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N-(2-Hydroxyethyl)pyrazine-2-carboxamide

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.134
Data-to-parameter ratio = 14.0

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

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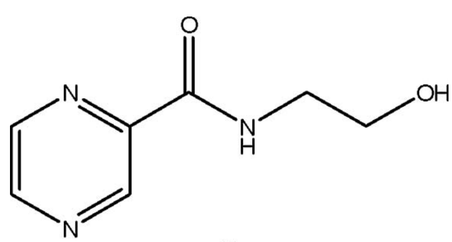
The title compound, $C_7H_9N_3O_2$, crystallizes with two independent molecules in the asymmetric unit. The amide group lies almost in the pyrazine plane. Each molecule is linked to three other molecules by means of hydrogen bonds, giving rise to a ladder-like two-dimensional network. Adjacent two-dimensional networks are linked by hydrogen bonds to form a three-dimensional structure.

Comment

In coordination chemistry, heterocyclic compounds containing N atoms are very useful ligands; for example, pyrazine, as a bridging group, is capable of coordinating to metal ions such as manganese (Coher & Mautner, 1999), forming an infinite ordered long-chain coordination polymer (Ding *et al.*, 2000; Holman *et al.*, 2005). The investigation of such compounds has attracted a great deal of interest in recent years. In order to prepare a new compound, we attempted to synthesize a pyrazine derivative with a substituent including N and O atoms, which can easily promote hydrogen bonding (Goswami *et al.*, 2005). For this, two isolated polymeric chains might be connected through weak hydrogen-bond interactions, forming a network which perhaps has some potential for future research. Therefore, we synthesized the title compound, (I), which is reported here. Compounds in which this ligand is coordinated to metal ions will be reported later.



(I)

Compound (I) contains two independent molecules in the asymmetric unit. In the two independent molecules, the C5—N3 and C12—N6 bond lengths are 1.327 (3) and 1.328 (3) Å, respectively, approximately equal to a C═N double-bond length (Shanmuga Sundara Raj *et al.*, 2000), indicating that atoms N3 and N6 of the amide groups must also be sp^2 hybridized. This conclusion is also supported by the O1—C5—C1 and O3—C12—C8 angles of 119.93 (19) and 119.6 (2)°, respectively, and by the fact that atoms N3, O1 and C5, and atoms N6, O3 and C12, lie almost in the pyrazine plane. In (I), other bond lengths and angles are norma.

In the conformation of (I), hydrogen bonds play an important role. Each molecule is linked to three other molecules by means of hydrogen bonds, giving rise to a two-

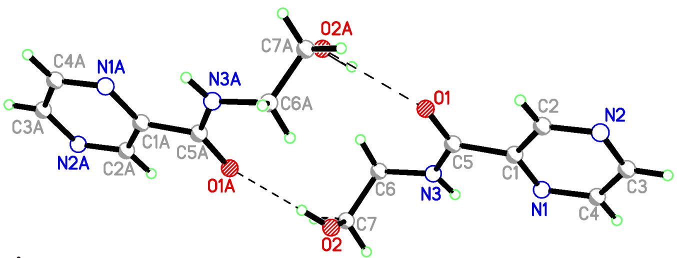


Figure 1
The structures of the two independent molecules in the asymmetric unit of (I), with displacement ellipsoids at the 30% probability level.

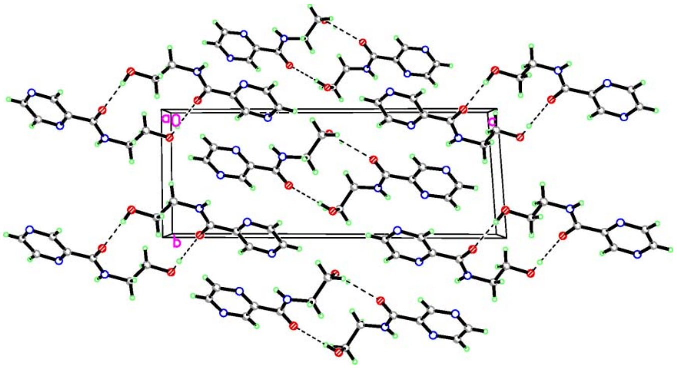


Figure 2
Part of the crystal structure of (I), showing the formation of $R_2^2(14)$ rings by two classical hydrogen bonds (dashed lines). H atoms have been omitted.

