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## 1-(3-Chlorophenyl)-3-(2,6-dichlorobenzoyl)thiourea

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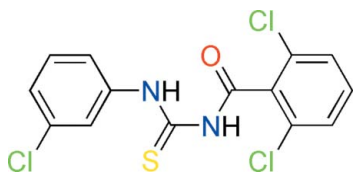
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Key indicators: single-crystal X-ray study;  $T = 173$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.037;  $wR$  factor = 0.094; data-to-parameter ratio = 25.5.

The structure of the title compound,  $\text{C}_{14}\text{H}_9\text{Cl}_3\text{N}_2\text{OS}$ , is composed of discrete molecules with bond lengths and angles quite typical for thiourea compounds of this class. The plane containing the thiocarbonyl and carbonyl groups subtends dihedral angles of  $48.19$  (3) and  $87.51$  (3)° with the planes formed by the 3-chloro and 2,6-dichlorophenyl rings, respectively; the dihedral angle between the two benzene ring planes is  $45.32$  (3)°. An intramolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bond stabilizes the molecular conformation and the molecules form intermolecular  $\text{N}-\text{H}\cdots\text{S}$  and  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds, generating a sheet along the  $a$  axis.

## Related literature

For related structures, see: Khawar Rauf *et al.*, (2006*a,b*; 2007). For a description of the Cambridge structural Database, see: Allen (2002).



## Experimental

## Crystal data

 $\text{C}_{14}\text{H}_9\text{Cl}_3\text{N}_2\text{OS}$  $M_r = 359.64$ 

Monoclinic,  $P2_1/c$   
 $a = 10.6589$  (5) Å  
 $b = 11.2114$  (5) Å  
 $c = 13.2919$  (6) Å  
 $\beta = 99.942$  (3)°  
 $V = 1564.55$  (12) Å<sup>3</sup>

$Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.72$  mm<sup>-1</sup>  
 $T = 173$  (2) K  
 $0.47 \times 0.47 \times 0.45$  mm

## Data collection

Stoe IPDS-II two-circle diffractometer  
 Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)  
 $T_{\min} = 0.729$ ,  $T_{\max} = 0.739$

39690 measured reflections  
 5066 independent reflections  
 4674 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.046$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.094$   
 $S = 1.06$   
 5066 reflections  
 199 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\max} = 0.65$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.66$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$                             | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{N2}-\text{H2}\cdots\text{O1}$             | 0.82 (2)     | 2.07 (2)           | 2.7190 (13) | 136.0 (18)           |
| $\text{N2}-\text{H2}\cdots\text{O1}^{\text{i}}$  | 0.82 (2)     | 2.37 (2)           | 3.0749 (14) | 145.5 (18)           |
| $\text{N1}-\text{H1}\cdots\text{S1}^{\text{ii}}$ | 0.86 (2)     | 2.47 (2)           | 3.2974 (10) | 163.6 (18)           |

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

Data collection: *X-Area* (Stoe & Cie, 2001); cell refinement: *X-Area*; data reduction: *X-Area*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003) and *XP* in *SHELXTL-Plus* (Sheldrick, 2008); software used to prepare material for publication: *PLATON* and *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2127).

## References

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**supplementary materials**

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## 1-(3-Chlorophenyl)-3-(2,6-dichlorobenzoyl)thiourea

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### Comment

The background to this study has been set out in our previous work on the structural chemistry of N,N'-disubstituted thioureas (Khawar Rauf et al., 2006a, 2007). Herein, as a continuation of these studies, the structure of the title compound, (I), is described.

In the structure of the title compound (Fig. 1), bond lengths and bond angles can be regarded as typical for N,N'-disubstituted thiourea compounds as found in the Cambridge Structural Database v5.28 (Allen, 2002) and some related structures (Khawar Rauf et al., 2006b). The molecule exists in the thione form with typical thiourea C—S and C—O bonds, as well as shortened C—N bonds. The thiocarbonyl and carbonyl groups are almost coplanar. The molecule features an intramolecular N—H···O hydrogen bond in the crystal structure. The molecules lying about inversion centers associate via N—H···S intermolecular hydrogen bonds to form dimers on one side and a similar association via N—H···O hydrogen bonding on the other side thus result in a sheet of molecules of (I) along the *a*-axis (Table 1; Fig. 2).

