Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl 2-benzamido-4,5,6,7-tetrahydro-1-benzothiophene-3-carboxylate

Asma Mukhtar,[a] M. Nawaz Tahir,[b]* Misbahul Ain Khan[a] and Muhammad Naeem Khan[c]

[a]Institute of Chemistry, University of the Punjab, Lahore, Pakistan, [b]Department of Physics, University of Sargodha, Sargodha, Pakistan, and [c]Applied Chemistry Research Center, PCSIR Laboratories Complex, Lahore 54600, Pakistan
Correspondence e-mail: dmntahir_uos@yahoo.com

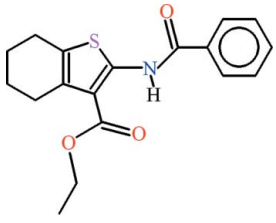
Received 19 September 2010; accepted 21 September 2010

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.042; wR factor = 0.117; data-to-parameter ratio = 14.1.

The molecule of the title compound, $C_{18}H_{19}NO_3S$, adopts an approximately planar conformation: the thiophene and phenyl rings form a dihedral angle of 8.13 (11)° while the ethyl ester group (r.m.s. deviation = 0.0217 Å) is inclined at 1.25 (14) and 8.61 (13)°, respectively, to the thiophene and phenyl rings. An intramolecular N—H···O hydrogen bond with an S(6) ring motif occurs as well as an intramolecular S···O hypervalent interaction [S···O = 2.7369 (18) Å]. The cyclohexene ring adopts a half-chair conformation and is disordered over two positions with site occupation factors of 0.641 (6) and 0.359 (6). In the crystal, inversion dimers linked by pairs of O—H···O hydrogen bonds generate $R_2^2(10)$ loops.

Related literature

For background on thiophene derivatives, see: Dupin *et al.* (2002); Khan & Rolim (1983); Sabnis *et al.* (1999). For related structures, see: Harrison *et al.* (2006); Yathirajan *et al.* (2007). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{18}H_{19}NO_3S$
M_r = 329.40
Monoclinic, $P2_1/c$
a = 8.1061 (2) Å
b = 10.6593 (3) Å
c = 19.0554 (5) Å
β = 92.500 (1)°
V = 1644.92 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 296 K
0.25 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.953, T_{max} = 0.958
12204 measured reflections
2964 independent reflections
2052 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.117
S = 1.01
2964 reflections
210 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 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—H1···O2	0.86	2.02	2.664 (2)	131
C6—H6···O1^{i}	0.93	2.44	3.242 (3)	145

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; 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 *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The authors acknowledge the provision of funds for the purchase of the diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2302).

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supporting information

Acta Cryst. (2010). E**66**, o2652 [doi:10.1107/S1600536810037761]

Ethyl 2-benzamido-4,5,6,7-tetrahydro-1-benzothiophene-3-carboxylate

Asma Mukhtar, M. Nawaz Tahir, Misbahul Ain Khan and Muhammad Naeem Khan

S1. Comment

Thiophenes and their condensed derivatives have been described in the literature (Khan & Rolim, 1983). Tetrahydro-1-benzothiophenes are intermediates for many useful products such as dyes and pharmaceuticals (Sabnis *et al.*, 1999) and compounds containing thrombolytic activity (Dupin *et al.*, 2002). The title compound (Fig. 1) has been prepared for the derivatization of other compounds.

The crystal structures of ethyl 2-acetylamino-4,5,6,7-tetrahydro-1-benzothiophene-3-carboxylate (Harrison *et al.*, 2006) and *i.e.* ethyl 2-(propionylamino)-4,5,6,7-tetrahydro-1-benzothiophene-3-carboxylate (Yathirajan *et al.*, 2007) have been published which are related to the title compound.

