



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 9, 2024 – 12:17 PM EST

PDB ID : 2CV9
Title : Crystal structure of a hypothetical protein from *Thermus thermophilus* HB8
Authors : Kanagawa, M.; Yokoyama, S.; Kuramitsu, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-06-01
Resolution : 2.50 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

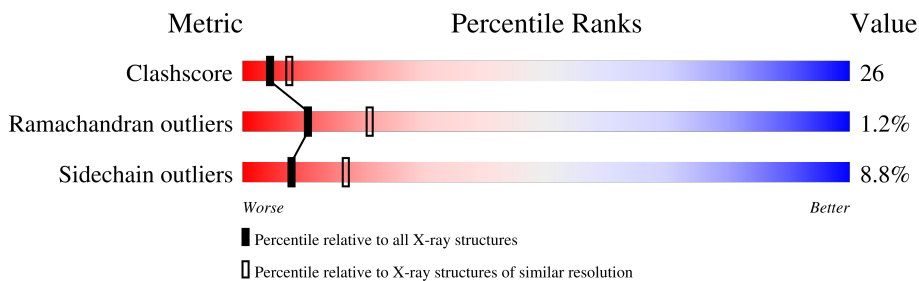
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)

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	252	 60% 33% 6%
1	B	252	 63% 31% 6%
1	C	252	 60% 34% 6%
1	D	252	 59% 36% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8338 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 TTHA0625.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total 1977	C 1259	N 351	O 361	Se 6	0	0	0
1	B	252	Total 1977	C 1259	N 351	O 361	Se 6	0	0	0
1	C	252	Total 1977	C 1259	N 351	O 361	Se 6	0	0	0
1	D	252	Total 1977	C 1259	N 351	O 361	Se 6	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q5SKL8
A	10	MSE	MET	modified residue	UNP Q5SKL8
A	113	MSE	MET	modified residue	UNP Q5SKL8
A	118	MSE	MET	modified residue	UNP Q5SKL8
A	153	MSE	MET	modified residue	UNP Q5SKL8
A	193	MSE	MET	modified residue	UNP Q5SKL8
B	1	MSE	MET	modified residue	UNP Q5SKL8
B	10	MSE	MET	modified residue	UNP Q5SKL8
B	113	MSE	MET	modified residue	UNP Q5SKL8
B	118	MSE	MET	modified residue	UNP Q5SKL8
B	153	MSE	MET	modified residue	UNP Q5SKL8
B	193	MSE	MET	modified residue	UNP Q5SKL8
C	1	MSE	MET	modified residue	UNP Q5SKL8
C	10	MSE	MET	modified residue	UNP Q5SKL8
C	113	MSE	MET	modified residue	UNP Q5SKL8
C	118	MSE	MET	modified residue	UNP Q5SKL8
C	153	MSE	MET	modified residue	UNP Q5SKL8
C	193	MSE	MET	modified residue	UNP Q5SKL8
D	1	MSE	MET	modified residue	UNP Q5SKL8
D	10	MSE	MET	modified residue	UNP Q5SKL8
D	113	MSE	MET	modified residue	UNP Q5SKL8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	118	MSE	MET	modified residue	UNP Q5SKL8
D	153	MSE	MET	modified residue	UNP Q5SKL8
D	193	MSE	MET	modified residue	UNP Q5SKL8

- Molecule 2 is water.

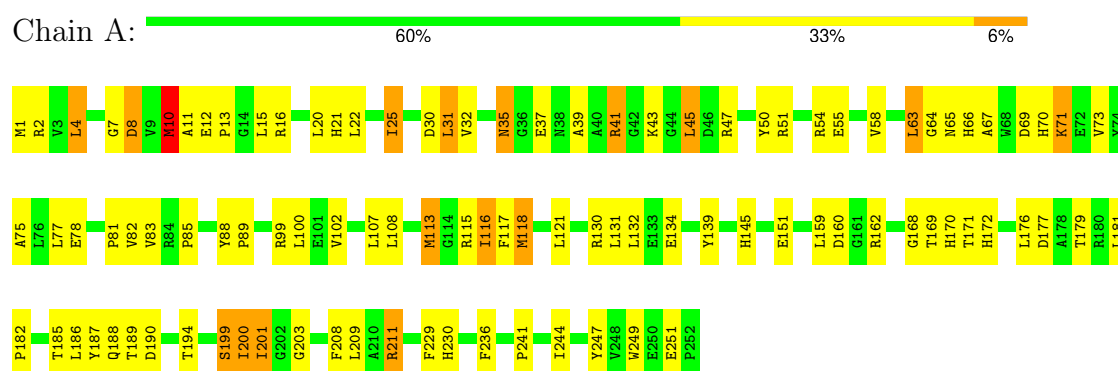
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	120	Total 120	O 120	0	0
2	B	108	Total 108	O 108	0	0
2	C	100	Total 100	O 100	0	0
2	D	102	Total 102	O 102	0	0

3 Residue-property plots

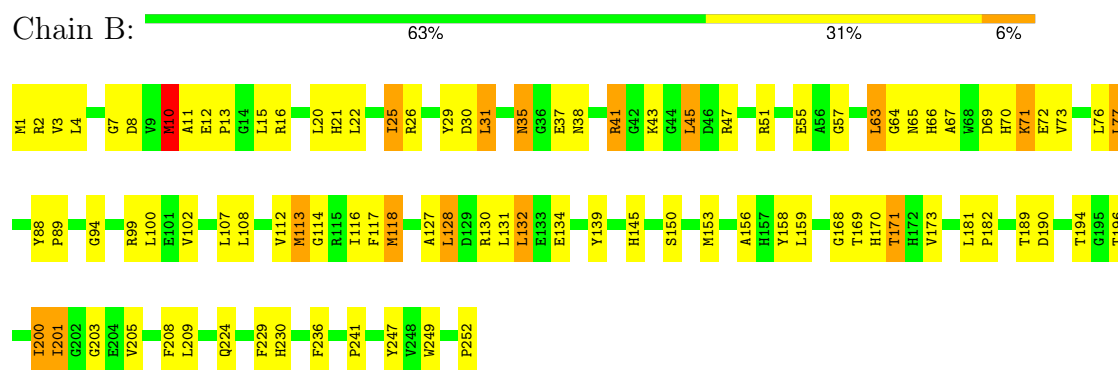
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

