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7-Hydroxy-1,2,3,4-tetrahydroquinolin-2-one dihydrate

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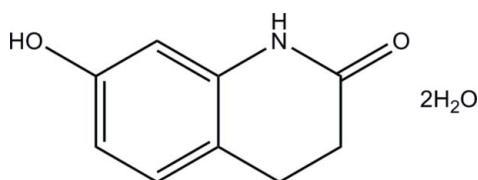
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.084; wR factor = 0.175; data-to-parameter ratio = 12.7.

The asymmetric unit of the title compound, $\text{C}_9\text{H}_9\text{NO}_2 \cdot 2\text{H}_2\text{O}$, comprises two independent organic molecules and four water molecules of crystallization. The heterocyclic rings are not planar: in one molecule, the C atom bearing the O atom and the adjacent methylene C atom are displaced by 0.320 (3) and 0.677 (3) Å, respectively, from the other eight atoms of the fused ring system. Equivalent values of 0.243 (3) and 0.659 (3) Å apply to the second molecule. In the crystal, the components are linked by $\text{N}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds, forming a three-dimensional network.

Related literature

For background to quinolin-2-ones as drugs, see: Braun *et al.* (2009a,b).



Experimental

Crystal data

 $\text{C}_9\text{H}_9\text{NO}_2 \cdot 2\text{H}_2\text{O}$ $M_r = 199.20$ Orthorhombic, $Pbca$ $a = 15.4597$ (16) Å $b = 12.7864$ (12) Å $c = 20.312$ (2) Å $V = 4015.1$ (7) Å³ $Z = 16$ Mo $K\alpha$ radiation $\mu = 0.10$ mm⁻¹ $T = 298$ K $0.20 \times 0.17 \times 0.15$ mm

Data collection

Bruker APEXII CCD

diffractometer

Absorption correction: multi-scan

(SADABS; Sheldrick, 2004)

 $T_{\min} = 0.980$, $T_{\max} = 0.985$

36302 measured reflections

3659 independent reflections

3061 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.058$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.084$ $wR(F^2) = 0.175$ $S = 1.30$

3659 reflections

287 parameters

14 restraints

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.15$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.17$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O7—H7B ⁱ ···O5	0.85 (1)	1.95 (1)	2.800 (4)	174 (3)
O5—H5A ⁱ ···O2 ⁱ	0.85 (1)	1.93 (1)	2.774 (3)	170 (3)
O8—H8B ⁱ ···O6 ⁱⁱ	0.85 (1)	1.90 (1)	2.751 (4)	177 (4)
O7—H7A ⁱ ···O6 ⁱⁱⁱ	0.85 (1)	1.94 (1)	2.791 (4)	172 (3)
O5—H5B ⁱ ···O1 ^{iv}	0.85 (1)	1.91 (1)	2.757 (3)	176 (3)
O8—H8A ⁱ ···O5 ^v	0.85 (1)	1.95 (1)	2.790 (4)	169 (4)
N2—H2 ⁱ ···O1 ^{vi}	0.90 (1)	1.98 (1)	2.867 (3)	169 (3)
N1—H1 ⁱ ···O3 ^{vii}	0.90 (1)	1.99 (1)	2.895 (3)	177 (3)
O4—H4 ⁱ ···O7 ^{viii}	0.82	1.86	2.668 (4)	170
O2—H2A ⁱ ···O8 ^{ix}	0.82	1.87	2.671 (4)	166
O6—H6A ⁱ ···O3	0.85 (1)	1.92 (1)	2.766 (3)	175 (4)

Symmetry codes: (i) $x, -y + \frac{1}{2}, z + \frac{1}{2}$; (ii) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (iii) $x + \frac{1}{2}, -y + \frac{1}{2}, -z + 1$; (iv) $x, y, z + 1$; (v) $-x + 1, -y + 1, -z + 1$; (vi) $-x + \frac{1}{2}, y - \frac{1}{2}, z$; (vii) $-x + \frac{1}{2}, y + \frac{1}{2}, z$; (viii) $-x + \frac{1}{2}, y - \frac{1}{2}, z - 1$; (ix) $x - \frac{1}{2}, y, -z + \frac{1}{2}$.

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); 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: HB6830).

