Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

OPEN ACCESS

ISSN 2056-9890

Crystal structure of quinolinium 2-carboxy-6-nitrobenzoate monohydrate

J. Mohana,[a] M. Divya Bharathi,[a] G. Ahila,[a] G. Chakkaravarthi[b]* and G. Anbalagan[a]*

[a]Department of Physics, Presidency College, Chennai 600 005, India, and [b]Department of Physics, CPCL Polytechnic College, Chennai 600 068, India. *Correspondence e-mail: chakkaravarthi_2005@yahoo.com, anbu24663@yahoo.co.in

Received 22 March 2015; accepted 25 March 2015

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

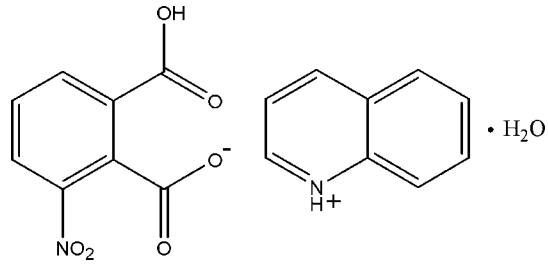
In the anion of the title hydrated molecular salt, $C_9H_8N^+\cdot C_8H_4NO_6^-\cdot H_2O$, the protonated carboxyl and nitro groups makes dihedral angles of 27.56 (5) and 6.86 (8)°, respectively, with the attached benzene ring, whereas the deprotonated carboxy group is almost orthogonal to it with a dihedral angle of 80.21 (1)°. In the crystal, the components are linked by O—H···O and N—H···O hydrogen bonds, generating [001] chains. The packing is consolidated by weak C—H···N and C—H···O interactions as well as aromatic π–π stacking [centroid-to-centroid distances: 3.7023 (8) & 3.6590 (9)Å] interactions, resulting in a three-dimensional network.

Keywords: crystal structure; molecular salt; quinolinium; 2-carboxy-6-nitrobenzoate; hydrogen bonding; π–π stacking interactions.

CCDC reference: 1015219

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); Divya Bharathi *et al.* (2015).



2. Experimental

2.1. Crystal data

$C_9H_8N^+\cdot C_8H_4NO_6^-\cdot H_2O$
M_r = 358.30
Monoclinic, $P2_1/c$
a = 14.7622 (8) Å
b = 14.2461 (8) Å
c = 7.6395 (4) Å
β = 104.434 (2)°
V = 1555.90 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 295 K
0.26 × 0.24 × 0.18 mm

2.2. Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.969, T_{max} = 0.979
32650 measured reflections
4728 independent reflections
3394 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.115
S = 1.04
4728 reflections
248 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7A···O4	0.83 (1)	1.92 (1)	2.7416 (14)	171 (19)
O7—H7B···O4^{i}	0.84 (1)	2.02 (1)	2.8459 (14)	169 (18)
O1—H1A···O7^{ii}	0.84 (1)	1.75 (1)	2.5818 (14)	173 (2)
N2—H2A···O3^{iii}	0.91 (1)	1.74 (1)	2.6425 (14)	176 (18)
C16—H16···O4^{iii}	0.93	2.49	3.1166 (17)	125
C16—H16···O2^{iv}	0.93	2.39	3.1278 (17)	136
C12—H12···N1	0.93	2.61	3.4866 (19)	157

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

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 wish to acknowledge the SAIF, IIT Madras, for the data collection.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7390).

References

Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Castañeda, R., Antal, S. A., Draguta, S., Timofeeva, T. V. & Khrustalev, V. N. (2014). *Acta Cryst.* E**70**, o924–o925.
Divya Bharathi, M., Ahila, G., Mohana, J., Chakkaravarthi, G. & Anbalagan, G. (2015). *Acta Cryst.* E**71**, o261–o262.
Font, M., Monge, A., Ruiz, I. & Heras, B. (1997). *Drug Des. Discov.* **14**, 259–272.
Kafka, S., Pevec, A., Proisl, K., Kimmel, R. & Košmrlj, J. (2012). *Acta Cryst.* E**68**, o3199–o3200.
Li, Z.-S. & Chai, J.-S. (2007). *Acta Cryst.* E**63**, o2857–o2859.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sloboda, A. E., Powell, D., Poletto, J. F., Pickett, W. C., Gibbons, J. J., Bell, D. H., Oronsky, A. L. & Kerwar, S. S. (1991). *J. Rheumatol.* **18**, 855–860.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2015). E**71**, o270–o271 [doi:10.1107/S2056989015006052]

