

## 3-[(*E*)-[1-(2-Hydroxyphenyl)ethylidene]-amino]-1-(2-methylphenyl)thiourea

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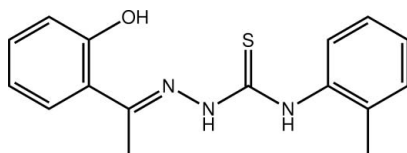
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Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.060;  $wR$  factor = 0.174; data-to-parameter ratio = 16.8.

In the title thiourea derivative,  $\text{C}_{16}\text{H}_{17}\text{N}_3\text{OS}$ , the hydroxy- and methyl-substituted benzene rings form dihedral angles of  $9.62$  (12) and  $55.69$  (6)°, respectively, with the central  $\text{CN}_3\text{S}$  chromophore (r.m.s. deviation =  $0.0117$  Å). An intramolecular  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bond ensures the coplanarity of the central atoms. The H atoms of the NH groups are *syn* and the conformation about the  $\text{N}=\text{C}$  double bond [ $1.295$  (4) Å] is *E*. In the crystal, helical supramolecular chains sustained primarily by  $\text{N}-\text{H}\cdots\text{S}$  hydrogen bonds are found. Additional stabilization is provided by  $\text{C}-\text{H}\cdots\pi$  and  $\pi-\pi$  [ring centroid(hydroxybenzene)  $\cdots$  ring centroid(methylbenzene) =  $3.8524$  (18) Å] interactions.

### Related literature

For pharmaceutical applications of thioruea derivatives, see: Venkatachalam *et al.* (2004); Bruce *et al.* (2007). For related thiourea structures, see: Normaya *et al.* (2011); Salam *et al.* (2011); Dzulkifli *et al.* (2011).



### Experimental

#### Crystal data

$\text{C}_{16}\text{H}_{17}\text{N}_3\text{OS}$   
 $M_r = 299.39$   
 Monoclinic,  $P2_1/c$   
 $a = 14.6966$  (8) Å  
 $b = 7.3586$  (4) Å  
 $c = 14.0926$  (8) Å  
 $\beta = 94.358$  (5)°

$V = 1519.66$  (15) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.22$  mm<sup>-1</sup>  
 $T = 100$  K  
 $0.30 \times 0.10 \times 0.05$  mm

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#### Data collection

Agilent Supernova Dual diffractometer with an Atlas detector  
 Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)  
 $T_{\min} = 0.419$ ,  $T_{\max} = 1.000$

7614 measured reflections  
 3375 independent reflections  
 2094 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.066$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.060$   
 $wR(F^2) = 0.174$   
 $S = 1.00$   
 3375 reflections  
 201 parameters  
 3 restraints

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.34$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.34$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$\text{Cg1}$  is the centroid of the  $\text{C10}-\text{C15}$  ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1o}\cdots\text{N1}$	0.84 (1)	1.81 (2)	2.551 (3)	145 (3)
$\text{N2}-\text{H2n}\cdots\text{S1}^i$	0.88 (1)	2.51 (2)	3.323 (2)	154 (3)
$\text{N3}-\text{H3n}\cdots\text{S1}^i$	0.88 (1)	2.49 (2)	3.286 (3)	151 (2)
$\text{C8}-\text{H8b}\cdots\text{Cg1}^i$	0.98	2.59	3.501 (3)	155

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

Data collection: *CrysAlis PRO* (Agilent, 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* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5025).

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**supplementary materials**

*Acta Cryst.* (2011). E67, o1164 [ doi:10.1107/S1600536811013729 ]

### 3-*{(E)-[1-(2-Hydroxyphenyl)ethylidene]amino}*-1-(2-methylphenyl)thiourea

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#### Comment

In continuation of structural investigations into the conformation and hydrogen bonding patterns in thiourea derivatives (Normaya *et al.* 2011; Salam *et al.*, 2011; Dzulkifli *et al.*, 2011), and also motivated by their pharmacological potential (Venkatachalam *et al.* 2004; Bruce *et al.*, 2007), the title compound, (I), was investigated.

