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3-Isopropyl-2-*p*-tolyloxy-5,6,7,8-tetrahydro-1-benzothieno[2,3-*d*]pyrimidin-4(3*H*)-one

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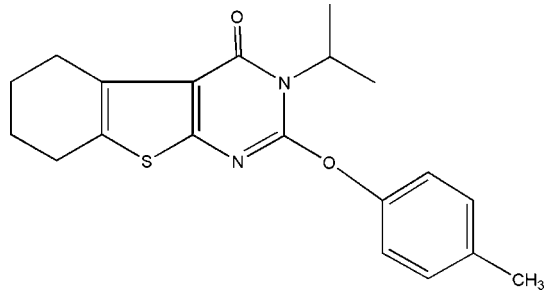
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.057; wR factor = 0.141; data-to-parameter ratio = 15.8.

In the title compound, $C_{20}H_{22}N_2O_2S$, the central thienopyrimidine ring system is essentially planar, with a maximum displacement of 0.023 (2) Å. The attached cyclohexene ring is disordered over two possible conformations, with an occupancy ratio of 0.776 (12):0.224 (12). Neither intermolecular hydrogen-bonding interactions nor π–π stacking interactions are present in the crystal structure. The molecular conformation and crystal packing are stabilized by three intramolecular C—H···O hydrogen bonds and two C—H···π interactions.

Related literature

For the biological activity of thienopyrimidin-4(3*H*)-one derivatives, see: De Laszlo *et al.* (1992*a*,*b*); Taguchi *et al.* (1993*a*,*b*); Walter (1999*a*,*b*,*c*,*d*); Walter & Zeun (2004); Ding *et al.* (2004); Santagati *et al.* (2003); Abbott GmbH Co KG (2004*a*, 2004*b*); Waehaelae *et al.* (2004*a*,*b*); Ford *et al.* (2004*a*,*b*); Duval *et al.* (2005). For a description of the Cambridge Structural Database, see: Allen (2002). For related structures, see: Xie *et al.* (2008); Xu *et al.* (2005); Zeng *et al.* (2005, 2006, 2007, 2008); Wang *et al.* (2006, 2007, 2008); Zheng *et al.* (2007).



Experimental

Crystal data

$C_{20}H_{22}N_2O_2S$
M_r = 354.47
Monoclinic, $P2_1$
a = 13.2367 (7) Å
b = 5.7493 (3) Å
c = 13.4306 (7) Å
β = 115.858 (4)°
V = 919.76 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 298 K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.963, T_{max} = 0.981
6373 measured reflections
3920 independent reflections
3370 reflections with $I > 2\sigma(I)$
R_{int} = 0.079

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.141
S = 1.01
3920 reflections
248 parameters
16 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Absolute structure: Flack (1983), 1702 Freidel pairs
Flack parameter: 0.16 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13*C*···O2	0.96	2.41	2.959 (4)	116
C12—H12*A*···O2	0.96	2.31	2.871 (4)	117
C11—H11···O1	0.98	2.20	2.725 (3)	112
C12—H12*C*···*Cg*1^{i}	0.96	2.94	3.838 (4)	156
C12—H12*C*···*Cg*2^{i}	0.96	2.72	3.413 (4)	130

Symmetry code: (i) $x, y-1, z$. *Cg*1 and *Cg*2 are the centroids of the thiophene (S1/C1/C6–C8) and pyrimidine (N1/N2/C7–C10) rings, respectively.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT* program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2765).

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supporting information

Acta Cryst. (2009). E**65**, o1142–o1143 [doi:10.1107/S1600536809014962]

3-Isopropyl-2-*p*-tolyloxy-5,6,7,8-tetrahydro-1-benzothieno[2,3-*d*]pyrimidin-4(3*H*)-one

Xiao-Hua Zeng, Shou-Heng Deng, Yong-Nian Qu and Hong-Mei Wang

S1. Comment

The derivatives of heterocycles containing thienopyrimidine system, which are well known bioisosteres of quinazolines, are of great importance because of their remarkable biological properties. Some of these activities include antimicrobial or antifungal activities (De Laszlo *et al.*, 1992*a*,*b*; Walter, 1999*a*,*b*,*c*,*d*); Ding *et al.*, 2004; Walter *et al.*, 2004), significant 5-HT_{1A} and 5-HT_{1B} receptor activities (Taguchi *et al.*, 1993*a*,*b*; Abbott GmbH & Co. KG., 2004*a*,*b*), potential selective COX-2 enzyme inhibitor activity (Santagati *et al.*, 2003), 17beta-hydroxysteroid dehydrogenase inhibitor activity (Waehaelae *et al.*, 2004*a*,*b*), potassium channel inhibitor activity (Ford *et al.*, 2004*a*,*b*), and tissue transglutaminase inhibitor activity (Duval *et al.*, 2005).

