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2-Chloroquinazolin-4(3*H*)-one

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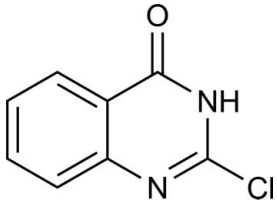
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.095; data-to-parameter ratio = 15.5.

In the title compound, $C_8H_5ClN_2O$, the quinazoline system is approximately planar with a maximum deviation from the least-squares plane of 0.034 (2) Å. In the crystal, classical N—H···O and weak non-classical C—H···N hydrogen bonds link the molecules.

Related literature

For the synthesis, see: Feng *et al.* (2007). For applications of related compounds, see: Labuda *et al.* (2009).



Experimental

Crystal data

$C_8H_5ClN_2O$
M_r = 180.59
Monoclinic, $C2/c$
a = 22.4315 (16) Å
b = 3.7666 (6) Å
c = 18.0640 (13) Å
β = 104.682 (7)°
V = 1476.4 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.46 mm^{-1}
T = 113 K
0.20 × 0.18 × 0.14 mm

Data collection

Rigaku Saturn CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.914, T_{max} = 0.939
6933 measured reflections
1749 independent reflections
1430 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.095
S = 1.03
1749 reflections
113 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.45 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
N2—H1···O1^{i}	0.92 (2)	1.88 (2)	2.7840 (17)	166.5 (19)
C3—H3···N1^{ii}	0.95	2.53	3.449 (2)	163

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

Data collection: *CrystalClear* (Rigaku/MSC, 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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2006).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2353).

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supporting information

Acta Cryst. (2012). E**68**, o1958 [doi:10.1107/S1600536812022891]

2-Chloroquinazolin-4(3*H*)-one

Dong-Lei Cao, Fan-Yong Yan, Meng Wang, Chu-Ying Li and Li Chen

S1. Comment

Quinazolin-4(3*H*)-ones and related quinazolines are classes of fused heterocycles that are of consider able interest because of the diverse range of their biological properties, for example, anticancer, anti-inflammatory, diuretic, anticonvulsant and antihypertensive activities (Labuda *et al.*, 2009). The title compound (Fig. 1) consists of a quinazoline ring with an Cl atom at C4. The quinazoline heterobicycle is nearly planar, with a maximum deviation from the least-squares plane of 0.034 (2)Å. All bond lengths and angles are normal, atoms O1 and Cl lie in the 2-chloroquinazolin ring (C1-C8/N1/N2) plane. In addition, two intermolecular hydrogen bonding (classical N–H···O and non-classical C–H···N) (Table 1, Fig. 2), are effective in stabilizing the crystal structure.

S2. Experimental

The title compound was prepared by following a reported procedure (Feng *et al.*, 2007). A suspension of 2,4-dichloro-quinazolines (2.0 g, 1 mmol) was stirred in 2% aqueous sodium hydroxide solution (3 ml) for 3 h. Reaction mixture was diluted with water (6 ml) and filtered to remove unreacted 2,4-dichloroquinazoline. Filtrate was neutralized with dilute acetic acid, precipitate thus obtained was filtered and washed with water. The product was recrystallized from acetone / ethyl acetate (5:1) over 5 d at ambient temperature, gave colourless single crystals of 2-chloroquinazolin-4(3*H*)-one, suitable for X-ray analysis.

S3. Refinement

The H atoms based on C atoms were positioned geometrically at distances C–H = 0.93Å and constrained to ride on their parent atoms with U_{iso}(H) = 1.2U_{eq}(C). The amino H atom was found from different Fourier map and refined isotropically.