### Experimental

Freshly prepared and steam distilled 2,6-dichlorobenzoyl isothiocyanate (2.32 g, 10 mmol) was stirred in acetone (30 ml) for 20 minutes. Neat 3-chloroaniline (1.27 g, 10 mmol) was then added and the resulting mixture was stirred for 1 h. The reaction mixture was then poured into acidified (pH 4) water (approx. 300 ml) and stirred well. The solid product was separated, washed with deionized water and purified by recrystallization from methanol/1,1-dichloromethane (1:10 v/v) to give fine crystals of (I), with an overall yield of 85%.

### Refinement

Hydrogen atoms bonded to C were included in calculated positions and refined as riding on their parent C atom with C—H = 0.95 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The H atoms bonded to N were freely refined.

### Figures

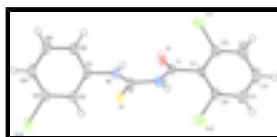


Fig. 1. Molecular structure of (I) showing atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

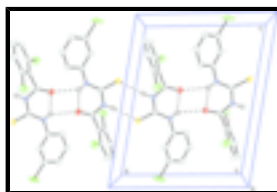


Fig. 2. A view of the unit cell of (I) showing hydrogen bonds as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

## 1-(3-Chlorophenyl)-3-(2,6-dichlorobenzoyl)thiourea

### Crystal data

|                                  |   |
|----------------------------------|---|
| $C_{14}H_9Cl_3N_2OS$             | $F_{000} = 728$                           |
| $M_r = 359.64$                   | $D_x = 1.527 \text{ Mg m}^{-3}$           |
| Monoclinic, $P2_1/c$             | Mo $K\alpha$ radiation                    |
| Hall symbol: -P 2ybc             | $\lambda = 0.71073 \text{ \AA}$           |
| $a = 10.6589 (5) \text{ \AA}$    | Cell parameters from 37695 reflections    |
| $b = 11.2114 (5) \text{ \AA}$    | $\theta = 3.7\text{--}31.2^\circ$         |
| $c = 13.2919 (6) \text{ \AA}$    | $\mu = 0.72 \text{ mm}^{-1}$              |
| $\beta = 99.942 (3)^\circ$       | $T = 173 (2) \text{ K}$                   |
| $V = 1564.55 (12) \text{ \AA}^3$ | Block, colourless                         |
| $Z = 4$                          | $0.47 \times 0.47 \times 0.45 \text{ mm}$ |

### Data collection

|  |  |
|--|--|
| Stoe IPDS-II two-circle diffractometer                                 | 5066 independent reflections           |
| Radiation source: fine-focus sealed tube                               | 4674 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite  | $R_{\text{int}} = 0.046$               |
| $T = 173(2) \text{ K}$   | $\theta_{\text{max}} = 31.3^\circ$     |
| $\omega$ scans   | $\theta_{\text{min}} = 3.6^\circ$      |
| Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995) | $h = -15 \rightarrow 15$               |
| $T_{\text{min}} = 0.729$ , $T_{\text{max}} = 0.739$                    | $k = -16 \rightarrow 16$               |
| 39690 measured reflections   | $l = -19 \rightarrow 19$               |

### Refinement

|  |  |
|--|--|
| Refinement on $F^2$  | Hydrogen site location: inferred from neighbouring sites   |
| Least-squares matrix: full                                     | H atoms treated by a mixture of independent and constrained refinement   |
| $R[F^2 > 2\sigma(F^2)] = 0.037$                                | $w = 1/[\sigma^2(F_o^2) + (0.0404P)^2 + 0.9365P]$  |
| $wR(F^2) = 0.094$  | where $P = (F_o^2 + 2F_c^2)/3$   |
| $S = 1.06$   | $(\Delta/\sigma)_{\text{max}} = 0.001$   |
| 5066 reflections   | $\Delta\rho_{\text{max}} = 0.65 \text{ e \AA}^{-3}$  |
| 199 parameters   | $\Delta\rho_{\text{min}} = -0.66 \text{ e \AA}^{-3}$   |
| Primary atom site location: structure-invariant direct methods | Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$ |
| Secondary atom site location: difference Fourier map           | Extinction coefficient: 0.0111 (12)  |

