Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Cinchonidinium chloride monohydrate

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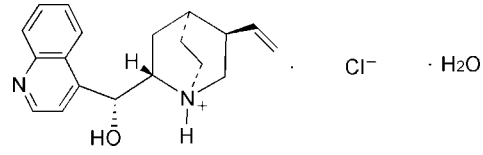
Received 23 November 2007; accepted 26 November 2007

Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.006 Å; disorder in main residue; R factor = 0.069; wR factor = 0.179; data-to-parameter ratio = 12.8.

In the title salt, $C_{19}H_{23}N_2O^+\cdot Cl^-\cdot H_2O$, the ions and the water molecule are held together by O—H···Cl, N—H···Cl, O—H···O, O—H···N and C—H···Cl hydrogen bonds, forming a three-dimensional framework. The vinyl group is disordered over two orientations with refined occupancies of 0.564 (16) and 0.436 (16). The cell parameters of the title compound have been reported previously [Griffiths (1952). *Acta Cryst.* **5**, 290–291].

Related literature

For the Cambridge Structural Database (Version 5.26), see: Allen (2002). For related literature, see: Griffiths (1952); Zhang, Lü *et al.* (2006); Zhang, Tu *et al.* (2006).



Experimental

Crystal data

$C_{19}H_{23}N_2O^+\cdot Cl^-\cdot H_2O$
M_r = 348.86
Orthorhombic, $P2_12_12_1$
a = 10.4924 (8) Å
b = 12.9049 (10) Å
c = 13.3936 (10) Å
V = 1813.5 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 273 (2) K
0.37 × 0.34 × 0.12 mm

Data collection

Siemens $P4$ diffractometer
Absorption correction: multi-scan (*SHELXTL*; Bruker, 1998)
T_{min} = 0.722, T_{max} = 0.895
(expected range = 0.785–0.973)
9572 measured reflections
3214 independent reflections
3090 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
3 standard reflections
every 97 reflections
intensity decay: 5.0%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.179
S = 1.18
3214 reflections
252 parameters
12 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Absolute structure: Flack (1983), 1369 Friedel pairs
Flack parameter: 0.04 (13)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82 (2)	1.84 (2)	2.653 (5)	172 (3)
O2—H2OB···N1^{ii}	0.82 (2)	2.07 (2)	2.867 (6)	165 (3)
O2—H2OA···Cl1	0.82 (2)	2.31 (2)	3.135 (5)	174 (6)
N2—H2···Cl1	0.96 (4)	2.08 (4)	3.034 (6)	175 (3)
C5—H5···Cl1	0.93	2.77	3.692 (5)	172

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

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2530).

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supporting information

Acta Cryst. (2008). E**64**, o193 [https://doi.org/10.1107/S160053680706343X]

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S1. Comment

The cell parameters (a = 12.8, b = 13.3, c = 10.6 Å) of the title compound have been reported previously (Griffiths, 1952; CSD refcode ZZZTZW, CSD, Version 5.26; Allen, 2002), but structural details are not available. Crystal structures of some compounds containing cinchonidine have also been reported, *e.g.* cinchonidinium bis(4-methylbenzenesulfonate) monohydrate (Zhang, Lü *et al.*, 2006), cinchonidinium bis(perchlorate) (Zhang, Tu *et al.*, 2006).

The geometry of the cinchonidinium unit is consistent with that observed in other cinchonidinium compounds (Zhang, Lv *et al.*, 2006; Zhang, Tu *et al.*, 2006), except for the disorder in the vinyl group. The C—C bond lengths in quinoline ring system range from 1.358 (6) to 1.429 (6) Å, comparable with the range of 1.344 (5)–1.422 (4) Å observed by Zhang, Lv *et al.* (2006).

As shown in Fig. 1, the chloride anion and cinchonidinium cation are linked by N—H···Cl and weak C—H···Cl hydrogen bonds, and the chloride ion and water molecule are connected by a O—H···Cl hydrogen bond (Table 1). The ionic pairs and water molecule are linked by O—H···N and O—H···O hydrogen bonds to form a three-dimensional framework (Fig. 2).