In the title compound, the heterocyclic ring A (S1/C8/C9/C10/C15) and the phenyl ring B (C1—C6) are planar. The dihedral angle between A/B is 8.13 (11)°. The ethyl ester group C (O2/C16/O3/C17/C18) is planar with r. m. s. deviation of 0.0217 Å and is inclined at 1.25 (14) and 8.61 (13)° with the rings A and B, respectively. In the title compound an S(6) ring motif (Bernstein *et al.*, 1995) is formed due to intramolecular H-bonding of N—H···O type (Table 1, Fig. 1). Two methylene groups of the cyclohexene ring in half-chair conformation are disordered over two positions with site occupation factors of 0.641 (6) and 0.359 (6).

S2. Experimental

Ethyl 2-amino-4,5,6,7-tetrahydro-1-benzothiophene-3-carboxylate (0.3 g, 1.0 mmol) was dissolved in 10 ml of chloroform. To this solution 0.15 ml of benzoyl chloride was added and heated under reflux for 9 h. The solvent was removed and the residue was recrystallized from ethanol to affoard the colorless prism.

S3. Refinement

In the cyclohexene ring two methylene groups are disordered over two positions with site occupation factors of 0.641 (6) and 0.359 (6). The disordered C atoms were refined anisotropically with equal displacement parameters (EADP instruction of SHELXL97).

The H atoms were positioned geometrically (N—H = 0.86, C–H = 0.93–0.97 Å) and refined as riding with U_{iso}(H) = xU_{eq}(C, N), where x = 1.5 for methyl and x = 1.2 for other H atoms.

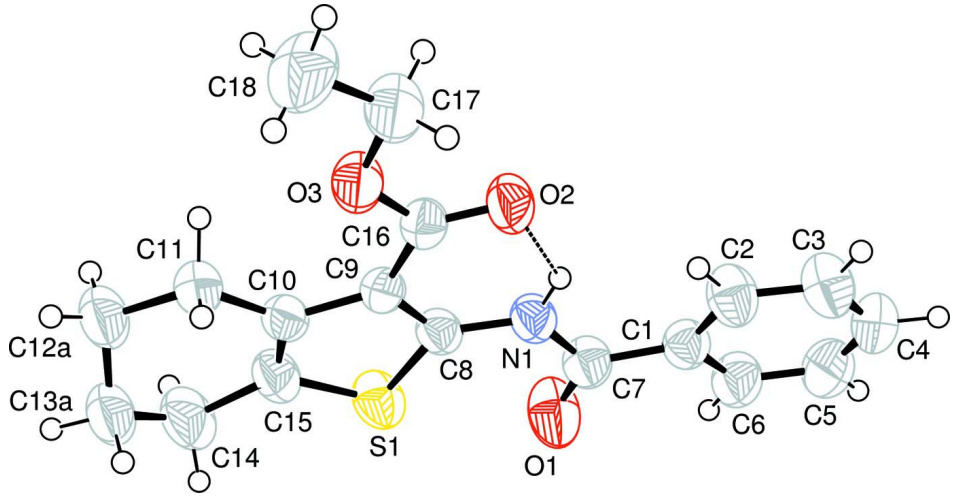

Figure 1

View of the title compound with the atom numbering scheme. The displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radii. The dotted line shows intramolecular hydrogen bonding.

