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# 3-Butyl-2-propylamino-1-benzothieno[3,2-*d*]pyrimidin-4(3*H*)-one

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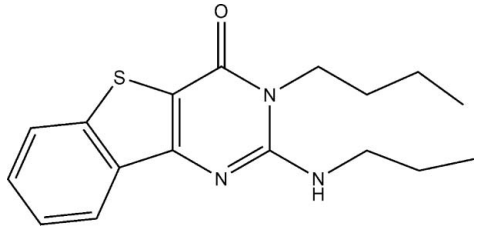
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.004 Å; disorder in main residue; $R$ factor = 0.058; $wR$ factor = 0.175; data-to-parameter ratio = 13.3.

In the title compound, $C_{17}H_{21}N_3OS$, the propyl and butyl groups are disordered over two positions; site occupation factors are 0.304 (10) and 0.696 (10). The three fused rings are coplanar. In the crystal structure, intermolecular N—H···O and C—H···O hydrogen bonds link the molecules. Further stability is provided by offset $\pi$–$\pi$ stacking interactions. Adjacent thienophene–pyrimidine and pyrimidine–benzene rings have centroid–centroid distances of 3.96 (1) and 3.55 (2) Å, respectively.

## Related literature

For general background, see: Chambhare *et al.* (2003); Janiak (2000). For related literature, see: Ding *et al.* (2004). For bond-length data, see: Allen *et al.* (1987).




## Experimental

### *Crystal data*

$C_{17}H_{21}N_3OS$ $M_r$ = 315.43
Monoclinic, $P2_1/c$
$a$ = 11.4322 (6) Å
$b$ = 14.2791 (8) Å
$c$ = 11.6704 (6) Å
$\beta$ = 116.606 (1)°
$V$ = 1703.36 (16) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.20 mm$^{-1}$
$T$ = 298 (2) K
0.30 × 0.20 × 0.20 mm

### *Data collection*

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: none
15640 measured reflections
3712 independent reflections
2599 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.054

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.175
$S$ = 1.04
3712 reflections
279 parameters
23 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C14—H14$A$···O1$^{i}$ | 0.97 | 2.52 | 3.478 (9) | 171 |
| N3—H3$A$···O1$^{i}$ | 0.86 | 2.46 | 3.140 (6) | 137 |

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2396).

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# supplementary materials

*Acta Cryst.* (2008). E**64**, o42 [ **doi:10.1107/S1600536807062484** ]

# 3-Butyl-2-propylamino-1-benzothieno[3,2-*d*]pyrimidin-4(3*H*)-one

**S. Xu**

## Comment

Thienopyrimidine derivatives are of interest as possible antiviral agents, and because of their other biological properties, including antibacterial, antifungal, antiallergic and anti inflammatory activities (Chambhare *et al.*, 2003). We have recently focused on the synthesis of the fused heterocyclic systems containing thienopyrimidine *via* aza-Wittig reactions at room temperature (Ding *et al.*, 2004). We report herein the structure of one such thienopyrimidine derivative, the title compound, (I).

In the molecule of (I), (Fig. 1) the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987). When the crystal structure was solved, propyl and butyl groups were found to be disordered.

Rings A (C1—C6), B (S1/C1/C6—C8) and C (N1/N2/C7—C10) are, of course, planar. The three fused rings A, B and C are also co-planar. The maximum deviation from the benzo[4,5]thieno[3,2-*e*]-pyrimidinone mean plane is 0.027 (3) Å (for atom C7).

In the crystal structure, intermolecular N—H···O and C—H···O hydrogen bonds (Table 1) link the molecules (Fig. 2), in which they may be effective in the stabilization of the structure. Further stability is provided by offset π-π stacking interactions (Janiak, 2000). The adjacent B, C and A, C rings have centroid-centroid distances of 3.96 (1) %A and 3.55 (2) %A, respectively, [symmetry code: −*x*, −*y*, 2 − *z*].

## Experimental

The title compound was synthesized according to a literature method (Ding *et al.*, 2004). The product was recrystallized from ethanol/dichloromethane (1:2 *v*/*v*) at room temperature to give crystals suitable for single-crystal X-ray analysis.

