

# Full wwPDB X-ray Structure Validation Report (i)

#### Oct 16, 2023 – 01:01 PM EDT

PDB ID	:	2DCT
Title	:	Crystal structure of the TT1209 from Thermus thermophilus HB8
Authors	:	Asada, Y.; Sugahara, M.; Shimizu, K.; Yamamoto, H.; Shimada,
		H.; Nakamoto, T.; Ono, N.; Kunishima, N.; RIKEN Structural Ge-
		nomics/Proteomics Initiative (RSGI)
Deposited on	:	2006-01-12
Resolution	:	1.45 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

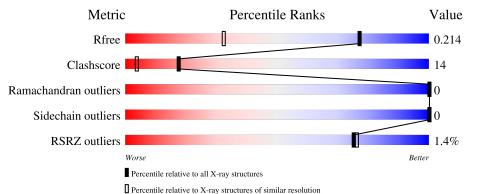
Refmac	: : :	
Ideal geometry (proteins) Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	:	Engh & Huber (2001) Parkinson et al. (1996)

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.45 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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 >=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 <=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	А	105	70%	30%	•			
1	В	105	3% 77%	23%	_			



#### $2\mathrm{DCT}$

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2000 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 hypothetical protein TTHA0104.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	105	Total 808	C 517	1,	0 147	$\frac{S}{4}$	0	0	0
1	В	105	Total 812	C 519	N 141	0 148	$\frac{S}{4}$	0	1	0

• Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Na 1 1	0	0

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	В	1	Total 1	Cl 1	0	0

• Molecule 4 is water.

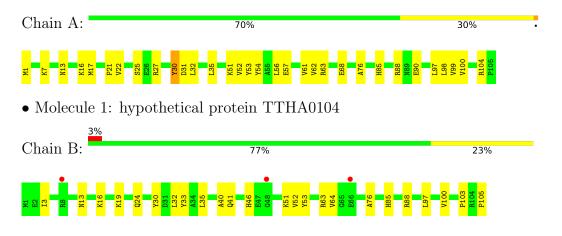
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	195	Total O 195 195	0	0
4	В	183	Total O 183 183	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: hypothetical protein TTHA0104





## 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 43 21 2	Depositor	
Cell constants	62.24Å 62.24Å 151.11Å	Deperitor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	28.78 - 1.45	Depositor	
Resolution (A)	28.78 - 1.40	EDS	
% Data completeness	100.0 (28.78-1.45)	Depositor	
(in resolution range)	96.9 (28.78-1.40)	EDS	
R <sub>merge</sub>	0.06	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$3.26 (at 1.40 \text{\AA})$	Xtriage	
Refinement program	CNS 1.1	Depositor	
D D.	0.199 , $0.209$	Depositor	
$R, R_{free}$	0.200 , $0.214$	DCC	
$R_{free}$ test set	2835 reflections $(4.96%)$	wwPDB-VP	
Wilson B-factor $(Å^2)$	15.3	Xtriage	
Anisotropy	0.291	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.39, $34.6$	EDS	
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
$F_o, F_c$ correlation	0.96	EDS	
Total number of atoms	2000	wwPDB-VP	
Average B, all atoms $(Å^2)$	19.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.28% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: CL, NA

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	А	0.43	0/826	0.77	1/1119~(0.1%)	
1	В	0.47	0/835	0.79	0/1131	
All	All	0.45	0/1661	0.78	1/2250~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	30	TYR	N-CA-C	-5.25	96.82	111.00

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	А	808	0	825	29	0
1	В	812	0	829	21	0
2	А	1	0	0	0	0
3	В	1	0	0	0	0
4	А	195	0	0	4	0
4	В	183	0	0	4	0
All	All	2000	0	1654	45	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 14.