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supporting information

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7-Hydroxy-1,2,3,4-tetrahydroquinolin-2-one dihydrate

Qian-Shou Zong and Jian-Yi Wu

S1. Comment

7-Hydroxy-3,4-dihydro-1*H*-quinolin-2-one is an important intermediate for the preparation of non-typical antipsychotic drugs (Braun *et al.*, 2009*a,b*). In this paper, the author reports the structure of the compound.

The asymmetric unit of the title compound comprises two independent 7-hydroxy-3,4-dihydro-1*H*-quinolin-2-one molecules and four water molecules of crystallization (Fig. 1). In the crystal, 7-hydroxy-3,4-dihydro-1*H*-quinolin-2-one molecules are linked by water molecules through hydrogen bonds (Table 1), to form a 3D network (Fig. 2).

S2. Experimental

7-Hydroxy-3,4-dihydro-1*H*-quinolin-2-one was obtained from Jiaying Taixin Pharmaceutical Chemical Co., Ltd, and recrystallized from aqueous solution as colourless blocks.

S3. Refinement

H1, H2 and the water H atoms were located from an electronic map and restrained with N—H, O—H, and H···H distances of 0.90 (1), 0.85 (1), and 1.37 (2) Å, respectively. All other H atoms were placed at calculated positions and refined using a riding model approximation, with C—H = 0.93 or 0.97 Å, O—H = 0.82 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{O})$.

