Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl 2-[3-(3,5-Dinitrobenzoyl)thioureido]benzoate

Sohail Saeed,[a]* Naghmana Rashid,[a] Moazzam H. Bhatti[a] and Wing-Tak Wong[b]

[a]Department of Chemistry, Research Complex, Allama Iqbal Open University, Islamabad 44000, Pakistan, and [b]Department of Chemistry, The University of Hong Kong, Pokfulam Road, Pokfulam, Hong Kong SAR, People's Republic of China
Correspondence e-mail: Sohail262001@yahoo.com

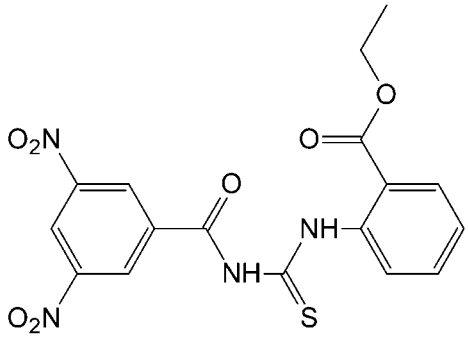
Received 14 March 2011; accepted 6 April 2011

Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.037; wR factor = 0.095; data-to-parameter ratio = 10.0.

In the title compound, $C_{17}H_{14}N_4O_7S$, the dihedral angle between the two benzene rings is 9.04 (15)°. The centroid–centroid distance of 3.9825 (19) Å between nearly parallel benzene rings of adjacent molecules suggests the existence of π-π stacking. Intermolecular and intra-molecular N—H···O hydrogen bonding is present in the structure. The ethoxy group is disordered over two sets of sites with an occupancy ratio of 0.580 (15):0.420 (15). The crystal studied was an inversion twin.

Related literature

For background to the chemistry of thiourea derivatives and their bioloical activity, and a related structure, see: Saeed *et al.* (2010).



Experimental

Crystal data

$C_{17}H_{14}N_4O_7S$ M_r = 418.38
Monoclinic, Cc
a = 11.7264 (19) Å
b = 16.617 (3) Å
c = 9.9630 (16) Å
β = 101.522 (2)°
V = 1902.3 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 299 K
0.27 × 0.16 × 0.08 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.943, T_{max} = 0.983
4944 measured reflections
3011 independent reflections
2727 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.095
S = 1.10
3011 reflections
301 parameters
42 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Absolute structure: Flack (1983), 1340 Friedel pairs
Flack parameter: 0.39 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.91 (3)	1.95 (3)	2.672 (3)	134 (2)
N1—H1···O3	0.91 (3)	2.01 (3)	2.700 (3)	131 (2)
N2—H2···O3^{i}	0.77 (3)	2.32 (3)	3.086 (3)	172 (2)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97*.

The authors are grateful to Allama Iqbal Open University, Islamabad, Pakistan, for the allocation of research and analytical laboratory facilities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5177).

References

Bruker. (1998). *SMART*, Madison, Wisconsin, USA.
Bruker. (2006). *SAINT*, Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Saeed, S., Rashid, N. & Wong, W.-T. (2010). *Acta Cryst.* E**66**, o980.
Sheldrick, G. M. (2004). *SADABS*, University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2011). E**67**, o1114 [doi:10.1107/S1600536811012918]

Ethyl 2-[3-(3,5-Dinitrobenzoyl)thioureido]benzoate

Sohail Saeed, Naghmana Rashid, Moazzam H. Bhatti and Wing-Tak Wong

S1. Comment

The background to this study has been set in our previous work on the structural chemistry of *N*,*N*′-disubstituted thiourea (Saeed *et al.*, 2010). Herein, as a continuation of these studies, the structure of the title compound, (I), $C_{17}H_{14}N_4O_7S$, is described.

The compound is slightly twisted. The nitro groups are 3.9 (5)° and 17 (1)° from the phenyl ring plane of C10—C15. The thiourea plane is making a dihedral angle of 5.3 (2)° with the amido group and makes a dihedral angle of 31.35 (17)° with the phenyl ring plane of C2—C7.

