6 Bibliography

[1] T. Wydrzynski, K. Satoh (Eds.), Photosystem II: The light-driven Water:Plastoquinone oxidoreductase, Springer, Dordrecht, The Netherlands, 2005.

[2] D.C. Catling, K.J. Zahnle, C. McKay, Biogenic methane, hydrogen escape, and the irreversible oxidation of early Earth, Science 293 (2001) 839-843.

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

[4] J.M. Olson, Early evolution of chlorophyll-based photosynthesis, Chemtracts-Biochem Mol Biol 12 (1999) 468-482.

[5] M.M. Tice, D.R. Lowe, Photosynthetic microbial mats in the 3,416-Myr-old ocean, Nature 431 (2004) 549-552.

[6] A.W.D. Larkum, The Evolution of Photosynthesis, in: G. Renger (Ed.), Primary Processes of Photosynthesis: Basic Priniciples and Apparatus, vol. II, Royal Society for Chemistry, Cambridge, 2007.

[7] R.E. Blankenship, Molecular mechanisms of photosynthesis, Blackwell Science, Oxford, 2002.

[8] A.W.D. Larkum, The Evolution of Photosynthesis, in: G. Renger (Ed.), Primary Processes of Photosynthesis: Principles and Apparatus, vol. II, Royal Society for Chemistry, Cambridge, 2008.

[9] Y. Zhang, L.J. Jermiin, A.W.D. Larkum, Phylogenetic analysis of light-harvesting antenna peptides from plants and bacteria, in: J. van der Erst, D. Bruce (Eds.), Photosynthesis: Fundamental Aspects to Global Perspectives, vol. 745-746, Alliance Communication Group, Kansas, 2004.

[10] H. Hartman, Photosynthesis and the origin of life, Orig life Evol Biosph 28 (1998) 515-521.

[11] L. Margulis, Archaeal-eubacterial mergers in the origin of Eukarya: phylogenetic classification of life, Proc. Natl. Acad. Sci. U. S. A. 93 (1996) 1071-1076.

[12] T. Cavalier-Smith, Membrane heredity and early chloroplast evolution, Trends Plant Sci. 5 (2000) 174-182.

[13] J.W. Stiller, B.D. Hall, The origin of red algae: implications for plastid evolution, Proc Natl Acad Sci USA 94 (1997) 4520-4525.

[14] W. Sidler, Phycobilisomes and Phycobiliprotein structures, in: D.A. Bryant (Ed.), The molecular biology of cyanobacteria, Kluwer Academic Publishers, Dordrecht, 1994, pp. 139-216.

[15] M. Mimuro, H. Kikuchi, A. Murakami, Structure and function of phycobilisomes, in: G.S. Singhal, G. Renger, S.K. Soropy, K.-D. Irrgang, Govindjee (Eds.), Photosynthesis and Photomorphogenesis, Narosa Publishing House, New Dehli, India, 1999, pp. 104-135.

[16] M. Mimuro, M. Kobayashi, A. Murakami, T. Tsuchiya, H. Miyashita, Oxygen-evolving Cyanobacteria, in: G. Renger (Ed.), Primary Processes of Photosynthesis: Principles and Apparatus, vol. 2, The Royal Society of Chemistry, Cambridge, 2008.

[17] T. Ritz, A. Damjanovic, K. Schulten, J.P. Zhang, Y. Koyama, Efficient light harvesting through carotenoids, Photosynth Res 66 (2000) 125-144.

[18] R.J. Cogdell, H.A. Frank, How Carotenoids Function in Photosynthetic Bacteria, Biochimica Et Biophysica Acta 895 (1987) 63-79.

[19] H.A. Frank, R.J. Cogdell, The photochemistry and function of carotenoids in photosynthesis, in: A. Young, G. Britton (Eds.), Carotenoids in Photosynthesis, Chapmen & Hall, London, 1993, pp. 252-326.

[20] Y. Koyama, Y. Kakitani, Y. Watanabe, Photophysical properties and light-harvesting and photoprotective functions of carotenoids in bacterial photosynthesis: structural selections, in: G. Renger (Ed.), Primary Processes of Photosynthesis: Principles and Apparatus, vol. 2, The Royal Society of Chemistry, Cambridge, 2008, pp. 151-201.

[21] H. Scheer, G. Hartwich, Bacterial reaction centers with modified tetrapyrolle chromophores, in: R. Blankenship, M.T. Madigan, C.E. Bauer (Eds.), Anoxygenic Photosynthetic Bacteria, Kluwer, Dordrecht, 1995, pp. 649-663.

[22] G. Renger (Ed.), Primary Processes of Photosynthesis: Basic Priniciples and Apparatus 2007.

[23] G. Renger, A.R. Holzwarth, Primary Electron Transfer, in: T. Wydrzynski, K. Satoh (Eds.), Photosystem II: The Water/Plastoquinone Oxido-Reductase in Photosynthesis, Kluwer Academic Publishers, Dordrecht, Netherlandss, 2005, pp. 139-175.

[24] G. Renger, Functional pattern of Photosystem II, in: G. Renger (Ed.), Primary Processes of Photosynthesis: Principles and Apparatus, vol. 2, The Royal Society of Chemistry, Cambridge, 2007, pp. 237-290.

[25] V.V. Klimov, A.V. Klevanik, V.A. Shuvalov, A.A. Krasnovsky, Reduction of pheophytin in the primary light reaction of photosystem II, FEBS Lett 82 (1977) 183-186.

[26] G. Raszewski, W. Saenger, T. Renger, Theory of optical spectra of photosystem II reaction centers: location of the triplet state and the identity of the primary electron donor, Biophys J 88 (2005) 986-998.

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

[28] E. Schlodder, T. Renger, G. Raszewski, W.J. Coleman, P.J. Nixon, R.O. Cohen, B.A. Diner, Site-directed mutations at D1-Thr179 of photosystem II in Synechocystis sp. PCC 6803 modify the spectroscopic properties of the accessory chlorophyll in the D1-branch of the reaction center, Biochemistry 47 (2008) 3143-3154.

[29] G. Raszewski, B.A. Diner, E. Schlodder, T. Renger, Spectroscopic properties of reaction center pigments in photosystem II core complexes: revision of the multimer model, Biophys J 95 (2008) 105-119.

[30] M.L. Groot, N.P. Pawlowicz, L. van Wilderen, J. Breton, I.H.M. van Stokkum, R. van Grondelle, Initial electron donor and acceptor in isolated Photosystem II reaction centers identified with femtosecond mid-IR spectroscopy, Proceedings of the National Academy of Sciences of the United States of America 102 (2005) 13087-13092.

[31] A.R. Holzwarth, M.G. Muller, M. Reus, M. Nowaczyk, J. Sander, M. Rögner, Kinetics and mechanism of electron transfer in intact photosystem II and in the isolated reaction center: pheophytin is the primary electron acceptor, Proc Natl Acad Sci U S A 103 (2006) 6895-6900.

[32] F. Rappaport, M. Guergova-Kuras, P.J. Nixon, B.A. Diner, J. Lavergne, Kinetics and pathways of charge recombination in photosystem II, Biochemistry 41 (2002) 8518-8527.

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

[34] G. Renger, Functional pattern of Photosystem II, in: G. Renger (Ed.), Primary Processes of Photosynthesis: Principles and Apparatus, vol. 2, The Royal Society of Chemistry, Cambridge, 2008, pp. 237-290.

[35] R.J. Debus, B.A. Barry, I. Sithole, G.T. Babcock, L. McIntosh, Directed mutageneis indicates that the donor to P680+ in photosystem II is tyrosine-161 of the D1 polypeptide, Biochemistry 27 (1988) 9071-9074.

[36] J.G. Metz, P.J. Nixon, M. Rögner, G.W. Brudvig, B.A. Diner, Directed Alteration of the D1 Polypeptide of Photosystem-II - Evidence That Tyrosine-161 Is the Redox Component, Z, Connecting the Oxygen-Evolving Complex to the Primary Electron- Donor, P680, Biochemistry 28 (1989) 6960-6969.

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

[38] A. Amunts, O. Drory, N. Nelson, The structure of a plant photosystem I supercomplex at 3.4 A resolution, Nature 447 (2007) 58-63.

[39] G. Kurisu, H. Zhang, J.L. Smith, W.A. Cramer, Structure of the cytochrome b6f complex of oxygenic photosynthesis: tuning the cavity, Science 302 (2003) 1009-1014.

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

[41] B. Loll, J. Kern, W. Saenger, A. Zouni, J. Biesiadka, Towards complete cofactor arrangement in the 3.0 Å resolution structure of photosystem II, Nature 438 (2005) 1040-1044.

[42] A. Guskov, J. Kern, A. Gabdulkhakov, M. Broser, A. Zouni, W. Saenger, Cyanobacterial photosystem II at 2.9 Å resolution: role of quinones, lipids, channels and chloride., Nat Struct Mol Biol 16 (2009) 334-342.

[43] E. Baena-Gonzalez, E.M. Aro, Biogenesis, assembly and turnover of photosystem II units, Philosophical Transactions of the Royal Society of London Series B-Biological Sciences 357 (2002) 1451-1459.

[44] I. Vass, E.M. Aro, Photoinhibition of photosynthetic electron transport, in: G. Renger (Ed.), Primary Processes of Photosynthesis: Principles and Apparatus, vol. 1, Royal Society of Chemistry, Cambridge, UK, 2008, pp. 393-425.

[45] Y. Nishiyama, S.I. Allakhverdiev, N. Murata, A new paradigm for the action of reactive oxygen species in the photoinhibition of photosystem II, Biochim Biophys Acta 1757 (2006) 742-749.

[46] D.H. Stewart, G.W. Brudvig, Cytochrome b559 of photosystem II, Biochim. Biophys. Acta 1367 (1998) 63-87.

[47] O. Kaminskaya, J. Kurreck, K.D. Irrgang, G. Renger, V.A. Shuvalov, Redox and spectral properties of cytochrome b559 in different preparations of photosystem II, Biochemistry 38 (1999) 16223-16235.

[48] C.A. Buser, B.A. Diner, G.W. Brudvig, Photooxidation of cytochrome b559 in oxygen-evolving photosystem II, Biochemistry 31 (1992) 11449-11459.

[49] C.A. Tracewell, G.W. Brudvig, Characterization of the secondary electron-transfer pathway intermediates of photosystem II containing low-potential cytochrome b559, Photosynth Res 98 (2008) 189-197.

[50] J.R. Shen, R.L. Burnap, Y. Inoue, 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 (1995) 12661-12668.

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

[52] I. Enami, A. Tohri, M. Kamo, H. Ohta, J.R. Shen, Identification of domains on the 43 kDa chlorophyll-carrying protein (CP43) that are shielded from tryptic attack by binding of the extrinsic 33 kDa protein with photosystem II complex, Biochim. Biophys. Acta 1320 (1997) 17-26.

[53] J. Hladik, D. Sofrova, Does the trimeric form of the Photosystem 1 reaction center of cyanobacteria in vivo exist?, Photosynth Res 29 (1991) 171-175.

[54] W.A. Cramer, H. Zhang, J. Yan, G. Kurisu, E. Yamashita, N. Dashdorj, H. Kim, S. Savikhin, Structure-function of the cytochrome b6f complex: a design that has worked for three billion years, in: G. Renger (Ed.), Primary Processes of Photosynthesis: Principles and Apparatus, vol. 2, The Royal Chemistry Society, Cambridge, 2007, pp. 417-446.

[55] Y. Munekage, M. Hashimoto, C. Miyake, K. Tomizawa, T. Endo, M. Tasaka, T. Shikanai, Cyclic electron flow around photosystem I is essential for photosynthesis, Nature 429 (2004) 579-582.

[56] A. Guskov, J. Kern, A. Zouni, W. Saenger, Current State of Crystallographic Studies on Cyanobacterial

Photosystem II – In Search for Better Resolution, in: J.F. Allen, E. Gantt, J.H. Golbeck, B. Osmond (Eds.), Photosynthesis. Energy from the Sun: 14th International Congress on Photosynthesis, Springer, Glasgow, 2007, pp. 409-412.

[57] C.F. Yocum, The calcium and chloride requirements of the O-2 evolving complex, Coordination Chemistry Reviews 252 (2008) 296-305.

[58] R.M. Garavito, S. Ferguson-Miller, Detergents as tools in membrane biochemistry, J Biol Chem 276 (2001) 32403-32406.

[59] J.P. Allen, G. Feher, Crystallization of reaction center from Rhodopseudomonas sphaeroides: preliminary characterization, Proc Natl Acad Sci U S A 81 (1984) 4795-4799.

[60] T. Tsukihara, H. Aoyama, E. Yamashita, T. Tomizaki, H. Yamaguchi, K. Shinzawa-Itoh, R. Nakashima, R. Yaono, S. Yoshikawa, The whole structure of the 13-subunit oxidized cytochrome c oxidase at 2.8 A, Science 272 (1996) 1136-1144.

[61] J. Kern, B. Loll, C. Lüneberg, D. DiFiore, J. Biesiadka, K.D. Irrgang, A. Zouni, Purification, characterisation and crystallisation of photosystem II from *Thermosynechococcus elongatus* cultivated in a new type of photobioreactor, Biochim Biophys Acta 1706 (2005) 147-157.

[62] N. Ishida, M. Sugiura, F. Rappaport, T.L. Lai, A.W. Rutherford, A. Boussac, Biosynthetic exchange of bromide for chloride and strontium for calcium in the photosystem II oxygen-evolving enzymes, J Biol Chem 283 (2008) 13330-13340.

[63] K.W. Miller, N.V. Reo, A.J. Schoot Uiterkamp, D.P. Stengle, T.R. Stengle, K.L. Williamson, Xenon NMR: chemical shifts of a general anesthetic in common solvents, proteins, and membranes, Proc Natl Acad Sci U S A 78 (1981) 4946-4949.

[64] T. Prange, M. Schiltz, L. Pernot, N. Colloc'h, S. Longhi, W. Bourguet, R. Fourme, Exploring hydrophobic sites in proteins with xenon or krypton, Proteins-Structure Function and Genetics 30 (1998) 61-73.

[65] M. Schiltz, T. Prange, R. Fourme, On the preparation and X-ray data collection of isomorphous xenon derivatives, J Appl Cryst 27 (1994) 950-960.

[66] C.U. Kim, Q. Hao, S.M. Gruner, Solution of protein crystallographic structures by high-pressure cryocooling and noble-gas phasing, Acta Cryst D 62 (2006) 687-694.

[67] A. Cohen, P. Ellis, N. Kresge, S.M. Soltis, MAD phasing with krypton, Acta Cryst D 57 (2000) 233-238.

[68] M.L. Quillin, W.A. Breyer, I.J. Griswold, B.W. Matthews, Size versus polarizability in protein-ligand interactions: binding of noble gases within engineered cavities in phage T4 lysozyme, Journal of molecular biology 302 (2000) 955-977.

