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3,6-Dimethyl-N^1,N^4-bis(pyridin-2-yl)-1,2,4,5-tetrazine-1,4-dicarboxamide

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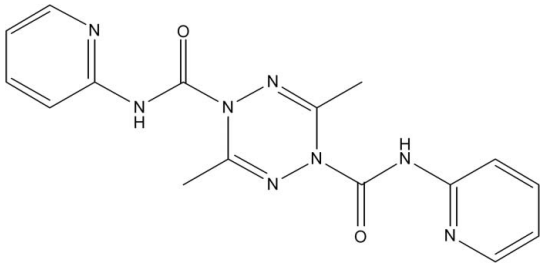
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.061; wR factor = 0.182; data-to-parameter ratio = 12.6.

In the title molecule, $C_{16}H_{16}N_8O_2$, four atoms of the tetrazine ring are coplanar, with the largest deviation from the plane being 0.0236 (12) Å; the other two atoms of the tetrazine ring deviate on the same side from this plane by 0.320 (4) and 0.335 (4) Å. Therefore, the central tetrazine ring exhibits a boat conformation. The dihedral angles between the mean plane of the four coplanar atoms of the tetrazine ring and the two pyridine rings are 26.22 (10) and 6.97 (5)°. The two pyridine rings form a dihedral angle of 31.27 (8)°. In the molecule, there are a number of short C—H···O interactions. In the crystal, molecules are linked *via* a C—H···O interaction to form zigzag chains propagating along the [010] direction.

Related literature

For the activities of 1,2,4,5-tetrazine derivatives in chemical reactions, see: Domingo *et al.* (2009); Lorincz *et al.* (2010). For biological activities in 1,2,4,5-tetrazine derivatives, see: Eremeev *et al.* (1978, 1980); Neunhoeffer (1984); Sauer (1996). For antitumor activities of 1,2,4,5-tetrazine derivatives, see: Hu *et al.* (2002, 2004); Rao & Hu (2005, 2006). For typical bond lengths for C=N double and C—N and N—N single bonds, see: Allen *et al.* (1987). For the synthesis of the title compound, see: Hu *et al.* (2004); Skorianetz & Kováts (1970, 1971); Sun *et al.* (2003).



Experimental

Crystal data

$C_{16}H_{16}N_8O_2$
M_r = 352.37
Monoclinic, $P2_1/c$
a = 11.753 (2) Å
b = 20.081 (4) Å
c = 7.2012 (14) Å
β = 96.273 (3)°
V = 1689.4 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 K
0.36 × 0.23 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.965, T_{max} = 0.981
7032 measured reflections
2985 independent reflections
2430 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.182
S = 1.07
2985 reflections
236 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···O2	0.96	2.07	2.778 (4)	130
C2—H2A···O1	0.96	2.09	2.777 (4)	127
C8—H8···O1	0.93	2.31	2.886 (3)	120
C16—H16···O1^{i}	0.93	2.39	3.229 (3)	150

Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); 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: ZJ2056).

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supplementary materials

Acta Cryst. (2012). E**68**, o702–o703 [doi:10.1107/S1600536812005405]

3,6-Dimethyl-N^1,N^4-bis(pyridin-2-yl)-1,2,4,5-tetrazine-1,4-dicarboxamide

Guo-Wu Rao, Yan-Mei Guo and Qun Shen

Comment

Tetrazine derivatives have high activities of chemical reaction (Domingo *et al.*, 2009; Lorincz *et al.*, 2010), and have been widely used in pesticides and medicines (Eremeev *et al.*, 1978, 1980; Neunhoeffer, 1984; Sauer, 1996). In a continuation of our studies of antitumor activities in 1,2,4,5-tetrazine derivatives (Hu *et al.*, 2002, 2004; Rao & Hu, 2005, 2006), we have obtained a colourless crystalline compound, (I). However, IR, NMR, and MS studies failed to prove whether the substituted groups of the nitrogen are located at the 1,4 or 1,2 position. The structure was confirmed by single-crystal X-ray diffraction.

