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Dimethyl and diethyl esters of 5,6-bis(pyridin-2-yl)-pyrazine-2,3-dicarboxylic acid: a comparison

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CCDC references: 1448182; 1448181

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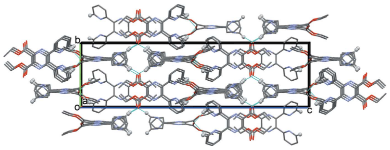
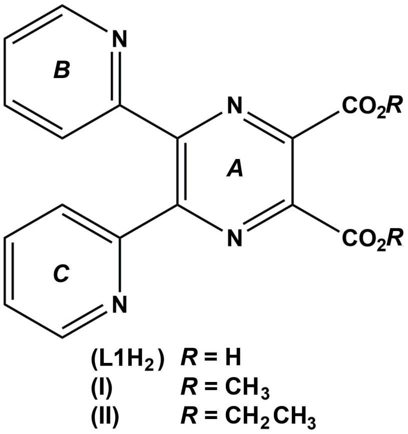


In dimethyl 5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylate, $C_{18}H_{14}N_4O_4$, (I), and diethyl 5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylate, $C_{20}H_{18}N_4O_4$, (II), the dimethyl and diethyl esters of 5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylic acid, the orientation of the two pyridine rings differ. In (I), pyridine ring *B* is inclined to pyrazine ring *A* by 44.8 (2)° and the pyridine and pyrazine N atoms are *trans* to one another, while pyridine ring *C* is inclined to the pyrazine ring by 50.3 (2)°, with the pyridine and pyrazine N atoms *cis* to one another. In compound (II), the diethyl ester, which possesses twofold rotation symmetry, the pyridine ring is inclined to the pyrazine ring by 40.7 (1)°, with the pyridine and pyrazine N atoms *trans* to one another. In the crystal of (I), molecules are linked by C—H···N hydrogen bonds, forming chains along [001]. The chains are linked by C—H···π interactions, forming a three-dimensional structure. In the crystal of (II), molecules are linked *via* C—H···O hydrogen bonds, forming a three-dimensional framework. There are C—H···π interactions present within the framework.

1. Chemical context

5,6-Bis(pyridin-2-yl)pyrazine-2,3-dicarboxylic acid (**L1H$_2$**) was synthesized to study its coordination behaviour with first row transitions metals (Alfonso, 1999). It exists as a zwitterion, with the adjacent pyridine and pyridinium rings almost coplanar due to the presence of an intramolecular N—H···N hydrogen bond. The crystal structures of the zwitterion and different charged forms of **L1H$_2$**, *viz.* the HCl, $HClO_4$ and HPF_6 salts, and details of the hydrogen bonding have been reported (Alfonso *et al.*, 2001).



Metal-catalysed hydrolysis of amino acid esters is a well documented phenomenon (Dugas, 1989). It has been shown previously that the reaction of copper(II) salts with the dimethyl esters of pyrazine-2,3-dicarboxylic acid (Neels *et al.*,

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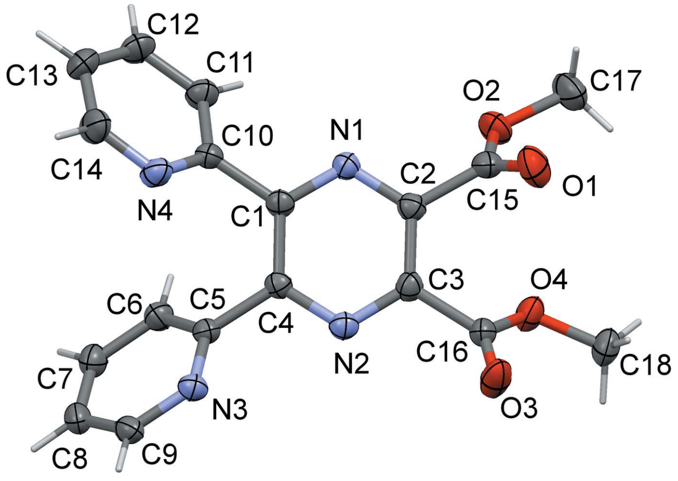

Figure 1
A view of the molecular structure of compound (I), showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

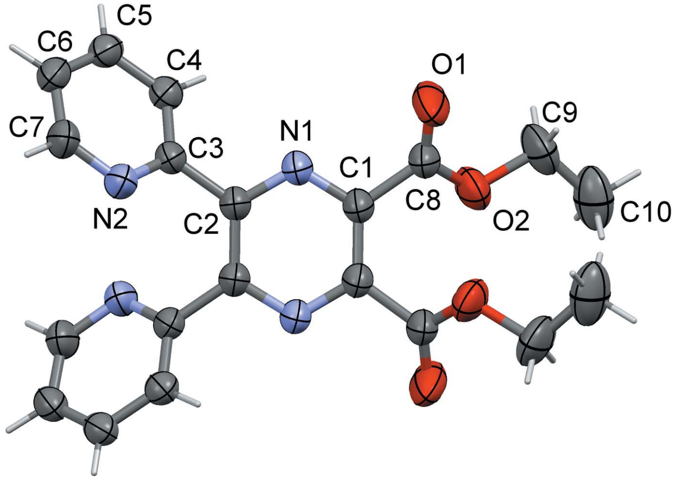

Figure 2
A view of the molecular structure of compound (II), showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level. Unlabelled atoms are related to labelled atoms by the symmetry code $(-x + 2, -y + \frac{3}{2}, z)$.

1997) and 2,5-dimethylpyrazine-3,6-dicarboxylic acid (Wang & Stoeckli-Evans, 1998) resulted in the partial hydrolysis of the ligand and the formation of a two-dimensional network in the first case and a mononuclear complex in the second. Hence, metal-ion-promoted ester hydrolysis leads to the formation of new ligands and may serve as a general route to prepare new coordination compounds. The title compounds, (I) and (II), were synthesized to study the hydrolysis of these esters with first row transition metals (Alfonso, 1999), and we report herein on their syntheses and crystal structures.

