ESRF BLOCK ALLOCATION GROUP EXPERIMENT REPORT

BAG RESPONSIBLE: Prof. Dr. Sinning
EXPERIMENT NO: LS-2175
LAST REVIEW DATE: -

Shift usage since last Review:

Allocated	9	Used	6	Cancelled by Users	3	Cancelled by ESRF	0
Total Number of Visits		2	Total Number of Visitors	6			

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

Principal Investigator	Institute
Prof. Dr. Irmgard Sinning	BZH University of Heidelberg
#Dr. F. Jon Kull	MPI Medizinische Forschung
Dr. Dean Madden	MPI Medizinische Forschung

Total Number of PDB submissions from data from ESRF beam lines since last report	0
Total Number of Publications resulting from data from ESRF beam lines since last report	0

List the <u>five</u> most important publications below (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**, 456-789[1].
2. A. N. Other *et al.,* (2000) An Interesting structure using data from ESRF and elsewhere. *Journal with High Impact Factor* **123**, 456-789[2].

Allocation has just started!

Summary (250 words maximum) of the results obtained during the past year of BAG operation:

The following experiments have already been carried out:
Sinning group: Mex-M/Mtr2 crystals (project 12) diffracted to around 7Å, crystal symmetry identified as c2221 – further data was not collected. Nup85/Seh1 crystals (project 13) exhibited fibre-like diffraction to 4Å. 180° collected and processing still underway. A number of native and substrate soak data sets have been collected of Tudor/Spice (project 14) protein with native (1 set), SDMA (3 sets – various SDMA concentrations) and SDMA8 (2 sets – various SDMA8 concentrations). The native structure is almost refined (1.6 A, R=17%). Further soaked and co-crystallization crystals screened. A 2.3 Å dataset could be obtained for project 15 (Fab). The structure could subsequently be solved by molecular replacement and the structure is under refinement.

Madden/Kull groups: First beamtime used while writing this report (24.02.02). ID13 data unusuable (see below).

Summary of project status during review period:

Protein Name[a]	Data set[$]	Beam-line	Date	Protein size	Unit cell dimensions (Å, °)	Space Group	Crystal size (mm^3)	Anom. Scatt.(s))	d_{min} (Å)	R_{sym} (%)	Structure Status[b]	Publication Status[c]	Comments
Tudor/Spice	native	ID29	09.08.01	7 kD	27, 110, 28, 90, 120.5, 90	P21	0.03,0.03,0.1		1.7	9.6	solved	submitted	NOT ID14-4, not submitted!
Tudor/Spice	ligand	ID29	09.08.01		27, 110, 28, 90, 120.5, 90	P21	0.03,0.03,0.1		1.8	10.6	under refinement	submitted	SDMA
Tudor/Spice	ligand	ID29	09.08.01		27, 110, 28, 90, 120.5, 90	P21	0.03,0.03,0.1		2.9	11.3	under refinement	submitted	SDMA8
Fab for AAC2	native	ID29	01.12.01	50 kD	90, 75, 103, 90, 93, 90	P21	0.4x0.2x0.1		2.3	6.4	under refinement	submitted	not submitted!
Tudor/Spice	native	ID14-EH1	30.11.01		27, 110, 28, 90, 120.5, 90	P21	0.03,0.03,0.1		1.6	10.2	solved	submitted	complete data
Tudor/Spice	ligand	ID14-EH1	30.11.01		27, 110, 28, 90, 120.5, 90	P21	0.03,0.03,0.1		1.8	11.6	under refinement	submitted	complete data, SDMA
myosin-dynamin fusion complexed with GTP-gammaN	unusable	ID14-EH1	31.01.02	120 kDa			.01x.01x.03				solved	submitted	ID13 microcrystal tested for first time; low resolution; no complete data set
myosinII F506G-2R	irrelevant	ID14-EH1	31.01.02	100 kDa	136; 155; 143; 90	P21212	0.1x0.1x0.02				solved	submitted	ID13; too low resolution; no complete data set
myosinII F487A-2R	irrelevant	ID14-EH1	31.01.02	100 kDa	136; 155; 143; 90	P21212	0.1x0.1x0.02				solved	submitted	ID13; too low resolution; no complete data set
myosin dynamin fusion; alternative crystal form	unusable	ID14-EH1	31.01.02	120 kDa	102; 50; 106; 92; 111; 89	?	.01x.01x0.1				solved	submitted	ID13; microcrystal tested for first time; resolution too low
	native	ID14-EH1									solved	submitted	
	native	ID14-EH1									solved	submitted	
	native	ID14-EH1									solved	submitted	
	native	ID14-EH1									solved	submitted	
	native	ID14-EH1									solved	submitted	
	native	ID14-EH1									solved	submitted	
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	native	ID14-EH1									solved	submitted	
	native	ID14-EH1									solved	submitted	
	native	ID14-EH1									solved	submitted	

[a]Include name of substrate/inhibitor ligand if applicable. [b]either "solved", "under refinement" or "completed". [c]Choose "submitted", "in press" or "published" as necessary. Also state if data set proved unusable or irrelevant and give reason under comments.
[$]Data set: describe as native, ligand, mutant, MAD, SAD, MIR.

List <u>all publications</u> resulting from the use of ESRF beam-lines since last report (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**, 456-789[1].
2. A. N. Other *et al.,* (2000) An Interesting structure using data from ESRF and elsewhere. *Journal with High Impact Factor* **123**, 456-789[2].
3. A. N. Other *et al.,* (2000) Interesting structure using data from ESRF. *Journal with High Impact Factor* **123**, 456-789[1].
4. A. N. Other *et al.,* (2000) Interesting structure using data from ESRF. *Journal with High Impact Factor* **123**, 456-789[1].
5 A. N. Other *et al.,* (2000) An Interesting structure using data from ESRF and elsewhere. *Journal with High Impact Factor* **123**, 456-789[2].

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Summary on ID13 time (31.01.02): Would have been the ideal beamline for small ***Nup85/Seh1/Nup120*** and ***Mex-M/Mtr2*** crystals grown (see above). However, a number of problems made it impossible to collect data.

1) Beamline dump evening of 31.01.2002
2) Beamline realigned incorrectly by beamline scientists such that true beam was (eventually) found over 30 micrometer from predicted beam centre. As the ***Mex-M/Mtr2*** and ***Nup85/Seh1/Nup120*** crystals are very small (both proteins give needles that have a dimension < 5 micrometer) they were unexposed to radiation. Fault was not noticed until a larger crystal was irradiated at the end of the shift.
3) Crystal to detector distance was not correctly calibrated, such that on other projects that did diffract the predicted distance and actual distance differed by > 20mm.

Beamline effectively unusable in this state. Local contact friendly, but unaware of the requirements of data collection for protein crystallography (original comment from user).