

N,N'-DibenzoylpiperazinePeng-Wu Zheng,^{a*} Wei Wang^b
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Key indicators

Single-crystal X-ray study

 $T = 294\text{ K}$ Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$ R factor = 0.038 wR factor = 0.106

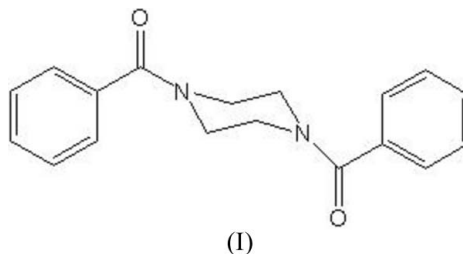
Data-to-parameter ratio = 15.6

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

In the title structure, $\text{C}_{18}\text{H}_{18}\text{N}_2\text{O}_2$, the piperazine ring adopts a chair conformation and the two phenyl rings are parallel. The molecule possesses a crystallographically imposed inversion centre. In the crystal structure, weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds link the molecules into ribbons along the b axis.

Comment

The structural study of piperazine derivatives is of interest because some of them constitute a novel class of mixed D2/D4 receptor antagonists (Zhao *et al.*, 2002). The *N,N'*-disubstituted piperazine derivatives exhibit antifilarial, antiamebic and spermicidal properties (Sonurlikar *et al.*, 1977). We report here the crystal structure of the title compound, (I).



The molecule of (I) possesses a crystallographically imposed inversion centre (Fig. 1). The piperazine ring exhibits a chair conformation with the usual bond lengths and angles (Table 1) (Martínez-Martínez *et al.*, 2004; Yogavel *et al.*, 2003). The sum of angles around atom N1 is 360.0° , and the $\text{N1}-\text{C7}$ bond length is $1.354(18)\text{ \AA}$, in accordance with the Nsp^2-

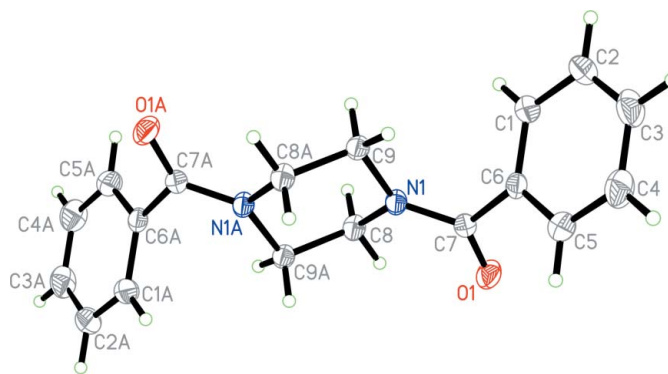


Figure 1

View of (I), showing the atom-labelling scheme and displacement ellipsoids drawn at the 30% probability level [symmetry code: (A) $1 - x, -y, 1 - z$].

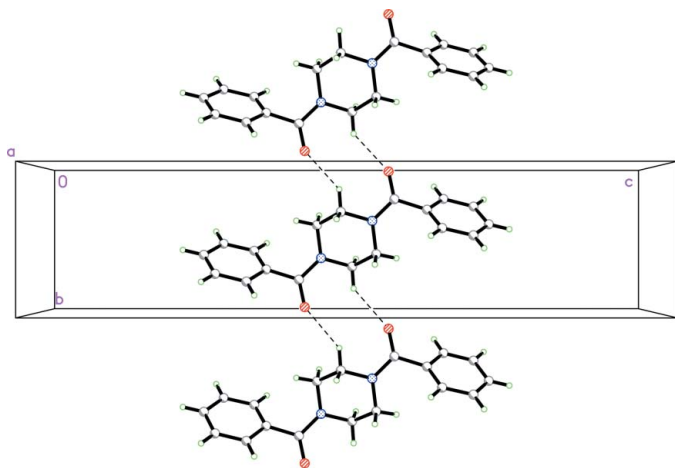


Figure 2
Hydrogen-bonded (dashed lines) ribbons of (I) in the crystal structure.

