Raw Diffraction Data Are Our Ground Truth from Which All Subsequent Workflows Develop

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Defining best practice in science is challenging. International consensus is facilitated by the International Science Council via its members like the International Union of Crystallography. The crystallographic community has many decades of tradition linking article with underpinning data, and is admired across all sciences accordingly. Crystallography is always at the forefront of harnessing new technologies. One such are the new vast data archiving opportunities allowing us to publish those raw diffraction data underpinning an article as well as the usual database depositions of a model's coordinates and associated structure factors. The raw diffraction data are our ground truth from which all subsequent workflows develop. Journal editorial boards are a practical forum for setting the criteria to decide if a study's files are truly the "version of record". Within that reality involves a variance of reasonable workflows. Workflows must be detailed carefully by authors in explaining what they have done.