Crystal structure of quinolinium 2-carboxy-6-nitrobenzoate monohydrate

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

S1. Chemical context

The quinoline derivatives are known to exhibit wide range of pharmacological activities such as antibacterial (Benzerka, *et al.*2012), anti-viral (Font *et al.*, 1997) and anti-inflammatory (Sloboda *et al.*, 1991). In view of the above importance, we have synthesized the title compound and report herein on its crystal structure.

S2. Structural commentary

The ORTEP diagram of the title compound (I) is shown in Fig.1. The asymmetric unit of the title compound consists of C_9 H_8 N^+ cation, C_8 H_4 N O_6^- anion and a water molecule. The geometric parameters of (I) (Fig. 1) are well agreed with the similar reported structures [Castañeda *et al.*, 2014; Kafka *et al.*, 2012; Li & Chai (2007)].

The quinolinium ring system is planar [r.m.s deviation = 0.0133 (12)Å] and protonated at N2 atom. In the anion, the carboxyl (O1/C7/O2), nitro (O5/N1/O6) and carboxy (O3/C8/O4) groups are inclined at an angle of 27.56 (5), 6.86 (8) and 80.21 (1)°, respectively with the attached benzene ring (C1—C6). The dihedral angle between the quinolinium ring system and benzene ring is 89.91 (5)°.

S3. Supramolecular features

The molecular structure is stabilized by weak intramolecular O—H···O and C—H···N hydrogen bonds (Table 1). The crystal structure is stabilized by weak intermolecular N—H···O, O—H···O and C—H···O hydrogen bonds (Table 1 & Fig. 2) which link adjacent anions and cations through water molecules into infinite one-dimensional chains along [001]. The crystal structure is further stabilized by weak $\pi\cdots\pi$ [Cg1···Cg1^{i} = 3.7023 (8); Cg3···Cg2^{ii} = 3.6590 (9)Å; (i) 1-x,-y,-z; (ii) x,1/2-y,-1/2+z; Cg1, Cg2 and Cg3 are the centroids of the rings (C1—C6), (C13/C14/C15/C16/c17/N2) and (C9—C13/c17), respectively] interactions.

S4. Synthesis and crystallization

Quinoline (3.22 g, 0.99 mol) was dissolved in hot water (25 ml) and after half an hour, a solution of 3-nitrophthalic acid (5.278 g, 0.38 mol) in methanol (25 ml) was added and stirred for about one hour. A white colour powder was formed. The product was dissolved in aqueous methanol solution (210 ml). Single crystals suitable for X-ray diffraction were obtained from the slow evaporation method at room temperature within a few days.

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 Uiso(H) = 1.5 Ueq(O). Distance restraints were applied for the distance O—H = 0.82 (1)Å. H atom for N atom was located from Fourier map and refined freely with distance restraint N—H = 0.88 (1)Å.

