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2-[3-(Methylphenoxymethyl)-5-phenyl-4*H*-1,2,4-triazol-4-yl]benzoic acid

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.047
wR factor = 0.115
Data-to-parameter ratio = 13.5

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

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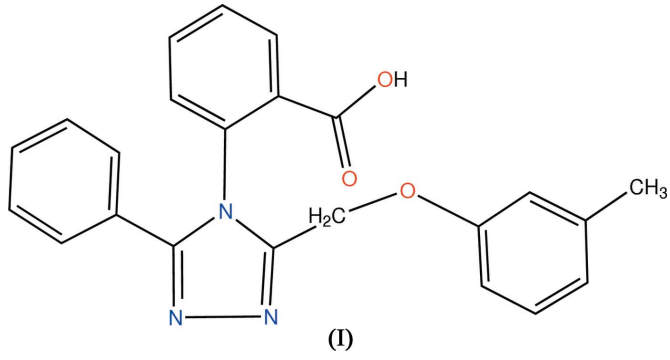
The structure of the title compound, $C_{23}H_{19}N_3O_3$, has been determined as part of our study on the synthesis and crystallography of triazole derivatives. The hydroxyl group is involved in an O—H···N intermolecular interaction.

Comment

Compounds containing a triazole ring are of considerable interest due to their antimicrobial, sedative, anticonvulsant, anti-inflammatory (Prasad *et al.*, 1989; El-masry *et al.*, 2000; Orabi *et al.*, 2000), antibacterial (Jantova *et al.*, 1998), antiviral and antifungal (Holla *et al.*, 1996) activities. The structure analysis of the title compound, (I), was undertaken due to the role of such derivatives as antidepressants and tranquilizers (Hirota *et al.*, 1991).



(I)

The N—N and C—N bond distances in the triazole ring are comparable with those found in analogous structures (Perman & Gleason, 1991; Palmer & Parsons, 1996; Puviarasan *et al.*, 1999; Rajakannan *et al.*, 2002). The molecules are linked by O—H···N hydrogen bonds (Table 1) to form a chain (Fig. 2).

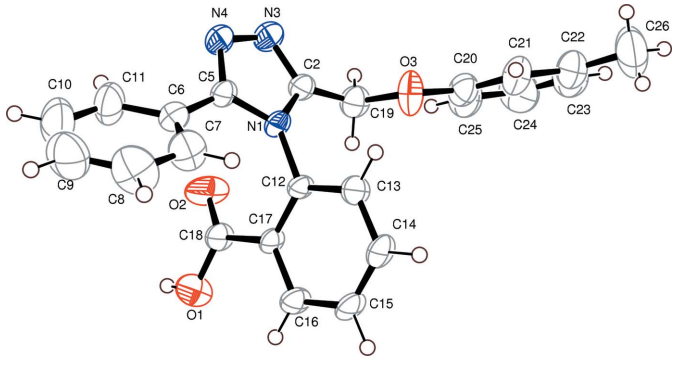


Figure 1
An *ORTEP-3* (Farrugia, 1997) drawing of the title compound, with displacement ellipsoids drawn at the 50% probability level.

Experimental

A mixture of anthranilic acid (0.1 mol) and benzoyl chloride (0.1 mol) in benzene (30 ml) and trimethylamine (0.5 ml) was heated on a water bath for 3 h. The solution then cooled and the separated solid was filtered off and further recrystallized from ethanol to give 2-phenyl-3,1-benzoxazin-4-one. A mixture of 2-phenyl-3-benzoxazin-4-one (0.1 mol) and m-methylphenoxyacetic acid hydrazide (0.1 mol) in methanol was refluxed for 6 h, cooled and the separated solid filtered off and recrystallized from ethanol.

Crystal data

$C_{23}H_{19}N_3O_3$
M_r = 385.41
Orthorhombic, *Pbca*
a = 13.589 (9) Å
b = 18.546 (6) Å
c = 16.075 (8) Å
V = 4051 (4) Å^3
Z = 8
D_x = 1.264 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 5.9–12.5°
μ = 0.09 mm^{-1}
T = 295 (2) K
Prism, light yellow
0.5 × 0.45 × 0.3 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
3548 measured reflections
3548 independent reflections
1595 reflections with $I > 2\sigma(I)$
θ_{max} = 25.0°
$h = 0 \rightarrow 16$
$k = 0 \rightarrow 22$
$l = 0 \rightarrow 19$
2 standard reflections
frequency: 60 min
intensity decay: <2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.115
S = 0.90
3548 reflections
263 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0538P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N4^{i}	0.82	1.87	2.644 (3)	158

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

H atoms were constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C,O) or 1.5U_{eq}(methyl C). Constrained distances were 0.82 Å for O—H and 0.93–0.97 Å for C—H.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *CAD-4 Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *PARST95* (Nardelli, 1995).

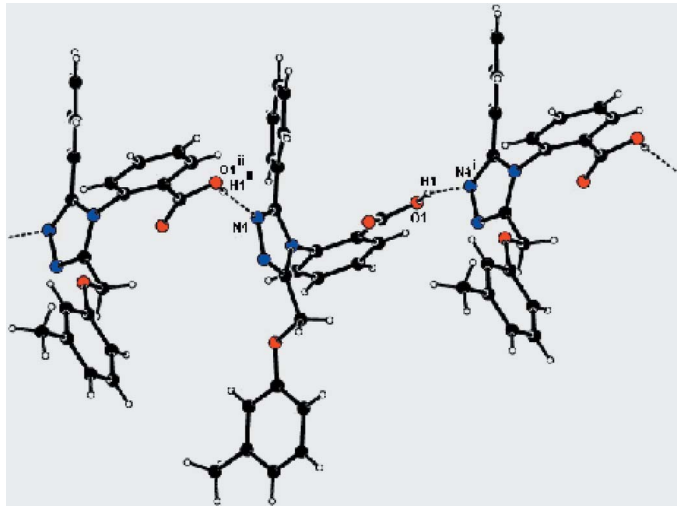


Figure 2
The hydrogen-bonded (dashed lines) chain of molecules [symmetry codes: (i) $x+\frac{1}{2}, y, -z+\frac{1}{2}$; (ii) $x-\frac{1}{2}, y, -z+\frac{1}{2}$].

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