References

Adam, Z. and Ostersetzer, O. (2001) Degradation of unassembled and damaged thylakoid proteins. *Biochem Soc Trans*, **29**, 427-430.

Adamian, L. and Liang, J. (2002) Interhelical hydrogen bonds and spatial motifs in membrane proteins: polar clamps and serine zippers. *Proteins*, **47**, 209-218.

Adir, N. (1999) Crystallization of the oxygen-evolving reaction centre of photosystem II in nine different detergent mixtures. *Acta Crystallogr D Biol Crystallogr*, **55**, 891-894.

Adir, N., Okamura, M.Y. and Feher, G. (1992) Crystallization of the PSII-reaction centre. In Murata, N. (ed.), *Research in Photosynthesis*. Kluwer Academic Press, Dordrecht, The Netherland, Vol. II, pp. 195-198.

Ahlbrink, R., Haumann, M., Cherepanov, D., Bogershausen, O., Mulkidjanian, A. and Junge, W. (1998) Function of tyrosine Z in water oxidation by photosystem II: electrostatical promotor instead of hydrogen abstractor. *Biochemistry*, **37**, 1131-1142.

Ahmed, A., Tajmir-Riahi, H.A. and Carpentier, R. (1995) A quantitative secondary structure analysis of the 33 kDa extrinsic polypeptide of photosystem II by FTIR spectroscopy. *FEBS Lett*, **363**, 65-68.

Akabori, K., Tsukamoto, H., J., T., Nagatsuka, T., Motokawa, O. and Toyashima, Y. (1988) Disintegration and reconstitution of photosystem II reaction centre core complex. I. Preparation and characterisation of 3 different types of subcomplex. *Biochim Biophys Acta*, **932**, 345-357.

Allen, J.P., Artz, K., Lin, X., Williams, J.C., Ivancich, A., Albouy, D., Mattioli, T.A., Fetsch, A., Kuhn, M. and Lubitz, W. (1996) Effects of hydrogen bonding to a bacteriochlorophyll-bacteriopheophytin dimer in reaction centers from *Rhodobacter sphaeroides*. *Biochemistry*, **35**, 6612-6619.

Ananyev, G.M., Sakiyan, I., Diner, B.A. and Dismukes, G.C. (2002) A Functional Role for Tyrosine-D in Assembly of the Inorganic Core of the Water Oxidase Complex of Photosystem II and the Kinetics of Water Oxidation. *Biochemistry*, **41**, 974-980.

Anbudurai, P.R., Mor, T.S., Ohad, I., Shestakov, S.V. and Pakrasi, H.B. (1994) The *ctpA* gene encodes the C-terminal processing protease for the D1 protein of the photosystem II reaction center complex. *Proc Natl Acad Sci U S A*, **91**, 8082-8086.

Aro, E.M., Virgin, I. and Andersson, B. (1993) Photoinhibition of Photosystem-2 - Inactivation, Protein Damage and Turnover. *Biochim Biophys Acta*, **1143**, 113-134.

Astashkin, A.V., Kodera, Y. and Kawamori, A. (1994) Distance between tyrosines Z^+ and D^+ in plant Photosystem II as determined by pulsed EPR. *Biochim Biophys Acta*, **1187**, 89-93.

Awramik, S.M. (1992) The oldest records of photosynthesis. *Photosynth Res*, **33**, 75-89.

Ban, N., Nissen, P., Hansen, J., Moore, P.B. and Steitz, T.A. (2000) The complete atomic structure of the large ribosomal subunit at 2.4 Å resolution. *Science*, **289**, 905-920.

Barbato, R., Race, H.L., Friso, G. and Barber, J. (1991) Chlorophyll levels in the pigment-binding proteins of photosystem II. A study based on the chlorophyll to cytochrome ratio in different photosystem II preparations. *FEBS Lett*, **286**, 86-90.

Barber, J. and Archer, M.D. (2001) P680, the primary electron donor of photosystem II. *J Photochem Photobiol A*, **142**, 97-106.

Barker, P.D. and Ferguson, S.J. (1999) Still a puzzle: why is haem covalently attached in *c*-type cytochromes? *Structure Fold Des*, **7**, 281-290.

Barter, L.M., Durrant, J.R. and Klug, D.R. (2003) A quantitative structure-function relationship for the Photosystem II reaction center: Supermolecular behavior in natural photosynthesis. *Proc Natl Acad Sci U S A*, **100**, 946-951.

Bassi, R., Pineau, B., Dainese, P. and Marquardt, J. (1993) Carotenoid-binding proteins of photosystem II. *Eur J Biochem*, **212**, 297-303.

Berglund, G.I., Carlsson, G.H., Smith, A.T., Szoke, H., Henriksen, A. and Hajdu, J. (2002) The catalytic pathway of horseradish peroxidase at high resolution. *Nature*, **417**, 463-468.

Berthomieu, C., Boussac, A., Mantele, W., Breton, J. and Nabedryk, E. (1992) Molecular changes following oxidoreduction of cytochrome *b*559 characterized by Fourier transform infrared difference spectroscopy and electron paramagnetic resonance: photooxidation in photosystem II and electrochemistry of isolated cytochrome *b*559 and iron protoporphyrin IX- bisimidazole model compounds. *Biochemistry*, **31**, 11460-11471.

Berthomieu, C. and Hienerwadel, R. (2001) Iron Coordination in Photosystem II: Interaction between bicarbonate and the Q_B pocket studied by Fourier transform Iinfrared spectroscopy. *Biochemistry*, **40**, 4044-4052.

Bibby, T.S., Nield, J. and Barber, J. (2001a) Iron deficiency induces the formation of an antenna ring around trimeric photosystem I in cyanobacteria. *Nature*, **412**, 743-745.

Bibby, T.S., Nield, J. and Barber, J. (2001b) Three-dimensional model and characterization of the iron stress-induced CP43'-photosystem I supercomplex isolated from the cyanobacterium Synechocystis PCC 6803. *J Biol Chem*, **276**, 43246-43252.

Bibby, T.S., Nield, J., Partensky, F. and Barber, J. (2001c) Oxyphotobacteria. Antenna ring around photosystem I. *Nature*, **413**, 590.

Biesiadka, J., Loll, B., Kern, J., Irrgang, K.-D. and Zouni, A. (2004) Crystal structure of cyanobacterial photosystem II at 3.2 Å resolution: a closer look at the Mn-cluster. *Phys Chem Chem Phys*, **6**, 4733-4736.

Boekema, E.J., Hifney, A., Yakushevska, A.E., Piotrowski, M., Keegstra, W., Berry, S., Michel, K.P., Pistorius, E.K. and Kruip, J. (2001) A giant chlorophyll-protein complex induced by iron deficiency in cyanobacteria. *Nature*, **412**, 745-748.

Boekema, E.J., van Breemen, J.F., van Roon, H. and Dekker, J.P. (2000) Arrangement of photosystem II supercomplexes in crystalline macrodomains within the thylakoid membrane of green plant chloroplasts. *J Mol Biol*, **301**, 1123-1133.

Boichenko, V.A., Hou, J.M. and Mauzerall, D. (2001) Thermodynamics of electron transfer in oxygenic photosynthetic reaction centers: volume change, enthalpy, and entropy of electron-transfer reactions in the intact cells of the cyanobacterium *Synechocystis* PCC 6803. *Biochemistry*, **40**, 7126-7132.

Boussac, A. and Rutherford, A.W. (1996) Nature of the inhibition of the oxygen-evolving enzyme of photosystem-II induced by NaCl washing and reversed by the addition of Ca^{2+} or Sr^{2+}. *Biochemistry*, **27**, 3476-3483.

Bricker, T.M. (1990) The structure and function of CPa-1 and CPa-2 in photosystem II. *Photosynth Res*, **24**, 1-13.

Bricker, T.M. and Frankel, L.K. (1987) Use of a monoclonal antibody in structural investigations of the 49-kDa polypeptide of photosystem II. *Arch Biochem Biophys*, **256**, 295-301.

Bricker, T.M. and Frankel, L.K. (1998) The structure and function of the 33 kDa extrinsic protein of photosystem II: a critical assessment. *Photosynth Res*, **56**, 157-173.

Bricker, T.M. and Frankel, L.K. (2002) The structure and function of CP47 and CP43 in Photosystem II. *Photosynthesis Research*, **72**, 131-146.

Bricker, T.M., Odom, W.R. and Queirolo, C.B. (1988) Close association of the 33-kDa extrinsic protein with the apoprotein of CPA1 in photosystem-II. *FEBS Lett*, **231**, 111-117.

Brünger, A.T., Adams, P.D., Clore, G.M., DeLano, W.L., Gros, P., Grosse-Kunstleve, R.W., Jiang, J.S., Kuszewski, J., Nilges, M., Pannu, N.S., Read, R.J., Rice, L.M., Simonson, T. and Warren, G.L. (1998) Crystallography & NMR system: A new software suite for macromolecular structure determination. *Acta Crystallogr D Biol*, **54 (Pt 5)**, 905-921.

