The Crystal Structure of Guaifenesin,
3-(2-methoxyphenoxy)-1,2-propanediol

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Guaifenesin finds common use as an expectorant in prescription and over-the-counter medications, but its crystal structure has never been reported. The synchrotron powder pattern (measured on the MR-CAT ID10 beamline at APS from a 2 mm capillary specimen using a wavelength of 0.459141 Å) could be indexed on a primitive orthorhombic unit cell having a = 7.6571(1), b = 25.6695(5), c = 4.9797(1) Å, and V = 978.77(3) Å; the space group is $P2_12_12_1$ (#19). The structure was solved using Monte Carlo simulated annealing techniques, and refined by the Rietveld method. The crystal structure contains double chains (along a) of hydrogen-bonded molecules. The strengths of the hydrogen bonds were quantified by a quantum calculation. The molecular conformation in the solid state is different from that expected in the gas phase, showing the importance of intermolecular interactions in determining the crystal structure.