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1*H*-1,2,4-Triazole-3-carboxamide

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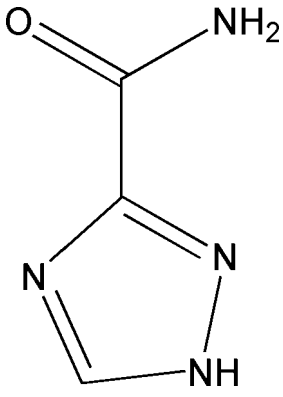
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.102; data-to-parameter ratio = 11.1.

Planar molecules of the title compound, $C_3H_4N_4O$, are organized into sheets by extensive N—H···O and N—H···N hydrogen bonding in the (101) plane of the crystal structure. These hydrogen bonds may also stabilize the molecule in the Z form. The title compound is in the amide form, as shown by the C=O bond length [1.252 (2) Å].

Related literature

Azo compounds are widely utilized as dyes and analytical reagents (Malinauskas *et al.*, 2000). The interactions of amide groups are of interest because of their importance in biochemical systems (Crespo *et al.*, 2005).



Experimental

Crystal data

$C_3H_4N_4O$ M_r = 112.10
Monoclinic, $P2_1/n$
a = 3.6944 (4) Å
b = 17.527 (3) Å
c = 7.0520 (17) Å
β = 94.4670 (10)° **precision OK?**
V = 455.24 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 298 (2) K
0.22 × 0.18 × 0.09 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.972, T_{max} = 0.988
2199 measured reflections
807 independent reflections
657 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.101
S = 1.05
807 reflections
73 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.86	2.21	3.065 (2)	173
N1—H1B···N4^{ii}	0.86	2.22	3.010 (2)	154
N2—H2···O1^{iii}	0.86	2.07	2.909 (2)	163
N2—H2···N3^{iii}	0.86	2.54	3.055 (2)	120

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

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: CS2075).

References

Bruker (2003). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Crespo, L., Sanclimens, G., Pons, M., Giralt, E., Royo, M. & Albericio, F. (2005). *Chem. Rev.* **105**, 1663–1681.
Malinauskas, A., Niaura, G. & Bloxham, S. (2000). *J. Colloid Interface Sci.* **230**, 122–127.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, o1110 [doi:10.1107/S1600536808014013]

1*H*-1,2,4-Triazole-3-carboxamide

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S1. Comment

The title compound was obtained by the reaction of methyl 1*H*-1,2,4-triazole-3-carboxylate and ammonium hydroxide. The C=O bond length of 1.2524 (18) Å suggests that the title compound is in the amide form. N—H···O and N—H···N hydrogen bonds link molecules into infinite sheets. These sheets provide the two-dimensional network in and paralell to the *{101}* plane of the cell.

S2. Experimental

Added 20 ml 25% ammonium hydroxide to methyl 1*H*-1,2,4-triazole-3-carboxylate (20 mmol, 2540 mg) while stirring for 8 h at 353 K. The resulting white precipitate was filtered and washed several times with ethanol and dried in vacuo (yield 85%). Single crystals of $C_3H_4N_4O$ suitable for X-ray diffraction were obtained by slow evaporation of an 50% ethanol solution at room temperature over a period of one week.

S3. Refinement

The C– and N-bound H atoms were placed in calculated positions and included in the refinement in the riding-model approximation with N—H = 0.86 Å and C—H = 0.93 Å, and with U_{iso}(H) 1.2U_{eq}(C,*N*).

