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4-Hydroxy-3-methoxybenzaldehyde (pyrazin-2-yl)hydrazone

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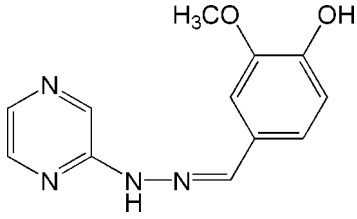
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.118; data-to-parameter ratio = 14.4.

The asymmetric unit of the title compound, $C_{12}H_{12}N_4O_2$, contains two independent molecules. The dihedral angles between the planar rings of the two molecules are 7.72 (3) and 40.24 (2)°. In the crystal structure, intramolecular O—H···O and intermolecular O—H···O, O—H···N and N—H···N hydrogen bonds form a network structure.

Related literature

For general backgroud, see: Desai *et al.* (2001); Isse *et al.* (1997); Bastos *et al.* (2000); Ma *et al.* (2001); Zhao *et al.* (2001); Allen *et al.* (1987); Kim *et al.* (2005).



Experimental

Crystal data

$C_{12}H_{12}N_4O_2$
M_r = 244.26
Monoclinic, $C2/c$
a = 43.862 (6) Å
b = 7.9026 (11) Å
c = 13.4958 (19) Å
β = 92.783 (3)°
V = 4672.4 (11) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
0.24 × 0.20 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.977, T_{max} = 0.988
12989 measured reflections
4741 independent reflections
2870 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.118
S = 0.99
4741 reflections
329 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.82	2.23	2.677 (2)	115
O1—H1···O4^{ii}	0.82	2.24	2.993 (2)	152
O3—H3···N1^{iii}	0.82	1.93	2.736 (2)	165
N3—H3B···N2^{iv}	0.86	2.25	3.060 (2)	157
N7—H7A···N6^{v}	0.86	2.23	3.044 (2)	159

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

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: HK2234).

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supplementary materials

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4-Hydroxy-3-methoxybenzaldehyde (pyrazin-2-yl)hydrazone

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Comment

In recent years, Schiff bases are applied in medicine (Desai *et al.*, 2001), catalytic chemistry (Isse *et al.*, 1997), analytical chemistry (Bastos *et al.*, 2000), corrosion (Ma *et al.*, 2001) and photochromism (Zhao *et al.*, 2001). The crystal structure determination of the title compound, (I), was carried out in order to elucidate its molecular conformation.

In the molecule of the title compound, (I), (Fig. 1), the asymmetric unit contains two independent molecules and the bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987).

Rings A (N1/N2/C1—C4), B (C6—C11), C (N5/N6/C13—C16) and D (C18—C23) are, of course, planar and the dihedral angles between them are A/B = 7.72 (3)° and C/D = 40.24 (2)°.

As can be seen from the packing diagram (Fig. 2), the intramolecular O—H···O and intermolecular O—H···O, O—H···N and N—H···N hydrogen bonds (Table 2) cause to the formation of a network structure, in which they may be effective in the stabilization of the crystal structure. Dipol-dipol and van der Waals interactions are also effective in the molecular packing.

Experimental

The title compound, (I), was synthesized by the reaction of 2-hydrazinopyrazine (100.0 mg, 0.91 mmol) (Kim *et al.*, 2005) with 3-methoxy-4-hydroxybenzaldehyde (138.2 mg, 0.91 mmol) in methanol (25 ml). The mixture was stirred and refluxed for 2 h, producing a light-yellow solution. Single crystals of (I) were obtained by slow evaporation of the methanol solution in 15 d (yield; 82.2 mg, 37%, m.p. 469-471 K).

Refinement

H atoms were positioned geometrically, with O—H = 0.82 Å (for OH), N—H = 0.86 Å (for NH) and C—H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C,O,N)$, where x = 1.5 for OH and methyl H and x = 1.2 for all other H atoms.

