

The 1.9Å structure of PA5083 – a 116 residue protein with 1 ordered sulfur - determined by Native-SAD using in-house data and phenix.autobuild recycling.

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The 1.9Å structure of PA5083 – a 116 residue protein with 1 ordered sulfur - determined by Native-SAD using in-house data and phenix.autobuild recycling.

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Abstract

PA5083 a Rid2 (Reactive Intermediate Deaminase) protein from *Pseudomonas aeruginosa* known to have broad imine deaminase activity against iminoarginine has been determined to 1.9Å resolution using Native-SAD. The Rid family enzymes are of interest since they play important roles in nutrition, amino acids biosynthesis, mitochondrial maintenance and other biological processes by reducing the accumulation of toxic metabolite intermediates.

The structure determination is noteworthy in that (1) the data were collected in-house ($\lambda = 1.5418$) and consisted of a single set of 1440 quarter degree images (total rotation 360°, multiplicity 16.6), (2) the 116 residue enzyme has only two sulfur containing residues (Met 1 and Cys 17) giving a Bijvoet ratio 0.374 assuming Met 1 is disordered (it was), (3) the initial results from phenix.autosol gave a "very low" (autosol) FOM of 0.16 with R and Rfree values of 0.5049 and 0.5505 respectively and (4) the structure was built from the initial autosol phases using several rounds of model building with phenix.autobuild. The R and Rfree values for the refined model are 0.200 and 0.233 respectively.

Details of the Native (sulfur atom)-SAD analysis and the PA5083 crystal structure will be presented.

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Keywords: Native (sulfur atom)-SAD; PA5083; Reactive Intermediate Deaminase; Rid2 Protein; Crystal Structure; Challenging Analysis