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

|     | <i>x</i>     | <i>y</i>     | <i>z</i>     | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|--------------|----------------------------------|
| S1  | 0.09625 (3)  | 0.60027 (3)  | 0.62517 (2)  | 0.02474 (9)                      |
| C11 | 0.19574 (4)  | 0.61905 (4)  | 0.23352 (3)  | 0.03999 (11)                     |
| C12 | 0.22323 (4)  | 0.18815 (4)  | 0.41908 (3)  | 0.03969 (11)                     |
| C13 | 0.33122 (7)  | 0.61484 (7)  | 0.99688 (3)  | 0.0735 (2)                       |
| C1  | 0.27158 (11) | 0.45474 (11) | 0.41547 (8)  | 0.0182 (2)                       |
| O1  | 0.38737 (8)  | 0.46303 (10) | 0.43625 (7)  | 0.0285 (2)                       |
| N1  | 0.19003 (9)  | 0.49493 (10) | 0.47738 (8)  | 0.01915 (19)                     |
| H1  | 0.1105 (19)  | 0.4841 (18)  | 0.4559 (15)  | 0.030 (5)*                       |
| C2  | 0.21866 (10) | 0.55197 (10) | 0.57210 (8)  | 0.0174 (2)                       |
| N2  | 0.34238 (9)  | 0.56439 (10) | 0.61243 (8)  | 0.01918 (19)                     |
| H2  | 0.394 (2)    | 0.5442 (19)  | 0.5770 (15)  | 0.032 (5)*                       |
| C11 | 0.20320 (10) | 0.39859 (11) | 0.31773 (8)  | 0.0179 (2)                       |
| C12 | 0.16489 (13) | 0.46736 (13) | 0.23029 (10) | 0.0251 (2)                       |
| C13 | 0.09985 (17) | 0.41613 (18) | 0.14040 (11) | 0.0394 (4)                       |
| H13 | 0.0745       | 0.4639       | 0.0814       | 0.047*                           |
| C14 | 0.07264 (17) | 0.29526 (19) | 0.13789 (12) | 0.0421 (4)                       |
| H14 | 0.0275       | 0.2606       | 0.0770       | 0.051*                           |
| C15 | 0.11043 (15) | 0.22420 (15) | 0.22299 (12) | 0.0337 (3)                       |
| H15 | 0.0923       | 0.1412       | 0.2208       | 0.040*                           |
| C16 | 0.17558 (12) | 0.27683 (12) | 0.31200 (10) | 0.0232 (2)                       |
| C21 | 0.39003 (11) | 0.62132 (11) | 0.70818 (9)  | 0.0195 (2)                       |
| C22 | 0.34464 (15) | 0.58955 (14) | 0.79662 (10) | 0.0289 (3)                       |
| H22 | 0.2822       | 0.5288       | 0.7953       | 0.035*                           |
| C23 | 0.39279 (16) | 0.64880 (16) | 0.88702 (10) | 0.0340 (3)                       |
| C24 | 0.48645 (15) | 0.73570 (15) | 0.89168 (11) | 0.0332 (3)                       |
| H24 | 0.5180       | 0.7752       | 0.9541       | 0.040*                           |
| C25 | 0.53305 (14) | 0.76367 (15) | 0.80313 (11) | 0.0318 (3)                       |
| H25 | 0.5984       | 0.8218       | 0.8053       | 0.038*                           |
| C26 | 0.48479 (12) | 0.70721 (13) | 0.71106 (10) | 0.0246 (2)                       |
| H26 | 0.5164       | 0.7273       | 0.6507       | 0.030*                           |

