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(*E*)-*N*′-(1,3-Benzodioxol-5-ylmethylene)-isonicotinohydrazide

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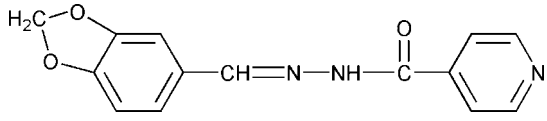
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.083; wR factor = 0.165; data-to-parameter ratio = 13.5.

The asymmetric unit of the title compound, $C_{14}H_{11}N_3O_3$, contains two similar molecules. Each molecule is almost planar; the dihedral angles between the pyridine ring and the benzene ring are 5.78 (15) and 8.24 (15)°. The crystal structure involves intermolecular N—H···N and C—H···N hydrogen bonds.

Related literature

For general background, see: Kahwa *et al.* (1986); Santos *et al.* (2001). For a related structure, see: Qian *et al.* (2006).



Experimental

Crystal data

$C_{14}H_{11}N_3O_3$
M_r = 269.26
Triclinic, $P\overline{1}$
a = 7.9190 (16) Å
b = 10.955 (2) Å
c = 15.479 (3) Å
α = 78.88 (3)°
β = 80.11 (3)°
γ = 69.08 (3)°
V = 1223.0 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 298 (2) K
0.27 × 0.23 × 0.20 mm

Data collection

Bruker SMART CCD area detector diffractometer
Absorption correction: none
13621 measured reflections
4961 independent reflections
3998 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.083
$wR(F^2)$ = 0.165
S = 1.17
4961 reflections
367 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N4^{i}	0.90 (2)	2.20 (3)	3.058 (4)	161 (3)
N5—H5A···N1^{ii}	0.90 (3)	2.24 (3)	3.135 (3)	170 (4)
C19—H19···N1^{ii}	0.93	2.49	3.396 (4)	164

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1998); 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: XU2324).

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supplementary materials

Acta Cryst. (2007). E**63**, o4109 [**doi:10.1107/S1600536807044881**]

(*E*)-*N*'-(1,3-Benzodioxol-5-ylmethylene)isonicotinohydrazide

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Comment

The chemistry of Schiff bases has attracted a great deal of interest in recent years. These compounds play an important role in the development of various proteins and enzymes (Kahwa *et al.*, 1986; Santos *et al.*, 2001). As part of our in the study of the coordination chemistry of Schiff bases, we synthesized the title compound and determined its crystal structure.

The molecular structure is shown in Fig. 1. Each molecule is almost coplanar, making the dihedral angle of 5.78 (15) and 8.24 (15)° between pyridine and benzene rings, respectively. Bond lengths and bond angles agree with the isonicotinohydrazide derivatives (Qian *et al.*, 2006).

In the crystal structure, there are intermolecular N—H···N and C—H···N hydrogen bonding (Table 1), which helps to stabilize the crystal structure (Fig. 2).

Experimental

Pyridine-4-carboxylic acid hydrazide (1 mmol, 0.137 g) was dissolved in anhydrous methanol (15 ml), then H_2SO_4 solution (98% 0.5 ml) was added to the above solution. The mixture was stirred for several minutes at 351 K, furylideneacetone (1 mmol 0.136 g) in methanol (8 ml) was added dropwise and the mixture was refluxed for 2 h. The solid product was isolated and recrystallized in dichloromethane, brown single crystals of the title compound were obtained after 1 d.

Refinement

Imino H atoms were located in a difference Fourier map and refined with a constraint of N—H = 0.90±0.01 Å, U_{iso}(H) = 0.08 Å^2. Other H atoms were placed in calculated positions, with C—H = 0.93 Å (aromatic) and 0.97 Å (methylene), and refined in riding mode with U_{iso}(H) = 1.2U_{eq}(C).

