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2-(2-Chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one

Ming-Jian Li and Chang-Jun Feng*

 School of Chemistry & Chemical Engineering, Xuzhou Institute of Technology, Xuzhou Jiangsu 221008, People's Republic of China
 Correspondence e-mail: feng.changjun@163.com

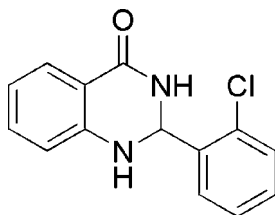
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 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.030; wR factor = 0.082; data-to-parameter ratio = 12.5.

The title compound, $\text{C}_{14}\text{H}_{11}\text{ClN}_2\text{O}$, was synthesized by the reaction of 2-chlorobenzaldehyde and 2-aminobenzamide in an ionic liquid. The pyrimidine ring adopts a skew-boat conformation and the two benzene rings make a dihedral angle of $87.1(1)^\circ$. In the crystal, $\text{N}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonding links the molecules along b .

Related literature

For quinazoline derivatives as antitumor agents, see: Feng *et al.* (2006); Keenan & Shakespear (2004); Mikiciuk-Olasik *et al.* (2004). For the biological activity of quinazoline derivatives, see: Bedi *et al.* (2004); Lin *et al.* (2006); Saleh *et al.* (2004).



Experimental

Crystal data

$\text{C}_{14}\text{H}_{11}\text{ClN}_2\text{O}$
 $M_r = 258.70$
 Triclinic, $P\bar{1}$
 $a = 6.9900(1)$ Å
 $b = 8.7488(2)$ Å
 $c = 10.4756(2)$ Å
 $\alpha = 100.639(1)^\circ$
 $\beta = 92.726(1)^\circ$

$\gamma = 101.786(1)^\circ$
 $V = 613.91(2)$ Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.30$ mm⁻¹
 $T = 296$ K
 $0.47 \times 0.15 \times 0.15$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (Jacobson, 1998)
 $T_{\min} = 0.901$, $T_{\max} = 0.950$
 8018 measured reflections
 2204 independent reflections
 2029 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.082$
 $S = 1.07$
 2204 reflections
 176 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.20$ e Å⁻³
 $\Delta\rho_{\min} = -0.19$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N2}-\text{H2A}\cdots\text{O1}^{\text{i}}$	0.831 (16)	2.461 (16)	3.1847 (16)	146.2 (14)
$\text{N1}-\text{H1A}\cdots\text{O1}^{\text{ii}}$	0.824 (18)	2.103 (18)	2.9146 (16)	168.4 (16)
$\text{C1}-\text{H1B}\cdots\text{N2}^{\text{iii}}$	0.948 (14)	2.635 (14)	3.4369 (17)	142.6 (11)

Symmetry codes: (i) $x - 1, y, z$; (ii) $-x + 2, -y + 2, -z$; (iii) $-x + 1, -y + 2, -z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE*; 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PB2004).

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supporting information

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2-(2-Chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one**Ming-Jian Li and Chang-Jun Feng****S1. Comment**

Quinazoline derivatives are well known compounds as antitumor agents (Feng *et al.*, 2006; Keenan *et al.*, 2004; Mikiciuk-Olasik *et al.*, 2004). In addition, it was reported that some quinazoline derivatives possessed biological activities, such as antimalarial activity (Lin *et al.*, 2006) antibacterial activity (Bedi *et al.*, 2004) and antifungal activity (Saleh *et al.*, 2004). We report here the crystal structure of 2-(2-chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one, (I).

The X-ray crystal structure determination indicates that the pyrimidine ring in the quinazoline moiety is slightly distorted, adopting a skew-boat conformation. The atoms of C2, C3, C8 and N2 are coplanar, with the atoms N1 and C1 deviating from the defined plane by 0.256 (2) and 0.623 (2) Å, respectively. The basal plane is nearly parallel to the benzene ring (C3—C8), forming a dihedral angle of 5.4 (1)°. And is nearly perpendicular to the benzene ring (C9—C14), forming a dihedral angle of 87.7 (1)°. Two benzene rings make a dihedral angle of 87.1 (1)°.