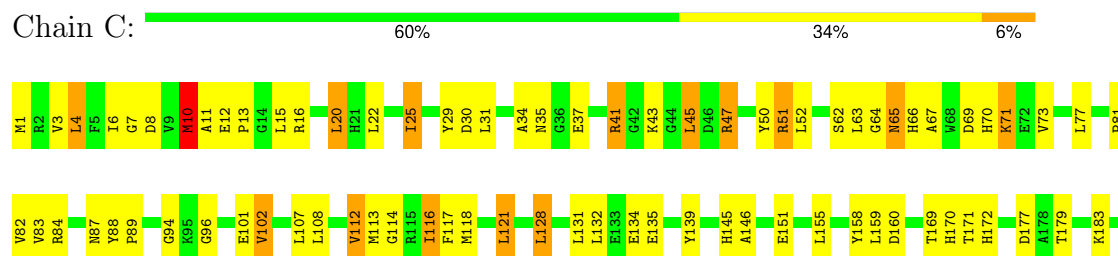
• Molecule 1: hypothetical protein TTHA0625

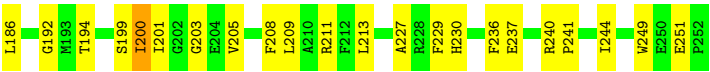


• Molecule 1: hypothetical protein TTHA0625

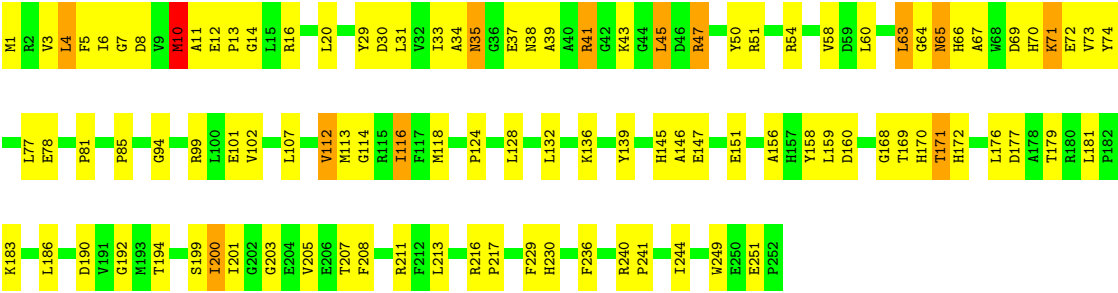


• Molecule 1: hypothetical protein TTHA0625





● Molecule 1: hypothetical protein TTHA0625



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	76.48Å 76.48Å 193.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.78 – 2.50	Depositor
% Data completeness (in resolution range)	97.7 (19.78-2.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8338	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality [i](#)

5.1 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	0.40	0/2021	0.65	1/2735 (0.0%)
1	B	0.39	0/2021	0.64	0/2735
1	C	0.37	0/2021	0.67	0/2735
1	D	0.37	0/2021	0.66	0/2735
All	All	0.38	0/8084	0.66	1/10940 (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	A	45	LEU	CA-CB-CG	6.29	129.76	115.30

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	1977	0	1958	100	0
1	B	1977	0	1958	105	0
1	C	1977	0	1958	113	0
1	D	1977	0	1958	98	0
2	A	120	0	0	7	0
2	B	108	0	0	7	0
2	C	100	0	0	4	0
2	D	102	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8338	0	7832	405	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 26.

The worst 5 of 405 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:B:171:THR:HB	1:B:190:ASP:OD1	1.59	1.00
1:D:194:THR:HG22	1:D:230:HIS:H	1.27	0.99
1:D:240:ARG:HD3	1:D:241:PRO:HD2	1.46	0.96
1:D:200:ILE:HD12	1:D:205:VAL:HA	1.49	0.94
1:D:1:MSE:HE1	1:D:107:LEU:HD22	1.53	0.90

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	250/252 (99%)	238 (95%)	8 (3%)	4 (2%)	8	15
1	B	250/252 (99%)	240 (96%)	7 (3%)	3 (1%)	11	21
1	C	250/252 (99%)	232 (93%)	15 (6%)	3 (1%)	11	21
1	D	250/252 (99%)	236 (94%)	12 (5%)	2 (1%)	16	31
All	All	1000/1008 (99%)	946 (95%)	42 (4%)	12 (1%)	11	21

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	MSE
1	B	10	MSE

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Mol	Chain	Res	Type
1	C	10	MSE
1	D	10	MSE
1	A	8	ASP

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	204/198 (103%)	187 (92%)	17 (8%)	9	19
1	B	204/198 (103%)	184 (90%)	20 (10%)	6	13
1	C	204/198 (103%)	186 (91%)	18 (9%)	8	17
1	D	204/198 (103%)	187 (92%)	17 (8%)	9	19
All	All	816/792 (103%)	744 (91%)	72 (9%)	8	17

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	35	ASN
1	D	207	THR
1	D	45	LEU
1	D	112	VAL
1	B	45	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	38	ASN
1	D	65	ASN
1	D	188	GLN
1	B	111	GLN
1	B	65	ASN

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](#)

There are no ligands in this entry.

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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.