

Acta Crystallographica Section E

## Structure Reports

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# *N,N'*-Bis(8-quinolyl)pyridine-2,6-dicarboxamide

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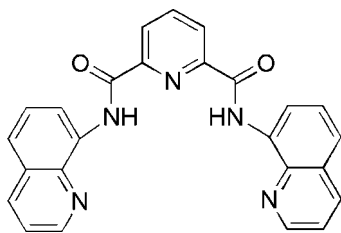
Received 29 October 2007; accepted 20 November 2007

 Key indicators: single-crystal X-ray study;  $T = 294$  K; mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å;  $R$  factor = 0.078;  $wR$  factor = 0.115; data-to-parameter ratio = 7.9.

In the molecule of the title compound,  $\text{C}_{25}\text{H}_{17}\text{N}_5\text{O}_2$ , the pyridyl ring is oriented at dihedral angles of 8.90 (3) and 28.67 (4)° with respect to the two planar quinolyl ring systems. Intramolecular  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bonds result in the formation of four planar five-membered rings, two of which are nearly coplanar with the adjacent quinolyl ring systems.

## Related literature

For related literature, see: Amirnasr *et al.* (2002); Meghdadi, Amirnasr *et al.* (2006); Meghdadi, Khavasi *et al.* (2006); Belda & Moberg (2005). For bond-length data, see: Allen *et al.* (1987).



## Experimental

### Crystal data

 $\text{C}_{25}\text{H}_{17}\text{N}_5\text{O}_2$   
 $M_r = 419.44$ 

 Orthorhombic,  $P2_12_12_1$   
 $a = 4.5443$  (13) Å

 $b = 17.030$  (6) Å  
 $c = 25.984$  (8) Å  
 $V = 2010.9$  (11) Å<sup>3</sup>  
 $Z = 4$ 

 Mo  $K\alpha$  radiation  
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 294$  (2) K  
 $0.35 \times 0.12 \times 0.01$  mm

### Data collection

 STOE IPDS II diffractometer  
 Absorption correction: none  
 20853 measured reflections

 2822 independent reflections  
 2161 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.108$ 

### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.078$   
 $wR(F^2) = 0.115$   
 $S = 1.34$   
 2822 reflections  
 357 parameters

 H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.19$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.19$  e Å<sup>-3</sup>

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

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N2}-\text{H2b}\cdots\text{N1}$	0.86 (4)	2.23 (4)	2.638 (5)	109 (3)
$\text{N2}-\text{H2b}\cdots\text{N3}$	0.86 (4)	2.19 (4)	2.666 (5)	115 (3)
$\text{N4}-\text{H4b}\cdots\text{N3}$	0.93 (4)	2.23 (3)	2.669 (5)	108 (2)
$\text{N4}-\text{H4b}\cdots\text{N5}$	0.93 (4)	2.23 (3)	2.667 (5)	108 (2)

Data collection: *X-Area* (Stoe & Cie, 2005); cell refinement: *X-Area*; data reduction: *X-RED32* (Stoe & Cie, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2359).

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## supporting information

*Acta Cryst.* (2008). E64, o431 [doi:10.1107/S1600536807055031]

***N,N'*-Bis(8-quinolyl)pyridine-2,6-dicarboxamide****Soraia Meghdadi, Saeid Nalchigar and Hamid Reza Khavasi****S1. Comment**

The carboxamide [C(O)NH] group, ubiquitous throughout the nature in the primary structure of proteins, is an important ligand construction unit for coordination chemists. Pyridine or quinolyl carboxamides, a burgeoning class of multidentate ligands containing this linkage, are available from condensation reactions between pyridyl or quinolyl-bearing amines and carboxylic acid, promoted by coupling agents such as triphenylphosphite (Amirnasr *et al.*, 2002; Meghdadi, Amirnasr *et al.* (2006); Meghdadi, Khavasi *et al.* (2006). These ligands have found use in asymmetric catalysis (Belda & Moberg, 2005). As part of our ongoing studies in this area, we report herein the crystal structure of the title compound, (I).

