Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl 2-{(2*Z*)-2-[(1-naphthylsulfonyl)-imino]-2,3-dihydro-1,3-thiazol-4-yl}-acetate monohydrate

Gabriel Navarrete-Vázquez,[a] Guadalupe Morales-Vilchis,[a] Samuel Estrada-Soto,[a] Verónica Rodríguez-López[a] and Hugo Tlahuext[b]*

[a]Facultad de Farmacia, Universidad Autónoma del Estado de Morelos, Av. Universidad 1001 Col Chamilpa CP 62209, Cuernavaca Mor., México, and [b]Centro de Investigaciones Químicas, Universidad Autónoma del Estado de Morelos. Av. Universidad 1001 Col., Chamilpa, CP 62209, Cuernavaca Mor., México
Correspondence e-mail: tlahuext@ciq.uaem.mx

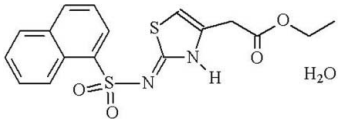
Received 29 September 2010; accepted 30 September 2010

Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.004 Å; R factor = 0.048; wR factor = 0.143; data-to-parameter ratio = 13.8.

The title compound, $C_{17}H_{16}N_2O_4S_2\cdot H_2O$, is of interest with respect to its antidiabetic and anti-obesity activity. In the crystal, the packing is stabilized by three cooperative interactions: offset π–π interactions [centroid–centroid distance = 3.604 (2) Å], as well as C—H···O and O—H···O hydrogen bonds. N—H···O interactions also occur.

Related literature

For similar structures and their antidiabetic activity, see: Navarrete-Vázquez *et al.* (2008); Alberts *et al.* (2002); Barf *et al.* (2002); Fotsch & Wang (2008); Saiah (2008); Vicker *et al.* (2007). For hydrogen bonds, see: Adams *et al.* (1996); Desiraju & Steiner (1999); Hanton *et al.* (1992).



Experimental

Crystal data

$C_{17}H_{16}N_2O_4S_2\cdot H_2O$
M_r = 394.45
Orthorhombic, *Pbcn*
a = 29.582 (6) Å
b = 7.9657 (17) Å
c = 15.676 (3) Å
V = 3694.0 (14) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 273 K
0.29 × 0.21 × 0.17 mm

Data collection

Bruker SMART APEX CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.913, T_{max} = 0.948
33131 measured reflections
3255 independent reflections
2488 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.143
S = 1.09
3255 reflections
236 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O5^{i}	0.86	1.91	2.767 (3)	177
O5—H5A···O2^{ii}	0.84	2.10	2.889 (3)	157
C13—H13···O2^{iii}	0.93	2.57	3.295 (4)	135
C14—H14A···O1^{iv}	0.97	2.34	3.295 (3)	167
C17—H17B···O2^{i}	0.96	2.57	3.466 (5)	155

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus-NT* (Bruker, 2001); data reduction: *SAINT-Plus-NT*; program(s) used to solve structure: *SHELXTL-NT* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL-NT*; molecular graphics: *SHELXTL-NT*; software used to prepare material for publication: *PLATON* (Spek, 2009), *DIAMOND* (Bergerhoff *et al.*, 1996) and *publCIF* (Westrip, 2010).

This work was supported by the Consejo Nacional de Ciencia y Tecnología (CONACyT) under grant No. 100608.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2215).

