STRUCTURAL
BIOLOGY

Volume 74 (2018)

Supporting information for article:

Thermus thermophilus cobalamin-dependent methionine synthase folate-binding module displays a distinct variation of the classical TIM barrel: a TIM barrel with a `twist'

Kazuhiro Yamada and Markos Koutmos

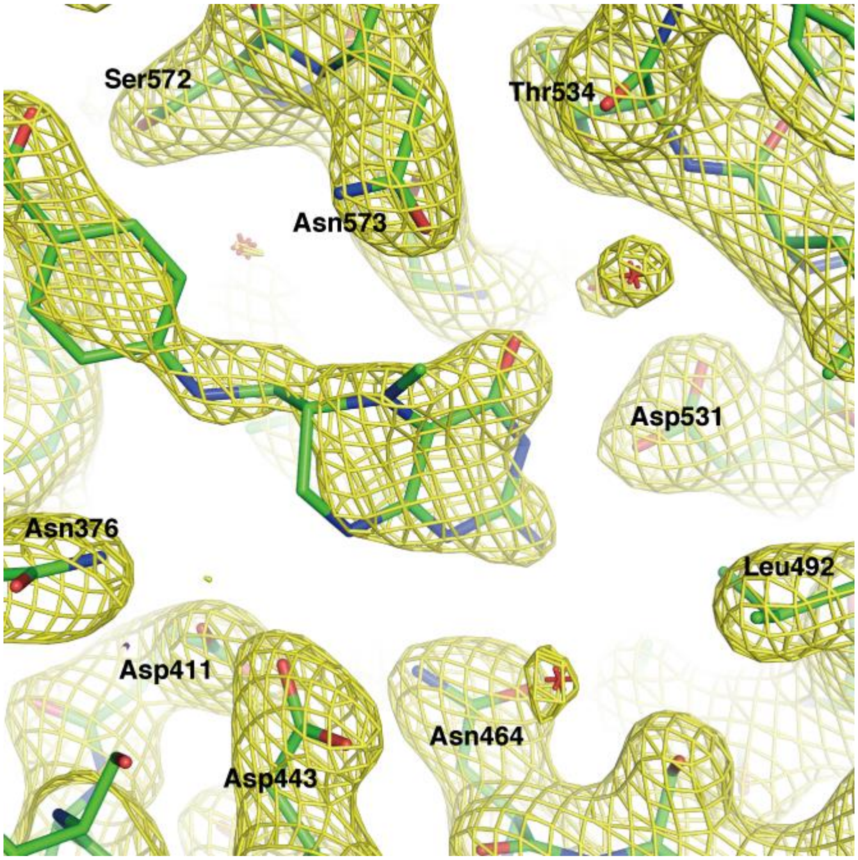

Figure S1 The composite omit electron density in yellow around the folate binding site is displayed in yellow. The Folate ligands as well as active site residues and waters are shown as sticks. The calculated refined composite omit 2Fo-Fc map is contoured at 1.5 σ.

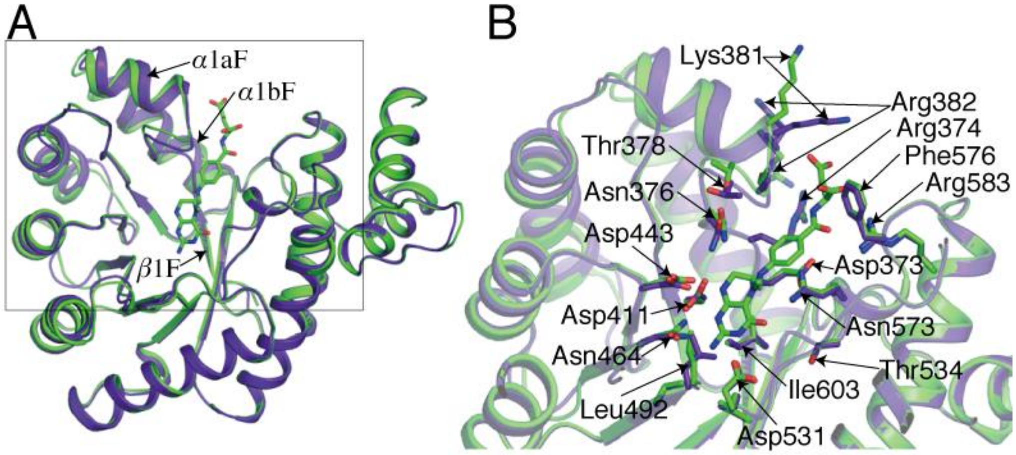

Figure S2 Comparison of the *T. thermophilus* MS Fol module structures with and without the CH_3-H_4folate substrate present. The substrate-bound form is displayed in green, and the substrate-free structure is shown in blue. The CH_3-H_4folate substrate is depicted in stick mode.