The molecular structure of (I) is illustrated in Fig. 1. The N2═C3 [1.279 (3) Å] and N5═C6 [1.278 (3) Å] bonds correspond to typical double bonds of C═N, and the C3—N4 [1.395 (3) Å], N4—N5 [1.419 (3) Å], C6—N1 [1.388 (3) Å] and N1—N2 [1.420 (3) Å] bond lengths correspond to typical single bonds (Allen *et al.*, 1987). Therefore, the tetrazine ring is the 1,4-dihydro structure with the N-substituted groups at the 1,4-positions and not the 1,2-positions, the compound being 3,6-dimethyl-N^1,N^4-di(pyridin-2-yl)-1,2,4,5-tetrazine-1,4-dicarboxamide, rather than the 3,6-dimethyl-N^1,N^2-di(pyridin-2-yl)-1,2,4,5-tetrazine-1,2-dicarboxamide.

In (I), atoms N2, C3, N5 and C6 are coplanar, with the largest deviation from this plane being ±0.0236 (12) Å. Atoms N1 and N4 deviate from this plane by -0.3202 (35) and -0.3345 (36) Å, respectively. The dihedral angle between the N2/C3/N5/C6 plane and the N1/N2/C6 plane is 26.25 (18)°, and between the N2/C3/N5/C6 plane and the N4/N5/C3 plane is 27.18 (19)°. Therefore, the central six-member ring of the compound, the tetrazine ring, has an obvious boat conformation. The dihedral angles between the N2/C3/N5/C6 plane and the two pyridyl rings are 26.22 (10) and 6.97 (5)°, respectively. And two pyridyl rings form a dihedral angle of 31.27 (8)°. In the molecule, there are a number of short C—H···O interactions. In the crystal, molecules are linked *via* a C—H···O interaction to form zigzag chains propagating along the [010] direction.

Experimental

The title compound was prepared according to the procedure of Hu *et al.* (2004), Sun *et al.* (2003) and Skorianetz & Kováts (1970, 1971). A saturated solution of the compound in ethanol and dichloromethane (4:1, *v*/*v*) of 298 K was concentrated gradually at room temperature to afford colourless blocks.

Refinement

H atoms were included in calculated positions and refined using a riding model. H atoms were given isotropic displacement parameters equal to 1.2 (or 1.5 for methyl H atoms) times the equivalent isotropic displacement parameters of their parent atoms, and C—H distances were set to 0.96 Å for methyl H atoms and 0.93 Å for pyridyl H atoms, while N—H distances were set to 0.86 Å.

Computing details

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

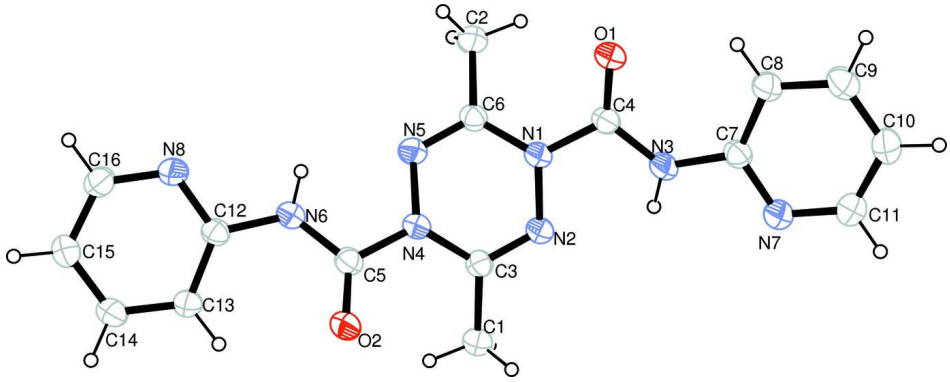

Figure 1

The structure of (I), shown with 30% probability displacement ellipsoids.