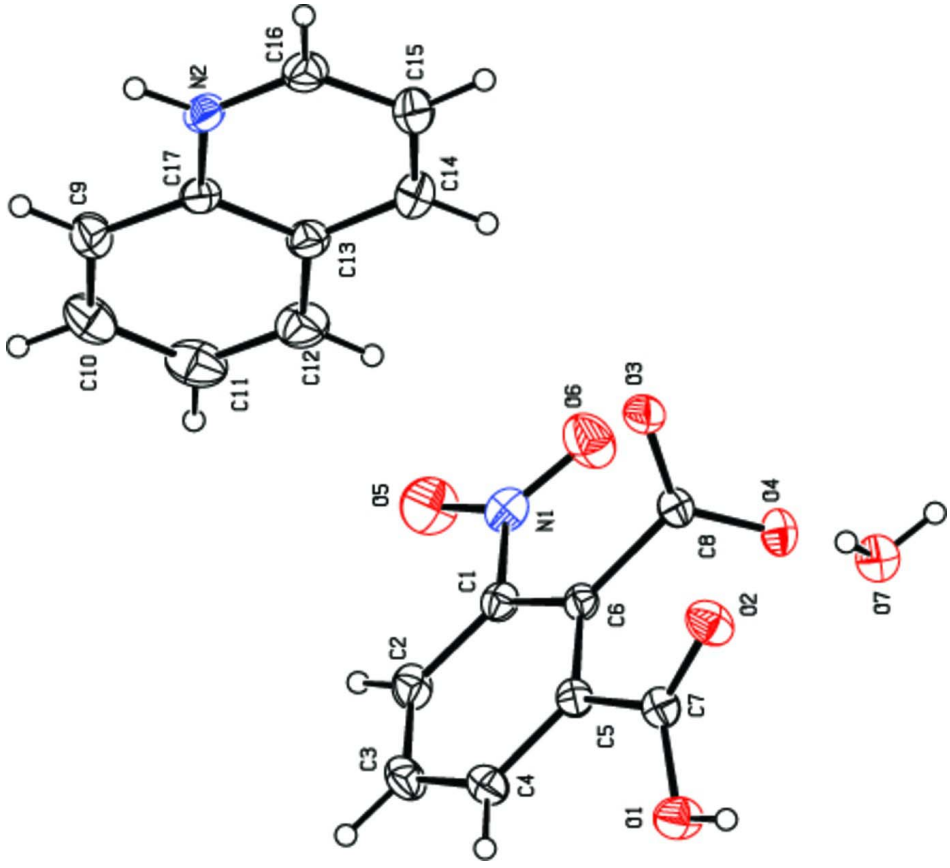


Figure 1

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

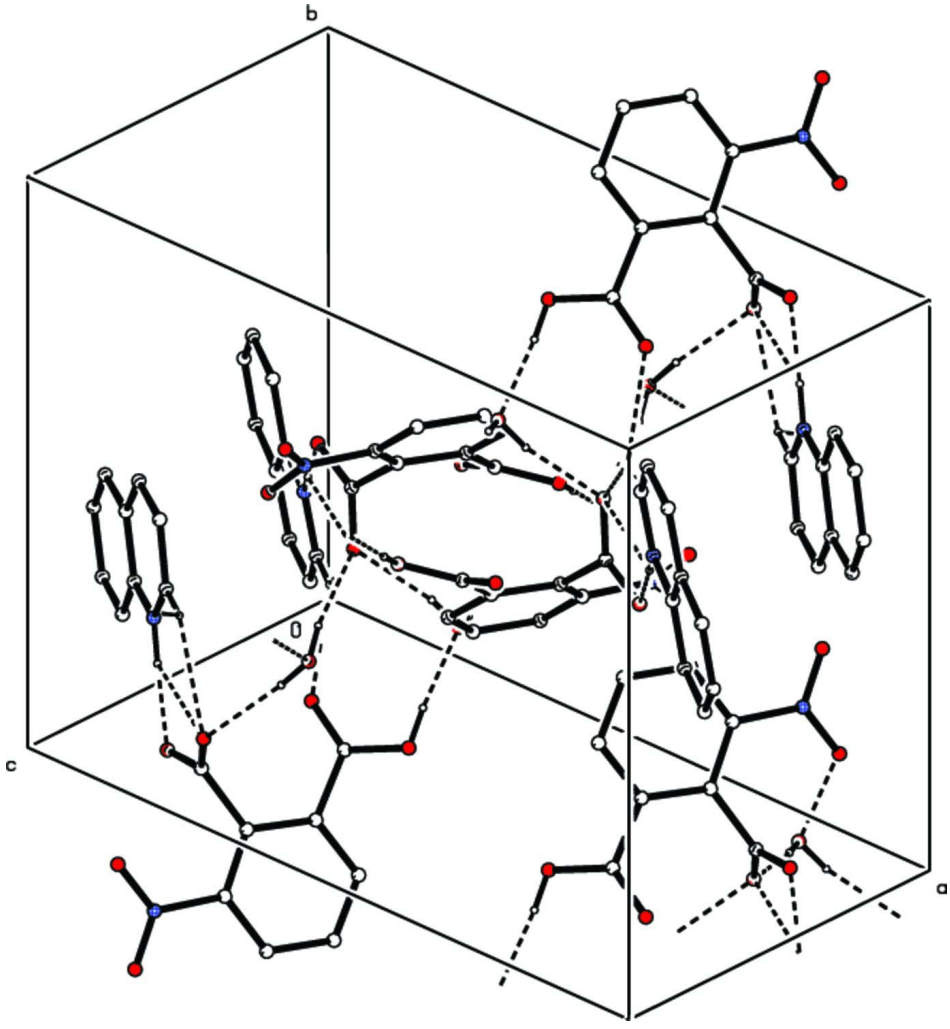


Figure 2

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

Quinolinium 2-carboxy-6-nitrobenzoate monohydrate

Crystal data

$C_9H_8N^+·C_8H_4NO_6^-·H_2O$
M_r = 358.30
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 14.7622 (8) Å
b = 14.2461 (8) Å
c = 7.6395 (4) Å
β = 104.434 (2)°
V = 1555.90 (15) Å^3
Z = 4
$F(000)$ = 744
D_x = 1.530 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9970 reflections
θ = 2.8–30.4°
μ = 0.12 mm^{-1}
T = 295 K
Block, colourless
0.26 × 0.24 × 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*; Bruker, 2004)
T_{min} = 0.969, T_{max} = 0.979
32650 measured reflections
4728 independent reflections
3394 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 30.8°, θ_{min} = 2.9°
h = −21→21
k = −20→20
l = −10→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.115
S = 1.04
4728 reflections
248 parameters
4 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
