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Crystal structure of 8-hydroxyquinolinium 2-carboxy-6-nitrobenzoate monohydrate

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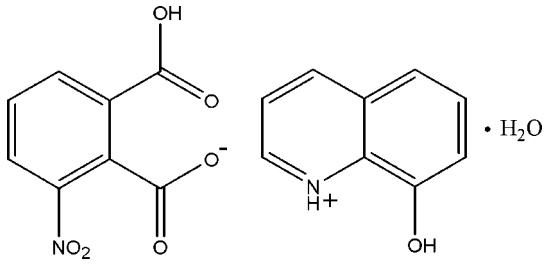
In the title hydrated salt, $C_9H_8NO^+\cdot C_8H_4NO_6^-\cdot H_2O$, the deprotonated carboxylate group is almost normal to its attached benzene ring [dihedral angle = 83.56 (8)°], whereas the protonated carboxylate group is close to parallel [dihedral angle = 24.56 (9)°]. In the crystal, the components are linked by N—H···O and O—H···O hydrogen bonds, generating [001] chains. The packing is consolidated by C—H···O and π–π [centroid-to-centroid distances = 3.6408 (9) and 3.6507 (9) Å] interactions, which result in a three-dimensional network.

Keywords: crystal structure; 8-hydroxyquinolinium; 2-carboxy-6-nitrobenzoate; hydrogen bonding; π–π interactions.

CCDC reference: 1055171

1. Related literature

For the biological activity of quinoline derivatives, see: Font *et al.* (1997); Sloboda *et al.* (1991). For similar structures, see: Castañeda *et al.* (2014); Kafka *et al.* (2012); Li & Chai (2007).



2. Experimental

2.1. Crystal data

$C_9H_8NO^+\cdot C_8H_4NO_6^-\cdot H_2O$
M_r = 374.30
Monoclinic, $P2_1/c$
a = 14.4283 (5) Å
b = 13.8196 (5) Å
c = 8.0483 (3) Å
β = 101.441 (2)°
V = 1572.89 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 295 K
0.26 × 0.22 × 0.18 mm

2.2. Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.968, T_{max} = 0.977
58922 measured reflections
7431 independent reflections
4272 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.176
S = 1.02
7431 reflections
260 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O3^{i}	0.89 (1)	2.00 (1)	2.8112 (16)	151 (2)
O5—H5A···O8^{ii}	0.82 (1)	1.78 (1)	2.5928 (18)	171 (3)
O7—H7···O3^{iii}	0.84 (1)	1.82 (1)	2.6482 (15)	168 (2)
O8—H8B···O4	0.83 (1)	2.07 (1)	2.8683 (17)	163 (2)
O8—H8A···O4^{ii}	0.83 (1)	2.01 (1)	2.8288 (18)	170 (2)
C11—H11···O1^{iv}	0.93	2.42	3.295 (2)	156
C12—H12···O6^{i}	0.93	2.48	3.343 (2)	155
C16—H16···O2^{v}	0.93	2.52	3.413 (2)	160

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (iii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $-x+1, -y+1, -z+1$; (v) $x, y, z+1$.

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: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

Acknowledgements

The authors thank SAIF, IIT Madras for the data collection.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7385).

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supporting information

Acta Cryst. (2015). E**71**, o261–o262 [doi:10.1107/S205698901500571X]

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M. Divya Bharathi, G. Ahila, J. Mohana, G. Chakkaravarthi and G. Anbalagan

S1. Chemical context

The quinoline nucleus is found in many synthetic and natural products having a wide range of pharmacological activities such as anti-viral (Font *et al.*, 1997), and anti-inflammatory (Sloboda *et al.*, 1991) activities.

S2. Structural commentary

We herewith report the crystal structure of the title compound (I), (Fig.1). The asymmetric unit of the title compound consists of C_9 H_8 N O^+ cation, C_8 H_4 N O_6^- anion and a water molecule. The geometric parameters of the title compound are comparable to the reported structures [Castañeda *et al.*, 2014; Kafka *et al.*, 2012; Li & Chai (2007)]. The benzene ring (C1—C6) of anion makes the dihedral angle of 58.18 (6)° with the quinolinium ring (C9—C12/N2/C13—C17) of cation.

