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Ethyl 4-(1,3-benzodioxol-5-yl)-6-methyl-2-sulfanylidene-1,2,3,4-tetrahydropyrimidine-5-carboxylate

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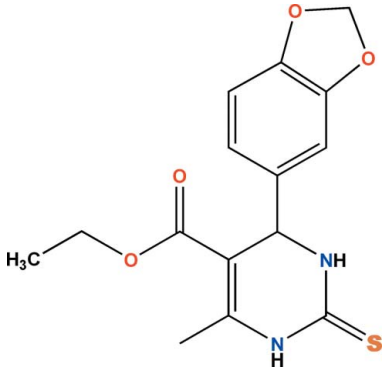
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.003 Å; R factor = 0.038; wR factor = 0.103; data-to-parameter ratio = 11.0.

In the title compound, $C_{15}H_{16}N_2O_4S$, the dihedral angles between the planes of the benzodioxole and ester groups and the plane of the six-membered tetrahydropyrimidine ring are 89.5 (1) and 20.2 (1)°, respectively. Intermolecular N—H···S hydrogen bonds assemble the molecules into dimers, which are further connected *via* N—H···O interactions into chains parallel to [010]. Weak C—H···S and C—H···π interactions enhance the stability of the crystal structure.

Related literature

For background to the applications of multi-functionalized dihydropyrimidines, see: Jauk *et al.* (2000); Kappe (2000); Mayer *et al.* (1999). For similar structures, see: Nayak *et al.* (2009, 2010, 2011).



Experimental

Crystal data

$C_{15}H_{16}N_2O_4S$
M_r = 320.37
Monoclinic, $P2_1/c$
a = 12.5102 (9) Å
b = 7.2054 (4) Å
c = 17.0881 (12) Å
β = 107.178 (8)°
V = 1471.62 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 120 K
0.28 × 0.22 × 0.19 mm

Data collection

Oxford Diffraction Xcalibur E diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min} = 0.936, T_{max} = 0.956
18163 measured reflections
2883 independent reflections
2349 reflections with $I > 2\sigma(I)$
R_{int} = 0.067

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.103
S = 1.09
2883 reflections
263 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the O3/C11/C12/O5/C15 and C9–C14 rings respectively.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1^{i}	0.84 (2)	2.14 (2)	2.9578 (19)	167 (2)
N2—H2N···S1^{ii}	0.76 (2)	2.57 (2)	3.3069 (17)	164 (2)
C10—H10···S1^{iii}	0.95 (2)	2.75 (2)	3.678 (2)	166.9 (18)
C15—H15*B*···*Cg*1^{iv}	0.98 (3)	2.95 (3)	3.890 (2)	160 (2)
C6—H6*A*···*Cg*2^{v}	0.98 (2)	2.87 (2)	3.691 (2)	142 (2)

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2009) and *PARST* (Nardelli, 1995).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2420).

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supporting information

Acta Cryst. (2011). E**67**, o3069–o3070 [doi:10.1107/S1600536811043649]

Ethyl 4-(1,3-benzodioxol-5-yl)-6-methyl-2-sulfanylidene-1,2,3,4-tetrahydropyrimidine-5-carboxylate

Susanta K. Nayak, K. N. Venugopala, Thavendran Govender, Hendrik G. Kruger, Glenn E. M. Maguire and Tayur N. Guru Row

S1. Comment

Biginelli compounds are multifunctionalized dihydropyrimidones (DHPM) (Kappe, 2000 and references therein), which have emerged as important target molecule for therapeutic and pharmacological properties such as anticarcinogenic (Kappe, 2000; Mayer *et al.*, 1999) and calcium channel modulators (Jauk *et al.*, 2000 and references therein). In view of the immense range of applications, we became interested in the DHPMS system (Nayak *et al.*,2009; 2010; 2011). Here we report a single-crystal structure of the title compound.

