

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Ethyl 2-amino-4-(3-nitrophenyl)-4H-1-benzothieno[3,2-*b*]pyran-3-carboxylateMohamed Bakhouch,^a Ghali Al Houari,^a Mohamed El Yazidi,^{a*} Mohamed Saadi^b and Lahcen El Ammari^b^aDépartement de Chimie, Faculté des Sciences, Dhar Mehraz, BP 1796 Atlas, 30000 Fes, Morocco, and ^bLaboratoire de Chimie du Solide Appliquée, Faculté des Sciences, Université Mohammed V-Agdal, Avenue Ibn Battouta, BP 1014, Rabat, Morocco

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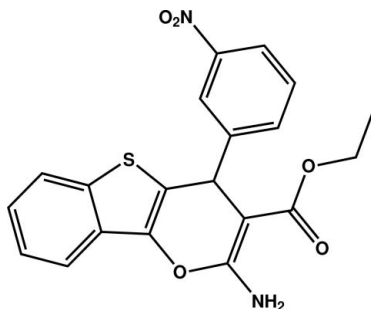
Received 9 April 2014; accepted 15 April 2014

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.044; wR factor = 0.137; data-to-parameter ratio = 19.2.

The molecule of the title compound, $\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}_5\text{S}$, is built up by one fused five-membered and two fused six-membered rings linked to ethoxycarbonyl and 3-nitrophenyl groups. The benzothienopyran ring system is nearly planar (r.m.s deviation = 0.0392 Å) and forms a dihedral angle of 86.90 (6)° with the aromatic ring of the nitrobenzene group. In the crystal, molecules are linked by $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds and by $\pi-\pi$ interactions between the phenyl ring and the six-membered heterocycle [intercentroid distance = 3.5819 (8) Å], forming a three-dimensional network.

Related literature

For background to the organic synthesis of the title compound, see: House (1972); Kabashima *et al.* (2000); Jung (1991). For the preparation of heterocyclic compounds using condensation reactions, see: Boughaleb *et al.* (2011); Cabiddu *et al.* (2002); Pradhan & Asish (2005).



Experimental

Crystal data

 $\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}_5\text{S}$ $M_r = 396.41$

Triclinic, $P\bar{1}$
 $a = 8.3670$ (2) Å
 $b = 9.4319$ (2) Å
 $c = 12.8948$ (4) Å
 $\alpha = 102.505$ (1)°
 $\beta = 106.493$ (1)°
 $\gamma = 94.840$ (1)°

$V = 940.96$ (4) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.21$ mm⁻¹
 $T = 296$ K
 $0.42 \times 0.31 \times 0.26$ mm

Data collection

Bruker X8 APEX diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker, 2009)
 $T_{\min} = 0.673$, $T_{\max} = 0.746$

20668 measured reflections
 4857 independent reflections
 3954 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.137$
 $S = 1.05$
 4857 reflections

253 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.37$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.25$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1B}\cdots\text{O2}$	0.86	2.09	2.6950 (17)	127
$\text{N1}-\text{H1B}\cdots\text{O2}^i$	0.86	2.30	3.0327 (17)	143
$\text{N1}-\text{H1A}\cdots\text{O5}^{ii}$	0.86	2.30	3.1489 (19)	169

Symmetry codes: (i) $-x + 1, -y + 2, -z$; (ii) $x + 1, y + 1, z$.

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, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009) and *pubCIF* (Westrip, 2010).

The authors thank the Unit of Support for Technical and Scientific Research (UATRS, CNRST) for the X-ray measurements.

Supporting information for this paper is available from the IUCr electronic archives (Reference: RZ5118).

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supporting information

Acta Cryst. (2014). E70, o587 [doi:10.1107/S1600536814008538]

Ethyl 2-amino-4-(3-nitrophenyl)-4*H*-1-benzothieno[3,2-*b*]pyran-3-carboxylate

Mohamed Bakhouch, Ghali Al Houari, Mohamed El Yazidi, Mohamed Saadi and Lahcen El Ammari