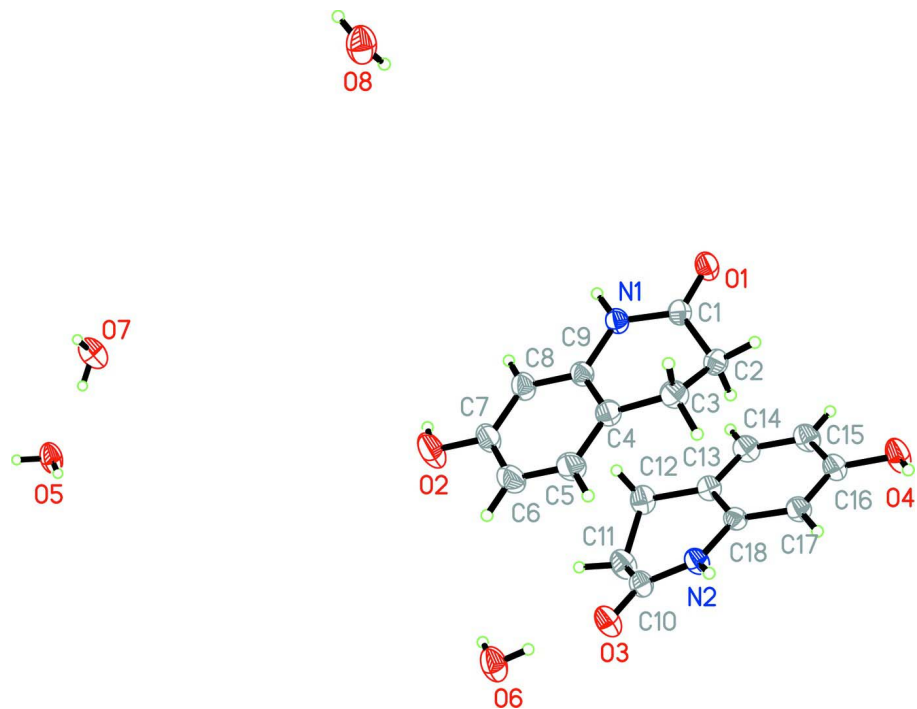


Figure 1

A view of the molecule of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

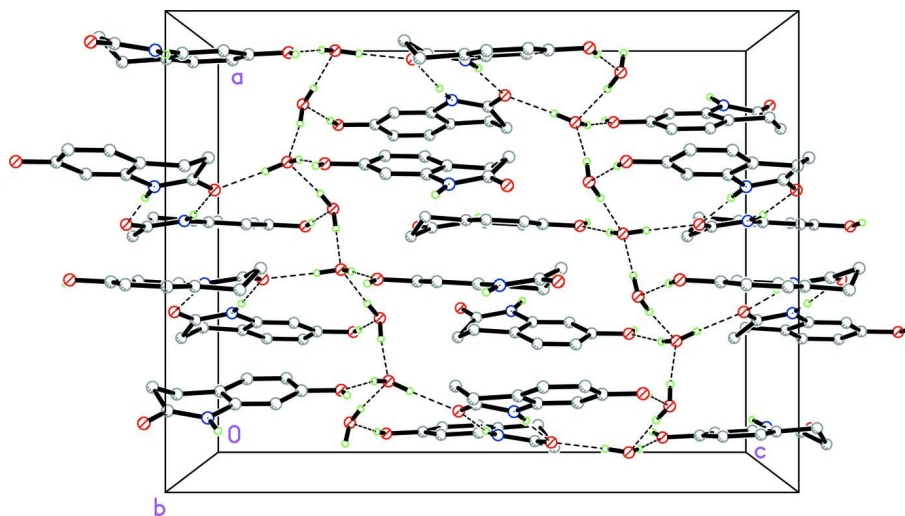


Figure 2

The crystal structure of the title compound, viewed along *b* axis. Hydrogen bonds are shown as dashed lines.

7-Hydroxy-1,2,3,4-tetrahydroquinolin-2-one dihydrate

Crystal data

$C_9H_9NO_2 \cdot 2H_2O$

$M_r = 199.20$

Orthorhombic, *Pbca*

$a = 15.4597(16) \text{ \AA}$

$b = 12.7864(12) \text{ \AA}$

$c = 20.312(2) \text{ \AA}$

$V = 4015.1(7) \text{ \AA}^3$

$Z = 16$

$F(000) = 1696$

$D_x = 1.318 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71070 \text{ \AA}$
 Cell parameters from 11198 reflections
 $\theta = 2.8\text{--}25.3^\circ$
 $\mu = 0.10 \text{ mm}^{-1}$

$T = 298 \text{ K}$
 Block, colorless
 $0.20 \times 0.17 \times 0.15 \text{ mm}$

Data collection

Bruker APEXII CCD
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 ω scan
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 2004)
 $T_{\min} = 0.980$, $T_{\max} = 0.985$

36302 measured reflections
 3659 independent reflections
 3061 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.058$
 $\theta_{\text{max}} = 25.4^\circ$, $\theta_{\text{min}} = 3.1^\circ$
 $h = -18 \rightarrow 18$
 $k = -15 \rightarrow 15$
 $l = -24 \rightarrow 22$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.084$
 $wR(F^2) = 0.175$
 $S = 1.30$
 3659 reflections
 287 parameters
 14 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
 $w = 1/[\sigma^2(F_o^2) + (0.0561P)^2 + 1.7267P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.15 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
H6B	0.044 (4)	0.0608 (19)	0.2751 (18)	0.17 (2)*
H6A	0.049 (3)	0.012 (3)	0.2142 (6)	0.098 (14)*
O1	0.36079 (14)	0.44183 (15)	-0.04017 (9)	0.0563 (6)
O2	0.3059 (2)	0.18779 (19)	0.26380 (11)	0.0877 (9)
H2A	0.3128	0.2485	0.2756	0.132*
O3	0.06233 (14)	0.02384 (15)	0.12063 (10)	0.0586 (6)
O4	0.06082 (19)	0.31032 (17)	-0.17569 (10)	0.0706 (7)
H4	0.0693	0.2514	-0.1903	0.106*
O5	0.29566 (19)	0.49405 (18)	0.83784 (11)	0.0750 (7)
O6	0.0409 (2)	0.00260 (19)	0.25515 (12)	0.0779 (8)
O7	0.4001 (2)	0.6303 (2)	0.76488 (14)	0.0886 (9)
O8	0.8445 (2)	0.3721 (2)	0.18171 (13)	0.0800 (8)

