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# 7-Chloro-4-[(*E*)-2-(2-methoxybenzylidene)hydrazin-1-yl]quinoline monohydrate

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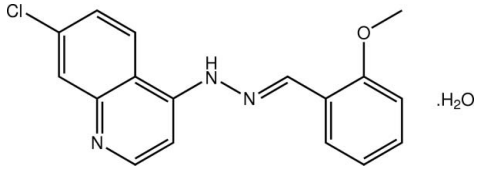
Key indicators: single-crystal X-ray study; $T$ = 120 K; mean $\sigma$(C–C) = 0.009 Å; $R$ factor = 0.093; $wR$ factor = 0.260; data-to-parameter ratio = 12.6.

In the title hydrate, $C_{17}H_{14}ClN_3O\cdot H_2O$, the dihedral angle between the quinoline fused-ring system and the benzene ring is 13.4 (2)° and the conformation about the C=N bond is *E*. In the crystal, $N_h$—H···$O_w$ and $O_w$—H···$N_q$ (h = hydrozone, w = water and q = quinoline) hydrogen bonds generate a two-dimenstional network in the *ac* plane. A weak C—H···O interaction helps to consolidate the packing.

## Related literature

For background to the pharmacological activity of quinoline derivatives, see: Warshakoon *et al.* (2006). For recent studies into quinoline-based anti-malarials, see: Andrade *et al.* (2007); de Souza *et al.* (2005). For related structures, see: Kaiser *et al.* (2009); de Souza *et al.* (2009, 2010). For the structure of the isomeric 2-methoxy structure, see: de Lima Ferreira *et al.* (2010).




## Experimental

### Crystal data

$C_{17}H_{14}ClN_3O\cdot H_2O$
$M_r$ = 329.78
Monoclinic, $P2_1/c$
$a$ = 3.9202 (2) Å
$b$ = 24.5084 (17) Å
$c$ = 16.1212 (11) Å
$\beta$ = 91.639 (4)°
$V$ = 1548.26 (17) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.26 mm$^{-1}$
$T$ = 120 K
0.62 × 0.03 × 0.02 mm

### Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
$T_{min}$ = 0.735, $T_{max}$ = 0.995
11507 measured reflections
2716 independent reflections
1769 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.096

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.093
$wR(F^2)$ = 0.260
$S$ = 1.04
2716 reflections
215 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.45 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2*N*···O1*W* | 0.88 | 2.08 | 2.928 (7) | 161 |
| O1*W*—H1*W*···N1$^{i}$ | 0.81 (9) | 2.30 (9) | 3.030 (8) | 150 (8) |
| O1*W*—H2*W*···N1$^{ii}$ | 0.82 (9) | 2.03 (9) | 2.820 (7) | 163 (8) |
| C5—H5···O1*W* | 0.95 | 2.43 | 3.358 (8) | 166 |

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

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5340).

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# supporting information

*Acta Cryst.* (2010). E**66**, o698–o699 [doi:10.1107/S1600536810006586]

## 7-Chloro-4-[(*E*)-2-(2-methoxybenzylidene)hydrazin-1-yl]quinoline monohydrate

**Marcus V. N. de Souza, R. Alan Howie, Edward R. T. Tiekink, James L. Wardell, Solange M. S. V. Wardell and Carlos R. Kaiser**

### S1. Comment

Quinoline derivatives are known to display pharmacological potential (Warshakoon *et al.*, 2006) and are being investigated for their anti-malarial activity (Andrade *et al.* 2007; de Souza *et al.*, 2005). Structural studies on quinoline derivatives augment the biological investigations (Kaiser *et al.*, 2009; de Souza *et al.*, 2009; de Souza *et al.*, 2010; de Lima Ferreira *et al.*, 2010) and as a part of these studies, the crystal structure of the title hydrate, (I), was investigated.

The most significant twist in the quinoline molecule of (I), Fig. 1, occurs around the C10–C11 bond as seen in the N3–C10–C11–C16 torsion angle of 6.9 (9) °. This accounts for the dihedral angle of 13.4 (2) ° formed between the quinoline fused-ring system and the benzene ring. The conformation about the C10═N3 bond [1.282 (8) Å] is *E*. The crystal packing is stabilised by a variety of hydrogen bonding interactions, Table 1. The water molecule accepts a hydrogen bond from the hydrazone-N2 atom and bridges two symmetry related molecules by forming donor interactions with quinoline-N1 atoms; the water-O atom also participates in a C–H···O contact, Table 1. The result of the hydrogen bonding is the formation of a 2-D supramolecular array in the *ac* plane, Fig. 2, and these stack along the *b* axis, Fig. 3.