S1. Comment

The Michael reaction is one of the most efficient methods for effecting carbon–carbon bond formation and has wide synthetic applications (House, 1972; Kabashima *et al.*, 2000). This reaction and its close variants have been extensively used in organic synthesis (Jung, 1991). Generally, Michael additions are conducted in a suitable solvent in the presence of a strong base either at room or at elevated temperatures. In continuing our previous works on the preparation of heterocyclic compounds by using condensation reactions (Boughaleb *et al.*, 2011), we now wish to describe the behavior of ethylcyanoacetate with respect to (*Z*)-2-(3-nitrobenzylidene)-1-benzo[*b*]thiophen-3(2*H*)-one and derivatives in ethanol, with the presence of piperidine as a basic catalyst (Cabiddu *et al.*, 2002; Pradhan & Asish, 2005). We have shown that cyclocondensation starts with a Michael 1,4-addition, followed by intramolecular cyclization *via* nucleophilic addition of the hydroxyl group to the cyano group and not onto the carboxylate, to afford the tricyclic heterocycle ethyl 2-amino-4-(3-nitrophenyl)-4*H*-1-benzothieno[3,2-*b*]pyran-3-carboxylate.

The molecule of the title compound, is formed by three fused rings linked to an ethyl-3-carboxylate and a 3-nitrophenyl group as shown in Fig. 1. The three fused rings (S1/C1–C11/O1) are almost coplanar, with the maximum deviation from the mean plane of $-0.089(2)$ Å at C9, and make a dihedral angle of $86.90(6)^\circ$ with the plane through the attached nitrophenyl group.

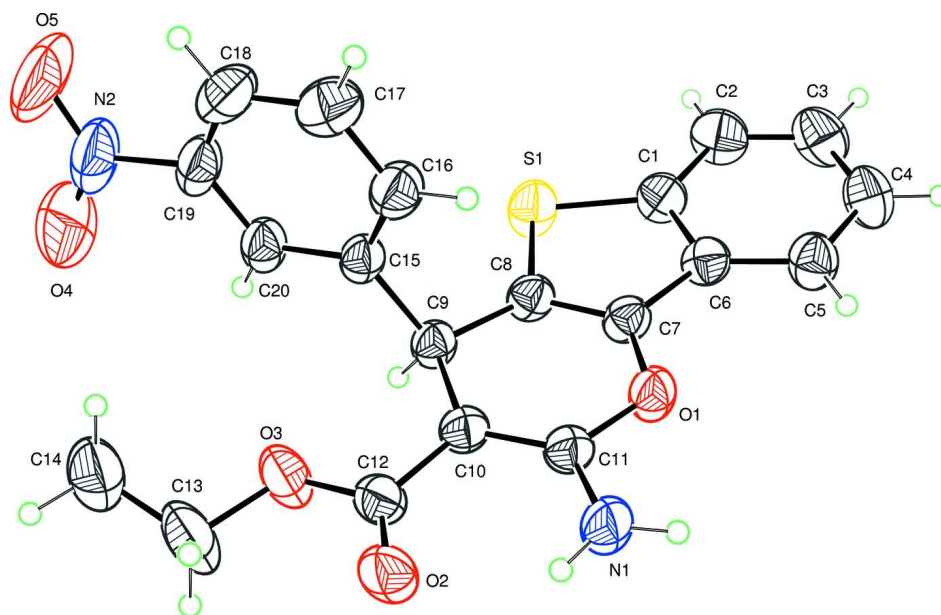
In the crystal, molecules are linked by N—H \cdots O hydrogen bonds and by π – π interactions in a three-dimensional network as shown in Fig. 2 and Table 1.

S2. Experimental

In a 100 ml flask equipped with a condenser was dissolved 4 mmol of (*Z*)-2-(3-nitrobenzylidene)-1-benzo[*b*]thiophen-3(2*H*)-one and 5 mmol of ethyl cyanoacetate in 30 ml of ethanol. Then, 1 ml of piperidine was added, and the reaction mixture was refluxed for 6 h. Thin layer chromatography revealed the formation of a single product. The organic phase was evaporated under reduced pressure. The resulting residue was recrystallized from ethanol (Yield: 68%; m.p.: 493 K).

S3. Refinement

H atoms were located in a difference map and treated as riding with C–H = 0.93–0.97 Å, N–H = 0.86 Å, and with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C}, \text{N})$ or $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{C})$ for methyl H atoms. Two outliers (0 0 1, 0 1 0) were omitted in the last cycles of refinement.

**Figure 1**

The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are represented as small circles.

