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6-Chloroquinolin-2(1*H*)-one

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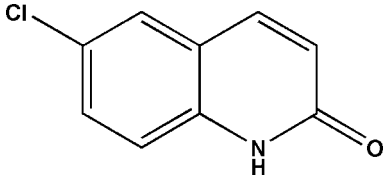
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.030; wR factor = 0.088; data-to-parameter ratio = 12.0.

In the title compound, C_9H_6ClNO, the Cl atom deviates by 0.142 (1) Å from the quinoline ring mean plane (r.m.s. deviation = 0.013 Å). In the crystal, N—H···O hydrogen bonds link the molecules into [010] $C(4)$ chains. Aromatic π–π stacking interactions [shortest centroid···centroid distance = 3.685 (3) Å] are also observed.

Related literature

For background to quinoline derivatives as pharmaceuticals, see: Luo *et al.* (2011).



Experimental

Crystal data

C_9H_6ClNO
M_r = 179.60
Orthorhombic, *Pccn*
a = 24.951 (19) Å
b = 7.733 (6) Å
c = 7.988 (6) Å
V = 1541 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.44 mm^{-1}
T = 296 K
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku SCXmini CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.917, T_{max} = 0.917
9911 measured reflections
1353 independent reflections
1161 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.088
S = 1.06
1353 reflections
113 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.887 (19)	1.98 (2)	2.859 (2)	168.7 (17)

Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{5}{2}$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *SHELXL97*.

We thank Southeast University for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6549).

References

Brandenburg, K. & Putz, H. (2005). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Luo, Y.-H., Qian, X.-M., Gao, G., Li, J.-F. & Mao, S.-L. (2011). *Acta Cryst.* E**67**, m172.
Rigaku. (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
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supporting information

Acta Cryst. (2012). E**68**, o188 [doi:10.1107/S1600536811053359]

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S1. Experimental

The title compound was purchased from ChemFuture PharmaTech, Ltd (Nanjing, Jiangsu). Pink prisms were obtained by slow evaporation of a methanol solution.

S2. Refinement

All H atoms attached to C atoms and O atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (CH) and N—H = 0.86 Å with U_{iso}(H) = 1.2U_{eq}.

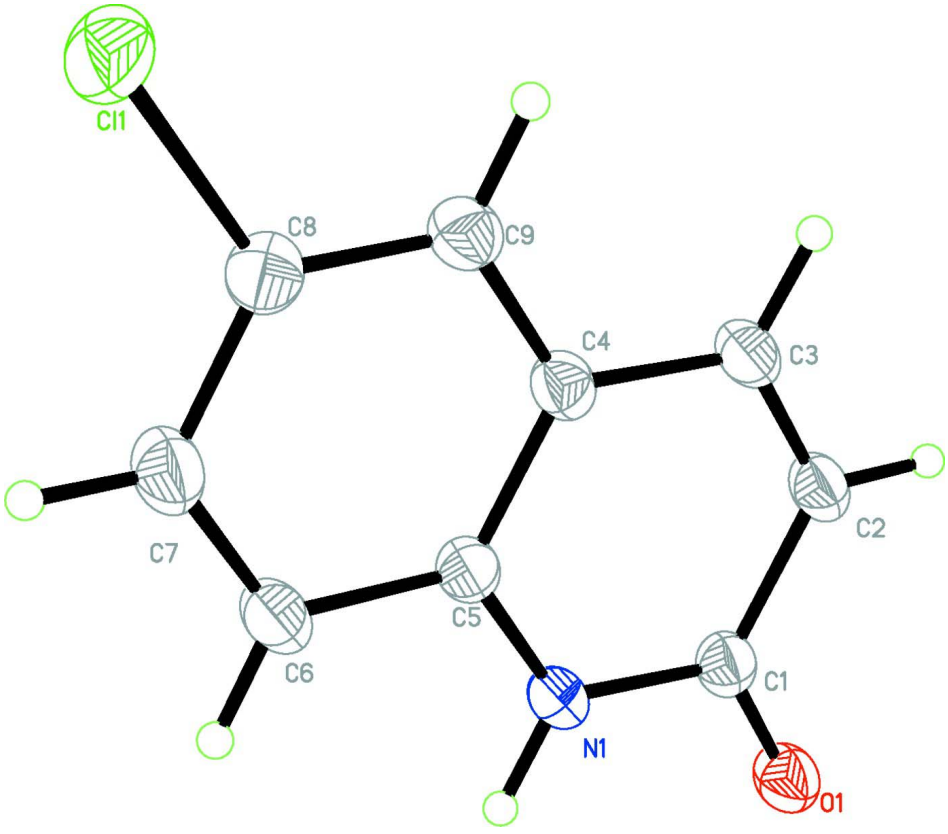

Figure 1

The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level.

