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1,3-Dicyclohexyl-1-isonicotinoylurea monohydrate

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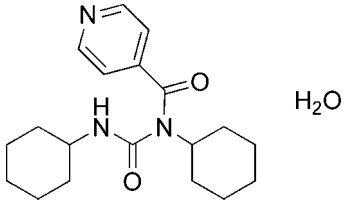
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.119; data-to-parameter ratio = 12.5.

The title organic compound, $C_{19}H_{27}N_3O_2\cdot H_2O$, was synthesized from methylene dicyclohexylamine, 4-pyridinecarboxylic acid and *N*,*N*′-dicyclohexylcarbodiimide. The water molecule is involved in intermolecular hydrogen bonds, linking symmetry-related urea molecules into a two-dimensional supramolecular ladder-like structure.

Related literature

For related literature, see: Iyer *et al.* (1971); Jew *et al.* (2003); Li *et al.* (2006); Mu & Qin (2003); Wachter *et al.* (1998).



Experimental

Crystal data

$C_{19}H_{27}N_3O_2\cdot H_2O$
M_r = 347.45
Triclinic, $P\overline{1}$
a = 6.6694 (13) Å
b = 11.106 (2) Å
c = 13.248 (3) Å
α = 98.55 (3)°
β = 94.11 (3)°
γ = 97.49 (3)°
V = 958.0 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
0.40 × 0.33 × 0.28 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.968, T_{max} = 0.977
9385 measured reflections
4284 independent reflections
2948 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.119
S = 1.04
4284 reflections
342 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.14 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
O3—H6···O1	0.89 (3)	1.95 (3)	2.7959 (18)	158 (2)
N2—H10···O3^{i}	0.91 (2)	1.89 (2)	2.7949 (19)	170 (2)
O3—H12···O2^{ii}	0.89 (2)	1.95 (3)	2.8319 (19)	171 (2)

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

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; 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: CS2080).

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1,3-Dicyclohexyl-1-isonicotinoylurea monohydrate

Cun-Kuan Wang and Feng-Yan Zhou

S1. Comment

Pyridine derivatives are important intermediates widely used in the synthesis of drugs (Wachter *et al.*, 1998; Jew *et al.*, 2003) and pesticides (Li *et al.*, 2006; Mu & Qin, 2003). The title organic compound, 1,3-dicyclohexyl-1-isonicotinoyl-urea, is an intermediate for the synthesis of an anti-tuberculosis drug (Iyer *et al.*, 1971). We report here its synthesis and the crystal structure of its hydrate.

The title compound was synthesized from methylene dicyclohexylamine, 4-pyridinecarboxylic acid and *N*,*N*′-dicyclo-hexylcarbodiimide. Asymmetric unit of the crystal structure consists of the organic molecule and one H_2O molecule, $C_{19}H_{27}N_3O_2.H_2O$. As shown in Fig. 1 and Table 1, the cyclohexyl groups display chair-type conformation. Interestingly, there are some strong intermolecular hydrogen bonds between the organic molecules and the crystal water. Thus each water effectively links two molecules as O–H···O donor to their O=C groups and accepts one N–H···O hydrogen bridge from a third molecule into a novel two-dimensional supramolecular ladder-like structure through both O—H···O and N—H···O hydrogen bonds (Fig.2 and Table 2).

S2. Experimental

Methylene dicyclohexylamine (0.21 g, 1 mmol), 4-pyridinecarboxylic acid (0.12 g, 1 mmol) and *N*,*N*′-dicyclohexyl-carbodiimide (0.25 g, 1.2 mmol) were added to a 50 ml round bottom flask, then added dichloromethane (25 ml). The mixture was stirred for 12 h at 298 K, after that the reaction mixture was washed with water (10 ml × 3). The organic layer was dried with anhydrous Na_2SO_4 and evaporated *in vacuo* to give a residue. The crude product was purified by column chromatography (SiO_2–EtOAc and hexane, 1:10) to afford the title compound as a colorless solid (yield 69%). ^{1}H NMR (400 MHz, $CDCl_3$): *d* 8.57 (d, *J* = 5.6 Hz, 2 H), 7.37 (d, *J* = 5.6 Hz, 2 H), 4.16–4.11 (m, 1 H), 3.27–3.22 (m, 1 H), 1.81–1.64 (m, 8 H), 1.60–1.57 (m, 2 H), 1.51–1.22 (m, 4 H), 1.17–1.08 (m, 2 H), 1.00–0.94 (m, 2 H), 0.85–0.76 (m, 2 H).

