From John R Helliwell Chairman of the IUCr DDD WG:-

Recent articles describing the metadata for processed and / or provision of raw diffraction/scattering data for specific techniques are listed below:-

*Acta Cryst.* (2012). D**68**, 620-626    [ [doi:10.1107/S0907444912012073](http://dx.doi.org/10.1107/S0907444912012073%22%20%5Co%20%22Open%20URL%20link) ]

**Publication guidelines for structural modelling of small-angle scattering data from biomolecules in solution**

[**D. A. Jacques**](http://scripts.iucr.org/cgi-bin/citedin?search_on=name&author_name=Jacques,%20D.A.)**,** [**J. M. Guss**](http://scripts.iucr.org/cgi-bin/citedin?search_on=name&author_name=Guss,%20J.M.)**,** [**D. I. Svergun**](http://scripts.iucr.org/cgi-bin/citedin?search_on=name&author_name=Svergun,%20D.I.) **and** [**J. Trewhella**](http://scripts.iucr.org/cgi-bin/citedin?search_on=name&author_name=Trewhella,%20J.)

**Abstract:** Small-angle scattering is becoming a mainstream technique for structural molecular biology. As such, it is important to establish guidelines for publication that will ensure that there is adequate reporting of the data and its treatment so that reviewers and readers can independently assess the quality of the data and the basis for any interpretations presented. This article presents a set of preliminary guidelines that emerged after consultation with the IUCr Commission on Small-Angle Scattering and other experts in the field and discusses the rationale for their application. At the 2011 Congress of the IUCr in Madrid, the Commission on Journals agreed to adopt these preliminary guidelines for the presentation of biomolecular structures from small-angle scattering data in IUCr publications. Here, these guidelines are outlined and the reasons for standardizing the way in which small-angle scattering data are presented.

**Keywords:** [**small-angle scattering**](http://scripts.iucr.org/cgi-bin/full_search?words=small-angle%20scattering&Action=Search)**;** [**publication guidelines**](http://scripts.iucr.org/cgi-bin/full_search?words=publication%20guidelines&Action=Search)**.**

*J. Synchrotron Rad.* (2012). **19**, 869-874  [ [doi:10.1107/S0909049512036886](http://dx.doi.org/10.1107/S0909049512036886) ]

### Towards data format standardization for X-ray absorption spectroscopy

### [B. Ravel](http://scripts.iucr.org/cgi-bin/citedin?search_on=name&author_name=Ravel%2C%20B%2E), [J. R. Hester](http://scripts.iucr.org/cgi-bin/citedin?search_on=name&author_name=Hester%2C%20J%2ER%2E), [V. A. Solé](http://scripts.iucr.org/cgi-bin/citedin?search_on=name&author_name=Sol%26eacute%3B%2C%20V%2EA%2E) and [M. Newville](http://scripts.iucr.org/cgi-bin/citedin?search_on=name&author_name=Newville%2C%20M%2E)

**Synopsis:** In this first report from an *ad hoc* working group on XAS data format standardization, concepts for addressing three XAS data storage needs are presented: a single spectrum interchange format, a hierarchical format for multispectral X-ray experiment, and a relational database format for XAS data libraries.

*J. Appl. Cryst.* (2013). **46**, 108-119    [ [doi:10.1107/S0021889812044172](http://dx.doi.org/10.1107/S0021889812044172%22%20%5Co%20%22Open%20URL%20link) ]

### Experience with exchange and archiving of raw data: comparison of data from two diffractometers and four software packages on a series of lysozyme crystals

### [S. W. M. Tanley](http://scripts.iucr.org/cgi-bin/citedin?search_on=name&author_name=Tanley,%20S.W.M.), [A. M. M. Schreurs](http://scripts.iucr.org/cgi-bin/citedin?search_on=name&author_name=Schreurs,%20A.M.M.), [J. R. Helliwell](http://scripts.iucr.org/cgi-bin/citedin?search_on=name&author_name=Helliwell,%20J.R.) and [L. M. J. Kroon-Batenburg](http://scripts.iucr.org/cgi-bin/citedin?search_on=name&author_name=Kroon-Batenburg,%20L.M.J.)

**Abstract:** The International Union of Crystallography has for many years been advocating archiving of raw data to accompany structural papers. Recently, it initiated the formation of the Diffraction Data Deposition Working Group with the aim of developing standards for the representation of these data. A means of studying this issue is to submit exemplar publications with associated raw data and metadata. A recent study on the effects of dimethyl sulfoxide on the binding of cisplatin and carboplatin to histidine in 11 different lysozyme crystals from two diffractometers led to an investigation of the possible effects of the equipment and X-ray diffraction data processing software on the calculated occupancies and *B* factors of the bound Pt compounds. 35.3 Gb of data were transferred from Manchester to Utrecht to be processed with *EVAL*. A systematic comparison shows that the largest differences in the occupancies and *B* factors of the bound Pt compounds are due to the software, but the equipment also has a noticeable effect. A detailed description of and discussion on the availability of metadata is given. By making these raw diffraction data sets available *via* a local depository, it is possible for the diffraction community to make their own evaluation as they may wish.

**Keywords:** [**data exchange**](http://scripts.iucr.org/cgi-bin/full_search?words=data%20exchange&Action=Search)**;** [**data archiving**](http://scripts.iucr.org/cgi-bin/full_search?words=data%20archiving&Action=Search)**;** [**metadata**](http://scripts.iucr.org/cgi-bin/full_search?words=metadata&Action=Search)**.**

For this latter article the raw data link is:-

[http://rawdata.chem.uu.nl/](https://outlook.manchester.ac.uk/owa/redir.aspx?C=b3f8939a55f3440b81a847e7bbc3a30f&URL=http%3a%2f%2frawdata.chem.uu.nl%2f)

And the screen shot of it is :-