## Refinement

When the crystal structure was solved, propyl and butyl groups were found to be disordered. During refinement with isotropic thermal parameters, the occupancies of disordered H atoms were refined as H3A, H11, H12A, H12B, H12C, H13A, H13B, H13C = 0.696 (10) and H3', H11', H12D, H12E, H12F, H13D, H13E, H13F = 0.304 (10), while the remaining site occupancy factors were also refined as N3, C11, C12,, C13 = 0.696 (10) and N3', C11', C12', C13' = 0.304 (10), during anisotropic refinement, for propyl group. On the other hand, for butyl group the occupancies of disordered H and non-H atoms were also refined in a similar way as H14A, H14B, H15A, H15B, H16A, H16B, H17A, H17B, H17C = 0.622 (11) and H14C, H14D, H15C, H15D, H16C, H16D, H17D, H17E, H17F = 0.378 (11), while the remaining site occupancy factors were also refined as C14, C15, C16,, C17 = 0.622 (11) and C14', C15', C16', C17' = 0.378 (11). H atoms were positioned geometrically, with N—H = 0.86 Å (for NH) and C—H = 0.93, 0.98, 0.96 and 0.97 Å, for aromatic, methine, methyl and methylene H atoms and constrained to ride on their parent atoms, with $U_{iso}$(H) = $xU_{eq}$(C,*N*), where $x$ = 1.5 for methyl H and $x$ = 1.2 for all other H atoms.

## Figures

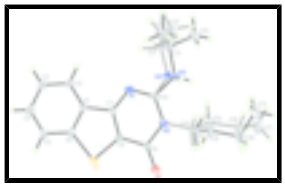

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

## 3-Butyl-2-propylamino-1-benzothieno[2,3-*d*]pyrimidin-4(3*H*)-one

*Crystal data*

| | |
|---|---|
| $C_{17}H_{21}N_3OS$ | $F_{000}$ = 672 |
| $M_r$ = 315.43 | $D_x$ = 1.230 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 4476 reflections |
| $a$ = 11.4322 (6) Å | θ = 2.4–24.2º |
| $b$ = 14.2791 (8) Å | μ = 0.20 mm$^{-1}$ |
| $c$ = 11.6704 (6) Å | $T$ = 298 (2) K |
| β = 116.606 (1)º | Block, colorless |
| $V$ = 1703.36 (16) Å$^3$ | 0.30 × 0.20 × 0.20 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART 4K CCD area-detector diffractometer | 2599 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int}$ = 0.054 |
| Monochromator: graphite | $\theta_{max}$ = 27.0º |
| $T$ = 298(2) K | $\theta_{min}$ = 2.0º |
| φ and ω scans | $h$ = −14→14 |
| Absorption correction: none | $k$ = −17→18 |
| 15640 measured reflections | $l$ = −14→14 |
| 3712 independent reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.058 | H-atom parameters constrained |
| $wR(F^2)$ = 0.175 | $w = 1/[\sigma^2(F_o^2) + (0.107P)^2]$ |

| | |
|---|---|
| | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.04$ | $(\Delta/\sigma)_{max} = 0.004$ |
| 3712 reflections | $\Delta\rho_{max} = 0.35$ e Å$^{-3}$ |
| 279 parameters | $\Delta\rho_{min} = -0.15$ e Å$^{-3}$ |
| 23 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

