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The Structure of the Yeast F_1 -ATPase at 2.8 Å Resolution. Venkatarman Kabaleeswaran¹, David M. Mueller¹, Neeti Puri¹, Cassandra Terry², Andrew G.W. Leslie³, John E. Walker², ¹Dept. Biochem. Molec. Biol., The Chicago Medical School, Rosalind Franklin Univ. of Medicine and Science, USA, ²MRC Dunn Human Nutrition Unit, Cambridge, UK, ³MRC Laboratory of Molecular Biology, Cambridge, UK.

The crystal structure of Yeast F_1 -ATPase has been obtained at 2.8 Å resolution. The enzyme was crystallized in presence of AMP-PNP, ADP, and Mg^{2+} , which gave crystals in space group P21 ($a=111.6$ Å $b=294.2$ Å $c=190.4$ Å and $\beta=101.6^\circ$). There are 3 F_1 molecules (>9,000 residues) in the asymmetric unit and 6 molecules in the unit cell. Thus, the crystal packing in these crystals is quite different from that of bovine F_1 . The structure was solved by molecular replacement using the structure of the bovine F_1 without the nucleotides (and missing much of the γ - and all of the δ - and ϵ - subunits) and the model has been refined to an Rfree of 24.2% and Rfactor of 20.0%. The 2Fo-Fc density map clearly shows the presence of 5 bound nucleotides per F_1 , with a nucleotide bound to three noncatalytic and to two catalytic sites with the remaining catalytic site (β_E) devoid of nucleotide. The conformations of the active sites are nearly identical to those of the bovine enzyme including the conformation of the β_E subunit. In addition to the nucleotides, the 2Fo-Fc map shows density for most of the γ -, δ -, and ϵ - subunits. It is clear that the structure of the yeast enzyme supports all of the major conclusions made from the structure of the bovine F_1 -ATPase. This is the first high-resolution structure of a non-bovine F_1 -ATPase, which shows the asymmetric features first observed in the bovine enzyme.

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