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2-(4-Aminophenyl)-1,3-benzoxazole

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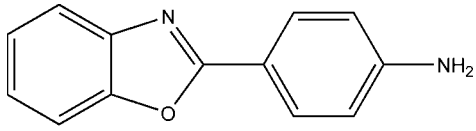
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.065; wR factor = 0.152; data-to-parameter ratio = 12.6.

In the title molecule, $C_{13}H_{10}N_2O$, the dihedral angle between the benzoxazole ring system and the benzene ring is 11.8 (1)°. In the crystal structure, molecules are linked by intermolecular N—H···N hydrogen bonds and $\pi\cdots\pi$ interactions [centroid–centroid distance = 3.6560 (15) Å] to form a two-dimensional network.

Related literature

For related literature, see: Prudhomme *et al.* (1986); Vinsova *et al.* (2005).



Experimental

Crystal data

$C_{13}H_{10}N_2O$
M_r = 210.23
Monoclinic, $P2_1/n$
a = 4.1461 (3) Å
b = 19.5420 (12) Å
c = 12.7705 (8) Å
β = 95.243 (1)°
V = 1030.38 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.30 × 0.20 × 0.15 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.974, T_{max} = 0.987
4628 measured reflections
1902 independent reflections
1315 reflections with $I > 2\sigma(I)$
R_{int} = 0.086

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.151
S = 1.08
1902 reflections
151 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···N1^{i}	0.868 (10)	2.174 (12)	3.028 (3)	168 (3)

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2630).

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2-(4-Aminophenyl)-1,3-benzoxazole

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S1. Comment

The benzoxazole rings sytem is one of the most common heterocycles in medicinal chemistry. Previous reports revealed that substituted benzoxazoles possess diverse chemotherapeutic activities including antibiotic, antimicrobial, antiviral and antitumor activities (Prudhomme *et al.*, 1986; Vinsova *et al.*, 2005). With this mind, the title compound, (I), was prepared in a series of syntheses to produce new benzoxazole derivatives, and we report the crystal stucture herein.

The molecular structure of (I) is illustrated in Fig. 1. In (I), the benzixazole rings system is not co-planar with the benzene ring, the dihedral angle being 11.8 (1)°. In the crystal structure, molecules are linked by N2—H2B···N1^{i} hydrogen bonds (symmetry code: (i) *x* -1/2, 3/2 - *y*, *z* - 1/2) into a one-dimensional chains along [101] (Fig. 2). Neighbouring chains are further linked into a two-dimensional network by $\pi..\pi$ interactions with Cg1···Cg2(-1+x, y, z) = 3.6560 (15) Å where Cg1 and Cg2 are the centroids defined by the ring atoms O1/C1/C6/N1/C7 and C1-C6 respectivley. There are no significant interactions between the adjacent layers.

S2. Experimental

All reagents and solvents were used as obtained without further purification. 4-aminobenzoic acid (13.7 g, 0.1 mol) and 2-aminophenol (10.9 g, 0.1 mmol) were mixed together with polyphosphoric acid (50 g) and heated to 493 K under N_2 atmosphere for 4 h. The reaction mixture was cooled to room temperature and poured into 10% K_2CO_3 solution. The precipitate was filtered under reduced pressure. Brown crystals were obtained by recrystallization from acetone-water.Yield: 88%; Analysis calculated for $C_{13}H_{10}N_2O$: C 74.29, H 4.76, N 13.33%; found: C 74.26, H 4.78, N 13.35%.

S3. Refinement

All the aromatic H atoms were located at the geometrical positions with C—H=0.93 Å(aromatic), and the U_{iso} values were set 1.2 times of their carrier atoms. H2A and H2B were found in difference Fourier maps and refined with the constraint of *N*—*H*=0.86 Å (amine) and U_{iso}(H)=1.2U_{eq}(N).

