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N′-[4-(Diethylamino)benzylidene]-pyrazine-2-carbohydrazide dihydrate

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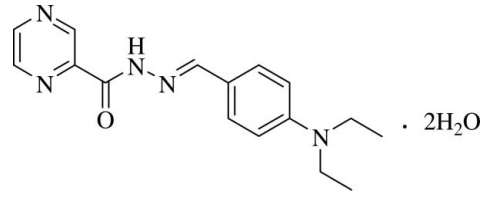
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.126; data-to-parameter ratio = 15.2.

The title compound, $C_{16}H_{19}N_5O\cdot 2H_2O$, was synthesized by the reaction of pyrazine-2-carbohydrazide with 4-(diethylamino)benzaldehyde in methanol. The molecule is nearly planar, with a dihedral angle of 11.95 (3)° between the pyrazine and benzene rings. The C—C—N—N torsion angles are 3.43 (3) and 4.46 (3)°. Molecules are linked by O—H···O and O—H···N hydrogen bonds involving all the potential donors. The pyrazine rings and the phenyl rings show weak face-to-face π–π stacking interactions.

Related literature

For related literature, see: Edwards *et al.* (1975); Gardner *et al.* (1956); Goswami & Ghosh (1997); Goswami *et al.* (1998); Hadjoudis *et al.* (1987); Parashar *et al.* (1988); Kushner *et al.* (1952); Shi & Zhang (2007).



Experimental

Crystal data

$C_{16}H_{19}N_5O\cdot 2H_2O$
M_r = 333.39
Monoclinic, $P2_1/c$
a = 13.422 (3) Å
b = 10.761 (3) Å
c = 12.820 (3) Å
β = 109.158 (4)°
V = 1749.1 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.26 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.977, T_{max} = 0.984
8345 measured reflections
3559 independent reflections
1920 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.126
S = 0.95
3559 reflections
234 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 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
N3—H3*C*···O2^{i}	0.926 (19)	2.11 (2)	2.987 (2)	158.1 (17)
O2—H2*A*···O1	0.89 (2)	2.27 (3)	3.049 (2)	146 (3)
O2—H2*A*···N4	0.89 (2)	2.49 (3)	3.262 (2)	145 (3)
O2—H2*B*···O3^{ii}	0.85 (2)	2.00 (2)	2.832 (2)	166 (3)
O3—H3*A*···O1	0.83 (2)	2.08 (2)	2.912 (2)	175 (3)
O3—H3*B*···N1^{ii}	0.86 (2)	2.00 (2)	2.853 (2)	175 (3)

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

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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2595).

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supplementary materials

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N'-[4-(Diethylamino)benzylidene]pyrazine-2-carbohydrazide dihydrate

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Comment

Hydrogen bonding plays a key role in molecular recognition (Goswami & Ghosh, 1997) and crystal engineering (Goswami *et al.*, 1998). The hydrazonecarbonyl compounds have been receiving considerable attention for a long time for their pharmacological activity (Parashar *et al.*, 1988) and their photochromic properties (Hadjoudis *et al.*, 1987). This type of pyrazine derivatives has wide application in the treatment of tuberculosis and also exhibits fungicidal activity (Edwards *et al.*, 1975, Kushner *et al.*, 1952). A series of similar pyrazinyl carboxylic acid hydrazone complexes had been reported previously (Gardner *et al.*, 1956). The present study has been undertaken as part of our research programme to explore hydrogen-bonding patterns involving pyrazinyl-water interactions (Shi & Zhang, 2007). Here we report the structure of pyrazine-2-carboxylic acid (4-diethylamino-benzylidene)hydrazide (I) dihydrate.

In the crystal, the molecular structure of (I), is nearly planar conformation with a dihedral angle of 11.95 (3)° between the pyrazinyl ring and phenyl ring. The torsion angles of C4—C5—N3—N4 and N3—N4—C6—C7 are 3.43 (3)° and 4.46 (3)°, respectively.

The carbonyl O atom acts as a H-receptor, involved in an intermolecular O—H···O hydrogen bond with H3A atom of an adjacent water molecule.

The molecules are linked through intermolecular hydrogen bonds. In addition, an adjacent molecule is staggered anti-parallel with centroid-centroid separation of pyrazinyl rings to phenyl ring by 3.795 (2)Å and 1.083 (2) Å offset distances indicating the presence of weak face-to-face π–π stacking interactions (Fig. 2).

