

	Experiment title: Structural studies of nucleotide diphosphate kinase in complex with inhibitors	Experiment number: LS-1685
Beamline ID-14.3	Date of experiment: June 23 rd , 2000	Date of report: August 28 th <i>Received at ESRF:</i>
Shifts:	Local contact(s):	
Names and affiliations of applicants (* indicates experimentalists): Alejandro Buschiazzo, Beatriz Gomes Guimaraes, Maria J. Mate Perez, Miguel Ortiz, Pedro M. Alzari Unité de Biochimie Structurale, Institut Pasteur, 25 rue du Dr. Roux, 75724 Paris, France		

Report:

Previous studies have suggested that nucleotide diphosphate kinase (NDPK) may play a role in the cellular metabolism of some anti-AIDS nucleoside drugs. To further investigate this issue, we are studying the structure of NDPK from *Dictyostelium discoideum* (wild-type and point mutants) in complex with potential inhibitors, substrates and anti-viral compounds.

During the last six months, we have collected diffraction data from three putative complexes, in some cases at atomic resolution: the NDPK double mutant (N119S, H122G) crystallized in the presence of ddGTP, the single mutant N119S in complex with ddGDP, and the single mutant H122G in complex with AZTDP. Data collection statistics is summarized in the table below. For the N119S single mutant, the diffraction data is still to be processed. The other two complexes have been solved by molecular replacement techniques and are currently being refined to high resolution. For the NDPK double mutant, the presence of the nucleotide in the crystals is not yet confirmed, and additional beam time could be required for this project.

Crystal form	Beam-line	λ (Å)	No. of images	Space group	a (Å)	b (Å)	c (Å)	Data resolution (Å)	Data complet. (%)	R merge (%)	Multiplicity
NDPK(N119S,H122G) - ddGTP	ID-14.3	0.931	212 + 212	P6 ₃ 22	71.036	71.036	106.199	1.15	96.2	0.04	9.1
NDPK (N119S) - ddGDP	ID-14.3	0.931	120	P6 ₃ 22	71	71	106	1.4	-	-	-
NDPK (H122G) - AZTDP	ID-14.3	0.931	100	R32	111.92	111.92	242.81	2.2	99.8	0.08	5.7

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