



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2FCA / pdb\_00002fca  
Title : The structure of BsTrmB  
Authors : Zegers, I.; Van Vliet, F.; Bujnicki, J.; Kosinski, J.; Gigot, D.; Droogmans, L.  
Deposited on : 2005-12-12  
Resolution : 2.10 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.

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

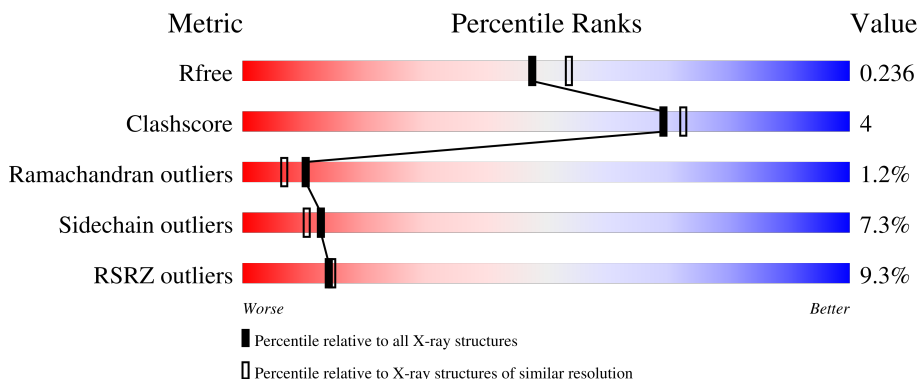
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

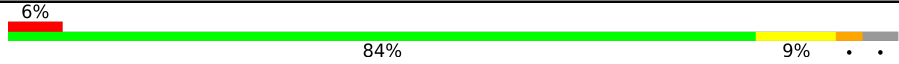
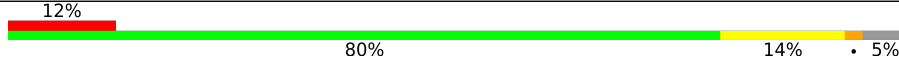
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	213	 6% 84% 9% • •
1	B	213	 12% 80% 14% • 5%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3648 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 tRNA (guanine-N(7)-)-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	205	1663	1065	277	318	3	0	0	0
1	B	203	1641	1050	274	314	3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	TRP	ALA	conflict	UNP O34522
B	9	TRP	ALA	conflict	UNP O34522

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	184	Total 184	O 184	0	0
3	B	157	Total 157	O 157	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.83Å 178.83Å 41.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.10) 99.7 (30.00-2.10)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 2.10Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.202 , 0.233 0.206 , 0.236	Depositor DCC
$R_{free}$ test set	1428 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtrriage
Anisotropy	0.665	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 34.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.015 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3648	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section:  
K

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	0.70	0/1703	1.06	6/2300 (0.3%)
1	B	0.69	0/1679	1.07	6/2266 (0.3%)
All	All	0.70	0/3382	1.07	12/4566 (0.3%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	GLY	N-CA-C	7.30	126.14	114.90
1	A	86	GLU	N-CA-C	6.32	124.26	110.80
1	A	180	LEU	N-CA-C	5.94	117.76	111.28
1	B	198	SER	N-CA-C	5.85	123.27	110.80
1	A	120	TRP	CA-C-N	5.67	125.78	119.32
1	A	120	TRP	C-N-CA	5.67	125.78	119.32
1	B	181	HIS	N-CA-C	5.57	118.12	111.71
1	B	180	LEU	N-CA-C	5.41	117.88	111.33
1	A	200	LEU	N-CA-C	-5.40	106.82	113.41
1	B	119	PRO	N-CA-C	5.31	120.82	113.65
1	B	133	SER	N-CA-C	5.25	117.68	111.33
1	A	50	GLY	N-CA-C	5.03	122.83	115.08

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	1663	0	1619	10	0
1	B	1641	0	1605	14	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	184	0	0	0	0
3	B	157	0	0	1	0
All	All	3648	0	3224	23	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 4.

