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# Crystal structures of *N*-(pyridin-2-ylmethyl)pyrazine-2-carboxamide (monoclinic polymorph) and *N*-(pyridin-4-ylmethyl)pyrazine-2-carboxamide

Dilovan S. Cati<sup>a</sup> and Helen Stoeckli-Evans<sup>b\*</sup>

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This work forms part of the PhD thesis (Neuchâtel, 2002) of DSC.

**Keywords:** crystal structure; pyrazine; pyridine; carboxamide

**CCDC references:** 1004272; 1004273

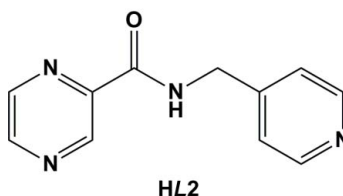
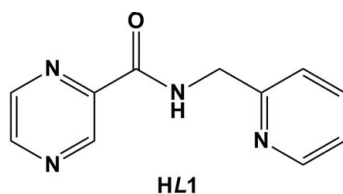
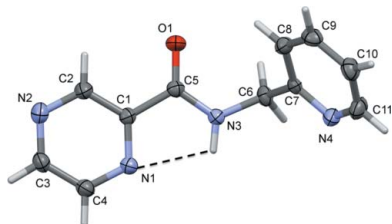
**Supporting information:** this article has supporting information at journals.iucr.org/e

<sup>a</sup>Debiopharm International S.A., Chemin Messidor 5-7, CP 5911, CH-1002 Lausanne, Switzerland, and <sup>b</sup>Institute of Physics, University of Neuchâtel, rue Emile-Argand 11, CH-2000 Neuchâtel, Switzerland. \*Correspondence e-mail: helen.stoeckli-evans@unine.ch

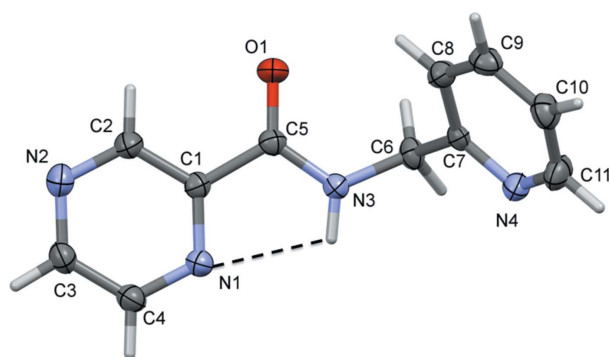
The title compounds, C<sub>11</sub>H<sub>10</sub>N<sub>4</sub>O (HL1) and C<sub>11</sub>H<sub>10</sub>N<sub>4</sub>O (HL2), are pyridine 2-ylmethyl and 4-ylmethyl derivatives, respectively, of pyrazine-2-carboxamide. HL1 was measured at 153 K and crystallized in the monoclinic space group *P*2<sub>1</sub>/*c* with *Z* = 4. There has been a report of the same structure measured at room temperature but assumed to crystallize in the triclinic space group *P* $\bar{1}$  with *Z* = 4 [Sasan *et al.* (2008). *Monatsh. Chem.* **139**, 773–780]. In HL1, the pyridine ring is inclined to the pyrazine ring by 61.34 (6)°, while in HL2 this dihedral angle is 84.33 (12)°. In both molecules, there is a short N–H···N interaction involving the pyrazine carboxamide unit. In the crystal of HL1, molecules are linked by N–H···N hydrogen bonds, forming inversion dimers with an *R*<sub>2</sub><sup>2</sup>(10) ring motif. The dimers are linked *via* bifurcated-acceptor C–H···O hydrogen bonds, forming sheets lying parallel to (102). The sheets are linked *via* C–H···N hydrogen bonds, forming a three-dimensional structure. In the crystal of HL2, molecules are linked by N–H···N and C–H···N hydrogen bonds to form chains propagating along [010]. The chains are linked *via* C–H···O hydrogen bonds, forming sheets lying parallel to (100). Within the sheets there are  $\pi$ – $\pi$  interactions involving neighbouring pyrazine rings [inter-centroid distance = 3.711 (15) Å]. Adjacent sheets are linked *via* parallel slipped  $\pi$ – $\pi$  interactions involving inversion-related pyridine rings [inter-centroid distance = 3.6395 (17) Å], forming a three-dimensional structure.

## 1. Chemical context

The title compounds form part of a series of ligands synthesized in order to study their coordination chemistry with 3*d* transition metals (Cati, 2002).



They have been used to construct coordination polymers and multi-nuclear compounds, and to study their magnetic


**Figure 1**

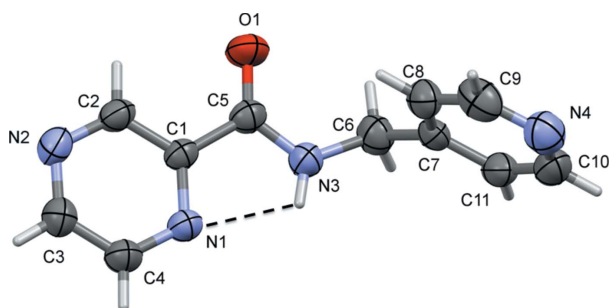
A view of the molecular structure of HL1, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level. The short intramolecular N—H···N interaction is shown as a dashed line (see Table 1 for details).

properties (Cati *et al.*, 2004). Similar ligands have been synthesized by other groups who have studied, for example, the magnetic properties of some copper(II) complexes (Hausmann *et al.*, 2003; Kingele *et al.*, 2007).