### S2. Experimental

A solution of 7-chloro-4-quinolinylhydrazine(0.2 g, 1.03 mmol) and 2-methoxybenzaldehyde (1.2 mmol) in EtOH (5 ml) was maintained at room temperature overnight and rotary evaporated. The solid residue, was washed with cold $Et_2O$ (3 x 10 ml) and recrystallised from EtOH; m.pt. 459-461 K, yield 82%. The sample for the X-ray study was slowly grown from moist EtOH and was found to be the monohydrate. MS/ESI: [M—H]: 310.8. IR *v*max (cm-1; KBr disc): 3190 (N—H), 1578 (C=N).

### S3. Refinement

The N- and C-bound H atoms were geometrically placed (N–H = 0.88 Å and C–H = 0.95–0.98 Å) and refined as riding with $U_{iso}$(H) = 1.2–1.5$U_{eq}$(C,*N*). The water-bound H atoms were located from a difference map and refined with $U_{iso}$(H) = 1.5$U_{eq}$(O).

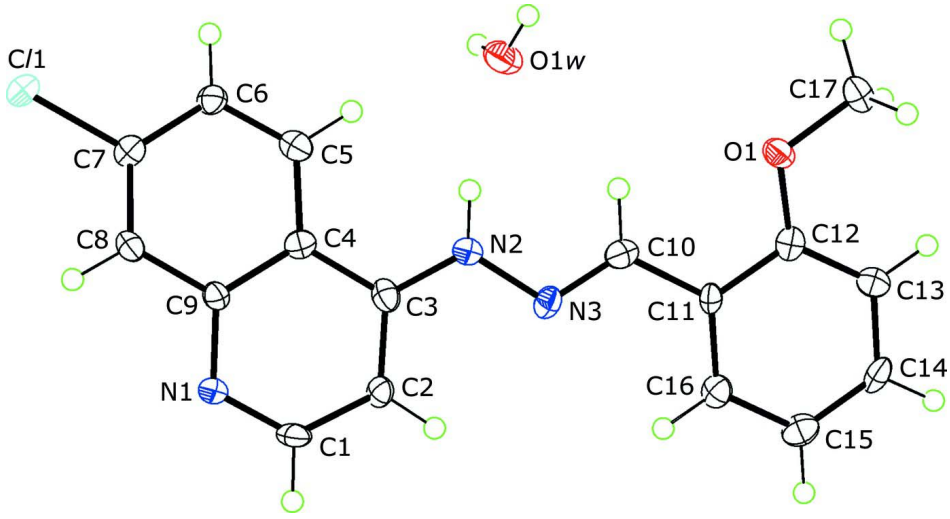


**Figure 1**

Molecular structures of the asymmetric unit in (I) showing displacement ellipsoids at the 50% probability level.

