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# (2*Z*)-3-(2,4-Dichlorophenyl)-3-hydroxy-*N*-phenylprop-2-enethioamide

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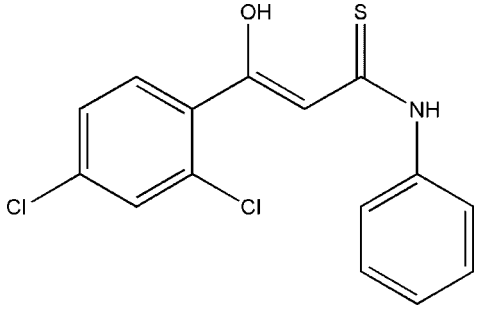
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.044; $wR$ factor = 0.091; data-to-parameter ratio = 15.3.

In the title molecule, $C_{15}H_{11}Cl_2NOS$, the dihedral angle between the phenyl and benzene rings is 72.24 (1)°. In the crystal, pairs of N—H···S hydrogen bonds form dimers with twofold rotational symmetry. The dimers are connected by weak C—H···O hydrogen bonds, forming a two-dimensional network parallel to (001). An intramolecular O—H···S hydrogen bond is also observed.

## Related literature

For the biological activity and applications of thioamides, see: Zahid *et al.* (2009); Jagodzinski (2003); Lebana *et al.* (2008). For the synthesis of thioamides, see: Bauer & Kuhlein (1985); Cava & Levinson (1985). For the synthesis of the title compound, see: Rudrof *et al.* (1979). For related structures, see: Xu *et al.* (2005); Cowley *et al.* (2002); Jiang (2009); Patil *et al.* (2011); Deshmukh *et al.* (2009). For standard bond-length data, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_{15}H_{11}Cl_2NOS$
$M_r$ = 324.21
Orthorhombic, *Pccn*
$a$ = 28.9562 (6) Å
$b$ = 13.2610 (3) Å
$c$ = 7.5284 (2) Å
$V$ = 2890.82 (12) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.59 mm$^{-1}$
$T$ = 293 K
0.3 × 0.2 × 0.1 mm

### Data collection

Agilent Xcalibur Sapphire3 diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
$T_{min}$ = 0.835, $T_{max}$ = 1.000
63107 measured reflections
2836 independent reflections
2275 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.067

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.091
$S$ = 1.11
2836 reflections
185 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···S1$^{i}$ | 0.86 | 2.61 | 3.4397 (18) | 162 |
| C3′—H3′···O1$^{ii}$ | 0.93 | 2.59 | 3.496 (3) | 164 |
| O1—H11···S1 | 0.89 (3) | 2.10 (3) | 2.9315 (18) | 157 (2) |

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *PLATON* (Spek, 2009).

RK is thankful to the Department of Science & Technology for the single-crystal X-ray diffractometer sanctioned as a National Facility under project No. SR/S2/ CMP-47/2003.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5625).

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# supporting information

*Acta Cryst.* (2013). E**69**, o1173–o1174 [https://doi.org/10.1107/S1600536813017339]

## (2*Z*)-3-(2,4-Dichlorophenyl)-3-hydroxy-*N*-phenylprop-2-enethioamide

**Dalbir Kour, Kuldeep Singh, Mayur M. Aitawade, Madhukar B. Deshmukh, Prashant V. Anbhule, Vivek K. Gupta and Rajni Kant**

### S1. Comment

Thioamides exhibit a wide range of applications, not only as synthetic intermediates in the synthesis of a variety of hetero-cyclic compounds (Zahid *et al.*, 2009), but also numerous biological activities have been associated with them (Jagodzinski, 2003). Moreover, thioamides are important ligands in the field of coordination chemistry (Lebana *et al.*, 2008). Several synthetic reports on thioamides have been published involving the uses of Lawesson's regent (Cava & Levinson, 1985) and phosphorus pentasulfide (Bauer & Kuhlein, 1985). Our ongoing research involves the development of newer synthetic methodologies for heterocyclic compounds (Patil *et al.*, 2011; Deshmukh *et al.*, 2009). The crystal structure of the title compound is described herein.