Experimental

For the synthesis of pyrazine-2-carboxylic acid (4-diethylamino-benzylidene)-hydrazide, (I), a mixture of pyrazine-2-carboxylic acid hydrazide (0.01 mol, 1.38 g) and 4-diethylamino-benzaldehyde (0.01 mol, 1.77 g) in methanol was refluxed for 2 h. The solid material obtained on cooling was filtered, washed with ethanol: ether =1:1, dried and crystallized from methanol (yield 62%). The compound (1.0 mmol, 0.268 g) was dissolved in 95% ethanol (30 ml) and kept at room temperature for one week, after which yellow block shaped single crystals formed and were collected and washed with ether for X-ray diffraction analysis.

Refinement

All H atoms were initially located in a difference Fourier map. The C—H atoms were then constrained to an ideal geometry, with C(CH_3)—H distances of 0.96 Å, *C*(phenyl)—H distances of 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The coordinates of the amino and water H atoms were refined using a restraints of 0.85 (3)Å for O—H and 0.93 (3)Å for N—H with U_{iso}(H) = 1.2U_{eq}(N) and U_{iso}(H) = 1.5U_{eq}(O).

Figures

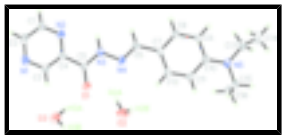

Fig. 1. The structure of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

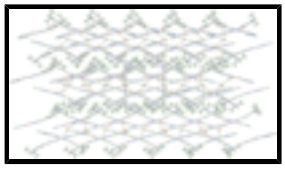

Fig. 2. Showing the hydrogen bonds and the packing of the molecules, viewed down the *c* axis.

N'-[4-(Diethylamino)benzylidene]pyrazine-2-carbohydrazide dihydrate

Crystal data

$C_{16}H_{19}N_5O_1{\cdot}2H_2O$	F_{000} = 712
M_r = 333.39	D_x = 1.266 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 13.422 (3) Å	Cell parameters from 1713 reflections
b = 10.761 (3) Å	θ = 2.5–25.1º
c = 12.820 (3) Å	μ = 0.09 mm^{-1}
β = 109.158 (4)º	T = 293 (2) K
V = 1749.1 (7) Å^3	Block, yellow
Z = 4	0.26 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3559 independent reflections
Radiation source: fine-focus sealed tube	1920 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.051
T = 293(2) K	θ_{max} = 26.4º
phi and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −16→14
T_{min} = 0.977, T_{max} = 0.984	k = −10→13
8345 measured reflections	l = −15→16

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.046	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.126	$w = 1/[\sigma^2(F_o^2) + (0.0589P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.95$	$(\Delta/\sigma)_{max} = 0.001$
3559 reflections	$\Delta\rho_{max} = 0.16$ e Å^{-3}
234 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}
4 restraints	Extinction correction: SHELXL
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.014 (5)

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}
O1	0.33520 (11)	0.91365 (14)	0.61157 (11)	0.0530 (4)
N1	0.42349 (14)	1.26849 (16)	0.54639 (16)	0.0512 (5)
N2	0.38454 (13)	1.07626 (16)	0.39227 (13)	0.0440 (4)
N3	0.32828 (13)	0.84807 (15)	0.44091 (14)	0.0386 (4)
H3C	0.3358 (14)	0.8688 (18)	0.3738 (16)	0.046*
N4	0.29365 (12)	0.73088 (15)	0.45891 (13)	0.0401 (4)
N5	0.07975 (14)	0.18864 (16)	0.35492 (14)	0.0530 (5)
C1	0.41266 (17)	1.1892 (2)	0.37146 (19)	0.0508 (6)
H1	0.4199	1.2048	0.3029	0.061*
C2	0.43160 (16)	1.2842 (2)	0.44711 (19)	0.0491 (6)
H2	0.4507	1.3618	0.4280	0.059*
C3	0.39436 (16)	1.15484 (19)	0.56756 (17)	0.0468 (6)
H3	0.3868	1.1397	0.6360	0.056*
C4	0.37526 (14)	1.05970 (18)	0.49196 (16)	0.0355 (5)
C5	0.34404 (14)	0.93349 (19)	0.52023 (16)	0.0372 (5)
C6	0.28043 (15)	0.65428 (18)	0.37889 (16)	0.0392 (5)
H6	0.2990	0.6788	0.3181	0.047*
C7	0.23762 (14)	0.53090 (17)	0.37987 (15)	0.0349 (5)
C8	0.21803 (15)	0.45612 (18)	0.28720 (16)	0.0394 (5)
H8	0.2387	0.4835	0.2286	0.047*
C9	0.16885 (15)	0.34244 (19)	0.27936 (16)	0.0410 (5)
H9	0.1584	0.2942	0.2165	0.049*
C10	0.13428 (15)	0.29828 (19)	0.36437 (16)	0.0400 (5)
C11	0.15718 (16)	0.3733 (2)	0.45958 (16)	0.0456 (6)
H11	0.1376	0.3461	0.5189	0.055*

