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N′-(2-Chlorobenzylidene)-2-hydroxy-3-methylbenzohydrazide

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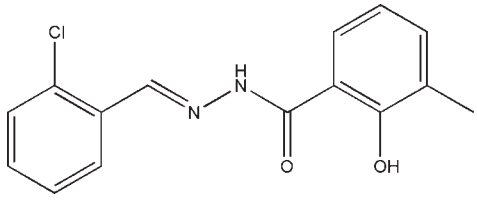
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.010 Å; R factor = 0.083; wR factor = 0.220; data-to-parameter ratio = 10.8.

In the title compound, $C_{15}H_{13}ClN_2O_2$, the dihedral angle between the two benzene rings is 3.4 (5)° and the molecule adopts an E configuration with respect to the C=N bond. There is an intramolecular O—H···O hydrogen bond in the molecule, which generates an S(6) loop. In the crystal structure, molecules are linked through intermolecular N—H···O hydrogen bonds, forming C(4) chains running along the a axis.

Related literature

For the biological properties of hydrazone compounds, see: Patil *et al.* (2010); Cukurovali *et al.* (2006). For related structures, see: Mohd Lair *et al.* (2009); Lin & Sang (2009); Suleiman Gwaram *et al.* (2010); Li & Ban (2009); Lo & Ng (2009); Ning & Xu (2009); Zhu *et al.* (2009). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{15}H_{13}ClN_2O_2$
M_r = 288.72
Monoclinic, Cc
a = 7.084 (2) Å
b = 27.010 (3) Å
c = 7.755 (2) Å
β = 111.229 (3)°
V = 1383.1 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 298 K
0.12 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.967, T_{max} = 0.973
3856 measured reflections
1981 independent reflections
1145 reflections with $I > 2\sigma(I)$
R_{int} = 0.151

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.083
$wR(F^2)$ = 0.220
S = 0.92
1981 reflections
183 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}
Absolute structure: Flack (1983), 470 Friedel pairs
Flack parameter: 0.29 (17)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.41	3.202 (7)	154
O2—H2···O1	0.82	1.92	2.641 (7)	146

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: HB5388).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–S19.
Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cukurovali, A., Yilmaz, I., Gur, S. & Kazaz, C. (2006). *Eur. J. Med. Chem.* **41**, 201–207.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Suleiman Gwaram, N., Khaledi, H., Mohd Ali, H., Robinson, W. T. & Abdulla, M. A. (2010). *Acta Cryst.* E**66**, o721.
Li, C.-M. & Ban, H.-Y. (2009). *Acta Cryst.* E**65**, o876.
Lin, X.-S. & Sang, Y.-L. (2009). *Acta Cryst.* E**65**, o1650.
Lo, K. M. & Ng, S. W. (2009). *Acta Cryst.* E**65**, o969.
Mohd Lair, N., Mohd Ali, H. & Ng, S. W. (2009). *Acta Cryst.* E**65**, o190.
Ning, J.-H. & Xu, X.-W. (2009). *Acta Cryst.* E**65**, o905–o906.
Patil, S. A., Naik, V. H., Kulkarni, A. D., Kamble, U., Bagihalli, G. B. & Badami, P. S. (2010). *J. Coord. Chem.* **63**, 688–699.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhu, C.-G., Wei, Y.-J. & Zhu, Q.-Y. (2009). *Acta Cryst.* E**65**, o85.

supporting information

Acta Cryst. (2010). E**66**, o1025 [https://doi.org/10.1107/S1600536810012110]

N′-(2-Chlorobenzylidene)-2-hydroxy-3-methylbenzohydrazide

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S1. Comment

Hydrazone compounds have been widely investigated for their biological properties (Patil *et al.*, 2010; Cukurovali *et al.*, 2006). Furthermore, the crystal structures of the hydrazone compounds have also attracted much attention in recent years (Mohd Lair *et al.*, 2009; Lin & Sang, 2009; Suleiman Gwaram *et al.*, 2010). In the present work, the title new hydrazone compound is reported.

In the molecule of the title compound, Fig. 1, the dihedral angle between the two benzene rings is 3.4 (5)°. The molecule adopts an *E* configuration with respect to the C═N bond. There is an intramolecular O–H···O hydrogen bond (Table 1) in the molecule. All the bond lengths are within normal ranges (Allen *et al.*, 1987), and are comparable with those in the similar compounds (Li & Ban, 2009; Lo & Ng, 2009; Ning & Xu, 2009; Zhu *et al.*, 2009).

