A case study in direct-space structure determination from powder X-ray diffraction data: Finding the hydrate structure of an organic molecule with significant conformational flexibility

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The structure of the monohydrate crystalline phase of 3,5-bis((3,4,5-trimethoxybenzyl)oxy)benzyl alcohol has been determined directly from powder X-ray diffraction data using the direct-space genetic algorithm technique for structure solution followed by Rietveld refinement. This work raises several issues of a general nature concerning the assessment of results obtained in the structure determination of organic molecular solids from powder X-ray diffraction data and serves as a case study that may find wider relevance in this field.
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