

## 3-Chloro-*N*-(2-methylphenyl)benzamide

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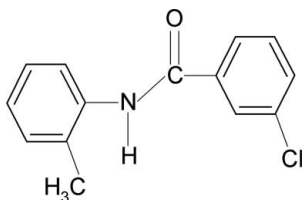
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.036;  $wR$  factor = 0.098; data-to-parameter ratio = 15.6.

In the molecular structure of the title compound,  $\text{C}_{14}\text{H}_{12}\text{ClNO}$ , the *meta*-Cl atom in the benzoyl ring is positioned *anti* to the  $\text{C}=\text{O}$  bond, while the *ortho*-methyl group in the aniline ring is positioned *syn* to the  $\text{N}-\text{H}$  bond. The two benzene rings are nearly coplanar [dihedral angle =  $3.48(5)^\circ$ ]. The crystal structure is stabilized by  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds, which link the molecules into chains along the  $b$  axis.

### Related literature

For the preparation of the title compound, see: Gowda *et al.* (2003). For our studies on the effects of substituents on the structures and other aspects of *N*-(aryl)-amides, see: Bowes *et al.* (2003); Gowda *et al.* (2000); Rodrigues *et al.* (2011); Saeed *et al.* (2010), on *N*-(aryl)-methanesulfonamides, see: Jayalakshmi & Gowda (2004) on *N*-(aryl)-arylsulfonamides, see: Shetty & Gowda (2005) and on *N*-chloroarylamides, see: Gowda *et al.* (1996).



### Experimental

#### Crystal data

$\text{C}_{14}\text{H}_{12}\text{ClNO}$   
 $M_r = 245.70$   
Monoclinic,  $P2_1/n$   
 $a = 11.1699(5)$  Å  
 $b = 4.9171(2)$  Å  
 $c = 21.4778(8)$  Å  
 $\beta = 90.339(3)^\circ$

$V = 1179.63(8)$  Å<sup>3</sup>  
 $Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 0.31$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.83 \times 0.55 \times 0.10$  mm

#### Data collection

|   |   |
|---|---|
| Oxford Diffraction Xcalibur Ruby Gemini diffractometer  | Reid (1995)                             |
| Absorption correction: analytical [CrysAlis RED (Oxford Diffraction, 2009), based on expressions derived from Clark & | $T_{\min} = 0.818$ , $T_{\max} = 0.970$ |
|   | 22104 measured reflections              |
|   | 2411 independent reflections            |
|   | 2154 reflections with $I > 2\sigma(I)$  |
|   | $R_{\text{int}} = 0.050$                |

#### Refinement

|                                 |   |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.036$ | 155 parameters                                |
| $wR(F^2) = 0.098$               | H-atom parameters constrained                 |
| $S = 1.04$                      | $\Delta\rho_{\max} = 0.18$ e Å <sup>-3</sup>  |
| 2411 reflections                | $\Delta\rho_{\min} = -0.24$ e Å <sup>-3</sup> |

**Table 1**

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$                    | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---|--------------|--------------------|-------------|----------------------|
| $\text{N1}-\text{H1A}\cdots\text{O1}^i$ | 0.86         | 2.11               | 2.9237 (18) | 158                  |

Symmetry code: (i)  $x, y - 1, z$ .

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2002); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2320).

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## supporting information

*Acta Cryst.* (2011). E67, o3381 [https://doi.org/10.1107/S1600536811048756]

### 3-Chloro-*N*-(2-methylphenyl)benzamide

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#### S1. Comment

The amide and sulfonamide moieties are the constituents of many biologically significant compounds. As part of our studies on the substituent effects on the structures and other aspects of *N*-(aryl)-amides (Bowes *et al.*, 2003; Gowda *et al.*, 2000; Rodrigues *et al.*, 2011; Saeed *et al.*, 2010), *N*-(aryl)-methanesulfonamides (Jayalakshmi & Gowda, 2004), *N*-(aryl)-arylsulfonamides (Shetty & Gowda, 2005) and *N*-chloro-arylamides (Gowda *et al.*, 1996), in the present work, the crystal structure of 3-Chloro-*N*-(2-methylphenyl)- benzamide (I) has been determined (Fig.1).