N1	0.35559 (16)	0.35016 (17)	0.05386 (11)	0.0456 (6)
N2	0.07165 (16)	0.11997 (17)	0.02837 (11)	0.0465 (6)
C1	0.33970 (18)	0.3603 (2)	-0.01053 (13)	0.0430 (7)
C2	0.29447 (19)	0.2720 (2)	-0.04418 (14)	0.0488 (7)
H2C	0.3106	0.2716	-0.0903	0.059*
H2B	0.2325	0.2833	-0.0417	0.059*
C3	0.3158 (2)	0.1665 (2)	-0.01435 (15)	0.0550 (8)
H3A	0.2761	0.1144	-0.0314	0.066*
H3B	0.3739	0.1463	-0.0271	0.066*
C4	0.30961 (19)	0.1692 (2)	0.05908 (14)	0.0481 (7)
C5	0.2861 (2)	0.0849 (2)	0.09787 (16)	0.0611 (9)
H5	0.2708	0.0224	0.0776	0.073*
C6	0.2847 (2)	0.0905 (3)	0.16567 (16)	0.0666 (9)
H6	0.2689	0.0324	0.1905	0.080*
C7	0.3070 (2)	0.1830 (2)	0.19654 (15)	0.0600 (9)
C8	0.3304 (2)	0.2690 (2)	0.15928 (14)	0.0547 (8)
H8	0.3453	0.3315	0.1797	0.066*
C9	0.33155 (18)	0.2613 (2)	0.09142 (13)	0.0442 (7)
C10	0.05833 (18)	0.1108 (2)	0.09337 (14)	0.0470 (7)
C11	0.0364 (2)	0.2089 (2)	0.13002 (15)	0.0596 (8)
H11A	0.0521	0.2004	0.1759	0.071*
H11B	-0.0256	0.2204	0.1279	0.071*
C12	0.0823 (2)	0.3036 (2)	0.10257 (15)	0.0559 (8)
H12A	0.0577	0.3663	0.1218	0.067*
H12B	0.1429	0.3007	0.1147	0.067*
C13	0.07463 (18)	0.3091 (2)	0.02891 (14)	0.0453 (7)
C14	0.0744 (2)	0.4010 (2)	-0.00691 (15)	0.0542 (8)
H14	0.0774	0.4645	0.0154	0.065*
C15	0.0699 (2)	0.4015 (2)	-0.07439 (15)	0.0569 (8)
H15	0.0700	0.4647	-0.0971	0.068*
C16	0.06517 (19)	0.3081 (2)	-0.10861 (14)	0.0500 (7)
C17	0.06498 (18)	0.2143 (2)	-0.07431 (14)	0.0470 (7)
H17	0.0615	0.1511	-0.0968	0.056*
C18	0.06997 (18)	0.2159 (2)	-0.00617 (13)	0.0415 (6)
H1	0.379 (2)	0.4051 (18)	0.0750 (15)	0.080*
H2	0.085 (2)	0.0608 (16)	0.0065 (15)	0.080*
H8A	0.7976 (12)	0.407 (2)	0.1786 (18)	0.080*
H5B	0.317 (2)	0.476 (2)	0.8746 (9)	0.080*
H7A	0.4461 (13)	0.595 (2)	0.7583 (18)	0.080*
H8B	0.8793 (16)	0.412 (2)	0.2025 (16)	0.080*
H5A	0.292 (2)	0.4385 (16)	0.8149 (13)	0.080*
H7B	0.3651 (16)	0.591 (2)	0.7857 (17)	0.080*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0830 (15)	0.0451 (12)	0.0409 (11)	-0.0094 (11)	-0.0055 (10)	0.0034 (9)
O2	0.156 (3)	0.0627 (15)	0.0439 (14)	-0.0189 (17)	-0.0015 (15)	0.0082 (11)

