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## Structure Reports

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## N-(2,5-Dichlorophenyl)acetamide

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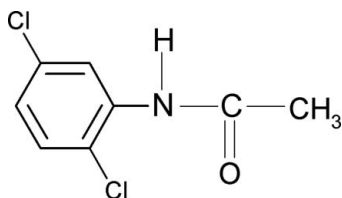
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Key indicators: single-crystal X-ray study;  $T = 299$  K; mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å;  $R$  factor = 0.055;  $wR$  factor = 0.108; data-to-parameter ratio = 14.0.

The conformation of the N—H bond in the title compound,  $\text{C}_8\text{H}_7\text{Cl}_2\text{NO}$ , is *syn* to the *ortho*-chloro group and *anti* to the *meta*-chloro group, in contrast to the *syn* conformation observed with respect to both *ortho*- and *meta*-chloro substituents in *N*-(2,3-dichlorophenyl)acetamide and the *anti* conformation with respect to the *meta*-chloro substituent in *N*-(3,4-dichlorophenyl)acetamide. The dihedral angle between the dichlorophenyl and acetamide groups is  $44.6(2)^\circ$ . Short Cl...Cl type II contacts ( $\text{Cl}\cdots\text{Cl} = 3.5$  Å) and intermolecular N—H...O hydrogen bonds link the molecules into chains.

## Related literature

For related literature, see: Allen *et al.* (1987); Gowda *et al.* (2007*a,b*); Gowda, Kozisek *et al.* (2007, and references therein); Jones *et al.* (1990); Pies *et al.* (1971); Shilpa & Gowda (2007); Wan *et al.* (2006).



## Experimental

## Crystal data

$\text{C}_8\text{H}_7\text{Cl}_2\text{NO}$   
 $M_r = 204.05$   
Monoclinic,  $P2_1/n$   
 $a = 5.8557(4)$  Å  
 $b = 4.7942(4)$  Å

$c = 31.822(2)$  Å  
 $\beta = 90.531(6)^\circ$   
 $V = 893.31(11)$  Å<sup>3</sup>  
 $Z = 4$   
Cu  $K\alpha$  radiation

$\mu = 6.13$  mm<sup>-1</sup>  
 $T = 299(2)$  K

0.15 × 0.10 × 0.03 mm

## Data collection

Enraf–Nonius CAD-4 diffractometer  
Absorption correction:  $\psi$  scan (North *et al.*, 1968)  
 $T_{\min} = 0.478$ ,  $T_{\max} = 0.832$   
3583 measured reflections

1569 independent reflections  
1017 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.213$   
3 standard reflections  
frequency: 120 min  
intensity decay: 1.0%

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.055$   
 $wR(F^2) = 0.108$   
 $S = 1.05$   
1569 reflections  
112 parameters  
1 restraint

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\max} = 0.28$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.48$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N4}-\text{H4N}\cdots\text{O3}^i$	0.841 (10)	2.099 (14)	2.921 (3)	166 (4)

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

Data collection: *CAD-4-PC* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GW2016).

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**supplementary materials**

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## *N*-(2,5-Dichlorophenyl)acetamide

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### Comment

The amide moiety is an important constituent of many biologically significant compounds. The structural studies of amides are therefore of interest (Gowda *et al.*, 2007*a,b*; Gowda, Kozisek *et al.*, 2007, and references therein; Jones *et al.*, 1990; Wan *et al.*, 2006). As part of a study of the effect of ring and side chain substitutions on the solid state structures of this class of compounds (Gowda *et al.*, 2007*a,b*; Gowda, Kozisek *et al.*, 2007, and references therein), the crystal structure of *N*-(2,5-dichlorophenyl)-acetamide (25DCPA) has been determined. The conformation of the N—H bond in 25DCPA is *syn* to the *ortho* chloro group and *anti* to the *meta* chloro group (Fig. 1), in contrast to the *syn* conformation observed with respect to both *ortho* and *meta* chloro substituents in *N*-(2,3-dichlorophenyl)-acetamide (Gowda *et al.*, 2007*b*) and *anti* conformation observed with respect to the *meta* chloro substituent in *N*-(3,4-dichlorophenyl)-acetamide (Jones *et al.*, 1990). The bond lengths and angles in 25DCPA show normal values (Allen *et al.*, 1987). The molecular skeleton is essentially planar. The dihedral angle between the mean planes of the dichlorophenyl and the acetamide moiety is 44.6 (2) °. The intermolecular N—H...O hydrogen bonds (Table 1) link the molecules into chains (Fig. 2). Further, a short ClA...Cl Type II contact (distance = 3.5 Å) controls the packing in the structure.