In the molecule of (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Rings A (N1/C1—C4/C9), B (C4—C9), C (N3/C11—C15), D (C17—C22) and E (N5/C17/C22—C25) are, of course, planar and rings A, B and D, E are also co-planar with dihedral angles of A/B = 1.01 (2)° and D/E = 0.52 (3)°. Ring C is oriented with respect to the co-planar rings at dihedral angles of 8.90 (4)° and 28.93 (3)°, respectively. The co-planar rings are oriented at a dihedral angle of 24.68 (3)°.

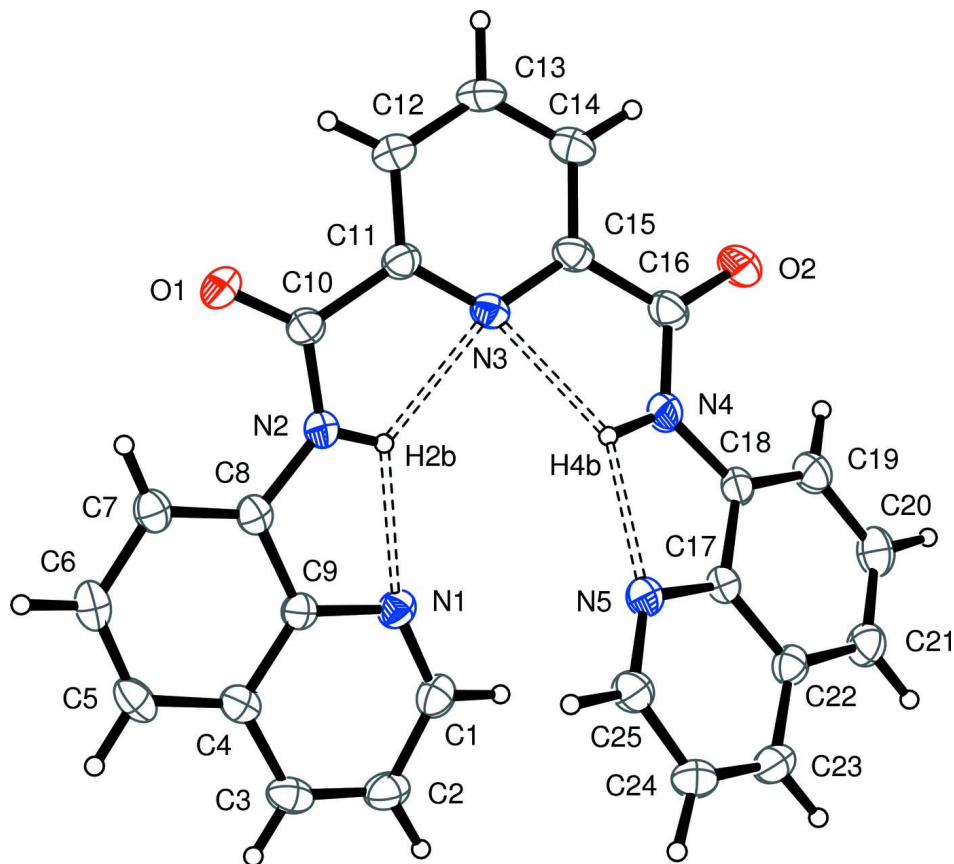
The intramolecular N—H···N hydrogen bonds (Table 1) result in the formation of the planar five-membered rings; F (N1/N2/C8/C9/H2b), G (N2/N3/C10/C11/H2b), H (N3/N4/C15/C16/H4b) and I (N4/N5/C17/C18/H4b), in which rings H and I are also nearly co-planar with the adjacent co-planar rings A, B and D, E at dihedral angles of 4.44 (4)° and 6.06 (5)°, respectively.

**S2. Experimental**

2,6-Pyridinedicarboxylic acid (1.00 g, 6 mmol) was suspended in pyridine (40 ml). 8-aminoquinoline (1.73 g, 12 mmol) was added to the mixture, and the mixture was stirred at 313–318 K, for 10 min. Triphenylphosphite (12 mmol, 3.2 ml) was added dropwise to the resulting solution. The temperature of the reaction mixture was increased to 363–373 K, and the mixture was magnetically stirred for 4 h. After cooling to room temperature, the reaction mixture was left in the hood for 24 h. The white precipitate was filtered off. Recrystallization was achieved by diethyl ether diffusion into a chloroform solution of the compound at room temperature (yield; 87%, m.p. 549 K).