The hydrogen bonds of N—H...O and C—H...N are presented in the crystal structure of (I) (Table 2). The intermolecular hydrogen bond (N1—H1A...O1) and hydrogen bond (C1—H1B...N2) link the adjacent molecules, forming dimers, respectively. The hydrogen bond of N2—H2A...O1 and above hydrogen bonds link the molecules forming polymers along *b* (Figure 2).

S2. Experimental

The title compound, (I), was prepared by the reaction of 2-chlorobenzaldehyde (2 mmol, 0.280 g), 2-aminobenzamide (2 mmol, 0.272 g) and ionic liquid of [Bmim]Br (2 ml) at 353 K. The isolated compound melts at 485–486 K. The single crystals suitable for X-ray diffraction were obtained by slow evaporation ethanol solution.

S3. Refinement

The H atoms were calculated geometrically and refined as riding, with C—H = 0.93 Å except for H1A, H1B and H2A, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$.

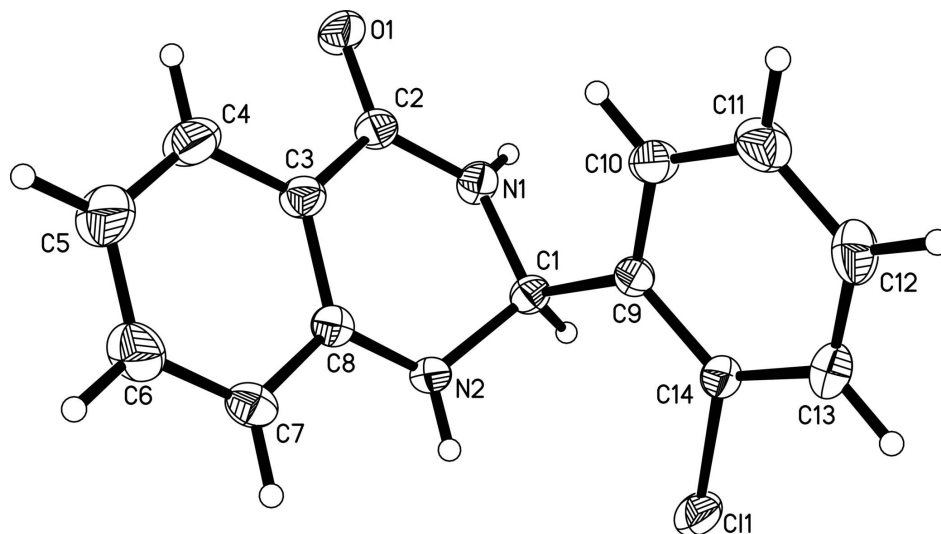


Figure 1

The molecular structure drawing for (I) showing 50% probability of displacement ellipsoids and the atom-numbering scheme.

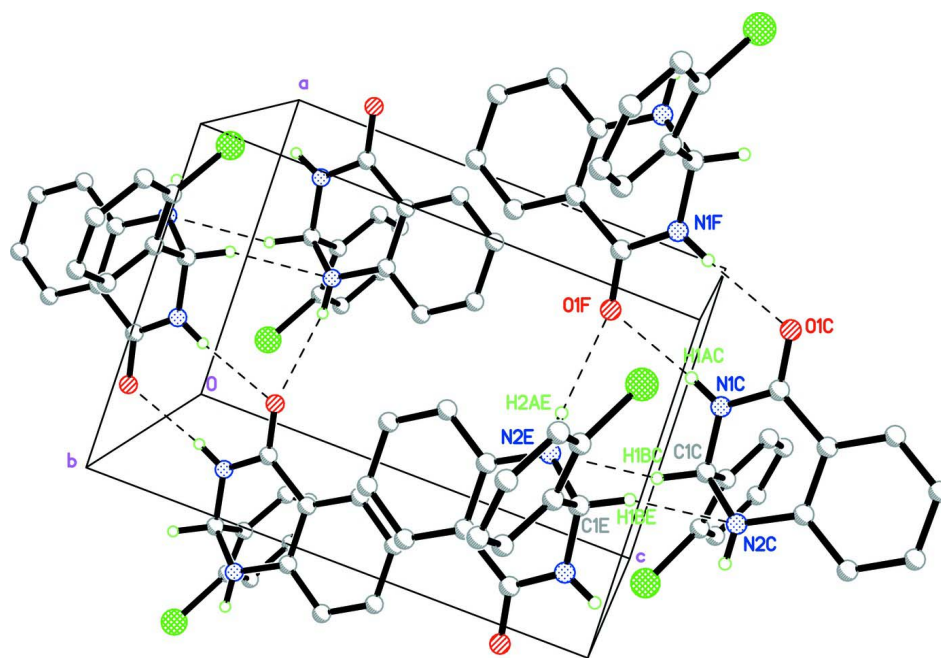


Figure 2

The molecular packing diagram showing the hydrogen-bonding network in the crystal for (I).

