Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-Butyl-2-morpholino-5,6,7,8-tetrahydrobenzothieno[2,3-*d*]pyrimidin-4(3*H*)-one

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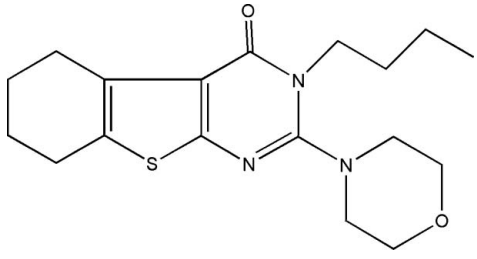
Received 6 October 2007; accepted 9 November 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.059; wR factor = 0.169; data-to-parameter ratio = 13.8.

In the title molecule, $C_{18}H_{25}N_3O_2S$, the central thienopyrimidine ring system is essentially planar. The cyclohexene ring, in which the four CH_2 groups are disordered in an approximately 1:1 ratio, adopts a half-chair conformation, while the morpholine ring is in a standard chair conformation. The butyl group is disordered in an approximately 2:1 ratio. In the crystal structure, weak intermolecular C—H···O hydrogen-bonding interactions stabilize the crystal structure.

Related literature

For related literature, see: Ding *et al.* (2004); Zeng *et al.* (2007).



Experimental

Crystal data

$C_{18}H_{25}N_3O_2S$
M_r = 347.47
Hexagonal, $R\overline{3}$
a = 27.2898 (17) Å
c = 13.3909 (9) Å
V = 8636.6 (8) Å^3
Z = 18
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 293 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.964, T_{max} = 0.982
27908 measured reflections
3789 independent reflections
1686 reflections with $I > 2\sigma(I)$
R_{int} = 0.088

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.169
S = 0.85
3789 reflections
275 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11A···O2^{i}	0.97	2.53	3.187 (4)	125
C14—H14B···O1^{ii}	0.97	2.46	3.343 (4)	152

Symmetry codes: (i) $-x+y+\frac{4}{3}, -x+\frac{2}{3}, z-\frac{1}{3}$; (ii) $y+1, -x+y+1, -z+2$.

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

The authors gratefully acknowledge financial support of this work by the National Basic Research Programme of China (grant No. 2003CB114400), the Key Science Research Project of Hubei Provincial Department of Education (No. D200524005) and the Science Foundation of Yunyang Medical College.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2529).

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  doi:10.1107/S1600536807057558

supplementary materials

Acta Cryst. (2007). E**63**, o4840 [**doi:10.1107/S1600536807057558**]

3-Butyl-2-morpholino-5,6,7,8-tetrahydrobenzothieno[2,3-*d*]pyrimidin-4(3*H*)-one

X.-H. Zeng, H.-M. Wang, A.-H. Zheng, J.-H. Tian and T.-Y. He

Comment

Pyrimidine derivatives are attracting the increasing attention of the synthetic community because of the important role played by such systems in many natural products, antibiotics and drugs (Ding *et al.*, 2004). In recent years, we have been engaged in the preparation of derivatives of heterocycles *via* the aza-Wittig reaction. The title compound, (I), was synthesized and structurally characterized in this context.

In the fused heterobicyclic ring of (I), bond lengths and angles are similar to those observed in closely related structures (Zeng *et al.*, 2007). All ring atoms in the thienopyrimidine system are essentially coplanar with the maximum displacement from the plane being 0.0884 (9) Å for atom C9.

In the title molecule (Fig. 1), the cyclohexene ring and butyl group exhibit orientational disorder. The cyclohexene ring adopts a half-chair conformation, while the morpholine ring is in a standard chair conformation.

The crystal packing is stabilized by intermolecular hydrogen bonding interactions. Atoms C11 and C14, as hydrogen-bond donors, respectively, link to the acceptor atoms, O1 and O2 (Fig. 2).

