



wwPDB X-ray Structure Validation Summary Report

Oct 23, 2024 – 04:42 AM EDT

PDB ID : 1WXW
Title : Crystal structure of Tt1595, a putative SAM-dependent methyltransferase from *Thermus thermophilus* HB8
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Deposited on : 2005-02-02
Resolution : 2.55 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) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

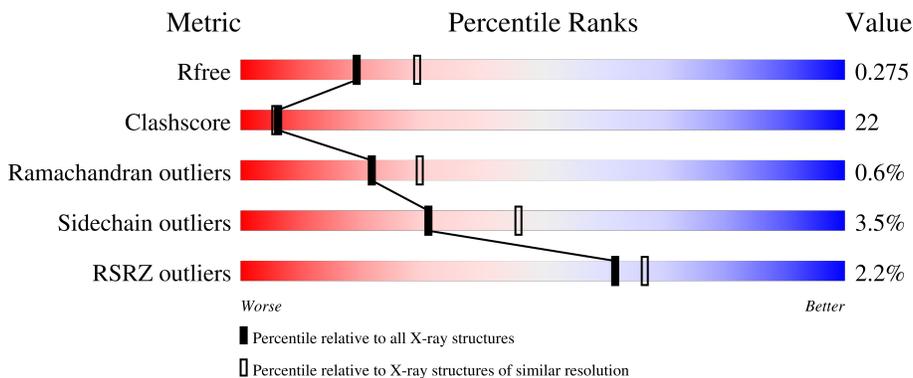
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	164625	1004 (2.54-2.54)
Clashscore	180529	1055 (2.54-2.54)
Ramachandran outliers	177936	1048 (2.54-2.54)
Sidechain outliers	177891	1048 (2.54-2.54)
RSRZ outliers	164620	1004 (2.54-2.54)

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 $\leq 5\%$. 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	382	 2% 64% 34% ..
1	B	382	 2% 59% 39% .
1	C	382	 % 63% 34% .
1	D	382	 3% 57% 41% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12185 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.

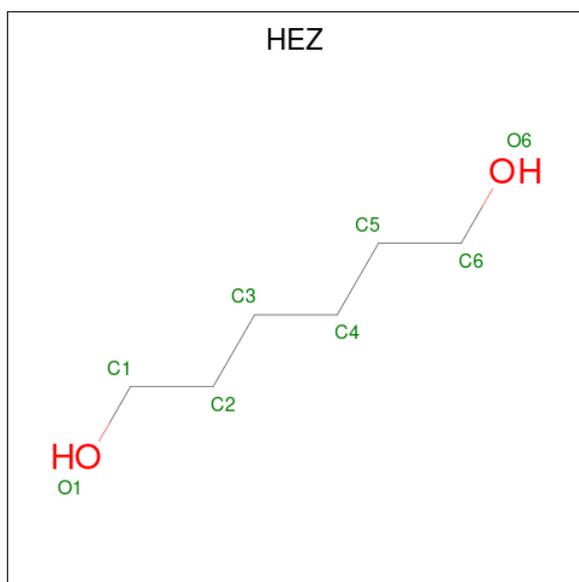
- Molecule 1 is a protein called hypothetical protein TTHA1280.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	377	3010	1917	560	528	1	4	0	0	0
1	B	382	3043	1936	567	535	1	4	0	0	0
1	C	382	3043	1936	567	535	1	4	0	0	0
1	D	382	3043	1936	567	535	1	4	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q5SIT4
A	205	MSE	MET	modified residue	UNP Q5SIT4
A	330	MSE	MET	modified residue	UNP Q5SIT4
A	338	MSE	MET	modified residue	UNP Q5SIT4
B	1	MSE	MET	modified residue	UNP Q5SIT4
B	205	MSE	MET	modified residue	UNP Q5SIT4
B	330	MSE	MET	modified residue	UNP Q5SIT4
B	338	MSE	MET	modified residue	UNP Q5SIT4
C	1	MSE	MET	modified residue	UNP Q5SIT4
C	205	MSE	MET	modified residue	UNP Q5SIT4
C	330	MSE	MET	modified residue	UNP Q5SIT4
C	338	MSE	MET	modified residue	UNP Q5SIT4
D	1	MSE	MET	modified residue	UNP Q5SIT4
D	205	MSE	MET	modified residue	UNP Q5SIT4
D	330	MSE	MET	modified residue	UNP Q5SIT4
D	338	MSE	MET	modified residue	UNP Q5SIT4

