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1-(1*H*-Benzimidazol-2-yl)-3-(3-chlorophenyl)prop-2-en-1-one

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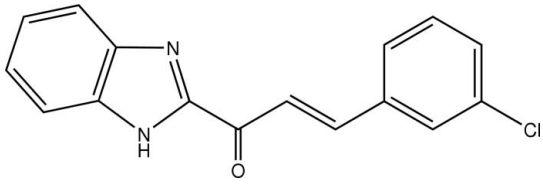
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.115; data-to-parameter ratio = 13.4.

In the title compound, $C_{16}H_{11}ClN_2O$, the dihedral angle between the benzimidazole and chlorophenyl ring systems is 5.92 (4)°. In the crystal packing, the molecules form centrosymmetric dimers *via* N—H···O hydrogen bonds. The dimers are arranged alternately in the [001] direction.

Related literature

For related structures, see: Eltayeb *et al.* (2007); Jian *et al.* (2007); Yıldırım *et al.* (2007); Bibila Mayaya Bisseyou *et al.* (2007). For related literature, see: Allen *et al.* (1987); Sissouma *et al.* (2005).



Experimental

Crystal data

$C_{16}H_{11}ClN_2O$
M_r = 282.73
Monoclinic, $P2_1/c$
a = 9.629 (2) Å
b = 5.617 (5) Å
c = 24.657 (4) Å
β = 92.379 (9)°
V = 1332.5 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 295 K
0.40 × 0.20 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan *DENZO/SCALEPACK* (Otwinowski & Minor, 1997)
T_{min} = 0.89, T_{max} = 0.95
8694 measured reflections
2429 independent reflections
1885 reflections with $I > 3\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.115
S = 1.01
2429 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H9···O1^{i}	0.88	2.03	2.853 (2)	156

Symmetry code: (i) $-x+1, -y-1, -z+1$.

Data collection: *COLLECT* (Nonius, 1997); cell refinement: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO/SCALEPACK*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *CRYSTALS*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2159).

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supplementary materials

Acta Cryst. (2007). E**63**, o4761 [**doi:10.1107/S1600536807053196**]

1-(1*H*-Benzimidazol-2-yl)-3-(3-chlorophenyl)prop-2-en-1-one

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Comment

Substituted benzimidazoles have considerable interest in pharmacology because of their various physiological actions. Several studies through the world showed that benzimidazole derivatives are therapeutic agents and possess versatile pharmacological properties such as anthelmintic, analgesic, antitumor, and vasodilator activities. The title compound is a 2-substituted benzimidazole obtained from a new method of synthesis (Sissouma *et al.*, 2005). The objective of the present study was to elucidate the crystal structure of this new benzimidazole, in conjunction with new investigations of benzimidazole derivative properties. The molecular structure of of the title compound is shown in Fig. 1. It consists of a benzimidazole ring system and chlorophenyl ring, linked by an enone group. The chlorophenyl ring and enone group (C6/C7/C8/C9/C10/O1) make dihedral angles of 5.92 (4) and 2.54 (5)°, respectively, with the benzimidazole ring system. In the benzimidazole ring system bond lengths and angles are in good agreement with the results obtained in previous studies of related benzimidazole derivatives (Eltayeb *et al.*, 2007; Jian *et al.*, 2007; Yıldırım *et al.*, 2007; Bibila Mayaya Bisseyou *et al.*, 2007). As for the phenyl ring also, bond lengths and angles are within normal ranges (Allen *et al.*, 1987). In the crystal structure, molecules form centrosymmetric dimers *via* N—H···O hydrogen bonds. The dimers are arranged in an alternate way along the [001] direction (Fig. 2).

Experimental

1 g (6.3 mmol) of 1-(1*H*-benzimidazol-2-yl)ethanone was added to a cold solution of ethanol (30 ml) and 1.88 g (470 mmol) of NaOH with stirring. To the solution, 1.07 g (7.6 mmol) of 3-chlorobenzaldehyde was added in small quantities. The mixture was agitated at ambient temperature for 3 h. 100 ml of water was added to the suspension. The resulting mixture was neutralized with 20% acetic acid. The precipitate was filtered, washed several times with water, dried and recrystallized from a mixture of hexane/dichloromethane (3:1). Yellow single crystals of parallelepiped shape were obtained for diffraction analysis (yield: 70%, m.p. 492 K). ^{1}H (DMSO-d$_6$) δ: 7.10 (d, 1H, H vinyl); 7.40 (m, 1H, H arom.); 7.50 (m, 3H, H arom.); 7.70 (m, 2H, H arom.); 8.60 (d, 1H, H vinyl); 13.60 (s, 1H, NH); ^{13}C (DMSO-d$_6$) δ: 117 (2 C arom.); 123 (2 C arom.); 124.40 (C vinyl); 127.20 (C arom.); 128.40 (C arom.); 131 (C arom.); 134 (C—Cl); 136 (C arom.); 139 (2 C arom.); 143 (C vinyl); 149 (C arom.), 181 (C=O). TOF+, SM: 282; m/*z* (%): *M*+1 = 283 (15), 282 (10), 253 (100), 118 (47), 102 (29).