In (I), the N—H and C=O bonds in the C—NH—C(O)—C segment are *anti* to each other. The *meta*-Cl atom in the benzoyl ring is positioned *anti* to the C=O bond, while the *ortho*-methyl group in the anilino ring is positioned *syn* to the N—H bond, in contrast to the *syn* conformation observed between the *meta*-Cl atom in the benzoyl ring and the C=O bond in 3-Chloro-*N*-(3-methylphenyl)benzamide (II) (Rodrigues *et al.*, 2011), while the *meta*-methyl group in the anilino ring is positioned *anti* to the N—H bond. Further, the two aromatic rings are nearly coplanar with the dihedral angle of 3.48 (5)°, compared to the value of 77.4 (1)° in (II).

In the crystal structure, intermolecular N—H···O hydrogen bonds link the molecules into infinite chains running along the *b*-axis. Part of the crystal structure is shown in Fig. 2.

#### S2. Experimental

The title compound was prepared according to the method described by Gowda *et al.* (2003). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra.

Rod like colorless single crystals of the title compound used in x-ray diffraction studies were obtained by slow evaporation of an ethanol solution of the compound (0.5 g in about 30 ml of ethanol) at room temperature.

#### S3. Refinement

All H atoms were visible in difference maps and then treated as riding atoms with C—H distances of 0.93 Å (C-aromatic), 0.96 Å (C-methyl) and N—H = 0.86 Å. The  $U_{iso}(H)$  values were set at 1.2  $U_{eq}(C\text{-aromatic}, N)$  and 1.5  $U_{eq}(C\text{-methyl})$ .

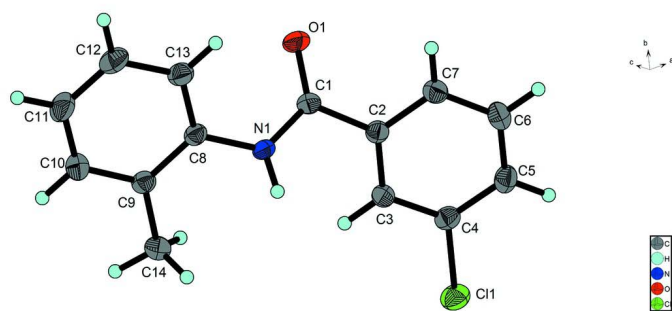


Figure 1

Molecular structure of the title compound showing the atom labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

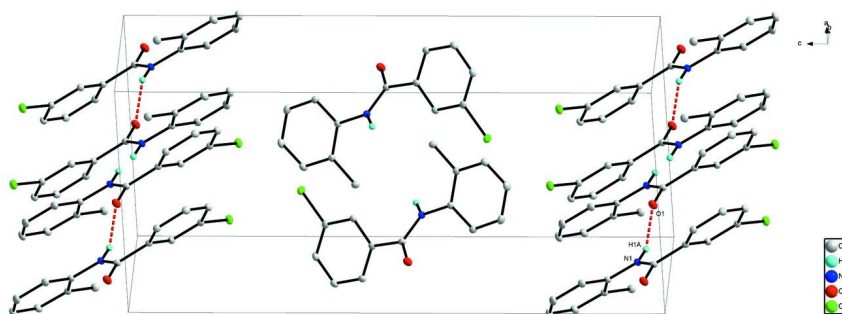


Figure 2

Part of the crystal structure of the title compound. Molecular chains are generated by N—H...O hydrogen bonds which are shown by dashed lines.

### 3-Chloro-*N*-(2-methylphenyl)benzamide

#### Crystal data

$C_{14}H_{12}ClNO$

$M_r = 245.70$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 11.1699 (5) \text{ \AA}$

$b = 4.9171 (2) \text{ \AA}$

$c = 21.4778 (8) \text{ \AA}$

$\beta = 90.339 (3)^\circ$

$V = 1179.63 (8) \text{ \AA}^3$

$Z = 4$

$F(000) = 512$

$D_x = 1.383 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 7179 reflections

$\theta = 3.4\text{--}26.4^\circ$

$\mu = 0.31 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Rod, colorless

$0.83 \times 0.55 \times 0.10 \text{ mm}$

*Data collection*

Oxford Diffraction Xcalibur Ruby Gemini diffractometer  
 Radiation source: Enhance (Mo) X-ray Source  
 Graphite monochromator  
 Detector resolution: 10.4340 pixels mm<sup>-1</sup>  
 $\omega$  scans  
 Absorption correction: analytical  
 [CrysAlis RED (Oxford Diffraction, 2009), based on expressions derived from Clark & Reid (1995)]

