



Crystal structure of 4-({(1*E*,2*E*)-3-[3-(4-fluorophenyl)-1-isopropyl-1*H*-indol-2-yl]allylidene}amino)-1*H*-1,2,4-triazole-5(4*H*)-thione

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Crystal structure of 4-({(1*E*,2*E*)-3-[3-(4-fluorophenyl)-1-isopropyl-1*H*-indol-2-yl]allylidene}amino)-1*H*-1,2,4-triazole-5(4*H*)-thione

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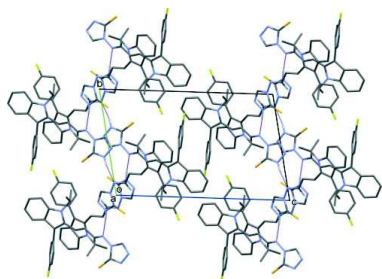
The asymmetric unit of the titled compound, C₂₂H₂₀FN₅S, comprises two independent molecules (*A* and *B*), both of which have a *trans* conformation with respect to the methene C=C [1.342 (2) and 1.335 (2) Å] and the acyclic N=C [1.283 (2) and 1.281 (2) Å] bonds. In molecule *A*, the triazole ring makes dihedral angles of 55.01 (12) and 18.17 (9)° with the benzene and indole rings, respectively. The corresponding dihedral angles for molecule *B* are 54.54 (11) and 14.60 (10)°, respectively. In the crystal, molecules are consolidated into –*A*–*B*–*A*–*B*– chains along [010] via N–H···N hydrogen bonds. The chains are further linked into layers parallel to the *ac* plane via π–π interactions involving inversion-related triazole rings [centroid–centroid distances = 3.3436 (11)–3.4792 (13) Å].

1. Chemical context

The chemistry of 1,2,4-triazole derivatives has attracted widespread attention due to their diverse biological activities and because they are a new class of antimicrobial agents (Sun *et al.*, 2004; Verreck *et al.*, 2003); for example fluconazole and itraconazole are used as antimicrobial drugs. Hence, metal complexes of Schiff bases derived from 1,2,4-triazole derivatives have been the subject of considerable study (Ozarowski *et al.*, 1991; Cornelissen *et al.*, 1992; Varma *et al.*, 1992; Mishra & Said, 1996). A number of metal complexes with 1,2,4-triazole Schiff bases have been reported from our laboratory (Yadawe & Patil, 1997; Avaji *et al.*, 2006; Kulkarni *et al.*, 2009, 2011). In addition to this isatin, which is an endogenous indole, and its derivatives have been shown to exhibit a wide range of biological activities (Daisley & Shah, 1984; Pandeya *et al.*, 1999*a,b*; Cerchiaro & Ferreira, 2006; Sridhar *et al.*, 2002). Since triazoles are heterocyclic compounds and Schiff bases derived from isatin often act as versatile chelating agents and exhibit promising bioactivities, it is likely that a Schiff base derived from fluvastatin–triazole might also exhibit useful biological activities. In this way, it was planned to prepare a Schiff base which possesses both nitrogen and sulfur coordination sites so that it might coordinate effectively to metal ions.

2. Structural commentary

The asymmetric unit of the title compound (Fig. 1) is comprised of two independent molecules (*A* and *B*). Both molecules have a *trans* conformation with respect to the



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