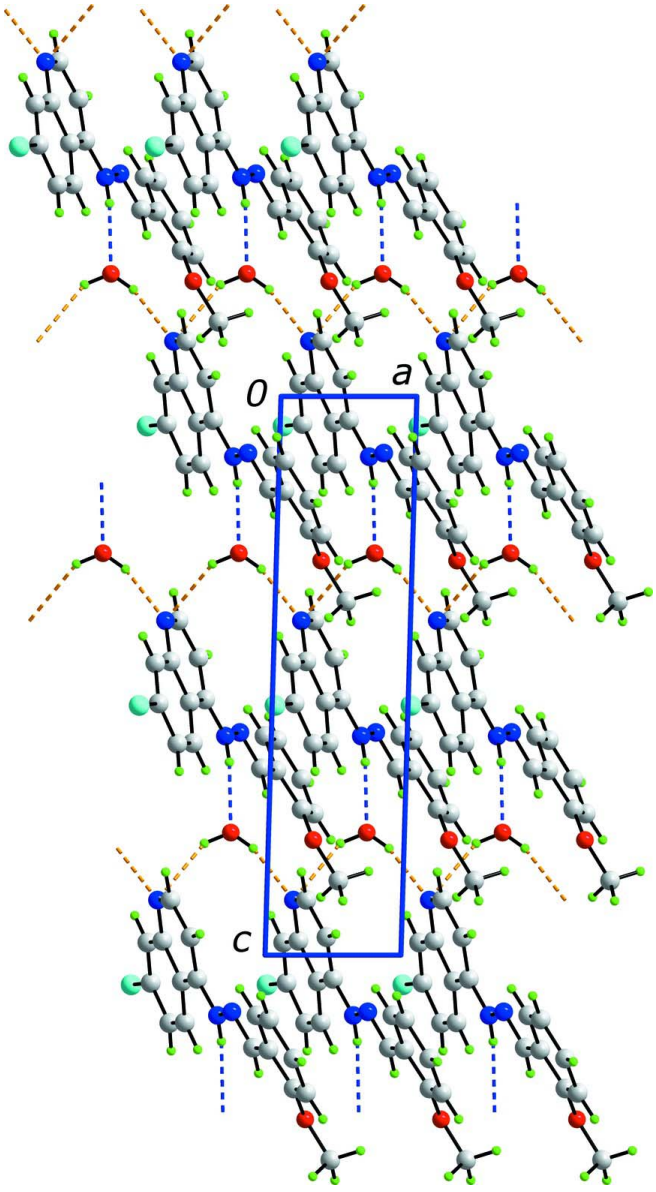


**Figure 2**

View of the 2-D supramolecular array in the *ac* plane of (I) showing the O–H···N and N–H···O hydrogen bonding as orange and blue dashed lines, respectively. Colour code: Cl, cyan; O, red; N, blue; C, grey; and H, green.

