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Key indicators

Single-crystal X-ray study
T = 160 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.122
Data-to-parameter ratio = 16.3

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

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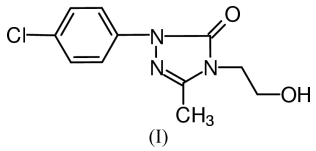
In the title compound, $C_{11}H_{12}ClN_3O_2$, the dihedral angle between the phenyl and triazole rings is 30.63 (9)°. An intermolecular O—H···O hydrogen bond is formed between the hydroxy group and the carbonyl group of the triazole moiety of a neighbouring molecule. This interaction links the molecules into chains, which run parallel to the *c* axis. C—H···O intermolecular hydrogen bonds are also observed.

Comment

Extensive studies have been carried out on substituted 1,2,4-triazole derivatives (Cornelissen *et al.*, 1992; Kunkeler *et al.*, 1996; Chinnakali *et al.*, 1999; Fun *et al.*, 1999; Kumaran *et al.*, 1999). Research findings indicate that the 1,2,4-triazole moiety is associated with diverse pharmacological activities, such as analgesic, anti-asthmatic, diuretic, antifungal, antibacterial, pesticidal and anti-inflammatory activities (Bennur *et al.*, 1976; Heubach *et al.*, 1980; Sharma & Babel, 1982; Mohamed *et al.*, 1993). In view of this, the crystal structure determination of the title compound, (I), has been carried out in order to elucidate the stereochemistry and the molecular conformation.



(I)

The bond lengths and angles in (I) are comparable with those reported for related structures (Chen *et al.*, 1998; Wang *et al.*, 1998). Unweighted least-squares planes calculations show that the phenyl group is oriented at an angle of 30.63 (9)° with respect to the plane of the triazole ring. The hydroxyethyl group projects roughly perpendicular to the triazole ring [C3—N4—C12—C13 = 80.7 (2)°]. The exocyclic angle N2—C3—O3 [128.58 (17)°] is significantly larger than the normal value of 120°, and this may be due to the short contact between atoms H11 of the phenyl ring and O3 (2.54 Å). The hydroxy group forms an intermolecular hydrogen bond with the carbonyl O atom of an adjacent molecule. This interaction links the molecules into chains, which run parallel to the *c* axis and have a graph-set motif of *C*(7) (Bernstein *et al.*, 1995). Several C—H···O intermolecular hydrogen bonds are also observed in (I) (Table 2).

Experimental

The title compound was prepared by heating 3-(4-chlorophenyl)-5-methyl-2-oxo-Δ^4-1,3,4-oxadiazole with ethanolamine. The solid obtained, (I), was crystallized from ethanol (m.p. 388–403 K).

Crystal data

$C_{11}H_{12}ClN_3O_2$
$M_r = 253.69$
Monoclinic, $P2_1/c$
$a = 12.6968$ (4) Å
$b = 11.1886$ (3) Å
$c = 7.9872$ (2) Å
$\beta = 95.446$ (1)°
$V = 1129.54$ (5) Å^3
$Z = 4$
$D_x = 1.492$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 13 330 reflections
$\theta = 2.0$–27.5°
$\mu = 0.33$ mm^{-1}
$T = 160$ (2) K
Tablet, pale yellow
0.28 × 0.20 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans with κ offsets
Absorption correction: multi-scan (Blessing, 1995)
$T_{min} = 0.895$, $T_{max} = 0.970$
23 311 measured reflections
2597 independent reflections
1777 reflections with $I > 2\sigma(I)$
$R_{int} = 0.081$
$\theta_{max} = 27.5°$
$h = -16 \rightarrow 16$
$k = -14 \rightarrow 14$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.122$
$S = 1.06$
2597 reflections
159 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C5	1.296 (2)	N4—C5	1.377 (2)
N1—N2	1.401 (2)	N4—C3	1.383 (2)
N2—C3	1.370 (2)		
C5—N1—N2	104.30 (15)	N2—C3—N4	103.37 (16)
C3—N2—N1	112.02 (15)	N1—C5—C15	124.96 (17)
C5—N4—C3	108.20 (16)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O14—H14···O3^{i}	0.86 (3)	1.91 (3)	2.7498 (19)	163 (3)
C12—H122···O14^{ii}	0.99	2.57	3.528 (2)	163
C12—H121···O14^{iii}	0.99	2.59	3.564 (2)	170
C15—H153···O14^{i}	0.98	2.49	3.463 (2)	174

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

The position of the hydroxy H atom was determined from a difference Fourier map and refined freely along with its isotropic displacement parameter. The methyl H atoms were constrained to an ideal geometry (C—H = 0.98 Å), with $U_{iso}(H) = 1.5U_{eq}(C)$, but were allowed to rotate freely about the parent C—C bond. All remaining H atoms were placed in geometrically idealized positions (C—H = 0.95–0.99 Å) and constrained to ride on their parent atoms with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO–SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO–SMN* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Version 1.07; Farrugia, 1997); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 2002).

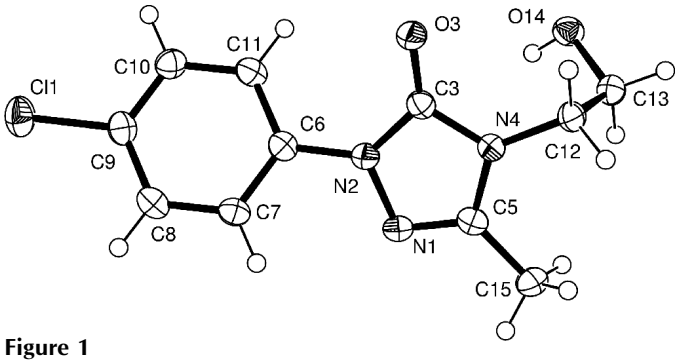


Figure 1
View of the asymmetric unit of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary radii.

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