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Crystal data

$C_{18}H_{19}NO_3S$
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$b = 10.6593$ (3) Å
$c = 19.0554$ (5) Å
$\beta = 92.500$ (1)°
$V = 1644.92$ (8) Å^3
$Z = 4$
$F(000) = 696$
$D_x = 1.330$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2052 reflections
$\theta = 2.5$–25.3°
$\mu = 0.21$ mm^{-1}
$T = 296$ K
Prism, colorless
0.25 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.10 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.953$, $T_{max} = 0.958$
12204 measured reflections
2964 independent reflections
2052 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 25.3°$, $\theta_{min} = 2.5°$
$h = -9\rightarrow9$
$k = -12\rightarrow12$
$l = -22\rightarrow22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.117$
$S = 1.01$
2964 reflections
210 parameters
6 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
$w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 0.4332P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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}	Occ. (<1)
S1	0.75739 (8)	0.64947 (6)	0.09851 (3)	0.0685 (2)	
O1	0.9000 (2)	0.82309 (16)	0.01442 (9)	0.0875 (7)	
O2	0.8026 (2)	0.41537 (14)	−0.09850 (7)	0.0658 (6)	
O3	0.6816 (2)	0.26412 (14)	−0.03830 (7)	0.0666 (6)	
N1	0.8625 (2)	0.63457 (16)	−0.03524 (8)	0.0527 (6)	
C1	0.9770 (3)	0.8019 (2)	−0.10411 (11)	0.0545 (7)	
C2	0.9702 (3)	0.7346 (2)	−0.16629 (12)	0.0679 (9)	
C3	1.0262 (3)	0.7864 (3)	−0.22706 (13)	0.0781 (10)	
C4	1.0909 (3)	0.9047 (3)	−0.22675 (14)	0.0804 (11)	
C5	1.1013 (3)	0.9711 (3)	−0.16569 (16)	0.0830 (11)	
C6	1.0438 (3)	0.9216 (2)	−0.10479 (13)	0.0697 (9)	
C7	0.9121 (3)	0.7563 (2)	−0.03689 (12)	0.0582 (8)	
C8	0.7865 (2)	0.5770 (2)	0.01970 (10)	0.0484 (7)	
C9	0.7256 (2)	0.45660 (19)	0.01795 (10)	0.0464 (7)	
C10	0.6520 (2)	0.4227 (2)	0.08292 (10)	0.0505 (7)	
C11	0.5695 (3)	0.2999 (2)	0.09967 (11)	0.0615 (8)	
C12A	0.5302 (8)	0.2864 (5)	0.1768 (3)	0.0771 (13)	0.641 (6)
C13A	0.4684 (7)	0.4071 (4)	0.2069 (3)	0.0771 (13)	0.641 (6)
C14	0.5952 (3)	0.5146 (3)	0.20270 (12)	0.0820 (10)	
C15	0.6620 (3)	0.5167 (2)	0.12986 (11)	0.0601 (8)	
C16	0.7408 (3)	0.3798 (2)	−0.04470 (11)	0.0518 (7)	
C17	0.6953 (4)	0.1819 (2)	−0.09806 (13)	0.0804 (10)	
C18	0.6130 (4)	0.0615 (3)	−0.08052 (16)	0.1017 (13)	
C12B	0.4639 (11)	0.3191 (11)	0.1642 (4)	0.0771 (13)	0.359 (6)
C13B	0.5564 (13)	0.3883 (8)	0.2231 (4)	0.0771 (13)	0.359 (6)
H1	0.88006	0.58943	−0.07157	0.0632*	
H4	1.12771	0.93963	−0.26797	0.0964*	
H2	0.92751	0.65362	−0.16705	0.0815*	
H3	1.01981	0.74051	−0.26860	0.0936*	
H11A	0.64111	0.23142	0.08692	0.0738*	
H11B	0.46774	0.29269	0.07120	0.0738*	
H12A	0.44709	0.22178	0.18136	0.0926*	0.641 (6)
H12B	0.62887	0.26010	0.20338	0.0926*	0.641 (6)

