EUROPEAN **S**YNCHROTRON **R**ADIATION **F**ACILITY

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Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF .

Once completed, the report should be submitted electronically to the User Office using the **Electronic Report Submission Application:**

http://193.49.43.2:8080/smis/servlet/UserUtils?start

Reports supporting requests for additional beam time

Reports can now be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

· fill in a separate form for each project or series of measurements.
· type your report, in English.
· include the reference number of the proposal to which the report refers.
· make sure that the text, tables and figures fit into the space available.
· if your work is published or is in press, you may prefer to paste in the

	Experiment title: Improving the structure of the anaerobic ribonucleotide reductase from bacteriophage T4	**Experiment number**: LS–1321
Beamline: ID14-3	**Date of experiment**: from: 19/4/1999 to: 20/4/1999	**Date of report**: 31/8/2001
Shifts: 3	**Local contact(s)**: Steffi Arzt	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

We collected several data sets from crystals of the anaerobic, class III ribonucleotide reductase from bacteriophage T4 soaked with the allosteric substrate specificity effectors dATP, dTTP and dGTP and with substrates. One of these was used in the published article but all were useful in preliminary analyses.

This work has been published in the following article:
Larsson K.-M., Andersson J., Sjöberg B.-M., Nordlund P & Logan D.T. (2001) Structural basis for allosteric substrate specificity regulation in anaerobic ribonucleotide reductases. ***Structure*** **9**, 739–750.

Abstract:

Background
The specificity of ribonucleotide reductases (RNRs) towards their four substrates is governed by binding of deoxyribonucleoside triphosphates (dNTPs) to the allosteric specificity site. Similar patterns in the kinetics of allosteric regulation have been a strong argument for a common evolutionary origin for the three otherwise widely divergent RNR classes. Recent structural information settled the case for divergent

currently poorly understood. A comparative study of the conformational effects of binding of different effectors has not yet been possible; in addition only one RNR class has been studied.

Results

We present structures of a class III, anaerobic RNR in complex with four dNTPs, allowing a full comparison of the protein conformations. Discrimination between the effectors is achieved by two side chains, Gln 114 and Glu 181, from separate monomers. Large conformational changes in the active site (loop 2), in particular Phe 194, are induced by effector binding. The overall differences are larger when comparing purine and pyrimidine effectors than when comparing purines or pyrimidines with each other.

Conclusions

The subtle differences in base size and hydrogen bonding pattern at the effector site are communicated to major conformational changes in the active site. We propose that the altered overlap of Phe 194 with the substrate base governs hydrogen bonding patterns with main- and side-chain hydrogen bonding groups in the active site. The relevance for evolution is discussed.