## 2. Structural commentary

The molecular structure of ligand HL1 is illustrated in Fig. 1. HL1 was measured at 153 K and crystallized in the monoclinic space group  $P2_1/c$  with  $Z = 4$ . The  $\beta$  angle is  $91.461(11)^\circ$  and the systematic absences, the  $R_{\text{int}}$  value (0.0348) and the successful refinement  $\{R1 [I > 2\sigma(I)] = 0.0319\}$  clearly show that at 153 K the space group is monoclinic  $P2_1/c$ . The same structure measured at room temperature was reported to crystallize in the triclinic space group  $P\bar{1}$  with  $Z = 4$  (Sasan *et al.*, 2008). However, the three cell angles are close  $90(2)^\circ$  [ $\alpha = 91.802(6)$ ,  $\beta = 89.834(7)$ ,  $\gamma = 91.845(6)^\circ$ ] and the crystal used was a very narrow needle. The final  $R1 [I > 2\sigma(I)]$  factor was rather high at 0.0699, hence it is possible that the choice of crystal system and space group are incorrect. However, this could not be confirmed when analysing the coordinates using the AddSymm routine in *PLATON* (Spek, 2009).

In the molecule of HL1 there is a short N—H···N hydrogen bond present in the pyrazine carboxamide unit (Table 1), and the amide group, C5(=O)N3, is approximately coplanar with


**Figure 2**

A view of the molecular structure of HL2, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level. The short intramolecular N—H···N interaction is shown as a dashed line (see Table 2 for details).

**Table 1**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ) for HL1.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3—H3N···N1	0.901 (16)	2.332 (15)	2.7136 (15)	105.4 (11)
N3—H3N···N4 <sup>i</sup>	0.901 (16)	2.206 (16)	2.9929 (14)	145.6 (13)
C3—H3···O1 <sup>ii</sup>	0.95	2.51	3.1544 (15)	125
C4—H4···O1 <sup>ii</sup>	0.95	2.56	3.1748 (15)	123
C10—H10···N2 <sup>iii</sup>	0.95	2.62	3.5678 (17)	174

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

**Table 2**

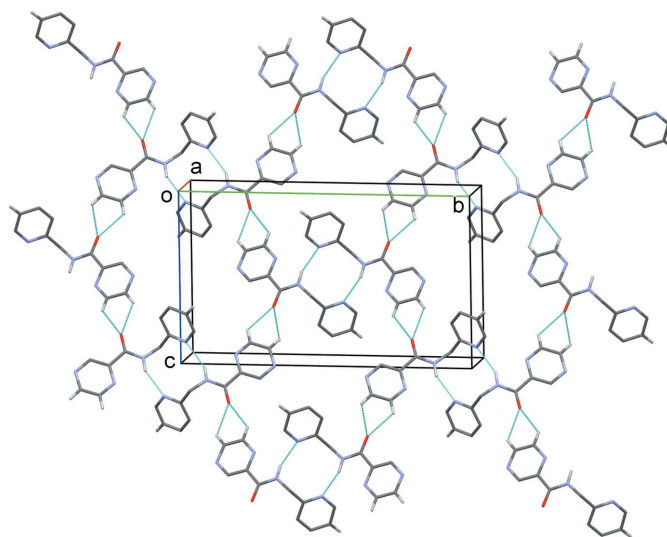
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ) for HL2.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3—H3N···N1	0.83 (3)	2.27 (3)	2.713 (3)	114 (2)
N3—H3N···N2 <sup>i</sup>	0.83 (3)	2.52 (3)	3.214 (3)	142 (2)
C2—H2···N1 <sup>ii</sup>	0.93	2.47	3.315 (3)	151
C8—H8···O1 <sup>iii</sup>	0.93	2.55	3.373 (3)	148

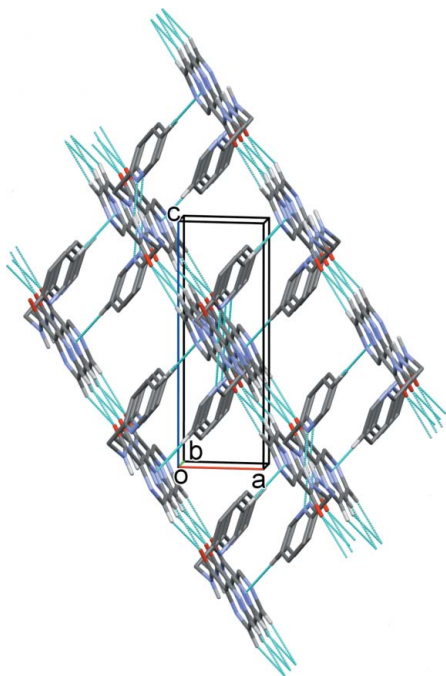
Symmetry codes: (i)  $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$ ; (ii)  $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$ ; (iii)  $x, -y + \frac{1}{2}, z - \frac{1}{2}$ .

the pyrazine (N1/N2/C1—C4) ring [dihedral angle =  $2.56(14)^\circ$ ]. The pyrazine and pyridine (N4/C7—C10) rings are inclined to one another by  $61.34(6)^\circ$ . In the triclinic structure mentioned above, the same angle in the two independent molecules is  $63.31(13)$  and  $61.94(13)^\circ$ .

The molecular structure of HL2 is illustrated in Fig. 2. Here too there is a short intramolecular N—H···N contact involving the pyrazine carboxamide unit (Table 2), and the amide group, C5(=O)N3, is almost coplanar with the pyrazine (N1/N2/C1—C4) ring with a dihedral angle of  $3.9(3)^\circ$ . Here the pyrazine and pyridine (N4/C7—C10) rings are almost normal to one another with a dihedral angle of  $84.33(12)^\circ$ .


**Figure 3**

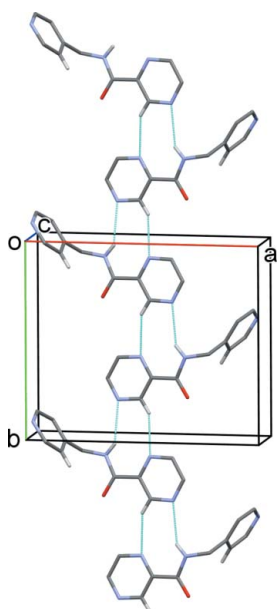
A partial view along the  $a$  axis of the crystal packing of compound HL1. The N—H···N, C—H···O and C—H···N hydrogen bonds are shown as dashed lines (see Table 1 for details).