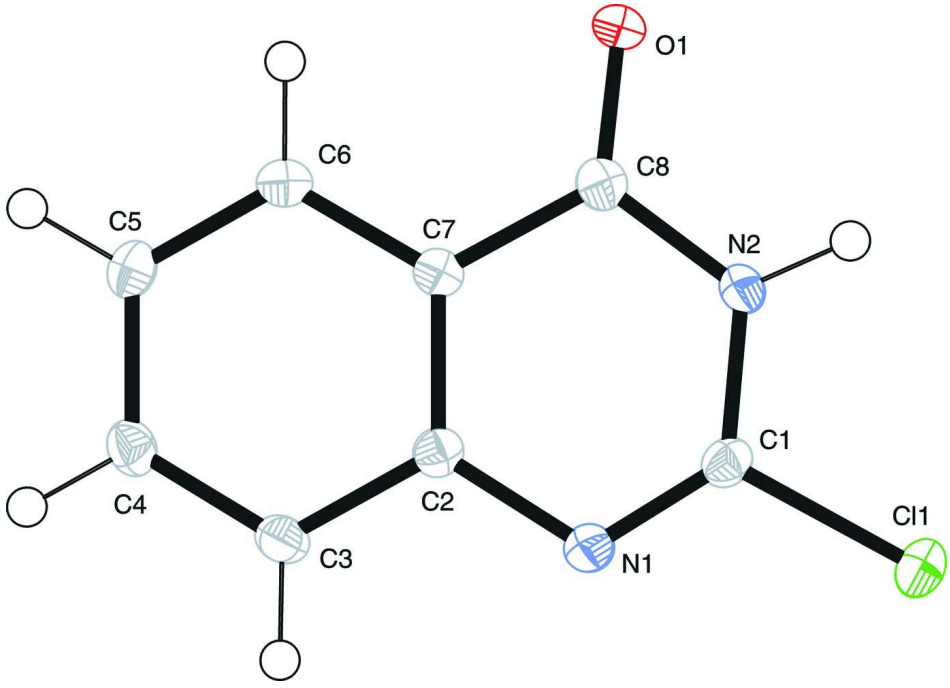

Figure 1

The molecular structure of title compound with the atom numbering scheme. Displacement ellipsoids are drawn with 50% probability level. H atoms are presented as spheres of arbitrary radius.

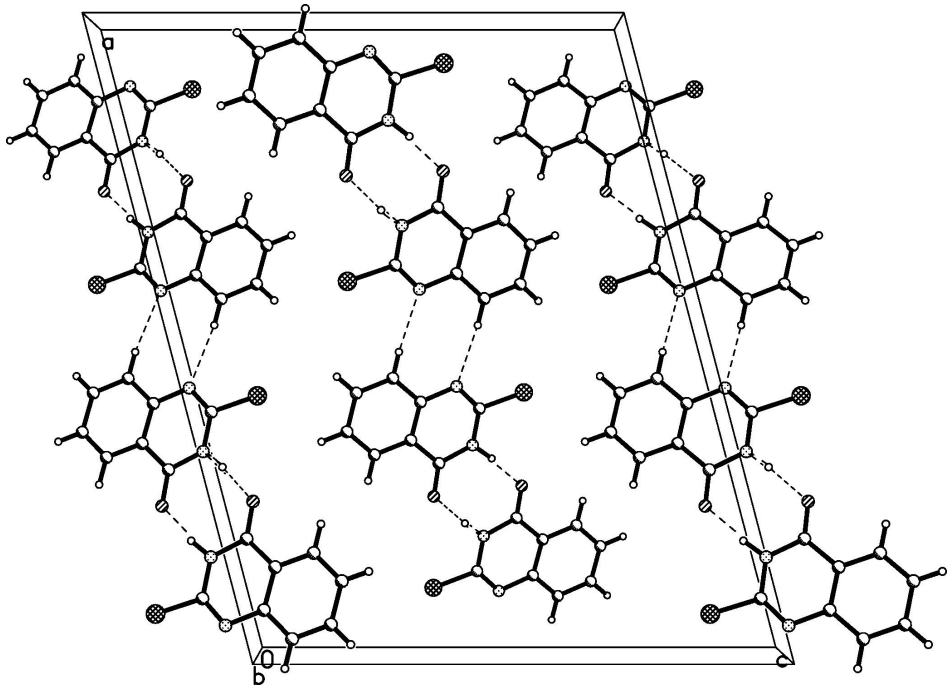

Figure 2

A packing diagram for title compound. Dashed lines indicate hydrogen bonds.