Refinement

The H atoms were all located in a difference map. They were initially refined with soft restraints on the bond lengths and angles to regularize their geometry, with C—H = 0.93–0.95 Å, N—H = 0.88 Å and U_{iso}(H) = 1.2U_{eq}(C,*N*), after which the positions were refined with riding constraints.

Figures

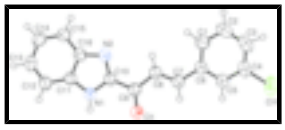

Fig. 1. The molecular structure with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitary radius.

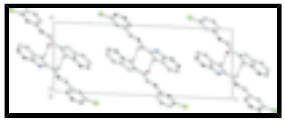

Fig. 2. Crystal packing of the title compound, viewed down the *b* axis, showing centrosymmetric dimers arranged in an alternate way along the *c* axis. H atoms not involved in hydrogen bonds have been omitted for clarity. Dashed lines indicate N—H···O hydrogen bonds.

1-(1*H*-Benzimidazol-2-yl)-3-(3-chlorophenyl)prop-2-en-1-one

Crystal data

$C_{16}H_{11}ClN_2O$	F_{000} = 584
M_r = 282.73	D_x = 1.409 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 492 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71070 Å
a = 9.629 (2) Å	Cell parameters from 8694 reflections
b = 5.617 (5) Å	θ = 3–26º
c = 24.657 (4) Å	μ = 0.28 mm^{-1}
β = 92.379 (9)º	T = 295 K
V = 1332.5 (12) Å^3	Parallelepiped, yellow
Z = 4	0.40 × 0.20 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer	1885 reflections with $I > 3\sigma(I)$
Monochromator: graphite	R_{int} = 0.038
T = 295 K	θ_{max} = 26.0º
φ scans	θ_{min} = 2.6º
Absorption correction: multi-scan DENZO/SCALEPACK (Otwinowski & Minor, 1997)	h = −11→11
T_{min} = 0.89, T_{max} = 0.95	k = −6→6
8694 measured reflections	l = −30→30
2429 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.046	$w = 1/[\sigma^2(F^2) + (0.06P)^2 + 0.69P]$, where $P = (\max(F_o^2,0) + 2F_c^2)/3$
$wR(F^2)$ = 0.115	$(\Delta/\sigma)_{max}$ = 0.001