2-(2-Chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one

Crystal data

$C_{14}H_{11}ClN_2O$

$M_r = 258.70$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 6.9900$ (1) Å

$b = 8.7488$ (2) Å

$c = 10.4756$ (2) Å

$\alpha = 100.639$ (1)°

$\beta = 92.726$ (1)°

$\gamma = 101.786$ (1)°

$V = 613.91 (2) \text{ \AA}^3$
 $Z = 2$
 $F(000) = 268$
 $D_x = 1.399 \text{ Mg m}^{-3}$
 Melting point = 485–486 K
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 5614 reflections

$\theta = 2.4\text{--}27.3^\circ$
 $\mu = 0.30 \text{ mm}^{-1}$
 $T = 296 \text{ K}$
 Block, colourless
 $0.47 \times 0.15 \times 0.15 \text{ mm}$

Data collection

Bruker SMART CCD area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω scans
 Absorption correction: multi-scan
 (Jacobson, 1998)
 $T_{\min} = 0.901, T_{\max} = 0.950$

8018 measured reflections
 2204 independent reflections
 2029 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$
 $\theta_{\max} = 25.2^\circ, \theta_{\min} = 2.0^\circ$
 $h = -8 \rightarrow 8$
 $k = -10 \rightarrow 10$
 $l = -12 \rightarrow 11$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.082$
 $S = 1.07$
 2204 reflections
 176 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
 $w = 1/[\sigma^2(F_o^2) + (0.0395P)^2 + 0.1722P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.20 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.19 \text{ e \AA}^{-3}$
 Extinction correction: *SHELXL97* (Sheldrick,
 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.028 (4)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.16029 (5)	0.69778 (5)	0.05650 (4)	0.05390 (17)
N2	0.50252 (18)	1.00296 (13)	0.18929 (11)	0.0344 (3)
C9	0.53903 (19)	0.72253 (15)	0.14393 (12)	0.0301 (3)
O1	1.08313 (14)	1.09067 (13)	0.17031 (11)	0.0497 (3)
C2	0.9066 (2)	1.04662 (16)	0.18541 (14)	0.0370 (3)
C8	0.61534 (19)	1.08206 (15)	0.30290 (12)	0.0319 (3)
N1	0.78205 (17)	0.94682 (14)	0.09040 (12)	0.0367 (3)
C14	0.3498 (2)	0.62845 (16)	0.12560 (13)	0.0345 (3)
C1	0.57649 (19)	0.88323 (15)	0.10227 (13)	0.0315 (3)