$T_{\min} = 0.818$ ,  $T_{\max} = 0.970$   
 22104 measured reflections  
 2411 independent reflections  
 2154 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.050$   
 $\theta_{\max} = 26.4^\circ$ ,  $\theta_{\min} = 3.4^\circ$   
 $h = -13 \rightarrow 13$   
 $k = -6 \rightarrow 6$   
 $l = -26 \rightarrow 26$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.098$   
 $S = 1.04$   
 2411 reflections  
 155 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-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 0.4496P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.18 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$

*Special details*

**Experimental.** CrysAlis RED (Oxford Diffraction, 2009) Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived (Clark & Reid, 1995).

**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 ( $\text{\AA}^2$ )*

|     | $x$          | $y$        | $z$         | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|------------|-------------|----------------------------------|
| C1  | 0.78713 (15) | 0.6810 (3) | 0.51026 (8) | 0.0347 (4)                       |
| C2  | 0.84225 (16) | 0.5801 (3) | 0.45112 (8) | 0.0342 (4)                       |
| C3  | 0.78692 (16) | 0.3823 (3) | 0.41438 (8) | 0.0357 (4)                       |
| H3A | 0.7150       | 0.3041     | 0.4267      | 0.043*                           |
| C4  | 0.84060 (17) | 0.3043 (3) | 0.35942 (8) | 0.0380 (4)                       |
| C5  | 0.94821 (18) | 0.4136 (4) | 0.34075 (9) | 0.0434 (4)                       |
| H5A | 0.9839       | 0.3563     | 0.3040      | 0.052*                           |
| C6  | 1.00224 (17) | 0.6092 (4) | 0.37740 (9) | 0.0452 (4)                       |
| H6A | 1.0750       | 0.6837     | 0.3652      | 0.054*                           |
| C7  | 0.94945 (17) | 0.6957 (4) | 0.43205 (8) | 0.0395 (4)                       |
| H7A | 0.9856       | 0.8308     | 0.4559      | 0.047*                           |
| C8  | 0.66916 (16) | 0.5439 (3) | 0.60171 (8) | 0.0333 (4)                       |
| C9  | 0.56240 (16) | 0.4044 (3) | 0.61282 (8) | 0.0362 (4)                       |

|      |              |              |             |              |
|------|--------------|--------------|-------------|--------------|
| C10  | 0.50367 (19) | 0.4563 (4)   | 0.66843 (9) | 0.0483 (5)   |
| H10A | 0.4327       | 0.3650       | 0.6769      | 0.058*       |
| C11  | 0.5475 (2)   | 0.6388 (5)   | 0.71132 (9) | 0.0547 (5)   |
| H11A | 0.5059       | 0.6712       | 0.7479      | 0.066*       |
| C12  | 0.6531 (2)   | 0.7737 (4)   | 0.69999 (9) | 0.0513 (5)   |
| H12A | 0.6831       | 0.8967       | 0.7290      | 0.062*       |
| C13  | 0.71473 (18) | 0.7262 (4)   | 0.64539 (8) | 0.0418 (4)   |
| H13A | 0.7865       | 0.8159       | 0.6379      | 0.050*       |
| C14  | 0.51064 (18) | 0.2054 (4)   | 0.56700 (9) | 0.0446 (4)   |
| H14C | 0.4336       | 0.1460       | 0.5811      | 0.053*       |
| H14B | 0.5630       | 0.0515       | 0.5635      | 0.053*       |
| H14A | 0.5022       | 0.2914       | 0.5271      | 0.053*       |
| N1   | 0.73102 (13) | 0.4923 (3)   | 0.54513 (6) | 0.0348 (3)   |
| H1A  | 0.7328       | 0.3269       | 0.5321      | 0.042*       |
| O1   | 0.79372 (14) | 0.9221 (2)   | 0.52456 (7) | 0.0504 (4)   |
| Cl1  | 0.77036 (5)  | 0.06380 (10) | 0.31224 (2) | 0.05338 (17) |