Figures

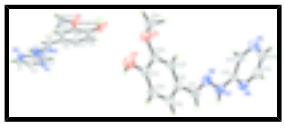

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

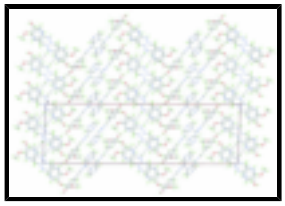

Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

4-Hydroxy-3-methoxybenzaldehyde (pyrazin-2-yl)hydrazone

Crystal data

$C_{12}H_{12}N_4O_2$	F_{000} = 2048
M_r = 244.26	D_x = 1.389 Mg m^{-3}
Monoclinic, *C*2/*c*	Melting point: 196 K
Hall symbol: -C 2yc	Mo *K*α radiation λ = 0.71073 Å
a = 43.862 (6) Å	Cell parameters from 2951 reflections
b = 7.9026 (11) Å	θ = 2.8–23.3º
c = 13.4958 (19) Å	μ = 0.10 mm^{-1}
β = 92.783 (3)º	*T* = 294 (2) K
V = 4672.4 (11) Å^3	Prism, orange
Z = 16	0.24 × 0.20 × 0.12 mm

Data collection

Bruker CCD area-detector diffractometer	4741 independent reflections
Radiation source: fine-focus sealed tube	2870 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.038
T = 294(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 0.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −45→54
T_{min} = 0.977, T_{max} = 0.988	*k* = −9→9
12989 measured reflections	*l* = −12→16

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 1.0712P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.042	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.118	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
S = 0.99	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
4741 reflections	Extinction correction: none
329 parameters	

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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	0.09624 (3)	−0.0018 (2)	0.35987 (9)	0.0491 (4)
H1	0.1125	−0.0479	0.3489	0.074*
O2	0.12414 (3)	−0.05024 (18)	0.19008 (9)	0.0412 (4)
O3	0.88212 (3)	0.37662 (18)	0.52439 (11)	0.0522 (4)
H3	0.8939	0.4482	0.5043	0.078*
O4	0.84359 (3)	0.17444 (17)	0.60218 (10)	0.0454 (4)
N1	−0.07790 (4)	0.4233 (2)	−0.07185 (13)	0.0457 (5)
N2	−0.03900 (4)	0.3369 (2)	−0.21998 (12)	0.0424 (4)
N3	−0.00114 (4)	0.2727 (3)	−0.10462 (12)	0.0508 (5)
H3B	0.0109	0.2598	−0.1525	0.061*
N4	0.00922 (4)	0.2394 (2)	−0.00933 (12)	0.0429 (4)
N5	0.77115 (4)	0.2428 (2)	1.12707 (13)	0.0466 (5)
N6	0.74870 (4)	0.5668 (2)	1.08398 (13)	0.0432 (4)
N7	0.78167 (4)	0.5929 (2)	0.95882 (13)	0.0448 (5)
H7A	0.7774	0.6990	0.9548	0.054*
N8	0.80002 (4)	0.5187 (2)	0.89084 (12)	0.0381 (4)
C1	−0.06743 (5)	0.3908 (3)	−0.24004 (16)	0.0482 (6)
H1A	−0.0744	0.3999	−0.3061	0.058*
C2	−0.08688 (5)	0.4334 (3)	−0.16788 (17)	0.0487 (6)
H2	−0.1065	0.4697	−0.1857	0.058*
C3	−0.04997 (4)	0.3702 (3)	−0.04990 (15)	0.0415 (5)
H3A	−0.0432	0.3618	0.0163	0.050*
C4	−0.03019 (4)	0.3260 (3)	−0.12424 (14)	0.0366 (5)
C5	0.03653 (5)	0.1859 (3)	0.00035 (14)	0.0407 (5)
H5	0.0476	0.1749	−0.0563	0.049*
C6	0.05136 (4)	0.1408 (3)	0.09534 (14)	0.0369 (5)
C7	0.03815 (5)	0.1649 (3)	0.18529 (15)	0.0467 (6)
H7	0.0189	0.2137	0.1868	0.056*