There are inter-molecular N—H···O H-bond interactions which link the molecules to form 1-D chain in the crystal lattice. There are also weak $\pi\cdots\pi$ between neighbouring rings in the crystal lattice.

S2. Experimental

A solution of 3,5-dinitrobenzoyl chloride (0.01 mol) in anhydrous acetone (75 ml) and 3% tetrabutylammonium bromide (TBAB) as a phase-transfer catalyst (PTC) in anhydrous acetone was added dropwise to a suspension of dry potassium thiocyanate (0.01 mol) in acetone (50 ml) and the reaction mixture was refluxed for 50 min. After cooling to room temperature, a solution of ethyl-orthoamino benzoate (0.01 mol) in anhydrous acetone (25 ml) was added dropwise and the resulting mixture refluxed for 3 h. Hydrochloric acid (0.1 N, 300 ml) was added, and the solution was filtered. The solid product was washed with water and purified by re-crystallization from ethyl acetate.

S3. Refinement

N-bound H-atoms were located in a difference Fourier map and refined isotropically. Other H atoms were placed at geometrical positions with C—H = 0.93–0.97 Å and refined using riding model with U_{iso}(H) =1.2U_{eq}(C). The ethoxy group is disordered over two sites, the occupancy ratio was refined to 0.580 (15):0.420 (15). Distance and displacement restraints were used for the disordered components.

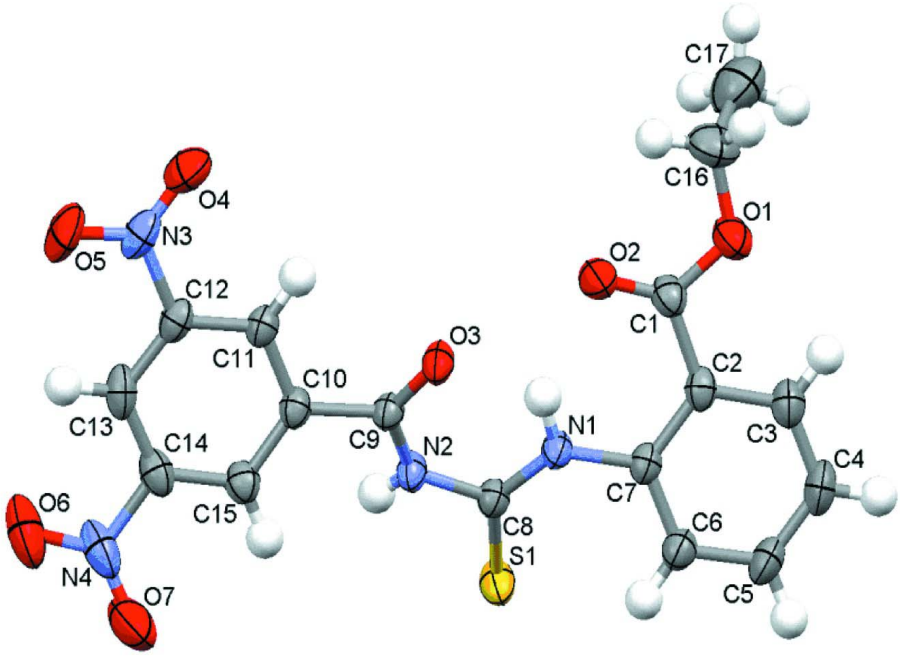


Figure 1

The *ORTEP* plot of the compound was shown at 50% probability thermal ellipsoids with the atom numbering scheme (only the major component was shown).

