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4-(1-Ethyl-1*H*-1,3-benzimidazol-2-yl)-*N*,*N*-diphenylaniline monohydrate

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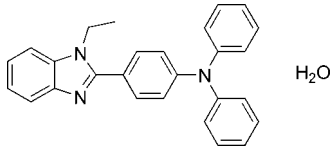
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.057; wR factor = 0.169; data-to-parameter ratio = 14.3.

In the title compound, $C_{27}H_{23}N_3O\cdot H_2O$, the benzimidazole ring system has an r.m.s. deviation of 0.0071 Å and makes dihedral angles of 34.51 (2), 55.22 (3) and 41.05 (5)° with the central and N-bonded phenyl rings, respectively. In the crystal, the water molecular is connected to the organic molecule by intermolecular O—H···N hydrogen bonds. Weak intermolecular C—H···O hydrogen bonds also occur.

Related literature

For the synthetic procedure, see: Vinodkumar *et al.* (2008). For bond-length data, see: Allen *et al.* (1987). For background to the use of the title compound as an intermediate in the preparation of OLED materials, see: Kakimoto *et al.* (2008).



Experimental

Crystal data

$C_{27}H_{23}N_3\cdot H_2O$
M_r = 407.50
Monoclinic, $P2_1/c$
a = 12.278 (3) Å
b = 9.2690 (19) Å
c = 19.468 (4) Å
β = 97.81 (3)°
V = 2195.0 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.978, T_{max} = 0.992
4223 measured reflections
4024 independent reflections
2487 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.169
S = 1.01
4024 reflections
281 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O*W*—H*WB*···N2	0.85	2.50	2.903 (3)	110
O*W*—H*WA*···N2	0.85	2.49	2.903 (3)	111
C24—H24*A*···O*W*^{i}	0.93	2.43	3.352 (4)	173

Symmetry code: (i) $x, y-1, z$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: BQ2268).

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supporting information

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4-(1-Ethyl-1*H*-1,3-benzimidazol-2-yl)-*N*,*N*-diphenylaniline monohydrate

Tao Wu, Kai Wang, Peng Jiang and Hong-Jun Zhu

S1. Comment

The title compound, (I), is a kind of important organic intermediate which can be used for many fields such as OLED materials. (Kakimoto *et al.*, 2008). We herein report its crystal structure.

In the molecule of (I), (Fig.1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. The benzimidazole ring (A) is obviously almost coplanar with an r.m.s. deviation of 0.0071 °. The dihedral angles between A and the rest three phenyl rings B (C13-C18), C (C7-C12) and D (C1-C6) are 34.51 (2) ° 55.22 (3) ° and 41.05 (5) °, respectively. The H_2O molecule stems from the solvent ethanol, and the water molecular is connected with the target molecular by intermolecular C—H···O and O—H···N hydrogen bonds (Table 1), which seems to be very effective in the stabilization of the crystal structure.

S2. Experimental

The title compound, (I) was synthesized according to the literature (Vinodkumar *et al.*, 2008) The crystals were obtained by dissolving (I) (0.52 g, 1.28 mmol) in 25 ml ethanol and evaporating the solvent slowly at room temperature for about 7 d.

S3. Refinement

H atoms bonded to N and O atoms were located in a difference map and refined with distance restraints of O—H = 0.85 (2) and N—H = 0.90 (2) Å, and with U_{iso}(H) = *1.2*U_{eq}(N,*O*). Other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 - 0.97 (2) Å, U_{iso}(H) = *1.2*U_{eq}(C).