2-Chloroquinazolin-4(3*H*)-one

Crystal data

$C_8H_5ClN_2O$
$M_r = 180.59$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 22.4315$ (16) Å
$b = 3.7666$ (6) Å
$c = 18.0640$ (13) Å
$\beta = 104.682$ (7)°
$V = 1476.4$ (3) Å^3
$Z = 8$
$F(000) = 736$
$D_x = 1.625$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2442 reflections
$\theta = 1.9$–27.9°
$\mu = 0.46$ mm^{-1}
$T = 113$ K
Prism, colourless
0.20 × 0.18 × 0.14 mm

Data collection

Rigaku Saturn CCD diffractometer
Radiation source: rotating anode
Multilayer monochromator
Detector resolution: 14.63 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min} = 0.914$, $T_{max} = 0.939$
6933 measured reflections
1749 independent reflections
1430 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 27.9°$, $\theta_{min} = 1.9°$
$h = -28 \rightarrow 27$
$k = -4 \rightarrow 4$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.095$
$S = 1.03$
1749 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
$w = 1/[\sigma^2(F_o^2) + (0.0578P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ 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 $F^2 > \sigma(F^2)$ 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}
Cl1	0.087385 (18)	0.57099 (12)	0.36030 (2)	0.02301 (15)
O1	0.25626 (5)	0.5555 (3)	0.58943 (6)	0.0200 (3)
N1	0.07663 (6)	0.3042 (4)	0.48893 (7)	0.0178 (3)

N2	0.17290 (6)	0.5527 (4)	0.48745 (7)	0.0165 (3)
C1	0.11297 (7)	0.4595 (4)	0.45572 (9)	0.0164 (3)
C2	0.10115 (7)	0.2222 (4)	0.56609 (8)	0.0155 (3)
C3	0.06280 (7)	0.0601 (4)	0.60639 (9)	0.0183 (3)
H3	0.0211	0.0084	0.5814	0.022*
C4	0.08592 (7)	−0.0240 (4)	0.68250 (9)	0.0186 (3)
H4	0.0597	−0.1318	0.7098	0.022*
C5	0.14730 (7)	0.0467 (4)	0.72020 (9)	0.0179 (3)
H5	0.1626	−0.0140	0.7726	0.021*
C6	0.18533 (7)	0.2042 (4)	0.68100 (9)	0.0172 (3)
H6	0.2272	0.2508	0.7063	0.021*
C7	0.16281 (6)	0.2959 (4)	0.60432 (8)	0.0144 (3)
C8	0.20165 (7)	0.4738 (4)	0.56241 (9)	0.0166 (3)
H1	0.1956 (9)	0.652 (6)	0.4567 (11)	0.042 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0253 (2)	0.0286 (3)	0.0141 (2)	−0.00270 (16)	0.00309 (15)	0.00145 (16)
O1	0.0127 (5)	0.0272 (6)	0.0195 (6)	−0.0031 (5)	0.0029 (4)	0.0031 (5)
N1	0.0165 (6)	0.0217 (7)	0.0150 (6)	−0.0028 (5)	0.0036 (5)	−0.0015 (6)
N2	0.0151 (6)	0.0201 (7)	0.0154 (6)	−0.0020 (5)	0.0061 (5)	−0.0002 (5)
C1	0.0171 (7)	0.0178 (8)	0.0136 (7)	0.0007 (6)	0.0028 (6)	−0.0023 (6)
C2	0.0166 (7)	0.0153 (8)	0.0147 (7)	0.0003 (6)	0.0040 (6)	−0.0022 (6)
C3	0.0152 (7)	0.0207 (8)	0.0196 (8)	−0.0032 (6)	0.0054 (6)	−0.0016 (7)
C4	0.0200 (8)	0.0203 (8)	0.0177 (8)	−0.0016 (6)	0.0087 (6)	−0.0003 (6)
C5	0.0220 (8)	0.0177 (8)	0.0141 (7)	0.0021 (6)	0.0047 (6)	0.0004 (6)
C6	0.0148 (7)	0.0178 (8)	0.0182 (7)	−0.0001 (6)	0.0028 (6)	−0.0020 (6)
C7	0.0145 (7)	0.0132 (8)	0.0161 (7)	0.0004 (6)	0.0049 (6)	−0.0021 (6)
C8	0.0174 (7)	0.0157 (8)	0.0176 (7)	0.0014 (6)	0.0060 (6)	−0.0010 (6)

