ESRF BLOCK ALLOCATION GROUP EXPERIMENT REPORT

BAG RESPONSIBLE: J.P. SAMAMA FORMTEXTE
EXPERIMENT NO: LS 2093 FORMTEXTE
LAST REVIEW DATE: 10/2001

Shift usage since last Review:

Allocated	9	Used	9	Cancelled by Users	0	Cancelled by ESRF	0
Total Number of Visits		3	Total Number of Visitors	11			

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

Principal Investigator	Institute
J. P. Samama	CNRS-Toulouse
Y. Mechulam	Ecole Polytechnique-Palaiseau
F. Rey #	CNRS-Gif sur Yvette

Total Number of PDB submissions from data from ESRF beam lines since last report	7
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- M. Ferri-Fioni, E. Schmitt, J. Soutourina, P. Plateau, Y. Mechulam and S. Blanquet (2001) Structure of crystalline D-Tyr-tRNATyr deacylase: a representative of a new class of tRNA-dependent hydrolase. J. Biol. Chem. 276, 47285-47290. [2]

2- E. Schmitt, S. Blanquet and Y. Mechulam. The large subunit of initiation factor aIF2 is a close structural homolog of elongation factors. (2002) EMBO J. (in press). [2]

3- L. Mourey, S. Da R , J-D. P delacq, T. Tolstykh, C. Faurie, J. B. Stock and J. P. Samama (2001) Crystal structure of the CheA histidine phosphotransfer domain that mediates response regulator phosphorylation in bacterial chemotaxis. J. Biol. Chem., 276, 31074-82.[1]

4- D. Golemi, L. Maveyraud, S. Vakulenko, J.P. Samama, S. Mobashery (2001) Critical involvement of a carbamylated lysine in catalytic function of class-D b-lactamase. P. N. A. S., 98, 14280-14285. [1]

5- S. Bressanelli et al., (2002) A structural analysis of the hepatitis C virus polymerase in complex with ribonucleotides. Journal of Virology, in press

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

Palaiseau group: That of D-tyr-tRNA deacylase from *E. coli* was solved (J. Biol. Chem., 2001). The structure of the large subunit of eIF2 from *P. abyssi*, was solved free and complexed with GDP and GDPNP (EMBO J., in press). Data were collected for dimeric MetRS from *P. abyssi* (attempts to solve by MR) and for E. coli MetRS complexed with di-fluoro-methionine (under refinement).

Toulouse group: The crystal structure of DivK in several conditions was solved (papers in preparation). The class D β-lactamase in complex with ligands has been determined to high resolution as well as the structure of a mutant protein carrying a mutation at an essential catalytic residue. The structure of the ATP binding domain of the histidine kinase YycG has been solved at 1.2 resolution by MAD (currently at the final stage of refinement).

Gif group: Complexes of the hepatitis C virus polymerase with nucleotides and divalent ions allowed a working model to be derived for the intiation of genome replication in this major public health problem. Progress was made on other important human or animal pathogens, ie Herpesviruses or Infectious Bursal Disease Virus, and model viruses such as Sindbis virus.

Summary of project status during review period:

Protein Name[a]	Data set[$]	Beam-line	Date	Protein size	Unit cell dimensions (, °)	Space Group	Crystal size (mm^3)	Anom. Scatt.(s))	d_{min} ( )	R_{sym} (%)	Structure Status[b]	Publication Status[c]	Comments
eIF2gamma GD235-GDP	FORMLISTEDEROUL	FORMLISTEDEROUL	FORMTEXTE 1 oct 2001	43 kD	51.5,87,58, 110, 90, 110,90	P21	0.3,0.1,0.05		2	3.9	completed	in press	soaking
eIF2gamma GD235-GDPNP	ligand	ID14-EH1	1 oct 2001	43 kD	51.5,87,58, 110, 90, 110,90	P21	0.3,0.1,0.05		1.8	4.3	completed	in press	co-crystallized
eIF2gamma GD235-GDP	ligand	ID14-EH1	1 oct 2001	43 kD	51.5,87,58, 110, 90, 110,90	P21	0.2,0.06,0.03		2.1	5.7	completed	in press	co-crystallized
eIF2gamma GD235-GDPNP	ligand	ID14-EH1	1 oct 2001	43 kD	51.5,87,58, 110, 90, 110,90	P21	0.3,0.1,0.05		2.2	5.0	completed	in press	soaking
eIF2gamma -GDP	ligand	ID14-EH1	1 oct 2001	43 kD	51.5,87,58, 110, 90, 110,90	P21	0.15,0.06,0.03		1.9	3.8	completed	in press	soaking
eIF2gamma GD235-ATP	irrelevant	ID14-EH1	1 oct 2001	43 kD	51.5,87,58, 110, 90, 110,90	P21	0.3,0.1,0.05		2.1	6.0	solved	in process	ligand not seen
MetRS P.abyssi	native	ID14-EH1	13 feb 2002	84 kD	117,117,288,90,90,90	I4122	0.2,0.05,0.03		4.5	8.0	solved	in process	
MetRS P.abyssi	native	ID14-EH1	13 feb 2002	84 kD	117,117,288,90,90,90	I4122	0.2,0.05,0.03		2.9	8.7	solved	in process	
MetRS-E.coli-DFM	native	ID14-EH1	13 feb 2002	64 kD	78,45,86,90,107,86	P21	0.4,0.4,0.03		1.7	5.2	under refinement	in process	
Herpesvirus-gD as a fusion protein with antibody fragment	MIR	ID14-EH1	01-10-01	170 kDa	43 76 103, 90 91.5 90	C2	.2x.1x.03	Pt	3.9	10	under refinement	in process	
HCVpolymerase-GTP-magnesium complex	ligand	ID14-EH1	01-10-01	62kDa	67 97 96.5, 90 90 90	P21212	.5x.2x.1		1.8	6.7	completed	in press	
HCVpolymerase-GTP-magnesium complex	ligand	ID14-EH1	17-11-01	62kDa	67 97 96.5, 90 90 90	P21212	.6x.2x.1		1.5	7.2	under refinement	in process	
Capsid protein of Infectious Bursal Disease Virus	native	ID14-EH1	17-11-01	10x45 kDa	261 261 353 90 90 120	P6322	.2 x .2 x .02		7	10	under refinement	in process	
Fusion protein of Sindbis Virus	native	ID14-EH1	17-11-01	43kDa	34 75 206, 90 90 90	P212121	.1x.08x.02		3.4	7.8	solved	in process	
Fab against gD of Herpesviruses	ligand	ID14-EH1	13-02-02	50 kDa	45.5 68 71, 90 106.4 90	P21	.4x.1x.05		1.7	6.9	solved	in process	
HCVpolymerase-inhibitor complex	ligand	ID14-EH1	13-02-02	62kDa	67 97 96.5, 90 90 90	P21212	.3x.1x.1		1.9	7.5	under refinement	in process	
Complex between antibody fragment and rheumatoid factor	native	ID14-EH1	13-02-02	100kDa	242 76 103, 90 91.5 90	C2	.2x.1x.03		3	6.9	under refinement	in process	
Capsid protein of Infectious Bursal Disease Virus	native	ID14-EH1	13-02-02	10x45 kDa	261 261 353 90 90 120	P6322	.2 x .2 x .1		4	9	solved	in process	
	native	ID14-EH1									solved	submitted	

FlhDC semeth E. coli	native	ID14-EH1	01-10-01	70 kD	85.2, 125.2, 179.03 90, 90, 90	I222	0.08x0.06x 0.06	Se	4.5	8.5	under refinement	in process	
FlhDC Salty	native	ID14-EH1	01-10-01	70 kD	150.5, 150.5, 115.9, 90, 90, 120	P61	0.05x0.05x 0.5	0	3.5	7.5	under refinement	in process	
YycG AMPPNP	SAD	ID14-EH4	17-11-01	18 kD	38.75, 48.52, 43.20 90, 112.54, 90	P21	0.15x0.04x 0.04	Zn	1.5	5.4	solved	in process	
Oxa-10 K70A	mutant	ID14-EH4	17-11-01	55 kD	79.1, 79.1, 105.4 90, 90, 120	P31	0.15x0.23x 0.1	0	2.2	7.1	solved	in process	
PleC-DivK Caucr	native	ID14-EH1	13-02-02	60 kD	171.5,171.5,255 90, 90, 120	P3	0.26x0.26x0. 2	0	3.7	8.3	under refinement	in process	
XCL Xerch	native	ID14-EH1	13-02-02	63 kD	83.8,83.8,71.5 90, 90, 120	P622	0.14x0.12x0. 12	0	2	9.8	under refinement	in process	
	native	ID14-EH1									solved	submitted	
	native	ID14-EH1									solved	submitted	
	native	ID14-EH1									solved	submitted	
	native	ID14-EH1									solved	submitted	
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[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.

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	native	ID14-EH1									solved	submitted	
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	native	ID14-EH1									solved	submitted	

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[$]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):

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