2. Structural commentary

As seen in compound (I), Fig. 1, the dimethyl ester of **L1H$_2$**, pyridine ring *B* (N4/C10–C14) is inclined to the pyrazine ring (*A*; N1/N2/C1–C4) by 44.8 (2)° and the pyridine and pyrazine N atoms, N1 and N4, are *trans* to one another. Pyridine ring *C* (N3/C5–C9) is inclined to pyrazine ring *A* by 50.3 (2)°. However, here the pyridine and pyrazine N atoms, N2 and N3, are *cis* to one another. The two pyridine rings, *B* and *C*, are inclined to one another by 60.2 (2)°. The acetate groups, O1/O2/C15/C17 and O3/O4/C16/C18, are almost planar with r.m.s. deviations of 0.027 and 0.007 Å, respectively. They are inclined to the pyrazine ring by 60.3 (3) and 49.8 (3)°, respectively, and to one another by 42.4 (3)°.

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

*Cg*2 is the centroid of the N3/C5–C9 pyridine ring.

D—H$\cdots$$A$	D—H	H$\cdots$$A$	$D\cdots A$	D—H$\cdots$$A$
C11—H11$\cdots$N3^{i}	0.93	2.57	3.334 (5)	140
C7—H7$\cdots$$Cg2^{ii}$	0.93	2.95	3.742 (5)	144
C17—H17C$\cdots$$Cg2^{iii}$	0.96	2.92	3.722 (6)	141

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

Compound (II), the diethyl ester of **L1H$_2$**, possesses twofold rotation symmetry, with the twofold rotation axis bisecting the $C_{ar}—C^{i}_{ar}$ bonds [ar = aromatic; symmetry code (i): $-x + 2, -y + \frac{3}{2}, z$], as shown in Fig. 2. The pyridine N atoms, N2 and N2^{i}, face one another with an N2$\cdots$N2^{i} separation of 3.043 (3) Å. The two pyridine rings are inclined to one another by 55.1 (1)° and to the pyrazine ring mean plane by 40.7 (1)°, with the pyrazine and pyridine N atoms, N1 and N2, *trans* to one another. The acetate group, O1/O2/C8/C9 [maximum deviation of 0.012 (3) Å for atom C8] is inclined to the pyrazine ring mean plane by 38.9 (1)°, and by 47.6 (2)° to the acetate group related by the twofold rotation axis. The oxygen atoms, O2 and O2^{i}, are separated by only 2.840 (3) Å. The pyrazine ring in (II) has a slight twist-boat conformation (r.m.s. deviation = 0.046 Å) with the N1/C1/C2 and N1^{i}/C1^{i}/C2^{i} planes inclined to one another by 3.9 (3)°.

As noted above the differences in the structures of the two compounds lies essentially in the orientation of the pyridine rings with respect to the pyrazine ring (*cf* Figs. 1 and 2). It is possible that the slight distortion of the planarity of the pyrazine ring in (II), mentioned above, is related to the short N2$\cdots$N2^{i} contact of 3.043 (3) Å of the adjacent pyridine rings and to the even shorter O2$\cdots$O2^{i} contact of 2.840 (3) Å of the adjacent acetate groups.

3. Supramolecular features

In the crystal of (I), molecules are linked by C—H$\cdots$N hydrogen bonds, forming chains along [001]; see Table 1 and Fig. 3. The chains are linked *via* C—H$\cdots$$\pi$ interactions (Table 1), forming a three-dimensional structure.

In the crystal of (II), molecules are linked *via* C—H$\cdots$O hydrogen bonds, forming a three-dimensional framework; see Table 2 and Fig. 4. Within the framework there are a number of C—H$\cdots$$\pi$ interactions present (Table 2).

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

*Cg*1 and *Cg*2 are the centroids of the pyrazine and pyridine rings N1/C1/C2/N1′/C1′/C2′ and N2/C3–C7, respectively [symmetry code (′): $-x+2, -y+\frac{3}{2}, z$].

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C7}-\text{H7}\cdots\text{O1}^{\text{i}}$	0.94	2.48	3.308 (3)	147
$\text{C4}-\text{H4}\cdots Cg2^{\text{ii}}$	0.94	2.92	3.739 (2)	147
$\text{C10}-\text{H10}B\cdots Cg1^{\text{iii}}$	0.97	2.56	3.409 (3)	146
$\text{C10}-\text{H10}B\cdots Cg1^{\text{iv}}$	0.97	2.56	3.409 (3)	146

Symmetry codes: (i) $-y+\frac{7}{4}, x+\frac{1}{4}, z+\frac{1}{4}$; (ii) $y-\frac{1}{4}, -x+\frac{5}{4}, -z+\frac{1}{4}$; (iii) $-x+2, -y+1, -z$; (iv) $x, y-\frac{1}{2}, -z$.

4. Database survey

Besides the structures of the zwitterion and different charged forms of **L1H$_2$**, *viz.* the HCl, $HClO_4$ and HPF_6 salts (Alfonso *et al.*, 2001), the crystal structures of two copper(II) complexes of **L1H$_2$** have been reported, *viz: catena*-[[[μ_3-5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylate]triaquadibromodicopper(II)] methanol solvate trihydrate] and *catena*-[[[μ_4-5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylate)diaquadibromodicopper(II) monohydrate] (Neels *et al.*, 2003).

