X-ray Structure Determination of Hydroxyphenylpyruvate Reductase at 1.47 Å Resolution

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Hydroxyphenylpyruvate reductase (HPPR) is involved in the biosynthesis of rosmarinic acid in plants. HPPR was identified, purified and cloned from suspension cultures of *Coleus blumei* [1] and subsequently expressed from E. *coli* and purified for crystallization. HPPR belongs to the family of D-isomer specific 2-hydroxyacid dehydrogenases and catalyzes the NAD(P)H dependent reduction of hydroxyphenylpyruvates to the corresponding lactates. HPPR shows only low sequence identity of about 30 % compared to other proteins from this enzyme family.

Suitable crystals of HPPR for X-ray diffraction were obtained from 30% MPD, 0.2 M NaCl, pH 7.5 and diffracted to 1.47 Å resolution at the Bessy synchrotron. The structure was determined by exhaustive molecular replacement methods. A potential solution obtained with the program PHASER resulted in reasonable electron density for 30% of the molecule. Iterative cycles of automated model building with ARP/wARP resulted in a virtually complete model. The obtained protein structure shows a high structural similarity to other oxidoreductases.

[1] Kim K.H., Janiak V., Petersen M., *Plant Mol. Biol.*, 2004, **54**, 311-323. Keywords: hydroxyphenylpyruvate reductase, biosynthesis, protein structure determination