Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 4-Bromo-2-{α-[1-(2-thienyl)benzimidazol-2-yl]benzyl}phenol

**Fengke Yang, Fang Chen and Hailian Xiao***

New Materials & Function, Coordination Chemistry Laboratory, Qingdao University of Science & Technology, Qingdao 266042, People's Republic of China
Correspondence e-mail: xiaohailian@163.com

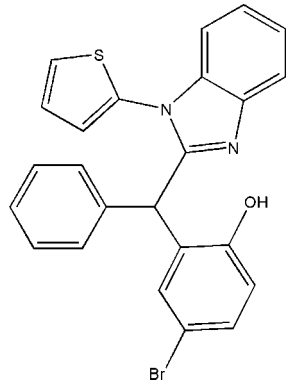
Received 24 April 2007; accepted 15 May 2007

Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.041; $wR$ factor = 0.112; data-to-parameter ratio = 14.7.

In the title compound, $C_{24}H_{17}BrN_2OS$, the benzimidazole ring system is planar. The dihedral angles formed by the bromophenol, phenyl and thienyl rings with the benzimidazole ring system are 78.4 (1), 80.2 (2) and 33.1 (1)°, respectively. The molecular structure and packing are stabilized by intra- and intermolecular O—H···N and C—H···N hydrogen-bonding interactions and C—H···π interactions.

## Related literature

For related literature, see: Fekner *et al.* (2004); Liu *et al.* (2005); Rivas *et al.* (2002); Woolley (1944).




## Experimental

*Crystal data*

$C_{24}H_{17}BrN_2OS$
$M_r$ = 461.37
Monoclinic, $P2_1/c$
$a$ = 13.623 (3) Å
$b$ = 9.6472 (19) Å
$c$ = 16.962 (3) Å
$\beta$ = 111.98 (3)°
$V$ = 2067.2 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 2.11 mm$^{-1}$
$T$ = 295 (2) K
0.25 × 0.20 × 0.18 mm

*Data collection*

Enraf-Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.609, $T_{max}$ = 0.684
8223 measured reflections
3632 independent reflections
2509 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033
3 standard reflections
every 100 reflections
intensity decay: none

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.112
$S$ = 1.02
3632 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.52 e Å$^{-3}$

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

*Cg*1 is the centroid of the C19–C24 ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C13—H13$A$···N2 | 0.93 | 2.50 | 2.843 (4) | 102 |
| O1—H1$A$···N1$^{i}$ | 0.82 | 1.94 | 2.753 (3) | 169 |
| C3—H3$A$···N1$^{ii}$ | 0.93 | 2.58 | 3.449 (5) | 155 |
| C12—H12$A$···$Cg$1$^{iii}$ | 0.93 | 3.15 | 3.916 (5) | 141 |

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2141).

## References

Enraf–Nonius (1989). *CAD-4 Software* (Version 5.0). Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Fekner, T., Gallucci, J. & Chan, M. K. (2004). *J. Am. Chem. Soc.* **126**, 223–236.
Gabe, E. J., Le Page, Y., Charland, J.-P., Lee, F. L. & White, P. S. (1989). *J. Appl. Cryst.* **22**, 384–387.
Liu, Q. D., Jia, W. L. & Wang, S. N. (2005). *Inorg. Chem.* **44**, 1332–1343.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Rivas, F. M., Giessert, A. J. & Diver, S. T. (2002). *J. Org. Chem.* **67**, 1708–1711.
Sheldrick, G. M. (1990). *SHELXTL/PC User's Manual*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Woolley, D. W. (1944). *J. Biol. Chem.* **162**, 225–232.