*Atomic displacement parameters (Å<sup>2</sup>)*

|     | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$    | $U^{13}$    | $U^{23}$    |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| C1  | 0.0383 (9)  | 0.0273 (8)  | 0.0386 (9)  | 0.0012 (7)  | 0.0004 (7)  | -0.0005 (7) |
| C2  | 0.0385 (9)  | 0.0286 (8)  | 0.0356 (8)  | 0.0035 (7)  | 0.0020 (7)  | 0.0037 (6)  |
| C3  | 0.0392 (9)  | 0.0319 (8)  | 0.0361 (8)  | -0.0009 (7) | 0.0040 (7)  | 0.0026 (7)  |
| C4  | 0.0462 (10) | 0.0328 (9)  | 0.0348 (9)  | 0.0036 (7)  | -0.0019 (7) | 0.0011 (7)  |
| C5  | 0.0481 (10) | 0.0468 (11) | 0.0353 (9)  | 0.0062 (8)  | 0.0088 (8)  | 0.0017 (8)  |
| C6  | 0.0383 (10) | 0.0503 (11) | 0.0469 (10) | -0.0025 (8) | 0.0074 (8)  | 0.0069 (9)  |
| C7  | 0.0415 (9)  | 0.0370 (9)  | 0.0401 (9)  | -0.0023 (7) | 0.0002 (7)  | 0.0013 (7)  |
| C8  | 0.0386 (9)  | 0.0278 (8)  | 0.0336 (8)  | 0.0039 (7)  | 0.0019 (7)  | -0.0005 (6) |
| C9  | 0.0406 (9)  | 0.0313 (8)  | 0.0369 (9)  | 0.0024 (7)  | 0.0002 (7)  | -0.0004 (7) |
| C10 | 0.0485 (11) | 0.0481 (11) | 0.0484 (11) | -0.0019 (9) | 0.0127 (9)  | -0.0004 (9) |
| C11 | 0.0669 (14) | 0.0582 (12) | 0.0393 (10) | 0.0033 (11) | 0.0142 (9)  | -0.0078 (9) |
| C12 | 0.0666 (13) | 0.0481 (11) | 0.0392 (10) | 0.0016 (10) | -0.0026 (9) | -0.0138 (8) |
| C13 | 0.0449 (10) | 0.0374 (9)  | 0.0429 (10) | -0.0016 (8) | -0.0011 (8) | -0.0074 (8) |
| C14 | 0.0440 (10) | 0.0418 (10) | 0.0479 (10) | -0.0062 (8) | 0.0002 (8)  | -0.0041 (8) |
| N1  | 0.0439 (8)  | 0.0258 (6)  | 0.0348 (7)  | 0.0000 (6)  | 0.0058 (6)  | -0.0047 (5) |
| O1  | 0.0717 (10) | 0.0252 (6)  | 0.0547 (8)  | -0.0019 (6) | 0.0158 (7)  | -0.0037 (5) |
| Cl1 | 0.0666 (3)  | 0.0502 (3)  | 0.0434 (3)  | -0.0055 (2) | -0.0005 (2) | -0.0113 (2) |

*Geometric parameters (Å, °)*

|        |           |          |           |
|--------|-----------|----------|-----------|
| C1—O1  | 1.227 (2) | C8—C9    | 1.398 (3) |
| C1—N1  | 1.349 (2) | C8—N1    | 1.424 (2) |
| C1—C2  | 1.499 (2) | C9—C10   | 1.390 (3) |
| C2—C7  | 1.389 (3) | C9—C14   | 1.501 (2) |
| C2—C3  | 1.395 (2) | C10—C11  | 1.374 (3) |
| C3—C4  | 1.381 (2) | C10—H10A | 0.9300    |
| C3—H3A | 0.9300    | C11—C12  | 1.376 (3) |
| C4—C5  | 1.378 (3) | C11—H11A | 0.9300    |