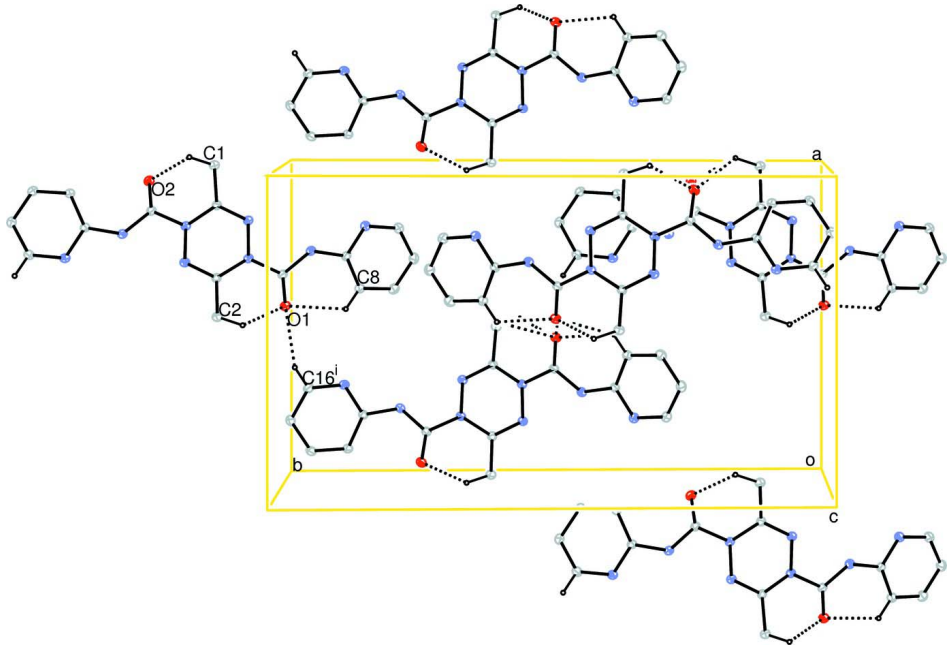

Figure 2

A portion of the crystal packing of (I). Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding were omitted for clarity.

3,6-Dimethyl-*N*^{1},*N*^{4}-bis(pyridin-2-yl)-1,2,4,5-tetrazine-1,4- dicarboxamide

Crystal data

$C_{16}H_{16}N_8O_2$
M_r = 352.37
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 11.753 (2) Å
b = 20.081 (4) Å

c = 7.2012 (14) Å
β = 96.273 (3)°
V = 1689.4 (6) Å^3
Z = 4
F(000) = 736
D_x = 1.385 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
θ = 3.0–28.2°
μ = 0.10 mm^{-1}
T = 298 K
Block, colourless
0.36 × 0.23 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.965, T_{max} = 0.981

7032 measured reflections
2985 independent reflections
2430 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 25.0°, θ_{min} = 1.7°
h = −13→11
k = −23→22
l = −8→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.182
S = 1.07
2985 reflections
236 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
$w = 1/[\sigma^2(F_o^2) + (0.0986P)^2 + 0.7423P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.012 (2)

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

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

	x	y	z	U_{iso}*/U_{eq}
N1	0.70522 (17)	0.06533 (10)	0.3165 (3)	0.0460 (5)
O2	0.94498 (16)	0.25045 (9)	0.2447 (3)	0.0587 (6)
O1	0.54879 (15)	0.00173 (9)	0.2281 (3)	0.0618 (6)
N4	0.80771 (16)	0.17897 (10)	0.3261 (3)	0.0464 (5)
N5	0.69810 (17)	0.17708 (10)	0.3912 (3)	0.0481 (6)
N2	0.82657 (17)	0.06420 (10)	0.3487 (3)	0.0480 (6)
N6	0.78462 (18)	0.29223 (10)	0.3540 (3)	0.0489 (6)
H6	0.7217	0.2801	0.3948	0.059*
N8	0.70889 (18)	0.39638 (11)	0.3514 (3)	0.0529 (6)

