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Supporting information for article:

Crystal structures of a subunit of the formylglycinamide ribonucleotide amidotransferase, PurS, from *Thermus thermophilus*, *Sulfolobus tokodaii* and *Methanocaldococcus jannaschii*

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	Tt PurS 2dgb	<i>Mj</i> PurS 2yx5	St PurS 2zw2	Bs PurS 1twj	Bs PurS 1t4a	MtPurS 1gtd	<i>Tm</i> PurS 1vq3	<i>Tm</i> PurS 3d54
Tt PurS 2cuw	0.553 (83)	1.124 (56)	0.937 (56)	0.939 (55)	1.038 (54)	1.113 (42)	0.843 (60)	1.005 (61)
Tt PurS 2dgb		1.064 (52)	1.072 (54)	0.853 (56)	1.090 (55)	1.191 (46)	0.755 (58)	0.942 (61)
Mj PurS 2yx5			0.936 (68)	1.136 (65)	1.268 (61)	1.268 (61)	1.145 (67)	1.135 (69)
St PurS 2zw2				1.063 (57)	1.152 (57)	1.151 (55)	1.105 (69)	1.108 (64)
Bs PurS 1twj					1.011 (78)	0.969 (66)	0.988 (60)	1.019 (60)
Bs PurS 1t4a						1.197 (60)	1.010 (61)	1.163 (66)
Mt PurS 1gtd							1.028 (52)	1.075 (53)
Tm PurS 1vq3								0.677 (82)

Supplementary Table S1. Tertiary structural similarity measured by C α rmsd (Å) Number of C α atoms used for rmsd calculation was shown in the parenthesis

	<i>Mj</i> PurS	St PurS	Bs PurS	Mt PurS	<i>Tm</i> PurS
Tt PurS	38	22	32	27	32
<i>Mj</i> PurS		27	39	45	32
St PurS			21	22	29
Bs PurS				28	28
Mt PurS					23

Supplementary Table S2. Sequence identities among PurS structures (%)



Supplemental Fig. S1 Structural fluctuations of PurSs A, B: TtPurS (2CUW), C, D: TtPurS (2DGB), E, F: MjPurS, G, H: StPurS,

- A, C, E, G: superimposed by a subunit, B, D, F, H: superimposed by a half of the molecule.



Supplemental Fig. S2 Structural fluctuations of PurSs A, B: TtPurS (2CUW), C, D: TtPurS (2DGB), E, F: MjPurS, G, H: StPurS.