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Ethyl 4-*tert*-butyl-2-(3-phenylureido)-1,3-thiazole-5-carboxylate

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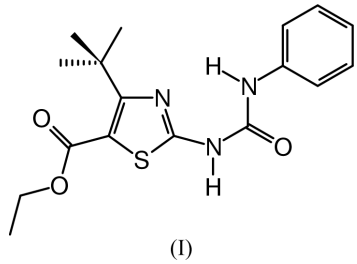
The structure of the title compound, $C_{17}H_{21}N_3O_3S$, (I), comprises an essentially flat molecule with a dihedral angle of 25.7 (2)° between the thiazole and phenyl rings. An intramolecular hydrogen bond exists between the phenyl amine and the thiazole N atom, while intermolecular hydrogen bonds exist to and from the other two components of the urea moiety.

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.006 Å
R factor = 0.050
wR factor = 0.136
Data-to-parameter ratio = 12.5

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



(I)

Experimental

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

Crystal data

$C_{17}H_{21}N_3O_3S$
M_r = 347.43
Orthorhombic, $P2_12_12_1$
a = 6.1391 (4) Å
b = 9.9755 (6) Å
c = 28.248 (2) Å
V = 1729.9 (2) Å^3
Z = 4
D_x = 1.334 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8676 reflections
θ = 2.9–27.5°
μ = 0.21 mm^{-1}
T = 120 (2) K
Block, colourless
0.10 × 0.07 × 0.06 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.980, T_{max} = 0.988
6163 measured reflections
2867 independent reflections
2175 reflections with $I > 2\sigma(I)$
R_{int} = 0.073
θ_{max} = 25.0°
$h = -6 \rightarrow 7$
$k = -11 \rightarrow 11$
$l = -33 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.136
S = 0.79
2867 reflections
229 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack (1983); 706 Friedel pairs
Flack parameter = 0.19 (13)

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N21—H21···O22^{i}	0.82 (4)	2.03 (4)	2.821 (5)	159 (4)
N23—H23···N3	0.99 (4)	1.79 (4)	2.677 (5)	148 (3)
C25—H25···O22	0.95	2.44	2.966 (5)	115
C43—H432···O51	0.98	2.50	3.262 (5)	135
C44—H442···O51	0.98	2.22	3.061 (5)	143

Symmetry code: (i) $x-\frac{1}{2}, -\frac{1}{2}-y, -z$.

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), except for the N—H atoms, which were located in difference syntheses and for which both positional and displacement parameters were refined.

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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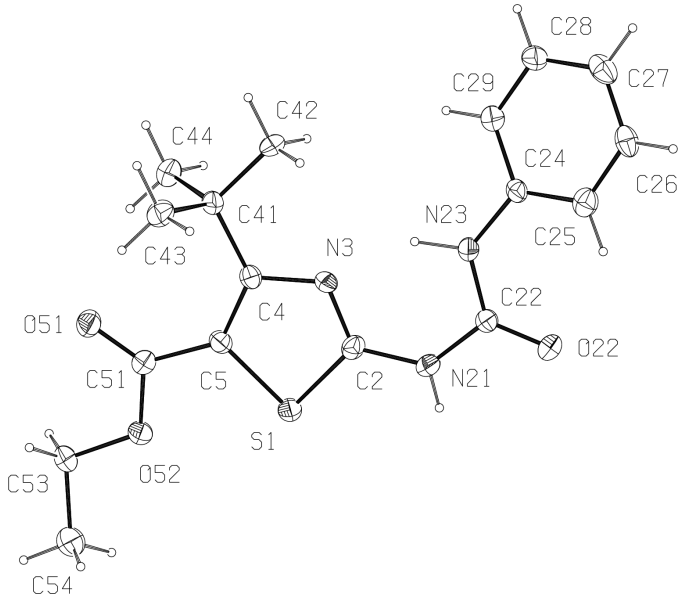

Figure 1
The molecular configuration and atom-numbering scheme for the title compound, showing 50% probability ellipsoids.

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