Figures

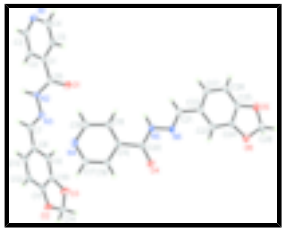

Fig. 1. The molecular structure of the title compound, displacement ellipsoids are drawn at the 50% probability level.

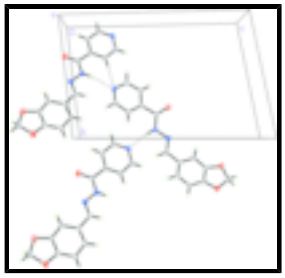

Fig. 2. Packing of (I), showing the intermolecular hydrogen bonds as dashed lines.

(*E*)-*N*'-(1,3-benzodioxol-5-ylmethylene)isonicotinohydrazide

Crystal data

$C_{14}H_{11}N_3O_3$	$Z = 4$
$M_r = 269.26$	$F_{000} = 560$
Triclinic, $P\overline{1}$	$D_x = 1.462$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.9190$ (16) Å	Cell parameters from 1205 reflections
$b = 10.955$ (2) Å	$\theta = 2.5$–23.5°
$c = 15.479$ (3) Å	$\mu = 0.11$ mm^{-1}
$\alpha = 78.88$ (3)°	$T = 298$ (2) K
$\beta = 80.11$ (3)°	Block, brown
$\gamma = 69.08$ (3)°	0.27 × 0.23 × 0.20 mm
$V = 1223.0$ (5) Å^3	

Data collection

Bruker SMART CCD area detector diffractometer	3998 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.051$
Monochromator: graphite	$\theta_{max} = 26.5^\circ$
$T = 298(2)$ K	$\theta_{min} = 2.6^\circ$
φ and ω scans	$h = -9 \rightarrow 9$
Absorption correction: none	$k = -13 \rightarrow 13$
13621 measured reflections	$l = -19 \rightarrow 18$
4961 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.083$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.165$	$w = 1/[\sigma^2(F_o^2) + (0.042P)^2 + 1.0203P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.17$	$(\Delta/\sigma)_{max} < 0.001$

4961 reflections	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
367 parameters	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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	0.9146 (4)	−0.2658 (2)	0.53135 (14)	0.0643 (8)
O2	0.3782 (3)	0.4409 (2)	0.74818 (15)	0.0521 (6)
O3	0.6028 (4)	0.2414 (2)	0.78416 (14)	0.0580 (7)
O4	0.8014 (3)	0.7100 (2)	0.02373 (13)	0.0481 (6)
O5	0.4833 (4)	0.0337 (2)	0.23747 (15)	0.0570 (7)
O6	0.4886 (3)	0.2214 (2)	0.28232 (14)	0.0517 (6)
N1	1.0747 (4)	−0.4254 (2)	0.23574 (16)	0.0423 (6)
N2	0.8450 (4)	−0.0721 (2)	0.43657 (15)	0.0383 (6)
N3	0.7771 (4)	0.0014 (2)	0.50607 (15)	0.0390 (6)
N4	1.0389 (4)	0.9103 (2)	−0.26796 (16)	0.0401 (6)
N5	0.8220 (3)	0.5591 (2)	−0.06345 (15)	0.0335 (6)
N6	0.7515 (3)	0.4833 (2)	0.00541 (15)	0.0339 (6)
C1	0.9666 (4)	−0.2782 (3)	0.37672 (18)	0.0329 (6)
C2	0.8959 (4)	−0.2270 (3)	0.29636 (19)	0.0376 (7)
H2	0.8112	−0.1425	0.2880	0.045*
C3	0.9532 (5)	−0.3036 (3)	0.2290 (2)	0.0431 (8)
H3	0.9042	−0.2683	0.1755	0.052*
C4	1.1388 (5)	−0.4734 (3)	0.3139 (2)	0.0499 (9)
H4	1.2223	−0.5586	0.3206	0.060*
C5	1.0899 (5)	−0.4056 (3)	0.3856 (2)	0.0431 (8)
H5	1.1387	−0.4445	0.4388	0.052*
C6	0.9083 (5)	−0.2058 (3)	0.45675 (19)	0.0401 (7)
C7	0.6917 (4)	0.1225 (3)	0.48411 (19)	0.0368 (7)
H7	0.6809	0.1557	0.4246	0.044*
C8	0.6098 (4)	0.2110 (3)	0.55047 (18)	0.0335 (6)
C9	0.6627 (4)	0.1724 (3)	0.63659 (19)	0.0358 (7)
H9	0.7533	0.0927	0.6519	0.043*