In recent years, we have been engaged in the preparation of the derivatives of heterocycles *via* aza-Wittig reaction. The title compound, (I), was synthesized and structurally characterized in this context.

The molecular structure indicates that the thieno[2,3-*d*]pyrimidine moiety is a conjugated system (Fig.1). All ring atoms in thieno[2,3-*d*]pyrimidine are essentially coplanar (Xu *et al.*, 2005; Zeng *et al.*, 2005, 2006, 2007, 2008; Wang *et al.*, 2006, 2007, 2008; Zheng *et al.*, 2007; Xie *et al.*, 2008). The bond lengths and angles are within experimental error, in the ranges of values in previously reported structures in the Cambridge Structural Database (Version 5.26; Allen, 2002).

The attached cyclohexene ring is disordered. There are two possible conformations, C2—C5 and C2/C3′/C4′/C5, with an occupancy ratio of 0.77:0.23. There exists no intermolecular hydrogen bonding interaction and no π-π stacking. The molecular conformation and crystal packing are stabilized by three intramolecular C—H···O hydrogen bonds and two C—H···π interactions.

S2. Experimental

To a solution of iminophosphorane (1.45 g, 3 mmol) in anhydrous dichloromethane (15 ml) was added iso-propyl isocyanate (3 mmol) under dry nitrogen at room temperature. After the reaction mixture was left unstirred for 48 h at room temperature, the solvent was removed off under reduced pressure and ether/petroleum ether (1:2 *v*/*v*, 20 ml) was added to precipitate triphenylphosphine oxide. After filtration, the solvent was removed, and the residue was dissolved in CH_3CN (15 ml). After adding 4-CH_3—PhOH (3.1 mmol) and excess K_2CO_3 to the solution of carbodiimide, the mixture was stirred for 15 h at room temperature. The solution was condensed and the residue was recrystallized by EtOH to give the title compound, (I), in yield of 65% (m.p. 436 K). Elemental analysis calculated for $C_{20}H_{22}N_2O_2S$: C 67.77, H 6.26, N 7.90%. Found: C 67.54, H 6.32, N 7.83%. Crystals suitable for single crystal X-ray diffraction were obtained by vapor diffusion of hexane and dichloromethane (1:3 *v*/*v*) at room temperature.

S3. Refinement

H atoms were placed at calculated positions and treated as riding atoms, with C—H = 0.93–0.98 Å, and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C).

