

s8b.m1.o3 Global Indicators of X-ray Data Quality.

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Keywords: diffraction data quality, merging R-factor, redundancy.

The quality of X-ray data is commonly assessed by calculating a number of statistical parameters. Unfortunately, the most popular and most widely used parameter, the symmetry or merging R-factor is a very poor indicator of data quality, especially when additional information is lacking.

In recent years, this problem has been realized by us and by others^{1,2} and improved global indicators of diffraction data quality such as the redundancy-independent merging R-factor ($R_{r.i.m.}$) or the precision-indicating merging R-factor ($R_{p.i.m.}$) have been proposed. These two as well as other quality indicators will be presented and discussed.

s8b.m1.o4 Macromolecular Structure Determination by MAD and OAS. S.M. McSweeney. *EMBL Grenoble Outstation, 6 Rue Jules Horowitz, BP 156, 38042 Grenoble Cedex 9, France.*

Keywords: Synchrotron radiation, MAD, SAS

The increased use of the Multi-wavelength Anomalous Dispersion, MAD, technique greatly reduces the time required to phase and solve a macromolecular structure. By utilizing the physics of anomalous dispersion to determine protein phases the technique is well suited to the spectral characteristics of a synchrotron source, and indeed each European Synchrotron facility has at least one MAD capable beamline.

In this presentation, we review the current state of the art in terms of instrumentation and practice at Synchrotron sources. Future developments and practical limitations are discussed.

[1] M.S. Weiss and R. Hilgenfeld (1997). On the use of the merging R-factor as a quality indicator for X-ray data. *J. Appl. Crystallogr.* 30, 203-205.

[2] K. Diederichs and P.A. Karplus (1997). Improved R-factors for diffraction data analysis in macromolecular crystallography. *Nature Struct. Biol.* 4, 269-275.