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N-[4-Acetyl-5-(2-methylprop-1-enyl)-5-(2-*p*-tolylpropyl)-4,5-dihydro-1,3,4-thiadiazol-2-yl]acetamide

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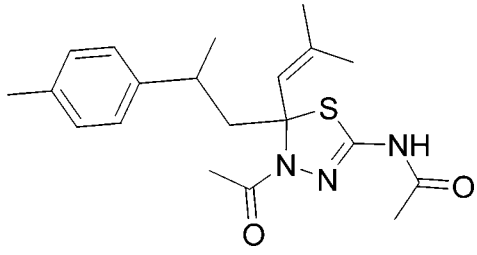
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.094; data-to-parameter ratio = 16.2.

The title heterocyclic compound, $C_{20}H_{27}N_3O_2S$, was synthesized from 2-(4-methylcyclohex-3-enyl)-6-methylhepta-2,5-dien-4-one, which was isolated from the essential oil *Cedrus atlantica*. The thiadiazole ring is essentially planar [maximum deviation 0.006 (2) Å] and it forms a dihedral angle of 18.08 (9)° with the benzene ring. The dihedral angle between the thiadiazole ring and the acetamide plane is 7.62 (10)°. In the crystal, molecules are linked into chains running along the c axis by intermolecular N—H···O hydrogen bonds.

Related literature

For the biological activity of 1,3,4-thiadiazole derivatives, see: Demirbas *et al.* (2005); Holla *et al.* (2002); Kritsanida *et al.* (2002); Nizamuddin *et al.* (1999); Sun *et al.* (1999); Udupi *et al.* (2000). For the synthesis, see: Beatriz *et al.* (2002); Sakthivel *et al.* (2008). For related structures, see: Loughzail *et al.* (2009); Tebaa *et al.* (2009).



Experimental

Crystal data

$C_{20}H_{27}N_3O_2S$
M_r = 373.51
Monoclinic, $P2_1/c$
a = 10.855 (2) Å
b = 14.193 (2) Å
c = 12.854 (4) Å
β = 90.955 (11)°
V = 1980.1 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 100 K
0.28 × 0.17 × 0.12 mm

Data collection

Bruker X8 APEX CCD area-detector diffractometer
Absorption correction: none
7884 measured reflections
4030 independent reflections
3365 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.094
S = 1.10
4030 reflections
249 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H2···O2^{i}	0.87 (2)	1.96 (2)	2.811 (2)	167 (2)

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2005); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXS97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2797).

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supporting information

Acta Cryst. (2009). E**65**, o1269–o1270 [doi:10.1107/S1600536809017127]

N-[4-Acetyl-5-(2-methylprop-1-enyl)-5-(2-*p*-tolylpropyl)-4,5-dihydro-1,3,4-thiadiazol-2-yl]acetamide

Noureddine Mazoir, Lahcen El Ammari, Nouzha Bouhmaida, Slimane Dahaoui, Ahmed Benharref and Moha Berraho

S1. Comment

1,3,4-Thiadiazole derivatives possess antimicrobial (Demirbas *et al.*, 2005) and antiviral (Kritsanida *et al.*, 2002) activities. They are also known for their broad-spectrum of biological activities such as antibacterial (Sun *et al.*, 1999), anti-inflammatory (Udupi *et al.*, 2000) and herbicidal (Nizamuddin *et al.*, 1999). In addition, [1,3,4]thiadiazoles exhibit various biological activities possibly due to the presence of the =N—C—S moiety (Holla *et al.*, 2002). In view of these findings and in continuation to our previous work on the synthesis of [1,3,4]thiadiazoles, we report herein the hemisynthesis of *N*-[4-acetyl-5-isobutenyl-5-(2-*p*-tolylpropyl)-4,5-dihydro-1,3,4-thiadiazol-2-yl]acetamide, (I), through chemical modification of 2-(4-methylcyclohex-3-enyl)-6-methylhepta-2,5-dien-4-one, which is isolated from Cedrus Atlantica essential oil. Thus, aromatization of this later, followed by condensation with thiosemicarbazide (Beatriz *et al.*, 2002; Sakthivel *et al.*, 2008) ending with treatment of acetic anhydride in the presence of pyridine yielded the diasterioisomers in high stereoselectivity.