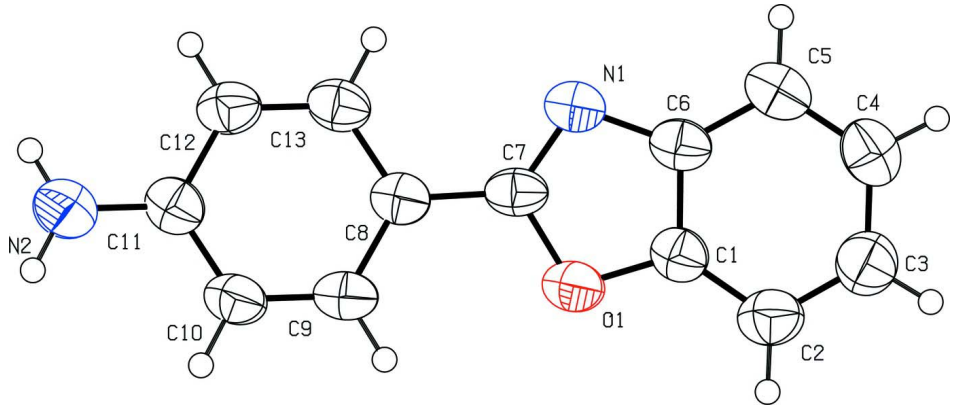

Figure 1

Molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

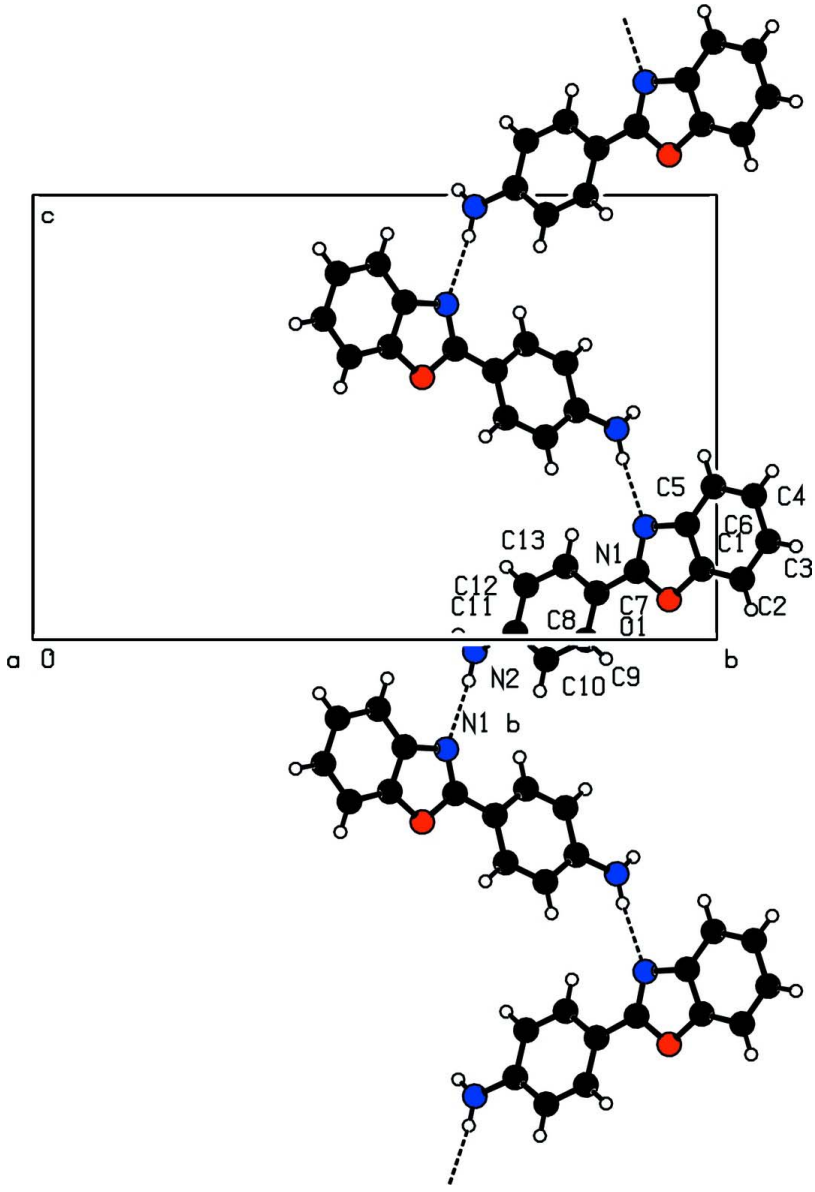

Figure 2

Part of the crystal packing showing the formation of the [101] chains linked by by N—H···N hydrogen bonds shown as dashed lines.

