ActaCrystallographica Section D research papers

SUPPLEMENTARY MATERIAL

Structural and Biochemical Characterization of N^5-Carboxyaminoimidazole RibonucleotideSynthetase and N^5-Carboxyaminoimidazole RibonucleotideMutase from *Staphylococcus aureus*

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CAPTIONS:

Scheme 1. *De novo* purine biosynthesis pathway

Scheme 2. Enzymatic assays used. **A:** Enzymatic assay for PurK. **B:** Enzymatic assay for PurE

Chart 1. Plot V_0 vs. [HCO_3^-] for PurK. Fit to a hyperbola using Origin.

Figure 1. Gel filtration chromatography for PurK, PurE and PurC

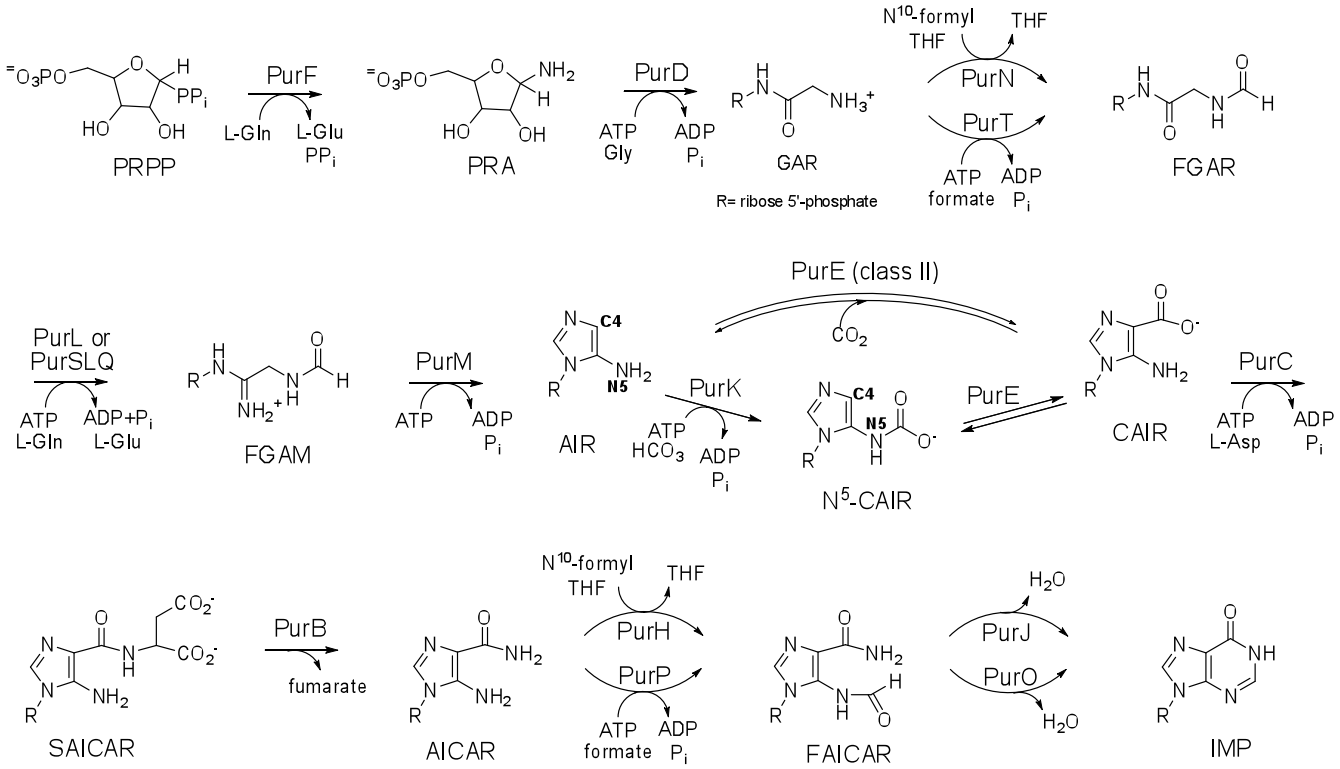
Figure 2.A: *S. aureus* PurK colored by B-factors. Blue indicates low B-factors, yellow indicates high B-factors. **B:** Superposition of the apo-PurK (grey) and PurK complexed with ADP structure (yellow). The RMSD for the A- and C- domains is 0.19 Å while the RMSD for domain B is 3.2 Å.