C12	0.8038 (2)	0.36064 (12)	0.3445 (3)	0.0434 (6)
C3	0.8743 (2)	0.12142 (12)	0.3484 (4)	0.0448 (6)
N7	0.7973 (2)	−0.14331 (12)	0.1576 (4)	0.0649 (7)
N3	0.72486 (18)	−0.04631 (10)	0.2546 (3)	0.0532 (6)
H3	0.7933	−0.0403	0.3073	0.064*
C6	0.6486 (2)	0.12036 (12)	0.3784 (3)	0.0432 (6)
C4	0.6513 (2)	0.00504 (12)	0.2642 (4)	0.0449 (6)
C5	0.8541 (2)	0.24270 (12)	0.3062 (4)	0.0453 (6)
C7	0.7024 (2)	−0.10818 (12)	0.1687 (4)	0.0470 (6)
C2	0.5324 (2)	0.11538 (14)	0.4433 (4)	0.0570 (7)
H2A	0.5046	0.0706	0.4263	0.086*
H2B	0.4811	0.1453	0.3721	0.086*
H2C	0.5369	0.1270	0.5733	0.086*
C13	0.9103 (2)	0.38885 (13)	0.3336 (4)	0.0503 (7)
H13	0.9753	0.3625	0.3325	0.060*
C8	0.5943 (2)	−0.13104 (13)	0.1018 (4)	0.0538 (7)
H8	0.5294	−0.1055	0.1130	0.065*
C16	0.7187 (2)	0.46207 (14)	0.3430 (4)	0.0585 (8)
H16	0.6530	0.4876	0.3476	0.070*
C9	0.5865 (3)	−0.19228 (15)	0.0190 (4)	0.0637 (8)
H9	0.5153	−0.2090	−0.0276	0.076*
C14	0.9165 (2)	0.45670 (14)	0.3243 (5)	0.0590 (8)
H14	0.9866	0.4773	0.3156	0.071*
C1	1.0012 (2)	0.12417 (14)	0.3833 (5)	0.0599 (8)
H1A	1.0262	0.1696	0.3778	0.090*
H1B	1.0340	0.0985	0.2900	0.090*
H1C	1.0255	0.1062	0.5047	0.090*
C15	0.8196 (2)	0.49461 (14)	0.3279 (4)	0.0617 (8)
H15	0.8225	0.5408	0.3204	0.074*
C11	0.7852 (3)	−0.20271 (15)	0.0760 (6)	0.0745 (10)
H11	0.8509	−0.2278	0.0673	0.089*
C10	0.6832 (3)	−0.22915 (15)	0.0042 (5)	0.0677 (9)
H10	0.6792	−0.2708	−0.0528	0.081*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0367 (11)	0.0442 (12)	0.0563 (13)	−0.0043 (8)	0.0015 (9)	−0.0017 (9)
O2	0.0514 (11)	0.0516 (11)	0.0763 (14)	−0.0098 (8)	0.0211 (10)	−0.0047 (9)
O1	0.0400 (11)	0.0556 (12)	0.0884 (15)	−0.0066 (8)	0.0015 (10)	−0.0091 (10)
N4	0.0383 (11)	0.0449 (12)	0.0569 (13)	−0.0051 (9)	0.0096 (9)	−0.0016 (9)
N5	0.0416 (12)	0.0473 (12)	0.0564 (13)	−0.0014 (9)	0.0106 (10)	0.0033 (10)
N2	0.0385 (11)	0.0458 (12)	0.0589 (14)	−0.0031 (9)	0.0014 (9)	−0.0054 (10)
N6	0.0411 (11)	0.0452 (12)	0.0612 (14)	−0.0053 (9)	0.0091 (10)	0.0018 (10)
N8	0.0386 (12)	0.0528 (13)	0.0662 (15)	−0.0012 (9)	0.0005 (10)	−0.0054 (11)
C12	0.0392 (13)	0.0466 (14)	0.0435 (14)	−0.0031 (10)	−0.0001 (10)	−0.0015 (10)
C3	0.0423 (13)	0.0445 (14)	0.0476 (14)	−0.0025 (10)	0.0042 (11)	−0.0062 (11)
N7	0.0469 (14)	0.0496 (13)	0.097 (2)	−0.0010 (10)	0.0032 (13)	−0.0065 (13)
N3	0.0397 (12)	0.0461 (12)	0.0713 (16)	−0.0053 (9)	−0.0047 (10)	−0.0034 (11)
C6	0.0417 (13)	0.0430 (13)	0.0446 (14)	−0.0024 (10)	0.0037 (10)	0.0049 (10)