C10	0.5752 (4)	0.2570 (3)	0.69660 (18)	0.0355 (7)
C11	0.4418 (4)	0.3763 (3)	0.67524 (19)	0.0356 (7)
C12	0.3882 (4)	0.4171 (3)	0.5921 (2)	0.0452 (8)
H12	0.2982	0.4976	0.5778	0.054*
C13	0.4758 (5)	0.3312 (3)	0.5298 (2)	0.0442 (8)
H13	0.4432	0.3557	0.4725	0.053*
C14	0.4804 (5)	0.3570 (4)	0.8169 (2)	0.0547 (9)
H14A	0.5475	0.4025	0.8375	0.066*
H14B	0.3991	0.3337	0.8665	0.066*
C15	0.9117 (4)	0.7499 (3)	−0.12767 (17)	0.0295 (6)
C16	0.9048 (4)	0.8749 (3)	−0.1192 (2)	0.0423 (8)
H16	0.8573	0.9079	−0.0659	0.051*
C17	0.9683 (5)	0.9503 (3)	−0.1899 (2)	0.0459 (8)
H17	0.9614	1.0343	−0.1826	0.055*
C18	1.0451 (5)	0.7897 (3)	−0.2758 (2)	0.0474 (8)
H18	1.0924	0.7595	−0.3300	0.057*
C19	0.9858 (5)	0.7067 (3)	−0.2083 (2)	0.0420 (8)
H19	0.9956	0.6227	−0.2171	0.050*
C20	0.8403 (4)	0.6714 (3)	−0.04863 (18)	0.0322 (6)
C21	0.7445 (4)	0.3777 (3)	−0.01433 (19)	0.0362 (7)
H21	0.7852	0.3584	−0.0718	0.043*
C22	0.6747 (4)	0.2859 (3)	0.05016 (18)	0.0321 (6)
C23	0.6145 (4)	0.3105 (3)	0.13782 (19)	0.0353 (7)
H23	0.6173	0.3852	0.1568	0.042*
C24	0.5518 (4)	0.2200 (3)	0.19372 (18)	0.0343 (6)
C25	0.5485 (4)	0.1076 (3)	0.1676 (2)	0.0390 (7)
C26	0.6067 (5)	0.0804 (3)	0.0828 (2)	0.0475 (8)
H26	0.6050	0.0044	0.0652	0.057*
C27	0.6692 (5)	0.1734 (3)	0.0240 (2)	0.0443 (8)
H27	0.7082	0.1593	−0.0346	0.053*
C28	0.4366 (5)	0.1062 (3)	0.3101 (2)	0.0500 (9)
H28A	0.4996	0.0525	0.3601	0.060*
H28B	0.3067	0.1315	0.3283	0.060*
H5A	0.857 (5)	0.529 (4)	−0.1163 (14)	0.080*
H2A	0.865 (5)	−0.033 (4)	0.3811 (12)	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.116 (2)	0.0410 (13)	0.0273 (12)	−0.0198 (14)	−0.0016 (13)	−0.0022 (10)
O2	0.0592 (15)	0.0428 (13)	0.0477 (13)	−0.0028 (11)	−0.0015 (11)	−0.0227 (11)
O3	0.0806 (18)	0.0473 (14)	0.0341 (12)	−0.0005 (13)	−0.0090 (12)	−0.0162 (10)
O4	0.0675 (16)	0.0477 (13)	0.0318 (11)	−0.0272 (12)	0.0101 (11)	−0.0108 (10)
O5	0.0817 (18)	0.0492 (14)	0.0454 (14)	−0.0393 (14)	0.0014 (13)	0.0073 (11)
O6	0.0680 (16)	0.0471 (13)	0.0353 (12)	−0.0234 (12)	0.0152 (11)	−0.0056 (10)
N1	0.0583 (17)	0.0368 (14)	0.0342 (14)	−0.0194 (13)	0.0041 (12)	−0.0126 (11)
N2	0.0561 (16)	0.0324 (13)	0.0263 (12)	−0.0163 (12)	0.0053 (12)	−0.0094 (10)
N3	0.0533 (16)	0.0356 (14)	0.0284 (13)	−0.0173 (12)	0.0070 (11)	−0.0109 (11)