With respect to the planar (r.m.s. = 0.0117 Å) central CN<sub>3</sub>S chromophore in (I), Fig. 1, the OH- and Me-benzene rings are twisted as seen in the respective dihedral angles of 9.62 (12) and 55.69 (6)°. The almost co-planarity of the central atoms is ascribed to the formation of an intramolecular hydroxyl-*O*—*H*⋯*N*-imine hydrogen bond, Table 1. The H atoms of the NH groups are *syn*, and the conformation about the N1=C7 double bond [1.295 (4) Å] is *E*. The *syn* arrangement in (I) contrast the *anti* arrangement often seen in such derivatives but is readily explained in terms of the intramolecular *O*—*H*⋯*N*-imine hydrogen bond in (I) by contrast to the normally observed intramolecular *N*—*H*⋯*N*-imine hydrogen bond (Normaya *et al.* 2011; Salam *et al.*, 2011; Dzulkifli *et al.*, 2011).

Helical supramolecular chains along the *b* axis dominate the crystal packing, Fig. 2 and Table 1. These arise as a result of the thione-S interacting with both N—H atoms of a neighbouring molecule thereby forming six-membered hydrogen bond mediated rings. Chains are stabilized by C—H⋯ $\pi$ , Table 1, and  $\pi$ — $\pi$  [ring centroid(C1⋯C6)⋯ring centroid(C10⋯C15)]<sup>i</sup> = 3.8524 (18) Å, dihedral angle = 2.37 (15)° for *i*: 1 - *x*, -1/2 + *y*, 1/2 - *z*] interactions, Fig. 3.

#### Experimental

2-Methylphenylisothiocyanate (0.746 g, 5 mmol) and hydrazine hydrate (0.253 g, 5 mmol), each dissolved in 10 ml ethanol, were mixed with constant stirring. The stirring was continued for 30 min and the white product formed was washed with ethanol and dried *in vacuo*. A solution of the isolated 2-methylphenylthiosemicarbazide (0.540 g, 3 mmol) in 10 ml methanol was then refluxed with a methanolic solution of 2-hydroxyacetophenone (0.408 g, 3 mmol) for 5 h after adding 1–2 drops of glacial acetic acid. On cooling, the solution to room temperature, a light-yellow powder separated and washed with methanol. The powder was recrystallized from methanol and dried *in vacuo* over silica gel. (*M.pt.* 451–453 K. Yield 0.740 g (78%). Elemental analysis: Calc. for C<sub>16</sub>H<sub>17</sub>N<sub>3</sub>OS: C, 64.21; H, 5.73; N, 14.04%. Found: C, 64.17; H, 5.67; N, 14.01%. FT—IR (KBr, cm<sup>-1</sup>)  $\nu_{\max}$ : 3175 (m, OH), 3000 (s, NH), 1583 (w, C=N), 943 (m, N—N), 1371, 861 (w, C=S).

#### Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H = 0.98 to 1.00 Å) and were included in the refinement in the riding model approximation, with  $U_{\text{iso}}(\text{H})$  set to 1.2–1.5 $U_{\text{eq}}(\text{C})$ . The O- and N-bound H-atoms were located in a difference Fourier map and were refined with distance restraints of O—H = 0.84±0.01 Å and N—H 0.88±0.01 Å, and with  $U_{\text{iso}}(\text{H}) = yU_{\text{eq}}(\text{parent atom})$  for  $y = 1.5$  (O) and 1.2 (N).

## Figures

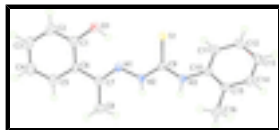


Fig. 1. The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

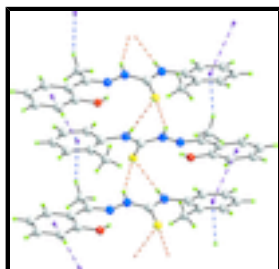


Fig. 2. A view of the helical supramolecular chain aligned along the *b* axis in (I). The N—H...S hydrogen bonds are shown as orange dashed lines. Further stabilization to the chain is provided by C—H... $\pi$  and  $\pi$ - $\pi$  interactions, shown as blue and purple dashed lines, respectively.



Fig. 3. A view in projection down the *c* axis of the crystal packing in (I) showing the stacking of layers comprising the helical supramolecular chains shown in Fig. 2. The O—H...O and N—H...S hydrogen bonds (orange), and C—H... $\pi$  (blue) and  $\pi$ - $\pi$  (purple) interactions are shown as dashed lines.