The molecular structure of (I) is shown in Fig. 1. The geometric parameters (bond lengths and angles) are very similar to those observed in previously reported structures (Loughzail *et al.*,2009; Tebaa *et al.*,2009). The thiadiazole ring system is essentially planar and it forms a dihedral angle of 18.08 (9)° with the benzene ring.

In the crystal structure, molecules are linked into chains (Fig. 2) running along the *c* axis by intermolecular N—H···O hydrogen bonds (Table 1) involving the carbonyl and the acetamide groups.

S2. Experimental

A mixture of 2-(4-methylcyclohex-3-enyl)-6-methylhepta-2,5-dien-4-one (0.5 g, 2.3 mmol) and Pd/C (10%) was heated at 423 K for 12 h. The product obtained was treated with equimolecular quantity of thiosemicarbazide and several drops of HCl were added. The reactional mixture was heated at reflux in ethanol for 5 h and then evaporated under reduced pressure and the residue obtained was purified on silica gel column using hexane–ethyl acetate (96:4) as an eluent. 0.25 mmol of the thiosemicarbazone obtained was dissolved in 2.5 ml of pyridine and 2.5 ml of acetic anhydride. The mixture was heated on a water bath for 1.5 h. The resulting residue was concentrated *in vacuo* and chromatographied on silica gel column with hexane–ethyl acetate (92:8) as an eluent. Suitable crystals were obtained by evaporation of an ethyl acetate solution at 277 K.

S3. Refinement

Atoms H2 and H9 were located in a difference map and refined freely. The remaining H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å (aromatic), 0.96 Å (methyl), 0.97 Å (methylene), 0.98 Å (methine), and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl}).

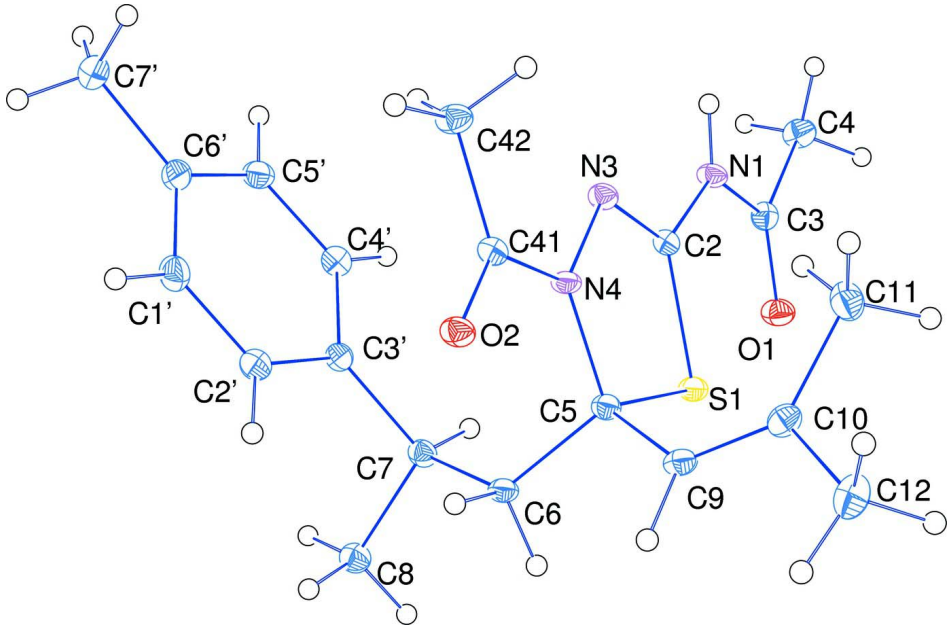

Figure 1

Molecular structure of the title compound, with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

