

Supplementary Materials

Crystal structure of the apo and the ADP-bound form of choline kinase from *Plasmodium falciparum*

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Contents

⌚ *Analytical Size Exclusion Chromatography protocol and results*

⌚ *Structural Superimposition between PfChoK and CKA-2 and human CKα1*

⌚ *ADP Omit map from 6YXT*

Analytical Size Exclusion Chromatography

Materials and Methods

The analytical size exclusion chromatography was performed on a Superdex 200 Increase 10/300 GL (GE Healthcare) using as buffer 20 mM Tris HCl pH 7.5, 150 mM NaCl and as analytes three different concentrations of PfChoK (2, 1 and 0.5 mg/mL) and as markers of known molecular weight human Albumin (66 kDa) and eGFP (26 kDa) at the concentration of 1 mg/mL. 500 µL was chosen as analyte volume, the flow rate was set at 0.5 mL/min and the protein elution was followed by monitoring the absorbance at 280 nm. Results of the different runs are shown below in FigS1.

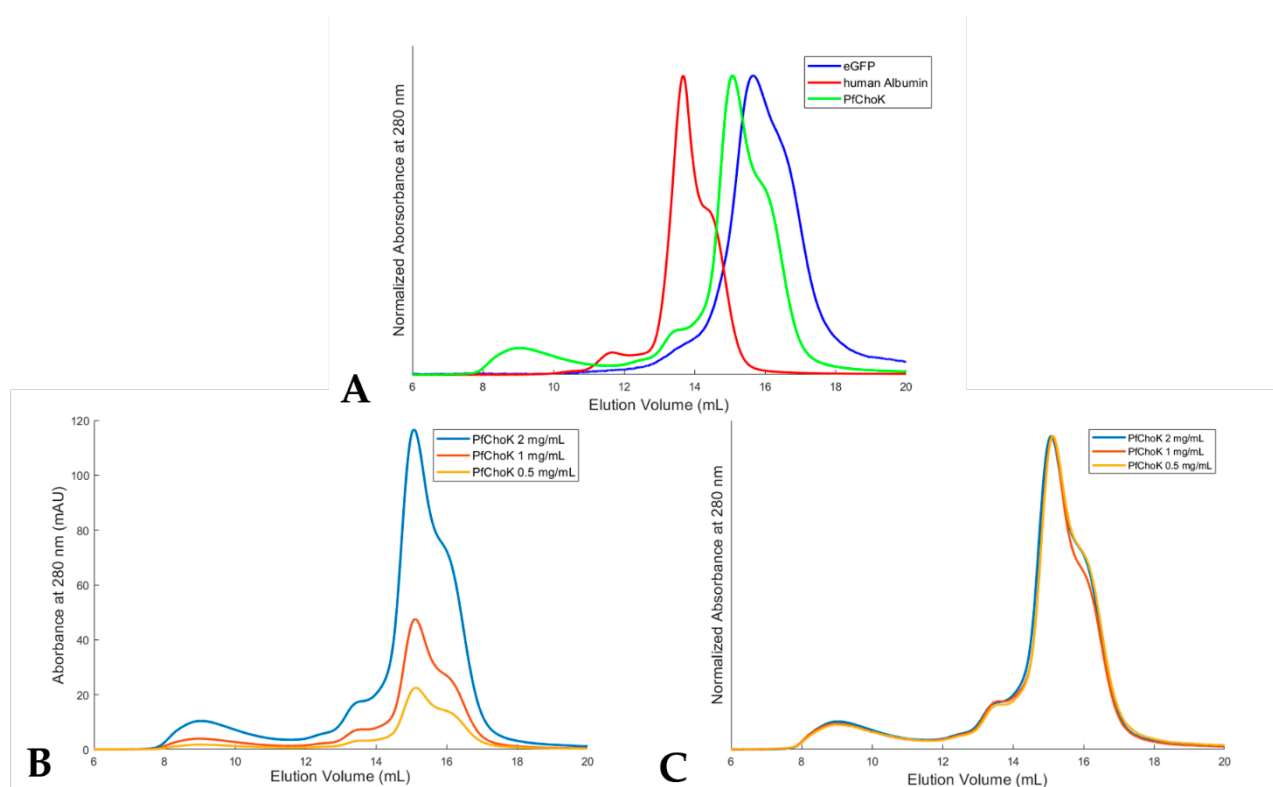


Fig S1. (A) Chromatograms of the normalized absorbance as a function of the elution volume of eGFP (blue line), human Albumin (red line) and PfChoK at the concentration of 2 mg/mL (green line) showing that the main PfChoK peak falls between the peaks of the two markers and therefore can be related to the molecular mass of the monomeric state (45 kDa). (B) Chromatograms of the PfChoK absorbance as a function of the elution volume at the three chosen concentrations (2 mg/mL as a blue line, 1 mg/mL as a red line and 0.5 mg/mL as an orange line) shows that the chromatogram morphology is the same regardless of the enzyme concentration. (C) Chromatograms of the normalized absorbance as a function of the elution volume at the three chosen concentrations (2 mg/mL as a blue line, 1 mg/mL as a red line and 0.5 mg/mL as an orange line) show that the relative height of the peaks remain the same at all the concentrations.



Fig S2. Cartoon diagram of the structural superimposition between PfChoK (green) (PDB code: 6YXS), CKA-2 (red) (PDB code: 1NW1) and human ChoK α 1 (PDB code: 2CKO).

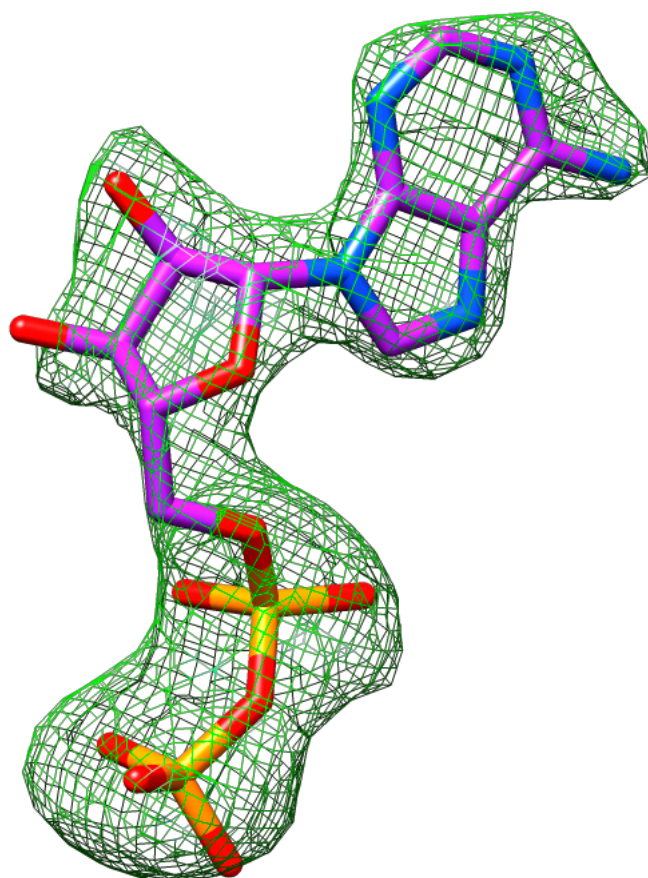


Figure 3. Omit map of the ADP molecule in the ADP-bound structure (6YXT). Electron density is shown as a green mesh contoured at the 4.0σ level. .