C4	0.0391 (14)	0.0456 (14)	0.0498 (15)	−0.0056 (10)	0.0033 (11)	0.0033 (11)
C5	0.0424 (14)	0.0458 (14)	0.0475 (14)	−0.0053 (11)	0.0048 (11)	−0.0032 (11)
C7	0.0438 (14)	0.0422 (14)	0.0546 (16)	−0.0047 (11)	0.0029 (11)	0.0049 (11)
C2	0.0475 (15)	0.0543 (16)	0.0718 (19)	−0.0021 (12)	0.0180 (13)	0.0038 (13)
C13	0.0383 (13)	0.0482 (15)	0.0634 (17)	−0.0017 (11)	0.0012 (12)	−0.0047 (12)
C8	0.0452 (15)	0.0504 (15)	0.0643 (18)	−0.0017 (11)	−0.0011 (13)	−0.0011 (13)
C16	0.0480 (15)	0.0530 (16)	0.074 (2)	0.0060 (12)	0.0023 (13)	−0.0084 (14)
C9	0.0574 (17)	0.0631 (18)	0.068 (2)	−0.0102 (14)	−0.0051 (14)	−0.0099 (15)
C14	0.0464 (15)	0.0530 (16)	0.079 (2)	−0.0108 (12)	0.0120 (14)	−0.0075 (14)
C1	0.0422 (15)	0.0531 (16)	0.083 (2)	−0.0020 (12)	0.0027 (14)	−0.0067 (14)
C15	0.0600 (18)	0.0449 (15)	0.081 (2)	−0.0065 (13)	0.0130 (15)	−0.0078 (14)
C11	0.0591 (19)	0.0521 (17)	0.113 (3)	0.0049 (14)	0.0123 (18)	−0.0106 (17)
C10	0.070 (2)	0.0518 (17)	0.081 (2)	−0.0028 (15)	0.0032 (16)	−0.0148 (15)

Geometric parameters (Å, º)

N1—C6	1.388 (3)	C6—C2	1.494 (3)
N1—C4	1.399 (3)	C7—C8	1.387 (4)
N1—N2	1.420 (3)	C2—H2A	0.9600
O2—C5	1.210 (3)	C2—H2B	0.9600
O1—C4	1.206 (3)	C2—H2C	0.9600
N4—C3	1.395 (3)	C13—C14	1.367 (4)
N4—C5	1.405 (3)	C13—H13	0.9300
N4—N5	1.419 (3)	C8—C9	1.366 (4)
N5—C6	1.278 (3)	C8—H8	0.9300
N2—C3	1.279 (3)	C16—C15	1.369 (4)
N6—C5	1.356 (3)	C16—H16	0.9300
N6—C12	1.395 (3)	C9—C10	1.370 (4)
N6—H6	0.8600	C9—H9	0.9300
N8—C16	1.326 (4)	C14—C15	1.372 (4)
N8—C12	1.332 (3)	C14—H14	0.9300
C12—C13	1.384 (3)	C1—H1A	0.9600
C3—C1	1.487 (3)	C1—H1B	0.9600
N7—C7	1.329 (3)	C1—H1C	0.9600
N7—C11	1.331 (4)	C15—H15	0.9300
N3—C4	1.353 (3)	C11—C10	1.360 (4)
N3—C7	1.400 (3)	C11—H11	0.9300
N3—H3	0.8600	C10—H10	0.9300
C6—N1—C4	123.8 (2)	C6—C2—H2B	109.5
C6—N1—N2	117.91 (19)	H2A—C2—H2B	109.5
C4—N1—N2	116.61 (19)	C6—C2—H2C	109.5
C3—N4—C5	123.2 (2)	H2A—C2—H2C	109.5
C3—N4—N5	117.25 (19)	H2B—C2—H2C	109.5
C5—N4—N5	115.78 (19)	C14—C13—C12	117.7 (2)
C6—N5—N4	115.0 (2)	C14—C13—H13	121.2
C3—N2—N1	114.7 (2)	C12—C13—H13	121.2
C5—N6—C12	127.2 (2)	C9—C8—C7	117.7 (3)
C5—N6—H6	116.4	C9—C8—H8	121.1
C12—N6—H6	116.4	C7—C8—H8	121.1