In the crystal structure, molecules are linked through intermolecular N–H···O hydrogen bonds (Table 1) to form chains running along the *a* axis (Fig. 2).

S2. Experimental

A mixture of 2-chlorobenzaldehyde (0.140 g, 1 mmol) and 2-hydroxy-3-methylbenzohydrazide (0.166 g, 1 mmol) in 50 ml me thanol was stirred at room temperature for 1 h. The mixture was filtered to remove impurities, and then left at room temperature. After a few days, colourless blocks of (I) were formed.

S3. Refinement

H atoms were positioned geometrically and refined using the riding-model approximation, with C–H = 0.93 or 0.96 Å, O–H = 0.82 Å, N–H = 0.86 Å, and U_{iso}(H) = 1.2U_{eq}(C,*N*) or U_{iso}(H) = 1.5U_{eq}(methyl C and O).

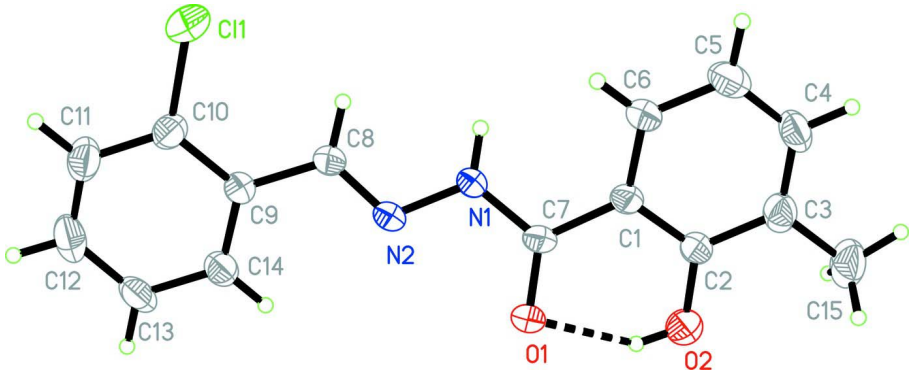

Figure 1

The molecular structure of (I) with 30% probability displacement ellipsoids for non-H atoms. Intramolecular O–H···O hydrogen bond is shown as a dashed line.

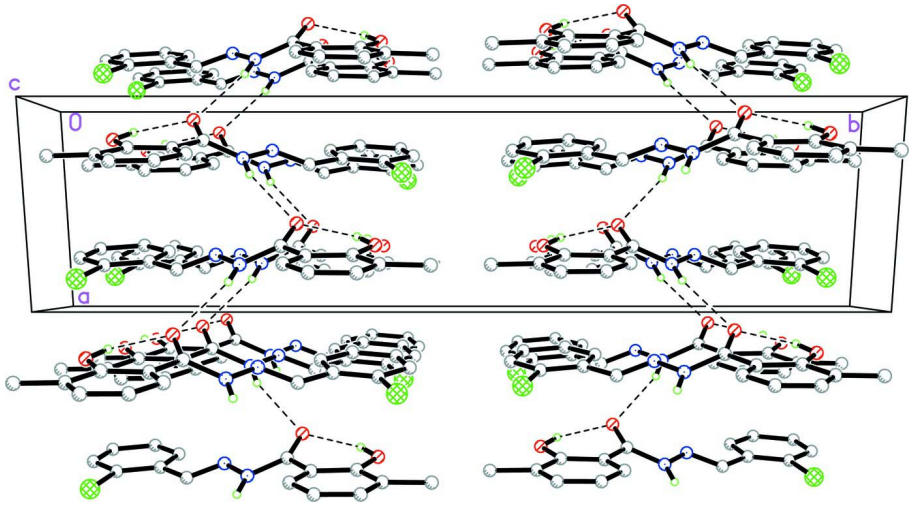

Figure 2

The packing of (I) viewed along the *c* axis. Hydrogen bonds are shown as dashed lines.

N′-(2-Chlorobenzylidene)-2-hydroxy-3-methylbenzohydrazide

Crystal data

$C_{15}H_{13}ClN_2O_2$
$M_r = 288.72$
Monoclinic, *Cc*
Hall symbol: C -2yc
$a = 7.084$ (2) Å
$b = 27.010$ (3) Å
$c = 7.755$ (2) Å
$\beta = 111.229$ (3)°
$V = 1383.1$ (6) Å^3
$Z = 4$
$F(000) = 600$
$D_x = 1.387$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 975 reflections
$\theta = 2.6$–24.5°
$\mu = 0.28$ mm^{-1}
$T = 298$ K
Block, colorless
0.12 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.967$, $T_{max} = 0.973$
3856 measured reflections
1981 independent reflections
1145 reflections with $I > 2\sigma(I)$
$R_{int} = 0.151$
$\theta_{max} = 27.0°$, $\theta_{min} = 3.0°$
$h = -4 \rightarrow 9$
$k = -34 \rightarrow 34$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.083$
$wR(F^2) = 0.220$
$S = 0.92$
1981 reflections
183 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1271P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.45$ e Å^{-3}