Figure 3. Sequence alignment of *S. aureus* PurK with *E. coli* PurK

Figure 4. Sequence alignment of *S. aureus* PurE with human PurE.

Figure 5. Overlay of *S. aureus* PurE (orange) and human bifunctional enzyme PurC-PurE. The PurE domain of the human enzyme is in the center and the PurC domain in the outside.

Scheme 1.*De novo* purine biosynthesis pathway



Scheme 2. Enzymatic assays used. **A:** Enzymatic assay for PurK. **B:** Enzymatic assay for PurE

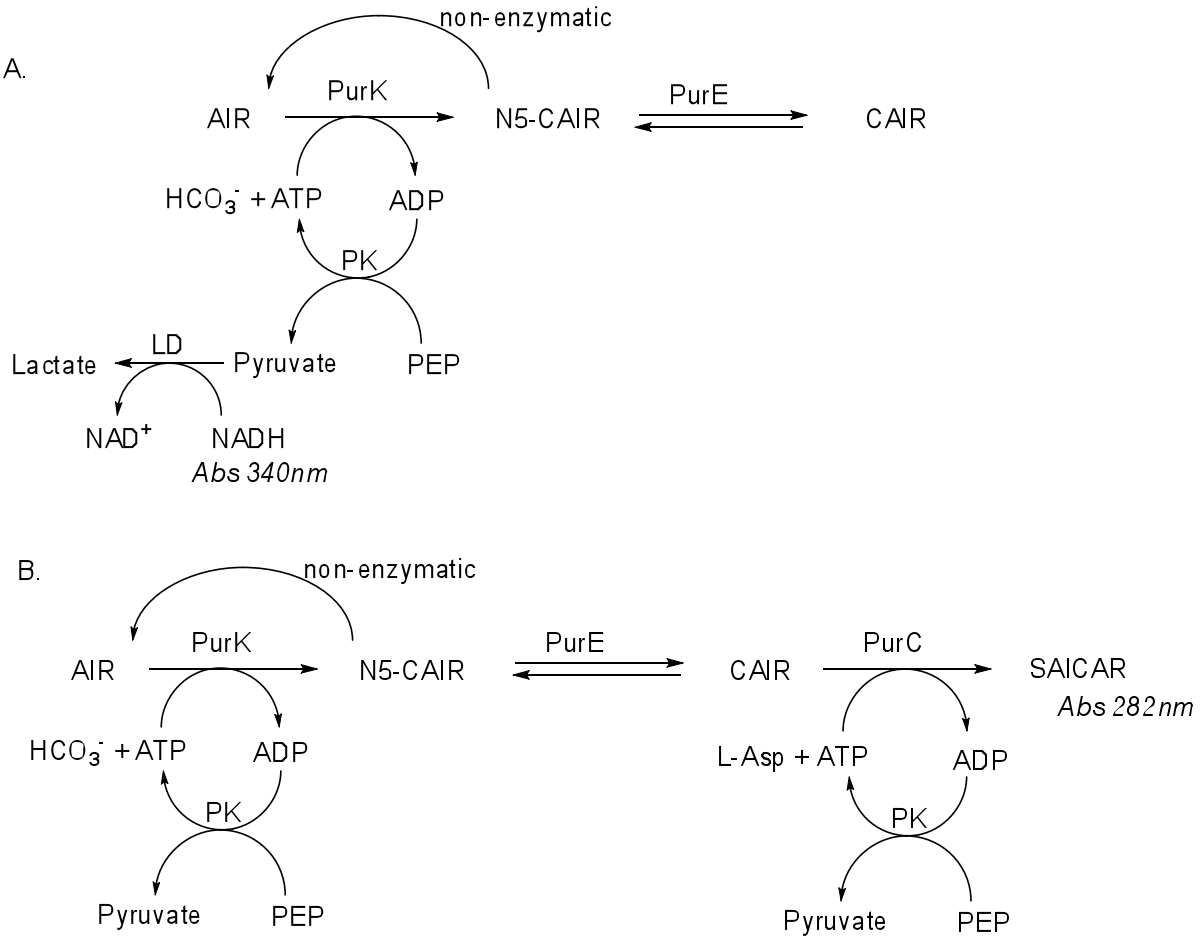
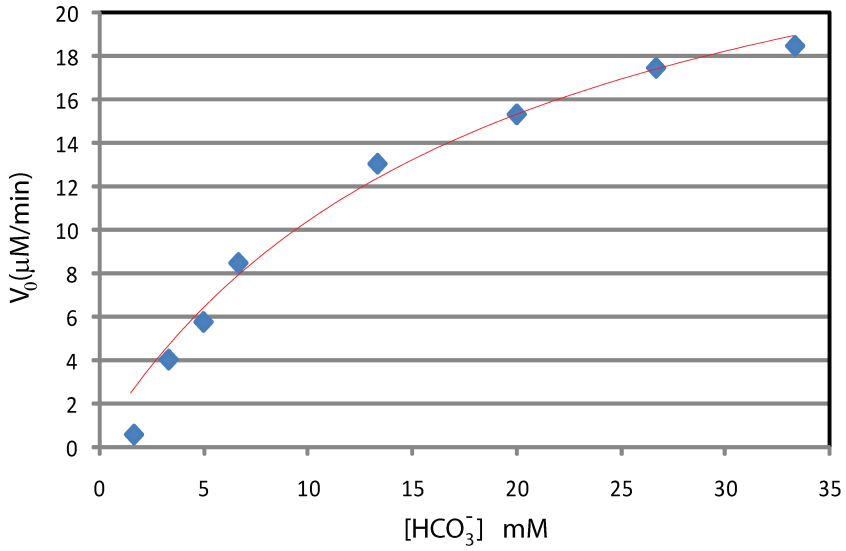