*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 $F^2 > 2\text{sigma}(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| S1 | 0.13711 (6) | 0.04643 (4) | 1.26890 (6) | 0.0767 (3) | |
| O1 | 0.22957 (17) | 0.23409 (10) | 1.18589 (13) | 0.0782 (5) | |
| N1 | 0.21439 (19) | −0.00118 (12) | 0.97855 (15) | 0.0679 (5) | |
| N2 | 0.25553 (18) | 0.16172 (11) | 1.02369 (15) | 0.0646 (5) | |
| N3 | 0.2992 (7) | 0.0903 (4) | 0.8663 (6) | 0.0835 (17) | 0.696 (10) |
| H3A | 0.3215 | 0.1450 | 0.8524 | 0.100* | 0.696 (10) |
| N3' | 0.2371 (11) | 0.0885 (9) | 0.8333 (9) | 0.057 (2) | 0.304 (10) |
| H3' | 0.2257 | 0.1427 | 0.7977 | 0.068* | 0.304 (10) |
| C1 | 0.14037 (18) | −0.08829 (14) | 1.11773 (18) | 0.0588 (5) | |
| C2 | 0.1241 (2) | −0.17839 (15) | 1.0674 (2) | 0.0775 (6) | |
| H2 | 0.1433 | −0.1913 | 0.9995 | 0.093* | |
| C3 | 0.0795 (3) | −0.24799 (17) | 1.1191 (3) | 0.0921 (8) | |
| H3 | 0.0683 | −0.3082 | 1.0855 | 0.110* | |
| C4 | 0.0510 (3) | −0.2299 (2) | 1.2203 (3) | 0.0969 (8) | |
| H4 | 0.0207 | −0.2780 | 1.2539 | 0.116* | |
| C5 | 0.0668 (3) | −0.14217 (19) | 1.2713 (3) | 0.0897 (7) | |
| H5 | 0.0479 | −0.1303 | 1.3396 | 0.108* | |
| C6 | 0.1117 (2) | −0.07033 (16) | 1.2202 (2) | 0.0663 (5) | |
| C7 | 0.18358 (19) | −0.00435 (13) | 1.07820 (16) | 0.0550 (5) | |
| C8 | 0.1850 (2) | 0.07176 (14) | 1.15013 (17) | 0.0569 (5) | |
| C9 | 0.2227 (2) | 0.16126 (14) | 1.12618 (17) | 0.0585 (5) | |
| C10 | 0.2479 (2) | 0.08120 (15) | 0.95393 (19) | 0.0708 (6) | |
| C11 | 0.3166 (9) | 0.0091 (5) | 0.7964 (8) | 0.115 (3) | 0.696 (10) |
| H11 | 0.3261 | −0.0490 | 0.8446 | 0.138* | 0.696 (10) |
| C11' | 0.2443 (15) | 0.0099 (9) | 0.7669 (9) | 0.085 (5) | 0.304 (10) |