S3. Supramolecular features

The molecular structure is stabilized by weak intramolecular N—H···O and O—H···O hydrogen bonds (Table 1). The crystal structure is formed by weak intermolecular N—H···O, O—H···O and C—H···O hydrogen bonds (Table 1 & Fig. 2) by linking the adjacent anions and cations by bridging water molecules through O—H···O hydrogen bonds into infinite two-dimensional network along [1 0 0] plane. The crystal structure is further stabilized by weak C—H···π (Table 1) and π–π [Cg1···Cg1^{i} = 3.6507 (9); Cg2···Cg2^{ii} = 3.6507 (9)Å; (i) -x,1-y,1-z; (ii) x,1/2-y,1/2+z; Cg1 and Cg2 are the centroids of the rings (C1—C6) and (N2/C12/C11/C10/C9/C13)] interactions.

S4. Synthesis and crystallization

The title compound was synthesized by taking at 1:1 ratio of 8-hydroxyquinoline and of 3-nitrophthalic acid was dissolved in a mixed solvent of methanol and water. The salt was formed while adding the base instanstaouly. The solution was stirred for about 2 h to get a homogenous solution. The solution was filtered off and kept aside for slow evaporation at room temperature which yields single crystals suitable for X-ray diffraction.

S5. Refinement

C-bound H atoms were positioned geometrically and refined using riding model with C—H = 0.93 Å and Uiso(H) = 1.2Ueq(C). H atoms for O atoms were located from Fourier map and refined with O—H = 0.82 (1)Å and Uiso(H) = 1.5 Ueq(O). H atom for N atom was located from Fourier map and refined freely with N—H = 0.88 (1)Å.

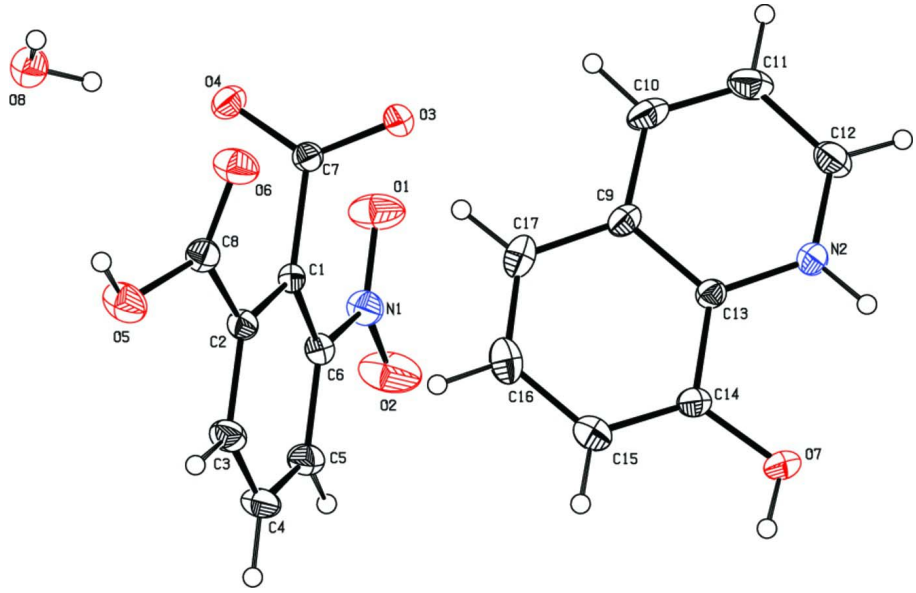

Figure 1

The molecular structure of (I), with 30% probability displacement ellipsoids for non-H atoms.

