



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4F71 / pdb\_00004f71  
Title : Crystal structure of had family enzyme bt-2542 (target efi-501088) from Bacteroides thetaiotaomicron, wild-type protein, complex with magnesium and inorganic phosphate  
Authors : Patskovsky, Y.; Toro, R.; Bhosle, R.; Hillerich, B.; Seidel, R.D.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Zencheck, W.D.; Imker, H.J.; Gerlt, J.A.; Allen, K.N.; Dunaway-Mariano, D.; Almo, S.C.; Enzyme Function Initiative (EFI)  
Deposited on : 2012-05-15  
Resolution : 2.27 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.

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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)

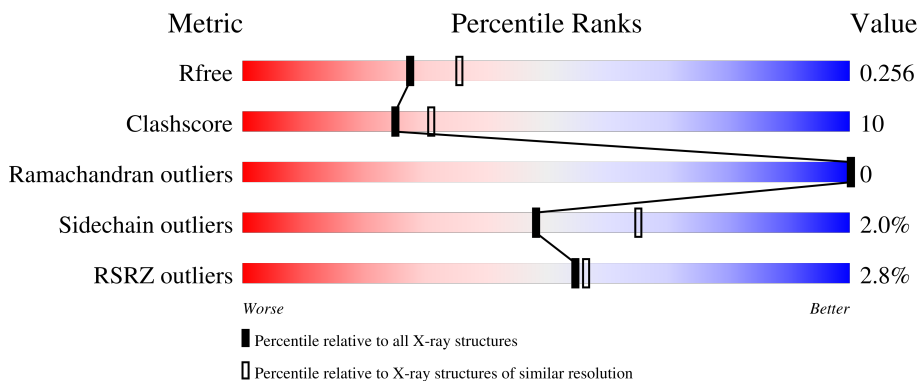
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.27 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))
$R_{free}$	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	229	 2% 72% 14% 14%
1	B	229	 3% 72% 14% 13%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.49

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3396 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 Putative haloacid dehalogenase-like hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	198	1640	1064	265	303	8	0	1	0
1	B	199	1647	1069	264	306	8	0	1	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q8A4Q5
A	-20	HIS	-	expression tag	UNP Q8A4Q5
A	-19	HIS	-	expression tag	UNP Q8A4Q5
A	-18	HIS	-	expression tag	UNP Q8A4Q5
A	-17	HIS	-	expression tag	UNP Q8A4Q5
A	-16	HIS	-	expression tag	UNP Q8A4Q5
A	-15	HIS	-	expression tag	UNP Q8A4Q5
A	-14	SER	-	expression tag	UNP Q8A4Q5
A	-13	SER	-	expression tag	UNP Q8A4Q5
A	-12	GLY	-	expression tag	UNP Q8A4Q5
A	-11	VAL	-	expression tag	UNP Q8A4Q5
A	-10	ASP	-	expression tag	UNP Q8A4Q5
A	-9	LEU	-	expression tag	UNP Q8A4Q5
A	-8	GLY	-	expression tag	UNP Q8A4Q5
A	-7	THR	-	expression tag	UNP Q8A4Q5
A	-6	GLU	-	expression tag	UNP Q8A4Q5
A	-5	ASN	-	expression tag	UNP Q8A4Q5
A	-4	LEU	-	expression tag	UNP Q8A4Q5
A	-3	TYR	-	expression tag	UNP Q8A4Q5
A	-2	PHE	-	expression tag	UNP Q8A4Q5
A	-1	GLN	-	expression tag	UNP Q8A4Q5
A	0	SER	-	expression tag	UNP Q8A4Q5
B	-21	MET	-	expression tag	UNP Q8A4Q5
B	-20	HIS	-	expression tag	UNP Q8A4Q5
B	-19	HIS	-	expression tag	UNP Q8A4Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	expression tag	UNP Q8A4Q5
B	-17	HIS	-	expression tag	UNP Q8A4Q5
B	-16	HIS	-	expression tag	UNP Q8A4Q5
B	-15	HIS	-	expression tag	UNP Q8A4Q5
B	-14	SER	-	expression tag	UNP Q8A4Q5
B	-13	SER	-	expression tag	UNP Q8A4Q5
B	-12	GLY	-	expression tag	UNP Q8A4Q5
B	-11	VAL	-	expression tag	UNP Q8A4Q5
B	-10	ASP	-	expression tag	UNP Q8A4Q5
B	-9	LEU	-	expression tag	UNP Q8A4Q5
B	-8	GLY	-	expression tag	UNP Q8A4Q5
B	-7	THR	-	expression tag	UNP Q8A4Q5
B	-6	GLU	-	expression tag	UNP Q8A4Q5
B	-5	ASN	-	expression tag	UNP Q8A4Q5
B	-4	LEU	-	expression tag	UNP Q8A4Q5
B	-3	TYR	-	expression tag	UNP Q8A4Q5
B	-2	PHE	-	expression tag	UNP Q8A4Q5
B	-1	GLN	-	expression tag	UNP Q8A4Q5
B	0	SER	-	expression tag	UNP Q8A4Q5