## supplementary materials

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

|     | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$      | $U^{13}$     | $U^{23}$      |
|-----|--------------|--------------|--------------|---------------|--------------|---------------|
| S1  | 0.01676 (13) | 0.03383 (17) | 0.02412 (15) | -0.00159 (11) | 0.00495 (10) | -0.01452 (12) |
| C11 | 0.0485 (2)   | 0.02974 (18) | 0.0415 (2)   | -0.00112 (15) | 0.00718 (16) | 0.00931 (14)  |
| C12 | 0.0507 (2)   | 0.02793 (17) | 0.0402 (2)   | 0.00109 (15)  | 0.00724 (16) | 0.00754 (14)  |
| C13 | 0.1095 (5)   | 0.0945 (5)   | 0.02015 (18) | -0.0585 (4)   | 0.0216 (2)   | -0.0165 (2)   |
| C1  | 0.0160 (4)   | 0.0228 (5)   | 0.0156 (4)   | 0.0010 (4)    | 0.0018 (4)   | -0.0044 (4)   |
| O1  | 0.0144 (4)   | 0.0461 (6)   | 0.0246 (4)   | 0.0004 (4)    | 0.0023 (3)   | -0.0134 (4)   |
| N1  | 0.0133 (4)   | 0.0275 (5)   | 0.0163 (4)   | -0.0008 (3)   | 0.0016 (3)   | -0.0081 (4)   |
| C2  | 0.0171 (5)   | 0.0197 (5)   | 0.0152 (4)   | -0.0009 (4)   | 0.0018 (4)   | -0.0037 (4)   |
| N2  | 0.0153 (4)   | 0.0266 (5)   | 0.0152 (4)   | -0.0008 (4)   | 0.0015 (3)   | -0.0061 (4)   |
| C11 | 0.0160 (4)   | 0.0231 (5)   | 0.0147 (4)   | -0.0007 (4)   | 0.0030 (4)   | -0.0051 (4)   |
| C12 | 0.0247 (6)   | 0.0317 (6)   | 0.0185 (5)   | -0.0009 (5)   | 0.0023 (4)   | 0.0000 (4)    |
| C13 | 0.0408 (8)   | 0.0571 (10)  | 0.0173 (6)   | -0.0037 (7)   | -0.0037 (5)  | -0.0014 (6)   |
| C14 | 0.0391 (8)   | 0.0612 (11)  | 0.0243 (6)   | -0.0127 (8)   | 0.0002 (6)   | -0.0189 (7)   |
| C15 | 0.0315 (7)   | 0.0355 (7)   | 0.0350 (7)   | -0.0098 (6)   | 0.0080 (5)   | -0.0185 (6)   |
| C16 | 0.0225 (5)   | 0.0246 (6)   | 0.0236 (5)   | -0.0020 (4)   | 0.0070 (4)   | -0.0059 (4)   |
| C21 | 0.0185 (5)   | 0.0235 (5)   | 0.0151 (4)   | -0.0003 (4)   | -0.0005 (4)  | -0.0049 (4)   |
| C22 | 0.0358 (7)   | 0.0330 (7)   | 0.0168 (5)   | -0.0123 (5)   | 0.0015 (5)   | -0.0041 (5)   |
| C23 | 0.0446 (8)   | 0.0414 (8)   | 0.0156 (5)   | -0.0123 (7)   | 0.0041 (5)   | -0.0064 (5)   |
| C24 | 0.0341 (7)   | 0.0410 (8)   | 0.0222 (6)   | -0.0079 (6)   | -0.0016 (5)  | -0.0123 (5)   |
| C25 | 0.0265 (6)   | 0.0382 (8)   | 0.0300 (6)   | -0.0108 (5)   | 0.0027 (5)   | -0.0129 (6)   |
| C26 | 0.0206 (5)   | 0.0305 (6)   | 0.0229 (5)   | -0.0044 (5)   | 0.0038 (4)   | -0.0076 (5)   |