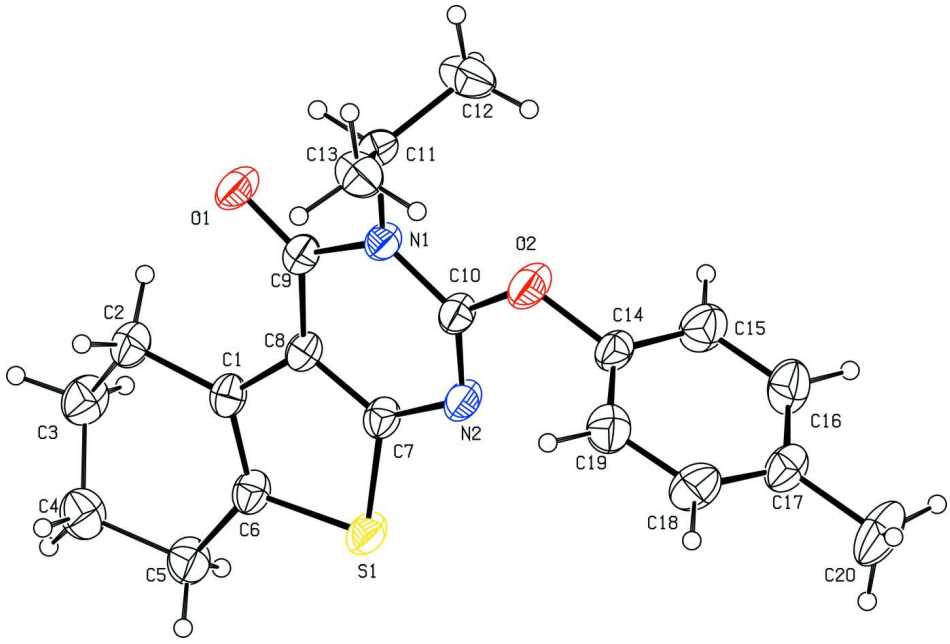

Figure 1

View of the molecule of showing the atom-labeling scheme. Displacement ellipsoids are drawn at 50% probability level. H-atoms are represented by circles of arbitrary size. Only the major component of the disordered cyclohexene ring is shown.

3-Isopropyl-2-*p*-tolyloxy-5,6,7,8-tetrahydro-1- benzothieno[2,3-*d*]pyrimidin-4(3*H*)-one

Crystal data

$C_{20}H_{22}N_2O_2S$
M_r = 354.47
Monoclinic, $P2_1$
Hall symbol: P 2yb
a = 13.2367 (7) Å
b = 5.7493 (3) Å
c = 13.4306 (7) Å
β = 115.858 (4)°
V = 919.76 (8) Å^3
Z = 2
$F(000)$ = 376
D_x = 1.280 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2048 reflections
θ = 2.9–24.5°
μ = 0.19 mm^{-1}
T = 298 K
Block, colourless
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.963, T_{max} = 0.981
6373 measured reflections
3920 independent reflections
3370 reflections with $I > 2\sigma(I)$
R_{int} = 0.079
θ_{max} = 27.0°, θ_{min} = 1.7°
h = −16→16
k = −7→7
l = −17→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.141$
$S = 1.01$
3920 reflections
248 parameters
16 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
$w = 1/[\sigma^2(F_o^2) + (0.0798P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}
Absolute structure: Flack (1983), 1702 Freidel pairs
Absolute structure parameter: 0.16 (10)

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}	Occ. (<1)
C1	0.20878 (19)	0.6656 (5)	0.88050 (19)	0.0448 (6)	
C2	0.0948 (2)	0.6877 (6)	0.8794 (2)	0.0563 (7)	
H2A	0.0446	0.7700	0.8132	0.068*	0.776 (12)
H2B	0.0639	0.5339	0.8776	0.068*	0.776 (12)
H2C	0.0817	0.5593	0.9191	0.068*	0.224 (12)
H2D	0.0370	0.6849	0.8037	0.068*	0.224 (12)
C3	0.1018 (4)	0.8162 (11)	0.9796 (5)	0.0662 (16)	0.776 (12)
H3A	0.1348	0.7157	1.0439	0.079*	0.776 (12)
H3B	0.0268	0.8576	0.9693	0.079*	0.776 (12)
C4	0.1717 (4)	1.0336 (10)	0.9996 (6)	0.0690 (17)	0.776 (12)
H4A	0.1703	1.1175	1.0616	0.083*	0.776 (12)
H4B	0.1383	1.1329	0.9349	0.083*	0.776 (12)
C3′	0.0904 (12)	0.916 (2)	0.9334 (14)	0.061 (5)	0.224 (12)
H3′1	0.0829	1.0405	0.8817	0.073*	0.224 (12)
H3′2	0.0230	0.9169	0.9448	0.073*	0.224 (12)
C4′	0.1882 (9)	0.974 (5)	1.0420 (11)	0.068 (6)	0.224 (12)
H4′1	0.1965	0.8556	1.0964	0.081*	0.224 (12)
H4′2	0.1758	1.1224	1.0692	0.081*	0.224 (12)
C5	0.2932 (2)	0.9853 (6)	1.0236 (3)	0.0615 (8)	
H5A	0.3283	1.1265	1.0144	0.074*	0.776 (12)
H5B	0.3346	0.9322	1.0993	0.074*	0.776 (12)
H5C	0.2996	1.1376	0.9958	0.074*	0.224 (12)
H5D	0.3578	0.9636	1.0943	0.074*	0.224 (12)

