

Figure 20. Low molecular weight subunits. A) side view onto the PSII homodimer, main proteins subunits in grey, whereas low molecular weight subunits are colour-coded as follows: PsbH in violet, PsbI in salmon red, PsbJ in dark green, PsbK in light blue, PsbL in brown, PsbM in cyan, PsbT in dark yellow, PsbX in light green, PsbY in dark red, ycf12 in marine, PsbZ in magenta; B) the same, but top view, small subunits are labelled.

It was shown that PsbH might influence the electron transfer between Q_A and Q_B [143, 144] and also the herbicide binding to PSII [145, 146] as well as the resistance to light stress [147]. Moreover, PsbH has the second highest turnover rate after subunit D1, which indicates that PsbH plays a significant role in the replacement of photodamaged D1. Several studies confirmed an importance of PsbH for the stability and assembly of the entire PSII complex [135, 148-150].

Subunit PsbI is located next to the TMH **a** of D1 and close to the monomer-monomer interface and to CP43 subunit. Its N-terminus starts at the luminal side, whereas the C-terminus protrudes slightly off the membrane towards the cytoplasm. The full length of PsbI is 38 residues, all were modelled except the last three residues. The TMH of PsbI is

significantly tilted (ca. 30° from the membrane normal) forming a pocket for ChlZ_{D1}. Additionally it contributes to the binding of MGDG20, DGDG1, β-DM30, β-DM32, Car_{D1} and Car17. PsbI forms several H-bonds with subunits D1 and CP43 (see Appendix Table 7.4).

The exact function of PsbI is not yet characterized. A change in the oxygen activity upon deletion of PsbI has been shown, albeit with different degree of suppression (25-40% less in *Synechocystis* PCC 6803 [151], 50% in tobacco [152] and up to 90% less in *Chlamydomonas reinhardtii* (*C. reinhardtii*) [153]). Obviously, this subunit is also involved in the stabilization of the PSII complex and in the D1-turnover as was confirmed recently [154].

Subunit PsbJ is located opposite to the α-subunit of *cyt-b559* and together with it forms channel I for the plastoquinone / plastoquinol exchange (see section 3.2.2.4). It is folded into a single TMH with N-terminus located at the cytoplasmic side. The polypeptide is 40 residues long, all are modelled except the first six residues. PsbJ forms only few H-bonds with subunit PsbE, and its C-terminus is stabilized by H-bonds with conserved Arg45 from subunit PsbF and Lys56 from subunit PsbV (see Appendix Table 7.4). PsbJ contributes to the binding sites of Car12, Car15, Car_{D2}, DGDG5, DGDG6 and Q_C.

The function of PsbJ is probably related with its structural role in channel formation. Indeed, studies with a deletion mutant [155] showed that electron flow from Q_A to Q_B was hindered indicating an interruption of PQ / PQH₂ exchange.

Subunit PsbK is located next to the TMH **a** of CP43, TMHs **a** and **b** of PsbZ and single TMHs of PsbJ and *ycf12*. It is folded into a single TMH with the N-terminus located at the luminal side. The TMH of PsbK is tilted about 35° from the membrane normal; thereby its C-terminus interacts with subunit PsbZ, whereas the N-terminus forms hydrogen bonds with subunit CP43. PsbK shows a hook-like folding of its N-terminus providing the binding-site for a calcium ion with unknown function (ligating residues with distances: K-Asp19OD2 ... Ca56, 2.81Å; K-Asp23OD1 ... Ca56, 2.91Å; K-Asp23OD2 ... Ca56, 3.02Å). PsbK forms only few H-bonds with neighbouring subunits (see Appendix Table 7.4), its C-terminus is fixed by H-bond with conserved Arg41 residue from CP43. PsbK contributes to the binding sites of Car13, MGDG19, Chl37, Chl46 and Chl47.

In terms of function, PsbK probably plays a strictly stabilization role as shown for example in *C. reinhardtii* [156].

Subunit PsbL is located in-between subunits PsbM and PsbT and close to the TMHs **d** and **e** of D2. It has 37 residues in its sequence with the N-terminus extending into the

cytoplasm. This strategic position allows H-bonds with many subunits: namely with D1, CP47, D2, PsbM and PsbT (see Appendix Table 7.4). PsbL contributes to the binding sites of SQDG13, MGDG17, Chl27, MGDG10, MGDG11, Q_A , Chl_{D1} and Chl27.

In terms of function, it is suggested that PsbL might play a role in the restoration of electron transfer activity in RCs [157, 158]. Recent mutagenesis studies [159] also showed that PsbL is essential for the normal PSII assembly and recovery from photodamage.

Subunit PsbM is located at the monomer-monomer interface and near subunit PsbL. PsbM is folded into a single TMH with N-terminus at the lumen. It was fully modelled, except two C-terminal serine residues. Intriguingly, PsbM forms most of inter-monomer interactions with its symmetry mate from the other monomer. Their single TMHs interlock with a heptad motif as found in membrane-spanning leucine zippers [160] (see Fig. 21). Additionally few H-bonds with PsbL and the symmetrically related PsbM subunit are present (see Appendix Table 7.4). Recent mutagenesis studies [161] confirmed that the formation of stable PSII homodimer is not possible in the absence of PsbM but with the incidental absence of PsbT.

