

Strategy of data collection based on statistic modelling, Alexander Popov^{a*} and Gleb Bourenkov^b,

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We present new developments in method and program BEST for optimal and automatic planning of data collection. The method is based on modelling of the statistical results of data collection taking into account characteristics of a particular crystal, X-ray equipment and time available for measurement [1]. Statistical methods are further developed for optimisation of anomalous data collection. A few initial images taken with short exposure time are required to make predictions. The set of parameters, which provide minimal data collection time or radiation dose is selected. Anisotropy in the diffraction, geometrical restrictions (e.g. spot overlapping) and already collected data are taken into account. On the basis of the resolution and I/σ ratio requested by the user, the program proposes the plan of data collection. The plan defines the total rotation range, scan speed and rotation range per frame, detector distance and the detector mode. Contrary to traditional data collection strategy, the rotation range per frame and scan speed vary with the rotation angle in a way to make the distribution of statistics over reciprocal space as uniform as possible. The program estimates the data statistics (mean intensity, mean sigma, R-merge, as a function of resolution) for the data that will be collected according to the plan. The program can also predict data statistics for any set of data collection parameters defined by the user. The software proved to be extremely useful in using the available data collection time in the most efficient way. The methods are directly applicable for ranking the crystals. Applications for automatic selection of the best quality crystal will be discussed.

[1] Popov, A.N. & Bourenkov, G.P. (2003). *Acta Cryst.* D59, 1145-1153.