S = 1.01	$\Delta\rho_{max}$ = 0.30 e Å^{-3}
2429 reflections	$\Delta\rho_{min}$ = −0.42 e Å^{-3}
181 parameters	Extinction correction: None
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cl1	1.14222 (8)	0.07072 (17)	0.26180 (3)	0.0894
O1	0.65896 (17)	−0.3629 (3)	0.47155 (6)	0.0665
N1	0.52500 (18)	−0.2698 (3)	0.56659 (7)	0.0495
N2	0.64559 (18)	0.0694 (3)	0.57681 (7)	0.0491
C1	1.0052 (2)	0.3141 (4)	0.42470 (9)	0.0567
C2	1.0999 (3)	0.4470 (5)	0.39692 (12)	0.0697
C3	1.1418 (3)	0.3739 (5)	0.34676 (11)	0.0686
C4	1.0902 (2)	0.1663 (5)	0.32496 (9)	0.0573
C5	0.9962 (2)	0.0307 (4)	0.35225 (8)	0.0500
C6	0.9524 (2)	0.1031 (4)	0.40244 (8)	0.0453
C7	0.8518 (2)	−0.0462 (4)	0.42944 (8)	0.0478
C8	0.7925 (2)	−0.0087 (4)	0.47603 (8)	0.0495
C9	0.6900 (2)	−0.1781 (4)	0.49582 (8)	0.0491
C10	0.6222 (2)	−0.1210 (4)	0.54655 (8)	0.0452
C11	0.4813 (2)	−0.1679 (4)	0.61334 (8)	0.0438
C12	0.3821 (2)	−0.2374 (4)	0.64994 (8)	0.0522
C13	0.3621 (2)	−0.0869 (5)	0.69252 (9)	0.0553
C14	0.4367 (2)	0.1244 (5)	0.69935 (9)	0.0606
C15	0.5344 (2)	0.1919 (4)	0.66327 (9)	0.0586
C16	0.5572 (2)	0.0432 (4)	0.61923 (8)	0.0453
H1	0.9765	0.3669	0.4586	0.0685*
H2	1.1355	0.5855	0.4138	0.0824*
H3	1.2036	0.4637	0.3260	0.0832*
H5	0.9619	−0.1115	0.3369	0.0597*
H7	0.8251	−0.1837	0.4108	0.0584*
H8	0.8127	0.1252	0.4971	0.0609*
H9	0.4907	−0.3996	0.5512	0.0615*
H12	0.3309	−0.3809	0.6456	0.0627*
H13	0.2977	−0.1296	0.7186	0.0671*
H14	0.4200	0.2206	0.7301	0.0734*
H15	0.5857	0.3349	0.6677	0.0711*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0859 (5)	0.1134 (7)	0.0720 (5)	0.0014 (4)	0.0408 (4)	0.0115 (4)
O1	0.0724 (11)	0.0732 (12)	0.0554 (9)	−0.0277 (9)	0.0190 (8)	−0.0162 (8)
N1	0.0534 (10)	0.0516 (11)	0.0442 (9)	−0.0146 (8)	0.0089 (8)	−0.0065 (8)
N2	0.0480 (10)	0.0497 (11)	0.0501 (10)	−0.0061 (8)	0.0090 (8)	−0.0010 (8)

C1	0.0635 (14)	0.0517 (14)	0.0548 (13)	−0.0067 (11)	0.0002 (10)	0.0003 (10)
C2	0.0708 (16)	0.0562 (16)	0.0812 (18)	−0.0205 (12)	−0.0065 (13)	0.0071 (13)
C3	0.0553 (14)	0.0727 (18)	0.0783 (17)	−0.0157 (12)	0.0092 (12)	0.0225 (14)
C4	0.0463 (12)	0.0696 (16)	0.0567 (13)	0.0011 (11)	0.0123 (10)	0.0151 (11)
C5	0.0462 (11)	0.0533 (13)	0.0509 (11)	−0.0026 (9)	0.0078 (9)	0.0029 (10)
C6	0.0423 (10)	0.0485 (13)	0.0454 (11)	−0.0020 (9)	0.0035 (8)	0.0049 (9)
C7	0.0482 (11)	0.0495 (13)	0.0459 (11)	−0.0071 (9)	0.0039 (9)	−0.0005 (9)
C8	0.0498 (11)	0.0540 (13)	0.0452 (11)	−0.0089 (9)	0.0061 (9)	−0.0023 (9)
C9	0.0470 (11)	0.0577 (14)	0.0427 (11)	−0.0066 (10)	0.0037 (9)	−0.0016 (10)
C10	0.0428 (11)	0.0513 (13)	0.0419 (10)	−0.0068 (9)	0.0054 (8)	0.0015 (9)
C11	0.0425 (10)	0.0487 (12)	0.0404 (10)	−0.0026 (9)	0.0040 (8)	0.0015 (8)
C12	0.0510 (12)	0.0586 (14)	0.0473 (11)	−0.0076 (10)	0.0068 (9)	0.0055 (10)
C13	0.0504 (12)	0.0711 (16)	0.0452 (11)	0.0009 (11)	0.0106 (9)	0.0049 (10)
C14	0.0567 (13)	0.0713 (17)	0.0545 (13)	0.0024 (12)	0.0108 (11)	−0.0128 (11)
C15	0.0569 (13)	0.0574 (15)	0.0621 (14)	−0.0068 (11)	0.0113 (10)	−0.0130 (11)
C16	0.0419 (10)	0.0470 (12)	0.0472 (11)	−0.0021 (9)	0.0043 (8)	0.0007 (9)

Geometric parameters (Å, °)