Experimental

To a solution of iminophosphorane(*a*) (1.45 g, 3 mmol) in anhydrous dichloromethane (15 ml) was added butyl isocyanate (3 mmol) under dry N_2 at room temperature. The reaction mixture was left unstirred for 48 h at room temperature, then the solvent was removed under reduced pressure and a ether/petroleum ether (1:3 *v*/*v*, 20 ml) mixture was added to precipitate triphenylphosphine oxide. After filtration the solvent was removed to give carbodiimide, which was used directly without further purification. To the solution of carbodiimide (15 ml), morpholine (3 mmol) was added. After the mixture was stirred for 6 h, the solvent was removed and anhydrous ethanol (10 ml) containing several drops of EtONa in EtOH was added. The mixture was stirred for 12 hr at room temperature. The solution was condensed and the residue was recrystallized from ethanol to give the title compound (I), in a yield of 51% (m.p. 391 K)·Spectroscopic analysis: IR (cm^{-1}, KBr), 1656 (C=O); ^{1}H NMR (CDCl3, 400 MHz), 4.09–4.05 (t, J = 7.4 Hz, 2H, NCH2), 3.85–3.83(t, J = 4.8 Hz, 4H, 2NCH2), 3.15–3.12 (t, J = 4.8 Hz, 4H, 2OCH2), 3.01–2.73 (m, 4H, 2CH2), 1.87–1.70 (m, 4H, 2CH2), 1.35–1.33 (m, 2H, CH2), 0.97–0.93 (t, J = 7.4 Hz, 3H, CH3); MS (m/*z*, %), 347 (*M*+, 100), 292 (12), 260 (16), 55 (14); Anal. Calcd. for $C_{18}H_{25}N_3O_2S$: C, 62.22; H, 7.25; N, 12.09;. Found: C, 62.09; H, 7.23; N, 12.15. Crystals suitable for single-crystal X-ray diffraction analysis were obtained by vapour diffusion of a hexane/dichloromethane solution (1:3 *v*/*v*) at room temperature.

Refinement

All H atoms were located in difference maps and then treated as riding atoms, with C—H = 0.96 (CH_3) or 0.97 Å (CH_2), and with U_{iso}(H) values of 1.2U_{eq}(C), or 1.5U_{eq}(C) for methyl groups. The cyclohexene ring and butyl group are dis-

ordered. There are two possible conformations, with atom sequences C2–C5 and C2/C3'/C4'/C5, with refined occupancies of 0.54 (3):0.46 (3), while atom sequences C15–C18 and C15'–C18' have refined occupancies of 0.74 (3):0.26 (3). The disorder has resulted in larger than normal displacement ellipsoids for the atoms involved. No significant electron density was located in the solvent accesible voids of appoximately 82 Å^3

Figures

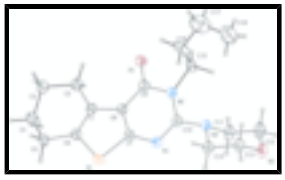

Fig. 1. The molecular structure with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H-atoms are represented by circles of arbitrary size. The disorder is not shown.

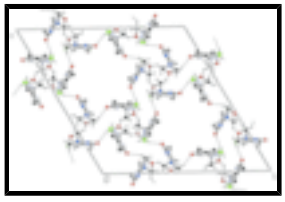

Fig. 2. Part of the crystal structure showing the formation of intermolecular hydrogen bonds (dashed lines). H atoms not involved in these interactions have been omitted for clarity. The disorder is not shown.

3-Butyl-2-morpholino-5,6,7,8-tetrahydrobenzothieno[2,3-*d*]pyrimidin-4(3*H*)-one

Crystal data

$C_{18}H_{25}N_3O_2S$	$Z = 18$
$M_r = 347.47$	$F_{000} = 3348$
Hexagonal, $R\overline{3}$	$D_x = 1.203$ Mg m^{-3}
Hall symbol: -R 3	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 27.2898$ (17) Å	Cell parameters from 2997 reflections
$b = 27.2898$ (9) Å	$\theta = 2.3$–17.9º
$c = 13.3909$ (9) Å	$\mu = 0.18$ mm^{-1}
$\alpha = 90$º	$T = 293$ (2) K
$\beta = 90$º	Block, colourless
$\gamma = 120$º	0.20 × 0.20 × 0.10 mm
$V = 8636.6$ (8) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3789 independent reflections
Radiation source: fine-focus sealed tube	1686 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.088$
$T = 292$(2) K	$\theta_{max} = 26.0$º
φ and ω scans	$\theta_{min} = 1.5$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -31 \rightarrow 33$
$T_{min} = 0.964$, $T_{max} = 0.982$	$k = -33 \rightarrow 31$