$w = 1/[\sigma^2(F_o^2) + (0.0472P)^2 + 0.4484P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Special details

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	0.64273 (8)	0.07483 (8)	−0.05905 (16)	0.0309 (2)
C2	0.57907 (9)	0.14414 (9)	−0.04652 (19)	0.0386 (3)
H2	0.5629	0.1900	−0.1354	0.046*
C3	0.54012 (9)	0.14429 (9)	0.09892 (19)	0.0405 (3)
H3	0.4982	0.1912	0.1106	0.049*
C4	0.56333 (9)	0.07465 (9)	0.22753 (18)	0.0361 (3)
H4	0.5351	0.0735	0.3236	0.043*
C5	0.62851 (8)	0.00608 (8)	0.21529 (16)	0.0295 (2)
C6	0.67125 (8)	0.00565 (8)	0.07151 (15)	0.0276 (2)
C7	0.65254 (8)	−0.06752 (8)	0.35872 (16)	0.0321 (2)
C8	0.74316 (8)	−0.06939 (8)	0.06354 (16)	0.0305 (2)
C9	0.95815 (10)	0.39076 (10)	0.1010 (2)	0.0450 (3)
H9	0.9905	0.4451	0.1463	0.054*
C10	0.87001 (11)	0.39591 (13)	−0.0086 (2)	0.0563 (4)
H10	0.8421	0.4543	−0.0379	0.068*
C11	0.82119 (11)	0.31475 (15)	−0.0772 (2)	0.0617 (5)
H11	0.7610	0.3196	−0.1515	0.074*
C12	0.86022 (10)	0.22927 (13)	−0.0373 (2)	0.0552 (4)
H12	0.8268	0.1759	−0.0848	0.066*