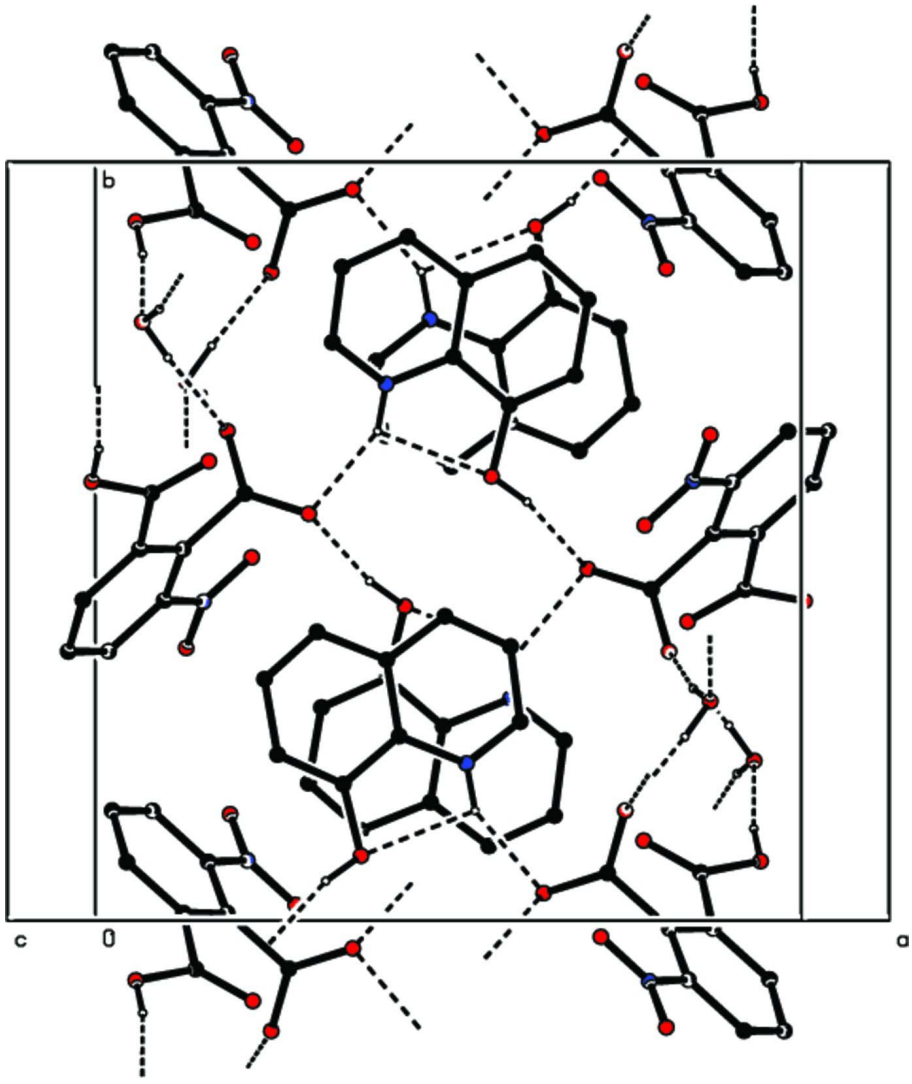

Figure 2

The packing of (I), viewed down *c* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

8-Hydroxyquinolinium 2-carboxy-6-nitrobenzoate monohydrate

Crystal data

$C_9H_8NO^+·C_8H_4NO_6^-·H_2O$
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β = 101.441 (2)°
V = 1572.89 (10) Å^3
Z = 4
$F(000)$ = 776
D_x = 1.581 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9900 reflections
θ = 2.8–33.4°
μ = 0.13 mm^{-1}
T = 295 K
Block, colourless
0.26 × 0.22 × 0.18 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.968, T_{max} = 0.977
58922 measured reflections
7431 independent reflections
4272 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 36.1°, θ_{min} = 2.1°
h = −23→23
k = −19→22
l = −13→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.176
S = 1.02
7431 reflections
260 parameters
5 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
$w = 1/[\sigma^2(F_o^2) + (0.0619P)^2 + 0.9848P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.17265 (9)	0.48978 (9)	0.55989 (18)	0.0237 (2)
C2	0.13410 (10)	0.48988 (10)	0.70682 (19)	0.0262 (3)
C3	0.06506 (11)	0.42272 (12)	0.7270 (2)	0.0331 (3)
H3	0.0403	0.4238	0.8252	0.040*
C4	0.03290 (11)	0.35481 (12)	0.6037 (2)	0.0370 (4)
H4	−0.0117	0.3091	0.6203	0.044*
C5	0.06716 (11)	0.35508 (12)	0.4557 (2)	0.0339 (3)
H5	0.0449	0.3108	0.3702	0.041*
C6	0.13531 (10)	0.42230 (10)	0.43632 (19)	0.0267 (3)
C7	0.24827 (10)	0.56315 (10)	0.53939 (18)	0.0249 (3)
C8	0.16432 (11)	0.56359 (11)	0.84160 (19)	0.0294 (3)
C9	0.46422 (11)	0.34368 (10)	0.87844 (19)	0.0288 (3)
C10	0.53122 (13)	0.40133 (12)	0.8201 (2)	0.0377 (4)
H10	0.5225	0.4680	0.8125	0.045*
C11	0.60883 (13)	0.36137 (14)	0.7744 (2)	0.0424 (4)