# supplementary materials

*Acta Cryst.* (2007). E**63**, o3041 [ **doi:10.1107/S1600536807023938** ]

# 4-Bromo-2-{α-[1-(2-thienyl)benzimidazol-2-yl]benzyl}phenol

**F. Yang, F. Chen and H. Xiao**

## Comment

The benzimidazole nucleus has been of considerable interest since it was noted that it inhibits the growth of certain yeasts and bacteria (Woolley, 1944). Over the past few years, benzimidazoles have been used as antifungals, antibacterials, antihelminthics, 5-HT receptor antagonists, and thrombin receptor antagonists (Rivas *et al.*, 2002). However, that structural modifications can produce marked effects on physiological activity has been shown by the test data on the substituted benzimidazoles. In recent chemical literature, introduction of bulky substituents in *ortho* to the amide groups significantly increases the barrier to racemization (Fekner *et al.*, 2004). For this reason, the efficient synthesis of important diversely functionalized substituted benzimidazoles have attracted considerable attention. In particular, the discovery of 1,2-bisubstituted benzimidazole has increased this interest, which can be attributed not only to a good nucleophile but to their diverse biological and pharmacological properties as well (Liu *et al.*, 2005). We describe here the structure of the title compound, I, whose ring system contains two nitrogen atoms, a tertiary basic nitrogen and the other attached to an active 2-hydroxy-5-bromophenyl)(phenyl)methyl group, bearing a chiral carbon atom.

In I, the benzimidazole ring is planar. The dihedral angles formed by the plane of the hydroxybromobenzene ring (p1) and thienyl ring (p2) with the phenyl ring are 73.6 (3) and 67.8 (2)°, respectively. The dihedral angles formed by the plane of benzimidazole with p1 and p2 are 78.4 (1) and 33.1 (1)°, respectively. The phenyl ring is almost perpendicular to the benzimidazole ring, as indicated by the dihedral angle of 80.2 (2)° between the two planes. The dihedral angle between p1 and p2 is 56.9 (2)°.

The molecular structure is stabilized by intra- and intermolecular O—H···N, C—H···N hydrogen-bonding interactions and by intermolecular C—H···π interactions (Table 2; *Cg*1 is the centroid of the C19—C24 ring).

## Experimental

5-Bromo-2-hydroxybenzophenone (HBBP) (27.7 g, 0.10 mol), 1,2-diaminobenzene (10.8 g, 0.10 mol), piperidine (10.2 g, 0.12 mol), and triethylorthoformate (12 ml) refluxed in absolute ethanol (120 ml) resulted in the red-orange product of HBBP-PHEN. The title compound was obtained by the reaction of HBBP-PHEN (22.0 g, 0.06 mol) with 2-thiopheneformaldehyde (7.3 g, 0.065 mol) and piperidine (8.5 g, 0.1 mol) in methanol (150 ml) under dry nitrogen at room temperature. The precipitated yellow solid was collected by filtration and washed twice with hot methanol. Single crystals suitable for X-ray measurements were obtained by slow evaporation of an absolute ethanol/acetic acid solution (1:1 *v*/*v*) at room temperature.

## Refinement

All H atoms were placed at calculated positions and allowed to ride on their attached atoms, with C—H = 0.93–0.98 Å and O—H = 0.82 Å, and with $U_{iso}$(H) = 1.2 $U_{eq}$(C) or 1.5 $U_{eq}$(O).

## Figures

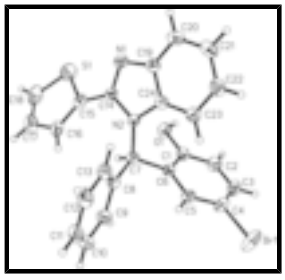


Fig. 1. The structure of the title compound showing 30% probability displacement ellipsoids and the atom-numbering scheme.

