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Small-angle scattering data representation in SASCIF and Integrative/hybrid methods dictionary

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Recent advances in the field of small angle scattering (SAS) have led to significant growth in the application of SAS data for structural characterization of macromolecules. Restraints derived from SAS experiments are frequently combined with data from other experimental methods to elucidate three-dimensional structures of biomolecules. Specifically, co-refinement of NMR and SAS data is found to yield accurate solution structures of a number of macromolecules. In 2013, the wwPDB SAS task force (https://www.wwpdb.org/task/sas) recommended that SAS data and models should be archived along with information required to carry out data quality assessments and model validation. Based on these recommendations, the SASCIF dictionary [1] has been developed as a compatible extension to the PDBx/mmCIF dictionary (http://mmcif.wwpdb.org/), which is the core data framework for the worldwide Protein Data Bank [2]. The establishment of common data standards have enabled the exchange of data between the wwPDB OneDep system for data deposition, validation, and annotation [3] and the SASBDB repository (https://www.sasbdb.org). Additionally, following the 2015 recommendations of the wwPDB integrative/hybrid (I/H) methods task force (https://www.wwpdb.org/task/hybrid), we have also developed an extension dictionary for I/H modeling methods, where spatial restraints derived from a variety of complementary experimental and computational techniques are combined to determine the structures of macromolecular assemblies. Restraints derived from SAS experiments play an important role in I/H modeling and are defined accordingly in the I/H methods dictionary (https://github.com/ihmwg/IHM-dictionary).

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