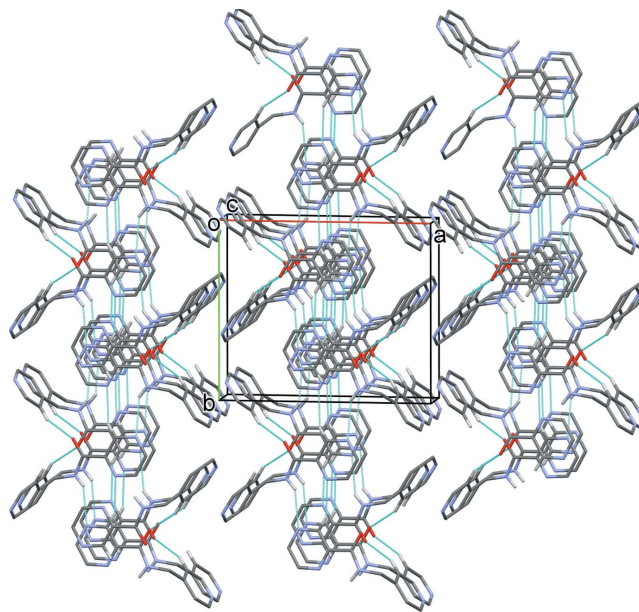
**Figure 4**  
The crystal packing of compound HL1 viewed along the *b* axis. The N—H···N, C—H···O and C—H···N hydrogen bonds are shown as dashed lines (see Table 1 for details).

### 3. Supramolecular features

In the crystal of HL1, molecules are linked by N—H···N hydrogen bonds, forming inversion dimers with an  $R_2^2(10)$  ring motif. The dimers are linked *via* bifurcated-acceptor C—H···O hydrogen bonds, forming sheets lying parallel to (102) (see Table 1 and Fig. 3). The sheets are linked *via* C—H···N hydrogen bonds, forming a three-dimensional structure (Table 1 and Fig. 4).



**Figure 5**  
A partial view along the *c* axis of the crystal packing of compound HL2. The N—H···N, and C—H···N hydrogen bonds are shown as dashed lines (see Table 2 for details).



**Figure 6**  
The crystal packing of compound HL2 viewed along the *c* axis. The N—H···N, C—H···O and C—H···N hydrogen bonds are shown as dashed lines (see Table 2 for details).

In the crystal of HL2, molecules are linked by N—H···N and C—H···N hydrogen bonds to form chains propagating along [010], as shown in Table 2 and Fig. 5. The chains are linked *via* C—H···O hydrogen bonds, forming sheets lying parallel to (100). Within the sheets there are  $\pi$ – $\pi$  interactions involving neighbouring pyrazine rings [ $Cg1 \cdots Cg1^i = 3.7113(15) \text{ \AA}$ ;  $Cg1$  is the centroid of the pyrazine ring N1/N2/C1–C4; symmetry code: (i)  $x, -y + \frac{1}{2}, z - \frac{1}{2}$ ]. The sheets are linked *via* slipped parallel  $\pi$ – $\pi$  interactions involving inversion-related pyridine rings [ $Cg2 \cdots Cg2^{ii} = 3.6395(11) \text{ \AA}$ , normal distance = 3.4164(11), slippage = 1.255  $\text{ \AA}$ ;  $Cg2$  is the centroid of pyridine ring N4/C7–C11; symmetry code: (ii)  $-x, -y, -z$ ], forming a three-dimensional structure (Table 2 and Fig. 6).

### 4. Database survey

A search of the Cambridge Structural Database (Version 5.35, last update November 2013; Allen, 2002) indicated the presence of 282 structures containing the pyrazine-2-carboxamide unit. 81 of these concern pyrazine-2-carboxamide itself. There were 10 hits for complexes of ligand HL1. These include a cobalt(III) (Hellyer *et al.*, 2009), a chromium(III) (Khavasi *et al.*, 2010) and four copper(II) complexes (Mohamadou *et al.*, 2012; Khavasi *et al.*, 2011), all of which are mononuclear with the ligand coordinating in a tridentate manner. There are also two polymeric mercury chloride complexes (Khavasi & Sadegh, 2010), a binuclear manganese chloride complex (Khavasi *et al.*, 2009), and a polymeric silver tetrafluoroborate complex (Hellyer *et al.*, 2009), where the ligand coordinates in a bis-monodentate manner. Plus the report of the ligand itself as mentioned above (Sasan *et al.*, 2008). For ligand HL2 there were no hits.

**Table 3**  
Experimental details.

	HL1	HL2
Crystal data		
Chemical formula	C <sub>11</sub> H <sub>10</sub> N <sub>4</sub> O	C <sub>11</sub> H <sub>10</sub> N <sub>4</sub> O
<i>M<sub>r</sub></i>	214.23	214.23
Crystal system, space group	Monoclinic, <i>P</i> <sub>2</sub> <sub>1</sub> / <i>c</i>	Monoclinic, <i>P</i> <sub>2</sub> <sub>1</sub> / <i>c</i>
Temperature (K)	153	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	4.1527 (4), 20.4629 (18), 12.0106 (11)	13.8564 (14), 11.1841 (11), 6.9122 (10)
$\beta$ (°)	91.461 (11)	104.356 (14)
<i>V</i> (Å <sup>3</sup> )	1020.28 (16)	1037.7 (2)
<i>Z</i>	4	4
Radiation type	Mo <i>K</i> $\alpha$	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	0.10	0.09
Crystal size (mm)	0.50 × 0.40 × 0.35	0.38 × 0.30 × 0.19
Data collection		
Diffractometer	Stoe <i>IPDS</i> 1	Stoe AED2 four-circle
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	7822, 1958, 1548	4132, 1937, 1198
<i>R</i> <sub>int</sub>	0.035	0.032
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.615	0.605
Refinement		
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.032, 0.088, 1.03	0.054, 0.127, 1.10
No. of reflections	1958	1937
No. of parameters	149	150
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}$ , $\Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	0.17, -0.17	0.17, -0.16