Absolute structure: Flack (1983), 470 Fridel pairs

Absolute structure parameter: 0.29 (17)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.3375 (3)	0.43050 (6)	0.8129 (3)	0.0785 (7)
N1	0.2710 (8)	0.24748 (18)	0.8198 (7)	0.0526 (14)
H1	0.3490	0.2572	0.9277	0.063*
N2	0.2275 (8)	0.2780 (2)	0.6677 (6)	0.0503 (13)
O1	0.0826 (8)	0.18614 (19)	0.6388 (6)	0.0704 (15)
O2	0.1832 (8)	0.09660 (18)	0.7787 (7)	0.0666 (14)
H2	0.1443	0.1174	0.6964	0.100*
C1	0.2311 (9)	0.1713 (2)	0.9627 (8)	0.0462 (15)
C2	0.2276 (10)	0.1188 (2)	0.9446 (8)	0.0505 (16)
C3	0.2680 (10)	0.0889 (3)	1.1021 (10)	0.0599 (19)
C4	0.3049 (11)	0.1111 (3)	1.2688 (9)	0.065 (2)
H4	0.3328	0.0912	1.3730	0.078*
C5	0.3026 (12)	0.1623 (3)	1.2901 (11)	0.067 (2)
H5	0.3253	0.1762	1.4055	0.081*
C6	0.2661 (9)	0.1919 (3)	1.1361 (8)	0.0550 (17)
H6	0.2648	0.2262	1.1484	0.066*
C7	0.1867 (9)	0.2013 (2)	0.7943 (8)	0.0489 (16)
C8	0.2946 (10)	0.3218 (3)	0.7035 (9)	0.0485 (15)
H8	0.3665	0.3312	0.8251	0.058*
C9	0.2591 (9)	0.3575 (2)	0.5540 (8)	0.0445 (14)
C10	0.2758 (10)	0.4085 (2)	0.5897 (9)	0.0548 (18)
C11	0.2424 (13)	0.4419 (3)	0.4451 (12)	0.070 (2)
H11	0.2509	0.4757	0.4689	0.084*
C12	0.1983 (14)	0.4256 (3)	0.2722 (13)	0.078 (2)
H12	0.1778	0.4485	0.1775	0.093*
C13	0.1823 (11)	0.3753 (3)	0.2297 (9)	0.066 (2)
H13	0.1523	0.3645	0.1087	0.079*
C14	0.2122 (10)	0.3417 (3)	0.3723 (9)	0.0555 (18)
H14	0.2008	0.3080	0.3462	0.067*
C15	0.2730 (15)	0.0336 (3)	1.0799 (14)	0.085 (3)
H15A	0.3750	0.0251	1.0306	0.127*
H15B	0.1433	0.0224	0.9969	0.127*
H15C	0.3037	0.0180	1.1982	0.127*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1018 (16)	0.0557 (10)	0.0756 (12)	−0.0051 (12)	0.0294 (10)	−0.0184 (10)
N1	0.063 (3)	0.044 (3)	0.035 (2)	−0.005 (3)	−0.001 (2)	0.005 (2)
N2	0.056 (3)	0.049 (3)	0.034 (2)	−0.002 (3)	0.002 (2)	0.002 (2)
O1	0.100 (4)	0.057 (3)	0.034 (2)	−0.024 (3)	0.001 (2)	−0.001 (2)
O2	0.087 (4)	0.049 (3)	0.058 (3)	−0.002 (3)	0.020 (3)	−0.005 (2)
C1	0.042 (3)	0.046 (3)	0.039 (3)	−0.001 (3)	0.001 (3)	0.001 (3)
C2	0.050 (4)	0.049 (3)	0.043 (3)	−0.003 (3)	0.005 (3)	0.006 (3)
C3	0.052 (4)	0.056 (4)	0.062 (5)	0.001 (3)	0.009 (3)	0.015 (3)
C4	0.063 (5)	0.075 (5)	0.050 (4)	−0.001 (4)	0.012 (4)	0.025 (4)
C5	0.066 (5)	0.089 (6)	0.043 (3)	−0.008 (4)	0.015 (3)	−0.003 (4)
C6	0.059 (4)	0.059 (4)	0.038 (3)	−0.007 (3)	0.007 (3)	0.001 (3)
C7	0.051 (4)	0.049 (3)	0.034 (3)	−0.005 (3)	0.001 (3)	−0.003 (3)
C8	0.048 (4)	0.049 (4)	0.039 (3)	−0.007 (3)	0.003 (2)	0.001 (3)
C9	0.046 (3)	0.043 (3)	0.041 (3)	0.002 (3)	0.011 (3)	0.003 (3)
C10	0.058 (4)	0.044 (3)	0.060 (4)	−0.003 (3)	0.018 (3)	−0.005 (3)
C11	0.078 (5)	0.047 (4)	0.082 (6)	0.009 (4)	0.024 (4)	0.012 (4)
C12	0.085 (6)	0.071 (5)	0.074 (5)	0.010 (5)	0.024 (4)	0.032 (5)
C13	0.066 (5)	0.082 (5)	0.038 (3)	0.001 (4)	0.006 (3)	0.012 (3)
C14	0.051 (4)	0.061 (4)	0.048 (4)	−0.004 (3)	0.011 (3)	0.008 (3)
C15	0.093 (6)	0.057 (4)	0.100 (7)	0.006 (5)	0.028 (5)	0.024 (5)