References

Adams, H., Carver, F. J., Hunter, C. A., Morales, J. C. & Seward, E. M. (1996). *Angew. Chem. Int. Ed. Engl.* **35**, 1542–1544.
Alberts, P., Engblom, L., Edling, N., Forsgren, M., Klingström, G., Larsson, C., Rönquist-Nii, Y., Öhman, B. & Abrahmsén, L. (2002). *Diabetologia*, **45**, 1528–1532.
Barf, T., Vallgarda, J., Emond, R., Haggström, C., Kurz, G., Nygren, A., Larwood, V., Mosialou, E., Axelsson, K., Olsson, R., Englom, L., Edling, N., Rönquist-Nii, Y., Öhman, B., Alberts, P. & Abrahmsén, L. (2002). *J. Med. Chem.* **45**, 3813–3815.
Bergerhoff, G., Berndt, M. & Brandenburg, K. (1996). *J. Res. Natl Inst. Stand. Technol.* **101**, 221–225.
Bruker (2000). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SAINT-Plus-NT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Desiraju, G. & Steiner, T. (1999). *The Weak Hydrogen Bond in Structural Chemistry and Biology*, pp. 5–6. New York: Oxford University Press.
Fotsch, C. & Wang, M. (2008). *J. Med. Chem.* **51**, 4851–4857.
Hanton, L. R., Hunter, C. A. & Purvis, D. H. (1992). *J. Chem. Soc. Chem. Commun.* pp. 1134–1136.
Navarrete-Vázquez, G., Moreno-Diaz, H., Villalobos-Molina, R., Estrada-Soto, S. & Tlahuext, H. (2008). *Acta Cryst.* E**64**, o227.
Saiah, E. (2008). *Curr. Med. Chem.* **15**, 642–649.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Vicker, N., Su, X., Ganeshapillai, D., Smith, A., Purohit, A., Reed, M. & Potter, B. V. L. (2007). *J. Steroid Biochem. Mol. Biol.* **104**, 123–129.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2010). E**66**, o2744 [https://doi.org/10.1107/S1600536810039279]

Ethyl 2-{(2*Z*)-2-[(1-naphthylsulfonyl)imino]-2,3-dihydro-1,3-thiazol-4-yl}acetate monohydrate

Gabriel Navarrete-Vázquez, Guadalupe Morales-Vilchis, Samuel Estrada-Soto, Verónica Rodríguez-López and Hugo Tlahuext

S1. Comment

The biochemistry and pharmacology of sulfur containing compounds are a subject of intense current interest, especially from the point of view of public health. Obesity and diabetes are major causes of morbidity and mortality in many countries (Saiah, 2008). Excessive levels of glucocorticoids into the body can cause both metabolic complications. The regulation of glucocorticoid production involves two 11*b*-hydroxysteroid dehydrogenase (11*b*-HSD) isozymes, that interconvert cortisone and cortisol. 11*b*-HSD1 is a reductase that amplifies glucocorticoid action in a tissue-specific manner (Fotsch *et al.*, 2008).

Recent studies suggest that inhibition of 11*b*-HSD1 increases hepatic insulin sensivity along with decreased glucose production (Alberts *et al.* 2002). Selective inhibitors of 11*b*-HSD1 have considerable potential as treatments of type 2 diabetes and obesity (Vicker *et al.*, 2007). BVT 14225 is a new selective 11*b*-HSD1 inhibitor, it belongs to a class of aryl-sulfonamidothiazoles with *in vitro* and *in vivo* antidiabetic effects (Barf *et al.*, 2002).

In order to assist our knowledge about the electronic and steric requirements in arylsulfonamidothiazoles that show antidiabetic and antiobesity activities (Navarrete-Vázquez *et al.*, 2008), we have synthesized and determined the crystal structure of the title compound (**I**), which is a precursor in the synthesis of an amide BVT14225 bioisoster.

In the crystal structure of (**I**), the molecules are linked by intermolecular C—H···O hydrogen bonds to give an overall two-dimensional hydrogen-bonded network paralell to plane *bc* (Fig. 2, Table 1) (Desiraju & Steiner, 1999). The crystal structure is further stabilized by C—H···O and O—H···O hydogen bonds with cocrystallized water molecules, thus generating the dimeric hydrogen-bonding motif outlined in Fig. 3 (Table 1). In addition, adjacent naphthyl groups show offset $\pi\cdots\pi$ interactions (Fig. 3), with a distance between the centroids C1—C5–10, C5—C10 (*Cg*1, *Cg*2) of the naphtyl rings of 3.604 (2) Å (Hanton *et al.*, 1992; Adams *et al.*, 1996).

S2. Experimental

Naphthalene-1-sulfonylchloride (1.2 g, 0.0053 mol), was suspended in dry methylene chloride (10 ml) under nitrogen atmosphere. Triethylamine (0.9 ml, 0.0064 mol) was added slowly and stirred with a catalytic amount of 4-*N*,*N*-dimethyl-aminopyridine (0.1 eq). After 30 minutes, ethyl (2-amino-1,3-thiazol-4-yl)acetate (1 g, 0.0053 mol) was added dropwise, resulting in a brown solution. When all started material had been consumed, the solvent was removed *in vacuo*, the residue was neutralized with sodium bicarbonate. The precipitate resulting was filtered off to give a brown solid (m.p. 371 K). Single crystals of (**I**) were obtained from ethanol.

