ESRF BLOCK ALLOCATION GROUP EXPERIMENT REPORT

BAG RESPONSIBLE: Prof. Dr. Sinning
EXPERIMENT NO: LS-2077
LAST REVIEW DATE: -

Shift usage since last Review:

Allocated	21	Used	12	Cancelled by Users	0	Cancelled by ESRF	9
Total Number of Visits		4	Total Number of Visitors	12			

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	3
Total Number of Publications resulting from data from ESRF beam lines since last report	3

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].

1. K. Wild, I. Sinning, S. Cusack. Crystal structure of an early protein-RNA assembly complex of the signal recognition particle. Science 294, 598-601 (2001)1.

2. K. Wild, O. Weichenrieder, K. Strub, I. Sinning, S. Cusack. Towards the assembly of the mammalian signal recognition particle. Curr. Opin. Struct. Biol. 12, 72-81 (2002)1.

3. Niemann, H.H., Knetsch, M.L., Scherer, A., Manstein, D.J. and Kull, F.J. (2001) Crystal structure of a dynamin GTPase domain in both nucleotide-free and GDP-bound forms. Embo J, 20, 5813-5821

Summary (250 words maximum) of the results obtained during the past year of BAG operation:
Two experiments from the Sinning group: the structure determination of 1) parts of the S domain of human SRP and 2) of parts from the archaeabacterial SRP. In the first project, we were able to solve the structure of protein SRP19 in complex with helix 6 of SRP RNA (Wild et al. 2001, Wild et al. 2002). Having these results in hand, we are now focusing on the larger assemblies. In the second project, the resolution of the crystals of SRP54 in complex with helix 8 could be increased to 2.5 Å, but unluckily difficult space group problems (no twinning!) made it impossible so far to solve this structure. Both projects will be continued during the actual allocation period (LS-2175) and are as well part of the continuing proposal. Due to late allocation, the beamtime has been used as well for LS-2175 projects (see report there).
Project: GluRB AMPA receptor Ligand-Binding Domain (Madden-Group): Three data sets were collected for this project (see table below (GluRB)). The structure was solved by molecular replacement with the released structure of the ligand-binding core. A soak in the antagonist NBQX resulted in an improved native data set, while short soaks aiming at freezing the intermediate docking complex with the full agonist glutamate resulted in apo structures. Project: Dynamin GTPase domain (Kull-Group) The structure has been solved at 2.3A in nucleotide-free and GDP-bound form (Niemann et al. 2001).

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
archaeal SRP	ligand	ID14-EH1	30.11.01	65 kD	102, 102, 122, 90, 90, 120	R3?	.03x.03x.03		2.9	7.1	solved	submitted	not solved yet
archaeal SRP	MIR	ID29	01.12.01	65 kD	98, 98, 119, 90, 90, 120	R3?	.03x.03x.03	hg	3.9	12.4	solved	submitted	not solved yet
archaeal SRP	MIR	ID29	01.12.01	65 kD	99, 99, 121, 90, 90, 120	R3?	.03x.03x.03	pt	3.9	7.5	solved	submitted	not solved yet
archaeal SRP	MIR	ID29	01.12.01	65 kD	99, 99, 121, 90, 90, 120	R3?	.03x.03x.03	pt	3.9	8.7	solved	submitted	not solved yet
GluRB, 531b16	ligand	ID14-EH1	24.09.01	45 kD	96x176x89	P21212	.04x.08x.08		2.75	6.1	under refinement	submitted	improved resolution
GluRB, 533b52	ligand	ID14-EH1	24.09.01	45 kD	96x176x89	P21212	.04x.08x.08		3.2	13.4	solved	submitted	
GluRB, 533b51	ligand	ID14-EH1	24.09.01	45 kD	96x176x89	P21212	.04x.08x.08		3.2	5.7	solved	submitted	
PCP AC, 7.6	unusable	ID14-EH1	24.09.01	40 kD							under refinement	submitted	high salt form under refinement at 2.2 A.
rest: see LS-2175	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	

[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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