C13	0.95129 (9)	0.22011 (10)	0.07584 (19)	0.0387 (3)
C14	0.99619 (11)	0.13384 (10)	0.1225 (2)	0.0488 (4)
H14	0.9653	0.0784	0.0797	0.059*
C15	1.08465 (11)	0.13063 (10)	0.2302 (2)	0.0497 (4)
H15	1.1152	0.0734	0.2584	0.060*
C16	1.12878 (9)	0.21365 (10)	0.2974 (2)	0.0429 (3)
H16	1.1887	0.2117	0.3734	0.051*
C17	0.99937 (8)	0.30253 (9)	0.14427 (17)	0.0331 (3)
N1	0.67819 (8)	0.07495 (8)	−0.22213 (15)	0.0389 (3)
H2A	1.1177 (11)	0.3480 (9)	0.304 (2)	0.060 (5)*
N2	1.08727 (7)	0.29511 (8)	0.25544 (16)	0.0364 (2)
O1	0.58421 (7)	−0.08353 (8)	0.43610 (14)	0.0457 (2)
H1A	0.6007 (14)	−0.1247 (11)	0.516 (2)	0.069*
O2	0.72664 (7)	−0.10794 (7)	0.39726 (13)	0.0445 (2)
O3	0.82733 (6)	−0.04668 (7)	0.11938 (14)	0.0408 (2)
O4	0.71315 (7)	−0.14892 (6)	0.01135 (13)	0.0386 (2)
O5	0.65803 (10)	0.14023 (9)	−0.32691 (17)	0.0659 (4)
O6	0.72700 (9)	0.01019 (9)	−0.24593 (16)	0.0611 (3)
O7	0.62094 (7)	−0.21451 (7)	−0.32298 (13)	0.0420 (2)
H7A	0.6537 (12)	−0.1934 (13)	−0.2261 (17)	0.063*
H7B	0.6482 (12)	−0.2591 (10)	−0.359 (2)	0.063*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0293 (5)	0.0308 (6)	0.0300 (6)	−0.0029 (4)	0.0026 (4)	0.0001 (4)
C2	0.0368 (6)	0.0332 (6)	0.0406 (7)	0.0043 (5)	0.0001 (5)	0.0069 (5)
C3	0.0350 (6)	0.0363 (7)	0.0469 (8)	0.0107 (5)	0.0042 (5)	−0.0002 (5)
C4	0.0322 (6)	0.0386 (6)	0.0368 (6)	0.0049 (5)	0.0073 (5)	−0.0027 (5)
C5	0.0273 (5)	0.0287 (5)	0.0296 (6)	0.0008 (4)	0.0014 (4)	−0.0015 (4)
C6	0.0245 (5)	0.0256 (5)	0.0300 (6)	−0.0016 (4)	0.0017 (4)	−0.0027 (4)
C7	0.0341 (6)	0.0325 (6)	0.0281 (6)	0.0010 (5)	0.0047 (5)	−0.0021 (5)
C8	0.0328 (6)	0.0293 (5)	0.0290 (6)	0.0023 (4)	0.0068 (4)	−0.0014 (4)
C9	0.0443 (7)	0.0386 (7)	0.0511 (8)	0.0053 (6)	0.0100 (6)	0.0017 (6)
C10	0.0489 (9)	0.0593 (10)	0.0580 (10)	0.0201 (7)	0.0085 (7)	0.0066 (8)
C11	0.0353 (7)	0.0846 (13)	0.0584 (10)	0.0099 (8)	−0.0011 (7)	−0.0028 (9)
C12	0.0359 (7)	0.0647 (10)	0.0604 (10)	−0.0080 (7)	0.0031 (7)	−0.0138 (8)
C13	0.0316 (6)	0.0414 (7)	0.0437 (7)	−0.0041 (5)	0.0105 (5)	−0.0058 (6)
C14	0.0479 (8)	0.0350 (7)	0.0644 (10)	−0.0077 (6)	0.0157 (7)	−0.0050 (6)
C15	0.0469 (8)	0.0350 (7)	0.0684 (10)	0.0049 (6)	0.0166 (7)	0.0093 (7)
C16	0.0311 (6)	0.0444 (7)	0.0519 (8)	0.0019 (5)	0.0080 (6)	0.0107 (6)
C17	0.0282 (5)	0.0364 (6)	0.0355 (6)	−0.0006 (5)	0.0094 (5)	0.0014 (5)
N1	0.0401 (6)	0.0412 (6)	0.0338 (6)	−0.0060 (5)	0.0061 (5)	0.0015 (5)
N2	0.0289 (5)	0.0362 (5)	0.0429 (6)	−0.0049 (4)	0.0068 (4)	0.0021 (5)
O1	0.0425 (5)	0.0521 (6)	0.0446 (6)	0.0056 (4)	0.0148 (4)	0.0143 (4)
O2	0.0439 (5)	0.0486 (6)	0.0404 (5)	0.0147 (4)	0.0095 (4)	0.0113 (4)
O3	0.0286 (4)	0.0385 (5)	0.0539 (6)	0.0020 (4)	0.0078 (4)	−0.0039 (4)
O4	0.0459 (5)	0.0293 (4)	0.0388 (5)	0.0001 (4)	0.0071 (4)	−0.0059 (4)

