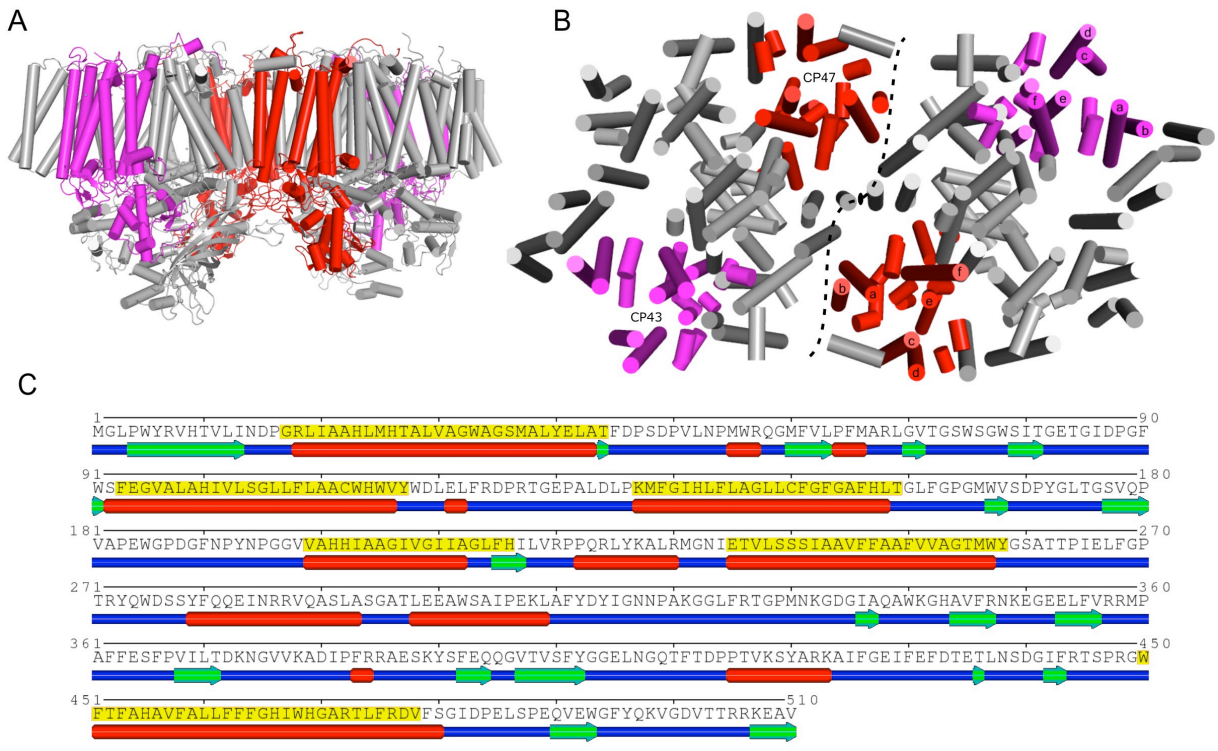
subunit D2, whereas CP43 is at the periphery of the complex and close to D1 (Fig. 15). The C- and N-termini of both subunits are at the cytoplasmic side, whereas its long hydrophilic loops are nestled near the lumen. CP47 and CP43 are each folded into six (**a** to **f**) TMHs, arranged as a trimer of two-TMH-bundles (Figs. 15; 18B,C,D).

In total these subunits bind 29 Chl *a* molecules: 16 are bound by CP47 and 13 by CP43 (Fig. 15). All Chl *a* molecules are arranged in three layers, similarly as in PSI [37] and almost all are ligated by conserved histidine residues, except for Chl17 and Chl37 that are ligated by ester carbonyl groups of lipids MGDG14 and DGDG5 respectively (see Appendix Table 7.2, for a list of Chl – protein interactions). In case of Chl11 and Chl43 probable axial ligands are water molecules, whereas for Chl47 the side chain oxygen of Asp39 from CP43.

Interestingly, almost each Chl *a* molecule (or at least clusters of Chl *a* molecules) is in van der Waals contact with carotenoid molecule(s) (see Appendix Table 7.2), which allows transfer of excitation energy from carotenoids to Chl *a* and photoprotection of PSII by rapid triplet transfer [41].

Both subunits were fully modelled, except for the flexible C-terminus of CP47 (last 19 residues; the full length of the mature form is 510 residues) and for the N-terminus of CP43 (first 26 residues; the full length of the mature form is 473 residues). The data also allowed modelling of missing side chains and better refinement in comparison with the previous 3.0 Å resolution structure [41] (see Appendix Table 7.1).



