

A new Crystal Form of the SR Ca^{2+} -ATPase in the $\text{Ca}_2\text{E1}$ State

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The sarco(endo)plasmic reticulum Ca^{2+} -ATPase (SERCA) is responsible for the re-uptake into the sarcoplasmic reticulum store of cytosolic Ca^{2+} released during muscle contraction. SERCA and the other cation pumps belong to the P-type ATPase family, whose functional cycle is fuelled by ATP hydrolysis via formation of a covalent aspartyl-phosphoanhydride intermediate. Several crystal structures representing different states of the functional cycle of the Ca^{2+} -ATPase have now been solved as recently updated [1]. The first structure to be solved was the $\text{Ca}_2\text{E1}$ state by Toyoshima et al. [2], which in comparison to later determined structures reveals an open arrangement of the cytoplasmic domains. We have obtained a new crystal form of the $\text{Ca}_2\text{E1}$ state in space group P1 with two molecules in the unit cell. Data were collected from a double crystal, allowing the processing and scaling of two independent datasets at 3.0 Å resolution, and phases from molecular replacement were refined by averaging. The structure appears to be almost identical to the original $\text{Ca}_2\text{E1}$ structure, indicating that the open domain arrangement is not the result of crystal packing effects. This provides further support to the use of this structure in describing the mechanism of activation upon binding of cytosolic Ca^{2+} .

[1] Olesen C, Sørensen, et al., *Science*, 2004, **306**, 2251. [2] Toyoshima C., et al., *Nature*, 2000, **405**, 647.

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