S2. Experimental

Cinchonidine (0.01 mol, 2.94 g) and 10% hydrochloric acid (3.65 g) were mixed together with enough water, and heated to a temperature where a clear solution was resulted. Colourless single crystals of the title compound were obtained by slow evaporation of the solution at room temperature for 7 d.

S3. Refinement

The vinyl group is disordered over two orientations with refined occupancies of 0.564 (16) and 0.436 (16); the corresponding C—C distances in the major and minor conformers were restrained to be equal. Atoms C18′ and C19′ were restrained to have the same U^{ij} components. N– and O-bound H atoms were located in a difference map and refined with the O—H and H···H (in water) distances restrained to 0.82 (2) and 1.39 (2) Å, respectively. C-bound H atoms were placed in calculated positions (C—H = 0.93–0.98 Å) and allowed to ride on their parent atoms, with U_{iso}(H) values set at 1.2 times U_{eq} of the parent atoms.

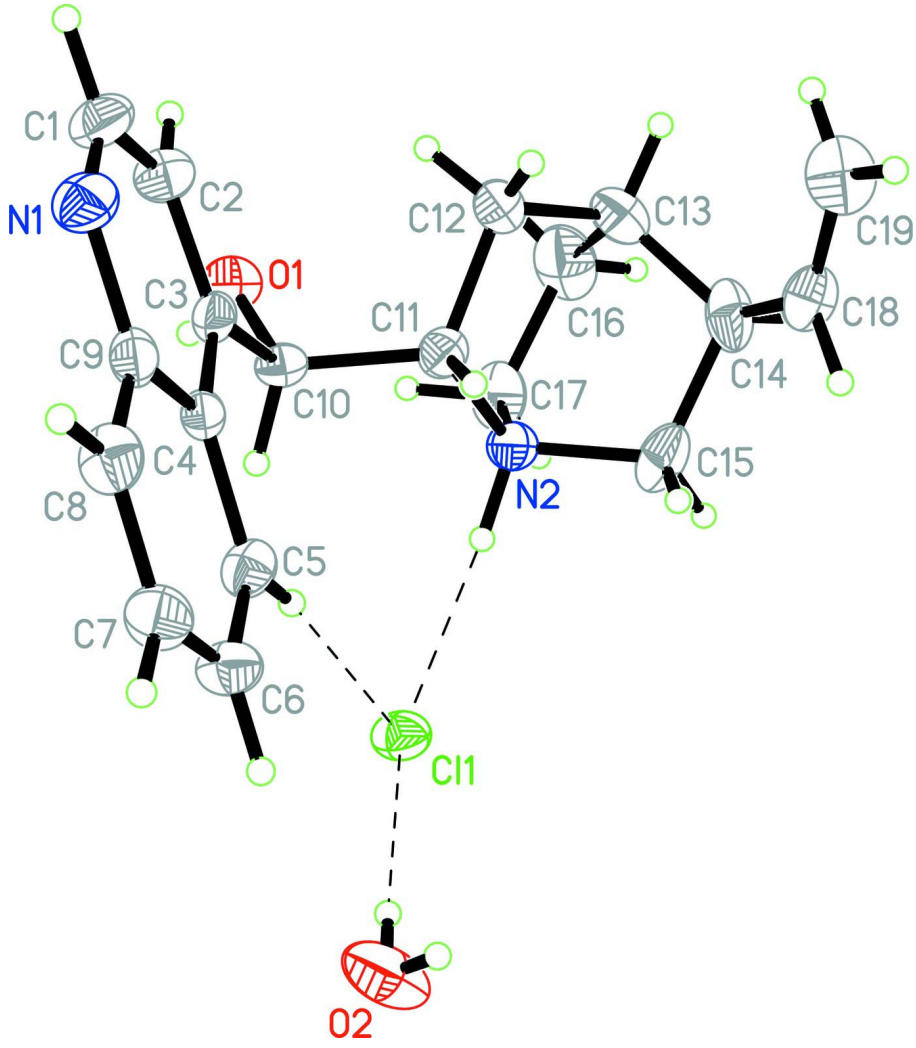

Figure 1

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 40% probability level. Hydrogen bonds are shown as dashed lines.