| | | | | | |
|---|---|---|---|---|---|
| H11' | 0.1795 | −0.0319 | 0.7733 | 0.102* | 0.304 (10) |
| C12 | 0.4388 (5) | 0.0288 (5) | 0.7817 (5) | 0.118 (2) | 0.696 (10) |
| H12A | 0.4292 | 0.0873 | 0.7377 | 0.177* | 0.696 (10) |
| H12B | 0.4525 | −0.0206 | 0.7332 | 0.177* | 0.696 (10) |
| H12C | 0.5125 | 0.0324 | 0.8648 | 0.177* | 0.696 (10) |
| C12' | 0.3646 (15) | −0.0512 (13) | 0.8141 (10) | 0.149 (9) | 0.304 (10) |
| H12D | 0.4229 | −0.0277 | 0.7820 | 0.223* | 0.304 (10) |
| H12E | 0.3395 | −0.1142 | 0.7843 | 0.223* | 0.304 (10) |
| H12F | 0.4080 | −0.0507 | 0.9061 | 0.223* | 0.304 (10) |
| C13 | 0.1988 (6) | 0.0047 (7) | 0.6697 (10) | 0.139 (4) | 0.696 (10) |
| H13A | 0.1233 | −0.0101 | 0.6821 | 0.208* | 0.696 (10) |
| H13B | 0.2109 | −0.0429 | 0.6179 | 0.208* | 0.696 (10) |
| H13C | 0.1862 | 0.0641 | 0.6274 | 0.208* | 0.696 (10) |
| C13' | 0.1899 (19) | 0.0248 (14) | 0.6251 (10) | 0.128 (8) | 0.304 (10) |
| H13D | 0.1081 | 0.0574 | 0.5945 | 0.193* | 0.304 (10) |
| H13E | 0.1764 | −0.0348 | 0.5829 | 0.193* | 0.304 (10) |
| H13F | 0.2504 | 0.0611 | 0.6072 | 0.193* | 0.304 (10) |
| C14 | 0.3278 (9) | 0.2503 (6) | 1.0136 (9) | 0.079 (3) | 0.622 (11) |
| H14A | 0.3095 | 0.2584 | 0.9247 | 0.095* | 0.622 (11) |
| H14B | 0.2914 | 0.3040 | 1.0374 | 0.095* | 0.622 (11) |
| C14' | 0.2809 (11) | 0.2515 (8) | 0.9807 (12) | 0.055 (2) | 0.378 (11) |
| H14C | 0.2538 | 0.3028 | 1.0179 | 0.066* | 0.378 (11) |
| H14D | 0.2356 | 0.2564 | 0.8881 | 0.066* | 0.378 (11) |
| C15 | 0.4741 (8) | 0.2515 (6) | 1.0939 (8) | 0.128 (3) | 0.622 (11) |
| H15A | 0.5120 | 0.1976 | 1.0725 | 0.154* | 0.622 (11) |
| H15B | 0.4941 | 0.2468 | 1.1838 | 0.154* | 0.622 (11) |
| C15' | 0.4291 (10) | 0.2516 (6) | 1.0287 (12) | 0.082 (3) | 0.378 (11) |
| H15C | 0.4555 | 0.1983 | 0.9941 | 0.099* | 0.378 (11) |
| H15D | 0.4733 | 0.2479 | 1.1215 | 0.099* | 0.378 (11) |
| C16 | 0.5353 (10) | 0.3408 (6) | 1.0727 (9) | 0.174 (4) | 0.622 (11) |
| H16A | 0.4767 | 0.3931 | 1.0603 | 0.209* | 0.622 (11) |
| H16B | 0.6166 | 0.3535 | 1.1483 | 0.209* | 0.622 (11) |
| C16' | 0.4644 (9) | 0.3432 (6) | 0.9833 (10) | 0.100 (3) | 0.378 (11) |
| H16C | 0.4288 | 0.3431 | 0.8907 | 0.120* | 0.378 (11) |
| H16D | 0.4274 | 0.3959 | 1.0083 | 0.120* | 0.378 (11) |
| C17 | 0.5612 (12) | 0.3325 (9) | 0.9614 (9) | 0.179 (4) | 0.622 (11) |
| H17A | 0.6154 | 0.2788 | 0.9714 | 0.269* | 0.622 (11) |
| H17B | 0.6053 | 0.3878 | 0.9543 | 0.269* | 0.622 (11) |
| H17C | 0.4800 | 0.3255 | 0.8854 | 0.269* | 0.622 (11) |
| C17' | 0.6098 (10) | 0.3518 (14) | 1.0427 (18) | 0.194 (9) | 0.378 (11) |
| H17D | 0.6484 | 0.3093 | 1.1136 | 0.291* | 0.378 (11) |
| H17E | 0.6347 | 0.4148 | 1.0725 | 0.291* | 0.378 (11) |
| H17F | 0.6399 | 0.3370 | 0.9801 | 0.291* | 0.378 (11) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.1169 (5) | 0.0600 (4) | 0.0808 (4) | −0.0027 (3) | 0.0688 (4) | −0.0042 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O1 | 0.1334 (13) | 0.0518 (9) | 0.0645 (8) | −0.0032 (8) | 0.0578 (9) | −0.0075 (7) |
| N1 | 0.1108 (14) | 0.0461 (10) | 0.0552 (9) | 0.0177 (9) | 0.0447 (9) | 0.0053 (7) |
| N2 | 0.1050 (12) | 0.0456 (9) | 0.0533 (9) | 0.0107 (8) | 0.0445 (9) | 0.0074 (7) |
| N3 | 0.142 (5) | 0.057 (2) | 0.080 (3) | 0.027 (3) | 0.075 (4) | 0.017 (2) |
| N3' | 0.087 (6) | 0.043 (3) | 0.047 (4) | 0.017 (4) | 0.035 (4) | 0.007 (3) |
| C1 | 0.0655 (11) | 0.0501 (11) | 0.0567 (10) | 0.0086 (9) | 0.0237 (9) | 0.0051 (8) |
| C2 | 0.1061 (17) | 0.0522 (13) | 0.0719 (13) | 0.0070 (11) | 0.0378 (12) | 0.0010 (10) |
| C3 | 0.1158 (19) | 0.0537 (14) | 0.0965 (18) | −0.0102 (13) | 0.0384 (16) | −0.0010 (13) |
| C4 | 0.112 (2) | 0.0737 (18) | 0.109 (2) | −0.0186 (15) | 0.0540 (17) | 0.0101 (15) |
| C5 | 0.1149 (19) | 0.0739 (17) | 0.1055 (19) | −0.0128 (14) | 0.0718 (16) | 0.0048 (14) |
| C6 | 0.0756 (13) | 0.0568 (12) | 0.0731 (12) | 0.0011 (9) | 0.0393 (11) | 0.0019 (10) |
| C7 | 0.0678 (11) | 0.0480 (11) | 0.0457 (9) | 0.0132 (8) | 0.0222 (8) | 0.0056 (8) |
| C8 | 0.0749 (12) | 0.0507 (11) | 0.0504 (10) | 0.0084 (9) | 0.0329 (9) | 0.0028 (8) |
| C9 | 0.0841 (13) | 0.0485 (11) | 0.0482 (10) | 0.0082 (9) | 0.0343 (9) | 0.0024 (8) |
| C10 | 0.1190 (17) | 0.0495 (12) | 0.0595 (11) | 0.0226 (11) | 0.0538 (12) | 0.0090 (9) |
| C11 | 0.212 (8) | 0.070 (3) | 0.125 (5) | 0.050 (5) | 0.132 (6) | 0.024 (3) |
| C11' | 0.175 (13) | 0.053 (6) | 0.055 (6) | 0.052 (8) | 0.078 (8) | 0.018 (4) |
| C12 | 0.126 (4) | 0.135 (5) | 0.105 (3) | 0.038 (3) | 0.063 (3) | −0.008 (3) |
| C12' | 0.204 (15) | 0.134 (14) | 0.103 (8) | 0.106 (12) | 0.065 (8) | 0.010 (7) |
| C13 | 0.131 (6) | 0.111 (6) | 0.210 (11) | −0.033 (4) | 0.109 (7) | −0.089 (7) |
| C13' | 0.221 (19) | 0.089 (10) | 0.040 (5) | 0.019 (10) | 0.028 (6) | −0.016 (5) |
| C14 | 0.126 (7) | 0.059 (3) | 0.053 (4) | 0.006 (4) | 0.041 (5) | 0.013 (2) |
| C14' | 0.088 (6) | 0.038 (3) | 0.049 (6) | 0.004 (4) | 0.039 (5) | 0.002 (3) |
| C15 | 0.113 (5) | 0.155 (6) | 0.090 (5) | −0.047 (4) | 0.022 (4) | 0.025 (4) |
| C15' | 0.078 (6) | 0.084 (5) | 0.080 (6) | −0.012 (4) | 0.032 (5) | 0.014 (4) |
| C16 | 0.145 (7) | 0.237 (10) | 0.135 (8) | −0.084 (6) | 0.058 (6) | −0.015 (6) |
| C16' | 0.112 (6) | 0.109 (6) | 0.073 (5) | −0.034 (5) | 0.034 (5) | −0.001 (4) |
| C17 | 0.162 (9) | 0.259 (12) | 0.140 (7) | −0.051 (8) | 0.088 (7) | 0.006 (8) |
| C17' | 0.157 (12) | 0.262 (19) | 0.145 (14) | −0.116 (13) | 0.052 (10) | 0.013 (14) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| N3—C11 | 1.482 (9) | C12'—H12D | 0.9600 |
| N3—H3A | 0.8600 | C12'—H12E | 0.9600 |
| N3'—C11' | 1.387 (16) | C12'—H12F | 0.9600 |
| N3'—H3' | 0.8600 | C13—H13A | 0.9600 |
| C1—C2 | 1.392 (3) | C13—H13B | 0.9600 |
| C1—C6 | 1.397 (3) | C13—H13C | 0.9600 |
| C1—C7 | 1.448 (3) | C13'—H13D | 0.9600 |
| C2—C3 | 1.374 (3) | C13'—H13E | 0.9600 |
| C2—H2 | 0.9300 | C13'—H13F | 0.9600 |
| C3—C4 | 1.384 (4) | C14—C15 | 1.507 (7) |
| C3—H3 | 0.9300 | C14—N2 | 1.544 (7) |
| C4—C5 | 1.364 (4) | C14—H14A | 0.9700 |
| C4—H4 | 0.9300 | C14—H14B | 0.9700 |
| C5—C6 | 1.395 (3) | C14'—N2 | 1.452 (9) |
| C5—H5 | 0.9300 | C14'—C15' | 1.528 (9) |
| C6—S1 | 1.743 (2) | C14'—H14C | 0.9700 |
| C7—N1 | 1.359 (3) | C14'—H14D | 0.9700 |