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

|           |             |             |             |
|-----------|-------------|-------------|-------------|
| S1—C2     | 1.6766 (12) | C13—H13     | 0.9500      |
| C11—C12   | 1.7313 (15) | C14—C15     | 1.385 (3)   |
| C12—C16   | 1.7386 (14) | C14—H14     | 0.9500      |
| C13—C23   | 1.7433 (15) | C15—C16     | 1.3951 (18) |
| C1—O1     | 1.2209 (14) | C15—H15     | 0.9500      |
| C1—N1     | 1.3721 (14) | C21—C26     | 1.3912 (18) |
| C1—C11    | 1.5128 (15) | C21—C22     | 1.3925 (18) |
| N1—C2     | 1.3980 (14) | C22—C23     | 1.3912 (18) |
| N1—H1     | 0.86 (2)    | C22—H22     | 0.9500      |
| C2—N2     | 1.3423 (14) | C23—C24     | 1.389 (2)   |
| N2—C21    | 1.4360 (14) | C24—C25     | 1.390 (2)   |
| N2—H2     | 0.82 (2)    | C24—H24     | 0.9500      |
| C11—C12   | 1.3957 (17) | C25—C26     | 1.3947 (17) |
| C11—C16   | 1.3957 (17) | C25—H25     | 0.9500      |
| C12—C13   | 1.3971 (19) | C26—H26     | 0.9500      |
| C13—C14   | 1.385 (3)   |             |             |
| O1—C1—N1  | 124.03 (10) | C14—C15—C16 | 118.77 (14) |
| O1—C1—C11 | 122.98 (10) | C14—C15—H15 | 120.6       |
| N1—C1—C11 | 112.99 (9)  | C16—C15—H15 | 120.6       |
| C1—N1—C2  | 128.90 (10) | C15—C16—C11 | 121.96 (13) |

|                 |              |                 |              |
|-----------------|--------------|-----------------|--------------|
| C1—N1—H1        | 116.6 (13)   | C15—C16—C12     | 118.99 (11)  |
| C2—N1—H1        | 114.5 (13)   | C11—C16—C12     | 119.05 (9)   |
| N2—C2—N1        | 116.98 (10)  | C26—C21—C22     | 120.68 (11)  |
| N2—C2—S1        | 125.50 (9)   | C26—C21—N2      | 118.43 (11)  |
| N1—C2—S1        | 117.52 (8)   | C22—C21—N2      | 120.88 (11)  |
| C2—N2—C21       | 124.95 (10)  | C23—C22—C21     | 118.48 (13)  |
| C2—N2—H2        | 117.2 (14)   | C23—C22—H22     | 120.8        |
| C21—N2—H2       | 117.5 (14)   | C21—C22—H22     | 120.8        |
| C12—C11—C16     | 117.79 (11)  | C24—C23—C22     | 121.91 (13)  |
| C12—C11—C1      | 120.90 (11)  | C24—C23—C13     | 119.18 (10)  |
| C16—C11—C1      | 121.31 (11)  | C22—C23—C13     | 118.89 (12)  |
| C11—C12—C13     | 121.04 (14)  | C23—C24—C25     | 118.67 (12)  |
| C11—C12—C11     | 119.67 (10)  | C23—C24—H24     | 120.7        |
| C13—C12—C11     | 119.28 (12)  | C25—C24—H24     | 120.7        |
| C14—C13—C12     | 119.59 (15)  | C24—C25—C26     | 120.60 (13)  |
| C14—C13—H13     | 120.2        | C24—C25—H25     | 119.7        |
| C12—C13—H13     | 120.2        | C26—C25—H25     | 119.7        |
| C13—C14—C15     | 120.85 (13)  | C21—C26—C25     | 119.62 (12)  |
| C13—C14—H14     | 119.6        | C21—C26—H26     | 120.2        |
| C15—C14—H14     | 119.6        | C25—C26—H26     | 120.2        |
| O1—C1—N1—C2     | 0.6 (2)      | C14—C15—C16—C11 | 0.2 (2)      |
| C11—C1—N1—C2    | -179.35 (12) | C14—C15—C16—C12 | 179.98 (12)  |
| C1—N1—C2—N2     | -4.11 (19)   | C12—C11—C16—C15 | -0.86 (18)   |
| C1—N1—C2—S1     | 175.27 (11)  | C1—C11—C16—C15  | 178.74 (12)  |
| N1—C2—N2—C21    | 179.40 (11)  | C12—C11—C16—C12 | 179.39 (9)   |
| S1—C2—N2—C21    | 0.07 (18)    | C1—C11—C16—C12  | -1.01 (16)   |
| O1—C1—C11—C12   | -90.46 (16)  | C2—N2—C21—C26   | -130.55 (14) |
| N1—C1—C11—C12   | 89.48 (14)   | C2—N2—C21—C22   | 50.86 (18)   |
| O1—C1—C11—C16   | 89.95 (16)   | C26—C21—C22—C23 | 2.4 (2)      |
| N1—C1—C11—C16   | -90.11 (14)  | N2—C21—C22—C23  | -179.07 (14) |
| C16—C11—C12—C13 | 0.68 (19)    | C21—C22—C23—C24 | -1.7 (3)     |
| C1—C11—C12—C13  | -178.93 (13) | C21—C22—C23—C13 | 176.96 (13)  |
| C16—C11—C12—C11 | 179.53 (10)  | C22—C23—C24—C25 | -0.1 (3)     |
| C1—C11—C12—C11  | -0.07 (16)   | C13—C23—C24—C25 | -178.76 (14) |
| C11—C12—C13—C14 | 0.1 (2)      | C23—C24—C25—C26 | 1.3 (3)      |
| C11—C12—C13—C14 | -178.73 (14) | C22—C21—C26—C25 | -1.2 (2)     |
| C12—C13—C14—C15 | -0.8 (3)     | N2—C21—C26—C25  | -179.82 (13) |
| C13—C14—C15—C16 | 0.6 (2)      | C24—C25—C26—C21 | -0.6 (2)     |