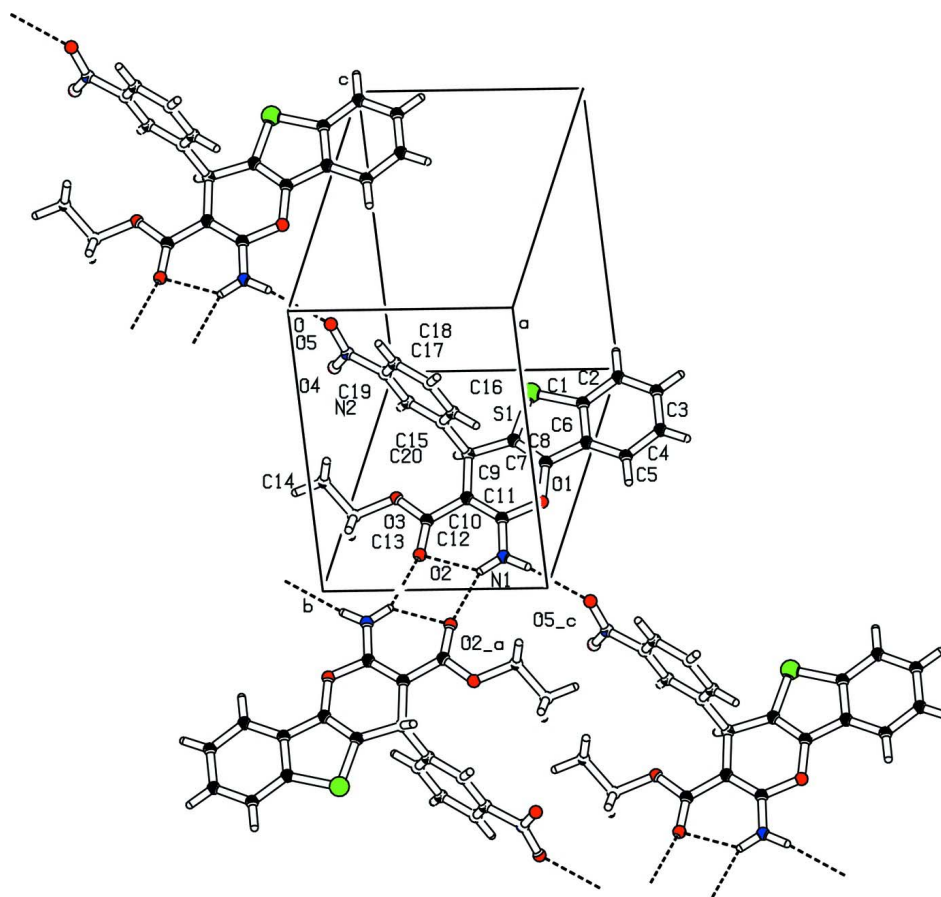


Figure 2

Partial crystal packing for the title compound showing molecules linked by hydrogen bonds (dashed lines).

Ethyl 2-amino-4-(3-nitrophenyl)-4H-1-benzothieno[3,2-b]pyran-3-carboxylate

Crystal data

$C_{20}H_{16}N_2O_5S$

$M_r = 396.41$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.3670$ (2) Å

$b = 9.4319$ (2) Å

$c = 12.8948$ (4) Å

$\alpha = 102.505$ (1)°

$\beta = 106.493$ (1)°

$\gamma = 94.840$ (1)°

$V = 940.96$ (4) Å³

$Z = 2$

$F(000) = 412$

$D_x = 1.399$ Mg m⁻³

Melting point: 493 K

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4857 reflections

$\theta = 2.5$ – 28.7 °

$\mu = 0.21$ mm⁻¹

$T = 296$ K

Block, colourless

$0.42 \times 0.31 \times 0.26$ mm

Data collection

Bruker X8 APEX
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2009)

$T_{\min} = 0.673$, $T_{\max} = 0.746$

20668 measured reflections

4857 independent reflections

3954 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.025$
 $\theta_{\text{max}} = 28.7^\circ$, $\theta_{\text{min}} = 2.5^\circ$
 $h = -11 \rightarrow 11$