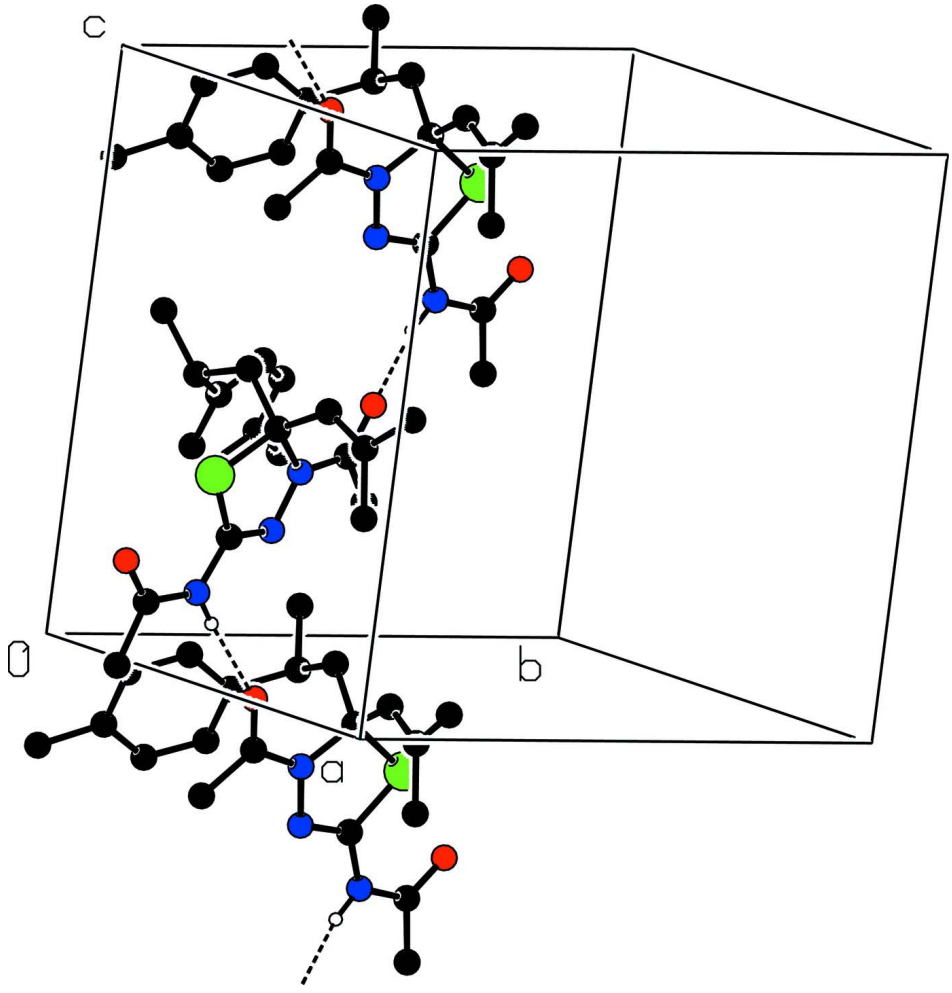

Figure 2

Partial packing view showing the N—H···O hydrogen bonds (dashed lines) and the formation of a chain along the *c* axis. H atoms not involved in hydrogen bonding have been omitted for clarity.

N-[4-Acetyl-5-(2-methylprop-1-enyl)-5-(2-*p*-tolylpropyl)-4,5-dihydro-1,3,4-thiadiazol-2-yl]acetamide

Crystal data

$C_{20}H_{27}N_3O_2S$
$M_r = 373.51$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.855\ (2)$ Å
$b = 14.193\ (2)$ Å
$c = 12.854\ (4)$ Å
$\beta = 90.955\ (11)°$
$V = 1980.1\ (8)$ Å^3
$Z = 4$
$F(000) = 800$
$D_x = 1.253$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8068 reflections
$\theta = 2.8–26.4°$
$\mu = 0.18$ mm^{-1}
$T = 100$ K
Prism, colourless
0.28 × 0.17 × 0.12 mm