[69] R.F. Tilton, Jr., I.D. Kuntz, Jr., G.A. Petsko, Cavities in proteins: structure of a metmyoglobin-xenon complex solved to 1.9 A, Biochemistry 23 (1984) 2849-2857.

[70] M. Schiltz, W. Shepard, R. Fourme, T. Prange, E. de La Fourtelle, G. Bricogne, High-Pressure Krypton Gas and Statistical Heavy-Atom Refinement: a Successful Combination of Tools for Macromolecular Structure Determination, Acta Cryst D 53 (1997) 78-92.

[71] P. Pirrat, M.A. Smith, A.R. Pearson, M.J. McPherson, S.E.V. Phillips, Structure of a xenon derivative of Escherichia coli copper amine oxidase: confirmation of the proposed oxygen-entry pathway, Acta Cryst F 64 (2008) 1105-1109.

[72] V.M. Luna, Y. Chen, J.A. Fee, C.D. Stout, Crystallographic studies of Xe and Kr binding within the large internal cavity of cytochrome ba3 from Thermus thermophilus: structural analysis and role of oxygen transport channels in the heme-Cu oxidases, Biochemistry 47 (2008) 4657-4665.

[73] J. Cohen, A. Arkhipov, R. Braun, K. Schulten, Imaging the migration pathways for O2, CO, NO, and Xe inside myoglobin, Biophysical journal 91 (2006) 1844-1857.

[74] M. Svensson-Ek, J. Abramson, G. Larsson, S. Tornroth, P. Brzezinski, S. Iwata, The X-ray crystal structures of wild-type and EQ(I-286) mutant cytochrome c oxidases from Rhodobacter sphaeroides, J Mol Biol 321 (2002) 329-339.

[75] D.J. Haas, M.G. Rosmann, Crystallographic studies on lactate dehydrogenase at -75°C, Acta Cryst B 26 (1970) 998-1004.

[76] S. Parkin, H. Hope, Macromolecular Crystallography: Cooling, Mounting, Storage and Transporation of Crystals, J Appl Cryst 31 (1998) 945-953.

[77] J.W. Pflugrath, Macromolecular cryocrystallography--methods for cooling and mounting protein crystals at cryogenic temperatures, Methods 34 (2004) 415-423.

[78] E. Garman, Cool data: quantity AND quality, Acta Crystallogr D Biol Crystallogr 55 (1999) 1641-1653.

[79] A. Riboldi-Tunnicliffe, R. Hilgenfeld, Cryocrystallography with oil - an old idea revived, J Appl Cryst 32 (1999) 1003-1005.

[80] J.R. Helliwell, Macromolecular crystallography with synchrotron radiation, Cambridge University Press, Cambridge, 1992.

[81] A. Gonzalez, C. Nave, Radiation damage in protein crystals at low temperature, Acta Cryst D 50 (1994) 874-877.

[82] E.F. Garman, R.L. Owen, Cryocooling and radiation damage in macromolecular crystallography, Acta Cryst D 62 (1996) 32-47.

[83] W.P. Burmeister, Structural changes in a cryo-cooled protein crystal owing to radiation damage, Acta Cryst D 56 (2000) 328-341.

[84] M. Weik, R.B. Ravelli, I. Silman, J.L. Sussman, P. Gros, J. Kroon, Specific protein dynamics near the solvent glass transition assayed by radiation-induced structural changes, Protein Sci 10 (2001) 1953-1961.

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

[86] P.O. Neill, D.L. Stevens, E. Garman, Physical and chemical considerations of damage induced in protein crystals by synchrotron radiation: a radiation chemical perspective, J. Synchrotron Rad. 9 (2002) 329-332.

[87] H.M. Swartz, S.M. Swartz, Biochemical and biophysical applications of electron spin resonance, Methods Biochem Anal 29 (1983) 207-323.

[88] R.J. Southworth-Davies, E.F. Garman, Radioprotectant screening for cryocrystallography, J Synchrotron Radiat 14 (2007) 73-83.

[89] L.A. Dick, I. Malfant, D. Kulia, S. Nebolsky, J.M. Nocek, B.M. Hoffmann, M. Rather, Cryogenic Electron Tunneling within Mixed-Metal Hemoglobin Hybrids: Protein Glassing and Electron-Transfer Energetics, J Am Chem Soc 120 (1998) 11401-11407.

[90] B. Kauffmann, M.S. Weiss, V.S. Lamzin, A. Schmidt, How to avoid premature decay of your macromolecular crystal: a quick soak for long life, Structure 14 (2006) 1099-1105.

[91] J. Murray, E. Garman, Investigation of possible free-radical scavengers and metrics for radiation damage in protein cryocrystallography, J Synchrotron Radiat 9 (2002) 347-354.

[92] J. Yano, J. Kern, K.D. Irrgang, M.J. Latimer, U. Bergmann, P. Glatzel, Y. Pushkar, J. Biesiadka, B. Loll, K. Sauer, J. Messinger, A. Zouni, V.K. Yachandra, X-ray damage to the Mn_4Ca complex in single crystals of photosystem II: A case study for metalloprotein crystallography, Proc Natl Acad Sci U S A 102 (2005) 12047-12052.

[93] Z. Dauter, Data-collection strategies, Acta Crystallogr D Biol Crystallogr 55 (1999) 1703-1717.

[94] W. Kabsch, Automatic processing of rotation diffraction data from crystals of initially unknown symmetry and cell constants, J. Appl. Cryst. 26 (1993) 795-800.

[95] A.G.W. Leslie, Recent changes to the MOSFLM package for processing film and image plate data, Jnt CCP4/ESF-EACMB. Newslett. Protein Crystallogr 26 (1992).

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

[97] K. Diederichs, P.A. Karplus, Improved R-factors for diffraction data analysis in macromolecular crystallography, Nat Struct Biol 4 (1997) 269-275.

[98] K. Diederichs, S. McSweeney, R.B. Ravelli, Zero-dose extrapolation as part of macromolecular synchrotron data reduction, Acta Crystallogr D Biol Crystallogr 59 (2003) 903-909.

[99] Collaborative_Computing_Project_4, Acta Crystallogr D Biol Crystallogr D50 (1994) 760-763.

[100] W.A. Hendrickson, E.E. Lattman, Representation of phase probability distributions for simplified combination of independent phase information, Acta Cryst B 26 (1970) 136-143.

[101] G. Taylor, The phase problem, Acta Crystallogr D Biol Crystallogr 59 (2003) 1881-1890.

[102] W.A. Hendrickson, J.R. Horton, D.M. LeMaster, Selenomethionyl proteins produced for analysis by multiwavelength anomalous diffraction (MAD): a vehicle for direct determination of three-dimensional structure, EMBO J 9 (1990) 1665-1672.

[103] W. Yang, W.A. Hendrickson, E.T. Kalman, R.J. Crouch, Expression, purification, and crystallization of natural and selenomethionyl recombinant ribonuclease H from Escherichia coli, J Biol Chem 265 (1990) 13553-13559.

[104] E. Dodson, Is it jolly SAD?, Acta Crystallogr D Biol Crystallogr 59 (2003) 1958-1965.

[105] M.G. Rossmann, D.M. Blow, The detection of sub-units within the crystallographic asymmetric unit, Acta Cryst 15 (1962) 24-31.

[106] H.M. Berman, J. Westbrook, Z. Feng, G. Gilliland, T.N. Bhat, H. Weissig, I.N. Shindyalov, P.E. Bourne, The Protein Data Bank, Nucleic Acids Res 28 (2000) 235-242.

[107] J. Navaza, AMoRe: an automated package for molecular replacement, Acta Cryst A 50 (1994) 157-163.

[108] A. Vagin, A. Teplyakov, MOLREP: an Automated Program for Molecular Replacement, J Appl Cryst 30 (1997) 1022-1025.

[109] A.J. McCoy, R.W. Grosse-Kunstleve, P.D. Adams, M.D. Winn, L.C. Storoni, R.J. Read, Phaser crystallographic software, J Appl Crystallogr 40 (2007) 658-674.

[110] F. Long, A.A. Vagin, P. Young, G.N. Murshudov, BALBES: a molecular-replacement pipeline, Acta Crystallogr D Biol Crystallogr 64 (2008) 125-132.

[111] R.M. Keegan, M.D. Winn, Automated search-model discovery and preparation for structure solution by molecular replacement, Acta Cryst D 63 (2007) 447-457.

[112] S.X. Cohen, M. Ben Jelloul, F. Long, A. Vagin, P. Knipscheer, J. Lebbink, T.K. Sixma, V.S. Lamzin, G.N. Murshudov, A. Perrakis, ARP/wARP and molecular replacement: the next generation, Acta Crystallogr D Biol Crystallogr 64 (2008) 49-60.

[113] G.J. Kleywegt, On vital aid: the why, what and how of validation, Acta Crystallogr D Biol Crystallogr 65 (2009) 134-139.

[114] D.E. Tronrud, Introduction to macromolecular refinement, Acta Crystallogr D Biol Crystallogr 60 (2004) 2156-2168.

[115] J.H. Konnert, A restrained-parameter structure-factor least-squares refinement procedure for large asymmetric units, Acta Cryst A 32 (1976) 614-617.

[116] S. Kirkpatrick, C.D. Gelatt, Jr., M.P. Vecchi, Optimization by Simulated Annealing, Science 220 (1983) 671-680.

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

[118] D.S. Sivia, Data analysis : a Bayesian tutorial, Clarendon Press ;
Oxford University Press, Oxford
New York, 1996.

[119] F.H. Allen, The Cambridge Structural Database: a quarter of a million crystal structures and rising, Acta Crystallogr B 58 (2002) 380-388.

[120] V. Schomaker, K.N. Trueblood, On the rigid-body motion of molecules in crystals, Acta Cryst B 24 (1968) 63-76.

[121] A.T. Brunger, Free R value: a novel statistical quantity for assessing the accuracy of crystal structures, Nature 355 (1992) 472-475.

[122] P. Emsley, K. Cowtan, Coot: model-building tools for molecular graphics, Acta Crystallogr. D60 (2004) 2126-2132.

[123] G.N. Ramachandran, C. Ramakrishnan, V. Sasisekharan, Stereochemistry of polypeptide chain configurations, J Mol Biol 7 (1963) 95-99.

[124] R.A. Engh, R. Huber, Accurate bond and angle parameters for X-ray protein structure refinement, Acta Cryst A 47 (1991) 392-400.

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

[126] R.A. Laskowski, D.S. Moss, J.M. Thornton, Main-chain bond lengths and bond angles in protein structures, J Mol Biol 231 (1993) 1049-1067.

[127] R. Chaloupkova, J. Sykorova, Z. Prokop, A. Jesenska, M. Monincova, M. Pavlova, M. Tsuda, Y. Nagata, J. Damborsky, Modification of activity and specificity of haloalkane dehalogenase from Sphingomonas paucimobilis UT26 by engineering of its entrance tunnel, J Biol Chem 278 (2003) 52622-52628.

[128] M. Petrek, M. Otyepka, P. Banas, P. Kosinova, J. Koca, J. Damborsky, CAVER: a new tool to explore routes from protein clefts, pockets and cavities, BMC Bioinformatics 7 (2006) 316.

[129] W.L. DeLano, The PyMOL Molecular Graphics System, DeLano Scientific LLC, Palo Alto, CA, USA, 2008.

[130] A.A. Vaguine, J. Richelle, S.J. Wodak, SFCHECK: a unified set of procedures for evaluating the quality of macromolecular structure-factor data and their agreement with the atomic model, Acta crystallographica 55 (1999) 191-205.

[131] W. Kabsch, XDS Program Package.

[132] J.E. Harlan, D. Picot, P.J. Loll, R.M. Garavito, Calibration of size-exclusion chromatography: use of a double Gaussian distribution function to describe pore sizes, Anal Biochem 224 (1995) 557-563.

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

[134] J. Deisenhofer, O. Epp, I. Sinning, H. Michel, Crystallographic Refinement at 2.3 Å Resolution and Refined Model of the Photosynthetic Reaction Center from *Rhodopseudomonas viridis*, J Mol Biol 246 (1995) 429-457.

[135] A. Rokka, M. Suorsa, A. Saleem, N. Battchikova, E.M. Aro, Synthesis and assembly of thylakoid protein complexes. Multiple assembly steps of photosystem II, Biochem J 388 (2005) 159-168.

[136] M. Roncel, J.M. Ortega, M. Losada, Factors determining the special redox properties of photosynthetic cytochrome b559, Eur. J. Biochem. 268 (2001) 4961-4968.

[137] L.K. Thompson, A.F. Miller, C.A. Buser, J.C. de Paula, G.W. Brudvig, Characterization of the multiple forms of cytochrome b559 in photosystem II, Biochemistry 28 (1989) 8048-8056.

[138] J.M. Ortega, M. Hervas, M. Losada, Redox and acid-base characterization of cytochrome b-559 in photosystem II particles, Eur J Biochem 171 (1988) 449-455.

[139] C. Berthomieu, A. Boussac, W. Mantele, J. Breton, E. Nabedryk, Molecular changes following oxidoreduction of cytochrome b559 characterized by Fourier transform infrared difference spectroscopy and electron paramagnetic resonance: photooxidation in photosystem II and electrochemistry of isolated cytochrome b559 and iron protoporphyrin IX- bisimidazole model compounds, Biochemistry 31 (1992) 11460-11471.

[140] G.T. Babcock, W.R. Widger, W.A. Cramer, W.A. Oertling, J.G. Metz, Axial ligands of chloroplast cytochrome b-559 - Identification and requirement for a haem-cross-linked polypeptide structure, Biochemistry 24 (1985) 3638-3645.

[141] L.I. Krishtalik, G.S. Tae, D.A. Cherepanov, W.A. Cramer, The redox properties of cytochromes b imposed by the membrane electrostatic environment, Biophys J 65 (1993) 184-195.

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

[143] J. Komenda, J. Barber, 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 (1995) 9625-9631.

[144] S.R. Mayes, J.M. Dubbs, I. Vass, E. Hideg, L. Nagy, J. Barber, Further characterization of the psbH locus of *Synechocystis sp.*PCC 6803: inactivation of psbH impairs Q_A to Q_B electron transport in photosystem 2, Biochemistry 32 (1993) 1454-1465.

[145] S. Chiaramonte, G.M. Giacometti, E. Bergantino, Construction and characterization of a functional mutant of *Synechocystis* 6803 harbouring a eukaryotic PSII-H subunit, Eur. J. Biochem. 260 (1999) 833-843.

[146] E. Bergantino, A. Brunetta, E. Touloupakis, A. Segalla, I. Szabo, G.M. Giacometti, Role of the PSII-H subunit in photoprotection: novel aspects of D1 turnover in Synechocystis 6803, J Biol Chem 278 (2003) 41820-41829.

