



# Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 01:01 AM GMT

PDB ID : 4A3S  
Title : Crystal structure of PFK from Bacillus subtilis  
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Deposited on : 2011-10-04  
Resolution : 2.30 Å (reported)

This is a full wwPDB validation 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 <http://wwpdb.org/ValidationPDFNotes.html>

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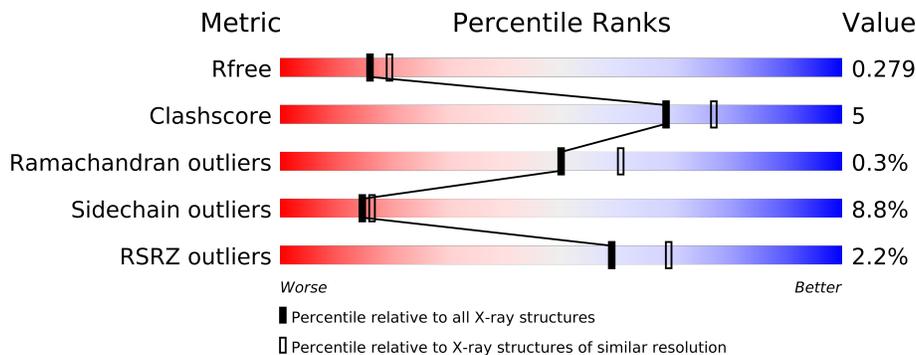
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	319	
1	B	319	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4992 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	319	2407	1508	429	461	9	0	0	0
1	B	319	2407	1508	429	461	9	0	0	0

- Molecule 2 is water.

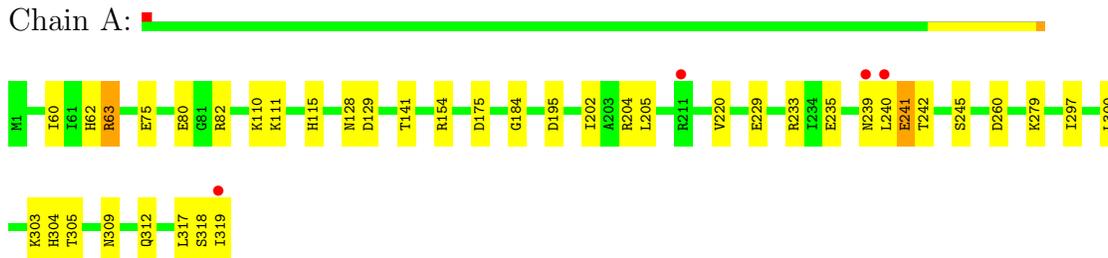
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total	O	0	0
			94	94		
2	B	84	Total	O	0	0
			84	84		

### 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 errors 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.

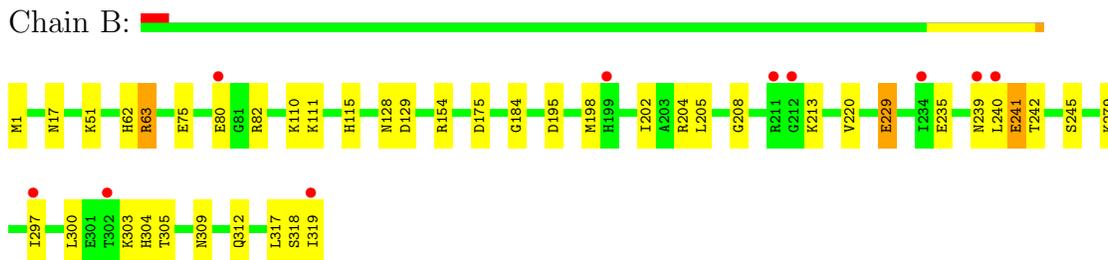
- Molecule 1: 6-PHOSPHOFRUCTOKINASE

Chain A:



- Molecule 1: 6-PHOSPHOFRUCTOKINASE

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.43Å 77.01Å 101.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.74 – 2.30 45.74 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (45.74-2.30) 79.6 (45.74-2.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.00Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.229 , 0.276 0.238 , 0.279	Depositor DCC
$R_{free}$ test set	2253 reflections (5.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.9	Xtrriage
Anisotropy	0.878	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 32.0	EDS
Estimated twinning fraction	0.084 for l,-k,h	Xtrriage
L-test for twinning	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtrriage
Outliers	0 of 43601 reflections	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4992	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.64 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.3156e-03.*

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

## 5 Model quality (i)

### 5.1 Standard geometry (i)

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	0.50	0/2441	0.61	3/3286 (0.1%)
1	B	0.53	0/2441	0.63	3/3286 (0.1%)
All	All	0.51	0/4882	0.62	6/6572 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	LEU	CA-CB-CG	5.59	128.16	115.30
1	A	205	LEU	CA-CB-CG	5.59	128.15	115.30
1	A	63	ARG	CB-CG-CD	5.26	125.27	111.60
1	B	63	ARG	CB-CG-CD	5.21	125.13	111.60
1	B	229	GLU	CA-CB-CG	5.07	124.56	113.40
1	A	63	ARG	CG-CD-NE	-5.02	101.26	111.80