Computer programs: *EXPOSE*, *CELL* and *INTEGRATE* in *IPDSI*, *STADIA* and *X-RED* (Stoe & Cie, 1997), *SHELXS97* and *SHELXL2013* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

## 5. Synthesis and crystallization

The precursor pyrazine-2-carboxylic acid methyl ester (2-pze) was prepared following the procedure described by Alvarez-Ibarra *et al.* (1994). 6.21 g (50 mmol) of pyrazine-2-carboxylic acid were added to 50 ml of absolute methanol in a two-necked flask (100 ml). The mixture was heated to 303 K and then 0.4 ml of concentrated sulfuric acid was added slowly. The mixture was heated for 23 h, at least. It was then poured over ice and made alkaline using NaOH (2 *N*), then extracted with CH<sub>2</sub>Cl<sub>2</sub>. The organic extract was dried over Na<sub>2</sub>SO<sub>4</sub>. The resulting yellow product was purified by recrystallization from hexane, or by column chromatography on silica gel using CH<sub>2</sub>Cl<sub>2</sub> as eluant, giving finally colourless crystals (yield 80%).

The ligand HL1 was prepared by refluxing 2-pze (1.80 g, 13 mmol) and an excess of 2-(aminomethyl)pyridine (1.84 g, 17 mmol) in 12 ml of methanol, for 6 h in a two-necked flask (50 ml). A yellowish oil remained when the methanol was evaporated off. The excess of 2-(aminomethyl)pyridine was eliminated by column chromatography on silica gel using CH<sub>2</sub>Cl<sub>2</sub> as eluant (*r* = 2 cm, *l* = 8 cm). A yellow band of 2-(aminomethyl)pyridine remained on the column. After evaporation, the ligand could be recrystallized from diethyl ether, acetonitrile or ethyl acetate. HL1 is very soluble in MeOH and in CH<sub>2</sub>Cl<sub>2</sub>. Recrystallization from diethyl ether gave colourless blocks of HL1 (yield 91%; m.p. 388 K). Analysis for C<sub>11</sub>H<sub>10</sub>N<sub>4</sub>O (*M<sub>r</sub>* = 214.46 g/mol) Calculated (%) C: 61.67 H: 4.71 N: 26.15; Found (%) C: 61.80 H: 4.76 N: 26.45. Spectroscopic data are available in the supporting information.

HL2 was prepared using the same procedure as for HL1. 2-pze (1.38 g, 10 mmol) with, this time, an excess of 4-(aminomethyl)pyridine (1.73 g, 16 mmol) were refluxed in 20 ml of methanol, for 20 h in a two-necked flask (50 ml). 4-(aminomethyl)pyridine (1g, 10 mmol) was then added to the red solution. After 4 h the solution was evaporated to about 8 ml. HL2 crystallized out at room temperature. About 20 ml of diethyl ether was added to filtrate the product. It was then recrystallized from a mixture of 3 ml of methanol and 40 ml of diethyl ether to give colourless blocks (yield 84%; m.p. 422 K). Anal. for C<sub>11</sub>H<sub>10</sub>N<sub>4</sub>O (*M<sub>r</sub>* = 214.46 g/mol) Calculated (%) C: 61.67 H: 4.71 N: 26.15 Found (%) C: 61.57 H: 4.75 N: 26.20. Spectroscopic data are available in the supporting information.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The NH H atoms were located in difference Fourier maps and freely refined. The C-bound H atoms were included in calculated positions and treated as riding atoms: C–H = 0.95 Å for HL1 and = 0.93 Å for HL2, with *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C).

## Acknowledgements

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## supporting information

*Acta Cryst.* (2014). E70, 18-22 [doi:10.1107/S1600536814009519]

## Crystal structures of *N*-(pyridin-2-ylmethyl)pyrazine-2-carboxamide (monoclinic polymorph) and *N*-(pyridin-4-ylmethyl)pyrazine-2-carboxamide

Dilovan S. Cati and Helen Stoeckli-Evans

### Computing details

Data collection: *EXPOSE* in *IPDSI* (Stoe & Cie, 1997) for HL1; *STADI4* (Stoe & Cie, 1997) for HL2. Cell refinement: *CELL* in *IPDSI* (Stoe & Cie, 1997) for HL1; *STADI4* (Stoe & Cie, 1997) for HL2. Data reduction: *INTEGRATE* in *IPDSI* (Stoe & Cie, 1997) for HL1; *X-RED* (Stoe & Cie, 1997) for HL2. For both compounds, program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2013* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

### (HL1) *N*-(Pyridin-2-ylmethyl)pyrazine-2-carboxamide

#### Crystal data

$C_{11}H_{10}N_4O$

$M_r = 214.23$

Monoclinic,  $P2_1/c$

$a = 4.1527$  (4) Å

$b = 20.4629$  (18) Å

$c = 12.0106$  (11) Å

$\beta = 91.461$  (11)°

$V = 1020.28$  (16) Å<sup>3</sup>

$Z = 4$

$F(000) = 448$

$D_x = 1.395$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 6532 reflections

$\theta = 2.0$ – $25.9^\circ$

$\mu = 0.10$  mm<sup>-1</sup>

$T = 153$  K

Block, colourless

$0.50 \times 0.40 \times 0.35$  mm

#### Data collection

Stoe IPDS 1

diffractometer

Radiation source: fine-focus sealed tube

Plane graphite monochromator

$\varphi$  rotation scans

7822 measured reflections

1958 independent reflections

1548 reflections with  $I > 2\sigma(I)$

$R_{int} = 0.035$

$\theta_{max} = 25.9^\circ$ ,  $\theta_{min} = 2.0^\circ$

$h = -5 \rightarrow 5$

$k = -25 \rightarrow 25$

$l = -14 \rightarrow 14$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.032$