Brünger, A.T., Krukowski, A. and Erickson, J.W. (1990) Slow-cooling protocols for crystallographic refinement by simulated annealing. *Acta Crystallogr A,* **46 (Pt 7)**, 585-593.

Burmeister, W.P. (2000) Structural changes in a cryo-cooled protein crystal owing to radiation damage. *Acta Crystallogr D Biol Crystallogr*, **56 (Pt 3)**, 328-341.

Burnap, R.L., Qian, M. and Pierce, C. (1996) The manganese stabilizing protein of photosystem II modifies the *in vivo* deactivation and photoactivation kinetics of the H_2O oxidation complex in *Synechocystis sp.* PCC6803. *Biochemistry*, **35**, 874-882.

Buser, C.A., Diner, B.A. and Brudvig, G.W. (1992) Photooxidation of cytochrome b_{559} in oxygen-evolving photosystem II. *Biochemistry*, **31**, 11449-11459.

Buser, C.A., Thompson, L.K., Diner, B.A. and Brudvig, G.W. (1990) Electron-transfer reactions in manganese-depleted photosystem II. *Biochemistry*, **29**, 8977-8985.

Bylina, E.J., C., K., McDowell, L., Holten, D. and Youvan, D.C. (1988) Influence of an amino-acid residue on the optical properties and electron transfer dynamics of a photosynthetic reaction centre complex. *Nature*, **336**, 182-184.

Camara-Artigas, A., Brune, D. and Allen, J.P. (2002) Interactions between lipids and bacterial reaction centers determined by protein crystallography. *Proc Natl Acad Sci U S A*, **99**, 11055-11060.

Campbell, K.A., Peloquin, J.M., Diner, B.A., Tang, X.-S., Chisholm, D.A. and Britt, R.D. (1997) The τ -nitrogen of D2 histidine 189 is the hydrogen bond donor to the tyrosine radical Y_D of Photosystem II. *J Am Chem Soc*, **119**, 4787 -4788.

Carrell, T.G., Tyryshkin, A.M. and Dismukes, G.C. (2002) An evaluation of structural models for the photosynthetic water-oxidizing complex derived from spectroscopic and X-ray diffraction signatures. *J Biol Inorg Chem*, **7**, 2-22.

Castenholz, R.W. (1988) Culturing Methods for Cyanobacteria. In *Methods Enzymol*, Vol. 58, pp. 68-100.

Cinco, R.M., Robblee, J.H., Messinger, J., Fernandez, C., McFarlane Holman, K.L., Sauer, K. and Yachandra, V.K. (2004) Orientation of calcium in the Mn_4Ca cluster of the oxygen-evolving complex determined using polarized strontium EXAFS of photosystem II membranes. *Biochemistry*, **43**, 13271-13282.

Cinco, R.M., Robblee, J.H., Rompel, A., Fernandez, C., Yachandra, V.K., Sauer, K. and Klein, M.P. (1998) Strontium EXAFS Reveals the Proximity of Calcium to the Manganese Cluster of Oxygen-Evolving Photosystem II. *J Phys Chem B*, **102**, 8248-8256.

Cohen, G.E. (1997) ALIGN: a program to superimpose protein coordinates, accounting for insertions and deletions. *J Appl Cryst*, **30**, 1160-1161.

Cowtan, K. (1999) Error estimation and bias correction in phase-improvement calculations. *Acta Crystallogr D Biol Crystallogr*, **55 (Pt 9)**, 1555-1567.

Cowtan, K. (2000) General quadratic functions in real and reciprocal space and their application to likelihood phasing. *Acta Crystallogr D Biol Crystallogr*, **56 Pt 12**, 1612-1621.

Cramer, P., Bushnell, D.A. and Kornberg, R.D. (2001) Structural basis of transcription: RNA polymerase II at 2.8 Å resolution. *Science*, **292**, 1863-1876.

Cuni, A., Xiong, L., Sayre, R., Rappaport, F. and Lavergne, J. (2004) Modification of the pheophytin midpoint potential in photosystem II: Modulation of the quantum yield of charge separation and of charge recombination pathways. *Phys Chem Chem Phys*, **6**, 4825-4831.

de Las Rivas, J., Andersson, B. and Barber, J. (1992) Two sites of primary degradation of the D1-protein induced by acceptor or donor side photo-inhibition in photosystem II core complexes. *FEBS Lett*, **301**, 246-252.

de Weerd, F.L., Palacios, M.A., Andrizhiyevskaya, E.G., Dekker, J.P. and van Grondelle, R. (2002a) Identifying the lowest electronic states of the chlorophylls in the CP47 core antenna protein of photosystem II. *Biochemistry*, **41**, 15224-15233.

de Weerd, F.L., van Stokkum, I.H., van Amerongen, H., Dekker, J.P. and van Grondelle, R. (2002b) Pathways for energy transfer in the core light-harvesting complexes CP43 and CP47 of photosystem II. *Biophys J*, **82**, 1586-1597.

Debenham, J.M., Hao, Q., Hasnain, S.S., Dodd, F.E., Abraham, Z.H.L. and Eady, R.R. (1996) Structure Solution of Azurin II from Alcaligenes xylosoxidans using the Laue Method: Possibility of Studying In Situ Redox Changes using X-rays. *J. Synchrotron Rad.*, **3**, 14-19.

Debus, R.J. (1992) The manganese and calcium ions of photosynthetic oxygen evolution. *Biochim Biophys Acta*, **1102**, 269-352.

Debus, R.J. (2001) Amino acid residues that modulate the properties of tyrosine Y(Z) and the manganese cluster in the water oxidizing complex of photosystem II. *Biochim Biophys Acta*, **1503**, 164-186.

Debus, R.J., Campbell, K.A., Pham, D.P., Hays, A.M. and Britt, R.D. (2000) Glutamate 189 of the D1 polypeptide modulates the magnetic and redox properties of the manganese cluster and tyrosine Y_Z in photosystem II. *Biochemistry*, **39**, 6275-6287.

Deisenhofer, J., Epp, O., Miki, K., Huber, R. and Michel, H. (1984) X-ray structure analysis of a membrane protein complex. Electron density map at 3 Å resolution and a model of the chromophores of the photosynthetic reaction center from *Rhodopseudomonas viridis*. *Journal of Molecular Biology*, **180**, 385-398.

Deisenhofer, J., Epp, O., Miki, K., Huber, R. and Michel, H. (1985) Structure of the protein subunits in the photosynthetic reaction centre of *Rhodopseudomonas viridis* at 3Å resolution. *Nature*, **318**, 618-624.

Deisenhofer, J., Epp, O., Sinning, I. and Michel, H. (1995) Crystallographic refinement at 2.3 Å resolution and refined model of the photosynthetic reaction centre from *Rhodopseudomonas viridis*. *J Mol Biol*, **246**, 429-457.

DeRose, V.J., Mukerji, I., Latimer, M.J., Yachandra, V.K., Sauer, K., Andrews, J.C. and Klein, M.P. (1994) Comparison of the manganese oxygen-evolving complex in photosystem II of spinach and *Synechococcus* sp. with multinuclear manganese model compounds by X-ray absorption spectroscopy. *J. Am. Chem. Soc.*, **116**, 5239-5249.

Desiraju, G.R. and Steiner, T. (1999) *The Weak Hydrogen Bond in Structural Chemistry and Biology*, (Oxford Univ. Press, Oxford).

Diner, B.A. (2001) Amino acid residues involved in the coordination and assembly of the manganese cluster of photosystem II. Proton-coupled electron transport of the redox-active tyrosines and its relationship to water oxidation. *Biochim Biophys Acta*, **1503**, 147-163.

Diner, B.A., Force, D.A., Randall, D.W. and Britt, R.D. (1998) Hydrogen bonding, solvent exchange, and coupled proton and electron transfer in the oxidation and reduction of redox-active tyrosine Y(Z) in Mn-depleted core complexes of photosystem II. *Biochemistry*, **37**, 17931-17943.

Diner, B.A., Schlodder, E., Nixon, P.J., Coleman, W.J., Rappaport, F., Lavergne, J., Vermaas, W.F.J. and Chisholm, D.A. (2001) Site-directed mutations at D1-His198 and D2-His197 of photosystem II in *Synechocystis* PCC 6803: Sites of primary charge separation and cation and triplet stabilization. *Biochemistry*, **40**, 9265-9281.

Doucet, J. and Benoit, J.P. (1987) Molecular dynamics studied by analysis of the X-ray diffuse scattering from lysozyme crystals. *Nature*, **325**, 643-646.

Eaton-Rye, J. and Vermaas, W. (1992) *Characterization of a histidine to glutamine substitution at residue 469 in Photosystem II*. Kluwer Academic Publishers, Dordrecht.

Eaton-Rye, J.J. and Murata, N. (1989) Evidence that the amino-terminus of the 33 kDa extrinsic is required for binding to the photosystem II complex. *Biochim Biophys Acta*, **977**, 219-226.

