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4-Amino-3,5-bis(1-hydroxyethyl)-4*H*-1,2,4-triazole

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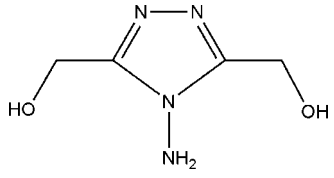
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.106; data-to-parameter ratio = 12.0.

In the title compound, $C_4H_8N_4O_2$, which was synthesized by the reaction of lactic acid with hydrazine hydrate under solvent-free conditions, all bond lengths and angles are normal. In the crystal structure, intermolecular O—H···N and N—H···O hydrogen bonds link the molecules into two-dimensional corrugated sheets parallel to the *bc* plane.

Related literature

In the complex $[Cu(L)_2]$ (H*L* = 4-salicylideneamino-3,5-dimethanol-1,2,4-triazole) (Yi *et al.*, 2004), all bond lengths and angles in *L* are comparable with those found in the title compound.



Experimental

Crystal data

$C_4H_8N_4O_2$
M_r = 144.14
Orthorhombic, *Pbca*
a = 8.7936 (17) Å
b = 8.8609 (18) Å
c = 16.058 (2) Å
V = 1251.3 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 298 (2) K
0.54 × 0.47 × 0.40 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.936, T_{max} = 0.952
4961 measured reflections
1107 independent reflections
853 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.106
S = 1.00
1107 reflections
92 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N2^{i}	0.82	2.02	2.820 (2)	164
N4—H4B···O1^{ii}	0.90	2.14	2.955 (2)	151
N4—H4A···O2^{iii}	0.90	2.25	3.058 (2)	150
O1—H1···N1^{iv}	0.82	1.98	2.782 (2)	165

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2290).

References

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Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
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supplementary materials

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4-Amino-3,5-bis(1-hydroxyethyl)-4*H*-1,2,4-triazole

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Comment

In this paper, we present the title compound, 4-amino-3,5-bis(1-hydroxyethyl)-l,2,4-triazole, (I), synthesized through the condensation of lactic acid and hydrazine hydrate under solvent-free conditions.

In (I) (Fig. 1), all bond lengths and angles are normal and comparable to those observed in the complex [Cu(L)$_2$] (HL=4-salicylideneamino-3,5-dimethanol-1,2,4-triazole) (Yi *et al.*, 2004)

In the crystal, there exist typical intermolecular N—H···O and O—H···N hydrogen bonds (Table 1), which assemble the molecules into infinite two-dimensional sheets (Fig. 2).

Experimental

A mixture of lactic acid (1 mmol) and hydrazine hydrate (1.05 mmol) was well stirred at room temperature for 10 minutes. The crude compound was purified by silica gel column chromatography. Elemental analysis: calculated for $C_4H_8N_4O_2$: C 33.33, H 5.59, N 38.87%; found: C 33.38, H 5.52, N 38.75%.

Refinement

The methylene H atoms were placed in idealized positions and constrained to ride on their parent atoms with methylene C—H distances of 0.97 Å. The U_{iso}(H) values were set at 1.2U_{eq}(C). The hydroxy H atoms were placed in idealized positions and constrained to ride on their parent atoms with O—H distances of 0.82 Å. The U_{iso}(H) values were set at 1.5 U_{eq}(O). The amino H atoms were placed in idealized positions and constrained to ride on their parent atoms with N—H distances of 0.90 Å. The U_{iso}(H) values were set at 1.2 U_{eq}(N).

Figures

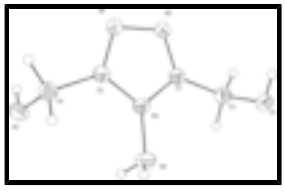

Fig. 1. *ORTEP* drawing of the title complex with atomic numbering scheme and thermal ellipsoids at 30% probability level.

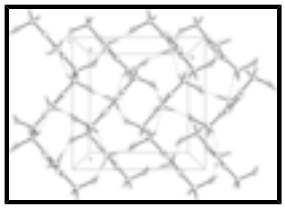

Fig. 2. A perspective view of the crystal packing of (I). Dashed lines denote intermolecular hydrogen bonds.