C8	0.05330 (5)	0.1172 (3)	0.27277 (15)	0.0461 (6)
H8	0.0442	0.1343	0.3328	0.055*
C9	0.08172 (5)	0.0447 (3)	0.27178 (14)	0.0367 (5)
C10	0.09553 (4)	0.0212 (2)	0.18214 (13)	0.0326 (4)
C11	0.08029 (4)	0.0694 (2)	0.09510 (14)	0.0362 (5)
H11	0.0895	0.0540	0.0352	0.043*
C12	0.13893 (5)	−0.0775 (3)	0.10010 (16)	0.0587 (7)
H12A	0.1268	−0.1518	0.0581	0.088*
H12B	0.1586	−0.1279	0.1144	0.088*
H12C	0.1415	0.0287	0.0670	0.088*
C13	0.73840 (5)	0.4715 (3)	1.15752 (16)	0.0477 (6)
H13	0.7233	0.5156	1.1959	0.057*
C14	0.74906 (5)	0.3134 (3)	1.17852 (17)	0.0481 (6)
H14	0.7408	0.2527	1.2299	0.058*
C15	0.78173 (5)	0.3346 (3)	1.05504 (15)	0.0402 (5)
H15	0.7972	0.2904	1.0182	0.048*
C16	0.77044 (4)	0.4973 (2)	1.03167 (14)	0.0345 (5)
C17	0.81365 (4)	0.6185 (3)	0.83397 (15)	0.0381 (5)
H17	0.8122	0.7344	0.8445	0.046*
C18	0.83143 (4)	0.5577 (2)	0.75289 (14)	0.0326 (5)
C19	0.85151 (4)	0.6639 (2)	0.70776 (15)	0.0371 (5)
H19	0.8536	0.7752	0.7294	0.045*
C20	0.86862 (4)	0.6076 (2)	0.63082 (15)	0.0374 (5)
H20	0.8821	0.6811	0.6018	0.045*
C21	0.86583 (4)	0.4434 (2)	0.59665 (14)	0.0348 (5)
C22	0.84495 (4)	0.3358 (2)	0.64100 (14)	0.0336 (5)
C23	0.82815 (4)	0.3918 (2)	0.71763 (14)	0.0332 (5)
H23	0.8145	0.3190	0.7464	0.040*
C24	0.81790 (5)	0.0741 (3)	0.62537 (17)	0.0499 (6)
H24A	0.8191	0.0467	0.6947	0.075*
H24B	0.8178	−0.0283	0.5871	0.075*
H24C	0.7995	0.1363	0.6099	0.075*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0538 (10)	0.0692 (11)	0.0248 (7)	0.0128 (8)	0.0052 (7)	0.0060 (7)
O2	0.0388 (8)	0.0572 (9)	0.0279 (7)	0.0093 (7)	0.0034 (6)	0.0001 (7)
O3	0.0597 (10)	0.0494 (9)	0.0501 (10)	−0.0084 (8)	0.0303 (8)	−0.0047 (8)
O4	0.0531 (9)	0.0357 (8)	0.0491 (9)	−0.0088 (7)	0.0210 (7)	−0.0077 (7)
N1	0.0412 (10)	0.0545 (12)	0.0422 (11)	0.0110 (9)	0.0109 (8)	0.0045 (9)
N2	0.0323 (9)	0.0624 (12)	0.0327 (10)	0.0062 (8)	0.0026 (7)	−0.0010 (9)
N3	0.0342 (10)	0.0897 (15)	0.0290 (10)	0.0161 (10)	0.0063 (8)	0.0048 (10)
N4	0.0385 (10)	0.0618 (12)	0.0284 (9)	0.0046 (9)	0.0011 (8)	0.0045 (9)
N5	0.0455 (11)	0.0450 (11)	0.0494 (11)	0.0031 (9)	0.0021 (9)	0.0082 (9)
N6	0.0496 (11)	0.0385 (10)	0.0428 (10)	0.0045 (8)	0.0156 (9)	−0.0022 (8)
N7	0.0555 (11)	0.0348 (10)	0.0459 (11)	0.0092 (8)	0.0213 (9)	0.0013 (8)
N8	0.0395 (10)	0.0408 (10)	0.0347 (9)	0.0067 (8)	0.0108 (8)	−0.0042 (8)

