



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 12:54 AM GMT

PDB ID : 4DDT  
Title : Thermotoga maritima reverse gyrase, C2 FORM 2  
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Deposited on : 2012-01-19  
Resolution : 3.20 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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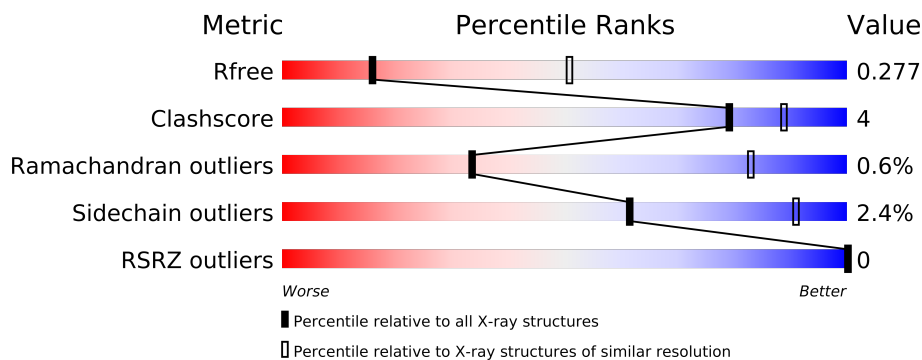
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.20 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))
$R_{free}$	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1104	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9032 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Reverse gyrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1102	Total	C	N	O	S	0	0	0
			9030	5759	1563	1682	26			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.94Å 104.43Å 96.74Å 90.00° 116.61° 90.00°	Depositor
Resolution (Å)	48.23 – 3.20 48.23 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.23-3.20) 94.6 (48.23-3.20)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	0.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_842)	Depositor
R, $R_{free}$	0.216 , 0.270 0.223 , 0.277	Depositor DCC
$R_{free}$ test set	1318 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.1	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 37.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 27506 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9032	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.24	0/9191	0.43	0/12356

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9030	0	0	32	0
2	A	2	0	0	0	0
All	All	9032	0	0	32	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (32) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:883:ARG:NH2	1:A:937:SER:O	2.14	0.81
1:A:206:ASP:OD2	1:A:260:ALA:N	2.32	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:482:LYS:O	1:A:529:ARG:NH1	2.35	0.59
1:A:1010:GLU:OE1	1:A:1014:ARG:NH1	2.37	0.57
1:A:674:GLU:OE1	1:A:693:ARG:NE	2.38	0.57
1:A:392:SER:OG	1:A:394:GLU:OE2	2.24	0.55
1:A:814:PRO:O	1:A:931:ARG:NH1	2.39	0.55
1:A:805:GLU:OE1	1:A:980:ARG:NH2	2.40	0.54
1:A:427:ILE:O	1:A:431:HIS:ND1	2.43	0.52
1:A:645:ASP:OD1	1:A:646:LYS:N	2.43	0.51
1:A:983:HIS:O	1:A:983:HIS:ND1	2.45	0.49
1:A:883:ARG:O	1:A:936:GLN:NE2	2.45	0.49
1:A:298:LYS:NZ	1:A:324:GLU:OE2	2.46	0.49
1:A:2:ALA:N	1:A:24:GLU:OE1	2.46	0.48
1:A:885:TRP:NE1	1:A:935:SER:OG	2.46	0.48
1:A:918:THR:OG1	1:A:921:HIS:ND1	2.46	0.48
1:A:695:GLU:OE1	1:A:712:ARG:NH2	2.46	0.47
1:A:452:ASP:OD1	1:A:452:ASP:N	2.48	0.47
1:A:342:GLU:O	1:A:346:ASN:ND2	2.48	0.47
1:A:286:ARG:NH1	1:A:508:GLU:OE1	2.49	0.46
1:A:529:ARG:O	1:A:532:SER:OG	2.34	0.46
1:A:623:ASP:OD2	1:A:640:SER:OG	2.33	0.45
1:A:378:ILE:O	1:A:529:ARG:NH2	2.50	0.45
1:A:78:ASP:OD1	1:A:79:LEU:N	2.51	0.44
1:A:668:ASP:O	1:A:693:ARG:NH2	2.51	0.44
1:A:286:ARG:NH2	1:A:466:ILE:O	2.52	0.42
1:A:213:ARG:O	1:A:217:THR:OG1	2.37	0.41
1:A:313:LEU:O	1:A:382:ILE:N	2.54	0.41
1:A:667:THR:OG1	1:A:673:GLY:O	2.38	0.41
1:A:879:ILE:O	1:A:938:ALA:N	2.54	0.41
1:A:22:ARG:NH2	1:A:33:LEU:O	2.54	0.41
1:A:1004:GLN:NE2	1:A:1037:GLU:OE2	2.54	0.40

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	1100/1104 (100%)	996 (90%)	97 (9%)	7 (1%)	33 83

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	537	THR
1	A	76	GLY
1	A	103	GLY
1	A	1022	TYR
1	A	309	ARG
1	A	101	PRO
1	A	785	VAL

### 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	992/993 (100%)	968 (98%)	24 (2%)	61 91

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	50	THR
1	A	158	MET
1	A	365	TYR
1	A	503	LEU
1	A	529	ARG
1	A	619	LYS
1	A	630	GLU
1	A	675	LYS
1	A	693	ARG
1	A	704	PHE
1	A	730	ARG
1	A	754	VAL
1	A	779	LEU
1	A	818	THR
1	A	851	TYR

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Mol	Chain	Res	Type
1	A	881	MET
1	A	931	ARG
1	A	935	SER
1	A	981	PHE
1	A	1020	SER
1	A	1030	PHE
1	A	1048	PHE
1	A	1086	TYR

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 chains 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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.

### 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 ⓘ

### 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	1102/1104 (99%)	-0.12	0 100 100	33, 82, 141, 227	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	A	1202	1/1	0.12	-0.58	74,74,74,74	0
2	ZN	A	1201	1/1	0.10	-1.71	106,106,106,106	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.