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# *N*-(3,5-Dichlorophenyl)-2,2,2-trimethylacetamide

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**Key indicators**

Single-crystal X-ray study
*T* = 299 K
Mean σ(C–C) = 0.008 Å
*R* factor = 0.094
*wR* factor = 0.206
Data-to-parameter ratio = 16.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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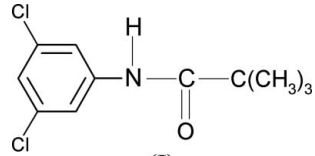
Molecules of the title compound, $C_{11}H_{13}Cl_2NO$, are linked into a chain running along the *b*-axis direction. The structure shows a close resemblance to those of related amides but with slightly different bond parameters.

## Comment

The amide unit is an important constituent of many biologically significant compounds. As part of a study of the effect of ring and side-chain substituents on the solid-state geometry of *N*-aromatic amides (Gowda *et al.*, 2006; Gowda, Kozisek *et al.*, 2007) we report here the crystal structure of *N*-(3,5-dichlorophenyl)-2,2,2-trimethylacetamide, (I) (35DCPTMA) (Fig. 1). Comparison of the bond parameters of 35DCPTMA with those of other amides, namely, *N*-(phenyl)-2,2,2-trimethylacetamide (PTMA) and *N*-(3,5-dimethylphenyl)-2,2,2-trimethylacetamide (35DMPTMA) (Gowda, Paulus *et al.*, 2007) are shown in Table 2. Comparison revealed that *meta*-dichloro ring substitution does not really affect the bond lengths, which are roughly identical within experimental error.




(I)

Molecules of the title compound are linked by N—H···O hydrogen bonds (Table 1), forming a chain running along the *b* axis (Fig. 2).

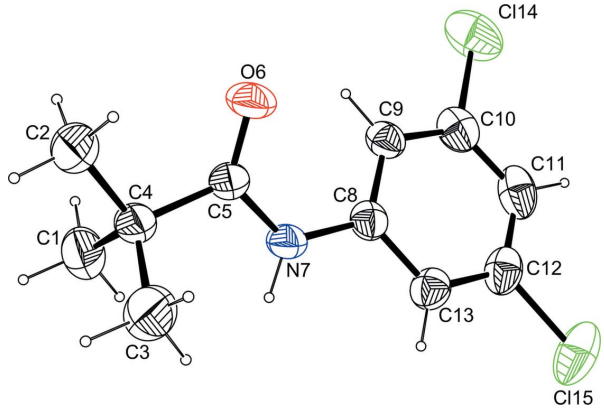



**Figure 1**
The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

## Experimental

The title compound was prepared according to the literature method of Shilpa & Gowda (2007). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Shilpa & Gowda, 2007). Single crystals of the title compound were obtained by slow evaporation of an ethanol solution.

*Crystal data*

$C_{11}H_{13}Cl_2NO$
$M_r$ = 246.12
Orthorhombic, *Pbca*
$a$ = 10.655 (2) Å
$b$ = 9.999 (3) Å
$c$ = 23.275 (9) Å
$V$ = 2479.7 (13) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.50 mm$^{-1}$
$T$ = 299 (2) K
0.40 × 0.14 × 0.03 mm

*Data collection*

Oxford Diffraction Xcalibur diffractometer
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2006)
$T_{min}$ = 0.855, $T_{max}$ = 0.976
14622 measured reflections
2250 independent reflections
1165 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.078

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.094
$wR(F^2)$ = 0.206
$S$ = 1.14
2250 reflections
139 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N7—H7···O6$^{i}$ | 0.86 | 2.08 | 2.900 (5) | 159 |