Csp^2 amide character [1.355 (14) Å; Allen *et al.*, 1987]. The two phenyl rings [C1–C6 and that related by the inversion centre C1ⁱ–C6ⁱ; symmetry code: (i) $1 - x, -y, 1 - z$] are parallel. In the crystal structure, weak intermolecular C–H \cdots O hydrogen bonds (Table 2) form a ten-membered ring described by the graph-set descriptor $R_2^2(10)$ and link the molecules into ribbons along the *b* axis (Fig. 2).

Experimental

The title compound was prepared by a modified method (Lewis *et al.*, 2003). To a solution of anhydrous piperazine (5 mmol, 0.43 g) in CH_2Cl_2 (20 ml) was added 2.2 equivalents of triethylamine (1.5 ml), followed by benzoyl chloride (10 mmol, 1.40 g) in CH_2Cl_2 (10 ml). After the mixture had been stirred for 10 min, the solvent was removed using a rotary evaporator. The solid residue was washed with water and recrystallized from ethanol–cyclohexane to give a colourless solid (85% yield; m.p. 471–472 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of the mother liquor.

Crystal data

$C_{18}H_{18}N_2O_2$	Mo $K\alpha$ radiation
$M_r = 294.34$	Cell parameters from 2532 reflections
Orthorhombic, <i>Pbca</i>	$\theta = 2.8$ – 26.4°
$a = 7.8486$ (13) Å	$\mu = 0.08$ mm ⁻¹
$b = 6.8254$ (12) Å	$T = 294$ (2) K
$c = 28.771$ (5) Å	Block, colourless
$V = 1541.3$ (5) Å ³	$0.26 \times 0.24 \times 0.20$ mm
$Z = 4$	
$D_x = 1.268$ Mg m ⁻³	

Data collection

Bruker SMART CCD area-detector diffractometer	1580 independent reflections
φ and ω scans	1168 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{int} = 0.037$
$T_{min} = 0.930, T_{max} = 0.983$	$\theta_{max} = 26.4^\circ$
7944 measured reflections	$h = -9 \rightarrow 5$
	$k = -8 \rightarrow 8$
	$l = -35 \rightarrow 35$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0513P)^2 + 0.3539P]$
$R[F^2 > 2\sigma(F^2)] = 0.038$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.106$	$(\Delta/\sigma)_{max} = 0.004$
$S = 1.02$	$\Delta\rho_{max} = 0.17$ e Å ⁻³
1580 reflections	$\Delta\rho_{min} = -0.14$ e Å ⁻³
101 parameters	Extinction correction: <i>SHELXL</i>
H-atom parameters constrained	Extinction coefficient: 0.060 (4)

Table 1

Selected geometric parameters (Å, °).

O1–C7	1.2284 (18)	N1–C9	1.4629 (17)
N1–C7	1.3539 (18)	C8–C9 ⁱ	1.511 (2)
N1–C8	1.4619 (17)		
C7–N1–C8	120.56 (12)	O1–C7–N1	122.27 (13)
C7–N1–C9	125.98 (12)	O1–C7–C6	119.23 (13)
C8–N1–C9	113.43 (11)	N1–C7–C6	118.45 (12)
C8–N1–C7–O1	–9.7 (2)	C8–N1–C7–C6	167.75 (12)
C9–N1–C7–O1	172.45 (14)	C9–N1–C7–C6	–10.1 (2)

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

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> –H \cdots <i>A</i>	<i>D</i> –H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> –H \cdots <i>A</i>
C8–H8A \cdots O1 ⁱⁱ	0.97	2.48	3.253 (3)	137

Symmetry codes (ii) $-x + 1, -y + 1, -z + 1$.

All H atoms were positioned geometrically and refined as riding, with C–H = 0.93–0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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