## 4-bromo-2-{α-[1-(2-thienyl)benzimidazol-2-yl]benzyl}phenol

*Crystal data*

| | |
|---|---|
| $C_{24}H_{17}BrN_2OS$ | $F_{000}$ = 936 |
| $M_r$ = 461.37 | $D_x$ = 1.482 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 25 reflections |
| $a$ = 13.623 (3) Å | θ = 4–14º |
| $b$ = 9.6472 (19) Å | μ = 2.11 mm$^{-1}$ |
| $c$ = 16.962 (3) Å | $T$ = 295 (2) K |
| β = 111.98 (3)º | Block, colourless |
| $V$ = 2067.2 (8) Å$^3$ | 0.25 × 0.20 × 0.18 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Enraf-Nonius CAD-4 diffractometer | $R_{int}$ = 0.033 |
| Radiation source: fine-focus sealed tube | $\theta_{max}$ = 25.0º |
| Monochromator: graphite | $\theta_{min}$ = 2.5º |
| $T$ = 295(2) K | $h$ = −15→16 |
| ω scans | $k$ = −11→7 |
| Absorption correction: ψ scan (North *et al.*, 1968) | $l$ = −20→18 |
| $T_{min}$ = 0.609, $T_{max}$ = 0.684 | 3 standard reflections |
| 8223 measured reflections | every 100 reflections |
| 3632 independent reflections | intensity decay: none |
| 2509 reflections with $I > 2\sigma(I)$ | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.042 | H-atom parameters constrained |

| | |
|---|---|
| $wR(F^2) = 0.112$ | $w = 1/[\sigma^2(F_o^2) + (0.0347P)^2 + 1.0362P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.02$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 3842 reflections | $\Delta\rho_{max} = 0.37$ e Å$^{-3}$ |
| 262 parameters | $\Delta\rho_{min} = -0.52$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 0.06574 (4) | 0.19632 (4) | 0.05538 (3) | 0.0884 (2) |
| S1 | 0.46731 (8) | −0.60807 (12) | 0.37058 (7) | 0.0777 (3) |
| O1 | 0.41657 (15) | −0.1640 (2) | 0.28505 (13) | 0.0519 (6) |
| H1A | 0.4732 | −0.1225 | 0.3019 | 0.078* |
| N1 | 0.39000 (19) | −0.5378 (3) | 0.17794 (16) | 0.0462 (6) |
| N2 | 0.27450 (17) | −0.3751 (2) | 0.18257 (14) | 0.0360 (5) |
| C1 | 0.3387 (2) | −0.0780 (3) | 0.23568 (18) | 0.0425 (7) |
| C2 | 0.3573 (3) | 0.0582 (4) | 0.2186 (2) | 0.0567 (9) |
| H2A | 0.4252 | 0.0949 | 0.2432 | 0.068* |
| C3 | 0.2769 (3) | 0.1391 (4) | 0.1658 (2) | 0.0606 (9) |
| H3A | 0.2903 | 0.2294 | 0.1534 | 0.073* |
| C4 | 0.1762 (3) | 0.0858 (3) | 0.1314 (2) | 0.0510 (8) |
| C5 | 0.1543 (2) | −0.0470 (3) | 0.14970 (18) | 0.0434 (7) |
| H5A | 0.0853 | −0.0804 | 0.1274 | 0.052* |
| C6 | 0.2360 (2) | −0.1312 (3) | 0.20179 (17) | 0.0358 (6) |
| C7 | 0.2183 (2) | −0.2816 (3) | 0.21980 (18) | 0.0366 (7) |
| H7A | 0.2518 | −0.2933 | 0.2815 | 0.044* |
| C8 | 0.1029 (2) | −0.3217 (3) | 0.19572 (18) | 0.0389 (7) |
| C9 | 0.0459 (3) | −0.2612 (4) | 0.2397 (2) | 0.0532 (8) |
| H9A | 0.0787 | −0.1977 | 0.2827 | 0.064* |
| C10 | −0.0591 (3) | −0.2948 (4) | 0.2199 (3) | 0.0675 (10) |
| H10A | −0.0965 | −0.2538 | 0.2496 | 0.081* |
| C11 | −0.1084 (3) | −0.3880 (4) | 0.1568 (3) | 0.0679 (11) |
| H11A | −0.1794 | −0.4096 | 0.1434 | 0.081* |
| C12 | −0.0535 (3) | −0.4490 (4) | 0.1138 (2) | 0.0635 (10) |