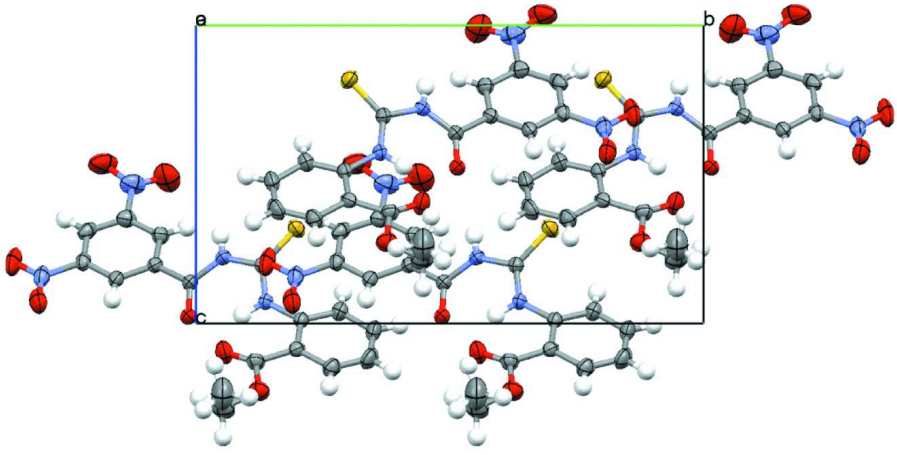


Figure 2

Packing diagram of the title compound viewed down the *a* axis.

Ethyl 2-[3-(3,5-Dinitrobenzoyl)thioureido]benzoate

Crystal data

$C_{17}H_{14}N_4O_7S$
$M_r = 418.38$
Monoclinic, *Cc*
Hall symbol: C -2yc
$a = 11.7264\ (19)$ Å
$b = 16.617\ (3)$ Å
$c = 9.9630\ (16)$ Å
$\beta = 101.522\ (2)°$
$V = 1902.3\ (5)$ Å^3
$Z = 4$

$F(000) = 864$
$D_x = 1.461$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6458 reflections
$\theta = 2.1$–$25.0°$
$\mu = 0.22$ mm^{-1}
$T = 299$ K
Block, yellow
0.27 × 0.16 × 0.08 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min} = 0.943$, $T_{max} = 0.983$
4944 measured reflections
3011 independent reflections
2727 reflections with $I > 2\sigma(I)$
$R_{int} = 0.014$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.7°$
$h = -13 \rightarrow 13$
$k = -19 \rightarrow 15$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.095$
$S = 1.10$
3011 reflections
301 parameters
42 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
$w = 1/[\sigma^2(F_o^2) + (0.0536P)^2 + 0.3273P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}
Absolute structure: Flack (1983), 1340 Friedel pairs
Absolute structure parameter: 0.39 (8)

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)
S1	0.94150 (8)	0.19793 (4)	0.68183 (8)	0.0759 (3)	
O2	0.8103 (2)	0.05570 (13)	1.0967 (3)	0.0866 (7)	
O3	0.99391 (19)	−0.01499 (10)	0.97679 (18)	0.0663 (5)	
O4	1.0187 (3)	−0.31100 (14)	0.9255 (4)	0.1022 (8)	
O5	1.1263 (3)	−0.35915 (14)	0.7937 (3)	0.1095 (10)	
O6	1.2496 (4)	−0.1832 (2)	0.4646 (3)	0.1355 (14)	
O7	1.2710 (4)	−0.0571 (3)	0.5114 (4)	0.1459 (15)	
N1	0.9176 (2)	0.13747 (12)	0.9269 (2)	0.0543 (5)	
H1	0.911 (2)	0.0912 (17)	0.974 (3)	0.064 (8)*	
H2	0.997 (2)	0.0472 (15)	0.704 (3)	0.045 (7)*	

