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3,3′-Diisopropyl-4,4′-(hexane-1,6-diyl)bis-[1*H*-1,2,4-triazol-5(4*H*)-one] dihydrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.127
Data-to-parameter ratio = 15.2

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

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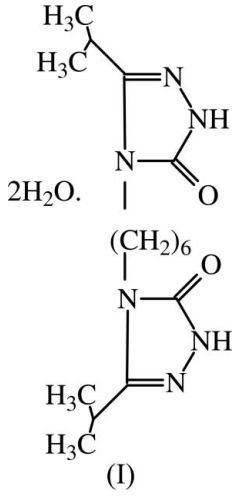
The triazole molecule of the title dihydrate, $C_{16}H_{28}N_6O_2\cdot 2H_2O$, possesses a crystallographically imposed centre of symmetry and shows normal values of bond lengths and angles. The uncoordinated water molecules are involved in intermolecular N—H···O, O—H···O and O—H···N hydrogen bonds, which stabilize the crystal packing.

Comment

1,2,4-Triazole and its derivatives exhibit various pharmacological properties such as antimicrobial (Holla *et al.*, 1998; Ersan *et al.*, 1998), anti-imflammatory, analgesic, antitumoral, antihypertensive and antiviral (Kritsanida *et al.*, 2002). In addition, compounds incorporating thidiazole and 1,2,4-triazole have been produced as antimicrobial agents (Holla *et al.*, 1998; Ersan *et al.*, 1998). Some of the azole derivatives used as common antibiotics, such as amphotericin B, exhibit toxic effects on humans along with antimicrobial effects (Collin *et al.*, 2003). Although different antimicrobial agents are used in the treatment of microbial infections, an increasing resistance to these drugs is observed (Collin *et al.*, 2003). Therefore, the search for and synthesis of new antibiotics different from commonly used ones is of current importance. We present here the crystal structure of the title compound, (I) (Fig. 1), a new 1,2,4-triazole derivative.



(I)

The triazole molecule possesses a crystallographically imposed centre of symmetry at the mid-point of the central C—C bond, and shows normal values of bond lengths and angles (Allen et al., 1987), cooresponding to those observed in 4,4′-(butane-1,4-diyl)bis[3-ethyl-1*H*-1,2,4-triazol-5(4*H*)-one] and 4-hydroxy-3-n-propyl-1*H*-1,2,4-triazol-5(4*H*)-one (Ocak

Ískeleli *et al.*, 2005). The uncoordinated water molecules are involved in intermolecular N—H···O, O—H···O and O—H···N hydrogen bonds (Table 1), which stabilize the crystal packing (Fig. 2).

Experimental

N′-(1-Ethoxy-2,2-dimethylethylidene)hydrazine carboxylic acid ethyl ester, (II), was obtained from the reaction of *N*′-(1-ethoxy-2,2-dimethylethylidene)imino ester hydrochloride (0.01 mol) with ethyl carbazate (0.01 mol). 1,6-Bis(3-isopropyl-4,5-dihydro-1*H*-1,2,4-triazole-5-one-4-yl)hexane was obtained from the reaction of (II) and 1,6-diaminohexane. To a solution of (II) (0.01 mol) in water (50 ml), 1,6-diaminohexane (0.01 mol) was added. The mixture was refluxed for 4 h and the resulting precipitate was filtered off. The solid obtained was recrystallized from water (yield 51.01%; m.p. 506–507 K).

Crystal data

$C_{16}H_{28}N_6O_2\cdot 2H_2O$
$M_r = 372.47$
Monoclinic, $P2_1/c$
$a = 7.7311\ (6)$ Å
$b = 10.7183\ (8)$ Å
$c = 12.691\ (1)$ Å
$\beta = 100.416\ (6)^\circ$
$V = 1034.30\ (14)$ Å^3
$Z = 2$
$D_x = 1.196$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 293\ (2)$ K
Prism, colourless
0.80 × 0.52 × 0.28 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min} = 0.976$, $T_{max} = 0.991$
14522 measured reflections
2033 independent reflections
1592 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 26.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.127$
$S = 0.92$
2033 reflections
134 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.077P)^2 + 0.2194P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···O33^{i}	0.86	1.89	2.7389 (18)	170
O33—H66···O1^{ii}	0.853 (16)	1.885 (16)	2.7372 (17)	176 (2)
O33—H77···N5	0.878 (16)	2.033 (17)	2.9105 (19)	177 (2)

Symmetry codes: (i) $-x, -y, -z+1$; (ii) $x+1, y, z$.

Water H atoms were located in a difference Fourier map and isotropically refined with O—H distance restraints of 0.85 (3) Å. The amino and C-bound H atoms were positioned geometrically (N—H = 0.86 Å and C—H = 0.93–0.97 Å) and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}$ or $1.5U_{eq}$(parent atom).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Johnson & Burnett, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PARST* (Nardelli, 1995).

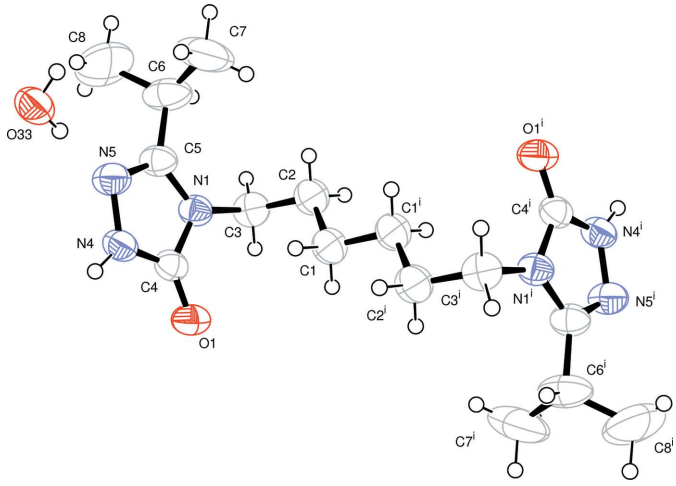


Figure 1
View of the title compound, showing the 50% probability displacement ellipsoids and the atom-numbering scheme [symmetry code: (i) $-1-x, -y, -z$].

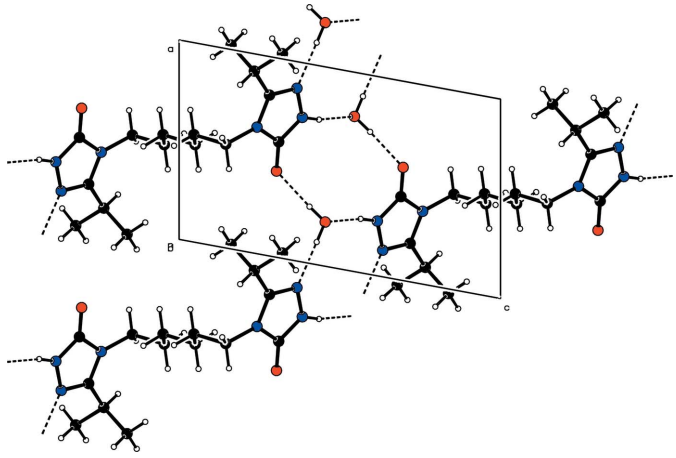


Figure 2
The packing, viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

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