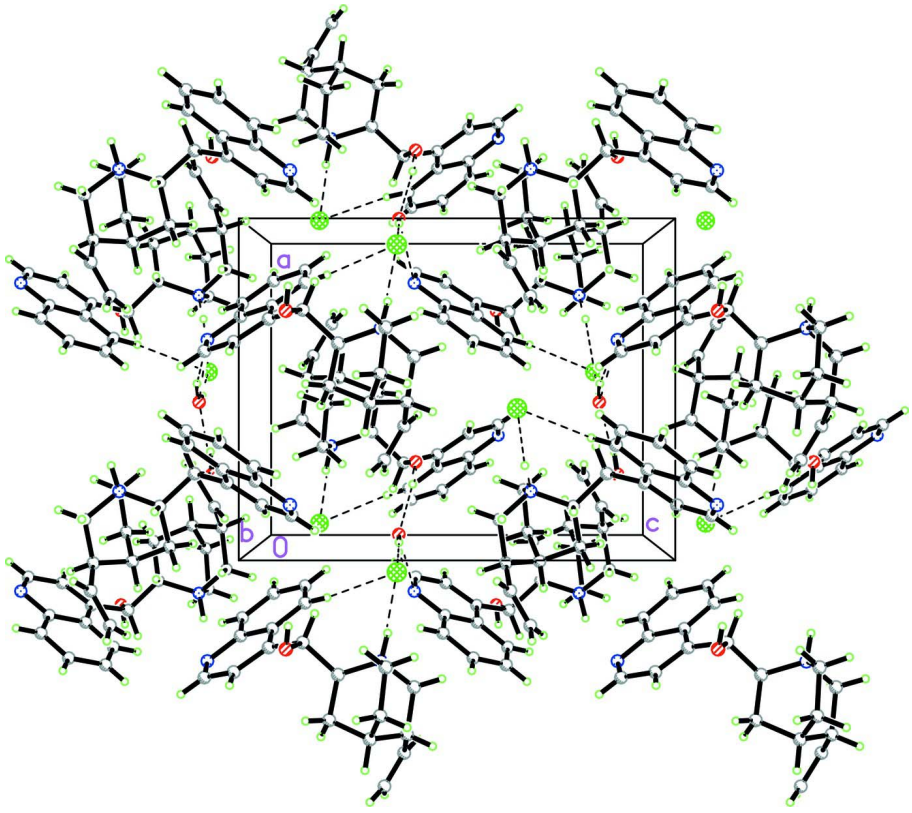

Figure 2

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

Cinchonidinium chloride monohydrate

Crystal data

$C_{19}H_{23}N_2O^+\cdot Cl^-\cdot H_2O$
$M_r = 348.86$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 10.4924\ (8)$ Å
$b = 12.9049\ (10)$ Å
$c = 13.3936\ (10)$ Å
$V = 1813.5\ (2)$ Å^3
$Z = 4$
$F(000) = 744$
$D_x = 1.278$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 31 reflections
$\theta = 3.3$–$18.6°$
$\mu = 0.22$ mm^{-1}
$T = 273$ K
Plate, colourless
0.37 × 0.34 × 0.12 mm

Data collection

Siemens P4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SHELXTL*; Bruker, 1998)
$T_{min} = 0.722$, $T_{max} = 0.895$
9572 measured reflections
3214 independent reflections
3090 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$
$h = -12 \rightarrow 11$
$k = -9 \rightarrow 15$
$l = -15 \rightarrow 15$
3 standard reflections every 97 reflections
intensity decay: 5.0%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.069$
$wR(F^2) = 0.179$
$S = 1.18$
3214 reflections
252 parameters
12 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
$w = 1/[\sigma^2(F_o^2) + (0.0981P)^2 + 0.5633P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}
Absolute structure: Flack (1983), with 1369 Friedel pairs
Absolute structure parameter: 0.04 (13)