$wR(F^2) = 0.088$

$S = 1.03$

1958 reflections

149 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 0.0704P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$

$$\Delta\rho_{\max} = 0.17 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.17 \text{ e } \text{\AA}^{-3}$$

### Special details

**Experimental.** Spectroscopic data for HL1:  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ; code Hh/NH, Hl/C3, Hn/C1, Hm/C2, Hb/C11, Hd/C9, He/C8, Hc/C10, Hg/C6): 9.50 (t, 1H, Jhg = 6.0, Hh); 9.23 (d, 1H, Jlm = 1.5, Hl); 8.91 (d, 1H, Jnm = 2.5, Hn); 8.78 (dd, 1H, Jmn = 2.5, Jml = 1.5, Hm); 8.53 (ddd, 1H, Jbc = 4.8, Jbd = 1.8, Jbe = 0.8, Hb); 7.76 (td, 1H, Jdc = 7.7, Jdb = 1.8, Hd); 7.35 (d, 1H, Jed = 7.9, He); 7.28 (dd, 1H, Jcd = 7.7, Jcb = 4.8, Hc); 4.64 (d, 2H, Jgh = 6.0, He).  $^{13}\text{C}$  NMR (400 MHz, DMSO- $d_6$ ): 163.9, 158.6, 149.7, 148.6, 145.5, 144.4, 144.3, 137.6, 123.1, 121.9, 45.0. IR (KBr pellet,  $\text{cm}^{-1}$ ): 3248 (m), 3066 (w), 3018 (w), 2949 (w), 1669 (versus), 1593 (m), 1570 (m), 1517 (versus), 1478 (m), 1462 (s), 1440 (s), 1423 (s), 1389 (s), 1350 (m), 1320 (m), 1287 (s), 1250 (m), 1221 (m), 1168 (s), 1148 (m), 1103 (m), 1055 (m), 1021 (s), 1000 (m), 975 (m), 870 (m), 840 (w), 776 (m), 753 (s), 707 (m), 634 (m), 611 (m), 528 (m), 444 (m).

**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 ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.7345 (3)	0.30055 (5)	0.42625 (8)	0.0260 (2)
N2	0.7780 (3)	0.16917 (5)	0.49125 (9)	0.0343 (3)
N3	0.4290 (2)	0.38859 (5)	0.55546 (8)	0.0224 (2)
H3N	0.514 (4)	0.3982 (7)	0.4892 (13)	0.037 (4)*
N4	0.5222 (3)	0.53951 (5)	0.66045 (8)	0.0293 (3)
O1	0.3074 (2)	0.30857 (4)	0.67870 (7)	0.0344 (2)
C1	0.6100 (3)	0.27903 (5)	0.52119 (9)	0.0215 (3)
C2	0.6318 (3)	0.21416 (6)	0.55317 (10)	0.0287 (3)
H2	0.5401	0.2011	0.6213	0.034*
C3	0.9010 (3)	0.19099 (6)	0.39702 (10)	0.0305 (3)
H3	1.0071	0.1609	0.3501	0.037*
C4	0.8800 (3)	0.25567 (6)	0.36486 (10)	0.0290 (3)
H4	0.9724	0.2686	0.2967	0.035*
C5	0.4355 (3)	0.32697 (6)	0.59277 (9)	0.0229 (3)
C6	0.2435 (3)	0.43932 (6)	0.60984 (10)	0.0263 (3)
H6A	0.0627	0.4186	0.6488	0.032*
H6B	0.1503	0.4688	0.5522	0.032*
C7	0.4391 (3)	0.47934 (5)	0.69249 (9)	0.0219 (3)
C8	0.5266 (3)	0.45428 (6)	0.79615 (10)	0.0271 (3)
H8	0.4640	0.4113	0.8163	0.033*
C9	0.7051 (3)	0.49220 (6)	0.86977 (10)	0.0312 (3)
H9	0.7682	0.4757	0.9410	0.037*
C10	0.7906 (4)	0.55455 (6)	0.83801 (11)	0.0350 (3)
H10	0.9115	0.5822	0.8870	0.042*
C11	0.6957 (4)	0.57556 (6)	0.73353 (11)	0.0376 (3)
H11	0.7569	0.6183	0.7117	0.045*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0305 (6)	0.0246 (5)	0.0231 (5)	-0.0011 (4)	0.0045 (4)	-0.0005 (4)
N2	0.0434 (7)	0.0239 (5)	0.0356 (6)	0.0046 (5)	0.0043 (5)	-0.0006 (4)
N3	0.0263 (5)	0.0207 (5)	0.0201 (5)	0.0007 (4)	0.0020 (4)	-0.0008 (4)
N4	0.0412 (7)	0.0219 (5)	0.0249 (5)	0.0016 (4)	0.0022 (4)	0.0007 (4)
O1	0.0454 (6)	0.0295 (5)	0.0288 (5)	0.0000 (4)	0.0154 (4)	0.0036 (4)
C1	0.0219 (6)	0.0217 (6)	0.0208 (5)	-0.0024 (5)	-0.0014 (4)	-0.0008 (4)
C2	0.0369 (8)	0.0247 (6)	0.0246 (6)	0.0006 (5)	0.0032 (5)	0.0016 (5)
C3	0.0327 (7)	0.0275 (6)	0.0313 (7)	0.0029 (5)	0.0039 (5)	-0.0067 (5)
C4	0.0321 (7)	0.0305 (6)	0.0246 (6)	-0.0012 (5)	0.0056 (5)	-0.0028 (5)
C5	0.0233 (6)	0.0242 (6)	0.0211 (6)	-0.0021 (5)	-0.0003 (5)	-0.0001 (4)
C6	0.0244 (7)	0.0248 (6)	0.0296 (6)	0.0062 (5)	-0.0010 (5)	-0.0021 (5)
C7	0.0210 (6)	0.0213 (6)	0.0235 (6)	0.0055 (5)	0.0057 (4)	-0.0011 (4)
C8	0.0275 (7)	0.0258 (6)	0.0281 (6)	0.0005 (5)	0.0024 (5)	0.0046 (5)
C9	0.0333 (7)	0.0374 (7)	0.0228 (6)	0.0044 (6)	-0.0001 (5)	0.0010 (5)
C10	0.0420 (8)	0.0310 (7)	0.0317 (7)	-0.0002 (6)	-0.0034 (6)	-0.0093 (5)
C11	0.0554 (9)	0.0207 (6)	0.0366 (7)	-0.0046 (6)	-0.0022 (6)	-0.0006 (5)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

