ESRF	**Experiment title:** Cytochrome b6f	**Experiment number:** 30-01-612
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Shifts: 6	**Local contact(s):** J.-L. Ferrer	*Received at ESRF:*

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Report:

The long term aim of this experiment was to determine the crystallographic structure of the membrane protein cytochrome b_6f complex which catalyses the transfer of electrons between the photosystem II and photosystem I in oxygenic photosynthesis, and couples this transfer with the translocation of proton through the thylacoid membrane. It is a membrane protein that contains 2x8 polypeptide chains with a molecular weight of ca 200000 Da. It is one of the last large complex protein of photosynthesis whose structure was missing. We have now succeeded in solving this structure.

The previous run we could collect data sets diffracting at 3.1 Åresolution and two heavy atoms $HgCl_2$ and $TbNO_3$, which diffracted not very strongly but which could be used for phasing with the help of solvent flattening which was quite efficient due to to an unusually high solvent content (82 % of the crystal volume).

One important finding in solving the structure was that it contains an unsuspected haem whose properties are quite atypical: *c*-type haem with only one thioether linkage and no amino acid as axial ligand, the latter has not been encountered previously in wild type proteins.

The main usage of these shifts was to collect anomalous signal around the Iron edge to eliminate other potential candidates (like Zn or Mn). It was difficult to obtain a strong signal but the experiments allow to show the presence that additional Iron. It is interesting to notice that this complex has undergone thorough spectroscopic investigation during the past 25 years without identifying this haem (except maybe one experiment in whole cell in 1986).

These results have been published: Stroebel D, Choquet Y, Popot JL, Picot D. (2003). An atypical haem in the cytochrome b6f complex. Nature. 426:413-408.

Abstract:
Photosystems I and II (PSI and II) are reaction centres that capture light energy in order to drive oxygenic photosynthesis; however, they can only do so by interacting with the multisubunit cytochrome b_6f complex. This complex receives electrons from PSII and passes them to PSI, pumping protons across the membrane and powering the Q-cycle. Unlike the mitochondrial and bacterial homologue cytochrome bc_1, cytochrome b_6f can switch to a cyclic mode of electron transfer around PSI using an unknown pathway. Here we present the X-ray structure at 3.1 Åof cytochrome b_6f from the alga Chlamydomonas reinhardtii. The structure bears similarities to cytochrome bc_1 but also exhibits some unique features, such as binding chlorophyll, beta-carotene and an unexpected haem sharing a quinone site. This haem is atypical as it is covalently bound by one thioether linkage and has no axial amino acid ligand. This haem may be the missing link in oxygenic photosynthesis.

Ligand studies
We have also started some ligands studies. The original structure has been obtained in the presence of stigmatellin. We have collected preliminary dataset in the absence of ligand and in the presence of several inhibitors. Interpretable maps have been obtained, but better data are needed. We also need to increase the resolution.