27908 measured reflections

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.059$

$wR(F^2) = 0.169$

$S = 0.85$

3789 reflections

275 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0933P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.25$ e Å^{-3}

$\Delta\rho_{min} = -0.17$ e Å^{-3}

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 $F^2 > 2\text{sigma}(F^2)$ 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)
C1	0.79829 (11)	0.00951 (13)	0.7454 (2)	0.0821 (8)	
C2	0.79786 (18)	−0.03694 (15)	0.6850 (3)	0.1148 (11)	
H2A	0.7593	−0.0681	0.6790	0.138*	0.54 (3)
H2B	0.8199	−0.0508	0.7191	0.138*	0.54 (3)
H2C	0.7656	−0.0729	0.7045	0.138*	0.46 (3)
H2D	0.8319	−0.0385	0.6994	0.138*	0.46 (3)
C3	0.8225 (15)	−0.0161 (16)	0.581 (3)	0.148 (9)	0.54 (3)
H3A	0.8633	0.0077	0.5852	0.177*	0.54 (3)
H3B	0.8143	−0.0482	0.5385	0.177*	0.54 (3)
C4	0.7974 (14)	0.0170 (9)	0.5349 (10)	0.142 (6)	0.54 (3)
H4A	0.7565	−0.0060	0.5345	0.171*	0.54 (3)
H4B	0.8102	0.0265	0.4664	0.171*	0.54 (3)
C3'	0.7955 (11)	−0.0280 (17)	0.573 (3)	0.127 (10)	0.46 (3)
H3C	0.8063	−0.0519	0.5368	0.152*	0.46 (3)
H3D	0.7570	−0.0389	0.5541	0.152*	0.46 (3)
C4'	0.8343 (12)	0.0328 (10)	0.5439 (13)	0.119 (6)	0.46 (3)
H4C	0.8341	0.0366	0.4719	0.143*	0.46 (3)

H4D	0.8727	0.0444	0.5646	0.143*	0.46 (3)
C5	0.81499 (16)	0.07103 (17)	0.5938 (2)	0.1111 (11)	
H5A	0.8548	0.0976	0.5827	0.133*	0.54 (3)
H5B	0.7934	0.0884	0.5714	0.133*	0.54 (3)
H5C	0.8439	0.1104	0.5854	0.133*	0.46 (3)
H5D	0.7806	0.0655	0.5623	0.133*	0.46 (3)
C6	0.80456 (11)	0.05727 (13)	0.7027 (2)	0.0827 (8)	
C7	0.79202 (11)	0.05670 (11)	0.8863 (2)	0.0724 (7)	
C8	0.79164 (11)	0.00962 (11)	0.8516 (2)	0.0751 (8)	
C9	0.78892 (13)	−0.03079 (13)	0.9234 (2)	0.0884 (9)	
C10	0.78204 (11)	0.03117 (12)	1.0477 (2)	0.0791 (8)	
C11	0.71695 (14)	0.00271 (13)	1.1876 (2)	0.1190 (13)	
H11A	0.7018	−0.0362	1.1662	0.143*	
H11B	0.6924	0.0162	1.1625	0.143*	
C12	0.71963 (17)	0.00613 (15)	1.2990 (3)	0.1355 (15)	
H12A	0.6819	−0.0171	1.3261	0.163*	
H12B	0.7430	−0.0088	1.3233	0.163*	
C13	0.79664 (14)	0.09788 (12)	1.2920 (2)	0.0981 (10)	
H13A	0.8223	0.0857	1.3165	0.118*	
H13B	0.8107	0.1365	1.3142	0.118*	
C14	0.79615 (12)	0.09645 (11)	1.1808 (2)	0.0859 (9)	
H14A	0.7720	0.1102	1.1552	0.103*	
H14B	0.8341	0.1206	1.1553	0.103*	
C15	0.8029 (10)	−0.0460 (5)	1.1006 (9)	0.111 (5)	0.74 (3)
H15A	0.7883	−0.0437	1.1654	0.133*	0.74 (3)
H15B	0.7852	−0.0856	1.0823	0.133*	0.74 (3)
C16	0.8634 (10)	−0.0230 (9)	1.1084 (16)	0.185 (7)	0.74 (3)
H16A	0.8809	0.0176	1.1165	0.222*	0.74 (3)
H16B	0.8766	−0.0296	1.0453	0.222*	0.74 (3)
C17	0.8844 (15)	−0.0440 (10)	1.187 (3)	0.296 (12)	0.74 (3)
H17A	0.9240	−0.0314	1.1745	0.355*	0.74 (3)
H17B	0.8638	−0.0850	1.1855	0.355*	0.74 (3)
C18	0.8790 (12)	−0.0248 (9)	1.2894 (15)	0.278 (9)	0.74 (3)
H18A	0.8814	0.0114	1.2847	0.417*	0.74 (3)
H18B	0.9090	−0.0218	1.3311	0.417*	0.74 (3)
H18C	0.8432	−0.0518	1.3177	0.417*	0.74 (3)
C15'	0.7750 (15)	−0.0584 (12)	1.100 (2)	0.070 (6)	0.26 (3)
H15C	0.7499	−0.0954	1.0718	0.084*	0.26 (3)
H15D	0.7553	−0.0528	1.1554	0.084*	0.26 (3)
C16'	0.826 (5)	−0.058 (4)	1.139 (9)	0.47 (7)	0.26 (3)
H16C	0.8151	−0.0818	1.1974	0.567*	0.26 (3)
H16D	0.8389	−0.0742	1.0887	0.567*	0.26 (3)
C17'	0.872 (2)	−0.0027 (18)	1.165 (4)	0.165 (14)	0.26 (3)
H17C	0.8584	0.0159	1.2097	0.198*	0.26 (3)
H17D	0.8864	0.0202	1.1054	0.198*	0.26 (3)
C18'	0.921 (3)	−0.007 (4)	1.217 (10)	0.34 (4)	0.26 (3)
H18D	0.9351	0.0195	1.2714	0.516*	0.26 (3)
H18E	0.9503	0.0021	1.1695	0.516*	0.26 (3)
H18F	0.9065	−0.0445	1.2416	0.516*	0.26 (3)

