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Diethyl 2-amino-5-[(*E*)-(furan-2-yl-methylidene)amino]thiophene-3,4-dicarboxylate

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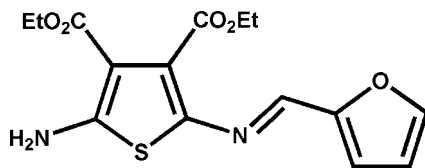
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 Key indicators: single-crystal X-ray study; $T = 123$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.037; wR factor = 0.102; data-to-parameter ratio = 14.3.

In the crystal structure of the title compound, $\text{C}_{15}\text{H}_{16}\text{N}_2\text{O}_5\text{S}$, the azomethine adopts the *E* configuration. The two heterocyclic rings adopt an antiperiplanar orientation. The mean planes of the thiophene and furan rings are twisted by $2.51(4)^\circ$. The crystal structure exhibits intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonding. $\pi-\pi$ stacking is also observed, the centroid-to-centroid distance being $3.770(4)$ Å.

Related literature

For general background, see: Dufresne & Skene (2008). For a related crystal structure, see: Skene *et al.* (2006)



Experimental

Crystal data

 $\text{C}_{15}\text{H}_{16}\text{N}_2\text{O}_5\text{S}$
 $M_r = 336.36$

 Monoclinic, $P2_1/n$
 $a = 9.3452(19)$ Å

 $b = 14.635(3)$ Å

 $c = 11.343(2)$ Å

 $\beta = 99.73(3)^\circ$
 $V = 1529.0(5)$ Å³
 $Z = 4$

 Cu $K\alpha$ radiation

 $\mu = 2.14$ mm⁻¹
 $T = 123$ K

 $0.14 \times 0.10 \times 0.04$ mm

Data collection

 Bruker SMART 6000 diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.728$, $T_{\max} = 0.920$

 6320 measured reflections
 3005 independent reflections
 2475 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.036$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.102$
 $S = 1.03$

3005 reflections

210 parameters

H-atom parameters constrained

 $\Delta\rho_{\max} = 0.29$ e Å⁻³
 $\Delta\rho_{\min} = -0.34$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1A}\cdots\text{O2}^{\text{i}}$	0.88	2.20	2.889 (2)	135
$\text{N1}-\text{H1B}\cdots\text{O4}^{\text{ii}}$	0.88	2.50	3.059 (3)	122

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

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *UdMX* (Marris, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2415).

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supporting information

Acta Cryst. (2010). E66, o3027 [https://doi.org/10.1107/S1600536810043746]

Diethyl 2-amino-5-[(*E*)-(furan-2-ylmethylidene)amino]thiophene-3,4-dicarboxylate

Stéphane Dufresne and W. G. Skene

S1. Comment

During the course of our ongoing conjugated azomethine research, we prepared the title compound. The X-ray crystallographic analysis not only confirmed the structure (Fig. 1), but that the energetically stable *E* isomer was formed. Neither solvent nor counter-ions were found in the structure.

The heterocyclic rings were found not to be coplanar; the angle between the heterocyclic mean planes is 2.51 (4)°. This angle is less than that in a previously reported azomethine thiophene system, whose angle is 7.25 (11)° (Skene *et al.*, 2006).

A major point of interest is the azomethine bond. The bond lengths for N2—C4, N2—C5 and C5—C6 are 1.382 (2), 1.289 (2) and 1.420 (2) Å, respectively. These are similar to the related azomethine thiophene compound (Skene *et al.*, 2006), whose homologous lengths are 1.381 (3), 1.283 (3) and 1.426 (3) Å.

Fig. 2 shows that two different hydrogen bonds occur in the crystal structure, viz. N1—H1A⋯O2ⁱⁱⁱ and N1—H1B⋯O4ⁱⁱ. The D—H⋯A angles are 135° and 122° and distances of 2.880 (3) Å and 3.059 (3) Å were measured between the nitrogen and oxygens (Table 1). Dimerization of two molecules occurs *via* H-bonding between N1—H1A⋯O2ⁱⁱⁱ. Additionally, π -stacking takes place between two different molecules, at $[x, y, z]$ and $[1 - x, -y, 1 - z]$. Fig. 3 shows the interactions, with the distance between the planes being 3.440 (4) Å. The centroid⋯centroid distance between the two rings is 3.770 (4) Å.

S2. Experimental

2-Furaldehyde (37 mg, 0.39 mmol) and 2,5-diamino-thiophene-3,4-dicarboxylic acid diethyl ester (100 mg, 0.39 mmol) were mixed in anhydrous 2-propanol with a catalytic amount of TFA and refluxed for 12 h. The reaction was then purified by flash chromatography to afford the title compound as a brownish yellow solid (110 mg, 85%). Single crystals were obtained by slow evaporation of an acetone solution.