C6	0.2953 (2)	0.8022 (5)	0.9451 (2)	0.0489 (6)
C7	0.3471 (2)	0.5369 (5)	0.8298 (2)	0.0457 (6)
C8	0.23832 (18)	0.5102 (5)	0.81357 (19)	0.0419 (5)
C9	0.1665 (2)	0.3547 (5)	0.7278 (2)	0.0440 (5)
C10	0.33155 (19)	0.2882 (5)	0.6970 (2)	0.0472 (6)
C11	0.1476 (2)	0.1089 (5)	0.5680 (2)	0.0476 (6)
H11	0.0727	0.1104	0.5658	0.057*
C12	0.1818 (3)	−0.1432 (6)	0.5773 (3)	0.0763 (10)
H12A	0.2536	−0.1556	0.5760	0.114*
H12B	0.1269	−0.2287	0.5163	0.114*
H12C	0.1867	−0.2060	0.6455	0.114*
C13	0.1348 (3)	0.2214 (6)	0.4619 (2)	0.0640 (8)
H13A	0.1085	0.3781	0.4587	0.096*
H13B	0.0817	0.1349	0.4001	0.096*
H13C	0.2061	0.2229	0.4591	0.096*
C14	0.4833 (2)	0.1798 (5)	0.6585 (2)	0.0515 (7)
C15	0.5521 (3)	0.0051 (7)	0.7178 (3)	0.0704 (9)
H15	0.5252	−0.1141	0.7466	0.084*
C16	0.6628 (3)	0.0076 (7)	0.7348 (3)	0.0743 (9)
H16	0.7098	−0.1137	0.7741	0.089*
C17	0.7055 (2)	0.1829 (6)	0.6956 (2)	0.0592 (8)
C18	0.6321 (3)	0.3536 (7)	0.6344 (3)	0.0721 (9)
H18	0.6583	0.4727	0.6050	0.086*
C19	0.5207 (3)	0.3543 (6)	0.6149 (3)	0.0710 (9)
H19	0.4724	0.4715	0.5730	0.085*
C20	0.8275 (2)	0.1872 (10)	0.7183 (3)	0.0936 (15)
H20A	0.8639	0.3178	0.7646	0.140*
H20B	0.8332	0.2006	0.6496	0.140*
H20C	0.8632	0.0460	0.7549	0.140*
N1	0.22102 (15)	0.2496 (4)	0.66777 (15)	0.0435 (4)
N2	0.39874 (17)	0.4226 (4)	0.77485 (19)	0.0524 (6)
O2	0.36853 (15)	0.1676 (4)	0.63340 (17)	0.0689 (7)
O1	0.06852 (14)	0.3137 (4)	0.70296 (16)	0.0607 (6)
S1	0.41623 (5)	0.74703 (15)	0.92707 (6)	0.0585 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0409 (13)	0.0542 (15)	0.0392 (12)	0.0072 (10)	0.0172 (10)	0.0072 (11)
C2	0.0453 (14)	0.068 (2)	0.0600 (16)	0.0029 (12)	0.0267 (12)	−0.0012 (14)
C3	0.062 (3)	0.086 (4)	0.062 (3)	−0.003 (2)	0.038 (2)	−0.010 (3)
C4	0.075 (3)	0.074 (4)	0.070 (4)	0.005 (2)	0.042 (3)	−0.014 (3)
C3′	0.053 (7)	0.072 (8)	0.060 (8)	0.002 (6)	0.026 (6)	0.000 (6)
C4′	0.075 (9)	0.081 (10)	0.056 (9)	0.012 (6)	0.036 (7)	0.012 (7)
C5	0.0554 (16)	0.071 (2)	0.0553 (16)	0.0041 (14)	0.0213 (13)	−0.0128 (15)
C6	0.0409 (12)	0.0616 (17)	0.0410 (12)	0.0051 (11)	0.0149 (10)	−0.0014 (12)
C7	0.0371 (13)	0.0556 (15)	0.0383 (12)	0.0036 (11)	0.0107 (10)	−0.0022 (11)
C8	0.0347 (11)	0.0508 (13)	0.0373 (12)	0.0014 (10)	0.0130 (10)	0.0026 (10)