4-Amino-3,5-bis(1-hydroxyethyl)-4*H*-1,2,4-triazole

Crystal data

$C_4H_8N_4O_2$	$D_x = 1.530$ Mg m^{-3}
$M_r = 144.14$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Orthorhombic, *Pbca*	Cell parameters from 2134 reflections
$a = 8.7936$ (17) Å	$\theta = 2.5$–27.6º
$b = 8.8609$ (18) Å	$\mu = 0.12$ mm^{-1}
$c = 16.058$ (2) Å	$T = 298$ (2) K
$V = 1251.3$ (4) Å^3	Block, colourless
$Z = 8$	0.54 × 0.47 × 0.40 mm
$F_{000} = 608$	

Data collection

Bruker SMART CCD area-detector diffractometer	1107 independent reflections
Radiation source: fine-focus sealed tube	853 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.048$
$T = 298$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 2.5$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -5 \rightarrow 10$
$T_{min} = 0.936$, $T_{max} = 0.952$	$k = -10 \rightarrow 9$
4961 measured reflections	$l = -19 \rightarrow 17$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.039$	$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 0.8519P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.106$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.00$	$\Delta\rho_{max} = 0.21$ e Å^{-3}
1107 reflections	$\Delta\rho_{min} = -0.19$ e Å^{-3}
92 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997a), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.061 (4)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	−0.06178 (18)	0.76742 (18)	0.23561 (10)	0.0344 (4)
N2	0.05790 (18)	0.66499 (18)	0.23983 (10)	0.0349 (4)
N3	0.01255 (17)	0.71644 (17)	0.10961 (9)	0.0307 (4)
N4	0.0336 (2)	0.7147 (2)	0.02318 (10)	0.0443 (5)
H4A	0.0599	0.8063	0.0037	0.053*
H4B	−0.0503	0.6824	−0.0034	0.053*
O1	0.16445 (16)	0.38730 (15)	0.11444 (8)	0.0402 (4)
H1	0.1196	0.3501	0.1542	0.060*
O2	−0.13453 (18)	1.04642 (15)	0.10268 (8)	0.0444 (5)
H2	−0.0956	1.0836	0.1443	0.067*
C1	0.1008 (2)	0.6365 (2)	0.16332 (11)	0.0307 (5)
C2	−0.0871 (2)	0.7968 (2)	0.15687 (11)	0.0304 (5)
C3	0.2228 (2)	0.5305 (2)	0.13717 (13)	0.0385 (5)
H3A	0.2771	0.5733	0.0902	0.046*
H3B	0.2945	0.5182	0.1825	0.046*
C4	−0.2009 (2)	0.9057 (2)	0.12349 (12)	0.0378 (5)
H4C	−0.2482	0.8629	0.0743	0.045*
H4D	−0.2798	0.9215	0.1648	0.045*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0390 (9)	0.0334 (9)	0.0310 (9)	0.0043 (7)	0.0023 (7)	0.0010 (7)
N2	0.0402 (10)	0.0332 (9)	0.0313 (9)	0.0032 (8)	0.0007 (7)	0.0027 (7)
N3	0.0347 (9)	0.0327 (9)	0.0246 (8)	−0.0026 (7)	0.0005 (6)	−0.0009 (7)
N4	0.0573 (12)	0.0504 (11)	0.0253 (9)	0.0000 (9)	0.0020 (8)	0.0000 (8)
O1	0.0542 (9)	0.0333 (8)	0.0331 (8)	0.0002 (7)	0.0046 (6)	−0.0030 (6)
O2	0.0614 (10)	0.0369 (9)	0.0350 (8)	−0.0017 (7)	−0.0072 (7)	0.0048 (6)
C1	0.0315 (10)	0.0287 (10)	0.0320 (10)	−0.0039 (8)	0.0007 (8)	0.0008 (8)
C2	0.0321 (10)	0.0280 (10)	0.0312 (10)	−0.0036 (8)	−0.0008 (8)	−0.0010 (8)
C3	0.0365 (11)	0.0379 (11)	0.0411 (11)	0.0003 (9)	0.0044 (9)	0.0007 (9)
C4	0.0378 (11)	0.0387 (11)	0.0369 (11)	0.0020 (9)	−0.0051 (9)	0.0007 (9)

Geometric parameters (Å, °)