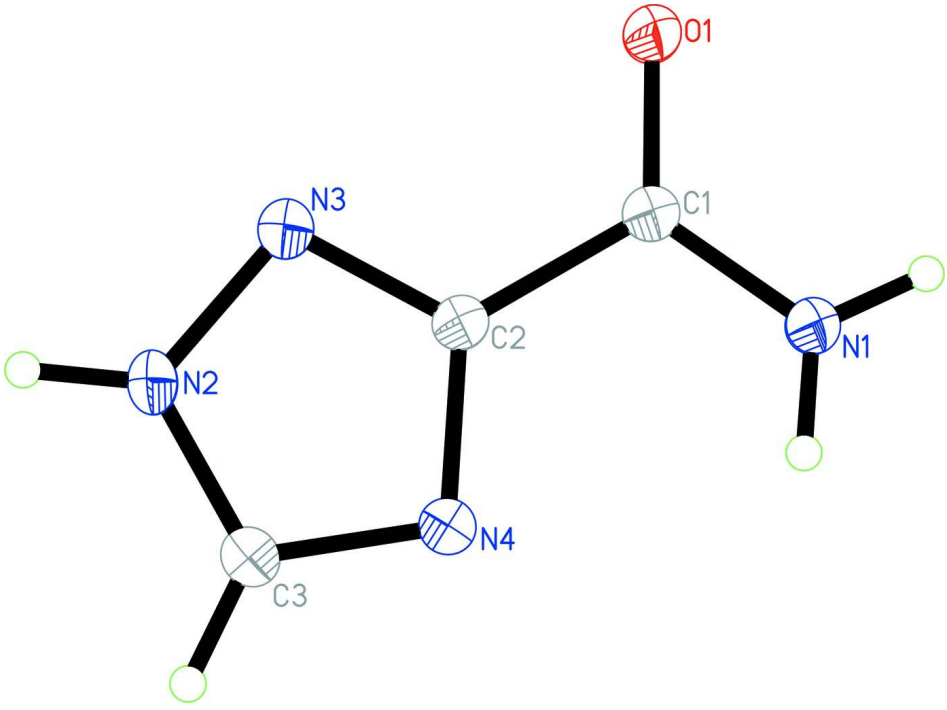

Figure 1

The structure of the title compound showing 30% probability displacement ellipsoids and the atom-numbering scheme.

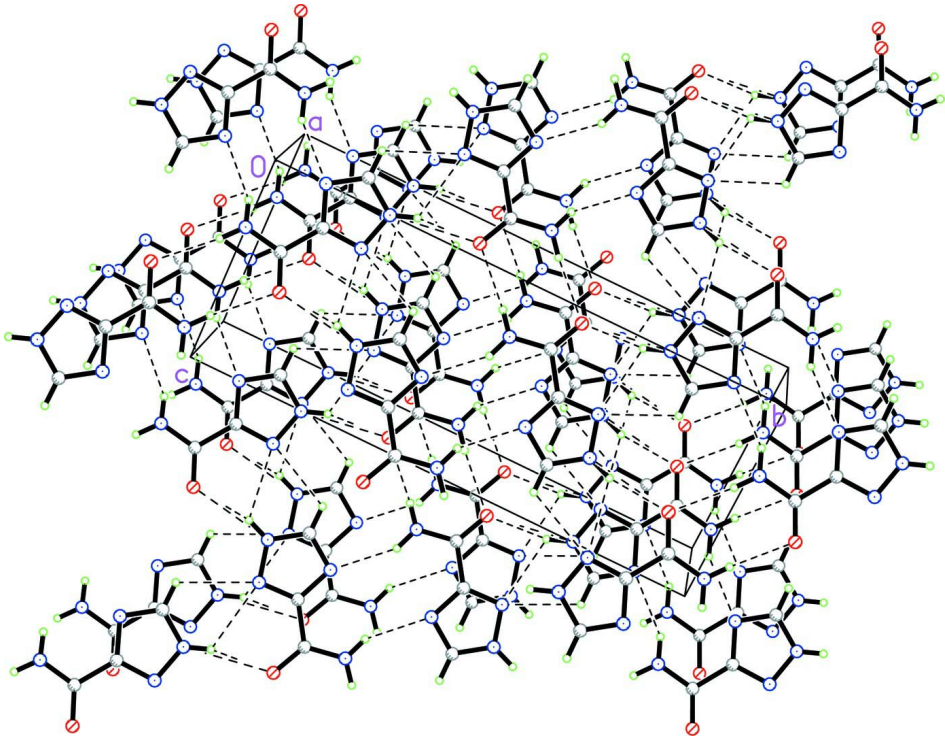

Figure 2

Crystal packing showing the hydrogen bonded interactions as dashed lines.