N4	0.0465 (15)	0.0399 (15)	0.0335 (14)	−0.0190 (12)	−0.0039 (12)	0.0038 (11)
N5	0.0407 (14)	0.0348 (13)	0.0263 (12)	−0.0192 (11)	0.0036 (11)	−0.0009 (10)
N6	0.0358 (13)	0.0324 (13)	0.0316 (13)	−0.0152 (11)	0.0005 (10)	0.0035 (10)
C1	0.0399 (16)	0.0302 (15)	0.0304 (15)	−0.0151 (12)	0.0003 (12)	−0.0056 (11)
C2	0.0463 (18)	0.0320 (15)	0.0316 (15)	−0.0100 (13)	−0.0029 (13)	−0.0051 (12)
C3	0.063 (2)	0.0418 (18)	0.0301 (16)	−0.0230 (16)	−0.0049 (14)	−0.0064 (13)
C4	0.063 (2)	0.0363 (17)	0.0462 (19)	−0.0102 (16)	−0.0023 (17)	−0.0117 (15)
C5	0.057 (2)	0.0357 (16)	0.0332 (16)	−0.0083 (15)	−0.0099 (14)	−0.0074 (13)
C6	0.058 (2)	0.0361 (16)	0.0279 (15)	−0.0182 (15)	0.0004 (14)	−0.0086 (12)
C7	0.0475 (18)	0.0387 (17)	0.0282 (15)	−0.0219 (14)	0.0045 (13)	−0.0073 (12)
C8	0.0426 (17)	0.0315 (15)	0.0299 (15)	−0.0184 (13)	0.0012 (12)	−0.0054 (12)
C9	0.0403 (16)	0.0266 (14)	0.0360 (16)	−0.0076 (12)	−0.0011 (13)	−0.0042 (12)
C10	0.0434 (17)	0.0357 (16)	0.0288 (14)	−0.0151 (13)	−0.0026 (13)	−0.0060 (12)
C11	0.0361 (16)	0.0336 (15)	0.0372 (16)	−0.0104 (13)	0.0019 (13)	−0.0132 (13)
C12	0.0479 (19)	0.0327 (16)	0.0478 (19)	−0.0019 (14)	−0.0096 (15)	−0.0073 (14)
C13	0.055 (2)	0.0407 (18)	0.0356 (17)	−0.0134 (15)	−0.0087 (15)	−0.0039 (14)
C14	0.059 (2)	0.056 (2)	0.044 (2)	−0.0083 (18)	−0.0002 (17)	−0.0221 (17)
C15	0.0278 (14)	0.0290 (14)	0.0286 (14)	−0.0072 (11)	−0.0035 (11)	−0.0010 (11)
C16	0.0530 (19)	0.0302 (16)	0.0388 (17)	−0.0126 (14)	0.0059 (14)	−0.0058 (13)
C17	0.054 (2)	0.0299 (16)	0.0491 (19)	−0.0154 (15)	0.0047 (16)	−0.0024 (14)
C18	0.063 (2)	0.056 (2)	0.0301 (16)	−0.0323 (18)	0.0055 (15)	−0.0100 (14)
C19	0.060 (2)	0.0407 (17)	0.0341 (16)	−0.0300 (16)	0.0053 (14)	−0.0105 (13)
C20	0.0288 (14)	0.0342 (15)	0.0298 (15)	−0.0072 (12)	−0.0016 (11)	−0.0036 (12)
C21	0.0402 (17)	0.0407 (17)	0.0276 (15)	−0.0161 (14)	−0.0034 (12)	−0.0003 (12)
C22	0.0334 (15)	0.0318 (15)	0.0300 (14)	−0.0114 (12)	−0.0054 (12)	0.0003 (11)
C23	0.0351 (16)	0.0281 (15)	0.0408 (17)	−0.0093 (12)	−0.0029 (13)	−0.0042 (12)
C24	0.0330 (15)	0.0348 (15)	0.0306 (15)	−0.0101 (12)	0.0004 (12)	−0.0001 (12)
C25	0.0420 (17)	0.0367 (16)	0.0385 (16)	−0.0188 (14)	−0.0053 (13)	0.0052 (13)
C26	0.069 (2)	0.0431 (19)	0.0409 (18)	−0.0310 (17)	−0.0065 (16)	−0.0061 (14)
C27	0.060 (2)	0.0452 (18)	0.0333 (16)	−0.0257 (16)	0.0005 (15)	−0.0081 (14)
C28	0.049 (2)	0.055 (2)	0.0440 (19)	−0.0255 (17)	0.0013 (15)	0.0072 (16)