N1	0.78524 (9)	0.06840 (9)	0.98258 (19)	0.0774 (6)
N2	0.78663 (10)	−0.01536 (10)	1.02424 (18)	0.0878 (7)
N3	0.77507 (10)	0.03834 (9)	1.14850 (17)	0.0846 (7)
O1	0.78962 (12)	−0.07423 (10)	0.90511 (17)	0.1210 (9)
O2	0.74223 (11)	0.06277 (9)	1.33329 (16)	0.1175 (9)
S1	0.80114 (4)	0.10249 (3)	0.78967 (6)	0.0921 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0744 (19)	0.080 (2)	0.084 (2)	0.0325 (16)	0.0062 (15)	−0.0022 (17)
C2	0.148 (3)	0.105 (3)	0.095 (3)	0.066 (2)	0.019 (2)	−0.006 (2)
C3	0.20 (2)	0.17 (3)	0.105 (8)	0.12 (2)	0.022 (19)	0.006 (13)
C4	0.184 (16)	0.150 (13)	0.087 (6)	0.079 (12)	−0.033 (9)	−0.006 (7)
C3'	0.138 (16)	0.126 (13)	0.103 (13)	0.055 (15)	0.028 (14)	−0.024 (10)
C4'	0.136 (12)	0.142 (14)	0.083 (7)	0.071 (12)	−0.017 (8)	−0.016 (7)
C5	0.119 (3)	0.135 (3)	0.083 (2)	0.065 (3)	−0.003 (2)	0.016 (2)
C6	0.0717 (19)	0.089 (2)	0.083 (2)	0.0371 (17)	−0.0069 (15)	0.0010 (17)
C7	0.0624 (17)	0.0609 (17)	0.081 (2)	0.0210 (14)	−0.0024 (14)	0.0001 (15)
C8	0.0722 (18)	0.0583 (18)	0.083 (2)	0.0238 (14)	0.0083 (14)	0.0005 (15)
C9	0.105 (2)	0.0592 (19)	0.091 (2)	0.0337 (17)	0.0122 (17)	−0.0005 (17)
C10	0.0740 (19)	0.0545 (18)	0.085 (2)	0.0140 (15)	0.0039 (15)	−0.0074 (16)
C11	0.119 (3)	0.072 (2)	0.099 (3)	−0.0025 (19)	0.031 (2)	−0.0140 (17)
C12	0.152 (3)	0.084 (3)	0.101 (3)	0.007 (2)	0.036 (2)	−0.008 (2)
C13	0.110 (3)	0.069 (2)	0.086 (2)	0.0223 (19)	0.0087 (19)	−0.0092 (16)
C14	0.086 (2)	0.0570 (18)	0.090 (2)	0.0169 (15)	0.0066 (16)	−0.0074 (15)
C15	0.140 (14)	0.069 (5)	0.093 (4)	0.029 (7)	0.014 (8)	0.021 (3)
C16	0.221 (17)	0.165 (12)	0.182 (12)	0.106 (11)	−0.081 (13)	0.033 (10)
C17	0.34 (3)	0.24 (2)	0.31 (3)	0.15 (2)	−0.06 (2)	−0.008 (18)
C18	0.36 (2)	0.247 (14)	0.233 (17)	0.158 (15)	0.028 (14)	0.052 (14)
C15'	0.077 (15)	0.048 (11)	0.086 (10)	0.032 (11)	0.021 (11)	0.015 (9)
C16'	0.47 (19)	0.47 (14)	0.48 (12)	0.24 (13)	0.00 (11)	0.01 (10)
C17'	0.19 (3)	0.15 (3)	0.17 (3)	0.10 (3)	−0.03 (3)	0.04 (2)
C18'	0.34 (9)	0.34 (10)	0.36 (10)	0.18 (7)	−0.01 (8)	−0.01 (8)
N1	0.0748 (16)	0.0598 (15)	0.0863 (17)	0.0251 (12)	0.0006 (12)	−0.0041 (13)
N2	0.113 (2)	0.0545 (15)	0.0820 (17)	0.0317 (14)	0.0154 (14)	0.0033 (13)
N3	0.0959 (18)	0.0550 (14)	0.0800 (17)	0.0206 (13)	0.0150 (13)	−0.0044 (11)
O1	0.195 (3)	0.0797 (15)	0.1035 (16)	0.0800 (17)	0.0203 (15)	0.0012 (12)
O2	0.132 (2)	0.0794 (15)	0.0932 (15)	0.0173 (14)	0.0287 (14)	−0.0123 (12)
S1	0.1001 (6)	0.0835 (6)	0.0969 (6)	0.0490 (5)	−0.0110 (4)	0.0068 (4)