O5	0.0789 (9)	0.0694 (8)	0.0530 (7)	0.0109 (6)	0.0232 (6)	0.0290 (6)
O6	0.0824 (9)	0.0594 (7)	0.0506 (6)	0.0141 (6)	0.0338 (6)	0.0025 (5)
O7	0.0478 (6)	0.0417 (5)	0.0355 (5)	0.0014 (4)	0.0086 (4)	0.0010 (4)

Geometric parameters (Å, º)

C1—C2	1.3828 (17)	C10—H10	0.9300
C1—C6	1.3907 (16)	C11—C12	1.349 (3)
C1—N1	1.4666 (16)	C11—H11	0.9300
C2—C3	1.372 (2)	C12—C13	1.4114 (19)
C2—H2	0.9300	C12—H12	0.9300
C3—C4	1.3780 (19)	C13—C14	1.400 (2)
C3—H3	0.9300	C13—C17	1.4039 (18)
C4—C5	1.3906 (16)	C14—C15	1.360 (2)
C4—H4	0.9300	C14—H14	0.9300
C5—C6	1.3965 (17)	C15—C16	1.386 (2)
C5—C7	1.4940 (16)	C15—H15	0.9300
C6—C8	1.5184 (16)	C16—N2	1.3141 (17)
C7—O2	1.2060 (15)	C16—H16	0.9300
C7—O1	1.3101 (16)	C17—N2	1.3663 (16)
C8—O4	1.2453 (14)	N1—O6	1.2120 (16)
C8—O3	1.2516 (14)	N1—O5	1.2146 (15)
C9—C10	1.362 (2)	N2—H2A	0.908 (9)
C9—C17	1.3996 (19)	O1—H1A	0.840 (9)
C9—H9	0.9300	O7—H7A	0.833 (9)
C10—C11	1.394 (3)	O7—H7B	0.836 (9)
C2—C1—C6	123.08 (12)	C12—C11—C10	120.79 (14)
C2—C1—N1	116.78 (11)	C12—C11—H11	119.6
C6—C1—N1	120.12 (11)	C10—C11—H11	119.6
C3—C2—C1	119.09 (12)	C11—C12—C13	120.66 (15)
C3—C2—H2	120.5	C11—C12—H12	119.7
C1—C2—H2	120.5	C13—C12—H12	119.7
C2—C3—C4	119.75 (12)	C14—C13—C17	118.44 (12)
C2—C3—H3	120.1	C14—C13—C12	123.75 (13)
C4—C3—H3	120.1	C17—C13—C12	117.82 (13)
C3—C4—C5	120.73 (12)	C15—C14—C13	120.41 (13)
C3—C4—H4	119.6	C15—C14—H14	119.8
C5—C4—H4	119.6	C13—C14—H14	119.8
C4—C5—C6	120.78 (11)	C14—C15—C16	119.16 (13)
C4—C5—C7	119.05 (11)	C14—C15—H15	120.4
C6—C5—C7	120.17 (10)	C16—C15—H15	120.4
C1—C6—C5	116.47 (10)	N2—C16—C15	121.06 (12)
C1—C6—C8	124.05 (11)	N2—C16—H16	119.5
C5—C6—C8	119.47 (10)	C15—C16—H16	119.5
O2—C7—O1	124.07 (12)	N2—C17—C9	120.40 (12)
O2—C7—C5	123.32 (11)	N2—C17—C13	118.71 (11)
O1—C7—C5	112.60 (10)	C9—C17—C13	120.89 (12)