The structure of the isoelectronic compound 3,6-bis(pyridin-2-yl)pyrazine-2,5-dicarboxylic acid (**L2H$_2$**), Fig. 5, has also been reported (Wang & Stoeckli-Evans, 2012*a*). It too exists as a zwitterion and the structures of its dihydrochloride salt and the dimethyl sulfonate disolvate have also been reported (Wang & Stoeckli-Evans, 2012*a*). The crystal structures of the dimethyl (III) and diethyl (IV) esters of **L2H$_2$** have been deposited as private communications (Wang & Stoeckli-Evans, 2012*b*,*c*) with the Cambridge Structural Database (CSD; Groom & Allen, 2014). Both compounds crystallize in the triclinic space group $P\overline{1}$ and possess inversion symmetry. The pyridine rings lie almost in the plane of the pyrazine ring and the N atoms are *trans* with respect to each other and to the nearest pyrazine N atom (as illustrated in Fig. 5). The ester groups are planar and in both compounds lie almost normal to the pyrazine ring. In the crystals of both compounds, inversion-related molecules are linked *via* pairs of $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, enclosing $R_2^2(10)$ ring motifs, forming chains propagating along [10$\overline{1}$].

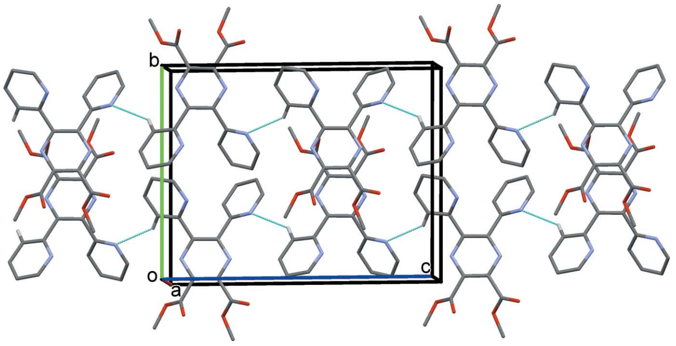

Figure 3
A view along the *a* axis of the crystal packing of compound (I). The hydrogen bonds are shown as dashed lines (see Table 1; only H atom H11 has been included).

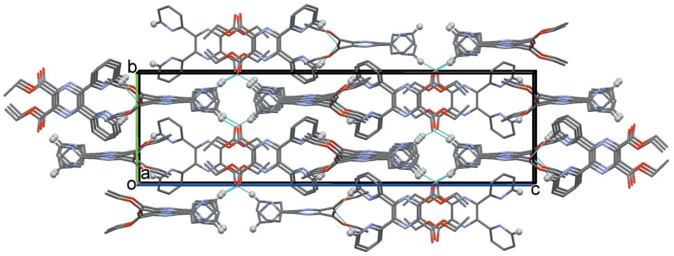

Figure 4
A view along the *a* axis of the crystal packing of compound (II). The hydrogen bonds are shown as dashed lines (see Table 2; only H atom H7 has been included).

5. Synthesis and crystallization

The synthesis of 5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylic acid (**L1H$_2$**) has been reported (Alfonso *et al.*, 2001). The dimethyl and diethyl esters, compounds (I) and (II), respectively, were obtained by the usual esterification procedure in acidic medium from the diacid and an excess of the corresponding alcohol.

Synthesis of compound (I): dimethyl-5,6-bis(pyridin-2-yl)-pyrazine-2,3-dicarboxylate L1H$_2$

(1.00 g, 3.11 mmol) was heated under reflux in freshly distilled MeOH (40ml) containing H_2SO_4 conc. (98%, 1 ml) during 16 h. After stopping the reaction, the temperature of the solution was allowed to cool to room temperature and then poured into an aqueous solution of NaOAc (6 g in 150 ml deionized water). The resulting solution was stirred in an ice bath containing NaCl to afford a white solid which was removed by filtration, washed with cold water and dried under vacuum. Single crystals suitable for X-ray analysis were obtained by the slow diffusion technique from CH_2Cl_2 and MeOH (yield: 0.77g, 65%; m.p. 410.2–411.7 K). Selected IR bands (KBr pellet, cm^{-1}): ν = 1743(*s*), 1729(*vs*), 1339(*s*), 1302(*s*), 1283(*vs*), 1164(*s*), 1089(*vs*). ^{1}H NMR (CDCl3, 400 MHz, p.p.m.): δ = 8.34(*dt*, 2H, *J* = 4.1Hz, *J* = 1.0 Hz, pyH),

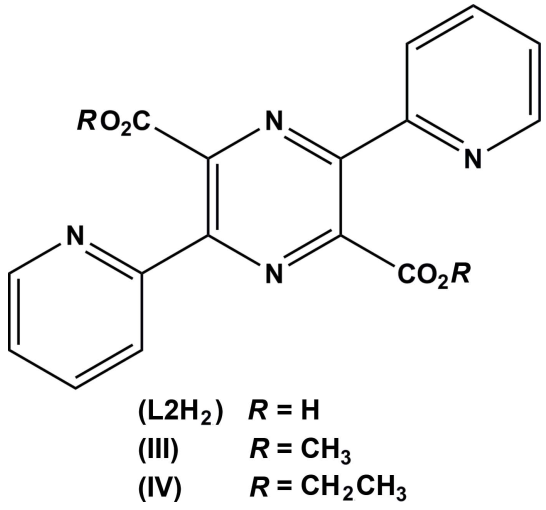

Figure 5
The chemical scheme for compound **L2H$_2$**.

Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{18}H_{14}N_4O_4$	$C_{20}H_{18}N_4O_4$
M_r	350.33	378.38
Crystal system, space group	Monoclinic, *Ia*	Tetragonal, $I4_1/a$
Temperature (K)	293	223
a, *b*, *c* (Å)	8.4249 (12), 12.2465 (10), 16.2561 (13)	10.2295 (6), 10.2295 (6), 36.281 (3)
α, β, γ (°)	90, 103.730 (8), 90	90, 90, 90
V ($Å^3$)	1629.3 (3)	3796.5 (5)
Z	4	8
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.10	0.10
Crystal size (mm)	0.70 × 0.50 × 0.38	0.65 × 0.50 × 0.50
Data collection		
Diffractometer	Stoe–Siemens AED2	Stoe IPDS 1
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3035, 3028, 2737	14760, 1851, 1153
R_{int}	0.012	0.043
$(\sin \theta/\lambda)_{max}$ ($Å^{-1}$)	0.606	0.616
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.135, 1.11	0.049, 0.149, 1.01
No. of reflections	3028	1851
No. of parameters	238	129
No. of restraints	2	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.19, −0.21	0.34, −0.19

Computer programs: *STADI4* (Stoe & Cie, 1997), *EXPOSE*, *CELL* and *INTEGRATE* in *IPDS-I* (Stoe & Cie, 2004), *X-RED* (Stoe & Cie, 1997), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *PLATON* (Spek, 2009), *Mercury* (Macrae *et al.*, 2008), and *publCIF* (Westrip, 2010).

7.99(*dt*, 2H, *J* = 7.7 Hz, *J* = 1.0 Hz, pyH), 7.82(*td*, 2H, *J* = 7.7 Hz, *J* = 1.0 Hz, pyH), 7.26(*td*, 2H, *J* = 7.7 Hz, *J* = 1.0 Hz, pyH), 4.04(*s*, 6H, CH_3). ^{13}C NMR ($CDCl_3$, 50 MHz, p.p.m.): δ = 165.53, 155.98, 153.35, 149.26, 142.92, 137.64, 125.41, 124.49, 54.11. DCI–MS *m*/*z*: 351(MH^+), 318, 279, 255, 208. Analysis for $C_{18}H_{14}N_4O_4$ (350.33), calculated C 61.70, H 4.04, N 15.99%, found C 61.4, H 3.91, N 15.65%.

Synthesis of compound (II): diethyl-5,6-bis(pyridin-2-yl)-pyrazine-2,3-dicarboxylate

This compound was prepared by the same method as for (I). $\mathbf{L1H_2}$ in freshly distilled EtOH containing catalytic amounts of H_2SO_4 conc. gave compound (II) as a white solid. Slow evaporation of an ethanolic solution afforded colourless crystals suitable for X-ray analysis (yield: 0.70g, 62%; m.p. 390.5–391.3 K). Selected IR bands (KBr pellet, cm^{-1}): ν = 3055(*w*), 1737(*s*), 1723(*vs*), 1368(*s*), 1301(*s*), 1276(vs), 1276(*vs*), 1161(*s*), 1086(*vs*). ^1H NMR ($CDCl_3$, 400 MHz, p.p.m.): δ = 8.33(*d*, 2H, *J* = 4 Hz, pyH), 8.01(*d*, 2H, *J* = 7.7 Hz, pyH), 7.81(*t*, 2H, *J* = 7.7 Hz, pyH), 7.24(*t*, 2H, *J* = 4.4 Hz, pyH), 4.52(*m*, 4H, *J* = 7 Hz, CH_2), 1.45(*t*, 6H, *J* = 7.4 Hz, CH_3). EI–MS *m*/*z*: 378 (34), 349 (9), 232 (95), 206 (66), 179 (25), 152 (11), 129 (9), 78(base), 46 (38). Analysis for $C_{20}H_{18}N_4O_4$ (378.38), calculated C 63.49, H 4.79, N 14.81%, found C 63.49, H 4.61, N 14.77%.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. For both compounds, the C-bound H-atoms were included in calculated positions and treated as riding atoms: C—H = 0.93–0.98 Å with $U_{iso}(H) = 1.5U_{eq}$(C-methyl) and $1.2U_{eq}(C)$ for other H atoms. For compound (I), the Flack parameter (Parsons *et al.*, 2013) is = −0.2 (10), but it has no physical meaning here.

Acknowledgements

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Dimethyl and diethyl esters of 5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylic acid: a comparison

Montserrat Alfonso and Helen Stoeckli-Evans

Computing details

Data collection: *STADI4* (Stoe & Cie, 1997) for (I); *EXPOSE* in *IPDS-I* (Stoe & Cie, 2004) for (II). Cell refinement: *STADI4* (Stoe & Cie, 1997) for (I); *CELL* in *IPDS-I* (Stoe & Cie, 2004) for (II). Data reduction: *X-RED* (Stoe & Cie, 1997) for (I); *INTEGRATE* in *IPDS-I* (Stoe & Cie, 2004) for (II). For both compounds, program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

(I) Dimethyl 5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylate

Crystal data

$C_{18}H_{14}N_4O_4$
$M_r = 350.33$
Monoclinic, *Ia*
$a = 8.4249$ (12) Å
$b = 12.2465$ (10) Å
$c = 16.2561$ (13) Å
$\beta = 103.730$ (8)°
$V = 1629.3$ (3) Å^3
$Z = 4$
$F(000) = 728$
$D_x = 1.428$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 33 reflections
$\theta = 14.1$–19.6°
$\mu = 0.10$ mm^{-1}
$T = 293$ K
Rod, colourless
0.70 × 0.50 × 0.38 mm