S3. Refinement

Carbon-bound H atoms were placed in calculated positions (Cmethyl—H = 0.98 Å, Cmethylene—H = 0.99 Å and Csp²—H = 0.95 Å) and included in the refinement in the riding-model approximation, with $U_{\text{iso}}(\text{H}) = kU_{\text{eq}}(\text{C})$, where $k = 1.5$ for Cmethyl and 1.2 for Cmethylene and Csp². The H atoms of the amino group were placed in calculated positions (N—H = 0.88 Å) and included in the refinement in the riding-model approximation, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$.

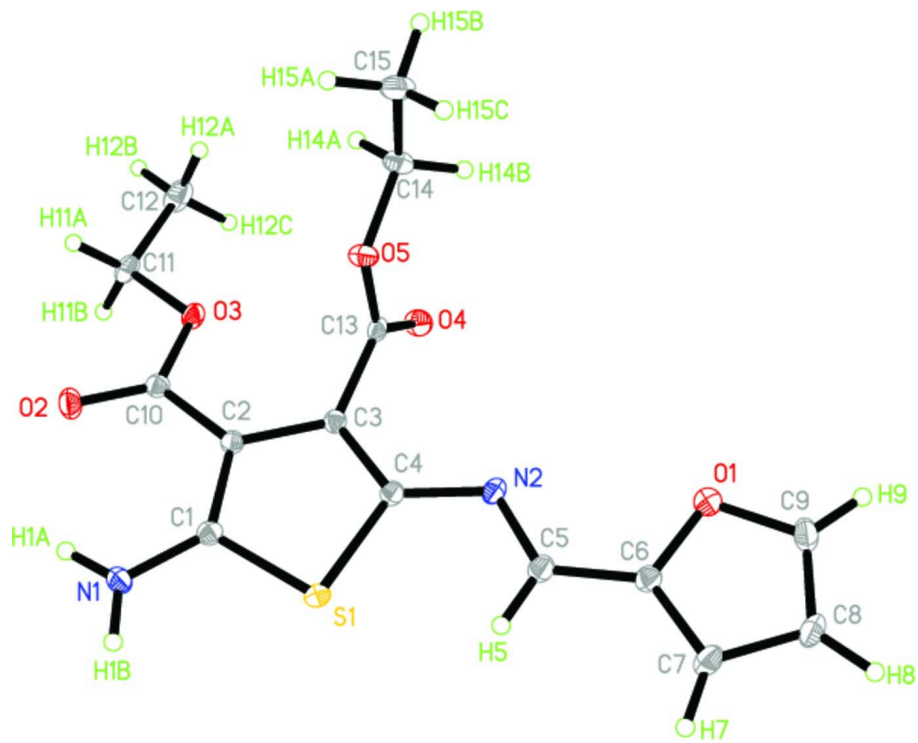


Figure 1

ORTEP-3 (Farrugia, 1997) representation of the molecular structure, with the numbering scheme adopted. Displacement ellipsoids are drawn at the 30% probability level. H atoms are shown as spheres of arbitrary radius.