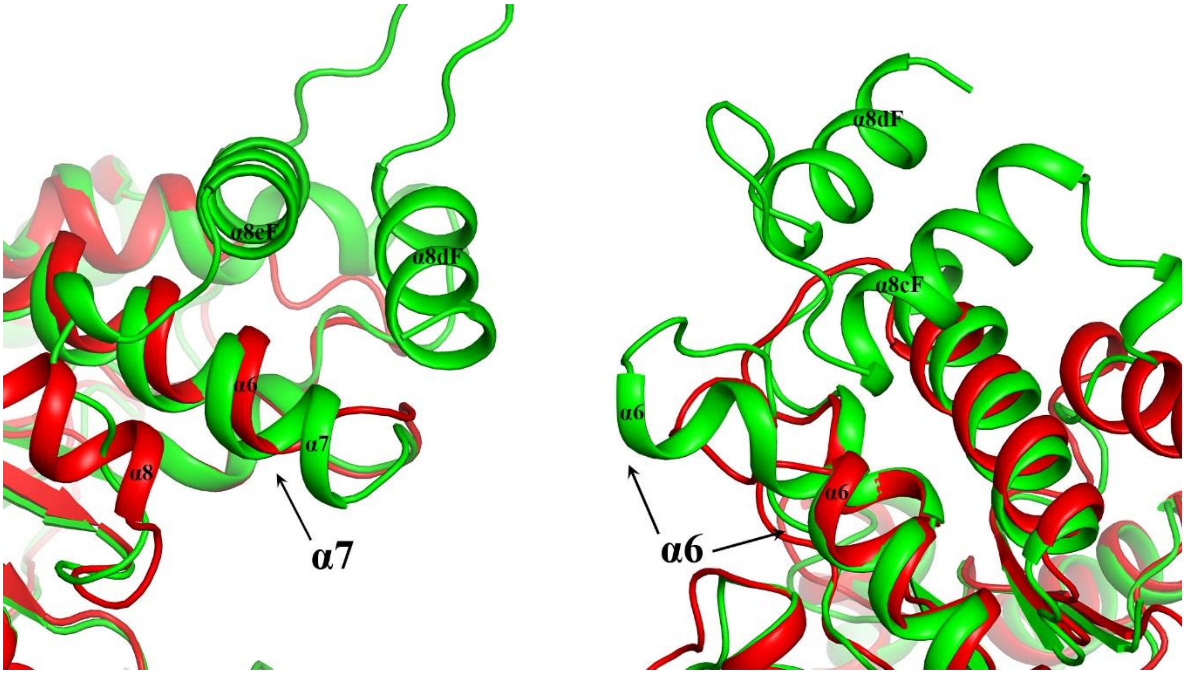

Figure S3 Two different close up views of the superimposed *T. maritima* (red) and *T. thermophilus* (green) Fol modules centered around helices α6 and α8. Both helices are longer in *T. thermophilus* MS as well as all the Fol modules with a $\beta_8\alpha_7$ fold.

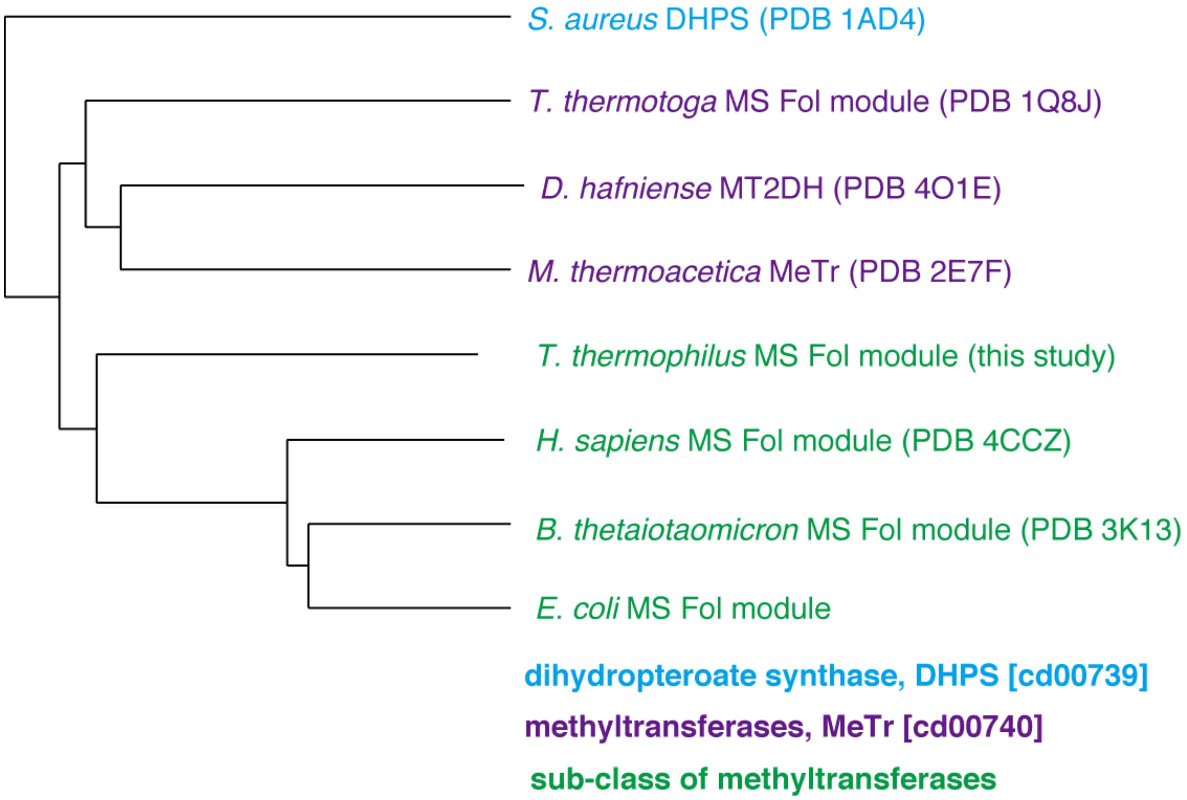

Figure S4 Phylogenetic tree analysis of Fol modules from different sources. Most MS Fol modules group separately from other pterin-binding modules. *T. maritima* MS Fol module is not grouped with other MSs.