



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 05:43 am BST

PDB ID : 2PBY  
Title : Probable Glutaminase from *Geobacillus kaustophilus* HTA426  
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Deposited on : 2007-03-29  
Resolution : 2.07 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](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	:	2.11
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)	:	2.11

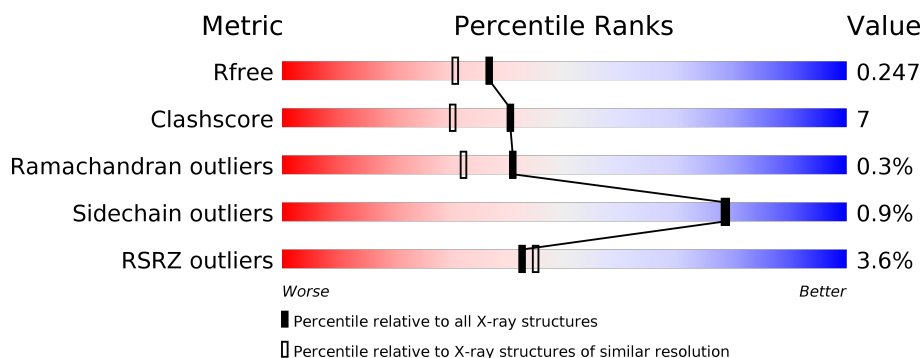
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	308	<div> <div>2%</div> <div>85%</div> <div>9%</div> <div>6%</div> </div>
1	B	308	<div> <div>5%</div> <div>74%</div> <div>19%</div> <div>6%</div> </div>
1	C	308	<div> <div>4%</div> <div>80%</div> <div>13%</div> <div>6%</div> </div>
1	D	308	<div> <div>2%</div> <div>84%</div> <div>9%</div> <div>7%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9310 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 Glutaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2229	1416	375	424	14			
1	B	290	Total	C	N	O	S	0	0	0
			2184	1384	367	419	14			
1	C	288	Total	C	N	O	S	0	0	0
			2196	1390	372	420	14			
1	D	286	Total	C	N	O	S	0	0	0
			2186	1385	369	418	14			

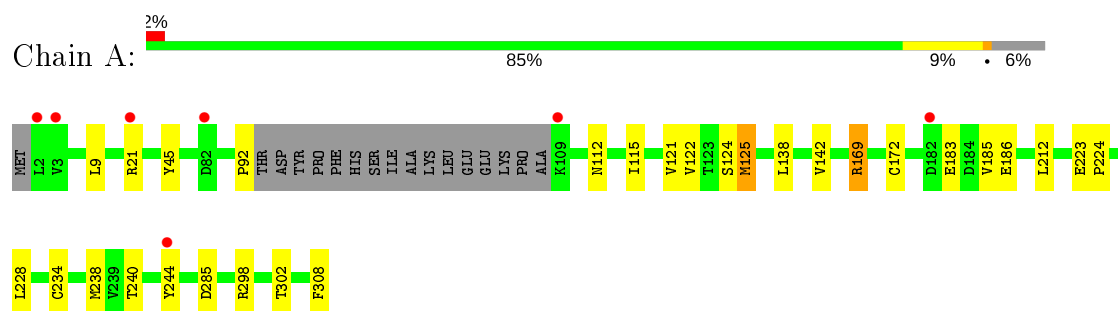
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	136	Total	O	0	0
			136	136		
2	B	98	Total	O	0	0
			98	98		
2	C	125	Total	O	0	0
			125	125		
2	D	156	Total	O	0	0
			156	156		