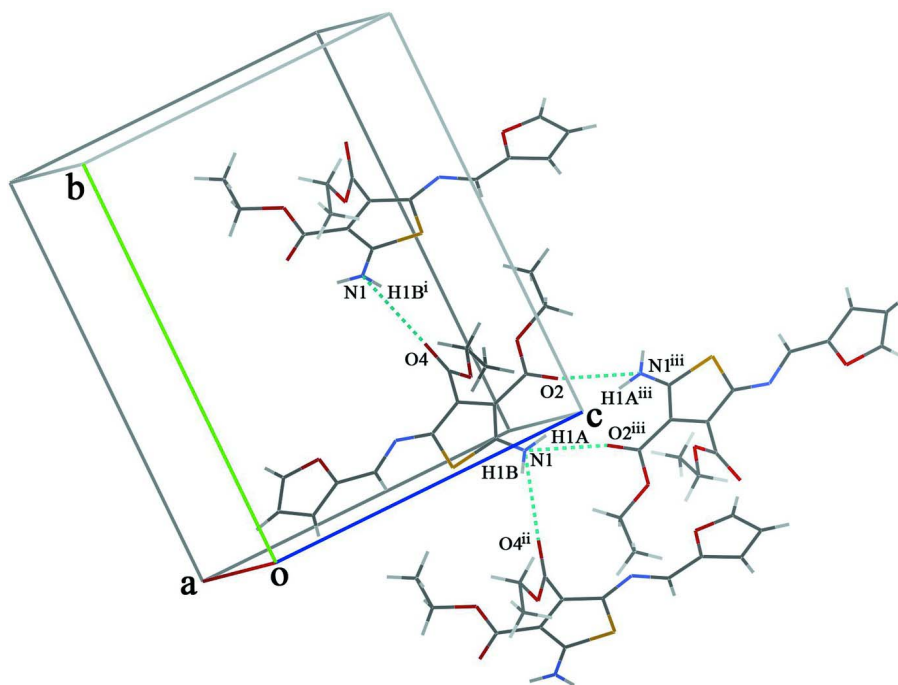


Figure 2

Supramolecular structure showing the intermolecular hydrogen bonding (dashed lines). [Symmetry codes: (i) $1/2 - x, 1/2 + y, 1.5 - z$; (ii) $1/2 - x, -1/2 + y, 1.5 - z$; (iii) $-x, -y, 2 - z$.]

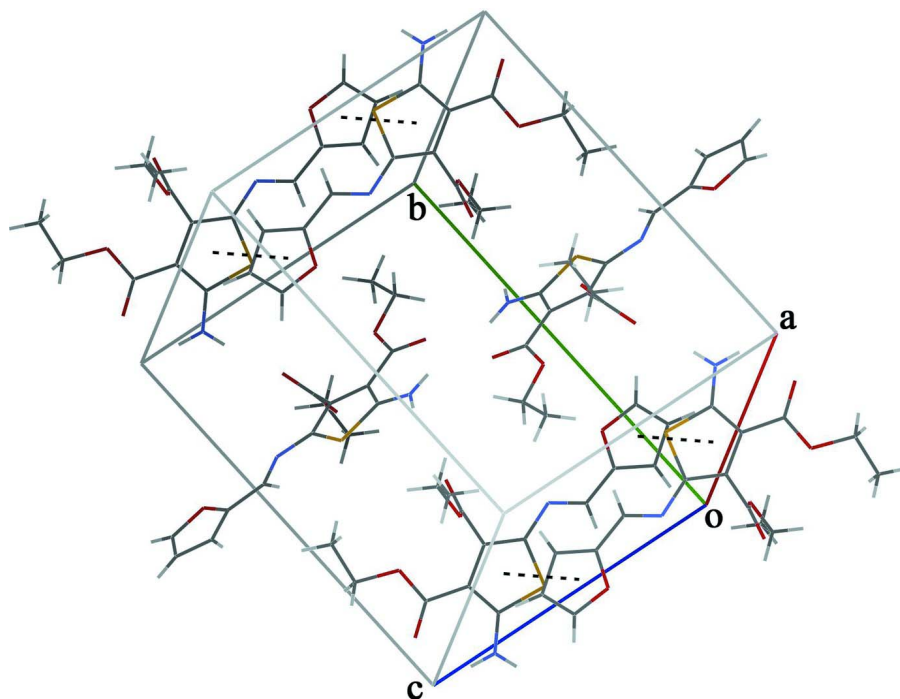


Figure 3

The three-dimensional network demonstrating the π -stacking (dashed lines) in the crystal structure.

Diethyl 2-amino-5-[(E)-(furan-2-ylmethylidene)amino]thiophene-3,4-dicarboxylate

Crystal data

$C_{15}H_{16}N_2O_5S$

$M_r = 336.36$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1/n$

$a = 9.3452\ (19)\ \text{\AA}$

$b = 14.635\ (3)\ \text{\AA}$

$c = 11.343\ (2)\ \text{\AA}$

$\beta = 99.73\ (3)^\circ$

$V = 1529.0\ (5)\ \text{\AA}^3$

$Z = 4$

$F(000) = 704$

$D_x = 1.461\ \text{Mg m}^{-3}$

Melting point: $425(2)\ \text{K}$

Cu $K\alpha$ radiation, $\lambda = 1.54178\ \text{\AA}$

Cell parameters from 3360 reflections

$\theta = 5.0\text{--}38.8^\circ$

$\mu = 2.14\ \text{mm}^{-1}$

$T = 123\ \text{K}$

Block, yellow

$0.14 \times 0.10 \times 0.04\ \text{mm}$

Data collection

Bruker SMART 6000

diffractometer

Radiation source: rotating anode

Montel 200 optics monochromator

Detector resolution: $5.5\ \text{pixels mm}^{-1}$

ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.728$, $T_{\max} = 0.920$

6320 measured reflections

3005 independent reflections

2475 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$

$\theta_{\max} = 72.3^\circ$, $\theta_{\min} = 5.0^\circ$

$h = -11 \rightarrow 11$

$k = -17 \rightarrow 18$

$l = -13 \rightarrow 13$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.037$ $wR(F^2) = 0.102$ $S = 1.03$