The preferred conformation of the molecule is that with the dihedral angles between the planes of benzodioxolyl and ester groups (O1/C5/O2/C6/C7) with the plane of the six-membered tetrahydropyrimidine ring of 89.5 (1) ° and 20.2 (1) °, respectively. The centrosymmetric N—H···S dimers of the title molecules are additionally organized into chains along the *b* axis via N—H···O hydrogen bonds. These chains are also stabilized by weak C—H···S interactions (Fig. 2). Additonal weak C—H···π interactions enhance the crystal stability.

S2. Experimental

A mixture of ethyl acetoacetate (0.1 mol), 3,4-(methylenedioxy)benzaldehyde (0.1 mol) and thiourea (0.1 mol) was refluxed in 50 ml of ethanol for 2 h in the presence of concentrated hydrochloric acid as a catalyst. The reaction was monitored with thin layer chromatography and the reaction medium was quenched in ice cold water. The precipitate obtained was filtered, dried and crystallized from methanol at room temperature to obtain the title compound.

S3. Refinement

All H atoms were located from difference Fourier map and refined freely.

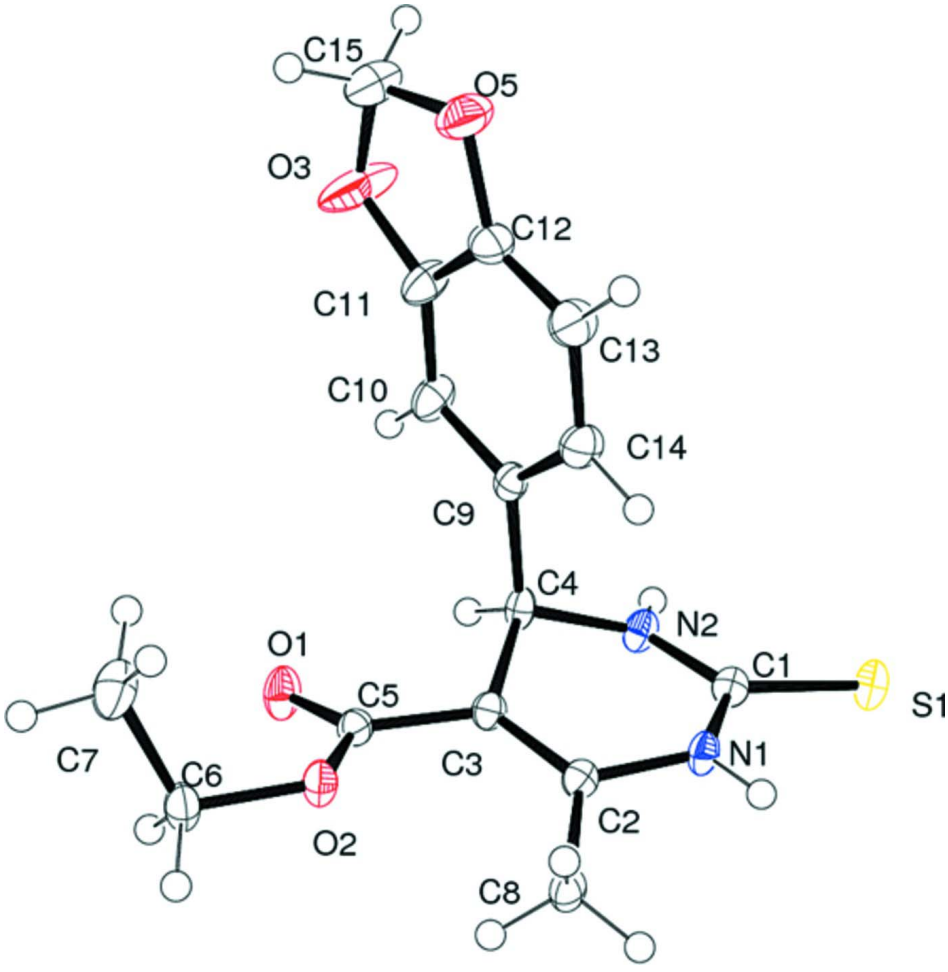

Figure 1

Molecular structure of the title compound with displacement ellipsoids for non-H atoms at the 50% probability level.

