

## *N'*-(1*E*)-1-(3,5-Dichloro-2-hydroxyphenyl)propylidene]-4-methoxybenzohydrazide monohydrate

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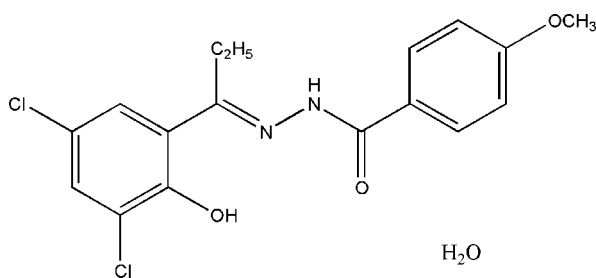
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 Key indicators: single-crystal X-ray study;  $T = 295$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.042;  $wR$  factor = 0.127; data-to-parameter ratio = 14.1.

The title compound,  $\text{C}_{17}\text{H}_{16}\text{Cl}_2\text{N}_2\text{O}_3 \cdot \text{H}_2\text{O}$ , displays a *trans* conformation with respect to the  $\text{C}=\text{N}$  double bond. The dihedral angle between the two benzene rings is  $30.77$  ( $5$ )° and there is one intramolecular  $\text{N}-\text{H} \cdots \text{O}$  hydrogen bond. In the crystal, molecules are linked by hydrogen bonding to the water molecules of crystallization, which acts as both an acceptor and a donor, into a three-dimensional network.

### Related literature

For further details of the chemistry of the title compound, see: Carcelli *et al.* (1995); Salem (1998). For a related structure, see: Chang & Ji (2007).



### Experimental

#### Crystal data

 $\text{C}_{17}\text{H}_{16}\text{Cl}_2\text{N}_2\text{O}_3 \cdot \text{H}_2\text{O}$ 
 $M_r = 385.23$ 

 Monoclinic,  $C2/c$   
 $a = 32.925$  (3) Å  
 $b = 7.3733$  (7) Å  
 $c = 15.1252$  (13) Å  
 $\beta = 92.319$  (2)°  
 $V = 3668.9$  (6) Å<sup>3</sup>
 $Z = 8$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.38$  mm<sup>-1</sup>  
 $T = 295$  K  
 $0.21 \times 0.16 \times 0.11$  mm

#### Data collection

 Bruker APEXII CCD area-detector diffractometer  
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)  
 $T_{\min} = 0.925$ ,  $T_{\max} = 0.960$ 

 9328 measured reflections  
 3242 independent reflections  
 2320 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.027$ 

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.127$   
 $S = 1.01$   
 3242 reflections

 230 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.29$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.39$  e Å<sup>-3</sup>
**Table 1**

Hydrogen-bond geometry (Å, °).

<i>D</i> — <i>H</i> ··· <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> — <i>H</i> ··· <i>A</i>
O1—H1···N1	0.82	1.77	2.494 (2)	146
N2—H2···O4 <sup>i</sup>	0.86	2.16	3.004 (2)	168
O4—H18···O2 <sup>ii</sup>	0.85	1.97	2.815 (2)	171
O4—H19···O1 <sup>iii</sup>	0.85	2.11	2.908 (2)	155

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2314).

### References

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 Carcelli, M., Mazza, P., Pelizzi, G. & Zani, F. (1995). *J. Inorg. Biochem.* **57**, 43–62.  
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**supplementary materials**

*Acta Cryst.* (2010). E66, o2620 [ doi:10.1107/S1600536810037293 ]

## *N'*-[(1*E*)-1-(3,5-Dichloro-2-hydroxyphenyl)propylidene]-4-methoxybenzohydrazide monohydrate

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### Comment

The chemistry of aroylhydrazones continues to attract much attention due to their ability to coordinate with metal ions (Salem, 1998) and their biological activity (Carcelli *et al.*, 1995). As an extension of work on the structural characterization of aroylhydrazone derivatives (Chang & Ji, 2007), the title compound, (I), was synthesized and its crystal structure is reported here.