Data collection

Stoe–Siemens AED2 diffractometer
ω/\2q scans
3035 measured reflections
3028 independent reflections
2737 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.012$
$\theta_{\max} = 25.5°$, $\theta_{\min} = 2.1°$
$h = -10 \rightarrow 10$
$k = 0 \rightarrow 14$
$l = -19 \rightarrow 19$
2 standard reflections every 60 min
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.135$
$S = 1.11$
3028 reflections
238 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0759P)^2 + 1.0624P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}
Extinction correction: *SHELXL2014* (Sheldrick, 2015), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0065 (18)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.8419 (5)	1.1583 (3)	0.0691 (2)	0.0470 (9)
O2	1.0295 (4)	1.1079 (3)	−0.0014 (2)	0.0395 (8)
O3	1.0067 (5)	1.1074 (3)	0.3016 (2)	0.0463 (10)
O4	1.1454 (4)	1.1588 (3)	0.2054 (2)	0.0355 (8)
N1	0.9519 (4)	0.8948 (3)	0.0567 (2)	0.0266 (8)
N2	1.0688 (4)	0.8934 (3)	0.2330 (2)	0.0272 (8)
N3	1.0738 (4)	0.6793 (3)	0.3087 (2)	0.0279 (8)
N4	0.8579 (5)	0.6232 (3)	0.0803 (2)	0.0348 (9)
C1	0.9822 (5)	0.8015 (3)	0.0992 (2)	0.0248 (9)
C2	0.9784 (5)	0.9878 (3)	0.1014 (2)	0.0259 (9)
C3	1.0319 (5)	0.9857 (3)	0.1896 (3)	0.0268 (9)
C4	1.0489 (5)	0.8006 (3)	0.1880 (2)	0.0227 (8)
C5	1.1158 (5)	0.6996 (3)	0.2355 (2)	0.0248 (9)
C6	1.2218 (5)	0.6347 (4)	0.2045 (3)	0.0311 (9)
H6	1.2486	0.6520	0.1537	0.037*
C7	1.2879 (6)	0.5430 (4)	0.2500 (3)	0.0349 (10)
H7	1.3595	0.4979	0.2303	0.042*
C8	1.2459 (6)	0.5200 (3)	0.3248 (3)	0.0345 (10)
H8	1.2879	0.4589	0.3565	0.041*
C9	1.1394 (5)	0.5903 (4)	0.3517 (3)	0.0312 (9)
H9	1.1118	0.5748	0.4025	0.037*
C10	0.9393 (5)	0.6998 (3)	0.0486 (2)	0.0255 (9)
C11	0.9763 (6)	0.6908 (4)	−0.0299 (3)	0.0334 (10)
H11	1.0322	0.7464	−0.0499	0.040*
C12	0.9291 (6)	0.5984 (4)	−0.0777 (3)	0.0389 (11)
H12	0.9543	0.5900	−0.1301	0.047*
C13	0.8443 (7)	0.5192 (4)	−0.0469 (3)	0.0413 (12)
H13	0.8098	0.4561	−0.0779	0.050*
C14	0.8113 (7)	0.5353 (4)	0.0320 (3)	0.0439 (13)
H14	0.7529	0.4814	0.0524	0.053*
C15	0.9399 (6)	1.0942 (4)	0.0546 (3)	0.0316 (10)
C16	1.0580 (5)	1.0903 (4)	0.2399 (3)	0.0287 (9)
C17	1.0131 (8)	1.2133 (4)	−0.0439 (3)	0.0525 (14)
H17A	1.0924	1.2190	−0.0774	0.079*
H17B	1.0307	1.2706	−0.0024	0.079*

H17C	0.9053	1.2199	−0.0798	0.079*
C18	1.1672 (6)	1.2674 (4)	0.2412 (3)	0.0386 (11)
H18A	1.2114	1.3143	0.2049	0.058*
H18B	1.2410	1.2645	0.2961	0.058*
H18C	1.0636	1.2955	0.2464	0.058*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.054 (2)	0.0354 (19)	0.054 (2)	0.0149 (17)	0.0183 (17)	0.0094 (17)
O2	0.055 (2)	0.0344 (19)	0.0313 (17)	−0.0011 (15)	0.0150 (15)	0.0089 (14)
O3	0.079 (3)	0.0309 (19)	0.037 (2)	−0.0093 (17)	0.0314 (19)	−0.0065 (14)
O4	0.0460 (18)	0.0266 (17)	0.0375 (16)	−0.0064 (13)	0.0171 (14)	−0.0077 (13)
N1	0.0339 (19)	0.0234 (19)	0.0235 (18)	−0.0009 (14)	0.0084 (14)	0.0004 (13)
N2	0.0320 (19)	0.027 (2)	0.0231 (18)	−0.0006 (14)	0.0081 (15)	−0.0003 (13)
N3	0.0337 (19)	0.0282 (19)	0.0223 (18)	−0.0009 (15)	0.0077 (14)	0.0010 (14)
N4	0.049 (2)	0.0326 (19)	0.0237 (17)	−0.0122 (17)	0.0103 (16)	−0.0023 (16)
C1	0.029 (2)	0.025 (2)	0.023 (2)	0.0003 (16)	0.0110 (17)	0.0009 (16)
C2	0.027 (2)	0.027 (2)	0.024 (2)	0.0006 (17)	0.0066 (16)	0.0011 (16)
C3	0.032 (2)	0.023 (2)	0.027 (2)	0.0005 (17)	0.0108 (18)	−0.0016 (16)
C4	0.0233 (19)	0.024 (2)	0.022 (2)	−0.0001 (15)	0.0082 (15)	0.0013 (15)
C5	0.029 (2)	0.024 (2)	0.0201 (19)	−0.0017 (16)	0.0032 (16)	−0.0009 (16)
C6	0.038 (2)	0.029 (2)	0.026 (2)	0.0039 (19)	0.0090 (18)	−0.0011 (18)
C7	0.040 (2)	0.027 (2)	0.036 (2)	0.0047 (19)	0.006 (2)	−0.0035 (19)
C8	0.043 (3)	0.022 (2)	0.034 (2)	0.0019 (19)	0.0007 (19)	0.0013 (18)
C9	0.038 (2)	0.029 (2)	0.024 (2)	−0.0046 (18)	0.0027 (18)	0.0040 (18)
C10	0.031 (2)	0.025 (2)	0.020 (2)	0.0015 (17)	0.0040 (16)	0.0015 (16)
C11	0.042 (3)	0.034 (2)	0.026 (2)	−0.0032 (18)	0.0130 (18)	−0.0015 (18)
C12	0.053 (3)	0.039 (3)	0.026 (2)	0.001 (2)	0.013 (2)	−0.007 (2)
C13	0.059 (3)	0.032 (3)	0.030 (2)	−0.003 (2)	0.003 (2)	−0.0083 (19)
C14	0.066 (3)	0.031 (2)	0.035 (3)	−0.018 (2)	0.012 (2)	0.002 (2)
C15	0.038 (2)	0.030 (2)	0.023 (2)	−0.002 (2)	0.0008 (17)	0.0001 (17)
C16	0.037 (2)	0.022 (2)	0.025 (2)	0.0026 (17)	0.0038 (17)	−0.0003 (17)
C17	0.069 (4)	0.039 (3)	0.045 (3)	−0.012 (3)	0.005 (3)	0.017 (2)
C18	0.047 (3)	0.024 (2)	0.046 (3)	−0.0043 (19)	0.013 (2)	−0.006 (2)