The molecular structure of the title compound (I) is shown in Fig. 1. The bond lengths (Allen, *et al.*, 1987) and angles observed in (I) show normal values and are comparable with related structures (Xu, *et al.*, 2005; Jiang, 2009). The dihedral angle between the phenyl and benzene rings [C1′-C6′ and C4-C9] is 72.24 (1)°. The two chlorine atoms Cl1 and Cl2 which were not included in the calculation of the least-squares plane of the C1′-C6′ ring, deviate from the plane by 0.1336 (1) and 0.0310 (1) Å. The C1—S1 bond length of 1.695 (2) Å is comparable with the value [1.688 (2) Å] in a related structure (Cowley *et al.*, 2002). In the crystal, pairs of N—H···S hydrogen bonds form dimers with twofold rotational symmetry. The dimers are connected by weak C—H···O hydrogen bonds to form a two-dimensional network parallel to (001). An intramolecular O—H···S hydrogen bond is also observed. The hydrogen bonds are shown in Fig. 2.

### S2. Experimental

(2*Z*)-3-(2,4-dichlorophenyl)-3-hydroxy-*N*-phenylprop-2-enethioamide was synthesized by a previously reported procedure (Rudrof *et al.*, 1979). The product dissolved in EtOH, on slow evaporation of the solvent formed crystals of the title compound. Yield: 85%. IR (KBr): 3442, 3207, 1607, 1364, 1224 cm-1. 1H NMR (300 MHz, CDCl3): dH = 5.97 (s, 1H, CH), 7.19–7.53 (m, 8H, Ar—H),8.29 (bs, 1H, NH), 14.75 (s, 1H, OH). 13 C NMR (CDCl3): dc = 136.3, 133.7, 132.6, 131.2, 137.0, 130.9, 129.4, 128.8, 127.5, 127.1, 126.8, 125.2, 123.1. (m/*z*) = 324.

### S3. Refinement

Hydrogen atom H11 bonded to O1 was located in a difference Fourier map and was refined independently with an isotropic displacement parameter. All other H atoms were positioned geometrically and were treated as riding on their parent atoms, with C—H = 0.93 Å, N—H = 0.86Å and $U_{iso}$(H)=1.2$U_{eq}$(C,N).

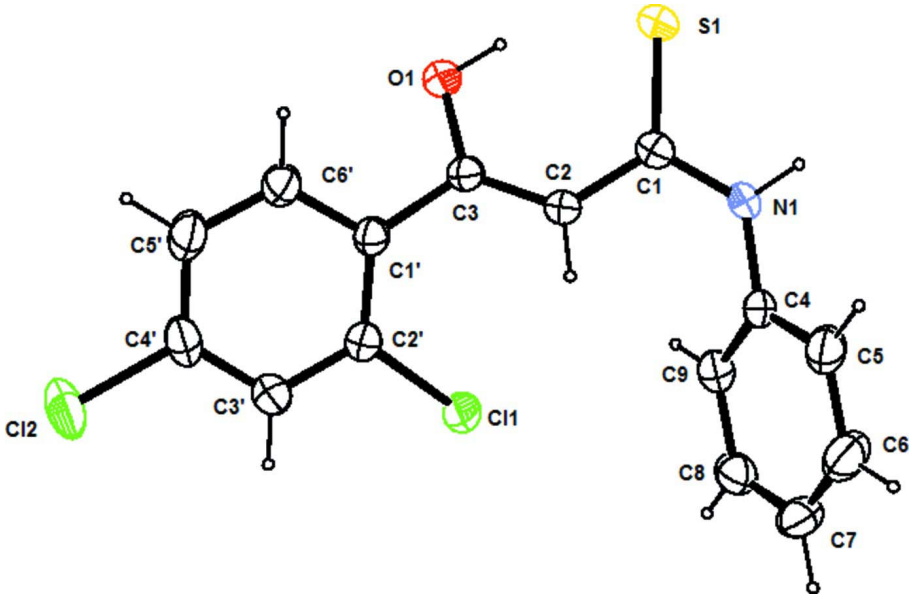


**Figure 1**

The molecular structure of (I) with displacement ellipsoids drawn at the 40% probability level. H atoms are shown as small spheres of arbitrary radii.