S3. Refinement

All H atoms were located in difference Fourier maps and refined independently with isotropic displacement parameters.

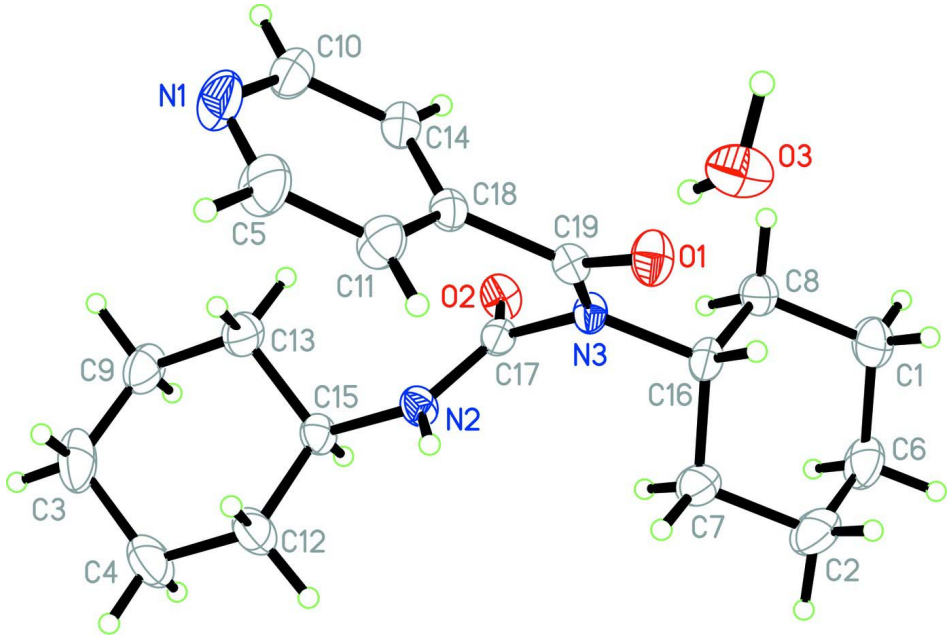

Figure 1

Perspective view of the title complex with the atom-numbering scheme. Atomic displacement ellipsoids are shown at the 30% probability level.

