

Reducing Data to $|F|$ and $\sigma(|F|)$ and Assessing Data Quality

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Intensities of X-ray reflections (I_{hkl}) are directly related to the amplitudes of structure factors $|F_{hkl}|$. During data acquisition, the intensity of each unique reflection is measured multiple times under different experimental conditions. Measured intensities are affected by multiple factors, e.g. time of the data point collection in the course of the experiment, reflections' positions at the detector's surface, the shape of the crystals, and many others systematic effects. Although symmetrically equivalent reflections should have, within experimental error, the same measured intensity, all these systematic effects modulate intensities of symmetrically equivalent reflections so that they are frequently significantly different from each other.

The process of scaling applies to each measured intensity a set of multiplicative scaling factors that correct some classes of systematic effects. The scaling is followed by the merging process, where the intensity of the symmetrically equivalent reflections are averaged and the differences between them are assessed.

The agreement between intensities of symmetrically equivalent reflections should follow the error model of a well-done experiment. Discrepancies should not only be explained by the error model, but also the estimates of error should allow for uncertainties to not be excessive. An excessive error model is likely an indicator of some other incorrect assignments, such as space group symmetry. A good assessment of the error model manifests with low $R_{\text{merge}}/R_{\text{pim}}/R_{\text{rim}}$ values in low resolution shells. However, it may happen that the applied error model was not close enough to the experimental reality and therefore the quality of scaling and merging is affected.

The best approaches to data reduction and quality assessment in various experimental situations will be discussed.