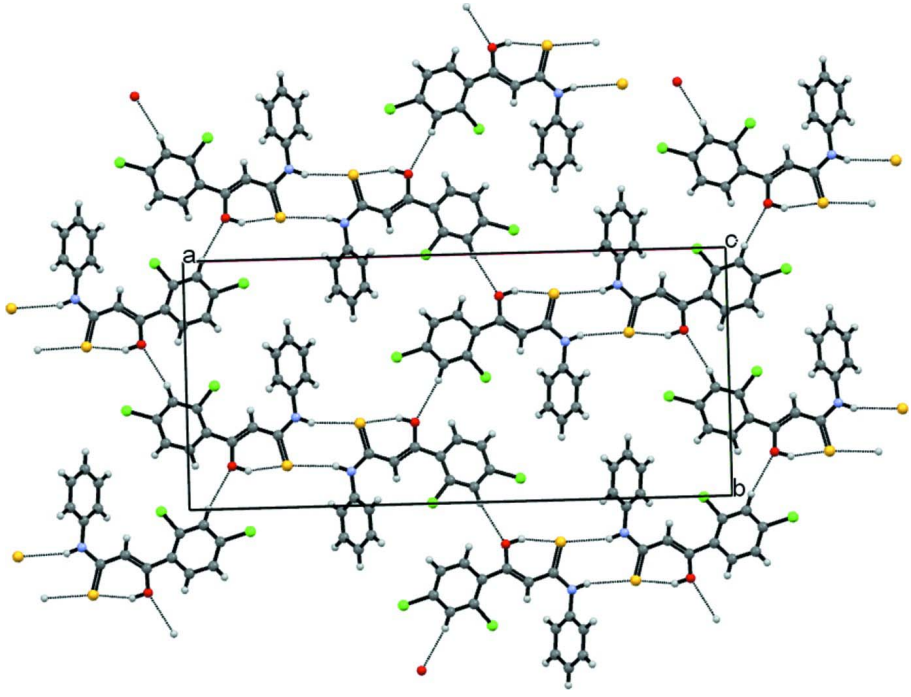


**Figure 2**

Part of the crystal structure with hydrogen bonds shown as dotted lines.

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*Crystal data*

$C_{15}H_{11}Cl_2NOS$
$M_r = 324.21$
Orthorhombic, *Pccn*
Hall symbol: -P 2ab 2ac
$a = 28.9562$ (6) Å
$b = 13.2610$ (3) Å
$c = 7.5284$ (2) Å
$V = 2890.82$ (12) Å$^3$
$Z = 8$
$F(000) = 1328$
$D_x = 1.490$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 24816 reflections
$\theta = 3.4$–$29.1°$
$\mu = 0.59$ mm$^{-1}$
$T = 293$ K
Block, orange
0.3 × 0.2 × 0.1 mm

*Data collection*

Agilent Xcalibur Sapphire3 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 16.1049 pixels mm$^{-1}$
$\omega$ scan
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
$T_{min} = 0.835$, $T_{max} = 1.000$
63107 measured reflections
2836 independent reflections
2275 reflections with $I > 2\sigma(I)$
$R_{int} = 0.067$
$\theta_{max} = 26.0°$, $\theta_{min} = 3.4°$
$h = -35 \rightarrow 35$
$k = -16 \rightarrow 16$
$l = -9 \rightarrow 9$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.091$
$S = 1.11$
2836 reflections
185 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
$w = 1/[\sigma^2(F_o^2) + (0.0293P)^2 + 2.0935P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å$^{-3}$
$\Delta\rho_{min} = -0.18$ e Å$^{-3}$

*Special details*

**Experimental**. *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27–08-2010 CrysAlis171. NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