| | | | |
|---|---|---|---|
| C7—C8 | 1.369 (3) | C15—C16 | 1.528 (7) |
| C8—C9 | 1.416 (3) | C15—H15A | 0.9700 |
| C8—S1 | 1.741 (2) | C15—H15B | 0.9700 |
| C9—O1 | 1.235 (2) | C15'—C16' | 1.531 (8) |
| C9—N2 | 1.405 (2) | C15'—H15C | 0.9700 |
| C10—N1 | 1.308 (3) | C15'—H15D | 0.9700 |
| C10—N3' | 1.361 (10) | C16—C17 | 1.461 (8) |
| C10—N2 | 1.389 (3) | C16—H16A | 0.9700 |
| C10—N3 | 1.394 (5) | C16—H16B | 0.9700 |
| C11—C13 | 1.490 (7) | C16'—C17' | 1.493 (9) |
| C11—C12 | 1.508 (7) | C16'—H16C | 0.9700 |
| C11—H11 | 0.9800 | C16'—H16D | 0.9700 |
| C11'—C13' | 1.499 (9) | C17—H17A | 0.9600 |
| C11'—C12' | 1.510 (9) | C17—H17B | 0.9600 |
| C11'—H11' | 0.9800 | C17—H17C | 0.9600 |
| C12—H12A | 0.9600 | C17'—H17D | 0.9600 |
| C12—H12B | 0.9600 | C17'—H17E | 0.9600 |
| C12—H12C | 0.9600 | C17'—H17F | 0.9600 |
| C8—S1—C6 | 90.27 (10) | C12'—C11'—H11' | 102.4 |
| C10—N1—C7 | 115.57 (16) | C11'—C12'—H12D | 109.5 |
| C10—N2—C9 | 121.65 (17) | C11'—C12'—H12E | 109.5 |
| C10—N2—C14' | 119.9 (6) | H12D—C12'—H12E | 109.5 |
| C9—N2—C14' | 118.0 (6) | C11'—C12'—H12F | 109.5 |
| C10—N2—C14 | 121.9 (4) | H12D—C12'—H12F | 109.5 |
| C9—N2—C14 | 115.1 (4) | H12E—C12'—H12F | 109.5 |
| C10—N3—C11 | 122.4 (6) | C11'—C13'—H13D | 109.5 |
| C10—N3—H3A | 118.8 | C11'—C13'—H13E | 109.5 |
| C11—N3—H3A | 118.8 | H13D—C13'—H13E | 109.5 |
| C10—N3'—C11' | 121.0 (10) | C11'—C13'—H13F | 109.5 |
| C10—N3'—H3' | 119.5 | H13D—C13'—H13F | 109.5 |
| C11'—N3'—H3' | 119.5 | H13E—C13'—H13F | 109.5 |
| C2—C1—C6 | 119.5 (2) | C15—C14—N2 | 116.4 (6) |
| C2—C1—C7 | 129.1 (2) | C15—C14—H14A | 108.2 |
| C6—C1—C7 | 111.39 (18) | N2—C14—H14A | 108.2 |
| C3—C2—C1 | 119.2 (2) | C15—C14—H14B | 108.2 |
| C3—C2—H2 | 120.4 | N2—C14—H14B | 108.2 |
| C1—C2—H2 | 120.4 | H14A—C14—H14B | 107.3 |
| C2—C3—C4 | 121.1 (2) | N2—C14'—C15' | 103.6 (7) |
| C2—C3—H3 | 119.5 | N2—C14'—H14C | 111.0 |
| C4—C3—H3 | 119.5 | C15'—C14'—H14C | 111.0 |
| C5—C4—C3 | 120.5 (2) | N2—C14'—H14D | 111.0 |
| C5—C4—H4 | 119.7 | C15'—C14'—H14D | 111.0 |
| C3—C4—H4 | 119.7 | H14C—C14'—H14D | 109.0 |
| C4—C5—C6 | 119.4 (3) | C14—C15—C16 | 111.7 (6) |
| C4—C5—H5 | 120.3 | C14—C15—H15A | 109.3 |
| C6—C5—H5 | 120.3 | C16—C15—H15A | 109.3 |
| C5—C6—C1 | 120.2 (2) | C14—C15—H15B | 109.3 |
| C5—C6—S1 | 127.07 (19) | C16—C15—H15B | 109.3 |
| C1—C6—S1 | 112.71 (16) | H15A—C15—H15B | 107.9 |

