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4,5-Dimethyl-1,2-bis(pyridine-3-carboxamido)benzene

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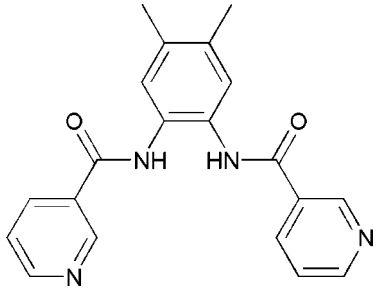
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.111; data-to-parameter ratio = 13.8.

In the title molecule, $C_{20}H_{18}N_4O_2$, the dihedral angles between the central benzene ring and the two pyridine rings are 12.07 (8) and 4.80 (1)°, and that between the two pyridine rings is 16.78 (9)°. An intramolecular N—H···O hydrogen bond may influence the molecular conformation. In the crystal structure, intermolecular N—H···O hydrogen bonds link molecules into centrosymmetric dimers, while weak intermolecuar C—H···O hydrogen bonds link these dimers into one-dimensional chains.

Related literature

The molecule of the corresponding H_2Me_2-bpzb compound [bpzb is 1,2-bis(2-pyrazine-3-carboxamido)-4,5-dimethylbenzene] is non-planar (Kim *et al.*, 2005). For background information, see: Batten & Robson (1998); Chi *et al.* (2006); Evans & Lin (2002); Hong *et al.* (2004); Janiak (2003); Janiak & Scharmann (2003); Kasai *et al.* (2000); Kitagawa *et al.* (2004); Luan *et al.* (2005, 2006); Moler *et al.* (2001); Moulton & Zaworotko (2001); Ryu *et al.* (2005); Sarkar & Biradha (2007); Wang *et al.* (2006).



Experimental

Crystal data

$C_{20}H_{18}N_4O_2$
M_r = 346.38
Monoclinic, $P2_1/c$
a = 8.086 (2) Å
b = 17.960 (5) Å
c = 12.135 (3) Å
β = 101.467 (5)°
V = 1727.2 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.25 × 0.25 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.978, T_{max} = 0.982
9503 measured reflections
3391 independent reflections
2300 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.111
S = 1.04
3391 reflections
246 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O1	0.93	2.51	2.921 (2)	107
N2—H2N···O2	0.90 (2)	1.88 (2)	2.701 (2)	150.8 (16)
C17—H17···O1^{i}	0.93	2.55	3.461 (3)	165
N3—H3N···O1^{ii}	0.907 (17)	2.066 (18)	2.9407 (19)	161.6 (15)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2501).

References

Batten, S. R. & Robson, R. (1998). *Angew. Chem. Int. Ed.* **37**, 1460–1494.
Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1998). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Chi, Y.-N., Huang, K.-L., Cui, F.-Y., Xu, Y.-Q. & Hu, C.-W. (2006). *Inorg. Chem.* **45**, 10605–10612.
Evans, O. R. & Lin, W. (2002). *Acc. Chem. Res.* **35**, 511–522.
Hong, S. J., Ryu, J. Y., Lee, J. Y., Kim, C., Kim, S.-J. & Kim, Y. (2004). *Dalton Trans.* pp. 2697–2701.
Janiak, C. (2003). *Dalton Trans.* pp. 2781–2804.
Janiak, C. & Scharmann, T. G. (2003). *Polyhedron*, **22**, 1123–1133.
Kasai, K., Aoyagi, M. & Fujita, M. (2000). *J. Am. Chem. Soc.* **122**, 2140–2141.
Kim, Y.-J., Kim, C. & Kim, Y. (2005). *Anal. Sci.* **21**, x23–x24.