**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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.31822 (2) | 0.16889 (5) | 0.20313 (10) | 0.04414 (18) |

| | | | | |
|---|---|---|---|---|
| O1 | 0.41937 (6) | 0.17165 (12) | 0.2188 (3) | 0.0476 (5) |
| N1 | 0.29969 (6) | 0.36160 (14) | 0.2171 (3) | 0.0391 (5) |
| H1 | 0.2719 | 0.3391 | 0.2114 | 0.047* |
| Cl1 | 0.44813 (2) | 0.49703 (5) | 0.15039 (11) | 0.0581 (2) |
| Cl2 | 0.61091 (2) | 0.40683 (7) | 0.43216 (13) | 0.0718 (3) |
| C1 | 0.33303 (8) | 0.29196 (17) | 0.2249 (3) | 0.0338 (5) |
| C1′ | 0.46507 (7) | 0.31015 (16) | 0.2953 (3) | 0.0320 (5) |
| C2 | 0.37934 (7) | 0.32640 (17) | 0.2576 (3) | 0.0333 (5) |
| H2 | 0.3828 | 0.3945 | 0.2840 | 0.040* |
| C2′ | 0.48099 (8) | 0.40787 (17) | 0.2622 (3) | 0.0360 (5) |
| C3 | 0.41830 (7) | 0.27056 (16) | 0.2540 (3) | 0.0315 (5) |
| C3′ | 0.52538 (8) | 0.43770 (19) | 0.3058 (3) | 0.0430 (6) |
| H3′ | 0.5351 | 0.5033 | 0.2834 | 0.052* |
| C4 | 0.30453 (7) | 0.46842 (17) | 0.2172 (3) | 0.0343 (5) |
| C4′ | 0.55494 (8) | 0.3693 (2) | 0.3827 (3) | 0.0440 (6) |
| C5 | 0.28010 (8) | 0.5236 (2) | 0.3398 (4) | 0.0463 (6) |
| H5 | 0.2619 | 0.4912 | 0.4241 | 0.056* |
| C5′ | 0.54086 (8) | 0.2721 (2) | 0.4168 (4) | 0.0478 (7) |
| H5′ | 0.5610 | 0.2261 | 0.4685 | 0.057* |
| C6 | 0.28268 (10) | 0.6273 (2) | 0.3371 (4) | 0.0565 (8) |
| H6 | 0.2661 | 0.6647 | 0.4200 | 0.068* |
| C6′ | 0.49660 (8) | 0.2442 (2) | 0.3733 (3) | 0.0404 (6) |
| H6′ | 0.4873 | 0.1784 | 0.3969 | 0.048* |
| C7 | 0.30932 (10) | 0.6760 (2) | 0.2137 (4) | 0.0534 (7) |
| H7 | 0.3111 | 0.7460 | 0.2134 | 0.064* |
| C8 | 0.33346 (9) | 0.6208 (2) | 0.0902 (4) | 0.0476 (7) |
| H8 | 0.3515 | 0.6537 | 0.0062 | 0.057* |
| C9 | 0.33111 (8) | 0.51666 (18) | 0.0900 (3) | 0.0401 (6) |
| H9 | 0.3472 | 0.4795 | 0.0055 | 0.048* |
| H11 | 0.3902 (11) | 0.152 (2) | 0.210 (4) | 0.070 (10)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0340 (3) | 0.0307 (3) | 0.0677 (4) | −0.0066 (3) | 0.0007 (3) | 0.0007 (3) |
| O1 | 0.0327 (10) | 0.0286 (9) | 0.0816 (13) | 0.0008 (7) | 0.0009 (9) | −0.0031 (9) |
| N1 | 0.0216 (10) | 0.0322 (10) | 0.0636 (14) | −0.0034 (8) | −0.0027 (9) | 0.0025 (10) |
| Cl1 | 0.0339 (3) | 0.0381 (3) | 0.1022 (6) | −0.0011 (3) | −0.0061 (4) | 0.0241 (4) |
| Cl2 | 0.0333 (4) | 0.0834 (6) | 0.0989 (6) | −0.0046 (4) | −0.0186 (4) | −0.0110 (5) |
| C1 | 0.0319 (13) | 0.0313 (12) | 0.0382 (13) | −0.0035 (10) | 0.0017 (10) | 0.0014 (10) |
| C1′ | 0.0279 (11) | 0.0327 (12) | 0.0354 (12) | 0.0031 (9) | 0.0028 (9) | 0.0003 (10) |
| C2 | 0.0292 (12) | 0.0258 (11) | 0.0451 (13) | −0.0016 (9) | 0.0008 (10) | 0.0000 (10) |
| C2′ | 0.0298 (12) | 0.0331 (12) | 0.0452 (13) | 0.0025 (10) | 0.0006 (10) | 0.0015 (11) |
| C3 | 0.0303 (12) | 0.0268 (12) | 0.0375 (12) | 0.0001 (9) | 0.0028 (10) | 0.0023 (10) |
