CURRENT DEVELOPMENT IN THE PROGRAM PACKAGE FROG FOR ATOMIC MODEL REFINEMENT

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After several years of being used only by the authors, the refinement package FROG (Urzhumtsev et al., 1989) has become a useful tool in other laboratories, in particular, in the UPR de Biologie Structurale, Strasbourg. Such features as simplicity, high speed and high convergence attracted the users attention. The same source files were easily compiled at different types of systems and computers, including different IBM-360/370, IBM PC, VAX- and UNIX-machines. This package is successfully used for cases of rigid-body or rigid groups refinement, e.g. for solutions of molecular replacement. In particular, for the case of $tRNA^{Asp}$ synthetase from *Th.thermophilus* FROG could refine a rigid-body model to its correct position, while an attempt using X-PLOR (Brünger et al., 1987) failed to do it (G.Webster, personal communication). The correctness of the solution was proven later by successful conventional refinement of the resulting model using X-PLOR at high resolution.

Since FROG proves to be an useful tool for atomic model refinement, but it was developed practically 10 years ago, several modifications have been done recently.

The very powerful R-free criterion by Brünger (1992a) has been inserted as an option in FROG refinement. A service program was also added which allows to reserve a prescribed percentage of randomly chosen reflections and to use them later in FROG.

At the stage of rigid body refinement, specially after molecular replacement search, it is meaningful to improve general packing without going into the fine details of interatomic interactions. To do so, an additional repulsion term of the form $-1/\Delta r^2$ was introduced in the refinement program. This criterion can be used instead of the Lennard-Jones potential and applied, for example, for C_α-atoms only or for main chain atoms at early stages of refinement.

A correlation coefficient between F_{obs} and F_{model} was introduced. It can be used both as a minimising criterion itself or, being taken with a zero weight, as an additional check of the model quality. The last option was found to be quite useful.

The stereochemical dictionary was completely updated. The information on bond lengths and angles was copied from a dictionary by Priestle (1993) and the information on dihedral angles, planes etc. was updated following X-PLOR (Brünger, 1992b).

The refinement program itself initially had the possibility of refining any type of molecules. However, the initial package of the service programs did not include enough options to work conveniently with nucleic acids. Currently, these options have been added.

The set of service programs was significantly changed since its first version. Different "bugs" have been fixed.

The program is available from the authors by the request to e-mail addresses sacha@ibmc.u-strasbg.fr or com@impb.serpukhov.su. Currently, a new, menu-based user-friendly version of FROG is being tested for IBM PC computers (by M.Ivanov et al., IMPB RAN).

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