Enami, I., Kamo, M., Ohta, H., Takahashi, S., Miura, T., Kusayanagi, M., Tanabe, S., Kamei, A., Motoki, A., Hirano, M., Tomo, T. and Satoh, K. (1998) Intramolecular cross-linking of the extrinsic 33-kDa protein leads to loss of oxygen evolution but not its ability of binding to photosystem II and stabilization of the manganese cluster. *J Biol Chem*, **273**, 4629-4634.

Enami, I., Kaneko, M., Kitamura, N., Koike, H., Sonoike, K., Inoue, Y. and Katoh, S. (1991) Total immobilisation of the extrinsic 33-kDa protein in spinach photosystem II membrane preparations. Protein stoichiometry and stabilisation of oxygen evolution. *Biochim Biophys Acta*, **1060**, 224-232.

Enami, I., Ohta, S., Mitsuhashi, S., Takahashi, S., Ikeuchi, M. and Katoh, S. (1992) Evidence from crosslinking for a close association of the extrinsic 33 kDa protein with the 9.4 kDa subunit of cytochrome *b*-559 and the 4.8 kDa product of the psbI gene in oxygen evolving photosystem II complexes from spinach. *Plant Cell Physiol*, **33**, 291-297.

Engh, R.A. and Huber, R. (1991) Accurate bond and angle parameters for X-ray protein-structure refinement. *Acta Cryst. A47*, **1320**, 392-400.

Faller, M., Niederweis, M. and Schulz, G.E. (2004) The structure of a mycobacterial outer-membrane channel. *Science*, **303**, 1189-1192.

Faller, P., Maly, T., Rutherford, A.W. and MacMillan, F. (2001) Chlorophyll and Carotenoid Radicals in Photosystem II Studied by Pulsed ENDOR. *Biochemistry*, **40**, 320-326.

Ferreira, K.N., Iverson, T.M., Maghlaoui, K., Barber, J. and Iwata, S. (2004) Architecture of the photosynthetic oxygen-evolving center. *Science*, **303**, 1831-1838.

Fleming, G.R., Martin, J.L. and Breton, J. (1988) Rates of primary electron-transfer in photosynthetic centers and their mechanistic implications. *Nature*, **333**, 190-192.

Frank, H.A. and Brudvig, G.W. (2004) Redox functions of carotenoids in photosynthesis. *Biochemistry*, **43**, 8607-8615.

Fritzsch, G., Koepke, J., Diem, R., Kuglstatter, A. and Baciou, L. (2002) Charge separation induces conformational changes in the photosynthetic reaction centre of purple bacteria. *Acta Crystallogr D Biol Crystallogr*, **58**, 1660-1663.

Fujiwara, M., Hayashi, H., Tasumi, M., Kanaji, M., Koyama, Y. and Satoh, K. (1987) Structural studies on a Photosystem II reaction center complex consisting of D-1 and D-2 polypeptides and cytochrome *b*-559 by resonance Raman spectroscopy and high-Performance liquid- chromatography. *Chemistry Letters*, 2005-2008.

Galtier, N., Gouy, M. and Gautier, C. (1996) SEAVIEW and PHYLO_WIN: two graphic tools for sequence alignment and molecular phylogeny. *Comput Appl Biosci*, **12**, 543-548.

Ghanotakis, D.F., Babcock, G.T. and Yocum, C.F. (1985) Structure of the oxygen-evolving complex of photosystem II: calcium and lanthanum compete for sites on the oxidizing side of photosystem II which control the binding of watersoluble polypeptides and regulate the activity of the manganese complex. *Biochim. Biophys. Acta*, **809**, 173-180.

Giorgi, L.B., Nixon, P.J., Merry, S.A., Joseph, D.M., Durrant, J.R., De Las Rivas, J., Barber, J., Porter, G. and Klug, D.R. (1996) Comparison of primary charge separation in the photosystem II reaction center complex isolated from wild-type and D1-130 mutants of the cyanobacterium *Synechocystis* PCC 6803. *J Biol Chem*, **271**, 2093-2101.

Gleiter, H.M., Haag, E., Shen, J.R., Eaton-Rye, J.J., Inoue, Y., Vermaas, W.F. and Renger, G. (1994) Functional characterization of mutant strains of the cyanobacterium *Synechocystis* sp. PCC 6803 lacking short domains within the large, lumen-exposed loop of the chlorophyll protein CP47 in photosystem II. *Biochemistry*, **33**, 12063-12071.

Gleiter, H.M., Haag, E., Shen, J.R., Eaton-Rye, J.J., Seeliger, A.G., Inoue, Y., Vermaas, W.F. and Renger, G. (1995) Involvement of the CP47 protein in stabilization and photoactivation of a functional water-oxidizing complex in the cyanobacterium *Synechocystis* sp. PCC 6803. *Biochemistry*, **34**, 6847-6856.

Glover, I.D., Harris, G.W., Helliwell, J.R. and Moss, D.S. (1991) The variety of X-ray diffuse scattering from macromolecular crystals and its respective components. *Acta Cryst B47*, 960–968.

Golden, S.S. (1995) Light-responsive gene expression in cyanobacteria. *J Bacteriol*, **177**, 1651-1654.

Golden, S.S., Brusslan, J. and Haselkorn, R. (1986) Expression of a family of *psbA* genes encoding a photosystem II polypeptide in the cyanobacterium *Anacystis nidulans* R2. *EMBO J*, **5**, 2789-2798.

Golden, S.S., Cho, D.S. and Nalty, M.S. (1989) Two functional *psbD* genes in the cyanobacterium *Synechococcus* sp. strain PCC 7942. *J Bacteriol*, **171**, 4707-4713.

Golden, S.S. and Stearns, G.W. (1988) Nucleotide sequence and transcript analysis of three photosystem II genes from the cyanobacterium *Synechococcus* sp. PCC7942. *Gene*, **67**, 85-96.

Gounaris, K., Chapman, D.J., Booth, P., Crystall, B., Giorgi, L.B., Klug, D.R., Porter, G. and Barber, J. (1990) Comparison of the D1/D2/Cytochrome-b_{559} reaction center complex of photosystem 2 isolated by two different methods. *Febs Letters*, **265**, 88-92.

Govindjee and Van Rensen, J. (1993) Photosystem II reaction center and bicarbonate. In Deisenhofer, J. and Norris, J. (eds.), *The Photosynthetic Reaction Center*. Academic Press, San Diego, CA, Vol. I, pp. 357-389.

Groot, M.L., Frese, R.N., de Weerd, F.L., Bromek, K., Pettersson, A., Peterman, E.J., van Stokkum, I.H., van Grondelle, R. and Dekker, J.P. (1999) Spectroscopic properties of the CP43 core antenna protein of photosystem II. *Biophys J*, **77**, 3328-3340.

Haag, E., Eaton-Rye, J.J., Renger, G. and Vermaas, W.F. (1993) Functionally important domains of the large hydrophilic loop of CP47 as probed by oligonucleotide-directed mutagenesis in *Synechocystis* sp. PCC 6803. *Biochemistry*, **32**, 4444-4454.

Hankamer, B., Nield, J., Zheleva, D., Boekema, E., Jansson, S. and Barber, J. (1997) Isolation and biochemical characterisation of monomeric and dimeric photosystem II complexes from spinach and their relevance to the organisation of photosystem II *in vivo*. *Eur J Biochem*, **243**, 422-429.

Harp, J.M., Hanson, B.L., Timm, D.E. and Bunick, G.J. (1999) Macromolecular crystal annealing: evaluation of techniques and variables. *Acta Crystallogr D Biol Crystallogr*, **55 (Pt 7)**, 1329-1334.

Hatanaka, H., Tanimura, R., Katoh, S. and Inagaki, F. (1997) Solution structure of ferredoxin from the thermophilic cyanobacterium *Synechococcus elongatus* and its thermostability. *J Mol Biol*, **268**, 922-933.

Hays, A.M., Vassiliev, I.R., Golbeck, J.H. and Debus, R.J. (1999) Role of D1-His190 in the proton-coupled oxidation of tyrosine Y_Z in manganese-depleted photosystem II. *Biochemistry*, **38**, 11851-11865.

Heras, B., Edeling, M.A., Byriel, K.A., Jones, A., Raina, S. and Martin, J.L. (2003) Dehydration converts DsbG crystal diffraction from low to high resolution. *Structure (Camb)*, **11**, 139-145.

Hill, R. and Bendall, F. (1960) Function of the two cytochrome components in chloroplasts: a working hypothesis. *Nature*, **186**, 136-137.

Hillier, W. and Wydrzynski, T. (1993) Increase in peroxide formation by the Photosystem II oxygen evolving reactions upon removal of the extrinsic 16, 22 and 33 kDa proteins are reversed by $CaCl_2$ addition. *Photosynthesis Research*, **38**, 417-423.

Hillmann, B., Brettel, K., van Mieghem, F., Kamlowski, A., Rutherford, A.W. and Schlodder, E. (1995) Charge recombination reactions in photosystem II. Transient absorbance difference spectra and their temperature dependence. *Biochemistry*, **34**, 4814-4827.