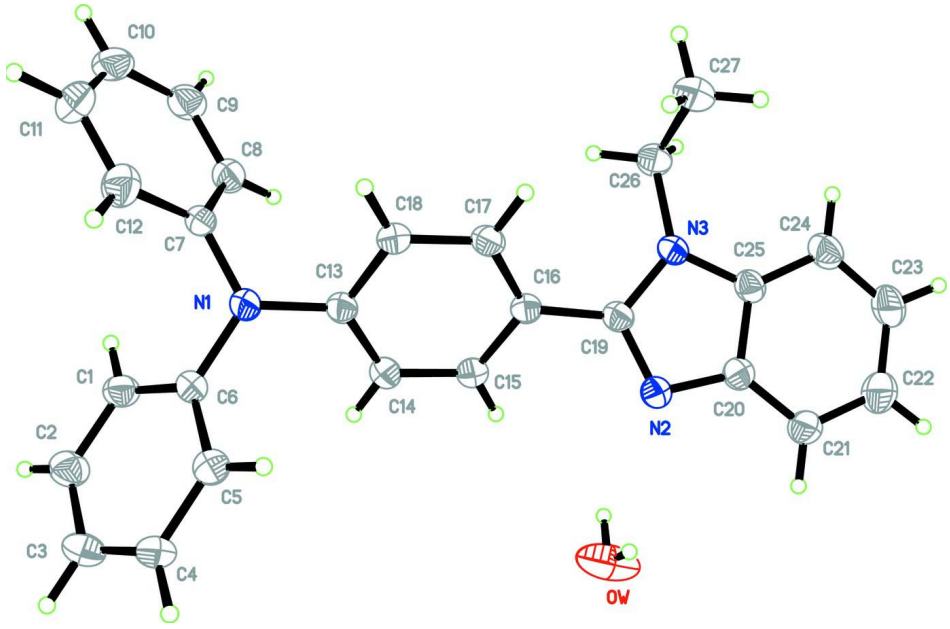

Figure 1

The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

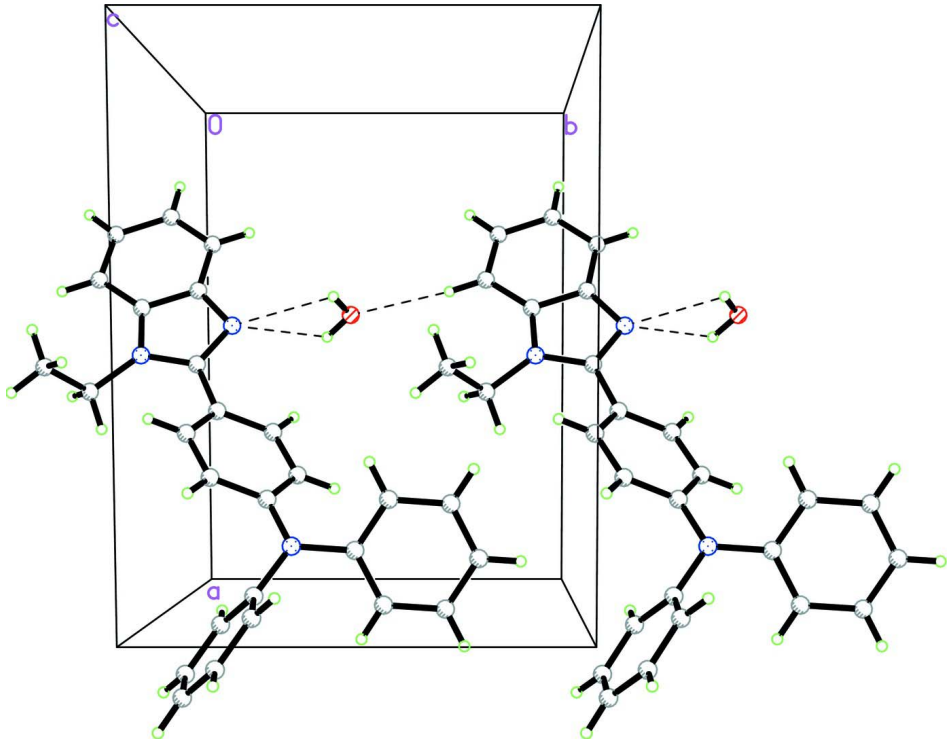

Figure 2

A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

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Crystal data

$C_{27}H_{23}N_3 \cdot H_2O$
$M_r = 407.50$
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Hall symbol: -P 2ybc
$a = 12.278$ (3) Å
$b = 9.2690$ (19) Å
$c = 19.468$ (4) Å
$\beta = 97.81$ (3)°
$V = 2195.0$ (8) Å^3
$Z = 4$
$F(000) = 864$
$D_x = 1.233$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 10$–14°
$\mu = 0.08$ mm^{-1}
$T = 293$ K
Block, colorless
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.978$, $T_{max} = 0.992$
4223 measured reflections
4024 independent reflections
2487 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 25.4°$, $\theta_{min} = 1.7°$
$h = 0 \rightarrow 14$
$k = 0 \rightarrow 11$
$l = -23 \rightarrow 23$
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.169$
$S = 1.01$
4024 reflections
281 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
$w = 1/[\sigma^2(F_o^2) + (0.090P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0093 (17)

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	0.12417 (17)	0.8084 (2)	−0.08205 (12)	0.0535 (6)
C1	0.0167 (2)	1.0299 (3)	−0.09280 (14)	0.0502 (7)

H1A	−0.0468	0.9764	−0.0906	0.060*
N2	0.53509 (16)	0.6320 (2)	0.14215 (10)	0.0457 (5)
C2	0.0102 (2)	1.1782 (3)	−0.10031 (16)	0.0599 (8)
H2B	−0.0578	1.2238	−0.1038	0.072*
N3	0.47737 (16)	0.4037 (2)	0.12179 (11)	0.0435 (5)
C3	0.1033 (3)	1.2582 (3)	−0.10260 (16)	0.0622 (8)
H3A	0.0986	1.3580	−0.1072	0.075*
C4	0.2031 (2)	1.1914 (3)	−0.09818 (15)	0.0567 (7)
H4A	0.2664	1.2461	−0.0993	0.068*