C12	0.20758 (15)	0.48508 (19)	0.46679 (16)	0.0424 (5)
H12	0.2221	0.5316	0.5312	0.051*
C13	0.03911 (18)	0.1227 (2)	0.25010 (18)	0.0572 (6)
H13A	0.0272	0.1822	0.1904	0.069*
H13B	−0.0285	0.0862	0.2447	0.069*
C14	0.1104 (2)	0.0223 (3)	0.2350 (2)	0.0835 (9)
H14A	0.1764	0.0580	0.2364	0.125*
H14B	0.0780	−0.0182	0.1654	0.125*
H14C	0.1226	−0.0373	0.2936	0.125*
C15	0.0437 (2)	0.1435 (2)	0.4438 (2)	0.0634 (7)
H15A	0.0987	0.1583	0.5138	0.076*
H15B	0.0331	0.0544	0.4357	0.076*
C16	−0.0573 (2)	0.2032 (3)	0.4471 (2)	0.0864 (9)
H16A	−0.0456	0.2902	0.4628	0.130*
H16B	−0.0789	0.1646	0.5037	0.130*
H16C	−0.1115	0.1926	0.3769	0.130*
O2	0.35713 (16)	0.65814 (18)	0.71961 (14)	0.0752 (6)
H2A	0.343 (2)	0.711 (3)	0.663 (2)	0.113*
H2B	0.390 (2)	0.596 (2)	0.705 (2)	0.113*
O3	0.50207 (14)	0.97928 (15)	0.81494 (13)	0.0592 (5)
H3A	0.4550 (19)	0.956 (2)	0.7582 (18)	0.089*
H3B	0.5231 (19)	0.913 (2)	0.853 (2)	0.089*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0742 (11)	0.0471 (10)	0.0457 (8)	−0.0120 (8)	0.0305 (8)	−0.0047 (7)
N1	0.0577 (13)	0.0324 (11)	0.0569 (12)	−0.0005 (9)	0.0100 (10)	−0.0016 (9)
N2	0.0532 (12)	0.0356 (11)	0.0455 (10)	−0.0008 (8)	0.0191 (9)	0.0025 (8)
N3	0.0487 (11)	0.0296 (10)	0.0383 (9)	−0.0050 (8)	0.0155 (8)	−0.0002 (8)
N4	0.0457 (11)	0.0297 (10)	0.0461 (10)	−0.0032 (8)	0.0166 (8)	0.0005 (8)
N5	0.0675 (13)	0.0423 (12)	0.0509 (11)	−0.0219 (10)	0.0217 (10)	−0.0054 (9)
C1	0.0599 (15)	0.0397 (14)	0.0551 (14)	0.0008 (11)	0.0221 (12)	0.0099 (11)
C2	0.0449 (14)	0.0300 (13)	0.0672 (16)	−0.0003 (10)	0.0114 (12)	0.0079 (12)
C3	0.0567 (14)	0.0359 (13)	0.0476 (13)	−0.0013 (11)	0.0171 (11)	−0.0028 (11)
C4	0.0330 (11)	0.0309 (11)	0.0405 (11)	0.0024 (9)	0.0091 (9)	−0.0003 (9)
C5	0.0352 (12)	0.0370 (13)	0.0403 (12)	0.0017 (9)	0.0134 (10)	−0.0014 (10)
C6	0.0390 (12)	0.0371 (12)	0.0436 (12)	0.0001 (9)	0.0163 (10)	0.0013 (10)
C7	0.0338 (11)	0.0297 (12)	0.0408 (11)	−0.0020 (9)	0.0118 (9)	0.0008 (9)
C8	0.0436 (12)	0.0365 (13)	0.0421 (12)	−0.0023 (10)	0.0193 (10)	0.0014 (9)
C9	0.0484 (13)	0.0378 (13)	0.0376 (11)	−0.0058 (10)	0.0153 (10)	−0.0051 (10)
C10	0.0406 (12)	0.0339 (12)	0.0437 (12)	−0.0049 (10)	0.0116 (10)	0.0012 (10)
C11	0.0556 (14)	0.0452 (14)	0.0384 (11)	−0.0108 (11)	0.0188 (10)	0.0013 (10)
C12	0.0483 (13)	0.0387 (13)	0.0399 (11)	−0.0060 (10)	0.0140 (10)	−0.0059 (10)
C13	0.0576 (15)	0.0523 (15)	0.0570 (14)	−0.0228 (12)	0.0124 (12)	−0.0047 (12)
C14	0.085 (2)	0.072 (2)	0.0893 (19)	−0.0046 (16)	0.0220 (16)	−0.0252 (17)
C15	0.092 (2)	0.0391 (14)	0.0670 (15)	−0.0213 (13)	0.0373 (14)	0.0046 (12)
C16	0.092 (2)	0.081 (2)	0.102 (2)	−0.0225 (17)	0.0551 (19)	−0.0114 (18)