(I) displays a *trans* conformation with respect to the C7=N1 double bond (Fig. 1). The N2-N1=C7-C6 torsion angle is  $-175.44$  (18)°. The dihedral angle between the two benzene rings is 30.77° (molecules are linked into a three dimensional network by intermolecular N-H...O, O-H...O Hydrogen bonds involving the water molecule which acts as both a donor and an acceptor. ( Table. 1, Fig. 1 and Fig. 2).

### Experimental

4-methoxybenzohydrazide (0.01 mol, 1.66 g) was dissolved in anhydrous ethanol (40 ml), and 1-(3,5-dichloro-2-hydroxyphenyl)propan-1-one (0.01 mol, 2.19 g) was added. The reaction mixture was refluxed for 6 h with stirring, then the resulting precipitate was collected by filtration, washed several times with ethanol and dried *in vacuo* (yield 82%). The compound (1.0 mmol, 0.37 g) was dissolved in dimethylformamide (15 ml) and kept at room temperature for 30 d to obtain colourless single crystals suitable for X-ray diffraction.

### Refinement

All H atoms were positioned geometrically and treated as riding on their parent atoms, with  $C-H(\text{methyl}) = 0.96$  Å,  $C-H(\text{methylene}) = 0.97$  Å,  $C-H(\text{aromatic}) = 0.93$  Å,  $O-H = 0.82$  Å,  $N-H = 0.86$  Å and with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C}_{\text{methyl}}, \text{O})$  and  $1.2U_{\text{eq}}(\text{C}_{\text{aromatic}}, \text{C}_{\text{methylene}}, \text{N})$ .

### Figures

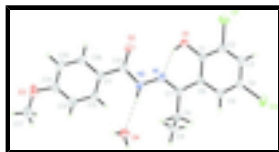


Fig. 1. The molecular structure of compound (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Dashed lines show intramolecular O-H...N hydrogen bonds.

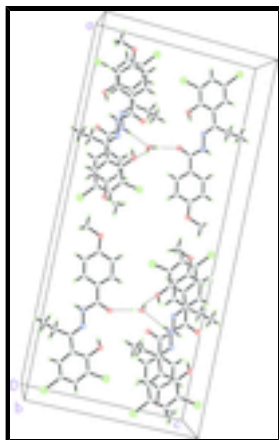


Fig. 2. Packing diagram of (I), showing intermolecular O—H...O and N—H...O hydrogen bonds with the water molecule (dashed lines).

***N*'-[(1*E*)-1-(3,5-Dichloro-2-hydroxyphenyl)propylidene]-4-methoxybenzohydrazide monohydrate**

*Crystal data*

$C_{17}H_{16}Cl_2N_2O_3 \cdot H_2O$

$M_r = 385.23$

Monoclinic,  $C2/c$

Hall symbol:  $-C\ 2yc$

$a = 32.925\ (3)\ \text{\AA}$

$b = 7.3733\ (7)\ \text{\AA}$

$c = 15.1252\ (13)\ \text{\AA}$

$\beta = 92.319\ (2)^\circ$

$V = 3668.9\ (6)\ \text{\AA}^3$

$Z = 8$

$F(000) = 1600$

$D_x = 1.395\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2261 reflections

$\theta = 2.7\text{--}22.8^\circ$

$\mu = 0.38\ \text{mm}^{-1}$

$T = 295\ \text{K}$

Block, colourless

$0.21 \times 0.16 \times 0.11\ \text{mm}$

*Data collection*

Bruker APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)

$T_{\min} = 0.925$ ,  $T_{\max} = 0.960$

9328 measured reflections

3242 independent reflections

2320 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\max} = 25.1^\circ$ ,  $\theta_{\min} = 2.5^\circ$

$h = -38 \rightarrow 31$

$k = -7 \rightarrow 8$

$l = -17 \rightarrow 18$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.127$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0624P)^2 + 2.1699P]$

