	Experiment title: BAG-LEBS-2004-2	Experiment number: MX-350
Beamline: ID14-EH1	**Date of experiment**: from: 30/11/2004 8h to: 01/12/2004 8h	**Date of report**: 22/2/05
Shifts: 3	**Local contact(s)**: Dr S. MONACO	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Lionel Trésaugues (Orsay University; PhD student)* , Marc Graille (IBBMC; post-doc)* Institut de Biochimie Moléculaire et Cellulaire (IBBMC), Equipe Génomique Structurale, CNRS UMR8619,

Université Paris-Sud, Orsay, France

Vincent CHAPTAL*, Solange MORERA*, Valérie BIOU, LEBS, Bat 34, CNRS UPR9063, 1 av. de la Terrasse, Gif-Sur-Yvette, France

Dumas Renaud*, Mas Corine*, LPCV-CEA, Grenoble, France

Report:

Lionel Trésaugues, Marc Graille (1 shift) : yeast *Saccharomyces cerevisiae* Structural Genomics project

The systematic names of the genes are used. More details on every orf can be found on http://genomics.eu.org:targets.html

PH0168
The report has been included at the end of the text of the proposal.

Vincent CHAPTAL, Solange MORERA (1 shift) : Hpr kinase/Phosphorylase (HprK/P):

HprK/P is a bifunctional enzyme that belongs to a new family of Ser/Thr kinases with a P-loop nucleotide binding site. We previously solved the structures of the native protein and its complex with Hpr. However, these two structures show HprK/P in its phosphorylase activity. We would like to get the kinase form of the enzyme using a mutant of HprK/P. All crystals diffracted badly. None were collected.

Dumas Renaud*, Mas Corine*, Valérie BIOU (1 shift) : Threonine synthase complex

All went well during the experiment.
Threonine synthase complex crystals are pseudo-hexagonal, but the real space group is C2 with 6 monomers in the asymmetric unit.
About 15 crystals were tested and data were collected on 3 crystals.
The statistics below correspond to the best data set.

N	1/d^2	Dmin(A)	Rmrg	Rfull	Rcum	Av_I	SIGMA I/sigma	sd Mn(I)/sd	Nmeas	Nref	Ncent	FRCBIAS	Nbias
1	.0174	7.59	.049	.049	.049	14555.	1255.4 11.6	956. 29.5	13172	3878	310	-.006	5457
2	.0347	5.37	.050	.048	.050	6260.	570.0 11.0	495. 24.9	26403	7248	377	-.016	11674
3	.0521	4.38	.050	.045	.050	6603.	570.3 11.6	589. 22.2	34542	9362	382	-.019	15645
4	.0694	3.79	.060	.047	.053	5755.	562.8 10.2	547. 19.3	41103	11133	388	-.020	18602
5	.0868	3.39	.091	.065	.058	3150.	443.5 7.1	381. 14.1	46225	12562	384	-.031	21043
6	.1042	3.10	.142	.113	.065	1566.	324.8 4.8	302. 9.1	50674	13773	380	-.040	22774
7	.1215	2.87	.229	.182	.072	825.	263.7 3.1	284. 5.7	55738	15118	383	-.071	25142
8	.1389	2.68	.335	.285	.079	509.	235.2 2.2	278. 3.8	59242	16101	381	-.075	26493
9	.1562	2.53	.495	.434	.086	332.	223.1 1.5	278. 2.6	63192	17174	386	-.090	28522
10	.1736	2.40	.680	.565	.094	236.	216.1 1.1	285. 1.8	66424	18125	382	-.095	29859
Overall:			.094	.077	.094	2539.	422.3 6.0	373. 10.0	456715	124474	3753	-.026	205211
			Rmrg	Rfull	Rcum	Av_I	SIGMA I/sigma	sd Mn(I)/sd	Nmeas	Nref	Ncent	FRCBIAS	Nbias

the data were later truncated to 2.6Å resolution.
Structure refinement is almost complete and shows the way threonine synthase interacts with its activator and its cofactor. A paper is being written.