[147] E. Bergantino, A. Brunetta, A. Segalla, I. Szabo, D. Carbonera, E. Bordignon, F. Rigoni, G.M. Giacometti, Structural and functional role of the PsbH protein in resistance to light stress in Synechocystis PCC 6803, Functional Plant Biology 29 (2002) 1181-1187.

[148] J. Komenda, L. Lupinkova, J. Kopecky, Absence of the psbH gene product destabilizes photosystem II complex and bicarbonate binding on its acceptor side in *Synechocystis* PCC 6803, Eur. J. Biochem. 269 (2002) 610-619.

[149] J. Komenda, M. Tichy, L.A. Eichacker, The PsbH Protein Is Associated with the Inner Antenna CP47 and Facilitates D1 Processing and Incorporation into Photosystem II in the Cyanobacterium Synechocystis PCC 6803, Plant Cell Physiol (2005).

[150] M. Iwai, M. Katayama, M. Ikeuchi, Absence of the psbH gene product destabilizes the Photosystem II complex and prevents association of the Photosystem II-X protein in the thermophilic cyanobacterium Thermosynechococcus elongatus BP-1, Photosynth Res 87 (2006) 313-322.

[151] M. Ikeuchi, V.K. Shukla, H.B. Pakrasi, Y. Inoue, Directed inactivation of the psbI gene does not affect photosystem II in the cyanobacterium *Synechocystis* sp. PCC 6803, Mol. Gen. Genet. 249 (1995) 622-628.

[152] S. Schwenkert, P. Umate, C. Dal Bosco, S. Volz, L. Mlcochova, M. Zoryan, L.A. Eichacker, I. Ohad, R.G. Herrmann, J. Meurer, PsbI affects the stability, function, and phosphorylation patterns of photosystem II assemblies in tobacco, J Biol Chem 281 (2006) 34227-34238.

[153] P. Künstner, A. Guardiola, Y. Takahashi, J.D. Rochaix, A mutant strain of *Chlamydomonas reinhardtii* lacking the chloroplast photosystem II psbI gene grows photoautotrophically, J. Biol. Chem. 270 (1995) 9651-9654.

[154] M. Dobakova, M. Tichy, J. Komenda, Role of the PsbI protein in photosystem II assembly and repair in the cyanobacterium Synechocystis sp. PCC 6803, Plant Physiol 145 (2007) 1681-1691.

[155] R.E. Regel, N.B. Ivleva, H. Zer, J. Meurer, S.V. Shestakov, R.G. Herrmann, H.B. Pakrasi, I. Ohad, Deregulation of electron flow within photosystem II in the absence of the PsbJ protein, J. Biol. Chem. 276 (2001) 41473-41478.

[156] Y. Takahashi, H. Matsumoto, M. Goldschmidt-Clermont, J.D. Rochaix, Directed disruption of the *Chlamydomonas* chloroplast psbK gene destabilizes the photosystem II reaction center complex, Plant Mol. Biol. 24 (1994) 779-788.

[157] H. Hoshida, R. Sugiyama, Y. Nakano, T. Shiina, Y. Toyoshima, Electron paramagnetic resonance and mutational analyses revealed the involvement of photosystem II-L subunit in the oxidation step of Tyr-Z by $P680^{+}$ to form the Tyr-Z^{+}P680$Pheo^{-}$ state in photosystem II, Biochemistry 36 (1997) 12053-12061.

[158] S. Ozawa, T. Kobayashi, R. Sugiyama, H. Hoshida, T. Shiina, Y. Toyoshima, Role of PSII-L protein (psbL gene product) on the electron transfer in photosystem II complex. 1. Over-production of wild-type and mutant versions of PSII-L protein and reconstitution into the PSII core complex, Plant Mol. Biol. 34 (1997) 151-161.

[159] H. Luo, J.J. Eaton-Rye, Directed mutagenesis of the transmembrane domain of the PsbL subunit of photosystem II in Synechocystis sp. PCC 6803, Photosynth Res 98 (2008) 337-347.

[160] R. Gurezka, R. Laage, B. Brosig, D. Langosch, A heptad motif of leucine residues found in membrane proteins can drive self-assembly of artificial transmembrane segments, J Biol Chem 274 (1999) 9265-9270.

[161] F.K. Bentley, H. Luo, P. Dilbeck, R.L. Burnap, J.J. Eaton-Rye, Effects of inactivating psbM and psbT on photodamage and assembly of photosystem II in Synechocystis sp. PCC 6803, Biochemistry 47 (2008) 11637-11646.

[162] N. Ohnishi, Y. Takahashi, PsbT polypeptide is required for efficient repair of photodamaged photosystem II reaction center, J Biol Chem 276 (2001) 33798-33804.

[163] N. Ohnishi, Y. Kashino, K. Satoh, S. Ozawa, Y. Takahashi, Chloroplast-encoded polypeptide PsbT is involved in the repair of primary electron acceptor QA of photosystem II during photoinhibition in Chlamydomonas reinhardtii, J Biol Chem 282 (2007) 7107-7115.

[164] M. Iwai, T. Suzuki, N. Dohmae, Y. Inoue, M. Ikeuchi, Absence of the PsbZ subunit prevents association of PsbK and Ycf12 with the PSII complex in the thermophilic cyanobacterium Thermosynechococcus elongatus BP-1, Plant Cell Physiol 48 (2007) 1758-1763.

[165] C.L. Bishop, S. Ulas, E. Baena-Gonzalez, E.M. Aro, S. Purton, J.H. Nugent, P. Maenpaa, The PsbZ subunit of Photosystem II in Synechocystis sp. PCC 6803 modulates electron flow through the photosynthetic electron transfer chain, Photosynth Res 93 (2007) 139-147.

[166] Y. Kashino, T. Takahashi, N. Inoue-Kashino, A. Ban, Y. Ikeda, K. Satoh, M. Sugiura, Ycf12 is a core subunit in the photosystem II complex, Biochim Biophys Acta 1767 (2007) 1269-1275.

[167] N. Inoue-Kashino, T. Takahashi, A. Ban, M. Sugiura, Y. Takahashi, K. Satoh, Y. Kashino, Evidence for a stable association of Psb30 (Ycf12) with photosystem II core complex in the cyanobacterium Synechocystis sp. PCC 6803, Photosynth Res 98 (2008) 323-335.

[168] C. Funk, Functional analysis of the PsbX protein by deletion of the corresponding gene in Synechocystis sp. PCC 6803, Plant Mol. Biol. 44 (2000) 815-827.

[169] H. Katoh, M. Ikeuchi, Targeted disruption of psbX and biochemical characterization of Photosystem II complex in the thermophilic cyanobacterium *Synechococcus elongatus*, Plant Cell Physiol. 42 (2001) 179-188.

[170] J.G. Garcia-Cerdan, D. Sveshnikov, D. Dewez, S. Jansson, C. Funk, W.P. Schroder, Antisense inhibition of the PsbX protein affects PSII integrity in the higher plant Arabidopsis thaliana, Plant Cell Physiol 50 (2009) 191-202.

[171] K. Kawakami, M. Iwai, M. Ikeuchi, N. Kamiya, J.R. Shen, Location of PsbY in oxygen-evolving photosystem II revealed by mutagenesis and X-ray crystallography, FEBS Lett 581 (2007) 4983-4987.

[172] H. Hayashi, Y. Fujimura, P. Mohanty, N. Murata, The Role of Cp-47 in the Evolution of Oxygen and the Binding of the Extrinsic 33-Kda Protein to the Core Complex of Photosystem-II as Determined by Limited Proteolysis, Photosynth. Res 36 (1993) 35-42.

[173] L.K. Frankel, T.M. Bricker, Interaction of the 33-kDa extrinsic protein with photosystem II: identification of domains on the 33-kDa protein that are shielded from NHS-biotinylation by photosystem II, Biochemistry 34 (1995) 7492-7497.

[174] W.R. Odom, T.M. Bricker, 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 (1992) 5616-5620.

[175] Y. Ishikawa, Y. Yamamoto, M. Otsubo, S.M. Theg, N. Tamura, Chemical Modification of Amine Groups on PS II Protein(s) Retards Photoassembly of the Photosynthetic Water-Oxidizing Complex, Biochemistry 41 (2002) 1972-1980.

[176] H.M. Gleiter, E. Haag, J.R. Shen, J.J. Eaton-Rye, Y. Inoue, W.F. Vermaas, G. Renger, 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 (1994) 12063-12071.

[177] C. Putnam-Evans, J. Wu, T.M. Bricker, Site-directed mutagenesis of the CP 47 protein of photosystem II: alteration of conserved charged residues which lie within lethal deletions of the large extrinsic loop E, Plant Mol Biol 32 (1996) 1191-1195.

[178] R. Mei, J.P. Green, R.T. Sayre, W.D. Frasch, Manganese-binding proteins of the oxygen-evolving complex, Biochemistry 28 (1989) 5560-5567.

[179] Z.L. Li, R.L. Burnap, Mutations of arginine 64 within the putative Ca(2+)-binding lumenal interhelical a-b loop of the photosystem II D1 protein disrupt binding of the manganese stabilizing protein and cytochrome c(550) in Synechocystis sp. PCC6803, Biochemistry 40 (2001) 10350-10359.

[180] T. Ono, Y. Inoue, Ca2+-dependent restoration of O2-evolving activity in CaCl2-washed PS II particles depleted of 33, 24 and 16 kDa proteins, FEBS Lett 168 (1984) 281-286.

[181] M. Miyao, N. Murata, Role of the 33-Kda Polypeptide in Preserving Mn in the Photosynthetic Oxygen-Evolution System and Its Replacement by Chloride-Ions, Febs Letters 170 (1984) 350-354.

[182] T.M. Bricker, R.L. Burnap, The extrinsic proteins of Photosystem II, in: T. Wydrzynski, K. Satoh (Eds.), Photosystem II: the light-driven water:plastoquinone oxidoreductase, Springer, Dordrecht, 2005, pp. 95-120.

[183] I. Enami, A. Okumura, R. Nagao, T. Suzuki, M. Iwai, J.R. Shen, Structures and functions of the extrinsic proteins of photosystem II from different species, Photosynth Res 98 (2008) 349-363.

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

[185] M. Roncel, A. Boussac, J.L. Zurita, H. Bottin, M. Sugiura, D. Kirilovsky, J.M. Ortega, Redox properties of the photosystem II cytochromes b559 and c550 in the cyanobacterium *Thermosynechococcus elongatus*, J. Biol. Inorg. Chem. 8 (2003) 206-216.

[186] J.L. Roose, K.M. Wegener, H.B. Pakrasi, The extrinsic proteins of Photosystem II, Photosynth Res 92 (2007) 369-387.

[187] F.A. Tezcan, J.R. Winkler, H.B. Gray, Effects of Ligation and Folding on Reduction Potentials of Heme Proteins, J Am Chem Soc 120 (1998) 13383-13388.

[188] H. Ishikita, E.W. Knapp, Redox potential of cytochrome c550 in the cyanobacterium Thermosynechococcus elongates, FEBS Lett 579 (2005) 3190-3194.

[189] H. Andrews, Z. Li, A. Altuve-Blanco, M. Rivera, R.L. Burnap, Expression, mutagenesis, and characterization of recombinant low-potential cytochrome c550 of photosystem II, Biochemistry 44 (2005) 6092-6100.

[190] D.W. Krogmann, The low-potential cytochrome c of cyanobacteria and algae, Biochim Biophys Acta 1058 (1991) 35-37.

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

[192] J.R. Shen, W. Vermaas, Y. Inoue, The role of cytochrome c-550 as studied through reverse genetics and mutant characterization in *Synechocystis* sp. PCC 6803, J Biol Chem 270 (1995) 6901-6907.

[193] A. Kimura, J.J. Eaton-Rye, E.H. Morita, Y. Nishiyama, H. Hayashi, 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 (2002) 932-938.

[194] N. Inoue-Kashino, Y. Kashino, K. Satoh, I. Terashima, H.B. Pakrasi, PsbU provides a stable architecture for the oxygen-evolving system in cyanobacterial Photosystem II, Biochemistry (2005).

[195] J. Veerman, F.K. Bentley, J.J. Eaton-Rye, C.W. Mullineaux, S. Vasil'ev, D. Bruce, The PsbU subunit of photosystem II stabilizes energy transfer and primary photochemistry in the phycobilisome - Photosystem II assembly of Synechocystis sp PCC 6803, Biochemistry 44 (2005) 16939-16948.

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

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

[198] J.R. Shen, M. Ikeuchi, Y. Inoue, 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 (1997) 17821-17826.

[199] I. Balint, J. Bhattacharya, A. Perelman, D. Schatz, Y. Moskovitz, N. Keren, R. Schwarz, Inactivation of the extrinsic subunit of photosystem II, PsbU, in Synechococcus PCC 7942 results in elevated resistance to oxidative stress, FEBS Lett 580 (2006) 2117-2122.

[200] I. Sakurai, J.R. Shen, J. Leng, S. Ohashi, M. Kobayashi, H. Wada, Lipids in Oxygen-Evolving Photosystem II Complexes of Cyanobacteria and Higher Plants, J Biochem (Tokyo) 140 (2006) 201-209.

[201] T. Ohno, K. Satoh, S. Katoh, Chemical composition of purified oxygen-evolving complexes from the thermophilic cyanobacterium *Synechococcus* sp., Biochim. Biophys. Acta 852 (1986) 1-8.

[202] E. Yamashita, H. Zhang, W.A. Cramer, Structure of the cytochrome b6f complex: quinone analogue inhibitors as ligands of heme cn, J Mol Biol 370 (2007) 39-52.

[203] M.R. Jones, Lipids in photosynthetic reaction centres: structural roles and functional holes, Prog Lipid Res 46 (2007) 56-87.

[204] C.R. Lancaster, C. Hunte, J. Kelley, 3rd, B.L. Trumpower, R. Ditchfield, A comparison of stigmatellin conformations, free and bound to the photosynthetic reaction center and the cytochrome bc1 complex, J Mol Biol 368 (2007) 197-208.

[205] K. Shinzawa-Itoh, H. Aoyama, K. Muramoto, H. Terada, T. Kurauchi, Y. Tadehara, A. Yamasaki, T. Sugimura, S. Kurono, K. Tsujimoto, T. Mizushima, E. Yamashita, T. Tsukihara, S. Yoshikawa, Structures and physiological roles of 13 integral lipids of bovine heart cytochrome c oxidase, Embo J 26 (2007) 1713-1725.

[206] A. Krieger-Liszkay, Singlet oxygen production in photosynthesis, J Exp Bot 56 (2005) 337-346.

[207] R. Barbato, G. Friso, F. Rigoni, F. Dalla Vecchia, G.M. Giacometti, Structural-Changes and Lateral Redistribution of Photosystem-II uring Donor Side Photoinhibition of Thylakoids, J. Cell Biol. 119 (1992) 325-335.