Data collection

Bruker X8 APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
7884 measured reflections
4030 independent reflections
3365 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.8°$
$h = 0 \rightarrow 13$
$k = -17 \rightarrow 17$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.094$
$S = 1.10$
4030 reflections
249 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0257P)^2 + 1.5568P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
H2	0.357 (2)	0.0915 (17)	0.0811 (19)	0.039 (7)*
H9	0.5323 (18)	0.1563 (13)	0.5491 (16)	0.018 (5)*
C1′	0.04998 (19)	0.36320 (14)	0.44410 (16)	0.0263 (4)
H1′	0.0473	0.4182	0.4833	0.032*
C2′	0.10902 (18)	0.28480 (14)	0.48503 (15)	0.0231 (4)
H2′	0.1442	0.2879	0.5514	0.028*
C2	0.37116 (16)	0.09545 (13)	0.23153 (13)	0.0180 (4)
C3′	0.11662 (17)	0.20141 (13)	0.42843 (14)	0.0188 (4)
C3	0.35748 (17)	−0.04166 (13)	0.11768 (14)	0.0204 (4)
C4	0.33879 (19)	−0.07060 (14)	0.00610 (14)	0.0252 (4)
H40	0.3814	−0.1287	−0.0061	0.038*
H41	0.3706	−0.0225	−0.0386	0.038*
H42	0.2524	−0.0790	−0.0083	0.038*
C4′	0.05884 (17)	0.19924 (14)	0.33050 (14)	0.0216 (4)
H4′	0.0611	0.1442	0.2913	0.026*
C5	0.41102 (17)	0.13772 (12)	0.42180 (14)	0.0178 (4)
C5′	−0.00180 (17)	0.27755 (14)	0.29079 (15)	0.0234 (4)
H5′	−0.0408	0.2737	0.2260	0.028*
C6	0.31344 (17)	0.12846 (13)	0.50691 (13)	0.0185 (4)
H60	0.3370	0.0759	0.5512	0.022*

H61	0.3176	0.1848	0.5495	0.022*
C6′	−0.00551 (18)	0.36170 (14)	0.34573 (16)	0.0247 (4)
C7	0.17835 (17)	0.11399 (13)	0.47324 (14)	0.0191 (4)
H7	0.1752	0.0644	0.4203	0.023*
C7′	−0.0625 (2)	0.44905 (15)	0.29915 (17)	0.0326 (5)
H70′	−0.0004	0.4848	0.2644	0.049*
H71′	−0.0974	0.4866	0.3533	0.049*
H72′	−0.1260	0.4315	0.2500	0.049*
C8	0.10620 (18)	0.07994 (13)	0.56829 (14)	0.0227 (4)
H80	0.1403	0.0215	0.5928	0.034*
H81	0.0213	0.0708	0.5487	0.034*
H82	0.1120	0.1263	0.6226	0.034*
C9	0.53585 (18)	0.15303 (13)	0.47409 (14)	0.0200 (4)
C10	0.64558 (18)	0.16273 (13)	0.43130 (15)	0.0226 (4)
C11	0.67035 (19)	0.16274 (15)	0.31623 (16)	0.0286 (5)
H111	0.7302	0.1151	0.3009	0.043*
H112	0.7013	0.2233	0.2961	0.043*
H113	0.5953	0.1498	0.2784	0.043*
C12	0.75806 (19)	0.17719 (15)	0.49976 (17)	0.0304 (5)
H121	0.7982	0.2348	0.4807	0.046*
H122	0.8138	0.1254	0.4911	0.046*
H123	0.7339	0.1807	0.5712	0.046*
C41	0.37297 (17)	0.30457 (13)	0.37021 (13)	0.0177 (4)
C42	0.33714 (19)	0.37167 (13)	0.28539 (14)	0.0231 (4)
H420	0.3991	0.3715	0.2330	0.035*
H421	0.3296	0.4340	0.3137	0.035*
H422	0.2597	0.3527	0.2550	0.035*
N1	0.35903 (15)	0.05391 (11)	0.13421 (12)	0.0192 (3)
N3	0.35840 (14)	0.18471 (10)	0.24065 (11)	0.0183 (3)
N4	0.38013 (14)	0.21218 (10)	0.34384 (11)	0.0174 (3)
O1	0.36850 (13)	−0.09778 (9)	0.18908 (10)	0.0256 (3)
O2	0.39419 (12)	0.32905 (9)	0.46085 (9)	0.0213 (3)
S1	0.40785 (4)	0.02872 (3)	0.34223 (3)	0.01914 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1′	0.0305 (11)	0.0224 (10)	0.0261 (10)	0.0034 (8)	0.0050 (8)	−0.0035 (8)
C2′	0.0251 (10)	0.0248 (10)	0.0195 (9)	0.0012 (8)	0.0007 (8)	−0.0015 (8)
C2	0.0184 (9)	0.0205 (9)	0.0153 (9)	0.0010 (7)	0.0019 (7)	0.0011 (7)
C3′	0.0175 (9)	0.0199 (9)	0.0192 (9)	−0.0004 (7)	0.0020 (7)	0.0011 (7)
C3	0.0198 (9)	0.0198 (9)	0.0215 (10)	0.0000 (8)	0.0010 (7)	−0.0005 (7)
C4	0.0334 (11)	0.0220 (10)	0.0201 (10)	0.0008 (8)	−0.0041 (8)	−0.0041 (8)
C4′	0.0212 (10)	0.0228 (9)	0.0207 (9)	−0.0018 (8)	0.0007 (7)	−0.0010 (8)
C5	0.0221 (9)	0.0169 (9)	0.0144 (8)	0.0007 (7)	0.0003 (7)	0.0003 (7)
C5′	0.0206 (10)	0.0304 (10)	0.0192 (9)	−0.0002 (8)	0.0002 (8)	0.0043 (8)
C6	0.0239 (10)	0.0187 (9)	0.0128 (8)	0.0013 (8)	−0.0008 (7)	0.0012 (7)
C6′	0.0196 (10)	0.0272 (10)	0.0276 (10)	0.0032 (8)	0.0058 (8)	0.0068 (8)