N1—C4	1.3323 (16)	C3—H3	0.9500
N1—C1	1.3386 (15)	C4—H4	0.9500
N2—C3	1.3307 (17)	C6—C7	1.5082 (16)
N2—C2	1.3387 (16)	C6—H6A	0.9900
N3—C5	1.3382 (15)	C6—H6B	0.9900
N3—C6	1.4570 (15)	C7—C8	1.3865 (17)
N3—H3N	0.901 (16)	C8—C9	1.3784 (18)
N4—C7	1.3379 (15)	C8—H8	0.9500
N4—C11	1.3422 (17)	C9—C10	1.3806 (18)
O1—C5	1.2319 (14)	C9—H9	0.9500
C1—C2	1.3842 (16)	C10—C11	1.3745 (19)
C1—C5	1.5028 (16)	C10—H10	0.9500
C2—H2	0.9500	C11—H11	0.9500
C3—C4	1.3808 (18)		
C4—N1—C1	115.80 (10)	N3—C6—C7	113.57 (9)
C3—N2—C2	115.53 (11)	N3—C6—H6A	108.9
C5—N3—C6	121.84 (10)	C7—C6—H6A	108.9
C5—N3—H3N	119.7 (9)	N3—C6—H6B	108.9
C6—N3—H3N	117.7 (9)	C7—C6—H6B	108.9
C7—N4—C11	117.12 (10)	H6A—C6—H6B	107.7
N1—C1—C2	121.86 (11)	N4—C7—C8	122.34 (11)
N1—C1—C5	118.36 (10)	N4—C7—C6	116.69 (10)
C2—C1—C5	119.76 (10)	C8—C7—C6	120.97 (11)
N2—C2—C1	122.19 (11)	C9—C8—C7	119.49 (11)
N2—C2—H2	118.9	C9—C8—H8	120.3



C1—C2—H2	118.9	C7—C8—H8	120.3
N2—C3—C4	122.47 (11)	C8—C9—C10	118.73 (11)
N2—C3—H3	118.8	C8—C9—H9	120.6
C4—C3—H3	118.8	C10—C9—H9	120.6
N1—C4—C3	122.14 (11)	C11—C10—C9	118.14 (12)
N1—C4—H4	118.9	C11—C10—H10	120.9
C3—C4—H4	118.9	C9—C10—H10	120.9
O1—C5—N3	124.27 (11)	N4—C11—C10	124.17 (12)
O1—C5—C1	120.30 (10)	N4—C11—H11	117.9
N3—C5—C1	115.43 (10)	C10—C11—H11	117.9
C4—N1—C1—C2	0.03 (17)	C2—C1—C5—N3	179.54 (11)
C4—N1—C1—C5	-178.51 (11)	C5—N3—C6—C7	95.48 (13)
C3—N2—C2—C1	0.06 (19)	C11—N4—C7—C8	-0.18 (18)
N1—C1—C2—N2	-0.1 (2)	C11—N4—C7—C6	179.86 (11)
C5—C1—C2—N2	178.43 (11)	N3—C6—C7—N4	104.41 (12)
C2—N2—C3—C4	0.03 (19)	N3—C6—C7—C8	-75.55 (14)
C1—N1—C4—C3	0.05 (18)	N4—C7—C8—C9	0.12 (18)
N2—C3—C4—N1	-0.1 (2)	C6—C7—C8—C9	-179.92 (11)
C6—N3—C5—O1	-5.16 (19)	C7—C8—C9—C10	0.33 (19)
C6—N3—C5—C1	174.05 (10)	C8—C9—C10—C11	-0.7 (2)
N1—C1—C5—O1	177.36 (11)	C7—N4—C11—C10	-0.2 (2)
C2—C1—C5—O1	-1.21 (18)	C9—C10—C11—N4	0.6 (2)
N1—C1—C5—N3	-1.88 (16)		

*Hydrogen-bond geometry* (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N3—H3 <i>N</i> ...N1	0.901 (16)	2.332 (15)	2.7136 (15)	105.4 (11)
N3—H3 <i>N</i> ...N4 <sup>i</sup>	0.901 (16)	2.206 (16)	2.9929 (14)	145.6 (13)
C3—H3...O1 <sup>ii</sup>	0.95	2.51	3.1544 (15)	125
C4—H4...O1 <sup>ii</sup>	0.95	2.56	3.1748 (15)	123
C10—H10...N2 <sup>iii</sup>	0.95	2.62	3.5678 (17)	174

Symmetry codes: (i)  $-x+1, -y+1, -z+1$ ; (ii)  $x+1, -y+1/2, z-1/2$ ; (iii)  $-x+2, y+1/2, -z+3/2$ .**(HL2) *N*-(Pyridin-4-ylmethyl)pyrazine-2-carboxamide***Crystal data*C<sub>11</sub>H<sub>10</sub>N<sub>4</sub>O $M_r = 214.23$ Monoclinic,  $P2_1/c$  $a = 13.8564$  (14) Å $b = 11.1841$  (11) Å $c = 6.9122$  (10) Å $\beta = 104.356$  (14)° $V = 1037.7$  (2) Å<sup>3</sup> $Z = 4$  $F(000) = 448$  $D_x = 1.371$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 20 reflections

