structure even in the absence of molecular symmetry. Here we evaluate the effectiveness of spherical averaged density matching as implemented in Molrep [3] in comparison to conventional molecular replacement methods in positioning a small domain in the electron density map of a multi-domain protein. We investigate how resolution, phase error and model error would influence the quality of density fitting.

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Keywords: low resolution crystallography; electron density fitting; algorithms

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Coordinate Variations in Structural Ensembles from Different Refinement Methods. Jacopo Negroni[a], Roberto Mosca[a], Thomas R. Schneider[a]. [a]*EMBL, Hamburg, Germany.*
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It is questionable whether a single model is an appropriate representation of the situation observed in a crystal of a biological macromolecule. In recent years, several authors have suggested procedures to produce ensembles of models that possibly yield a better description of the variability observed in a crystal [1,2].
In principle, the spread observed for a particular atomic position in an ensemble obtained by a particular method can provide a measure of the *precision* of the position. It may be possible to obtain a first-order approximation of the *accuracy* of an atomic position by comparing several ensembles obtained using different refinement methods. Accurate estimates of the accuracy of atomic coordinates would in fact be very useful as these could then be taken into account in structure analysis.
To compare the coordinate variability between different models produced by the same refinement method ('ensemble') and between models produced by different refinement methods, we have created a series of ensembles and single models for the tetragonal crystal form of Lysozyme.
We found that, within ensembles created by one method the coordinate variability is rather small, while between ensembles or models created by different methods, larger differences can be observed.

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Keywords: structure analysis; coordinate error estimation; precision

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Advancement of the Main Chain Tracing in ARP/wARP. Helene Dörksen[a], Victor S. Lamzin[b]. [a,b]*EMBL-Hamburg, Germany.*
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Comprehensive structural interpretation of the crystallographic experimental X-ray data, having both observed structure factor amplitudes and phase estimates, remains one of the most challenging tasks in the protein crystallography. Our on-going development is addressed to the problem of performing accuracy and completeness of the protein structure provided by the protein chain tracing module of ARP/wARP software. The success of the model building strongly depends on the level of the informational content of the data, where a low level is indicated by noisy structure factors leading to a hardly interpretable electron density map or by the data, whose resolution is limited. We combine several methods including weighted template matching technique and optimisation of the density template alignment. We apply a number of rotation invariant characteristics defined on the density values and centre-atomic distances. This leads to the completeness of the model that is growing from iteration to iteration. We also introduce a resolution dependent parameter, which further increase the completeness of the provided structure. Overall the improvement of the built main chain by 12-25% is achieved compared to the protein chain tracing in earlier ARP/wARP version 7.0.

Keywords: software development; density modification; model building

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Intensity to Amplitude Conversion Using Ctruncate. Norman Stein[a], Charles Ballard[a]. [a]*CCP4, Daresbury Laboratory, Warrington, WA4 4AD, UK.*
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In protein crystallography, calculation of structure factor amplitudes from intensity measurements is complicated by the fact that some weak reflections will have negative intensities, due to the background subtraction process. Ctruncate is a new CCP4 program, ultimately intended to replace the original Truncate program, which uses Bayesian statistics to calculate positive structure factors from negative input intensities, using the French and Wilson algorithm. Ctruncate detects significant anisotropy in the data and performs anisotropy correction. The corrected data is used to calculate a number of data quality indicators, such as moments of intensity and cumulative intensity distributions. Potential twinning operators are calculated from first principles, thus allowing detection of cases of pseudomerohedral twinning which might otherwise be missed. A number of quantitative tests for twinning such as the H test and the L test have been introduced. Ctruncate also checks for the presence of translational Non Crystallographic Symmetry (tNCS) using a Patterson function. The optical resolution is used to give a guide to the limiting resolution of the data. The prior distribution used in Ctruncate is the Wilson distribution, which is only really appropriate in the absence of twinning and tNCS. It is hoped to extend this work to give a quantitative treatment of the modifications to the Wilson distribution induced by these effects.

Keywords: software; protein structure determination; twinning