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Crystal Structure and Hirshfeld Surface Analysis of a Tosyl group Substituent Indole Derivative

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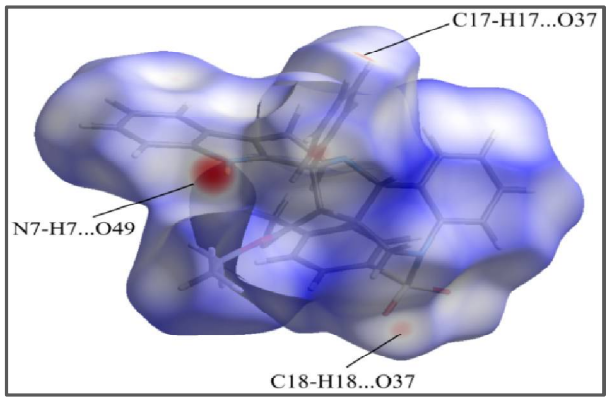
ABSTRACT

The crystal structure of (6bR,14bR,15R,15aS)-ethyl 14b-phenyl-2-tosyl-2,6b,8,9,14,14b,15,15a-octahydro-1H-indolo[3',2':7]indolizino[2,3-c]quinoline-15-carboxylate is determined by single crystal X-ray diffraction technique. The compound crystallizes in the triclinic crystal system in the space group $P\bar{1}$. The unit cell parameters are: a = 11.4998(7) Å, b = 12.4129(7) Å, c = 13.5102(8) Å, α = 75.678(2)°, β = 79.099(2)°, γ = 74.438(2)°. Two molecules comprise the asymmetric unit. In the structure C-H...N, C-H...O and N-H...O hydrogen bond interactions are observed. Hirshfeld surface analysis was carried out to understand the intermolecular interactions.

Graphical Abstract



Hirshfeld surface mapped with the normalized contact distance d_{norm}.

Keywords: Crystal structure, Indole, Cytotoxic, Graph-set motif, Hirshfeld surface.