Geometric parameters (Å, º)

Cl1—C10	1.730 (7)	C5—H5	0.9300
N1—C7	1.365 (8)	C6—H6	0.9300
N1—N2	1.379 (7)	C8—C9	1.458 (9)
N1—H1	0.8600	C8—H8	0.9300
N2—C8	1.268 (8)	C9—C14	1.392 (10)
O1—C7	1.234 (7)	C9—C10	1.400 (8)
O2—C2	1.350 (8)	C10—C11	1.392 (10)
O2—H2	0.8200	C11—C12	1.336 (12)
C1—C6	1.392 (9)	C11—H11	0.9300
C1—C2	1.423 (8)	C12—C13	1.392 (12)
C1—C7	1.472 (9)	C12—H12	0.9300
C2—C3	1.405 (9)	C13—C14	1.387 (10)
C3—C4	1.362 (10)	C13—H13	0.9300
C3—C15	1.506 (12)	C14—H14	0.9300
C4—C5	1.394 (11)	C15—H15A	0.9600
C4—H4	0.9300	C15—H15B	0.9600
C5—C6	1.382 (10)	C15—H15C	0.9600
C7—N1—N2	118.1 (4)	N2—C8—H8	120.0
C7—N1—H1	121.0	C9—C8—H8	120.0
N2—N1—H1	121.0	C14—C9—C10	118.3 (6)
C8—N2—N1	114.9 (5)	C14—C9—C8	120.7 (6)

C2—O2—H2	109.5	C10—C9—C8	121.0 (6)
C6—C1—C2	119.0 (6)	C11—C10—C9	120.0 (6)
C6—C1—C7	122.8 (6)	C11—C10—Cl1	119.4 (5)
C2—C1—C7	118.1 (5)	C9—C10—Cl1	120.6 (5)
O2—C2—C3	118.4 (6)	C12—C11—C10	120.3 (7)
O2—C2—C1	121.8 (5)	C12—C11—H11	119.8
C3—C2—C1	119.8 (6)	C10—C11—H11	119.8
C4—C3—C2	118.7 (7)	C11—C12—C13	121.9 (7)
C4—C3—C15	122.7 (7)	C11—C12—H12	119.1
C2—C3—C15	118.5 (7)	C13—C12—H12	119.1
C3—C4—C5	122.9 (7)	C14—C13—C12	118.3 (7)
C3—C4—H4	118.6	C14—C13—H13	120.9
C5—C4—H4	118.6	C12—C13—H13	120.9
C6—C5—C4	118.6 (7)	C13—C14—C9	121.2 (7)
C6—C5—H5	120.7	C13—C14—H14	119.4
C4—C5—H5	120.7	C9—C14—H14	119.4
C5—C6—C1	121.0 (7)	C3—C15—H15A	109.5
C5—C6—H6	119.5	C3—C15—H15B	109.5
C1—C6—H6	119.5	H15A—C15—H15B	109.5
O1—C7—N1	121.4 (6)	C3—C15—H15C	109.5
O1—C7—C1	122.9 (6)	H15A—C15—H15C	109.5
N1—C7—C1	115.7 (5)	H15B—C15—H15C	109.5
N2—C8—C9	120.0 (6)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	2.41	3.202 (7)	154
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