ESRF ~~BIENNIAL~~ BLOCK ALLOCATION GROUP ~~REVIEW~~EXPERIMENT REPORT

BAG RESPONSIBLE: **Inger Andersson**
EXPERIMENT NO: **LS-2080/LS-1934**
LAST REVIEW DATE: **March 2001**

Shift usage since last ~~Biennial~~ Review:

Allocated	39	Used	30	Cancelled by Users	0	Cancelled by ESRF	____
Total Number of Visits		7	Total Number of Visitors	13			

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

Principal Investigator	Institute
Ulla Uhlin	Dept. of Molecular Biology, SLU
Janos Hajdu	Dept. of Biochemistry, Uppsala University
Inger Andersson	Dept. of Molecular Biology, SLU
_____	_____
_____	_____
_____	_____
_____	_____
_____	_____

Total Number of PDB submissions from data from ESRF beam lines since last report	9
Total Number of Publications resulting from data from ESRF beam lines since last report	7

List the five most important publications below (indicate [1] ESRF data only; [2] data from more than one source):

1. K. Johansson et al. (2001). Structural basis for substrate specificities of cellular deoxyribonucleoside kinases. *Nature Struct. Biol.* **8**, 616-620[1].
2. N.E. Mikkelsen et al. (2001). Aminoglycoside binding displaces a divalent metal ion in a tRNA-neomycin B complex. Nature Struct. Biol. **8**, 510-514 [2].
3. T.C. Taylor et al. (2001). First crystal structure of Rubisco from a green alga, *Chlamydomonas reinhardtii*. *J. Biol. Chem.* **276**, 48159-48164[1].
4. A.C. Terwisscha van Scheltingaet al. (2001). Multiple isomorphous replacement on merohedral twins: structure determination of deacetoxycephalosporin C synthase. *Acta Crystallogr.* **D57**, 1776-1785[2].
5. A. Karlsson et al. (2002) X-ray Crystal Structure of Benzoate 1,2-Dioxygenase Reductase from *Acinetobacter* sp. Strain ADP1. *J. Mol. Biol.* (in press)[2].

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

The total beam time allocated to this BAG (LS-1934 and LS-2080) was 39 shifts, 9+6 on ID14 1, 3+6 on ID14-3, 6 on ID14-4, and 6+ 3 on ID29. The group consists of 15 scientists (fluctuating number) from two Departments at two different Universities comprising around ten different research projects. The advantages of sharing the beam time under the hat of a BAG proposal are several: first and foremost it enables efficient use of allocated beam time, but also it promotes collaboration between groups and efficient training for students. The disadvantage is the additional work necessary for a) organisation of travel, b) maintenance of a data base of collected data, c) reporting and d) applications, and which has to be done by the responsible scientist.
Highlights of the past year include the structure determination of Benzoate 1,2-Dioxygenase Reductase from *Acinetobacter* sp. from MAD data, and the structure determination of the subunits of ribonucleotide reductase from Salmonella tyhimurium by molecular replacement.

~~Global Summary:~~

~~This should occupy one A4 page at maximum. As well as a more complete overview of the activities of the BAG during the period under review, this section should also contain comments on the overall usefulness of the scheme to your BAG. These may include suggestions at to how the scheme can be improved and should be made in a constructive manner.~~