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}	Occ. (<1)
Cl1	0.94217 (9)	0.75097 (9)	0.35617 (7)	0.0500 (3)	
O1	0.7326 (3)	0.9410 (2)	0.1041 (2)	0.0511 (8)	
O2	1.0407 (3)	0.5216 (3)	0.3556 (4)	0.0858 (13)	
N1	0.6545 (4)	0.6294 (3)	−0.1087 (2)	0.0510 (9)	
N2	0.6840 (3)	0.8504 (3)	0.3211 (2)	0.0454 (8)	
C1	0.6176 (4)	0.7257 (4)	−0.1063 (3)	0.0533 (12)	
H1A	0.5696	0.7497	−0.1599	0.064*	
C2	0.6443 (4)	0.7957 (4)	−0.0297 (3)	0.0478 (10)	
H2A	0.6143	0.8634	−0.0333	0.057*	
C3	0.7148 (3)	0.7642 (3)	0.0508 (3)	0.0381 (9)	
C4	0.7589 (3)	0.6594 (3)	0.0517 (3)	0.0346 (8)	
C5	0.8343 (4)	0.6152 (3)	0.1287 (3)	0.0422 (9)	
H5	0.8546	0.6549	0.1844	0.051*	
C6	0.8775 (4)	0.5162 (3)	0.1227 (3)	0.0482 (10)	
H6	0.9271	0.4890	0.1739	0.058*	
C7	0.8475 (4)	0.4552 (4)	0.0401 (3)	0.0527 (11)	
H7	0.8781	0.3877	0.0361	0.063*	
C8	0.7738 (4)	0.4939 (4)	−0.0349 (3)	0.0489 (10)	
H8	0.7533	0.4522	−0.0892	0.059*	
C9	0.7288 (4)	0.5953 (3)	−0.0310 (3)	0.0397 (9)	
C10	0.7394 (3)	0.8374 (3)	0.1368 (3)	0.0363 (8)	
H10	0.8246	0.8241	0.1638	0.044*	
C11	0.6392 (4)	0.8168 (3)	0.2187 (3)	0.0410 (9)	

H11	0.6269	0.7416	0.2216	0.049*	
C12	0.5101 (4)	0.8640 (5)	0.2001 (4)	0.0668 (15)	
H12A	0.4511	0.8109	0.1780	0.080*	
H12B	0.5163	0.9162	0.1482	0.080*	
C13	0.4614 (5)	0.9137 (5)	0.2972 (4)	0.0701 (15)	
H13	0.3743	0.9388	0.2869	0.084*	
C14	0.4621 (5)	0.8368 (4)	0.3821 (3)	0.0615 (13)	
H14	0.4334	0.8725	0.4426	0.074*	
C15	0.5996 (5)	0.8022 (4)	0.3980 (3)	0.0620 (13)	
H15A	0.6277	0.8227	0.4642	0.074*	
H15B	0.6048	0.7273	0.3934	0.074*	
C16	0.5460 (6)	1.0037 (4)	0.3240 (5)	0.0831 (18)	
H16A	0.5175	1.0346	0.3861	0.100*	
H16B	0.5420	1.0560	0.2721	0.100*	
C17	0.6826 (5)	0.9649 (4)	0.3353 (4)	0.0613 (13)	
H17A	0.7369	0.9978	0.2860	0.074*	
H17B	0.7147	0.9822	0.4011	0.074*	
C18	0.3877 (9)	0.7331 (8)	0.3733 (7)	0.050 (3)	0.564 (16)
H18	0.4218	0.6754	0.4051	0.061*	0.564 (16)
C19	0.2832 (9)	0.7210 (9)	0.3257 (8)	0.067 (3)	0.564 (16)
H19A	0.2460	0.7768	0.2929	0.081*	0.564 (16)
H19B	0.2443	0.6562	0.3239	0.081*	0.564 (16)
C18′	0.3393 (10)	0.7759 (9)	0.3550 (12)	0.080 (6)	0.436 (16)
H18′	0.2713	0.8063	0.3215	0.096*	0.436 (16)
C19′	0.338 (2)	0.6812 (10)	0.3823 (11)	0.079 (5)	0.436 (16)
H19C	0.4083	0.6535	0.4158	0.094*	0.436 (16)
H19D	0.2680	0.6398	0.3687	0.094*	0.436 (16)
H2	0.765 (4)	0.820 (3)	0.336 (3)	0.035 (10)*	
H1	0.803 (3)	0.967 (4)	0.111 (4)	0.062 (16)*	
H2OA	1.020 (4)	0.5832 (15)	0.358 (5)	0.081 (18)*	
H2OB	0.982 (3)	0.480 (2)	0.354 (4)	0.061 (15)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0518 (5)	0.0549 (6)	0.0432 (5)	0.0083 (5)	−0.0100 (4)	−0.0045 (5)
O1	0.0510 (18)	0.0404 (16)	0.0618 (18)	−0.0074 (14)	−0.0066 (15)	0.0044 (14)
O2	0.0468 (19)	0.051 (2)	0.160 (4)	0.0026 (17)	0.002 (3)	0.012 (3)
N1	0.053 (2)	0.059 (2)	0.0405 (18)	−0.0011 (18)	−0.0096 (16)	−0.0068 (17)
N2	0.0440 (19)	0.053 (2)	0.0387 (17)	0.0083 (17)	−0.0003 (14)	−0.0012 (16)
C1	0.056 (2)	0.066 (3)	0.038 (2)	0.000 (2)	−0.0127 (19)	0.006 (2)
C2	0.051 (2)	0.044 (2)	0.048 (2)	0.002 (2)	−0.005 (2)	0.0043 (18)
C3	0.0346 (18)	0.047 (2)	0.0329 (18)	−0.0061 (18)	0.0032 (14)	0.0078 (17)
C4	0.0298 (17)	0.045 (2)	0.0294 (18)	−0.0013 (16)	0.0031 (14)	0.0000 (16)
C5	0.047 (2)	0.045 (2)	0.0344 (19)	−0.0088 (18)	−0.0041 (17)	−0.0029 (17)
C6	0.051 (2)	0.045 (2)	0.048 (2)	0.0081 (19)	−0.008 (2)	0.0003 (19)
C7	0.057 (3)	0.042 (2)	0.059 (3)	0.011 (2)	0.004 (2)	−0.001 (2)
C8	0.056 (2)	0.050 (2)	0.041 (2)	−0.005 (2)	−0.0007 (19)	−0.0162 (19)