C9	0.0369 (12)	0.0502 (14)	0.0449 (13)	0.0016 (10)	0.0179 (10)	0.0058 (11)
C10	0.0360 (11)	0.0563 (16)	0.0490 (13)	0.0013 (11)	0.0182 (10)	−0.0032 (12)
C11	0.0381 (13)	0.0495 (15)	0.0485 (14)	−0.0052 (11)	0.0127 (11)	−0.0059 (12)
C12	0.095 (3)	0.0463 (17)	0.072 (2)	−0.0096 (16)	0.0220 (19)	0.0016 (16)
C13	0.0728 (18)	0.0565 (18)	0.0483 (15)	0.0039 (15)	0.0130 (13)	−0.0016 (14)
C14	0.0381 (13)	0.0631 (18)	0.0561 (15)	−0.0044 (11)	0.0232 (12)	−0.0184 (13)
C15	0.0602 (18)	0.075 (2)	0.082 (2)	−0.0034 (17)	0.0366 (17)	0.0130 (19)
C16	0.0570 (18)	0.083 (2)	0.077 (2)	0.0165 (17)	0.0243 (16)	0.0157 (19)
C17	0.0473 (14)	0.085 (2)	0.0514 (15)	−0.0026 (14)	0.0276 (12)	−0.0128 (15)
C18	0.0622 (19)	0.085 (2)	0.076 (2)	−0.0121 (18)	0.0372 (17)	0.0070 (18)
C19	0.0608 (18)	0.067 (2)	0.083 (2)	0.0070 (16)	0.0292 (17)	0.0075 (18)
C20	0.0496 (17)	0.166 (5)	0.073 (2)	0.002 (2)	0.0332 (16)	−0.020 (3)
N1	0.0338 (9)	0.0498 (11)	0.0439 (10)	−0.0019 (10)	0.0143 (8)	−0.0033 (10)
N2	0.0319 (10)	0.0662 (15)	0.0566 (13)	−0.0020 (10)	0.0169 (9)	−0.0152 (11)
O2	0.0398 (10)	0.0937 (17)	0.0744 (13)	−0.0097 (10)	0.0261 (9)	−0.0374 (12)
O1	0.0361 (9)	0.0808 (15)	0.0670 (11)	−0.0103 (9)	0.0242 (8)	−0.0142 (11)
S1	0.0359 (3)	0.0722 (5)	0.0603 (4)	−0.0040 (3)	0.0144 (3)	−0.0216 (4)

Geometric parameters (Å, º)

C1—C6	1.347 (4)	C9—O1	1.213 (3)
C1—C8	1.437 (4)	C9—N1	1.429 (3)
C1—C2	1.508 (3)	C10—N2	1.292 (3)
C2—C3	1.502 (5)	C10—O2	1.348 (3)
C2—C3′	1.515 (10)	C10—N1	1.358 (3)
C2—H2A	0.9700	C11—N1	1.503 (3)
C2—H2B	0.9700	C11—C13	1.506 (4)
C2—H2C	0.9700	C11—C12	1.508 (5)
C2—H2D	0.9700	C11—H11	0.9800
C3—C4	1.508 (7)	C12—H12A	0.9600
C3—H3A	0.9700	C12—H12B	0.9600
C3—H3B	0.9700	C12—H12C	0.9600
C4—C5	1.521 (5)	C13—H13A	0.9600
C4—H4A	0.9700	C13—H13B	0.9600
C4—H4B	0.9700	C13—H13C	0.9600
C3′—C4′	1.505 (10)	C14—C15	1.356 (5)
C3′—H3′1	0.9700	C14—C19	1.359 (4)
C3′—H3′2	0.9700	C14—O2	1.407 (3)
C4′—C5	1.515 (9)	C15—C16	1.382 (4)
C4′—H4′1	0.9700	C15—H15	0.9300
C4′—H4′2	0.9700	C16—C17	1.368 (5)
C5—C6	1.499 (4)	C16—H16	0.9300
C5—H5A	0.9700	C17—C18	1.373 (5)
C5—H5B	0.9700	C17—C20	1.508 (4)
C5—H5C	0.9700	C18—C19	1.381 (4)
C5—H5D	0.9700	C18—H18	0.9300
C6—S1	1.749 (3)	C19—H19	0.9300
C7—C8	1.368 (3)	C20—H20A	0.9600

C7—N2	1.372 (3)	C20—H20B	0.9600
C7—S1	1.721 (3)	C20—H20C	0.9600
C8—C9	1.440 (4)		