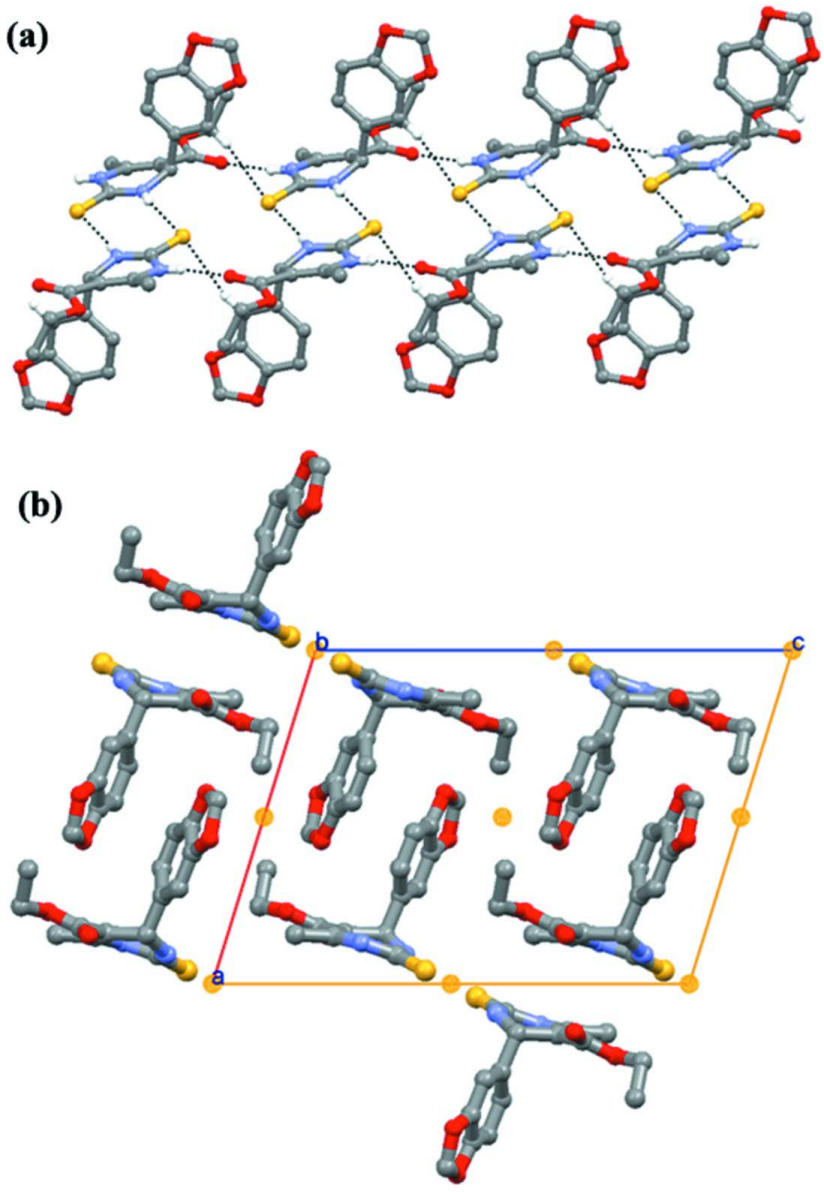

Figure 2

(*a*) The crystal packing diagram showing hydrogen-bonded chains formed by hydrogen-bonded dimers. (*b*) View of the crystal packing along the *b* axis (yellow circle represents centre of inversion).