Geometric parameters (Å, º)

O1—C15	1.202 (6)	C6—C7	1.387 (6)
O2—C15	1.324 (6)	C6—H6	0.9300
O2—C17	1.455 (5)	C7—C8	1.373 (7)
O3—C16	1.200 (6)	C7—H7	0.9300
O4—C16	1.325 (6)	C8—C9	1.387 (7)
O4—C18	1.446 (5)	C8—H8	0.9300
N1—C1	1.329 (5)	C9—H9	0.9300
N1—C2	1.340 (5)	C10—C11	1.388 (6)
N2—C3	1.331 (6)	C11—C12	1.377 (7)
N2—C4	1.341 (5)	C11—H11	0.9300

N3—C9	1.340 (5)	C12—C13	1.368 (7)
N3—C5	1.343 (5)	C12—H12	0.9300
N4—C10	1.335 (6)	C13—C14	1.389 (7)
N4—C14	1.336 (6)	C13—H13	0.9300
C1—C4	1.419 (5)	C14—H14	0.9300
C1—C10	1.489 (6)	C17—H17A	0.9600
C2—C3	1.397 (5)	C17—H17B	0.9600
C2—C15	1.505 (6)	C17—H17C	0.9600
C3—C16	1.508 (6)	C18—H18A	0.9600
C4—C5	1.495 (6)	C18—H18B	0.9600
C5—C6	1.377 (6)	C18—H18C	0.9600

C15—O2—C17	115.7 (4)	N4—C10—C11	123.2 (4)
C16—O4—C18	116.2 (3)	N4—C10—C1	117.0 (3)
C1—N1—C2	117.5 (3)	C11—C10—C1	119.7 (4)
C3—N2—C4	116.6 (3)	C12—C11—C10	119.1 (4)
C9—N3—C5	116.7 (4)	C12—C11—H11	120.5
C10—N4—C14	116.5 (4)	C10—C11—H11	120.5
N1—C1—C4	121.1 (4)	C13—C12—C11	118.8 (4)
N1—C1—C10	116.2 (3)	C13—C12—H12	120.6
C4—C1—C10	122.7 (4)	C11—C12—H12	120.6
N1—C2—C3	120.9 (4)	C12—C13—C14	118.3 (4)
N1—C2—C15	118.3 (3)	C12—C13—H13	120.9
C3—C2—C15	120.8 (4)	C14—C13—H13	120.9
N2—C3—C2	122.5 (4)	N4—C14—C13	124.2 (4)
N2—C3—C16	116.7 (3)	N4—C14—H14	117.9
C2—C3—C16	120.8 (4)	C13—C14—H14	117.9
N2—C4—C1	121.1 (4)	O1—C15—O2	125.6 (4)
N2—C4—C5	115.8 (3)	O1—C15—C2	122.9 (4)
C1—C4—C5	122.8 (4)	O2—C15—C2	111.6 (4)
N3—C5—C6	123.2 (4)	O3—C16—O4	126.2 (4)
N3—C5—C4	117.7 (3)	O3—C16—C3	124.5 (4)
C6—C5—C4	119.1 (4)	O4—C16—C3	109.4 (3)
C5—C6—C7	119.0 (4)	O2—C17—H17A	109.5
C5—C6—H6	120.5	O2—C17—H17B	109.5
C7—C6—H6	120.5	H17A—C17—H17B	109.5
C8—C7—C6	118.9 (4)	O2—C17—H17C	109.5
C8—C7—H7	120.5	H17A—C17—H17C	109.5
C6—C7—H7	120.5	H17B—C17—H17C	109.5
C7—C8—C9	118.3 (4)	O4—C18—H18A	109.5
C7—C8—H8	120.9	O4—C18—H18B	109.5
C9—C8—H8	120.9	H18A—C18—H18B	109.5
N3—C9—C8	123.9 (4)	O4—C18—H18C	109.5
N3—C9—H9	118.1	H18A—C18—H18C	109.5
C8—C9—H9	118.1	H18B—C18—H18C	109.5

C2—N1—C1—C4	−3.6 (5)	C5—N3—C9—C8	0.1 (6)
C2—N1—C1—C10	175.4 (3)	C7—C8—C9—N3	0.4 (7)

