ESRF	**Experiment title:** **Structural studies on signal transduction pathways and cell cycle control.**	**Experiment number**: **LS-1526**
Beamline: ID14-EH3 ID14-EH4	**Date of experiment**: from: 24-09-99 to: 26-09-99 from: 13-11-99 to: 15-11-99	**Date of report**: August 31st, 2000
Shifts: 6	**Local contact(s)**: Dr. E. Mitchell	*Received at ESRF:*

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The Structure of Arylamine N-acetyltransferase

Enzymes of the arylamine N-acetyltransferase (NAT) family are found in species ranging from Escherichia coli to humans. In humans they are known to be responsible for the acetylation of a number of arylamine and hydrazine drugs, and they are strongly linked to the carcinogenic potentiation of certain foreign substances. In prokaryotes their substrate specificities may vary and members of the gene family have been linked to pathways including amide synthesis during rifamycin production. We have determined the crystal structure at 2.8 Å resolution of a representative member of this family from Salmonella typhimurium in the presence and absence of a covalently bound product analog. The structure revealed surprising mechanistic information including the presence of a Cys-His-Asp catalytic triad. The fold can be described in terms of three domains of roughly equal length with the second and third domains linked by an interdomain helix. The first two domains, a

Table 1 – Data collection and refinement statistics for SeMet datset collected on ID14-EH3

Figure 1 – Fold of Arylamine N-acetyltransferase from S. typhimurium showing position of catalytic triad

Table 1

Resolution: 30-2.8 Å

Observed reflections: 235,995

Unique reflections: 73,897

Completeness: 94.7%

Mean I / Mean s(I): 8.3

R-factor: 26.4%

R-free: 33.2%

RMSD bond lengths: 0.017 Å

RMSD angles: 1.81˚

No. atoms (Protein/Solvent): 17,792 / 472

Figure 1