S3. Refinement

H atoms were positioned geometrically and constrained using the riding-model approximation [C-$H_{thiazolyl\ and\ naphtyl}$ = 0.93 Å, $U_{iso}(H_{thiazolyl\ and\ naphtyl})$= 1.2 U_{eq}(C)]; [C-$H_{methylene}$ = 0.97 Å, $U_{iso}(H_{methylene})$= 1.2 U_{eq}(C)], [C-H_{methyl} = 0.96 Å, $U_{iso}(H_{methyl})$= 1.5 U_{eq}(C)]. The hydrogen atoms bonded to O5 and N2 were located by difference Fourier maps. Its coordinates were refined with a distance restraint: O—H = 0.84 Å and [U_{iso}(H) = 1.5 U_{eq}(O)], N—H = 0.86 Å and [U_{iso}(H) = 1.2 U_{eq}(N)].

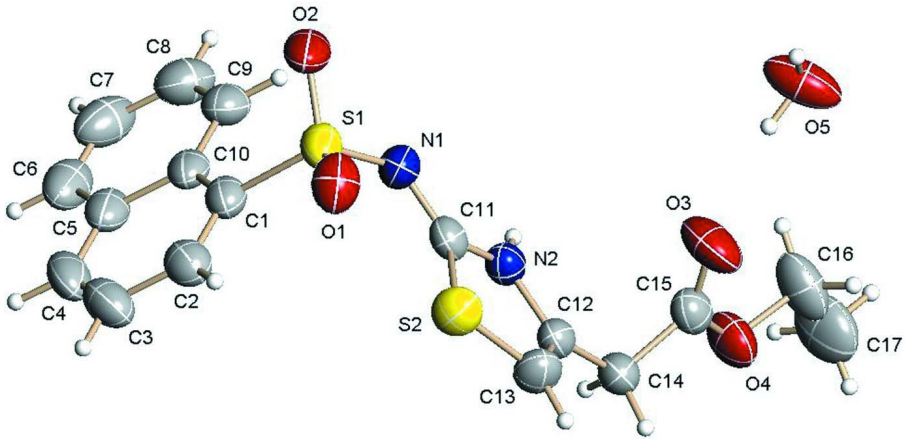


Figure 1

The molecular structure of (**I**) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radius.

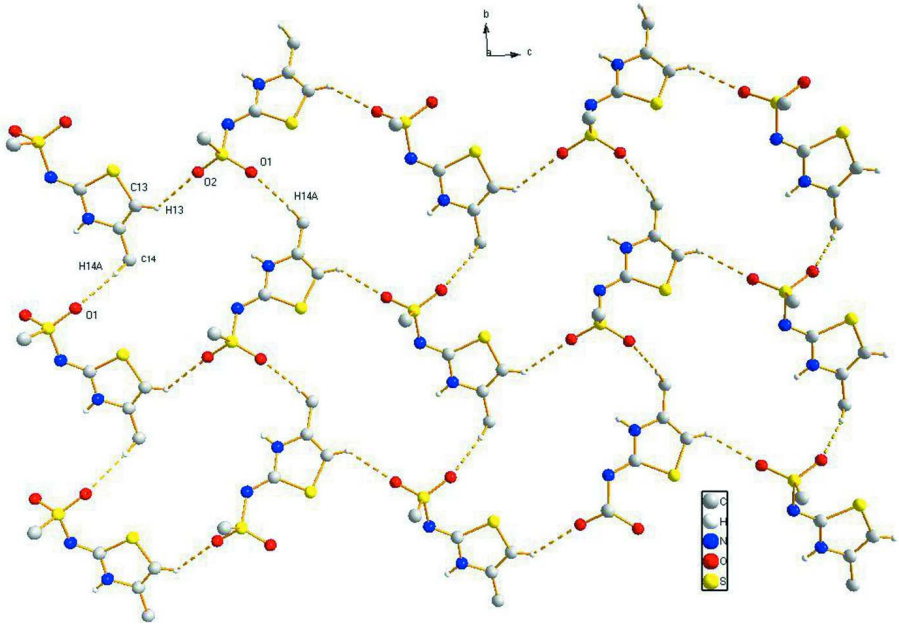


Figure 2

View of the C—H···O hydrogen bonds (dashed lines) in (**I**) to give an overall two-dimensional hydrogen-bonded network paralell to plane *bc*. H atoms not involved in hydrogen-bonding, as well as napthyl and ethoxy carbonylmethyl groups have been omitted for clarity.

