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1,2-Bis[5-oxo-3-(*n*-propyl)-4,5-dihydro-3*H*-1,2,4-triazol-4-yl]ethane dihydrate

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.046
wR factor = 0.119
Data-to-parameter ratio = 12.7

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

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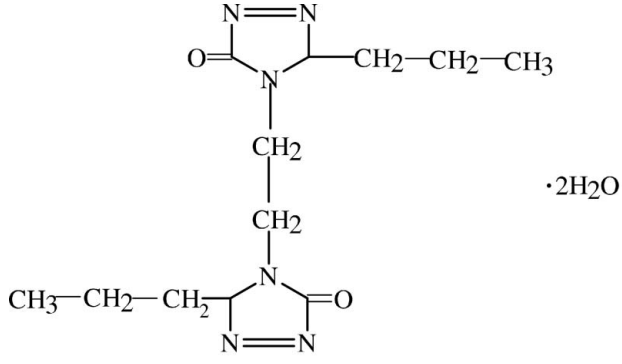
The molecule of the title compound, $C_{12}H_{20}N_6O_2\cdot 2H_2O$, contains two planar triazole rings. The molecule has crystallographic twofold rotation symmetry. The crystal structure is stabilized by intermolecular hydrogen bonds, which form a three-dimensional network.

Comment

Triazole ring systems are planar and partially aromatic. Several articles have been devoted to the syntheses and pharmacological investigations of triazole compounds (Lønning *et al.*, 1998). Apart from its extensive chemical significance, the 1,2,4-triazole nucleus is also found to be associated with diverse medicinal properties, such as analgesic, anti-asthmatic, diuretic and antifungal activities (Mohamed *et al.*, 1993). 1,2,4-Triazole rings interact strongly with heme iron, and aromatic substituents on the triazoles are very effective for interacting with the active site of aromatase (Chen *et al.*, 1997).

The title compound, (I), is shown in Fig. 1. The molecule has twofold rotation symmetry. Selected bond lengths and angles are listed in Table 1. In the crystal structure, there are intermolecular N—H···O, O—H···O and O—H···N hydrogen bonds (Table 2). The structures of the closely related compounds 4,4′-butane-1,4-diylbis[3-ethyl-1*H*-1,2,4-triazole-5(4*H*)-one] and 4-hydroxy-3-*n*-propyl-1*H*-1,2,4-triazole-5(4*H*)-one were recently reported (Ocak Ískeleli *et al.*, 2005).



(I)

Experimental

1,2-Bis[(3-n-propyl)-4,5-dihydro-1H-1,2,4-triazole-5-one-4-yl]ethane dihydrate (4.04 g, 0.02 mol) was treated with a solution of 1,3-diaminopropane (0.83 ml, 0.74 g, 0.01 mol) in water (50 ml), and the mixture was refluxed for 6 h. After cooling, the precipitate that formed was recrystallized from ethanol to give (I) (yield 44%, m.p.

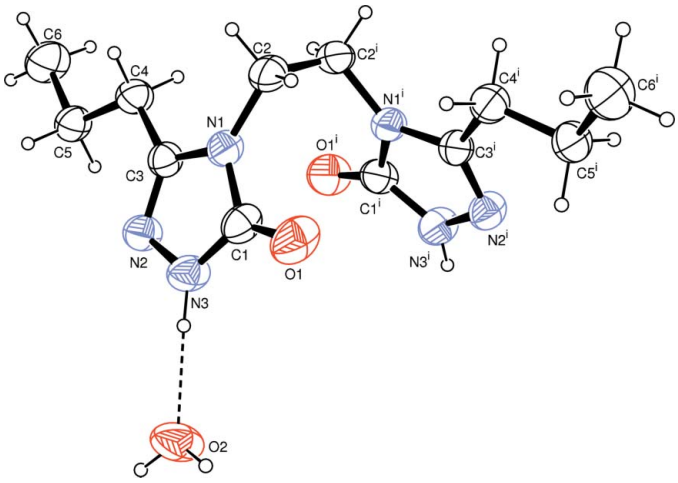


Figure 1
An *ORTEP-3* (Farrugia, 1997) view of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids for non-H atoms [symmetry code: (i) $1-x, y, \frac{3}{2}-z$]. The dashed line represents the N—H···O hydrogen bond.

