



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2025 – 12:03 PM EDT

PDB ID : 3TN5  
Title : Crystal structure of GkaP mutant Y99L from *Geobacillus kaustophilus* HTA426  
Authors : An, J.; Zhang, Z.; Zhang, Y.; Feng, Y.; Wu, G.  
Deposited on : 2011-09-01  
Resolution : 1.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

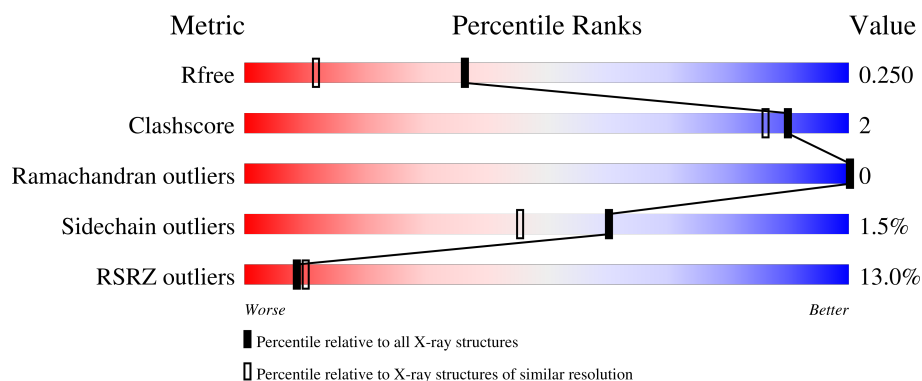
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

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  $\geq 3$ , 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	360	<div> <div>16%</div> <div> <div></div> <div>85%</div> <div>5%</div> <div>10%</div> </div> </div>
1	B	360	<div> <div>8%</div> <div> <div></div> <div>84%</div> <div>6%</div> <div>10%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5597 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 Phosphotriesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2544	1617	436	475	16			
1	B	324	Total	C	N	O	S	0	0	0
			2544	1617	436	475	16			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	expression tag	UNP Q5KZU5
A	-32	GLY	-	expression tag	UNP Q5KZU5
A	-31	SER	-	expression tag	UNP Q5KZU5
A	-30	SER	-	expression tag	UNP Q5KZU5
A	-29	HIS	-	expression tag	UNP Q5KZU5
A	-28	HIS	-	expression tag	UNP Q5KZU5
A	-27	HIS	-	expression tag	UNP Q5KZU5
A	-26	HIS	-	expression tag	UNP Q5KZU5
A	-25	HIS	-	expression tag	UNP Q5KZU5
A	-24	HIS	-	expression tag	UNP Q5KZU5
A	-23	SER	-	expression tag	UNP Q5KZU5
A	-22	SER	-	expression tag	UNP Q5KZU5
A	-21	GLY	-	expression tag	UNP Q5KZU5
A	-20	LEU	-	expression tag	UNP Q5KZU5
A	-19	VAL	-	expression tag	UNP Q5KZU5
A	-18	PRO	-	expression tag	UNP Q5KZU5
A	-17	ARG	-	expression tag	UNP Q5KZU5
A	-16	GLY	-	expression tag	UNP Q5KZU5
A	-15	SER	-	expression tag	UNP Q5KZU5
A	-14	HIS	-	expression tag	UNP Q5KZU5
A	-13	MET	-	expression tag	UNP Q5KZU5
A	-12	ALA	-	expression tag	UNP Q5KZU5
A	-11	SER	-	expression tag	UNP Q5KZU5
A	-10	MET	-	expression tag	UNP Q5KZU5
A	-9	THR	-	expression tag	UNP Q5KZU5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP Q5KZU5
A	-7	GLY	-	expression tag	UNP Q5KZU5
A	-6	GLN	-	expression tag	UNP Q5KZU5
A	-5	GLN	-	expression tag	UNP Q5KZU5
A	-4	MET	-	expression tag	UNP Q5KZU5
A	-3	GLY	-	expression tag	UNP Q5KZU5
A	-2	ARG	-	expression tag	UNP Q5KZU5
A	-1	GLY	-	expression tag	UNP Q5KZU5
A	0	SER	-	expression tag	UNP Q5KZU5
A	99	LEU	TYR	engineered mutation	UNP Q5KZU5
B	-33	MET	-	expression tag	UNP Q5KZU5
B	-32	GLY	-	expression tag	UNP Q5KZU5
B	-31	SER	-	expression tag	UNP Q5KZU5
B	-30	SER	-	expression tag	UNP Q5KZU5
B	-29	HIS	-	expression tag	UNP Q5KZU5
B	-28	HIS	-	expression tag	UNP Q5KZU5
B	-27	HIS	-	expression tag	UNP Q5KZU5
B	-26	HIS	-	expression tag	UNP Q5KZU5
B	-25	HIS	-	expression tag	UNP Q5KZU5
B	-24	HIS	-	expression tag	UNP Q5KZU5
B	-23	SER	-	expression tag	UNP Q5KZU5
B	-22	SER	-	expression tag	UNP Q5KZU5
B	-21	GLY	-	expression tag	UNP Q5KZU5
B	-20	LEU	-	expression tag	UNP Q5KZU5
B	-19	VAL	-	expression tag	UNP Q5KZU5
B	-18	PRO	-	expression tag	UNP Q5KZU5
B	-17	ARG	-	expression tag	UNP Q5KZU5
B	-16	GLY	-	expression tag	UNP Q5KZU5
B	-15	SER	-	expression tag	UNP Q5KZU5
B	-14	HIS	-	expression tag	UNP Q5KZU5
B	-13	MET	-	expression tag	UNP Q5KZU5
B	-12	ALA	-	expression tag	UNP Q5KZU5
B	-11	SER	-	expression tag	UNP Q5KZU5
B	-10	MET	-	expression tag	UNP Q5KZU5
B	-9	THR	-	expression tag	UNP Q5KZU5
B	-8	GLY	-	expression tag	UNP Q5KZU5
B	-7	GLY	-	expression tag	UNP Q5KZU5
B	-6	GLN	-	expression tag	UNP Q5KZU5
B	-5	GLN	-	expression tag	UNP Q5KZU5
B	-4	MET	-	expression tag	UNP Q5KZU5
B	-3	GLY	-	expression tag	UNP Q5KZU5
B	-2	ARG	-	expression tag	UNP Q5KZU5