### Experimental

The title compound was prepared according to the literature method of Shilpa and Gowda (Shilpa & Gowda, 2007). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared, NMR (Shilpa & Gowda, 2007) and NQR spectra (Pies *et al.*, 1971). Single crystals of the title compound were obtained from a slow evaporation of its ethanolic solution (2 g in about 30 ml ethanol) and used for X-ray diffraction studies at room temperature.

### Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (CH aromatic) or 0.96 Å (CH<sub>3</sub>) and  $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{CH}_3)$ . N—H distance was restrained to 0.86 (1) Å.

### Figures

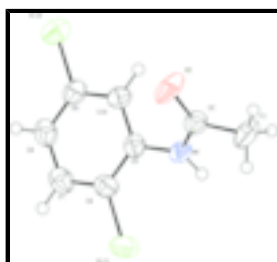


Fig. 1. Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

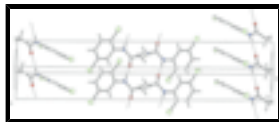


Fig. 2. Crystal packing of the title compound. Hydrogen bonds are shown as dashed lines.

## *N*-(2,5-Dichlorophenyl)acetamide

### Crystal data

$C_8H_7Cl_2NO$	$F_{000} = 416$
$M_r = 204.05$	$D_x = 1.517 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Cu $K\alpha$ radiation
Hall symbol: -P 2yn	$\lambda = 1.54180 \text{ \AA}$
$a = 5.8557 (4) \text{ \AA}$	Cell parameters from 25 reflections
$b = 4.7942 (4) \text{ \AA}$	$\theta = 5.6\text{--}25.3^\circ$
$c = 31.822 (2) \text{ \AA}$	$\mu = 6.13 \text{ mm}^{-1}$
$\beta = 90.531 (6)^\circ$	$T = 299 (2) \text{ K}$
$V = 893.31 (11) \text{ \AA}^3$	Prism, white
$Z = 4$	$0.15 \times 0.10 \times 0.03 \text{ mm}$

### Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{\text{int}} = 0.213$
Radiation source: fine-focus sealed tube	$\theta_{\text{max}} = 66.9^\circ$
Monochromator: graphite	$\theta_{\text{min}} = 2.8^\circ$
$T = 299(2) \text{ K}$	$h = -6 \rightarrow 6$
$\omega/2\theta$ scans	$k = -5 \rightarrow 1$
Absorption correction: $\psi$ scan (North <i>et al.</i> , 1968)	$l = -37 \rightarrow 37$
$T_{\text{min}} = 0.478$ , $T_{\text{max}} = 0.832$	3 standard reflections
3583 measured reflections	every 120 min
1569 independent reflections	intensity decay: 1.0%
1017 reflections with $I > 2\sigma(I)$	

### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.055$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.108$	$w = 1/[\sigma^2(F_o^2)]$
$S = 1.05$	$(\Delta/\sigma)_{\text{max}} < 0.001$
1569 reflections	$\Delta\rho_{\text{max}} = 0.29 \text{ e \AA}^{-3}$
112 parameters	$\Delta\rho_{\text{min}} = -0.48 \text{ e \AA}^{-3}$
1 restraint	Extinction correction: none

Primary atom site location: structure-invariant direct methods

*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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.2319 (10)	0.7304 (5)	0.01550 (14)	0.058 (2)
H1A	0.1171	0.5979	0.0234	0.069*
H1B	0.3502	0.6368	0.0003	0.069*
H1C	0.1643	0.8718	-0.0020	0.069*
C2	0.3318 (8)	0.8623 (5)	0.05414 (13)	0.0379 (12)
C5	0.5242 (9)	0.7740 (5)	0.12195 (12)	0.0357 (12)
C6	0.7266 (8)	0.6682 (5)	0.13610 (12)	0.0395 (12)
C7	0.8178 (9)	0.7474 (6)	0.17467 (15)	0.0468 (14)
H7	0.9556	0.6719	0.1840	0.056*
C8	0.7039 (9)	0.9384 (6)	0.19928 (14)	0.0459 (14)
H8	0.7638	0.9938	0.2251	0.055*
C9	0.5013 (9)	1.0442 (5)	0.18487 (13)	0.0396 (12)
C10	0.4075 (9)	0.9656 (5)	0.14680 (13)	0.0386 (12)
H10	0.2685	1.0392	0.1378	0.046*
N4	0.4305 (7)	0.6906 (4)	0.08251 (10)	0.0371 (10)
H4N	0.424 (7)	0.522 (3)	0.0752 (12)	0.045*
O3	0.3239 (7)	1.1152 (3)	0.05928 (9)	0.0610 (13)
Cl11	0.8771 (2)	0.43003 (17)	0.10588 (4)	0.0553 (4)
Cl12	0.3522 (2)	1.28471 (15)	0.21550 (3)	0.0535 (4)

