s8a.m7.o3 **Dioxygen reduction in strict anaerobes. Crystal structure of rubredoxin:oxygen oxidoreductase (ROO) from *Desulfovibrio gigas*.** C. Frazão[1], G. Silva[1], C. M. Gomes[1], P. Matias[1], R. Coelho[1], L. Sieker[1], S. Macedo[1], M. Y. Liu[2], S. Oliveira[1, 3], M. Teixeira[1], A. V. Xavier[1], C. Rodrigues-Pousada[1], M. A. Carrondo[1], and J. Le Gall[1,2]. *[1]Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Av. da República, Apartado 127, 2781-901 Oeiras, Portugal; [2]Department of Biochemistry and Molecular Biology, University of Georgia, Athens, Georgia 30602; [3]Universidade de Évora, 7001 Évora, Portugal*
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With the rise of atmospheric oxygen, living systems evolved enzymatic systems for its reduction to water, which provided a high energy yielding process. However, the presence of oxygen in the cell leads to production of highly toxic Reactive Oxygen Species (ROS), for which defense mechanisms had to be developed, even by the strict anaerobes that can tolerate transient contact with oxygen. For these organisms, the safer way to deal with the deleterious effects of ROS is to efficiently decrease the concentration of oxygen in the cell. A new metabolic pathway enabling such a process was established for the sulfate-reducing bacterium *Desulfovibrio* (*D.*) *gigas*[1]. The 3D structure of the terminal reductase of that pathway, rubredoxin:oxygen oxidoreductase (ROO)[2,3] reveals a novel assembly of cofactors and structural domains that accomplishes the direct reduction of dioxygen to water. The enzyme is a homodimer, with each monomer shown to be built by two structural domains: one β-lactamase-like, containing a diiron center, and another flavodoxin-like, harboring a flavin-mononucleotide. The enzyme quaternary structure assures a direct electron transfer between the flavin moiety – the primary electron acceptor from rubredoxin – and the diiron catalytic reaction center. *D. gigas* ROO is a member of a superfamily of highly homologous enzymes widespread in anaerobic prokaryotes, showing the biological relevance of this dioxygen reducing mechanism.

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s8a.m7.o4 **Zinc ion mediated amino acid recognition by threonyl-tRNA synthetase**. R. Sankaranarayanan[1], A-C. Dock Bregeon[1], B. Rees[1], M. Bovee[2], J. Caillet[3], P. Romby[4], C. Francklyn[2] and D. Moras[1]. *[1]UPR 9004 du Biologie Structurale, IGBMC, CNRS/INSERM/ULP, BP163-67404 Illkirch Cedex, [2]Department of Biochemistry, College of Medicine, University of Vermont, Burlington VT054045, USA, [3]UPR 9073 du CNRS, IBPC, 13 rue P. et M. Curie, 75005 Paris and [4]UPR 9002 du CNRS, IBMC, 15 rue Rene Descartes, 67084 Strasbourg Cedex, France.*
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Aminoacyl-tRNA synthetases play a crucial role in the translation of the genetic code by performing a two step aminoacylation reaction[1]. Threonyl-tRNA synthetase (ThrRS) from *E. coli* is a class II enzyme that represses the translation of its own mRNA[2]. The crystal structure of the enzyme in complex with its tRNA showed an unusual interaction of two adjacent anticodon bases which accounts for their prominent role in tRNA identity and translational regulation[3]. The threonyl system specific N-terminal extension envelops the acceptor stem recognizing the identity determinants from the minor groove side. A zinc ion, found for the first time in the active site of an aaRS, was implicated in amino acid recognition[3].

To understand the exact role played by the zinc ion and to investigate the basis of amino acid recognition, we have determined the crystal structures of complexes of an active truncated form of the enzyme in complex with a threonyl adenylate analog and threonine. The structures showed that the zinc ion is directly involved in threonine recognition by forming a pentacoordinate intermediate with both the amino and the side chain hydroxyl groups. With such a geometry of binding, the isosteric amino acid valine should be directly rejected by the enzyme. This is confirmed by amino acid activation experiments which show no activation of valine. However, the enzyme activates serine 1000-fold less than that of cognate threonine. The study demonstrates that with the use of a zinc ion the enzyme ensures that only threonine is activated to a meaningful extent *in vivo*.

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