[208] O. Kruse, B. Hankamer, C. Konczak, C. Gerle, E. Morris, A. Radunz, G.H. Schmid, J. Barber, Phosphatidylglycerol Is Involved in the Dimerization of Photosystem II, J. Biol. Chem. 275 (2000) 6509-6514.

[209] Z. Gombos, Z. Varkonyi, M. Hagio, M. Iwaki, L. Kovacs, K. Masamoto, S. Itoh, H. Wada, Phosphatidylglycerol requirement for the function of electron acceptor plastoquinone Q(B) in the photosystem II reaction center, Biochemistry 41 (2002) 3796-3802.

[210] H. Laczkó-Dobos, B. Ughy, S.Z. Tóth, J. Komenda, O. Zsiros, I. Domonkos, Á. Párducz, B. Bogos, M. Komura, S. Itoh, Z. Gombos, Role of phosphatidylglycerol in the function and assembly of Photosystem II reaction center, studied in a cdsA-inactivated PAL mutant strain of Synechocystis sp. PCC6803 that lacks phycobilisomes, Biochim Biophys Acta 1777 (2008) 1184-1194.

[211] J. Leng, I. Sakurai, H. Wada, J.R. Shen, Effects of phospholipase and lipase treatments on photosystem II core dimer from a thermophilic cyanobacterium., Photosynth Res in press (2008) doi 10.1007/s11120-11008-19335-11129.

[212] B. Loll, J. Kern, W. Saenger, A. Zouni, J. Biesiadka, Lipids in photosystem II: interactions with protein and cofactors, Biochim Biophys Acta 1767 (2007) 509-519.

[213] O. Kruse, G.H. Schmid, The role of phosphatidylglycerol as a functional effector and membrane anchor of the D1-core peptide from photosystem II-particles of the cyanobacterium *Oscillatoria chalybea*, Z. Naturforsch. 50c (1995) 380-390.

[214] B. Pineau, J. Girard-Bascou, S. Eberhard, Y. Choquet, A. Tremolieres, C. Gerard-Hirne, A. Bennardo-Connan, P. Decottignies, S. Gillet, F.A. Wollman, A single mutation that causes phosphatidylglycerol deficiency impairs synthesis of photosystem II cores in Chlamydomonas reinhardtii, Eur. J. Biochem. 271 (2004) 329-338.

[215] F. Reifarth, G. Christen, A.G. Seeliger, P. Dormann, C. Benning, G. Renger, Modification of the water oxidizing complex in leaves of the dgd1 mutant of *Arabidopsis thaliana* deficient in the galactolipid digalactosyldiacylglycerol, Biochemistry 36 (1997) 11769-11776.

[216] R. Steffen, A.A. Kelly, J. Huyer, P. Doermann, G. Renger, Investigations on the reaction pattern of photosystem II in leaves from Arabidopsis thaliana wild type plants and mutants with genetically modified lipid content, Biochemistry 44 (2005) 3134-3142.

[217] I. Sakurai, N. Mizusawa, H. Wada, N. Sato, Digalactosyldiacylglycerol is required for stabilization of the oxygen-evolving complex in photosystem II, Plant Physiol 145 (2007) 1361-1370.

[218] A. Minoda, K. Sonoike, K. Okada, N. Sato, M. Tsuzuki, Decrease in the efficiency of the electron donation to tyrosine Z of photosystem II in an SQDG-deficient mutant of *Chlamydomonas*, FEBS Lett. 553 (2003) 109-112.

[219] A. Ligeza, A.N. Tikhonov, J.S. Hyde, W.K. Subczynski, Oxygen permeability of thylakoid membranes: electron paramagnetic resonance spin labeling study, Biochim Biophys Acta 1365 (1998) 453-463.

[220] W.K. Subczynski, A. Wisniewska, Physical properties of lipid bilayer membranes: relevance to membrane biological functions, Acta biochimica Polonica 47 (2000) 613-625.

[221] D. Marsh, T. Pali, Lipid conformation in crystalline bilayers and in crystals of transmembrane proteins, Chem Phys Lipids 141 (2006) 48-65.

[222] G. Renger, Oxidative photosynthetic water splitting: energetics, kinetics and mechanism, Photosynth Res 92 (2007) 407-425.

[223] J.W. Murray, K. Maghlaoui, J. Kargul, M. Sugiura, J. Barber, Analysis of xenon binding to photosystem II by X-ray crystallography, Photosynth Res 98 (2008) 523-527.

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

[225] R. de Wijn, H.J. van Gorkom, Kinetics of electron transfer from Q(a) to Q(b) in photosystem II, Biochemistry 40 (2001) 11912-11922.

[226] V. Petrouleas, A.R. Crofts, The iron-quinone acceptor complex, in: T. Wydrzynski, K. Satoh (Eds.), Photosystem II: The Water/ Plastoquinone Oxido-Reductase in Photosynthesis, Kluwer Academic Publishers, Dordrecht, The Netherlands, 2005, pp. 177-206.

[227] B.A. Diner, P.J. Nixon, J.W. Farchaus, Site -directed mutagenesis of photosynthetic reaction centers., Curr. Opin. Struct. Biol. 1 (1991) 546-554.

[228] C. Kirmaier, D. Holten, R.J. Debus, G. Feher, M.Y. Okamura, Primary photochemistry of iron-depleted and zinc-reconstituted reaction centers from Rhodopseudomonas sphaeroides, Proc Natl Acad Sci U S A 83 (1986) 6407-6411.

[229] R.J. Debus, G. Feher, M.Y. Okamura, Iron-depleted reaction centers from Rhodopseudomonas sphaeroides R-26.1: characterization and reconstitution with Fe2+, Mn2+, Co2+, Ni2+, Cu2+, and Zn2+, Biochemistry 25 (1986) 2276-2287.

[230] J. Kern, G. Renger, Photosystem II: Structure and mechanism of the water:plastoquinone oxidoreductase, Photosynth Res 94 (2007) 183-202.

[231] H. Cheap, J. Tandori, V. Derrien, M. Benoit, P. de Oliveira, J. Koepke, J. Lavergne, P. Maroti, P. Sebban, Evidence for delocalized anticooperative flash induced proton binding as revealed by mutants at the M266His iron ligand in bacterial reaction centers, Biochemistry 46 (2007) 4510-4521.

[232] R. Krivanek, J. Kern, A. Zouni, H. Dau, M. Haumann, Spare quinones in the QB cavity of crystallized photosystem II from Thermosynechococcus elongatus, Biochim Biophys Acta 1767 (2007) 520-527.

[233] C. Fufezan, C.X. Zhang, A. Krieger-Liszkay, A.W. Rutherford, Secondary quinone in photosystem II of Thermosynechococcus elongatus: Semiquinone-iron EPR signals and temperature dependence of electron transfer, Biochemistry 44 (2005) 12780-12789.

[234] K. Zimmermann, M. Heck, J. Frank, J. Kern, I. Vass, A. Zouni, Herbicide binding and thermal stability of photosystem II isolated from Thermosynechococcus elongatus, Biochim Biophys Acta 1757 (2006) 106-114.

[235] O. Kaminskaya, V.A. Shuvalov, G. Renger, Evidence for a novel quinone-binding site in the photosystem II (PS II) complex that regulates the redox potential of cytochrome b559, Biochemistry 46 (2007) 1091-1105.

[236] J. Kruk, K. Strzalka, Redox changes of cytochrome b(559) in the presence of plastoquinones, J Biol Chem 276 (2001) 86-91.

[237] J.W. Murray, K. Maghlaoui, J. Barber, The structure of allophycocyanin from Thermosynechococcus elongatus at 3.5 A resolution, Acta Crystallogr Sect F Struct Biol Cryst Commun 63 (2007) 998-1002.

[238] B. Hankamer, E. Morris, J. Nield, C. Gerle, J. Barber, Three-Dimensional Structure of the Photosystem II Core Dimer of Higher Plants Determined by Electron Microscopy, J Struct Biol 135 (2001) 262-269.

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

[240] J. Nield, J. Barber, Refinement of the structural model for the Photosystem II supercomplex of higher plants, Biochim Biophys Acta 1757 (2006) 353-361.

[241] M.F. Blackwell, C. Gibas, S. Gygax, D. Roman, B. Wagner, The plastoquinone diffusion coefficient in chloroplasts and its mechanistic implications, Biochem Biophys Acta 1183 (1994) 533-543.

[242] H. Kirchhoff, U. Mukherjee, H.J. Galla, Molecular architecture of the thylakoid membrane: lipid diffusion space for plastoquinone, Biochemistry 41 (2002) 4872-4882.

[243] I.G. Tremmel, H. Kirchhoff, E. Weis, G.D. Farquhar, Dependence of plastoquinol diffusion on the shape, size, and density of integral thylakoid proteins, Biochim Biophys Acta 1607 (2003) 97-109.

[244] P. Joliot, J. lavergne, D. Beal, Plastoquinone compartmentation in chloroplasts. I. Evidence for domains with different rates of photo-reduction, Biochem Biophys Acta 1101 (1992) 1-12.

[245] J. lavergne, J.-P. Bouchard, P. Joliot, Plastoquinone compartmentation in chloroplasts. II. Theoretical aspects, Biochim Biophys Acta 1101 (1992) 13-22.

[246] H. Kirchhoff, S. Horstmann, E. Weis, Control of the photosynthetic electron transport by PQ diffusion microdomains in thylakoids of higher plants, Biochim Biophys Acta 1459 (2000) 148-168.

[247] H. Kirchhoff, Molecular crowding and order in photosynthetic membranes, Trends Plant Sci 13 (2008) 201-207.

[248] H. Kirchhoff, Significance of protein crowding, order and mobility for photosynthetic membrane functions, Biochem Soc Trans 36 (2008) 967-970.

[249] I.M. Folea, P. Zhang, E.M. Aro, E.J. Boekema, Domain organization of photosystem II in membranes of the cyanobacterium Synechocystis PCC6803 investigated by electron microscopy, FEBS Lett 582 (2008) 1749-1754.

[250] H. Kuhl, M. Rögner, J.F. Van Breemen, E.J. Boekema, Localization of cyanobacterial photosystem II donor-side subunits by electron microscopy and the supramolecular organization of photosystem II in the thylakoid membrane, Eur. J. Biochem. 266 (1999) 453-459.

[251] J.P. Dekker, E.J. Boekema, Supramolecular organization of thylakoid membrane proteins in green plants, Biochim Biophys Acta 1706 (2005) 12-39.

[252] H. Kirchhoff, S. Lenhert, C. Buchel, L. Chi, J. Nield, Probing the organization of photosystem II in photosynthetic membranes by atomic force microscopy, Biochemistry 47 (2008) 431-440.

[253] G. Renger, Ed., Primary Processes of Photosynthesis – Principles and Apparatus RCS Publishing, , Cambridge, 2008.

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

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

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

[257] J. Yano, J. Kern, K. Sauer, M.J. Latimer, Y. Pushkar, J. Biesiadka, B. Loll, W. Saenger, J. Messinger, A. Zouni, V.K. Yachandra, Where water is oxidized to dioxygen: structure of the photosynthetic Mn_4Ca cluster, Science 314 (2006) 821-825.

[258] K. Lindberg, T. Vanngard, L.-E. Andreasson, Studies of the slowly exchanging chloride in Photosystem II of higher plants, Photosynth Res 38 (1993) 401-408.

[259] K. Lindberg, L.E. Andreasson, A one-site, two-state model for the binding of anions in photosystem II, Biochemistry 35 (1996) 14259-14267.

[260] D.I. Bryson, N. Doctor, R. Johnson, S. Baranov, A. Haddy, Characteristics of iodide activation and inhibition of oxygen evolution by photosystem II, Biochemistry 44 (2005) 7354-7360.

[261] K. Olesen, L.E. Andreasson, The function of the chloride ion in photosynthetic oxygen evolution, Biochemistry 42 (2003) 2025-2035.

[262] P.M. Kelley, S. Izawa, The role of Cl− in photosystem II. I. Effects of chloride ion on photosystem II electron transport and on hydroxylamine inhibition, Biochim Biophys Acta 502 (1978) 198-210.

[263] H. Wincencjusz, C.F. Yocum, H.J. van Gorkom, Activating anions that replace Cl- in the O2-evolving complex of photosystem II slow the kinetics of the terminal step in water oxidation and destabilize the S2 and S3 states, Biochemistry 38 (1999) 3719-3725.

[264] M. Haumann, M. Barra, P. Loja, S. Loscher, R. Krivanek, A. Grundmeier, L.E. Andreasson, H. Dau, Bromide does not bind to the Mn4Ca complex in its S1 state in Cl(-)-depleted and Br(-)-reconstituted oxygen-evolving photosystem II: evidence from X-ray absorption spectroscopy at the Br K-edge, Biochemistry 45 (2006) 13101-13107.

[265] J.A. Laszlo, G.M. Baker, R.A. Dilley, Nonequilibration of membrane-associated protons with the internal aqueous space in dark-maintained chloroplast thylakoids, J Bioenerg Biomembr 16 (1984) 37-51.

[266] R.J. Debus, The catalytic manganese cluster: Protein ligation, in: T. Wydrzynski, K. Satoh (Eds.), Photosystem II: The light driven water:Plastoquinone oxidoreductase, Springer, The Netherlands, 2005, pp. 261-284.

[267] R.J. Debus, Protein Ligation of the Photosynthetic Oxygen-Evolving Center, Coord Chem Rev 252 (2008) 244-258.

[268] P.O. Sandusky, C.F. Yocum, The Chloride Requirement for Photosynthetic Oxygen Evolution - Analysis of the Effects of Chloride and Other Anions on Amine Inhibition of the Oxygen-Evolving Complex, Biochimica Et Biophysica Acta 766 (1984) 603-611.

[269] J. Clausen, W. Junge, Detection of an intermediate of photosynthetic water oxidation, Nature 430 (2004) 480-483.

[270] J. Clausen, W. Junge, H. Dau, M. Haumann, Photosynthetic water oxidation at high O-2 backpressure monitored by delayed chlorophyll fluorescence, Biochemistry 44 (2005) 12775-12779.

[271] J.M. Anderson, Does functional photosystem II complex have an oxygen channel?, FEBS Lett 488 (2001) 1-4.

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

[273] A.W. Rutherford, P. Faller, The heart of photosynthesis in glorious 3D, TIBS 26 (2001) 341-344.

[274] J.W. Murray, J. Barber, Structural characteristics of channels and pathways in photosystem II including the identification of an oxygen channel, J Struct Biol 159 (2007) 228-237.

[275] F.M. Ho, S. Styring, Access channels and methanol binding site to the CaMn4 cluster in Photosystem II based on solvent accessibility simulations, with implications for substrate water access, Biochim Biophys Acta 1777 (2008) 140-153.

[276] J. Barber, K.N. Ferreira, K. Maghlaoui, S. Iwata, Structural model of the oxygen-evolving centre of photosystem II with mechanistic implications, Physical Chemistry Chemical Physics 6 (2004) 4737-4742.

