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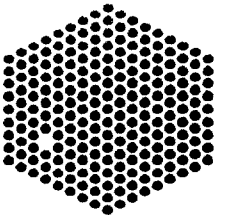

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Structure of native chaperone GroEL in solution

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GroEL [1] is a very large protein complex of 800,000 mass, which is a essential cell component localized in the cytoplasm of many organisms, e.g. *Escherichia coli*. It is a homolgoue of the HSP70 of higher organisms, e.g. man. GroEL and its homologs have the function of folding or modifying the fold of other proteins, whether they have been demaged during the life of the cell or after protein biosynthesis or modification.

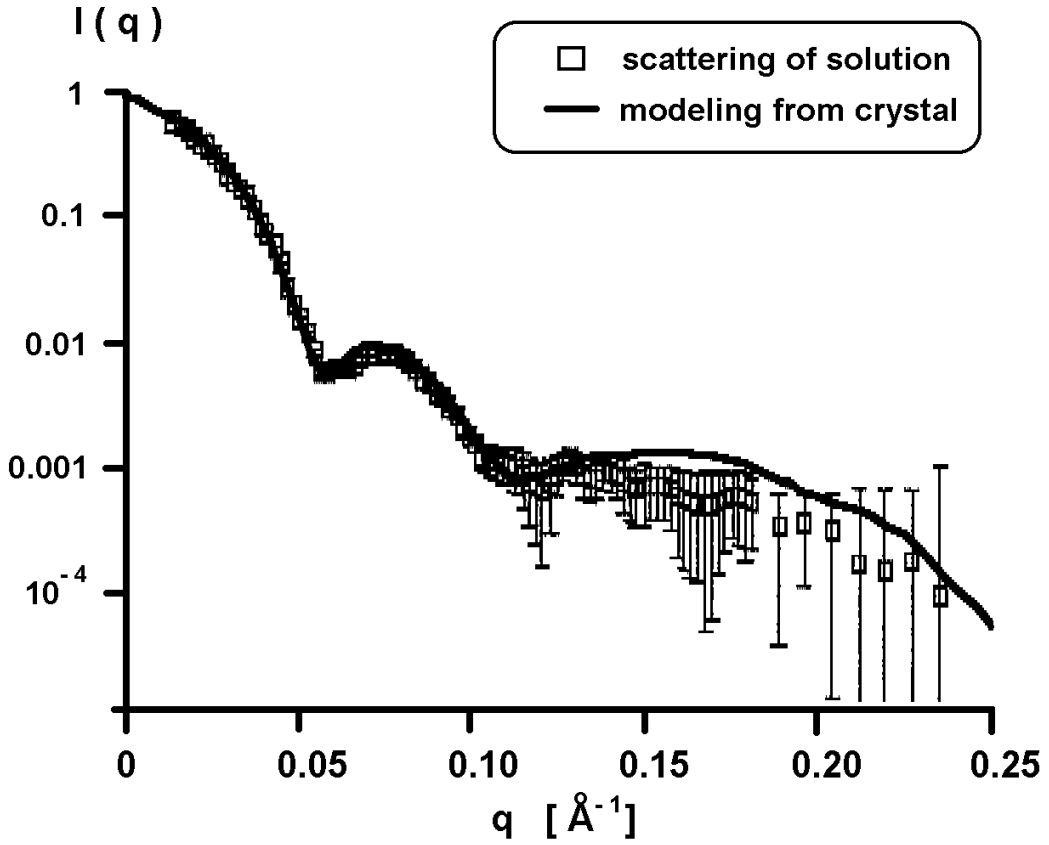
GroEL is a homo-oligomer of 2 x 7 identical subunits, which form a pair of hollow cylinders associated end by end. During folding catalysis the substrate protein is included in the GroEL cylinder after ATP hydrolsis, while a further protein named GroES covers the assembly as a lid (70,000 mass). The structure of resting GroEL is known from X-ray crystallography, whereas the structure of the native complex in solution and the reaction mechanism, which is suggested to be accompanied by large transient structural changes, is unknown.

We have investigated the structure of purified GroEL and GroEL-GroES complex from *Escherichia coli* in aqueous solution by X-ray small angle scattering at the JUSIFA camera at the beamline B1 at DESY / HASYLAB, Hamburg. The solution was irradiated at 4°C in a quartz flow-through capillary using a 0.9 x 1.1 mm^2 beam of 8 keV (1.5 Å) photons. Scattering profiles of protein solution (10 g/l) and buffer were taken at 0.9 and 3.6 m distance from the sample using a 2D-detector (256 x 256 pixel) in 3 h for each specimen.

The X-ray scattering of a GroEL solution consists of a central signal and a series of sharp side maxima (fig.). The profile is characteristic for the hollow protein cylinder, which is assembled by a highly symmetrical complex of identical subunits. Thus the position and intensity of the side maxima allows the comparison of GroEL in solution and after crystallization by modelling and the detection of structural dynamics after binding of GroES and substrates.

In the figure the experimental scattering of the native protein in aqueous solution is compared with the modelled scattering profile from the structure of crystallized GroEL. The comparison shows that: i) the over all structure (size, expansion) of the chaperone is very similar in solution and after crystallization, whereas ii) the subunit organization of GroEL appears to be different, which is indicated by the shifts in the position of the side maxima 2 to n. The modelled scattering curve of crystallized GroEL shows a minimum at the position of the third side maximum (q_S = 1.1 nm^{-1}) of the protein solution. The strongest (second) side maximum is shifted from q_S = 0.7 to 0.75 nm^{-1}, which corresponds to a decrease of the average subunit spacing from d_S = 9.0 to 8.4 nm according to Bragg's law ($d_S = 2\pi / q_S$).

1) Hartl, F.U. (1996) Nature 381, 571-580



The experimental X-ray small angle scattering of the chaperone GroEL from *Escherichia coli* in aqueous solution (10 g/l) fits the modelled profile of crystallyzed protein in the central signal, whereas the side maxima 2 to n are shifted in position. This indicates subunit displacements in the complex.