Hol, W.G. (1985) The role of the alpha-helix dipole in protein function and structure. *Prog Biophys Mol Biol*, **45**, 149-195.

Hooft, R.W., Vriend, G., Sander, C. and Abola, E.E. (1996) Errors in protein structures. *Nature*, **381**, 272.

Hope, H. (1990) Crystallography of Biological Macromolecules at Ultra-Low Temperature. *Annu Rev Biophys Biophys Chem*, **19**, 107-126.

Huppman, P., Arlt, T., Penzkofer, H., Schmidt, S., Bibikova, M., Dohse, B., Oesterhelt, D., Wachtveit, J. and Zinth, W. (2002) Kinetics, energetics, and electronic coupling of the primary electron transfer reactions in mutated reaction centers of *Blastochloris viridis*. *Biophys J*, **82**, 3186-3197.

Inoue, T., Sugawara, H., Hamanaka, S., Tsukui, H., Suzuki, E., Kohzuma, T. and Kai, Y. (1999) Crystal structure determinations of oxidized and reduced plastocyanin from the cyanobacterium *Synechococcus* sp. PCC 7942. *Biochemistry*, **38**, 6063-6069.

Ishikita, H., Loll, B., Biesiadka, J., Saenger, W. and Knapp, E.W. (2004) Redox potentials of chlorophylls in photosystem II reaction center. *submitted*.

Iwata, M., Imamura, H., Stambouli, E., Ikeda, C., Tamakoshi, M., Nagata, K., Makyio, H., Hankamer, B., Barber, J., Yoshida, M., Yokoyama, K. and Iwata, S. (2004) Crystal structure of a central stalk subunit C and reversible association/dissociation of vacuole-type ATPase. *Proc Natl Acad Sci U S A*, **101**, 59-64.

Iwata, S., Ostermeier, C., Ludwig, B. and Michel, H. (1995) Structure at 2.8 Å resolution of cytochrome *c* oxidase from *Paracoccus denitrificans*. *Nature*, **376**, 660-669.

Jeans, C., Schilstra, M.J. and Klug, D.R. (2002) The temperature dependence of $P680^+$ reduction in oxygen-evolving photosystem II. *Biochemistry*, **41**, 5015-5023.

Jiang, L. and Lai, L. (2002) CH...O hydrogen bonds at protein-protein interfaces. *J Biol Chem*, **277**, 37732-37740.

Jones, T.A., Zou, J.Y., Cowan, S.W. and Kjeldgaard, M. (1991) Improved methods for binding protein models in electron density maps and the location of errors in these models. *Acta Cryst A*, **A47**, 110-119.

Jordan, P. (2001) Röntgenstrukturanalyse des trimeren Photosystem I aus dem Cyanobakterium *Synechococcus elongatus* bei 2.5 Å. *[PhD Thesis] Freie Universität Berlin*.

Jordan, P., Fromme, P., Witt, H.T., Klukas, O., Saenger, W. and Krauss, N. (2001) Three-dimensional structure of cyanobacterial photosystem I at 2.5 Å resolution. *Nature*, **411**, 909-917.

Kamiya, N. and Shen, J.R. (2003) Crystal structure of oxygen-evolving photosystem II from *Thermosynechococcus vulcanus* at 3.7-Å resolution. *Proc Natl Acad Sci U S A*, **100**, 98-103.

Kasting, J.F. and Siefert, J.L. (2002) Life and the evolution of Earth's atmosphere. *Science*, **296**, 1066-1068.

Katoh, H., Itoh, S., Shen, J.R. and Ikeuchi, M. (2001) Functional analysis of psbV and a novel *c*-type cytochrome gene *psbV2* of the thermophilic cyanobacterium *Thermosynechococcus elongatus* strain BP- 1. *Plant Cell Physiol*, **42**, 599-607.

Ke, B. (2001) *Photosynthesis - Photobiochemistry and Photobiophysics*. Kluwer Academic, Dordrecht.

Keilty, A.T., Vavilin, D.V. and Vermaas, W.F. (2001) Functional Analysis of Combinatorial Mutants with Changes in the C- Terminus of the CD Loop of the D2 Protein in Photosystem II of *Synechocystis* sp. PCC 6803. *Biochemistry*, **40**, 4131-4139.

Kerfeld, C.A. and Krogmann, D.W. (1998) Photosynthetic cytochromes *c* in cyanobacteria, algae and plants. *Annu Rev Plant Physiol Plant Mol Biol*, **49**, 397-425.

Kerfeld, C.A., Sawaya, M.R., Bottin, H., Tran, K.T., Sugiura, M., Cascio, D., Desbois, A., Yeates, T.O., Kirilovsky, D. and Boussac, A. (2003) Structural and EPR characterization of the soluble form of cytochrome *c*-550 and of the *psbV2* gene product from the cyanobacterium *Thermosynechococcus elongatus*. *Plant Cell Physiol*, **44**, 697-706.

Kern, J., Loll, B., Lüneberg, C., DiFiore, D., Biesiadka, J., Irrgang, K.-D. and Zouni, A. (2004a) Purification, Characterisation and Crystallisation of Photosystem II from *Thermosynechococcus elongatus* cultivated in a new type of photobioreactor. *Biochim Biophys Acta*, in press.

Kern, J., Zouni, A., Franke, P., Schröder, W. and Irrgang, K.-D. (2004b) Subunit composition of photosystem II core complexes from the cyanobacterium *Thermeosynechococcus elongatus* and the higher plant *spinacia oleracea*. *submitted*.

Kiefersauer, R., Tha, M.E., Dobbek, H., Gremer, L., Melero, M., Strobl, S., Dias, J.M., Soulimane, T. and Huber, R. (2000) A novel free-mounting system for protein crystals: transformation and improvement of diffraction power by accurately controlled humidity changes. *J Appl Cryst*, **33**, 1223-1230.

Kimura, A., Eaton-Rye, J.J., Morita, E.H., Nishiyama, Y. and Hayashi, H. (2002) Protection of the oxygen-evolving machinery by the extrinsic proteins of photosystem II is essential for development of cellular thermotolerance in Synechocystis sp. PCC 6803. *Plant Cell Physiol*, **43**, 932-938.

Kleiger, G., Grothe, R., Mallick, P. and Eisenberg, D. (2002) GxxxG and AxxxA: common alpha-helical interaction motifs in proteins, particularly in extremophiles. *Biochemistry*, **41**, 5990-5997.

Kleywegt, G.J. and Jones, T.A. (1998) Databases in protein crystallography. *Acta Crystallogr D Biol Crystallogr*, **54**, 1119-1131.

Kok, B., Forbush, B. and McGloin, M. (1970) Cooperation of charges in photosynthetic evolution: I. A linear four step mechanism. *Photochem Photobiol*, **11**, 457-475.

Komenda, J. and Barber, J. (1995) Comparison of *psbO* and *psbH* deletion mutants of *Synechocystis* PCC 6803 indicates that degradation of D1 protein is regulated by the Q_B site and dependent on protein synthesis. *Biochemistry*, **34**, 9625-9631.

Kriminski, S., Caylor, C.L., Nonato, M.C., Finkelstein, K.D. and Thorne, R.E. (2002) Flash-cooling and annealing of protein crystals. *Acta Crystallogr D Biol Crystallogr*, **58**, 459-471.

Kuhl, H., Kruip, J., Seidler, A., Krieger-Liszkay, A., Bunker, M., Bald, D., Scheidig, A.J. and Rögner, M. (2000) Towards structural determination of the water-splitting enzyme. Purification, crystallization, and preliminary crystallographic studies of photosystem II from a thermophilic cyanobacterium. *J Biol Chem*, **275**, 20652-20659.

Kühlbrandt, W., Wang, D.N. and Fujiyoshi, Y. (1994) Atomic Model of Plant Light-Harvesting Complex by Electron Crystallography. *Nature*, **367**, 614-621.

Kuhn, M.G. and Vermaas, W.F. (1993) Deletion mutations in a long hydrophilic loop in the photosystem II chlorophyll-binding protein CP43 in the cyanobacterium *Synechocystis* sp. PCC 6803. *Plant Mol Biol*, **23**, 123-133.

Kuo, A., Bowler, M.W., Zimmer, J., Antcliff, J.F. and Doyle, D.A. (2003) Increasing the diffraction limit and internal order of a membrane protein crystal by dehydration. *J Struct Biol*, **141**, 97-102.

Kurisu, G., Zhang, H., Smith, J.L. and Cramer, W.A. (2003) Structure of the cytochrome b_6f complex of oxygenic photosynthesis: tuning the cavity. *Science*, **302**, 1009-1014.

Kyte, J. and Doolittle, R.F. (1982) A simple method for displaying the hydropathic character of a protein. *J Mol Biol*, **157**, 105-132.

Lakshmi, K.V., Eaton, S.S., Eaton, G.R. and Brudvig, G.W. (1999) Orientation of the tetranuclear manganese cluster and tyrosine Z in the O_2-evolving complex of photosystem II: An EPR study of the S_2Y_Z* state in oriented acetate-inhibited photosystem II membranes. *Biochemistry*, **38**, 12758-12767.