C7	0.0231 (10)	0.0181 (9)	0.0160 (9)	−0.0001 (7)	0.0011 (7)	−0.0020 (7)
C7′	0.0328 (12)	0.0314 (11)	0.0338 (12)	0.0119 (9)	0.0082 (9)	0.0077 (9)
C8	0.0248 (10)	0.0216 (9)	0.0216 (10)	−0.0014 (8)	0.0009 (8)	0.0000 (8)
C9	0.0245 (10)	0.0197 (9)	0.0157 (9)	0.0011 (7)	−0.0032 (7)	0.0018 (7)
C10	0.0253 (10)	0.0171 (9)	0.0254 (10)	0.0020 (8)	−0.0015 (8)	0.0013 (7)
C11	0.0258 (11)	0.0285 (11)	0.0316 (11)	−0.0001 (9)	0.0064 (9)	−0.0002 (9)
C12	0.0229 (11)	0.0271 (11)	0.0410 (12)	0.0019 (9)	−0.0029 (9)	−0.0013 (9)
C41	0.0193 (9)	0.0187 (9)	0.0153 (9)	−0.0014 (7)	0.0009 (7)	−0.0003 (7)
C42	0.0332 (11)	0.0183 (9)	0.0176 (9)	0.0004 (8)	−0.0029 (8)	−0.0003 (7)
N1	0.0274 (9)	0.0185 (8)	0.0117 (7)	0.0001 (7)	0.0000 (6)	−0.0010 (6)
N3	0.0230 (8)	0.0188 (8)	0.0130 (7)	0.0003 (6)	−0.0009 (6)	−0.0019 (6)
N4	0.0240 (8)	0.0174 (7)	0.0107 (7)	0.0021 (6)	−0.0006 (6)	0.0014 (6)
O1	0.0358 (8)	0.0201 (7)	0.0208 (7)	0.0013 (6)	0.0010 (6)	0.0016 (6)
O2	0.0277 (7)	0.0211 (7)	0.0149 (6)	0.0000 (6)	−0.0011 (5)	−0.0019 (5)
S1	0.0254 (2)	0.0175 (2)	0.0145 (2)	0.00277 (19)	0.00084 (17)	0.00137 (18)

Geometric parameters (Å, º)

