A New Crystal Form of Ribonucleotide Reductase R2 from *Escherichia coli*

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Ribonucleotide reductase (RNR) catalyzes the reduction of ribonucleotides to the corresponding deoxyribonucleotides using a radical reaction mechanism. This reaction is essential for DNA replication and repair in all organisms. Class I RNRs consist of two homodimeric subunits, R1 and R2. R1 contains the substrate and allosteric effector binding sites and R2 houses a dinuclear iron center, which generates a catalytically essential tyrosine radical. Crystal structures of RNR R2 from several organisms have provided a wealth of information on the protein fold and on details of the active site spurring numerous inorganic modeling approaches and theoretical calculations addressing the reaction mechanism. Do protein X-ray crystal structures reveal a model that is close to the physiological situation of a soluble protein? Here, a new crystal form providing a new, independent view on the structure of the same protein is of value. The benefits of a new crystal form include a reduction of model bias due to crystal packing effects and restrictions due to particular crystal growing conditions. Maybe new electron density for amino acid residues unordered in the previous crystal form can be discovered. In case of RNR R2, the conformation of the active site was found to be dependent on the method used to generate the diferrous state in the crystal[1]. An alternative crystal form could help to clarify the preferred conformation of the active site.

A new crystallization condition for RNR R2 from *E. coli* has been identified. This condition is based on ammonium sulfate instead of polyethylene glycol as the main precipitating agent. Large crystals with dimensions of 0.5 x 0.5 x 1 mm can be obtained. The space group is $P6_1$ with unit cell dimensions of $a = b = 93$ Å, $c = 200$ Å. Using synchrotron radiation the resolution limit is currently 2.3 Å. A molecular replacement solution was obtained and carefully examined with simulated annealing omit maps.

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[1] Voegtli W.C., Sommerhalter M., Saleh L., Baldwin J., Bollinger J.M.Jr., Rosenzweig A.C., *J. Am. Chem. Soc.*, **2003**, 125(51), 15822-15830.