$S = 1.01$	where $P = (F_o^2 + 2F_c^2)/3$
3242 reflections	$(\Delta/\sigma)_{\max} = 0.001$
230 parameters	$\Delta\rho_{\max} = 0.28 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\min} = -0.39 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008) Extinction coefficient: 0.0014 (2)

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

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.90858 (2)	0.20782 (14)	0.56665 (4)	0.0858 (3)
Cl2	0.96867 (2)	0.10906 (15)	0.90003 (5)	0.0939 (4)
N1	0.78571 (6)	0.0580 (3)	0.76338 (12)	0.0430 (5)
N2	0.74565 (5)	0.0416 (3)	0.78172 (11)	0.0449 (5)
H2	0.7378	0.0201	0.8342	0.054*
O1	0.83142 (5)	0.1268 (2)	0.64024 (10)	0.0538 (5)
H1	0.8097	0.1104	0.6635	0.081*
O2	0.73122 (5)	0.0679 (2)	0.63564 (10)	0.0550 (5)
O3	0.55192 (6)	0.1318 (3)	0.76671 (15)	0.0877 (7)
O4	0.28854 (6)	0.0811 (2)	0.04707 (10)	0.0605 (5)
H18	0.2830	0.0895	-0.0081	0.091*
H19	0.3050	0.1670	0.0597	0.091*
C1	0.86185 (7)	0.1190 (3)	0.70224 (14)	0.0445 (6)
C2	0.90114 (8)	0.1561 (4)	0.67682 (15)	0.0528 (6)
C3	0.93372 (8)	0.1525 (4)	0.73556 (18)	0.0636 (7)
H3	0.9597	0.1786	0.7172	0.076*
C4	0.92734 (8)	0.1095 (4)	0.82283 (17)	0.0596 (7)
C5	0.88941 (7)	0.0692 (3)	0.85008 (16)	0.0503 (6)
H5	0.8860	0.0387	0.9090	0.060*
C6	0.85555 (7)	0.0729 (3)	0.79125 (14)	0.0409 (5)
C7	0.81465 (7)	0.0354 (3)	0.82230 (14)	0.0397 (5)
C8	0.80792 (7)	-0.0152 (3)	0.91630 (14)	0.0437 (5)
H8A	0.8310	-0.0844	0.9394	0.052*
H8B	0.7840	-0.0916	0.9186	0.052*
C9	0.80230 (9)	0.1511 (4)	0.97375 (16)	0.0606 (7)