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
Chlamydomonas Rubisco	ligand	ID14-EH1	2001-11-15	550 kDa	???	???	0.05x0.05x0.01	_____	3.5	-	under refinement	in process	crystal died during data collection
Salmonella RNR, small subunit nrdE with AMP-PNP and dUDP	native	ID14-EH1	2001-06-28	79 kDa	99x99x290	P43212	_____	_____	2.8	0.077	completed	in process	_____
Salmonella RNR, small subunit nrdE with AMP-PNP and dUDP	native	ID14-EH1	2001-06-28	79 kDa	99x99x290	P43212	_____	_____	3.2	_____	under refinement	in process	_____
Salmonella RNR, small subunit nrdE with AMP-PNP	ligand	ID14-EH4	2001-09-23	79 kDa	99x99x290	P43212	_____	_____	3	_____	solved	in process	_____
Salmonella RNR, small subunit nrdE with AMP-PNP and CDP	ligand	ID14-EH4	2001-09-23	79 kDa	99x99x290	P43212	_____	_____	3.4	_____	solved	in process	_____
Salmonella RNR, small subunit nrdE with AMP-PNP and UDP	ligand	ID14-EH2	_____	79 kDa	99x99x290	P43212	_____	_____	3.2	0.12	under refinement	in process	_____
Salmonella RNR, small and big subunits nrdE and nrdF with AMP-PNP and CDP	native	ID14-EH2	_____	79 + 40 kDa	276x276x269	P212121	_____	_____	4	14	solved	in process	_____
Drosophila nucleotide kinase with dThd	ligand	ID14-EH4	2002-01-30	44 kDa	120x62x68	P212121	0.1x0.05x0.05	_____	2.9	0.059	under refinement	in process	_____
Drosophila nucleotide kinase with dTTP	ligand	ID29	2001-04-13	44 kDa	67x120x69	P21	0.1x0.05x0.05	_____	2.6	_____	solved	in process	_____
Drosophila nucleotide kinase with dCyd	ligand	ID14-EH2	_____	44 kDa	119.5x60.8x67.3	P212121	0.1x0.05x0.05	_____	2.5	_____	solved	in process	_____
human thymidine kinase	native	ID14-EH4	2002-01-30	25.7 kDa	123.7x115.5x123.4	P21	0.2x0.2x0.05	_____	3	_____	under refinement	in process	need phases (MIR/MAD)
tRNA Phe	ligand	ID14-EH4	2001-11-20	25 kDa	55x33x62	P21	0.1x0.05x0.01	_____	3.5	_____	under refinement	in process	_____
succinate dehydrogenase	native	ID14-EH1	2001-06-28	130 kDa	124x124x212	P63	0.2x0.2x0.05	_____	4.0	7.7	under refinement	published	_____
anthranilate dioxygenase	native	ID14-EH4	2001-04-14	70 kDa	130x130x175	I4	0.05	_____	2.8	0.11	under refinement	in process	crystal died during data collection
anthranilate dioxygenase	native	ID14-EH4	2001-04-14	70 kDa	130x130x175	I4	0.05	_____	3.4	0.088	under refinement	in process	crystal died during data collection