| | | | |
|---|---|---|---|
| N1—C7—C8 | 124.20 (18) | C14'—C15'—C16' | 107.1 (7) |
| N1—C7—C1 | 123.82 (17) | C14'—C15'—H15C | 110.3 |
| C8—C7—C1 | 111.94 (18) | C16'—C15'—H15C | 110.3 |
| C7—C8—C9 | 121.09 (18) | C14'—C15'—H15D | 110.3 |
| C7—C8—S1 | 113.69 (15) | C16'—C15'—H15D | 110.3 |
| C9—C8—S1 | 125.23 (15) | H15C—C15'—H15D | 108.5 |
| O1—C9—N2 | 120.20 (18) | C17—C16—C15 | 111.5 (7) |
| O1—C9—C8 | 126.63 (18) | C17—C16—H16A | 109.3 |
| N2—C9—C8 | 113.17 (16) | C15—C16—H16A | 109.3 |
| N1—C10—N3' | 113.4 (6) | C17—C16—H16B | 109.3 |
| N1—C10—N2 | 124.28 (18) | C15—C16—H16B | 109.3 |
| N3'—C10—N2 | 119.7 (5) | H16A—C16—H16B | 108.0 |
| N1—C10—N3 | 120.3 (3) | C17'—C16'—C15' | 108.7 (7) |
| N2—C10—N3 | 114.6 (3) | C17'—C16'—H16C | 109.9 |
| N3—C11—C13 | 107.2 (6) | C15'—C16'—H16C | 109.9 |
| N3—C11—C12 | 106.0 (6) | C17'—C16'—H16D | 109.9 |
| C13—C11—C12 | 111.5 (5) | C15'—C16'—H16D | 109.9 |
| N3—C11—H11 | 110.7 | H16C—C16'—H16D | 108.3 |
| C13—C11—H11 | 110.7 | C16'—C17'—H17D | 109.5 |
| C12—C11—H11 | 110.7 | C16'—C17'—H17E | 109.5 |
| N3'—C11'—C13' | 113.8 (11) | H17D—C17'—H17E | 109.5 |
| N3'—C11'—C12' | 122.5 (11) | C16'—C17'—H17F | 109.5 |
| C13'—C11'—C12' | 110.1 (8) | H17D—C17'—H17F | 109.5 |
| N3'—C11'—H11' | 102.4 | H17E—C17'—H17F | 109.5 |
| C13'—C11'—H11' | 102.4 | | |
| C6—C1—C2—C3 | 0.3 (3) | C14—C15—C16—C17 | −84.7 (12) |
| C7—C1—C2—C3 | −178.9 (2) | N2—C14'—C15'—C16' | 178.1 (8) |
| C1—C2—C3—C4 | −0.2 (4) | C14'—C15'—C16'—C17' | 172.6 (15) |
| C2—C3—C4—C5 | −0.1 (4) | N3'—C10—N1—C7 | −160.1 (5) |
| C3—C4—C5—C6 | 0.3 (4) | N2—C10—N1—C7 | 1.3 (3) |
| C4—C5—C6—C1 | −0.1 (4) | N3—C10—N1—C7 | 170.8 (4) |
| C4—C5—C6—S1 | 179.2 (2) | C8—C7—N1—C10 | 0.5 (3) |
| C2—C1—C6—C5 | −0.2 (3) | C1—C7—N1—C10 | 178.05 (18) |
| C7—C1—C6—C5 | 179.2 (2) | N1—C10—N2—C9 | −2.2 (3) |
| C2—C1—C6—S1 | −179.60 (17) | N3'—C10—N2—C9 | 158.1 (6) |
| C7—C1—C6—S1 | −0.2 (2) | N3—C10—N2—C9 | −172.3 (4) |
| C2—C1—C7—N1 | 1.2 (3) | N1—C10—N2—C14' | −173.8 (6) |
| C6—C1—C7—N1 | −178.14 (17) | N3'—C10—N2—C14' | −13.5 (8) |
| C2—C1—C7—C8 | 178.9 (2) | N3—C10—N2—C14' | 16.1 (7) |
| C6—C1—C7—C8 | −0.4 (2) | N1—C10—N2—C14 | 164.2 (4) |
| N1—C7—C8—C9 | −1.5 (3) | N3'—C10—N2—C14 | −35.5 (7) |
| C1—C7—C8—C9 | −179.22 (17) | N3—C10—N2—C14 | −5.9 (6) |
| N1—C7—C8—S1 | 178.56 (15) | O1—C9—N2—C10 | −179.5 (2) |
| C1—C7—C8—S1 | 0.8 (2) | C8—C9—N2—C10 | 1.1 (3) |
| C7—C8—C9—O1 | −178.78 (19) | O1—C9—N2—C14' | −7.7 (6) |
| S1—C8—C9—O1 | 1.2 (3) | C8—C9—N2—C14' | 172.9 (5) |
| C7—C8—C9—N2 | 0.5 (3) | O1—C9—N2—C14 | 13.3 (4) |
| S1—C8—C9—N2 | −179.48 (14) | C8—C9—N2—C14 | −166.1 (4) |
| N1—C10—N3—C11 | 0.8 (8) | C15'—C14'—N2—C10 | −80.9 (8) |