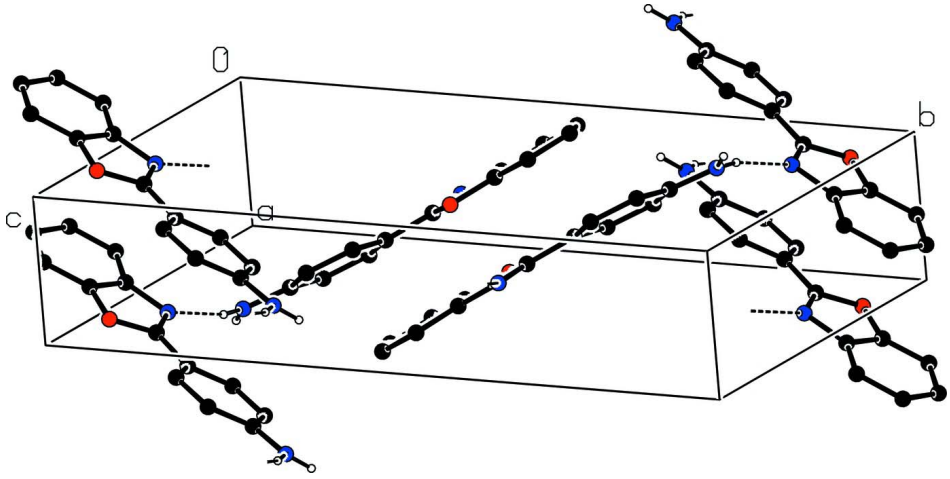

Figure 3

Part of the crystal packing showing the formation of the two-dimensional layers formed by by N—H···N hydrogen bonds shown as dashed lines and $\pi\cdots\pi$ interactions. For clarity, H atoms not involved in the motif have been omitted.

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Crystal data

$C_{13}H_{10}N_2O$
$M_r = 210.23$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 4.1461\ (3)$ Å
$b = 19.5420\ (12)$ Å
$c = 12.7705\ (8)$ Å
$\beta = 95.243\ (1)°$
$V = 1030.38\ (12)$ Å^3
$Z = 4$
$F(000) = 440$
$D_x = 1.355$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1089 reflections
$\theta = 2.6–22.6°$
$\mu = 0.09$ mm^{-1}
$T = 298$ K
Block, brown
0.30 × 0.20 × 0.15 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.974$, $T_{max} = 0.987$
4628 measured reflections
1902 independent reflections
1315 reflections with $I > 2\sigma(I)$
$R_{int} = 0.086$
$\theta_{max} = 25.5°$, $\theta_{min} = 1.9°$
$h = -4\rightarrow5$
$k = -23\rightarrow17$
$l = -14\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.151$
$S = 1.09$
1902 reflections
151 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 atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 0.0374P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	1.1291 (4)	0.93054 (9)	0.09030 (12)	0.0548 (5)
N1	1.0571 (5)	0.89549 (10)	0.25399 (15)	0.0508 (6)
C8	0.8394 (6)	0.82440 (13)	0.10509 (18)	0.0471 (6)
C7	1.0044 (6)	0.88277 (13)	0.15444 (18)	0.0472 (6)
C13	0.6743 (6)	0.77900 (13)	0.16499 (19)	0.0522 (7)
H13	0.6617	0.7882	0.2360	0.063*
C11	0.5492 (6)	0.70536 (14)	0.01598 (19)	0.0511 (7)
C1	1.2748 (6)	0.97814 (13)	0.15893 (18)	0.0488 (7)
N2	0.4179 (7)	0.64627 (14)	−0.02632 (19)	0.0746 (8)
H2B	0.430 (7)	0.6376 (13)	−0.0924 (9)	0.090 (1)*
H2A	0.300 (6)	0.6220 (12)	0.0115 (19)	0.090 (1)*
C6	1.2309 (6)	0.95673 (13)	0.25916 (18)	0.0487 (7)
C12	0.5301 (6)	0.72124 (13)	0.1221 (2)	0.0561 (7)
H12	0.4183	0.6923	0.1638	0.067*
C9	0.8540 (6)	0.80871 (14)	−0.00072 (18)	0.0529 (7)
H9	0.9622	0.8382	−0.0428	0.064*
C2	1.4362 (7)	1.03717 (14)	0.1363 (2)	0.0630 (8)
H2	1.4620	1.0504	0.0676	0.076*
C5	1.3567 (7)	0.99539 (15)	0.3444 (2)	0.0615 (8)
H5	1.3315	0.9819	0.4130	0.074*
C10	0.7122 (6)	0.75067 (14)	−0.04423 (19)	0.0556 (7)
H10	0.7254	0.7415	−0.1152	0.067*
C3	1.5567 (7)	1.07529 (15)	0.2214 (2)	0.0664 (8)
H3	1.6650	1.1159	0.2103	0.080*
C4	1.5205 (7)	1.05458 (16)	0.3237 (2)	0.0640 (8)
H4	1.6088	1.0812	0.3795	0.077*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0637 (12)	0.0592 (12)	0.0423 (10)	0.0044 (9)	0.0097 (8)	0.0024 (9)
N1	0.0542 (13)	0.0567 (15)	0.0422 (12)	0.0052 (11)	0.0075 (9)	0.0029 (10)