H13A	0.44302	0.39369	0.25557	0.0926*	0.641 (6)
H13B	0.36703	0.43138	0.18147	0.0926*	0.641 (6)
H14A	0.54276	0.59409	0.21247	0.0985*	
H14B	0.68476	0.50168	0.23738	0.0985*	
H17A	0.81052	0.16736	−0.10724	0.0962*	
H17B	0.64183	0.21915	−0.13955	0.0962*	
H18A	0.66559	0.02642	−0.03888	0.1525*	
H18B	0.62180	0.00366	−0.11881	0.1525*	
H18C	0.49861	0.07682	−0.07259	0.1525*	
H5	1.14776	1.05084	−0.16517	0.0996*	
H6	1.04969	0.96880	−0.06371	0.0837*	
H12C	0.36549	0.36616	0.15021	0.0926*	0.359 (6)
H12D	0.42929	0.23798	0.18130	0.0926*	0.359 (6)
H13C	0.48949	0.39036	0.26402	0.0926*	0.359 (6)
H13D	0.65770	0.34371	0.23564	0.0926*	0.359 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0836 (4)	0.0704 (4)	0.0522 (3)	−0.0085 (3)	0.0127 (3)	−0.0147 (3)
O1	0.1332 (16)	0.0676 (12)	0.0634 (10)	−0.0298 (11)	0.0243 (10)	−0.0167 (9)
O2	0.0950 (11)	0.0567 (10)	0.0472 (9)	−0.0046 (8)	0.0196 (8)	−0.0014 (7)
O3	0.0983 (12)	0.0495 (9)	0.0532 (9)	−0.0073 (8)	0.0168 (8)	−0.0036 (7)
N1	0.0610 (11)	0.0512 (11)	0.0463 (10)	−0.0008 (8)	0.0086 (8)	−0.0027 (8)
C1	0.0553 (12)	0.0529 (13)	0.0555 (13)	−0.0032 (10)	0.0045 (10)	0.0017 (11)
C2	0.0746 (15)	0.0689 (16)	0.0609 (14)	−0.0185 (12)	0.0098 (12)	−0.0028 (13)
C3	0.0868 (18)	0.089 (2)	0.0591 (15)	−0.0080 (15)	0.0115 (13)	−0.0011 (14)
C4	0.0936 (19)	0.0776 (19)	0.0714 (17)	0.0040 (15)	0.0196 (14)	0.0237 (16)
C5	0.101 (2)	0.0565 (16)	0.093 (2)	−0.0055 (14)	0.0221 (16)	0.0151 (15)
C6	0.0878 (17)	0.0550 (15)	0.0670 (15)	−0.0053 (12)	0.0108 (13)	0.0003 (12)
C7	0.0642 (14)	0.0529 (14)	0.0576 (13)	−0.0069 (11)	0.0053 (10)	−0.0027 (12)
C8	0.0476 (11)	0.0559 (13)	0.0418 (11)	0.0043 (10)	0.0031 (9)	−0.0007 (9)
C9	0.0489 (11)	0.0482 (12)	0.0420 (11)	0.0049 (9)	0.0025 (9)	0.0029 (9)
C10	0.0485 (12)	0.0593 (14)	0.0439 (11)	0.0080 (10)	0.0039 (9)	0.0047 (10)
C11	0.0621 (13)	0.0656 (15)	0.0576 (13)	0.0034 (11)	0.0117 (10)	0.0105 (11)
C12A	0.076 (3)	0.098 (2)	0.0587 (18)	0.004 (2)	0.0198 (18)	0.0171 (15)
C13A	0.076 (3)	0.098 (2)	0.0587 (18)	0.004 (2)	0.0198 (18)	0.0171 (15)
C14	0.0943 (18)	0.105 (2)	0.0479 (13)	0.0045 (16)	0.0172 (12)	−0.0045 (14)
C15	0.0626 (14)	0.0730 (16)	0.0452 (12)	0.0009 (11)	0.0096 (10)	−0.0011 (11)
C16	0.0594 (13)	0.0505 (13)	0.0456 (12)	0.0025 (10)	0.0044 (10)	0.0043 (10)
C17	0.127 (2)	0.0565 (15)	0.0587 (15)	−0.0111 (15)	0.0169 (14)	−0.0116 (12)
C18	0.154 (3)	0.0614 (18)	0.090 (2)	−0.0203 (18)	0.0097 (19)	−0.0084 (16)
C12B	0.076 (3)	0.098 (2)	0.0587 (18)	0.004 (2)	0.0198 (18)	0.0171 (15)
C13B	0.076 (3)	0.098 (2)	0.0587 (18)	0.004 (2)	0.0198 (18)	0.0171 (15)

Geometric parameters (Å, º)