Geometric parameters (Å, °)

O1—C6	1.213 (4)	C8—C13	1.385 (4)
O2—C11	1.374 (3)	C8—C9	1.407 (4)
O2—C14	1.421 (4)	C9—C10	1.361 (4)
O3—C10	1.378 (3)	C9—H9	0.9300
O3—C14	1.415 (4)	C10—C11	1.379 (4)
O4—C20	1.224 (3)	C11—C12	1.366 (4)
O5—C25	1.364 (3)	C12—C13	1.396 (4)
O5—C28	1.423 (4)	C12—H12	0.9300
O6—C24	1.378 (3)	C13—H13	0.9300
O6—C28	1.431 (4)	C14—H14A	0.9700
N1—C4	1.332 (4)	C14—H14B	0.9700
N1—C3	1.334 (4)	C15—C19	1.380 (4)
N2—C6	1.358 (4)	C15—C16	1.382 (4)
N2—N3	1.386 (3)	C15—C20	1.503 (4)
N2—H2A	0.90 (2)	C16—C17	1.376 (4)

N3—C7	1.264 (4)	C16—H16	0.9300
N4—C17	1.327 (4)	C17—H17	0.9300
N4—C18	1.333 (4)	C18—C19	1.382 (4)
N5—C20	1.354 (4)	C18—H18	0.9300
N5—N6	1.387 (3)	C19—H19	0.9300
N5—H5A	0.90 (3)	C21—C22	1.460 (4)
N6—C21	1.274 (4)	C21—H21	0.9300
C1—C5	1.386 (4)	C22—C27	1.386 (4)
C1—C2	1.386 (4)	C22—C23	1.403 (4)
C1—C6	1.516 (4)	C23—C24	1.361 (4)
C2—C3	1.379 (4)	C23—H23	0.9300
C2—H2	0.9300	C24—C25	1.378 (4)
C3—H3	0.9300	C25—C26	1.367 (4)
C4—C5	1.377 (4)	C26—C27	1.400 (4)
C4—H4	0.9300	C26—H26	0.9300
C5—H5	0.9300	C27—H27	0.9300
C7—C8	1.457 (4)	C28—H28A	0.9700
C7—H7	0.9300	C28—H28B	0.9700
C11—O2—C14	105.5 (2)	C12—C13—H13	118.8
C10—O3—C14	105.6 (2)	O3—C14—O2	109.2 (3)
C25—O5—C28	106.3 (2)	O3—C14—H14A	109.8
C24—O6—C28	105.7 (2)	O2—C14—H14A	109.8
C4—N1—C3	116.1 (3)	O3—C14—H14B	109.8
C6—N2—N3	117.8 (2)	O2—C14—H14B	109.8
C6—N2—H2A	121 (3)	H14A—C14—H14B	108.3
N3—N2—H2A	121 (3)	C19—C15—C16	117.0 (3)
C7—N3—N2	115.2 (2)	C19—C15—C20	125.2 (3)
C17—N4—C18	116.1 (3)	C16—C15—C20	117.8 (3)
C20—N5—N6	119.5 (2)	C17—C16—C15	119.7 (3)
