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Ethyl 2-amino-4-phenyl-1,3-thiazole-5-carboxylate

Daniel E. Lynch[a]* and Ian McClenaghan[b]†

[a]School of Natural and Environmental Sciences, Coventry University, Coventry CV1 5FB, England, and [b]Spa Contract Synthesis, School of Natural and Environmental Sciences, Coventry University, Coventry CV1 5FB, England
Correspondence e-mail: apx106@coventry.ac.uk

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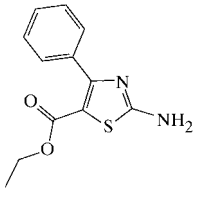
The structure of the title compound, $C_{12}H_{12}N_2O_2S$, (I), comprises molecules that form dimers *via* N—H···N hydrogen-bonding interactions and then construct the overall network through N—H···O associations. The dihedral angle between the phenyl and thiazole rings is 42.41 (6)°.



(I)

Experimental

Crystals of (I) obtained from Spa Contract Synthesis.

Crystal data

$C_{12}H_{12}N_2O_2S$
M_r = 248.30
Monoclinic, $P2_1/n$
a = 10.3124 (2) Å
b = 8.6888 (3) Å
c = 13.3156 (3) Å
β = 97.2427 (15)°
V = 1183.59 (5) Å^3
Z = 4
D_x = 1.393 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3395 reflections
θ = 2.91–27.48°
μ = 0.264 mm^{-1}
T = 150 (2) K
Block, colourless
0.20 × 0.15 × 0.15 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.949, T_{max} = 0.961
7275 measured reflections
2633 independent reflections
2361 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 27.5°
$h = -12 \rightarrow 12$
$k = -11 \rightarrow 11$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.102
S = 1.013
2633 reflections
163 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 0.3670P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N21—H21···N3^{i}	0.89 (2)	2.09 (2)	2.9797 (17)	176.4 (19)
N21—H22···O40^{ii}	0.838 (19)	2.15 (2)	2.9302 (16)	154.0 (18)

Symmetry codes: (i) $-x, -y, 2-z$; (ii) $\frac{1}{2}-x, y-\frac{1}{2}, \frac{3}{2}-z$.

All H atoms were included in the refinement, at calculated positions, as riding models with C—H set to 0.95 (Ar-H), 0.98 (CH_3) and 0.99 Å (CH_2), except for the two amine H atoms which were located on difference syntheses and for which both the 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); software used to prepare material for publication: *SHELXL*97.

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† Contact e-mail: 106355.1670@compuserve.com.