Lakshmi, K.V., Poluektov, O.G., Reifler, M.J., Wagner, A.M., Thurnauer, M.C. and Brudvig, G.W. (2003) Pulsed high-frequency EPR study on the location of carotenoid and chlorophyll cation radicals in photosystem II. *J Am Chem Soc*, **125**, 5005-5014.

Latimer, M.J., DeRose, V.J., Mukerji, I., Yachandra, V.K., Sauer, K. and Klein, M.P. (1995) Evidence for the proximity of calcium to the manganese cluster of photosystem II: determination by X-ray absorption spectroscopy. *Biochemistry*, **34**, 10898-10909.

Lince, M.T. and Vermaas, W. (1998) Association of His117 in the D2 protein of photosystem II with a chlorophyll that affects excitation-energy transfer efficiency to the reaction center. *Eur J Biochem*, **256**, 595-602.

Liu, Z., Yan, H., Wang, K., Kuang, T., Zhang, J., Gui, L., An, X. and Chang, W. (2004) Crystal structure of spinach major light-harvesting complex at 2.72 Å resolution. *Nature*, **428**, 287-292.

Loll, B., Gerold, G., Slowik, D., Voelter, W., Jung, C., Saenger, W. and Irrgang, K.-D. (2005) Thermostability and Ca^{2+}-binding Properties of Wild Type and Heterologously Expressed PsbO Protein from Cyanobacterial PhotosystemII. *Biochemistry*, in press

Loll, B., Raszewski, G., Saenger, W. and Biesiadka, J. (2003) Functional role of C(α)-H···O hydrogen bonds between transmembrane α-helices in photosystem I. *J Mol Biol*, **328**, 737-747.

Lydakis-Simantiris, N., Hutchison, R.S., Betts, S.D., Barry, B.A. and Yocum, C.F. (1999) Manganese stabilizing protein of photosystem II is a thermostable, natively unfolded polypeptide. *Biochemistry*, **38**, 404-414.

Mamedov, F., Sayre, R.T. and Styring, S. (1998) Involvement of histidine 190 on the D1 protein in electron/proton transfer reactions on the donor side of photosystem II. *Biochemistry*, **37**, 14245-14256.

Manna, P., LoBrutto, R., Eijckelhoff, C., Dekker, J.P. and Vermaas, W. (1998) Role of Arg180 of the D2 protein in photosystem II structure and function. *Eur J Biochem*, **251**, 142-154.

Manna, P. and Vermaas, W. (1997) Mutational studies on conserved histidine residues in the chlorophyll- binding protein CP43 of photosystem II. *Eur J Biochem*, **247**, 666-672.

Margulis, L. (1981) *Symbiosis in Cell Evolution*. W. H. Freeman and Company, San Francisco.

Mayes, S.R., Cook, K.M., Self, S.J., Zhang, Z. and Barber, J. (1991) Deletion of the gene encoding the PSII 33kDa protein from *Synechocystis* PCC 6803 does not inactivate water splitting but increases vulnerability to photoinhibition. *Biochim Biophys Acta*, **1060**, 1-12.

McDonald, I.K. and Thornton, J.M. (1994) Satisfying hydrogen bonding potential in proteins. *J Mol Biol*, **238**, 777-793.

Merry, S.A.P., Nixon, P.J., Barter, L.M.C., Schilstra, M., Porter, G., Barber, J., Durrant, J.R. and Klug, D.R. (1998) Modulation of quantum yield of primary radical pair formation in photosystem II by site-directed mutagenesis affecting radical cations and anions. *Biochemistry*, **37**, 17439-17447.

Michel, H. (1983) Crystallization of membrane proteins. *Trends in Biochemical Science*, **8**, 56-59.

Michel, H. and Deisenhofer, J. (1988) Relevance of the photosynthetic reaction center from purple bacteria to the structure of photosystem II. *Biochemistry*, **27**, 1-7.

Miyao, M. and Murata, N. (1983) Partial reconstitution of photosynthetic oxygen evolution system by rebinding of the 33 kDa polypeptide. *FEBS Lett*, **164**, 375-378.

Motoki, A., Usui, M., Shimazu, T., Hirano, M. and Katoh, S. (2002) A domain of the Mn-stabilizing protein from *Synechococcus elongatus* involved in functional binding to phtosystem II. *J Biol Chem*, **23**, 23.

Muirhead, H., Cox, J.M., Mazzarella, L. and Perutz, M.F. (1967) Structure and function of haemoglobin IV. A three-dimensional fourier synthesis of human deoxyhaemoglobin at 5.5 Å resolution. *J Mol Biol*, **28**, 117-156.

Mulkidjanian, A.Y. (1999) Photosystem II of green plants: on the possible role of retarded protonic relaxation in water oxidation. *Biochim Biophys Acta*, **1410**, 1-6.

Nakamura, Y., Kaneko, T., Sato, S., Ikeuchi, M., Katoh, H., Sasamoto, S., Watanabe, A., Iriguchi, M., Kawashima, K., Kimura, T., Kishida, Y., Kiyokawa, C., Kohara, M., Matsumoto, M., Matsuno, A., Nakazaki, N., Shimpo, S., Sugimoto, M., Takeuchi, C., Yamada, M. and Tabata, S. (2002) Complete genome structure of the thermophilic cyanobacterium *Thermosynechococcus elongatus* BP-1. *DNA Res*, **9**, 123-130.

Navarro, J.A., Hervas, M., De la Cerda, B. and De la Rosa, M.A. (1995) Purification and physicochemical properties of the low-potential cytochrome c-549 from the cyanobacterium *Synechocystis* sp. PCC 6803. *Arch Biochem Biophys*, **318**, 46-52.

Nedbal, L., Samson, G. and Whitmarsh, J. (1992) Redox state of a one-electron component controls the rate of photoinhibition of photosystem II. *Proc Natl Acad Sci U S A*, **89**, 7929-7933.

Nield, J., Orlova, E.V., Morris, E.P., Gowen, B., van Heel, M. and Barber, J. (2000) 3D map of the plant photosystem II supercomplex obtained by cryoelectron microscopy and single particle analysis. *Nat Struct Biol*, **7**, 44-47.

Nishiyama, Y., Hayashi, H., Watanabe, T. and Murata, N. (1994) Photosynthetic Oxygen evolution is stabilized by cytochrome *c*550 against heat inactivation in *Synechococcus* sp. PCC 7002. *Plant Physiol*, **105**, 1313-1319.

Nishiyama, Y., Los, D.A., Hayashi, H. and Murata, N. (1997) Thermal protection of the oxygen-evolving machinery by PsbU, an extrinsic protein of photosystem II, in *Synechococcus* species PCC 7002. *Plant Physiol*, **115**, 1473-1480.

Nishiyama, Y., Los, D.A. and Murata, N. (1999) PsbU, a protein associated with photosystem II, is required for the acquisition of cellular thermotolerance in *Synechococcus* species PCC 7002. *Plant Physiol*, **120**, 301-308.

Nitschke, W. and Rutherford, A.W. (1991) Photosynthetic reaction centres: variations on a common structural theme? *Trends Biochem Sci*, **16**, 241-245.

Nixon, P.J., Trost, J.T. and Diner, B.A. (1992) Role of the carboxy terminus of polypeptide D1 in the assembly of a functional water-oxidizing manganese cluster in photosystem II of the cyanobacterium *Synechocystis* sp. PCC 6803: assembly requires a free carboxyl group at C-terminal position 344. *Biochemistry*, **31**, 10859-10871.

Niyogi, K.K. (1999) Photoprotection revisited: Genetic and Molecular Approaches. *Annu Rev Plant Physiol Plant Mol Biol*, **50**, 333-359.

Odom, W.R. and Bricker, T.M. (1992) Interaction of CPa-1 with the manganese-stabilizing protein of photosystem II: identification of domains cross-linked by 1-ethyl-3-[3-(dimethylamino)propyl]carbodiimide. *Biochemistry*, **31**, 5616-5620.

Oettmeier, W. (1999) Herbicide resistance and supersensitivity in photosystem II. *Cell Mol Life Sci*, **55**, 1255-1277.

Ohyama, K., Fukuzawa, H., Kohchi, T., Shirai, H., Sano, T., Sano, S., Umesono, K., Shiki, Y., Takeuchi, M., Chang, Z., Aota, S., Inokuchi, H. and Ozeki, H. (1986) Chloroplast gene organization deduced from complete sequence of liverwort *Marchantia polymorpha* chloroplast DNA. *Nature*, **322**, 572-574.

Ortega, J.M., Roncel, M. and Losada, M. (1999) Light-induced degradation of cytochrome *b*559 during photoinhibition of the photosystem II reaction center. *FEBS Lett*, **458**, 87-92.

Otwinowski, Z. and Minor, W. (1996) Processing of X-ray diffraction data collected in oscillation mode. *Methods Enzymol*, **276**, 307-326.