Geometric parameters (Å, °)

C1—C6	1.353 (4)	C11—H11A	0.9700
C1—C8	1.433 (4)	C11—H11B	0.9700
C1—C2	1.499 (4)	C12—O2	1.424 (4)
C2—C3'	1.53 (4)	C12—H12A	0.9700
C2—C3	1.53 (3)	C12—H12B	0.9700
C2—H2A	0.9700	C13—O2	1.416 (3)

C2—H2B	0.9700	C13—C14	1.489 (4)
C2—H2C	0.9700	C13—H13A	0.9700
C2—H2D	0.9700	C13—H13B	0.9700
C3—C4	1.51 (5)	C14—N3	1.456 (3)
C3—H3A	0.9700	C14—H14A	0.9700
C3—H3B	0.9700	C14—H14B	0.9700
C4—C5	1.522 (17)	C15—C16	1.45 (3)
C4—H4A	0.9700	C15—N2	1.520 (15)
C4—H4B	0.9700	C15—H15A	0.9700
C3'—C4'	1.50 (5)	C15—H15B	0.9700
C3'—H3C	0.9700	C16—C17	1.45 (4)
C3'—H3D	0.9700	C16—H16A	0.9700
C4'—C5	1.538 (18)	C16—H16B	0.9700
C4'—H4C	0.9700	C17—C18	1.50 (3)
C4'—H4D	0.9700	C17—H17A	0.9700
C5—C6	1.497 (4)	C17—H17B	0.9700
C5—H5A	0.9700	C18—H18A	0.9600
C5—H5B	0.9700	C18—H18B	0.9600
C5—H5C	0.9700	C18—H18C	0.9600
C5—H5D	0.9700	C15'—N2	1.46 (3)
C6—S1	1.733 (3)	C15'—C16'	1.47 (14)
C7—C8	1.362 (4)	C15'—H15C	0.9700
C7—N1	1.363 (3)	C15'—H15D	0.9700
C7—S1	1.728 (3)	C16'—C17'	1.44 (13)
C8—C9	1.437 (4)	C16'—H16C	0.9700
C9—O1	1.220 (3)	C16'—H16D	0.9700
C9—N2	1.425 (4)	C17'—C18'	1.55 (10)
C10—N1	1.308 (3)	C17'—H17C	0.9700
C10—N2	1.373 (4)	C17'—H17D	0.9700
C10—N3	1.391 (3)	C18'—H18D	0.9600
C11—N3	1.481 (3)	C18'—H18E	0.9600
C11—C12	1.495 (4)	C18'—H18F	0.9600
C6—C1—C8	111.8 (3)	N3—C11—C12	108.0 (3)
C6—C1—C2	122.0 (3)	N3—C11—H11A	110.1
C8—C1—C2	126.1 (3)	C12—C11—H11A	110.1
C1—C2—C3'	112.2 (16)	N3—C11—H11B	110.1
C1—C2—C3	111.2 (14)	C12—C11—H11B	110.1
C1—C2—H2A	109.4	H11A—C11—H11B	108.4
C3'—C2—H2A	86.8	O2—C12—C11	111.7 (3)
C3—C2—H2A	109.4	O2—C12—H12A	109.3
C1—C2—H2B	109.4	C11—C12—H12A	109.3
C3'—C2—H2B	127.5	O2—C12—H12B	109.3
C3—C2—H2B	109.4	C11—C12—H12B	109.3
H2A—C2—H2B	108.0	H12A—C12—H12B	107.9
C1—C2—H2C	109.2	O2—C13—C14	112.3 (3)
C3'—C2—H2C	109.7	O2—C13—H13A	109.1
C3—C2—H2C	129.0	C14—C13—H13A	109.1
H2B—C2—H2C	84.5	O2—C13—H13B	109.1