C16—N8—C12	117.2 (2)	N8—C16—C15	124.0 (3)
N8—C12—C13	123.2 (2)	N8—C16—H16	118.0
N8—C12—N6	112.9 (2)	C15—C16—H16	118.0
C13—C12—N6	123.9 (2)	C8—C9—C10	120.2 (3)
N2—C3—N4	120.3 (2)	C8—C9—H9	119.9
N2—C3—C1	117.7 (2)	C10—C9—H9	119.9
N4—C3—C1	121.9 (2)	C13—C14—C15	120.2 (3)
C7—N7—C11	116.9 (2)	C13—C14—H14	119.9
C4—N3—C7	127.5 (2)	C15—C14—H14	119.9
C4—N3—H3	116.2	C3—C1—H1A	109.5
C7—N3—H3	116.2	C3—C1—H1B	109.5
N5—C6—N1	120.2 (2)	H1A—C1—H1B	109.5
N5—C6—C2	117.5 (2)	C3—C1—H1C	109.5
N1—C6—C2	122.3 (2)	H1A—C1—H1C	109.5
O1—C4—N3	125.2 (2)	H1B—C1—H1C	109.5
O1—C4—N1	121.2 (2)	C16—C15—C14	117.7 (3)
N3—C4—N1	113.6 (2)	C16—C15—H15	121.2
O2—C5—N6	125.4 (2)	C14—C15—H15	121.2
O2—C5—N4	121.5 (2)	N7—C11—C10	124.4 (3)
N6—C5—N4	113.0 (2)	N7—C11—H11	117.8
N7—C7—C8	123.1 (3)	C10—C11—H11	117.8
N7—C7—N3	112.3 (2)	C11—C10—C9	117.6 (3)
C8—C7—N3	124.6 (2)	C11—C10—H10	121.2
C6—C2—H2A	109.5	C9—C10—H10	121.2

C3—N4—N5—C6	−32.6 (3)	C6—N1—C4—N3	−164.0 (2)
C5—N4—N5—C6	168.6 (2)	N2—N1—C4—N3	0.8 (3)
C6—N1—N2—C3	−31.4 (3)	C12—N6—C5—O2	−0.8 (4)
C4—N1—N2—C3	162.8 (2)	C12—N6—C5—N4	−177.8 (2)
C16—N8—C12—C13	1.6 (4)	C3—N4—C5—O2	25.5 (4)
C16—N8—C12—N6	−179.9 (2)	N5—N4—C5—O2	−177.0 (2)
C5—N6—C12—N8	162.7 (2)	C3—N4—C5—N6	−157.3 (2)
C5—N6—C12—C13	−18.8 (4)	N5—N4—C5—N6	0.1 (3)
N1—N2—C3—N4	2.8 (3)	C11—N7—C7—C8	0.7 (5)
N1—N2—C3—C1	179.3 (2)	C11—N7—C7—N3	−179.2 (3)
C5—N4—C3—N2	−173.6 (2)	C4—N3—C7—N7	169.7 (3)
N5—N4—C3—N2	29.3 (3)	C4—N3—C7—C8	−10.2 (4)
C5—N4—C3—C1	10.0 (4)	N8—C12—C13—C14	−1.9 (4)
N5—N4—C3—C1	−147.1 (3)	N6—C12—C13—C14	179.8 (3)
N4—N5—C6—N1	4.2 (3)	N7—C7—C8—C9	−0.8 (4)
N4—N5—C6—C2	−179.5 (2)	N3—C7—C8—C9	179.1 (3)
C4—N1—C6—N5	−167.2 (2)	C12—N8—C16—C15	−0.1 (4)
N2—N1—C6—N5	28.1 (3)	C7—C8—C9—C10	0.1 (5)
C4—N1—C6—C2	16.6 (4)	C12—C13—C14—C15	0.7 (4)
N2—N1—C6—C2	−148.0 (2)	N8—C16—C15—C14	−1.0 (5)
C7—N3—C4—O1	13.6 (5)	C13—C14—C15—C16	0.7 (5)
C7—N3—C4—N1	−164.6 (2)	C7—N7—C11—C10	0.1 (5)
C6—N1—C4—O1	17.6 (4)	N7—C11—C10—C9	−0.7 (6)
N2—N1—C4—O1	−177.6 (2)	C8—C9—C10—C11	0.6 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···O2	0.96	2.07	2.778 (4)	130
C2—H2*A*···O1	0.96	2.09	2.777 (4)	127
C8—H8···O1	0.93	2.31	2.886 (3)	120
C16—H16···O1^{i}	0.93	2.39	3.229 (3)	150

Symmetry code: (i) −*x*+1, *y*+1/2, −*z*+1/2.