Advances in automated data analysis and processing within autoPROC, combined with improved characterisation, mitigation and visualisation of the anisotropy of diffraction limits using STARANISO.

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Current trends towards ever higher levels of automation require not only improvements in the efficiency and speed of data processing programs and pipelines, but also new and improved approaches to data analysis and to the visual presentation of its results. This is not just a matter of producing ever more "pretty pictures", but of helping automated processes - as well as ordinary users - make use of the most appropriate quality metrics in evaluating experimental protocols and in designing optimal experiments for given instrument capabilities and crystal characteristics. In the context of serial crystallography this provides improved diagnostics and criteria for guiding the handling of individual datasets and producing optimal groupings among them.

Well designed visualisation tools are essential in enabling the rapid assessment of the characteristics and quality of conventional (single crystal/sweep) datasets, as well as of combinations of partial datasets originating from multi-sweep and/or multi-crystal datasets and/or serial experiments. The proper perception of the relationships between partial datasets, or different image ranges of a single dataset, and of the manner in which combinations of them succeed or not in filling 3D reciprocal space, requires a full 3D visualisation of local geometric properties such as redundancy and of statistical properties such as local averages of I/sig(I). To that end we have developed the STARANISO program [1] for analysing and mitigating anisotropy in diffraction data. This capability is available both via autoPROC [2] (our package for automated data processing and analysis) and the public STARANISO webserver [3] (processing, analysis and visualisation of user-provided datasets, either as merged or unmerged intensity data). A recent additional capability has been provided by the "PDBpeep" server, allowing, with extreme simplicity, the analysis and 3D visual examination of diffraction datasets deposited with PDB entries [4].

[1] Tickle, I.J. et al (2016). STARANISO. Global Phasing Ltd., Cambridge, UK.
[2] Vonrhein, C. et al (2011). Data processing and analysis with the autoPROC toolbox. Acta Cryst. D67, 293-302.
[3] http://staraniso.globalphasing.org/
[4] http://staraniso.globalphasing.org/cgi-bin/PDBpeep.cgi