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The Challenging Structure Determination of Tomato Fruit Polygalacturonase: Space Group Ambiguity Arising from Pseudo-Symmetry. Susan Heffron[a], Stephan Watkins[a], Rhonda Moeller[a], Aise Huma Taban[b], Rafal Butowt[b], Dean DellaPenna[c], Frances Jurnak[a], [a]Dept. of Physiology & Biophysics, Univ. of California Irvine, Irvine, CA 92697, [b]Univ. of Nevada, Reno, NV, [c]Michigan State Univ., East Lansing, MI.

Polygalacturonase (PG) is a naturally occurring enzyme involved in the ripening process of many fruits and vegetables. PG is also secreted by several plant pathogenic fungi and bacteria to initiate soft-rot diseases. The first crystal structure of a plant PG, tomato fruit PG2, has been determined to a resolution 1.87 Å. The data were initially indexed in space group $P2_12_12_1$, (with R_{sym} of 0.053), and a plausible molecular replacement solution was found, but did not refine well. After considerable trials in alternative space groups, the correct space group was eventually determined to be $P2_1$ (R_{sym}=0.047), with $\beta = 90.04°$. An examination of the contents of the correct and incorrect asymmetric units revealed two factors contributing to the space group ambiguity: 1) a pseudo-symmetry axis parallel to a crystallographic axis, and 2) the repetitive nature of the beta-helical PG2 structure itself. Two structures of PG2 have been successfully refined and will be presented, one of which is a complex with several galacturonic acid monomers in the active site groove.