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

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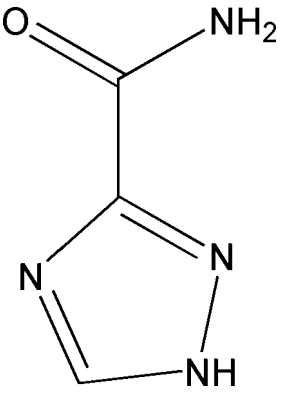
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.102; data-to-parameter ratio = 11.1.

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)°
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).

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