  doi:10.1107/S1600536807044492

Kitagawa, S., Kitaura, R. & Noro, S.-I. (2004). *Angew. Chem. Int. Ed.* **43**, 2334–2375.
Luan, X.-J., Cai, X.-H., Wang, Y.-Y., Li, D.-S., Wang, C.-J., Liu, P., Hu, H.-M., Shi, Q.-Z. & Peng, S.-M. (2006). *Chem. Eur. J.* **12**, 6281–6289.
Luan, X.-J., Wang, Y.-Y., Li, D.-S., Liu, P., Hu, H.-M., Shi, Q.-Z. & Peng, S.-M. (2005). *Angew. Chem. Int. Ed.* **44**, 3864–3867.
Moler, D. B., Chen, H., Li, B., Reineke, T. M., O'Keeffe, M. & Yaghi, O. M. (2001). *Acc. Chem. Res.* **34**, 319–330.
Moulton, B. & Zaworotko, M. J. (2001). *Chem. Rev.* **101**, 1629–1658.
Ryu, J. Y., Han, J. H., Lee, J. Y., Hong, S. J., Choi, S. H., Kim, C., Kim, S.-J. & Kim, Y. (2005). *Inorg. Chim. Acta*, **358**, 3659–3670.
Sarkar, M. & Biradha, K. (2007). *Cryst. Growth Des.* **7**, 1318–1331.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Wang, X.-Y., Wang, L., Wang, Z.-M. & Gao, S. (2006). *J. Am. Chem. Soc.* **128**, 674–675.

supplementary materials

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4,5-Dimethyl-1,2-bis(pyridine-3-carboxamido)benzene

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Comment

The rational design and construction of novel discrete and polymeric metal–organic complexes has been the subject of enormous studies in recent years, not only due to their structural and topological novelty (Batten & Robson, 1998; Moler *et al.*, 2001; Moulton & Zaworotko, 2001), but also for their potential applications as functional materials in areas such as catalysis, molecular recognition, separation, and nonlinear optics (Hong *et al.*, 2004; Evans & Lin, 2002; Kasai *et al.*, 2000; Kitagawa *et al.*, 2004). The structure of metal–organic complexes is highly influenced by many factors such as the coordination geometry of metal ions (Chi *et al.*, 2006), the structure of organic ligands (Wang *et al.*, 2006), the solvent system (Ryu *et al.*, 2005), the counteranion (Luan *et al.*, 2006), and the ratio of ligands to metal ions. In addition, the secondary forces such as hydrogen-bonding, pi–pi stacking, and host–guest interactions must be considered as well (Luan *et al.*, 2005; Janiak & Scharmann, 2003; Janiak, 2003). For obtaining novel structural motifs with predictable properties, a large number of organic ligands have been designed and utilized. Recently, much attention was paid to ligands with amide moieties that can assemble into higher dimensional architectures *via* hydrogen-bonded interactions (Sarkar & Biradha, 2007). In order to further investigate the influence of the ligand with amide moieties on the crystal structure, we synthesized the title compound an we report its crystal structure herein.

The asymmetric unit of the monoclinic unit cell contains one whole molecule [$P2_1/c$ and $Z = 4$]. The molecule is not planar, having twisted angles between the central benzene ring and two pyridyl rings. The dihedral angles between the central benzene ring and the two pyridyl rings are 12.07 (8)° and 4.80 (1)° (Fig. 1). An intramolecular N—H···O hydrogen bond may influence the molecular conformation. In the crystal structure, intermolecular N—H···O hydrogen bonds link molecules into centrosymmetric dimers while weak intermolecuar C—H···O hydrogen bonds link these dimers into one-dimensional chains (Fig. 2).

Experimental

4,5-Dimethyl-1,2-phenylenediamine (1.39 g, 10.0 mmol) and triethylamine (4.2 ml, 30.0 mmol) were dissolved in pyridine and stirred for 10 min. Nicotinoyl chloride (3.67 g, 20.0 mmol) dissolved in pyridine was added slowly to the resulting solution at 272 K. After the reaction mixture was stirred for 4 h at room temperature, solvent was removed with a evaporator. The product was dissolved in chloroform and extracted with brine and water. The extracted solution was dried over anhydrous Na_2SO_4. The powered product was obtained in a mixture of ether and chloroform (4:1). Colorless block crystals were obtained from an acetone–hexane solution at room temperature by slow evaporation for X-ray experiments.