C5	0.2108 (2)	1.0429 (3)	−0.09211 (14)	0.0522 (7)
H5A	0.2787	0.9977	−0.0905	0.063*
C6	0.1169 (2)	0.9614 (3)	−0.08850 (13)	0.0442 (6)
C7	0.03574 (19)	0.7225 (3)	−0.11420 (13)	0.0419 (6)
C8	−0.0220 (2)	0.6349 (3)	−0.07465 (15)	0.0514 (7)
H8A	−0.0017	0.6299	−0.0269	0.062*
C9	−0.1095 (2)	0.5549 (3)	−0.10554 (18)	0.0625 (8)
H9A	−0.1477	0.4955	−0.0786	0.075*
C10	−0.1405 (3)	0.5620 (3)	−0.1750 (2)	0.0737 (10)
H10A	−0.2004	0.5088	−0.1956	0.088*
C11	−0.0834 (3)	0.6476 (4)	−0.21467 (17)	0.0733 (9)
H11A	−0.1042	0.6516	−0.2624	0.088*
C12	0.0048 (2)	0.7282 (3)	−0.18469 (14)	0.0609 (8)
H12A	0.0433	0.7861	−0.2121	0.073*
C13	0.20766 (19)	0.7440 (3)	−0.03508 (13)	0.0431 (6)
C14	0.2497 (2)	0.8104 (3)	0.02666 (13)	0.0461 (6)
H14A	0.2234	0.9005	0.0375	0.055*
C15	0.3298 (2)	0.7442 (3)	0.07189 (13)	0.0443 (6)
H15A	0.3578	0.7910	0.1128	0.053*
C16	0.37033 (19)	0.6077 (3)	0.05776 (13)	0.0408 (6)
C17	0.32912 (19)	0.5432 (3)	−0.00436 (13)	0.0435 (6)
H17A	0.3560	0.4536	−0.0154	0.052*
C18	0.2488 (2)	0.6091 (3)	−0.05033 (13)	0.0446 (6)
H18A	0.2220	0.5633	−0.0917	0.053*
C19	0.4598 (2)	0.5481 (3)	0.10699 (13)	0.0419 (6)
C20	0.6054 (2)	0.5389 (3)	0.18193 (13)	0.0457 (6)
C21	0.6991 (2)	0.5681 (3)	0.22815 (14)	0.0560 (7)
H21A	0.7225	0.6625	0.2371	0.067*
C22	0.7562 (3)	0.4543 (4)	0.26021 (16)	0.0706 (9)
H22A	0.8196	0.4716	0.2910	0.085*
C23	0.7204 (3)	0.3122 (3)	0.24720 (16)	0.0681 (9)
H23A	0.7611	0.2374	0.2697	0.082*
C24	0.6278 (2)	0.2793 (3)	0.20264 (15)	0.0587 (8)
H24A	0.6040	0.1847	0.1947	0.070*
C25	0.5710 (2)	0.3962 (3)	0.16973 (13)	0.0443 (6)
C26	0.4069 (2)	0.2785 (3)	0.10055 (15)	0.0556 (7)
H26A	0.3350	0.3125	0.0803	0.067*
H26B	0.3975	0.2221	0.1413	0.067*
C27	0.4534 (3)	0.1826 (3)	0.04887 (17)	0.0717 (9)