### 3-*{(E)-[1-(2-Hydroxyphenyl)ethylidene]amino}*-1-(2-methylphenyl)thiourea

#### Crystal data

$C_{16}H_{17}N_3OS$

$M_r = 299.39$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 14.6966$  (8) Å

$b = 7.3586$  (4) Å

$c = 14.0926$  (8) Å

$\beta = 94.358$  (5)°

$V = 1519.66$  (15) Å<sup>3</sup>

$Z = 4$

$F(000) = 632$

$D_x = 1.309$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 1905 reflections

$\theta = 2.8$ – $29.3$ °

$\mu = 0.22$  mm<sup>-1</sup>

$T = 100$  K

Prism, light-yellow

$0.30 \times 0.10 \times 0.05$  mm

#### Data collection

Agilent Supernova Dual  
diffractometer with an Atlas detector

Radiation source: SuperNova (Mo) X-ray Source

Mirror

Detector resolution: 10.4041 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: multi-scan  
(*CrysAlis PRO*; Agilent, 2010)

$T_{\min} = 0.419$ ,  $T_{\max} = 1.000$

7614 measured reflections

3375 independent reflections

2094 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.066$

$\theta_{\text{max}} = 27.5$ °,  $\theta_{\text{min}} = 2.8$ °

$h = -14 \rightarrow 19$

$k = -9 \rightarrow 7$

$l = -18 \rightarrow 15$

Refinement

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.060$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.174$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.0769P)^2]$
3375 reflections	where $P = (F_o^2 + 2F_c^2)/3$
201 parameters	$(\Delta/\sigma)_{\max} < 0.001$
3 restraints	$\Delta\rho_{\max} = 0.34 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -0.34 \text{ e } \text{\AA}^{-3}$

Special details

**Geometry.** All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.46230 (5)	0.24817 (10)	0.38597 (5)	0.0188 (2)
O1	0.21619 (14)	0.2307 (3)	0.31997 (15)	0.0250 (5)
H1O	0.2693 (11)	0.261 (4)	0.308 (2)	0.038*
N1	0.33770 (15)	0.3710 (3)	0.22261 (17)	0.0182 (6)
N2	0.42781 (16)	0.4196 (3)	0.21980 (18)	0.0190 (6)
H2N	0.4433 (19)	0.497 (3)	0.1764 (16)	0.023*
N3	0.57409 (16)	0.4362 (3)	0.27942 (17)	0.0197 (6)
H3N	0.5801 (19)	0.496 (4)	0.2259 (13)	0.024*
C1	0.1592 (2)	0.2588 (4)	0.2410 (2)	0.0229 (7)
C2	0.0685 (2)	0.2066 (5)	0.2458 (3)	0.0309 (8)
H2	0.0496	0.1544	0.3027	0.037*
C3	0.0062 (2)	0.2298 (5)	0.1692 (3)	0.0331 (9)
H3A	-0.0553	0.1927	0.1732	0.040*
C4	0.0327 (2)	0.3073 (5)	0.0857 (3)	0.0320 (8)
H4	-0.0104	0.3236	0.0327	0.038*
C5	0.1220 (2)	0.3603 (4)	0.0806 (2)	0.0260 (8)
H5A	0.1396	0.4142	0.0236	0.031*

