Crystal Structure of The Ternary Complex of *E. coli* ADP-ribose pyrophosphatase, an ADP-ribose Analog and Magnesium: A Step Towards Its Mechanism.

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Beamline(s): X25

**Introduction:** *E. coli* ADPR-ase, a housecleaning Nudix enzyme, catalyses the hydrolysis of ADP-ribose to AMP and ribose-5-P.

**Methods and Materials:** The ternary complex of ADPR-ase with the non hydrolyzable α,β-methylene ADP-ribose analog, AMPCPR, and Mg^{2+} was determined with data to 2.0Å resolution collected on a CCD detector (Brandeis B4) at Beamline X25 at NSLS, Brookhaven National Laboratory. Diffraction data, processed with Denzo and Scalepack, have an R_{sym} of 11%. The model was refined using the CNS suite with a residual target to R_{crys}=19% (R_{free}=24%).

**Results:** The structure of the ternary complex of ADPR-ase with the non hydrolysable AMPCPR and Mg^{2+} shows that the attacking water molecule is activated by bridging two Magnesium atoms with a glutamate functioning as the catalytic base. The oxygen of the attacking water is in molecular contact (3.0Å) with the phosphorous of the adenosyl phosphate forming an angle of 177° with the scicile bond. These observations suggest that the reaction occurs via an associative mechanism.

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**References:**