C20—N5—H5A	123 (3)	C17—C16—H16	120.1
N6—N5—H5A	118 (3)	C15—C16—H16	120.1
C21—N6—N5	114.9 (2)	N4—C17—C16	123.9 (3)
C5—C1—C2	117.8 (3)	N4—C17—H17	118.0
C5—C1—C6	118.4 (3)	C16—C17—H17	118.0
C2—C1—C6	123.7 (3)	N4—C18—C19	124.0 (3)
C3—C2—C1	118.9 (3)	N4—C18—H18	118.0
C3—C2—H2	120.5	C19—C18—H18	118.0
C1—C2—H2	120.5	C15—C19—C18	119.2 (3)
N1—C3—C2	124.0 (3)	C15—C19—H19	120.4
N1—C3—H3	118.0	C18—C19—H19	120.4
C2—C3—H3	118.0	O4—C20—N5	123.7 (3)
N1—C4—C5	124.5 (3)	O4—C20—C15	120.4 (3)
N1—C4—H4	117.7	N5—C20—C15	116.0 (2)
C5—C4—H4	117.7	N6—C21—C22	122.3 (3)
C4—C5—C1	118.6 (3)	N6—C21—H21	118.9
C4—C5—H5	120.7	C22—C21—H21	118.9
C1—C5—H5	120.7	C27—C22—C23	120.1 (3)
O1—C6—N2	124.8 (3)	C27—C22—C21	119.3 (3)
O1—C6—C1	121.0 (3)	C23—C22—C21	120.6 (3)

N2—C6—C1	114.2 (2)	C24—C23—C22	116.9 (3)
N3—C7—C8	121.1 (3)	C24—C23—H23	121.6
N3—C7—H7	119.4	C22—C23—H23	121.6
C8—C7—H7	119.4	C23—C24—C25	122.8 (3)
C13—C8—C9	119.9 (3)	C23—C24—O6	127.6 (3)
C13—C8—C7	120.2 (3)	C25—C24—O6	109.7 (2)
C9—C8—C7	119.9 (3)	O5—C25—C26	128.1 (3)
C10—C9—C8	117.0 (3)	O5—C25—C24	110.1 (3)
C10—C9—H9	121.5	C26—C25—C24	121.8 (3)
C8—C9—H9	121.5	C25—C26—C27	116.2 (3)
C9—C10—O3	127.8 (3)	C25—C26—H26	121.9
C9—C10—C11	122.5 (3)	C27—C26—H26	121.9
O3—C10—C11	109.7 (3)	C22—C27—C26	122.2 (3)
C12—C11—O2	128.2 (3)	C22—C27—H27	118.9
C12—C11—C10	121.9 (3)	C26—C27—H27	118.9
O2—C11—C10	109.9 (3)	O5—C28—O6	108.0 (2)
C11—C12—C13	116.3 (3)	O5—C28—H28A	110.1
C11—C12—H12	121.8	O6—C28—H28A	110.1
C13—C12—H12	121.8	O5—C28—H28B	110.1
C8—C13—C12	122.3 (3)	O6—C28—H28B	110.1
C8—C13—H13	118.8	H28A—C28—H28B	108.4