## supplementary materials

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H9A	0.8275	0.2160	0.9799	0.091*
H9B	0.7939	0.1141	1.0311	0.091*
H9C	0.7819	0.2284	0.9466	0.091*
C10	0.71868 (7)	0.0615 (3)	0.71071 (14)	0.0418 (5)
C11	0.67535 (7)	0.0788 (3)	0.72990 (14)	0.0422 (5)
C12	0.66180 (7)	0.1335 (3)	0.81114 (15)	0.0505 (6)
H12	0.6807	0.1569	0.8570	0.061*
C13	0.62131 (8)	0.1540 (4)	0.82595 (17)	0.0584 (7)
H13	0.6130	0.1909	0.8812	0.070*
C14	0.59297 (8)	0.1198 (4)	0.75892 (19)	0.0593 (7)
C15	0.60576 (8)	0.0678 (4)	0.67635 (18)	0.0621 (7)
H15	0.5867	0.0458	0.6306	0.075*
C16	0.64623 (7)	0.0488 (3)	0.66187 (16)	0.0522 (6)
H16	0.6545	0.0154	0.6061	0.063*
C17	0.53716 (10)	0.1785 (6)	0.8521 (2)	0.1014 (12)
H17A	0.5465	0.0903	0.8950	0.152*
H17B	0.5080	0.1802	0.8491	0.152*
H17C	0.5472	0.2962	0.8692	0.152*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cl1	0.0798 (6)	0.1289 (8)	0.0498 (4)	-0.0187 (5)	0.0173 (4)	-0.0021 (4)
Cl2	0.0387 (4)	0.1699 (10)	0.0722 (5)	0.0028 (4)	-0.0099 (3)	0.0112 (5)
N1	0.0393 (11)	0.0532 (12)	0.0363 (10)	0.0011 (9)	-0.0018 (8)	0.0007 (9)
N2	0.0402 (11)	0.0603 (13)	0.0340 (10)	-0.0005 (9)	-0.0003 (8)	0.0058 (9)
O1	0.0489 (10)	0.0745 (12)	0.0378 (9)	-0.0036 (9)	-0.0019 (7)	0.0026 (8)
O2	0.0523 (10)	0.0788 (12)	0.0337 (9)	0.0002 (9)	-0.0012 (7)	0.0023 (8)
O3	0.0422 (11)	0.1199 (19)	0.1009 (17)	0.0046 (11)	0.0012 (11)	-0.0046 (14)
O4	0.0738 (12)	0.0694 (12)	0.0379 (9)	-0.0159 (9)	-0.0028 (8)	0.0036 (8)
C1	0.0480 (14)	0.0468 (13)	0.0385 (12)	0.0019 (11)	-0.0019 (10)	-0.0035 (10)
C2	0.0504 (15)	0.0648 (16)	0.0439 (13)	0.0003 (12)	0.0082 (11)	-0.0045 (12)
C3	0.0432 (15)	0.085 (2)	0.0629 (17)	0.0017 (13)	0.0084 (13)	-0.0052 (15)
C4	0.0411 (14)	0.082 (2)	0.0554 (15)	0.0071 (13)	-0.0029 (12)	-0.0018 (14)
C5	0.0442 (14)	0.0633 (16)	0.0432 (13)	0.0097 (11)	-0.0017 (11)	0.0019 (11)
C6	0.0415 (13)	0.0423 (13)	0.0388 (12)	0.0050 (10)	-0.0013 (9)	-0.0020 (10)
C7	0.0445 (13)	0.0384 (12)	0.0359 (11)	0.0038 (10)	-0.0023 (10)	-0.0016 (9)
C8	0.0425 (13)	0.0489 (13)	0.0395 (12)	0.0017 (10)	-0.0031 (10)	0.0053 (10)
C9	0.0770 (18)	0.0666 (17)	0.0383 (13)	-0.0001 (14)	0.0055 (12)	-0.0033 (12)
C10	0.0462 (13)	0.0414 (13)	0.0374 (13)	-0.0004 (10)	-0.0044 (10)	0.0002 (10)
C11	0.0426 (13)	0.0409 (12)	0.0425 (12)	-0.0026 (10)	-0.0062 (10)	0.0040 (10)
C12	0.0459 (14)	0.0614 (16)	0.0436 (13)	0.0016 (12)	-0.0049 (11)	-0.0010 (11)
C13	0.0532 (16)	0.0683 (18)	0.0541 (15)	0.0056 (13)	0.0049 (13)	0.0004 (13)
C14	0.0417 (14)	0.0641 (17)	0.0719 (18)	0.0013 (12)	0.0004 (13)	0.0059 (14)
C15	0.0477 (16)	0.0732 (19)	0.0638 (17)	-0.0041 (13)	-0.0179 (13)	-0.0016 (14)
C16	0.0525 (15)	0.0557 (15)	0.0476 (14)	-0.0007 (12)	-0.0073 (11)	-0.0025 (11)
C17	0.0529 (19)	0.139 (3)	0.114 (3)	0.009 (2)	0.0225 (19)	-0.006 (3)