C1—N1—C2—C3	−1.6 (5)	C14—N4—C10—C11	−0.4 (7)
C1—N1—C2—C15	−178.2 (4)	C14—N4—C10—C1	176.0 (4)
C4—N2—C3—C2	−1.4 (5)	N1—C1—C10—N4	−133.7 (4)
C4—N2—C3—C16	−178.6 (4)	C4—C1—C10—N4	45.3 (5)
N1—C2—C3—N2	4.3 (6)	N1—C1—C10—C11	42.8 (5)
C15—C2—C3—N2	−179.2 (4)	C4—C1—C10—C11	−138.2 (4)
N1—C2—C3—C16	−178.6 (4)	N4—C10—C11—C12	−0.7 (7)
C15—C2—C3—C16	−2.1 (6)	C1—C10—C11—C12	−177.0 (4)
C3—N2—C4—C1	−3.8 (5)	C10—C11—C12—C13	1.2 (7)
C3—N2—C4—C5	170.5 (3)	C11—C12—C13—C14	−0.6 (8)
N1—C1—C4—N2	6.5 (5)	C10—N4—C14—C13	1.0 (8)
C10—C1—C4—N2	−172.4 (4)	C12—C13—C14—N4	−0.5 (8)
N1—C1—C4—C5	−167.4 (4)	C17—O2—C15—O1	4.4 (7)
C10—C1—C4—C5	13.7 (5)	C17—O2—C15—C2	−174.1 (4)
C9—N3—C5—C6	−0.6 (6)	N1—C2—C15—O1	120.0 (5)
C9—N3—C5—C4	−177.9 (4)	C3—C2—C15—O1	−56.6 (6)
N2—C4—C5—N3	50.7 (5)	N1—C2—C15—O2	−61.5 (5)
C1—C4—C5—N3	−135.1 (4)	C3—C2—C15—O2	121.9 (4)
N2—C4—C5—C6	−126.6 (4)	C18—O4—C16—O3	−6.2 (7)
C1—C4—C5—C6	47.6 (6)	C18—O4—C16—C3	173.9 (4)
N3—C5—C6—C7	0.7 (7)	N2—C3—C16—O3	−50.9 (6)
C4—C5—C6—C7	177.9 (4)	C2—C3—C16—O3	131.8 (5)
C5—C6—C7—C8	−0.2 (7)	N2—C3—C16—O4	128.9 (4)
C6—C7—C8—C9	−0.4 (7)	C2—C3—C16—O4	−48.3 (5)

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the N3/C5–C9 pyridine ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···N3^{i}	0.93	2.57	3.334 (5)	140
C7—H7···*Cg*2^{ii}	0.93	2.95	3.742 (5)	144
C17—H17*C*···*Cg*2^{iii}	0.96	2.92	3.722 (6)	141

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

(II) Diethyl 5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylate

Crystal data

$C_{20}H_{18}N_4O_4$
M_r = 378.38
Tetragonal, $I4_1/a$
a = 10.2295 (6) Å
c = 36.281 (3) Å
V = 3796.5 (5) Å^3
Z = 8
F(000) = 1584

D_x = 1.324 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 5000 reflections
θ = 3.3–52.1°
μ = 0.10 mm^{-1}
T = 223 K
Block, colourless
0.65 × 0.50 × 0.50 mm

Data collection

Stoe IPDS 1 diffractometer
Radiation source: fine-focus sealed tube
Plane graphite monochromator
φ rotation scans
14760 measured reflections
1851 independent reflections
1153 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.043$
$\theta_{\text{max}} = 26.0°$, $\theta_{\text{min}} = 2.1°$
$h = -12 \rightarrow 12$
$k = -12 \rightarrow 12$
$l = -44 \rightarrow 44$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.149$
$S = 1.01$
1851 reflections
129 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0925P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\text{max}} < 0.001$
$\Delta\rho_{\text{max}} = 0.34$ e Å^{-3}
$\Delta\rho_{\text{min}} = -0.19$ e Å^{-3}
Extinction correction: *SHELXL2014* (Sheldrick, 2015), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0049 (10)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.7424 (2)	0.7559 (3)	0.00480 (5)	0.1009 (9)
O2	0.91015 (17)	0.64422 (18)	−0.01674 (4)	0.0693 (5)
N1	0.86590 (16)	0.73125 (18)	0.07318 (4)	0.0478 (5)
N2	0.88149 (17)	0.8399 (2)	0.16340 (5)	0.0583 (6)
C1	0.9332 (2)	0.7371 (2)	0.04156 (5)	0.0473 (5)
C2	0.93113 (19)	0.7446 (2)	0.10488 (5)	0.0450 (5)
C3	0.84753 (19)	0.7504 (2)	0.13824 (5)	0.0452 (5)
C4	0.7388 (2)	0.6719 (2)	0.14134 (5)	0.0466 (5)
H4	0.7174	0.6124	0.1225	0.056*
C5	0.6613 (2)	0.6817 (2)	0.17249 (5)	0.0503 (5)
H5	0.5874	0.6282	0.1755	0.060*
C6	0.6952 (2)	0.7712 (2)	0.19868 (6)	0.0569 (6)
H6	0.6448	0.7803	0.2202	0.068*
C7	0.8042 (2)	0.8481 (3)	0.19322 (6)	0.0637 (7)
H7	0.8256	0.9098	0.2114	0.076*
C8	0.8508 (2)	0.7155 (3)	0.00796 (5)	0.0558 (6)
C9	0.8402 (3)	0.6183 (4)	−0.05106 (7)	0.0978 (11)
H9A	0.7744	0.5501	−0.0471	0.117*
H9B	0.7956	0.6977	−0.0594	0.117*

