Cytochrome b6f is part of the electron transport chain involved in transferring electrons from PSII to PSI during photosynthesis. To accomplish this, the protein oxidizes plastoquinol and reduces plastocyanin or cytochrome c6. It transfers one electron from reduced dihydro-plastoquinone (PQH2) to the electron transport chain containing the Rieske iron-sulfur protein and cytochrome f, which results in two protons being released into the lumen. Plastocyanin is then released and transfers electrons to PSI. The second electron from the reduced dihydro-plastoquinone is transferred through two b-hemes, CytbL and CytbH (these are low L and high H potential hemes), in cytochrome b6 and is taken up on the electronegative side of the membrane where it eventually reenters the cycle. Protons released into the lumen create a proton gradient and are used to fuel the production of ATP via ATP synthase to create energy for cellular metabolic processes and for the fixation of CO2 into sugars via the Calvin cycle.

The resolution of this structure is 3Å. The structure, solved using x-ray diffraction, includes 16 polypeptide chains. This is a breakdown of the number of residues per chain - A: 215, B: 160, C: 289, D: 179, E: 32, F: 35, G: 37, H: 29, I: 215, J: 160, K: 289, L: 179, M: 32, N: 35, O: 37, P: 29. The protein contains 15,091 atoms in total. In each monomer there are four large subunits; cytochrome f, cytochrome b6, the Rieske iron-sulfur protein, and subunit 4. There are also four smaller subunits. The overall molecular weight of the dimer is 217 kDa.

In this picture, the heme groups are represented as round red balls, and each of the chains is colored differently. The part of the protein that in this diagram faces the top right side is the side that is exposed to the lumen in nature. The side facing the bottom left is the side that faces the stroma in nature.
In this representation, the pigment molecules present in the protein are visible - in teal are the chlorophyll a molecules, the light green molecules are beta-carotene, and the bright green molecules are TDS, a quinone-analog inhibitor that was added to solve the protein structure. This inhibitor may prevent binding of quinone by preventing access to the cavity containing the binding site. In addition to these pigments, the purple diamond shaped molecules are iron-sulfur clusters, and the pink and white cluster of molecules are lipids that were added to solve the structure. The function of the pigment molecules present in this protein is largely unknown, though they may serve to provide structural support.

The two images shown below represent the protein chains in teal, and the heme groups in red. The heme on the lumen side is where one of the PQH2 electrons travels after going through the iron sulfur complex and before being transferred to plastocyanin. The heme near the center of the protein is the first stop for the other electron from PQH2, this electron then is transferred to one of the two hemes nearer to the stromal side before leaving the protein. The other of these two hemes proximal to the stromal side is known as heme x, and is an unknown heme type.

Images created using Visual Molecular Dynamics (VMD).

VMD was developed by the Theoretical and Computational Biophysics Group in the Beckman Institute for Advanced Science and Technology at the University of Illinois at Urbana-Champaign.

http://www.ks.uiuc.edu/Research/vmd/