**S3. Refinement**

H atoms were located in difference syntheses and refined isotropically [C—H = 0.92 (4)–1.00 (4) Å and  $U_{\text{iso}}(\text{H}) = 0.025 (10)$ – $0.077 (17)$  Å<sup>2</sup>; N—H = 0.86 (4) and 0.93 (4) Å,  $U_{\text{iso}}(\text{H}) = 0.029 (10)$  and  $0.035 (11)$  Å<sup>2</sup>].



**Figure 1**

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen bonds are shown as dashed lines.

### *N,N'*-Bis(8-quinoly)pyridine-2,6-dicarboxamide

#### Crystal data

$C_{25}H_{17}N_5O_2$

$M_r = 419.44$

Orthorhombic,  $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 4.5443$  (13) Å

$b = 17.030$  (6) Å

$c = 25.984$  (8) Å

$V = 2010.9$  (11) Å<sup>3</sup>

$Z = 4$

$F(000) = 872$

$D_x = 1.385$  Mg m<sup>-3</sup>

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

Cell parameters from 2000 reflections

$\mu = 0.09$  mm<sup>-1</sup>

$T = 294$  K

Plate, colorless

$0.35 \times 0.12 \times 0.01$  mm

#### Data collection

STOE IPDS II

diffractometer

rotation method scans

20853 measured reflections

2822 independent reflections

2161 reflections with  $I > 2\sigma(I)$

$R_{int} = 0.108$

$\theta_{max} = 28.1^\circ$ ,  $\theta_{min} = 1.6^\circ$

$h = -5 \rightarrow 5$

$k = -22 \rightarrow 22$

$l = -34 \rightarrow 34$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.078$   
 $wR(F^2) = 0.115$   
 $S = 1.34$   
 2822 reflections  
 357 parameters  
 0 restraints

H atoms treated by a mixture of independent  
 and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0157P)^2 + 0.8034P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.19 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.19 \text{ e } \text{\AA}^{-3}$

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	-1.1830 (9)	0.20409 (17)	-0.25242 (11)	0.0583 (9)
O2	-0.7396 (9)	0.11039 (19)	-0.00052 (11)	0.0661 (10)
N1	-0.4455 (8)	-0.00267 (19)	-0.23061 (13)	0.0428 (9)
N2	-0.8476 (9)	0.1090 (2)	-0.23237 (13)	0.0403 (8)
H2B	-0.772 (10)	0.087 (2)	-0.2057 (14)	0.035 (11)*
N3	-0.9289 (8)	0.13333 (18)	-0.13200 (13)	0.0394 (8)
N4	-0.6766 (10)	0.02863 (19)	-0.06957 (12)	0.0482 (10)
H4B	-0.737 (9)	0.0212 (19)	-0.1036 (14)	0.029 (10)*
N5	-0.6672 (9)	-0.10469 (19)	-0.12342 (12)	0.0433 (9)
C1	-0.2521 (11)	-0.0600 (3)	-0.22863 (18)	0.0497 (12)
H1	-0.158 (9)	-0.0703 (19)	-0.1965 (13)	0.025 (10)*
C2	-0.1689 (12)	-0.1062 (3)	-0.2710 (2)	0.0546 (12)
H2	-0.030 (12)	-0.147 (3)	-0.2656 (17)	0.062 (15)*
C3	-0.2898 (12)	-0.0903 (2)	-0.31741 (19)	0.0485 (11)
H3	-0.242 (11)	-0.118 (2)	-0.3467 (16)	0.045 (12)*
C4	-0.4986 (10)	-0.0292 (2)	-0.32281 (15)	0.0398 (10)
C5	-0.6346 (12)	-0.0079 (3)	-0.36987 (16)	0.0501 (13)
H5	-0.586 (9)	-0.0384 (19)	-0.4011 (14)	0.029 (10)*
C6	-0.8307 (12)	0.0518 (3)	-0.37084 (17)	0.0498 (12)
H6	-0.923 (11)	0.063 (2)	-0.4024 (18)	0.058 (14)*
C7	-0.9085 (11)	0.0937 (3)	-0.32581 (16)	0.0425 (11)
H7	-1.047 (10)	0.134 (2)	-0.3262 (15)	0.045 (13)*
C8	-0.7823 (10)	0.0742 (2)	-0.27974 (15)	0.0369 (9)
C9	-0.5688 (10)	0.0130 (2)	-0.27723 (15)	0.0359 (9)
C10	-1.0437 (11)	0.1664 (2)	-0.22071 (16)	0.0403 (10)
C11	-1.0722 (10)	0.1816 (2)	-0.16408 (16)	0.0402 (10)
C12	-1.2395 (12)	0.2443 (3)	-0.14696 (19)	0.0534 (13)
H12	-1.337 (12)	0.277 (3)	-0.1714 (17)	0.062 (15)*
C13	-1.2533 (13)	0.2591 (3)	-0.0948 (2)	0.0595 (14)
H13	-1.357 (13)	0.304 (3)	-0.0808 (18)	0.077 (17)*

