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(*E*)-4-Chloro-*N*′-(4-hydroxybenzylidene)-benzohydrazide

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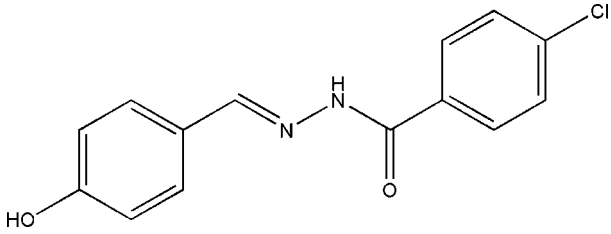
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.116; data-to-parameter ratio = 12.3.

The molecule of the title compound, $C_{14}H_{11}ClN_2O_2$, displays a *trans* configuration with respect to the C=N double bond. The dihedral angle between the two benzene rings is 12.8 (3)°. In the crystal structure, molecules are linked through intermolecular O—H···O and N—H···O hydrogen bonds and C—H···π interactions, forming a three-dimensional network.

Related literature

For related structures, see: Yang (2007, 2008*a*,*b*). For bond-length data, see: Allen *et al.* (1987). For related literature, see: Bernardo *et al.* (1996); Musie *et al.* (2001); Paul *et al.* (2002).



Experimental

Crystal data

$C_{14}H_{11}ClN_2O_2$
M_r = 274.70
Orthorhombic, *Pbca*
a = 26.251 (3) Å
b = 12.376 (3) Å
c = 7.786 (2) Å
V = 2529.5 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 298 (2) K
0.13 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.963, T_{max} = 0.971
11323 measured reflections
2164 independent reflections
1462 reflections with $I > 2\sigma(I)$
R_{int} = 0.078

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.116
S = 1.02
2164 reflections
176 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2^{i}	0.90 (1)	2.078 (11)	2.970 (3)	171 (3)
O1—H1···O2^{ii}	0.82	1.91	2.725 (3)	170
C6—H6···$Cg1^{iii}$	0.93	2.88	3.726 (3)	152

Symmetry codes: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $-x+\frac{1}{2}, y+\frac{1}{2}, z$; (iii) $-x+\frac{1}{2}, -y+2, z-\frac{1}{2}$. $Cg1$ is the C1–C6 ring centroid.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2657).

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supporting information

Acta Cryst. (2008). E**64**, o1849 [doi:10.1107/S1600536808027013]

(*E*)-4-Chloro-*N*′-(4-hydroxybenzylidene)benzohydrazide

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S1. Comment

Schiff base compounds have been of great interest for a long time. These compounds play an important role in the development of coordination chemistry (Musie *et al.*, 2001; Bernardo *et al.*, 1996; Paul *et al.*, 2002). Recently, we have reported a few Schiff base compounds (Yang, 2007, 2008*a*,b). As a further investigation of this work, the crystal structure of the title compound is reported here.

The molecule of the title compound displays a *trans* configuration with respect to the C═N double bond (Fig. 1). The dihedral angle between the two benzene rings is 12.8 (3)°. All the bonds are within normal ranges (Allen *et al.*, 1987). The C7?N1 bond length of 1.268 (3) Å conforms to the value for a double bond. The bond length of 1.339 (3) Å between atoms C8 and N2 is intermediate between a C—N single bond and a C?N double bond, because of conjugation effects in the molecule.

In the crystal structure, molecules are linked through intermolecular O—H···O and N—H···O hydrogen bonds, and C—H···π interactions (Table 1), forming a three-dimensional network (Fig. 2).

S2. Experimental

4-Hydroxybenzaldehyde (0.1 mmol, 12.2 mg) and 4-chlorobenzohydrazide (0.1 mmol, 17.0 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature to give a clear colourless solution. Crystals of the title compound were formed by gradual evaporation of the solvent over a period of 5 days at room temperature.

S3. Refinement

Atom H2A was located in a difference Fourier map and refined isotropically, with N—H distance restrained to 0.90 (1) Å and with a U_{iso} of 0.08 Å^2. Other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with O—H distance of 0.82 Å, C—H distances of 0.93 Å, and with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O).