Refinement

H atoms were placed in calculated positions with C—H distances of 0.93 A% (benzene and pyridine) and 0.96 A% (methyl). They were included in the refinement in riding–motion approximation with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C)$. The H atoms bonded to N atoms were refined independently with isotropic displacement parameters.

Figures

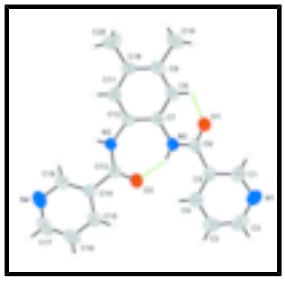

Fig. 1. The molecular structure of the title compound showing the atom-labeling scheme. Displacement ellipsoids are shown at the 50% probability level. Hydrogen bonds are shown as dashed lines.

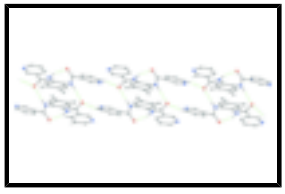

Fig. 2. Part of the crystal structure showing hydrogen bonds as dashed lines.

4,5-Dimethyl-1,2-bis(pyridine-3-carboxamido)benzene

Crystal data

$C_{20}H_{18}N_4O_2$	F_{000} = 728
M_r = 346.38	D_x = 1.332 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1519 reflections
a = 8.086 (2) Å	θ = 2.3–21.6º
b = 17.960 (5) Å	μ = 0.09 mm^{-1}
c = 12.135 (3) Å	T = 293 (2) K
β = 101.467 (5)º	Block, colourless
V = 1727.2 (8) Å^3	0.25 × 0.25 × 0.20 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	3391 independent reflections
Radiation source: fine-focus sealed tube	2300 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.030
T = 293(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	h = −9→9
T_{min} = 0.978, T_{max} = 0.982	k = −22→22
9503 measured reflections	l = −8→14

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.043$	$w = 1/[\sigma^2(F_o^2) + (0.0396P)^2 + 0.2189P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.111$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.04$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
3391 reflections	$\Delta\rho_{min} = -0.15$ e Å^{-3}
246 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0233 (19)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.5376 (2)	0.74635 (9)	0.34859 (15)	0.0654 (5)
N2	0.28726 (18)	0.52612 (8)	0.46355 (13)	0.0414 (4)
H2N	0.356 (2)	0.5308 (10)	0.5311 (17)	0.054 (5)*
N3	0.16193 (17)	0.45162 (7)	0.64598 (11)	0.0395 (3)
H3N	0.069 (2)	0.4465 (9)	0.6770 (14)	0.048 (5)*
N4	0.1892 (2)	0.45996 (12)	0.99772 (15)	0.0791 (6)
O1	0.16797 (14)	0.58349 (6)	0.29969 (9)	0.0481 (3)
O2	0.42842 (14)	0.49969 (7)	0.68104 (10)	0.0513 (3)
C1	0.4360 (2)	0.68713 (10)	0.33456 (16)	0.0535 (5)
H1	0.3927	0.6719	0.2612	0.064*
C2	0.5950 (3)	0.76727 (11)	0.45490 (19)	0.0619 (5)
H2	0.6652	0.8087	0.4676	0.074*
C3	0.5569 (2)	0.73150 (10)	0.54635 (17)	0.0566 (5)
H3	0.6001	0.7486	0.6187	0.068*
C4	0.4536 (2)	0.66975 (9)	0.52960 (16)	0.0496 (5)