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2407	0	0	11	0
1	B	2407	0	0	12	0
2	A	94	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	84	0	0	3	0
All	All	4992	0	0	23	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (23) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:204:ARG:NH1	1:A:318:SER:OG	2.24	0.70
1:B:1:MET:N	2:B:2001:HOH:O	2.27	0.66
1:A:154:ARG:NH2	1:A:184:GLY:O	2.29	0.66
1:B:154:ARG:NH2	1:B:184:GLY:O	2.30	0.65
1:B:204:ARG:NH1	1:B:318:SER:OG	2.31	0.64
1:A:129:ASP:CA	1:A:304:HIS:CD2	2.88	0.56
1:B:129:ASP:CA	1:B:304:HIS:CD2	2.91	0.54
1:B:62:HIS:CE1	1:B:63:ARG:CZ	2.92	0.53
1:B:198:MET:N	2:B:2062:HOH:O	2.41	0.53
1:A:63:ARG:NH1	2:A:2027:HOH:O	2.44	0.51
1:A:62:HIS:CE1	1:A:63:ARG:CZ	2.95	0.50
1:B:17:ASN:ND2	2:B:2011:HOH:O	2.49	0.46
1:A:141:THR:OG1	1:A:260:ASP:OD2	2.35	0.45
1:A:304:HIS:ND1	1:A:305:THR:N	2.65	0.44
1:A:128:ASN:O	1:A:304:HIS:NE2	2.52	0.43
1:B:304:HIS:ND1	1:B:305:THR:N	2.67	0.42
1:B:82:ARG:CZ	1:B:115:HIS:CE1	3.03	0.42
1:A:60:ILE:N	2:A:2026:HOH:O	2.52	0.41
1:B:128:ASN:O	1:B:304:HIS:NE2	2.54	0.41
1:A:82:ARG:CZ	1:A:115:HIS:CE1	3.03	0.41
1:B:240:LEU:O	1:B:241:GLU:C	2.58	0.41
1:B:208:GLY:O	1:B:213:LYS:N	2.55	0.40
1:A:240:LEU:O	1:A:241:GLU:C	2.59	0.40

There are no symmetry-related clashes.

## 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	317/319 (99%)	301 (95%)	15 (5%)	1 (0%)	50	60
1	B	317/319 (99%)	299 (94%)	17 (5%)	1 (0%)	50	60
All	All	634/638 (99%)	600 (95%)	32 (5%)	2 (0%)	50	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	GLU
1	B	241	GLU

### 5.3.2 Protein sidechains ❶

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	251/251 (100%)	229 (91%)	22 (9%)	14	16
1	B	251/251 (100%)	229 (91%)	22 (9%)	14	16
All	All	502/502 (100%)	458 (91%)	44 (9%)	14	16

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	GLU
1	A	80	GLU
1	A	110	LYS
1	A	111	LYS
1	A	175	ASP
1	A	195	ASP
1	A	202	ILE
1	A	220	VAL
1	A	229	GLU
1	A	233	ARG
1	A	235	GLU
1	A	239	ASN
1	A	242	THR

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Mol	Chain	Res	Type
1	A	245	SER
1	A	279	LYS
1	A	297	ILE
1	A	300	LEU
1	A	303	LYS
1	A	309	ASN
1	A	312	GLN
1	A	317	LEU
1	A	319	ILE
1	B	51	LYS
1	B	75	GLU
1	B	80	GLU
1	B	110	LYS
1	B	111	LYS
1	B	175	ASP
1	B	195	ASP
1	B	202	ILE
1	B	220	VAL
1	B	229	GLU
1	B	235	GLU
1	B	239	ASN
1	B	242	THR
1	B	245	SER
1	B	279	LYS
1	B	297	ILE
1	B	300	LEU
1	B	303	LYS
1	B	309	ASN
1	B	312	GLN
1	B	317	LEU
1	B	319	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
1	A	319/319 (100%)	-0.02	4 (1%) 74 82	15, 34, 79, 96	0
1	B	319/319 (100%)	0.01	10 (3%) 47 56	18, 35, 79, 96	0
All	All	638/638 (100%)	-0.00	14 (2%) 59 69	15, 35, 79, 96	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	240	LEU	6.8
1	A	319	ILE	5.4
1	B	212	GLY	4.3
1	B	199	HIS	3.1
1	B	240	LEU	3.0
1	A	239	ASN	3.0
1	B	211	ARG	2.7
1	B	234	ILE	2.6
1	B	80	GLU	2.6
1	B	319	ILE	2.5
1	B	239	ASN	2.2
1	B	302	THR	2.1
1	A	211	ARG	2.0
1	B	297	ILE	2.0

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

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

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.