O3	0.0874 (16)	0.0441 (12)	0.0443 (12)	0.0079 (11)	0.0094 (10)	0.0045 (9)
O4	0.115 (2)	0.0526 (13)	0.0444 (13)	0.0070 (14)	-0.0001 (12)	0.0085 (10)
O5	0.119 (2)	0.0561 (14)	0.0498 (14)	0.0043 (14)	-0.0149 (14)	-0.0023 (11)
O6	0.130 (2)	0.0563 (14)	0.0474 (14)	0.0020 (15)	-0.0051 (15)	-0.0005 (12)
O7	0.124 (3)	0.0710 (18)	0.0709 (18)	0.0040 (16)	0.0160 (17)	0.0059 (14)
O8	0.108 (2)	0.0669 (16)	0.0649 (16)	0.0013 (15)	-0.0148 (15)	-0.0050 (13)
N1	0.0596 (16)	0.0379 (13)	0.0392 (13)	-0.0049 (11)	-0.0025 (11)	0.0006 (10)
N2	0.0634 (16)	0.0349 (13)	0.0413 (14)	0.0017 (11)	0.0053 (11)	-0.0006 (10)
C1	0.0461 (16)	0.0432 (16)	0.0395 (16)	0.0036 (13)	0.0015 (12)	-0.0038 (12)
C2	0.0556 (17)	0.0494 (17)	0.0413 (16)	-0.0053 (14)	-0.0023 (13)	-0.0060 (13)
C3	0.071 (2)	0.0421 (16)	0.0520 (19)	-0.0070 (15)	0.0026 (15)	-0.0079 (13)
C4	0.0549 (18)	0.0424 (16)	0.0470 (17)	-0.0011 (13)	-0.0012 (14)	-0.0023 (13)
C5	0.082 (2)	0.0413 (17)	0.060 (2)	-0.0107 (16)	-0.0020 (17)	-0.0019 (14)
C6	0.092 (3)	0.0486 (19)	0.059 (2)	-0.0148 (17)	-0.0024 (18)	0.0111 (15)
C7	0.085 (2)	0.0513 (19)	0.0436 (18)	-0.0088 (17)	-0.0035 (16)	0.0070 (14)
C8	0.074 (2)	0.0465 (17)	0.0437 (17)	-0.0039 (15)	-0.0055 (15)	-0.0001 (13)
C9	0.0499 (16)	0.0404 (15)	0.0423 (16)	-0.0009 (13)	-0.0009 (13)	0.0018 (12)
C10	0.0536 (18)	0.0463 (17)	0.0412 (16)	0.0042 (14)	0.0030 (13)	0.0000 (13)
C11	0.082 (2)	0.0498 (17)	0.0472 (18)	0.0075 (16)	0.0098 (16)	-0.0024 (14)
C12	0.074 (2)	0.0450 (17)	0.0490 (18)	0.0065 (15)	-0.0014 (16)	-0.0089 (13)
C13	0.0483 (16)	0.0404 (15)	0.0471 (16)	0.0055 (13)	0.0016 (13)	-0.0021 (12)
C14	0.069 (2)	0.0369 (16)	0.0571 (19)	0.0032 (14)	0.0042 (15)	-0.0038 (13)
C15	0.073 (2)	0.0368 (16)	0.060 (2)	0.0052 (15)	0.0011 (16)	0.0072 (14)
C16	0.0597 (19)	0.0469 (16)	0.0435 (16)	0.0026 (14)	0.0017 (14)	0.0049 (13)
C17	0.0560 (18)	0.0382 (15)	0.0469 (17)	-0.0011 (13)	0.0015 (13)	-0.0012 (12)
C18	0.0449 (16)	0.0377 (15)	0.0419 (16)	-0.0012 (12)	0.0018 (12)	0.0018 (12)

Geometric parameters (Å, °)

O1—C1	1.247 (3)	C3—H3B	0.9700
O2—C7	1.368 (4)	C4—C5	1.384 (4)
O2—H2A	0.8200	C4—C9	1.390 (4)
O3—C10	1.244 (3)	C5—C6	1.379 (4)
O4—C16	1.364 (3)	C5—H5	0.9300
O4—H4	0.8200	C6—C7	1.382 (4)
O5—H5B	0.851 (10)	C6—H6	0.9300
O5—H5A	0.851 (10)	C7—C8	1.383 (4)
O6—H6B	0.850 (10)	C8—C9	1.382 (4)
O6—H6A	0.850 (10)	C8—H8	0.9300
O7—H7A	0.854 (10)	C10—C11	1.498 (4)
O7—H7B	0.853 (10)	C11—C12	1.509 (4)
O8—H8A	0.853 (10)	C11—H11A	0.9700
O8—H8B	0.854 (10)	C11—H11B	0.9700
N1—C1	1.337 (3)	C12—C13	1.502 (4)
N1—C9	1.419 (3)	C12—H12A	0.9700
N1—H1	0.902 (10)	C12—H12B	0.9700
N2—C10	1.341 (3)	C13—C14	1.382 (4)
N2—C18	1.414 (3)	C13—C18	1.390 (4)