H27A	0.4046	0.1029	0.0370	0.108*
H27B	0.5241	0.1471	0.0689	0.108*
H27C	0.4611	0.2371	0.0079	0.108*
OW	0.5578 (2)	0.9300 (3)	0.18768 (15)	0.1158 (10)
HWB	0.5151	0.8673	0.2015	0.139*
HWA	0.5919	0.8888	0.1579	0.139*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0452 (12)	0.0373 (12)	0.0720 (15)	−0.0054 (10)	−0.0136 (11)	0.0103 (11)
C1	0.0447 (15)	0.0436 (16)	0.0618 (18)	−0.0048 (12)	0.0060 (13)	−0.0013 (13)
N2	0.0466 (12)	0.0395 (12)	0.0487 (13)	0.0007 (10)	−0.0017 (10)	0.0037 (10)
C2	0.0593 (18)	0.0438 (17)	0.076 (2)	0.0047 (14)	0.0084 (15)	−0.0064 (14)
N3	0.0456 (12)	0.0314 (11)	0.0524 (13)	−0.0009 (9)	0.0030 (10)	0.0064 (9)
C3	0.076 (2)	0.0335 (15)	0.076 (2)	−0.0049 (15)	0.0059 (17)	−0.0042 (14)
C4	0.0601 (18)	0.0439 (17)	0.0637 (18)	−0.0169 (14)	−0.0005 (14)	0.0051 (14)
C5	0.0432 (14)	0.0482 (16)	0.0631 (18)	−0.0050 (13)	−0.0007 (13)	0.0064 (14)
C6	0.0455 (14)	0.0373 (14)	0.0476 (15)	−0.0025 (12)	−0.0012 (12)	0.0054 (12)
C7	0.0381 (13)	0.0333 (13)	0.0520 (16)	−0.0002 (11)	−0.0019 (12)	0.0013 (11)
C8	0.0511 (15)	0.0469 (16)	0.0554 (17)	−0.0007 (13)	0.0041 (13)	0.0050 (13)
C9	0.0478 (16)	0.0487 (17)	0.090 (2)	−0.0096 (14)	0.0067 (16)	0.0052 (16)
C10	0.0583 (19)	0.0508 (19)	0.104 (3)	−0.0061 (16)	−0.0186 (19)	−0.0158 (19)
C11	0.085 (2)	0.071 (2)	0.0557 (19)	0.004 (2)	−0.0171 (18)	−0.0122 (17)
C12	0.0669 (19)	0.0648 (19)	0.0495 (17)	−0.0021 (16)	0.0026 (15)	0.0044 (14)
C13	0.0378 (13)	0.0357 (14)	0.0544 (16)	−0.0037 (11)	0.0013 (12)	0.0076 (12)
C14	0.0448 (14)	0.0386 (14)	0.0537 (16)	0.0036 (12)	0.0025 (12)	−0.0012 (12)
C15	0.0458 (14)	0.0399 (14)	0.0458 (15)	−0.0016 (12)	0.0009 (12)	−0.0031 (11)
C16	0.0377 (13)	0.0367 (14)	0.0476 (15)	−0.0032 (11)	0.0040 (11)	0.0025 (11)
C17	0.0415 (13)	0.0332 (13)	0.0560 (16)	−0.0002 (11)	0.0073 (12)	−0.0011 (12)
C18	0.0450 (14)	0.0381 (14)	0.0487 (15)	−0.0049 (12)	−0.0003 (12)	−0.0016 (12)
C19	0.0430 (13)	0.0360 (14)	0.0469 (14)	−0.0002 (12)	0.0063 (11)	0.0028 (12)
C20	0.0463 (15)	0.0440 (15)	0.0460 (15)	0.0011 (12)	0.0041 (12)	0.0036 (12)
C21	0.0570 (17)	0.0506 (17)	0.0563 (17)	−0.0022 (14)	−0.0067 (14)	0.0013 (14)
C22	0.0651 (19)	0.076 (2)	0.064 (2)	0.0051 (18)	−0.0142 (16)	0.0095 (17)
C23	0.072 (2)	0.061 (2)	0.067 (2)	0.0176 (17)	−0.0079 (17)	0.0206 (16)
C24	0.0676 (19)	0.0433 (16)	0.0645 (19)	0.0062 (14)	0.0067 (16)	0.0122 (14)
C25	0.0469 (14)	0.0404 (14)	0.0458 (15)	0.0033 (12)	0.0072 (12)	0.0076 (12)
C26	0.0544 (16)	0.0392 (15)	0.0715 (19)	−0.0095 (13)	0.0032 (14)	0.0105 (14)
C27	0.077 (2)	0.0437 (17)	0.091 (2)	−0.0017 (16)	−0.0020 (18)	−0.0060 (16)
OW	0.154 (2)	0.0616 (15)	0.146 (2)	−0.0265 (16)	0.073 (2)	−0.0184 (15)