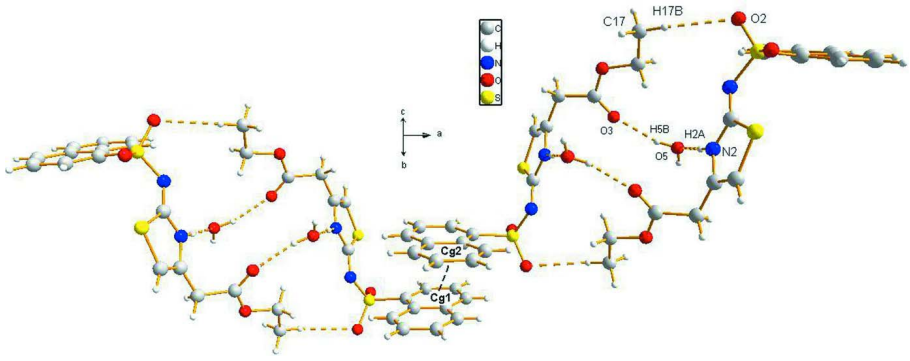


Figure 3

View of the dimeric hydrogen-bonding motif generated by C—H···O and O—H···O hydogen bonds (dashed lines) with cocrystallized water molecules. Also, the offset $\pi\cdots\pi$ [*Cg*1, *Cg*2^{i}; symmetry code: (i) 1/2 - *x*, 1/2 + *y*, *z*] interaction is illustrated (dashed line).

Ethyl 2-{(2*Z*)-2-[(1-naphthylsulfonyl)imino]-2,3-dihydro- 1,3-thiazol-4-yl}acetate monohydrate

Crystal data

$C_{17}H_{16}N_2O_4S_2{\cdot}H_2O$
M_r = 394.45
Orthorhombic, *Pbcn*
Hall symbol: -P 2n 2ab
a = 29.582 (6) Å
b = 7.9657 (17) Å
c = 15.676 (3) Å
V = 3694.0 (14) Å^3
Z = 8
F(000) = 1648
D_x = 1.419 Mg m^{-3}
Melting point: 371 K
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 7399 reflections
θ = 2.6–23.6°
μ = 0.32 mm^{-1}
T = 273 K
Rectangular prism, colourless
0.29 × 0.21 × 0.17 mm

Data collection

Bruker SMART APEX CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3 pixels mm^{-1}
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.913, T_{max} = 0.948
33131 measured reflections
3255 independent reflections
2488 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 25.0°, θ_{min} = 1.4°
h = −35→35
k = −9→9
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.143
S = 1.09
3255 reflections
236 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0753P)^2 + 1.2945P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 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}
C1	0.30111 (9)	1.0099 (3)	−0.01807 (17)	0.0476 (7)
C2	0.27124 (10)	1.0650 (4)	0.0426 (2)	0.0579 (8)
H2	0.2818	1.1180	0.0915	0.069*
C3	0.22466 (11)	1.0411 (4)	0.0306 (3)	0.0694 (9)
H3	0.2044	1.0776	0.0719	0.083*
C4	0.20921 (10)	0.9652 (4)	−0.0408 (2)	0.0679 (9)
H4	0.1782	0.9534	−0.0487	0.081*
C5	0.23901 (10)	0.9033 (4)	−0.1037 (2)	0.0562 (8)
C6	0.22292 (12)	0.8195 (5)	−0.1765 (2)	0.0724 (10)
H6	0.1919	0.8057	−0.1838	0.087*
C7	0.25155 (14)	0.7585 (5)	−0.2363 (2)	0.0794 (11)
H7	0.2402	0.7041	−0.2842	0.095*
C8	0.29822 (13)	0.7776 (5)	−0.2257 (2)	0.0733 (9)
H8	0.3178	0.7355	−0.2669	0.088*
C9	0.31544 (11)	0.8571 (4)	−0.15595 (18)	0.0573 (7)
H9	0.3466	0.8675	−0.1499	0.069*
C10	0.28653 (9)	0.9240 (3)	−0.09264 (18)	0.0484 (7)
C11	0.38848 (8)	0.8134 (3)	0.08417 (17)	0.0433 (6)
C12	0.40857 (8)	0.5962 (3)	0.17449 (16)	0.0436 (6)
C13	0.39714 (10)	0.7109 (4)	0.23161 (18)	0.0557 (7)
H13	0.3984	0.6930	0.2902	0.067*
C14	0.42320 (9)	0.4204 (3)	0.18915 (18)	0.0496 (7)
H14A	0.4013	0.3457	0.1630	0.060*
H14B	0.4230	0.3986	0.2500	0.060*
C15	0.46919 (9)	0.3790 (4)	0.15489 (18)	0.0508 (7)
C16	0.51735 (11)	0.1490 (5)	0.1211 (3)	0.0821 (11)
H16A	0.5425	0.1802	0.1575	0.099*
H16B	0.5228	0.1929	0.0643	0.099*
C17	0.51244 (15)	−0.0349 (5)	0.1183 (3)	0.1036 (14)
H17A	0.5089	−0.0774	0.1752	0.155*
H17B	0.5389	−0.0835	0.0928	0.155*
H17C	0.4863	−0.0637	0.0850	0.155*
N1	0.38373 (7)	0.8826 (3)	0.00845 (14)	0.0499 (6)
N2	0.40331 (7)	0.6559 (3)	0.09207 (13)	0.0428 (5)
H2A	0.4093	0.5947	0.0483	0.051*

