



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

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*Acta Cryst.* (2015). E71, 1411–1413



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

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Received 12 October 2015

Accepted 24 October 2015

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

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**Keywords:** crystal structure; 1,2,4-triazole-5(4H)-thione; indole; Schiff base; N—H⋯S hydrogen bonds; C—H⋯π and π—π interactions

**CCDC reference:** 1433130

**Supporting information:** this article has supporting information at journals.iucr.org/e

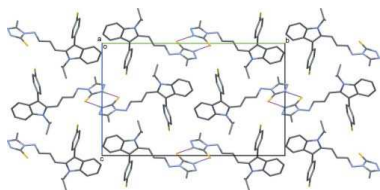
The title compound, C<sub>23</sub>H<sub>22</sub>FN<sub>5</sub>S, exists in a *trans* conformation with respect to the methene C=C and the acyclic N=C bonds. The 1,2,4-triazole-5(4H)-thione ring makes dihedral angles of 88.66 (9) and 84.51 (10)°, respectively, with the indole and benzene rings. In the crystal, molecules are linked by pairs of N—H⋯S hydrogen bonds, forming inversion dimers with an R<sub>2</sub><sup>2</sup>(8) ring motif. The dimers are linked via C—H⋯π interactions, forming chains along [11̄0]. The chains are linked via π—π interactions involving inversion-related triazole rings [centroid–centroid distance = 3.4340 (13) Å], forming layers parallel to the *ab* plane.

## 1. Chemical context

The synthesis and functionalization of indoles has been a major area of focus for researchers for several decades. Indoles are of great importance in view of their natural occurrence as a prominent sub-structure of a large number of alkaloids (Somei & Yamada, 2003; Hibino & Choshi, 2002) and wide-ranging biological activities (Gribble, 1995). They also constitute an important moiety of various drugs. In addition, 1,2,4-triazoles are an important class of heterocyclic compounds which are well known for their potential antimicrobial properties. Substituted 1,2,4-triazoles are associated with diverse biological activities such as fungicidal, antimicrobial, anticonvulsant and antiviral activities (Walser et al., 1991; Eweiss et al., 1986; Bhat et al., 2001; Kitazaki et al., 1996; Todoulou et al., 1994). The proper design of indoles and triazoles can be used to prepare Schiff bases. The wide spectrum of biological applications of 1,2,4-triazoles prompted us to synthesize Schiff bases derived from triazole and indole derivatives. The formation of the azomethine functional group CH=N is thought to be the main reason for the biological properties of Schiff bases. We have reported a number of metal complexes of Schiff bases, recently, which possess very good antimicrobial properties (Kulkarni et al., 2009a,b, 2011).

## 2. Structural commentary

The title compound, Fig. 1, exists in a *trans* conformation with respect to the methene C<sup>9</sup>=C<sup>10</sup> [1.322 (2) Å] and acyclic N<sup>2</sup>=C<sup>11</sup> bonds [1.278 (2) Å]. The triazole ring is almost planar [maximum deviation of 0.011 (2) Å for atom C<sup>13</sup>], as is the indole ring [maximum deviation of 0.031 (2) Å for atom



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