| | | | |
|---|---|---|---|
| N3'—C10—N3—C11 | −81.1 (18) | C15'—C14'—N2—C9 | 107.1 (8) |
| N2—C10—N3—C11 | 171.4 (5) | C15'—C14'—N2—C14 | 21 (2) |
| C10—N3—C11—C13 | 95.4 (8) | C15—C14—N2—C10 | −82.4 (8) |
| C10—N3—C11—C12 | −145.4 (7) | C15—C14—N2—C9 | 84.8 (8) |
| N1—C10—N3'—C11' | −25.1 (12) | C15—C14—N2—C14' | −172 (3) |
| N2—C10—N3'—C11' | 172.6 (9) | C7—C8—S1—C6 | −0.77 (16) |
| N3—C10—N3'—C11' | 86.3 (17) | C9—C8—S1—C6 | 179.24 (19) |
| C10—N3'—C11'—C13' | 161.8 (14) | C5—C6—S1—C8 | −178.8 (2) |
| C10—N3'—C11'—C12' | −61.6 (18) | C1—C6—S1—C8 | 0.55 (16) |
| N2—C14—C15—C16 | 178.0 (7) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C14—H14A···O1$^{i}$ | 0.97 | 2.52 | 3.478 (9) | 171 |
| N3—H3A···O1$^{i}$ | 0.86 | 2.46 | 3.140 (6) | 137 |