|               |              |                 |              |
|---------------|--------------|-----------------|--------------|
| C4—C11        | 1.7412 (18)  | C12—C13         | 1.383 (3)    |
| C5—C6         | 1.380 (3)    | C12—H12A        | 0.9300       |
| C5—H5A        | 0.9300       | C13—H13A        | 0.9300       |
| C6—C7         | 1.384 (3)    | C14—H14C        | 0.9600       |
| C6—H6A        | 0.9300       | C14—H14B        | 0.9600       |
| C7—H7A        | 0.9300       | C14—H14A        | 0.9600       |
| C8—C13        | 1.392 (2)    | N1—H1A          | 0.8600       |
| O1—C1—N1      | 123.60 (16)  | C10—C9—C8       | 117.66 (17)  |
| O1—C1—C2      | 120.50 (16)  | C10—C9—C14      | 120.08 (17)  |
| N1—C1—C2      | 115.91 (14)  | C8—C9—C14       | 122.26 (16)  |
| C7—C2—C3      | 119.89 (16)  | C11—C10—C9      | 121.86 (19)  |
| C7—C2—C1      | 118.25 (16)  | C11—C10—H10A    | 119.1        |
| C3—C2—C1      | 121.82 (16)  | C9—C10—H10A     | 119.1        |
| C4—C3—C2      | 118.93 (17)  | C10—C11—C12     | 119.91 (18)  |
| C4—C3—H3A     | 120.5        | C10—C11—H11A    | 120.0        |
| C2—C3—H3A     | 120.5        | C12—C11—H11A    | 120.0        |
| C5—C4—C3      | 121.61 (17)  | C11—C12—C13     | 119.99 (18)  |
| C5—C4—C11     | 119.08 (14)  | C11—C12—H12A    | 120.0        |
| C3—C4—C11     | 119.31 (14)  | C13—C12—H12A    | 120.0        |
| C4—C5—C6      | 119.01 (17)  | C12—C13—C8      | 119.91 (18)  |
| C4—C5—H5A     | 120.5        | C12—C13—H13A    | 120.0        |
| C6—C5—H5A     | 120.5        | C8—C13—H13A     | 120.0        |
| C5—C6—C7      | 120.75 (18)  | C9—C14—H14C     | 109.5        |
| C5—C6—H6A     | 119.6        | C9—C14—H14B     | 109.5        |
| C7—C6—H6A     | 119.6        | H14C—C14—H14B   | 109.5        |
| C6—C7—C2      | 119.78 (17)  | C9—C14—H14A     | 109.5        |
| C6—C7—H7A     | 120.1        | H14C—C14—H14A   | 109.5        |
| C2—C7—H7A     | 120.1        | H14B—C14—H14A   | 109.5        |
| C13—C8—C9     | 120.67 (16)  | C1—N1—C8        | 125.45 (14)  |
| C13—C8—N1     | 120.84 (16)  | C1—N1—H1A       | 117.3        |
| C9—C8—N1      | 118.48 (15)  | C8—N1—H1A       | 117.3        |
| O1—C1—C2—C7   | 36.2 (2)     | N1—C8—C9—C10    | 179.64 (16)  |
| N1—C1—C2—C7   | -144.13 (16) | C13—C8—C9—C14   | -179.74 (17) |
| O1—C1—C2—C3   | -141.61 (19) | N1—C8—C9—C14    | -0.6 (3)     |
| N1—C1—C2—C3   | 38.0 (2)     | C8—C9—C10—C11   | 0.3 (3)      |
| C7—C2—C3—C4   | 0.2 (3)      | C14—C9—C10—C11  | -179.4 (2)   |
| C1—C2—C3—C4   | 177.98 (15)  | C9—C10—C11—C12  | -0.7 (3)     |
| C2—C3—C4—C5   | 1.2 (3)      | C10—C11—C12—C13 | 0.3 (3)      |
| C2—C3—C4—C11  | -178.37 (13) | C11—C12—C13—C8  | 0.6 (3)      |
| C3—C4—C5—C6   | -1.2 (3)     | C9—C8—C13—C12   | -1.0 (3)     |
| C11—C4—C5—C6  | 178.37 (15)  | N1—C8—C13—C12   | 179.91 (17)  |
| C4—C5—C6—C7   | -0.2 (3)     | O1—C1—N1—C8     | 1.9 (3)      |
| C5—C6—C7—C2   | 1.6 (3)      | C2—C1—N1—C8     | -177.71 (15) |
| C3—C2—C7—C6   | -1.5 (3)     | C13—C8—N1—C1    | -40.0 (3)    |
| C1—C2—C7—C6   | -179.42 (16) | C9—C8—N1—C1     | 140.87 (17)  |
| C13—C8—C9—C10 | 0.5 (3)      |                 |              |

*Hydrogen-bond geometry (Å, °)*

| <i>D</i> —H $\cdots$ <i>A</i>   | <i>D</i> —H | H $\cdots$ <i>A</i> | <i>D</i> $\cdots$ <i>A</i> | <i>D</i> —H $\cdots$ <i>A</i> |
|---------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| N1—H1A $\cdots$ O1 <sup>i</sup> | 0.86        | 2.11                | 2.9237 (18)                | 158                           |

Symmetry code: (i)  $x, y-1, z$ .