| | | | | |
|---|---|---|---|---|
| H12A | −0.0872 | −0.5129 | 0.0712 | 0.076* |
| C13 | 0.0529 (2) | −0.4170 (3) | 0.13276 (19) | 0.0499 (8) |
| H13A | 0.0899 | −0.4596 | 0.1031 | 0.060* |
| C14 | 0.3385 (2) | −0.4836 (3) | 0.22301 (18) | 0.0384 (7) |
| C15 | 0.3489 (2) | −0.5363 (3) | 0.30641 (19) | 0.0468 (8) |
| C16 | 0.2737 (3) | −0.5468 (3) | 0.3435 (2) | 0.0547 (8) |
| H16A | 0.2042 | −0.5158 | 0.3186 | 0.066* |
| C17 | 0.3172 (4) | −0.6111 (4) | 0.4243 (2) | 0.0753 (11) |
| H17A | 0.2790 | −0.6267 | 0.4589 | 0.090* |
| C18 | 0.4191 (4) | −0.6472 (5) | 0.4460 (2) | 0.0829 (13) |
| H18A | 0.4589 | −0.6895 | 0.4973 | 0.099* |
| C19 | 0.3577 (2) | −0.4605 (3) | 0.10344 (19) | 0.0419 (7) |
| C20 | 0.3864 (3) | −0.4754 (4) | 0.0331 (2) | 0.0557 (9) |
| H20A | 0.4330 | −0.5446 | 0.0311 | 0.067* |
| C21 | 0.3433 (3) | −0.3840 (4) | −0.0334 (2) | 0.0613 (10) |
| H21A | 0.3620 | −0.3904 | −0.0807 | 0.074* |
| C22 | 0.2729 (3) | −0.2831 (4) | −0.0307 (2) | 0.0576 (9) |
| H22A | 0.2453 | −0.2229 | −0.0765 | 0.069* |
| C23 | 0.2417 (2) | −0.2681 (3) | 0.03740 (18) | 0.0487 (8) |
| H23A | 0.1934 | −0.2005 | 0.0381 | 0.058* |
| C24 | 0.2862 (2) | −0.3589 (3) | 0.10480 (17) | 0.0370 (7) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.0952 (4) | 0.0492 (2) | 0.0888 (3) | 0.0169 (2) | −0.0023 (2) | 0.0140 (2) |
| S1 | 0.0674 (6) | 0.0854 (8) | 0.0717 (7) | 0.0199 (5) | 0.0162 (5) | 0.0253 (6) |
| O1 | 0.0355 (11) | 0.0475 (13) | 0.0650 (14) | −0.0063 (10) | 0.0098 (10) | 0.0043 (11) |
| N1 | 0.0377 (13) | 0.0423 (15) | 0.0585 (16) | 0.0047 (12) | 0.0180 (12) | 0.0007 (13) |
| N2 | 0.0336 (12) | 0.0317 (13) | 0.0416 (14) | 0.0028 (10) | 0.0126 (10) | −0.0009 (10) |
| C1 | 0.0426 (17) | 0.0406 (17) | 0.0450 (17) | −0.0007 (14) | 0.0172 (14) | −0.0005 (14) |
| C2 | 0.0488 (19) | 0.0442 (19) | 0.075 (2) | −0.0122 (16) | 0.0210 (17) | −0.0047 (17) |