C1	0.0371 (12)	0.0716 (16)	0.0355 (12)	0.0075 (11)	−0.0017 (10)	0.0006 (11)
C2	0.0339 (12)	0.0659 (16)	0.0464 (14)	0.0119 (11)	0.0020 (10)	0.0043 (12)
C3	0.0387 (12)	0.0557 (14)	0.0305 (11)	0.0088 (10)	0.0063 (9)	0.0039 (10)
C4	0.0307 (11)	0.0482 (13)	0.0311 (11)	0.0015 (9)	0.0025 (8)	0.0016 (10)
C5	0.0348 (12)	0.0593 (14)	0.0284 (11)	0.0038 (10)	0.0051 (9)	0.0005 (10)
C6	0.0342 (11)	0.0457 (12)	0.0310 (11)	−0.0003 (9)	0.0029 (9)	0.0031 (9)
C7	0.0377 (12)	0.0658 (15)	0.0373 (12)	0.0090 (11)	0.0095 (10)	0.0021 (11)
C8	0.0477 (13)	0.0641 (15)	0.0273 (11)	0.0084 (11)	0.0121 (10)	−0.0004 (10)
C9	0.0432 (12)	0.0429 (12)	0.0241 (10)	−0.0017 (10)	0.0028 (9)	0.0045 (9)
C10	0.0346 (11)	0.0367 (11)	0.0268 (10)	−0.0015 (9)	0.0046 (8)	−0.0009 (9)
C11	0.0377 (11)	0.0468 (13)	0.0247 (10)	0.0006 (9)	0.0073 (9)	−0.0005 (9)
C12	0.0466 (14)	0.093 (2)	0.0370 (13)	0.0214 (13)	0.0094 (11)	0.0002 (13)
C13	0.0515 (13)	0.0475 (14)	0.0455 (13)	0.0008 (11)	0.0180 (11)	−0.0005 (11)
C14	0.0483 (13)	0.0517 (14)	0.0449 (13)	−0.0022 (11)	0.0091 (11)	0.0079 (11)
C15	0.0405 (12)	0.0417 (13)	0.0385 (12)	0.0068 (10)	0.0038 (9)	−0.0016 (10)
C16	0.0372 (11)	0.0345 (11)	0.0321 (11)	−0.0003 (9)	0.0034 (9)	−0.0055 (9)
C17	0.0391 (11)	0.0328 (11)	0.0427 (12)	0.0067 (9)	0.0042 (10)	−0.0003 (10)
C18	0.0311 (10)	0.0338 (11)	0.0331 (11)	0.0049 (8)	0.0036 (8)	0.0010 (9)
C19	0.0393 (12)	0.0314 (11)	0.0408 (12)	0.0005 (9)	0.0026 (9)	0.0015 (9)
C20	0.0367 (11)	0.0366 (12)	0.0393 (12)	−0.0060 (9)	0.0064 (9)	0.0084 (9)
C21	0.0345 (11)	0.0398 (12)	0.0307 (10)	0.0001 (9)	0.0071 (9)	0.0009 (9)
C22	0.0334 (11)	0.0326 (11)	0.0352 (11)	−0.0011 (9)	0.0053 (9)	−0.0004 (9)
C23	0.0306 (10)	0.0350 (11)	0.0346 (11)	−0.0010 (9)	0.0074 (9)	0.0050 (9)
C24	0.0515 (14)	0.0405 (13)	0.0585 (15)	−0.0121 (11)	0.0113 (11)	−0.0041 (11)

Geometric parameters (Å, °)

O1—C9	1.371 (2)	C6—C7	1.384 (3)
O1—H1	0.8200	C6—C11	1.389 (3)
O2—C10	1.375 (2)	C7—C8	1.379 (3)
O2—C12	1.421 (2)	C7—H7	0.9300
O3—C21	1.344 (2)	C8—C9	1.373 (3)
O3—H3	0.8200	C8—H8	0.9300
O4—C22	1.379 (2)	C9—C10	1.391 (3)
O4—C24	1.425 (2)	C10—C11	1.377 (3)
N1—C3	1.315 (2)	C11—H11	0.9300
N1—C2	1.338 (3)	C12—H12A	0.9600
N2—C1	1.333 (2)	C12—H12B	0.9600
N2—C4	1.333 (2)	C12—H12C	0.9600
N3—C4	1.355 (2)	C13—C14	1.358 (3)
N3—N4	1.368 (2)	C13—H13	0.9300
N3—H3B	0.8600	C14—H14	0.9300
N4—C5	1.271 (2)	C15—C16	1.408 (3)
N5—C15	1.315 (3)	C15—H15	0.9300
N5—C14	1.341 (3)	C17—C18	1.456 (3)
N6—C16	1.332 (2)	C17—H17	0.9300
N6—C13	1.342 (3)	C18—C19	1.379 (3)
N7—C16	1.351 (2)	C18—C23	1.400 (3)
N7—N8	1.380 (2)	C19—C20	1.384 (3)