| C3′ | 0.0322 (13) | 0.0378 (13) | 0.0591 (16) | −0.0023 (11) | −0.0001 (12) | −0.0034 (12) |
| C4 | 0.0236 (11) | 0.0310 (12) | 0.0484 (14) | 0.0020 (9) | −0.0073 (10) | 0.0016 (11) |
| C4′ | 0.0270 (13) | 0.0569 (16) | 0.0480 (15) | −0.0003 (11) | −0.0039 (11) | −0.0075 (13) |
| C5 | 0.0357 (14) | 0.0479 (15) | 0.0552 (16) | 0.0073 (11) | 0.0058 (12) | 0.0036 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C5′ | 0.0363 (14) | 0.0518 (17) | 0.0552 (16) | 0.0091 (12) | −0.0079 (12) | 0.0076 (13) |
| C6 | 0.0555 (18) | 0.0457 (16) | 0.069 (2) | 0.0163 (14) | −0.0018 (15) | −0.0087 (15) |
| C6′ | 0.0343 (13) | 0.0391 (13) | 0.0477 (14) | 0.0028 (11) | 0.0003 (11) | 0.0094 (12) |
| C7 | 0.0519 (17) | 0.0324 (14) | 0.076 (2) | 0.0054 (12) | −0.0157 (15) | 0.0011 (14) |
| C8 | 0.0381 (14) | 0.0434 (15) | 0.0613 (17) | −0.0052 (11) | −0.0074 (13) | 0.0148 (13) |
| C9 | 0.0301 (13) | 0.0420 (14) | 0.0481 (14) | 0.0000 (10) | −0.0002 (11) | 0.0021 (12) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C1 | 1.695 (2) | C3′—H3′ | 0.9300 |
| O1—C3 | 1.339 (3) | C4—C5 | 1.374 (3) |
| O1—H11 | 0.89 (3) | C4—C9 | 1.385 (3) |
| N1—C1 | 1.337 (3) | C4′—C5′ | 1.376 (4) |
| N1—C4 | 1.423 (3) | C5—C6 | 1.377 (4) |
| N1—H1 | 0.8600 | C5—H5 | 0.9300 |
| Cl1—C2′ | 1.735 (2) | C5′—C6′ | 1.374 (3) |
| Cl2—C4′ | 1.736 (2) | C5′—H5′ | 0.9300 |
| C1—C2 | 1.438 (3) | C6—C7 | 1.369 (4) |
| C1′—C6′ | 1.394 (3) | C6—H6 | 0.9300 |
| C1′—C2′ | 1.398 (3) | C6′—H6′ | 0.9300 |
| C1′—C3 | 1.485 (3) | C7—C8 | 1.374 (4) |
| C2—C3 | 1.350 (3) | C7—H7 | 0.9300 |
| C2—H2 | 0.9300 | C8—C9 | 1.382 (3) |
| C2′—C3′ | 1.384 (3) | C8—H8 | 0.9300 |
| C3′—C4′ | 1.375 (3) | C9—H9 | 0.9300 |
| | | | |
| C3—O1—H11 | 106 (2) | C3′—C4′—C5′ | 120.8 (2) |
| C1—N1—C4 | 128.05 (19) | C3′—C4′—Cl2 | 118.8 (2) |
| C1—N1—H1 | 116.0 | C5′—C4′—Cl2 | 120.3 (2) |
| C4—N1—H1 | 116.0 | C4—C5—C6 | 119.6 (3) |
| N1—C1—C2 | 117.5 (2) | C4—C5—H5 | 120.2 |
| N1—C1—S1 | 118.57 (17) | C6—C5—H5 | 120.2 |
| C2—C1—S1 | 123.93 (17) | C6′—C5′—C4′ | 119.0 (2) |
| C6′—C1′—C2′ | 116.2 (2) | C6′—C5′—H5′ | 120.5 |
| C6′—C1′—C3 | 117.6 (2) | C4′—C5′—H5′ | 120.5 |
| C2′—C1′—C3 | 126.2 (2) | C7—C6—C5 | 120.7 (3) |
| C3—C2—C1 | 127.0 (2) | C7—C6—H6 | 119.6 |
| C3—C2—H2 | 116.5 | C5—C6—H6 | 119.6 |
| C1—C2—H2 | 116.5 | C5′—C6′—C1′ | 122.8 (2) |
| C3′—C2′—C1′ | 121.9 (2) | C5′—C6′—H6′ | 118.6 |
| C3′—C2′—Cl1 | 115.43 (18) | C1′—C6′—H6′ | 118.6 |
| C1′—C2′—Cl1 | 122.49 (18) | C6—C7—C8 | 119.7 (3) |
| O1—C3—C2 | 124.1 (2) | C6—C7—H7 | 120.2 |
| O1—C3—C1′ | 111.51 (18) | C8—C7—H7 | 120.2 |
| C2—C3—C1′ | 124.3 (2) | C7—C8—C9 | 120.5 (3) |
| C4′—C3′—C2′ | 119.3 (2) | C7—C8—H8 | 119.7 |
| C4′—C3′—H3′ | 120.3 | C9—C8—H8 | 119.7 |
| C2′—C3′—H3′ | 120.3 | C8—C9—C4 | 119.2 (2) |