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.090 (5)	0.0300 (13)	0.053 (3)	0.0036 (19)	-0.022 (3)	-0.0087 (15)
C2	0.043 (4)	0.0297 (12)	0.041 (3)	-0.0012 (17)	-0.001 (2)	0.0017 (15)
C5	0.038 (3)	0.0292 (12)	0.040 (3)	-0.0044 (15)	-0.007 (2)	0.0057 (14)
C6	0.036 (3)	0.0314 (13)	0.052 (3)	0.0000 (17)	0.001 (2)	0.0075 (15)
C7	0.041 (4)	0.0488 (16)	0.051 (3)	0.002 (2)	-0.007 (3)	0.0082 (18)
C8	0.045 (4)	0.0496 (17)	0.043 (3)	-0.004 (2)	-0.011 (2)	0.0026 (18)
C9	0.048 (4)	0.0286 (13)	0.043 (3)	-0.0049 (17)	0.000 (2)	0.0020 (14)
C10	0.042 (3)	0.0298 (12)	0.044 (3)	0.0028 (17)	-0.001 (2)	0.0013 (15)

## supplementary materials

N4	0.043 (3)	0.0235 (10)	0.045 (2)	0.0026 (14)	-0.0064 (18)	-0.0024 (11)
O3	0.108 (4)	0.0222 (8)	0.052 (2)	0.0035 (14)	-0.015 (2)	-0.0009 (11)
C111	0.0448 (10)	0.0533 (5)	0.0679 (9)	0.0153 (5)	0.0043 (6)	-0.0026 (5)
C112	0.0659 (12)	0.0473 (4)	0.0474 (8)	0.0051 (5)	0.0033 (6)	-0.0066 (4)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

C1—C2	1.497 (4)	C6—C111	1.738 (5)
C1—H1A	0.9600	C7—C8	1.381 (7)
C1—H1B	0.9600	C7—H7	0.9300
C1—H1C	0.9600	C8—C9	1.366 (6)
C2—O3	1.225 (3)	C8—H8	0.9300
C2—N4	1.348 (4)	C9—C10	1.378 (5)
C5—C6	1.362 (5)	C9—C112	1.748 (5)
C5—C10	1.395 (6)	C10—H10	0.9300
C5—N4	1.423 (4)	N4—H4N	0.841 (10)
C6—C7	1.387 (5)		
C2—C1—H1A	109.5	C8—C7—C6	120.0 (4)
C2—C1—H1B	109.5	C8—C7—H7	120.0
H1A—C1—H1B	109.5	C6—C7—H7	120.0
C2—C1—H1C	109.5	C9—C8—C7	118.6 (3)
H1A—C1—H1C	109.5	C9—C8—H8	120.7
H1B—C1—H1C	109.5	C7—C8—H8	120.7
O3—C2—N4	122.1 (3)	C8—C9—C10	122.1 (4)
O3—C2—C1	120.9 (3)	C8—C9—C112	119.6 (3)
N4—C2—C1	117.0 (2)	C10—C9—C112	118.3 (4)
C6—C5—C10	119.1 (3)	C9—C10—C5	119.0 (4)
C6—C5—N4	121.0 (4)	C9—C10—H10	120.5
C10—C5—N4	119.9 (4)	C5—C10—H10	120.5
C5—C6—C7	121.2 (4)	C2—N4—C5	125.3 (2)
C5—C6—C111	120.4 (3)	C2—N4—H4N	113 (2)
C7—C6—C111	118.4 (3)	C5—N4—H4N	122 (2)
C10—C5—C6—C7	0.1 (6)	C8—C9—C10—C5	-0.7 (7)
N4—C5—C6—C7	-179.5 (4)	C112—C9—C10—C5	180.0 (3)
C10—C5—C6—C111	-179.8 (3)	C6—C5—C10—C9	0.5 (6)
N4—C5—C6—C111	0.6 (6)	N4—C5—C10—C9	-179.9 (4)
C5—C6—C7—C8	-0.5 (7)	O3—C2—N4—C5	3.6 (8)
C111—C6—C7—C8	179.3 (3)	C1—C2—N4—C5	-176.7 (5)
C6—C7—C8—C9	0.4 (7)	C6—C5—N4—C2	-137.7 (5)
C7—C8—C9—C10	0.2 (7)	C10—C5—N4—C2	42.7 (7)
C7—C8—C9—C112	179.6 (3)		