H11	0.6521	0.4002	0.7341	0.051*
C12	0.62252 (11)	0.26245 (14)	0.7886 (2)	0.0390 (4)
H12	0.6752	0.2346	0.7575	0.047*
C13	0.48139 (9)	0.24333 (10)	0.89029 (18)	0.0247 (3)
C14	0.41699 (10)	0.18003 (10)	0.94525 (19)	0.0284 (3)
C15	0.33963 (11)	0.21885 (13)	0.9934 (2)	0.0364 (3)
H15	0.2978	0.1785	1.0346	0.044*
C16	0.32192 (13)	0.31850 (15)	0.9818 (2)	0.0432 (4)
H16	0.2680	0.3428	1.0140	0.052*
C17	0.38181 (13)	0.38061 (12)	0.9246 (2)	0.0390 (4)
H17	0.3685	0.4465	0.9160	0.047*
N1	0.16655 (10)	0.42040 (10)	0.27386 (18)	0.0337 (3)
N2	0.56126 (9)	0.20732 (9)	0.84612 (17)	0.0305 (3)
H2	0.5741 (15)	0.1450 (8)	0.866 (3)	0.047 (6)*
O1	0.22455 (12)	0.47889 (11)	0.24810 (18)	0.0545 (4)
O2	0.13344 (13)	0.35960 (13)	0.1701 (2)	0.0684 (5)
O3	0.33312 (7)	0.53639 (8)	0.57868 (15)	0.0318 (2)
O4	0.22067 (8)	0.64521 (8)	0.49029 (15)	0.0326 (2)
O5	0.09894 (10)	0.57856 (11)	0.93152 (18)	0.0465 (3)
H5A	0.1152 (18)	0.6216 (15)	1.002 (3)	0.070*
O6	0.23875 (9)	0.60562 (10)	0.86357 (17)	0.0435 (3)
O7	0.43930 (9)	0.08565 (8)	0.94455 (17)	0.0378 (3)
H7	0.3990 (13)	0.0519 (15)	0.981 (3)	0.057*
O8	0.13275 (9)	0.78915 (10)	0.66412 (16)	0.0392 (3)
H8A	0.1644 (15)	0.8061 (18)	0.7569 (18)	0.059*
H8B	0.1616 (16)	0.7423 (13)	0.635 (3)	0.059*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0214 (5)	0.0215 (5)	0.0289 (6)	0.0023 (4)	0.0070 (5)	0.0021 (5)
C2	0.0244 (6)	0.0266 (6)	0.0286 (7)	0.0001 (5)	0.0074 (5)	0.0023 (5)
C3	0.0308 (7)	0.0365 (8)	0.0344 (8)	−0.0042 (6)	0.0123 (6)	0.0047 (6)
C4	0.0300 (7)	0.0364 (8)	0.0457 (9)	−0.0096 (6)	0.0101 (7)	0.0028 (7)
C5	0.0298 (7)	0.0321 (7)	0.0395 (8)	−0.0067 (6)	0.0064 (6)	−0.0041 (6)
C6	0.0244 (6)	0.0262 (6)	0.0304 (7)	0.0012 (5)	0.0076 (5)	−0.0007 (5)
C7	0.0269 (6)	0.0238 (6)	0.0262 (6)	−0.0013 (5)	0.0109 (5)	−0.0016 (5)
C8	0.0323 (7)	0.0301 (7)	0.0269 (7)	0.0003 (5)	0.0084 (5)	0.0024 (5)
C9	0.0337 (7)	0.0212 (6)	0.0294 (7)	0.0003 (5)	0.0014 (5)	0.0015 (5)
C10	0.0465 (9)	0.0239 (7)	0.0395 (8)	−0.0065 (6)	0.0006 (7)	0.0066 (6)
C11	0.0365 (8)	0.0441 (9)	0.0449 (10)	−0.0124 (7)	0.0041 (7)	0.0152 (8)
C12	0.0267 (7)	0.0467 (9)	0.0441 (9)	−0.0008 (6)	0.0088 (6)	0.0120 (7)
C13	0.0249 (6)	0.0221 (6)	0.0264 (6)	−0.0004 (4)	0.0034 (5)	0.0023 (5)
C14	0.0289 (7)	0.0256 (6)	0.0303 (7)	−0.0042 (5)	0.0052 (5)	0.0017 (5)
C15	0.0316 (7)	0.0420 (9)	0.0371 (8)	−0.0043 (6)	0.0103 (6)	0.0004 (7)
C16	0.0377 (8)	0.0510 (10)	0.0427 (9)	0.0119 (7)	0.0126 (7)	−0.0041 (8)
C17	0.0446 (9)	0.0305 (7)	0.0415 (9)	0.0111 (7)	0.0072 (7)	−0.0023 (7)
N1	0.0339 (7)	0.0353 (7)	0.0334 (7)	−0.0031 (5)	0.0103 (5)	−0.0067 (5)