O1	0.36124 (7)	1.1601 (2)	0.07509 (14)	0.0648 (6)
O2	0.37576 (7)	1.1370 (3)	−0.07715 (14)	0.0639 (6)
O3	0.49668 (8)	0.4789 (3)	0.13212 (19)	0.0858 (8)
O4	0.47548 (7)	0.2156 (3)	0.15495 (15)	0.0698 (6)
O5	0.57738 (8)	0.5513 (3)	0.04480 (16)	0.0876 (8)
H5A	0.5842	0.6535	0.0484	0.131*
H5B	0.5518	0.5450	0.0679	0.131*
S1	0.35869 (2)	1.05939 (9)	−0.00081 (5)	0.0514 (2)
S2	0.37963 (3)	0.89724 (10)	0.18608 (5)	0.0577 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0426 (14)	0.0430 (14)	0.0572 (16)	−0.0020 (12)	−0.0018 (12)	0.0115 (13)
C2	0.0547 (18)	0.0499 (17)	0.0692 (19)	0.0008 (13)	0.0047 (15)	0.0069 (15)
C3	0.0510 (18)	0.063 (2)	0.094 (3)	0.0032 (15)	0.0181 (18)	0.0091 (19)
C4	0.0385 (15)	0.067 (2)	0.098 (3)	−0.0065 (14)	0.0017 (17)	0.023 (2)
C5	0.0482 (17)	0.0538 (17)	0.0665 (18)	−0.0140 (13)	−0.0068 (14)	0.0201 (15)
C6	0.062 (2)	0.074 (2)	0.082 (2)	−0.0258 (18)	−0.0198 (19)	0.026 (2)
C7	0.097 (3)	0.078 (2)	0.063 (2)	−0.034 (2)	−0.019 (2)	0.0146 (19)
C8	0.087 (3)	0.075 (2)	0.058 (2)	−0.0155 (19)	0.0034 (18)	0.0084 (17)
C9	0.0561 (17)	0.0624 (19)	0.0534 (17)	−0.0079 (14)	0.0026 (14)	0.0120 (15)
C10	0.0447 (15)	0.0450 (15)	0.0555 (16)	−0.0063 (12)	−0.0026 (13)	0.0184 (13)
C11	0.0314 (12)	0.0479 (15)	0.0505 (16)	−0.0008 (11)	−0.0009 (11)	−0.0038 (12)
C12	0.0347 (13)	0.0540 (17)	0.0422 (14)	0.0008 (11)	0.0002 (11)	0.0044 (12)
C13	0.0617 (17)	0.0663 (19)	0.0391 (15)	0.0072 (15)	0.0040 (13)	0.0001 (14)
C14	0.0413 (15)	0.0563 (17)	0.0512 (16)	0.0022 (12)	0.0036 (12)	0.0065 (13)
C15	0.0423 (15)	0.0605 (19)	0.0494 (16)	0.0001 (14)	−0.0031 (12)	−0.0024 (14)
C16	0.0498 (18)	0.092 (3)	0.105 (3)	0.0127 (17)	0.0076 (18)	−0.036 (2)
C17	0.088 (3)	0.086 (3)	0.137 (4)	0.028 (2)	0.028 (3)	−0.019 (3)
N1	0.0469 (13)	0.0547 (14)	0.0480 (13)	0.0037 (11)	−0.0023 (10)	0.0069 (11)
N2	0.0409 (12)	0.0480 (13)	0.0395 (11)	0.0024 (10)	0.0001 (9)	−0.0034 (9)
O1	0.0653 (14)	0.0492 (12)	0.0798 (15)	0.0002 (9)	−0.0171 (11)	−0.0087 (11)
O2	0.0493 (11)	0.0649 (13)	0.0774 (14)	−0.0120 (10)	−0.0017 (10)	0.0266 (11)
O3	0.0549 (13)	0.0784 (16)	0.124 (2)	−0.0084 (13)	0.0285 (13)	−0.0052 (15)
O4	0.0510 (12)	0.0629 (14)	0.0955 (17)	0.0114 (10)	0.0146 (11)	−0.0053 (12)
O5	0.0865 (17)	0.0755 (16)	0.1008 (18)	−0.0314 (13)	0.0476 (14)	−0.0389 (14)
S1	0.0429 (4)	0.0474 (4)	0.0641 (5)	−0.0047 (3)	−0.0060 (3)	0.0101 (3)
S2	0.0665 (5)	0.0547 (5)	0.0520 (4)	0.0092 (4)	0.0064 (3)	−0.0083 (3)

