Validation of the Molecular Replacement Solutions with the OMIT Procedure

Yanina Vekhter, John H. Konnert, *Laboratory for the Structure of Matter, Naval Research Laboratory, Washington, DC 20375-5000, USA*. E-mail: vekhter@ccs.nrl.navy.mil

In the method of molecular replacement, the phases for the initial map of the unknown structure are computed by rotating and translating a trial molecular entity to estimate it's location and orientation within the unit cell of the unknown structure.

The usefulness of this initial map is determined by the molecular entity actually being present in the unknown structure, by the fraction of the unknown that this entity represents, and by accuracy with which it is positioned within the cell. With the omit validation procedure a small fraction of the trial model is deleted before the translation-rotation search. The validity and usefulness of the search resalts are judged by quantitatively evaluating the region of the molecular-replacement map corresponding to the omitted entity. This procedure was found to be useful when evaluating the structure of the maltose binding protein that was thought to have a Ru(II) group bound to it. The validation procedure indicated that the Ru(II) group was not bound to the maltose binding protein molecule in an ordered fashion.

Keywords: molecular replacement, model building, ligand