C14	-1.1027 (13)	0.2106 (3)	-0.06103 (19)	0.0559 (14)
H14	-1.103 (12)	0.221 (2)	-0.0244 (17)	0.065 (15)*
C15	-0.9457 (11)	0.1478 (2)	-0.08149 (16)	0.0422 (10)
C16	-0.7765 (12)	0.0943 (2)	-0.04607 (15)	0.0484 (12)
C17	-0.5007 (9)	-0.1025 (2)	-0.07963 (14)	0.0359 (9)
C18	-0.5091 (11)	-0.0328 (2)	-0.04887 (15)	0.0392 (10)
C19	-0.3521 (12)	-0.0288 (3)	-0.00420 (16)	0.0513 (12)
H19	-0.354 (10)	0.018 (2)	0.0165 (14)	0.046 (12)*
C20	-0.1806 (13)	-0.0928 (3)	0.01167 (18)	0.0579 (13)
H20	-0.092 (12)	-0.090 (2)	0.0438 (17)	0.060 (14)*
C21	-0.1634 (12)	-0.1597 (3)	-0.01678 (18)	0.0526 (12)
H21	-0.059 (12)	-0.206 (2)	-0.0069 (18)	0.068 (16)*
C22	-0.3258 (11)	-0.1664 (2)	-0.06304 (15)	0.0426 (10)
C23	-0.3234 (12)	-0.2336 (3)	-0.09477 (18)	0.0506 (12)
H23	-0.205 (11)	-0.277 (2)	-0.0844 (15)	0.053 (13)*
C24	-0.4870 (12)	-0.2346 (3)	-0.13880 (19)	0.0508 (12)
H24	-0.480 (10)	-0.280 (2)	-0.1630 (15)	0.041 (11)*
C25	-0.6587 (12)	-0.1694 (3)	-0.15076 (17)	0.0496 (12)
H25	-0.769 (11)	-0.170 (2)	-0.1836 (14)	0.045 (12)*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.073 (2)	0.0501 (17)	0.0519 (17)	0.0201 (19)	-0.008 (2)	0.0062 (14)
O2	0.094 (3)	0.067 (2)	0.0376 (16)	0.015 (2)	-0.006 (2)	-0.0164 (14)
N1	0.038 (2)	0.0422 (19)	0.048 (2)	0.0026 (18)	-0.0001 (19)	0.0046 (16)
N2	0.047 (2)	0.0407 (18)	0.0333 (18)	0.0031 (19)	-0.0024 (18)	0.0000 (15)
N3	0.042 (2)	0.0364 (17)	0.0394 (18)	-0.0006 (17)	0.0025 (18)	-0.0065 (14)
N4	0.070 (3)	0.0424 (19)	0.0318 (18)	0.002 (2)	-0.006 (2)	-0.0033 (15)
N5	0.050 (2)	0.0441 (19)	0.0360 (18)	0.0030 (19)	-0.0062 (18)	-0.0019 (15)
C1	0.046 (3)	0.049 (3)	0.054 (3)	0.001 (2)	0.002 (3)	0.011 (2)
C2	0.050 (3)	0.045 (3)	0.069 (3)	0.008 (3)	0.015 (3)	0.003 (2)
C3	0.046 (3)	0.041 (2)	0.058 (3)	-0.007 (2)	0.017 (3)	-0.010 (2)
C4	0.040 (2)	0.037 (2)	0.042 (2)	-0.011 (2)	0.010 (2)	-0.0033 (17)
C5	0.059 (3)	0.055 (3)	0.036 (2)	-0.018 (3)	0.014 (2)	-0.009 (2)
C6	0.054 (3)	0.061 (3)	0.035 (2)	-0.014 (3)	-0.005 (3)	0.004 (2)
C7	0.043 (3)	0.046 (2)	0.039 (2)	-0.008 (2)	0.002 (2)	0.0035 (19)
C8	0.037 (2)	0.036 (2)	0.038 (2)	-0.0098 (19)	0.003 (2)	0.0023 (16)
C9	0.036 (2)	0.0315 (19)	0.040 (2)	-0.0049 (19)	0.007 (2)	0.0035 (16)
C10	0.046 (3)	0.033 (2)	0.042 (2)	-0.002 (2)	0.002 (2)	-0.0006 (17)
C11	0.042 (3)	0.034 (2)	0.044 (2)	0.002 (2)	0.002 (2)	0.0016 (17)
C12	0.062 (3)	0.042 (2)	0.057 (3)	0.012 (3)	0.004 (3)	0.000 (2)
C13	0.070 (4)	0.041 (2)	0.067 (3)	0.019 (3)	0.011 (3)	-0.012 (2)
C14	0.069 (4)	0.049 (3)	0.049 (3)	0.003 (3)	0.003 (3)	-0.015 (2)
C15	0.048 (3)	0.034 (2)	0.044 (2)	-0.004 (2)	0.007 (2)	-0.0079 (17)
C16	0.061 (3)	0.045 (2)	0.039 (2)	-0.005 (2)	0.002 (2)	-0.0093 (18)
C17	0.035 (2)	0.040 (2)	0.032 (2)	-0.0021 (19)	0.0022 (18)	0.0007 (16)
C18	0.047 (3)	0.041 (2)	0.0297 (19)	-0.001 (2)	0.002 (2)	0.0025 (16)