All (45) 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:16:LYS:HD3	4:A:1097:HOH:O	1.74	0.88
1:B:24:GLN:NE2	4:B:2181:HOH:O	2.21	0.73
1:A:7:LYS:HD3	4:B:2034:HOH:O	1.94	0.68
1:B:24:GLN:HG3	4:B:2181:HOH:O	1.97	0.63
1:A:13:ASN:HB3	1:A:16:LYS:O	2.00	0.62
1:A:27:ARG:HD2	1:B:103:PRO:HD3	1.82	0.62
1:B:46:HIS:NE2	1:B:105:PRO:HB3	2.15	0.61
1:A:7:LYS:NZ	4:A:1123:HOH:O	2.25	0.60
1:A:7:LYS:HE3	1:A:56:LEU:HB3	1.86	0.57
1:A:30:TYR:CZ	1:B:52:VAL:HG11	2.42	0.55
1:A:30:TYR:CE2	1:A:98:LEU:HD11	2.42	0.55
1:A:16:LYS:HE2	4:A:1183:HOH:O	2.07	0.55
1:B:63:ARG:O	1:B:85:HIS:HA	2.06	0.54
1:A:1:MET:HG3	1:B:64:VAL:HB	1.88	0.54
1:A:25:SER:O	1:A:104:ARG:HD2	2.10	0.52
1:A:17:MET:HG3	1:A:35:LEU:HG	1.93	0.50
1:A:22:VAL:CG2	1:A:32:LEU:HG	2.42	0.50
1:A:54:TYR:HE2	1:A:56:LEU:HD23	1.77	0.50
1:B:41[B]:GLN:NE2	1:B:53:TYR:OH	2.44	0.50
1:A:7:LYS:CE	1:A:56:LEU:HB3	2.42	0.49
1:B:53:TYR:O	1:B:76:ALA:HA	2.13	0.49
1:A:52:VAL:HG11	1:B:30:TYR:CZ	2.47	0.49
1:A:63:ARG:O	1:A:85:HIS:HA	2.15	0.47
1:A:54:TYR:CE2	1:A:56:LEU:HD23	2.50	0.46
1:A:61:VAL:HG21	1:A:90:GLU:OE1	2.16	0.46
1:B:32:LEU:HA	1:B:97:LEU:O	2.15	0.46
1:A:61:VAL:HG11	1:A:88:ARG:HH21	1.80	0.45
1:A:51:LYS:HA	1:A:100:VAL:O	2.16	0.45
1:A:21:PRO:HA	1:A:31:ASP:OD1	2.15	0.45
1:B:19:LYS:NZ	4:B:2135:HOH:O	2.49	0.45
1:A:104:ARG:NH1	4:A:1019:HOH:O	2.49	0.45
1:B:40:ALA:HB2	1:B:88:ARG:HA	1.99	0.44
1:A:53:TYR:O	1:A:76:ALA:HA	2.17	0.44
1:B:40:ALA:CB	1:B:88:ARG:HA	2.48	0.44
1:B:13:ASN:HB3	1:B:16:LYS:O	2.17	0.43
1:A:51:LYS:HE2	1:A:99:VAL:HG11	1.99	0.43
1:B:33:TYR:HB3	1:B:35:LEU:HD11	2.01	0.43

Continued on next page...



01	DOT	٦
21		-

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LEU:HD23	1:B:40:ALA:HA	2.00	0.42
1:A:76:ALA:O	1:B:3:ILE:HA	2.19	0.42
1:A:7:LYS:HE2	1:A:57:GLU:HG3	2.02	0.42
1:A:62:VAL:O	1:A:68:GLU:HA	2.19	0.42
1:A:32:LEU:HA	1:A:97:LEU:O	2.21	0.41
1:B:51:LYS:HA	1:B:100:VAL:O	2.21	0.41
1:B:53:TYR:OH	1:B:85:HIS:HD2	2.03	0.41
1:B:40:ALA:HB2	1:B:88:ARG:HG3	2.04	0.40

Continued from previous page...

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	rs Percentil	
1	А	103/105~(98%)	103 (100%)	0	0	100	100
1	В	104/105~(99%)	104 (100%)	0	0	100	100
All	All	207/210~(99%)	207 (100%)	0	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	А	83/83~(100%)	83 (100%)	0	100 100

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	В	84/83~(101%)	84 (100%)	0	100 100	
All	All	167/166~(101%)	167 (100%)	0	100 100	

There are no protein residues with a non-rotameric sidechain to report.

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such side chains are listed below:

Mol	Chain	Res	Type
1	А	44	HIS
1	В	85	HIS

#### 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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

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.

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,  $95^{th}$  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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	105/105~(100%)	-0.01	0 100 100	10, 14, 23, 27	0
1	В	105/105~(100%)	0.30	3 (2%) 51 53	10, 16, 24, 29	0
All	All	210/210~(100%)	0.15	3 (1%) 75 76	10, 15, 23, 29	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	66	GLU	3.0
1	В	48	GLY	2.9
1	В	8	ARG	2.2

## 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 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,  $95^{th}$  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	$\mathbf{Res}$	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
2	NA	А	1001	1/1	0.91	0.22	30,30,30,30	0
3	CL	В	2001	1/1	0.98	0.05	17,17,17,17	1



## 6.5 Other polymers (i)

There are no such residues in this entry.