[277] J. De Las Rivas, J. Barber, Analysis of the Structure of the PsbO Protein and its Implications, Photosynthesis research 81 (2004) 329-343.

[278] H. Ishikita, W. Saenger, B. Loll, J. Biesiadka, E.W. Knapp, Energetics of a Possible Proton Exit Pathway for Water Oxidation in Photosystem II, Biochemistry 45 (2006) 2063-2071.

[279] F.M. Ho, Uncovering channels in photosystem II by computer modelling: current progress, future prospects, and lessons from analogous systems, Photosynthesis research 98 (2008) 503-522.

[280] A. Okumura, H. Ohta, Y. Inoue, I. Enami, Identification of functional domains of the extrinsic 12 kDa protein in red algal PSII by limited proteolysis and directed mutagenesis, Plant Cell Physiol 42 (2001) 1331-1337.

[281] J. Norberg, L. Nilsson, Solvent influence on base stacking, Biophysical journal 74 (1998) 394-402.

[282] D.A. Force, D.W. Randall, G.A. Lorigan, K.L. Clemens, R.D. Britt, ESEEM Studies of Alcohol Binding to the Manganese Cluster of the Oxygen Evolving Complex of Photosystem II, J. Am. Chem. Soc 120 (1998) 13321–13333.

[283] A. Boussac, H. Kuhl, E. Ghibaudi, M. Rögner, A.W. Rutherford, Detection of an electron paramagnetic resonance signal in the S0 state of the manganese complex of photosystem II from *Synechococcus elongatus*, Biochemistry 38 (1999) 11942-11948.

[284] W.D. Frasch, R. Mei, M. Sanders, Oxidation of alcohols catalyzed by the oxygen-evolving complex, Biochemistry 27 (1988) 3715–3719.

[285] K.A. Ahrling, M.C. Evans, J.H. Nugent, R.J. Ball, R.J. Pace, ESEEM studies of substrate water and small alcohol binding to the oxygen-evolving complex of photosystem II during functional turnover, Biochemistry 45 (2006) 7069-7082.

[286] B. Noring, D. Shevela, G. Renger, J. Messinger, Effects of methanol on the Si-state transitions in photosynthetic water-splitting, Photosynthesis research 98 (2008) 251-260.

[287] P. Brzezinski, P. Adelroth, Design principles of proton-pumping haem-copper oxidases, Current opinion in structural biology 16 (2006) 465-472.

[288] S. Cukierman, Et tu, Grotthuss! and other unfinished stories, Biochimica et biophysica acta 1757 (2006) 876-885.

[289] H.A. Chu, A.P. Nguyen, R.J. Debus, Amino acid residues that influence the binding of manganese or calcium to photosystem II. 1. The lumenal interhelical domains of the D1 polypeptide, Biochemistry 34 (1995) 5839-5858.

[290] M. Brunori, F. Cutruzzola, C. Savino, C. Travaglini-Allocatelli, B. Vallone, Q.H. Gibson, Structural dynamics of ligand diffusion in the protein matrix: A study on a new myoglobin mutant Y(B10) Q(E7) R(E10), Biophysical journal 76 (1999) 1259-1269.

[291] J.W. Murray, K. Maghlaoui, J. Kargul, M. Sugiura, J. Barber, Analysis of xenon binding to photosystem II by X-ray crystallography, Photosynthesis research 98 (2008) 523-527.

[292] D. Marsh, B.G. Dzikovski, V.A. Livshits, Oxygen profiles in membranes, Biophysical journal 90 (2006) L49-51.

[293] S.C. Lovell, I.W. Davis, W.B. Arendall, 3rd, P.I. de Bakker, J.M. Word, M.G. Prisant, J.S. Richardson, D.C. Richardson, Structure validation by Calpha geometry: phi,psi and Cbeta deviation, Proteins 50 (2003) 437-450.

7 Appendices

7.1 Nomenclature conversion

Established nomenclature	New nomenclature from pdb
Cla 1 (P_{D1})	Cla 362A
Cla 2 (P_{D2})	Cla 354D
Cla 3 (Chl_{D1})	Cla 363A
Cla 4 (Chl_{D2})	Cla 364D
Pho 5 (Phe_{D1})	Pho 365A
Pho 6 (Phe_{D2})	Pho 355D
Cla 7 (Chl_{ZD1})	Cla 366A
Cla 8 (Chl_{ZD2})	Cla 356D
Cla 11 (Chl11)	Cla 511B
Cla 12	Cla 512B
Cla 13	Cla 513B
Cla 14	Cla 514B
Cla 15	Cla 515B
Cla 16	Cla 516B
Cla 17	Cla 517B
Cla 21	Cla 518B
Cla 22	Cla 519B
Cla 23	Cla 520B
Cla 24	Cla 521B
Cla 25	Cla 522B
Cla 26	Cla 523B
Cla 27	Cla 524B
Cla 28	Cla 525B
Cla 29	Cla 526B
Cla 33	Cla 474C
Cla 34	Cla 475C
Cla 35	Cla 476C
Cla 37	Cla 477C

Cla 41	Cla 478C
Cla 42	Cla 479C
Cla 43	Cla 480C
Cla 44	Cla 481C
Cla 45	Cla 482C
Cla 46	Cla 483C
Cla 47	Cla 484C
Cla 48	Cla 485C
Cla 49	Cla 486C
Hem 51	Hem 85E
Hem 52	Hem 164V
PQ9 53 (Q_A)	PL9 357D
PQ9 54 (Q_B)	PL9 367A
OEC 55 (Mn_4Ca)	OEC 368A
Ca 56 (Ca^{2+}-PsbK)	Ca 56K
Fe 57	Fe 361A
BCT 58 (bicarbonate)	BCT 353D
PQ9 59 (Q_C)[#]	PL9 59J
Ca 60 (Ca^{2+}-PsbO)[#]	Ca 273O
Bcr 101 (Car_{D1})	Bcr 369A
Bcr 103	Bcr 527B
Bcr 104	Bcr 528B
Bcr 105	Bcr 529B
Bcr 106	Bcr 530B
Bcr 107	Bcr 107H
Bcr 111 (Car_{D2})	Bcr 358D
Bcr 112	Bcr 112K
Bcr 113	Bcr 487C
Bcr 115 (Car15)[#]	Bcr 115J
Bcr 116	Bcr 116Z
Bcr 117	Bcr 488C
DGD 201 (DGDG1)	DGD 370A
DGD 202	DGD 489C
LHG 203 (PG3)	LHG 371A

SQD 204 (SQDG4)	SQD 372A
DGD 205	DGD 490C
DGD 206	DGD 491C
MGE 207 (MGDG7)	LMG 359D
DGD 208	DGD 208H
MGE 209	LMG 531B
MGE 210	LMG 373A
MGE 211	LMG 360D
SQD 212	SQD 532B
SQD 213	SQD 213T
MGE 214	LMG 533B
MGE 215#	LMG 534B
SQD 216#	SQD 361D
MGE 217#	LMG 217M
MGE 218#	LMG 218E
MGE 219#	LMG 492C
MGE 220#	LMG 220I
MGE 221#	LMG 493C
LHG 222#	LHG 374A
DGD 223#	DGD 375A
SQD 224#	SQD 224F
DGD 225#	DGD 362D
LMT 226 (β–DM26)	LMT 226H
LMT 227	LMT 227T
LMT 228#	LMT 535B
LMT 229#	LMT 363D
LMT 230#	LMT 230I
LMT 231#	LMT 536B
LMT 232#	LMT 274O

Nomenclature of cofactors as used in previous atom coordinate files (pdb code: 2AXT) in comparison with the numbering of cofactors used in the present coordinate file (pdb code: 3BZ1 and 3BZ2). The common names/abbreviations used in the text are given in parentheses, newly identified cofactors in the 2.9 Å resolution structure (in comparison with 3.0 Å structure) are indicated by #.

7.2 Ramachandran plots data

Comparison of the quality of refinements at 2.9 Å and 3.0 Å resolution. Data derived with Rampage [293].

Ramachandran plot data	2.9 Å resolution	3.0 Å resolution
Reaction Centre		
Number of residues in favored region for D1, for D2	300 (90.1%) 297 (87.9%)	286 (85.9%) 282 (83.4%)
Number of residues in allowed region for D1, for D2	30 (9.0%) 36 (10.7%)	34 (10.2%) 45 (13.3%)
Number of residues in outlier region for D1, for D2	3 (0.9%) 5 (1.5%)	13 (3.9%) 11 (3.3%)
Antenna subinits		
Number of residues in favored region for CP47, for CP43	436 (89.3%) 384 (86.3%)	424 (87.2%) 358 (80.4%)
Number of residues in allowed region for CP47, for CP43	42 (8.6%) 51 (11.5%)	50 (10.3%) 70 (15.7%)
Number of residues in outlier region for CP47, for CP43	10 (2.0%) 10 (2.2%)	12 (2.5%) 17 (3.8%)
Cyt b-559		
Number of residues in favored region for PsbE, for PsbF	73 (91.2%) 25 (75.8%)	61 (76.2%) 28 (84.8%)
Number of residues in allowed region for PsbE, for PsbF	4 (5.0%) 8 (24.2%)	15 (18.8%) 4 (12.2%)
Number of residues in outlier region for PsbE, for PsbF	3 (3.8%) 0 (0.0%)	4 (5.0%) 1 (3.0%)
Low molecular weight subunits		
Number of residues in favored region for PsbH, for PsbI for PsbJ for PsbK for PsbL for PsbM for PsbT for PsbX for PsbY for ycf12 for PsbZ	51 (81%) 24 24 (72.7%) 26 (81.2%) 30 (85.7%) 34 (97.1%) 26 (81.2%) 25 (83.3%) 29 (82.9%) n.a. (poly-Ala) 16 (61.5%) 50 (83.3%)	49 (79%) 24 (72.7%) 27 (84.4%) 31 (88.6%) 30 (85.7%) 28 (82.4%) 26 (92.9%) not assigned not assigned not assigned 49 (81.7%)
Number of residues in allowed region for PsbH, for PsbI for PsbJ for PsbK for PsbL	9 (14.3%) 7 (21.2%) 4 (12.5%) 3 (8.6%) 1 (2.9%)	9 (14.5%) 8 (24.2%) 4 (12.5%) 2 (5.7%) 3 (8.6%)

for PsbM	6 (18.8%)	4 (11.8%)
for PsbT	4 (13.4%)	2 (7.1%)
for PsbX	5 (14.2%)	not assigned
for PsbY	n.a. (poly-Ala)	not assigned
for ycf12	9 (34.6%)	not assigned
for PsbZ	7 (11.7%)	9 (15.0%)
Number of residues in outlier region for PsbH,	3 (4.8 %)	4 (6.5%)
for PsbI	2 (6.1%)	1 (3.0%)
for PsbJ	2 (6.2 %)	1 (3.1%)
for PsbK	2 (5.7%)	2 (5.7%)
for PsbL	0 (0.0%)	2 (5.7%)
for PsbM	0 (0.0%)	2 (5.9%)
for PsbT	1 (3.3%)	0 (0.0%)
for PsbX	1 (2.9%)	not assigned
for PsbY	n.a. (poly-Ala)	not assigned
for ycf12	1 (3.8%)	not assigned
for PsbZ	3 (5.0%)	2 (3.3%)
Membrane extrinsic subunits		
Number of residues in favored region for PsbO,	205 (85.1%)	191 (79.6%)
for PsbU	81 (85.3%)	71 (74%)
for PsbV	115 (85.2%)	113 (81.7%)
Number of residues in allowed region for PsbO,	30 (12.4%)	35 (14.6%)
for PsbU	11 (11.6%)	20 (20.8%)
for PsbV	19 (14.1%)	19 (14.1%)
Number of residues in outlier region for PsbO,	6 (2.5%)	14 (5.8%)
for PsbU	3 (3.1%)	5 (5.2%)
for PsbV	1 (0.7%)	3 (2.2 %)
Overall		
Number of residues in favored region	4454 (86.7%)	4145 (82.7%)
Number of residues in allowed region	572 (11.1%)	682 (13.6%)
Number of residues in outlier region	112 (2.2%)	183 (3.7%)

7.3 Chlorophyll-protein contacts

Chl *a* molecule	Axial ligand	Distance, Å	Neighbouring carotenoid (edge to edge distance, Å)
CP47			
Chl11	B-Trp185 (main chain carbonyl) or bridged with putative water	4.19 *	Bcr107 (4.15)
Chl12	B-His201	2.36	Bcr107 (4.26)
Chl13	B-His202	2.36	Bcr107 (8.26)
Chl14	B-His455	2.40	Bcr105 (4.91)
Chl15	B-His100	2.51	Bcr106 (4.55)
Chl16	B-His157	2.35	Bcr106 (7.22)
Chl17	MGDG14 (ester carbonyl)	3.92	Bcr103 (4.43) Bcr104 (4.33) Bcr105 (4.57)
Chl21	B-His466	2.37	Bcr107 (6.15)
Chl22	B-His216	2.36	Bcr107 (3.06)
Chl23	Putative water	*	Bcr107 (4.30)
Chl24	B-His469	2.37	Bcr105 (14.76)
Chl25	B-His23	2.75	Bcr103 (7.84)
Chl26	B-His26	3.06	Bcr 103 (3.99) Bcr105 (4.02)
Chl27	B-His9	2.28	Bcr103 (3.66)
Chl28	B-His142	3.05	Bcr106 (8.43)
Chl29	B-His114	2.88	Bcr106 (3.99)
CP43			
Chl33	C-His237	2.23	Bcr117 (3.35)
Chl34	C-His430	2.41	Bcr117 (11.56)
Chl35	C-His118	2.29	Bcr116 (8.02)
Chl37	DGDG5 (ester carbonyl)	3.47	Bcr115 (8.78)
Chl41	C-His441	2.22	Bcr117 (4.04)
Chl42	C-His251	2.34	Bcr117 (7.19)
Chl43	Putative water	*	Bcr117 (4.69)
Chl44	C-His444	2.34	Bcr113 (14.11)
Chl45	C-His53	2.84	Bcr113 (7.07)
Chl46	C-His56	2.88	Bcr113 (6.67)

Chl47	C-Asn39 (side chain carboxyl)	2.24	Bcr113 (3.73)
Chl48	C-His164	2.95	Bcr116 (3.38)
Chl49	C-His132	2.23	Bcr116 (3.35)

* Putative waters were not placed into the final model due to the limited resolution