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

**Table 2**
Comparison of selected geometric parameters (Å, °) of the title compound with those in other related amides.

| Parameter | 35DCPTMA | PTMA | 35DMPTMA |
|---|---|---|---|
| Space group | *Pbca* | *Pca*2$_1$ | *Pbca* |
| Z | 8 | 4 | 8 |
| C($r$)—C($r$)$_{mean}$ | 1.370 (6) | 1.377 (4) | 1.381 (4) |
| C($r$)—C($r$)$_{min}$ | 1.357 (6) | 1.362 (5) | 1.363 (5) |
| C($r$)—C($r$)$_{max}$ | 1.387 (6) | 1.384 (3) | 1.393 (4) |
| C($r$)—N | 1.414 (6) | 1.420 (2) | 1.417 (3) |
| N—C(O) | 1.363 (5) | 1.348 (3) | 1.342 (3) |
| C—O | 1.192 (5) | 1.219 (2) | 1.223 (3) |
| C(O)—C(side) | 1.515 (6) | 1.532 (2) | 1.523 (4) |
| C(2$r$)—C(1$r$)—C(6$r$) | 119.9 (4) | 119.7 (2) | 119.6 (3) |
| C(2$r$)—C(1$r$)—N | 123.1 (4) | 122.4 (2) | 122.1 (3) |
| C(6$r$)—C(1$r$)—N | 117.0 (4) | 117.9 (2) | 118.2 (3) |
| C(1$r$)—N—C(O) | 126.9 (4) | 126.8 (2) | 127.2 (2) |
| N—C(O)—C(side) | 115.4 (4) | 116.1 (2) | 116.8 (2) |
| N—C(O)—O | 120.5 (4) | 122.1 (2) | 120.9 (3) |
| O—C(O)—C(side) | 124.1 (4) | 121.9 (2) | 122.2 (2) |

Note: $r$ = ring and side = side chain.

All H atoms were positioned geometrically and treated as riding with C—H = 0.93 Å (CH aromatic) or 0.96 Å ($CH_3$) and N—H = 0.86 Å, with $U_{iso}$(H) = 1.2$U_{eq}$(CH or NH) and $U_{iso}$(H) = 1.5$U_{eq}$($CH_3$).

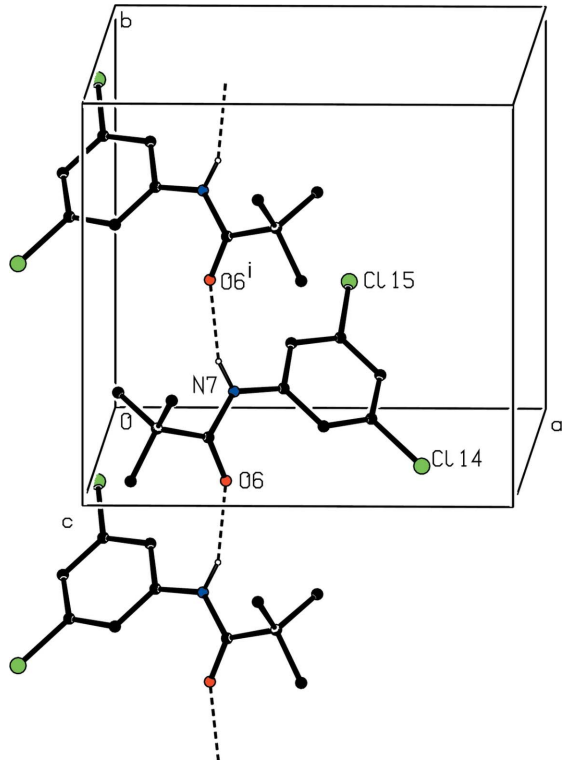



**Figure 2**
Partial packing view, showing the N—H···O hydrogen bonds linking the molecules into a chain. H bonds are shown as dashed lines. For the sake of clarity, H atoms not involved in hydrogen bonding have been omitted. [Symmetry code: (i) $\frac{1}{2}-x, \frac{1}{2}+y, z$]

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997), *PLATON* and *WinGX* (Farrugia, 1999).

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