Geometric parameters (Å, º)

N1—C13	1.410 (3)	C13—C14	1.386 (4)
N1—C7	1.421 (3)	C13—C18	1.396 (3)
N1—C6	1.426 (3)	C14—C15	1.373 (3)
C1—C6	1.377 (3)	C14—H14A	0.9300

C1—C2	1.383 (4)	C15—C16	1.401 (3)
C1—H1A	0.9300	C15—H15A	0.9300
N2—C19	1.324 (3)	C16—C17	1.382 (3)
N2—C20	1.381 (3)	C16—C19	1.464 (3)
C2—C3	1.369 (4)	C17—C18	1.380 (3)
C2—H2B	0.9300	C17—H17A	0.9300
N3—C19	1.380 (3)	C18—H18A	0.9300
N3—C25	1.381 (3)	C20—C21	1.388 (3)
N3—C26	1.473 (3)	C20—C25	1.398 (4)
C3—C4	1.365 (4)	C21—C22	1.369 (4)
C3—H3A	0.9300	C21—H21A	0.9300
C4—C5	1.384 (4)	C22—C23	1.401 (4)
C4—H4A	0.9300	C22—H22A	0.9300
C5—C6	1.388 (3)	C23—C24	1.368 (4)
C5—H5A	0.9300	C23—H23A	0.9300
C7—C12	1.374 (4)	C24—C25	1.397 (3)
C7—C8	1.380 (3)	C24—H24A	0.9300
C8—C9	1.375 (4)	C26—C27	1.511 (4)
C8—H8A	0.9300	C26—H26A	0.9700
C9—C10	1.356 (5)	C26—H26B	0.9700
C9—H9A	0.9300	C27—H27A	0.9600
C10—C11	1.365 (5)	C27—H27B	0.9600
C10—H10A	0.9300	C27—H27C	0.9600
C11—C12	1.378 (4)	OW—HWB	0.8499
C11—H11A	0.9300	OW—HWA	0.8501
C12—H12A	0.9300		