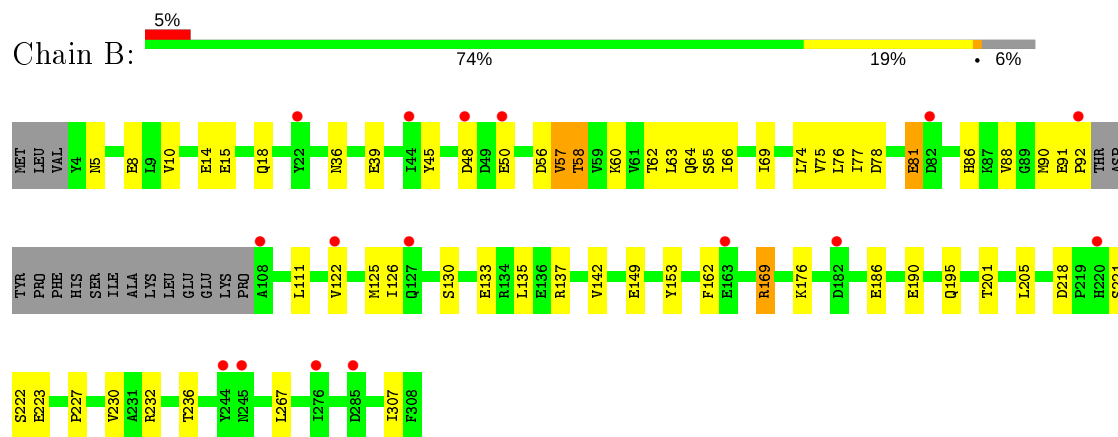
### 3 Residue-property plots [i](#)

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.

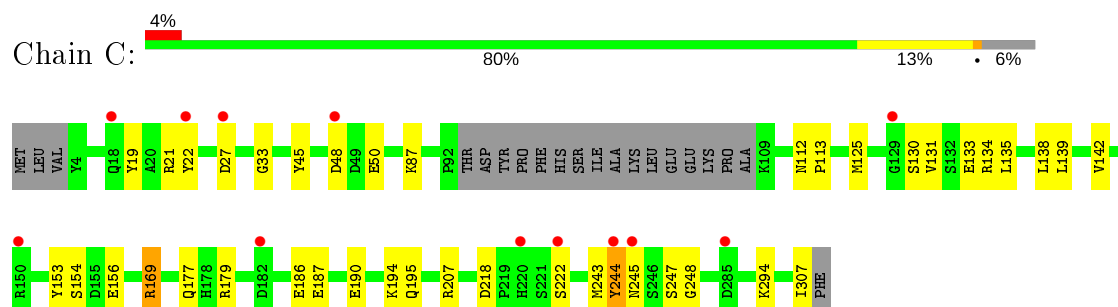
#### • Molecule 1: Glutaminase



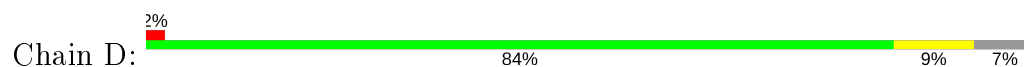
#### • Molecule 1: Glutaminase

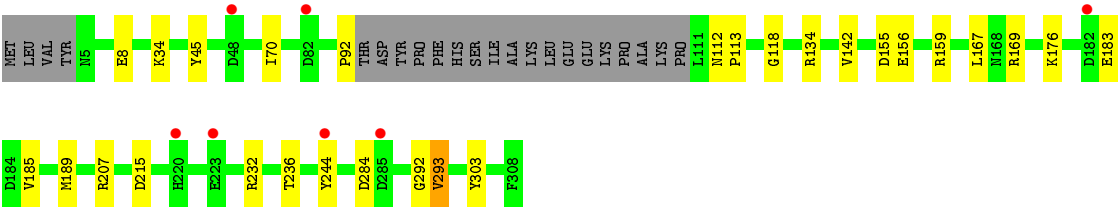


#### • Molecule 1: Glutaminase



#### • Molecule 1: Glutaminase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.50Å 86.79Å 106.88Å 90.00° 109.76° 90.00°	Depositor
Resolution (Å)	19.86 – 2.07 19.86 – 2.07	Depositor EDS
% Data completeness (in resolution range)	97.3 (19.86-2.07) 97.3 (19.86-2.07)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.98 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.195 , 0.249 0.195 , 0.247	Depositor DCC
$R_{free}$ test set	3706 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 48.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9310	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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