| C3 | 0.069 (2) | 0.0340 (17) | 0.081 (2) | −0.0033 (17) | 0.029 (2) | 0.0054 (17) |
| C4 | 0.058 (2) | 0.0359 (17) | 0.0536 (19) | 0.0106 (15) | 0.0142 (16) | 0.0016 (15) |
| C5 | 0.0436 (17) | 0.0371 (16) | 0.0465 (17) | 0.0006 (14) | 0.0134 (14) | −0.0035 (14) |
| C6 | 0.0383 (15) | 0.0311 (15) | 0.0395 (15) | 0.0004 (12) | 0.0162 (13) | −0.0027 (12) |
| C7 | 0.0360 (15) | 0.0353 (16) | 0.0380 (15) | 0.0012 (12) | 0.0134 (12) | −0.0021 (12) |
| C8 | 0.0361 (15) | 0.0343 (15) | 0.0457 (17) | 0.0009 (13) | 0.0148 (13) | 0.0040 (13) |
| C9 | 0.0472 (19) | 0.053 (2) | 0.062 (2) | −0.0007 (16) | 0.0243 (16) | −0.0044 (17) |
| C10 | 0.050 (2) | 0.072 (3) | 0.090 (3) | 0.006 (2) | 0.038 (2) | 0.010 (2) |
| C11 | 0.0390 (19) | 0.071 (3) | 0.090 (3) | −0.0083 (19) | 0.020 (2) | 0.017 (2) |
| C12 | 0.053 (2) | 0.060 (2) | 0.069 (2) | −0.0222 (18) | 0.0127 (18) | −0.0024 (19) |
| C13 | 0.0494 (19) | 0.0466 (19) | 0.0515 (19) | −0.0067 (15) | 0.0164 (15) | −0.0014 (15) |
| C14 | 0.0324 (15) | 0.0317 (15) | 0.0483 (18) | −0.0008 (12) | 0.0119 (13) | −0.0020 (13) |
| C15 | 0.0488 (18) | 0.0363 (17) | 0.0502 (18) | −0.0002 (14) | 0.0128 (15) | 0.0018 (14) |
| C16 | 0.060 (2) | 0.049 (2) | 0.058 (2) | 0.0038 (17) | 0.0249 (17) | 0.0157 (17) |
| C17 | 0.091 (3) | 0.071 (3) | 0.072 (3) | −0.005 (2) | 0.040 (2) | 0.020 (2) |
| C18 | 0.098 (3) | 0.074 (3) | 0.064 (3) | 0.009 (2) | 0.015 (2) | 0.028 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C19 | 0.0349 (16) | 0.0408 (17) | 0.0501 (18) | −0.0050 (13) | 0.0161 (14) | −0.0059 (14) |
| C20 | 0.0451 (19) | 0.062 (2) | 0.065 (2) | 0.0026 (17) | 0.0266 (17) | −0.0123 (19) |
| C21 | 0.060 (2) | 0.080 (3) | 0.052 (2) | −0.009 (2) | 0.0306 (18) | −0.013 (2) |
| C22 | 0.063 (2) | 0.067 (2) | 0.0412 (19) | 0.0014 (19) | 0.0179 (16) | 0.0049 (17) |
| C23 | 0.0525 (19) | 0.0496 (19) | 0.0422 (18) | 0.0052 (15) | 0.0157 (15) | −0.0016 (15) |