N2	0.9902 (2)	0.05353 (12)	0.7789 (2)	0.0555 (5)	
N3	1.0798 (3)	−0.30348 (14)	0.8423 (3)	0.0773 (8)	
N4	1.2402 (3)	−0.1244 (3)	0.5338 (3)	0.0976 (10)	
C1	0.7736 (3)	0.11786 (17)	1.1281 (3)	0.0647 (7)	
C2	0.8103 (2)	0.19844 (15)	1.0865 (3)	0.0563 (6)	
C3	0.7770 (3)	0.26756 (18)	1.1485 (3)	0.0713 (8)	
H3	0.7296	0.2626	1.2125	0.086*	
C4	0.8124 (4)	0.3418 (2)	1.1176 (4)	0.0842 (10)	
H4	0.7885	0.3870	1.1596	0.101*	
C5	0.8830 (3)	0.35007 (17)	1.0248 (3)	0.0782 (9)	
H5	0.9080	0.4010	1.0051	0.094*	
C6	0.9179 (3)	0.28322 (16)	0.9596 (3)	0.0657 (7)	
H6	0.9662	0.2896	0.8968	0.079*	
C7	0.8809 (2)	0.20717 (14)	0.9882 (2)	0.0531 (6)	
C8	0.9476 (2)	0.13033 (14)	0.8043 (3)	0.0525 (6)	
C9	1.0156 (2)	−0.01157 (13)	0.8622 (2)	0.0518 (6)	
C10	1.0713 (2)	−0.08065 (14)	0.8043 (3)	0.0539 (6)	
C11	1.0528 (2)	−0.15737 (14)	0.8509 (3)	0.0555 (6)	
H11	1.0103	−0.1650	0.9193	0.067*	
C12	1.0991 (2)	−0.22190 (15)	0.7933 (3)	0.0595 (7)	
C13	1.1609 (3)	−0.21360 (18)	0.6905 (3)	0.0695 (8)	
H13	1.1890	−0.2582	0.6508	0.083*	
C14	1.1797 (3)	−0.1366 (2)	0.6489 (3)	0.0677 (8)	
C15	1.1379 (3)	−0.07002 (16)	0.7053 (3)	0.0618 (7)	
H15	1.1542	−0.0186	0.6775	0.074*	
O1	0.7136 (10)	0.1247 (5)	1.2262 (9)	0.083 (2)	0.580 (15)
C16	0.6730 (10)	0.0532 (7)	1.2838 (13)	0.113 (4)	0.580 (15)
H16A	0.6931	0.0548	1.3830	0.135*	0.580 (15)
H16B	0.7077	0.0056	1.2523	0.135*	0.580 (15)
C17	0.5404 (10)	0.0522 (6)	1.2345 (19)	0.161 (6)	0.580 (15)
H17A	0.5070	0.0125	1.2851	0.193*	0.580 (15)
H17B	0.5219	0.0392	1.1387	0.193*	0.580 (15)
H17C	0.5093	0.1042	1.2489	0.193*	0.580 (15)
O1′	0.6758 (12)	0.1178 (7)	1.1805 (14)	0.085 (3)	0.420 (15)
C16′	0.6436 (15)	0.0411 (7)	1.2287 (14)	0.084 (4)	0.420 (15)
H16C	0.7119	0.0073	1.2549	0.101*	0.420 (15)
H16D	0.5889	0.0139	1.1571	0.101*	0.420 (15)
C17′	0.5883 (19)	0.0568 (8)	1.3511 (18)	0.134 (6)	0.420 (15)
H17D	0.5738	0.0065	1.3920	0.161*	0.420 (15)
H17E	0.5162	0.0850	1.3219	0.161*	0.420 (15)
H17F	0.6399	0.0888	1.4169	0.161*	0.420 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.1117 (6)	0.0590 (4)	0.0655 (4)	0.0263 (4)	0.0381 (4)	0.0158 (3)
O2	0.1105 (17)	0.0589 (12)	0.1056 (17)	0.0112 (11)	0.0580 (14)	0.0120 (11)
O3	0.1054 (16)	0.0478 (10)	0.0498 (10)	0.0112 (9)	0.0252 (10)	−0.0004 (7)