Chart 1. Plot V_0 vs. $[HCO_3^-]$ for PurK. Fit to a hyperbola using Origin.



$$V_0 = \frac{V_{max}[S]}{K_m + [S]} \qquad V_{max} = 29.6 \pm 3\ \mu M/min \qquad K_m = 18.8 \pm 3.9\ mM$$

Figure 1. Gel filtration chromatography for PurE (octamer), PurK (dimer) and PurC (dimer).

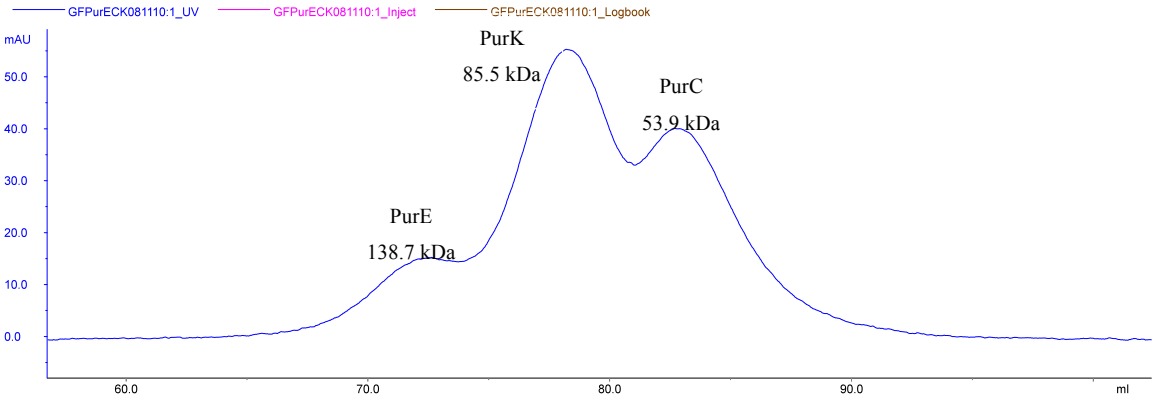


Figure 2.A: *S. aureus* PurK colored by B-factors. Blue indicates low B-factors, yellow indicates high B-factors. **B:** Superposition of the apo-PurK (grey) and PurK complexed with ADP structure (yellow). The RMSD for the A- and C- domains is 0.19 Å while the RMSD for domain B is 3.2 Å.