H4	0.4272	0.6442	0.5905	0.060*
C5	0.3900 (2)	0.64649 (9)	0.42080 (14)	0.0408 (4)
C6	0.2720 (2)	0.58253 (9)	0.38911 (14)	0.0402 (4)
C7	0.19937 (19)	0.45736 (9)	0.44661 (14)	0.0381 (4)
C8	0.1681 (2)	0.42332 (9)	0.34149 (14)	0.0458 (4)
H8	0.2085	0.4458	0.2830	0.055*
C9	0.0792 (2)	0.35732 (10)	0.32058 (14)	0.0468 (4)
C10	0.0223 (2)	0.32184 (9)	0.40926 (15)	0.0452 (4)
C11	0.0582 (2)	0.35489 (9)	0.51430 (14)	0.0424 (4)
H11	0.0227	0.3312	0.5737	0.051*
C12	0.14512 (19)	0.42190 (8)	0.53512 (13)	0.0363 (4)
C13	0.2963 (2)	0.48389 (9)	0.71203 (14)	0.0391 (4)
C14	0.2776 (2)	0.49965 (9)	0.82949 (14)	0.0403 (4)
C15	0.3483 (2)	0.56311 (10)	0.88388 (16)	0.0549 (5)
H15	0.4049	0.5970	0.8468	0.066*
C16	0.3339 (3)	0.57546 (12)	0.99318 (17)	0.0670 (6)
H16	0.3776	0.6185	1.0306	0.080*
C17	0.2542 (3)	0.52323 (14)	1.04615 (19)	0.0740 (6)
H17	0.2447	0.5322	1.1201	0.089*
C18	0.1988 (2)	0.45048 (11)	0.89029 (16)	0.0588 (5)
H18	0.1495	0.4081	0.8538	0.071*
C19	0.0500 (3)	0.32368 (11)	0.20413 (17)	0.0689 (6)
H19A	0.0737	0.3602	0.1516	0.103*
H19B	−0.0654	0.3079	0.1827	0.103*
H19C	0.1231	0.2816	0.2041	0.103*
C20	−0.0709 (3)	0.24884 (10)	0.39309 (19)	0.0696 (6)
H20A	−0.0907	0.2315	0.4642	0.104*
H20B	−0.0045	0.2128	0.3627	0.104*
H20C	−0.1769	0.2556	0.3421	0.104*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0692 (11)	0.0592 (10)	0.0661 (12)	−0.0163 (9)	0.0091 (9)	0.0101 (9)
N2	0.0444 (8)	0.0462 (8)	0.0336 (8)	−0.0022 (7)	0.0081 (7)	0.0015 (7)
N3	0.0380 (8)	0.0476 (8)	0.0345 (8)	−0.0027 (6)	0.0110 (6)	−0.0021 (6)
N4	0.0844 (13)	0.1113 (15)	0.0429 (11)	−0.0207 (12)	0.0157 (9)	0.0045 (11)
O1	0.0473 (7)	0.0567 (7)	0.0388 (7)	−0.0034 (6)	0.0049 (6)	0.0052 (6)
O2	0.0395 (7)	0.0726 (8)	0.0426 (7)	−0.0055 (6)	0.0098 (5)	−0.0003 (6)
C1	0.0585 (11)	0.0526 (10)	0.0480 (11)	−0.0062 (9)	0.0070 (9)	0.0062 (9)
C2	0.0574 (12)	0.0503 (11)	0.0749 (15)	−0.0081 (9)	0.0058 (11)	0.0001 (11)
C3	0.0560 (12)	0.0520 (11)	0.0584 (13)	0.0014 (9)	0.0033 (10)	−0.0086 (10)
C4	0.0533 (11)	0.0491 (10)	0.0467 (11)	0.0029 (9)	0.0105 (9)	0.0017 (8)
C5	0.0391 (9)	0.0417 (9)	0.0420 (10)	0.0035 (7)	0.0087 (7)	0.0033 (8)
C6	0.0398 (9)	0.0474 (9)	0.0356 (10)	0.0023 (8)	0.0126 (7)	0.0008 (8)
C7	0.0372 (9)	0.0411 (9)	0.0371 (9)	0.0035 (7)	0.0099 (7)	−0.0004 (7)
C8	0.0521 (10)	0.0506 (10)	0.0366 (10)	0.0051 (8)	0.0138 (8)	−0.0009 (8)
C9	0.0502 (10)	0.0488 (10)	0.0403 (10)	0.0076 (9)	0.0063 (8)	−0.0086 (8)