O4	0.131 (2)	0.0570 (13)	0.122 (2)	−0.0046 (13)	0.031 (2)	0.0083 (13)
O5	0.118 (2)	0.0524 (12)	0.153 (3)	0.0257 (13)	0.0147 (19)	−0.0192 (14)
O6	0.172 (3)	0.163 (3)	0.0823 (18)	0.073 (3)	0.052 (2)	−0.0065 (18)
O7	0.179 (4)	0.131 (3)	0.163 (3)	0.028 (3)	0.119 (3)	0.026 (2)
N1	0.0734 (15)	0.0413 (10)	0.0509 (12)	0.0056 (9)	0.0185 (10)	−0.0003 (8)
N2	0.0776 (15)	0.0480 (11)	0.0434 (12)	0.0094 (10)	0.0178 (11)	−0.0029 (9)
N3	0.0820 (18)	0.0479 (13)	0.092 (2)	0.0105 (12)	−0.0056 (16)	−0.0079 (13)
N4	0.099 (2)	0.123 (3)	0.0795 (19)	0.049 (2)	0.0396 (17)	0.0068 (19)
C1	0.076 (2)	0.0658 (17)	0.0559 (15)	0.0108 (14)	0.0209 (14)	0.0059 (12)
C2	0.0635 (17)	0.0569 (14)	0.0459 (13)	0.0114 (11)	0.0046 (12)	−0.0053 (10)
C3	0.081 (2)	0.0679 (18)	0.0663 (18)	0.0144 (14)	0.0178 (16)	−0.0096 (14)
C4	0.103 (3)	0.0639 (19)	0.086 (2)	0.0187 (17)	0.0186 (19)	−0.0250 (16)
C5	0.103 (2)	0.0453 (14)	0.084 (2)	0.0031 (14)	0.0121 (18)	−0.0134 (13)
C6	0.080 (2)	0.0526 (14)	0.0644 (17)	−0.0012 (12)	0.0144 (15)	−0.0065 (12)
C7	0.0631 (16)	0.0459 (12)	0.0478 (13)	0.0070 (10)	0.0049 (12)	−0.0029 (10)
C8	0.0577 (15)	0.0476 (13)	0.0520 (13)	0.0034 (10)	0.0100 (11)	−0.0010 (10)
C9	0.0643 (17)	0.0453 (13)	0.0462 (14)	0.0029 (10)	0.0119 (12)	−0.0023 (10)
C10	0.0649 (17)	0.0507 (13)	0.0445 (12)	0.0062 (11)	0.0069 (12)	−0.0030 (10)
C11	0.0637 (17)	0.0486 (13)	0.0516 (13)	0.0047 (11)	0.0056 (12)	−0.0062 (10)
C12	0.0622 (17)	0.0462 (13)	0.0641 (17)	0.0098 (11)	−0.0015 (14)	−0.0033 (11)
C13	0.0718 (19)	0.0740 (18)	0.0574 (16)	0.0290 (14)	0.0001 (14)	−0.0162 (14)
C14	0.0655 (18)	0.082 (2)	0.0568 (16)	0.0240 (14)	0.0151 (14)	0.0023 (14)
C15	0.0686 (18)	0.0592 (14)	0.0581 (15)	0.0113 (13)	0.0138 (13)	0.0029 (12)
O1	0.103 (6)	0.083 (3)	0.075 (4)	0.006 (3)	0.043 (4)	0.008 (3)
C16	0.130 (8)	0.116 (7)	0.104 (7)	−0.012 (5)	0.053 (6)	0.018 (5)
C17	0.191 (12)	0.086 (5)	0.212 (14)	−0.002 (6)	0.056 (10)	0.002 (7)
O1′	0.087 (6)	0.081 (4)	0.093 (7)	0.005 (4)	0.035 (5)	−0.008 (4)
C16′	0.090 (7)	0.070 (5)	0.108 (8)	−0.013 (4)	0.055 (6)	0.007 (5)
C17′	0.209 (14)	0.092 (7)	0.135 (10)	0.039 (8)	0.116 (10)	0.024 (7)

Geometric parameters (Å, º)

S1—C8	1.649 (2)	C6—C7	1.385 (4)
O2—C1	1.185 (3)	C6—H6	0.9300
O3—C9	1.219 (3)	C9—C10	1.493 (3)
O4—N3	1.205 (4)	C10—C15	1.386 (4)
O5—N3	1.222 (4)	C10—C11	1.388 (3)
O6—N4	1.213 (4)	C11—C12	1.377 (4)
O7—N4	1.210 (5)	C11—H11	0.9300
N1—C8	1.342 (3)	C12—C13	1.375 (4)
N1—C7	1.416 (3)	C13—C14	1.376 (5)
N1—H1	0.91 (3)	C13—H13	0.9300
N2—C9	1.360 (3)	C14—C15	1.375 (4)
N2—C8	1.412 (3)	C15—H15	0.9300
N2—H2	0.77 (3)	O1—C16	1.442 (8)
N3—C12	1.474 (4)	C16—C17	1.535 (9)
N4—C14	1.478 (4)	C16—H16A	0.9700
C1—O1	1.318 (10)	C16—H16B	0.9700