Cl1—C4	1.741 (2)	C6—C7	1.462 (3)
O1—C9	1.229 (3)	C7—C8	1.321 (3)
N1—C10	1.363 (3)	C7—H7	0.929
N1—C11	1.369 (2)	C8—C9	1.469 (3)
N1—H9	0.880	C8—H8	0.930
N2—C10	1.318 (3)	C9—C10	1.470 (3)
N2—C16	1.383 (3)	C11—C12	1.397 (3)
C1—C2	1.382 (3)	C11—C16	1.398 (3)
C1—C6	1.393 (3)	C12—C13	1.368 (3)
C1—H1	0.939	C12—H12	0.948
C2—C3	1.379 (4)	C13—C14	1.394 (4)
C2—H2	0.940	C13—H13	0.942
C3—C4	1.369 (4)	C14—C15	1.375 (3)
C3—H3	0.946	C14—H14	0.951
C4—C5	1.379 (3)	C15—C16	1.395 (3)
C5—C6	1.385 (3)	C15—H15	0.947
C5—H5	0.938		
C10—N1—C11	106.79 (18)	C7—C8—H8	121.8
C10—N1—H9	127.1	C9—C8—H8	117.7
C11—N1—H9	125.8	C8—C9—O1	122.57 (19)
C10—N2—C16	104.25 (17)	C8—C9—C10	118.00 (19)
C2—C1—C6	120.1 (2)	O1—C9—C10	119.42 (19)
C2—C1—H1	119.6	C9—C10—N1	120.70 (19)
C6—C1—H1	120.2	C9—C10—N2	125.98 (18)
C1—C2—C3	120.5 (2)	N1—C10—N2	113.32 (18)
C1—C2—H2	117.7	N1—C11—C12	132.1 (2)
C3—C2—H2	121.9	N1—C11—C16	105.33 (17)
C2—C3—C4	119.4 (2)	C12—C11—C16	122.61 (19)
C2—C3—H3	122.6	C11—C12—C13	116.4 (2)
C4—C3—H3	117.9	C11—C12—H12	122.0

Cl1—C4—C3	120.05 (19)	C13—C12—H12	121.6
Cl1—C4—C5	119.0 (2)	C12—C13—C14	122.0 (2)
C3—C4—C5	120.9 (2)	C12—C13—H13	118.9
C4—C5—C6	120.3 (2)	C14—C13—H13	119.0
C4—C5—H5	120.1	C13—C14—C15	121.3 (2)
C6—C5—H5	119.6	C13—C14—H14	118.5
C1—C6—C5	118.8 (2)	C15—C14—H14	120.2
C1—C6—C7	123.1 (2)	C14—C15—C16	118.2 (2)
C5—C6—C7	118.1 (2)	C14—C15—H15	121.9
C6—C7—C8	128.5 (2)	C16—C15—H15	119.9
C6—C7—H7	115.3	C11—C16—C15	119.37 (19)
C8—C7—H7	116.2	C11—C16—N2	110.30 (18)
C7—C8—C9	120.4 (2)	C15—C16—N2	130.3 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H9···O1^{i}	0.88	2.03	2.853 (2)	156

Symmetry codes: (i) −*x*+1, −*y*−1, −*z*+1.

Fig. 1

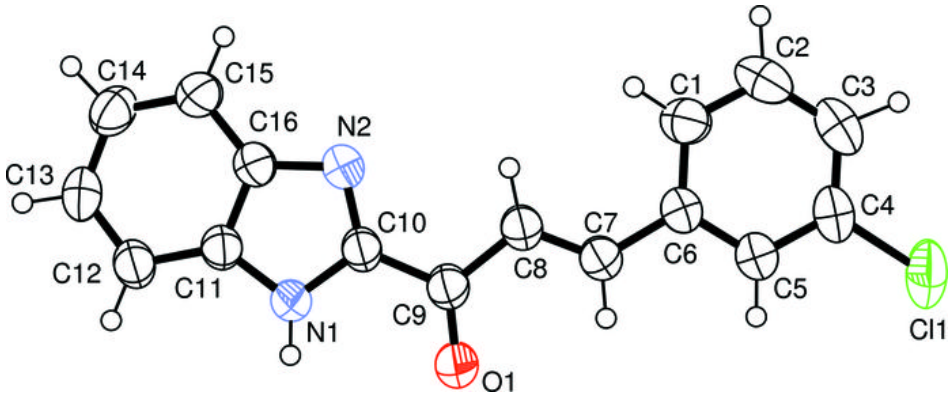

Fig. 2