C10	0.6833 (2)	0.66331 (18)	0.20113 (14)	0.0411 (3)
H10A	0.8115	0.7230	0.2153	0.049*
C13	0.3048 (2)	0.48197 (17)	0.16089 (15)	0.0451 (4)
H13A	0.1769	0.4217	0.1469	0.054*
C3	0.8198 (2)	1.10531 (17)	0.30508 (13)	0.0384 (3)
C7	0.5326 (2)	1.14921 (18)	0.41197 (14)	0.0419 (3)
H7A	0.3970	1.1339	0.4120	0.050*
C11	0.6398 (3)	0.5163 (2)	0.23777 (16)	0.0521 (4)
H11A	0.7385	0.4786	0.2765	0.063*
C4	0.9362 (2)	1.1958 (2)	0.41504 (17)	0.0613 (5)
H4A	1.0720	1.2122	0.4163	0.074*
C12	0.4514 (3)	0.42650 (18)	0.21692 (16)	0.0517 (4)
H12A	0.4232	0.3277	0.2409	0.062*
C6	0.6509 (3)	1.2379 (2)	0.51937 (16)	0.0582 (5)
H6A	0.5944	1.2828	0.5916	0.070*
C5	0.8526 (3)	1.2615 (3)	0.52208 (17)	0.0722 (6)
H5A	0.9312	1.3214	0.5957	0.087*
H2A	0.382 (2)	0.9860 (18)	0.1921 (14)	0.037 (4)*
H1A	0.823 (2)	0.9236 (19)	0.0184 (18)	0.045 (4)*
H1B	0.510 (2)	0.8682 (16)	0.0185 (14)	0.027 (3)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0326 (2)	0.0464 (2)	0.0788 (3)	0.00346 (16)	-0.01097 (18)	0.01200 (19)
N2	0.0259 (6)	0.0347 (6)	0.0423 (7)	0.0069 (5)	0.0038 (5)	0.0067 (5)
C9	0.0304 (7)	0.0324 (6)	0.0270 (6)	0.0067 (5)	0.0065 (5)	0.0041 (5)
O1	0.0298 (5)	0.0554 (7)	0.0566 (7)	-0.0007 (5)	0.0140 (5)	0.0007 (5)
C2	0.0310 (7)	0.0380 (7)	0.0418 (8)	0.0051 (6)	0.0087 (6)	0.0084 (6)
C8	0.0330 (7)	0.0308 (6)	0.0347 (7)	0.0076 (5)	0.0059 (5)	0.0119 (5)
N1	0.0338 (6)	0.0396 (6)	0.0339 (6)	0.0012 (5)	0.0126 (5)	0.0050 (5)
C14	0.0329 (7)	0.0334 (7)	0.0350 (7)	0.0055 (6)	0.0015 (5)	0.0034 (5)
C1	0.0292 (7)	0.0347 (7)	0.0298 (7)	0.0041 (5)	0.0032 (5)	0.0073 (5)
C10	0.0342 (8)	0.0447 (8)	0.0456 (8)	0.0101 (6)	0.0034 (6)	0.0105 (6)
C13	0.0473 (9)	0.0339 (7)	0.0481 (9)	-0.0027 (6)	0.0017 (7)	0.0063 (6)
C3	0.0327 (7)	0.0448 (8)	0.0368 (7)	0.0081 (6)	0.0049 (6)	0.0060 (6)
C7	0.0395 (8)	0.0473 (8)	0.0431 (8)	0.0148 (6)	0.0130 (6)	0.0118 (6)
C11	0.0576 (10)	0.0484 (9)	0.0569 (10)	0.0218 (8)	-0.0019 (8)	0.0175 (7)
C4	0.0382 (9)	0.0858 (13)	0.0502 (10)	0.0114 (9)	-0.0030 (7)	-0.0067 (9)
C12	0.0676 (11)	0.0326 (7)	0.0546 (9)	0.0063 (7)	0.0013 (8)	0.0139 (7)
C6	0.0641 (11)	0.0729 (12)	0.0372 (8)	0.0220 (9)	0.0126 (7)	0.0002 (8)
C5	0.0615 (12)	0.0989 (15)	0.0431 (10)	0.0171 (11)	-0.0070 (8)	-0.0161 (9)

Geometric parameters (Å, °)

C11—C14	1.7453 (14)	C10—C11	1.388 (2)
N2—C8	1.3787 (17)	C10—H10A	0.9300
N2—C1	1.4523 (17)	C13—C12	1.372 (2)

