s7'.m2.o5 **SAXS and shape determination studies of *Escherichia coli* L-asparaginase II in solution.** M. Kozak, D. Svergun*, M. Malfois*, M.H.J. Koch*, S. Jurga, *Department of Macromolecular Physics, A. Mickiewicz University, Umultowska 85, 61-614 Poznan, Poland, *EMBL-Outstation, Notkestrasse 85, 22603 Hamburg, Germany*
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Asparaginases are hydrolytic enzymes that hydrolyse the amide bond in L-asparagine converting it to L-aspartic acid and ammonia. Type II asparaginases from *Escherichia coli* (EcAII) and *Erwinia chrysanthemi* (ErA) are successful drugs in the treatment of leukemia. The crystal structure of EcAII were determined at 2.3 A resolution[1]. The active form of the enzyme is a homotetramer with nearly ideal 222 symmetry. The identical subunits (in EcAII 326 amino acids each) composing the tetramer are denoted A, B, C, D. The active site is created by subunits A and C (or B and D). Here we report a SAXS study of the global conformation of EcAII in solution.

The synchrotron radiation small angle X-ray scattering data were recorded using a position sensitive delay line readout detector. The experimental data collected at lower concentrations (6 and 9 mg/ml) were merged with the data at higher concentration (21 mg/ml) to obtain the final scattering curve. The theoretical scattering curve for EcAII was evaluated from the crystal structure (PDB entry: 3ECA) and fitted to the experimental scattering data by the program CRYSOL[2]. The shape of the molecule in solution was determined using the program DAMMIN[3] and rigid-body modeling was done with the graphical package ASSA[4].

The scattering curve from the native EcAII was compared to that evaluated from the crystal structure. The best fit was obtained for an excluded volume V=174 nm^3 and radii of gyration of 3.37 nm and 3.03 nm for the experimental and crystallographic data respectively. The agreement between the theoretical and scattering curves is quite reasonable (?= 2.48). Comparison of the P(r) functions calculated for the crystal structure and solution scattering data suggests that the overall quaternary tetrameric structure in the crystal and in solution are similar but that the enzyme is less compact in solution than in the crystal. In the poster we also report the results of shape determination and rigid body modeling studies.

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