N7—H7A	0.8600	C19—H19	0.9300
N8—C17	1.270 (2)	C20—C21	1.381 (3)
C1—C2	1.367 (3)	C20—H20	0.9300
C1—H1A	0.9300	C21—C22	1.405 (3)
C2—H2	0.9300	C22—C23	1.372 (3)
C3—C4	1.402 (3)	C23—H23	0.9300
C3—H3A	0.9300	C24—H24A	0.9600
C5—C6	1.453 (3)	C24—H24B	0.9600
C5—H5	0.9300	C24—H24C	0.9600
C9—O1—H1	109.5	C10—C11—H11	119.5
C10—O2—C12	116.66 (15)	C6—C11—H11	119.5
C21—O3—H3	109.5	O2—C12—H12A	109.5
C22—O4—C24	116.84 (15)	O2—C12—H12B	109.5
C3—N1—C2	117.65 (17)	H12A—C12—H12B	109.5
C1—N2—C4	116.21 (17)	O2—C12—H12C	109.5
C4—N3—N4	120.62 (16)	H12A—C12—H12C	109.5
C4—N3—H3B	119.7	H12B—C12—H12C	109.5
N4—N3—H3B	119.7	N6—C13—C14	123.07 (19)
C5—N4—N3	115.40 (16)	N6—C13—H13	118.5
C15—N5—C14	116.28 (19)	C14—C13—H13	118.5
C16—N6—C13	115.85 (18)	N5—C14—C13	121.6 (2)
C16—N7—N8	119.42 (16)	N5—C14—H14	119.2
C16—N7—H7A	120.3	C13—C14—H14	119.2
N8—N7—H7A	120.3	N5—C15—C16	122.44 (19)
C17—N8—N7	116.43 (17)	N5—C15—H15	118.8
N2—C1—C2	122.9 (2)	C16—C15—H15	118.8
N2—C1—H1A	118.5	N6—C16—N7	116.79 (18)
C2—C1—H1A	118.5	N6—C16—C15	120.69 (18)
N1—C2—C1	120.71 (19)	N7—C16—C15	122.47 (17)
N1—C2—H2	119.6	N8—C17—C18	122.33 (18)
C1—C2—H2	119.6	N8—C17—H17	118.8
N1—C3—C4	121.36 (19)	C18—C17—H17	118.8
N1—C3—H3A	119.3	C19—C18—C23	118.48 (17)
C4—C3—H3A	119.3	C19—C18—C17	120.55 (18)
N2—C4—N3	115.78 (17)	C23—C18—C17	120.96 (17)
N2—C4—C3	121.12 (18)	C18—C19—C20	121.13 (18)
N3—C4—C3	123.09 (18)	C18—C19—H19	119.4
N4—C5—C6	123.47 (18)	C20—C19—H19	119.4
N4—C5—H5	118.3	C21—C20—C19	120.69 (18)
C6—C5—H5	118.3	C21—C20—H20	119.7
C7—C6—C11	118.67 (18)	C19—C20—H20	119.7
C7—C6—C5	123.47 (18)	O3—C21—C20	124.72 (17)
C11—C6—C5	117.86 (17)	O3—C21—C22	116.88 (17)
C8—C7—C6	120.58 (19)	C20—C21—C22	118.39 (17)
C8—C7—H7	119.7	C23—C22—O4	124.72 (17)
C6—C7—H7	119.7	C23—C22—C21	120.75 (18)
C9—C8—C7	120.39 (18)	O4—C22—C21	114.52 (16)
C9—C8—H8	119.8	C22—C23—C18	120.54 (17)
C7—C8—H8	119.8	C22—C23—H23	119.7