N2	0.0281 (6)	0.0267 (6)	0.0368 (7)	0.0031 (4)	0.0069 (5)	0.0071 (5)
O1	0.0734 (10)	0.0545 (8)	0.0431 (7)	−0.0271 (7)	0.0301 (7)	−0.0107 (6)
O2	0.0782 (11)	0.0794 (12)	0.0555 (9)	−0.0402 (9)	0.0328 (8)	−0.0384 (8)
O3	0.0249 (5)	0.0287 (5)	0.0439 (6)	0.0004 (4)	0.0122 (4)	−0.0032 (4)
O4	0.0375 (6)	0.0241 (5)	0.0365 (6)	0.0007 (4)	0.0084 (5)	0.0031 (4)
O5	0.0434 (7)	0.0575 (8)	0.0442 (7)	−0.0089 (6)	0.0222 (6)	−0.0169 (6)
O6	0.0428 (7)	0.0496 (7)	0.0410 (7)	−0.0147 (6)	0.0153 (5)	−0.0122 (6)
O7	0.0393 (6)	0.0232 (5)	0.0537 (7)	−0.0050 (4)	0.0161 (5)	0.0044 (5)
O8	0.0429 (7)	0.0397 (7)	0.0361 (6)	0.0043 (5)	0.0104 (5)	0.0014 (5)

Geometric parameters (Å, º)

C1—C6	1.392 (2)	C11—C12	1.383 (3)
C1—C2	1.4030 (19)	C11—H11	0.9300
C1—C7	1.5222 (18)	C12—N2	1.318 (2)
C2—C3	1.394 (2)	C12—H12	0.9300
C2—C8	1.489 (2)	C13—N2	1.3655 (18)
C3—C4	1.378 (2)	C13—C14	1.4097 (19)
C3—H3	0.9300	C14—O7	1.3437 (18)
C4—C5	1.377 (2)	C14—C15	1.362 (2)
C4—H4	0.9300	C15—C16	1.400 (3)
C5—C6	1.384 (2)	C15—H15	0.9300
C5—H5	0.9300	C16—C17	1.362 (3)
C6—N1	1.4654 (19)	C16—H16	0.9300
C7—O4	1.2404 (17)	C17—H17	0.9300
C7—O3	1.2577 (17)	N1—O1	1.2106 (18)
C8—O6	1.2028 (19)	N1—O2	1.2137 (19)
C8—O5	1.3142 (19)	N2—H2	0.889 (9)
C9—C10	1.403 (2)	O5—H5A	0.823 (10)
C9—C13	1.4085 (19)	O7—H7	0.841 (9)
C9—C17	1.410 (2)	O8—H8A	0.828 (10)
C10—C11	1.363 (3)	O8—H8B	0.829 (10)
C10—H10	0.9300		

C6—C1—C2	116.16 (12)	C10—C11—C12	119.32 (15)
C6—C1—C7	123.58 (12)	C10—C11—H11	120.3
C2—C1—C7	120.21 (12)	C12—C11—H11	120.3
C3—C2—C1	120.61 (14)	N2—C12—C11	120.37 (16)
C3—C2—C8	118.90 (13)	N2—C12—H12	119.8
C1—C2—C8	120.46 (12)	C11—C12—H12	119.8
C4—C3—C2	121.06 (14)	N2—C13—C9	119.16 (13)
C4—C3—H3	119.5	N2—C13—C14	119.89 (13)
C2—C3—H3	119.5	C9—C13—C14	120.94 (13)
C5—C4—C3	119.59 (14)	O7—C14—C15	126.44 (14)
C5—C4—H4	120.2	O7—C14—C13	115.32 (13)
C3—C4—H4	120.2	C15—C14—C13	118.23 (14)
C4—C5—C6	118.98 (15)	C14—C15—C16	121.17 (15)
C4—C5—H5	120.5	C14—C15—H15	119.4