All (23) 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:23:ASN:H	1:A:23:ASN:HD22	1.21	0.83
1:A:23:ASN:HD22	1:A:23:ASN:N	1.92	0.65
1:B:72:LYS:HD3	1:B:72:LYS:H	1.63	0.64
1:B:23:ASN:HD22	1:B:23:ASN:H	1.48	0.60
1:A:156:ARG:NH1	1:B:183:SER:OG	2.38	0.57
1:B:32:ASN:HD22	1:B:32:ASN:N	2.07	0.53
1:B:83:LYS:NZ	3:B:448:HOH:O	2.43	0.52
1:B:65:TYR:HB2	1:B:90:VAL:HG22	1.92	0.51
1:B:72:LYS:HD3	1:B:72:LYS:N	2.25	0.51
1:B:23:ASN:HD22	1:B:23:ASN:N	2.08	0.51
1:A:175:TYR:HB3	1:A:208:GLU:HB2	1.93	0.49
1:A:151:PHE:HZ	1:A:158:LEU:HD13	1.79	0.48
1:B:32:ASN:HD22	1:B:32:ASN:H	1.61	0.47
1:A:23:ASN:N	1:A:23:ASN:ND2	2.63	0.47
1:B:72:LYS:H	1:B:72:LYS:CD	2.27	0.44
1:B:185:LEU:HD22	1:B:188:ASN:HD21	1.83	0.44
1:A:119:PRO:HA	1:A:158:LEU:HG	2.00	0.44
1:A:192:GLU:CD	1:A:192:GLU:H	2.26	0.43
1:B:125:HIS:CD2	1:B:128:ARG:HE	2.37	0.42
1:B:24:PRO:HB3	1:B:93:LEU:HD22	2.01	0.42
1:A:52:PHE:HB2	1:A:191:THR:HG22	2.03	0.41
1:A:171:LEU:HB3	1:A:209:VAL:HG13	2.02	0.41
1:B:175:TYR:HB3	1:B:208:GLU:HB2	2.03	0.41

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	203/213 (95%)	194 (96%)	7 (3%)	2 (1%)	12	9
1	B	201/213 (94%)	192 (96%)	6 (3%)	3 (2%)	8	4
All	All	404/426 (95%)	386 (96%)	13 (3%)	5 (1%)	10	7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	GLU
1	B	198	SER
1	A	185	LEU
1	B	187	GLY
1	B	86	GLU

### 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	180/188 (96%)	167 (93%)	13 (7%)	13	11
1	B	178/188 (95%)	165 (93%)	13 (7%)	13	10
All	All	358/376 (95%)	332 (93%)	26 (7%)	13	10

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	63	ILE
1	A	74	VAL
1	A	90	VAL
1	A	111	ARG
1	A	114	LEU
1	A	136	LEU
1	A	156	ARG
1	A	158	LEU
1	A	163	LEU
1	A	185	LEU
1	A	200	LEU
1	A	202	GLN
1	B	13	LEU
1	B	23	ASN
1	B	32	ASN
1	B	37	ASN
1	B	58	LYS
1	B	112	VAL
1	B	124	ARG
1	B	136	LEU
1	B	156	ARG
1	B	172	LEU
1	B	188	ASN
1	B	197	PHE
1	B	202	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	23	ASN
1	A	51	GLN
1	A	80	GLN
1	A	94	ASN
1	A	184	ASN
1	B	23	ASN
1	B	32	ASN
1	B	37	ASN
1	B	64	ASN
1	B	125	HIS
1	B	134	HIS
1	B	182	ASN
1	B	188	ASN

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Mol	Chain	Res	Type
1	B	202	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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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

### 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	205/213 (96%)	0.40	13 (6%) 26 27	28, 36, 65, 83	0
1	B	203/213 (95%)	0.57	25 (12%) 8 8	28, 39, 76, 91	0
All	All	408/426 (95%)	0.49	38 (9%) 14 15	28, 37, 73, 91	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	LEU	6.8
1	B	185	LEU	6.7
1	A	9	TRP	5.7
1	B	200	LEU	5.6
1	A	199	ALA	5.3
1	A	185	LEU	4.5
1	B	199	ALA	4.4
1	B	197	PHE	4.2
1	A	197	PHE	3.6
1	A	184	ASN	3.6
1	B	195	GLU	3.4
1	B	198	SER	3.4
1	A	85	SER	3.3
1	A	213	THR	3.1
1	B	184	ASN	3.1
1	A	201	GLY	3.0
1	B	86	GLU	3.0
1	B	12	PHE	3.0
1	A	86	GLU	2.8
1	B	201	GLY	2.8
1	B	189	ILE	2.7
1	A	196	LYS	2.7
1	A	198	SER	2.5
1	B	13	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	79	VAL	2.4
1	B	191	THR	2.4
1	B	186	GLU	2.3
1	B	182	ASN	2.3
1	B	82	VAL	2.2
1	B	73	SER	2.1
1	B	58	LYS	2.1
1	A	82	VAL	2.1
1	B	213	THR	2.1
1	B	192	GLU	2.0
1	B	123	LYS	2.0
1	B	196	LYS	2.0
1	B	14	ALA	2.0
1	B	193	TYR	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 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(Å <sup>2</sup> )	Q<0.9
2	K	A	250	1/1	0.99	0.02	37,37,37,37	0
2	K	A	252	1/1	0.99	0.10	38,38,38,38	0
2	K	B	251	1/1	0.99	0.07	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.