Geometric parameters (Å, º)

C1—C2	1.370 (4)	C12—N2	1.385 (3)
C1—C10	1.421 (4)	C12—C14	1.484 (4)
C1—S1	1.769 (3)	C13—S2	1.727 (3)
C2—C3	1.404 (4)	C13—H13	0.9300
C2—H2	0.9300	C14—C15	1.499 (4)
C3—C4	1.352 (5)	C14—H14A	0.9700

C3—H3	0.9300	C14—H14B	0.9700
C4—C5	1.411 (5)	C15—O3	1.193 (3)
C4—H4	0.9300	C15—O4	1.315 (3)
C5—C6	1.406 (4)	C16—O4	1.448 (4)
C5—C10	1.426 (4)	C16—C17	1.473 (5)
C6—C7	1.353 (5)	C16—H16A	0.9700
C6—H6	0.9300	C16—H16B	0.9700
C7—C8	1.399 (5)	C17—H17A	0.9600
C7—H7	0.9300	C17—H17B	0.9600
C8—C9	1.363 (4)	C17—H17C	0.9600
C8—H8	0.9300	N1—S1	1.598 (2)
C9—C10	1.414 (4)	N2—H2A	0.8600
C9—H9	0.9300	O1—S1	1.437 (2)
C11—N1	1.316 (3)	O2—S1	1.439 (2)
C11—N2	1.335 (3)	O5—H5A	0.8399
C11—S2	1.751 (3)	O5—H5B	0.8400
C12—C13	1.323 (4)		

C2—C1—C10	121.9 (3)	C12—C13—H13	123.5
C2—C1—S1	116.3 (2)	S2—C13—H13	123.5
C10—C1—S1	121.7 (2)	C12—C14—C15	114.6 (2)
C1—C2—C3	119.8 (3)	C12—C14—H14A	108.6
C1—C2—H2	120.1	C15—C14—H14A	108.6
C3—C2—H2	120.1	C12—C14—H14B	108.6
C4—C3—C2	120.2 (3)	C15—C14—H14B	108.6
C4—C3—H3	119.9	H14A—C14—H14B	107.6
C2—C3—H3	119.9	O3—C15—O4	124.4 (3)
C3—C4—C5	121.5 (3)	O3—C15—C14	125.4 (3)
C3—C4—H4	119.2	O4—C15—C14	110.2 (2)
C5—C4—H4	119.2	O4—C16—C17	106.9 (3)
C6—C5—C4	121.4 (3)	O4—C16—H16A	110.3
C6—C5—C10	119.2 (3)	C17—C16—H16A	110.3
C4—C5—C10	119.4 (3)	O4—C16—H16B	110.3
C7—C6—C5	121.4 (3)	C17—C16—H16B	110.3
C7—C6—H6	119.3	H16A—C16—H16B	108.6
C5—C6—H6	119.3	C16—C17—H17A	109.5
C6—C7—C8	119.8 (3)	C16—C17—H17B	109.5
C6—C7—H7	120.1	H17A—C17—H17B	109.5
C8—C7—H7	120.1	C16—C17—H17C	109.5
C9—C8—C7	120.9 (3)	H17A—C17—H17C	109.5
C9—C8—H8	119.5	H17B—C17—H17C	109.5
C7—C8—H8	119.5	C11—N1—S1	120.0 (2)
C8—C9—C10	120.8 (3)	C11—N2—C12	116.5 (2)
C8—C9—H9	119.6	C11—N2—H2A	121.8
C10—C9—H9	119.6	C12—N2—H2A	121.8
C9—C10—C1	125.1 (3)	C15—O4—C16	118.9 (3)
C9—C10—C5	117.9 (3)	H5A—O5—H5B	104.1
C1—C10—C5	117.0 (3)	O1—S1—O2	115.50 (13)

