



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1WDJ / pdb_00001wdj
Title : Crystal structure of TT1808 from *Thermus thermophilus* HB8
Authors : Idaka, M.; Wada, T.; Murayama, K.; Terada, T.; Kuramitsu, S.; Shirouzu, M.;
Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2004-05-17
Resolution : 2.00 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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

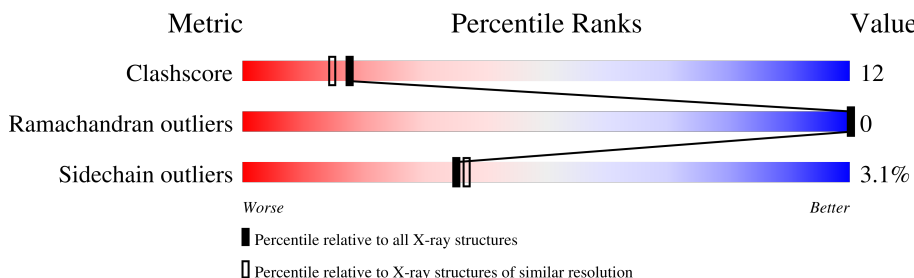
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	187	 71% 26% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4363 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 TT1808.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1463	935	256	271	1			
1	B	152	Total	C	N	O	S	0	0	0
			1182	760	204	217	1			
1	C	186	Total	C	N	O	S	0	0	0
			1463	935	256	271	1			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	84	Total	O	0	0
			84	84		
2	B	75	Total	O	0	0
			75	75		
2	C	96	Total	O	0	0
			96	96		

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.68Å 95.17Å 99.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.04 – 2.00	Depositor
% Data completeness (in resolution range)	94.7 (20.04-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.189 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4363	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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	0.53	0/1503	0.90	2/2043 (0.1%)
1	B	0.52	0/1215	0.92	1/1652 (0.1%)
1	C	0.54	0/1503	0.96	4/2043 (0.2%)
All	All	0.53	0/4221	0.93	7/5738 (0.1%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	173	ASP	N-CA-C	-7.48	99.76	110.08
1	C	23	ASN	CA-C-N	6.66	126.91	119.32
1	C	23	ASN	C-N-CA	6.66	126.91	119.32
1	A	71	SER	N-CA-C	5.95	120.01	112.87
1	A	8	ALA	N-CA-C	-5.73	106.62	113.21

There are no chirality outliers.

There are no planarity outliers.

4.2 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	1463	0	1448	44	0
1	B	1182	0	1171	29	0
1	C	1463	0	1448	37	0
2	A	84	0	0	2	0
2	B	75	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	96	0	0	2	0
All	All	4363	0	4067	101	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 12.

The worst 5 of 101 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:104:GLU:HG2	1:B:38:VAL:HG22	1.41	1.01
1:A:51:GLN:HE21	1:A:55:GLN:HE21	1.09	0.94
1:C:27:GLN:NE2	2:C:188:HOH:O	2.13	0.81
1:C:99:SER:OG	1:C:102:GLU:HG3	1.83	0.78
1:C:51:GLN:HE21	1:C:55:GLN:HE21	1.33	0.77

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 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	57/187 (30%)	55 (96%)	2 (4%)	0	100	100
1	B	69/187 (37%)	66 (96%)	3 (4%)	0	100	100
1	C	99/187 (53%)	99 (100%)	0	0	100	100
All	All	225/561 (40%)	220 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

4.3.2 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	154/155 (99%)	149 (97%)	5 (3%)	34	35
1	B	123/155 (79%)	119 (97%)	4 (3%)	33	34
1	C	148/155 (96%)	144 (97%)	4 (3%)	39	42
All	All	425/465 (91%)	412 (97%)	13 (3%)	35	37

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	164	LEU
1	B	173	ASP
1	C	162	LEU
1	C	47	ARG
1	C	91	GLU

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

Mol	Chain	Res	Type
1	A	51	GLN
1	B	51	GLN
1	C	51	GLN

4.3.3 RNA

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

5.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

5.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

5.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.