1*H*-1,2,4-Triazole-3-carboxamide

Crystal data

$C_3H_4N_4O$
$M_r = 112.10$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 3.6944$ (4) Å
$b = 17.527$ (3) Å
$c = 7.0520$ (17) Å
$\beta = 94.467$ (1)°
$V = 455.24$ (14) Å^3
$Z = 4$
$F(000) = 232$
$D_x = 1.636$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1200 reflections
$\theta = 2.3$–$27.5°$
$\mu = 0.13$ mm^{-1}
$T = 298$ K
Prism, colourless
0.22 × 0.18 × 0.09 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.972$, $T_{max} = 0.988$
2199 measured reflections
807 independent reflections
657 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.3°$
$h = -4 \rightarrow 3$
$k = -20 \rightarrow 18$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.101$
$S = 1.05$
807 reflections
73 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 0.058P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.2702 (4)	0.99272 (7)	0.7168 (2)	0.0381 (4)
H1A	0.3404	1.0240	0.6332	0.046*
H1B	0.1763	1.0098	0.8163	0.046*
N2	0.0498 (4)	0.77481 (8)	1.00884 (19)	0.0330 (4)
H2	0.0162	0.7288	1.0460	0.040*
N3	0.1784 (4)	0.79443 (7)	0.84073 (18)	0.0329 (4)
N4	0.0595 (4)	0.89955 (8)	1.01228 (18)	0.0349 (4)
O1	0.4402 (3)	0.88844 (6)	0.55202 (16)	0.0386 (4)
C1	0.3067 (4)	0.91813 (8)	0.6923 (2)	0.0289 (4)
C2	0.1793 (4)	0.87021 (8)	0.8491 (2)	0.0271 (4)
C3	−0.0168 (5)	0.83716 (9)	1.1079 (2)	0.0360 (4)
H3	−0.1048	0.8370	1.2279	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0594 (10)	0.0241 (8)	0.0333 (8)	0.0011 (6)	0.0202 (7)	0.0017 (5)
N2	0.0449 (9)	0.0220 (7)	0.0331 (8)	−0.0010 (5)	0.0098 (6)	0.0056 (5)
N3	0.0434 (8)	0.0250 (8)	0.0314 (7)	−0.0006 (5)	0.0093 (6)	0.0010 (5)
N4	0.0494 (9)	0.0259 (8)	0.0310 (8)	0.0004 (6)	0.0145 (6)	0.0004 (5)
O1	0.0566 (8)	0.0267 (6)	0.0347 (7)	0.0030 (5)	0.0176 (5)	−0.0001 (5)
C1	0.0339 (9)	0.0259 (9)	0.0274 (8)	0.0006 (6)	0.0055 (6)	−0.0007 (6)
C2	0.0307 (8)	0.0243 (8)	0.0268 (8)	0.0016 (6)	0.0052 (6)	−0.0009 (6)
C3	0.0495 (10)	0.0292 (9)	0.0308 (8)	−0.0012 (7)	0.0131 (7)	0.0013 (7)

Geometric parameters (Å, º)

N1—C1	1.3270 (19)	N3—C2	1.3294 (19)
N1—H1A	0.8600	N4—C3	1.326 (2)
N1—H1B	0.8600	N4—C2	1.366 (2)
N2—C3	1.330 (2)	O1—C1	1.2524 (18)
N2—N3	1.3553 (19)	C1—C2	1.493 (2)
N2—H2	0.8600	C3—H3	0.9300
C1—N1—H1A	120.0	O1—C1—C2	121.15 (14)
C1—N1—H1B	120.0	N1—C1—C2	114.62 (14)
H1A—N1—H1B	120.0	N3—C2—N4	114.43 (13)
C3—N2—N3	110.03 (13)	N3—C2—C1	121.94 (13)
C3—N2—H2	125.0	N4—C2—C1	123.62 (14)
N3—N2—H2	125.0	N4—C3—N2	110.81 (15)
C2—N3—N2	102.40 (13)	N4—C3—H3	124.6
C3—N4—C2	102.33 (13)	N2—C3—H3	124.6
O1—C1—N1	124.23 (15)		
C3—N2—N3—C2	−0.33 (17)	N1—C1—C2—N3	176.10 (15)
N2—N3—C2—N4	0.05 (17)	O1—C1—C2—N4	174.46 (15)
N2—N3—C2—C1	179.30 (13)	N1—C1—C2—N4	−4.7 (2)
C3—N4—C2—N3	0.23 (18)	C2—N4—C3—N2	−0.43 (18)
C3—N4—C2—C1	−179.00 (14)	N3—N2—C3—N4	0.50 (19)
O1—C1—C2—N3	−4.7 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1^{i}	0.86	2.21	3.065 (2)	173
N1—H1*B*···N4^{ii}	0.86	2.22	3.010 (2)	154
N2—H2···O1^{iii}	0.86	2.07	2.909 (2)	163
N2—H2···N3^{iii}	0.86	2.54	3.055 (2)	120

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+1; (ii) −*x*, −*y*+2, −*z*+2; (iii) *x*−1/2, −*y*+3/2, *z*+1/2.