Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

N-(1-Benzylpiperidin-4-yl)-*N*′-(4-methoxybenzoyl)-thiourea

Sukeri M. Yusof and Bohari M. Yamin*

School of Chemical Sciences and Food Technology, Universiti Kebangsaan Malaysia, 43600 Bangi, Selangor, Malaysia

Correspondence e-mail: bohari@pkrisc.cc.ukm.my

In the title compound, $C_{21}H_{25}N_3O_2S$, the *p*-anisoyl group is inclined to the central thiourea N_2CS unit by 31.939 (11)° and the piperidine ring adopts a chair conformation. The molecule is stabilized by intra- and intermolecular interactions to form polymeric chains parallel to the *ac* plane.

Received 10 June 2005
Accepted 20 June 2005
Online 24 June 2005

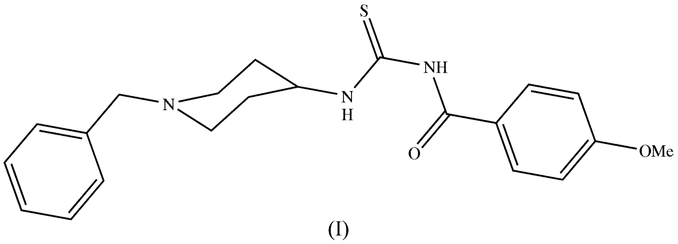
Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.004 Å
R factor = 0.068
wR factor = 0.133
Data-to-parameter ratio = 15.4

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

Comment

Bond lengths and angles in the molecule of the title compound (I) (Fig. 1) are in normal ranges (Allen *et al.*, 1987) and in agreement with those found in *N*-(2-chlorophenyl)-*N*′-(4-methoxybenzoyl)thiourea (Yusof & Yamin, 2004).



(I)

The piperidine ring adopts a chair conformation. The methoxybenzoyl and 1-benzyl-1-piperidine fragments are *trans* and *cis*, respectively, with respect to the C8═S1 thiono group across the C8—N1 and C8—N2 bonds. The dihedral angle between the central thiourea unit, S1/C8/N1/N2 [maximum deviation 0.007 (3) Å at C8] and the benzene ring C1–C6/C7/O2/C21 [maximum deviation 0.017 (3) Å at C21] is 31.93 (11)°. The benzyl fragment C14–C20 [maximum deviation 0.049 (2)° at C14] is inclined to the central thiourea unit and the C1–C7/O2/C21 ring by 38.17 (12) and 48.40 (11)°,

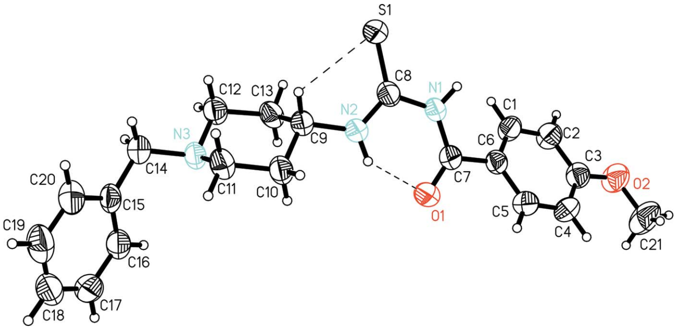


Figure 1
A drawing of the molecule of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Intramolecular hydrogen bonds are shown as dashed lines.

respectively. There are two intramolecular interactions, *viz*. C9—H9*A*···S1 and N2—H2*A*···O1, resulting in the formation of pseudo-five-membered and six-membered rings S1···H2*A*—C9—N2—C8—S1 and O1···H2*A*—N2—C8—N1—C7—O1, respectively. In the crystal structure, the molecules are linked by intermolecular interactions, *viz*. N1—H1*A*···S1^{i} and C21—H21*C*···O2^{ii} (symmetry codes as in Table 2), to form polymeric chains parallel to the *ac* plane.