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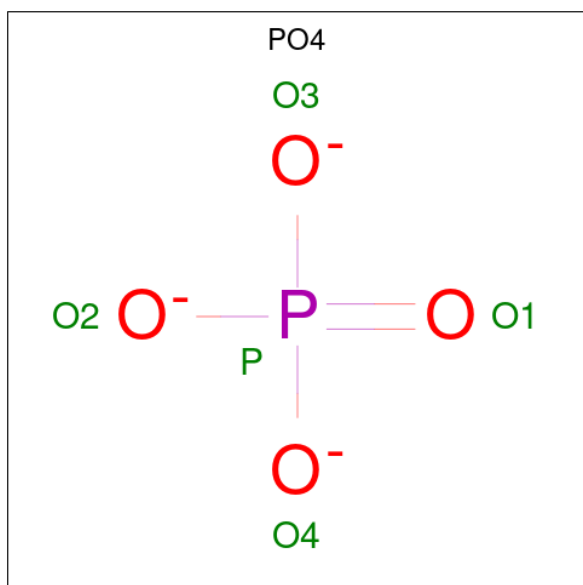
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP Q5KZU5
B	0	SER	-	expression tag	UNP Q5KZU5
B	99	LEU	TYR	engineered mutation	UNP Q5KZU5

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Co	0	0
			2	2		
2	B	2	Total	Co	0	0
			2	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	248	Total	O	0	0
			248	248		
4	B	252	Total	O	0	0
			252	252		



- Molecule 1: Phosphotriesterase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.36Å 80.30Å 92.20Å 90.00° 99.35° 90.00°	Depositor
Resolution (Å)	50.00 – 1.75 50.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.75) 99.6 (50.00-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.222 , 0.249 0.222 , 0.250	Depositor DCC
$R_{free}$ test set	3732 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5597	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

Bond lengths and bond angles in the following residue types are not validated in this section: CO, KCX, PO4

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	0.32	0/2589	0.46	0/3503
1	B	0.32	0/2589	0.48	0/3503
All	All	0.32	0/5178	0.47	0/7006

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	2544	0	2493	7	0
1	B	2544	0	2493	10	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	B	5	0	0	0	0
4	A	248	0	0	0	0
4	B	252	0	0	0	0
All	All	5597	0	4986	17	0

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 2.



The worst 5 of 17 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:236:MET:HG2	1:B:282:PHE:HZ	1.39	0.85
1:B:236:MET:HG2	1:B:282:PHE:CZ	2.23	0.73
1:B:265:HIS:HB2	1:B:267:THR:HG23	1.88	0.53
1:B:27:LEU:HD23	1:B:270:VAL:HB	1.92	0.52
1:A:220:LEU:HD21	1:A:226:ILE:HG12	1.98	0.46

There are no symmetry-related clashes.

## 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	321/360 (89%)	318 (99%)	3 (1%)	0	100	100
1	B	321/360 (89%)	315 (98%)	6 (2%)	0	100	100
All	All	642/720 (89%)	633 (99%)	9 (1%)	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	263/290 (91%)	259 (98%)	4 (2%)	60	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	263/290 (91%)	259 (98%)	4 (2%)	60	45
All	All	526/580 (91%)	518 (98%)	8 (2%)	60	45

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	264	SER
1	B	236	MET
1	B	99	LEU
1	A	264	SER
1	B	168	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	304	ASN
1	B	195	HIS
1	A	304	ASN
1	A	195	HIS
1	B	168	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	KCX	B	145	2,1	10,11,12	0.92	0	6,12,14	1.59	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	KCX	A	145	2,1	10,11,12	0.94	0	6,12,14	1.48	1 (16%)

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
1	KCX	B	145	2,1	-	0/9/10/12	-
1	KCX	A	145	2,1	-	0/9/10/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	KCX	OQ1-CX-NZ	-3.82	119.11	124.92
1	A	145	KCX	OQ1-CX-NZ	-3.58	119.49	124.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PO4	B	329	-	4,4,4	0.94	0	6,6,6	0.46	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.

No monomer is involved in short contacts.

## 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<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	323/360 (89%)	1.17	56 (17%) 5 5	19, 29, 40, 44	6 (1%)
1	B	323/360 (89%)	0.64	28 (8%) 17 20	13, 22, 32, 43	2 (0%)
All	All	646/720 (89%)	0.90	84 (13%) 9 10	13, 26, 38, 44	8 (1%)

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	238	GLY	7.6
1	B	237	VAL	6.8
1	A	237	VAL	6.2
1	A	280	GLU	5.9
1	A	238	GLY	5.6

### 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	KCX	A	145	12/13	0.93	0.08	19,19,19,20	0
1	KCX	B	145	12/13	0.95	0.06	12,12,12,13	0

### 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<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	PO4	B	329	5/5	0.75	0.22	75,75,75,75	0
2	CO	B	327	1/1	0.99	0.02	14,14,14,14	0
2	CO	B	328	1/1	0.99	0.03	16,16,16,16	0
2	CO	A	328	1/1	0.99	0.06	21,21,21,21	0
2	CO	A	327	1/1	1.00	0.01	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.