C1′—C2′	1.384 (3)	C6′—C7′	1.505 (3)
C1′—C6′	1.392 (3)	C7—C8	1.540 (3)
C1′—H1′	0.93	C7—H7	0.98
C2′—C3′	1.392 (3)	C7′—H70′	0.96
C2′—H2′	0.93	C7′—H71′	0.96
C2—N3	1.280 (2)	C7′—H72′	0.96
C2—N1	1.387 (2)	C8—H80	0.96
C2—S1	1.7497 (18)	C8—H81	0.96
C3′—C4′	1.397 (3)	C8—H82	0.96
C3′—C7	1.519 (2)	C9—C10	1.327 (3)
C3—O1	1.219 (2)	C9—H9	0.97 (2)
C3—N1	1.373 (2)	C10—C12	1.507 (3)
C3—C4	1.502 (3)	C10—C11	1.508 (3)
C4—H40	0.96	C11—H111	0.96
C4—H41	0.96	C11—H112	0.96
C4—H42	0.96	C11—H113	0.96
C4′—C5′	1.385 (3)	C12—H121	0.96
C4′—H4′	0.93	C12—H122	0.96
C5—N4	1.491 (2)	C12—H123	0.96
C5—C9	1.518 (3)	C41—O2	1.234 (2)
C5—C6	1.541 (2)	C41—N4	1.357 (2)
C5—S1	1.8545 (18)	C41—C42	1.494 (2)
C5′—C6′	1.388 (3)	C42—H420	0.96
C5′—H5′	0.93	C42—H421	0.96
C6—C7	1.536 (3)	C42—H422	0.96
C6—H60	0.97	N1—H2	0.87 (2)
C6—H61	0.97	N3—N4	1.399 (2)
C2′—C1′—C6′	121.60 (18)	C6′—C7′—H70′	109.5
C2′—C1′—H1′	119.2	C6′—C7′—H71′	109.5

C6′—C1′—H1′	119.2	H70′—C7′—H71′	109.5
C1′—C2′—C3′	121.06 (18)	C6′—C7′—H72′	109.5
C1′—C2′—H2′	119.5	H70′—C7′—H72′	109.5
C3′—C2′—H2′	119.5	H71′—C7′—H72′	109.5
N3—C2—N1	119.63 (16)	C7—C8—H80	109.5
N3—C2—S1	119.00 (14)	C7—C8—H81	109.5
N1—C2—S1	121.35 (14)	H80—C8—H81	109.5
C2′—C3′—C4′	117.38 (17)	C7—C8—H82	109.5
C2′—C3′—C7	121.72 (16)	H80—C8—H82	109.5
C4′—C3′—C7	120.80 (16)	H81—C8—H82	109.5
O1—C3—N1	121.87 (17)	C10—C9—C5	129.19 (17)
O1—C3—C4	123.36 (17)	C10—C9—H9	117.4 (12)
N1—C3—C4	114.76 (16)	C5—C9—H9	113.5 (12)
C3—C4—H40	109.5	C9—C10—C12	119.73 (18)
C3—C4—H41	109.5	C9—C10—C11	125.62 (18)
H40—C4—H41	109.5	C12—C10—C11	114.63 (17)
C3—C4—H42	109.5	C10—C11—H111	109.5
H40—C4—H42	109.5	C10—C11—H112	109.5
H41—C4—H42	109.5	H111—C11—H112	109.5
C5′—C4′—C3′	121.18 (18)	C10—C11—H113	109.5
C5′—C4′—H4′	119.4	H111—C11—H113	109.5
C3′—C4′—H4′	119.4	H112—C11—H113	109.5
N4—C5—C9	112.66 (15)	C10—C12—H121	109.5
N4—C5—C6	112.84 (14)	C10—C12—H122	109.5
C9—C5—C6	108.48 (15)	H121—C12—H122	109.5
N4—C5—S1	102.63 (11)	C10—C12—H123	109.5
C9—C5—S1	111.83 (13)	H121—C12—H123	109.5
C6—C5—S1	108.29 (12)	H122—C12—H123	109.5
C4′—C5′—C6′	121.37 (18)	O2—C41—N4	119.83 (16)
C4′—C5′—H5′	119.3	O2—C41—C42	123.49 (16)
C6′—C5′—H5′	119.3	N4—C41—C42	116.67 (15)
C7—C6—C5	118.41 (15)	C41—C42—H420	109.5
C7—C6—H60	107.7	C41—C42—H421	109.5
C5—C6—H60	107.7	H420—C42—H421	109.5
C7—C6—H61	107.7	C41—C42—H422	109.5
C5—C6—H61	107.7	H420—C42—H422	109.5
H60—C6—H61	107.1	H421—C42—H422	109.5
C5′—C6′—C1′	117.35 (18)	C3—N1—C2	124.06 (16)
C5′—C6′—C7′	121.43 (18)	C3—N1—H2	119.1 (16)
C1′—C6′—C7′	121.17 (19)	C2—N1—H2	116.7 (16)
C3′—C7—C6	114.25 (15)	C2—N3—N4	110.24 (14)
C3′—C7—C8	109.29 (15)	C41—N4—N3	119.79 (14)
C6—C7—C8	108.32 (15)	C41—N4—C5	122.03 (14)
C3′—C7—H7	108.3	N3—N4—C5	118.18 (14)
C6—C7—H7	108.3	C2—S1—C5	89.94 (8)
C8—C7—H7	108.3		