Ethyl 4-(1,3-benzodioxol-5-yl)-6-methyl-2-sulfanylidene-1,2,3,4- tetrahydropyrimidine-5-carboxylate

Crystal data

$C_{15}H_{16}N_2O_4S$
$M_r = 320.37$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.5102\ (9)$ Å
$b = 7.2054\ (4)$ Å
$c = 17.0881\ (12)$ Å
$\beta = 107.178\ (8)°$
$V = 1471.62\ (17)$ Å^3
$Z = 4$
$F(000) = 672$
$D_x = 1.446$ Mg m^{-3}
Melting point: 447(2) K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 430 reflections
$\theta = 1.0–27.9°$

μ = 0.24 mm^{-1}
T = 120 K

Block, colorless
0.28 × 0.22 × 0.19 mm

Data collection

Oxford Diffraction Xcalibur E diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.0839 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min} = 0.936, T_{max} = 0.956

18163 measured reflections
2883 independent reflections
2349 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 26.0°, θ_{min} = 2.5°
h = −15→15
k = −8→8
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.103
S = 1.09
2883 reflections
263 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
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.044P)^2 + 0.4413P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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}
S1	0.03990 (4)	0.22578 (6)	0.06240 (3)	0.02136 (16)
O2	0.21637 (11)	0.77438 (16)	0.39149 (7)	0.0190 (3)
C4	0.14810 (16)	0.7167 (2)	0.17046 (11)	0.0167 (4)
O1	0.14472 (12)	0.97853 (17)	0.29048 (8)	0.0246 (3)
C9	0.26335 (16)	0.7523 (2)	0.16168 (10)	0.0164 (4)
N1	0.12326 (13)	0.3507 (2)	0.21437 (9)	0.0178 (4)
N2	0.08802 (14)	0.5707 (2)	0.11385 (10)	0.0179 (4)
C2	0.14299 (15)	0.4837 (2)	0.27642 (11)	0.0161 (4)
C5	0.16897 (15)	0.8200 (2)	0.31311 (11)	0.0164 (4)
C3	0.15224 (15)	0.6627 (2)	0.25676 (10)	0.0157 (4)
C8	0.14782 (18)	0.4050 (3)	0.35838 (12)	0.0194 (4)
C1	0.08656 (15)	0.3933 (2)	0.13312 (11)	0.0173 (4)
C6	0.23338 (18)	0.9229 (3)	0.45154 (12)	0.0214 (4)