| C24 | 0.0339 (15) | 0.0379 (15) | 0.0373 (16) | −0.0045 (13) | 0.0111 (13) | −0.0048 (13) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Br1—C4 | 1.900 (3) | C9—H9A | 0.9300 |
| S1—C18 | 1.686 (4) | C10—C11 | 1.365 (5) |
| S1—C15 | 1.718 (3) | C10—H10A | 0.9300 |
| O1—C1 | 1.360 (3) | C11—C12 | 1.360 (5) |
| O1—H1A | 0.8200 | C11—H11A | 0.9300 |
| N1—C14 | 1.323 (4) | C12—C13 | 1.396 (4) |
| N1—C19 | 1.389 (4) | C12—H12A | 0.9300 |
| N2—C14 | 1.371 (3) | C13—H13A | 0.9300 |
| N2—C24 | 1.396 (3) | C14—C15 | 1.459 (4) |
| N2—C7 | 1.470 (3) | C15—C16 | 1.392 (4) |
| C1—C2 | 1.390 (4) | C16—C17 | 1.417 (5) |
| C1—C6 | 1.395 (4) | C16—H16A | 0.9300 |
| C2—C3 | 1.370 (5) | C17—C18 | 1.341 (5) |
| C2—H2A | 0.9300 | C17—H17A | 0.9300 |
| C3—C4 | 1.374 (5) | C18—H18A | 0.9300 |
| C3—H3A | 0.9300 | C19—C24 | 1.387 (4) |
| C4—C5 | 1.376 (4) | C19—C20 | 1.395 (4) |
| C5—C6 | 1.394 (4) | C20—C21 | 1.377 (5) |
| C5—H5A | 0.9300 | C20—H20A | 0.9300 |
| C6—C7 | 1.521 (4) | C21—C22 | 1.379 (5) |
| C7—C8 | 1.519 (4) | C21—H21A | 0.9300 |
| C7—H7A | 0.9800 | C22—C23 | 1.379 (4) |
| C8—C13 | 1.380 (4) | C22—H22A | 0.9300 |
| C8—C9 | 1.390 (4) | C23—C24 | 1.387 (4) |
| C9—C10 | 1.379 (5) | C23—H23A | 0.9300 |
| C18—S1—C15 | 91.77 (19) | C10—C11—H11A | 120.1 |
| C1—O1—H1A | 109.5 | C11—C12—C13 | 120.8 (3) |
| C14—N1—C19 | 104.9 (2) | C11—C12—H12A | 119.6 |
| C14—N2—C24 | 106.4 (2) | C13—C12—H12A | 119.6 |
| C14—N2—C7 | 126.1 (2) | C8—C13—C12 | 119.6 (3) |
| C24—N2—C7 | 126.9 (2) | C8—C13—H13A | 120.2 |
| O1—C1—C2 | 122.9 (3) | C12—C13—H13A | 120.2 |
| O1—C1—C6 | 117.4 (3) | N1—C14—N2 | 112.8 (2) |
| C2—C1—C6 | 119.7 (3) | N1—C14—C15 | 122.8 (3) |
| C3—C2—C1 | 120.7 (3) | N2—C14—C15 | 124.3 (3) |
| C3—C2—H2A | 119.6 | C16—C15—C14 | 130.0 (3) |
| C1—C2—H2A | 119.6 | C16—C15—S1 | 111.1 (2) |
| C2—C3—C4 | 119.4 (3) | C14—C15—S1 | 118.8 (2) |
| C2—C3—H3A | 120.3 | C15—C16—C17 | 110.9 (3) |
| C4—C3—H3A | 120.3 | C15—C16—H16A | 124.5 |