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	0.93	0/2262	0.82	4/3056 (0.1%)
1	B	1.02	4/2214 (0.2%)	0.90	3/2990 (0.1%)
1	C	0.91	0/2227	0.84	4/3008 (0.1%)
1	D	0.94	0/2217	0.86	5/2994 (0.2%)
All	All	0.95	4/8920 (0.0%)	0.86	16/12048 (0.1%)

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	B	0	1
1	D	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	GLU	CD-OE1	15.56	1.42	1.25
1	B	81	GLU	CD-OE2	10.95	1.37	1.25
1	B	65	SER	CB-OG	5.16	1.49	1.42
1	B	64	GLN	CG-CD	5.09	1.62	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	GLU	OE1-CD-OE2	-15.56	104.62	123.30
1	B	169	ARG	NE-CZ-NH1	-10.50	115.05	120.30
1	A	169	ARG	NE-CZ-NH1	-10.14	115.23	120.30
1	C	243	MET	CG-SD-CE	-9.03	85.76	100.20
1	A	169	ARG	NE-CZ-NH2	7.64	124.12	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	57	VAL	Peptide
1	D	292	GLY	Peptide

## 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	2229	0	2276	22	0
1	B	2184	0	2171	64	0
1	C	2196	0	2240	33	0
1	D	2186	0	2227	16	0
2	A	136	0	0	0	0
2	B	98	0	0	4	0
2	C	125	0	0	5	0
2	D	156	0	0	1	0
All	All	9310	0	8914	128	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 7.

The worst 5 of 128 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:76:LEU:HD21	1:B:227:PRO:CD	1.84	1.06
1:B:169:ARG:NH1	1:B:186:GLU:OE2	1.90	1.05
1:B:74:LEU:HD11	1:B:122:VAL:O	1.63	0.97
1:B:76:LEU:HD21	1:B:227:PRO:HD2	1.42	0.97
1:B:90:MET:HE2	2:C:416:HOH:O	1.66	0.94

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	287/308 (93%)	276 (96%)	10 (4%)	1 (0%)	41	32
1	B	286/308 (93%)	276 (96%)	10 (4%)	0	100	100
1	C	284/308 (92%)	275 (97%)	8 (3%)	1 (0%)	34	25
1	D	282/308 (92%)	271 (96%)	10 (4%)	1 (0%)	34	25
All	All	1139/1232 (92%)	1098 (96%)	38 (3%)	3 (0%)	41	32

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	TYR
1	D	293	VAL
1	C	244	TYR

### 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	244/259 (94%)	242 (99%)	2 (1%)	81	81
1	B	229/259 (88%)	226 (99%)	3 (1%)	69	67
1	C	240/259 (93%)	239 (100%)	1 (0%)	91	91
1	D	239/259 (92%)	236 (99%)	3 (1%)	69	67
All	All	952/1036 (92%)	943 (99%)	9 (1%)	78	78

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	149	GLU
1	D	244	TYR
1	D	45	TYR
1	B	45	TYR
1	C	45	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	B	64	GLN
1	C	127	GLN

### 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 [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	291/308 (94%)	0.03	7 (2%) 59 61	14, 25, 41, 58	0
1	B	290/308 (94%)	0.20	16 (5%) 25 26	16, 27, 45, 52	0
1	C	288/308 (93%)	0.02	12 (4%) 36 38	15, 27, 42, 53	0
1	D	286/308 (92%)	-0.06	7 (2%) 59 61	14, 23, 40, 53	0
All	All	1155/1232 (93%)	0.05	42 (3%) 42 45	14, 26, 42, 58	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	TYR	8.8
1	B	108	ALA	3.8
1	B	220	HIS	3.6
1	A	109	LYS	3.6
1	A	2	LEU	3.5

### 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 carbohydrates 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.