O4—C8—O3	126.02 (11)	O6—N1—O5	122.75 (13)
O4—C8—C6	117.19 (10)	O6—N1—C1	118.55 (11)
O3—C8—C6	116.67 (10)	O5—N1—C1	118.69 (12)
C10—C9—C17	119.08 (14)	C16—N2—C17	122.19 (11)
C10—C9—H9	120.5	C16—N2—H2A	118.7 (12)
C17—C9—H9	120.5	C17—N2—H2A	119.1 (12)
C9—C10—C11	120.77 (15)	C7—O1—H1A	109.7 (14)
C9—C10—H10	119.6	H7A—O7—H7B	110.4 (18)
C11—C10—H10	119.6		

C6—C1—C2—C3	−1.47 (19)	C17—C9—C10—C11	−0.1 (3)
N1—C1—C2—C3	176.70 (11)	C9—C10—C11—C12	−0.2 (3)
C1—C2—C3—C4	−1.4 (2)	C10—C11—C12—C13	0.3 (3)
C2—C3—C4—C5	2.4 (2)	C11—C12—C13—C14	−179.82 (16)
C3—C4—C5—C6	−0.64 (18)	C11—C12—C13—C17	−0.1 (2)
C3—C4—C5—C7	179.28 (12)	C17—C13—C14—C15	−0.7 (2)
C2—C1—C6—C5	3.15 (17)	C12—C13—C14—C15	179.01 (16)
N1—C1—C6—C5	−174.97 (10)	C13—C14—C15—C16	1.9 (2)
C2—C1—C6—C8	−178.10 (11)	C14—C15—C16—N2	−1.5 (2)
N1—C1—C6—C8	3.78 (17)	C10—C9—C17—N2	−179.26 (14)
C4—C5—C6—C1	−2.06 (16)	C10—C9—C17—C13	0.3 (2)
C7—C5—C6—C1	178.02 (10)	C14—C13—C17—N2	−0.92 (19)
C4—C5—C6—C8	179.13 (11)	C12—C13—C17—N2	179.37 (13)
C7—C5—C6—C8	−0.78 (16)	C14—C13—C17—C9	179.54 (14)
C4—C5—C7—O2	−153.38 (13)	C12—C13—C17—C9	−0.2 (2)
C6—C5—C7—O2	26.54 (18)	C2—C1—N1—O6	−173.03 (12)
C4—C5—C7—O1	27.15 (16)	C6—C1—N1—O6	5.20 (17)
C6—C5—C7—O1	−152.93 (11)	C2—C1—N1—O5	7.53 (17)
C1—C6—C8—O4	−100.90 (14)	C6—C1—N1—O5	−174.24 (12)
C5—C6—C8—O4	77.82 (14)	C15—C16—N2—C17	−0.1 (2)
C1—C6—C8—O3	82.81 (15)	C9—C17—N2—C16	−179.12 (13)
C5—C6—C8—O3	−98.48 (13)	C13—C17—N2—C16	1.3 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7*A*···O4	0.83 (1)	1.92 (1)	2.7416 (14)	171 (19)
O7—H7*B*···O4^{i}	0.84 (1)	2.02 (1)	2.8459 (14)	169 (18)
O1—H1*A*···O7^{ii}	0.84 (1)	1.75 (1)	2.5818 (14)	173 (2)
N2—H2*A*···O3^{iii}	0.91 (1)	1.74 (1)	2.6425 (14)	176 (18)
C16—H16···O4^{iii}	0.93	2.49	3.1166 (17)	125
C16—H16···O2^{iv}	0.93	2.39	3.1278 (17)	136
C12—H12···N1	0.93	2.61	3.4866 (19)	157

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