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	37	Total O 37 37	0	0
6	B	47	Total O 47 47	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.59Å 76.82Å 118.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.27 50.00 – 2.27	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-2.27) 95.9 (50.00-2.27)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 2.27Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.206 , 0.258 0.205 , 0.256	Depositor DCC
$R_{free}$ test set	747 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.2	Xtrriage
Anisotropy	0.407	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 28.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3396	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	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 22.43 % 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 5.7057e-03. 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, GOL, CL

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	0.51	0/1679	0.71	0/2260
1	B	0.45	0/1686	0.71	1/2269 (0.0%)
All	All	0.48	0/3365	0.71	1/4529 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	ARG	CB-CA-C	-5.16	110.21	117.23

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	1640	0	1637	40	0
1	B	1647	0	1643	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
4	A	6	0	8	1	0
4	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
6	A	37	0	0	1	0
6	B	47	0	0	0	0
All	All	3396	0	3296	64	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 10.

The worst 5 of 64 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:49:ILE:HD11	1:A:70:MET:CE	2.07	0.84
1:A:71:MET:HE1	1:A:75:VAL:HG11	1.67	0.77
1:A:72:GLY:O	1:A:73:LYS:HG3	1.87	0.74
1:A:149:MET:HE1	1:A:155:GLU:CD	2.14	0.73
1:A:51:LEU:O	1:A:51:LEU:HD13	1.89	0.71

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	195/229 (85%)	190 (97%)	5 (3%)	0	100	100
1	B	196/229 (86%)	189 (96%)	7 (4%)	0	100	100
All	All	391/458 (85%)	379 (97%)	12 (3%)	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	179/207 (86%)	175 (98%)	4 (2%)	45	62
1	B	180/207 (87%)	177 (98%)	3 (2%)	53	70
All	All	359/414 (87%)	352 (98%)	7 (2%)	48	66

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	MET
1	B	120	LYS
1	B	169	LYS
1	B	130	ARG
1	A	70	MET

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	185	GLN
1	B	53	GLN
1	B	45	GLN
1	B	8	ASN
1	B	52	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	A	302	2	4,4,4	0.65	0	6,6,6	0.44	0
4	GOL	B	303	-	5,5,5	0.29	0	5,5,5	0.42	0
3	PO4	B	302	2	4,4,4	0.99	0	6,6,6	0.32	0
4	GOL	A	303	-	5,5,5	0.30	0	5,5,5	0.56	0

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
4	GOL	A	303	-	-	4/4/4/4	-
4	GOL	B	303	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	GOL	O1-C1-C2-C3
4	B	303	GOL	C1-C2-C3-O3
4	A	303	GOL	C1-C2-C3-O3
4	A	303	GOL	O2-C2-C3-O3
4	B	303	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	PO4	1	0
4	A	303	GOL	1	0

## 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	198/229 (86%)	0.16	5 (2%) 58 60	30, 48, 76, 96	1 (0%)
1	B	199/229 (86%)	0.08	6 (3%) 52 54	30, 48, 77, 109	1 (0%)
All	All	397/458 (86%)	0.12	11 (2%) 55 56	30, 48, 77, 109	2 (0%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	46	LEU	4.3
1	A	46	LEU	4.1
1	A	73	LYS	3.4
1	A	41	PHE	3.3
1	B	45	GLN	3.3

### 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 oligosaccharides 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( $\text{\AA}^2$ )	Q<0.9
4	GOL	B	303	6/6	0.90	0.18	48,62,69,74	0
4	GOL	A	303	6/6	0.93	0.14	40,66,70,75	0
5	CL	A	304	1/1	0.94	0.09	70,70,70,70	0
3	PO4	B	302	5/5	0.96	0.09	37,38,44,53	0
3	PO4	A	302	5/5	0.97	0.12	38,39,40,52	0
2	MG	B	301	1/1	0.99	0.07	38,38,38,38	0
2	MG	A	301	1/1	0.99	0.04	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.