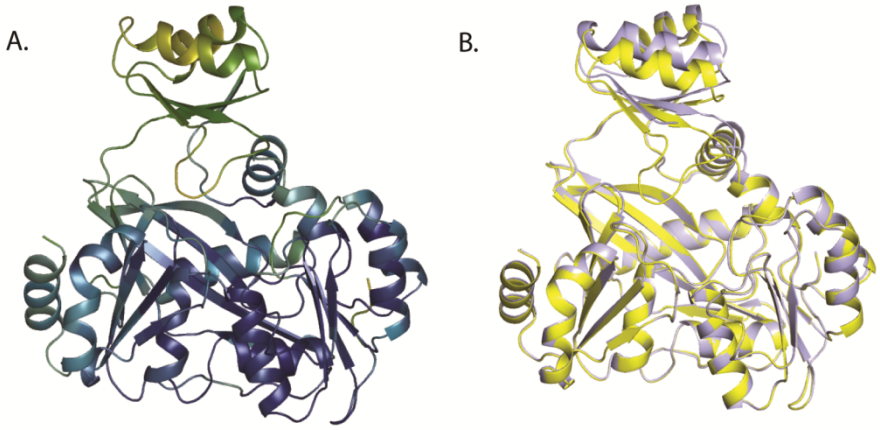


Figure 3. Sequence alignment of *S. aureus* PurK with *E. coli* PurK

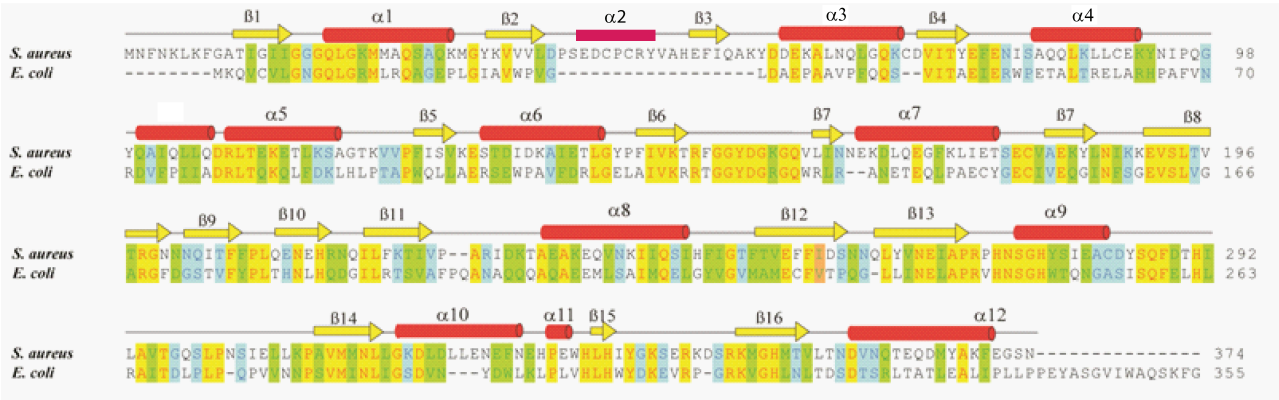


Figure 4. Sequence alignment of *S. aureus* PurE with human PurE.

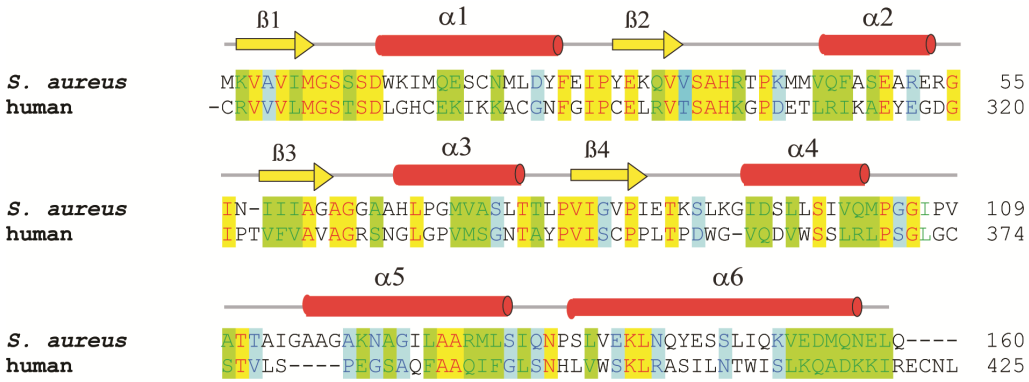


Figure 5. Overlay of *S. aureus* PurE (orange) and human bifunctional enzyme PurC-PurE (PDB ID: 2H31). The PurE domain of the human enzyme is in the center and the PurC domain in the outside.