| | | | |
|---|---|---|---|
| C5—C4—C9 | 120.3 (2) | C8—C9—H9 | 120.4 |
| C5—C4—N1 | 118.7 (2) | C4—C9—H9 | 120.4 |
| C9—C4—N1 | 120.9 (2) | | |
| | | | |
| C4—N1—C1—C2 | 7.8 (4) | C1—N1—C4—C9 | 56.9 (4) |
| C4—N1—C1—S1 | −174.3 (2) | C2′—C3′—C4′—C5′ | −0.1 (4) |
| N1—C1—C2—C3 | −173.3 (2) | C2′—C3′—C4′—Cl2 | 178.55 (19) |
| S1—C1—C2—C3 | 8.9 (4) | C9—C4—C5—C6 | −0.9 (4) |
| C6′—C1′—C2′—C3′ | −0.6 (3) | N1—C4—C5—C6 | −177.1 (2) |
| C3—C1′—C2′—C3′ | 180.0 (2) | C3′—C4′—C5′—C6′ | −0.2 (4) |
| C6′—C1′—C2′—Cl1 | 174.85 (18) | Cl2—C4′—C5′—C6′ | −178.9 (2) |
| C3—C1′—C2′—Cl1 | −4.6 (3) | C4—C5—C6—C7 | 0.0 (4) |
| C1—C2—C3—O1 | −0.2 (4) | C4′—C5′—C6′—C1′ | 0.1 (4) |
| C1—C2—C3—C1′ | −177.8 (2) | C2′—C1′—C6′—C5′ | 0.3 (4) |
| C6′—C1′—C3—O1 | −29.6 (3) | C3—C1′—C6′—C5′ | 179.7 (2) |
| C2′—C1′—C3—O1 | 149.8 (2) | C5—C6—C7—C8 | 0.5 (4) |
| C6′—C1′—C3—C2 | 148.2 (2) | C6—C7—C8—C9 | −0.1 (4) |
| C2′—C1′—C3—C2 | −32.4 (4) | C7—C8—C9—C4 | −0.8 (4) |
| C1′—C2′—C3′—C4′ | 0.5 (4) | C5—C4—C9—C8 | 1.3 (4) |
| Cl1—C2′—C3′—C4′ | −175.2 (2) | N1—C4—C9—C8 | 177.4 (2) |
| C1—N1—C4—C5 | −126.9 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···S1$^{i}$ | 0.86 | 2.61 | 3.4397 (18) | 162 |
| C3′—H3′···O1$^{ii}$ | 0.93 | 2.59 | 3.496 (3) | 164 |
| O1—H11···S1 | 0.89 (3) | 2.10 (3) | 2.9315 (18) | 157 (2) |

Symmetry codes: (i) −*x*+1/2, −*y*+1/2, *z*; (ii) −*x*+1, *y*+1/2, −*z*+1/2.