C8	0.0499 (15)	0.0475 (16)	0.0443 (14)	0.0116 (12)	0.0062 (11)	0.0034 (12)
C7	0.0491 (15)	0.0520 (17)	0.0419 (14)	0.0135 (13)	0.0115 (11)	0.0073 (12)
C13	0.0545 (16)	0.0579 (19)	0.0453 (15)	0.0110 (14)	0.0119 (12)	−0.0013 (13)
C11	0.0529 (16)	0.0502 (17)	0.0502 (15)	0.0121 (13)	0.0053 (12)	−0.0028 (13)
C1	0.0528 (16)	0.0470 (16)	0.0469 (15)	0.0099 (13)	0.0059 (11)	−0.0013 (12)
N2	0.097 (2)	0.0717 (19)	0.0584 (15)	−0.0086 (15)	0.0221 (14)	−0.0112 (14)
C6	0.0493 (15)	0.0537 (17)	0.0439 (14)	0.0127 (13)	0.0082 (11)	0.0023 (12)
C12	0.0601 (17)	0.0587 (19)	0.0518 (16)	0.0057 (14)	0.0173 (13)	0.0044 (13)
C9	0.0594 (17)	0.0594 (18)	0.0410 (14)	0.0089 (14)	0.0103 (11)	0.0072 (12)
C2	0.071 (2)	0.063 (2)	0.0568 (17)	0.0044 (16)	0.0167 (14)	0.0039 (15)
C5	0.0651 (18)	0.072 (2)	0.0468 (16)	0.0091 (16)	0.0051 (13)	−0.0044 (14)
C10	0.0680 (18)	0.0591 (19)	0.0408 (14)	0.0067 (15)	0.0111 (13)	−0.0006 (13)
C3	0.067 (2)	0.063 (2)	0.070 (2)	−0.0023 (15)	0.0143 (15)	−0.0052 (16)
C4	0.0577 (18)	0.069 (2)	0.0643 (19)	0.0032 (16)	0.0024 (14)	−0.0143 (15)

Geometric parameters (Å, º)

