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Report:

We are elucidating the three-dimensional structure of the photosystem II (PSII) purified from the thermophilic cyanobacterium *Synechococcus elongatus*. For that reason we wanted to collect additional derivatives. For that reason we wanted tocollect additional derivatives. The crystals were soaked in 1 M $CaBr_2$ to replace the native chlorine by bromine. It is known that oxygen production also involves Ca^{2+} and Cl^- ions, but these have not been located in the current electron density map. It is of special interest to find the binding sites of these ions.

A rapid soak of protein crystals containing up to 1 M bromide anions can often lead to incorporation of these anomalously scattering centers into the ordered solvent region around protein molecules. These ions bind through electrostatic interactions with hydrophilic regions of the protein surface.

Bromide ions have suitable anomalous scattering properties to provide phasing for protein structure solution. Halides, being small monoatomic ions, are able to substitute for solvent water molecules around the protein surface and do not show strong preference for specific coordination geometry. Because halide soaking might result in many poorly occupied sites, it might often be difficult to determine the position of these sites with standard Patterson or direct techniques. This approach can be used in combination with other phasing vehicles to augment the phase calculations, however, with the site positions determined using difference Fourier analysis.

We could collect two complete data sets:

the first crystal had cell parameters with a=132.7 Å, b=228.1 Å and c=310.6 Å in the same space group ($P2_12_12_1$) as the native ones. This crystal diffract to ~ 3.7 Å resolution. The resulting data set after processing with DENZO and SCALEPACK, the data set had a maximum resolution of 3.8 Å with Rsym=0.06 and <I/σ(I)>=2.1 (Rsym=0.5 <I/σ(I)>=1.2) and a completeness of 84.7 %.
From the second crystal we collected a data set to 3.9 Å resolution with a completeness of 94.5 %. The data were processed with DENZO and SCALEPACK and led to the following statistics: Rsym=0.06 and <I/σ(I)>=3.4 (Rsym=0.5 <I/σ(I)>=1.4). In the difference electron density map, we identified additional density. We saw one peak in the density belonging to the bromine atom. The bromine is located close to the Mn cluster. Up to now, we could not adjudge whether the bromine has the same binding site as the native chlorine. To answer this question, it is essential to collect a native data set at higher resolution.