N1—C2	1.310 (2)	O1—H1	0.8200
N1—N2	1.391 (2)	O2—C4	1.417 (2)
N2—C1	1.310 (2)	O2—H2	0.8200
N3—C1	1.359 (2)	C1—C3	1.486 (3)
N3—C2	1.361 (2)	C2—C4	1.489 (3)
N3—N4	1.400 (2)	C3—H3A	0.9700
N4—H4A	0.9000	C3—H3B	0.9700
N4—H4B	0.9000	C4—H4C	0.9700
O1—C3	1.417 (2)	C4—H4D	0.9700
C2—N1—N2	107.79 (14)	N1—C2—C4	126.18 (17)
C1—N2—N1	107.30 (15)	N3—C2—C4	124.81 (17)
C1—N3—C2	106.64 (15)	O1—C3—C1	112.19 (16)
C1—N3—N4	123.21 (16)	O1—C3—H3A	109.2
C2—N3—N4	130.08 (16)	C1—C3—H3A	109.2
N3—N4—H4A	111.6	O1—C3—H3B	109.2
N3—N4—H4B	111.4	C1—C3—H3B	109.2
H4A—N4—H4B	109.5	H3A—C3—H3B	107.9
C3—O1—H1	109.5	O2—C4—C2	112.22 (16)
C4—O2—H2	109.5	O2—C4—H4C	109.2
N2—C1—N3	109.32 (16)	C2—C4—H4C	109.2
N2—C1—C3	126.46 (17)	O2—C4—H4D	109.2
N3—C1—C3	124.19 (17)	C2—C4—H4D	109.2
N1—C2—N3	108.94 (16)	H4C—C4—H4D	107.9

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···N2^{i}	0.82	2.02	2.820 (2)	164
N4—H4B···O1^{ii}	0.90	2.14	2.955 (2)	151
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Symmetry codes: (i) −*x*, *y*+1/2, −*z*+1/2; (ii) −*x*, −*y*+1, −*z*; (iii) −*x*, −*y*+2, −*z*; (iv) −*x*, *y*−1/2, −*z*+1/2.

Fig. 1

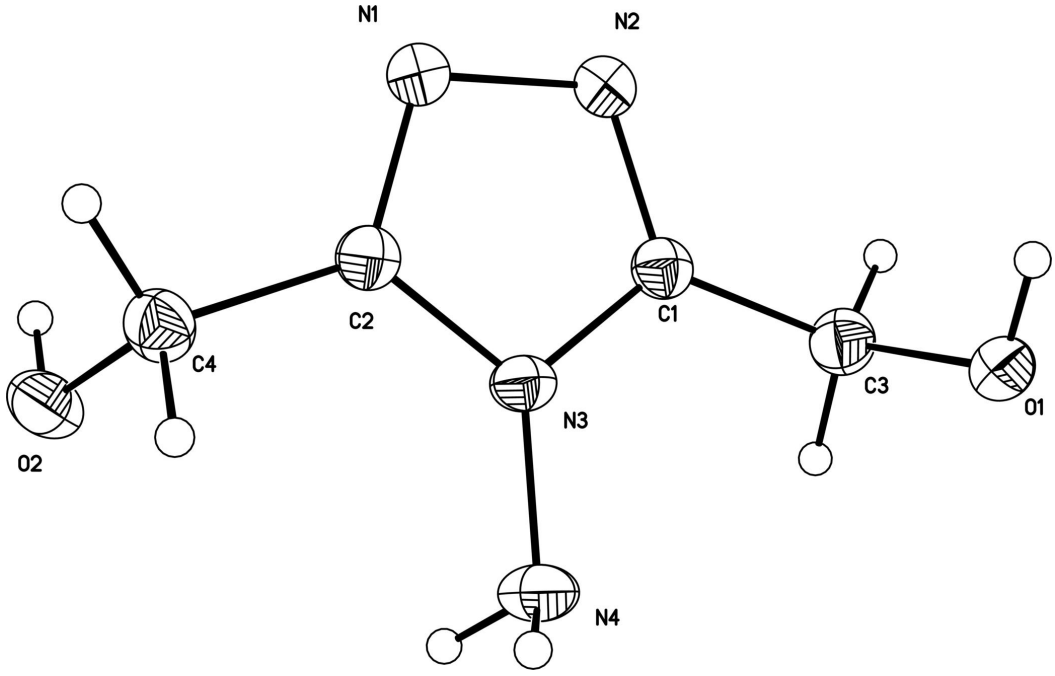

Fig. 2