C13—N1—C7	119.5 (2)	C13—C14—H14A	119.7
C13—N1—C6	120.7 (2)	C14—C15—C16	121.4 (2)
C7—N1—C6	118.9 (2)	C14—C15—H15A	119.3
C6—C1—C2	120.2 (3)	C16—C15—H15A	119.3
C6—C1—H1A	119.9	C17—C16—C15	117.7 (2)
C2—C1—H1A	119.9	C17—C16—C19	124.3 (2)
C19—N2—C20	105.2 (2)	C15—C16—C19	117.8 (2)
C3—C2—C1	120.4 (3)	C18—C17—C16	121.4 (2)
C3—C2—H2B	119.8	C18—C17—H17A	119.3
C1—C2—H2B	119.8	C16—C17—H17A	119.3
C19—N3—C25	106.37 (19)	C17—C18—C13	120.4 (2)
C19—N3—C26	129.6 (2)	C17—C18—H18A	119.8
C25—N3—C26	123.6 (2)	C13—C18—H18A	119.8
C4—C3—C2	119.9 (3)	N2—C19—N3	112.5 (2)
C4—C3—H3A	120.0	N2—C19—C16	121.7 (2)
C2—C3—H3A	120.0	N3—C19—C16	125.7 (2)
C3—C4—C5	120.4 (3)	N2—C20—C21	129.9 (2)
C3—C4—H4A	119.8	N2—C20—C25	110.1 (2)
C5—C4—H4A	119.8	C21—C20—C25	120.0 (2)
C4—C5—C6	119.9 (3)	C22—C21—C20	118.2 (3)
C4—C5—H5A	120.1	C22—C21—H21A	120.9

C6—C5—H5A	120.1	C20—C21—H21A	120.9
C1—C6—C5	119.2 (2)	C21—C22—C23	120.9 (3)
C1—C6—N1	120.6 (2)	C21—C22—H22A	119.6
C5—C6—N1	120.2 (2)	C23—C22—H22A	119.6
C12—C7—C8	119.1 (2)	C24—C23—C22	122.6 (3)
C12—C7—N1	120.6 (2)	C24—C23—H23A	118.7
C8—C7—N1	120.3 (2)	C22—C23—H23A	118.7
C9—C8—C7	120.3 (3)	C23—C24—C25	116.0 (3)
C9—C8—H8A	119.9	C23—C24—H24A	122.0
C7—C8—H8A	119.9	C25—C24—H24A	122.0
C10—C9—C8	120.4 (3)	N3—C25—C24	131.8 (2)
C10—C9—H9A	119.8	N3—C25—C20	105.8 (2)
C8—C9—H9A	119.8	C24—C25—C20	122.4 (2)
C9—C10—C11	119.8 (3)	N3—C26—C27	112.9 (2)
C9—C10—H10A	120.1	N3—C26—H26A	109.0
C11—C10—H10A	120.1	C27—C26—H26A	109.0
C10—C11—C12	120.6 (3)	N3—C26—H26B	109.0
C10—C11—H11A	119.7	C27—C26—H26B	109.0
C12—C11—H11A	119.7	H26A—C26—H26B	107.8
C7—C12—C11	119.8 (3)	C26—C27—H27A	109.5
C7—C12—H12A	120.1	C26—C27—H27B	109.5
C11—C12—H12A	120.1	H27A—C27—H27B	109.5
C14—C13—C18	118.6 (2)	C26—C27—H27C	109.5
C14—C13—N1	121.8 (2)	H27A—C27—H27C	109.5
C18—C13—N1	119.6 (2)	H27B—C27—H27C	109.5
C15—C14—C13	120.5 (2)	HWB—OW—HWA	106.9
C15—C14—H14A	119.7		

