



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 08:12 PM BST

PDB ID : 6VBJ  
Title : CRYSTAL STRUCTURE OF THE HYBRID C-TERMINAL DOMAIN OF ENZYME I OF THE BACTERIAL PHOSPHOTRANSFERASE SYSTEM FORMED BY HYBRIDIZING THE SCAFFOLD OF THE THERMOANAEROBACTER TENGCONGENSIS ENZYME WITH THE ACTIVE SITE LOOPS FROM THE ESCHERICHIA COLI ENZYME  
Authors : Stewart Jr., C.E.  
Deposited on : 2019-12-19  
Resolution : 2.00 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](mailto: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 ⓘ symbol.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

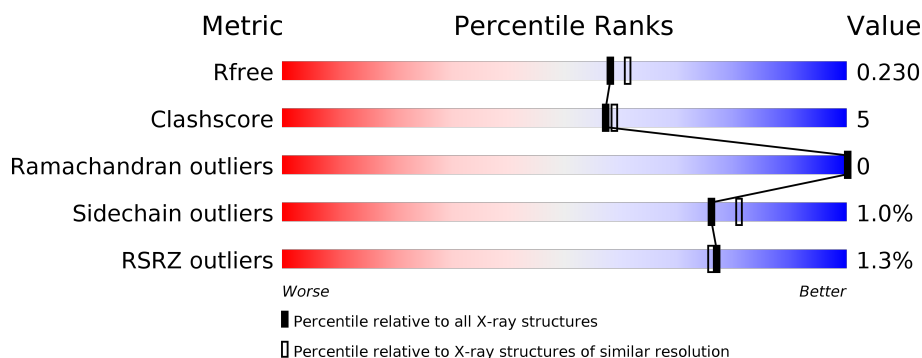
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	314	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 10px; right: 0;">89%</div> <div style="position: absolute; top: 10px; right: 10px;">11%</div> </div> </div>
1	B	314	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">2%</div> <div style="position: absolute; top: 10px; right: 0;">93%</div> <div style="position: absolute; top: 10px; right: 10px;">6%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10266 atoms, of which 4962 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 Phosphoenolpyruvate-protein phosphotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	313	Total	C	H	N	O	S	0	0	0
			4909	1540	2478	405	466	20			
1	B	313	Total	C	H	N	O	S	0	1	0
			4924	1545	2484	406	469	20			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	260	MET	-	initiating methionine	UNP Q8R7R4
A	278	VAL	PRO	engineered mutation	UNP Q8R7R4
A	279	ARG	LYS	engineered mutation	UNP Q8R7R4
A	301	PHE	TYR	engineered mutation	UNP Q8R7R4
A	305	ASP	ASN	engineered mutation	UNP Q8R7R4
A	306	ALA	SER	engineered mutation	UNP Q8R7R4
A	309	THR	SER	engineered mutation	UNP Q8R7R4
A	334	MET	LEU	engineered mutation	UNP Q8R7R4
A	345	MET	LEU	engineered mutation	UNP Q8R7R4
A	346	ASN	ASP	engineered mutation	UNP Q8R7R4
A	347	PHE	MET	engineered mutation	UNP Q8R7R4
A	351	GLU	MET	engineered mutation	UNP Q8R7R4
A	357	TRP	TYR	engineered mutation	UNP Q8R7R4
A	466	GLY	MET	engineered mutation	UNP Q8R7R4
A	468	ASP	GLU	engineered mutation	UNP Q8R7R4
A	469	MET	HIS	engineered mutation	UNP Q8R7R4
A	470	ILE	VAL	engineered mutation	UNP Q8R7R4
A	471	SER	LYS	engineered mutation	UNP Q8R7R4
A	472	HIS	GLU	engineered mutation	UNP Q8R7R4
A	473	LEU	TYR	engineered mutation	UNP Q8R7R4
A	477	MET	PHE	engineered mutation	UNP Q8R7R4
A	478	SER	HIS	engineered mutation	UNP Q8R7R4
B	260	MET	-	initiating methionine	UNP Q8R7R4
B	278	VAL	PRO	engineered mutation	UNP Q8R7R4
B	279	ARG	LYS	engineered mutation	UNP Q8R7R4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	301	PHE	TYR	engineered mutation	UNP Q8R7R4
B	305	ASP	ASN	engineered mutation	UNP Q8R7R4
B	306	ALA	SER	engineered mutation	UNP Q8R7R4
B	309	THR	SER	engineered mutation	UNP Q8R7R4
B	334	MET	LEU	engineered mutation	UNP Q8R7R4
B	345	MET	LEU	engineered mutation	UNP Q8R7R4
B	346	ASN	ASP	engineered mutation	UNP Q8R7R4
B	347	PHE	MET	engineered mutation	UNP Q8R7R4
B	351	GLU	MET	engineered mutation	UNP Q8R7R4
B	357	TRP	TYR	engineered mutation	UNP Q8R7R4
B	466	GLY	MET	engineered mutation	UNP Q8R7R4
B	468	ASP	GLU	engineered mutation	UNP Q8R7R4
B	469	MET	HIS	engineered mutation	UNP Q8R7R4
B	470	ILE	VAL	engineered mutation	UNP Q8R7R4
B	471	SER	LYS	engineered mutation	UNP Q8R7R4
B	472	HIS	GLU	engineered mutation	UNP Q8R7R4
B	473	LEU	TYR	engineered mutation	UNP Q8R7R4
B	477	MET	PHE	engineered mutation	UNP Q8R7R4
B	478	SER	HIS	engineered mutation	UNP Q8R7R4