C6—C1—C8	112.2 (2)	H5A—C5—H5D	88.0
C6—C1—C2	121.6 (2)	H5B—C5—H5D	23.0
C8—C1—C2	126.2 (2)	H5C—C5—H5D	107.8
C3—C2—C1	111.2 (3)	C1—C6—C5	126.2 (2)
C3—C2—C3′	31.2 (6)	C1—C6—S1	112.19 (19)
C1—C2—C3′	108.4 (7)	C5—C6—S1	121.6 (2)
C3—C2—H2A	109.4	C8—C7—N2	126.7 (2)
C1—C2—H2A	109.4	C8—C7—S1	111.93 (19)
C3′—C2—H2A	82.1	N2—C7—S1	121.34 (18)
C3—C2—H2B	109.4	C7—C8—C1	112.7 (2)
C1—C2—H2B	109.4	C7—C8—C9	118.6 (2)
C3′—C2—H2B	134.4	C1—C8—C9	128.4 (2)
H2A—C2—H2B	108.0	O1—C9—N1	120.3 (2)
C3—C2—H2C	80.7	O1—C9—C8	126.4 (2)
C1—C2—H2C	110.4	N1—C9—C8	113.2 (2)
C3′—C2—H2C	110.1	N2—C10—O2	120.6 (2)
H2A—C2—H2C	131.4	N2—C10—N1	127.4 (2)
H2B—C2—H2C	31.3	O2—C10—N1	112.1 (2)
C3—C2—H2D	131.3	N1—C11—C13	112.0 (2)
C1—C2—H2D	109.7	N1—C11—C12	112.9 (2)
C3′—C2—H2D	109.9	C13—C11—C12	113.4 (3)
H2A—C2—H2D	30.2	N1—C11—H11	105.9
H2B—C2—H2D	80.0	C13—C11—H11	105.9
H2C—C2—H2D	108.4	C12—C11—H11	105.9
C2—C3—C4	111.1 (5)	C11—C12—H12A	109.5
C2—C3—H3A	109.4	C11—C12—H12B	109.5
C4—C3—H3A	109.4	H12A—C12—H12B	109.5
C2—C3—H3B	109.4	C11—C12—H12C	109.5
C4—C3—H3B	109.4	H12A—C12—H12C	109.5
H3A—C3—H3B	108.0	H12B—C12—H12C	109.5
C3—C4—C5	113.3 (4)	C11—C13—H13A	109.5
C3—C4—H4A	108.9	C11—C13—H13B	109.5
C5—C4—H4A	108.9	H13A—C13—H13B	109.5
C3—C4—H4B	108.9	C11—C13—H13C	109.5
C5—C4—H4B	108.9	H13A—C13—H13C	109.5
H4A—C4—H4B	107.7	H13B—C13—H13C	109.5
C4′—C3′—C2	117.3 (15)	C15—C14—C19	121.5 (3)
C4′—C3′—H3′1	108.0	C15—C14—O2	118.8 (3)
C2—C3′—H3′1	108.0	C19—C14—O2	119.4 (3)
C4′—C3′—H3′2	108.0	C14—C15—C16	118.8 (3)
C2—C3′—H3′2	108.0	C14—C15—H15	120.6
H3′1—C3′—H3′2	107.2	C16—C15—H15	120.6
C3′—C4′—C5	108.3 (10)	C17—C16—C15	122.0 (3)
C3′—C4′—H4′1	110.0	C17—C16—H16	119.0

C5—C4′—H4′1	110.0	C15—C16—H16	119.0
C3′—C4′—H4′2	110.0	C16—C17—C18	117.0 (3)
C5—C4′—H4′2	110.0	C16—C17—C20	121.3 (3)
H4′1—C4′—H4′2	108.4	C18—C17—C20	121.6 (3)
C6—C5—C4′	112.6 (9)	C17—C18—C19	122.2 (3)
C6—C5—C4	108.8 (3)	C17—C18—H18	118.9
C4′—C5—C4	23.5 (6)	C19—C18—H18	118.9
C6—C5—H5A	109.9	C14—C19—C18	118.4 (3)
C4′—C5—H5A	125.5	C14—C19—H19	120.8
C4—C5—H5A	109.9	C18—C19—H19	120.8
C6—C5—H5B	109.9	C17—C20—H20A	109.5
C4′—C5—H5B	87.4	C17—C20—H20B	109.5
C4—C5—H5B	109.9	H20A—C20—H20B	109.5
H5A—C5—H5B	108.3	C17—C20—H20C	109.5
C6—C5—H5C	109.4	H20A—C20—H20C	109.5
C4′—C5—H5C	110.0	H20B—C20—H20C	109.5
C4—C5—H5C	90.9	C10—N1—C9	120.8 (2)
H5A—C5—H5C	21.3	C10—N1—C11	122.9 (2)
H5B—C5—H5C	125.7	C9—N1—C11	116.21 (18)
C6—C5—H5D	108.6	C10—N2—C7	113.1 (2)
C4′—C5—H5D	108.3	C10—O2—C14	118.4 (2)
C4—C5—H5D	129.0	C7—S1—C6	90.97 (12)