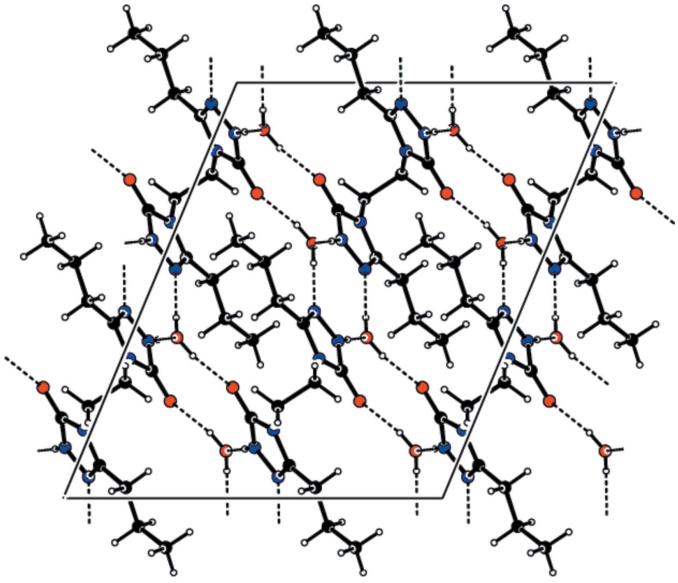


Figure 2
A packing diagram of (I), viewed along the *b* axis. Hydrogen bonds are shown by dashed lines.

462 K). IR: 3520–3440 (OH), 3240 (NH), 1690 (C═O), 1393 (C═N) cm^{-1}; ^1H NMR: δ 11.35 [*s*, 2H(2NH)], 3.60 [*t*, 6H($3CH_2$)], 2.40 [*t*, 4H($2CH_2$)], 2.10 [*s*, 2H(H_2O)], 1.35 [*q*, 4H($2CH_2$)], 0.85 [*t*, 6H($2CH_3$)].

Crystal data

$C_{12}H_{20}N_6O_2\cdot 2H_2O$
$M_r = 316.37$
Monoclinic, $C2/c$
$a = 13.0125\ (12)$ Å
$b = 8.5957\ (6)$ Å
$c = 15.4586\ (12)$ Å
$\beta = 112.655\ (6)^\circ$
$V = 1595.7\ (2)$ Å^3
$Z = 4$
$D_x = 1.317$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1008 reflections
$\theta = 2.9$–27.9°
$\mu = 0.10$ mm^{-1}
$T = 296\ (2)$ K
Prism, colourless
0.50 × 0.43 × 0.23 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: integration (*X-RED*; Stoe & Cie, 2002)
$T_{min} = 0.954$, $T_{max} = 0.985$
5349 measured reflections
1887 independent reflections
1470 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 27.9^\circ$
$h = -17 \rightarrow 17$
$k = -11 \rightarrow 11$
$l = -15 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.120$
$S = 1.04$
1887 reflections
149 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0836P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.047 (4)

Table 1
Selected geometric parameters (Å, °).

N1—C3	1.3725 (15)	O1—C1	1.2261 (16)
N1—C1	1.3838 (15)	N3—C1	1.3410 (17)
N2—C3	1.2966 (15)	C2—C2^{i}	1.515 (3)
N2—N3	1.3810 (14)		
N1—C2—C2^{i}	112.85 (9)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O2	0.86 (2)	1.90 (2)	2.7576 (16)	177 (2)
O2—H11*B*···O1^{ii}	0.85 (2)	1.91 (3)	2.7457 (16)	165 (2)
O2—H11*A*···N2^{iii}	0.85 (3)	2.03 (3)	2.8815 (16)	178 (2)

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

All H atoms were refined isotropically [C—H = 0.935 (17)–1.03 (2) Å].

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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