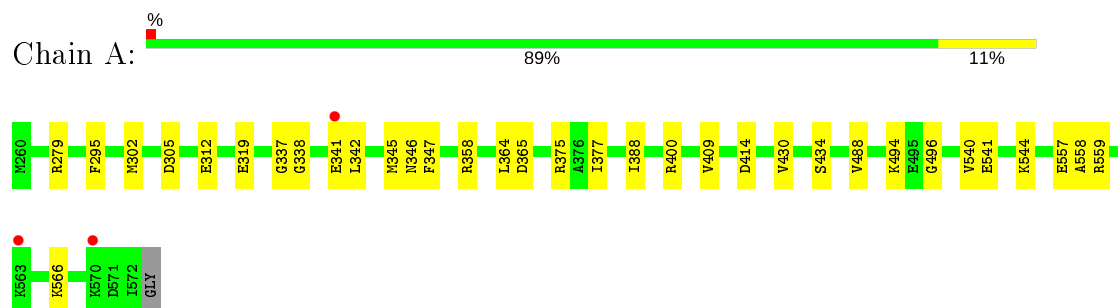
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	232	Total O 232 232	0	0
2	B	201	Total O 201 201	0	0

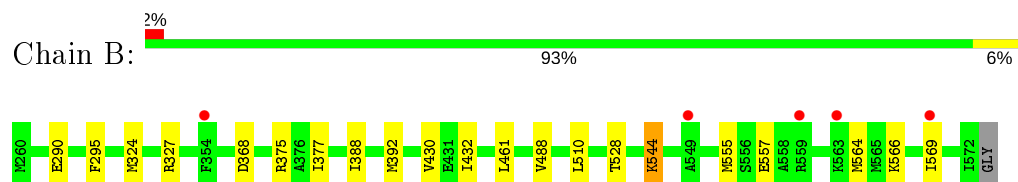
### 3 Residue-property plots [i](#)

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: Phosphoenolpyruvate-protein phosphotransferase



- Molecule 1: Phosphoenolpyruvate-protein phosphotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.43Å 85.42Å 95.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.71 – 2.00 42.71 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (42.71-2.00) 97.9 (42.71-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, $R_{free}$	0.191 , 0.230 0.191 , 0.230	Depositor DCC
$R_{free}$ test set	1997 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10266	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.31 % 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 2.4096e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	0.26	0/2466	0.43	0/3320
1	B	0.25	0/2475	0.42	0/3332
All	All	0.26	0/4941	0.42	0/6652

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2431	2478	2475	33	0
1	B	2440	2484	2480	18	0
2	A	232	0	0	21	2
2	B	201	0	0	6	1
All	All	5304	4962	4955	48	2

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 5.