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

**Fig. 1**

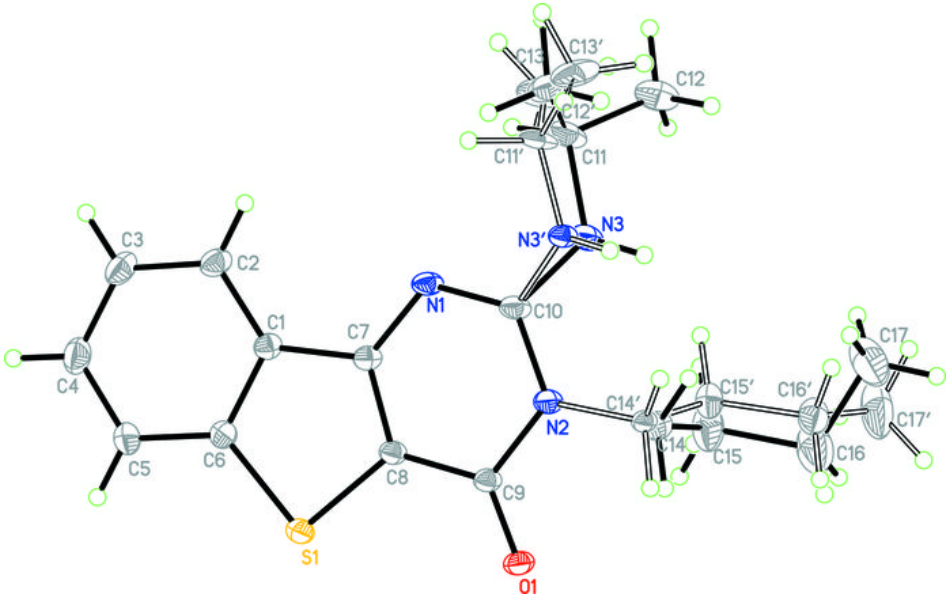
C13
C13′
C12
C12′
C11′
C11
N3′
N3
C3
C2
N1
C10
C1
C7
C17
C15′
C16′
C4
C14′
N2
C17′
C14
C15
C16
C5
C6
C8
C9
S1
O1

**Fig. 2**