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N4—H4N $\cdots$ O3 <sup>i</sup>	0.841 (10)	2.099 (14)	2.921 (3)	166 (4)

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

Fig. 1

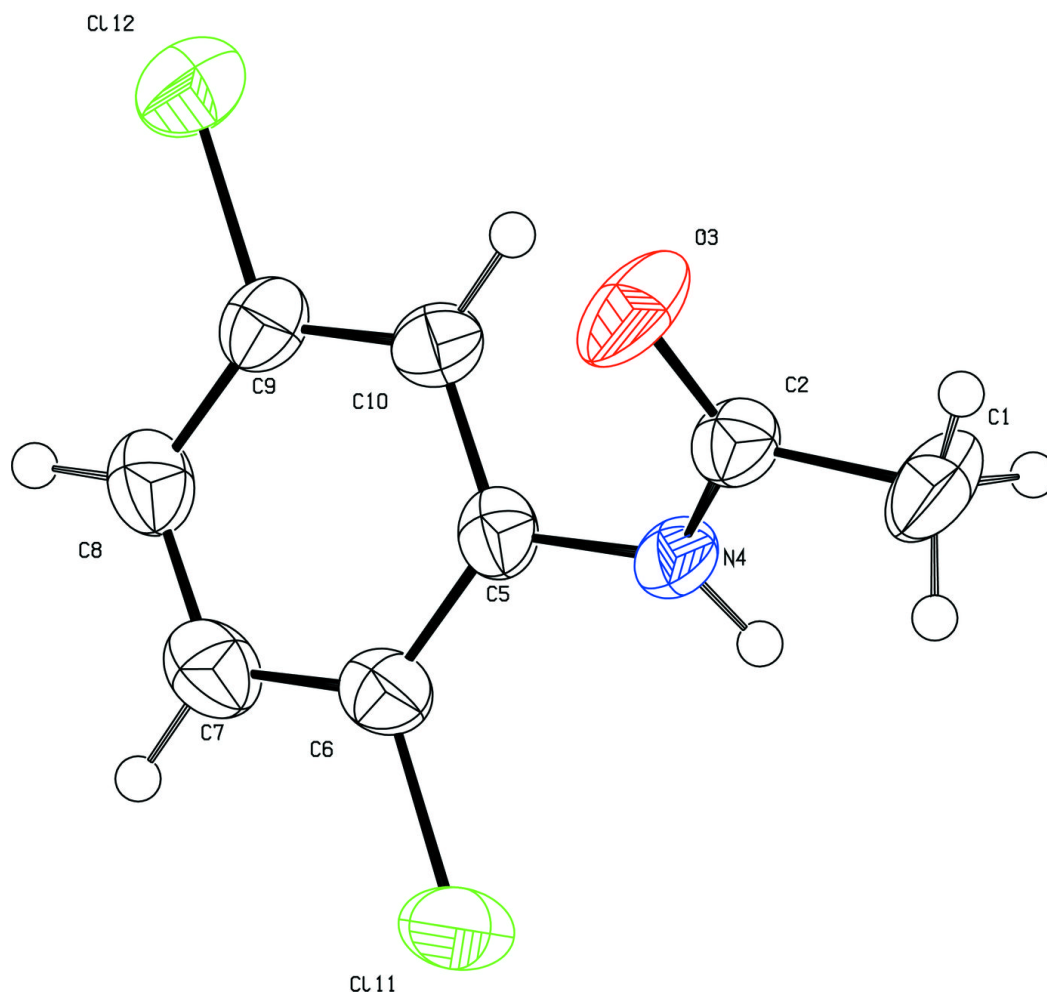


Fig. 2