S1—C8	1.714 (2)	C13B—C14	1.440 (9)
S1—C15	1.732 (2)	C14—C15	1.512 (3)
O1—C7	1.217 (3)	C17—C18	1.491 (4)
O2—C16	1.221 (3)	C2—H2	0.9300
O3—C16	1.331 (3)	C3—H3	0.9300
O3—C17	1.445 (3)	C4—H4	0.9300
N1—C7	1.359 (3)	C5—H5	0.9300
N1—C8	1.381 (2)	C6—H6	0.9300
N1—H1	0.8600	C11—H11A	0.9700
C1—C2	1.384 (3)	C11—H11B	0.9700
C1—C6	1.386 (3)	C12A—H12A	0.9700
C1—C7	1.488 (3)	C12A—H12B	0.9700
C2—C3	1.378 (3)	C12B—H12D	0.9700
C3—C4	1.366 (4)	C12B—H12C	0.9700
C4—C5	1.361 (4)	C13A—H13B	0.9700
C5—C6	1.375 (4)	C13A—H13A	0.9700
C8—C9	1.375 (3)	C13B—H13C	0.9700
C9—C10	1.444 (3)	C13B—H13D	0.9700
C9—C16	1.457 (3)	C14—H14A	0.9700
C10—C15	1.343 (3)	C14—H14B	0.9700
C10—C11	1.510 (3)	C17—H17A	0.9700
C11—C12A	1.524 (6)	C17—H17B	0.9700
C11—C12B	1.542 (8)	C18—H18B	0.9600
C12A—C13A	1.503 (7)	C18—H18C	0.9600
C12B—C13B	1.514 (12)	C18—H18A	0.9600
C13A—C14	1.544 (6)		
C8—S1—C15	90.83 (10)	C1—C6—H6	120.00
C16—O3—C17	116.70 (17)	C5—C6—H6	120.00
C7—N1—C8	125.72 (18)	C10—C11—H11A	109.00
C7—N1—H1	117.00	C10—C11—H11B	109.00
C8—N1—H1	117.00	C12A—C11—H11A	109.00
C2—C1—C6	118.0 (2)	C12A—C11—H11B	109.00
C2—C1—C7	124.4 (2)	H11A—C11—H11B	108.00
C6—C1—C7	117.5 (2)	C12B—C11—H11A	131.00
C1—C2—C3	120.6 (2)	C12B—C11—H11B	88.00
C2—C3—C4	120.5 (2)	C11—C12A—H12A	109.00
C3—C4—C5	119.6 (3)	C11—C12A—H12B	109.00
C4—C5—C6	120.8 (3)	C13A—C12A—H12A	109.00
C1—C6—C5	120.5 (2)	C13A—C12A—H12B	109.00
O1—C7—C1	123.0 (2)	H12A—C12A—H12B	108.00
O1—C7—N1	120.4 (2)	C13B—C12B—H12C	109.00
N1—C7—C1	116.61 (19)	C11—C12B—H12C	109.00
S1—C8—C9	112.26 (14)	C11—C12B—H12D	109.00
S1—C8—N1	123.14 (16)	C13B—C12B—H12D	109.00
N1—C8—C9	124.60 (18)	H12C—C12B—H12D	108.00