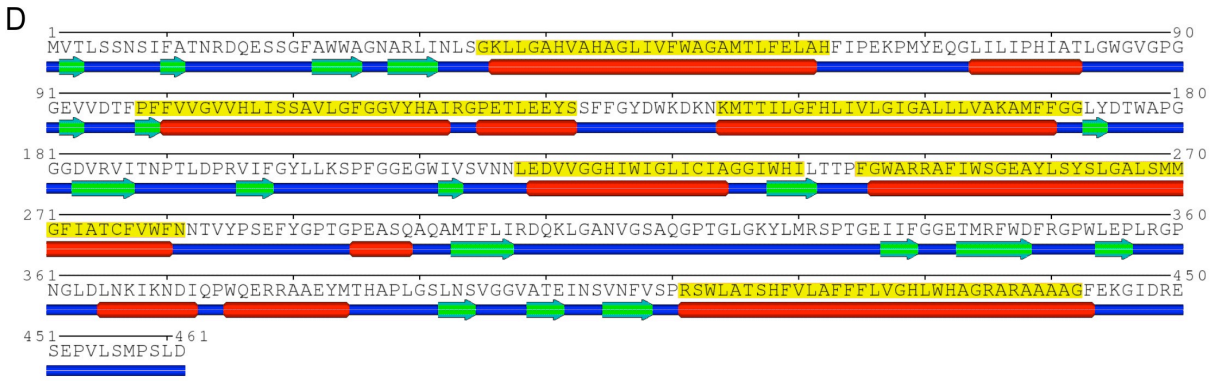


Figure 18. Antenna subunits: A) side view of PSII homodimer, all proteins subunits in grey, except CP43 in magenta, CP47 in red; B) top view onto PSII homodimer from the cytoplasmic side, colours same as in panel A, TMHs of CP43 and CP47 are labelled from a to f; C) secondary structure and sequence details of CP47, TMHs are highlighted in yellow, α-helices in red, β-strands in green, coil in blue; D) the same for CP43.

3.1.1.3 Cytochrome b-559

Two protein subunits PsbE (α-subunit) and PSbF (β-subunit) each provide one conserved histidine residue to ligate the haem group (Fig. 19), known as cytochrome *b-559* (*cyt b-559*).

Cyt b-559 is located at the periphery of PSII and close to the TMH **a** of D1 and the single TMH of PsbY (Fig. 15). Each subunit shows only one TMH, the N-termini located at the cytoplasmic side. The haem group is located about 30 Å from the head group of Q_B and about 17 Å from the head group of the novel plastoquinone Q_C (see section 3.2.2.3).

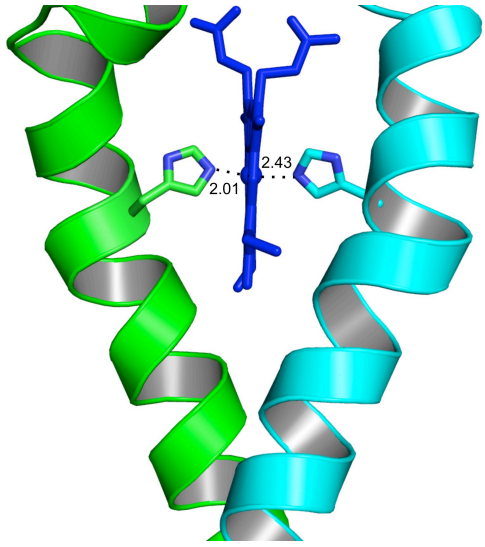


Figure 19. Ligating haem in *cyt b-559*. Subinits α and β are coloured green and cyan respectively. The haem group is shown as sticks in blue. Distances are given in Å.

This haem possesses unusual redox properties and has been found to be present in three forms [47, 136-138]: (i) dominant high potential form with midpoint potential (E_m) about +400mV; (ii) intermediate potential form with E_m about +200mV; (iii) low potential form, E_m is about +50 to +100mV. Several hypotheses explaining this variety of redox potential emerged: (i) modification of hydrogen-bonding pattern of the axial ligands [136, 139]; different orientation of ligating histidines [140]; changes in the electrostatic environment [141].

In terms of function, *cyt-b559* is also puzzling. The most accepted role is participation in the cyclic electron pathway, protecting PSII against photodamage [46]. It has been suggested that the oxidized form of *cyt-b559* accepts electrons from the reduced plastoquinol or semi-plastoquinol, and then the electron is passed to excited $P680^{+\cdot}$ presumably via Car_{D2} and $ChlZ_{D2}$ [41, 142].

Both α- and β-subunits were fully modelled, except for the two N-terminal residues for PsbE (the full length of the mature form is 83 residues, the first methionine is cleaved) and for the flexible N-terminus of PsbF (first ten N-terminal residues are missing; the full length of the mature form is 44 residues, the first methionine is cleaved). The data also allowed modelling of missing side chains and better refinement in comparison with the previous 3.0 Å resolution structure [41] (see Appendix Table 7.1).

3.1.1.4 Low-molecular weight subunits

The remaining intrinsic protein subunits have low molecular weight and show only one TMH (except PsbZ, which shows two), their functions are mostly unknown. The general overview of their location in PSII is presented in Figure 20 (see also Fig. 15).

Subunit PsbH is located next to TMH **d** of CP47, TMHs **a** and **b** of D1 and TMH of PsbX (Fig. 15). Its N-terminus is located at the cytoplasmic side and the overall length of polypeptide is 66 residues, all are modelled except initiatory methionine Met1, which was post-translationally removed. PsbH forms hydrogen bonds mostly of non-specific nature (i.e. main chain – main chain or side chain – main chain interactions) mainly with subunit CP47 (see Appendix Table 7.4 for a list of contacts), but its C-terminus also stabilizes the N-terminus of subunit PsbX and interacts with D2 and the α-subunit of *cyt b-559*. PsbH also provides binding surface and contributes to the binding sites for Chl11, 12, 22, 29; Car7 and lipid DGDG8 (for lipid-protein interactions see Appendix Table 7.6).