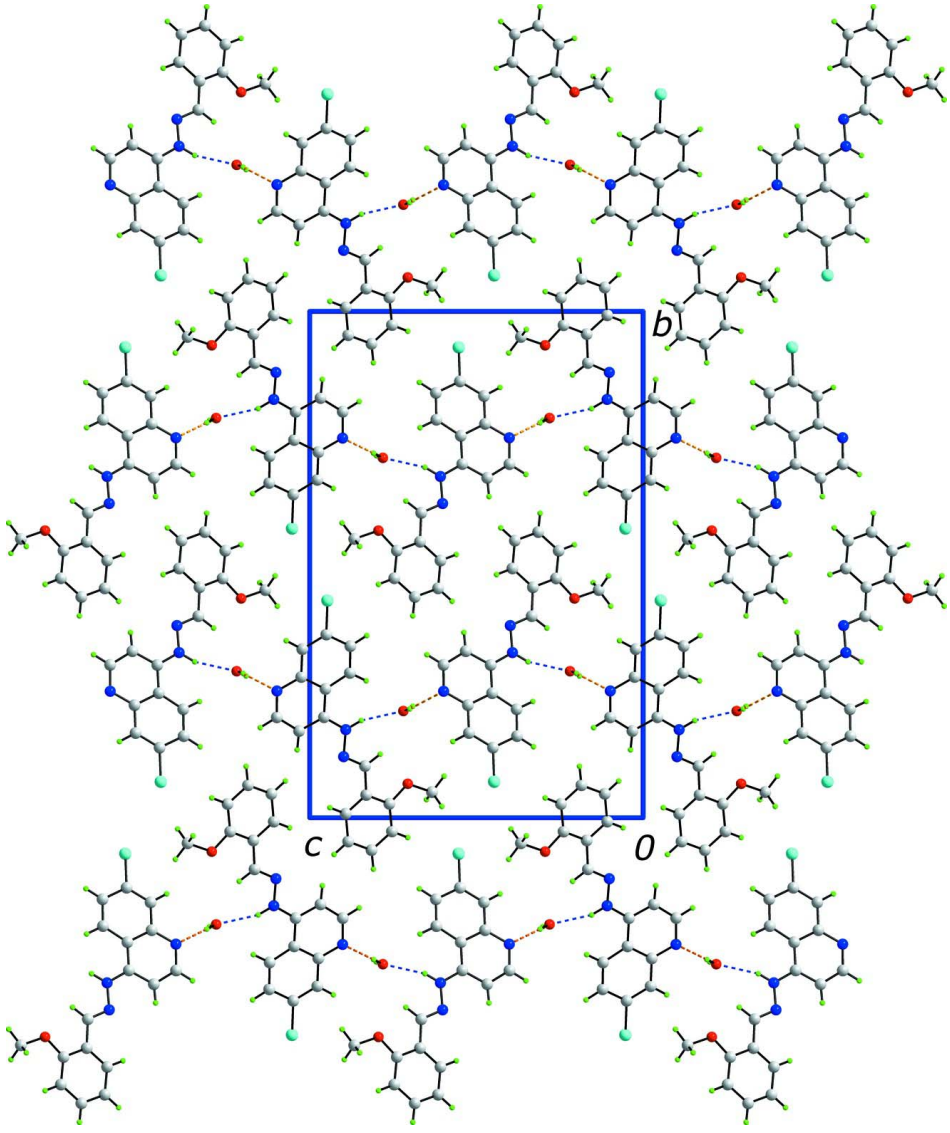


**Figure 3**

A view of the stacking of layers in (I). The O–H···N and N–H···O hydrogen bonding as orange and blue dashed lines, respectively. Colour code: Cl, cyan; O, red; N, blue; C, grey; and H, green.

### 7-Chloro-4-[(*E*)-2-(2-methoxybenzylidene)hydrazin-1-yl]quinoline monohydrate

*Crystal data*

$C_{17}H_{14}ClN_3O·H_2O$
$M_r$ = 329.78
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 3.9202 (2) Å
$b$ = 24.5084 (17) Å
$c$ = 16.1212 (11) Å
$\beta$ = 91.639 (4)°
$V$ = 1548.26 (17) Å$^3$
$Z$ = 4
$F(000)$ = 688
$D_x$ = 1.415 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9260 reflections
$\theta$ = 2.9–27.5°
$\mu$ = 0.26 mm$^{-1}$
$T$ = 120 K
Needle, colourless
0.62 × 0.03 × 0.02 mm

*Data collection*

Nonius KappaCCD diffractometer
Radiation source: Enraf Nonius FR591 rotating anode
10 cm confocal mirrors monochromator
Detector resolution: 9.091 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
$T_{min}$ = 0.735, $T_{max}$ = 0.995
11507 measured reflections
2716 independent reflections
1769 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.096
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 3.0°
$h$ = −4→4
$k$ = −29→29
$l$ = −19→19

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.093
$wR(F^2)$ = 0.260
$S$ = 1.04
2716 reflections
215 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
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 10.4045P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.40 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.45 e Å$^{-3}$

*Special details*

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.0208 (4) | 0.57108 (6) | 0.05313 (10) | 0.0256 (5) |
| O1 | 1.3298 (11) | 0.93299 (18) | 0.2940 (3) | 0.0232 (10) |
| N1 | 0.1966 (13) | 0.7497 (2) | −0.0985 (3) | 0.0201 (12) |
| N2 | 0.6619 (13) | 0.8261 (2) | 0.1080 (3) | 0.0214 (12) |
| H2N | 0.6968 | 0.8080 | 0.1547 | 0.026* |
| N3 | 0.7680 (12) | 0.8795 (2) | 0.1015 (3) | 0.0195 (12) |
| C1 | 0.2920 (16) | 0.8018 (3) | −0.0989 (4) | 0.0232 (15) |
| H1 | 0.2504 | 0.8220 | −0.1484 | 0.028* |
| C2 | 0.4479 (15) | 0.8288 (2) | −0.0322 (4) | 0.0183 (13) |
| H2 | 0.5157 | 0.8658 | −0.0377 | 0.022* |
| C3 | 0.5046 (15) | 0.8016 (2) | 0.0426 (4) | 0.0203 (14) |
| C4 | 0.3926 (15) | 0.7459 (2) | 0.0470 (4) | 0.0176 (13) |
| C5 | 0.4234 (15) | 0.7141 (3) | 0.1204 (4) | 0.0223 (14) |
| H5 | 0.5240 | 0.7296 | 0.1692 | 0.027* |
| C6 | 0.3094 (16) | 0.6611 (2) | 0.1217 (4) | 0.0206 (14) |

