MS22.O06

Coping with translational non-crystallographic symmetry in molecular replacement

R. Read[1], P. Adams[2], A. McCoy[1]

[1]University of Cambridge, Department of Haematology, Cambridge, UK, [2]Lawrence Berkeley National Laboratory, Berkeley, CA, USA

In translational noncrystallographic symmetry (tNCS), two or more copies of a component are present in a similar orientation in the asymmetric unit of the crystal. This causes systematic modulations of the intensities in the diffraction pattern, leading to problems with methods that assume, either implicitly or explicitly, that the distribution of intensities is a function only of resolution. To characterize the statistical effects of tNCS accurately, it is necessary to determine the translation relating the copies, any small rotational differences in their orientations, and the size of random coordinate differences caused by conformational differences. An algorithm has been developed to estimate these parameters and refine their values against a likelihood function. By accounting for the statistical effects of tNCS, it is possible to unmask the competing statistical effects of twinning and tNCS and to more robustly assess the crystal for the presence of twinning. Modified likelihood functions that account for the statistical effects of tNCS have been developed for use in molecular replacement and implemented in Phaser. With the use of these new targets, it is now possible to solve structures that eluded earlier versions of the program. Pseudosymmetry and space group ambiguities often accompany tNCS, but the new version of Phaser is less likely to fall into the traps that these set.

Keywords: translational non-crystallographic symmetry, molecular replacement, intensity statistics