C1—C2—H2D	109.1	C14—C13—H13B	109.1

C3'—C2—H2D	108.7	H13A—C13—H13B	107.9
C3—C2—H2D	86.8	N3—C14—C13	108.6 (2)
H2A—C2—H2D	128.4	N3—C14—H14A	110.0
H2C—C2—H2D	107.9	C13—C14—H14A	110.0
C4—C3—C2	110 (2)	N3—C14—H14B	110.0
C4—C3—H3A	109.6	C13—C14—H14B	110.0
C2—C3—H3A	109.6	H14A—C14—H14B	108.4
C4—C3—H3B	109.6	C16—C15—N2	113.2 (10)
C2—C3—H3B	109.6	C16—C15—H15A	108.9
H3A—C3—H3B	108.1	N2—C15—H15A	108.9
C3—C4—C5	111 (2)	C16—C15—H15B	108.9
C3—C4—H4A	109.5	N2—C15—H15B	108.9
C5—C4—H4A	109.5	H15A—C15—H15B	107.7
C3—C4—H4B	109.5	C15—C16—C17	118 (2)
C5—C4—H4B	109.5	C15—C16—H16A	107.7
H4A—C4—H4B	108.1	C17—C16—H16A	107.7
C4'—C3'—C2	112 (2)	C15—C16—H16B	107.7
C4'—C3'—H3C	109.3	C17—C16—H16B	107.7
C2—C3'—H3C	109.3	H16A—C16—H16B	107.1
C4'—C3'—H3D	109.3	C16—C17—C18	114 (3)
C2—C3'—H3D	109.3	C16—C17—H17A	108.9
H3C—C3'—H3D	108.0	C18—C17—H17A	108.9
C3'—C4'—C5	110 (2)	C16—C17—H17B	108.9
C3'—C4'—H4C	109.6	C18—C17—H17B	108.9
C5—C4'—H4C	109.6	H17A—C17—H17B	107.7
C3'—C4'—H4D	109.6	N2—C15'—C16'	114 (5)
C5—C4'—H4D	109.6	N2—C15'—H15C	108.7
H4C—C4'—H4D	108.2	C16'—C15'—H15C	108.7
C6—C5—C4	109.5 (7)	N2—C15'—H15D	108.7
C6—C5—C4'	109.8 (8)	C16'—C15'—H15D	108.7
C6—C5—H5A	109.8	H15C—C15'—H15D	107.6
C4—C5—H5A	109.8	C17'—C16'—C15'	115 (8)
C6—C5—H5B	109.8	C17'—C16'—H16C	108.4
C4—C5—H5B	109.8	C15'—C16'—H16C	108.4
C4'—C5—H5B	134.1	C17'—C16'—H16D	108.4
H5A—C5—H5B	108.2	C15'—C16'—H16D	108.4
C6—C5—H5C	109.7	H16C—C16'—H16D	107.5
C4—C5—H5C	134.4	C16'—C17'—C18'	112 (7)
C4'—C5—H5C	109.5	C16'—C17'—H17C	109.3
H5B—C5—H5C	77.4	C18'—C17'—H17C	109.3
C6—C5—H5D	109.7	C16'—C17'—H17D	109.3
C4—C5—H5D	79.2	C18'—C17'—H17D	109.3
C4'—C5—H5D	109.9	H17C—C17'—H17D	107.9
H5A—C5—H5D	133.2	C17'—C18'—H18D	109.5
H5C—C5—H5D	108.2	C17'—C18'—H18E	109.5
C1—C6—C5	124.7 (3)	H18D—C18'—H18E	109.5
C1—C6—S1	112.1 (2)	C17'—C18'—H18F	109.5
C5—C6—S1	123.2 (3)	H18D—C18'—H18F	109.5
C8—C7—N1	127.3 (3)	H18E—C18'—H18F	109.5