All (48) 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:A:279:ARG:N	2:A:604:HOH:O	1.97	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:GLU:OE1	2:A:602:HOH:O	1.95	0.85
1:A:557:GLU:OE1	2:A:601:HOH:O	1.93	0.84
1:A:345:MET:O	2:A:603:HOH:O	1.95	0.83
1:A:496:GLY:O	2:A:605:HOH:O	2.00	0.79
1:B:510:LEU:HD23	1:B:569:ILE:HD11	1.66	0.77
1:A:400:ARG:NH1	1:B:557:GLU:OE2	2.21	0.73
1:B:368:ASP:OD1	2:B:602:HOH:O	2.06	0.73
1:A:341:GLU:O	1:A:342:LEU:HD23	1.91	0.70
1:A:365:ASP:OD1	2:A:607:HOH:O	2.09	0.69
1:B:510:LEU:HD21	1:B:566:LYS:HE2	1.78	0.65
1:B:430:VAL:HG11	1:B:488:VAL:HG21	1.82	0.62
1:A:400:ARG:NH1	2:A:606:HOH:O	2.09	0.60
2:A:606:HOH:O	1:B:557:GLU:OE2	2.17	0.60
1:A:566:LYS:O	2:A:608:HOH:O	2.17	0.58
1:A:364:LEU:O	2:A:610:HOH:O	2.17	0.57
1:A:414:ASP:OD1	2:A:609:HOH:O	2.17	0.57
1:A:544:LYS:NZ	2:A:623:HOH:O	2.41	0.53
1:B:324:MET:HE3	1:B:327:ARG:HD2	1.89	0.53
1:B:528:THR:HG23	2:B:743:HOH:O	2.08	0.53
1:B:555:MET:SD	1:B:564:MET:HE1	2.49	0.52
1:A:341:GLU:O	2:A:611:HOH:O	2.19	0.52
1:B:377:ILE:HG21	1:B:388:ILE:HG12	1.93	0.51
1:A:319:GLU:OE2	2:A:612:HOH:O	2.19	0.51
1:A:375:ARG:HG2	1:A:409:VAL:HG13	1.93	0.50
1:A:430:VAL:HG11	1:A:488:VAL:HG21	1.93	0.50
1:B:375:ARG:NH2	2:B:607:HOH:O	2.31	0.49
1:A:358:ARG:NH1	2:A:625:HOH:O	2.45	0.49
1:B:290:GLU:OE1	2:B:604:HOH:O	2.19	0.49
1:B:510:LEU:HD23	1:B:569:ILE:CD1	2.41	0.48
1:A:337:GLY:HA3	2:A:617:HOH:O	2.13	0.48
1:A:434:SER:HB3	1:B:461:LEU:HD23	1.97	0.47
1:A:341:GLU:O	1:A:341:GLU:HG2	2.13	0.47
1:A:541:GLU:HB2	1:A:544:LYS:HE3	1.97	0.47
1:A:305:ASP:HB3	2:A:651:HOH:O	2.13	0.46
1:B:544:LYS:NZ	2:B:601:HOH:O	2.03	0.45
1:B:392:MET:HG3	1:B:432:ILE:HD11	1.98	0.44
1:A:434:SER:CB	1:B:461:LEU:HD23	2.48	0.44
1:A:338:GLY:HA2	1:A:347:PHE:CG	2.54	0.43
1:A:540:VAL:HG13	1:A:540:VAL:O	2.19	0.43
1:A:375:ARG:NH2	2:A:619:HOH:O	2.36	0.42
1:A:279:ARG:HB2	2:A:604:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LEU:HD23	2:A:611:HOH:O	2.19	0.42
1:A:377:ILE:HG21	1:A:388:ILE:HG12	2.00	0.42
1:B:544:LYS:CE	2:B:601:HOH:O	2.61	0.42
1:A:558:ALA:O	2:A:613:HOH:O	2.21	0.41
1:A:302:MET:HA	1:A:342:LEU:HD21	2.02	0.40
1:A:345:MET:O	1:A:346:ASN:HB3	2.22	0.40

All (2) 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:A:603:HOH:O	2:B:701:HOH:O 3_545]	2.13	0.07
2:A:726:HOH:O	2:A:796:HOH:O 4_556]	2.19	0.01

## 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	311/314 (99%)	304 (98%)	7 (2%)	0	100	100
1	B	312/314 (99%)	307 (98%)	5 (2%)	0	100	100
All	All	623/628 (99%)	611 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	Rotameric	Outliers	Percentiles	
1	A	260/260 (100%)	257 (99%)	3 (1%)	71	76
1	B	261/260 (100%)	259 (99%)	2 (1%)	81	86
All	All	521/520 (100%)	516 (99%)	5 (1%)	76	81

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	PHE
1	A	494	LYS
1	A	559	ARG
1	B	295	PHE
1	B	544	LYS

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 molecules 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 monosaccharides 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 [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<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	313/314 (99%)	0.08	3 (0%) 82 81	17, 28, 66, 96	0
1	B	313/314 (99%)	0.08	5 (1%) 72 70	18, 29, 63, 105	0
All	All	626/628 (99%)	0.08	8 (1%) 77 76	17, 29, 65, 105	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	563	LYS	3.0
1	A	563	LYS	2.7
1	A	341	GLU	2.7
1	B	569	ILE	2.6
1	B	559	ARG	2.4
1	A	570	LYS	2.4
1	B	354	PHE	2.3
1	B	549	ALA	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.