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

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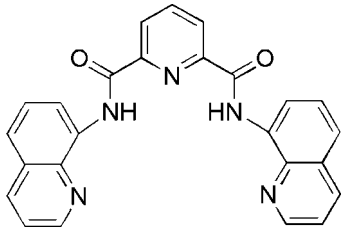
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.006 Å; R factor = 0.078; wR factor = 0.115; data-to-parameter ratio = 7.9.

In the molecule of the title compound, $C_{25}H_{17}N_5O_2$, 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 N—H···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

$C_{25}H_{17}N_5O_2$
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^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
0.35 × 0.12 × 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_{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
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
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)

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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supplementary materials

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

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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 qunolyl carboxamides, a burgeoning class of multidentate ligands containing this linkage, are available from condensation reactions between pyridyl or qunolyl-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.

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).

Refinement

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

Figures

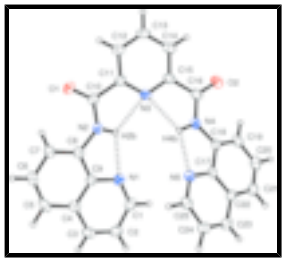


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen bonds are shown as dashed lines.

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

Crystal data

$C_{25}H_{17}N_5O_2$	F_{000} = 872
M_r = 419.44	D_x = 1.385 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 2000 reflections
a = 4.5443 (13) Å	μ = 0.09 mm^{-1}
b = 17.030 (6) Å	T = 294 (2) K
c = 25.984 (8) Å	Plate, colorless
V = 2010.9 (11) Å^3	0.35 × 0.12 × 0.01 mm
Z = 4	

Data collection

STOE IPDS II diffractometer	R_{int} = 0.108
rotation method scans	θ_{max} = 28.1º
Absorption correction: none	θ_{min} = 1.6º
20853 measured reflections	h = −5→5
2822 independent reflections	k = −22→22
2161 reflections with $I > 2\sigma(I)$	l = −34→34

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0157P)^2 + 0.8034P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.078	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.115	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
S = 1.34	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
2822 reflections	Extinction correction: none
357 parameters	

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	−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^2)

	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)

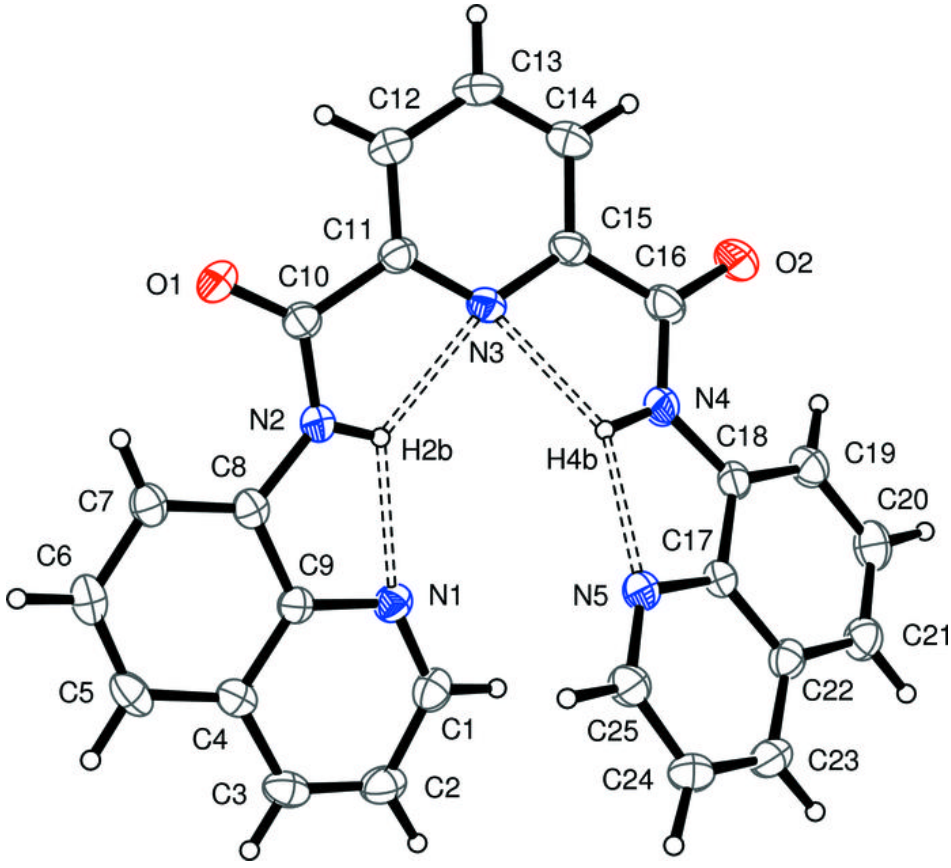
C8—C7—H7	118 (3)	C20—C21—H21	125 (3)
C6—C7—H7	122 (3)	C22—C21—H21	115 (3)
C7—C8—N2	125.3 (4)	C23—C22—C17	116.7 (4)
C7—C8—C9	120.2 (4)	C23—C22—C21	123.9 (4)
N2—C8—C9	114.5 (4)	C17—C22—C21	119.4 (4)
N1—C9—C4	123.4 (4)	C24—C23—C22	119.8 (4)
N1—C9—C8	117.7 (3)	C24—C23—H23	123 (3)
C4—C9—C8	119.0 (4)	C22—C23—H23	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, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
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)

Fig. 1


C13
C12
C14
C11
C15
O1
C10
C16
O2
N3
N2
H2b
H4b
N4
C18
C19
C8
C7
C20
C17
C6
C9
N1
N5
C21
C5
C22
C1
C25
C4
C23
C3
C2
C24