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···N4^{i}	0.90 (2)	2.20 (3)	3.058 (4)	161 (3)
N5—H5A···N1^{ii}	0.90 (3)	2.24 (3)	3.135 (3)	170 (4)
C19—H19···N1^{ii}	0.93	2.49	3.396 (4)	164

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

Fig. 1

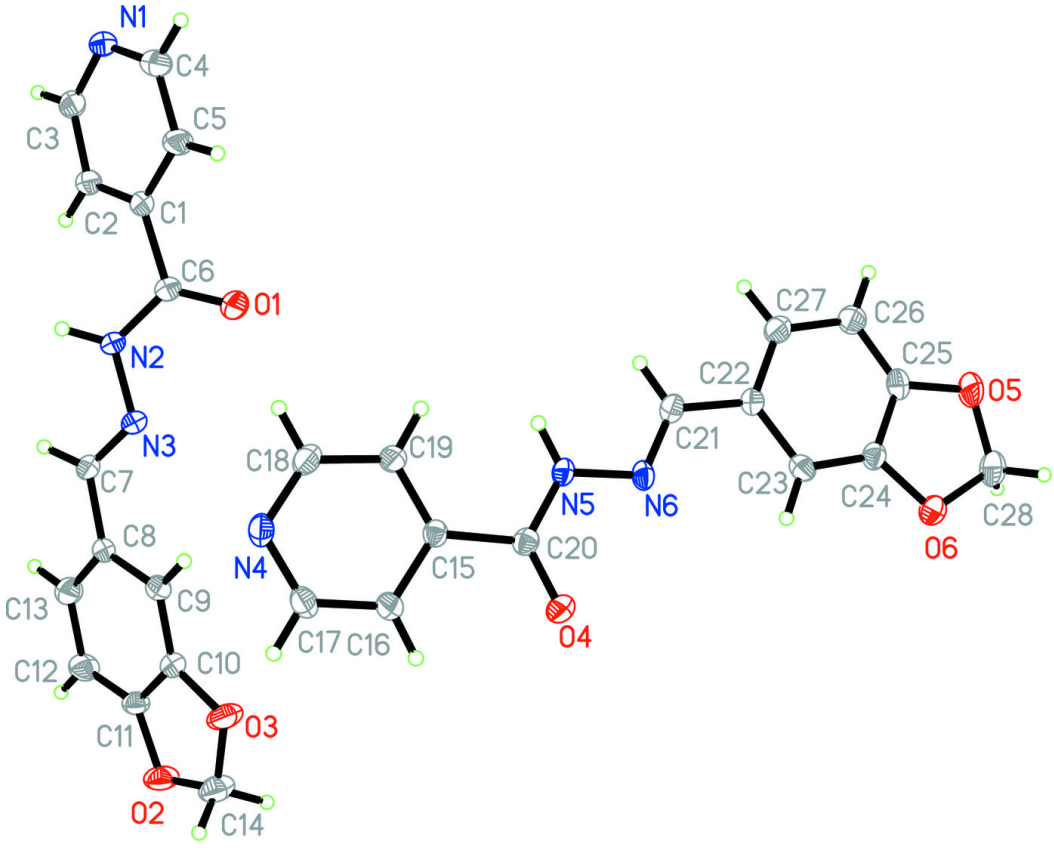
N1
C4
C5
C3
C2
C1
C6
O1
N2
N3
C7
C8
C13
C9
C12
C10
C11
O3
O2
C14
C18
C19
N4
C15
C17
C16
C20
O4
N5
N6
C21
C22
C27
C26
C25
O5
C23
C24
C28
O6

Fig. 2