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2-Amino-5-(2-phenyl-1,2,3-triazol-4-yl)-1,3,4-oxadiazole

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In the structure of the the title compound, $C_{10}H_8N_6O$, the triazole and oxadiazole rings are almost coplanar. The oxadiazole ring participates in intermolecular N—H···N hydrogen bonds, forming an infinite network in the *ac* plane. π–π stacking between parallel oxadiazole rings contributes to the stabilization of the crystal packing.

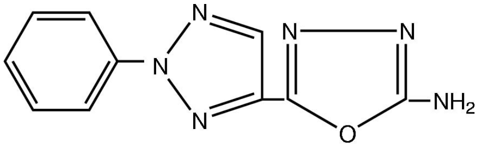
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.124
Data-to-parameter ratio = 14.3

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

Comment

1,2,3-Triazole and 1,3,4-oxadiazole have been reported to exihibit a broad spectrum of biological activities (Fei *et al.*, 1999; Wang & Qin, 2004. To extend our knowledge about such compounds, the title compound (I) was prepared and its crystal structure determined (Fig. 1).



(I)

The torsion angle around the C8—C9 bond of 6.3 (3)° reveals the near coplanarity of the triazole and oxadiazole rings, while the phenyl ring is rotated by 19.6 (3)° about the C1—N2 bond. The interplanar distance of 3.220 Å between parallel oxadiazole rings suggests the existence of π–π stacking (Fig. 2; Christoph, 2000). The oxadiazole ring participates as a double donor (substituted amino group) and as a double acceptor (ring atoms N4 and N5) in intermolecular hydrogen bonds (Table 2, Fig. 2). Each molecule connects three neighbouring molecules by N6—H6*A*···N5 and N6—H6*B*···N4 interactions, generating a nine-membered ring of graph set $R_3^3(9)$ (Bernstein *et al.*, 1995).

Experimental

A precursor, 2-phenyl-4-formyloxotriazole, obtained as described in the literature (Raymond & Hudson, 1944), was converted to its semicarbazone *via* reaction with semicarbazide hydrochloride. The semicarbazone (0.01 mol) was reacted with Br_2 (0.57 ml), NaOAc (0.38 ml) and HOAc (12 ml) in an ice bath for 4 h. The reaction gave a mixture containing (I). The title compound was separated by recrystallization from ethanol and water (1:1 *v*/*v*). However, suitable crystals for data collection (m.p. 548–549 K) were obtained by evaporation of an ethanol:DMF solution (1:1). Spectroscopic analysis: ^{1}H NMR (DMSO, 400 MHz) 8.82 (*s*, 1 H, CH), 7.51–8.12 (*m*, 5H, C6H5) 6.43 (*s*, 2H, NH2) MS (*m*/*z*, relative intensity %): 227 (M+, 100.00), 184 (61.86), 76 (62.06); Anal. Calcd. For $C_{10}H_8N_6O$: C 52.63, H 3.51, N 36.84%, found C 52.80, H 3.72, N 36.98%.

Crystal data

$C_{10}H_8N_6O$
$M_r = 228.22$
Monoclinic, $P2_1/c$
$a = 13.616 (2)$ Å
$b = 5.9421 (9)$ Å
$c = 12.7479 (19)$ Å
$\beta = 99.952 (3)^\circ$
$V = 1015.9 (3)$ Å^3
$Z = 4$
$D_x = 1.492$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1227 reflections
$\theta = 3.0$–23.5°
$\mu = 0.11$ mm^{-1}
$T = 292 (2)$ K
Plate, colourless
$0.34 \times 0.22 \times 0.04$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.996$, $T_{\max} = 0.996$
5611 measured reflections
2203 independent reflections
1433 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.034$
$\theta_{\max} = 27.0^\circ$
$h = -17 \rightarrow 13$
$k = -7 \rightarrow 7$
$l = -16 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.124$
$S = 0.95$
2203 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0706P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.23$ e Å^{-3}
$\Delta\rho_{\min} = -0.19$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—N2	1.4243 (19)	C10—N6	1.3219 (19)
C8—C9	1.448 (2)	N2—N3	1.3295 (17)
C9—O1	1.3722 (18)	N4—N5	1.4095 (17)
C7—C8—C9	128.64 (16)	N6—C10—O1	117.65 (14)
N4—C9—C8	128.77 (16)	N3—N2—C1	123.07 (14)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N6—H6$A\cdots$N5$^{\rm i}$	0.86	2.14	2.977 (2)	165.9
N6—H6$B\cdots$N4$^{\rm ii}$	0.86	2.14	2.991 (2)	169.2

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

The H atoms attached to C and N atoms were placed in geometrically idealized positions with Csp^2—H = 0.93 Å, and Nsp^2—H = 0.86 Å and constrained to ride on their parent atoms, with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$.(carrier atom)

Data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1995); software used to prepare material for publication: *SHELXTL*.

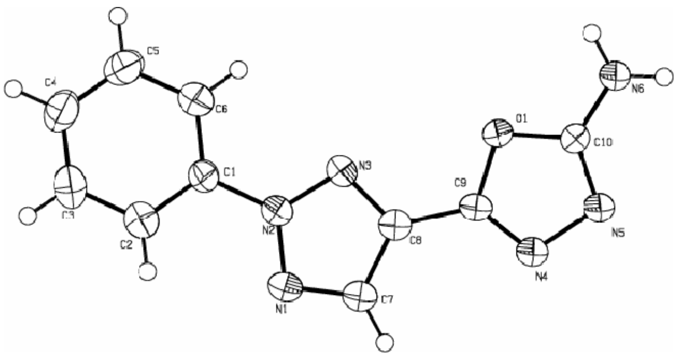


Figure 1
View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

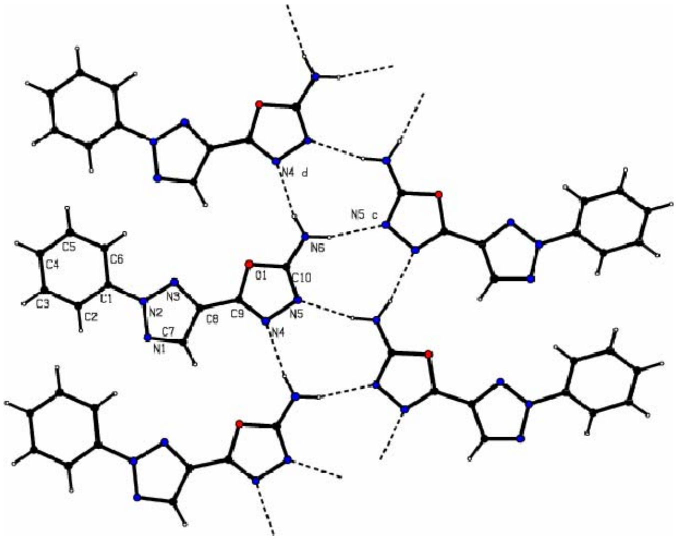


Figure 2
The molecular packing of (I), viewed along the b axis, illustrating the $R^3_3(9)$ ring motif. Dashed lines indicate hydrogen bonds. [Symmetry codes: (c) $1 - x, \frac{1}{2} + y, -\frac{1}{2} - z$; ($d$) $x, 1 + y, z$.]

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