N2—H2	0.902 (10)	C14—C15	1.372 (4)
C1—C2	1.494 (4)	C14—H14	0.9300
C2—C3	1.516 (4)	C15—C16	1.384 (4)
C2—H2C	0.9700	C15—H15	0.9300
C2—H2B	0.9700	C16—C17	1.387 (4)
C3—C4	1.495 (4)	C17—C18	1.386 (4)
C3—H3A	0.9700	C17—H17	0.9300
C7—O2—H2A	109.5	C9—C8—C7	119.5 (3)
C16—O4—H4	109.5	C9—C8—H8	120.3
H5B—O5—H5A	106 (2)	C7—C8—H8	120.3
H6B—O6—H6A	109 (2)	C8—C9—C4	121.9 (3)
H7A—O7—H7B	107 (2)	C8—C9—N1	118.8 (2)
H8A—O8—H8B	105 (2)	C4—C9—N1	119.2 (2)
C1—N1—C9	123.8 (2)	O3—C10—N2	120.6 (2)
C1—N1—H1	118 (2)	O3—C10—C11	122.6 (3)
C9—N1—H1	118 (2)	N2—C10—C11	116.8 (2)
C10—N2—C18	124.2 (2)	C10—C11—C12	112.4 (2)
C10—N2—H2	117 (2)	C10—C11—H11A	109.1
C18—N2—H2	119 (2)	C12—C11—H11A	109.1
O1—C1—N1	120.4 (2)	C10—C11—H11B	109.1
O1—C1—C2	122.2 (2)	C12—C11—H11B	109.1
N1—C1—C2	117.4 (2)	H11A—C11—H11B	107.8
C1—C2—C3	112.9 (2)	C13—C12—C11	111.6 (3)
C1—C2—H2C	109.0	C13—C12—H12A	109.3
C3—C2—H2C	109.0	C11—C12—H12A	109.3
C1—C2—H2B	109.0	C13—C12—H12B	109.3
C3—C2—H2B	109.0	C11—C12—H12B	109.3
H2C—C2—H2B	107.8	H12A—C12—H12B	108.0
C4—C3—C2	111.4 (2)	C14—C13—C18	117.3 (3)
C4—C3—H3A	109.4	C14—C13—C12	124.4 (3)
C2—C3—H3A	109.4	C18—C13—C12	118.3 (2)
C4—C3—H3B	109.4	C15—C14—C13	122.0 (3)
C2—C3—H3B	109.4	C15—C14—H14	119.0
H3A—C3—H3B	108.0	C13—C14—H14	119.0
C5—C4—C9	117.0 (3)	C14—C15—C16	120.0 (3)
C5—C4—C3	124.5 (3)	C14—C15—H15	120.0
C9—C4—C3	118.4 (3)	C16—C15—H15	120.0
C6—C5—C4	122.2 (3)	O4—C16—C15	119.1 (3)
C6—C5—H5	118.9	O4—C16—C17	121.3 (3)
C4—C5—H5	118.9	C15—C16—C17	119.6 (3)
C5—C6—C7	119.6 (3)	C18—C17—C16	119.2 (3)
C5—C6—H6	120.2	C18—C17—H17	120.4
C7—C6—H6	120.2	C16—C17—H17	120.4
O2—C7—C6	119.2 (3)	C17—C18—C13	121.9 (2)
O2—C7—C8	120.9 (3)	C17—C18—N2	118.9 (2)
C6—C7—C8	119.8 (3)	C13—C18—N2	119.2 (2)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O7—H7B \cdots O5	0.85 (1)	1.95 (1)	2.800 (4)	174 (3)
O5—H5A \cdots O2 ⁱ	0.85 (1)	1.93 (1)	2.774 (3)	170 (3)
O8—H8B \cdots O6 ⁱⁱ	0.85 (1)	1.90 (1)	2.751 (4)	177 (4)
O7—H7A \cdots O6 ⁱⁱⁱ	0.85 (1)	1.94 (1)	2.791 (4)	172 (3)
O5—H5B \cdots O1 ^{iv}	0.85 (1)	1.91 (1)	2.757 (3)	176 (3)
O8—H8A \cdots O5 ^v	0.85 (1)	1.95 (1)	2.790 (4)	169 (4)
N2—H2 \cdots O1 ^{vi}	0.90 (1)	1.98 (1)	2.867 (3)	169 (3)
N1—H1 \cdots O3 ^{vii}	0.90 (1)	1.99 (1)	2.895 (3)	177 (3)
O4—H4 \cdots O7 ^{viii}	0.82	1.86	2.668 (4)	170
O2—H2A \cdots O8 ^{ix}	0.82	1.87	2.671 (4)	166
O6—H6A \cdots O3	0.85 (1)	1.92 (1)	2.766 (3)	175 (4)

Symmetry codes: (i) $x, -y+1/2, z+1/2$; (ii) $-x+1, y+1/2, -z+1/2$; (iii) $x+1/2, -y+1/2, -z+1$; (iv) $x, y, z+1$; (v) $-x+1, -y+1, -z+1$; (vi) $-x+1/2, y-1/2, z$; (vii) $-x+1/2, y+1/2, z$; (viii) $-x+1/2, y-1/2, z-1$; (ix) $x-1/2, y, -z+1/2$.