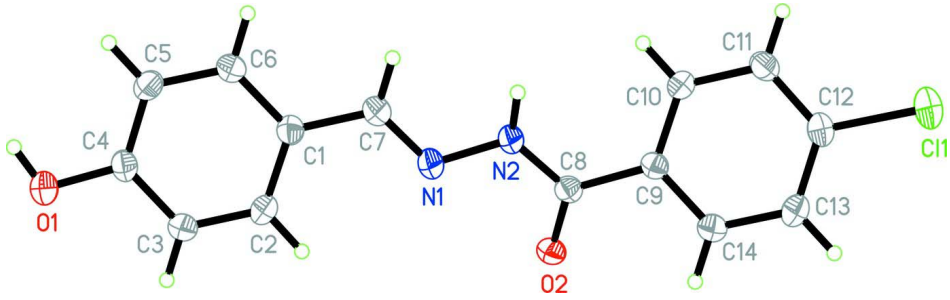

Figure 1

The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

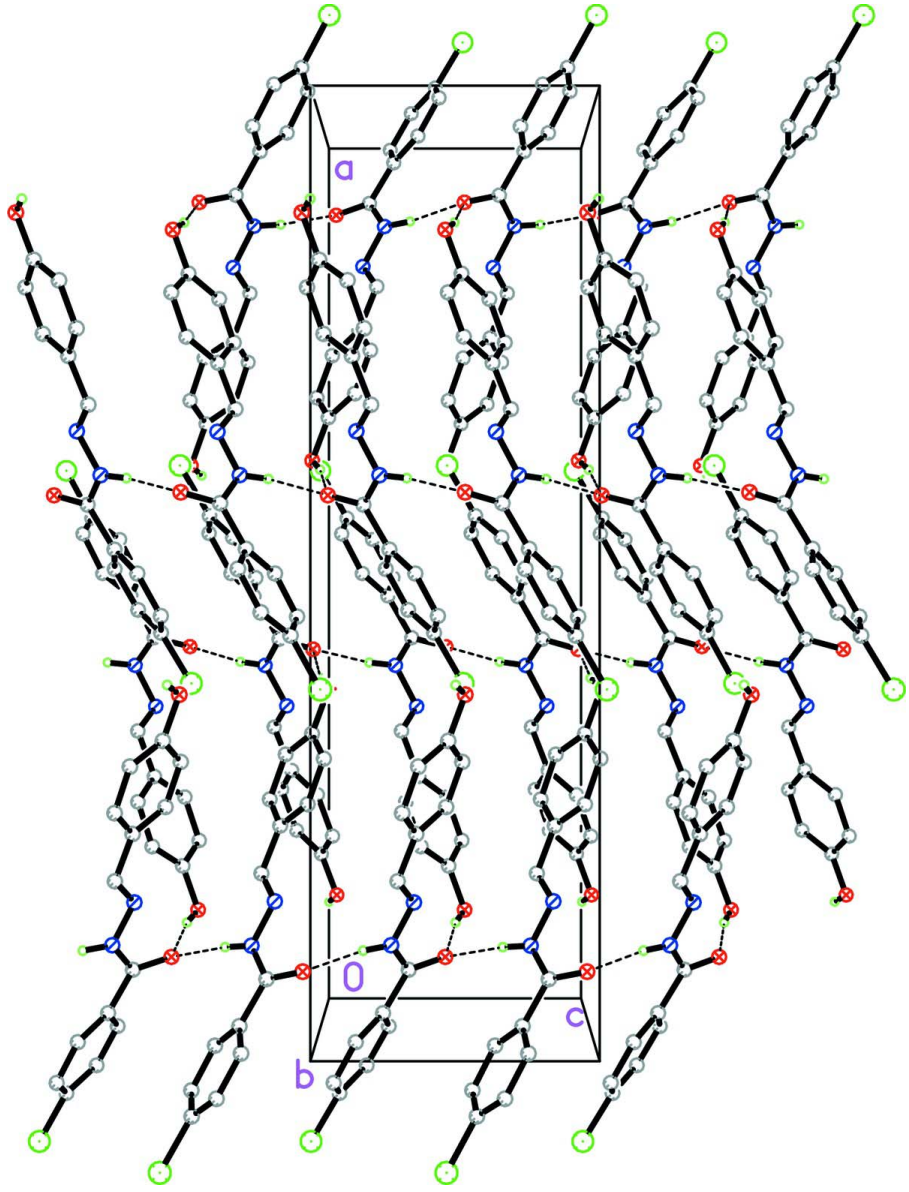

Figure 2

Molecular packing as viewed along the *b* axis. H atoms not involved hydrogen bonding (dashed lines) have been omitted for clarity.