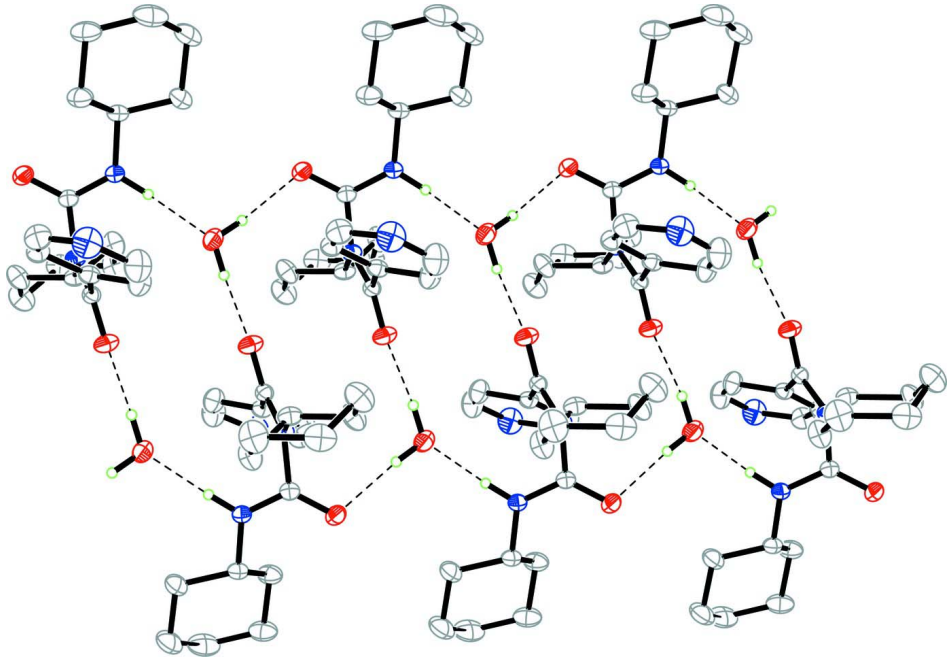

Figure 2

View of the two-dimensional hydrogen-bonded supramolecular structure.

1,3-Dicyclohexyl-1-isonicotinoylurea monohydrate

Crystal data

$C_{19}H_{27}N_3O_2 \cdot H_2O$
$M_r = 347.45$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.6694$ (13) Å
$b = 11.106$ (2) Å
$c = 13.248$ (3) Å
$\alpha = 98.55$ (3)°
$\beta = 94.11$ (3)°
$\gamma = 97.49$ (3)°
$V = 958.0$ (3) Å^3
$Z = 2$
$F(000) = 376$
$D_x = 1.205$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3059 reflections
$\theta = 3.1$–$27.5°$
$\mu = 0.08$ mm^{-1}
$T = 298$ K
Block, colorless
0.40 × 0.33 × 0.28 mm

Data collection

Bruker SMART CCD APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.40 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.968$, $T_{max} = 0.977$
9385 measured reflections
4284 independent reflections
2948 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -8 \rightarrow 7$
$k = -14 \rightarrow 14$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.119$
$S = 1.05$
4284 reflections
342 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.054P)^2 + 0.1047P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.25983 (16)	0.03443 (9)	0.01466 (8)	0.0451 (3)
O2	0.57498 (15)	0.02624 (10)	0.32408 (8)	0.0437 (3)
O3	0.11137 (18)	−0.00473 (13)	−0.19210 (11)	0.0546 (3)
N1	0.2456 (3)	−0.40235 (13)	0.05844 (13)	0.0635 (4)
N2	0.23694 (19)	−0.04403 (11)	0.29989 (9)	0.0357 (3)
N3	0.38649 (17)	0.06272 (10)	0.18085 (8)	0.0325 (3)
C1	0.6570 (4)	0.39594 (16)	0.21113 (19)	0.0636 (5)
C2	0.3121 (3)	0.39686 (17)	0.2711 (2)	0.0667 (6)
C3	0.0813 (4)	−0.32783 (19)	0.47794 (19)	0.0731 (6)
C4	−0.0296 (4)	−0.2166 (2)	0.48890 (18)	0.0690 (6)
C5	0.0909 (3)	−0.34257 (17)	0.03668 (17)	0.0650 (5)

