Supporting Information

Zhao et al. 10.1073/pnas.1400166111

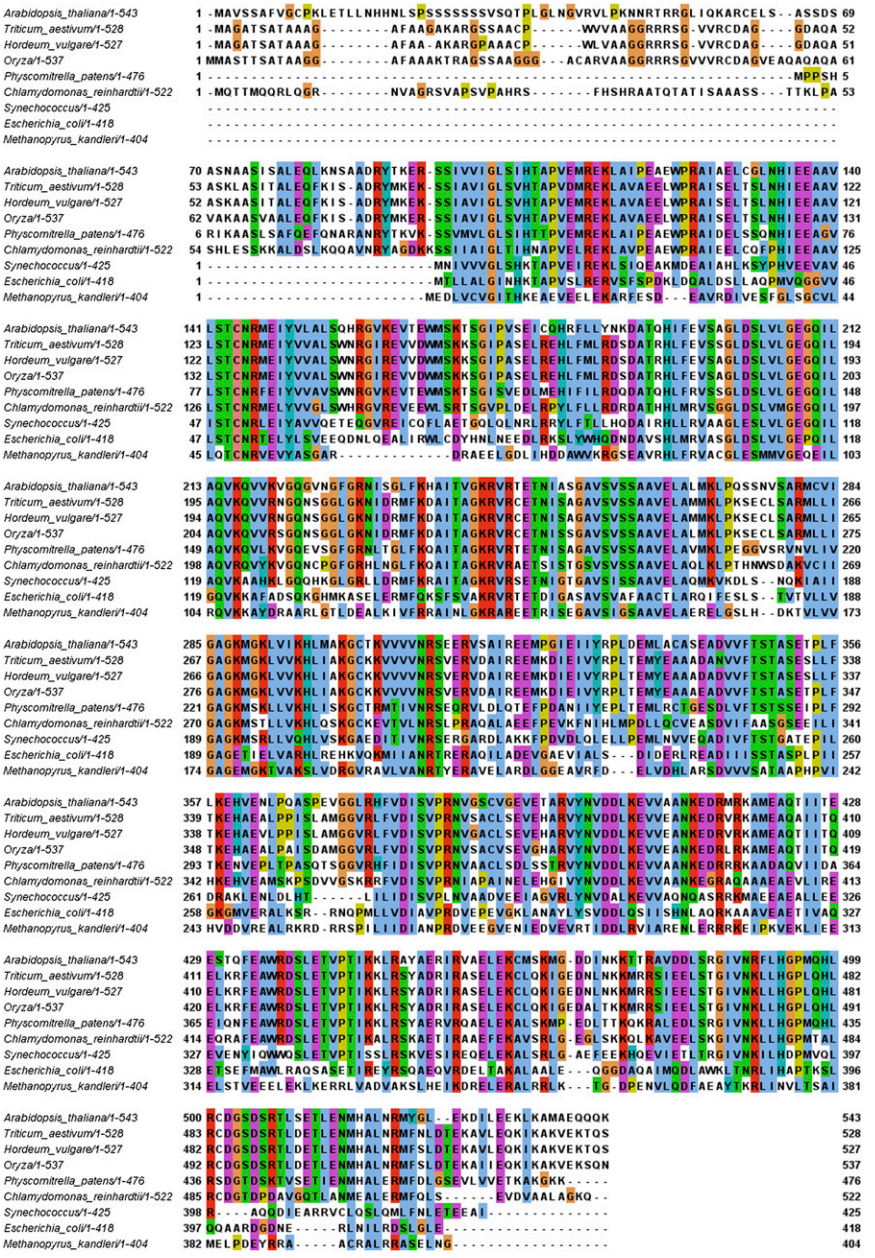

Fig. S1. Sequence alignment of *Arabidopsis* glutamyl-tRNA reductase (GluTR) with *Methanopyrus* and other homologs. The alignment is colored by conservation.