C19	0.063 (3)	0.054 (3)	0.037 (2)	-0.002 (3)	-0.006 (3)	-0.006 (2)
C20	0.061 (3)	0.074 (3)	0.039 (2)	-0.004 (3)	-0.016 (3)	0.005 (2)
C21	0.050 (3)	0.059 (3)	0.049 (3)	0.008 (3)	-0.005 (3)	0.007 (2)
C22	0.040 (3)	0.044 (2)	0.044 (2)	-0.001 (2)	0.003 (2)	0.0070 (18)
C23	0.051 (3)	0.040 (2)	0.061 (3)	0.007 (2)	0.003 (3)	0.004 (2)
C24	0.057 (3)	0.039 (2)	0.056 (3)	0.000 (2)	0.000 (3)	-0.010 (2)
C25	0.055 (3)	0.050 (3)	0.044 (2)	-0.001 (3)	-0.009 (3)	-0.0064 (19)

*Geometric parameters (Å, °)*

C1—N1	1.314 (6)	C14—C15	1.392 (6)
C1—C2	1.406 (6)	C14—H14	0.97 (4)
C1—H1	0.95 (4)	C15—N3	1.338 (5)
C2—C3	1.352 (7)	C15—C16	1.506 (6)
C2—H2	0.94 (5)	C16—O2	1.227 (5)
C3—C4	1.416 (6)	C16—N4	1.353 (5)
C3—H3	0.92 (4)	C17—N5	1.367 (5)
C4—C5	1.418 (6)	C17—C22	1.414 (6)
C4—C9	1.421 (5)	C17—C18	1.432 (5)
C5—C6	1.351 (7)	C18—C19	1.364 (6)
C5—H5	0.99 (4)	C18—N4	1.401 (5)
C6—C7	1.416 (6)	C19—C20	1.402 (7)
C6—H6	0.94 (5)	C19—H19	0.96 (4)
C7—C8	1.369 (6)	C20—C21	1.360 (7)
C7—H7	0.93 (4)	C20—H20	0.93 (5)
C8—N2	1.398 (5)	C21—C22	1.415 (6)
C8—C9	1.425 (6)	C21—H21	0.95 (5)
C9—N1	1.361 (5)	C22—C23	1.411 (6)
C10—O1	1.222 (5)	C23—C24	1.365 (7)
C10—N2	1.357 (5)	C23—H23	0.95 (4)
C10—C11	1.500 (6)	C24—C25	1.392 (7)
C11—N3	1.339 (5)	C24—H24	1.00 (4)
C11—C12	1.385 (6)	C25—N5	1.312 (5)
C12—C13	1.381 (6)	C25—H25	0.99 (4)
C12—H12	0.95 (5)	N2—H2B	0.86 (4)
C13—C14	1.385 (7)	N4—H4B	0.93 (4)
C13—H13	0.97 (5)		
N1—C1—C2	124.4 (5)	N3—C15—C14	123.1 (4)
N1—C1—H1	118 (2)	N3—C15—C16	117.3 (4)
C2—C1—H1	118 (2)	C14—C15—C16	119.6 (4)
C3—C2—C1	118.5 (5)	O2—C16—N4	125.1 (4)
C3—C2—H2	123 (3)	O2—C16—C15	121.6 (4)
C1—C2—H2	118 (3)	N4—C16—C15	113.3 (3)
C2—C3—C4	120.5 (4)	N5—C17—C22	123.0 (4)
C2—C3—H3	123 (3)	N5—C17—C18	118.2 (4)
C4—C3—H3	117 (3)	C22—C17—C18	118.8 (4)
C3—C4—C5	124.5 (4)	C19—C18—N4	125.0 (4)

C3—C4—C9	116.1 (4)	C19—C18—C17	120.1 (4)
C5—C4—C9	119.4 (4)	N4—C18—C17	114.8 (4)
