s1.m7.p1 **Crystal structure of an intact group I self-splicing intron in complex with both introns.** Peter L. Adams, Mary R. Stahley, Anne B. Kosek, Jimin Wang and Scott A. Strobel, *Department of Molecular Biophysics and Biochemistry, 260 Whitney Ave., Yale University, New Haven, CT 06520-8114. E-mail: padams@csb.yale.edu*

Keywords: RNA; Catalysis; Splicing

The group I intron is a metalloenyzme that catalyzes two consecutive phosphotransfer reactions in the course of exon ligation. We have determined a 3.1Å crystal structure of the group I self-splicing intron from the pre-tRNA^{Ile} anticodon loop of the purple bacterium *Azoarcus*. It has been crystallized in the state prior to the exon ligation step. The intron is complexed with both the 5′ and 3′ exons (222 nucleotides total) and shows both the basis for splice site selection and the location of metal ion co-factors. The 5′ splice site is mediated by an extensive network of secondary and tertiary interactions. All the tertiary contacts to the 5′ exon are non-sequence specific interactions with the ribose backbone. There no tertiary contacts with the 3' exon. The 3' splice site appears to be selected primarily by interactions with the last G of the intron, □G (G206). G206 is sandwiched between A127 and G128, and the Watson-Crick face of G206 hydrogen bonds with the Hoogsteen edge of the universally conserved G130 in the P7 helix. There is a complete reversal in strand direction at the splice junction between the intron and the 3′ exon, which aligns the scissile phosphate for in-line nucleophilic attack by the 5′ exon. Two metal ions co-factors (5.4 Å apart) flank the scissile phosphate and are positioned by a unique arrangement of the phosphate backbone. A magnesium ion, equivalent to the biochemically defined MA, is coordinated by five pro-Sp oxygens, including that of the scissile phosphate. The second site, which is in some ways analogous to the biochemically defined metal MC, is occupied by a potassium ion. Overall, the intron has a compact structure consisting of three main helical elements (P10/1/2, P4/5/6 and P3/8/7/9.0) that are linked by extensive tertiary interactions, via the joiner segments and metal ions. This is the first crystal structure of RNA splicing complex. The second step of splicing visualized in this structure is analogous to in the reaction catalyzed during group II intron and nuclear pre-RNA splicing.

s1.m7.p2 **Crystal structure of photosystem II at 3.2 A provides new details of protein-cofactor interactions.** Jacek Biesiadka,[a] Bernhard Loll,[a] Jan Kern,[b] Klaus-Dieter Irrgang,[b] Athina Zouni[b] and Wolfram Saenger[a], [a]*Institute for Chemistry/Crystallography, Free University Berlin, Takustrasse 6, D-14195 Berlin, Germany, and* [b]*Institute for Chemistry/Max Volmer Laboratory for Biophysical Chemistry, Technical University Berlin, Strasse des 17. Juni 135, D-10623 Berlin, Germany. E-mail: jabies@chemie.fu-berlin.de*

Keywords: Photosynthesis; Photosystem; Membrane protein complex

The photosystem II (PSII), a multi subunit protein-pigment complex located in the thylakoid membrane of plants, green algae and cyanobacteria, carries out the light driven oxidation of water, evolving oxygen. We isolated PSII from the photoautotrophic thermophilic cyanobacterium *Thermosynechococcus elongatus*. The crystals are capable in water oxidation [1], confirming that this sensitive molecular apparatus has not changed structurally during the crystallisation.

PSII occurs as homodimer [2] with the monomers related by a non-crystallographic twofold axis. Of the at least 14 membrane-intrinsic protein subunits in the monomer, six were identified: the reaction center proteins D1 and D2, core antennae CP43 and CP47, and α- and β-chains of cytochrome *b-559*. The remaining 12 transmembrane α-helices belong to smaller subunits, some of which were tentatively assigned based on biochemical data. The membrane-extrinsic subunits PsbO, PsbU and PsbV (cytochrome *c-550*) were localized on the lumenal side of PSII.

A big variety of prosthetic groups take part in the electron transfer: chlorophyll, pheophytine, heme, quinone, β-carotene and a manganese cluster.

PSII captures sun light by two membrane-intrinsic antenna proteins habouring chlorophyll *a* (Chl*a*) molecules arranged in two layers. The excitation energy is transferred to the photochemical reaction center with primary electron donor P680 formed by Chl*a* molecule(s). The primary donor is oxidized to $P680^{+\cdot}$, and the released electron travels along the electron transfer chain featuring two pairs of Chla, one pair of pheophytin a and two plastoquinones (Q_A and Q_B). Doubly reduced and protonated Q_B leaves PSII as plastoquinol Q_BH_2, and the reducing equivalents finally convert $NADP^+$ to NADPH. $P680^{+\cdot}$ is re-reduced via redox-active tyrosine Tyr_Z by an electron from a Mn-cluster catalyzing oxidation of water to atmospheric oxygen.

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[2] A. Zouni, HT. Witt, J.Kern, P. Fromme, N. Krauss, W. Saenger, P. Orth (2001), *Nature* **409**, 739.