

## Resolution and validation of SAS-based structural models

The possibility to reconstruct *ab initio* three-dimensional structures from one-dimensional small-angle-scattering (SAS) profiles of particles in solutions was a major breakthrough in the scattering techniques nearly two decades ago, and since then SAS has become a standard method for structural studies of macromolecules and their complexes. However, the models generated from SAS data are still reported without quantifying their resolution. This situation contrasts with other structural methods such as X-ray crystallography and electron microscopy. The lack of an objective quality measure for SAS-derived models has limited their validation and further use. We have recently developed a method for resolution assessment of *ab initio* SAS models based on the average variability within a structural ensemble (Tuukkanen *et al.* 2016, *IUCrJ* 3, 440). Here, we shall demonstrate the practical use of the novel measure and discuss the approaches for the validation of SAS-based *ab initio* and hybrid rigid body models. We expect the presented developments to have a significant impact on the archiving of SAS models and on their further use with other structural biology information.

Anne Tuukkanen  
Gerard J. Kleywegt  
Dmitri Svergun

Germany  
United Kingdom  
Germany

EMBL-Hamburg / EMBL-EBI  
European Bioinformatics Institute  
EMBL Hamburg