C10	0.9335 (4)	0.5760 (3)	−0.07867 (8)	0.0965 (11)
H10A	0.8877	0.5552	−0.1013	0.145*
H10B	0.9793	0.4990	−0.0699	0.145*
H10C	0.9960	0.6455	−0.0833	0.145*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0662 (13)	0.187 (2)	0.0499 (11)	0.0406 (14)	−0.0132 (9)	−0.0026 (12)
O2	0.0689 (11)	0.0889 (12)	0.0500 (9)	0.0023 (9)	−0.0168 (8)	−0.0172 (8)
N1	0.0424 (9)	0.0665 (12)	0.0347 (9)	0.0012 (8)	−0.0018 (7)	0.0026 (8)
N2	0.0464 (10)	0.0866 (14)	0.0418 (9)	−0.0104 (10)	0.0042 (8)	−0.0093 (9)
C1	0.0440 (10)	0.0630 (13)	0.0348 (10)	0.0039 (10)	−0.0018 (8)	0.0012 (9)
C2	0.0418 (10)	0.0581 (13)	0.0350 (10)	−0.0016 (9)	−0.0010 (8)	0.0011 (9)
C3	0.0379 (10)	0.0629 (13)	0.0348 (10)	0.0007 (9)	−0.0026 (8)	0.0026 (9)
C4	0.0421 (11)	0.0541 (12)	0.0437 (11)	0.0028 (9)	−0.0017 (8)	0.0041 (9)
C5	0.0407 (11)	0.0630 (13)	0.0471 (12)	0.0017 (10)	0.0035 (9)	0.0086 (10)
C6	0.0450 (12)	0.0826 (17)	0.0431 (11)	0.0052 (12)	0.0067 (9)	0.0062 (11)
C7	0.0553 (14)	0.0941 (18)	0.0416 (11)	−0.0080 (13)	0.0046 (10)	−0.0127 (12)
C8	0.0467 (13)	0.0851 (17)	0.0357 (11)	0.0035 (12)	−0.0008 (9)	0.0047 (11)
C9	0.095 (2)	0.141 (3)	0.0578 (16)	−0.007 (2)	−0.0290 (15)	−0.0268 (18)
C10	0.157 (3)	0.0720 (18)	0.0605 (17)	−0.020 (2)	−0.0135 (19)	−0.0139 (14)

Geometric parameters (Å, º)

O1—C8	1.189 (3)	C4—H4	0.9400
O2—C8	1.305 (3)	C5—C6	1.364 (3)
O2—C9	1.460 (3)	C5—H5	0.9400
N1—C2	1.337 (2)	C6—C7	1.379 (3)
N1—C1	1.339 (2)	C6—H6	0.9400
N2—C3	1.339 (3)	C7—H7	0.9400
N2—C7	1.343 (3)	C9—C10	1.450 (5)
C1—C1$^{\text{i}}$	1.392 (4)	C9—H9A	0.9800
C1—C8	1.499 (3)	C9—H9B	0.9800
C2—C2$^{\text{i}}$	1.413 (4)	C10—H10A	0.9700
C2—C3	1.483 (3)	C10—H10B	0.9700
C3—C4	1.377 (3)	C10—H10C	0.9700
C4—C5	1.384 (3)		

C8—O2—C9	117.3 (2)	C7—C6—H6	120.4
C2—N1—C1	118.40 (17)	N2—C7—C6	123.8 (2)
C3—N2—C7	116.06 (19)	N2—C7—H7	118.1
N1—C1—C1$^{\text{i}}$	120.88 (11)	C6—C7—H7	118.1
N1—C1—C8	113.63 (18)	O1—C8—O2	124.2 (2)
C1$^{\text{i}}$—C1—C8	125.48 (12)	O1—C8—C1	123.5 (2)
N1—C2—C2$^{\text{i}}$	120.38 (11)	O2—C8—C1	112.27 (19)
N1—C2—C3	114.72 (17)	C10—C9—O2	108.7 (3)
C2$^{\text{i}}$—C2—C3	124.88 (11)	C10—C9—H9A	109.9

N2—C3—C4	123.56 (18)	O2—C9—H9A	109.9
N2—C3—C2	115.71 (18)	C10—C9—H9B	109.9
C4—C3—C2	120.65 (18)	O2—C9—H9B	109.9
C3—C4—C5	119.1 (2)	H9A—C9—H9B	108.3
C3—C4—H4	120.4	C9—C10—H10A	109.5
C5—C4—H4	120.4	C9—C10—H10B	109.5
C6—C5—C4	118.2 (2)	H10A—C10—H10B	109.5
C6—C5—H5	120.9	C9—C10—H10C	109.5
C4—C5—H5	120.9	H10A—C10—H10C	109.5
C5—C6—C7	119.20 (19)	H10B—C10—H10C	109.5
C5—C6—H6	120.4		

C2—N1—C1—C1^{i}	−3.1 (4)	C3—C4—C5—C6	1.1 (3)
C2—N1—C1—C8	177.7 (2)	C4—C5—C6—C7	0.1 (3)
C1—N1—C2—C2^{i}	−4.4 (4)	C3—N2—C7—C6	−0.2 (4)
C1—N1—C2—C3	174.09 (19)	C5—C6—C7—N2	−0.6 (4)
C7—N2—C3—C4	1.6 (3)	C9—O2—C8—O1	3.0 (4)
C7—N2—C3—C2	178.3 (2)	C9—O2—C8—C1	−179.0 (2)
N1—C2—C3—N2	−137.7 (2)	N1—C1—C8—O1	37.9 (4)
C2^{i}—C2—C3—N2	40.8 (4)	C1^{i}—C1—C8—O1	−141.2 (3)
N1—C2—C3—C4	39.1 (3)	N1—C1—C8—O2	−140.1 (2)
C2^{i}—C2—C3—C4	−142.4 (3)	C1^{i}—C1—C8—O2	40.8 (4)
N2—C3—C4—C5	−2.1 (3)	C8—O2—C9—C10	162.0 (3)
C2—C3—C4—C5	−178.62 (19)		

Symmetry code: (i) −*x*+2, −*y*+3/2, *z*.

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of the pyrazine and pyridine rings N1/C1/C2/N1′/C1′/C2′ and N2/C3–C7, respectively [symmetry code (′): -*x* + 2, -*y* + 3/2, *z*].

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O1^{ii}	0.94	2.48	3.308 (3)	147
C4—H4···*Cg*2^{iii}	0.94	2.92	3.739 (2)	147
C10—H10*B*···*Cg*1^{iv}	0.97	2.56	3.409 (3)	146
C10—H10*B*···*Cg*1^{v}	0.97	2.56	3.409 (3)	146

Symmetry codes: (ii) −*y*+7/4, *x*+1/4, *z*+1/4; (iii) *y*−1/4, −*x*+5/4, −*z*+1/4; (iv) −*x*+2, −*y*+1, −*z*; (v) *x*, *y*−1/2, −*z*.