C9	0.0357 (19)	0.049 (2)	0.0347 (18)	−0.0030 (18)	0.0058 (16)	−0.0030 (17)
C10	0.0369 (18)	0.0347 (18)	0.0374 (18)	−0.0003 (16)	−0.0076 (16)	0.0005 (16)
C11	0.042 (2)	0.043 (2)	0.038 (2)	−0.0058 (18)	−0.0023 (16)	0.0026 (17)
C12	0.040 (2)	0.113 (4)	0.047 (3)	0.007 (3)	0.0029 (19)	0.009 (3)
C13	0.045 (3)	0.092 (4)	0.073 (3)	0.019 (3)	0.008 (2)	0.005 (3)
C14	0.061 (3)	0.076 (3)	0.048 (3)	−0.011 (3)	0.021 (2)	−0.015 (2)
C15	0.090 (4)	0.060 (3)	0.036 (2)	0.002 (3)	0.011 (2)	0.003 (2)
C16	0.086 (4)	0.053 (3)	0.110 (5)	0.019 (3)	0.031 (4)	0.006 (3)
C17	0.073 (3)	0.056 (3)	0.055 (3)	−0.011 (2)	0.011 (2)	−0.013 (2)
C18	0.068 (6)	0.026 (6)	0.058 (5)	−0.010 (5)	0.005 (4)	0.008 (4)
C19	0.078 (7)	0.051 (7)	0.072 (7)	−0.015 (5)	0.003 (5)	−0.019 (5)
C18′	0.108 (15)	0.040 (8)	0.092 (11)	0.033 (9)	0.034 (11)	−0.006 (9)
C19′	0.115 (13)	0.046 (8)	0.075 (10)	−0.012 (9)	−0.007 (9)	−0.010 (7)

Geometric parameters (Å, º)