| | | | | |
|---|---|---|---|---|
| H6 | 0.3293 | 0.6402 | 0.1712 | 0.025* |
| C7 | 0.1640 (15) | 0.6384 (2) | 0.0496 (4) | 0.0176 (13) |
| C8 | 0.1307 (16) | 0.6672 (3) | −0.0225 (4) | 0.0213 (14) |
| H8 | 0.0329 | 0.6504 | −0.0707 | 0.026* |
| C9 | 0.2419 (15) | 0.7222 (2) | −0.0257 (4) | 0.0180 (13) |
| C10 | 0.9303 (15) | 0.8980 (3) | 0.1657 (4) | 0.0211 (14) |
| H10 | 0.9774 | 0.8745 | 0.2115 | 0.025* |
| C11 | 1.0442 (14) | 0.9551 (2) | 0.1693 (4) | 0.0164 (13) |
| C12 | 1.2380 (14) | 0.9726 (2) | 0.2387 (4) | 0.0181 (14) |
| C13 | 1.3295 (16) | 1.0271 (3) | 0.2466 (4) | 0.0237 (15) |
| H13 | 1.4596 | 1.0391 | 0.2938 | 0.028* |
| C14 | 1.2299 (16) | 1.0641 (3) | 0.1851 (4) | 0.0222 (14) |
| H14 | 1.2908 | 1.1014 | 0.1909 | 0.027* |
| C15 | 1.0422 (16) | 1.0471 (3) | 0.1152 (4) | 0.0249 (15) |
| H15 | 0.9778 | 1.0725 | 0.0731 | 0.030* |
| C16 | 0.9495 (15) | 0.9922 (2) | 0.1078 (4) | 0.0212 (14) |
| H16 | 0.8211 | 0.9802 | 0.0604 | 0.025* |
| C17 | 1.5235 (16) | 0.9495 (3) | 0.3666 (4) | 0.0242 (15) |
| H17A | 1.7439 | 0.9642 | 0.3501 | 0.036* |
| H17B | 1.5613 | 0.9179 | 0.4030 | 0.036* |
| H17C | 1.3976 | 0.9777 | 0.3962 | 0.036* |
| O1W | 0.7223 (14) | 0.7893 (2) | 0.2807 (3) | 0.0304 (12) |
| H1W | 0.53 (2) | 0.785 (3) | 0.300 (5) | 0.046* |
| H2W | 0.89 (2) | 0.780 (3) | 0.309 (5) | 0.046* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0319 (9) | 0.0186 (8) | 0.0263 (9) | −0.0044 (7) | −0.0002 (7) | 0.0044 (7) |
| O1 | 0.028 (2) | 0.023 (2) | 0.018 (2) | 0.0005 (19) | −0.0047 (18) | −0.001 (2) |
| N1 | 0.027 (3) | 0.019 (3) | 0.015 (3) | −0.002 (2) | −0.003 (2) | 0.002 (2) |
| N2 | 0.027 (3) | 0.020 (3) | 0.017 (3) | −0.002 (2) | −0.003 (2) | 0.002 (2) |
| N3 | 0.022 (3) | 0.015 (3) | 0.022 (3) | −0.002 (2) | 0.004 (2) | −0.002 (2) |
| C1 | 0.026 (3) | 0.026 (4) | 0.017 (4) | 0.000 (3) | −0.005 (3) | 0.008 (3) |
| C2 | 0.023 (3) | 0.015 (3) | 0.017 (3) | −0.001 (2) | 0.004 (3) | −0.004 (3) |
| C3 | 0.018 (3) | 0.020 (3) | 0.022 (4) | 0.002 (3) | −0.003 (3) | −0.004 (3) |
| C4 | 0.016 (3) | 0.020 (3) | 0.017 (3) | 0.001 (2) | 0.005 (2) | 0.001 (3) |
| C5 | 0.023 (3) | 0.025 (3) | 0.019 (4) | 0.002 (3) | −0.002 (3) | 0.000 (3) |
| C6 | 0.029 (3) | 0.015 (3) | 0.018 (4) | 0.002 (3) | 0.001 (3) | −0.001 (3) |
| C7 | 0.019 (3) | 0.017 (3) | 0.018 (3) | 0.002 (2) | 0.008 (2) | −0.002 (3) |
| C8 | 0.023 (3) | 0.024 (3) | 0.017 (4) | −0.004 (3) | −0.004 (3) | −0.001 (3) |
| C9 | 0.023 (3) | 0.016 (3) | 0.015 (3) | 0.000 (2) | −0.002 (3) | −0.002 (3) |
| C10 | 0.019 (3) | 0.021 (3) | 0.023 (4) | 0.001 (3) | 0.002 (3) | 0.005 (3) |