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> |
|---------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| N2—H2 $\cdots$ O1               | 0.82 (2)    | 2.07 (2)            | 2.7190 (13)                | 136.0 (18)                    |
| N2—H2 $\cdots$ O1 <sup>i</sup>  | 0.82 (2)    | 2.37 (2)            | 3.0749 (14)                | 145.5 (18)                    |
| N1—H1 $\cdots$ S1 <sup>ii</sup> | 0.86 (2)    | 2.47 (2)            | 3.2974 (10)                | 163.6 (18)                    |

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

Fig. 1

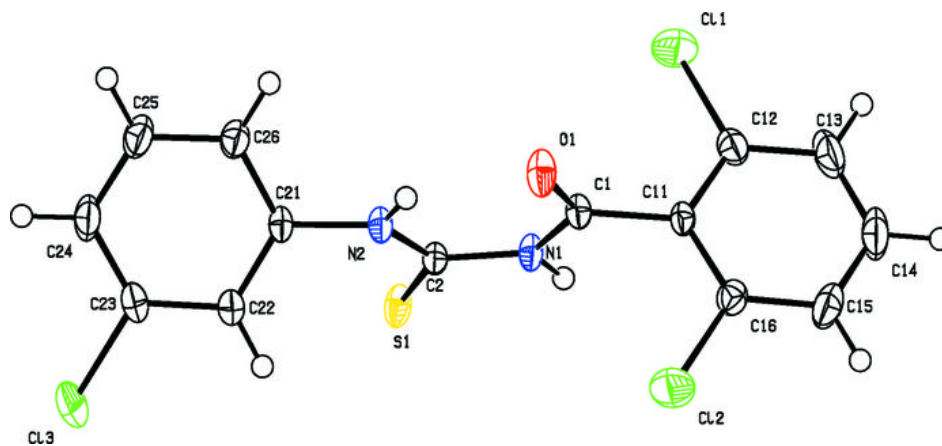


Fig. 2