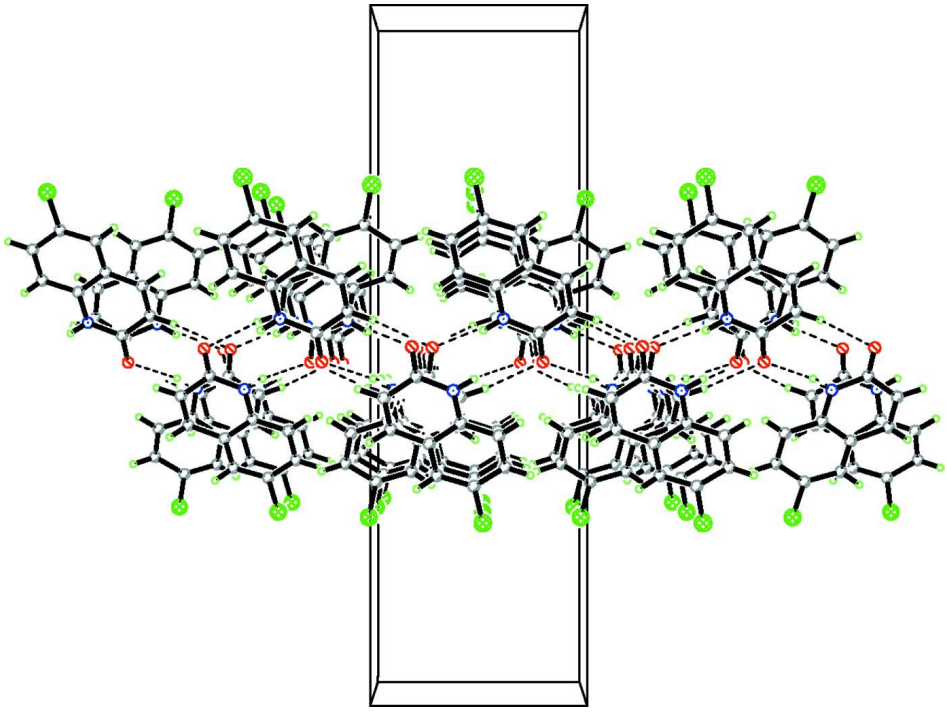

Figure 2

A packing view down the *a* axis showing hydrogen bonds as dashed lines.

6-Chloroquinolin-2(1*H*)-one

Crystal data

C_9H_6ClNO
$M_r = 179.60$
Orthorhombic, *Pccn*
Hall symbol: -P 2ab 2ac
$a = 24.951$ (19) Å
$b = 7.733$ (6) Å
$c = 7.988$ (6) Å
$V = 1541$ (2) Å^3
$Z = 8$
$F(000) = 736$
$D_x = 1.548$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1357 reflections
$\theta = 1.6$–25.0°
$\mu = 0.44$ mm^{-1}
$T = 296$ K
Prism, pink
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku SCXmini CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD_Profile_fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.917$, $T_{max} = 0.917$
9911 measured reflections
1353 independent reflections
1161 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.6°$
$h = -29 \rightarrow 29$
$k = -9 \rightarrow 9$
$l = -8 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.088$
$S = 1.06$
1353 reflections
113 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
$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 0.4479P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.73621 (2)	1.01875 (7)	0.69204 (7)	0.0614 (2)
N1	0.54956 (5)	0.88864 (17)	1.12378 (17)	0.0369 (3)
O1	0.49027 (5)	0.70991 (15)	1.25021 (16)	0.0472 (3)
C1	0.53024 (6)	0.7277 (2)	1.1598 (2)	0.0369 (4)
C5	0.59440 (6)	0.9205 (2)	1.02710 (19)	0.0349 (4)
C2	0.55943 (7)	0.5842 (2)	1.0882 (2)	0.0398 (4)
H2	0.5477	0.4719	1.1079	0.048*
C4	0.62280 (6)	0.7806 (2)	0.95924 (19)	0.0357 (4)
C9	0.66766 (7)	0.8129 (2)	0.8591 (2)	0.0409 (4)
H9	0.6871	0.7214	0.8140	0.049*
C7	0.65567 (7)	1.1184 (2)	0.8970 (2)	0.0487 (5)
H7	0.6671	1.2308	0.8759	0.058*
C8	0.68283 (7)	0.9794 (2)	0.8280 (2)	0.0426 (4)
C3	0.60308 (7)	0.6101 (2)	0.9940 (2)	0.0404 (4)
H3	0.6211	0.5151	0.9500	0.049*
C6	0.61155 (7)	1.0894 (2)	0.9970 (2)	0.0453 (4)
H6	0.5933	1.1821	1.0443	0.054*
H1	0.5337 (8)	0.980 (2)	1.170 (2)	0.044 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0512 (3)	0.0595 (3)	0.0736 (4)	0.0024 (2)	0.0190 (2)	0.0143 (2)
N1	0.0428 (8)	0.0276 (7)	0.0404 (8)	0.0031 (6)	0.0035 (6)	−0.0012 (6)