Pace, N.R. (1997) A molecular view of microbial diversity and the biosphere. *Science*, **276**, 734-740.

Pace, R.J. and Ahrling, K.A. (2004) Water oxidation in PSII-H atom abstraction revisited. *Biochim Biophys Acta*, **1655**, 172-178.

Pakrasi, H.B. and Vermaas, W.F.J. (1992) The Photosystems: Structure, Function and Molecular Biology. In Barber, J. (ed.). Elsevier Science Publishers, Amsterdam, pp. 2331-2357.

Papiz, M.Z., Prince, S.M., Howard, T., Cogdell, R.J. and Isaacs, N.W. (2003) The structure and thermal motion of the B800-850 LH2 complex from *Rps. acidophila* at 2.0Å resolution and 100K: new structural features and functionally relevant motions. *J Mol Biol*, **326**, 1523-1538.

Pazos, F., Heredia, P., Valencia, A. and de las Rivas, J. (2001) Threading structural model of the manganese-stabilizing protein PsbO reveals presence of two possible β-sandwich domains. *Proteins*, **45**, 372-381.

Pebay-Peyroula, E., Rummel, G., Rosenbusch, J.P. and Landau, E.M. (1997) X-ray structure of bacteriorhodopsin at 2.5 Å from microcrystals grown in lipidic cubic phases. *Science*, **277**, 1676-1681.

Peterman, E.J.G., van Amerongen, H., van Grondelle, R. and Dekker, J.P. (1998) The nature of the excited state of the reaction center of photosystem II of green plants: A high-resolution fluorescence spectroscopy study. *Proc Natl Acad Sci U S A*, **95**, 6128-6133.

Pfister, K., Steinback, K.E., Gardner, G. and Arntzen, C.J. (1981) Photoaffinity Labeling of an Herbicide Receptor Protein in Chloroplast Membranes *Proc. Natl. Acad. Sci. USA*, **78**, 981-985.

Popelkova, H., Im, M.M. and Yocum, C.F. (2003) Binding of manganese stabilizing protein to photosystem II: identification of essential N-terminal threonine residues and domains that prevent nonspecific binding. *Biochemistry*, **42**, 6193-6200.

Pueyo, J.J., Alfonso, M., Andres, C. and Picorel, R. (2002) Increased tolerance to thermal inactivation of oxygen evolution in spinach Photosystem II membranes by substitution of the extrinsic 33-kDa protein by its homologue from a thermophilic cyanobacterium. *Biochim Biophys Acta*, **1554**, 29-35.

Putnam-Evans, C. and Bricker, T.M. (1992) Site-directed mutagenesis of the CPa-1 protein of photosystem II: alteration of the basic residue pair 384, 385R to 384, 385G leads to a defect associated with the oxygen-evolving complex. *Biochemistry*, **31**, 11482-11488.

Putnam-Evans, C., Wu, J. and Bricker, T.M. (1996) Site-directed mutagenesis of the CP47 protein of photosystem II: alteration of conserved charged residues which lie within lethal deletions of the large extrinsic loop E. *Plant Mol Biol*, **32**, 1191-1195.

Qian, M., Al-Khaldi, S.F., Putnam-Evans, C., Bricker, T.M. and Burnap, R.L. (1997) Photoassembly of the photosystem II $(Mn)_4$ cluster in site-directed mutants impaired in the binding of the manganese-stabilizing protein. *Biochemistry*, **36**, 15244-15252.

Rakhimberdieva, M.G., Boichenko, V.A., Karapetyan, N.V. and Stadnichuk, I.N. (2001) Interaction of Phycobilisomes with Photosystem II Dimers and Photosystem I Monomers and Trimers in the Cyanobacterium *Spirulina platensis*. *Biochemistry*, **40**, 15780-15788.

Rayment, I. (2002) Small-scale batch crystallization of proteins revisited: an underutilized way to grow large protein crystals. *Structure (Camb)*, **10**, 147-151.

Reifarth, F. and Renger, G. (1998) Indirect evidence for structural changes coupled with $Q_B^{-\cdot}$ formation in photosystem II. *FEBS Lett*, **428**, 123-126.

Rhee, K.H. (2001) Photosystem II: the solid structural era. *Annu Rev Biophys Biomol Struct*, **30**, 307-328.

Rhee, K.H., Morris, E.P., Barber, J. and Kühlbrandt, W. (1998) Three-dimensional structure of the plant photosystem II reaction centre at 8 Å resolution. *Nature*, **396**, 283-286.

Rigby, S.E., Nugent, J.H.A. and O'Malley, P.J. (1994) The dark stable tyrosine radical of photosystem 2 studied in three species using ENDOR and EPR spectroscopies. *Biochemistry*, **33**, 1734-1742.

Riggs-Gelasco, P.J., Mei, R., Ghanotakis, D.F., Yocum, C.F. and Penner-Hahn, J.E. (1996) X-ray Absorption Spectroscopy of calcium-substituted Derivatives of the oxygen-evolving complex of Photosystem II. *J Am Chem Soc*, **118**, 2400-2410.

Robblee, J.H., Cinco, R.M. and Yachandra, V.K. (2001) X-ray spectroscopy-based structure of the Mn cluster and mechanism of photosynthetic oxygen evolution. *Biochim Biophys Acta*, **1503**, 7-23.

Rochaix, J.D. (1992) Post-transcriptional steps in the expression of chloroplast genes. *Annu Rev Cell Biol*, **8**, 1-28.

Rochaix, J.D., Kuchka, M., Mayfield, S., Schirmer-Rahire, M., Girard-Bascou, J. and Bennoun, P. (1989) Nuclear and chloroplast mutations affect the synthesis or stability of the chloroplast *psbC* gene product in *Chlamydomonas reinhardtii*. *EMBO J*, **8**, 1013-1021.

Rögner, M., Chisholm, D.A. and Diner, B.A. (1991) Site-directed mutagenesis of the psbC gene of photosystem II: isolation and functional characterization of CP43-less photosystem II core complexes. *Biochemistry*, **30**, 5387-5395.

Roncel, M., Boussac, A., Zurita, J.L., Bottin, H., Sugiura, M., Kirilovsky, D. and Ortega, J.M. (2003) Redox properties of the photosystem II cytochromes *b*559 and *c*550 in the cyanobacterium *Thermosynechococcus elongatus*. *J Biol Inorg Chem*, **8**, 206-216.

Roose, J.L. and Pakrasi, H.B. (2004) Evidence that D1 processing is required for manganese binding and extrinsic protein assembly into photosystem II. *J Biol Chem*.

Rosenberg, C., Christian, J., Bricker, T.M. and Putnam-Evans, C. (1999) Site-directed mutagenesis of glutamate residues in the large extrinsic loop of the photosystem II protein CP 43 affects oxygen-evolving activity and PS II assembly. *Biochemistry*, **38**, 15994-16000.

Rost, B., Fariselli, P. and Casadio, R. (1996) Topology prediction for helical transmembrane proteins at 86% accuracy. *Protein Sci*, **5**, 1704-1718.

Roszak, A.W., McKendrick, K., Gardiner, A.T., Mitchell, I.A., Isaacs, N.W., Cogdell, R.J., Hashimoto, H. and Frank, H.A. (2004) Protein regulation of carotenoid binding; gatekeeper and locking amino acid residues in reaction centers of *Rhodobacter sphaeroides*. *Structure*, **12**, 765-773.

Russ, W.P. and Engelman, D.M. (2000) The GxxxG motif: a framework for transmembrane helix-helix association. *J Mol Biol*, **296**, 911-919.

Sane, P.V., Ivanov, A.G., Sveshnikov, D., Huner, N.P. and Oquist, G. (2002) A transient exchange of the photosystem II reaction center protein D1:1 with D1:2 during low temperature stress of *Synechococcus* sp. PCC 7942 in the light lowers the redox potential of Q_B. *J Biol Chem*, **277**, 32739-32745.

Schatz, G.H. and Witt, H.T. (1984) Extraction and characterisation of oxygen-evolving Photosystem II complexes from a thermophilic cyanobacterium *Synechococcus* spec. *Photobiochemistry and Photobiophysics*, **7**, 1-14.

Scheller, H.V. (1996) In Vitro Cyclic Electron Transport in Barley Thylakoids follows Two Independent Pathways. *Plant Physiol*, **110**, 187-194.

Schelvis, J.P.M., van Noort, P.I., Aartsma, T.J. and van Gorkom, H.J. (1994) Energy transfer, charge separation and pigment arrangement in the reaction center of Photosystem II. *Biochim Biophys Acta*, **1184**, 242-250.

Schirmer, T., Bode, W. and Huber, R. (1987) Refined three-dimensional structures of two cyanobacterial C-phycocyanins at 2.1 and 2.5 Å resolution. A common principle of phycobilin-protein interaction. *J Mol Biol*, **196**, 677-695.

Schubert, W.D., Klukas, O., Saenger, W., Witt, H.T., Fromme, P. and Krauss, N. (1998) A common ancestor for oxygenic and anoxygenic photosynthetic systems: a comparison based on the structural model of photosystem I. *J Mol Biol*, **280**, 297-314.