$k = -12 \rightarrow 12$
 $l = -17 \rightarrow 17$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.137$
 $S = 1.05$
 4857 reflections
 253 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
 $w = 1/[\sigma^2(F_o^2) + (0.0782P)^2 + 0.1615P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.37 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.25 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	1.03581 (19)	0.74569 (16)	0.51586 (12)	0.0444 (3)
C2	1.1714 (2)	0.7184 (2)	0.59752 (14)	0.0572 (4)
H2	1.1539	0.6646	0.6469	0.069*
C3	1.3318 (2)	0.7739 (2)	0.60256 (14)	0.0596 (4)
H3	1.4239	0.7566	0.6561	0.072*
C4	1.3590 (2)	0.8552 (2)	0.52938 (14)	0.0553 (4)
H4	1.4689	0.8908	0.5347	0.066*
C5	1.22638 (19)	0.88383 (17)	0.44927 (13)	0.0472 (3)
H5	1.2455	0.9388	0.4010	0.057*
C6	1.06239 (17)	0.82841 (14)	0.44214 (11)	0.0388 (3)
C7	0.90329 (17)	0.83869 (14)	0.36665 (11)	0.0366 (3)
C8	0.76677 (17)	0.76734 (14)	0.37893 (11)	0.0373 (3)
C9	0.59063 (16)	0.75463 (14)	0.30354 (11)	0.0356 (3)
H9	0.5205	0.7943	0.3487	0.043*
C10	0.59569 (16)	0.84817 (14)	0.22130 (11)	0.0361 (3)
C11	0.74244 (17)	0.91953 (14)	0.21693 (11)	0.0371 (3)
C12	0.43789 (18)	0.86851 (15)	0.14814 (12)	0.0418 (3)
C13	0.1380 (2)	0.8102 (3)	0.0990 (2)	0.0859 (7)
H13A	0.1389	0.8011	0.0228	0.103*
H13B	0.1031	0.9034	0.1248	0.103*
C14	0.0200 (2)	0.6887 (2)	0.1031 (2)	0.0785 (6)
H14A	-0.0914	0.6910	0.0564	0.118*