## supplementary materials

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C6	0.18777 (19)	0.3372 (4)	0.1568 (2)	0.0200 (7)
C7	0.28345 (19)	0.3879 (4)	0.1464 (2)	0.0189 (7)
C8	0.3131 (2)	0.4548 (4)	0.0530 (2)	0.0229 (7)
H8A	0.3795	0.4432	0.0525	0.034*
H8B	0.2957	0.5827	0.0445	0.034*
H8C	0.2834	0.3824	0.0012	0.034*
C9	0.48965 (19)	0.3751 (4)	0.2920 (2)	0.0174 (7)
C10	0.65424 (19)	0.4166 (4)	0.3422 (2)	0.0172 (7)
C11	0.6563 (2)	0.4776 (4)	0.4351 (2)	0.0201 (7)
H11	0.6024	0.5242	0.4592	0.024*
C12	0.7355 (2)	0.4712 (4)	0.4928 (2)	0.0252 (7)
H12A	0.7364	0.5112	0.5570	0.030*
C13	0.8147 (2)	0.4057 (4)	0.4568 (2)	0.0253 (7)
H13	0.8703	0.4035	0.4960	0.030*
C14	0.8128 (2)	0.3441 (4)	0.3647 (2)	0.0231 (7)
H14	0.8671	0.2974	0.3414	0.028*
C15	0.73287 (19)	0.3485 (4)	0.3047 (2)	0.0195 (7)
C16	0.7318 (2)	0.2841 (4)	0.2034 (2)	0.0260 (8)
H16A	0.7815	0.1969	0.1974	0.039*
H16B	0.7401	0.3882	0.1615	0.039*
H16C	0.6733	0.2253	0.1851	0.039*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0225 (4)	0.0163 (4)	0.0179 (4)	-0.0009 (3)	0.0039 (3)	-0.0001 (3)
O1	0.0214 (11)	0.0291 (13)	0.0247 (13)	-0.0029 (10)	0.0027 (10)	-0.0005 (10)
N1	0.0150 (12)	0.0148 (13)	0.0247 (15)	-0.0010 (10)	0.0019 (10)	-0.0010 (11)
N2	0.0179 (13)	0.0166 (14)	0.0222 (15)	-0.0023 (10)	0.0002 (11)	0.0044 (11)
N3	0.0187 (13)	0.0205 (14)	0.0199 (15)	-0.0006 (11)	0.0016 (11)	0.0052 (11)
C1	0.0245 (16)	0.0172 (16)	0.0269 (18)	0.0046 (13)	0.0018 (13)	-0.0085 (14)
C2	0.0234 (17)	0.030 (2)	0.040 (2)	-0.0028 (14)	0.0098 (15)	-0.0020 (16)
C3	0.0198 (17)	0.031 (2)	0.049 (2)	-0.0018 (14)	0.0039 (16)	-0.0077 (17)
C4	0.0248 (18)	0.0298 (19)	0.040 (2)	0.0018 (15)	-0.0039 (15)	0.0006 (17)
C5	0.0242 (17)	0.0207 (17)	0.032 (2)	0.0010 (14)	-0.0026 (14)	-0.0014 (15)
C6	0.0174 (15)	0.0158 (16)	0.0266 (18)	-0.0010 (12)	0.0003 (13)	-0.0037 (13)
C7	0.0209 (15)	0.0104 (15)	0.0250 (18)	0.0038 (12)	0.0004 (13)	-0.0030 (13)
C8	0.0248 (16)	0.0192 (17)	0.0247 (18)	-0.0002 (13)	0.0021 (13)	-0.0036 (14)
C9	0.0180 (15)	0.0151 (15)	0.0197 (16)	0.0034 (12)	0.0045 (12)	-0.0028 (13)
C10	0.0185 (15)	0.0126 (15)	0.0205 (17)	-0.0006 (12)	0.0014 (12)	0.0014 (12)
C11	0.0272 (16)	0.0095 (14)	0.0239 (18)	0.0015 (13)	0.0045 (13)	-0.0009 (13)
C12	0.0354 (19)	0.0158 (16)	0.0235 (18)	-0.0033 (14)	-0.0037 (14)	0.0013 (14)
C13	0.0249 (17)	0.0192 (17)	0.030 (2)	-0.0021 (13)	-0.0091 (14)	0.0055 (14)
C14	0.0171 (15)	0.0183 (16)	0.034 (2)	0.0001 (13)	0.0034 (13)	0.0026 (15)
C15	0.0262 (16)	0.0132 (15)	0.0200 (17)	-0.0058 (13)	0.0063 (13)	-0.0003 (13)
C16	0.0275 (17)	0.0240 (18)	0.0276 (19)	-0.0018 (14)	0.0094 (14)	-0.0020 (14)