7.4 Intersubunit H-bonds for low molecular weight subunits

Interacting residues (residue-atom ··· atom-residue-subunit)	Distance, Å
PsbH	
Ala2-N ··· OD2-Asp119-B	3.36
Arg3-N ··· O-Asp119-B	3.25
Arg3-O ··· N-Glu121-B	3.16
Thr5-OG1 ···OBD-Chl29	3.02
Arg12-NH2 ··· O-Arg124-B	2.82
Leu14-O ··· NZ-Lys137-B	2.54
ASN15-OD1 ··· N-Asp134-B	2.81
ASN15-ND2 ··· O-Ala132-B	3.36
Tyr18-OH ··· O-Gly232-B	3.54
Lys20-O ··· Arg220-NH1-B	2.59
Ala22-O ··· N-Gln223-B	2.71
Gly24-O ··· N-Gln223-B	3.50
Tyr49-OH ··· O-Gly259-B	2.85
Asn50-ND2 ··· O-His87-D	3.50
Asn50-OD1 ··· N-Leu89-D	3.08
Asn50-O ··· NH1-Arg69-E	3.54
Ser51-O ··· NH2-Arg69-E	3.60
Ile54-N ··· OG-Ser15-X	2.99
Ile54-O ··· OG1-Thr13-X	2.97
Asp56-OD1 ··· N-Thr11-X	3.35
Asn59-N ··· OD1-Asp188-B	3.41
Lys63-NZ ··· OH-Tyr172-B	3.13
PsbI	
Gly22-O ··· NE1-Trp32-A	3.30
Ser25-OG ··· NE-Trp32-A	3.15
Asp27-OD1 ··· NH2-Arg136-A	2.47
Asp27-OD2 ··· NH1-Arg136-A	2.99
Asp27-OD2 ··· NH2-Arg449-C	3.39
Pro28-O ··· OH-Tyr135-A	2.89

Arg34-N ···O-Ala453-C	3.36
PsbJ	
Arg7-NH1 ··· OD1-Asp12-E	3.38
Arg7-NH2 ··· O-Asp12-E	3.67
Ile8-O ··· OG1-Thr15-E	3.66
Leu40-O ··· NH2-Arg45-F	2.66
Leu40-OXT ··· NZ-Lys56-V	3.42
PsbK	
Lys10-N ··· O-Phe75-C	3.44
Tyr15-OH ··· ND2-Asn58-Z	2.42
Asp23-OD2 ··· NE2-Gly21-y	286
Arg46-O ··· NH2-Arg41-C	3.24
Arg46-OXT ··· NH1-Arg41-C	3.36
PsbL	
Asn4-ND2 ··· OD2-Asp15-B	2.99
Asn6-ND2 ··· O-Asn14-B	3.37
Pro9-O ··· N-Leu3-B	2.91
Glu11-OE1 ··· N-Gly2-B	2.77
Glu11-OE2 ··· OH-Tyr235-A	2.52
Glu11-N ··· O-Leu3-B	3.02
Leu12-N ··· OG1-Thr29-M	2.84
Arg14-N ··· OE2-Glu25-T	3.48
Arg14-NH1 ··· O-Phe23-T	2.92
Arg14-NE ··· OH-Tyr26-M	3.22
Thr15-N ··· OE2-Glu25-T	3.54
Tyr18-OH ··· O-Phe23-T	3.24
Tyr18-OH ··· O-Phe19-T	3.39
Ser33-OG ··· N-Ile78-A	3.67
Tyr34-OH ··· O-Leu193-D	2.50
Phe35-O ··· ND2-Asn4-M	3.23
Phe36-O ··· N-Asn4-M	2.87
Asn37-OD1 ··· N-Ile229-D	2.95
Asn37-ND2 ··· O-Phe325-B	3.10
Asn37-O ··· N-Ser300-D	3.33

Asn37-OXT ··· OG-Ser300-D	2.85
PsbM	
Asn4-N ··· O-Phe36-L	2.87
Asn4-ND2 ··· O-Phe35-L	3.23
Tyr26-OH ··· NE-Arg14-L	3.22
Gln28-OE1 ··· OG-Ser31-M*	3.47
Gln32-NE2 ··· O-Val10-L	3.63
Gln33-NE2 ··· O-Gln33-M*	3.64
PsbT	
Glu2-OE1 ··· N-Met1-M	3.82
Ile21-O ··· NH2-Arg27-A	2.87
Phe23-O ··· NH1-Arg14-C	2.92
Arg24-NH1 ··· OG-Ser254-D	3.00
Arg24-NH2 ··· OXT-Asp473-C	3.04
Arg24-NE ··· OXT-Asp473-C	2.86
Arg28-NH1 ··· OG-Ser471-C	3.07
Arg28-NH2 ··· OD2-Asp-C	3.35
Thr30-N ··· O-Phe239-A	2.76
Lys32-OXT ··· NZ-Lys238-A	3.08
ycf12	
Gln21-NE2 ··· OD2-Asp23-K	2.80
Asn45-ND2 ··· O-Ala28-Z	3.23
Leu46-O ··· NH2-Arg46-K	3.08
PsbX	
Thr11-N ··· OD1-Asp56-H	3.35
Thr13-OG1 ··· O-Ile54-H	2.90
Ser15-OG ··· N-Ile54-H	2.99
Gly18-O ··· NE1-Trp93-D	3.69
Asp44-OD2 ··· NH2-Arg-D	3.40
PsbZ	
Ala28-O ··· ND2-Asp45y	3.23
Asn58-ND2 ··· Oh-Tyr15-K	2.42

* from the other monomer

7.5 Intersubunit H-bonds for extrinsic subunits

Interacting residues (residue-atom ··· atom-residue-subunit)	Distance, Å
PsbO	
Asp34-OD1 ··· NH2-Arg362-C	3.44
Asp34-OD2 ··· NH1-Arg362-C	3.52
Gly38-O ··· OE2-Glu348-C	2.94
Ala42-O ··· ND2-Asn373-C	3.20
Asn43-OD1 ··· NH1-Arg343-C	3.27
Lys83-NZ ··· OD2-Asp49-B*	3.08
Lys83-NZ ··· O-Ala337-B*	2.63
Asn84-ND2 ··· OE1-Glu431-B*	3.51
Val97-O ··· ND2-Asn108-A	3.45
Glu100-N ··· O-Pro345-C	3.36
Glu100-O ··· N-Gly347-C	3.06
Ser103-O ··· NH2-Arg343-C	3.00
Gln106-OE1 ··· N-Leu377-C	3.64
Asp125-OD2 ··· NZ-Lys381-C	2.64
Asp125-OD1 ··· OG-Ser330-C	2.65
Pro131-O ··· NH1-Arg64-A	2.90
Gln135-NE2 ··· OD2-Asp103-A	2.93
Arg141-NH2 ··· O-Pro57-A	3.35
Ser176-O ··· NE2-Gln332-C	2.97
Tyr177-O ··· NE2-Gln332-C	2.79
Arg178-NH2 ··· O-Arg64-A	2.51
Asn181-ND2 ··· O-Asn130-U	3.07
Asn181-ND2 ··· OD1-Asn350-D	3.00
Leu183-N ··· OD1-Asn335-A	2.75
Leu183-O ··· ND2-Asn335-A	3.14
Pro184-O ··· NH1-Arg334-A	2.67
Lys186-NZ ··· OE1-Glu302-D	2.49
Arg188-NH1 ··· O-Ala306-D	3.17
Arg188-NH2 ··· O-Ala305-D	3.10

Leu190-O ··· ND2-Asn41-U	2.79
Ser192-OG ··· O-Phe383-B	3.56
Gly193-O ···NH1-Arg385-B	2.93
Tyr194-OH ···OE1-Glu323-D	3.66
Asp195-OD2 ··· NH2-Arg422-B	2.83
Ser196-OG ··· NH1-Arg422-B	3.59
Pro201-O ··· NZ-Lys423-B	3.18
Gln202-OE1 ··· OH-Tyr314-B	3.21
Lys204-NZ ··· OG1-Thr34-B	3.42
Glu205-OE2 ··· NH1-Arg422-B	3.05
His254NE2 ··· OE2-Glu310D	3.04
PsbU	
Asn41-ND2 ··· O-Leu190-O	2.79
Gly52-O ···NE2-Gln394-B	2.96
Arg69-NH1 ··· O-Ala86-V	2.86
Gly70-N ··· OG1-Thr89-V	3.21
Thr74-OG1 ··· OD2-Asp109-V	3.07
Thr74-N ··· OD2-Asp109-V	2.92
Lys77-NZ ··· O-Lys323-C	2.94
Glu124-O ··· NZ-Lys339-C	3.54
Asp126-OD1 ··· NZ-Lys339-C	3.24
Tyr128-OH ··· O-Gly325-C	3.30
Asn129-ND2 ··· OD2-Asp321-C	2.73
Asn130-O ··· ND2-Asn181-O	3.07
Gly131-O ··· N-Ala351-D	2.99
Tyr133-OH ··· O-Asn338-A	2.97
Lys134-O ··· NH1-Arg348-D	3.57
Lys134-NZ ··· OD2-Asp79-V	3.26
PsbV	
Ala27-O ··· N-Lys310-A	3.55
Ala-27-N ··· O-Asp53E	3.45
Glu28-N ··· OE1-Gln58-E	3.14
Glu28-O ··· NE2-Gln58-E	3.01
Lys56-NZ ··· OXT-Leu40-J	3.42

Ser65-OG ··· OG1-Thr397-C	3.49
Lys73-NZ ··· OE2-Glu413-C	2.78
Asn75-OD1 ··· NH1-Arg320-C	3.05
Asp79-OD2 ··· Lys134-U	3.26
Ala86-O ··· NH1-Arg69-U	2.86
Thr89-OG1 ··· N-Gly70-U	3.21
Asp109-OD2 ··· N-Thr74-U	2.92
Asp109-OD2 ··· OG1-Thr74-U	3.07
Glu116-OE2 ··· NH1-Arg390-C	3.04
Lys129-NZ ··· OE1-Glu83-C	2.67
Arg131-NH1 ··· OE1-Glu104-C	3.08
Leu152-O ··· NH2-Arg61-E	3.40
Lys160-NZ ··· OE2-Glu329-A	3.05
Lys160-NZ ··· O-Leu352-D	3.12
Lys160-O ··· NH1-Arg323-A	3.44
Val161-O ··· NH1-Arg323-A	2.90
Tyr162-OH ··· OE2-Glu343-D	3.12
Tyr163-O ··· NE2-His304-A	2.62
Tyr163-OXT ··· NH1-Arg323-A	3.07
Tyr163-OH ··· OE1-Glu413-C	2.58

* from the other monomer

7.6 Lipid and detergent positions

Nr	lipid type	orientation of head group / position in complex	neighbouring subunits	polar interactions (≤3.5 Å) with protein / with cofactors Interacting atom of cofactor—protein chain-residue -interacting atom (distance in Å)	hydrophobic interactions (≤5 Å)with protein / with cofactors
1	DGDG	lumenal / intrinsic	D1, CP43, PsbI, PsbO	O2E—A-*Glu98*OE2 (2.49)* O3E— A-*Glu98*OE1 (2.84)* O4E—O-Gly38O (2.87)* O2D—I-*Tyr9*OH (2.61)* O3D—A-*Trp97*NE1 (2.53)* O4D—I-*Lys5*NZ(2.75)* O1A—C-Ser216N (3.27)* O3G—C-Ser216OG (3.40)*	A-Phe93, A-Phe117, A-Leu121, A-Phe155, C-Pro217, C-Phe218, C-Trp223, C-Met281, C-Phe284, C-Ile285 / Chl_{ZD1}, Chl41, Chl42, DGDG2
2	DGDG	lumenal / intrinsic	D1, CP43	O2E—C-Ser226O (3.68)** O3E—C-Arg362O (3.76)** O4E—C-Arg362O (2.13)* O4E—C-Arg362N (3.15)* O4E—C-*Asn294*ND2 (3.15)* O5E—C-Phe292O (3.90)** O2D—C-Phe218O (3.17)* O2D—C-Gly219N (3.60)** O4D—C-Gly220N (2.73)* O4D—C-Gly220O (3.18)*	A-Ala152, A-Phe155, A-Ile160, A-Ile163, C-Pro217, C-Phe218, C-Phe284, C-Ile285, C-Cys288, C-Phe431, C-Phe435, C-Leu438 / DGDG1, Chl41
3	PG	cytoplasmic / intrinsic, Q_B cavity	D1, D2, CP43	O1—C-*Arg447*NE (2.99)* O1—C-*Arg447*NH1 (3.25)* O1—C-*Arg447*NH2 (3.70)** O3—A-*Arg140*NH2 (2.78) O5—A-*Arg140*NH1 (2.65)[#] O5—A-*Arg140*NH2 (3.17)[#] O5—D-Thr231OG1 (2.55)* O5—D-Thr231N (3.26)* O10—D-*Asn220*ND2 (3.32)* / O1—Chl44O1D (3.23)* O1—Chl44O2D (3.05)* O2—Chl44O1D (3.58)** O2—Chl44OBD (3.81)**	A- Phe273, A-Phe285, A-Val281, C-Trp36, C-Phe436, C-Trp443 / Chl37, Chl44, Chl46, SQDG4
4	SQDG	cytoplasmic / intrinsic, PQ cavity	D1, D2, CP43 PsbK	O2—A-Ser270OG (3.17)* O3—A-*Asn267*ND2 (3.42)* O3—A-Ser270OG (3.74)** O4—A-*Asn267*ND2 (3.41)* O8—D-Arg223NE (3.39)[#] O8—D-Arg223NH1 (3.50)[#] O8—D-Arg223NH2 (3.48)[#] O9—C-*Trp36*NE1 (2.93)*	A-Phe265, A-Phe274, A-Trp278, C-Trp35, C-Trp36, D-Phe232, K-Leu33, K-Phe37 / LHG3, LHG22, Q_C, Car_{D2}, Car15, Chl44, DGDG5, DGDG6, MGDG7, MGDG18,
5	DGDG	lumenal / intrinsic, PQ cavity	D1, CP43, PsbJ	O2E—C-*Asn418*ND2 (2.98)* O3E—C-Glu83O (3.07)* O4E—C-Glu83O (2.88)* O3E—C-Gln84O (3.68)** O4E—C-Gln84N (3.16)* O4E—C-Tyr82O (3.66)** O5E—C-Val420O (2.58)* O5E—C-Gly85N (3.61)** O4D—C-*Asn418*ND2 (3.16)*	A-Phe197, A-Leu297, C-Leu404, C-Val432, J-Phe29 / SQDG4, DGDG6, MGDG19, LHG22, Car15, Chl37, Chl44