O2	0.1169 (16)	0.0646 (13)	0.0523 (10)	0.0316 (11)	0.0390 (11)	0.0090 (9)
O3	0.0790 (13)	0.0441 (11)	0.0549 (10)	−0.0007 (9)	0.0223 (9)	0.0058 (8)

Geometric parameters (Å, °)

O1—C5	1.234 (2)	C8—H8	0.9300
N1—C2	1.323 (3)	C9—C10	1.400 (3)
N1—C3	1.339 (3)	C9—H9	0.9300
N2—C1	1.325 (3)	C10—C11	1.411 (3)
N2—C4	1.336 (2)	C11—C12	1.368 (3)
N3—C5	1.335 (2)	C11—H11	0.9300
N3—N4	1.389 (2)	C12—H12	0.9300
N3—H3C	0.926 (19)	C13—C14	1.498 (3)
N4—C6	1.282 (2)	C13—H13A	0.9700
N5—C10	1.373 (2)	C13—H13B	0.9700
N5—C13	1.458 (3)	C14—H14A	0.9600
N5—C15	1.459 (3)	C14—H14B	0.9600
C1—C2	1.374 (3)	C14—H14C	0.9600
C1—H1	0.9300	C15—C16	1.514 (3)
C2—H2	0.9300	C15—H15A	0.9700
C3—C4	1.375 (3)	C15—H15B	0.9700
C3—H3	0.9300	C16—H16A	0.9600
C4—C5	1.500 (3)	C16—H16B	0.9600
C6—C7	1.448 (3)	C16—H16C	0.9600
C6—H6	0.9300	O2—H2A	0.89 (2)
C7—C8	1.387 (3)	O2—H2B	0.85 (2)
C7—C12	1.394 (3)	O3—H3A	0.83 (2)
C8—C9	1.378 (3)	O3—H3B	0.86 (2)
C2—N1—C3	115.66 (19)	N5—C10—C9	121.75 (18)
C1—N2—C4	115.91 (19)	N5—C10—C11	121.78 (18)
C5—N3—N4	118.46 (17)	C9—C10—C11	116.46 (18)
C5—N3—H3C	120.2 (13)	C12—C11—C10	121.61 (19)
N4—N3—H3C	121.2 (12)	C12—C11—H11	119.2
C6—N4—N3	114.63 (16)	C10—C11—H11	119.2
C10—N5—C13	121.80 (17)	C11—C12—C7	121.56 (19)
C10—N5—C15	121.41 (18)	C11—C12—H12	119.2
C13—N5—C15	115.97 (18)	C7—C12—H12	119.2
N2—C1—C2	122.6 (2)	N5—C13—C14	114.10 (19)
N2—C1—H1	118.7	N5—C13—H13A	108.7
C2—C1—H1	118.7	C14—C13—H13A	108.7
N1—C2—C1	122.0 (2)	N5—C13—H13B	108.7
N1—C2—H2	119.0	C14—C13—H13B	108.7
C1—C2—H2	119.0	H13A—C13—H13B	107.6
N1—C3—C4	122.5 (2)	C13—C14—H14A	109.5
N1—C3—H3	118.8	C13—C14—H14B	109.5
C4—C3—H3	118.8	H14A—C14—H14B	109.5
N2—C4—C3	121.38 (19)	C13—C14—H14C	109.5
N2—C4—C5	118.22 (18)	H14A—C14—H14C	109.5
C3—C4—C5	120.40 (18)	H14B—C14—H14C	109.5