 $\theta = 10.4$ – $17.6$ ° $\mu = 0.09$  mm<sup>-1</sup> $T = 293$  K

Block, colourless

 $0.38 \times 0.30 \times 0.19$  mm

Data collection

Stoe AED2 four-circle  
diffractometer  
Radiation source: fine-focus sealed tube  
Plane graphite monochromator  
2 $\theta$ / $\omega$  scans  
4132 measured reflections  
1937 independent reflections  
1198 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.032$   
 $\theta_{\text{max}} = 25.5^\circ$ ,  $\theta_{\text{min}} = 2.4^\circ$   
 $h = -16 \rightarrow 16$   
 $k = -13 \rightarrow 0$   
 $l = -8 \rightarrow 8$   
2 standard reflections every 60 min  
intensity decay: 2%

Refinement

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.054$   
 $wR(F^2) = 0.127$   
 $S = 1.10$   
1937 reflections  
150 parameters  
0 restraints  
Hydrogen site location: mixed

H atoms treated by a mixture of independent  
and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0426P)^2 + 0.1904P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.17 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.16 \text{ e } \text{\AA}^{-3}$   
Extinction correction: *SHELXL2013* (Sheldrick,  
2008),  $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$   
Extinction coefficient: 0.014 (2)

Special details

**Experimental.** Spectroscopic data for HL2: <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>; code Hh/NH, Hl/C3, Hn/C1, Hm/C2, Hb/C11, Hd/C9, Ha/C11/, He/C8, Hg/C6): 9.63 (t, 1H, J<sub>hg</sub> = 6.3, Hh); 9.21 (d, 1H, J<sub>lm</sub> = 1.5, Hl); 8.90 (d, 1H, J<sub>nm</sub> = 2.5, Hn); 8.77 (dd, 1H, J<sub>mn</sub> = 2.5, J<sub>ml</sub> = 1.5, Hm); 8.49 (dd, 2H, J<sub>ba</sub> = 4.4, J<sub>be</sub> = 1.6, Hb = Hd); 7.31 (dd, 2H, J<sub>ab</sub> = 4.4, J<sub>ad</sub> = 1.6, Ha = He); 4.54 (d, 2H, J<sub>gh</sub> = 6.3, Hg). <sup>13</sup>C NMR (400 MHz, DMSO-d<sub>6</sub>): 164.2, 150.4, 149.0, 148.5, 145.4, 144.5, 144.3, 123.0, 42.4. IR (KBr pellet, cm<sup>-1</sup>): 3366 (*versus*), 3089 (*s*), 3050 (*m*), 3031 (*s*), 2967 (*m*), 2935 (*s*), 1966 (*w*), 1924 (*w*), 1834 (*w*), 1674 (*versus*), 1634 (*s*), 1602 (*versus*), 1585 (*s*), 1564 (*s*) 1526 (*versus*), 1467 (*versus*), 1429 (*versus*), 1415 (*versus*), 1399 (*versus*), 1359 (*s*), 1329 (*s*), 1288 (*versus*), 1240 (*m*), 1216 (*versus*), 1167 (*s*), 1155 (*s*), 1059 (*versus*), 1025 (*versus*), 1020 (*versus*), 993 (*s*), 981 (*s*), 968 (*s*), 887 (*m*), 870 (*s*), 842 (*s*), 832 (*s*), 804 (*versus*), 775 (*s*), 731 (*m*), 652 (*versus*), 608 (*s*), 517 (*s*), 479 (*m*), 445 (*versus*), 411 (*m*).

**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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.32038 (14)	0.28041 (15)	0.2248 (3)	0.0618 (6)
N1	0.52051 (15)	0.08089 (17)	0.2297 (3)	0.0456 (6)
N2	0.61838 (17)	0.29856 (19)	0.2153 (3)	0.0530 (6)
N3	0.32823 (16)	0.0787 (2)	0.2548 (3)	0.0495 (6)
H3N	0.367 (2)	0.022 (2)	0.251 (4)	0.057 (9)*
N4	0.04496 (18)	-0.1046 (2)	-0.2659 (4)	0.0677 (7)
C1	0.47371 (18)	0.1855 (2)	0.2255 (3)	0.0389 (6)
C2	0.5226 (2)	0.2927 (2)	0.2174 (4)	0.0477 (7)
H2	0.4870	0.3635	0.2132	0.057*
C3	0.6641 (2)	0.1935 (2)	0.2189 (4)	0.0531 (7)
H3	0.7309	0.1925	0.2166	0.064*
C4	0.61612 (19)	0.0861 (2)	0.2258 (4)	0.0510 (7)