| C11 | 0.014 (3) | 0.016 (3) | 0.018 (3) | −0.004 (2) | 0.001 (2) | −0.003 (3) |
| C12 | 0.014 (3) | 0.019 (3) | 0.022 (4) | 0.001 (2) | 0.006 (2) | −0.004 (3) |
| C13 | 0.027 (3) | 0.026 (3) | 0.018 (4) | −0.001 (3) | 0.000 (3) | 0.001 (3) |
| C14 | 0.026 (3) | 0.015 (3) | 0.026 (4) | −0.007 (3) | 0.011 (3) | −0.003 (3) |
| C15 | 0.027 (3) | 0.019 (3) | 0.029 (4) | 0.006 (3) | 0.003 (3) | 0.003 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C16 | 0.024 (3) | 0.018 (3) | 0.021 (4) | 0.001 (3) | 0.004 (3) | −0.004 (3) |
| C17 | 0.022 (3) | 0.030 (4) | 0.021 (4) | −0.002 (3) | −0.002 (3) | −0.005 (3) |
| O1W | 0.028 (3) | 0.039 (3) | 0.024 (3) | 0.000 (2) | −0.005 (2) | 0.004 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C7 | 1.744 (6) | C7—C8 | 1.362 (9) |
| O1—C12 | 1.360 (7) | C8—C9 | 1.419 (9) |
| O1—C17 | 1.434 (7) | C8—H8 | 0.9500 |
| N1—C1 | 1.330 (8) | C10—C11 | 1.471 (8) |
| N1—C9 | 1.361 (8) | C10—H10 | 0.9500 |
| N2—C3 | 1.348 (8) | C11—C16 | 1.388 (9) |
| N2—N3 | 1.379 (7) | C11—C12 | 1.401 (8) |
| N2—H2N | 0.8800 | C12—C13 | 1.388 (9) |
| N3—C10 | 1.282 (8) | C13—C14 | 1.391 (9) |
| C1—C2 | 1.389 (9) | C13—H13 | 0.9500 |
| C1—H1 | 0.9500 | C14—C15 | 1.391 (9) |
| C2—C3 | 1.391 (9) | C14—H14 | 0.9500 |
| C2—H2 | 0.9500 | C15—C16 | 1.399 (9) |
| C3—C4 | 1.436 (8) | C15—H15 | 0.9500 |
| C4—C9 | 1.420 (8) | C16—H16 | 0.9500 |
| C4—C5 | 1.420 (9) | C17—H17A | 0.9800 |
| C5—C6 | 1.372 (9) | C17—H17B | 0.9800 |
| C5—H5 | 0.9500 | C17—H17C | 0.9800 |
| C6—C7 | 1.396 (9) | O1W—H1W | 0.81 (9) |
| C6—H6 | 0.9500 | O1W—H2W | 0.82 (9) |
| | | | |
| C12—O1—C17 | 117.2 (5) | N1—C9—C4 | 123.4 (5) |
| C1—N1—C9 | 116.6 (5) | C8—C9—C4 | 118.6 (6) |
| C3—N2—N3 | 119.7 (5) | N3—C10—C11 | 120.7 (6) |
| C3—N2—H2N | 120.2 | N3—C10—H10 | 119.6 |
| N3—N2—H2N | 120.2 | C11—C10—H10 | 119.6 |
| C10—N3—N2 | 114.6 (5) | C16—C11—C12 | 119.9 (6) |
| N1—C1—C2 | 124.9 (6) | C16—C11—C10 | 121.4 (5) |
| N1—C1—H1 | 117.6 | C12—C11—C10 | 118.7 (5) |
| C2—C1—H1 | 117.6 | O1—C12—C13 | 124.3 (6) |
| C1—C2—C3 | 119.9 (6) | O1—C12—C11 | 115.7 (5) |
| C1—C2—H2 | 120.1 | C13—C12—C11 | 120.0 (6) |
| C3—C2—H2 | 120.1 | C12—C13—C14 | 119.6 (6) |
| N2—C3—C2 | 121.6 (6) | C12—C13—H13 | 120.2 |
| N2—C3—C4 | 121.2 (6) | C14—C13—H13 | 120.2 |
| C2—C3—C4 | 117.2 (5) | C15—C14—C13 | 120.9 (6) |
| C9—C4—C5 | 119.1 (5) | C15—C14—H14 | 119.5 |
| C9—C4—C3 | 117.9 (5) | C13—C14—H14 | 119.5 |
| C5—C4—C3 | 122.9 (6) | C14—C15—C16 | 119.1 (6) |
| C6—C5—C4 | 120.8 (6) | C14—C15—H15 | 120.4 |
| C6—C5—H5 | 119.6 | C16—C15—H15 | 120.4 |
| C4—C5—H5 | 119.6 | C11—C16—C15 | 120.3 (6) |

