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Ethyl 4-phenyl-2-(*N*-pyrrolyl)-1,3-thiazole-5-carboxylate

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.006 Å
R factor = 0.080
wR factor = 0.206
Data-to-parameter ratio = 13.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The structure of the title compound, $C_{16}H_{14}N_2O_2S$, comprises a twisted molecule with dihedral angles of 11.3 (2) and 45.8 (1)° between the thiazole and, respectively, the pyrrole and phenyl rings.

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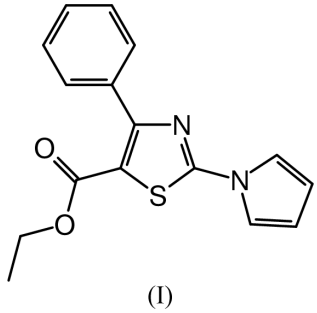
Comment

The title compound, (I), has been studied as part of a larger investigation into the solid-state packing of 2-aminothiazoles and their carboxylic acid cocrystals. The structure of (I) (Fig. 1)



(I)

comprises a twisted molecule with dihedral angles of 11.3 (2) and 45.8 (1)° between the thiazole and, respectively, the pyrrole and phenyl rings.

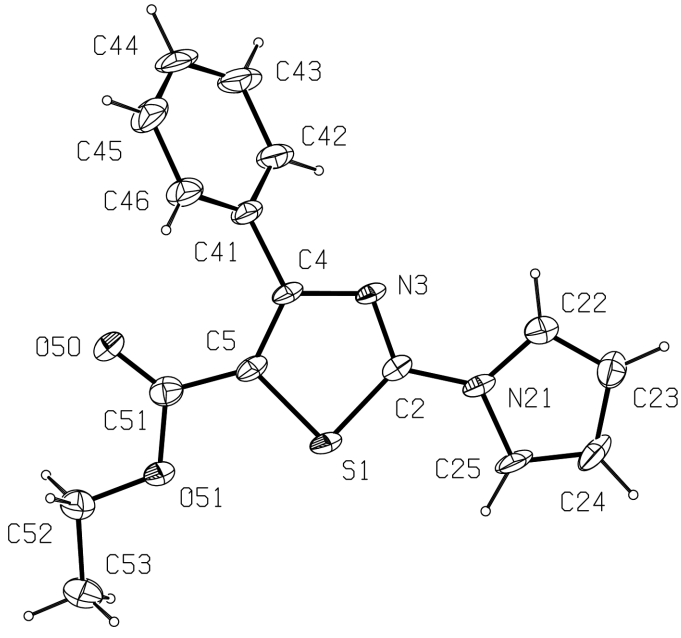


Figure 1
The molecular configuration and the atom-numbering scheme for (I), showing 50% probability ellipsoids.

Experimental

The title compound was obtained from Key Organics Ltd and crystals were grown from an ethanol solution.

Crystal data

$C_{16}H_{14}N_2O_2S$
$M_r = 298.35$
Monoclinic, $P2_1/c$
$a = 10.2375\ (4)$ Å
$b = 3.9460\ (2)$ Å
$c = 35.075\ (2)$ Å
$\beta = 91.979\ (2)^\circ$
$V = 1416.1\ (1)$ Å^3
$Z = 4$
$D_x = 1.399$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6999 reflections
$\theta = 2.9$–27.5°
$\mu = 0.23$ mm^{-1}
$T = 150\ (2)$ K
Needle, colourless
$0.30 \times 0.08 \times 0.03$ mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
$T_{min} = 0.933$, $T_{max} = 0.993$
6999 measured reflections
2486 independent reflections
1643 reflections with $I > 2\sigma(I)$
$R_{int} = 0.171$
$\theta_{max} = 25.0^\circ$
$h = -12 \rightarrow 12$
$k = -4 \rightarrow 4$
$l = -37 \rightarrow 41$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.080$
$wR(F^2) = 0.206$
$S = 1.04$
2486 reflections
191 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1059P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.26$ e Å^{-3}
$\Delta\rho_{min} = -0.95$ e Å^{-3}

All H atoms were included in the refinement, at calculated positions, as riding models, with C—H distances set to 0.95 (Ar-H), 0.99 (CH_2) and 0.98 Å (CH_3). An R_{int} value of 0.171 was the result of weak high-angle data. An unassigned maximum (positive) residual density of 1.26 e Å^{-3} and a minimum (negative) residual density of −0.95 e Å^{-3} are both observed, approximately 0.9 Å from the S atom but 1.37 Å apart.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON*97 (Spek, 1997); software used to prepare material for publication: *SHELXL*97.

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