C6—C1—C2—C3	−17.9 (5)	C19—C14—C15—C16	0.6 (5)
C8—C1—C2—C3	164.4 (4)	O2—C14—C15—C16	174.8 (3)
C6—C1—C2—C3′	15.2 (8)	C14—C15—C16—C17	1.4 (5)
C8—C1—C2—C3′	−162.5 (8)	C15—C16—C17—C18	−2.5 (5)
C1—C2—C3—C4	46.7 (6)	C15—C16—C17—C20	177.8 (3)
C3′—C2—C3—C4	−44.0 (11)	C16—C17—C18—C19	1.7 (5)
C2—C3—C4—C5	−62.5 (8)	C20—C17—C18—C19	−178.6 (3)
C3—C2—C3′—C4′	53.3 (13)	C15—C14—C19—C18	−1.4 (5)
C1—C2—C3′—C4′	−47.5 (19)	O2—C14—C19—C18	−175.5 (3)
C2—C3′—C4′—C5	61 (3)	C17—C18—C19—C14	0.2 (5)
C3′—C4′—C5—C6	−39 (2)	N2—C10—N1—C9	−2.7 (4)
C3′—C4′—C5—C4	46.5 (12)	O2—C10—N1—C9	177.7 (2)
C3—C4—C5—C6	43.0 (7)	N2—C10—N1—C11	173.4 (3)
C3—C4—C5—C4′	−61 (2)	O2—C10—N1—C11	−6.3 (4)
C8—C1—C6—C5	179.2 (3)	O1—C9—N1—C10	−177.9 (3)
C2—C1—C6—C5	1.2 (4)	C8—C9—N1—C10	3.8 (3)
C8—C1—C6—S1	0.0 (3)	O1—C9—N1—C11	5.8 (4)
C2—C1—C6—S1	−178.0 (2)	C8—C9—N1—C11	−172.6 (2)
C4′—C5—C6—C1	11.4 (9)	C13—C11—N1—C10	−64.3 (3)
C4—C5—C6—C1	−13.4 (5)	C12—C11—N1—C10	65.2 (3)
C4′—C5—C6—S1	−169.5 (9)	C13—C11—N1—C9	112.0 (3)
C4—C5—C6—S1	165.8 (3)	C12—C11—N1—C9	−118.6 (3)
N2—C7—C8—C1	−176.8 (3)	O2—C10—N2—C7	178.4 (3)
S1—C7—C8—C1	0.7 (3)	N1—C10—N2—C7	−1.2 (4)
N2—C7—C8—C9	−2.7 (4)	C8—C7—N2—C10	4.0 (4)

S1—C7—C8—C9	174.81 (19)	S1—C7—N2—C10	−173.3 (2)
C6—C1—C8—C7	−0.4 (3)	N2—C10—O2—C14	4.1 (4)
C2—C1—C8—C7	177.4 (2)	N1—C10—O2—C14	−176.3 (2)
C6—C1—C8—C9	−173.8 (2)	C15—C14—O2—C10	98.6 (3)
C2—C1—C8—C9	4.1 (4)	C19—C14—O2—C10	−87.0 (3)
C7—C8—C9—O1	−179.5 (3)	C8—C7—S1—C6	−0.6 (2)
C1—C8—C9—O1	−6.5 (4)	N2—C7—S1—C6	177.0 (2)
C7—C8—C9—N1	−1.3 (3)	C1—C6—S1—C7	0.4 (2)
C1—C8—C9—N1	171.7 (2)	C5—C6—S1—C7	−178.9 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13*C*···O2	0.96	2.41	2.959 (4)	116
C12—H12*A*···O2	0.96	2.31	2.871 (4)	117
C11—H11···O1	0.98	2.20	2.725 (3)	112
C12—H12*C*···*Cg*1^{i}	0.96	2.94	3.838 (4)	156
C12—H12*C*···*Cg*2^{i}	0.96	2.72	3.413 (4)	130

Symmetry code: (i) *x*, *y*−1, *z*.