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| C5—C6—C7 | 119.3 (6) | C11—C16—H16 | 119.8 |
| C5—C6—H6 | 120.3 | C15—C16—H16 | 119.8 |
| C7—C6—H6 | 120.3 | O1—C17—H17A | 109.5 |
| C8—C7—C6 | 122.0 (6) | O1—C17—H17B | 109.5 |
| C8—C7—Cl1 | 119.7 (5) | H17A—C17—H17B | 109.5 |
| C6—C7—Cl1 | 118.3 (5) | O1—C17—H17C | 109.5 |
| C7—C8—C9 | 120.1 (6) | H17A—C17—H17C | 109.5 |
| C7—C8—H8 | 119.9 | H17B—C17—H17C | 109.5 |
| C9—C8—H8 | 119.9 | H1W—O1W—H2W | 118 (9) |
| N1—C9—C8 | 118.0 (5) | | |

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| C3—N2—N3—C10 | −176.6 (6) | C7—C8—C9—C4 | 1.1 (9) |
| C9—N1—C1—C2 | 3.4 (9) | C5—C4—C9—N1 | 178.9 (6) |
| N1—C1—C2—C3 | −2.1 (10) | C3—C4—C9—N1 | −0.4 (9) |
| N3—N2—C3—C2 | 0.5 (9) | C5—C4—C9—C8 | −0.8 (9) |
| N3—N2—C3—C4 | 179.6 (5) | C3—C4—C9—C8 | 179.9 (6) |
| C1—C2—C3—N2 | 178.5 (6) | N2—N3—C10—C11 | −177.0 (5) |
| C1—C2—C3—C4 | −0.6 (9) | N3—C10—C11—C16 | 6.9 (9) |
| N2—C3—C4—C9 | −177.4 (6) | N3—C10—C11—C12 | −176.3 (6) |
| C2—C3—C4—C9 | 1.7 (8) | C17—O1—C12—C13 | 2.3 (9) |
| N2—C3—C4—C5 | 3.3 (9) | C17—O1—C12—C11 | −178.9 (5) |
| C2—C3—C4—C5 | −177.6 (6) | C16—C11—C12—O1 | −177.5 (5) |
| C9—C4—C5—C6 | 0.0 (9) | C10—C11—C12—O1 | 5.6 (8) |
| C3—C4—C5—C6 | 179.3 (6) | C16—C11—C12—C13 | 1.3 (9) |
| C4—C5—C6—C7 | 0.5 (9) | C10—C11—C12—C13 | −175.6 (6) |
| C5—C6—C7—C8 | −0.1 (9) | O1—C12—C13—C14 | 178.2 (6) |
| C5—C6—C7—Cl1 | −179.9 (5) | C11—C12—C13—C14 | −0.5 (9) |
| C6—C7—C8—C9 | −0.7 (10) | C12—C13—C14—C15 | −0.6 (10) |
| Cl1—C7—C8—C9 | 179.1 (5) | C13—C14—C15—C16 | 0.9 (10) |
| C1—N1—C9—C8 | 177.7 (6) | C12—C11—C16—C15 | −1.0 (9) |
| C1—N1—C9—C4 | −2.0 (9) | C10—C11—C16—C15 | 175.8 (6) |
| C7—C8—C9—N1 | −178.6 (6) | C14—C15—C16—C11 | −0.1 (10) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*N*···O1*W* | 0.88 | 2.08 | 2.928 (7) | 161 |
| O1*W*—H1*W*···N1$^{i}$ | 0.81 (9) | 2.30 (9) | 3.030 (8) | 150 (8) |
| O1*W*—H2*W*···N1$^{ii}$ | 0.82 (9) | 2.03 (9) | 2.820 (7) | 163 (8) |
| C5—H5···O1*W* | 0.95 | 2.43 | 3.358 (8) | 166 |

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