H14B	0.0192	0.6988	0.1787	0.118*
H14C	0.0549	0.5969	0.0770	0.118*
C15	0.51766 (16)	0.59335 (14)	0.24462 (11)	0.0363 (3)
C16	0.5980 (2)	0.50862 (16)	0.17907 (13)	0.0486 (3)
H16	0.6969	0.5507	0.1710	0.058*
C17	0.5336 (2)	0.36266 (18)	0.12555 (16)	0.0598 (4)
H17	0.5895	0.3077	0.0820	0.072*
C18	0.3863 (2)	0.29794 (17)	0.13649 (15)	0.0592 (5)
H18	0.3414	0.2000	0.1008	0.071*
C19	0.30905 (19)	0.38353 (17)	0.20176 (14)	0.0516 (4)
C20	0.37110 (17)	0.52953 (16)	0.25679 (12)	0.0439 (3)
H20	0.3155	0.5835	0.3010	0.053*
N1	0.75846 (17)	0.99963 (14)	0.14576 (11)	0.0500 (3)
H1A	0.8569	1.0394	0.1494	0.060*
H1B	0.6704	1.0114	0.0963	0.060*
N2	0.1493 (2)	0.3189 (2)	0.21188 (16)	0.0745 (5)
O1	0.89774 (12)	0.91629 (11)	0.28705 (8)	0.0435 (2)
O2	0.41926 (14)	0.93260 (13)	0.07393 (10)	0.0551 (3)
O3	0.30471 (13)	0.80479 (15)	0.16981 (11)	0.0597 (3)
O4	0.0661 (2)	0.3993 (2)	0.2526 (2)	0.1098 (7)
O5	0.1064 (2)	0.1868 (2)	0.17700 (19)	0.1165 (7)
S1	0.82193 (5)	0.68473 (5)	0.48947 (3)	0.05225 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0450 (7)	0.0467 (7)	0.0397 (7)	0.0057 (6)	0.0084 (6)	0.0138 (6)
C2	0.0577 (10)	0.0676 (10)	0.0468 (8)	0.0126 (8)	0.0067 (7)	0.0273 (7)
C3	0.0479 (9)	0.0773 (11)	0.0482 (9)	0.0150 (8)	0.0012 (7)	0.0211 (8)
C4	0.0391 (8)	0.0712 (10)	0.0487 (9)	0.0056 (7)	0.0063 (6)	0.0119 (7)
C5	0.0410 (7)	0.0539 (8)	0.0423 (7)	0.0017 (6)	0.0072 (6)	0.0130 (6)
C6	0.0404 (7)	0.0371 (6)	0.0342 (6)	0.0037 (5)	0.0068 (5)	0.0064 (5)
C7	0.0392 (7)	0.0346 (6)	0.0343 (6)	0.0025 (5)	0.0082 (5)	0.0107 (5)
C8	0.0394 (7)	0.0373 (6)	0.0343 (6)	0.0030 (5)	0.0083 (5)	0.0126 (5)
C9	0.0349 (6)	0.0380 (6)	0.0360 (6)	0.0032 (5)	0.0121 (5)	0.0129 (5)
C10	0.0377 (7)	0.0355 (6)	0.0373 (6)	0.0054 (5)	0.0113 (5)	0.0139 (5)
C11	0.0380 (6)	0.0356 (6)	0.0386 (7)	0.0054 (5)	0.0106 (5)	0.0131 (5)
C12	0.0388 (7)	0.0452 (7)	0.0477 (8)	0.0116 (5)	0.0156 (6)	0.0197 (6)
C13	0.0361 (9)	0.1282 (19)	0.1168 (18)	0.0216 (10)	0.0176 (10)	0.0839 (16)
C14	0.0483 (10)	0.0803 (13)	0.0881 (15)	0.0057 (9)	0.0018 (10)	0.0096 (11)
C15	0.0341 (6)	0.0387 (6)	0.0365 (6)	0.0011 (5)	0.0075 (5)	0.0166 (5)
C16	0.0476 (8)	0.0441 (7)	0.0552 (9)	0.0014 (6)	0.0198 (7)	0.0119 (6)
C17	0.0684 (11)	0.0455 (8)	0.0610 (10)	0.0067 (7)	0.0188 (9)	0.0067 (7)
C18	0.0655 (10)	0.0412 (7)	0.0560 (9)	−0.0078 (7)	−0.0024 (8)	0.0160 (7)
C19	0.0409 (7)	0.0545 (8)	0.0533 (8)	−0.0106 (6)	−0.0014 (6)	0.0292 (7)
C20	0.0358 (7)	0.0509 (7)	0.0467 (8)	−0.0001 (6)	0.0094 (6)	0.0228 (6)
N1	0.0416 (6)	0.0573 (7)	0.0569 (8)	0.0010 (5)	0.0113 (6)	0.0342 (6)
N2	0.0517 (9)	0.0814 (11)	0.0832 (11)	−0.0221 (8)	0.0030 (8)	0.0424 (9)

O1	0.0356 (5)	0.0502 (5)	0.0465 (5)	-0.0001 (4)	0.0085 (4)	0.0239 (4)
O2	0.0458 (6)	0.0699 (7)	0.0608 (7)	0.0148 (5)	0.0145 (5)	0.0404 (6)
O3	0.0343 (5)	0.0866 (8)	0.0737 (8)	0.0155 (5)	0.0171 (5)	0.0496 (7)
O4	0.0650 (10)	0.1204 (15)	0.1621 (19)	-0.0096 (10)	0.0533 (12)	0.0581 (14)
O5	0.0925 (12)	0.0841 (11)	0.1571 (18)	-0.0447 (9)	0.0255 (12)	0.0378 (11)
S1	0.0472 (2)	0.0633 (3)	0.0485 (2)	-0.00050 (17)	0.00801 (16)	0.03121 (18)

Geometric parameters (Å, °)