Schweitzer, R.H. and Brudvig, G.W. (1997) Fluorescence quenching by chlorophyll cations in photosystem II. *Biochemistry*, **36**, 11351-11359.

Seidler, A. (1996) The extrinsic polypeptides of Photosystem II. *Biochim Biophys Acta*, **1277**, 35-60.

Senes, A., Gerstein, M. and Engelman, D.M. (2000) Statistical analysis of amino acid patterns in transmembrane helices: the GxxxG motif occurs frequently and in association with beta-branched residues at neighboring positions. *J Mol Biol*, **296**, 921-936.

Senes, A., Ubarretxena-Belandia, I. and Engelman, D.M. (2001) The Cα ---H¨O hydrogen bond: a determinant of stability and specificity in transmembrane helix interactions. *Proc Natl Acad Sci U S A*, **98**, 9056-9061.

Shen, G., Eaton-Rye, J.J. and Vermaas, W.F.J. (1993) Mutation of histidine residues in CP47 leads to destabilization of the photosystem II complex and impairment of light energy transfer. *Biochemistry*, **32**, 5105-5115.

Shen, G. and Vermaas, W.F.J. (1994) Mutation of Chlorophyll Ligands in the Chlorophyll-Binding CP47-Protein as Studied in a *Synechocystis* sp PCC 6803 Photosystem-I-Less Background. *Biochemistry*, **33**, 7379-7388.

Shen, J.R., Burnap, R.L. and Inoue, Y. (1995) An independent role of cytochrome *c*-550 in cyanobacterial photosystem II as revealed by double-deletion mutagenesis of the *psbO* and *psbV* genes in *Synechocystis* sp. PCC 6803. *Biochemistry*, **34**, 12661-12668.

Shen, J.R., Ikeuchi, M. and Inoue, Y. (1997) Analysis of the *psbU* gene encoding the 12-kDa extrinsic protein of photosystem II and studies on its role by deletion mutagenesis in *Synechocystis* sp. PCC 6803. *J Biol Chem*, **272**, 17821-17826.

Shen, J.-R. and Inoue, Y. (1993) Binding and Functional Propterties of Two New Extrinsic Components, Cytochrome *c*-550 and a 12-kDa Protein, in Cyanobacterial Photosystem II. *Biochemistry*, **32**, 1825-1832.

Shen, J.R., Qian, M., Inoue, Y. and Burnap, R.L. (1998) Functional characterization of *Synechocystis* sp. PCC 6803 Δ*psbU* and Δ*psbV* mutants reveals important roles of cytochrome *c*-550 in cyanobacterial oxygen evolution. *Biochemistry*, **37**, 1551-1558.

Shutova, T., Irrgang, K., Klimov, V.V. and Renger, G. (2000) Is the manganese stabilizing 33 kDa protein of photosystem II attaining a 'natively unfolded' or 'molten globule' structure in solution? *FEBS Lett*, **467**, 137-140.

Shutova, T., Irrgang, K.D., Shubin, V., Klimov, V.V. and Renger, G. (1997) Analysis of pH-induced structural changes of the isolated extrinsic 33 kilodalton protein of photosystem II. *Biochemistry*, **36**, 6350-6358.

Siegbahn, P.E. and Blomberg, M.R. (2004) Important roles of tyrosines in photosystem II and cytochrome oxidase. *Biochim Biophys Acta*, **1655**, 45-50.

Sonoyama, M., Motoki, A., Okamoto, G., Hirano, M., Ishida, H. and Katoh, S. (1996) Secondary structure and thermostability of the photosystem II manganese-stabilizing protein of the thermophilic cyanobacterium *Synechococcus elongatus*. *Biochim Biophys Acta*, **1297**, 167-170.

Stewart, D.H. and Brudvig, G.W. (1998) Cytochrome b_{559} of photosystem II. *Biochim Biophys Acta*, **1367**, 63-87.

Stiller, J.W. and Hall, B.D. (1997) The origin of red algae: implications for plastid evolution. *Proc Natl Acad Sci U S A*, **94**, 4520-4525.

Stock, D., Leslie, A.G. and Walker, J.E. (1999) Molecular architecture of the rotary motor in ATP synthase. *Science*, **286**, 1700-1705.

Stowell, M.H., McPhillips, T.M., Rees, D.C., Soltis, S.M., Abresch, E. and Feher, G. (1997) Light-induced structural changes in photosynthetic reaction center: implications for mechanism of electron-proton transfer. *Science*, **276**, 812-816.

Stroebel, D., Choquet, Y., Popot, J.L. and Picot, D. (2003) An atypical haem in the cytochrome b_6f complex. *Nature*, **426**, 413-418.

Sui, H., Han, B.G., Lee, J.K., Walian, P. and Jap, B.K. (2001) Structural basis of water-specific transport through the AQP1 water channel. *Nature*, **414**, 872-878.

Svensson, B., Tiede, D.M., Nelson, D.R. and Barry, B.A. (2004) Structural studies of the manganese stabilizing subunit in photosystem II. *Biophys J*, **86**, 1807-1812.

Svensson, B., Vass, I., Cendergren, E. and Styring, S. (1990) Structure of donor side components in photosystem II predicted by computer modelling. *EMBO J*, **9**, 2051-2059.

Tanaka, S. and Wada, K. (1988) The status of cysteine residues in the extrinsic 33kDa protein of spinach photosystem II complexes. *Photosynth Res*, **17**, 255-266.

Tang, X.S. and Satoh, K. (1984) Characterization of a 47-kilodalton chlorophyll-binding polypeptide (CP-47) Isolated from a photosystem II core complex. *Plant Cell Physiol*, **25**, 935-945.

Telfer, A. (2002) What is β-carotene doing in the photosystem II reaction centre? *Philos Trans R Soc London Ser B*, **357**, 1431-1440.

Tetenkin, V.L., Gulyaev, B.A., Seibert, M. and Rubin, A. (1989) Spectral properties of stabilized D1/D2/cytochrome *b*-559 photosystem II reaction center complex Effects of Triton X-100, the redox state of pheophytin, and β -carotene. *FEBS Lett*, **250**, 459-463.

Thompson, J.D., Higgins, D.G. and Gibson, T.J. (1994) CLUSTAL W: improving the sensitivity of progressive multiple sequence alignment through sequence weighting, position-specific gap penalties and weight matrix choice. *Nucleic Acids Res*, **22**, 4673-4680.

Thompson, L.K. and Brudvig, G.W. (1988) Cytochrome *b*-559 may function to protect photosystem II from photoinhibition. *Biochemistry*, **27**, 6653-6658.

Thornton, L.E., Ohkawa, H., Roose, J.L., Kashino, Y., Keren, N. and Pakrasi, H.B. (2004) Homologs of Plant PsbP and PsbQ Proteins Are Necessary for Regulation of Photosystem II Activity in the Cyanobacterium *Synechocystis* 6803. *Plant Cell*, **16**, 2164-2175.

Timmins, P.A., Hauk, J., Wacker, T. and Welte, W. (1991) The influence of heptane-1,2,3-triol on the size and shape of LDAO micelles. Implications for the crystallisation of membrane proteins. *FEBS Lett*, **280**, 115-120.

Timmins, P.A., Pebay-Peyroula, E. and Welte, W. (1994) Detergent organisation in solution and in crystals of membrane proteins. *Biophys Chem*, **53**, 27-36.

Tohri, A., Suzuki, T., Okuyama, S., Kamino, K., Motoki, A., Hirano, M., Ohta, H., Shen, J.R., Yamamoto, Y. and Enami, I. (2002) Comparison of the structure of the extrinsic 33 kDa protein from different organisms. *Plant Cell Physiol*, **43**, 429-439.

Tommos, C. (2002) Electron, proton and hydrogen-atom transfers in photosynthetic water oxidation. *Philos Trans R Soc London Ser B*, **357**, 1383-1394.

Tommos, C. and Babcock, G.T. (1998) Oxygen production in nature: A light-driven metalloradical enzyme process. *Acc chem Res*, **31**, 18-25.

Tommos, C. and Babcock, G.T. (2000) Proton and hydrogen currents in photosynthetic water oxidation. *Biochim Biophys Acta*, **1458**, 199-219.

Tracewell, C.A. and Brudvig, G.W. (2003) Two Redox-Active β-Carotene Molecules in Photosystem II. *Biochemistry*, **42**, 9127-9136.

Tracewell, C.A., Cua, A., Stewart, D.H., Bocian, D.F. and Brudvig, G.W. (2001a) Characterization of Carotenoid and Chlorophyll Photooxidation in Photosystem II. *Biochemistry*, **40**, 193-203.

Tracewell, C.A., Vrettos, J.S., Bautista, J.A., Frank, H.A. and Brudvig, G.W. (2001b) Carotenoid photooxidation in photosystem II. *Arch Biochem Biophys*, **385**, 61-69.