C12	0.47322 (16)	0.8166 (3)	0.14736 (12)	0.0242 (4)
C10	0.28717 (17)	0.9248 (3)	0.13323 (12)	0.0240 (4)
O5	0.57092 (12)	0.8812 (2)	0.13570 (10)	0.0348 (4)
C14	0.34567 (17)	0.6153 (3)	0.18099 (12)	0.0236 (4)
C13	0.45264 (18)	0.6459 (3)	0.17449 (13)	0.0268 (5)
O3	0.43410 (14)	1.1070 (2)	0.09967 (13)	0.0551 (6)
C11	0.39210 (18)	0.9510 (3)	0.12682 (13)	0.0267 (5)
C7	0.3423 (2)	1.0191 (3)	0.46053 (15)	0.0316 (5)
C15	0.54868 (19)	1.0701 (3)	0.10926 (16)	0.0341 (5)
H8A	0.1201 (17)	0.491 (3)	0.3892 (13)	0.022 (5)*
H6B	0.1710 (17)	1.006 (3)	0.4352 (12)	0.017 (5)*
H10	0.2310 (19)	1.017 (3)	0.1214 (13)	0.030 (6)*
H8B	0.1075 (18)	0.292 (3)	0.3532 (12)	0.022 (5)*
H13	0.5136 (19)	0.551 (3)	0.1892 (13)	0.030 (6)*
H2N	0.0633 (19)	0.599 (3)	0.0693 (14)	0.023 (6)*
H1N	0.122 (2)	0.240 (3)	0.2286 (14)	0.031 (7)*
H4	0.1015 (16)	0.829 (3)	0.1527 (11)	0.015 (5)*
H6A	0.2297 (16)	0.861 (3)	0.5017 (12)	0.016 (5)*
H14	0.326 (2)	0.496 (3)	0.2002 (14)	0.042 (7)*
H7A	0.408 (2)	0.932 (4)	0.4772 (16)	0.050 (7)*
H7B	0.3470 (19)	1.077 (3)	0.4079 (14)	0.033 (6)*
H8C	0.222 (2)	0.379 (3)	0.3889 (15)	0.038 (7)*
H15A	0.593 (2)	1.155 (4)	0.1543 (16)	0.048 (7)*
H7C	0.349 (2)	1.111 (4)	0.5042 (16)	0.051 (8)*
H15B	0.556 (2)	1.086 (4)	0.0541 (17)	0.053 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0238 (3)	0.0142 (3)	0.0213 (3)	0.00006 (18)	−0.0006 (2)	−0.00166 (17)
O2	0.0258 (8)	0.0137 (7)	0.0154 (6)	−0.0003 (5)	0.0032 (6)	−0.0012 (5)
C4	0.0206 (10)	0.0107 (9)	0.0162 (9)	0.0004 (7)	0.0014 (7)	−0.0004 (7)
O1	0.0350 (8)	0.0129 (7)	0.0225 (7)	0.0038 (6)	0.0033 (6)	0.0012 (5)
C9	0.0188 (10)	0.0162 (9)	0.0129 (8)	−0.0021 (7)	0.0023 (7)	−0.0014 (7)
N1	0.0230 (9)	0.0095 (8)	0.0194 (8)	0.0010 (6)	0.0040 (7)	0.0005 (6)
N2	0.0211 (9)	0.0136 (8)	0.0157 (9)	−0.0001 (6)	0.0004 (7)	0.0027 (6)
C2	0.0143 (9)	0.0145 (9)	0.0188 (9)	0.0018 (7)	0.0037 (7)	0.0009 (7)
C5	0.0159 (9)	0.0144 (9)	0.0194 (9)	0.0008 (7)	0.0060 (7)	−0.0001 (7)
C3	0.0159 (9)	0.0139 (9)	0.0162 (9)	0.0008 (7)	0.0033 (7)	0.0003 (7)
C8	0.0258 (12)	0.0126 (10)	0.0199 (10)	0.0005 (8)	0.0067 (9)	0.0011 (7)
C1	0.0127 (9)	0.0169 (10)	0.0205 (9)	0.0017 (7)	0.0020 (7)	−0.0002 (7)
C6	0.0301 (12)	0.0165 (10)	0.0164 (9)	−0.0008 (8)	0.0050 (8)	−0.0028 (7)
C12	0.0177 (10)	0.0290 (11)	0.0262 (10)	−0.0032 (8)	0.0070 (8)	−0.0042 (8)
C10	0.0209 (11)	0.0165 (10)	0.0321 (11)	0.0008 (8)	0.0040 (9)	0.0037 (8)
O5	0.0236 (8)	0.0302 (9)	0.0538 (10)	−0.0040 (6)	0.0162 (7)	0.0021 (7)
C14	0.0266 (11)	0.0175 (10)	0.0283 (10)	0.0020 (8)	0.0102 (9)	0.0049 (8)
C13	0.0232 (11)	0.0219 (11)	0.0360 (11)	0.0047 (8)	0.0099 (9)	0.0034 (9)
O3	0.0303 (10)	0.0329 (10)	0.1070 (16)	−0.0001 (7)	0.0281 (10)	0.0314 (10)

C11	0.0264 (11)	0.0187 (10)	0.0345 (11)	−0.0037 (8)	0.0083 (9)	0.0061 (8)
C7	0.0301 (13)	0.0261 (12)	0.0348 (13)	−0.0056 (10)	0.0036 (10)	−0.0075 (10)
C15	0.0274 (13)	0.0331 (13)	0.0427 (14)	−0.0071 (9)	0.0117 (11)	0.0052 (10)