Geometric parameters (Å, º)

Cl1—C1	1.7249 (16)	C3—C4	1.378 (2)
O1—C8	1.2370 (18)	C3—H3	0.9500
N1—C1	1.2706 (19)	C4—C5	1.398 (2)
N1—C2	1.3971 (19)	C4—H4	0.9500
N2—C1	1.3669 (19)	C5—C6	1.374 (2)
N2—C8	1.3766 (19)	C5—H5	0.9500
N2—H1	0.92 (2)	C6—C7	1.392 (2)
C2—C3	1.400 (2)	C6—H6	0.9500
C2—C7	1.408 (2)	C7—C8	1.455 (2)
C1—N1—C2	115.79 (13)	C3—C4—H4	119.4
C1—N2—C8	121.52 (13)	C5—C4—H4	119.4
C1—N2—H1	119.1 (12)	C6—C5—C4	119.64 (14)
C8—N2—H1	119.2 (12)	C6—C5—H5	120.2
N1—C1—N2	126.93 (14)	C4—C5—H5	120.2

N1—C1—Cl1	119.55 (12)	C5—C6—C7	120.25 (14)
N2—C1—Cl1	113.53 (11)	C5—C6—H6	119.9
N1—C2—C3	118.46 (13)	C7—C6—H6	119.9
N1—C2—C7	122.36 (14)	C6—C7—C2	120.18 (14)
C3—C2—C7	119.18 (14)	C6—C7—C8	121.19 (13)
C4—C3—C2	119.58 (14)	C2—C7—C8	118.62 (14)
C4—C3—H3	120.2	O1—C8—N2	120.31 (14)
C2—C3—H3	120.2	O1—C8—C7	124.97 (14)
C3—C4—C5	121.16 (14)	N2—C8—C7	114.72 (13)
C2—N1—C1—N2	0.1 (2)	C5—C6—C7—C8	177.88 (14)
C2—N1—C1—Cl1	179.76 (11)	N1—C2—C7—C6	−179.03 (14)
C8—N2—C1—N1	1.8 (3)	C3—C2—C7—C6	0.8 (2)
C8—N2—C1—Cl1	−177.85 (11)	N1—C2—C7—C8	2.0 (2)
C1—N1—C2—C3	178.19 (13)	C3—C2—C7—C8	−178.21 (13)
C1—N1—C2—C7	−2.0 (2)	C1—N2—C8—O1	178.72 (13)
N1—C2—C3—C4	179.88 (14)	C1—N2—C8—C7	−1.7 (2)
C7—C2—C3—C4	0.1 (2)	C6—C7—C8—O1	0.5 (2)
C2—C3—C4—C5	−0.6 (2)	C2—C7—C8—O1	179.48 (15)
C3—C4—C5—C6	0.3 (2)	C6—C7—C8—N2	−179.07 (14)
C4—C5—C6—C7	0.5 (2)	C2—C7—C8—N2	−0.1 (2)
C5—C6—C7—C2	−1.1 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H1···O1^{i}	0.92 (2)	1.88 (2)	2.7840 (17)	166.5 (19)
C3—H3···N1^{ii}	0.95	2.53	3.449 (2)	163

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