*Geometric parameters (Å, °)*

C11—C2	1.736 (2)	C7—C8	1.495 (3)
C12—C4	1.757 (3)	C8—C9	1.519 (3)
N1—C7	1.289 (3)	C8—H8A	0.9700
N1—N2	1.364 (3)	C8—H8B	0.9700
N2—C10	1.374 (3)	C9—H9A	0.9600
N2—H2	0.8600	C9—H9B	0.9600
O1—C1	1.346 (3)	C9—H9C	0.9600
O1—H1	0.8200	C10—C11	1.473 (3)
O2—C10	1.225 (3)	C11—C12	1.384 (3)
O3—C14	1.364 (3)	C11—C16	1.395 (3)
O3—C17	1.440 (4)	C12—C13	1.369 (3)
O4—H18	0.8499	C12—H12	0.9300
O4—H19	0.8500	C13—C14	1.373 (4)
C1—C2	1.392 (3)	C13—H13	0.9300
C1—C6	1.412 (3)	C14—C15	1.388 (4)
C2—C3	1.365 (3)	C15—C16	1.366 (4)
C3—C4	1.382 (4)	C15—H15	0.9300
C3—H3	0.9300	C16—H16	0.9300
C4—C5	1.364 (3)	C17—H17A	0.9600
C5—C6	1.398 (3)	C17—H17B	0.9600
C5—H5	0.9300	C17—H17C	0.9600
C6—C7	1.470 (3)		
C7—N1—N2	122.80 (18)	C8—C9—H9A	109.5
N1—N2—C10	115.55 (18)	C8—C9—H9B	109.5
N1—N2—H2	122.2	H9A—C9—H9B	109.5
C10—N2—H2	122.2	C8—C9—H9C	109.5
C1—O1—H1	109.5	H9A—C9—H9C	109.5
C14—O3—C17	117.7 (2)	H9B—C9—H9C	109.5
H18—O4—H19	106.0	O2—C10—N2	119.8 (2)
O1—C1—C2	118.2 (2)	O2—C10—C11	123.0 (2)
O1—C1—C6	122.7 (2)	N2—C10—C11	117.13 (19)
C2—C1—C6	119.0 (2)	C12—C11—C16	117.7 (2)
C3—C2—C1	122.1 (2)	C12—C11—C10	123.3 (2)
C3—C2—C11	119.4 (2)	C16—C11—C10	118.9 (2)
C1—C2—C11	118.50 (18)	C13—C12—C11	121.9 (2)
C2—C3—C4	118.7 (2)	C13—C12—H12	119.1
C2—C3—H3	120.6	C11—C12—H12	119.1
C4—C3—H3	120.6	C12—C13—C14	119.7 (2)
C5—C4—C3	121.0 (2)	C12—C13—H13	120.1
C5—C4—C12	119.5 (2)	C14—C13—H13	120.1
C3—C4—C12	119.5 (2)	O3—C14—C13	124.8 (3)
C4—C5—C6	121.3 (2)	O3—C14—C15	115.7 (2)
C4—C5—H5	119.3	C13—C14—C15	119.5 (2)
C6—C5—H5	119.3	C16—C15—C14	120.4 (2)
C5—C6—C1	117.9 (2)	C16—C15—H15	119.8
C5—C6—C7	120.7 (2)	C14—C15—H15	119.8

