SAXS-WAXS STUDIES OF THE LOW RESOLUTION STRUCTURE IN SOLUTION OF GLUCOSE ISOMERASE FROM STREPTOMYCES RUBIGINOSUS

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Glucose isomerase (D-xylose ketol-isomerase; EC. 5.3.1.5) is an enzyme catalysing the reaction of isomerisation of D-glucose to D-fructose. The protein molecule (MW = 172 kDa) is a homotetramer built of four identical subunits [1,2]. Each monomer consists of two domains of which the larger contains the (α/β) 8 motif of the TIM barrel type. The crystal structure of glucose isomerase has been determined by X-ray diffraction techniques to a high resolution (0.099 nm) [PDB code: 1MNZ].

The structure and conformation of isomerase molecule in solution (at pH 6 and 7.6; with and without of substrate) has been studied by small and wide angle scattering of synchrotron radiation (SAXS-WAXS). Solution scattering measurements were performed on the EMBL X33 at DESY, Hamburg (Germany). A linear gas proportional detector with delay line readout has been used. Camera length, *i.e.*, sample-to-detector distance, was 2.2 m, corresponding to the scattering vector range: $0.12 < s < 9.8 \text{ nm}^{-1}$ ($s = 4\pi \sin\theta / \lambda$ with 2θ the scattering angle and the X-ray wavelength, 0.15 nm).

On the basis of SAXS-WAXS data, the lowresolution structure in solution has been reconstructed using *ab inito* methods and programs DAMMIN [3] and GASBOR [4]. A comparison of the models of glucose isomerase shows only insignificant differences between the model in solution and the crystal structure.

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