C10	0.0454 (10)	0.0402 (9)	0.0491 (11)	0.0042 (8)	0.0071 (8)	−0.0063 (8)
C11	0.0459 (10)	0.0396 (9)	0.0423 (10)	0.0006 (8)	0.0105 (8)	0.0009 (8)
C12	0.0363 (9)	0.0397 (9)	0.0330 (9)	0.0043 (7)	0.0071 (7)	−0.0014 (7)
C13	0.0387 (9)	0.0409 (9)	0.0374 (10)	0.0019 (7)	0.0065 (7)	0.0020 (7)
C14	0.0395 (9)	0.0472 (9)	0.0335 (9)	0.0018 (7)	0.0054 (7)	0.0020 (8)
C15	0.0683 (13)	0.0517 (11)	0.0449 (11)	−0.0074 (9)	0.0119 (9)	−0.0019 (9)
C16	0.0866 (16)	0.0660 (13)	0.0464 (12)	0.0005 (11)	0.0087 (11)	−0.0159 (10)
C17	0.0796 (15)	0.1054 (18)	0.0397 (12)	0.0062 (14)	0.0183 (11)	−0.0067 (13)
C18	0.0662 (13)	0.0698 (12)	0.0400 (11)	−0.0193 (10)	0.0097 (9)	0.0008 (10)
C19	0.0869 (15)	0.0688 (13)	0.0510 (12)	0.0008 (11)	0.0137 (11)	−0.0189 (11)
C20	0.0813 (15)	0.0554 (12)	0.0711 (15)	−0.0131 (11)	0.0128 (12)	−0.0160 (11)

Geometric parameters (Å, °)

N1—C1	1.334 (2)	C8—C9	1.383 (2)
N1—C2	1.335 (3)	C8—H8	0.9300
N2—C6	1.347 (2)	C9—C10	1.404 (2)
N2—C7	1.419 (2)	C9—C19	1.512 (2)
N2—H2N	0.90 (2)	C10—C11	1.384 (2)
N3—C13	1.346 (2)	C10—C20	1.506 (2)
N3—C12	1.428 (2)	C11—C12	1.391 (2)
N3—H3N	0.907 (17)	C11—H11	0.9300
N4—C18	1.332 (2)	C13—C14	1.490 (2)
N4—C17	1.338 (3)	C14—C15	1.382 (2)
O1—C6	1.2340 (19)	C14—C18	1.384 (2)
O2—C13	1.2345 (19)	C15—C16	1.372 (3)
C1—C5	1.386 (2)	C15—H15	0.9300
C1—H1	0.9300	C16—C17	1.369 (3)
C2—C3	1.369 (3)	C16—H16	0.9300
C2—H2	0.9300	C17—H17	0.9300
C3—C4	1.379 (2)	C18—H18	0.9300
C3—H3	0.9300	C19—H19A	0.9600
C4—C5	1.383 (2)	C19—H19B	0.9600
C4—H4	0.9300	C19—H19C	0.9600
C5—C6	1.494 (2)	C20—H20A	0.9600
C7—C8	1.392 (2)	C20—H20B	0.9600
C7—C12	1.392 (2)	C20—H20C	0.9600
C1—N1—C2	115.76 (17)	C9—C10—C20	121.80 (16)
C6—N2—C7	125.53 (15)	C10—C11—C12	122.98 (15)
C6—N2—H2N	120.0 (12)	C10—C11—H11	118.5
C7—N2—H2N	114.5 (12)	C12—C11—H11	118.5
C13—N3—C12	129.50 (14)	C11—C12—C7	118.73 (15)
C13—N3—H3N	115.5 (11)	C11—C12—N3	116.38 (14)
C12—N3—H3N	114.9 (11)	C7—C12—N3	124.75 (14)
C18—N4—C17	116.35 (19)	O2—C13—N3	124.23 (15)
N1—C1—C5	125.06 (18)	O2—C13—C14	120.41 (15)
N1—C1—H1	117.5	N3—C13—C14	115.36 (14)
C5—C1—H1	117.5	C15—C14—C18	117.49 (16)
N1—C2—C3	124.06 (18)	C15—C14—C13	120.17 (15)

