the USAXS images, and offer a complementary view of the small-angle X-ray scattering contrast mechanism. The ray-tracing analysis indicates that refraction, in the form of Porod scattering, and, to a much lesser extent, X-ray reflection, fully account for USAXS imaging contrast.

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Analysis of solution small-angle scattering using the program package ATSAS

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Small-angle scattering (SAS) of X-rays and neutrons is a universal technique serving as a nanometer structure probe for a wide variety of non-crystalline objects (e.g. solutions of biological macromolecules, nanocomposites, alloys, synthetic polymers etc). The program package ATSAS [1] implements advanced methods for the data analysis from isotropic systems, developed for but not limited to, biological mactomolecules in solution The package allows one to perform major analysis steps of the scattering data from data reduction to automated three-dimensional (3D) modelling. With the present ATSAS 2.2 version it is possible:
to compute overall structural parameters and characteristic functions;
to reconstruct ab initio 3D low resolution shapes;
to calculate the scattering profiles from atomic models of macromolecular structures;
to perform rigid body modelling of macromolecular complexes;
to jointly employ X-ray and contrast variation neutron scattering data;
to quantitatively analyze interacting and flexible systems and mixtures.
The use of the ATSAS package is illustrated by the recent examples of its application to study oligomeric state and conformation changes of proteins [2,3], macromolecular complexes and large assemblies [4,5].
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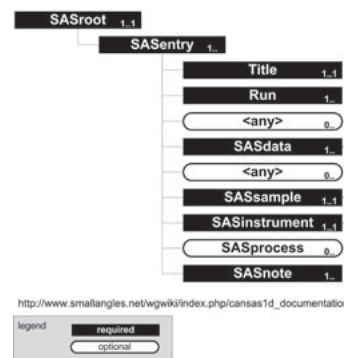
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The canSAS standard for storing reduced one-dimensional small-angle scattering data in XML files

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One of the first aims of the canSAS (Collective Action for Nomadic Small-Angle Scatterers, www.smallangles.net) forum of users and facility staff was to discuss better sharing of SAS data analysis software. CanSAS identified that a significant need within the SAS community is satisfied by standardizing a robust, self-describing, text-based format to communicate reduced one-dimensional small-angle scattering data, I(Q), between users of our facilities. Our goal has been to define such a format with minimal verbosity that leaves the data file instantly human-readable, editable in simple editors, and importable by simple text import filters in programs that need not recognise advanced structure in the file nor require advanced programming interfaces. The file should contain the primary data, I(Q), and also any other descriptive information (metadata) about the sample, measurement, instrument, processing, or analysis steps. The cansas1d/1.0 standard meets the objectives for a 1D standard, incorporating experiment metadata, and parameters and results of processing or analysis steps. Even multiple measurements may be included within a single XML (or SASXML) file.

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Software for automated high-throughput biological small-angle X-ray scattering

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Small-Angle X-ray Scattering (SAXS) is a fundamental tool in the study of proteins and macromolecular complexes. SAXS is employed for screening large numbers of samples and for studying these samples under different conditions, including space- and time-resolved analysis. These measurements produce immense amounts of data, especially on modern third-generation synchrotron radiation sources. Automation of data analysis becomes an indispensable prerequisite for adequate evaluation of high-throughput SAXS experiments. We have developed a set of tools to perform major analysis tasks automatically, starting from the raw data processing and finishing with three-dimensional modelling. Automated data analysis starts from raw data reduction including radial averaging of scattering intensities, normalization, radiation damage check, and subtraction of the background. The radius of gyration (Rg) is