C6	0.5319 (3)	0.45402 (16)	0.29056 (16)	0.0602 (5)
C7	0.2898 (3)	0.25718 (15)	0.26796 (16)	0.0536 (5)
C8	0.6370 (3)	0.25617 (14)	0.20801 (17)	0.0513 (4)
C9	0.3026 (3)	−0.29165 (18)	0.46441 (15)	0.0593 (5)
C10	0.4223 (3)	−0.33354 (15)	0.09157 (14)	0.0524 (4)
C11	0.1057 (3)	−0.21635 (15)	0.04690 (14)	0.0498 (4)
C12	−0.0014 (3)	−0.1451 (2)	0.40009 (15)	0.0539 (4)
C13	0.3287 (3)	−0.22376 (17)	0.37377 (14)	0.0505 (4)
C14	0.4515 (3)	−0.20672 (14)	0.10728 (12)	0.0414 (4)
C15	0.2219 (2)	−0.11014 (14)	0.38727 (11)	0.0371 (3)
C16	0.4161 (2)	0.19968 (12)	0.18824 (12)	0.0376 (3)
C17	0.4089 (2)	0.01254 (12)	0.27488 (10)	0.0326 (3)
C18	0.2898 (2)	−0.14614 (12)	0.08435 (10)	0.0351 (3)
C19	0.3093 (2)	−0.00917 (12)	0.09085 (10)	0.0324 (3)
H1	0.289 (2)	−0.0558 (14)	0.4476 (12)	0.039 (4)*
H2	0.365 (2)	0.2150 (14)	0.1216 (13)	0.045 (4)*
H3	0.579 (3)	−0.1618 (15)	0.1334 (12)	0.047 (4)*
H4	−0.010 (3)	−0.1756 (17)	0.0266 (14)	0.064 (5)*
H5	0.260 (3)	−0.2770 (17)	0.3092 (15)	0.063 (5)*
H6	0.153 (4)	−0.014 (2)	−0.128 (2)	0.093 (8)*
H7	−0.061 (3)	−0.1957 (18)	0.3374 (16)	0.064 (6)*
H8	0.341 (3)	0.2358 (16)	0.3374 (15)	0.060 (5)*
H9	0.542 (3)	0.5415 (19)	0.2889 (15)	0.074 (6)*
H10	0.118 (3)	−0.0381 (17)	0.2633 (15)	0.063 (5)*
H11	0.686 (3)	0.2370 (19)	0.2787 (17)	0.078 (6)*
H12	0.212 (4)	−0.019 (2)	−0.2310 (18)	0.084 (7)*
H13	0.538 (3)	−0.3773 (17)	0.1074 (14)	0.063 (5)*
H14	0.599 (3)	0.4149 (19)	0.1418 (19)	0.084 (7)*
H15	0.373 (3)	−0.2369 (19)	0.5286 (17)	0.075 (6)*
H16	0.706 (3)	0.2202 (18)	0.1530 (16)	0.072 (6)*
H17	0.473 (3)	−0.1978 (17)	0.3659 (14)	0.065 (6)*
H18	0.587 (3)	0.4396 (17)	0.3617 (16)	0.067 (6)*
H19	0.015 (3)	−0.387 (2)	0.4148 (18)	0.086 (7)*
H20	−0.041 (3)	−0.3951 (19)	0.0133 (16)	0.078 (6)*
H21	0.258 (3)	0.4170 (19)	0.2025 (18)	0.079 (7)*
H22	0.150 (3)	0.2190 (17)	0.2552 (14)	0.066 (6)*
H23	0.067 (3)	−0.369 (2)	0.5385 (18)	0.087 (7)*
H24	0.018 (4)	−0.160 (2)	0.554 (2)	0.094 (8)*
H25	0.379 (3)	−0.3669 (19)	0.4574 (15)	0.072 (6)*
H26	0.235 (3)	0.431 (2)	0.3277 (19)	0.093 (7)*
H27	−0.064 (3)	−0.0673 (19)	0.4108 (15)	0.071 (6)*
H28	−0.174 (4)	−0.239 (2)	0.4927 (19)	0.099 (8)*
H29	0.800 (4)	0.430 (2)	0.2219 (18)	0.091 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0575 (7)	0.0422 (6)	0.0340 (6)	0.0022 (5)	−0.0074 (5)	0.0113 (5)

