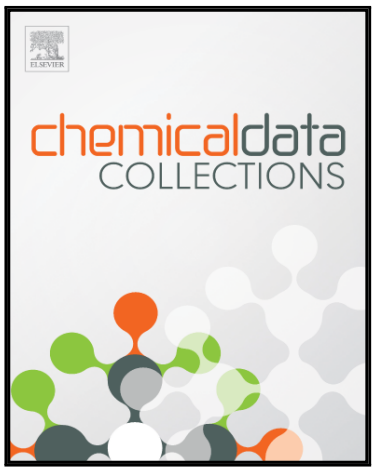

Investigation of supramolecular synthons in the crystals of N-(aryl)-succinamic acids and N-(aryl)-maleamic acids: A case study of 4-oxo-4-(pyridin-2-ylamino)butanoic acid

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PII: S2405-8300(18)30011-9
DOI: 10.1016/j.cdc.2018.02.002
Reference: CDC 96

To appear in: *Chemical Data Collections*

Received date: 17 January 2018
Revised date: 18 February 2018
Accepted date: 22 February 2018

Please cite this article as: Prakash Shet M , Naveen Shivalingegowda , Suresha Erachikkaiah , Lokanath Neratur Krishnappagowda , Parameshwar Adimoole Suchetan , 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, *Chemical Data Collections* (2018), doi: 10.1016/j.cdc.2018.02.002

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