Geometric parameters (Å, º)

S1—C1	1.6854 (18)	C8—H8C	0.94 (3)
O2—C5	1.336 (2)	C6—C7	1.496 (3)
O2—C6	1.454 (2)	C6—H6B	0.96 (2)
C4—N2	1.476 (2)	C6—H6A	0.98 (2)
C4—C3	1.511 (2)	C12—C13	1.365 (3)
C4—C9	1.515 (3)	C12—C11	1.372 (3)
C4—H4	0.99 (2)	C12—O5	1.376 (2)
O1—C5	1.215 (2)	C10—C11	1.362 (3)
C9—C14	1.394 (3)	C10—H10	0.94 (2)
C9—C10	1.398 (3)	O5—C15	1.435 (3)
N1—C1	1.362 (2)	C14—C13	1.393 (3)
N1—C2	1.396 (2)	C14—H14	0.97 (2)
N1—H1N	0.84 (2)	C13—H13	1.00 (2)
N2—C1	1.322 (2)	O3—C11	1.378 (2)
N2—H2N	0.76 (2)	O3—C15	1.419 (3)
C2—C3	1.346 (2)	C7—H7A	1.01 (3)
C2—C8	1.495 (3)	C7—H7B	1.01 (2)
C5—C3	1.462 (2)	C7—H7C	0.98 (3)
C8—H8A	0.94 (2)	C15—H15A	1.01 (3)
C8—H8B	0.95 (2)	C15—H15B	0.98 (3)
C5—O2—C6	117.10 (14)	O2—C6—H6B	108.5 (12)
N2—C4—C3	108.68 (15)	C7—C6—H6B	112.3 (12)
N2—C4—C9	111.78 (15)	O2—C6—H6A	104.3 (11)
C3—C4—C9	112.39 (15)	C7—C6—H6A	113.5 (11)
N2—C4—H4	104.0 (11)	H6B—C6—H6A	107.2 (17)
C3—C4—H4	110.9 (11)	C13—C12—C11	121.57 (19)
C9—C4—H4	108.7 (11)	C13—C12—O5	128.22 (19)
C14—C9—C10	119.55 (18)	C11—C12—O5	110.21 (18)
C14—C9—C4	120.99 (17)	C11—C10—C9	117.43 (18)
C10—C9—C4	119.46 (16)	C11—C10—H10	124.0 (14)
C1—N1—C2	123.39 (16)	C9—C10—H10	118.6 (14)
C1—N1—H1N	118.8 (16)	C12—O5—C15	105.58 (16)
C2—N1—H1N	116.7 (16)	C13—C14—C9	121.93 (19)
C1—N2—C4	124.61 (16)	C13—C14—H14	120.6 (15)
C1—N2—H2N	118.7 (17)	C9—C14—H14	117.4 (15)
C4—N2—H2N	116.1 (17)	C12—C13—C14	116.87 (18)
C3—C2—N1	118.48 (16)	C12—C13—H13	119.6 (13)
C3—C2—C8	127.90 (17)	C14—C13—H13	123.6 (13)
N1—C2—C8	113.59 (15)	C11—O3—C15	106.32 (17)
O1—C5—O2	123.07 (16)	C10—C11—C12	122.62 (19)
O1—C5—C3	123.06 (16)	C10—C11—O3	127.79 (19)

