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Supporting information for article:

**Crystal structure of SAM-dependent methyltransferase from
*Pyrococcus horikoshii***

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Table S1 Hydrogen bonding distance between SAM and the residues.

SAM atoms	Interacting residues	Distance in Å
N6	Asp93 (OD1)	3.0
	Gln19 (O1)	2.9
N1	Ala94(N)	3.0
O2	Asp67(OD1)	2.5
O3	Asp67(OD2)	2.8
	Tyr7(OH)	3.5
CE	Tyr7(OH)	3.4
N	Ala46	2.8
	Ile110(O)	2.9
O	Tyr21(OH)	3.2
OXT	Arg24(NH2)	2.4

Table S2 Various interactions in monomeric *PhSAM*-MT coordinates.

Residue 1	Residue 2	Distance in Å
Residue (Atom)	Residue (atom)	
Ionic interactions		
Arg24 (NH2)	Asp111(OD2)	2.78
Arg74(NH1)	Asp71(OD1)	2.66
Arg74(NH2)	Asp71(OD1)	3.13
Arg95 (NH2)	Asp93(OD1)	3.83
Arg95 (NH2)	Asp93(OD2)	2.66
Lys96 (133)	Glu210(OE1)	3.05
Arg130(NH1)	Asp101(OD1)	2.62
Arg130(NH2)	Glu127(OE1)	2.70
Lys133(NZ)	Asp105(OD1)	3.26
Lys133(NZ)	Asp105(OD2)	3.83
Lys137(NZ)	Glu210(OE1)	3.95
Arg146(NH2)	Asp144(OD2)	3.05
Arg146(NH2)	Asp144(OD2)	3.51
Lys161 (NZ)	Asp185(OD2)	3.57
Lys196(NZ)	Glu200(OE1)	3.95
Lys196(NZ)	Gu212(OE1)	3.55
Lys204(NZ)	Glu200(OE1)	3.56
Lys209(NZ)	Glu200(OE1)	3.53
Lys209(NZ)	Glu212(OE1)	3.97
Aromatic-Aromatic interactions (4.5-6.0 Å)		
Phe3	Phe187	
Tyr6	Phe10	
Tyr6	Tyr7	
Tyr6	Phe191	
Tyr6	Tyr13	
Phe10	Phe180	
Phe54	Phe89	
Phe61	Tyr106	

Phe99	Phe104	
Phe125	Phe138	
Phe138	Phe207	
Tyr162	Phe187	
Phe180	Phe187	
Phe207	Tyr224	
Phe109	Phe116	
Intra-protein cation-pi interactions (within 6Å)		
Tyr13	Arg24	
Tyr21	Arg24	
Phe52	Arg24	
Phe54	Arg83	
Phe61	Arg39	
Phe104	Lys41	
Tyr106	Lys137	
Tyr162	Lys161	
Trp194	Arg174	
Tyr218	Lys214	
Tyr220	Lys196	
Tyr220	Lys214	

Table S3 Structure comparison for two domains with other coordinates in the PDB.

PDB ID	Z	Rmsd (Å)	Residues fitted	Sequence identity (%)	Source
Domain I					
1WZN	22.8	2.2	245	33	SAM-dependent methyltransferase from <i>Pyrococcus horikoshii</i>
3SM3	22.7	1.5	212	28	SAM-dependent methyltransferases from <i>Methanosarcina mazei</i>
1XXL	22.6	1.6	234	25	YcgJ protein from <i>Bacillus subtilis</i>
4KDR	22.6	1.9	208	14	UBIG/SAH complex
2GLU	22.6	1.6	234	25	YcgJ protein from <i>Bacillus subtilis</i>
5GM1	22.4	1.8	281	22	methyltransferase TleD complexed with SAH
5FCD	21.6	1.8	228	27	MccD protein
Domain II					
2ARH	4.6	2.5	198	8	Unknown function AQ1966 from <i>Aquifex aeolicus</i>
1VL4	4.3	1.7	428	15	Putative modulator of a DNA gyrase (tm0727) from <i>Thermotoga maritima</i>
2P25	4.1	2.2	126	5	Glyoxalase family protein from <i>Enterococcus faecalis</i>
4Q51	4.0	3.1	264	7	Putative molybdenum cofactor biosynthesis protein F from <i>Burkholderia cenocepacia</i>
4MTT	4.0	2.3	128	17	Ni- and Zn-bound GloA2
3DB7	3.9	2.3	127	7	Calcium-regulated periplasmic protein (bt0923) from <i>Bacteroides thetaiotaomicron</i>