O1—C5—N3	124.28 (19)	N5—C15—C16	114.2 (2)
O1—C5—C4	120.49 (18)	N5—C15—H15A	108.7
N3—C5—C4	115.23 (17)	C16—C15—H15A	108.7
N4—C6—C7	122.24 (19)	N5—C15—H15B	108.7
N4—C6—H6	118.9	C16—C15—H15B	108.7
C7—C6—H6	118.9	H15A—C15—H15B	107.6
C8—C7—C12	117.15 (18)	C15—C16—H16A	109.5
C8—C7—C6	119.26 (18)	C15—C16—H16B	109.5
C12—C7—C6	123.43 (18)	H16A—C16—H16B	109.5
C9—C8—C7	121.96 (18)	C15—C16—H16C	109.5
C9—C8—H8	119.0	H16A—C16—H16C	109.5
C7—C8—H8	119.0	H16B—C16—H16C	109.5
C8—C9—C10	121.18 (18)	H2A—O2—H2B	108 (3)
C8—C9—H9	119.4	H3A—O3—H3B	105 (3)
C10—C9—H9	119.4		
C5—N3—N4—C6	−179.99 (17)	C12—C7—C8—C9	1.4 (3)
C4—N2—C1—C2	0.2 (3)	C6—C7—C8—C9	−174.18 (18)
C3—N1—C2—C1	−0.8 (3)	C7—C8—C9—C10	1.4 (3)
N2—C1—C2—N1	0.4 (3)	C13—N5—C10—C9	−10.6 (3)
C2—N1—C3—C4	0.8 (3)	C15—N5—C10—C9	−179.8 (2)
C1—N2—C4—C3	−0.2 (3)	C13—N5—C10—C11	168.5 (2)
C1—N2—C4—C5	−179.75 (18)	C15—N5—C10—C11	−0.7 (3)
N1—C3—C4—N2	−0.3 (3)	C8—C9—C10—N5	176.12 (19)
N1—C3—C4—C5	179.26 (18)	C8—C9—C10—C11	−3.0 (3)
N4—N3—C5—O1	4.0 (3)	N5—C10—C11—C12	−177.2 (2)
N4—N3—C5—C4	−176.57 (15)	C9—C10—C11—C12	2.0 (3)
N2—C4—C5—O1	179.51 (17)	C10—C11—C12—C7	0.8 (3)
C3—C4—C5—O1	0.0 (3)	C8—C7—C12—C11	−2.5 (3)
N2—C4—C5—N3	0.0 (3)	C6—C7—C12—C11	172.94 (19)
C3—C4—C5—N3	−179.50 (17)	C10—N5—C13—C14	95.3 (3)
N3—N4—C6—C7	−175.54 (16)	C15—N5—C13—C14	−95.0 (3)
N4—C6—C7—C8	175.21 (18)	C10—N5—C15—C16	80.8 (3)
N4—C6—C7—C12	−0.1 (3)	C13—N5—C15—C16	−89.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3C···O2^{i}	0.926 (19)	2.11 (2)	2.987 (2)	158.1 (17)
O2—H2A···O1	0.89 (2)	2.27 (3)	3.049 (2)	146 (3)
O2—H2A···N4	0.89 (2)	2.49 (3)	3.262 (2)	145 (3)
O2—H2B···O3^{ii}	0.85 (2)	2.00 (2)	2.832 (2)	166 (3)
O3—H3A···O1	0.83 (2)	2.08 (2)	2.912 (2)	175 (3)
O3—H3B···N1^{ii}	0.86 (2)	2.00 (2)	2.853 (2)	175 (3)

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

Fig. 1

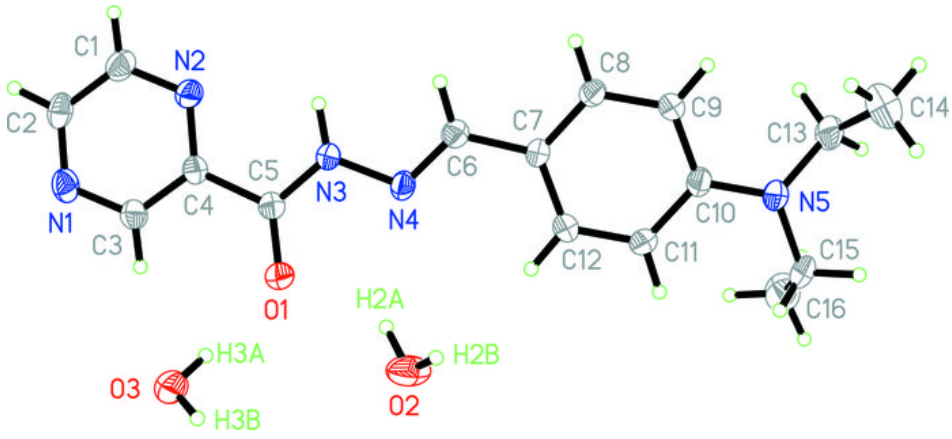
C1
N2
C2
N1
C3
C4
C5
N3
N4
C6
C7
C8
C9
C10
C11
C12
C13
C14
N5
C15
C16
O1
H2A
H2B
O2
H3A
O3
H3B

Fig. 2