N2—H2A	0.831 (16)	C13—H13A	0.9300
C9—C10	1.3839 (19)	C3—C4	1.388 (2)
C9—C14	1.3915 (19)	C7—C6	1.371 (2)
C9—C1	1.5240 (18)	C7—H7A	0.9300
O1—C2	1.2421 (17)	C11—C12	1.373 (2)
C2—N1	1.3405 (18)	C11—H11A	0.9300
C2—C3	1.4716 (19)	C4—C5	1.375 (2)
C8—C7	1.3924 (19)	C4—H4A	0.9300
C8—C3	1.4001 (19)	C12—H12A	0.9300
N1—C1	1.4511 (17)	C6—C5	1.380 (3)
N1—H1A	0.824 (18)	C6—H6A	0.9300
C14—C13	1.378 (2)	C5—H5A	0.9300
C1—H1B	0.948 (14)		
C8—N2—C1	118.48 (11)	C11—C10—H10A	119.5
C8—N2—H2A	116.8 (10)	C12—C13—C14	118.97 (14)
C1—N2—H2A	116.0 (10)	C12—C13—H13A	120.5
C10—C9—C14	116.97 (12)	C14—C13—H13A	120.5
C10—C9—C1	123.74 (12)	C4—C3—C8	119.58 (13)
C14—C9—C1	119.28 (11)	C4—C3—C2	121.32 (14)
O1—C2—N1	121.40 (13)	C8—C3—C2	118.80 (12)
O1—C2—C3	122.54 (13)	C6—C7—C8	120.05 (14)
N1—C2—C3	116.00 (12)	C6—C7—H7A	120.0
N2—C8—C7	121.83 (12)	C8—C7—H7A	120.0
N2—C8—C3	118.83 (12)	C12—C11—C10	120.13 (14)
C7—C8—C3	119.18 (13)	C12—C11—H11A	119.9
C2—N1—C1	124.90 (12)	C10—C11—H11A	119.9
C2—N1—H1A	117.9 (12)	C5—C4—C3	120.63 (16)
C1—N1—H1A	117.1 (12)	C5—C4—H4A	119.7
C13—C14—C9	122.57 (13)	C3—C4—H4A	119.7
C13—C14—C11	118.17 (11)	C13—C12—C11	120.28 (14)
C9—C14—C11	119.26 (10)	C13—C12—H12A	119.9
N1—C1—N2	108.17 (11)	C11—C12—H12A	119.9
N1—C1—C9	113.41 (11)	C7—C6—C5	121.06 (15)
N2—C1—C9	112.80 (10)	C7—C6—H6A	119.5
N1—C1—H1B	106.9 (8)	C5—C6—H6A	119.5
N2—C1—H1B	107.8 (8)	C4—C5—C6	119.49 (16)
C9—C1—H1B	107.5 (8)	C4—C5—H5A	120.3
C9—C10—C11	121.08 (14)	C6—C5—H5A	120.3
C9—C10—H10A	119.5		
C1—N2—C8—C7	-154.80 (12)	C11—C14—C13—C12	-179.15 (12)
C1—N2—C8—C3	29.94 (17)	N2—C8—C3—C4	174.78 (14)
O1—C2—N1—C1	176.67 (13)	C7—C8—C3—C4	-0.6 (2)
C3—C2—N1—C1	-5.9 (2)	N2—C8—C3—C2	0.93 (19)
C10—C9—C14—C13	-0.6 (2)	C7—C8—C3—C2	-174.45 (13)
C1—C9—C14—C13	-179.95 (12)	O1—C2—C3—C4	-9.3 (2)
C10—C9—C14—C11	178.92 (10)	N1—C2—C3—C4	173.25 (15)

C1—C9—C14—C11	-0.48 (16)	O1—C2—C3—C8	164.39 (14)
C2—N1—C1—N2	33.01 (17)	N1—C2—C3—C8	-13.0 (2)
C2—N1—C1—C9	-92.90 (15)	N2—C8—C7—C6	-174.73 (14)
C8—N2—C1—N1	-44.49 (15)	C3—C8—C7—C6	0.5 (2)
C8—N2—C1—C9	81.78 (14)	C9—C10—C11—C12	0.3 (2)
C10—C9—C1—N1	17.84 (18)	C8—C3—C4—C5	0.6 (3)
C14—C9—C1—N1	-162.81 (11)	C2—C3—C4—C5	174.27 (18)
C10—C9—C1—N2	-105.57 (14)	C14—C13—C12—C11	0.3 (2)
C14—C9—C1—N2	73.78 (15)	C10—C11—C12—C13	-0.6 (3)
C14—C9—C10—C11	0.2 (2)	C8—C7—C6—C5	-0.4 (3)
C1—C9—C10—C11	179.58 (13)	C3—C4—C5—C6	-0.5 (3)
C9—C14—C13—C12	0.3 (2)	C7—C6—C5—C4	0.4 (3)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N2—H2 <i>A</i> ...O1 ⁱ	0.831 (16)	2.461 (16)	3.1847 (16)	146.2 (14)
N1—H1 <i>A</i> ...O1 ⁱⁱ	0.824 (18)	2.103 (18)	2.9146 (16)	168.4 (16)
C1—H1 <i>B</i> ...N2 ⁱⁱⁱ	0.948 (14)	2.635 (14)	3.4369 (17)	142.6 (11)

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+2, -y+2, -z$; (iii) $-x+1, -y+2, -z$.