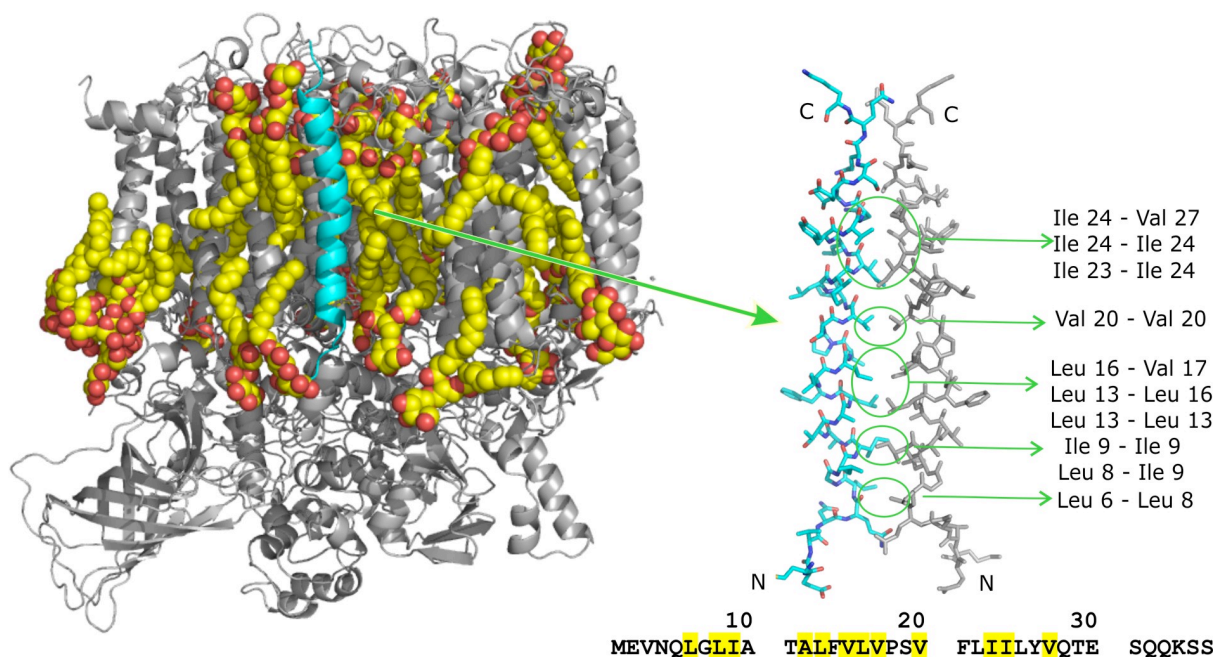


Figure 21. PsbM interactions. Left, view of one monomer looking onto the monomer-monomer interface along the membrane plane, with the cytoplasm above and the lumen below. Proteins are shown in cartoon presentation in grey, and subunit PsbM in cyan; lipid and detergent molecules are in space-filling presentation (carbon, yellow; oxygen, red). Right, interactions between PsbM (cyan) of monomer I and PsbM* (grey) of monomer II. The N- and C-termini are labelled; specific protein-protein interactions are indicated by circles and involve residues highlighted (yellow) in the amino acid sequence of PsbM given below.

Subunit PsbT is located near subunits PsbL and PsbM. It is 32 residues long, all of which were modelled. This subunit is folded into a single TMH, with N-terminus located at the lumen, forms several strong H-bonds with its neighbouring subunits (see Appendix Table 7.4), and its highly conserved Arg24 residue fixes the C-terminus of CP43. The C-terminus of PsbT is fixed by H-bond with conserved Lys238 from subunit D1. It contributes to the binding sites of Q_A , β -DM26, β -DM27, Car4, MGDG11 and SQDG13.

It was shown that PsbT is required for PSII recovery after photodamage [162] and for the stabilization of the Q_A -binding site [163] as well as for the stabilization of homodimer [161].

Subunit PsbZ is located at the periphery of PSII, close to subunits PsbK and CP43. It is folded into two TMHs, with full length of 62 residues, all of which were modelled. The N- and C-termini are located at the lumen. Interestingly, this subunit shows almost no inter-subunit H-bonds (see Appendix Table 7.4), and is probably bound by hydrophobic forces. It contributes to the binding sites of three carotenoids (Car12, Car13 and Car16), lipid molecule MGDG21 and Chl47.

Mutagenesis studies showed [164] that the absence of PsbZ leads to nearly complete loss of subunits PsbK and ycf12, therefore PsbZ is essential for the structural integrity of the PSII complex. Additionally it was shown that lack of PsbZ might influence the rate of cyclic electron flow around PSI [165].

The most exciting output of the electron density was the possibility to assign three previously not assigned subunits (Fig. 22), termed X1, X2 and X3 in the 3.0 Å resolution structure [41] to subunits ycf12, PsbY and PSbX, respectively.

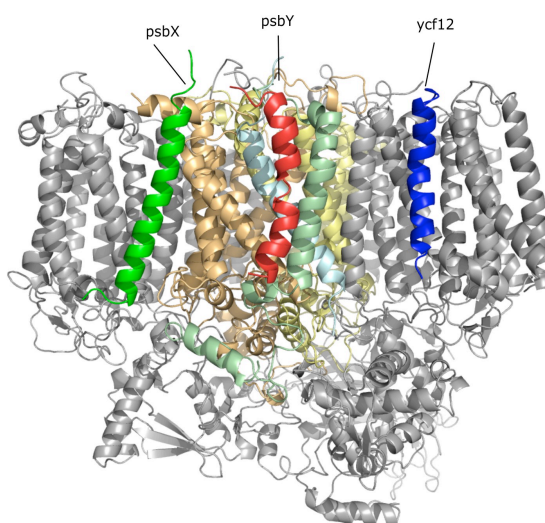


Figure 22. Newly assigned subunits. Side view of one PSII monomer, cytoplasmic side at the top and lumenal side at the bottom. All 20 protein subunits are shown in cartoon mode; cofactors are omitted. The three newly