

JOINT CCP4 AND ESF-EACBM NEWSLETTER ON PROTEIN CRYSTALLOGRAPHY

An informal Newsletter associated with the BBSRC Collaborative Computational Project No. 4 on Protein Crystallography and the ESF Network of the European Association of the Crystallography of Biological Macromolecules.

Number 31

June 1995

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FROG PC - a menu-based environment for atomic model refinement program on a personal computer

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The decrease in price and increase in power of personal computers makes them suitable workstations, both in the laboratory and at home. Currently many useful crystallographic programs, including very elaborate ones (e.g., PROTEIN) have been effectively adapted to these machines (Steigemann, 1994). Due to high-quality graphics, these programs can be dressed up in a user-friendly menu-driven shell (e.g., FROG PC series of programs by Vernoslova & Lunin, 1994).

The refinement program FROG (Urzhumtsev et al., 1989) has proven to be a quite compact, high-speed one, and was used effectively on IBM PC 486/487 in its original form for several years. The FROG package consists of the main refinement program and several service programs and, being developed for general purpose machines, exchanges data between them using a file system.

A menu-driven shell for the program FROG has been developed to simplify the file and data management. Operating with this menu, there is no need to learn any special macrolanguage. This option together with the help, dependent on the content of the screen, make the program specially useful for beginners allowing them to execute basic steps of the atomic model refinement. It should be noted that an advanced user can prepare very complicated script files and run them without the menu if necessary.

With the user-friendly menu there is no need to type command lines in order to:

- a) choose necessary files;
- b) prepare control data;
- c) run the programs;
- d) look at the results of the calculations.

The necessary input files can be chosen from directories and their content can be checked and edited. Similarly, the names for the output files can be assigned. The presentation of the files in a single scheme (Fig.1a) makes their connection well illustrated and helps their management.

The shell uses a common stack of parameters (e.g., unit cell values) so after being defined once they can be used later by other programs. The parameters are defined under a program control and default values are available for most of them. The program indicates whether some necessary parameters were not defined. The input information is presented both in numerical and schematic form. In particular, the schematical presentation is used to assign rigid groups for the refinement (Fig.1b).

For each type of object a list of possible operations can be obtained by clicking the corresponding window. For example, for the atomic model these operations include rigid group assignment, calculation of geometrical statistics, calculation of structure factors or refinement itself (Fig.1c).

The current version of the program has not yet a graphical presentation of the output results. However, the output files can be viewed directly inside the system, without exiting to the MS DOS shell.

Currently the package runs on an IBM PC or compatible computers, under MS DOS version 3.3 or higher. An EGA (640x350) display or better is necessary. The original refinement package FROG has two modes: a file mode, for the case of small memory but large available disk space, and a memory mode, for the case of an available memory large enough to keep both atomic and reciprocal space information. The FROG PC package can operate in both modes; to run the file mode, about 300kb of RAM is necessary. One refinement cycle for a middle-size protein at a resolution of about 2Å takes a few minutes of CPU time on the IBM PC 486/487 computer.

The program is available by request from one of authors (M.I.). The e-mail address is ivanov@impb.serpukhov.su

The authors thank Dr. V.Lunin for his support and interest in the work and Dr. A.Podjarny for his reading and criticism of the manuscript. The work was supported by the grant 94-04-12844 of the Russian Foundation for Fundamental Research and by the grant RMZ000 from the International Science Foundation.

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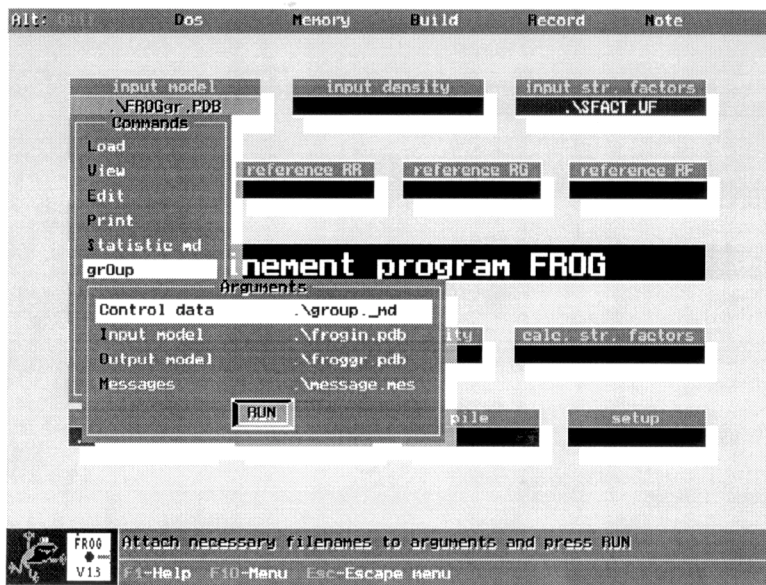
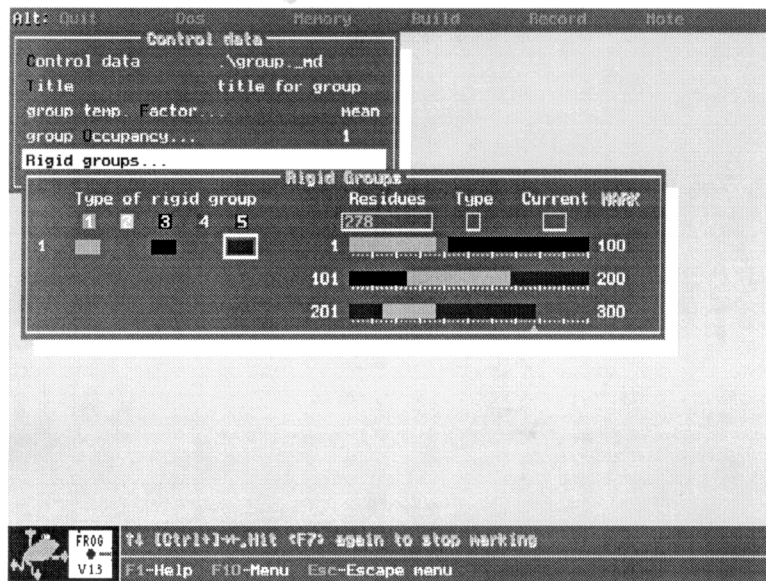


Figure 1. Different screen scenes during the run of the program FROG PC:

- initial scene;
- determination of the rigid groups;
- running the program.