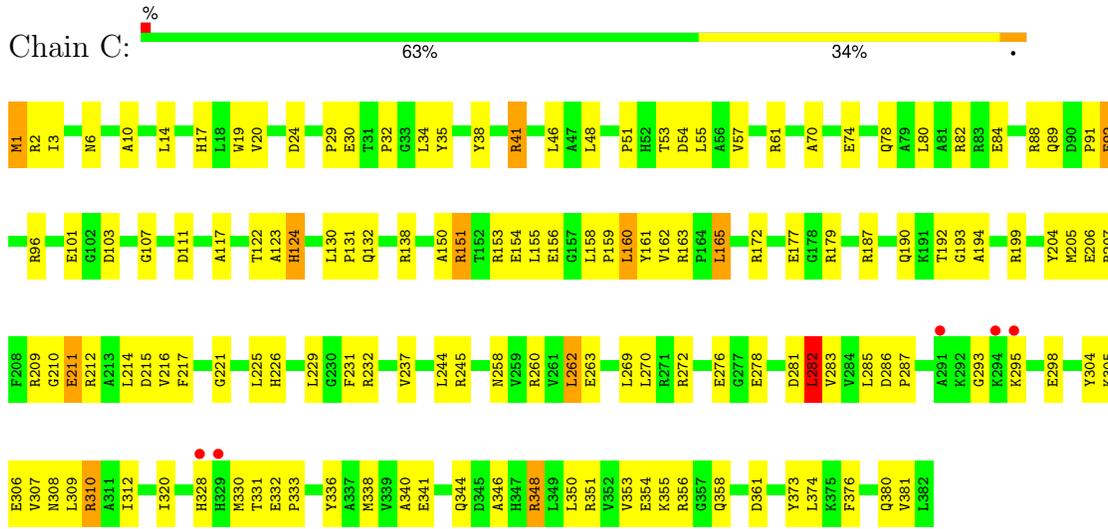
- Molecule 2 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: C₆H₁₄O₂).



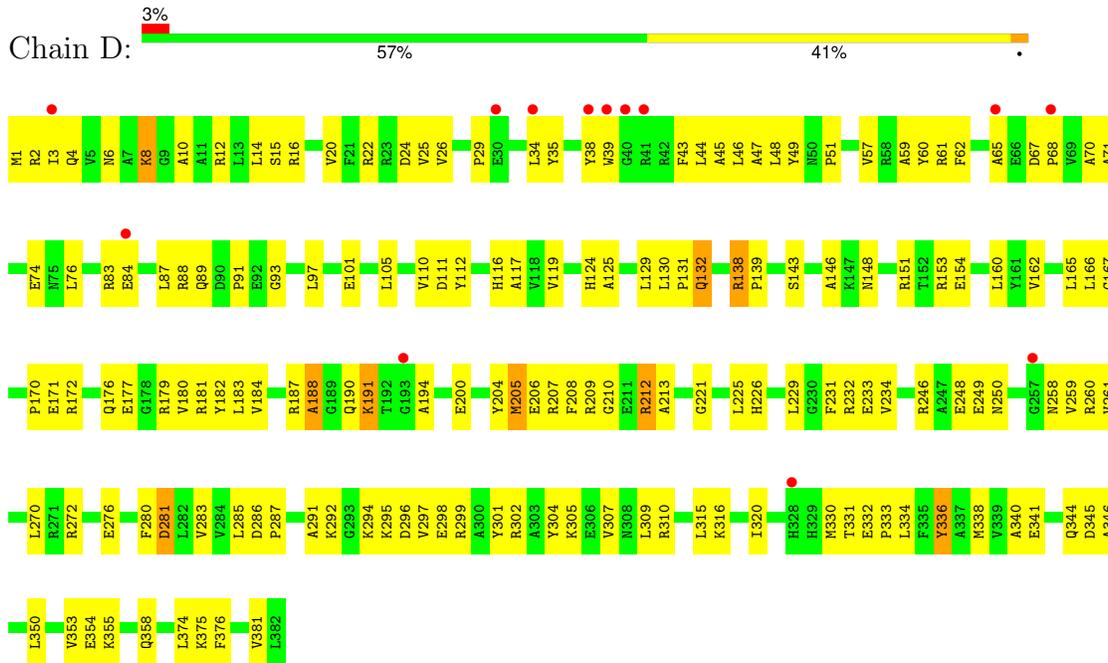
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	C O	0	0
			8	6 2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	B	10	Total	O	0	0
			10	10		
3	C	16	Total	O	0	0
			16	16		
3	D	7	Total	O	0	0
			7	7		