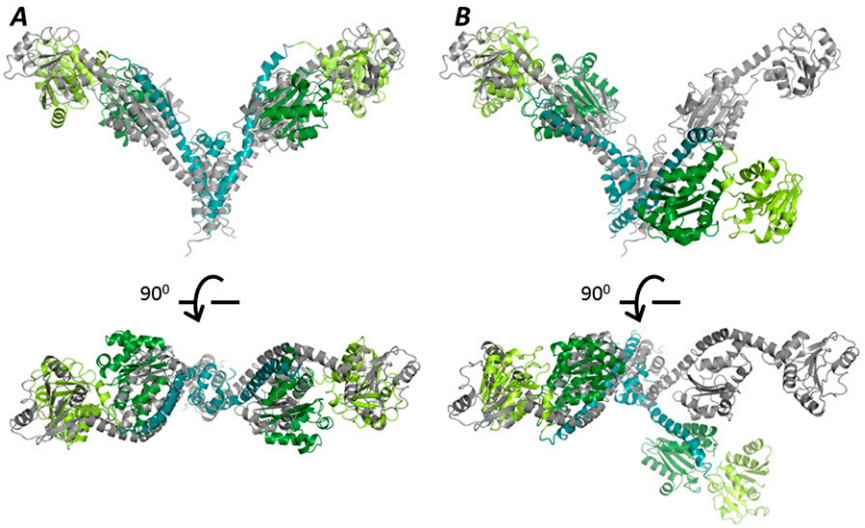

Fig. S2. Structure comparison of *Methanopyrus kandleri* GluTR (*Mk*GluTR) and *Arabidopsis* GluTR (*At*GluTR). (*A*) Superposition of the two dimers. (*B*) Superposition of the monomeric halves. *Mk*GluTR is colored gray and *Arabidopsis* GluTR is colored the same as in Fig. 1.

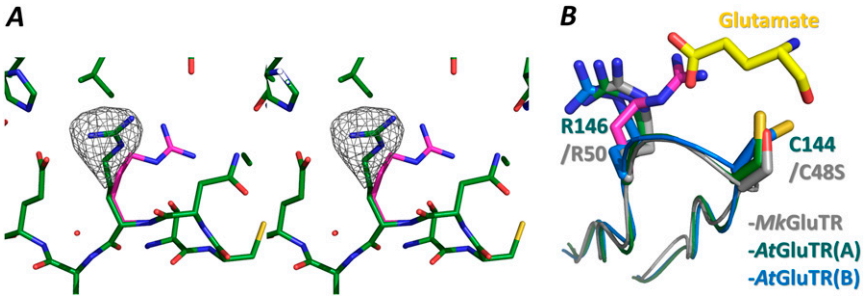

Fig. S3. Alternative conformations of GluTR Arg146. (*A*) Stereo view of the double conformations of Arg146 on chain A of GluTR. The alternative conformation of Arg146 on chain A is displayed together with electron density calculated by using the Fo−Fc coefficient and contoured at 3.0σ as a gray mesh. Arg146 on chain B does not have double conformations. (*B*) Superposition of Arg146 conformations and *Mk*GluTR Arg50. Carbon atoms are colored as indicated, with the glutamate moiety of glutamycin in the *Mk*GluTR structure shown in yellow (O, red; N, blue; S, orange).

Table S1. Data collection, phasing, and refinement statistics for GluTR-GluBP structures

	GluTR–GluBP	GluTR–seGluBP*	seGluTR–seGluBP†
Data collection			
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
Cell dimensions			
a, *b*, *c*, Å	59.4, 84.8, 360.0	60.0, 84.0, 360.2	60.1, 84.1, 362.0
α, β, γ, °	90, 90, 90	90, 90, 90	90, 90, 90
Wavelength, Å	0.9793	0.9793	0.9793
Resolution, Å‡	2.80 (2.90–2.80)	4.20 (4.35–4.20)	3.10 (3.21–3.10)
R_{sym} or R_{merge}	0.104 (0.551)	0.212 (0.529)	0.183 (0.574)
$I/\sigma I$	17.7 (3.8)	38.7 (15)	12.5 (4.1)
Completeness, %	94.3 (93.4)	100 (100)	99.8 (100)
Redundancy	7.1 (7.5)	25.1 (25.9)	8.4 (8.8)
Refinement			
Resolution, Å	49.56–2.80	—	—
No. reflections	43,245	—	—
R_{work}/R_{free}	0.221/0.272	—	—
No. atoms			
Protein	9,920	—	—
Ligand/ion	0		
Water	47		
β-Factors			
Protein	62.3		
Ligand/ion	None		
Water	31.7		
rmsds			
Bond lengths, Å	0.003		
Bond angles, °	0.969		

GluBP, glutamyl-tRNA reductase binding protein.
*Methionines were replaced by selenomethionines in GluBP only.
†Methionines were replaced by selenomethionines in GluTR and GluBP.
‡Values in parentheses are for highest-resolution shell.