	Experiment title: Diffraction data of protein kinase CK2 with substrates	**Experiment number**: MX-342
Beamline: ID29	**Date of experiment**: from: 17-2-05 to: 18-2-05	**Date of report**: 12-04-05
Shifts: 3	**Local contact(s)**:	*Received at ESRF:*

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Report:

The goal of the experimebnt was to soak the crystal of protein kinase CK2 (whise structure, alone and in complex with inhibitors is already known) with ATP, Mg2+ and a peptide substrate. Since the kinetics, at the ionic strength of crystallization, is quite slow, wee hope to cacth the structure of an intermediate of the reaction. For this, three data sets at different timesd (3 min, 5min and 10 min) were measured. I report here only the statistics for the 3 min data set.

N	1/d^2	Dmin(A)	Rmrg	Rfull	Rcum	Ranom	Nanom	Av_I	SIGMA	I/sigma	sd	Mn(I)/sd	Nmeas	Nref	Ncent	FRCBIAS	Nbias
1	0.0472	4.60	0.067	0.077	0.067	0.000	0	10494.	1432.0	7.3	1521.	11.4	3683	1248	106	-0.096	1170
2	0.0945	3.25	0.073	0.089	0.072	0.000	0	16800.	2583.2	6.5	2379.	12.2	8790	2764	147	-0.087	2578
3	0.1417	2.66	0.094	0.108	0.081	0.000	0	9649.	1676.7	5.8	1398.	12.4	14161	4109	168	-0.110	4073
4	0.1889	2.30	0.120	0.133	0.091	0.000	0	6087.	1319.7	4.6	951.	11.5	17608	4909	205	-0.132	4930
5	0.2362	2.06	0.136	0.149	0.099	0.000	0	4908.	1206.4	4.1	843.	10.5	20450	5567	221	-0.150	5743
6	0.2834	1.88	0.155	0.168	0.106	0.000	0	3090.	877.3	3.5	598.	8.9	22239	6099	211	-0.149	6281
7	0.3307	1.74	0.178	0.193	0.109	0.000	0	1856.	651.2	2.8	431.	6.2	14838	5192	165	-0.180	4125
8	0.3779	1.63	0.211	0.235	0.111	0.000	0	1267.	523.9	2.4	366.	4.6	8991	3713	127	-0.226	2295
9	0.4251	1.53	0.230	0.242	0.112	0.000	0	949.	428.0	2.2	342.	3.4	4801	2233	60	-0.271	1128
10	0.4724	1.45	0.250	0.311	0.112	0.000	0	659.	305.1	2.2	311.	2.4	1309	647	14	-0.244	305
Overall:			0.112	0.130	0.112	0.000	0	5507.	1286.1	4.3	901.	8.9	116870	36481	1424	-0.122	32628

	Rmrg	Rfull	Rcum	Ranom	Nanom	Av_I	SIGMA	I/sigma	sd	Mn(I)/sd	Nmeas	Nref	Ncent	FRCBIAS	Nbias

: Rmeas, Rsym & PCV v Resolution :N:2,13,14,15,16,17: $$

N	1/resol^2	Dmin	Nmeas	Nref	Ncent	%poss	C%poss	MlplctAnoCmpl	AnoFrc	AnoMlt	Rmeas	Rmeas0 (Rsym)	PCV	PCV0
1	0.047	4.60	4034	1599	168	87.3	87.3	2.5	0.0	0.0	0.0	0.084	0.084	0.067	0.093	0.093
2	0.094	3.25	9151	3125	193	96.0	92.9	2.9	0.0	0.0	0.0	0.091	0.091	0.073	0.102	0.102
3	0.142	2.66	14273	4221	216	99.7	96.0	3.4	0.0	0.0	0.0	0.113	0.113	0.094	0.128	0.128
4	0.189	2.30	17654	4955	229	99.9	97.4	3.6	0.0	0.0	0.0	0.142	0.142	0.120	0.163	0.163
5	0.236	2.06	20469	5586	230	100.0	98.1	3.7	0.0	0.0	0.0	0.159	0.159	0.136	0.185	0.185
6	0.283	1.88	22297	6157	224	99.5	98.4	3.6	0.0	0.0	0.0	0.182	0.182	0.155	0.210	0.210
7	0.331	1.74	15107	5461	175	81.1	94.9	2.8	0.0	0.0	0.0	0.223	0.223	0.178	0.265	0.265
8	0.378	1.63	9249	3971	132	55.1	87.7	2.3	0.0	0.0	0.0	0.276	0.276	0.211	0.318	0.318
9	0.425	1.53	5114	2546	78	33.1	78.8	2.0	0.0	0.0	0.0	0.315	0.315	0.230	0.366	0.366
10	0.472	1.45	1613	951	23	11.8	69.0	1.7	0.0	0.0	0.0	0.352	0.352	0.250	0.411	0.411
Overall			118961	38572	1668	69.0	69.0	3.1	0.0	0.0	0.0	0.135	0.135	0.112	0.154	0.154

	Nmeas	Nref	Ncent	%poss	C%poss	MlplctAnoCmpl	AnoFrc	AnoMlt	Rmeas	Rmeas0 (Rsym)	PCV	PCV0

Data processing is in progress, but preliminary analysis of the electron density map indicates that teh peptide is not yet bound. Data sets at a longer soaking time are probably necessary.