N1—C2—H2	118.0	C18—C14—C13	122.24 (16)
C3—C2—H2	118.0	C16—C15—C14	119.24 (18)
C2—C3—C4	119.02 (18)	C16—C15—H15	120.4
C2—C3—H3	120.5	C14—C15—H15	120.4
C4—C3—H3	120.5	C17—C16—C15	118.8 (2)
C3—C4—C5	118.88 (17)	C17—C16—H16	120.6
C3—C4—H4	120.6	C15—C16—H16	120.6
C5—C4—H4	120.6	N4—C17—C16	123.8 (2)
C4—C5—C1	117.21 (16)	N4—C17—H17	118.1
C4—C5—C6	125.11 (15)	C16—C17—H17	118.1
C1—C5—C6	117.65 (15)	N4—C18—C14	124.24 (19)
O1—C6—N2	123.77 (15)	N4—C18—H18	117.9
O1—C6—C5	120.29 (15)	C14—C18—H18	117.9
N2—C6—C5	115.94 (15)	C9—C19—H19A	109.5
C8—C7—C12	118.58 (15)	C9—C19—H19B	109.5
C8—C7—N2	120.63 (15)	H19A—C19—H19B	109.5
C12—C7—N2	120.78 (14)	C9—C19—H19C	109.5
C9—C8—C7	122.53 (16)	H19A—C19—H19C	109.5
C9—C8—H8	118.7	H19B—C19—H19C	109.5
C7—C8—H8	118.7	C10—C20—H20A	109.5
C8—C9—C10	119.05 (15)	C10—C20—H20B	109.5
C8—C9—C19	119.53 (16)	H20A—C20—H20B	109.5
C10—C9—C19	121.40 (17)	C10—C20—H20C	109.5
C11—C10—C9	118.08 (15)	H20A—C20—H20C	109.5
C11—C10—C20	120.10 (16)	H20B—C20—H20C	109.5
C2—N1—C1—C5	−1.1 (3)	C9—C10—C11—C12	1.1 (2)
C1—N1—C2—C3	0.7 (3)	C20—C10—C11—C12	179.44 (16)
N1—C2—C3—C4	0.3 (3)	C10—C11—C12—C7	−0.3 (2)
C2—C3—C4—C5	−0.8 (3)	C10—C11—C12—N3	175.65 (14)
C3—C4—C5—C1	0.4 (2)	C8—C7—C12—C11	−1.6 (2)
C3—C4—C5—C6	−177.68 (15)	N2—C7—C12—C11	179.49 (14)
N1—C1—C5—C4	0.6 (3)	C8—C7—C12—N3	−177.19 (14)
N1—C1—C5—C6	178.84 (17)	N2—C7—C12—N3	3.9 (2)
C7—N2—C6—O1	6.3 (3)	C13—N3—C12—C11	138.35 (17)
C7—N2—C6—C5	−174.10 (13)	C13—N3—C12—C7	−45.9 (2)
C4—C5—C6—O1	148.83 (17)	C12—N3—C13—O2	7.3 (3)
C1—C5—C6—O1	−29.3 (2)	C12—N3—C13—C14	−172.16 (14)
C4—C5—C6—N2	−30.8 (2)	O2—C13—C14—C15	36.5 (2)
C1—C5—C6—N2	151.08 (16)	N3—C13—C14—C15	−144.00 (16)
C6—N2—C7—C8	37.4 (2)	O2—C13—C14—C18	−139.76 (18)
C6—N2—C7—C12	−143.67 (16)	N3—C13—C14—C18	39.7 (2)
C12—C7—C8—C9	2.8 (2)	C18—C14—C15—C16	−1.6 (3)
N2—C7—C8—C9	−178.30 (15)	C13—C14—C15—C16	−178.07 (17)
C7—C8—C9—C10	−2.0 (3)	C14—C15—C16—C17	1.9 (3)
C7—C8—C9—C19	179.94 (16)	C18—N4—C17—C16	−2.8 (3)
C8—C9—C10—C11	0.0 (2)	C15—C16—C17—N4	0.3 (3)
C19—C9—C10—C11	178.07 (17)	C17—N4—C18—C14	3.1 (3)
C8—C9—C10—C20	−178.29 (17)	C15—C14—C18—N4	−1.0 (3)
C19—C9—C10—C20	−0.2 (3)	C13—C14—C18—N4	175.37 (18)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O1	0.93	2.51	2.921 (2)	107
N2—H2N···O2	0.90 (2)	1.88 (2)	2.701 (2)	150.8 (16)
C17—H17···O1^{i}	0.93	2.55	3.461 (3)	165
N3—H3N···O1^{ii}	0.907 (17)	2.066 (18)	2.9407 (19)	161.6 (15)

