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Supporting information for article:

Crystal structure of adenylosuccinate lyase from the thermophilic bacterium *Thermus thermophilus* HB8

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Supplementary figures

Supplementary Fig. S1. Alignment of PurB

Supplementary Fig. S2. Subunit interface of PurB

Supplementary Fig. S3. Ligplot image

References

1. Gouet, P., Courcells. E., Stuart, D. I. and Métoz, F. (1999). *Bioinformatics*, **15**, 305-308.

2. Laskowski, R. A. and Swindells, M. B. (2011). *J. Chem. Inf. Model.,* **51**, 2778-2786.

3. Larkin, M. A., Blackshields, G., Brown, N.P., Chenna, R., McGettigan, P.A., McWilliam, H., Valentin, F., Wallace, I. M., Wilm, A., Lopez, R., Thompson, J. D., Gibson, T. J. and Higgins, D.G. (2007). *Bioinformatics,* **23**, 2947-2948.
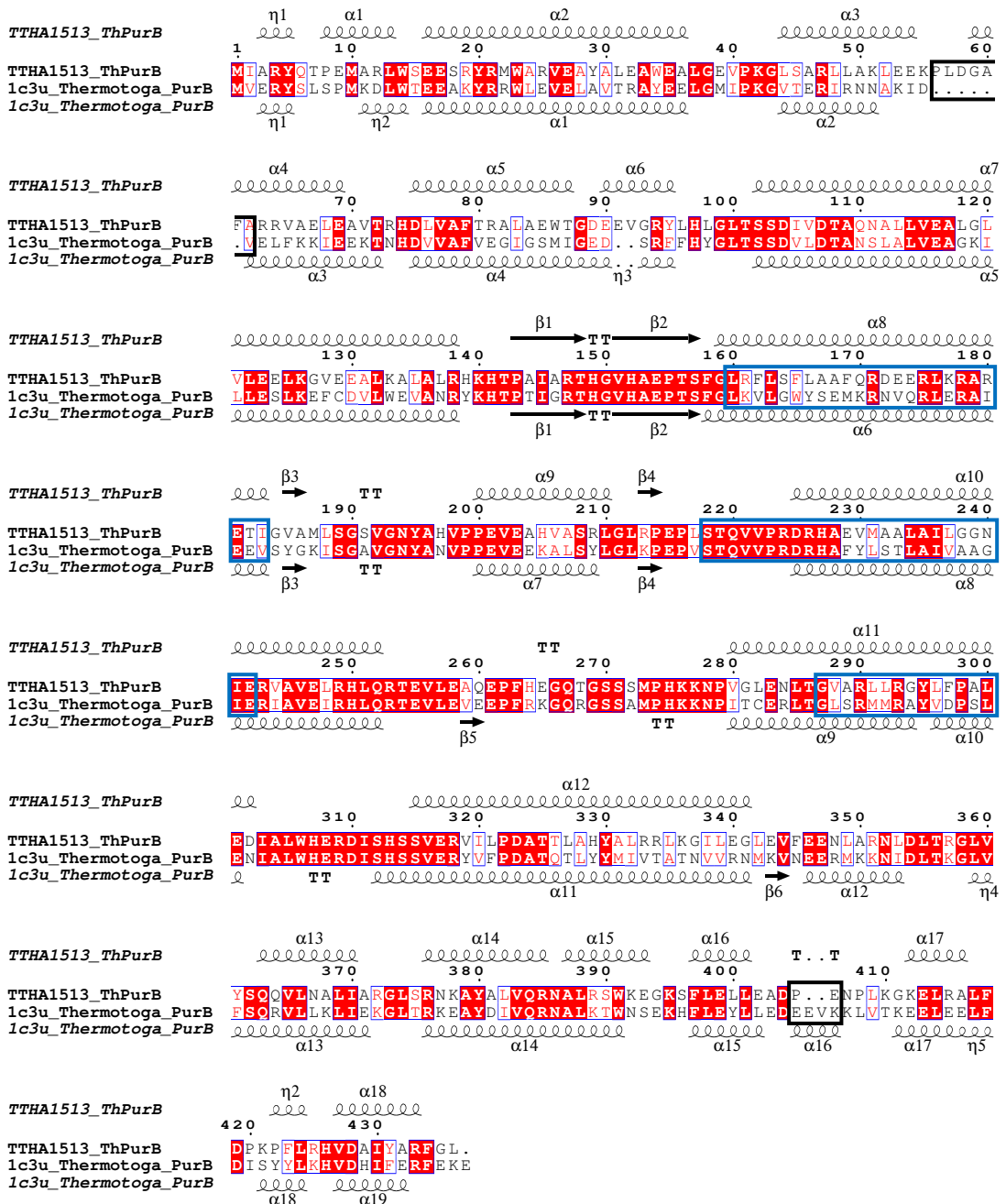
Supplementary Figure S1. Alignment of PurB
Amino-acid sequence alignment of *Tt*PurB and *Tm*PurB proteins. Alignment was performed by CLUSTAL W (Larkin et al., 2007). Conserved residues are highlighted with red boxes and similar residues are shown in red text. The secondary