (Å)	Clash overlap (Å)
2:D:389:HOH:O	2:D:389:HOH:O[4_556]	1.95	0.25
1:C:236:LYS:NZ	1:D:232:HIS:CD2[4_546]	2.07	0.13
1:A:279:TYR:OH	1:C:87:GLU:OE2[4_556]	2.10	0.10

5.3 Torsion angles

5.3.1 Protein backbone

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	299/320 (93%)	288 (96%)	10 (3%)	1 (0%)	44	60
1	B	299/320 (93%)	293 (98%)	6 (2%)	0	100	100
1	C	300/320 (94%)	292 (97%)	8 (3%)	0	100	100
1	D	303/320 (95%)	290 (96%)	13 (4%)	0	100	100
All	All	1201/1280 (94%)	1163 (97%)	37 (3%)	1 (0%)	55	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	MET

5.3.2 Protein sidechains

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	233/255 (91%)	214 (92%)	19 (8%)	13	20
1	B	227/255 (89%)	210 (92%)	17 (8%)	16	24
1	C	233/255 (91%)	216 (93%)	17 (7%)	16	26
1	D	236/255 (92%)	221 (94%)	15 (6%)	20	32
All	All	929/1020 (91%)	861 (93%)	68 (7%)	16	26

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	131	LYS
1	C	51	GLN
1	D	178	LEU
1	B	158	SER
1	B	240	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	288	ASN
1	C	161	GLN
1	D	161	GLN
1	B	232	HIS
1	C	288	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.