naphtalene dioxygenase reaction intermediates	ligand	ID14-EH1	2002-01-31	70 kDa	140x140x210	R32	0.5	_____	1.4	0.08	solved	in process	_____
naphtalene dioxygenase reaction intermediates	ligand	ID14-EH1	2002-01-31	70 kDa	140x140x210	R32	0.5	_____	1.8	0.07	solved	in process	_____
naphtalene dioxygenase reaction intermediates	ligand	ID14-EH1	2002-01-31	70 kDa	140x140x210	R32	0.5	_____	1.8	0.083	solved	in process	_____
naphtalene dioxygenase reaction intermediates	ligand	ID14-EH1	2002-01-31	70 kDa	140x140x210	R32	0.5	_____	1.85	0.084	solved	in process	_____
naphtalene dioxygenase reaction intermediates	ligand	ID14-EH1	2002-01-31	70 kDa	140x140x210	R32	0.5	_____	1.95	0.090	solved	in process	_____
Clavaldehyde Dehydrogenase	native	ID14-EH1	2002-01-31	_____	???	???	0.12x0.12	_____	6	_____	under refinement	in process	_____
DAOCS with ampicillin	ligand	ID14-EH1	2001-02-24	35 kDa	139x139x48	P3121	0.2x0.1x0.15	_____	3.3	0.15	under refinement	in process	_____
DAOCS with Fe(II)	ligand	ID29	2001-04-13	35 kDa	139x139x48	P3121	0.2x0.1x0.15	_____	2.5	0.05	completed	in process	_____
DAOCS with 2-oxo-glutarate	ligand	ID14-EH4	2001-09-23	35 kDa	136x136x48	P3121	0.2x0.1x0.15	_____	3.1	0.10	under refinement	in process	_____
DAOCS with 2-oxo-glutarate	ligand	ID14-EH4	2001-09-23	35 kDa	137x137x48	P3121	0.2x0.1x0.15	_____	3.1	0.10	under refinement	in process	_____
DAOCS with 2-oxo-glutarate	ligand	ID14-EH4	2001-09-23	35 kDa	137x137x48	P3121	0.2x0.1x0.15	_____	2.9	0.07	under refinement	in process	_____
DAOCS with succinate	ligand	ID14-EH4	2001-09-23	35 kDa	138x138x48	P3121	0.2x0.1x0.15	_____	3.0	0.10	under refinement	in process	_____
DAOCS with DAOC	ligand	ID14-EH1	2001-02-24	35 kDa	139x139x48	P3121	0.2x0.1x0.15	_____	3.0	0.10	under refinement	in process	_____
DAOCS	ligand	ID14-EH1	2001-02-24	35 kDa	107.2x107.2x70.7	R3	0.2x0.2x0.1	_____	1.95	0.074	completed	in process	_____
DAOCS	ligand	ID14-EH1	2001-02-24	35 kDa	106.6x106.6x71.7	R3	0.2x0.2x0.1	_____	1.7	0.051	completed	in process	_____
DAOCS	ligand	ID14-EH1	2001-02-24	35 kDa	107.2x107.2x70.5	R3	0.2x0.2x0.1	_____	1.9	0.085	completed	in process	_____
DAOCS	ligand	ID29	2001-04-13	35 kDa	106.7x106.7x71.2	R3	0.2x0.2x0.1	_____	1.55	_____	completed	in process	_____
DAOCS	ligand	ID14-EH4	2001-09-23	35 kDa	106.8x106.8x71.8	R3	0.2x0.2x0.1	_____	1.7	_____	completed	in process	scaling impossible due to shutter problems
DAOCS	ligand	ID14-EH4	2001-09-23	35 kDa	106.8x106.8x71.1	R3	0.2x0.2x0.1	_____	1.6	_____	completed	in process	_____
DAOCS	ligand	ID14-EH4	2001-09-23	35 kDa	107.0x107.0x71.3	R3	0.2x0.2x0.1	_____	1.7	_____	completed	in process	_____

[a]Include name of substrate/inhibitor ligand if applicable. [b]either "solved", "under refinement" or "completed". [c]Choose "submitted", "in press", "published" or “in press” 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.

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
DAOCS	ligand	ID14-EH4	2001-09-23	35 kDa	107.5x107.5x70.8	R3	0.2x0.2x0.1	_____	2.1	_____	completed	in process	scaling impossible due to shutter problems
_____	native	ID14-EH1	_____	_____	_____	_____	_____	_____	_____	_____	solved	submitted	_____

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. K. Johansson et al. (2001). Structural basis for substrate specificities of cellular deoxyribonucleoside kinases. *Nature Struct. Biol.* **8**, 616-620[1].

2. N.E. Mikkelsen et al. (2001). Aminoglycoside binding displaces a divalent metal ion in a tRNA-neomycin B complex. Nature Struct. Biol. **8**, 510-514 [2].

3. T.C. Taylor et al. (2001). First crystal structure of Rubisco from a green alga, *Chlamydomonas reinhardtii*. *J. Biol. Chem.* **276**, 48159-48164[1].

4. A.C. Terwisscha van Scheltingaet al. (2001). Multiple isomorphous replacement on merohedral twins: structure determination of deacetoxycephalosporin C synthase. *Acta Crystallogr.* **D57**, 1776-1785[2].

5. S. Törnroth et al. (2002). Purification, crystallisation and preliminary crystallographic studies of succinta:ubiquinone from *E. coli*. *BBA* **1553**, 171-176[1].

6. A. Karlsson et al. (2002). X-ray Crystal Structure of Benzoate 1,2-Dioxygenase Reductase from *Acinetobacter* sp. Strain ADP1. *J. Mol. Biol.* (in press)[2].

7. B. Dalhus et al. (2002). Structural basis for thermophilic protein stability: structures of thermophilic and mesophilic malate dehydrogenases. *J. Mol. Biol.* (in press)[2].