C8—C7—S1	110.9 (2)	C10—N1—C7	114.4 (2)
N1—C7—S1	121.7 (2)	C10—N2—C9	121.8 (3)
C7—C8—C1	113.6 (3)	C10—N2—C15'	120.0 (10)
C7—C8—C9	117.9 (3)	C9—N2—C15'	116.4 (11)
C1—C8—C9	128.3 (3)	C10—N2—C15	122.8 (5)
O1—C9—N2	120.1 (3)	C9—N2—C15	114.0 (6)
O1—C9—C8	126.3 (3)	C10—N3—C14	115.7 (2)
N2—C9—C8	113.6 (3)	C10—N3—C11	115.3 (2)
N1—C10—N2	124.4 (3)	C14—N3—C11	108.7 (2)
N1—C10—N3	119.9 (3)	C13—O2—C12	110.3 (2)
N2—C10—N3	115.7 (3)	C7—S1—C6	91.58 (15)
C6—C1—C2—C3'	−9.3 (12)	N2—C15'—C16'—C17'	47 (10)
C8—C1—C2—C3'	169.8 (11)	C15'—C16'—C17'—C18'	173 (8)
C6—C1—C2—C3	17.1 (15)	N2—C10—N1—C7	1.9 (4)
C8—C1—C2—C3	−163.8 (15)	N3—C10—N1—C7	−180.0 (2)
C1—C2—C3—C4	−47 (3)	C8—C7—N1—C10	5.1 (4)
C3'—C2—C3—C4	50 (6)	S1—C7—N1—C10	−176.3 (2)
C2—C3—C4—C5	65 (4)	N1—C10—N2—C9	−7.4 (4)
C1—C2—C3'—C4'	43 (3)	N3—C10—N2—C9	174.4 (2)
C3—C2—C3'—C4'	−50 (5)	N1—C10—N2—C15'	−171.8 (17)
C2—C3'—C4'—C5	−64 (3)	N3—C10—N2—C15'	9.9 (17)
C3—C4—C5—C6	−49 (3)	N1—C10—N2—C15	158.3 (10)
C3—C4—C5—C4'	48 (3)	N3—C10—N2—C15	−19.9 (10)
C3'—C4'—C5—C6	49 (3)	O1—C9—N2—C10	−175.7 (3)
C3'—C4'—C5—C4	−47 (2)	C8—C9—N2—C10	5.8 (4)
C8—C1—C6—C5	177.1 (3)	O1—C9—N2—C15'	−10.7 (16)
C2—C1—C6—C5	−3.7 (5)	C8—C9—N2—C15'	170.8 (15)
C8—C1—C6—S1	−1.2 (3)	O1—C9—N2—C15	17.5 (9)
C2—C1—C6—S1	178.0 (3)	C8—C9—N2—C15	−161.1 (9)
C4—C5—C6—C1	19.5 (15)	C16'—C15'—N2—C10	−107 (5)
C4'—C5—C6—C1	−16.2 (13)	C16'—C15'—N2—C9	88 (5)
C4—C5—C6—S1	−162.4 (14)	C16'—C15'—N2—C15	−3(5)
C4'—C5—C6—S1	161.9 (12)	C16—C15—N2—C10	−88.6 (12)
N1—C7—C8—C1	178.2 (2)	C16—C15—N2—C9	78.1 (14)
S1—C7—C8—C1	−0.5 (3)	C16—C15—N2—C15'	180 (4)
N1—C7—C8—C9	−6.1 (4)	N1—C10—N3—C14	−26.2 (4)
S1—C7—C8—C9	175.2 (2)	N2—C10—N3—C14	152.1 (2)
C6—C1—C8—C7	1.1 (4)	N1—C10—N3—C11	102.2 (3)
C2—C1—C8—C7	−178.1 (3)	N2—C10—N3—C11	−79.4 (3)
C6—C1—C8—C9	−174.0 (3)	C13—C14—N3—C10	−168.1 (3)
C2—C1—C8—C9	6.8 (5)	C13—C14—N3—C11	60.3 (3)
C7—C8—C9—O1	−178.1 (3)	C12—C11—N3—C10	167.7 (3)
C1—C8—C9—O1	−3.2 (5)	C12—C11—N3—C14	−60.5 (4)
C7—C8—C9—N2	0.3 (4)	C14—C13—O2—C12	56.7 (4)
C1—C8—C9—N2	175.3 (3)	C11—C12—O2—C13	−57.0 (4)
N3—C11—C12—O2	59.1 (4)	C8—C7—S1—C6	−0.2 (2)
O2—C13—C14—N3	−59.0 (3)	N1—C7—S1—C6	−179.0 (2)
N2—C15—C16—C17	172 (2)	C1—C6—S1—C7	0.8 (2)
C15—C16—C17—C18	−71 (4)	C5—C6—S1—C7	−177.5 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11A···O2^{i}	0.97	2.53	3.187 (4)	125
C14—H14B···O1^{ii}	0.97	2.46	3.343 (4)	152