C6—C5—H5	120.5	C16—C15—H15	119.4
C5—C6—C1	123.52 (14)	C17—C16—C15	121.51 (16)
C5—C6—N1	116.10 (13)	C17—C16—H16	119.2
C1—C6—N1	120.38 (12)	C15—C16—H16	119.2
O4—C7—O3	125.72 (13)	C16—C17—C9	119.08 (15)
O4—C7—C1	116.86 (12)	C16—C17—H17	120.5
O3—C7—C1	117.37 (12)	C9—C17—H17	120.5
O6—C8—O5	124.10 (15)	O1—N1—O2	122.38 (15)
O6—C8—C2	124.14 (14)	O1—N1—C6	119.10 (13)
O5—C8—C2	111.75 (13)	O2—N1—C6	118.52 (14)
C10—C9—C13	117.26 (14)	C12—N2—C13	122.68 (14)
C10—C9—C17	123.74 (14)	C12—N2—H2	119.6 (14)
C13—C9—C17	119.00 (14)	C13—N2—H2	117.5 (14)
C11—C10—C9	121.17 (15)	C8—O5—H5A	110.8 (19)
C11—C10—H10	119.4	C14—O7—H7	110.7 (17)
C9—C10—H10	119.4	H8A—O8—H8B	105 (2)

C6—C1—C2—C3	2.4 (2)	C9—C10—C11—C12	−1.1 (3)
C7—C1—C2—C3	−179.76 (13)	C10—C11—C12—N2	−0.1 (3)
C6—C1—C2—C8	−175.78 (13)	C10—C9—C13—N2	0.3 (2)
C7—C1—C2—C8	2.0 (2)	C17—C9—C13—N2	−179.84 (14)
C1—C2—C3—C4	0.0 (2)	C10—C9—C13—C14	−179.04 (14)
C8—C2—C3—C4	178.20 (15)	C17—C9—C13—C14	0.8 (2)
C2—C3—C4—C5	−2.1 (3)	N2—C13—C14—O7	−2.0 (2)
C3—C4—C5—C6	1.7 (3)	C9—C13—C14—O7	177.38 (14)
C4—C5—C6—C1	0.8 (2)	N2—C13—C14—C15	177.96 (14)
C4—C5—C6—N1	−178.24 (15)	C9—C13—C14—C15	−2.7 (2)
C2—C1—C6—C5	−2.9 (2)	O7—C14—C15—C16	−177.32 (17)
C7—C1—C6—C5	179.40 (14)	C13—C14—C15—C16	2.8 (2)
C2—C1—C6—N1	176.16 (13)	C14—C15—C16—C17	−1.0 (3)
C7—C1—C6—N1	−1.6 (2)	C15—C16—C17—C9	−1.0 (3)
C6—C1—C7—O4	96.24 (16)	C10—C9—C17—C16	−179.12 (17)
C2—C1—C7—O4	−81.38 (17)	C13—C9—C17—C16	1.0 (2)
C6—C1—C7—O3	−85.96 (18)	C5—C6—N1—O1	178.42 (16)
C2—C1—C7—O3	96.42 (16)	C1—C6—N1—O1	−0.7 (2)
C3—C2—C8—O6	157.79 (16)	C5—C6—N1—O2	−2.0 (2)
C1—C2—C8—O6	−24.0 (2)	C1—C6—N1—O2	178.93 (17)
C3—C2—C8—O5	−23.5 (2)	C11—C12—N2—C13	1.5 (3)
C1—C2—C8—O5	154.77 (14)	C9—C13—N2—C12	−1.6 (2)
C13—C9—C10—C11	1.0 (2)	C14—C13—N2—C12	177.75 (15)
C17—C9—C10—C11	−178.83 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O3^{i}	0.89 (1)	2.00 (1)	2.8112 (16)	151 (2)
O5—H5*A*···O8^{ii}	0.82 (1)	1.78 (1)	2.5928 (18)	171 (3)
O7—H7···O3^{iii}	0.84 (1)	1.82 (1)	2.6482 (15)	168 (2)

O8—H8*B*···O4	0.83 (1)	2.07 (1)	2.8683 (17)	163 (2)
O8—H8*A*···O4^{ii}	0.83 (1)	2.01 (1)	2.8288 (18)	170 (2)
C11—H11···O1^{iv}	0.93	2.42	3.295 (2)	156
C12—H12···O6^{i}	0.93	2.48	3.343 (2)	155
C16—H16···O2^{v}	0.93	2.52	3.413 (2)	160

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+3/2; (ii) *x*, −*y*+3/2, *z*+1/2; (iii) *x*, −*y*+1/2, *z*+1/2; (iv) −*x*+1, −*y*+1, −*z*+1; (v) *x*, *y*, *z*+1.