

Supplementary Table S1 Abbreviations of modified nucleosides.

Abbreviation	Modified nucleosides
s ⁴ U	4-thiouridine
D	dihydrouridine
m ¹ A	N ¹ -methyladenosine
Cm	2'-O-methylcytidine
ms ² i ⁶ A	2-methylthio-N ⁶ -isopentenyladenosine
Ψ	pseudouridine
m ⁵ U	5-methyluridine
Gm	2'-O-methylguanosine
m ⁷ G	7-methylguanosine
Q	queuosine
m ⁶ A	N ⁶ -methyladenosine
m ² G	N ² -methylguanosine
m ² ₂ G	N ² ,N ² -dimethylguanosine
i ⁶ A	N ⁶ -isopentenyladenosine
m ⁵ s ² U	5-methyl-2-thiouridine
G ⁺	archaeosine
t ⁶ A	N ⁶ -threonylcarbamoyladenine
ncm ⁵ U	5-carbamoylmethyluridine
m ¹ G	1-methylguanosine
m ⁵ C	5-methylcytidine
Um	2'-O-methyluridine
m ¹ I	1-methylinosine
s ² C	2-thiocytidine
m ⁵ Cm	5, 2'-O-dimethylcytidine
mimG	methylwyosine
m ¹ Im	1, 2'-O-dimethylinosine
m ² ₂ Gm	N ² , N ² , 2'-O-trimethylguanosine
m ² , ⁷ Gm	N ² , 7, 2'-O-trimethylguanosine

Am	2'-O-methyladenosine
I	inosine
k ² C	lysidine
agm ² C	agmatidine
mn ⁵ U	5-methylaminomethyluridine
cm ⁵ U	5-carboxymethyluridine
cnm ⁵ U	5-cyanomethyluridine
cmnm ⁵ Um	5-carboxymethylaminomethyl-2'-O-methyluridine
m ¹ Ψ	1-methylpseudouridine
ac ⁶ A	N ⁶ -acetyladenosine
hn ⁶ A	N ⁶ -hydroxynorvalylcarbamoyladenine
ms ² hn ⁶ A	2-methylthio- N ⁶ -hydroxynorvalylcarbamoyladenine
methyl-hn ⁶ A	methylated hn ⁶ A*
s ² Um	2-thio-2'-O-methyluridine
ac ⁴ Cm	4-acetyl-2'-O-methylcytidine
oQ	epoxyqueosine
imG2	isowyosine
yW-86	7-aminocarboxypropyldemethylwyosine
imG-14	4-demethylwyosine

* Precise structure is unknown.

Supplementary Table S2 Crystal structural studies on tRNA modification enzymes from thermophiles.