Symmetry codes: (i) −*x*+*y*+4/3, −*x*+2/3, *z*−1/3; (ii) *y*+1, −*x*+*y*+1, −*z*+2.

Fig. 1

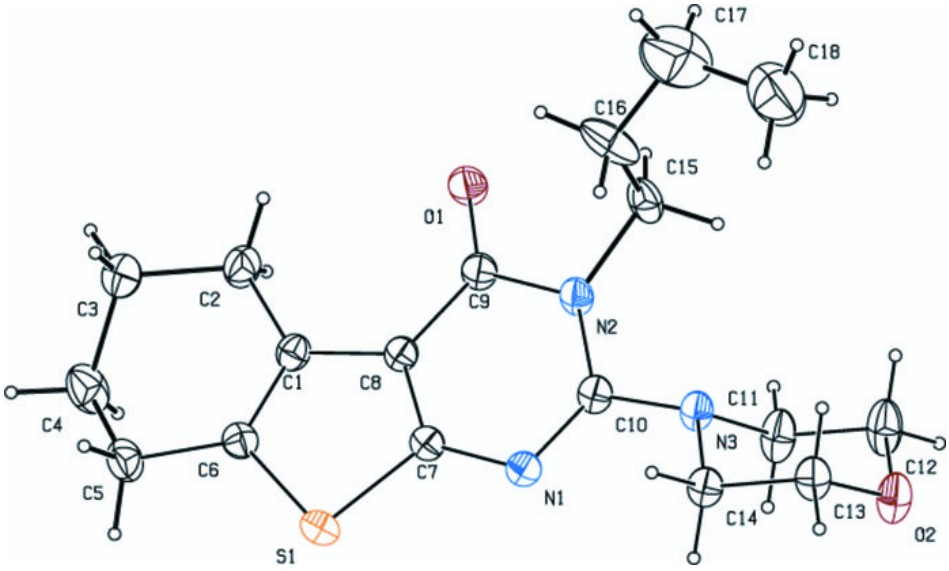
C17
C18
C16
C15
O1
C9
N2
C3
C2
C1
C8
C10
C11
C4
N3
C12
C6
C7
C5
N1
C14
C13
O2
S1

Fig. 2