N1—C11—N2	120.8 (2)	O1—S1—N1	113.12 (12)
N1—C11—S2	130.3 (2)	O2—S1—N1	106.95 (13)
N2—C11—S2	108.83 (19)	O1—S1—C1	107.55 (13)
C13—C12—N2	111.4 (2)	O2—S1—C1	107.85 (13)
C13—C12—C14	128.4 (2)	N1—S1—C1	105.29 (12)
N2—C12—C14	120.1 (2)	C13—S2—C11	90.25 (13)
C12—C13—S2	113.0 (2)		

C10—C1—C2—C3	−1.8 (4)	N2—C12—C14—C15	62.3 (3)
S1—C1—C2—C3	175.5 (2)	C12—C14—C15—O3	14.1 (4)
C1—C2—C3—C4	−0.5 (5)	C12—C14—C15—O4	−167.2 (2)
C2—C3—C4—C5	2.1 (5)	N2—C11—N1—S1	170.26 (19)
C3—C4—C5—C6	177.9 (3)	S2—C11—N1—S1	−11.7 (3)
C3—C4—C5—C10	−1.3 (4)	N1—C11—N2—C12	178.0 (2)
C4—C5—C6—C7	−179.3 (3)	S2—C11—N2—C12	−0.4 (3)
C10—C5—C6—C7	−0.1 (5)	C13—C12—N2—C11	0.4 (3)
C5—C6—C7—C8	0.4 (5)	C14—C12—N2—C11	177.6 (2)
C6—C7—C8—C9	0.0 (5)	O3—C15—O4—C16	−3.5 (5)
C7—C8—C9—C10	−0.7 (5)	C14—C15—O4—C16	177.7 (3)
C8—C9—C10—C1	−179.5 (3)	C17—C16—O4—C15	−172.3 (3)
C8—C9—C10—C5	0.9 (4)	C11—N1—S1—O1	26.1 (3)
C2—C1—C10—C9	−177.0 (3)	C11—N1—S1—O2	154.4 (2)
S1—C1—C10—C9	5.7 (4)	C11—N1—S1—C1	−91.0 (2)
C2—C1—C10—C5	2.5 (4)	C2—C1—S1—O1	−3.2 (2)
S1—C1—C10—C5	−174.7 (2)	C10—C1—S1—O1	174.1 (2)
C6—C5—C10—C9	−0.5 (4)	C2—C1—S1—O2	−128.4 (2)
C4—C5—C10—C9	178.6 (3)	C10—C1—S1—O2	48.9 (2)
C6—C5—C10—C1	179.9 (3)	C2—C1—S1—N1	117.7 (2)
C4—C5—C10—C1	−1.0 (4)	C10—C1—S1—N1	−65.0 (2)
N2—C12—C13—S2	−0.2 (3)	C12—C13—S2—C11	0.0 (2)
C14—C12—C13—S2	−177.1 (2)	N1—C11—S2—C13	−177.9 (3)
C13—C12—C14—C15	−121.0 (3)	N2—C11—S2—C13	0.27 (19)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O5^{i}	0.86	1.91	2.767 (3)	177
O5—H5*A*···O2^{ii}	0.84	2.10	2.889 (3)	157
C13—H13···O2^{iii}	0.93	2.57	3.295 (4)	135
C14—H14*A*···O1^{iv}	0.97	2.34	3.295 (3)	167
C17—H17*B*···O2^{i}	0.96	2.57	3.466 (5)	155

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