C6—C1—C2—C3	−0.9 (4)	C19—C16—C17—C18	−176.2 (2)
C1—C2—C3—C4	0.7 (5)	C16—C17—C18—C13	0.4 (4)
C2—C3—C4—C5	0.7 (4)	C14—C13—C18—C17	0.5 (4)
C3—C4—C5—C6	−1.8 (4)	N1—C13—C18—C17	−178.8 (2)
C2—C1—C6—C5	−0.3 (4)	C20—N2—C19—N3	0.0 (3)
C2—C1—C6—N1	−178.8 (3)	C20—N2—C19—C16	−179.3 (2)
C4—C5—C6—C1	1.6 (4)	C25—N3—C19—N2	−0.2 (3)
C4—C5—C6—N1	−179.8 (3)	C26—N3—C19—N2	172.0 (2)
C13—N1—C6—C1	−136.8 (3)	C25—N3—C19—C16	179.0 (2)
C7—N1—C6—C1	32.2 (4)	C26—N3—C19—C16	−8.7 (4)
C13—N1—C6—C5	44.7 (4)	C17—C16—C19—N2	142.4 (3)
C7—N1—C6—C5	−146.3 (2)	C15—C16—C19—N2	−32.3 (3)
C13—N1—C7—C12	−130.9 (3)	C17—C16—C19—N3	−36.8 (4)
C6—N1—C7—C12	59.9 (3)	C15—C16—C19—N3	148.5 (2)
C13—N1—C7—C8	50.7 (3)	C19—N2—C20—C21	179.5 (3)
C6—N1—C7—C8	−118.5 (3)	C19—N2—C20—C25	0.2 (3)
C12—C7—C8—C9	−0.2 (4)	N2—C20—C21—C22	−178.5 (3)
N1—C7—C8—C9	178.2 (2)	C25—C20—C21—C22	0.6 (4)
C7—C8—C9—C10	−0.5 (4)	C20—C21—C22—C23	−0.6 (5)
C8—C9—C10—C11	1.0 (5)	C21—C22—C23—C24	−0.2 (5)

C9—C10—C11—C12	−0.7 (5)	C22—C23—C24—C25	0.8 (5)
C8—C7—C12—C11	0.5 (4)	C19—N3—C25—C24	−179.4 (3)
N1—C7—C12—C11	−177.9 (3)	C26—N3—C25—C24	7.8 (4)
C10—C11—C12—C7	−0.1 (5)	C19—N3—C25—C20	0.4 (3)
C7—N1—C13—C14	−137.3 (3)	C26—N3—C25—C20	−172.5 (2)
C6—N1—C13—C14	31.7 (4)	C23—C24—C25—N3	178.9 (3)
C7—N1—C13—C18	42.1 (3)	C23—C24—C25—C20	−0.8 (4)
C6—N1—C13—C18	−149.0 (2)	N2—C20—C25—N3	−0.4 (3)
C18—C13—C14—C15	−0.3 (4)	C21—C20—C25—N3	−179.7 (2)
N1—C13—C14—C15	179.0 (2)	N2—C20—C25—C24	179.4 (2)
C13—C14—C15—C16	−0.9 (4)	C21—C20—C25—C24	0.0 (4)
C14—C15—C16—C17	1.8 (4)	C19—N3—C26—C27	110.2 (3)
C14—C15—C16—C19	176.8 (2)	C25—N3—C26—C27	−78.7 (3)
C15—C16—C17—C18	−1.6 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O*W*—H*WB*···N2	0.85	2.50	2.903 (3)	110
O*W*—H*WA*···N2	0.85	2.49	2.903 (3)	111
C24—H24*A*···O*W*^{i}	0.93	2.43	3.352 (4)	173

Symmetry code: (i) *x*, *y*−1, *z*.