

Supporting information

The crystal structures of $Z\text{-Gly-Aib-O}^- \times \frac{1}{2}\text{Ca}^{2+} \times \text{H}_2\text{O}$ and $Z\text{-Gly-Aib-OH}$

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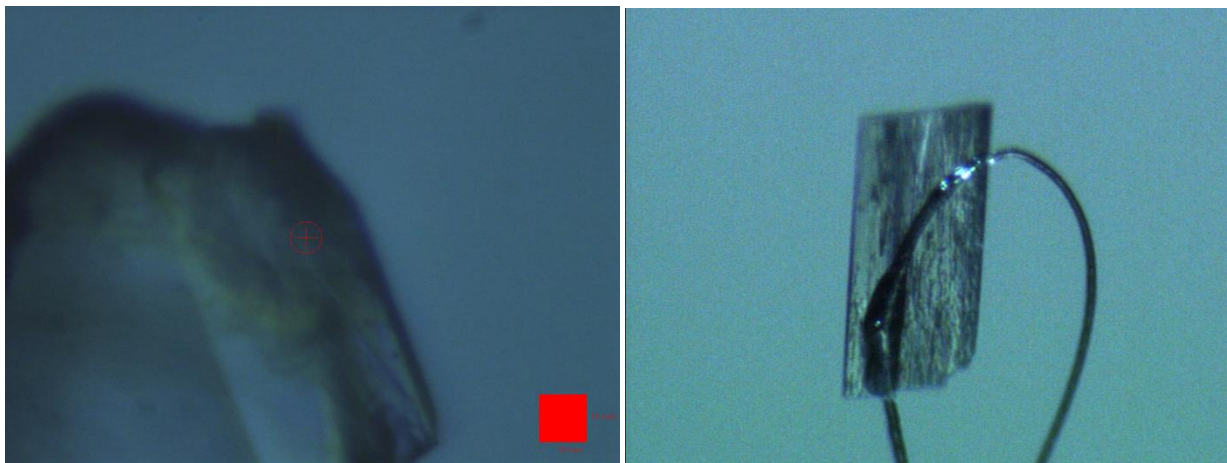


Figure S1. The crystals used for data collection.

Left: The complex of the dipeptide with Ca^{2+} and H_2O ($Z\text{-Gly-Aib-O}^- \times \frac{1}{2}\text{Ca}^{2+} \times \text{H}_2\text{O}$, **I**).

Right: The free form of the dipeptide ($Z\text{-Gly-Aib-OH}$, **II**).

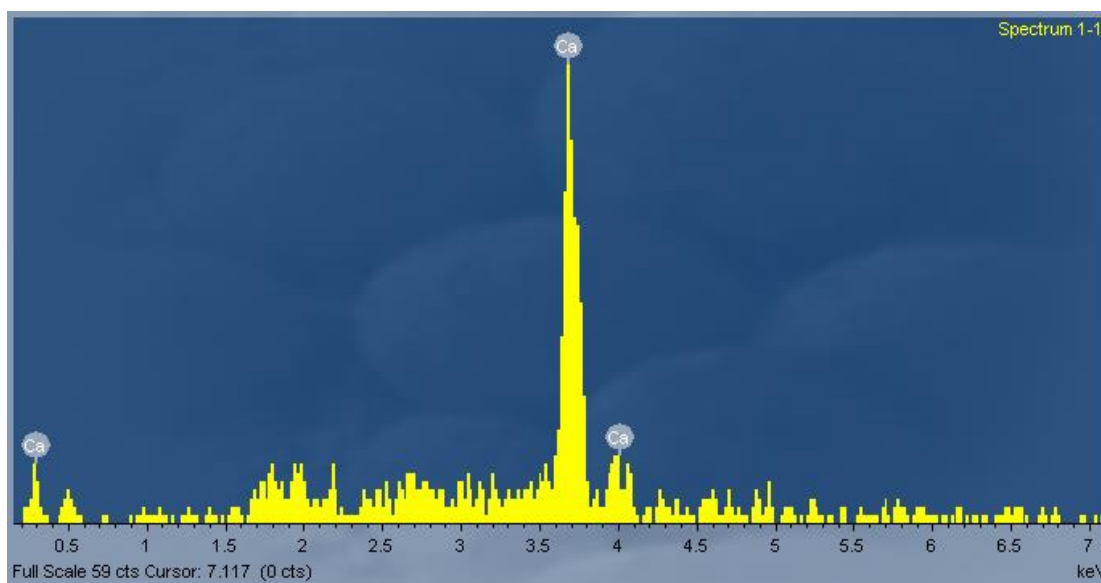


Figure S2. Energy-dispersive X-ray emission spectrum of a crystal selected from the same crystallization batch as the one that provided structure **I** showing peaks at 0.3, 3.7 and 4.0 keV, which are identified as the L, $K\alpha$ and $K\beta$ lines of calcium.