

The Refinement of the Yeast Phosphofructokinase-1 Atomic Model

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6-Phosphofructo-1-kinase (Pfk), a key enzyme in glycolysis, is a heterooctamer ($\alpha_4\beta_4$) of about 800 kDa (21S). The crystal structure of the limited proteolysis product (600 kDa, 12S Pfk) was determined to 2.9 Å resolution. The total number of atoms of the Pfk model exceeds 44,000 and subsequently the number of parameters to be refined is four times as many. Owing to the low data to parameter ratio at this resolution (172,763 unique reflections have been obtained) the refinement has been carried out under tight restraints and with careful monitoring of the R/R_{free} ratio. The bulk of the molecule has clear electron density.

Fructose-6-phosphate was present in the crystallization medium. The electron density clearly shows the mode of binding of the ligand in the active site and in the binding site of the allosteric effector: fructose-2,6-bisphosphate, unique to eukaryotic Pfk. The Pfk molecule appears to be in the allosteric R-state.

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