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Photosystem II at 2.9 Å Resolution - Quinones, Lipids, Channels and Chloride Ion. Wolfram Saenger[a], Albert Guskov[a], Azat Gabdulkhakov[a], Matthias Broser[b], Jan Kern[b], Athina Zouni[b]. [a]*Freie Universitaet Berlin, Institute for Chemistry and Biochemistry/Crystallography, Berlin, Germany.* [b]*Technische Universitaet Berlin, Max Volmer Laboratory for Biophysical Chemistry, Berlin, Germany.*
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Photosystem II (PSII) is a large homodimeric protein-cofactor complex that acts as light-driven water:plastoquinone oxidoreductase and is located in the photosynthetic thylakoid membrane of plants, green algae and cyanobacteria. The principal function of PSII is to oxidize two water molecules at the unique Mn_4Ca cluster to molecular (atmospheric) oxygen, 4 protons and 4 electrons. The protons serve to drive ATP synthetase and the electrons reduce plastoquinone (Q_B) to plastoquinol (Q_BH_2) that is exported and delivers the electrons (through the cytochrome b_6f complex) to photosystem I. Here the electrons gain a high reducing potential and serve at NADP reductase to generate NADPH that together with ATP reduces CO_2 to carbohydrates in the Calvin cycle.
The crystal structure of PSII from *Thermosynechococcus elongatus* at 2.9-Å resolution [1] allowed the unambiguous assignment of all 20 protein subunits and complete modeling of all 35 chlorophyll *a*, 2 pheophytin, 2 cytochrome, 2 plastoquinone, and 12 carotenoid molecules, 25 integral lipids, 1 chloride ion and the Mn_4Ca cluster per PSII monomer. The presence of a third plastoquinone Q_C and a second plastoquinone-transfer channel, which were not observed before, suggest mechanisms for plastoquinol-plastoquinone exchange, and we calculated other possible water or dioxygen and proton channels. Putative oxygen positions obtained from Xenon derivative crystals indicate a role for lipids in oxygen diffusion to the cytoplasmic side of PSII. The chloride position suggests a role in proton-transfer reactions because it is bound through a putative water molecule to the Mn_4Ca cluster at a distance of 6.5 Å and is close to two possible proton transfer channels.

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Structure and Molecular Mechanism of a Nucleobase -Cation-Symport-1 Family Transporter. Simone Weyand[a,b,c], Tatsuro Shimamura[b,c,d], Shunsuke Yajima[b,c], Shun'ichi Suzuki[e], Osman Mirza[b], Kuakarun Krusong[b], Elisabeth P. Carpenter[a,b], Nicholas G. Rutherford[e], Jonathan M. Hadden[e], John O'Reilly[e], Pikyee Ma[e], Massoud Saidijam[e], Simon G. Patching[e], Ryan J. Hope[e], Halina T. Norbertczak[e], Peter C. J. Roach[e], So Iwata[a,b,c,d,f], Peter J. F. Henderson[e], Alexander D. Cameron[a,b,c]. [a]*Membrane Protein Laboratory, Diamond Light Source, Harwell Science and Innovation Campus, Chilton, Didcot, Oxfordshire OX11 0DE, UK.* [b]*Division of Molecular Biosciences, Membrane Protein Crystallography Group, Imperial College, London SW7 2AZ, UK.* [c]*Human Receptor Crystallography Project, ERATO, Japan Science and Technology Agency, Yoshidakonoe-cho, Sakyo-ku, Kyoto 606- 8501, Japan.* [d]*Department of Cell Biology, Graduate School of Medicine, Kyoto University, Yoshida-Konoe, Sakyo-Ku, Kyoto 606-8501, Japan.* [e]*Astbury Centre for Structural Molecular Biology, Institute for Membrane and Systems Biology, University of Leeds, Leeds LS2 9JT, UK.* [f]*Systems and Structural Biology Center, RIKEN, 1-7-22 Suehiro-cho Tsurumi-ku, Yokohama 230-0045 Japan.*
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Membrane transport proteins are usually classified into three groups: the primary active transporters, the secondary active transporters and those using diffusion without energy. The molecular mechanism of all of them is based on the alternating access model [1]. Mhp1 belongs to the nucleobase–cation–symport-1 family of secondary active transporters enabling the uptake of indolyl methyl- and benzyl-hydantoins into M. liquefaciens. This is part of a metabolic salvage pathway for their conversion to amino acids [2].
Mhp1 has been cloned, heterologously expressed in E.coli, purified and crystallized. The strucure was solved by MIRAS and refined at 2.85 Å resolution to R=24% and R free=28.1% [3]. A second structure with the substrate bound was solved by molecular replacement.
The overall architecture of the protein shows a monomer with 12 transmembrane helices. The helices are arranged in two repeating units (1-5 and 6-10), showing an opposite topology with respect to the membrane and are related to each other by a rotation of 168° around an axis in the center of the membrane and parallel to its plane. The substratesand cation-binding sites are all located in between a central four-helix bundle and the surrounding helix coat.
The outward-facing open and outward-facing occluded structures of this protein give detailed insights in the closing mechanism of the substrate binding site. A comparison to proteins with similar fold, LeuT Aa and vSGLT, discloses the symmetrically inverted arrangement of the cavities in the outward and inward facing conformations. The reciprocal opening and closing of these cavities is synchronized by the inverted repeat helices 3 and 8.
These results give for the first time structural insight in the molecular mechanism of the alternate access model [3].