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Investigation of supramolecular synthons in the crystals of N-(aryl)-succinamic acids and N-(aryl)-maleamic acids: A case study of 4-oxo-4-(pyridin-2-ylamino)butanoic acid

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Abstract

4-Oxo-4-(pyridin-2-ylamino) butanoic acid crystallizes with two symmetry independent molecules (A and B) in the asymmetric unit. The crystal structure features hetero $R_2^2(8)$ synthon comprising of N-H...O=C(acid) and O-H...N_{pyridyl} hydrogen bonds between the molecules A and B resulting in one-dimensional (1D) helical columns running down the a axis which are further stabilized by C-H...O=C(acid) interactions. The C-H...O=C(amide) interactions characterized by $R_2^2(14)$ rings between the molecules of the neighbouring channels result in a 1D architecture. Hirshfeld surface analysis comprising of d_{norm} surface and 2D Fingerprint plot (FP) analyses revealed that the maximum contribution to the Hirshfeld surfaces of A and B are from H...H contacts followed by O...H/H...O contacts. In the crystal structure of the reported N-(aryl)-succinamic/maleamic acids, the most repetitive supramolecular synthons are either amide...acid C(7) chains or a combination of acid...acid $R_2^2(8)$ homodimers and amide...amide C(4) chains, which are very different from the one observed in the present structure.

Graphical abstract

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