

ESRF BLOCK ALLOCATION GROUP PROGRESS REPORT

BAG RESPONSIBLE: Oded Livnah
EXPERIMENT NO: MX-390
LAST REVIEW DATE: not reviewed yet

Shift usage since last Biennial Review:

Allocated	42	Used	39	Cancelled by Users	3	Cancelled by ESRF	
Total Number of Visits		11	Total Number of Visitors		26		

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

Principal Investigator	Institute
Noam Adir	Technion
Joel Hirsch	Tel Aviv University
Nathan Nelson	Tel Aviv University
Yael Domovich	The Hebrew U of Jerusalem
Joel Sussman	Weizmann Inst. Sci.
Deborah Fass	Weizmann Inst. Sci.
Mark Safo	Weizmann Inst. Sci.
Zipora Shakked	Weizmann Inst. Sci.
Linda Shimon	Weizmann Inst. Sci.
Ada Yonath	Weizmann Inst. Sci.

Total Number of PDB submissions from data from ESRF beam lines since last report	15
Total Number of Publications resulting from data from ESRF beam lines since last report	17

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):

- ¹Drory, O., Frolow, F. and Nelson, N. (2004). Crystal structure of yeast V-ATPase subunit C reveals its stator function. **EMBO Rep.** 5, 1148-1152.
- ¹Fish A., Danieli T., Ohad I., Nechushtai R., Livnah O. Structural basis for the thermostability of ferredoxin from cyanobacterium *Mastigicladus laminosus* (2005) *J. Mol. Biol.* 350, 599-608.
- ¹Noach, I., Frolow, F., Jakoby, H., Rosenheck, S., Shimon, L. J. W., Lamed, R. & Bayer, E. A. (2005). Crystal structure of a type-II cohesin module from the *Bacteroides cellulosolvens* cellulosome reveals novel and distinctive secondary structural elements. *J. Mol. Biol.* 348, 1-12.
- ¹The MntC crystal structure suggests that import of Mn²⁺ in cyanobacteria is redox controlled. Valeria Rukhman, Rina Anati, Meira Melamed-Frank and Noam Adir, *J. Mol. Biol.* 348, 961-969 (2005).

Summary (250 words maximum) of the results obtained since last biennial review: Due to space limitation names of Livnah and Frolow were not included in the PI table. During the 6 months that the BIG, extended Israeli BAG exists, we have visited ESRF 11 times, utilizing 39 shifts. We collected numerous fixed wavelength data sets and several MAD/SAD data sets on stations ID14-1, ID14-3, ID14-4, ID23-1, ID29, and BM16. . In most cases, data processing was completed in-situ, verifying data quality and completeness. Many of the data sets collected during these sessions were solved the structures are being currently refined. After revealing the first structure of super complex of plant photosystem I (PSI) to 4.4 Å we attempted to increase the resolution of the crystals in order to reveal more structural details. We have identified crystals that diffract to higher resolution (3.5-3.7 Å) yet complete data sets have not collected yet. Considerable progress was achieved by determining the structure of the G-domain (Ras homology domain) of Gem in complex with GDP to 2.4Å from SAD data. In addition, the structure of galectin-1 protein was solved to 1.4 Å using SAD. As for now, the BIG-BAG constellation has proven itself as a very good approach although we feel that we will need more beam time allocation in the future. In general the BAG format at ESRF is highly important to the success of our structural research.

Beamtime Request Justification: No more than half an A4 page. If the number of shifts requested in your current application is significantly higher or lower than that requested in the previous year, please comment here on the reasons for this.

The extended BAG comprises 12 PI's and was allocated 39-42 shifts per period (6 months), of which 27 shifts are designated for Ribosome and PSI. The remaining 12-15 shifts must be shared amongst 10 PI's! This will be inadequate. Initially, the BAG was able to manage as Prof. Yonath (15 shifts) temporarily declined use of her time. In the next term, with larger detectors installed at stations ID23-1 and ID14-4, she plans to fully utilize her shifts: the general allocation is insufficient to meet the needs of the remaining PI's.

The severe limitation on each PI's shifts will make the necessary instruction of graduate students nearly impossible. During this time, 13 students visited ESRF; this is a high educational priority.

Beam line performance: No more than half an A4 page. Please comment on the beam line performance during your visits, together with any constructive suggestions about possible enhancements to the facilities.

During our visits to ESRF, in the framework of BAG program covered by this report, we have experienced excellent performance of all beam lines used. The outstanding operation of the beam lines through improved goniostats, development of the centering software and improvements in hardware, as well as the highly professional support of local contacts have significantly improve user's performance. Moreover, we thank the ESRF staff and management for purchasing larger (3x3) CCD detectors that will permit high resolution data collection.