• Molecule 1: hypothetical protein TTHA1280



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	252.70Å 45.96Å 139.64Å 90.00° 100.08° 90.00°	Depositor
Resolution (Å)	45.83 – 2.55 45.83 – 2.55	Depositor EDS
% Data completeness (in resolution range)	92.5 (45.83-2.55) 95.3 (45.83-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.54Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.279 0.218 , 0.275	Depositor DCC
R_{free} test set	2425 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtrriage
Anisotropy	0.277	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12185	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1221e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: HEZ

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	0.39	0/3073	0.63	0/4160
1	B	0.39	0/3107	0.66	1/4206 (0.0%)
1	C	0.43	0/3107	0.68	1/4206 (0.0%)
1	D	0.39	0/3107	0.64	0/4206
All	All	0.40	0/12394	0.65	2/16778 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	282	LEU	CA-CB-CG	5.64	128.27	115.30
1	B	282	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	336	TYR	Sidechain

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	3010	0	3030	117	0
1	B	3043	0	3065	139	0
1	C	3043	0	3065	129	0
1	D	3043	0	3065	159	0
2	C	8	0	14	0	0
3	A	5	0	0	0	0
3	B	10	0	0	1	0
3	C	16	0	0	0	0
3	D	7	0	0	0	0
All	All	12185	0	12239	536	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 22.

The worst 5 of 536 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:134:ALA:HB2	1:A:165:LEU:HD23	1.40	1.04
1:D:294:LYS:H	1:D:294:LYS:HD2	1.27	0.99
1:D:46:LEU:HD11	1:D:65:ALA:HB3	1.40	0.98
1:B:98:VAL:HB	1:B:110:VAL:HG22	1.44	0.97
1:D:67:ASP:HB3	1:D:70:ALA:HB3	1.44	0.97

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	373/382 (98%)	351 (94%)	19 (5%)	3 (1%)	16	23
1	B	380/382 (100%)	353 (93%)	26 (7%)	1 (0%)	37	46
1	C	380/382 (100%)	354 (93%)	24 (6%)	2 (0%)	25	34
1	D	380/382 (100%)	349 (92%)	28 (7%)	3 (1%)	16	23
All	All	1513/1528 (99%)	1407 (93%)	97 (6%)	9 (1%)	22	29

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	188	ALA
1	D	68	PRO
1	A	186	LEU
1	B	294	LYS
1	C	124	HIS

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	302/301 (100%)	294 (97%)	8 (3%)	41	59
1	B	305/301 (101%)	296 (97%)	9 (3%)	36	52
1	C	305/301 (101%)	289 (95%)	16 (5%)	19	27
1	D	305/301 (101%)	296 (97%)	9 (3%)	36	52
All	All	1217/1204 (101%)	1175 (96%)	42 (4%)	31	46

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	281	ASP
1	D	124	HIS
1	C	282	LEU
1	C	348	ARG
1	D	191	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	132	GLN
1	C	132	GLN
1	B	344	GLN
1	C	17	HIS
1	B	308	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEZ	C	400	-	7,7,7	0.89	0	6,6,6	4.02	2 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEZ	C	400	-	-	4/5/5/5	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	HEZ	O6-C6-C5	7.39	158.36	111.44
2	C	400	HEZ	C4-C3-C2	6.49	147.18	114.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	400	HEZ	C4-C5-C6-O6
2	C	400	HEZ	C3-C4-C5-C6
2	C	400	HEZ	C2-C3-C4-C5
2	C	400	HEZ	C1-C2-C3-C4

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, 95th 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 ²)	Q<0.9
1	A	373/382 (97%)	0.21	8 (2%) 63 68	23, 54, 88, 118	0
1	B	378/382 (98%)	0.19	7 (1%) 66 69	21, 50, 90, 115	0
1	C	378/382 (98%)	-0.15	5 (1%) 74 77	19, 40, 79, 103	0
1	D	378/382 (98%)	0.31	13 (3%) 48 53	25, 54, 89, 114	0
All	All	1507/1528 (98%)	0.14	33 (2%) 62 67	19, 50, 87, 118	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	ALA	3.6
1	A	195	TYR	3.3
1	C	291	ALA	3.3
1	A	188	ALA	3.3
1	B	236	ALA	3.1

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, 95th 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(\AA^2)	Q<0.9
2	HEZ	C	400	8/8	0.78	0.20	57,58,59,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.