O2—C5—C3	113.85 (15)	C12—C11—O3	109.59 (18)
C2—C3—C5	125.78 (16)	C6—C7—H7A	112.5 (15)
C2—C3—C4	120.63 (16)	C6—C7—H7B	113.0 (13)
C5—C3—C4	113.58 (15)	H7A—C7—H7B	105 (2)
C2—C8—H8A	110.8 (12)	C6—C7—H7C	104.9 (15)
C2—C8—H8B	111.5 (12)	H7A—C7—H7C	109 (2)
H8A—C8—H8B	110.1 (18)	H7B—C7—H7C	112.7 (19)
C2—C8—H8C	110.8 (15)	O3—C15—O5	108.02 (17)
H8A—C8—H8C	106.6 (19)	O3—C15—H15A	106.3 (15)
H8B—C8—H8C	106.9 (19)	O5—C15—H15A	108.9 (15)
N2—C1—N1	116.51 (16)	O3—C15—H15B	104.3 (16)
N2—C1—S1	122.78 (14)	O5—C15—H15B	110.3 (16)
N1—C1—S1	120.71 (14)	H15A—C15—H15B	118 (2)
O2—C6—C7	110.65 (17)		

N2—C4—C9—C14	−64.5 (2)	C4—N2—C1—S1	−167.04 (14)
C3—C4—C9—C14	58.0 (2)	C2—N1—C1—N2	11.3 (3)
N2—C4—C9—C10	115.08 (18)	C2—N1—C1—S1	−167.60 (15)
C3—C4—C9—C10	−122.40 (18)	C5—O2—C6—C7	−86.5 (2)
C3—C4—N2—C1	−30.0 (2)	C14—C9—C10—C11	−0.9 (3)
C9—C4—N2—C1	94.6 (2)	C4—C9—C10—C11	179.58 (18)
C1—N1—C2—C3	−16.3 (3)	C13—C12—O5—C15	−178.2 (2)
C1—N1—C2—C8	162.00 (17)	C11—C12—O5—C15	2.3 (2)
C6—O2—C5—O1	3.2 (3)	C10—C9—C14—C13	1.4 (3)
C6—O2—C5—C3	−178.61 (16)	C4—C9—C14—C13	−179.05 (18)
N1—C2—C3—C5	177.79 (17)	C11—C12—C13—C14	−0.5 (3)
C8—C2—C3—C5	−0.2 (3)	O5—C12—C13—C14	179.97 (19)
N1—C2—C3—C4	−3.5 (3)	C9—C14—C13—C12	−0.7 (3)
C8—C2—C3—C4	178.49 (18)	C9—C10—C11—C12	−0.3 (3)
O1—C5—C3—C2	−157.7 (2)	C9—C10—C11—O3	179.2 (2)
O2—C5—C3—C2	24.2 (3)	C13—C12—C11—C10	1.0 (3)
O1—C5—C3—C4	23.5 (3)	O5—C12—C11—C10	−179.37 (19)
O2—C5—C3—C4	−154.60 (16)	C13—C12—C11—O3	−178.55 (19)
N2—C4—C3—C2	23.6 (2)	O5—C12—C11—O3	1.0 (2)
C9—C4—C3—C2	−100.7 (2)	C15—O3—C11—C10	176.5 (2)
N2—C4—C3—C5	−157.57 (15)	C15—O3—C11—C12	−4.0 (3)
C9—C4—C3—C5	78.17 (19)	C11—O3—C15—O5	5.3 (3)
C4—N2—C1—N1	14.1 (3)	C12—O5—C15—O3	−4.7 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O1^{i}	0.84 (2)	2.14 (2)	2.9578 (19)	167 (2)
N2—H2*N*···S1^{ii}	0.76 (2)	2.57 (2)	3.3069 (17)	164 (2)
C10—H10···S1^{iii}	0.95 (2)	2.75 (2)	3.678 (2)	166.9 (18)

C15—H15*B*···*Cg*1^{iv}	0.98 (3)	2.95 (3)	3.890 (2)	160 (2)
C6—H6*A*···*Cg*2^{v}	0.98 (2)	2.87 (2)	3.691 (2)	142 (2)

Symmetry codes: (i) $x, y-1, z$; (ii) $-x, -y+1, -z$; (iii) $x, y+1, z$; (iv) $-x+1, -y+2, -z$; (v) $x, -y+3/2, z+1/2$.