

## Supplementary Material Section

# High-Confidence Placement of Fragments into Electron Density Using Anomalous Diffraction—A Case Study Using Hits Targeting SARS-CoV-2 Non-Structural Protein 1

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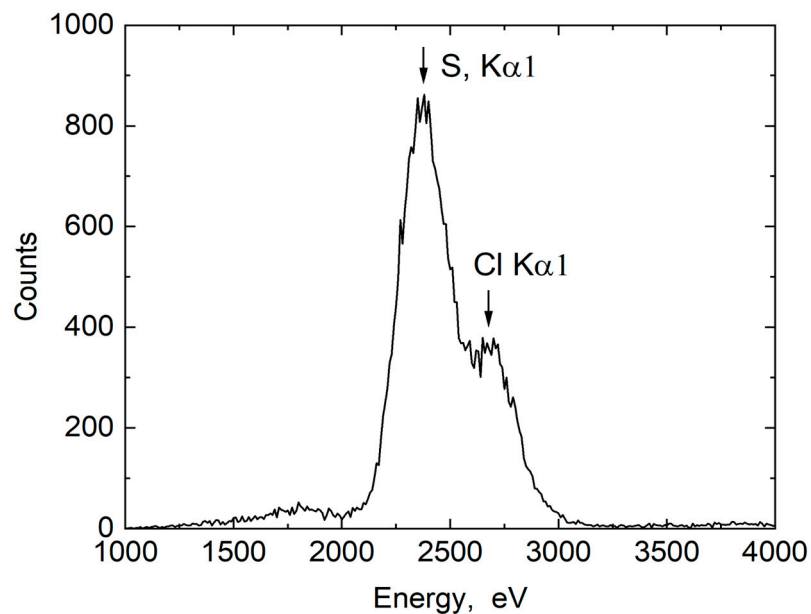
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## Content

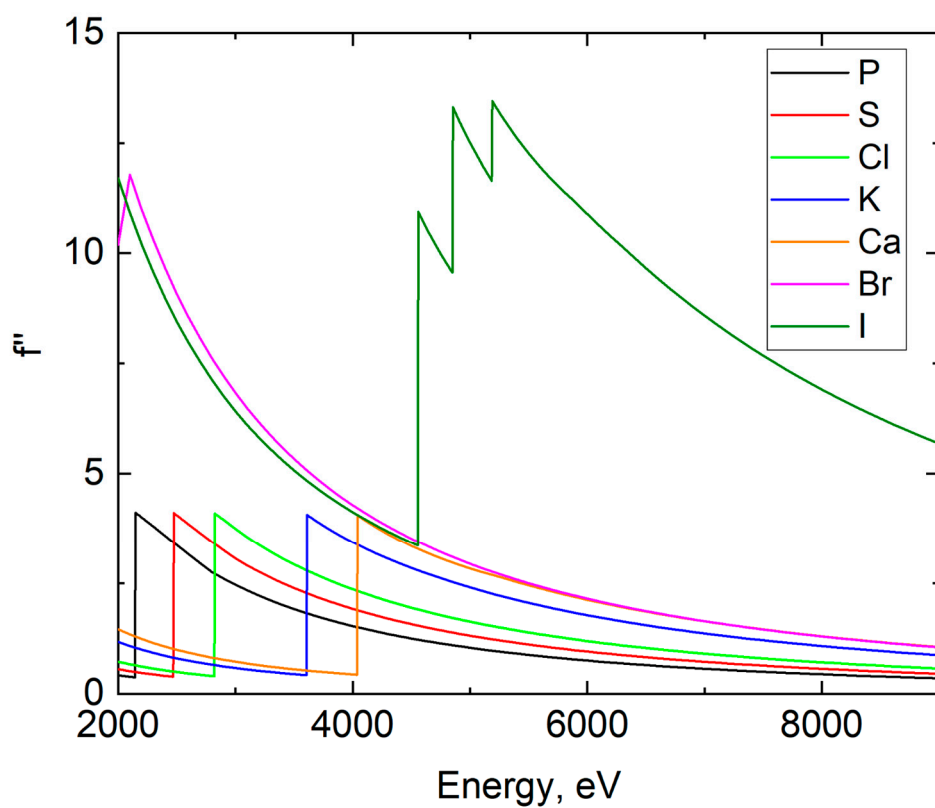
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**Figure S1**



**Figure S1.** X-ray fluorescence spectra of the nsp1-11C6 crystal sample. The peaks at 2308 and 2622 keV correspond to  $K_{\alpha 1}$  emission lines of sulphur and chlorine. The elevation at low energy is a background predominantly caused by X-ray emission of silicon from the detector.

**Figure S2**



**Figure S2.** Energy dependence of the anomalous contribution to the structural factor  $f''$  for biologically relevant light ions and halides (data from [www.bmsc.washington.edu](http://www.bmsc.washington.edu)). The value of  $f''$  manifests a sharp increase at the K-edge of light atoms (P, S, Cl, K, Ca) or L-edges of Br and I thus enabling positive identification of the ions.