O2	0.0385 (6)	0.0526 (6)	0.0395 (6)	0.0011 (5)	−0.0045 (5)	0.0143 (5)
O3	0.0408 (6)	0.0825 (9)	0.0413 (7)	0.0172 (6)	−0.0019 (5)	0.0078 (6)
N1	0.0736 (11)	0.0339 (7)	0.0786 (11)	−0.0003 (8)	0.0038 (9)	0.0040 (7)
N2	0.0354 (7)	0.0420 (7)	0.0322 (6)	0.0058 (5)	0.0029 (5)	0.0134 (5)
N3	0.0406 (7)	0.0281 (6)	0.0287 (6)	0.0027 (5)	0.0015 (5)	0.0066 (4)
C1	0.0734 (14)	0.0375 (9)	0.0786 (15)	−0.0047 (9)	0.0201 (11)	0.0097 (9)
C2	0.0732 (14)	0.0413 (10)	0.0859 (16)	0.0170 (10)	0.0152 (12)	−0.0004 (10)
C3	0.1100 (19)	0.0512 (11)	0.0591 (13)	−0.0050 (12)	0.0115 (12)	0.0254 (10)
C4	0.0696 (14)	0.0793 (15)	0.0660 (14)	0.0037 (12)	0.0264 (11)	0.0335 (12)
C5	0.0594 (12)	0.0423 (10)	0.0837 (14)	−0.0081 (9)	−0.0013 (10)	−0.0042 (9)
C6	0.0873 (15)	0.0319 (9)	0.0589 (12)	0.0045 (9)	0.0076 (10)	0.0019 (8)
C7	0.0506 (11)	0.0397 (9)	0.0706 (13)	0.0082 (8)	0.0159 (9)	0.0022 (8)
C8	0.0533 (10)	0.0342 (8)	0.0661 (12)	−0.0008 (7)	0.0210 (9)	0.0059 (8)
C9	0.0894 (15)	0.0476 (10)	0.0478 (11)	0.0204 (10)	0.0105 (10)	0.0192 (8)
C10	0.0619 (11)	0.0392 (9)	0.0578 (11)	0.0116 (9)	0.0042 (9)	0.0102 (8)
C11	0.0461 (9)	0.0397 (9)	0.0580 (11)	−0.0006 (8)	−0.0036 (8)	−0.0007 (7)
C12	0.0492 (10)	0.0645 (12)	0.0537 (11)	0.0056 (9)	0.0152 (9)	0.0253 (9)
C13	0.0656 (12)	0.0488 (9)	0.0435 (10)	0.0182 (9)	0.0106 (9)	0.0172 (8)
C14	0.0468 (9)	0.0357 (8)	0.0411 (8)	0.0023 (7)	0.0018 (7)	0.0082 (6)
C15	0.0449 (8)	0.0391 (8)	0.0289 (7)	0.0050 (7)	0.0041 (6)	0.0108 (6)
C16	0.0530 (9)	0.0272 (7)	0.0323 (8)	0.0048 (6)	0.0011 (6)	0.0064 (6)
C17	0.0387 (8)	0.0289 (7)	0.0302 (7)	0.0056 (6)	0.0026 (6)	0.0049 (5)
C18	0.0427 (8)	0.0320 (7)	0.0291 (7)	0.0006 (6)	0.0047 (6)	0.0039 (5)
C19	0.0321 (7)	0.0336 (7)	0.0309 (7)	0.0013 (6)	0.0026 (6)	0.0067 (6)

Geometric parameters (Å, º)

O1—C19	1.2253 (16)	C5—H20	0.99 (2)
O2—C17	1.2239 (17)	C6—H9	0.97 (2)
O3—H6	0.89 (3)	C6—H18	1.03 (2)
O3—H12	0.89 (2)	C7—C16	1.516 (2)
N1—C10	1.325 (2)	C7—H8	1.030 (19)
N1—C5	1.335 (3)	C7—H22	0.96 (2)
N2—C17	1.3222 (19)	C8—C16	1.513 (2)
N2—C15	1.4628 (18)	C8—H11	1.03 (2)
N2—H10	0.91 (2)	C8—H16	0.95 (2)
N3—C19	1.3587 (18)	C9—C13	1.518 (2)
N3—C17	1.4443 (17)	C9—H15	1.01 (2)
N3—C16	1.4957 (17)	C9—H25	1.03 (2)
C1—C6	1.511 (3)	C10—C14	1.379 (2)
C1—C8	1.535 (2)	C10—H13	0.988 (19)
C1—H14	1.03 (2)	C11—C18	1.382 (2)
C1—H29	0.97 (2)	C11—H4	0.98 (2)
C2—C6	1.508 (3)	C12—C15	1.518 (2)
C2—C7	1.533 (2)	C12—H7	0.96 (2)
C2—H21	1.02 (2)	C12—H27	1.00 (2)
C2—H26	0.99 (2)	C13—C15	1.522 (2)
C3—C9	1.509 (3)	C13—H5	1.008 (19)