				O4D—C-*Asn418*OD1 (3.48)* O1B—J-*Tyr33*OH (3.36)* / O2E—MGDG19O3 (2.94)* O3E—MGDG19O3 (3.50)* O4D—DGDG6O5E (3.03)* O1A—Chl37Mg (3.47)[§]	
6	DGDG	lumenal / intrinsic, PQ cavity	D1, CP43, PsbJ, cyt-c550	O2E—C-*Asn415*OD1 (2.89)* O3E—C-Ser416N (3.00)* O3E—C-Ser416O (3.26)* O4E—V-Gln60OE1 (3.12)* O4E—C-Ser416O (3.76)** O2D—J-Gly37O (3.39)* O2D—J-Ala32O (3.80)** O3D—J-Gly37O (2.73)* O3D—J-Ser38O (2.76)* O3D—J-Ser39N (3.31)* O4D—A-*Ser305*OG (3.13)* O4D—A-Asn301O (3.77)** O4D—C-*Asn405*ND2 (3.84)** O4D—C-*Asn415*OD1 (3.32)* O4D—C-*Asn415*ND2 (3.76)** O6D—C-*Asn405*ND2 (3.06)* / O5E—DGDG5O4D (3.03)*	A-Pro196, A-Leu200, A-Ala203, A-Trp278, A-Val281, A-Phe300, A-Phe302, C-Leu404, J-Phe29 / SQDG4, DGDG5, MGDG7, Chl_{D2}, Chl37, Q_C
7	MGDG	lumenal / intrinsic, PQ cavity	D2, PsbF, PsbJ	O3—D-Gly70O (2.98)* O4—J-Gly31O (2.39)* O4—F-*Gln41*OE1 (3.24)* O5—D-Tyr67O (2.80)* O6—F-*Gln41*NE2 (2.72)*	D-Leu45, D-Trp48, D-Leu49, D-Phe73, J-Phe28, J-Phe29, F-Leu26 / SQDG4, DGDG6, Car_{D2}, Q_C, P_{D2}, Chl_{D2}
8	DGDG	lumenal / intrinsic	D2, CP47, PsbH	O2E—B193TyrOH (2.90)* O3E—H-Ser61OG (2.84)* O3E—H-Val60O (2.86)* O4E—H-Ser61OG (3.09)* O4E—H-*Trp62*N (3.71)** O5E—B-Ser277OG (3.05)* O5E—B-Tyr273O (3.34)* O6E—H-*Trp62*NE1 (3.43)* O2D—D-*His87*N (3.47)* O2D—D-*His87*ND1 (3.77)** O3D—D-Ser165O (3.21)* O3D—D-*His87*ND1 (3.58)**	B-Phe246, B-Phe250, B-Val251, B-Trp257, B-Tyr258, B-Ala456, B-Phe463, D-Leu89, D-Leu116, D-Phe120, D-Ile123, D-Leu158, D-Leu162, D-Leu291, D-Trp167, H-Tyr49 / Chl12, Chl21, Chl22
9	MGDG	cytoplasmic / intrinsic	D1, D2, CP47, PsbL, PsbM	O2—D-*Tyr141*OH (2.53)* O3—B-*Arg7*NH2 (2.46)* O4—D-*Tyr141*OH (2.61)* O5—A-*Asn234*OD1(3.85)**/ O5—MGDG10O2 (3.21)* O5—MGDG10O3 (3.69)**	B-Trp5, B-Tyr6, B-Leu461, B-Phe464, D-Ile144, D-Phe269, D-Leu272, D-Phe273, D-Val276, D-Trp280, D-Met281, L-Leu23, L-Leu27, M-Phe14, M-Val17, M-Pro18 / MGDG10, MGDG14, Chl17, Chl24, Chl26
10	MGDG	cytoplasmic / intrinsic	D1, D2, CP47, PsbL, PsbM	O2—A-*Asn234*OD1 (2.64)* O3—B-*Tyr6*OH (2.56)* O4—A-*Ser232*OG (2.73)* O4—A-*Asn234*OD1 (3.75)** O5—L-*Glu11*OE2 (3.34)* O5—L-Glu11O (3.26)* O5—L-*Asn13*ND2 (3.90)**	D-Ala202, D-Trp266, D-Phe269, D-Phe273, L-Leu19, L-Leu22, L-Leu23, L-Ile24, L-Val26, M-Val17, M-Pro18, M-Phe21, M-Leu22 / Chl_{D1}, Chl24, Chl27, Car3,

				O6—L-*Ser16*OG (3.01) O6—L-*Asn13*ND2 (3.68)** O9—B-*Trp5*NE1 (3.12)* O10—B-*Trp5*NE1 (3.10)* / O2—MGDG9O5 (3.21)* O3—MGDG9O5 (3.69)*	Car5, MGDG9, MGDG11, MGDG14, Q_A
11	MGDG	cytoplasmic / intrinsic	D1, D2, PsbL, PsbT	O1—L-Thr15OG1 (3.04)* O2—D-Ser262OG (2.66)* O2—D-Ser262N (3.22)* O2—D-Ala260O (3.34)* O3—D-Ser262N (2.67)* O3—D-Asn263N (3.12)* O4—D-Ser262OG (2.80)* O4—D-Ser262O (3.02)* O4—D-Asn263N (3.73)** O6—L-Thr15OG1 (3.06)* O9—D-*Trp266*NE1 (2.88)* O10—L-Leu19N (3.35)*	A-Tyr126, D-Phe257, D-Phe261, D-Phe270, L-Leu19, L-Leu22, L-Val26, L-Leu29, T-Phe10, T-Ile13, T-Phe17, T-Ile21 / Q_A, Phe_{D1}, **Car4**, **SQDG12**, P_{D1}, MGDG10, Chl_{D1}
12	SQDG	cytoplasmic / monomer interface	**D1**, CP47, **PsbI**, **PsbT**	O2—**A**-*Asn26*OD1 (3.34)* O2—**A**-*Trp20*NE1 (2.75)* O3—**A**-*Trp20*NE1 (3.19)* O8—B-*Trp113*NE1 (2.70)* O9—B-Tyr117OH (2.79)* O49—**A**-Arg27N (3.08)* O49—**A**-Leu28N (3.25)*	**A**-Leu28, **A**-Val30, **A**-Ile38, **A**-Leu41, **A**-Leu42, B-Leu109, **I**-Val11, **I**-Phe15, **T**-Phe22 / Car4, Car6, Chl16, Chl29, **Phe_{D1}**, **Chl_{D1}**, **MGDG11**, **Car_{D1}**, **MGDG20**, **Chl_{ZD1}**
13	SQDG	cytoplasmic / monomer interface	**CP47**, PsbL, **PsbL**, PsbM, PsbT, **PsbT**	O2—L-*Arg14*NH1 (3.52)* O3—L-*Arg14*NH2 (3.20)* O3—L-*Arg14*NH1 (3.65)** O7—**B**-*Arg18*NH1 (3.67) [#] O8—**L**-Asn4N (3.59)** O9—**B**-*Arg18*NH2 (2.65) [#] O10—M-*Tyr26*OH (3.36)*	**B**-Ala28, **B**-Leu29, **B**-Phe108, L-Leu17, L-Tyr18, L-Leu21, T-Leu16, T-Phe19, T-Phe23 / MGDG17, **Chl27**, **Car3**, **Car4**, **Car5**
14	MGDG	lumenal / monomer interface	D2, CP47, PsbL, PsbM,	O2—B-Thr327OG1 (2.75)* O2—B-Gly328N (3.26)* O5—B-*Tyr40*OH (3.76) ** O9—M-*Asn4*ND2 (3.78)** / O3—**LMT26**O2' (3.17)* O5—Chl17OBD (3.16)* O10—Chl17Mg (3.92) [§]	B-Phe196, B-Trp450, B-Phe453, B-Ala454, B-Val457, B-Phe458, B-Leu461, D-Met281, D-Ile284, L-Phe35, M-Ala10, M-Leu13, M-Phe14, M-Val17 / Chl17, Chl24, Chl26, Car3, Car5, MGDG9, MGDG10
15	MGDG	lumenal / monomer interface	**D1**, **D2**, CP47, **PsbO**	O3—**D**-*Arg304*NH1 (3.19)* O3—**D**-*Arg304*NH2 (3.23)* O4—**D**-*Arg304*NH2 (3.45)* O10—B-*Trp78*NE1 (3.55)** O10—B-Ser76OG (3.27)* / O2—**LMT27**O3 (3.84)** O9—**LMT27**O2'(3.69)**	B-Leu39, B-Leu42, B-Ala43, B-Trp75, B-Leu98, B-Ile101, **A**-Ile50, **A**-Ala54, **A**-Leu72, **A**-Leu102, **A**-Leu106 / **Car_{D1}**, **DGDG23**
16	SQDG	cytoplasmic / intrinsic	D2, CP47, PsbH, PsbX	O3—D-Lys23NZ (3.22)* O7—B-Lys227NZ (4.17) [#] O8—B-Ala228N (3.41)* O9—B-*Arg230*NH1 (3.39) [#] O9—B-*Arg230*NH2 (3.84) [#] O10—D-*Trp32*NE1 (2.97)* O49—B-*Arg230*NH1 (3.46)*/ O7—LMT31O2' (3.49)* O8—LMT31O2' (3.36)*	B-Leu229, B-Leu474, D-Phe15, D-Trp32, H-Leu39, X-Leu30, X-Phe34 / Chl21, Chl22, LMT31

17	MGDG	cytoplasmic / monomer interface	PsbM, **PsbM PsbL**	O3—M-Glu30O (2.99)* O5—M-Ser31O (3.02)* O5—M-Gln33N (3.55)**	M-Leu16, M-Ile23, M-Tyr26, M-Val27, **L**-Val10, **M**-Val20, **M**-Phe21, **M**-Ile24, **M**-Leu25 / SQDG13, **Chl27**
18	MGDG	cytoplasmic / intrinsic, PQ cavity	D1, D2, PsbE, PsbF	O2—E-Ser11OG (3.55)** O3—E-Phe10N (2.95)* O4—E-Phe10N (3.00)* O4—E-Ser11N (2.84)* O4—E-Ser11OG (2.84)* O5—A-*Tyr262*OH (3.71)** O6—E-Ser11OG (3.43)*	A-Ile259, A-Phe260, A-Tyr262, A-Ala263, D-Phe27, D-Val28, D-Phe38, E-Phe10, F-Ala22, F-Val23, F-Leu26 / Q_B, Q_C, SQDG4, LHG22, Car_{D2}, Car15, Chl_{D2}
19	MGDG	lumenal / intrinsic PQ cavity	CP43, PsbJ, PsbK, ycf12	/ O2—Chl37O2D (2.94)* O3—DGDG5O2E (3.00)* O3—DGDG5O3E (3.50)*	C-Leu433, J-Ile22, K-Val24, K-Val27, K-Val30, K-Leu31, y-Ile25 /DGDG5, Car15, Chl37, Chl44, Chl46
20	MGDG	lumenal / monomer interface	PsbI, **CP47**	O5—I-*Thr3*OG1 (2.67)* O5—I-Thr3N (3.78)**/ O2—DGDG23O5D (3.17)* O2—DGDG23O2E (3.30)* O3—LMT32O2‘ (2.83)* O5—LMT30O6B (3.83)** O9—DGDG23O3E (3.84)**	I-Thr3, I-Leu4, I-Thr7 / LMT30, LMT32, **SQDG12**, DGDG23, Car_{D1}, Chl_{ZD1}
21	MGDG	lumenal / membrane exposed	CP43, PsbZ	O5—C-*Asp107*OD1 (3.19)* O5—C-*Asp107*OD2 (3.88)** O9—C-*Trp97*NE1 (3.66)**	C-Val61, C-Trp97, C-Phe109, C-Val113, C-Val114, C-Val117, Z-Phe59 /Car16, Chl34, Chl35, Chl48
22	PG	cytoplasmic / intrinsic, PQ cavity	D1, CP43, PsbK	O1—A-*Asn266*ND2 (3.53)** O2—A-Tyr262O (3.68)** O10—C-*Trp35*NE1 (3.21)*	C-Trp35,K-Phe37, K-Phe45 /SQDG4, DGDG5, MGDG18, Car_{D2}, Car12, Car15
23	DGDG	lumenal / monomer interface	D1, **CP47**	O2D—**B**-*Trp75*NE1 (3.31)* O4D—**B**-Asp87OD1 (3.21)* O4D—**B**-Asp87OD2 (3.51)** / O3E—MGDG20O9 (3.84)** O4E—**LMT28**O5B (3.02)* O3D—LMT32O6‘ (3.20)* O5D—MGDG20O2 (3.17)*	A-Ile46, A-Ile50, A-Leu102, **B**-Trp75, **B**-Phe90, **B**-Trp91, **B**-Leu98, **B**-Val102 / LMT32, MGDG20, Car_{D1},**Car5**, **Car6**, **Chl16**
24	SQDG	cytoplasmic / membrane exposed	D2, PsbE, PsbF, PsbX, PsbY	O4—D-*Arg24*NH1 (3.68)** O7—D-*Arg26*NH2 (3.57) # O7—D-*Arg26*NE (2.62) # O8—F-Val18N (2.89)*	D-Trp21, F-Phe16, F-Trp20, F-Val21, X-Leu32, X-Val36, X-Leu37, X-Ile40 / Q_B, DGDG25
25	DGDG	lumenal / membrane exposed	D2, PsbE, PsbY	O2E—D-Asp100OD2 (2.54)* O2E—D-Asp100OD1 (3.44)* O5D—D-Thr102OG1 (3.78)** / O1A—LMT29O6’ (3.00)*	D-Tyr42, D-Phe101, E-Val46, E-Phe47, F-Pro29, F-Phe33 / Car_{D2}, LMT29, Chl_{ZD2}, SQDG24
26	β-DM	lumenal / monomer interface	**CP47**, PsbM, **PsbM**, PsbT	O1B—**M**-Gln5NE2 (3.24)* O2B—**M**-Gln5NE2 (2.55)* O3B—**M**-Gln5NE2 (3.86)** O6B—M-Met1N (3.76)** O3’—**M**-Gln5NE2 (3.37)* O4’—M-Met1O (3.40)* / O2’—**MGDG14**O3 (3.08)*	**B**-Tyr40, M-Leu8, M-Ala12, **M**-Leu6, **M**-Ile9, T-Met1, T-Ile4, T-Phe8 /, **MGDG14**, **Car3**, **Car4**, **Chl17**, **Chl27**

27	β-DM	lumenal / monomer interface	D1, **CP47**, PsbT	O2B—**B**-Thr44O (3.87)**/ O2'—**MGDG15**O9 (3.64)** O3'—**MGDG15**O2 (3.90)**	A-Leu72, **B**-Leu39, **B**-Tyr40, T-Thr3, T-Ile4, T-Val7, T-Ala11 / **Car4**, **Car5**
28	β-DM	lumenal / monomer interface	CP47	/ O5B—**DGDG23**O4E (3.47)* O6'—Chl16OBD (2.55)*	B-Trp91, B-Leu149, B-Phe162 / Chl14, Chl15, Chl16, Chl28, Car6
29	β-DM	lumenal / membrane exposed	D2, PsbX	O2'—X-*Ser25*OG (3.42)* O2'—X-Ile21O (3.61) ** / O6'—DGDG25O1A (3.00)*	D-Leu92, D-Trp93, X-Val29, X-Leu30 / DGDG25, Chl_{ZD2}, Chl21
30	β-DM	lumenal / membrane exposed (close to monomer interface)	PsbI	O2'—I-*Thr3*OG1 (3.64)** / O6B—MGDG20O5 (3.83)**	I-Thr3, I-Thr7, I-Ile10, I-Val11, I-Phe14, I-Phe15 / MGDG20
31	β-DM	cytoplasmic / intrinsic	D2, CP47, PsbH	O1'—B-*Arg224*NE (3.74)** O2'—B-Arg224O (3.42)* O3'—B-Lys227NZ (2.66)* O5'—B-*Arg224*NH2 (3.16) O6'—D-*Asp19*OD2 (3.01)* / O2'—SQDG16O8 (3.36)*	B-Leu225, D-Phe15, H-Trp15, H-Met31, H-Ala32, H-Met35 / SQDG16, Chl22
32	β-DM	lumenal / monomer interface	D1, **CP47**, PsbI, PsbO	O1B—O-*Lys95*NZ (3.32)* O2B—**B**-Asp87OD2 (3.08)* O3B—**B**-Gly85O (3.15)* O3'—A-Ala100O (3.81)** O6'—**B**-Asp87OD2 (3.08)* / O2'—MGDG20O3 (2.83)* O6'—DGDG23O3D (3.20)*	A-Ile96, A-Leu102, I-Met1, I-Leu4 / MGDG20, DGDG23, Car_{D1}, Chl_{ZD1}

Subunit or cofactor of the other monomer is in **bold**; * potential hydrogen bond; ** potential hydrogen bond if a distance longer than 3.5 Å is accepted; # potential salt bridge; § axial coordination of Chl Mg^{2+}. Conserved amino acids in *italic*. Atomic nomenclature is as in PDB files (3BZ1 and 3BZ2). LMT is the pdb file-format name for β-dM (see also Appendix Table 7.1). Here, intrinsic lipid means a lipid within PSII complex, not at periphery and not at the monomer-monomer interface.