C1—C2	1.396 (2)	C12—O3	1.3482 (17)
C1—C6	1.405 (2)	C13—O3	1.446 (2)
C1—S1	1.7449 (16)	C13—C14	1.469 (3)
C2—C3	1.377 (3)	C13—H13A	0.9700
C2—H2	0.9300	C13—H13B	0.9700
C3—C4	1.392 (3)	C14—H14A	0.9600
C3—H3	0.9300	C14—H14B	0.9600
C4—C5	1.376 (2)	C14—H14C	0.9600
C4—H4	0.9300	C15—C20	1.3843 (18)
C5—C6	1.397 (2)	C15—C16	1.388 (2)
C5—H5	0.9300	C16—C17	1.383 (2)
C6—C7	1.4338 (18)	C16—H16	0.9300
C7—C8	1.3423 (18)	C17—C18	1.386 (3)
C7—O1	1.3768 (15)	C17—H17	0.9300
C8—C9	1.4959 (18)	C18—C19	1.371 (3)
C8—S1	1.7378 (14)	C18—H18	0.9300
C9—C10	1.5261 (17)	C19—C20	1.384 (2)
C9—C15	1.5308 (17)	C19—N2	1.473 (2)
C9—H9	0.9800	C20—H20	0.9300
C10—C11	1.3712 (18)	N1—H1A	0.8600
C10—C12	1.4436 (19)	N1—H1B	0.8600
C11—N1	1.3356 (17)	N2—O4	1.208 (3)
C11—O1	1.3633 (16)	N2—O5	1.214 (2)
C12—O2	1.2195 (17)		
C2—C1—C6	120.99 (15)	O3—C13—C14	108.58 (16)
C2—C1—S1	127.04 (13)	O3—C13—H13A	110.0
C6—C1—S1	111.96 (11)	C14—C13—H13A	110.0
C3—C2—C1	117.84 (16)	O3—C13—H13B	110.0
C3—C2—H2	121.1	C14—C13—H13B	110.0
C1—C2—H2	121.1	H13A—C13—H13B	108.4
C2—C3—C4	121.46 (15)	C13—C14—H14A	109.5
C2—C3—H3	119.3	C13—C14—H14B	109.5
C4—C3—H3	119.3	H14A—C14—H14B	109.5
C5—C4—C3	121.21 (16)	C13—C14—H14C	109.5
C5—C4—H4	119.4	H14A—C14—H14C	109.5
C3—C4—H4	119.4	H14B—C14—H14C	109.5
C4—C5—C6	118.47 (15)	C20—C15—C16	119.01 (13)
C4—C5—H5	120.8	C20—C15—C9	120.39 (12)

C6—C5—H5	120.8	C16—C15—C9	120.59 (11)
C5—C6—C1	120.03 (13)	C17—C16—C15	121.20 (15)
C5—C6—C7	130.31 (13)	C17—C16—H16	119.4
C1—C6—C7	109.65 (12)	C15—C16—H16	119.4
C8—C7—O1	124.23 (12)	C16—C17—C18	120.27 (17)
C8—C7—C6	115.68 (12)	C16—C17—H17	119.9
O1—C7—C6	120.09 (11)	C18—C17—H17	119.9
C7—C8—C9	124.19 (12)	C19—C18—C17	117.59 (14)
C7—C8—S1	111.37 (10)	C19—C18—H18	121.2
C9—C8—S1	124.38 (10)	C17—C18—H18	121.2
C8—C9—C10	107.83 (10)	C18—C19—C20	123.38 (14)
C8—C9—C15	110.43 (11)	C18—C19—N2	118.73 (15)
C10—C9—C15	112.40 (10)	C20—C19—N2	117.87 (17)
C8—C9—H9	108.7	C19—C20—C15	118.54 (15)
C10—C9—H9	108.7	C19—C20—H20	120.7
C15—C9—H9	108.7	C15—C20—H20	120.7
C11—C10—C12	118.22 (12)	C11—N1—H1A	120.0
C11—C10—C9	123.25 (12)	C11—N1—H1B	120.0
C12—C10—C9	118.45 (11)	H1A—N1—H1B	120.0
N1—C11—O1	109.61 (11)	O4—N2—O5	123.09 (19)
N1—C11—C10	127.07 (13)	O4—N2—C19	118.92 (16)
O1—C11—C10	123.32 (12)	O5—N2—C19	118.0 (2)
O2—C12—O3	121.52 (13)	C11—O1—C7	116.95 (10)
O2—C12—C10	126.91 (13)	C12—O3—C13	117.57 (13)
O3—C12—C10	111.56 (12)	C8—S1—C1	91.31 (7)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1B \cdots O2	0.86	2.09	2.6950 (17)	127
N1—H1B \cdots O2 ⁱ	0.86	2.30	3.0327 (17)	143
N1—H1A \cdots O5 ⁱⁱ	0.86	2.30	3.1489 (19)	169

Symmetry codes: (i) $-x+1, -y+2, -z$; (ii) $x+1, y+1, z$.