C8—C9—C16	120.08 (17)	C12A—C13A—H13A	109.00
C10—C9—C16	127.95 (18)	C14—C13A—H13A	109.00
C8—C9—C10	111.98 (17)	C14—C13A—H13B	109.00
C11—C10—C15	121.34 (18)	C12A—C13A—H13B	109.00
C9—C10—C11	126.98 (18)	H13A—C13A—H13B	108.00
C9—C10—C15	111.67 (19)	C14—C13B—H13C	109.00
C10—C11—C12B	108.7 (5)	C14—C13B—H13D	109.00
C10—C11—C12A	113.5 (3)	C12B—C13B—H13C	109.00
C11—C12A—C13A	112.0 (4)	C12B—C13B—H13D	109.00
C11—C12B—C13B	112.4 (7)	H13C—C13B—H13D	108.00
C12A—C13A—C14	112.4 (4)	C13A—C14—H14A	110.00
C12B—C13B—C14	111.2 (7)	C13A—C14—H14B	110.00
C13A—C14—C15	108.9 (3)	C15—C14—H14A	110.00
C13B—C14—C15	110.7 (4)	C13B—C14—H14A	131.00
S1—C15—C10	113.26 (16)	C13B—C14—H14B	81.00
S1—C15—C14	120.80 (18)	C15—C14—H14B	110.00
C10—C15—C14	125.9 (2)	H14A—C14—H14B	108.00
O2—C16—C9	124.47 (19)	C18—C17—H17A	110.00
O3—C16—C9	113.69 (18)	O3—C17—H17A	110.00
O2—C16—O3	121.84 (19)	O3—C17—H17B	110.00
O3—C17—C18	107.2 (2)	H17A—C17—H17B	109.00
C1—C2—H2	120.00	C18—C17—H17B	110.00
C3—C2—H2	120.00	C17—C18—H18C	109.00
C2—C3—H3	120.00	C17—C18—H18B	109.00
C4—C3—H3	120.00	H18B—C18—H18C	109.00
C3—C4—H4	120.00	H18A—C18—H18B	109.00
C5—C4—H4	120.00	H18A—C18—H18C	109.00
C4—C5—H5	120.00	C17—C18—H18A	109.00
C6—C5—H5	120.00		

C15—S1—C8—N1	179.88 (17)	S1—C8—C9—C10	0.33 (19)
C15—S1—C8—C9	−0.02 (15)	S1—C8—C9—C16	−179.36 (15)
C8—S1—C15—C10	−0.32 (18)	N1—C8—C9—C10	−179.57 (16)
C8—S1—C15—C14	−178.7 (2)	N1—C8—C9—C16	0.8 (3)
C17—O3—C16—O2	0.5 (3)	C8—C9—C10—C11	178.53 (18)
C17—O3—C16—C9	−178.9 (2)	C8—C9—C10—C15	−0.6 (2)
C16—O3—C17—C18	−176.8 (2)	C16—C9—C10—C11	−1.8 (3)
C8—N1—C7—O1	4.4 (3)	C16—C9—C10—C15	179.1 (2)
C8—N1—C7—C1	−174.38 (19)	C8—C9—C16—O2	−1.6 (3)
C7—N1—C8—S1	−5.3 (3)	C8—C9—C16—O3	177.88 (18)
C7—N1—C8—C9	174.55 (19)	C10—C9—C16—O2	178.8 (2)
C6—C1—C2—C3	−0.9 (4)	C10—C9—C16—O3	−1.8 (3)
C7—C1—C2—C3	176.9 (2)	C9—C10—C11—C12A	170.4 (3)
C2—C1—C6—C5	0.0 (4)	C15—C10—C11—C12A	−10.6 (4)
C7—C1—C6—C5	−178.0 (2)	C9—C10—C15—S1	0.6 (2)
C2—C1—C7—O1	−170.1 (2)	C9—C10—C15—C14	178.9 (2)
C2—C1—C7—N1	8.6 (3)	C11—C10—C15—S1	−178.60 (16)
C6—C1—C7—O1	7.7 (4)	C11—C10—C15—C14	−0.3 (3)

C6—C1—C7—N1	−173.6 (2)	C10—C11—C12A—C13A	39.9 (5)
C1—C2—C3—C4	0.7 (4)	C11—C12A—C13A—C14	−59.8 (6)
C2—C3—C4—C5	0.6 (4)	C12A—C13A—C14—C15	46.7 (5)
C3—C4—C5—C6	−1.6 (4)	C13A—C14—C15—S1	160.7 (3)
C4—C5—C6—C1	1.3 (4)	C13A—C14—C15—C10	−17.5 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.86	2.02	2.664 (2)	131
C6—H6···O1^{i}	0.93	2.44	3.242 (3)	145
C11—H11*A*···O3	0.97	2.45	2.845 (3)	104

Symmetry code: (i) −*x*+2, −*y*+2, −*z*.