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ESRF FULL 2-YEAR BLOCK ALLOCATION GROUP REVIEW REPORT

BAG RESPONSIBLE: Felix Frolow
EXPERIMENT NO: MX-117, MX-271
LAST REVIEW DATE: September 2003

Shift usage since last Biennial Review:

Allocated	66	Used	66	Cancelled by Users	0	Cancelled by ESRF	0
Total Number of Visits		7	Total Number of Visitors		22		

BAG Principle Investigators (indicate by # those left since last review, * those new since last review.)

Principal Investigator	Institute
Felix Frolow	Tel Aviv University
Nathan Nelson	Tel Aviv University
Linda Shimon	The Weizmann Institute of Science
Zipora Shakked	The Weizmann Institute of Science
Oded Livnah	The Hebrew University of Jerusalem
Orly Dym	The Hebrew University of Jerusalem
Yael Domovich*	The Hebrew University of Jerusalem
Joel Hirsch	Tel Aviv University

Total Number of PDB submissions from data from ESRF beam lines since last report	8
Total Number of Publications resulting from data from ESRF beam lines since last report	8

List below the **five** most important publications directly resulting from data recorded either wholly or partially on ESRF beamlines (**you must indicate** ¹ ESRF data only; ² data from more than one source):

1. A. N. Other *et al.*, (2000) Interesting structure using data from ESRF. *Journal with High Impact Factor* **123**, 456-789¹.
2. A. N. Other *et al.*, (2000) An Interesting structure using data from ESRF and elsewhere. *Journal with High Impact Factor* **123**, 456-789². (Please delete the examples.)

Summary: During last two years we have visited ESRF a total of 7 times as a BAG LS-2200, MX-117 and BAG MX-271. We were allocated 63 shifts and we used them all. During this time we have used ID14-4, ID14-2, BM30A and ID29 stations. We have collected 120 single wavelength data sets (ID14-4, ID14-2 and BM30A) and 7 complete MAD SeMet and MAD Lu data sets (BM30A, ID29, ID14-4). During these visits we collected also a lower resolution data sweeps when needed in order to clean data from overexposed reflections. All data processing was completed during the experiment to ensure completeness and quality of each measurement. Many of our systems were of low crystallographic symmetry (mainly P2₁) and required about 180° rotation in the space. Among these data sets are 36 full data sets from complete photosystem I which were used to solve the structure and to improve low order and high order resolution as well. Many of these structures, including PSI are already solved and under refinement (see the following Table). During this time 8 students were given initial training to use synchrotron for the protein data collection

Global Summary:

The TJW Block Allocation Group comprises 6 principle investigators from Tel Aviv University, Hebrew University of Jerusalem and The Weizmann Institute of Science. We have found Block Allocation Group approach extremely important factor for advance of our scientific research. The expedient flexibility built into the BAG system combined with the high degree of cooperation amongst principal investigators and students from all 3 institutions participating in this BAG dramatically enhances the scientific impact ESRF has on our research. We have always found the local contacts to be extremely professional and helpful. Our long time and repeated association with the local scientific and technical staff of ESRF allows for very efficient and valuable use of our time.

During last two years members of our BAG made considerable progress in their research program solving many structures including a membrane higher plant PSI complete complex with core and light harvesting antenna and chlorophyll cofactors. We believe that our rapid progress with this project was made possible because we have used a BAG scheme for it. Every member of our BAG even not specifically associated with the project contributed his specific expertise to the experiment. Considerable progress understanding tetramer alcohol dehydrogenases from bacteria and malignant parasites was made during the time covered by this report. On the basis of these structures, mutants, chimera constructs and mixed species hybrid tetramers were designed, crystallized and their structures solved. A number of scorpion toxin structures and their various mutants have been solved to atomic resolutions and give insight about structural features of the sodium channels. Components of cellulosome assembly such as cohesions and cellulose binding modules have been studied and provide detailed information about intra-cellulosome inter-subunit interactions at high resolution. Structural factors that unravel the pseudo-catalytic properties of avidin molecule were deduced from the series of the atomic resolution structures.

We hope that in the future the BAG mode of operation ingeniously introduced by ESRF will continue. We see the BAG access to ESRF as one of the most important factors that contribute to the success of our research.