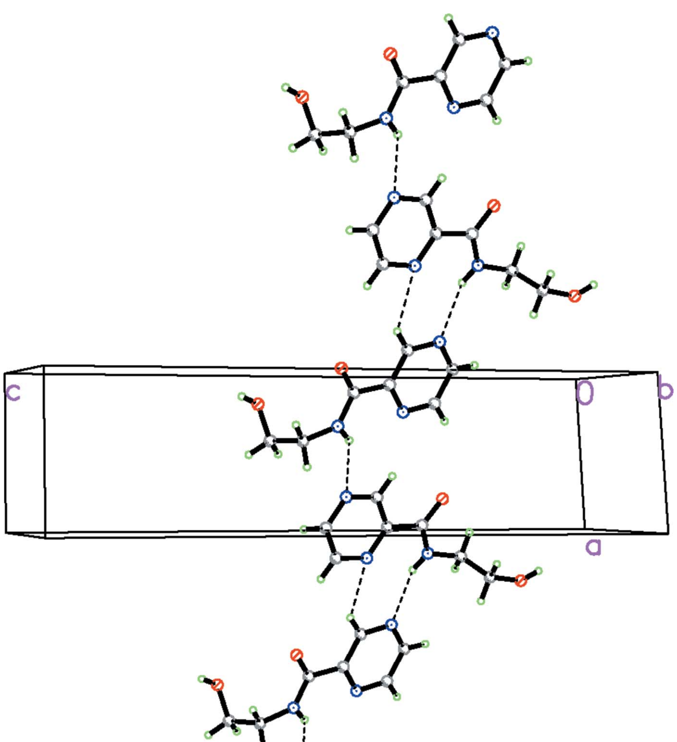


Figure 3
Part of the crystal structure of (I), showing the formation of a chain of pairs of molecules by hydrogen bonds (dashed lines) along the [101] direction.

dimensional (Tonogaki *et al.*, 1993; Glidewell *et al.*, 2002) hydrogen-bonded structure (Fig. 2, Table 2), each of which

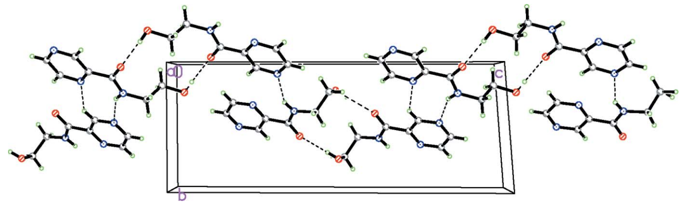


Figure 4
Part of the crystal structure of (I), showing the formation of a [001] chain. Hydrogen bonds are shown as dashed lines.

generates a centrosymmetric $R_2^2(14)$ ring possessing a stabilized chair conformation. In addition to these two classical hydrogen bonds, two other hydrogen bonds exist, of classical N—H···N and non-classical C—H···N types, which produce $R_2^2(8)$ rings coplanar with two adjacent pyrazine rings. Additionally, there exists one N—H···N hydrogen bond, which connects the molecules together. Thus an infinite chain of pairs of molecules running parallel to [100] is generated (Fig. 3). Furthermore, propagation of the hydrogen bonds mentioned above produces a one-dimensional chain along the [001] direction (Fig. 4). The combination of the [100] and [001] chains generates a molecular ladder-like two-dimensional network; adjacent ladders are linked linked by hydrogen bonds to form a three-dimensional structure.

Experimental

The title compound was synthesized according to the method described by Darmstadt & Munick (1935). Single crystals of (I) were grown from a solution in methanol by slow evaporation (yield 79%, m.p. 391 K).

Crystal data

$C_7H_9N_3O_2$
M_r = 167.17
Triclinic, $P\bar{1}$
a = 5.3054 (12) Å
b = 7.8287 (19) Å
c = 19.880 (5) Å
α = 86.953 (4)°
β = 87.262 (4)°
γ = 74.451 (4)°
V = 793.9 (3) Å^3
Z = 4
D_x = 1.399 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1336 reflections
θ = 2.7–25.6°
μ = 0.11 mm^{-1}
T = 294 (2) K
Block, colourless
0.28 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.962, T_{max} = 0.983
4504 measured reflections
3197 independent reflections
1895 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 26.4°
$h = -6 \rightarrow 6$
$k = -9 \rightarrow 8$
$l = -24 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.134
S = 1.05
3197 reflections
228 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0576P)^2 + 0.0883P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.042 (5)

Table 1
Selected geometric parameters (Å, °).

N3—C5	1.327 (3)	C1—C5	1.504 (3)
O1—C5	1.232 (2)		
O1—C5—N3	125.3 (2)	N3—C5—C1	114.78 (19)
O1—C5—C1	119.93 (19)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O3^{i}	0.82	1.94	2.763 (3)	176
O2—H2···O1^{ii}	0.82	2.01	2.813 (2)	166
N6—H6···N2^{iii}	0.83 (3)	2.31 (3)	3.062 (3)	151 (3)
N3—H3···N5^{iv}	0.84 (2)	2.36 (2)	3.090 (3)	145 (2)
N3—H3···N1	0.84 (2)	2.28 (2)	2.699 (3)	111 (2)

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

Atoms H3 and H6 bound to the atoms N3 and N6 were found in a difference Fourier map and refined isotropically. The other H atoms were positioned geometrically and refined as riding (C—H = 0.93–0.97 Å and O—H = 0.82 Å), with U_{iso}(H) values set equal to 1.2 (CH and CH_2) or 1.5 (CH_3 and OH) times U_{eq} of the parent atom.

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

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