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Absorption Correction and Optimal Planning of Data Collection Based on a 3D Sample Model.
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A reconstruction using visual images has been used to produce a 3D model of a macromolecular crystal sample, with the crystal, supporting loop and buffer identified as separate components. The model allows path lengths through crystal, solvent and crystal mount system to be determined, as well as the calculation of the diffraction volume.
A software package, named 3DAC, was developed for building a 3D model of a macromolecular crystal, and treating X-ray diffraction data for absorption effects using the sample shape information [1]. The method offers an effective absorption correction. At lower levels of data redundancy, the algorithm provided a clear advantage, illustrating that it may be of considerable value in situations where data acquisition is limited by crystal lifetime.
The previously published work is now gradually being improved towards the automation and general use: the absorption correction work is being taken forward with a systematic study of several crystal systems and more precise measurements and descriptions of the beam profile; the software package producing the 3D model is also being enriched with a new user interface. In difficult cases (e.g. when the crystal is not fully visible), the user can now fit a polyhedron to the crystal sample.
The 3D model is also being applied to data collection strategies using the BEST software [2][3] by allowing the crystal cross-section to be included in the strategy calculations.
The methods described here are of general interest, particularly for long wavelength X-ray work and very sensitive crystal samples.

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Keywords: 3D modeling; absorption correction; data collection strategy

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Recent Advances in CRANK.
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CRANK is a software suite for automatic macromolecular structure solution. The first release of CRANK was shown to effectively detect and phase anomalous scatterers from SAD data [1]. The current release can successfully build over 200 real SAD, SIRAS, MAD and MAD+native data sets. Improvements in the latest version of CRANK have sped-up and increased the robustness of the automatic structure solution process. As of CRANK version 1.3.x the quality and completeness of an obtained substructure are validated using the Luzzati parameters refined in the program BP3. This approach allows for early termination of the substructure detection stage in a common situation where the figure of merit alone is insufficient to safely decide whether a correct solution has been reached. Furthermore, algorithmic improvements in BP3 have led to about a three-fold speed improvement in substructure refinement and phasing. Additionally, automatic model building has been improved by using SAD data directly in model refinement, made possible by the new interface for ARP/wARP and REFMAC. A modified version of REFMAC, implementing a multivariate SAD likelihood function, extends resolution and phase quality limits required for automatic model building with iterative refinement [2]. In combination with the SHELX[C/D/E] pipeline, this approach has recently been found to be very effective. The addition of Baubles markup has made CRANK log files more insightful and user friendly. These and other improvements are in the latest version of CRANK, packaged with CCP4 6.1.2 and freely available from http://www.bfsc.leidenuniv.nl/software/crank.

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Using Molrep for Fragment-based Electron Density Interpretation at Low Resolution
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Despite the technological advances in X-ray crystallography and electron microscopy, the electron density of large macromolecular complexes is often available to low resolution and is difficult to interpret by conventional methods. Fortunately, a complex often already contains known structural components, which can be further divided into rigid fragments [1,2]. To efficiently position a fragment in an experimentally phased density map at low resolution requires density fitting in real space. Such real space molecular replacement should have a minimal signal interference from the vast "missing part" of the target structure, tolerate reasonable errors in homology models and experimental phases, and be able to find multiple copies of the similar modular domain present in the target