C3—C4	1.515 (3)	C13—H17	0.98 (2)
C3—H19	1.02 (2)	C14—C18	1.382 (2)
C3—H23	0.99 (2)	C14—H3	0.943 (17)
C4—C12	1.523 (3)	C15—H1	0.969 (16)
C4—H24	0.99 (3)	C16—H2	0.970 (17)
C4—H28	0.97 (3)	C18—C19	1.4988 (19)
C5—C11	1.378 (2)		

H6—O3—H12	107 (2)	C1—C8—H16	109.9 (12)
C10—N1—C5	116.45 (15)	H11—C8—H16	114.0 (16)
C17—N2—C15	124.07 (13)	C3—C9—C13	111.55 (18)
C17—N2—H10	118.8 (12)	C3—C9—H15	110.0 (12)
C15—N2—H10	117.0 (12)	C13—C9—H15	108.9 (12)
C19—N3—C17	121.70 (11)	C3—C9—H25	111.3 (11)
C19—N3—C16	119.75 (11)	C13—C9—H25	110.8 (11)
C17—N3—C16	117.70 (11)	H15—C9—H25	104.0 (16)
C6—C1—C8	111.14 (16)	N1—C10—C14	124.03 (17)
C6—C1—H14	105.6 (12)	N1—C10—H13	116.8 (11)
C8—C1—H14	109.7 (12)	C14—C10—H13	119.1 (11)
C6—C1—H29	113.1 (14)	C5—C11—C18	118.67 (17)
C8—C1—H29	108.9 (14)	C5—C11—H4	121.7 (11)
H14—C1—H29	108.3 (19)	C18—C11—H4	119.6 (11)
C6—C2—C7	111.16 (17)	C15—C12—C4	111.31 (16)
C6—C2—H21	107.2 (12)	C15—C12—H7	106.9 (12)
C7—C2—H21	110.3 (12)	C4—C12—H7	109.6 (12)
C6—C2—H26	109.6 (13)	C15—C12—H27	107.6 (11)
C7—C2—H26	107.3 (13)	C4—C12—H27	111.5 (11)
H21—C2—H26	111.3 (18)	H7—C12—H27	109.9 (16)
C9—C3—C4	111.04 (17)	C9—C13—C15	110.16 (14)
C9—C3—H19	109.2 (13)	C9—C13—H5	109.9 (11)
C4—C3—H19	107.8 (12)	C15—C13—H5	105.7 (10)
C9—C3—H23	110.5 (13)	C9—C13—H17	111.8 (11)
C4—C3—H23	109.8 (13)	C15—C13—H17	108.5 (11)
H19—C3—H23	108.4 (18)	H5—C13—H17	110.5 (16)
C3—C4—C12	111.67 (18)	C10—C14—C18	118.81 (16)
C3—C4—H24	111.1 (14)	C10—C14—H3	120.8 (10)
C12—C4—H24	108.5 (14)	C18—C14—H3	120.3 (10)
C3—C4—H28	112.3 (14)	N2—C15—C12	108.20 (13)
C12—C4—H28	108.1 (15)	N2—C15—C13	112.09 (12)
H24—C4—H28	105 (2)	C12—C15—C13	110.68 (15)
N1—C5—C11	123.98 (18)	N2—C15—H1	108.0 (9)
N1—C5—H20	115.5 (11)	C12—C15—H1	110.7 (9)
C11—C5—H20	120.5 (12)	C13—C15—H1	107.1 (9)
C2—C6—C1	110.99 (17)	N3—C16—C8	112.88 (13)
C2—C6—H9	109.3 (12)	N3—C16—C7	110.71 (13)
C1—C6—H9	109.7 (12)	C8—C16—C7	111.38 (14)
C2—C6—H18	108.5 (11)	N3—C16—H2	105.2 (9)
C1—C6—H18	108.6 (11)	C8—C16—H2	108.1 (9)