## supplementary materials

C1—C6—C7	121.45 (19)	C15—C16—C11	120.7 (2)
N1—C7—C6	114.57 (19)	C15—C16—H16	119.6
N1—C7—C8	123.8 (2)	C11—C16—H16	119.6
C6—C7—C8	121.57 (18)	O3—C17—H17A	109.5
C7—C8—C9	111.64 (19)	O3—C17—H17B	109.5
C7—C8—H8A	109.3	H17A—C17—H17B	109.5
C9—C8—H8A	109.3	O3—C17—H17C	109.5
C7—C8—H8B	109.3	H17A—C17—H17C	109.5
C9—C8—H8B	109.3	H17B—C17—H17C	109.5
H8A—C8—H8B	108.0		
C7—N1—N2—C10	-177.1 (2)	C1—C6—C7—C8	179.4 (2)
O1—C1—C2—C3	179.5 (2)	N1—C7—C8—C9	-88.7 (3)
C6—C1—C2—C3	-1.2 (4)	C6—C7—C8—C9	88.0 (3)
O1—C1—C2—C11	-0.7 (3)	N1—N2—C10—O2	9.7 (3)
C6—C1—C2—C11	178.64 (18)	N1—N2—C10—C11	-168.88 (19)
C1—C2—C3—C4	0.4 (4)	O2—C10—C11—C12	-157.1 (2)
C11—C2—C3—C4	-179.4 (2)	N2—C10—C11—C12	21.4 (3)
C2—C3—C4—C5	0.7 (4)	O2—C10—C11—C16	19.2 (3)
C2—C3—C4—C12	-178.6 (2)	N2—C10—C11—C16	-162.3 (2)
C3—C4—C5—C6	-1.1 (4)	C16—C11—C12—C13	1.4 (4)
C12—C4—C5—C6	178.2 (2)	C10—C11—C12—C13	177.8 (2)
C4—C5—C6—C1	0.3 (4)	C11—C12—C13—C14	0.0 (4)
C4—C5—C6—C7	-177.8 (2)	C17—O3—C14—C13	-1.9 (4)
O1—C1—C6—C5	-179.9 (2)	C17—O3—C14—C15	177.7 (3)
C2—C1—C6—C5	0.8 (3)	C12—C13—C14—O3	178.4 (2)
O1—C1—C6—C7	-1.8 (3)	C12—C13—C14—C15	-1.1 (4)
C2—C1—C6—C7	178.9 (2)	O3—C14—C15—C16	-178.9 (3)
N2—N1—C7—C6	-175.44 (18)	C13—C14—C15—C16	0.7 (4)
N2—N1—C7—C8	1.4 (3)	C14—C15—C16—C11	0.8 (4)
C5—C6—C7—N1	174.4 (2)	C12—C11—C16—C15	-1.9 (4)
C1—C6—C7—N1	-3.6 (3)	C10—C11—C16—C15	-178.4 (2)
C5—C6—C7—C8	-2.6 (3)		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 $\cdots$ N1	0.82	1.77	2.494 (2)	146
N2—H2 $\cdots$ O4 <sup>i</sup>	0.86	2.16	3.004 (2)	168
O4—H18 $\cdots$ O2 <sup>ii</sup>	0.85	1.97	2.815 (2)	171
O4—H19 $\cdots$ O1 <sup>iii</sup>	0.85	2.11	2.908 (2)	155

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



Fig. 1

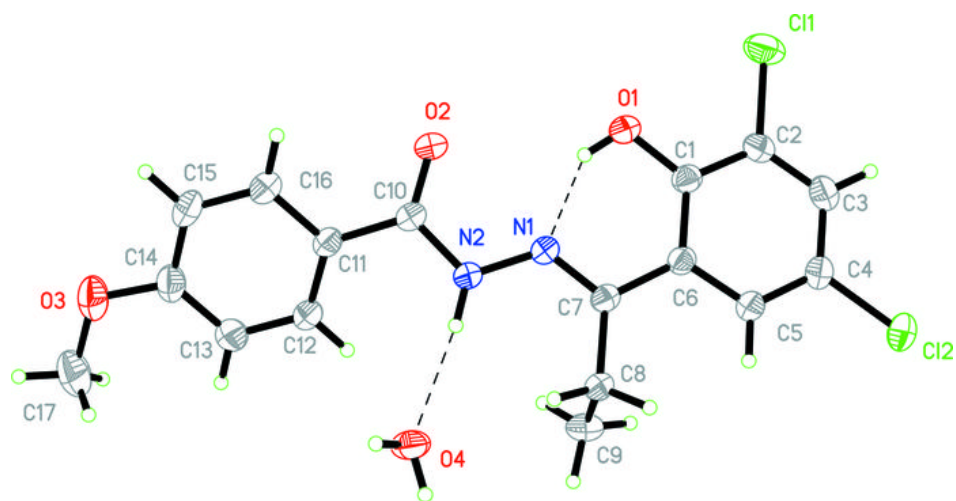


Fig. 2