(*E*)-4-Chloro-*N*′-(4-hydroxybenzylidene)benzohydrazide

Crystal data

$C_{14}H_{11}ClN_2O_2$
$M_r = 274.70$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 26.251\ (3)$ Å
$b = 12.376\ (3)$ Å
$c = 7.786\ (2)$ Å
$V = 2529.5\ (9)$ Å^3
$Z = 8$

$F(000) = 1136$
$D_x = 1.443$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1916 reflections
$\theta = 2.3–24.5°$
$\mu = 0.30$ mm^{-1}
$T = 298$ K
Block, colourless
0.13 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.963, T_{max} = 0.971
11323 measured reflections
2164 independent reflections
1462 reflections with $I > 2\sigma(I)$
R_{int} = 0.078
θ_{max} = 24.9°, θ_{min} = 1.6°
h = −30→31
k = −14→11
l = −8→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.116
S = 1.02
2164 reflections
176 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0433P)^2 + 1.3235P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Cl1	−0.11993 (3)	0.56136 (8)	−0.02967 (12)	0.0721 (3)
N1	0.15097 (8)	0.76262 (18)	0.3530 (3)	0.0421 (6)
N2	0.10461 (9)	0.74598 (18)	0.2709 (3)	0.0401 (6)
O1	0.37436 (7)	0.92023 (16)	0.5358 (3)	0.0554 (6)
H1	0.3853	0.9786	0.5022	0.083*
O2	0.08473 (7)	0.61751 (14)	0.4644 (2)	0.0412 (5)
C1	0.22762 (10)	0.8643 (2)	0.3633 (3)	0.0378 (7)
C2	0.25323 (10)	0.7913 (2)	0.4685 (4)	0.0450 (7)
H2	0.2372	0.7273	0.5004	0.054*
C3	0.30150 (10)	0.8119 (2)	0.5258 (4)	0.0463 (8)
H3	0.3178	0.7630	0.5979	0.056*
C4	0.32601 (10)	0.9058 (2)	0.4761 (3)	0.0394 (7)
C5	0.30142 (10)	0.9795 (2)	0.3730 (4)	0.0427 (7)
H5	0.3176	1.0435	0.3418	0.051*
C6	0.25282 (10)	0.9580 (2)	0.3163 (4)	0.0440 (7)

H6	0.2366	1.0075	0.2449	0.053*
C7	0.17709 (10)	0.8413 (2)	0.2970 (4)	0.0430 (7)
H7	0.1636	0.8853	0.2116	0.052*
C8	0.07391 (10)	0.6686 (2)	0.3321 (3)	0.0351 (6)
C9	0.02586 (9)	0.6472 (2)	0.2385 (3)	0.0335 (6)
C10	−0.00001 (10)	0.7240 (2)	0.1430 (4)	0.0409 (7)
H10	0.0134	0.7933	0.1331	0.049*
C11	−0.04545 (10)	0.6992 (2)	0.0619 (4)	0.0441 (7)
H11	−0.0628	0.7512	−0.0013	0.053*
C12	−0.06436 (10)	0.5965 (2)	0.0767 (3)	0.0435 (7)
C13	−0.03996 (10)	0.5193 (2)	0.1731 (4)	0.0476 (8)
H13	−0.0536	0.4502	0.1827	0.057*
C14	0.00479 (10)	0.5449 (2)	0.2554 (3)	0.0425 (7)
H14	0.0210	0.4934	0.3229	0.051*
H2A	0.1010 (12)	0.783 (2)	0.172 (2)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0490 (5)	0.0779 (6)	0.0895 (7)	−0.0117 (4)	−0.0259 (5)	0.0004 (5)
N1	0.0359 (13)	0.0460 (15)	0.0443 (14)	−0.0041 (11)	−0.0089 (11)	0.0015 (12)
N2	0.0355 (13)	0.0423 (14)	0.0424 (13)	−0.0048 (11)	−0.0094 (11)	0.0047 (11)
O1	0.0404 (13)	0.0531 (14)	0.0726 (15)	−0.0084 (9)	−0.0133 (11)	0.0061 (12)
O2	0.0436 (11)	0.0403 (11)	0.0398 (10)	0.0025 (9)	−0.0063 (9)	0.0053 (9)
C1	0.0356 (16)	0.0400 (16)	0.0379 (15)	−0.0022 (13)	−0.0013 (13)	−0.0006 (13)
C2	0.0419 (17)	0.0391 (16)	0.0539 (18)	−0.0091 (13)	−0.0022 (15)	0.0060 (14)
C3	0.0428 (18)	0.0409 (17)	0.0552 (19)	−0.0001 (13)	−0.0092 (15)	0.0096 (15)
C4	0.0321 (16)	0.0425 (17)	0.0437 (16)	−0.0009 (12)	−0.0019 (13)	−0.0058 (14)
C5	0.0437 (17)	0.0371 (16)	0.0472 (17)	−0.0063 (13)	0.0020 (14)	0.0023 (14)
C6	0.0423 (17)	0.0450 (18)	0.0447 (17)	−0.0012 (14)	−0.0075 (14)	0.0094 (13)
C7	0.0400 (17)	0.0448 (18)	0.0442 (17)	−0.0007 (14)	−0.0071 (13)	0.0045 (14)
C8	0.0365 (16)	0.0323 (15)	0.0365 (15)	0.0047 (13)	−0.0008 (12)	−0.0052 (13)
C9	0.0318 (15)	0.0361 (16)	0.0325 (14)	0.0037 (12)	0.0025 (12)	0.0007 (12)
C10	0.0392 (16)	0.0353 (16)	0.0480 (16)	−0.0046 (13)	−0.0025 (14)	0.0027 (13)
C11	0.0391 (16)	0.0483 (18)	0.0449 (17)	0.0014 (14)	−0.0064 (14)	0.0077 (14)
C12	0.0333 (16)	0.0520 (19)	0.0451 (17)	−0.0032 (14)	−0.0032 (13)	−0.0031 (15)
C13	0.0441 (18)	0.0426 (18)	0.0560 (19)	−0.0116 (14)	−0.0027 (15)	0.0030 (15)
C14	0.0431 (17)	0.0408 (17)	0.0438 (16)	−0.0003 (14)	−0.0046 (14)	0.0064 (14)