7.7 The substrate/product channels at the lumenal side of PSII

Channel	Starting point	End point	Narrowest radius (Å)	Residues at the narrowest point	Length (Å)	Residues with the dominance of polar groups in channel	Residues with the dominance of hydrophobic groups in channel
A1	CP43, D1	Ca, Mn1, Mn2	1.24	C-Asp360, DGDG2	25	A-Asp342, A-Ala344, A-Gln165, A-His190, A-Asn296, A-Gly164, A-Gly166, A-Ile163, C-Asp360, DGDG2, C-Gly220, C-Glu221, C-Lys215, C-Arg362, C-Ser226, C-Asn228	C-Leu401, A-Leu343, C-Phe358, C-Gly306, C-Trp291, C-Pro307, C-Phe292, A-Leu91
A2	D1, CP43, PsbO	Ca, Mn1, Mn2	1.38	A-His92, C-Trp359, A-Ile89	35	A-Asp342, A-Ala344, A-Gln165, A-His190, A-Asn296, A-Gly164, A-Gly166, A-Ile163, DGDG2, A-His92, C-Arg357, C-Asp360, C-Trp359, A-Ala88, O-Arg99, DGDG1, A-Glu98, O-Thr39, O-Gly38, O-Glu100	C-Leu401, A-Leu343, C-Phe358, C-Trp291, C-Gly306, C-Gly219, C-Pro307, C-Phe292, A-Leu91, A-Ile89, C-Pro345, C-Thr346
B1	Ca, Mn1, Mn2	CP43, D1, PsbV,	1.44 1.55	C-Val410, A-Glu329, A-Asp342 C-His398, C-Val417, V-Ser65	33.5	A-Asp342A, A-Glu329, A-Pro340, V-Lys160, C-Glu413, C-His398, V-Lys73, C-Met396, C-Asn418, C-Ala399, C-Glu83, ***V-Gln60***, C-Lys79, DGDG5, DGDG6	A-Glu189, C-Val410, A-Leu341, C-Gly409, A-Leu343, ***V-Ser65***, C-Gly408, C-Leu401, ***V-Lys129, V-Tyr61***, C-Thr397, C-Val417, ***C-Phe419***, V-Ala64, D-Leu352, C-Thr412, A-Ala188
B2	Ca, Mn1, Mn2	PsbU, PsbV	1.44 1.75	C-Val410, A-Glu329, A-Asp342 U-Lys134, V-Pro76, V-Asp79	29.5	A-Asp342, A-Glu329, A-Pro340, A-Ala344, C-Glu413, V-Tyr163, ***V-Asp79***, ***V-Ser77***, V-Gly157	A-Glu189, C-Val410, D-Leu352, A-Leu342, V-Lys160, V-Lys73, V-Ile71, U-Tyr133, V-Pro76, V-Gly159, ***U-Lys134***
C	Mn3, Mn4	D1, D2, PsbO	0.66	A-Glu65, A-Arg334, A-Asn335	31.5	A-Asn181, A-Asp61, A-Arg334, A-Asn335, A-Glu65, A-Phe182, D-Glu312, O-Arg178, D-Glu310, O-Asp183, O-Asp250, D-Pro309, A-Arg64, O-Arg141	A-His332, A-Pro173, A-Glu333, D-Phe314, A-Ile60, D-Lys317, A-Val185, D-Leu320, D-Leu321, O-Asp184, O-Pro185, O-Phe182, A-Pro66, A-Pro57, D-Phe311, A-Ile63, O-Pro143
D	Mn3, Mn4	D1, D2, PsbO,	0.72 1.01	O-Tyr177, O-Arg178, A-Arg64 A-Ile63, C-Leu337, C-Thr335	30	A-Glu333, C-Glu354, C-Arg357, A-Ser169, A-Asp61, Asn338, C-Thr335, O-Tyr177, O-Arg178, A-Arg64A	A-Ala336, C-Gly353, C-Met356, A-Gly62, C-Gly338, A-Ile63, C-Leu337
E	Mn3, Mn4	CP47, PsbU	1.08	C-Pro334, D-Asn350, A-Asn335	52	A-Glu333, C-Glu354, C-Arg357, A-Asp170, ***A-Asn87***, A-Ser169, A-Asp61, C-Thr335, A-Asn338, A-Asn335, D-Asn350, ***O-Asn181***, B-Arg384, ***O-Ser192***, ***U-Asn130***, ***U-Asn61***, ***U-Thr60***, ***U-Tyr51***	A-Ala336, C-Met356, A-Ile63, C-Gly338, C-Leu337, C-Pro334, D-Gly349, O-Leu183, ***U-Leu132***, ***O-Ala191***, B-Ala386
F	Mn3, Mn4	CP47, PsbU	0.96 1.12	A-Asn338, C-Pro334, C-Lys339 U-Asp126, U-Asn130, O-Asn181	42	A-Glu333, C-Glu354, C-Arg357, A-Ser169, A-Asp61, A-Ile63, C-Thr335, C-Lys339, A-Asn338, D-Asn350, ***O-Asn181***, U-Asp126, ***U-Asn130***, ***U-Asn61***, ***U-Tyr51***	A-Gly62, A-Ala336, C-Gly353, C-Met356, C-Met342, C-Leu337, C-Pro334, C-Gly333, ***O-Ala191***, U-Leu121, B-Ala386
G	Mn3, Mn4	PsbO	0.88	D-Thr316, D-Leu320, O-Pro185	51	A-Glu333, A-His332, A-Asn181, D-Lys317, A-Arg334, D-Thr316, O-Lys186, ***O-Ala199***, D-Glu323, D-Glu302, D-Tyr296, B-Glu364, ***B-Ser365***, ***O-Glu205***, O-Asn212, B-Arg422	A-Val185, D-Leu321, D-Leu320, O-Pro185, ***D-Leu319***, ***O-Ile198***, ***O-Pro201***, O-Ala197

Non-conserved residues are marked by ***bold italic***, all other residues listed are strictly conserved. Residues are labelled first with PSII subunit name, their three-letter code and sequence number.

7.8 Crystallographic statistics for Xe and Kr derivative datasets

Noble gas	Xe	Xe	Xe	Kr
Pressure [bar]	10	14	30	40
Incubation time (min)	5	5	5	8
Wavelength [Å]	2.1	2.1	2.1	0.86
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
Unit cell parameters				
a [Å]	127.6	128.7	127.9	131.45
b [Å]	224.8	226.3	224.5	226.90
c [Å]	306.5	306.5	306.0	307.06
α=β=γ(°)	90	90	90	90
Resolution [Å]	30-4.2 (4.3-4.2)*	30-4.5 (4.6-4.5)*	30-4.5 (4.6-4.5)*	30-4.5 (4.6-4.5)*
Measured reflections	442227	225447	306108	267126
Unique reflections	117764	90277	94705	105238
Redundancy	3.75	2.49	3.23	2.53
R_{sym}	0.108 (0.465)*	0.110 (0.473)*	0.106 (0.491)*	0.121(0.525)*
Completeness [%]	94.8 (90.3)*	88.0 (73.9)*	93.8 (88.1)*	88.3 (69.1)*
Number of Xe/Kr sites in PSII dimer	19	35	53	23

* values for high resolution shells

7.9 Positions of Xe and Kr atoms found in the difference electron density map

Site	Noble gas position	Neighbouring residues	Sigma level Xe site			Sigma level Kr site
			30 bar	14 bar	10 bar	40 bar
1	Near B-tail of DGDG2, 12 Å away from channels A1, A2	DGDG2, C-Phe431, C-Phe284, A-Ile160, A-Phe295, C-Cys288, A-Ile163, B-Thr287	17.98	19.52	23.68	6.65
2	ß-barrel inside PsbO	O-Leu69, O-Phe121, O-Ile237, O-Phe168, O-Phe265, O-Leu225, O-Ile66, O-Ile269, O-Leu111, O-Ala267, O-Ala153	16.49	18.29	22.19	7.98
3	Near A-tail of DGDG8	DGDG8, D-Leu122, D-Phe153, D-Ile150, D-Val154, Chl21, D-Ile123, D-Ala119	16.38	14.21	16.39	
4	In chlorophyll cluster of CP47	B-Ala244, B-Val245, B-Ala248, Chl15 tail, Chl13 tail, Chl23 tail, Chl25 tail	15.44	13.67	18.48	5.94
5	C_2 fold axis, at monomer interface	M-Leu13, M-Leu13*, M-Ala12, M-Ile9, M-Ile9*, M-Leu16, M-Leu16*	15.29	12.11	15.65	6.56
6	In D1	A-Leu200, A-Gly204, A-Trp278, A-Val281, A-Gly282, A-Phe285, DGDG6 tail, Chl37	15.11	12.78	13.43	6.51
7	Near Q_C	Car_{D2}, Q_C, J-Val21, J-Ile24, J-Val25, F-Leu34	14.95	10.93	13.29	
8	Near middle of A-tail of DGDG8	In the middle of DGDG8, D-Leu89, D-Trp111, D-Thr112, D-Leu116, D-Leu158, D-Trp167	14.84	11.46		
9	At the monomer interface	Car3 chain, Car4 chain, Car5 chain, Chl27, SQDG13* tail	14.19	9.38	13.03	
10	At the monomer interface	β-DM26 tail, M-Thr11, M-Ala12, M-Val15, T-Thr5, T-Phe8, Chl27*	13.64	9.77	11.60	
11	In chlorophyll cluster of CP47	Chl12, Chl13, Chl21, Chl22, B-Phe247	13.20	11.03		6.48
12	Near channel II (Q_B) exit	X-Val36, X-Thr33, D-Pro39, SQDG24 tail, Chl8 head group, Q_B tail	12.01	11.40	10.70	
13	Near A-tail of DGDG2	A-tail DGDG2, A-Ala152, A-Ala156, C-Phe431, C-Phe435	11.63	9.96		6.93
14	At the monomer interface	SQDG13, B-Leu29, B-Phe108	11.45	10.06		
15	At N terminus of PsbX	Car7, X-Leu16, X-Phe19, H-Ile44, H-Leu53	11.28	10.11		6.72
16	Near DGDG9	B-Trp468, B-Ala471, B-Phe479, D-Pro140, D-Tyr141	10.73	9.23		
17	Between PsbK and PsbX	X-Leu10, X-Val13, X-Leu14, K-Val24, K-Val27	10.51			
18	Near Car16	Z-Trp47, Z-Ile48, Z-Val51, Car16	10.31	10.02		
19	Near PG3	PG3, Chl44, C-Trp443	10.17	9.87		
20	Near monomer interface	MGDG14, L-Phe35, Car5*	10.01			
21	At the monomer interface	T-Ile14, Chl_{D1}, SQDG12*	9.89			
22	Near Q_A head	Q_A, D-Leu210, D-Phe261, D-Leu267	9.81			
23	Near A-tail of DGDG1	DGDG1, A-Phe93, A-Phe117, C-Phe218, Chl_{ZD1}	9.75			
24	At the monomer interface	T-Val7, T-Phe10, T-Ala11, DGDG15*	9.66			
25	At the monomer interface	T-Val7, T-Phe8, T-Ala11, β-DM27, Car4*	9.36			
26	Near A-tail of DGDG2	A-Met127, A-Ser148, C-Leu438, C-Leu442, Chl41, DGDG2	9.29			
27	Near A-tail of DGDG23	DGDG23, C-Val432, C-Leu433, Chl37	9.10			
28	Oxygen channel B2	V-Ile71, V-Lys73, V-Pro76, A-Pro340				6.41
29	Oxygen channel B1	C-Val407, C-Gly408, C-Val417, C-Phe419				6.31
30	Near chlorophyll cluster of CP43	C-Pro90, C-Thr94, C-Phe301, C-Tyr302				6.24
31	In chlorophyll cluster of CP47	B-Leu149, Chl13, Chl14, Chl16, Chl23				6.07

* from the other monomer. Sites that coincide with those in ref [291] are marked by ***bold italic***.

8 Publications

Guskov A., Kern J., Gabdulkhakov A., Broser M., Zouni A., Saenger W. (2009). Cyanobacterial photosystem II at 2.9 Å resolution and the role of quinones, lipids, channels and chloride. *Nat Struct Mol Biol*. Mar;16(3):334-42

Gabdulkhakov A., Guskov A., Broser M., Kern J., Müh F., Saenger W., Zouni A. (2009). Probing the accessibility of the Mn4Ca cluster in photosystem II: Channels calculation, noble gas derivatization and co-crystallization with DMSO. Structure, Sep 9; 17 (9), 1223-34.

Guskov A., Kern J., Zouni A., Saenger W. (2008). Current State of Crystallographic Studies on Cyanobacterial Photosystem II – In Search for Better Resolution in Photosynthesis. Energy from the Sun: 14th International Congress on Photosynthesis (eds. Allen J.F., Gantt E., Golbeck J.H., Osmond B.).p. 409-412. Springer, Netherlands.