H9—C6—H18	109.8 (16)	C7—C16—H2	108.2 (9)
C16—C7—C2	110.43 (16)	O2—C17—N2	126.20 (13)
C16—C7—H8	107.0 (10)	O2—C17—N3	120.23 (13)
C2—C7—H8	111.0 (10)	N2—C17—N3	113.55 (12)
C16—C7—H22	110.3 (11)	C11—C18—C14	118.01 (14)
C2—C7—H22	112.4 (11)	C11—C18—C19	118.81 (14)
H8—C7—H22	105.5 (15)	C14—C18—C19	123.02 (13)
C16—C8—C1	110.19 (16)	O1—C19—N3	122.14 (13)
C16—C8—H11	105.7 (12)	O1—C19—C18	119.26 (12)
C1—C8—H11	109.8 (12)	N3—C19—C18	118.59 (12)
C16—C8—H16	107.1 (12)		

C9—C3—C4—C12	54.2 (3)	C1—C8—C16—N3	178.11 (14)
C10—N1—C5—C11	−0.1 (3)	C1—C8—C16—C7	−56.6 (2)
C7—C2—C6—C1	56.2 (3)	C2—C7—C16—N3	−177.01 (16)
C8—C1—C6—C2	−56.5 (3)	C2—C7—C16—C8	56.5 (2)
C6—C2—C7—C16	−56.0 (3)	C15—N2—C17—O2	−6.0 (2)
C6—C1—C8—C16	56.4 (2)	C15—N2—C17—N3	175.33 (11)
C4—C3—C9—C13	−56.0 (2)	C19—N3—C17—O2	123.81 (15)
C5—N1—C10—C14	2.1 (3)	C16—N3—C17—O2	−66.79 (17)
N1—C5—C11—C18	−1.7 (3)	C19—N3—C17—N2	−57.40 (17)
C3—C4—C12—C15	−54.4 (3)	C16—N3—C17—N2	111.99 (14)
C3—C9—C13—C15	57.5 (2)	C5—C11—C18—C14	1.6 (2)
N1—C10—C14—C18	−2.2 (3)	C5—C11—C18—C19	177.11 (16)
C17—N2—C15—C12	171.48 (14)	C10—C14—C18—C11	0.2 (2)
C17—N2—C15—C13	−66.20 (19)	C10—C14—C18—C19	−175.11 (14)
C4—C12—C15—N2	179.01 (16)	C17—N3—C19—O1	168.24 (12)
C4—C12—C15—C13	55.8 (2)	C16—N3—C19—O1	−0.9 (2)
C9—C13—C15—N2	−178.00 (15)	C17—N3—C19—C18	−13.44 (19)
C9—C13—C15—C12	−57.1 (2)	C16—N3—C19—C18	177.38 (12)
C19—N3—C16—C8	−115.27 (16)	C11—C18—C19—O1	−52.43 (19)
C17—N3—C16—C8	75.12 (17)	C14—C18—C19—O1	122.84 (16)
C19—N3—C16—C7	119.10 (16)	C11—C18—C19—N3	129.19 (15)
C17—N3—C16—C7	−50.51 (18)	C14—C18—C19—N3	−55.53 (19)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H6···O1	0.89 (3)	1.95 (3)	2.7959 (18)	158 (2)
N2—H10···O3^{i}	0.91 (2)	1.89 (2)	2.7949 (19)	170 (2)
O3—H12···O2^{ii}	0.89 (2)	1.95 (3)	2.8319 (19)	171 (2)

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