C6—C5—C4	119.7 (4)	C18—C19—C20	120.2 (4)
C6—C5—H5	122 (2)	C18—C19—H19	121 (3)
C4—C5—H5	118 (2)	C20—C19—H19	119 (3)
C5—C6—C7	121.9 (5)	C21—C20—C19	121.6 (5)
C5—C6—H6	118 (3)	C21—C20—H20	121 (3)
C7—C6—H6	120 (3)	C19—C20—H20	118 (3)
C8—C7—C6	119.7 (4)	C20—C21—C22	119.9 (5)
C8—C7—H7	118 (3)	C20—C21—H21	125 (3)
C6—C7—H7	122 (3)	C22—C21—H21	115 (3)
C7—C8—N2	125.3 (4)	C23—C22—C17	116.7 (4)
C7—C8—C9	120.2 (4)	C23—C22—C21	123.9 (4)
N2—C8—C9	114.5 (4)	C17—C22—C21	119.4 (4)
N1—C9—C4	123.4 (4)	C24—C23—C22	119.8 (4)
N1—C9—C8	117.7 (3)	C24—C23—H23	123 (3)
C4—C9—C8	119.0 (4)	C22—C23—H23	118 (3)
O1—C10—N2	124.7 (4)	C23—C24—C25	118.8 (4)
O1—C10—C11	121.7 (4)	C23—C24—H24	121 (2)
N2—C10—C11	113.6 (4)	C25—C24—H24	120 (2)
N3—C11—C12	122.7 (4)	N5—C25—C24	124.4 (4)
N3—C11—C10	117.6 (4)	N5—C25—H25	118 (2)
C12—C11—C10	119.7 (4)	C24—C25—H25	118 (2)
C13—C12—C11	118.8 (5)	C1—N1—C9	117.1 (4)
C13—C12—H12	122 (3)	C10—N2—C8	129.9 (4)
C11—C12—H12	119 (3)	C10—N2—H2B	113 (3)
C12—C13—C14	119.3 (4)	C8—N2—H2B	116 (3)
C12—C13—H13	122 (3)	C15—N3—C11	118.0 (4)
C14—C13—H13	118 (3)	C16—N4—C18	128.8 (4)
C13—C14—C15	118.0 (4)	C16—N4—H4B	116 (2)
C13—C14—H14	121 (3)	C18—N4—H4B	115 (2)
C15—C14—H14	121 (3)	C25—N5—C17	117.2 (4)
N1—C1—C2—C3	1.4 (7)	N5—C17—C18—N4	-4.1 (6)
C1—C2—C3—C4	-0.9 (7)	C22—C17—C18—N4	177.1 (4)
C2—C3—C4—C5	179.4 (5)	N4—C18—C19—C20	-177.0 (5)
C2—C3—C4—C9	0.1 (6)	C17—C18—C19—C20	0.3 (7)
C3—C4—C5—C6	-179.7 (4)	C18—C19—C20—C21	0.6 (8)
C9—C4—C5—C6	-0.5 (7)	C19—C20—C21—C22	-1.3 (8)
C4—C5—C6—C7	-0.7 (7)	N5—C17—C22—C23	1.5 (6)
C5—C6—C7—C8	0.3 (7)	C18—C17—C22—C23	-179.7 (4)
C6—C7—C8—N2	-177.6 (4)	N5—C17—C22—C21	-179.0 (4)
C6—C7—C8—C9	1.3 (6)	C18—C17—C22—C21	-0.2 (6)
C3—C4—C9—N1	0.4 (6)	C20—C21—C22—C23	-179.5 (5)
C5—C4—C9—N1	-178.9 (4)	C20—C21—C22—C17	1.1 (7)
C3—C4—C9—C8	-178.6 (4)	C17—C22—C23—C24	-0.5 (7)
C5—C4—C9—C8	2.0 (6)	C21—C22—C23—C24	-179.9 (5)
C7—C8—C9—N1	178.4 (4)	C22—C23—C24—C25	-1.5 (8)