*Geometric parameters (Å, °)*

S1—C9	1.694 (3)	C6—C7	1.473 (4)
O1—C1	1.357 (4)	C7—C8	1.500 (4)
O1—H1O	0.842 (10)	C8—H8A	0.9800
N1—C7	1.295 (4)	C8—H8B	0.9800
N1—N2	1.375 (3)	C8—H8C	0.9800
N2—C9	1.352 (4)	C10—C11	1.383 (4)
N2—H2N	0.880 (10)	C10—C15	1.400 (4)
N3—C9	1.344 (3)	C11—C12	1.369 (4)
N3—C10	1.426 (4)	C11—H11	0.9500
N3—H3N	0.882 (10)	C12—C13	1.391 (4)
C1—C2	1.394 (4)	C12—H12A	0.9500
C1—C6	1.411 (4)	C13—C14	1.373 (4)
C2—C3	1.372 (5)	C13—H13	0.9500
C2—H2	0.9500	C14—C15	1.395 (4)
C3—C4	1.390 (5)	C14—H14	0.9500
C3—H3A	0.9500	C15—C16	1.503 (4)
C4—C5	1.376 (4)	C16—H16A	0.9800
C4—H4	0.9500	C16—H16B	0.9800
C5—C6	1.400 (4)	C16—H16C	0.9800
C5—H5A	0.9500		
C1—O1—H1O	108 (2)	H8A—C8—H8B	109.5
C7—N1—N2	119.0 (2)	C7—C8—H8C	109.5
C9—N2—N1	120.6 (2)	H8A—C8—H8C	109.5
C9—N2—H2N	119 (2)	H8B—C8—H8C	109.5
N1—N2—H2N	119.3 (19)	N3—C9—N2	113.2 (2)
C9—N3—C10	127.7 (2)	N3—C9—S1	124.3 (2)
C9—N3—H3N	115.6 (19)	N2—C9—S1	122.4 (2)
C10—N3—H3N	116.7 (19)	C11—C10—C15	121.0 (3)
O1—C1—C2	116.8 (3)	C11—C10—N3	120.9 (3)
O1—C1—C6	123.2 (3)	C15—C10—N3	117.9 (3)
C2—C1—C6	120.0 (3)	C12—C11—C10	120.5 (3)
C3—C2—C1	120.8 (3)	C12—C11—H11	119.7
C3—C2—H2	119.6	C10—C11—H11	119.7
C1—C2—H2	119.6	C11—C12—C13	119.5 (3)
C2—C3—C4	120.2 (3)	C11—C12—H12A	120.2
C2—C3—H3A	119.9	C13—C12—H12A	120.2
C4—C3—H3A	119.9	C14—C13—C12	120.1 (3)
C5—C4—C3	119.4 (3)	C14—C13—H13	120.0
C5—C4—H4	120.3	C12—C13—H13	120.0
C3—C4—H4	120.3	C13—C14—C15	121.5 (3)
C4—C5—C6	122.1 (3)	C13—C14—H14	119.3
C4—C5—H5A	119.0	C15—C14—H14	119.3
C6—C5—H5A	119.0	C14—C15—C10	117.4 (3)
C5—C6—C1	117.6 (3)	C14—C15—C16	121.1 (3)
C5—C6—C7	120.1 (3)	C10—C15—C16	121.5 (3)
C1—C6—C7	122.3 (3)	C15—C16—H16A	109.5

## supplementary materials

N1—C7—C6	115.1 (3)	C15—C16—H16B	109.5
N1—C7—C8	123.9 (3)	H16A—C16—H16B	109.5
C6—C7—C8	120.9 (3)	C15—C16—H16C	109.5
C7—C8—H8A	109.5	H16A—C16—H16C	109.5
C7—C8—H8B	109.5	H16B—C16—H16C	109.5
C7—N1—N2—C9	-168.5 (3)	C10—N3—C9—N2	178.6 (3)
O1—C1—C2—C3	-179.9 (3)	C10—N3—C9—S1	-3.6 (4)
C6—C1—C2—C3	0.3 (5)	N1—N2—C9—N3	-178.5 (2)
C1—C2—C3—C4	-0.5 (5)	N1—N2—C9—S1	3.7 (4)
C2—C3—C4—C5	0.1 (5)	C9—N3—C10—C11	-56.4 (4)
C3—C4—C5—C6	0.6 (5)	C9—N3—C10—C15	129.0 (3)
C4—C5—C6—C1	-0.8 (5)	C15—C10—C11—C12	-0.5 (4)
C4—C5—C6—C7	177.0 (3)	N3—C10—C11—C12	-174.9 (3)
O1—C1—C6—C5	-179.4 (3)	C10—C11—C12—C13	1.1 (4)
C2—C1—C6—C5	0.3 (4)	C11—C12—C13—C14	-1.5 (5)
O1—C1—C6—C7	2.8 (5)	C12—C13—C14—C15	1.2 (5)
C2—C1—C6—C7	-177.4 (3)	C13—C14—C15—C10	-0.6 (4)
N2—N1—C7—C6	-178.4 (2)	C13—C14—C15—C16	178.8 (3)
N2—N1—C7—C8	1.2 (4)	C11—C10—C15—C14	0.2 (4)
C5—C6—C7—N1	176.2 (3)	N3—C10—C15—C14	174.8 (3)
C1—C6—C7—N1	-6.1 (4)	C11—C10—C15—C16	-179.2 (3)
C5—C6—C7—C8	-3.4 (4)	N3—C10—C15—C16	-4.6 (4)
C1—C6—C7—C8	174.3 (3)		

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

<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>
O1—H1o $\cdots$ N1	0.842 (10)	1.81 (2)	2.551 (3)	145 (3)
N2—H2n $\cdots$ S1 <sup>i</sup>	0.880 (10)	2.508 (16)	3.323 (2)	154 (3)
N3—H3n $\cdots$ S1 <sup>i</sup>	0.882 (10)	2.485 (17)	3.286 (3)	151 (2)
C8—H8b $\cdots$ Cg1 <sup>i</sup>	0.98	2.59	3.501 (3)	155

Symmetry codes: (i)  $-x+1, y+1/2, -z+1/2$ .