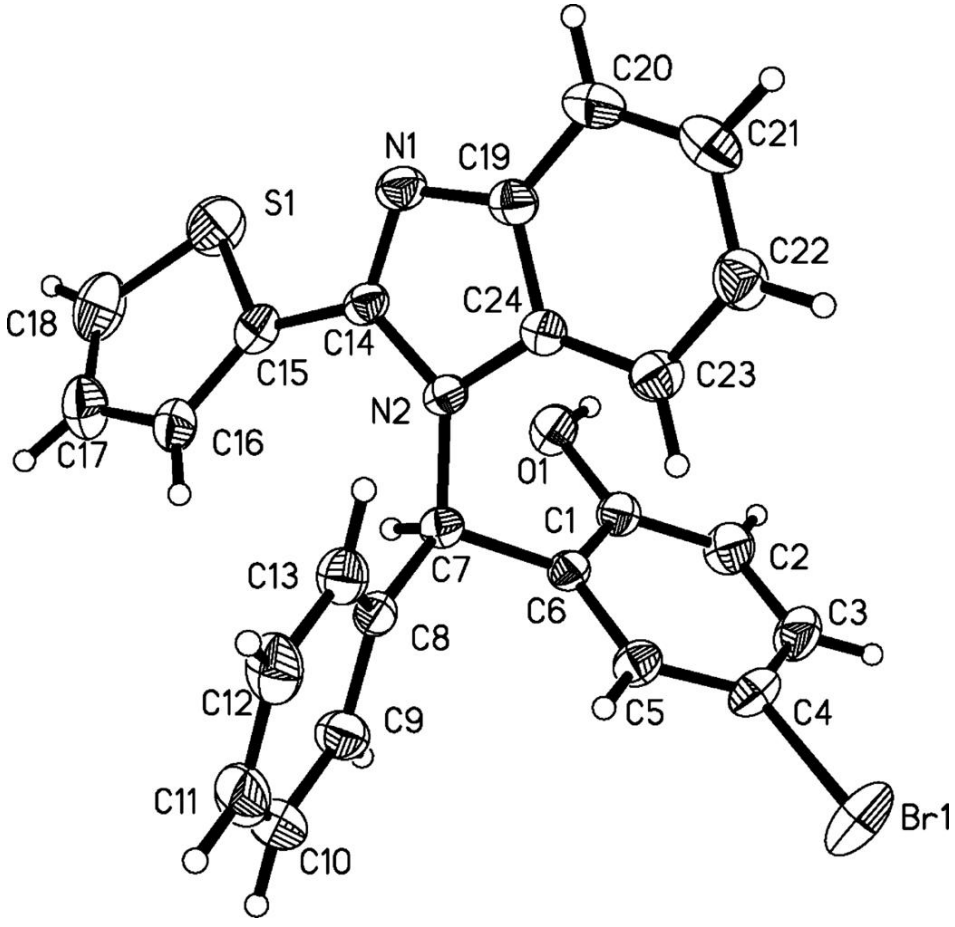
| | | | |
|---|---|---|---|
| C3—C4—C5 | 121.2 (3) | C17—C16—H16A | 124.5 |
| C3—C4—Br1 | 119.3 (3) | C18—C17—C16 | 113.2 (4) |
| C5—C4—Br1 | 119.5 (2) | C18—C17—H17A | 123.4 |
| C4—C5—C6 | 119.8 (3) | C16—C17—H17A | 123.4 |
| C4—C5—H5A | 120.1 | C17—C18—S1 | 113.0 (3) |
| C6—C5—H5A | 120.1 | C17—C18—H18A | 123.5 |
| C5—C6—C1 | 119.1 (3) | S1—C18—H18A | 123.5 |
| C5—C6—C7 | 122.3 (2) | C24—C19—N1 | 110.5 (2) |
| C1—C6—C7 | 118.5 (2) | C24—C19—C20 | 120.6 (3) |
| N2—C7—C8 | 112.4 (2) | N1—C19—C20 | 128.9 (3) |
| N2—C7—C6 | 110.6 (2) | C21—C20—C19 | 117.7 (3) |
| C8—C7—C6 | 114.5 (2) | C21—C20—H20A | 121.2 |
| N2—C7—H7A | 106.2 | C19—C20—H20A | 121.2 |
| C8—C7—H7A | 106.2 | C20—C21—C22 | 120.9 (3) |
| C6—C7—H7A | 106.2 | C20—C21—H21A | 119.6 |
| C13—C8—C9 | 118.8 (3) | C22—C21—H21A | 119.6 |
| C13—C8—C7 | 122.6 (3) | C23—C22—C21 | 122.5 (3) |
| C9—C8—C7 | 118.6 (3) | C23—C22—H22A | 118.7 |
| C10—C9—C8 | 120.5 (3) | C21—C22—H22A | 118.7 |
| C10—C9—H9A | 119.8 | C22—C23—C24 | 116.6 (3) |
| C8—C9—H9A | 119.8 | C22—C23—H23A | 121.7 |
| C11—C10—C9 | 120.5 (4) | C24—C23—H23A | 121.7 |
| C11—C10—H10A | 119.8 | C23—C24—C19 | 121.7 (3) |
| C9—C10—H10A | 119.8 | C23—C24—N2 | 132.9 (3) |
| C12—C11—C10 | 119.8 (3) | C19—C24—N2 | 105.4 (2) |
| C12—C11—H11A | 120.1 | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C13—H13A···N2 | 0.93 | 2.50 | 2.843 (4) | 102 |
| O1—H1A···N1$^{i}$ | 0.82 | 1.94 | 2.753 (3) | 169 |
| C3—H3A···N1$^{ii}$ | 0.93 | 2.58 | 3.449 (5) | 155 |
| C12—H12A···Cg1$^{iii}$ | 0.93 | 3.15 | 3.916 (5) | 141 |

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

**Fig. 1**


C20
C21
N1
C19
S1
C22
C24
C18
C14
C15
C23
N2
C17
C16
O1
C1
C13
C7
C2
C6
C3
C8
C12
C9
C5
C4
C11
Br1
C10