N2—C8—C9—N1	-2.5 (5)	C23—C24—C25—N5	2.7 (8)
C7—C8—C9—C4	-2.5 (6)	C2—C1—N1—C9	-0.9 (7)
N2—C8—C9—C4	176.6 (4)	C4—C9—N1—C1	0.0 (6)
O1—C10—C11—N3	174.9 (4)	C8—C9—N1—C1	179.0 (4)
N2—C10—C11—N3	-6.4 (6)	O1—C10—N2—C8	-7.7 (7)
O1—C10—C11—C12	-5.9 (7)	C11—C10—N2—C8	173.6 (4)
N2—C10—C11—C12	172.8 (4)	C7—C8—N2—C10	1.2 (7)
N3—C11—C12—C13	1.7 (7)	C9—C8—N2—C10	-177.8 (4)
C10—C11—C12—C13	-177.5 (5)	C14—C15—N3—C11	-0.4 (7)
C11—C12—C13—C14	-0.6 (8)	C16—C15—N3—C11	-178.4 (4)
C12—C13—C14—C15	-0.9 (8)	C12—C11—N3—C15	-1.2 (7)
C13—C14—C15—N3	1.5 (8)	C10—C11—N3—C15	178.0 (4)
C13—C14—C15—C16	179.4 (5)	O2—C16—N4—C18	-1.6 (9)
N3—C15—C16—O2	167.9 (5)	C15—C16—N4—C18	178.9 (4)
C14—C15—C16—O2	-10.1 (7)	C19—C18—N4—C16	-17.5 (8)
N3—C15—C16—N4	-12.6 (6)	C17—C18—N4—C16	165.1 (5)
C14—C15—C16—N4	169.3 (5)	C24—C25—N5—C17	-1.7 (7)
N5—C17—C18—C19	178.4 (4)	C22—C17—N5—C25	-0.5 (6)
C22—C17—C18—C19	-0.5 (6)	C18—C17—N5—C25	-179.3 (4)

*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>
N2—H2b...N1	0.86 (4)	2.23 (4)	2.638 (5)	109 (3)
N2—H2b...N3	0.86 (4)	2.19 (4)	2.666 (5)	115 (3)
N4—H4b...N3	0.93 (4)	2.23 (3)	2.669 (5)	108 (2)
N4—H4b...N5	0.93 (4)	2.23 (3)	2.667 (5)	108 (2)