O1—C7	1.374 (3)	N2—H2B	0.868 (10)
O1—C1	1.379 (3)	N2—H2A	0.859 (10)
N1—C7	1.294 (3)	C6—C5	1.387 (3)
N1—C6	1.395 (3)	C12—H12	0.9300
C8—C13	1.392 (3)	C9—C10	1.372 (3)
C8—C9	1.392 (3)	C9—H9	0.9300
C8—C7	1.445 (4)	C2—C3	1.373 (4)
C13—C12	1.368 (3)	C2—H2	0.9300
C13—H13	0.9300	C5—C4	1.379 (4)
C11—N2	1.367 (4)	C5—H5	0.9300
C11—C10	1.388 (3)	C10—H10	0.9300
C11—C12	1.399 (3)	C3—C4	1.389 (4)
C1—C6	1.374 (3)	C3—H3	0.9300
C1—C2	1.378 (4)	C4—H4	0.9300
C7—O1—C1	104.26 (18)	C5—C6—N1	131.3 (2)
C7—N1—C6	104.6 (2)	C13—C12—C11	120.6 (2)
C13—C8—C9	117.4 (2)	C13—C12—H12	119.7
C13—C8—C7	120.0 (2)	C11—C12—H12	119.7
C9—C8—C7	122.4 (2)	C10—C9—C8	121.4 (2)
N1—C7—O1	114.6 (2)	C10—C9—H9	119.3
N1—C7—C8	127.7 (2)	C8—C9—H9	119.3
O1—C7—C8	117.7 (2)	C3—C2—C1	115.9 (3)
C12—C13—C8	121.7 (2)	C3—C2—H2	122.0
C12—C13—H13	119.2	C1—C2—H2	122.0
C8—C13—H13	119.2	C4—C5—C6	117.5 (2)
N2—C11—C10	121.1 (2)	C4—C5—H5	121.2
N2—C11—C12	121.0 (2)	C6—C5—H5	121.2
C10—C11—C12	117.9 (2)	C9—C10—C11	121.0 (2)
C6—C1—C2	123.9 (2)	C9—C10—H10	119.5
C6—C1—O1	107.4 (2)	C11—C10—H10	119.5

C2—C1—O1	128.7 (2)	C2—C3—C4	121.6 (3)
C11—N2—H2B	119.6 (19)	C2—C3—H3	119.2
C11—N2—H2A	118 (2)	C4—C3—H3	119.2
H2B—N2—H2A	122 (3)	C5—C4—C3	121.5 (3)
C1—C6—C5	119.5 (3)	C5—C4—H4	119.3
C1—C6—N1	109.2 (2)	C3—C4—H4	119.3
C6—N1—C7—O1	0.1 (3)	C7—N1—C6—C5	−179.6 (3)
C6—N1—C7—C8	178.5 (2)	C8—C13—C12—C11	1.1 (4)
C1—O1—C7—N1	−0.1 (3)	N2—C11—C12—C13	177.1 (3)
C1—O1—C7—C8	−178.7 (2)	C10—C11—C12—C13	−1.4 (4)
C13—C8—C7—N1	9.5 (4)	C13—C8—C9—C10	−0.2 (4)
C9—C8—C7—N1	−166.4 (2)	C7—C8—C9—C10	175.9 (2)
C13—C8—C7—O1	−172.1 (2)	C6—C1—C2—C3	0.1 (4)
C9—C8—C7—O1	12.0 (3)	O1—C1—C2—C3	179.7 (2)
C9—C8—C13—C12	−0.3 (4)	C1—C6—C5—C4	0.4 (4)
C7—C8—C13—C12	−176.4 (2)	N1—C6—C5—C4	179.9 (2)
C7—O1—C1—C6	0.1 (2)	C8—C9—C10—C11	−0.1 (4)
C7—O1—C1—C2	−179.6 (2)	N2—C11—C10—C9	−177.6 (3)
C2—C1—C6—C5	−0.7 (4)	C12—C11—C10—C9	0.9 (4)
O1—C1—C6—C5	179.6 (2)	C1—C2—C3—C4	0.9 (4)
C2—C1—C6—N1	179.7 (2)	C6—C5—C4—C3	0.5 (4)
O1—C1—C6—N1	0.0 (3)	C2—C3—C4—C5	−1.2 (4)
C7—N1—C6—C1	−0.1 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···N1^{i}	0.87 (1)	2.17 (1)	3.028 (3)	168 (3)

Symmetry code: (i) *x*−1/2, −*y*+3/2, *z*−1/2.