O1	0.0483 (7)	0.0359 (7)	0.0574 (8)	−0.0015 (5)	0.0130 (7)	0.0020 (6)
C1	0.0406 (9)	0.0330 (9)	0.0371 (9)	−0.0011 (7)	−0.0033 (7)	0.0012 (7)
C5	0.0383 (8)	0.0322 (8)	0.0342 (8)	0.0014 (7)	−0.0020 (7)	−0.0001 (7)
C2	0.0470 (10)	0.0269 (8)	0.0454 (9)	0.0006 (7)	−0.0023 (8)	−0.0004 (7)
C4	0.0394 (8)	0.0317 (9)	0.0359 (9)	0.0045 (6)	−0.0050 (7)	0.0004 (7)
C9	0.0399 (9)	0.0400 (9)	0.0428 (10)	0.0078 (7)	−0.0007 (8)	−0.0004 (8)
C7	0.0499 (10)	0.0343 (9)	0.0618 (11)	−0.0035 (8)	0.0056 (9)	0.0036 (9)
C8	0.0368 (9)	0.0450 (10)	0.0461 (10)	0.0016 (7)	0.0009 (7)	0.0049 (8)
C3	0.0475 (10)	0.0298 (8)	0.0440 (10)	0.0078 (7)	−0.0022 (8)	−0.0025 (7)
C6	0.0506 (10)	0.0294 (9)	0.0558 (11)	0.0031 (7)	0.0071 (9)	−0.0024 (8)

Geometric parameters (Å, º)

Cl1—C8	1.745 (2)	C4—C9	1.398 (2)
N1—C1	1.365 (2)	C4—C3	1.434 (2)
N1—C5	1.382 (2)	C9—C8	1.365 (3)
N1—H1	0.887 (19)	C9—H9	0.9300
O1—C1	1.239 (2)	C7—C6	1.379 (3)
C1—C2	1.445 (2)	C7—C8	1.385 (3)
C5—C6	1.395 (2)	C7—H7	0.9300
C5—C4	1.402 (2)	C3—H3	0.9300
C2—C3	1.339 (2)	C6—H6	0.9300
C2—H2	0.9300		
C1—N1—C5	124.49 (14)	C8—C9—C4	119.66 (15)
C1—N1—H1	118.7 (12)	C8—C9—H9	120.2
C5—N1—H1	116.7 (12)	C4—C9—H9	120.2
O1—C1—N1	120.54 (15)	C6—C7—C8	119.65 (16)
O1—C1—C2	123.46 (15)	C6—C7—H7	120.2
N1—C1—C2	116.00 (15)	C8—C7—H7	120.2
N1—C5—C6	120.77 (14)	C9—C8—C7	121.59 (17)
N1—C5—C4	119.20 (14)	C9—C8—Cl1	119.31 (14)
C6—C5—C4	120.03 (16)	C7—C8—Cl1	119.06 (14)
C3—C2—C1	121.17 (15)	C2—C3—C4	121.70 (15)
C3—C2—H2	119.4	C2—C3—H3	119.2
C1—C2—H2	119.4	C4—C3—H3	119.2
C9—C4—C5	119.21 (15)	C7—C6—C5	119.83 (16)
C9—C4—C3	123.33 (15)	C7—C6—H6	120.1
C5—C4—C3	117.44 (15)	C5—C6—H6	120.1

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.887 (19)	1.98 (2)	2.859 (2)	168.7 (17)

Symmetry code: (i) −*x*+1, *y*+1/2, −*z*+5/2.