



	Experiment title: Ribose 5-phosphate B from <i>M. tuberculosis</i> in complex with potential inhibitor #1.	Experiment number: MX-133
Beamline: ID29	Date of experiment: 3rd April 2004	Date of report: 30 th Aug 2004
Shifts: 1/3	Local contact(s): William Shepard	
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Report:

Ribose-5-phosphate isomerase is an enzyme involved in the pentose phosphate pathway where it catalyses the interconversion of ribose-5-phosphate to ribulose-5-phosphate. Two non-homologous enzymes have been identified that perform this catalysis, RpiA and RpiB. Humans have the RpiA form whereas the pathogenic bacterium *M. tuberculosis* only has RpiB. Therefore this enzyme could be a good potential drug target. We solved the structure in 2003 (Roos et al.) and are now pursuing ligand complex structures to learn more about the reaction mechanism and to find possible inhibitory molecules. Potential inhibitor #1 has been designed by our collaborators at Organic Pharmaceutical Chemistry, Uppsala University by docking into the active site and is thought to be a starting template for designing a new drug. NMR studies have shown that #1 binds to RpiB.

A data set of a crystal cocrystallised with inhibitor #1 was collected on ID29 to 2.0 Ångström but no density for the ligand could be seen in the electron density map.

Roos, A.K., Andersson, C.E., Bergfors, T., Jacobsson, M., Karlen, A., Unge, T., Jones, T.A. and Mowbray, S.L. (2004). *Mycobacterium tuberculosis* ribose-5-phosphate isomerase has a known fold, but a novel active site. *J Mol Biol* **335**, 799-809.