

MacCHESS Director's report

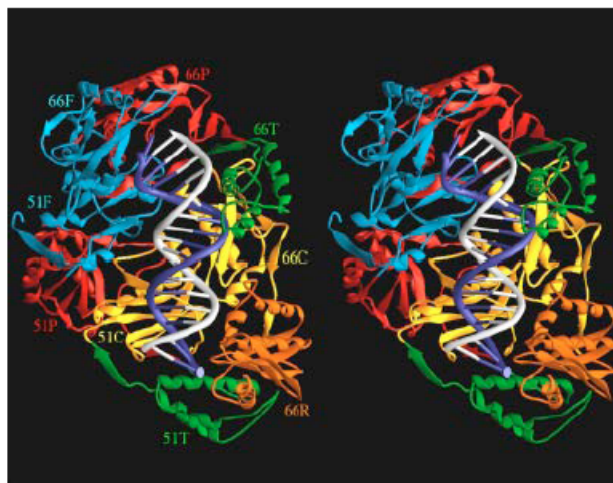
Steven Ealick

Activities in structural biology continue as a strong component of the overall research program at CHESS. After successfully competing for a five year renewal of the MacCHESS NIH Research Resource grant we have now set our sights on a research and development program that will benefit from a significant increase in our equipment budget. We have also received a generous award from the W.M. Keck Foundation and several other funding requests are pending. These new funds, coupled with the recent upgrade of station A-1, will provide substantial new capabilities for the macromolecular crystallography user community.

Currently, stations A-1 and F-1 are routinely used for macromolecular crystallography, while station F-2 has been used to develop capabilities for MAD phasing experiments. Station A-1 is now a doubly focused, tunable station and the beam intensity (as measured through a 0.3 mm collimator) is at least as high as that of station F-1. It is anticipated that a large fraction of the time on station A-1 will be available for structural biology.

Demand for beam time from macromolecular crystallographers remains high both for regular proposals and express mode proposals. The considerable back log of user requests that accumulated during the A line construction period has begun to show signs of letting up now that the A-1 station is fully operational. Nevertheless, new structural biology proposals are arriving at a record pace and it is likely that additional new resources will be needed to fully satisfy all of our user requests.

We have now added a second FUJI BAS-2000 image plate scanner, primarily for use on station A-1. With this addition we can now finally phase out the Kodak scanner and the PDP-11 computer which was required to control it. We will continue to provide 8" x 10" image plates,



Stereoview of HIV-RT taken by the Arnold group at Rutgers. See article on page 12.

however users are encouraged to purchase their own personal set to ensure the highest quality data. It seems that FUJI image plates are one item that we have not been able to make user proof. We have also purchased a Molecular Structure Corporation flash freezing system and a second MSC device has now been ordered (see article on shock freezing on page 44). We strongly encourage users to freeze crystals and will provide training and guidance to those who need assistance.

During the next few years the main MacCHESS development efforts will be in three areas: (1) CCD-based detector development, (2) MAD phasing and (3) on site data reduction. The CCD detector work is carried out in collaboration with Dr. Sol Gruner at Princeton University and has already paid off in the form of a 1K x 1K detector which is currently installed on the A-1 station (see separate article in this report by Rick Walter, page 36). Future plans include the construction of a 2K x 2K

detector and a 16 module mosaic detector.

We have now used station F-2 for several MAD phasing runs which have resulted in three new structures with several others in progress (see MAD article on page 22). Although we plan additional developments, we urge users to submit proposals for MAD phasing experiments which require the flux and energy resolution provided by station F-2.

Finally we have taken steps to ensure that users can more efficiently process the data collected at CHESS (see page 40). We now have two DEC Alpha workstations on site and plan to add additional workstations as funds become available. Both the DENZO (now DENVIEW) and MOSCO packages are implemented and users are encouraged to process their data before returning home. Drs. Wlodek Minor and Zbyszek Otwinowski have kindly agreed to provide a temporary site license for those users who need to process CHESS data in the home laboratory

CONTINUED ON PAGE 4

with DENVIEW. We have also entered into a collaboration with the Cornell Theory Center with the ultimate goal of real time data processing. We plan to use an IBM SP-1 scalable parallel computer for data management and processing.

Now that our funding is secure for the next five years, the MacCHESS staff is beginning a process of refurbishment and development. Our goal is to have reliable station hardware for stations A-1, F-1 and F-2 with at least one backup for every key component. We have also begun to assess documentation. Much of the station documentation is out of date and new developments have made additional documentation necessary. As part of this process, we are developing a troubleshooting guide which will be available to users on each station.

I would like to close this report by stating that macromolecular crystallography is alive and well at CHESS. New funding, new staff and new development initiatives are providing opportunities both for our user community and Cornell research programs. With announced plans to increase ring currents to 500 mA, the intensity of the CHESS wiggler beams will be comparable to those of the APS wigglers. It is my belief that if our current progress continues, CHESS will remain a leader in structural biology for many years to come.