Experimental

A solution of 4-amino-*N*-benzylpiperidine (0.5 g, 1.31 mol) in acetone (50 ml) was added dropwise to an acetone solution (50 ml) containing an equimolar amount of *p*-methoxybenzoyl isothiocyanate. The solution was refluxed for 2 h and then poured into a beaker containing some crushed ice. The white precipitate was washed with cold ethanol and distilled water, then dried in a vacuum (yield 80%). Recrystallization from acetone gave single cystals suitable for X-ray analysis (m.p. 412.2–413.1 K). Analysis calculated: C 65.7, H 6.57, N 10.96, S 8.36, O 8.34%; found: C 66.3, H 6.40, N 10.69, S 7.50, O 9.13%.

Crystal data

$C_{21}H_{25}N_3O_2S$
$M_r = 383.50$
Monoclinic, $P2_1/n$
$a = 11.775$ (2) Å
$b = 7.0646$ (14) Å
$c = 24.362$ (5) Å
$\beta = 94.777$ (4)°
$V = 2019.6$ (7) Å^3
$Z = 4$
$D_x = 1.261$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 1914 reflections
$\theta = 1.6$–25.5°
$\mu = 0.18$ mm^{-1}
$T = 273$ (2) K
Plate, colourless
0.46 × 0.20 × 0.09 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.921$, $T_{\max} = 0.983$
10172 measured reflections
3754 independent reflections
2953 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.036$
$\theta_{\max} = 25.5°$
$h = -13 \rightarrow 14$
$k = -8 \rightarrow 8$
$l = -29 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.133$
$S = 1.18$
3754 reflections
244 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0387P)^2 + 0.7201P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.23$ e Å^{-3}
$\Delta\rho_{\min} = -0.16$ e Å^{-3}

Table 1
Selected bond lengths (Å).

S1—C8	1.667 (3)	N2—C8	1.321 (3)
O1—C7	1.221 (3)	N2—C9	1.465 (3)
O2—C3	1.364 (3)	N3—C11	1.456 (3)
O2—C21	1.409 (4)	N3—C14	1.462 (3)
N1—C7	1.373 (3)	N3—C12	1.463 (3)
N1—C8	1.391 (3)		

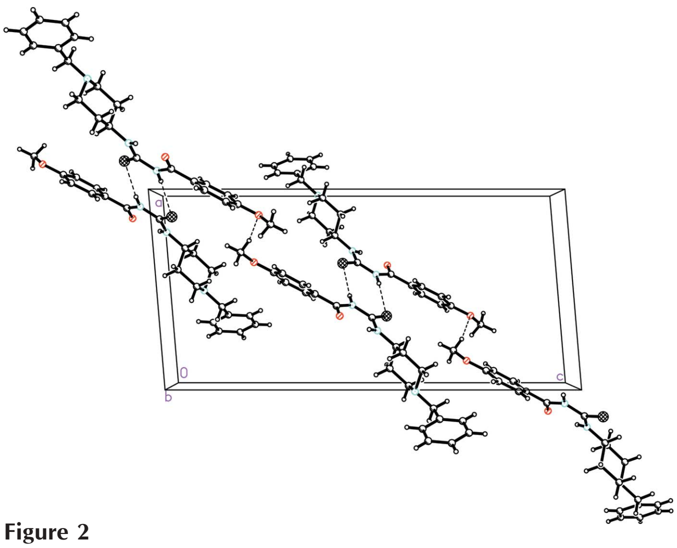


Figure 2
The crystal packing of (I), viewed along the *b* axis. Dashed lines indicate hydrogen bonds.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1^{i}	0.86	1.94	2.627 (3)	136
C9—H9*A*···S1^{i}	0.98	2.80	3.120 (3)	100
N1—H1*A*···S1^{ii}	0.86	2.66	3.516 (2)	172
C21—H21*C*···O2^{iii}	0.96	2.56	3.438 (4)	152

Symmetry codes: (i) x, y, z; (ii) $-x+2, -y+2, -z+2$; (iii) $-x+\frac{5}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

After their location in a difference map, all H atoms were positioned geometrically and allowed to ride on the parent atom with C—H = 0.93–0.96 Å and N—H = 0.86 Å, and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$($CH_2$ and NH) or $1.5U_{\rm eq}$(CH_3).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

The authors thank the Malaysian Government for the research grant IRPA No. 09–02-02–0163.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L. Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Yusof, M. S. M. & Yamin, B. M. (2004). *Acta Cryst.* E**60**, o1998–o1999.