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Structural insights in the SoxY protein of Chlorobium limicola f. thiosulfatophilum

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Dissimilatory oxidation of thiosulfate in *Chlorobium limicola* f. *thiosulfatophilum* is performed by a sulfur oxidizing multi-enzyme (Sox) system. The system is widespread in several Green Sulfur bacteria and phototrophic and non-phototrophic Proteobacteria, and becomes physiologically and genetically ever better understood [1, 2]. A few gaps in our knowledge of the structural biology of this system nevertheless need to be clarified. Here we present the first crystal structure of the SoxY component of the Sox-system. SoxY is involved in the initial phase of the reaction cycle and is responsible for the covalent binding of thiosulfate via a reactive cysteine. The resulting complex then serves as a substrate for the other components of the enzyme system. The structure determination of SoxY reveals a tetrameric organization. Each monomer consists of an N-terminal α-helix and an s-type immunoglobulin domain of which both β-sheets are associated with the β-sheets of a second, two-fold NCS-axis orientated monomer. A combination of main chain hydrogen bonds between the edge strands of both sheets and the hydrophobic effect of the inward pointing aliphatic and aromatic side chains enables the formation of a stable, extended dimeric β-sandwich. This secondary structure has the two α-helices on one side and interacts on the other side with a second dimeric β-sandwich via two identical binding patches. The tetramer contains, furthermore, a disulfide bridge between the reactive cysteines in the proximity of each dimeric interaction region. The structural information now obtained sets the stage for further biochemical and biophysical studies of the Sox-based reaction cycle.

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4',4',6',6'-tetrachloro-3,4-dihydro-3-(6-methylpyridin-2-yl)spiro[1,3,2-benzoxazaphosphinine-2,2'-(2λ^5,4λ^5,6λ^5-cyclotriphosphazene)]

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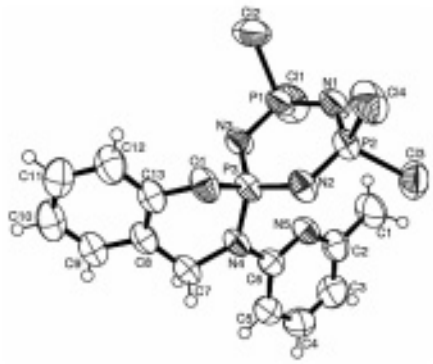
The crystal structure of $C_{13}H_{12}Cl_4N_5OP_3$ was determined from the intensity data measured with CuK_α radiation on a Nonius CAD-4 diffractometer. The crystals are triclinic, space group P -1 with a = 8.9834 (1), b = 9.5110 (2), c = 11.9857 (2) Å, α = 82.131 (2), β= 87.598 (1), γ= 81.992 (2)° and Z = 2. The parameters obtained by direct methods using SHELXS97 [1] were full-matrix least squares refined by using SHELXL97 [1] to an R value of 0.063 for 3274 reflections. During data collection 4003 reflections were measured where 3909 of them are independent. Molecular graphics were drawn by using ORTEP-3 for Windows [2].
$C_{13}H_{12}Cl_4N_5OP_3$ is a phosphazene derivative with a bulky substituted spirocyclic ring. The phosphazene ring is not completely planar, having a total puckering amplitude, Q_T, of 0.078(2) Å [3] and a flattened boat form (ϕ = 64.3 (16)° and θ = 96.1°). In the phosphazene ring, the P-N bond lengths are in the range 1.558 (3)-1.584 (3) Å. The P-N bonds of the phosphazene ring have double-bond character. However, the exocyclic P3-N4 bond [1.642 (3) Å] is at the lower limit for a single bond. The shortness of the P3-N4 bond indicates that electron release has occurred from the lone pairs of electrons of atom N4 to the phosphazene ring.
In the phosphazene ring, the endocyclic N2-P3-N3 angle [116.45 (14)°] is smaller than and the exocyclic O1-P3-N4 angle [101.66 (13)°] is almost the same as those of the 'standard' compound $N_3P_3Cl_6$ [4]; these values are consistent with electron donation and withdrawal by the substituents in $C_{13}H_{12}Cl_4N_5OP_3$.



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