

Crystal structure of the Zn/Co containing Adenylate Kinase from *D. gigas*., José Trincão,* Sergey Bursakov, José J.G. Moura, Isabel Moura and Maria João Romão, *REQUIMTE/CQFB, Departamento de Química, FCT, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal, Portugal.* E-mail: trincao@dq.fct.unl.pt

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Adenylate kinase (AK) mediates the reversible transfer of phosphate groups from ATP to AMP. It contributes to the maintenance of a constant cellular level of ADP, necessary for energetic metabolism and nucleic acid synthesis. In contrast to the AK from Gram-negative bacteria, which requires only the presence of Mg^{2+} ion for this reaction, the enzyme from Gram-positive organisms also harbours a Zn^{2+} (or Co^{2+}) ion, believed to have a structural role. AK from *D. gigas* is a monomer in solution and has a molecular mass of 24.7 kDa^[1]. Due to difficulties in obtaining a MR solution using models of AK from other organisms, the structure of AK from *D. gigas* was solved by MAD using the bound Zn as the anomalous scatterer. A single crystal was used to collect data to 2.1 Å at the Zn peak, at the edge and at a remote wavelength. The crystal belongs to space group I222, with unit cell **a** = 39.6 Å, **b** = 119.8 Å and **c** = 150 Å. The structure was refined to a final R factor of 19.9 % (R_{free} = 23.4 %). It shows a single molecule in the asymmetric unit. The crystal structure was used to confirm, correct and complete the available partial sequence of the AK from *D. gigas*.

Structural data will also be obtained for the Co-containing AK, as well as for complexes of the enzyme with substrate-analogues, which will help to gather a better understanding of the structural and catalytic properties of this class of adenylate kinases.

[1] Gavel, O.Y., Bursakov, S.A., Pina, D.G., Zhaden, G.G., Moura, J.J.G., Moura, I., Shnyrov, V.L. (2004) *Bioph. Chem.*, in press.