C1—O1′	1.351 (14)	C17—H17A	0.9600
C1—C2	1.490 (4)	C17—H17B	0.9600
C2—C3	1.396 (4)	C17—H17C	0.9600
C2—C7	1.410 (4)	O1′—C16′	1.440 (9)
C3—C4	1.356 (5)	C16′—C17′	1.514 (9)
C3—H3	0.9300	C16′—H16C	0.9700
C4—C5	1.365 (5)	C16′—H16D	0.9700
C4—H4	0.9300	C17′—H17D	0.9600
C5—C6	1.389 (4)	C17′—H17E	0.9600
C5—H5	0.9300	C17′—H17F	0.9600

C8—N1—C7	128.5 (2)	N2—C9—C10	115.8 (2)
C8—N1—H1	117.1 (18)	C15—C10—C11	120.2 (2)
C7—N1—H1	114.0 (18)	C15—C10—C9	122.0 (2)
C9—N2—C8	130.7 (2)	C11—C10—C9	117.9 (2)
C9—N2—H2	115.4 (18)	C12—C11—C10	118.4 (3)
C8—N2—H2	113.8 (19)	C12—C11—H11	120.8
O4—N3—O5	124.6 (3)	C10—C11—H11	120.8
O4—N3—C12	118.4 (2)	C13—C12—C11	122.8 (3)
O5—N3—C12	117.1 (3)	C13—C12—N3	118.5 (2)
O7—N4—O6	125.1 (4)	C11—C12—N3	118.6 (3)
O7—N4—C14	118.6 (3)	C12—C13—C14	117.2 (2)
O6—N4—C14	116.2 (4)	C12—C13—H13	121.4
O2—C1—O1	123.2 (5)	C14—C13—H13	121.4
O2—C1—O1′	118.9 (6)	C15—C14—C13	122.3 (3)
O2—C1—C2	124.7 (3)	C15—C14—N4	118.1 (3)
O1—C1—C2	110.8 (4)	C13—C14—N4	119.5 (3)
O1′—C1—C2	115.0 (5)	C14—C15—C10	119.0 (3)
C3—C2—C7	118.5 (2)	C14—C15—H15	120.5
C3—C2—C1	119.6 (3)	C10—C15—H15	120.5
C7—C2—C1	121.9 (2)	C1—O1—C16	119.4 (9)
C4—C3—C2	121.5 (3)	O1—C16—C17	106.0 (9)
C4—C3—H3	119.2	O1—C16—H16A	110.5
C2—C3—H3	119.2	C17—C16—H16A	110.5
C3—C4—C5	120.0 (3)	O1—C16—H16B	110.5
C3—C4—H4	120.0	C17—C16—H16B	110.5
C5—C4—H4	120.0	H16A—C16—H16B	108.7
C4—C5—C6	120.7 (3)	C1—O1′—C16′	115.3 (10)
C4—C5—H5	119.6	O1′—C16′—C17′	107.4 (10)
C6—C5—H5	119.6	O1′—C16′—H16C	110.2
C7—C6—C5	120.0 (3)	C17′—C16′—H16C	110.2
C7—C6—H6	120.0	O1′—C16′—H16D	110.2
C5—C6—H6	120.0	C17′—C16′—H16D	110.2
C6—C7—C2	119.3 (2)	H16C—C16′—H16D	108.5
C6—C7—N1	121.5 (2)	C16′—C17′—H17D	109.5
C2—C7—N1	119.1 (2)	C16′—C17′—H17E	109.5
N1—C8—N2	114.2 (2)	H17D—C17′—H17E	109.5
N1—C8—S1	129.22 (19)	C16′—C17′—H17F	109.5

N2—C8—S1	116.62 (19)	H17D—C17′—H17F	109.5
O3—C9—N2	123.2 (2)	H17E—C17′—H17F	109.5
O3—C9—C10	121.0 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.91 (3)	1.95 (3)	2.672 (3)	134 (2)
N1—H1···O3	0.91 (3)	2.01 (3)	2.700 (3)	131 (2)
N2—H2···O3^{i}	0.77 (3)	2.32 (3)	3.086 (3)	172 (2)

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