Fig. 1

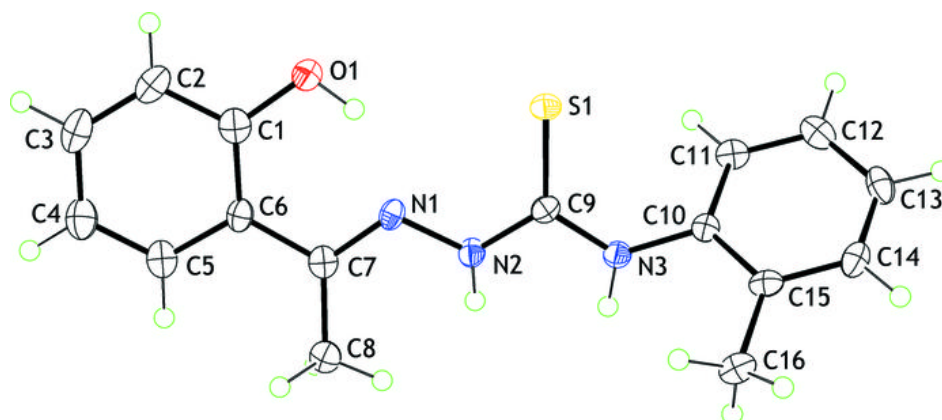


Fig. 2

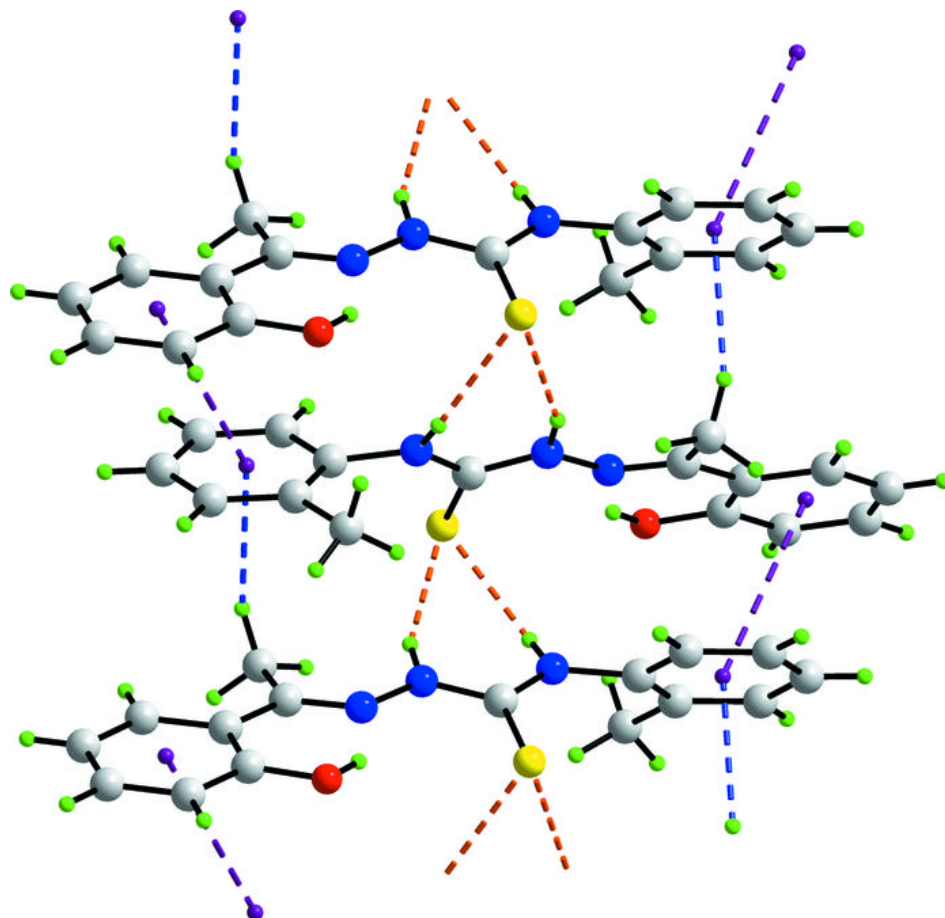


Fig. 3