Trebst, A. (1986) The topology of the plastoquinone and herbicide binding peptides of photosystem II in the thylakoid membrane. *Z Naturforsch*, **41c**, 240-245.

Trissl, H.W. (1990) Photoelectric measurements of purple membranes. *Photochem Photobiol*, **51**, 793-818.

Trumpower, B.L. (1990) The protonmotive Q cycle. Energy transduction by coupling of proton translocation to electron transfer by the cytochrome bc_1 complex. *J Biol Chem*, **265**, 11409-11412.

Tsiotis, G., Walz, T., Spyridaki, A., Lustig, A., Engel, A. and Ghanotakis, D. (1996) Tubular crystals of a photosystem II core complex. *J Mol Biol*, **259**, 241-248.

van den Berg, B., Clemons, W.M., Jr., Collinson, I., Modis, Y., Hartmann, E., Harrison, S.C. and Rapoport, T.A. (2004) X-ray structure of a protein-conducting channel. *Nature*, **427**, 36-44.

van Dorssen, R.J., Breton, J., Plijter, J.J., Satoh, K., Van Gorkom, H.J. and Amesz, J. (1987) Spectroscopic properties of the reaction center and of the 47 kDa chlorophyll protein of photosysetm II. *Biochim Biophys Acta*, **893**, 267-274.

van Mieghem, F., Satoh, K. and Rutherford, A. (1991) A chlorophyll tilted 30° realtive to the membrane in the Photosystem II reaction centre. *Biochim Biophys Acta*, **1058**, 379-385.

van Rensen, J.J.S. (2002) Role of bicarbonate at the acceptor side of Photosystem II. *Photosynthesis Research*, **73**, 185-192.

Vasil'ev, S. and Bruce, D. (2000) Picosecond time-resolved fluorescence studies on excitation energy transfer in a histidine 117 mutant of the D2 protein of photosystem II in synechocystis 6803. *Biochemistry*, **39**, 14211-14218.

Vasil'ev, S. and Bruce, D. (2004) Optimization and Evolution of Light Harvesting in Photosynthesis: The Role of Antenna Chlorophyll Conserved between Photosystem II and Photosystem I. *Plant Cell*, **16**, 3059-3068.

Vasil'ev, S., Brudvig, G.W. and Bruce, D. (2003) The X-ray structure of photosystem II reveals a novel electron transport pathway between P680, cytochrome b_{559} and the energy-quenching cation, Chl_Z^+. *FEBS Lett*, **543**, 159-163.

Vasil'ev, S., Orth, P., Zouni, A., Owens, T.G. and Bruce, D. (2001) Excited-state dynamics in photosystem II: insights from the x-ray crystal structure. *Proc Natl Acad Sci U S A*, **98**, 8602-8607.

Vermaas, W.F.J., Rutherford, A.W. and Hansson, Ö. (1988) Site-Directed Mutagenesis in Photosystem-II of the Cyanobacterium *Synechocystis* Sp PCC-6803 - Donor-D Is a Tyrosine Residue in the D2-Protein. *Proc Natl Acad Sci USA*, **85**, 8477-8481.

von Heijne, G. (1989) Control of topology and mode of assembly of a polytopic membrane protein by positively charged residues. *Nature*, **341**, 456-458.

Vrettos, J.S., Reifler, M.J., Kievit, O., Lakshmi, K.V., de Paula, J.C. and Brudvig, G.W. (2001) Factors that determine the unusually low reduction potential of cytochrome c_{550} in cyanobacterial photosystem II. *J Biol Inorg Chem*, **6**, 708-716.

Wall, M.E., Clarage, J.B. and Phillips, G.N. (1997) Motions of calmodulin characterized using both Bragg and diffuse X-ray scattering. *Structure*, **5**, 1599-1612.

Wang, B.C. (1985) *Diffraction Methods for Biological Macromolecules*. Academic Press.

Weik, M., Kryger, G., Schreurs, A.M., Bouma, B., Silman, I., Sussman, J.L., Gros, P. and Kroon, J. (2001) Solvent behaviour in flash-cooled protein crystals at cryogenic temperatures. *Acta Crystallogr D Biol Crystallogr*, **57**, 566-573.

Weik, M., Ravelli, R.B., Kryger, G., McSweeney, S., Raves, M.L., Harel, M., Gros, P., Silman, I., Kroon, J. and Sussman, J.L. (2000) Specific chemical and structural damage to proteins produced by synchrotron radiation. *Proc Natl Acad Sci U S A*, **97**, 623-628.

Weng, J., Tan, C., Shen, J.R., Yu, Y., Zeng, X., Xu, C. and Ruan, K. (2004) pH-induced conformational changes in the soluble manganese-stabilizing protein of photosystem II. *Biochemistry*, **43**, 4855-4861.

Whitmarsh, J. and Pakrasi, H.B. (1996) Form and function of cytochrome b559. In Ort, D.R. and Yocum, C.F. (eds.), *Oxygenic Photosynthesis: The Light Reactions*. Kluwer Academic Publishers, Dordrecht, The Netherlands, pp. 249-264.

Wiklund, R., Salih, G.F., Maenpaa, P. and Jansson, C. (2001) Engineering of the protein environment around the redox-active TyrZ in photosystem II The role of F186 and P162 in the D1 protein of Synechocystis 6803. *Eur J Biochem*, **268**, 5356-5364.

Witt, H.T., Müller, A. and Rumberg, B. (1961) Experimental Evidence for the Mechanism of Photosynthesis. *Nature*, **191**, 194-195.

Woese, C.R., Kandler, O. and Wheelis, M.L. (1990) Towards a natural system of organisms: proposal for the domains Archaea, Bacteria, and Eucarya. *Proc Natl Acad Sci U S A*, **87**, 4576-4579.

Xiong, J., Subramaniam, S. and Govindjee. (1996) Modeling of the D1/D2 proteins and cofactors of the photosystem II reaction center: implications for herbicide and bicarbonate binding. *Protein Sci*, **5**, 2054-2073.

Xiong, J., Subramaniam, S. and Govindjee. (1998) A knowledge-based three dimensional model of the photosystem II reaction center of *Chlamydomonas reinhardti*. *Photosynth Res*, **56**, 229-254.

Xu, Q., Nelson, J. and Bricker, T.M. (1994) Secundary structure of the 33 kDa, extrinsic protein of Photosystem II: a far-UV circular dichroism study. *Biochim Biophys Acta*, **1188**, 427-431.

Yachandra, V.K., DeRose, V.J., Latimer, M.J., Mukerji, I., Sauer, K. and Klein, M.P. (1993) Where Plants make Oxygen: A Structural Model for the Photosynthetic Oxygen-Evolving Manganese Cluster. *Science*, **260**, 675-679.

Yakushevska, A.E., Jensen, P.E., Keegstra, W., van Roon, H., Scheller, H.V., Boekema, E.J. and Dekker, J.P. (2001) Supermolecular organization of photosystem II and its associated light harvesting antenna in *Arabidopsis thaliana*. *Eur J Biochem*, **268**, 6020-6028.

Yang, C. and Pflugrath, J.W. (2001) Applications of anomalous scattering from S atoms for improved phasing of protein diffraction data collected at Cu Kα wavelength. *Acta Crystallogr D Biol Crystallogr*, **57**, 1480-1490.

Zech, S.G., Kurreck, J., Eckert, H.J., Renger, G., Lubitz, W. and Bittl, R. (1997) Pulsed EPR measurement of the distance between $P680^{+\cdot}$ and $Q_A^{-\cdot}$ in photosystem II. *FEBS Lett*, **414**, 454-456.

Zech, S.G., Kurreck, J., Renger, G., Lubitz, W. and Bittl, R. (1999) Determination of the distance between Y_Z^{ox*} and Q_A^{-*} in photosystem II by pulsed EPR spectroscopy on light-induced radical pairs. *FEBS Lett*, **442**, 79-82.

Zhang, H., Kurisu, G., Smith, J.L. and Cramer, W.A. (2003) A defined protein-detergent-lipid complex for crystallization of integral membrane proteins: The cytochrome b_6f complex of oxygenic photosynthesis. *Proc Natl Acad Sci U S A*, **100**, 5160-5163.

Zhang, K.H.J. and Main, P. (1990) Histogram matching as a new density modification technique for phase refinement and extension of protein molecules. *Acta Crystallogr A*, **46**, 41-46.

Zolla, L., Bianchetti, M. and Rinalducci, S. (2002) Functional studies of the *Synechocystis* phycobilisomes organization by high performance liquid chromatography on line with a mass spectrometer. *Eur J Biochem*, **269**, 1534-1542.

Zouni, A., Jordan, R., Schlodder, E., Fromme, P. and Witt, H.T. (2000) First photosystem II crystals capable of water oxidation. *Biochim Biophys Acta*, **1457**, 103-105.

Zouni, A., Witt, H.T., Kern, J., Fromme, P., Krauss, N., Saenger, W. and Orth, P. (2001) Crystal structure of photosystem II from *Synechococcus elongatus* at 3.8 Å resolution. *Nature*, **409**, 739-743.