O1—C9—C8	119.17 (17)	C18—C23—H23	119.7
O1—C9—C10	120.96 (18)	O4—C24—H24A	109.5
C8—C9—C10	119.87 (18)	O4—C24—H24B	109.5
O2—C10—C11	125.68 (16)	H24A—C24—H24B	109.5
O2—C10—C9	114.90 (16)	O4—C24—H24C	109.5
C11—C10—C9	119.42 (18)	H24A—C24—H24C	109.5
C10—C11—C6	121.07 (17)	H24B—C24—H24C	109.5
C4—N3—N4—C5	178.2 (2)	C5—C6—C11—C10	−178.98 (18)
C16—N7—N8—C17	−169.45 (19)	C16—N6—C13—C14	−0.2 (3)
C4—N2—C1—C2	0.0 (3)	C15—N5—C14—C13	−0.4 (3)
C3—N1—C2—C1	−0.5 (3)	N6—C13—C14—N5	0.9 (4)
N2—C1—C2—N1	0.4 (4)	C14—N5—C15—C16	−0.7 (3)
C2—N1—C3—C4	0.1 (3)	C13—N6—C16—N7	−178.42 (19)
C1—N2—C4—N3	−179.34 (19)	C13—N6—C16—C15	−0.9 (3)
C1—N2—C4—C3	−0.4 (3)	N8—N7—C16—N6	−168.35 (17)
N4—N3—C4—N2	−172.90 (19)	N8—N7—C16—C15	14.2 (3)
N4—N3—C4—C3	8.1 (3)	N5—C15—C16—N6	1.4 (3)
N1—C3—C4—N2	0.3 (3)	N5—C15—C16—N7	178.8 (2)
N1—C3—C4—N3	179.2 (2)	N7—N8—C17—C18	−174.17 (17)
N3—N4—C5—C6	−178.85 (19)	N8—C17—C18—C19	−164.76 (19)
N4—C5—C6—C7	−5.5 (3)	N8—C17—C18—C23	16.5 (3)
N4—C5—C6—C11	174.3 (2)	C23—C18—C19—C20	−1.4 (3)
C11—C6—C7—C8	−0.7 (3)	C17—C18—C19—C20	179.80 (18)
C5—C6—C7—C8	179.1 (2)	C18—C19—C20—C21	0.5 (3)
C6—C7—C8—C9	−0.2 (3)	C19—C20—C21—O3	−178.01 (19)
C7—C8—C9—O1	−179.9 (2)	C19—C20—C21—C22	0.8 (3)
C7—C8—C9—C10	0.9 (3)	C24—O4—C22—C23	16.6 (3)
C12—O2—C10—C11	−0.7 (3)	C24—O4—C22—C21	−164.40 (18)
C12—O2—C10—C9	179.54 (19)	O3—C21—C22—C23	177.75 (18)
O1—C9—C10—O2	−0.1 (3)	C20—C21—C22—C23	−1.2 (3)
C8—C9—C10—O2	179.09 (18)	O3—C21—C22—O4	−1.3 (3)
O1—C9—C10—C11	−179.95 (18)	C20—C21—C22—O4	179.83 (17)
C8—C9—C10—C11	−0.7 (3)	O4—C22—C23—C18	179.11 (18)
O2—C10—C11—C6	−179.95 (18)	C21—C22—C23—C18	0.2 (3)
C9—C10—C11—C6	−0.1 (3)	C19—C18—C23—C22	1.1 (3)
C7—C6—C11—C10	0.9 (3)	C17—C18—C23—C22	179.84 (18)

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

D-H···A	D-H	H···A	D···A	D-H···A
O1-H1···O2	0.82	2.23	2.677 (2)	115
O1-H1···O4^{ii}	0.82	2.24	2.993 (2)	152
O3-H3···N1^{iii}	0.82	1.93	2.736 (2)	165
N3-H3B···N2^{iv}	0.86	2.25	3.060 (2)	157
N7-H7A···N6^{v}	0.86	2.23	3.044 (2)	159

Symmetry codes: (ii) 1 - x, -y, 1 - z; (iii) 1 + x, 1 - y, 1/2 + z; (iv) -x, y, -z - 1/2; (v) 3/2 - x, 3/2 - y, 2 - z

Fig. 1

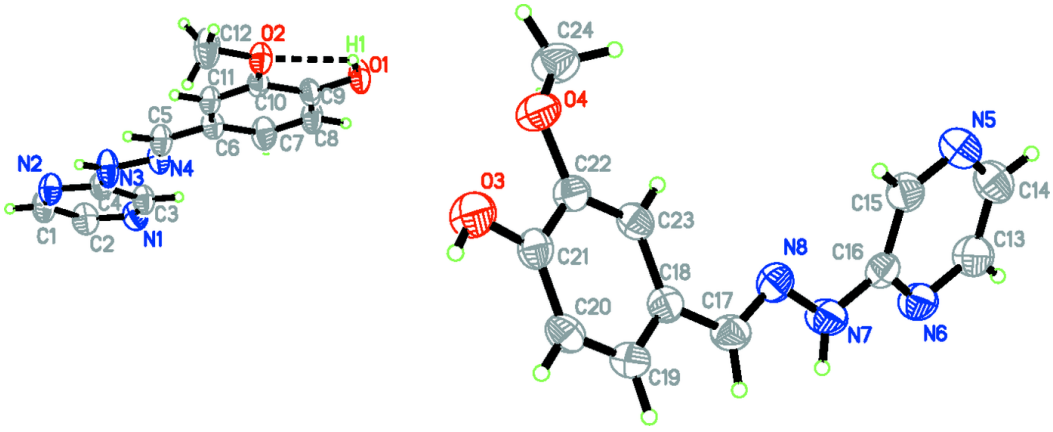
C12
O2
H1
O1
C11
C10
C9
C5
C6
C7
C8
N2
N3
N4
C4
C3
C1
C2
N1
C24
O4
C22
O3
C23
C21
C18
C17
N8
C16
N5
C15
C14
C13
C20
N7
N6
C19

Fig. 2