H4	0.6515	0.0153	0.2279	0.061*
C5	0.36661 (19)	0.1863 (2)	0.2342 (4)	0.0442 (6)
C6	0.22661 (19)	0.0590 (2)	0.2660 (4)	0.0548 (7)
H6A	0.1972	0.1350	0.2877	0.066*
H6B	0.2267	0.0080	0.3795	0.066*
C7	0.16399 (17)	0.0020 (2)	0.0798 (4)	0.0431 (6)
C8	0.1571 (2)	0.0498 (2)	-0.1071 (4)	0.0534 (7)
H8	0.1922	0.1187	-0.1216	0.064*
C9	0.0979 (2)	-0.0052 (3)	-0.2711 (5)	0.0652 (8)
H9	0.0943	0.0291	-0.3953	0.078*
C10	0.0528 (2)	-0.1497 (2)	-0.0853 (5)	0.0627 (8)
H10	0.0171	-0.2188	-0.0752	0.075*
C11	0.11055 (19)	-0.1010 (2)	0.0887 (4)	0.0517 (7)
H11	0.1134	-0.1374	0.2110	0.062*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0615 (13)	0.0417 (11)	0.0868 (15)	0.0116 (10)	0.0272 (11)	-0.0013 (10)
N1	0.0459 (13)	0.0334 (12)	0.0586 (14)	0.0012 (10)	0.0149 (10)	-0.0024 (10)
N2	0.0553 (15)	0.0427 (14)	0.0610 (15)	-0.0100 (11)	0.0144 (11)	-0.0006 (11)
N3	0.0421 (14)	0.0421 (14)	0.0663 (16)	-0.0008 (11)	0.0170 (11)	-0.0043 (11)
N4	0.0590 (16)	0.0684 (18)	0.0749 (19)	0.0011 (13)	0.0148 (14)	-0.0111 (15)
C1	0.0441 (14)	0.0323 (13)	0.0399 (14)	-0.0006 (11)	0.0101 (11)	-0.0028 (11)
C2	0.0560 (18)	0.0325 (15)	0.0531 (17)	0.0008 (12)	0.0109 (13)	-0.0023 (12)
C3	0.0488 (17)	0.0505 (16)	0.0607 (17)	-0.0050 (14)	0.0149 (13)	0.0007 (14)
C4	0.0496 (16)	0.0406 (15)	0.0646 (18)	0.0044 (13)	0.0174 (13)	-0.0019 (13)
C5	0.0501 (16)	0.0376 (14)	0.0447 (15)	0.0009 (13)	0.0117 (12)	-0.0045 (12)
C6	0.0471 (16)	0.0585 (18)	0.0625 (19)	-0.0012 (13)	0.0206 (14)	-0.0040 (14)
C7	0.0321 (13)	0.0416 (14)	0.0582 (18)	0.0048 (11)	0.0162 (12)	0.0016 (12)
C8	0.0442 (15)	0.0551 (17)	0.0646 (19)	-0.0022 (13)	0.0204 (14)	0.0059 (15)
C9	0.0589 (19)	0.084 (2)	0.056 (2)	0.0091 (17)	0.0214 (16)	0.0066 (17)
C10	0.0530 (18)	0.0444 (16)	0.092 (3)	-0.0008 (14)	0.0204 (17)	-0.0063 (17)
C11	0.0457 (15)	0.0439 (15)	0.0674 (19)	0.0043 (13)	0.0179 (13)	0.0087 (14)

*Geometric parameters (Å, °)*

O1—C5	1.225 (3)	C3—H3	0.9300
N1—C4	1.333 (3)	C4—H4	0.9300
N1—C1	1.334 (3)	C6—C7	1.504 (3)
N2—C3	1.332 (3)	C6—H6A	0.9700
N2—C2	1.333 (3)	C6—H6B	0.9700
N3—C5	1.338 (3)	C7—C11	1.379 (3)
N3—C6	1.446 (3)	C7—C8	1.379 (4)
N3—H3N	0.83 (3)	C8—C9	1.369 (4)
N4—C10	1.325 (4)	C8—H8	0.9300
N4—C9	1.337 (4)	C9—H9	0.9300
C1—C2	1.385 (3)	C10—C11	1.381 (4)

C1—C5	1.500 (3)	C10—H10	0.9300
C2—H2	0.9300	C11—H11	0.9300
C3—C4	1.379 (3)		
C4—N1—C1	116.2 (2)	N3—C6—C7	112.4 (2)
C3—N2—C2	115.2 (2)	N3—C6—H6A	109.1
C5—N3—C6	124.1 (2)	C7—C6—H6A	109.1
C5—N3—H3N	113.8 (19)	N3—C6—H6B	109.1
C6—N3—H3N	121.9 (19)	C7—C6—H6B	109.1
C10—N4—C9	115.1 (3)	H6A—C6—H6B	107.9
N1—C1—C2	121.3 (2)	C11—C7—C8	116.9 (3)
N1—C1—C5	119.0 (2)	C11—C7—C6	121.2 (2)
C2—C1—C5	119.6 (2)	C8—C7—C6	121.9 (2)
N2—C2—C1	122.8 (2)	C9—C8—C7	119.3 (3)
N2—C2—H2	118.6	C9—C8—H8	120.3
C1—C2—H2	118.6	C7—C8—H8	120.3
N2—C3—C4	122.5 (3)	N4—C9—C8	124.8 (3)
N2—C3—H3	118.7	N4—C9—H9	117.6
C4—C3—H3	118.7	C8—C9—H9	117.6
N1—C4—C3	121.9 (2)	N4—C10—C11	124.4 (3)
N1—C4—H4	119.0	N4—C10—H10	117.8
C3—C4—H4	119.0	C11—C10—H10	117.8
O1—C5—N3	124.2 (2)	C7—C11—C10	119.5 (3)
O1—C5—C1	120.9 (2)	C7—C11—H11	120.3
N3—C5—C1	114.9 (2)	C10—C11—H11	120.3
C4—N1—C1—C2	0.1 (3)	C2—C1—C5—N3	-175.8 (2)
C4—N1—C1—C5	-178.6 (2)	C5—N3—C6—C7	108.0 (3)
C3—N2—C2—C1	0.9 (4)	N3—C6—C7—C11	126.7 (3)
N1—C1—C2—N2	-0.7 (4)	N3—C6—C7—C8	-53.3 (3)
C5—C1—C2—N2	178.0 (2)	C11—C7—C8—C9	0.8 (4)
C2—N2—C3—C4	-0.5 (4)	C6—C7—C8—C9	-179.2 (2)
C1—N1—C4—C3	0.3 (4)	C10—N4—C9—C8	0.0 (4)
N2—C3—C4—N1	-0.1 (4)	C7—C8—C9—N4	-0.3 (4)
C6—N3—C5—O1	0.9 (4)	C9—N4—C10—C11	-0.1 (4)
C6—N3—C5—C1	-179.9 (2)	C8—C7—C11—C10	-0.9 (4)
N1—C1—C5—O1	-177.8 (2)	C6—C7—C11—C10	179.1 (2)
C2—C1—C5—O1	3.4 (4)	N4—C10—C11—C7	0.6 (4)
N1—C1—C5—N3	2.9 (3)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N3—H3N...N1	0.83 (3)	2.27 (3)	2.713 (3)	114 (2)
N3—H3N...N2 <sup>i</sup>	0.83 (3)	2.52 (3)	3.214 (3)	142 (2)

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C2—H2···N1 <sup>ii</sup>	0.93	2.47	3.315 (3)	151
C8—H8···O1 <sup>iii</sup>	0.93	2.55	3.373 (3)	148

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