C6′—C1′—C2′—C3′	0.9 (3)	O1—C3—N1—C2	−1.0 (3)

C1′—C2′—C3′—C4′	−2.1 (3)	C4—C3—N1—C2	177.88 (17)
C1′—C2′—C3′—C7	−178.47 (17)	N3—C2—N1—C3	−172.52 (18)
C2′—C3′—C4′—C5′	1.0 (3)	S1—C2—N1—C3	9.3 (3)
C7—C3′—C4′—C5′	177.45 (17)	N1—C2—N3—N4	−177.12 (15)
C3′—C4′—C5′—C6′	1.3 (3)	S1—C2—N3—N4	1.1 (2)
N4—C5—C6—C7	53.5 (2)	O2—C41—N4—N3	−178.76 (15)
C9—C5—C6—C7	179.04 (15)	C42—C41—N4—N3	2.1 (2)
S1—C5—C6—C7	−59.41 (18)	O2—C41—N4—C5	1.1 (3)
C4′—C5′—C6′—C1′	−2.5 (3)	C42—C41—N4—C5	−178.05 (16)
C4′—C5′—C6′—C7′	175.03 (18)	C2—N3—N4—C41	179.12 (16)
C2′—C1′—C6′—C5′	1.4 (3)	C2—N3—N4—C5	−0.7 (2)
C2′—C1′—C6′—C7′	−176.10 (19)	C9—C5—N4—C41	−59.4 (2)
C2′—C3′—C7—C6	−57.9 (2)	C6—C5—N4—C41	63.9 (2)
C4′—C3′—C7—C6	125.84 (18)	S1—C5—N4—C41	−179.78 (14)
C2′—C3′—C7—C8	63.6 (2)	C9—C5—N4—N3	120.51 (17)
C4′—C3′—C7—C8	−112.64 (19)	C6—C5—N4—N3	−116.23 (16)
C5—C6—C7—C3′	−73.3 (2)	S1—C5—N4—N3	0.08 (18)
C5—C6—C7—C8	164.63 (15)	N3—C2—S1—C5	−0.96 (16)
N4—C5—C9—C10	−55.8 (3)	N1—C2—S1—C5	177.27 (16)
C6—C5—C9—C10	178.55 (19)	N4—C5—S1—C2	0.41 (12)
S1—C5—C9—C10	59.2 (2)	C9—C5—S1—C2	−120.59 (14)
C5—C9—C10—C12	−179.85 (17)	C6—C5—S1—C2	119.95 (13)
C5—C9—C10—C11	1.5 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H2···O2^{i}	0.87 (2)	1.96 (2)	2.811 (2)	167 (2)

Symmetry code: (i) x, $-y+1/2$, $z-1/2$.