Geometric parameters (Å, º)

Cl1—C12	1.733 (3)	C5—C6	1.376 (4)
N1—C7	1.268 (3)	C5—H5	0.93
N1—N2	1.390 (3)	C6—H6	0.93
N2—C8	1.339 (3)	C7—H7	0.93
N2—H2A	0.899 (10)	C8—C9	1.481 (3)
O1—C4	1.363 (3)	C9—C10	1.385 (3)
O1—H1	0.82	C9—C14	1.387 (4)

O2—C8	1.242 (3)	C10—C11	1.384 (4)
C1—C6	1.385 (4)	C10—H10	0.93
C1—C2	1.392 (4)	C11—C12	1.369 (4)
C1—C7	1.451 (4)	C11—H11	0.93
C2—C3	1.367 (4)	C12—C13	1.373 (4)
C2—H2	0.93	C13—C14	1.375 (4)
C3—C4	1.383 (4)	C13—H13	0.93
C3—H3	0.93	C14—H14	0.93
C4—C5	1.377 (4)		

C7—N1—N2	115.4 (2)	N1—C7—H7	119.3
C8—N2—N1	118.0 (2)	C1—C7—H7	119.3
C8—N2—H2A	127 (2)	O2—C8—N2	121.5 (2)
N1—N2—H2A	114 (2)	O2—C8—C9	120.8 (2)
C4—O1—H1	109.5	N2—C8—C9	117.8 (2)
C6—C1—C2	117.9 (2)	C10—C9—C14	118.8 (2)
C6—C1—C7	120.4 (2)	C10—C9—C8	124.0 (2)
C2—C1—C7	121.6 (2)	C14—C9—C8	117.2 (2)
C3—C2—C1	121.2 (3)	C11—C10—C9	121.0 (2)
C3—C2—H2	119.4	C11—C10—H10	119.5
C1—C2—H2	119.4	C9—C10—H10	119.5
C2—C3—C4	119.8 (3)	C12—C11—C10	118.7 (3)
C2—C3—H3	120.1	C12—C11—H11	120.6
C4—C3—H3	120.1	C10—C11—H11	120.6
O1—C4—C5	123.3 (2)	C11—C12—C13	121.5 (3)
O1—C4—C3	116.6 (2)	C11—C12—Cl1	119.8 (2)
C5—C4—C3	120.1 (3)	C13—C12—Cl1	118.7 (2)
C6—C5—C4	119.6 (3)	C12—C13—C14	119.5 (3)
C6—C5—H5	120.2	C12—C13—H13	120.2
C4—C5—H5	120.2	C14—C13—H13	120.2
C5—C6—C1	121.3 (3)	C13—C14—C9	120.4 (3)
C5—C6—H6	119.3	C13—C14—H14	119.8
C1—C6—H6	119.3	C9—C14—H14	119.8
N1—C7—C1	121.5 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O2^{i}	0.90 (1)	2.08 (1)	2.970 (3)	171 (3)
O1—H1···O2^{ii}	0.82	1.91	2.725 (3)	170
C6—H6···*Cg*1^{iii}	0.93	2.88	3.726 (3)	152

Symmetry codes: (i) *x*, −*y*+3/2, *z*−1/2; (ii) −*x*+1/2, *y*+1/2, *z*; (iii) −*x*+1/2, −*y*+2, *z*−1/2.