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Crystal structure of 3-{5-[3-(4-fluorophenyl)-1-isopropyl-1H-indol-2-yl]-1H-pyrazol-1-yl}indolin-2-one ethanol monosolvate

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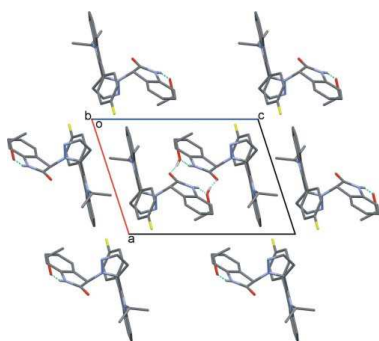
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The title indolin-2-one compound, C₂₈H₂₃FN₄O·C₂H₆O, crystallizes as a 1:1 ethanol solvate. The ethanol molecule is disordered over two positions with refined site occupancies of 0.560 (14) and 0.440 (14). The pyrazole ring makes dihedral angles of 84.16 (10) and 85.33 (9)° with the indolin-2-one and indole rings, respectively, whereas the dihedral angle between indolin-2-one and indole rings is 57.30 (7)°. In the crystal, the components are linked by N—H⋯O and O—H⋯O hydrogen bonds, forming an inversion molecule–solvate 2:2 dimer with R₄⁴(12) ring motifs. The crystal structure is consolidated by π–π interaction between pairs of inversion-related indolin-2-one rings [interplanar spacing = 3.599 (2) Å].

1. Chemical context

Heterocyclic compounds containing the pyrazolone nucleus, indole, and its derivatives play an important role in biological activities. The synthesis and biological activity of some new indole derivatives containing a pyrazole moiety have been reported (Raju et al., 2013). Pyrazole and its analogues have been found to exhibit industrial and biologically active applications (el-Kashef et al., 2000; Taha et al., 2001; Brzozowski & Sączewski, 2002). Consequently, synthesis of indole derivatives has been a major topic in organic and medicinal chemistry over the past few decades. Nitrogen-containing heterocycles are universal systems in nature and are consequently considered as privileged structures in drug discovery (Raju et al., 2013). A literature survey shows that some pyrazoles play an essential role in biologically active compounds and also in medicinal chemistry (Penning et al., 2006), exhibiting phenomena such as antibacterial (Pevarello et al., 2006), antifungal, antiviral (Meghashyam et al., 2011), anti-oxidant (Singarave & Sarkkarai, 2011), anti-inflammatory (Mana et al., 2010), and anticancer (Pathak et al., 2010) effects etc. Certain indole derivatives have also been reported to exhibit wide-spectrum activities such as antiparkinsonian and anti-convulsant effects (Siddiqui et al., 2008; Archana et al., 2002). In addition, pyrazoles have played a crucial role in the development of theory in heterocyclic chemistry, and are also used extensively as useful synthons in organic synthesis. Isatin, an endogenous indole and its derivatives have been shown to exhibit a wide range of biological activities (Daisley & Shah,



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