tRNA modification enzyme(s)	Source (thermophile species)	PDB ID	Reference(s)
Archaeal Trm14	<i>Pyrococcus furiosus</i>	3TLJ, 3TM4, 3TM5	[15]
TrmN	<i>Thermus thermophilus</i>	3TMA	[15]
CDAT8	<i>Methanopyrus kandleri</i>	3G8Q	[16]
ThiI	<i>Thermotoga maritima</i>	4KR6, 4KR7, 4KR9	[32]
Archaeal Trm10	<i>Sulfolobus acidocaldarius</i>	5A7Z, 5A7Y, 5A7T	[38]
	<i>Thermococcus kodakarensis</i>	6EMS, 6EMT, 6EMU, 6EMV	[39]
Archaeal Trm11	<i>Thermococcus kodakarensis</i>	5E71, 5E72	[43]
ArcTGT	<i>Pyrococcus horikoshii</i>	1IT7, 1IT8, 1IQ8	[54,55]
TrmH	<i>Thermus thermophilus</i>	1V2X	[75]
	<i>Aquifex aeolicus</i>	1ZJR	[77]
DusA	<i>Thermus thermophilus</i>	3B0V, 3B0U, 3B0P	[84]
TrmI	<i>Pyrococcus horikoshii</i>	2DUL, 2DYY, 2EJT, 2EJU, 2YTZ	[93]
	<i>Aquifex aeolicus</i>	3AXS, 3AXT	[95]
Archaeal TrmJ	<i>Sulfolobus acidocaldarius</i>	4CNF, 4CNG	[96]
TadA	<i>Aquifex aeolicus</i>	1WWR	[104,105]
TilS	<i>Aquifex aeolicus</i>	1WY5, 2E21, 2E89	[112,113]
TiaS	<i>Archaeoglobus fulgidus</i>	3AU7, 3AMU, 3AMT	[119]
MnmC2	<i>Aquifex aeolicus</i>	3VYW	[136]
MnmE	<i>Thermotoga maritima</i>	1XZP, 1XZQ	[138]
MnmG	<i>Aquifex aeolicus</i>	2ZXI, 2ZXH	[141]
TrmL	<i>Thermus thermophilus</i>	5CO4	[144]
QueA	<i>Thermotoga maritima</i>	1VKY	[151]
TrmD	<i>Aquifex aeolicus</i>	1OY5	[160]
Archaeal Trm5	<i>Methanocaldococcus janaschii</i>	3AY0, 2YX1, 2ZZN	[166–168]
Trm5a	<i>Pyrococcus abyssi</i>	5WT1, 5WT3	[177]
Trm5b	<i>Pyrococcus abyssi</i>	5YAC	[180]
Taw1	<i>Pyrococcus horikoshii</i>	2YX0	[172]
	<i>Methanocaldococcus janaschii</i>	2Z2U	[173]
Taw2	<i>Pyrococcus horikoshii</i>	3A25, 3A26	[174]
	<i>Methanocaldococcus janaschii</i>	3A27	[174]
Taw3	<i>Sulfolobus solfataricus</i>	1TLJ	[178]
KEOPS complex	<i>Methanocaldococcus janaschii</i> and	3ENQ, 3ENC, 3ENH, 3ENO, 2VWB	[184,185]

	<i>Pyrococcus furiosus</i>		
Sua5	<i>Pyrococcus abyssi</i>	6F89, 6F87, 6F8Y	[189]
	<i>Sulfolobus tokodaii</i>	2EQA, 2YV4, 3AJE, 4E1B	[327,328]
TruA	<i>Thermus thermophilus</i>	1VS3	[202]
Archaeal Trm4	<i>Methanocaldococcus janaschii</i>	3A4T, 3AJD	[210]
TrmY	<i>Methanocaldococcus janaschii</i>	3AI9, 3AIA	[215]
TrmFO	<i>Thermus thermophilus</i>	3G5Q, 3G5R, 3G5S	[223]
TtuA	<i>Thermus thermophilus</i>	5B4F, 5B4E	[236]
	<i>Thermotoga maritima</i>	5MKQ, 5MKO	[134]
	<i>Pyrococcus horikoshii</i>	3VRH	[233]
TtuA and TtuB complex	<i>Thermus thermophilus</i>	5GHA	[236]
Archaeal TrmA	<i>Pyrococcus abyssi</i>	2JJQ, 2VS1	[238]
TruB	<i>Thermotoga maritima</i>	1R3E, 1R3F, 1ZE1, 1ZE2, 2AB4	[244,246,247]
Trm56	<i>Pyrococcus horikoshii</i>	2YY8	[251]
Archaeal TrmI	<i>Pyrococcus abyssi</i>	3LGA, 3LHD, 3MB5	[256]
TrmI	<i>Thermus thermophilus</i>	5C0O, 5C1I, 2PWY	[261,264]
	<i>Aquifex aeolicus</i>	2YVL	[262]
Box C/D RNP	<i>Sulfolobus solfataricus</i>	5GIN, 5GIO, 5GIP	[326]

In this table, only the published crystal structures from thermophiles are listed. Numerous unpublished protein structures, which seem to be related to tRNA modifications, are deposited in Protein Data Bank. In this table, the structures of tRNA modification enzymes from mesophiles are not cited.