O1—C10	1.409 (5)	C11—C12	1.505 (6)
O1—H1	0.82 (2)	C11—H11	0.98
O2—H2OA	0.823 (19)	C12—C13	1.538 (7)
O2—H2OB	0.816 (18)	C12—H12A	0.97
N1—C1	1.302 (6)	C12—H12B	0.97
N1—C9	1.372 (5)	C13—C16	1.506 (9)
N2—C17	1.490 (6)	C13—C14	1.508 (7)
N2—C15	1.495 (6)	C13—H13	0.98
N2—C11	1.512 (5)	C14—C15	1.524 (7)
N2—H2	0.96 (4)	C14—C18′	1.552 (12)
C1—C2	1.395 (6)	C14—C18	1.554 (9)
C1—H1A	0.93	C14—H14	0.98
C2—C3	1.370 (6)	C15—H15A	0.97
C2—H2A	0.93	C15—H15B	0.97
C3—C4	1.429 (6)	C16—C17	1.525 (8)
C3—C10	1.512 (5)	C16—H16A	0.97
C4—C9	1.419 (5)	C16—H16B	0.97
C4—C5	1.419 (5)	C17—H17A	0.97
C5—C6	1.358 (6)	C17—H17B	0.97
C5—H5	0.93	C18—C19	1.278 (11)
C6—C7	1.394 (6)	C18—H18	0.93
C6—H6	0.93	C19—H19A	0.93
C7—C8	1.363 (6)	C19—H19B	0.93
C7—H7	0.93	C18′—C19′	1.277 (12)
C8—C9	1.391 (6)	C18′—H18′	0.93
C8—H8	0.93	C19′—H19C	0.93
C10—C11	1.543 (5)	C19′—H19D	0.93
C10—H10	0.98		

C10—O1—H1	108 (4)	C13—C12—H12A	109.9
H2OA—O2—H2OB	116 (3)	C11—C12—H12B	109.9
C1—N1—C9	117.1 (3)	C13—C12—H12B	109.9

C17—N2—C15	108.6 (4)	H12A—C12—H12B	108.3
C17—N2—C11	113.4 (3)	C16—C13—C14	109.0 (5)
C15—N2—C11	108.8 (3)	C16—C13—C12	109.1 (5)
C17—N2—H2	113 (2)	C14—C13—C12	111.2 (4)
C15—N2—H2	102 (2)	C16—C13—H13	109.2
C11—N2—H2	110 (2)	C14—C13—H13	109.2
N1—C1—C2	125.2 (4)	C12—C13—H13	109.2
N1—C1—H1A	117.4	C13—C14—C15	107.6 (4)
C2—C1—H1A	117.4	C13—C14—C18′	98.8 (7)
C3—C2—C1	119.6 (4)	C15—C14—C18′	132.1 (6)
C3—C2—H2A	120.2	C13—C14—C18	120.4 (5)
C1—C2—H2A	120.2	C15—C14—C18	103.5 (5)
C2—C3—C4	117.6 (4)	C13—C14—H14	108.2
C2—C3—C10	120.4 (4)	C15—C14—H14	108.2
C4—C3—C10	122.0 (3)	C18′—C14—H14	100.1
C9—C4—C5	117.2 (4)	C18—C14—H14	108.2
C9—C4—C3	118.2 (3)	N2—C15—C14	110.0 (4)
C5—C4—C3	124.5 (3)	N2—C15—H15A	109.7
C6—C5—C4	121.4 (4)	C14—C15—H15A	109.7
C6—C5—H5	119.3	N2—C15—H15B	109.7
C4—C5—H5	119.3	C14—C15—H15B	109.7
C5—C6—C7	120.2 (4)	H15A—C15—H15B	108.2
C5—C6—H6	119.9	C13—C16—C17	108.9 (4)
C7—C6—H6	119.9	C13—C16—H16A	109.9
C8—C7—C6	120.4 (4)	C17—C16—H16A	109.9
C8—C7—H7	119.8	C13—C16—H16B	109.9
C6—C7—H7	119.8	C17—C16—H16B	109.9
C7—C8—C9	120.6 (4)	H16A—C16—H16B	108.3
C7—C8—H8	119.7	N2—C17—C16	108.8 (4)
C9—C8—H8	119.7	N2—C17—H17A	109.9
N1—C9—C8	117.8 (4)	C16—C17—H17A	109.9
N1—C9—C4	122.1 (4)	N2—C17—H17B	109.9
C8—C9—C4	120.1 (4)	C16—C17—H17B	109.9
O1—C10—C3	110.4 (3)	H17A—C17—H17B	108.3
O1—C10—C11	110.5 (3)	C19—C18—C14	125.1 (11)
C3—C10—C11	108.5 (3)	C19—C18—H18	117.4
O1—C10—H10	109.1	C14—C18—H18	117.4
C3—C10—H10	109.1	C18—C19—H19A	120.0
C11—C10—H10	109.1	C18—C19—H19B	120.0
C12—C11—N2	108.3 (4)	H19A—C19—H19B	120.0
C12—C11—C10	115.2 (3)	C19′—C18′—C14	115.1 (13)
N2—C11—C10	112.6 (3)	C19′—C18′—H18′	122.4
C12—C11—H11	106.8	C14—C18′—H18′	122.4
N2—C11—H11	106.8	C18′—C19′—H19C	120.0
C10—C11—H11	106.8	C18′—C19′—H19D	120.0
C11—C12—C13	109.1 (4)	H19C—C19′—H19D	120.0
C11—C12—H12A	109.9		