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

Fig. 1

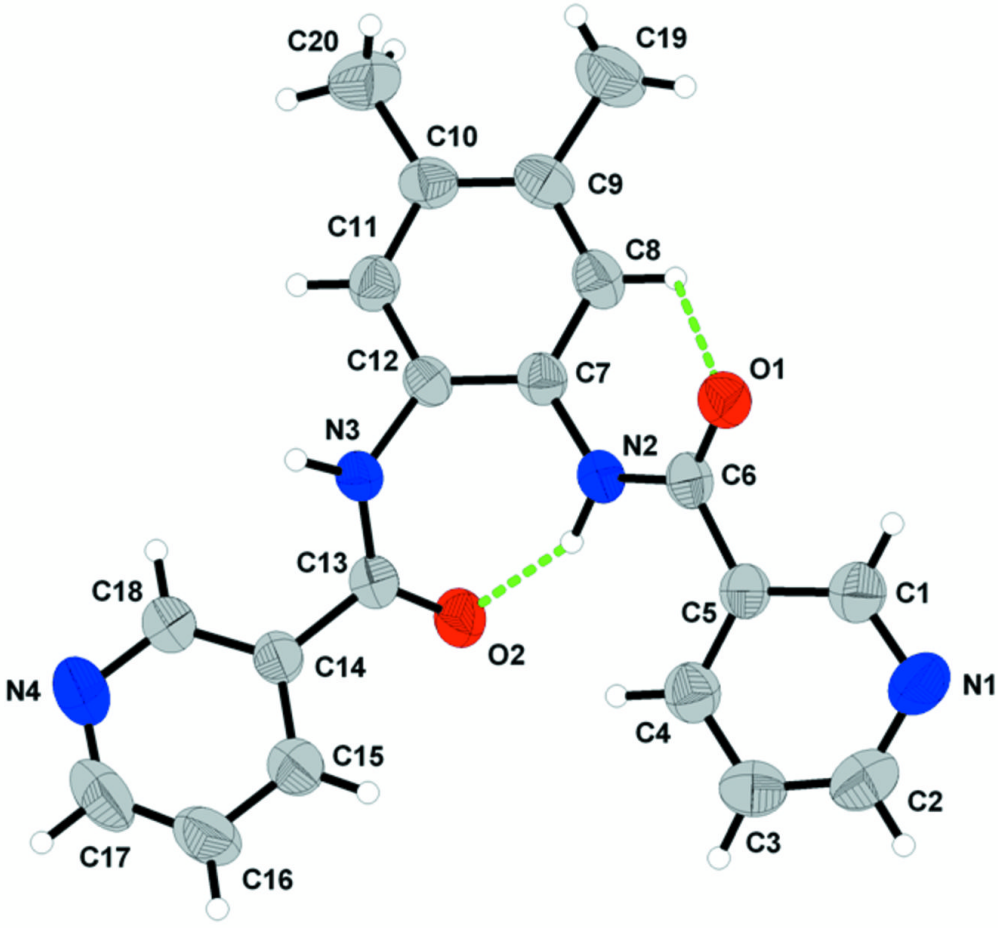
C20
C19
C10
C9
C11
C8
C12
C7
O1
N3
N2
C6
C13
C18
C5
C1
O2
C14
N4
N1
C4
C15
C2
C17
C3
C16

Fig. 2