structure of both PurBs is indicated by helices (α-helices), arrows (β-strands) and TT (β-turn). The regions with differences in secondary structure of are surrounded by black boxes. Three regions, which form the interaction surface between subunit A and subunit B are surrounded by blue boxes. The alignment figure was prepared by *ESPript* 3.0 (Gouet et al., 1999).
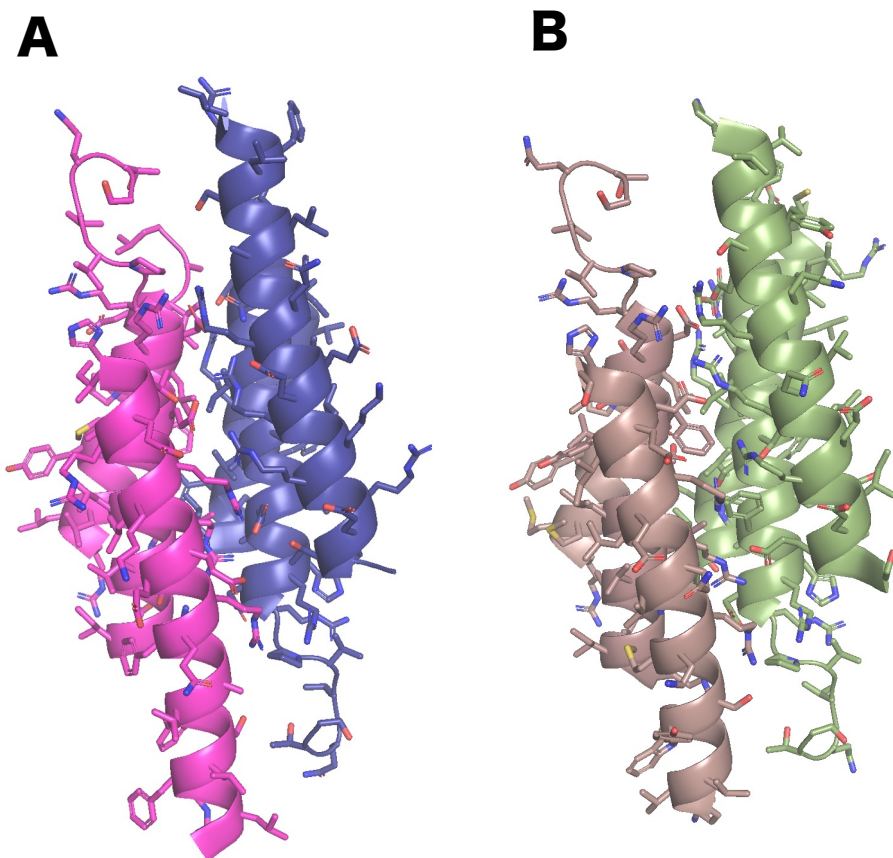
Supplementary Figure S2. Subunit interface of PurB
Subunit interface between subunit A and B of (A) *Tt*PurB and (B) *Tm*PurB proteins. Subunit interface residues (blue boxes in Supplemental Fig. S1) were shown by wire and cartoon. The helices of subunit A and B are both α8 (α6), α10 (α8) and α11(α9-10) of *Tt*PurB (*Tm*PurB) from the front. The structures are colored as follows: the subunit A and B of *Tt*PurB; blue and red, : the subunit A and B of *Tm*PurB; green and dark salmon.

Supplementary Fig. S3. Ligplot image
(A) SAICAR, (B) SAMP. Intermolecular interaction was analyzed by Ligplot (Laskowski and Swindells, 2011). Residue numbers of each subunits are as follows. Subunit A, B, C, and D; 1-436, 437-872, 873-1308, 1309-1744, respectively.