C9—N1—C1—C2	−2.0 (7)	C3—C10—C11—C12	−79.1 (5)
N1—C1—C2—C3	0.1 (7)	O1—C10—C11—N2	−82.8 (4)
C1—C2—C3—C4	0.4 (6)	C3—C10—C11—N2	156.1 (3)
C1—C2—C3—C10	−177.1 (4)	N2—C11—C12—C13	−9.2 (5)
C2—C3—C4—C9	0.9 (5)	C10—C11—C12—C13	−136.2 (4)
C10—C3—C4—C9	178.5 (3)	C11—C12—C13—C16	65.9 (6)
C2—C3—C4—C5	179.0 (4)	C11—C12—C13—C14	−54.3 (6)
C10—C3—C4—C5	−3.4 (5)	C16—C13—C14—C15	−59.0 (5)
C9—C4—C5—C6	0.9 (6)	C12—C13—C14—C15	61.3 (5)
C3—C4—C5—C6	−177.2 (4)	C16—C13—C14—C18′	161.5 (6)
C4—C5—C6—C7	−0.3 (6)	C12—C13—C14—C18′	−78.3 (6)
C5—C6—C7—C8	−0.6 (7)	C16—C13—C14—C18	−177.2 (6)
C6—C7—C8—C9	1.0 (7)	C12—C13—C14—C18	−56.9 (7)
C1—N1—C9—C8	−177.1 (4)	C17—N2—C15—C14	64.0 (5)
C1—N1—C9—C4	3.5 (6)	C11—N2—C15—C14	−59.8 (5)
C7—C8—C9—N1	−179.7 (4)	C13—C14—C15—N2	−3.6 (5)
C7—C8—C9—C4	−0.3 (6)	C18′—C14—C15—N2	116.6 (9)
C5—C4—C9—N1	178.8 (4)	C18—C14—C15—N2	125.0 (5)
C3—C4—C9—N1	−3.0 (5)	C14—C13—C16—C17	63.4 (6)
C5—C4—C9—C8	−0.6 (5)	C12—C13—C16—C17	−58.2 (6)
C3—C4—C9—C8	177.6 (4)	C15—N2—C17—C16	−59.6 (5)
C2—C3—C10—O1	−25.4 (5)	C11—N2—C17—C16	61.4 (5)
C4—C3—C10—O1	157.1 (3)	C13—C16—C17—N2	−2.9 (6)
C2—C3—C10—C11	95.8 (4)	C13—C14—C18—C19	−33.2 (12)
C4—C3—C10—C11	−81.6 (4)	C15—C14—C18—C19	−153.4 (10)
C17—N2—C11—C12	−53.9 (5)	C18′—C14—C18—C19	13.9 (13)
C15—N2—C11—C12	67.0 (5)	C13—C14—C18′—C19′	150.7 (12)
C17—N2—C11—C10	74.6 (4)	C15—C14—C18′—C19′	27.2 (17)
C15—N2—C11—C10	−164.5 (3)	C18—C14—C18′—C19′	10.5 (12)
O1—C10—C11—C12	42.0 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.82 (2)	1.84 (2)	2.653 (5)	172 (3)
O2—H2*OB*···N1^{ii}	0.82 (2)	2.07 (2)	2.867 (6)	165 (3)
O2—H2*OA*···Cl1	0.82 (2)	2.31 (2)	3.135 (5)	174 (6)
N2—H2···Cl1	0.96 (4)	2.08 (4)	3.034 (6)	175 (3)
C5—H5···Cl1	0.93	2.77	3.692 (5)	172

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