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

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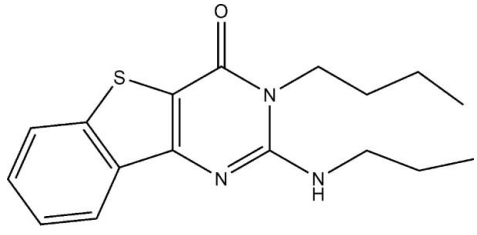
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.058; wR factor = 0.175; data-to-parameter ratio = 13.3.

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 π–π 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
β = 116.606 (1)°
V = 1703.36 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 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—H14A···O1^{i}	0.97	2.52	3.478 (9)	171
N3—H3A···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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supporting information

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

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S1. 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*].

S2. 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.

S3. 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.

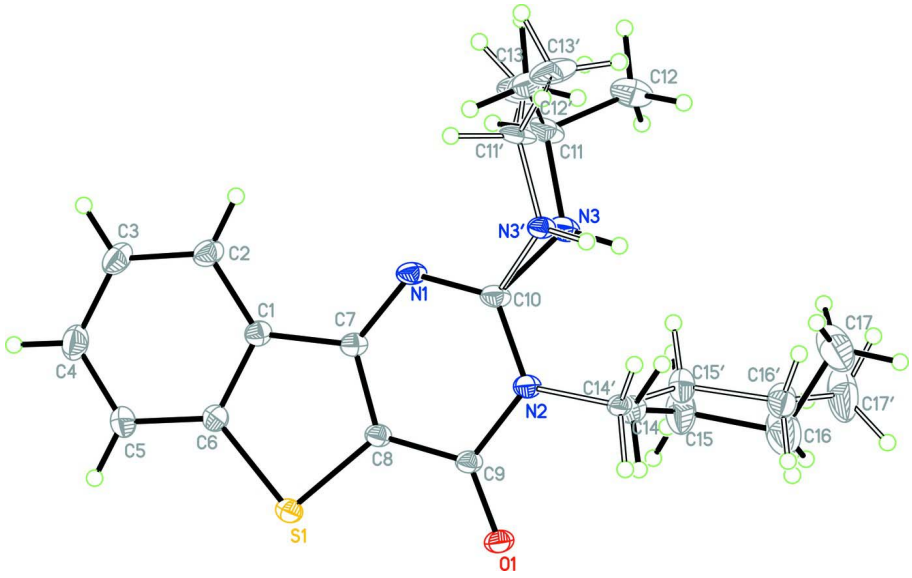

Figure 1

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

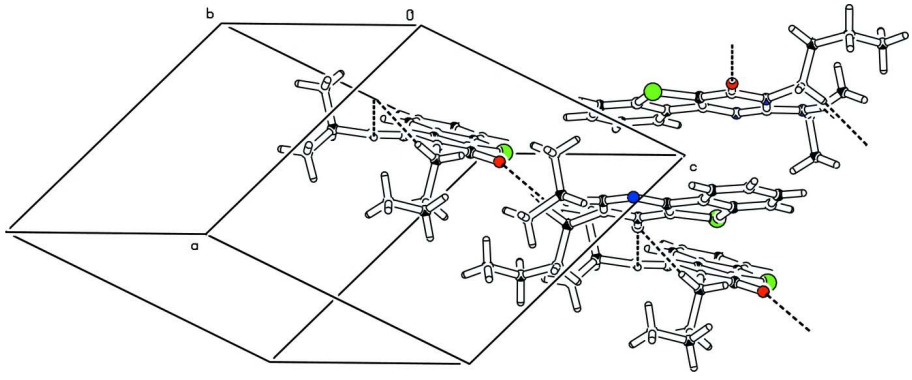

Figure 2

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

$C_{17}H_{21}N_3OS$
$M_r = 315.43$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.4322\ (6)$ Å
$b = 14.2791\ (8)$ Å
$c = 11.6704\ (6)$ Å
$\beta = 116.606\ (1)°$
$V = 1703.36\ (16)$ Å^3
$Z = 4$

$F(000) = 672$
$D_x = 1.230$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4476 reflections
$\theta = 2.4–24.2°$
$\mu = 0.20$ mm^{-1}
$T = 298$ K
Block, colorless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
15640 measured reflections
3712 independent reflections
2599 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.0°$
$h = -14 \rightarrow 14$
$k = -17 \rightarrow 18$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.175$
$S = 1.04$
3712 reflections
279 parameters
23 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.107P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ 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 (Å²)

	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 (Å²)

	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, º)

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, º)

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*+1/2, *z*−1/2.