3005 reflections

210 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0643P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.29 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.34 \text{ e } \text{\AA}^{-3}$ *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	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.15876 (5)	0.01058 (3)	0.62132 (4)	0.02153 (13)
O3	0.26457 (13)	0.20322 (8)	0.97617 (10)	0.0216 (3)
O5	0.53448 (13)	0.16250 (8)	0.86520 (11)	0.0229 (3)
O1	0.53601 (14)	0.14839 (10)	0.36188 (11)	0.0299 (3)
O4	0.42258 (13)	0.28091 (8)	0.76310 (11)	0.0261 (3)
O2	0.11370 (14)	0.08821 (9)	1.00209 (11)	0.0280 (3)
N2	0.37833 (15)	0.11513 (10)	0.55344 (12)	0.0201 (3)
N1	0.01952 (16)	-0.02136 (10)	0.80267 (14)	0.0247 (3)
H1A	-0.0029	-0.0108	0.8737	0.030*
H1B	-0.0274	-0.0637	0.7563	0.030*
C13	0.42543 (18)	0.20165 (12)	0.79259 (14)	0.0180 (3)
C2	0.21155 (17)	0.09610 (11)	0.82328 (15)	0.0177 (3)
C4	0.29499 (18)	0.09523 (12)	0.63985 (15)	0.0194 (4)
C10	0.19189 (18)	0.12672 (12)	0.94126 (15)	0.0192 (4)
C3	0.30893 (17)	0.13360 (12)	0.75044 (14)	0.0175 (3)
C14	0.65332 (19)	0.22184 (13)	0.91629 (17)	0.0274 (4)
H14A	0.6231	0.2619	0.9780	0.033*
H14B	0.6830	0.2608	0.8533	0.033*
C1	0.12570 (18)	0.02730 (12)	0.76478 (15)	0.0191 (4)
C6	0.42538 (19)	0.08612 (12)	0.35493 (16)	0.0218 (4)
C5	0.35120 (19)	0.07232 (12)	0.45285 (15)	0.0225 (4)
H5	0.2757	0.0281	0.4435	0.027*
C11	0.2356 (2)	0.24369 (13)	1.08714 (15)	0.0259 (4)
H11A	0.2526	0.1984	1.1528	0.031*
H11B	0.1335	0.2646	1.0776	0.031*

C8	0.5077 (2)	0.08255 (14)	0.18213 (16)	0.0284 (4)
H8	0.5204	0.0675	0.1031	0.034*
C7	0.4049 (2)	0.04441 (13)	0.24649 (16)	0.0272 (4)
H7	0.3351	-0.0014	0.2191	0.033*
C9	0.5836 (2)	0.14410 (15)	0.25473 (17)	0.0316 (5)
H9	0.6604	0.1800	0.2343	0.038*
C15	0.7766 (2)	0.16205 (14)	0.97085 (18)	0.0320 (4)
H15A	0.7455	0.1231	1.0321	0.048*
H15B	0.8583	0.2002	1.0075	0.048*
H15C	0.8068	0.1237	0.9087	0.048*
C12	0.3367 (2)	0.32281 (13)	1.11445 (17)	0.0351 (5)
H12A	0.4372	0.3007	1.1284	0.053*
H12B	0.3167	0.3543	1.1862	0.053*
H12C	0.3227	0.3653	1.0467	0.053*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0226 (2)	0.0245 (2)	0.0170 (2)	-0.00387 (17)	0.00208 (16)	-0.00373 (16)
O3	0.0288 (7)	0.0215 (6)	0.0158 (6)	-0.0027 (5)	0.0072 (5)	-0.0041 (5)
O5	0.0206 (6)	0.0213 (6)	0.0245 (7)	-0.0023 (5)	-0.0025 (5)	-0.0003 (5)
O1	0.0275 (7)	0.0373 (8)	0.0254 (7)	-0.0063 (6)	0.0062 (6)	-0.0053 (6)
O4	0.0286 (7)	0.0206 (7)	0.0278 (7)	-0.0032 (5)	0.0013 (5)	0.0036 (5)
O2	0.0310 (7)	0.0308 (7)	0.0253 (7)	-0.0070 (6)	0.0134 (6)	-0.0019 (6)
N2	0.0221 (7)	0.0234 (8)	0.0148 (7)	0.0023 (6)	0.0036 (6)	0.0009 (6)
N1	0.0242 (8)	0.0269 (8)	0.0239 (8)	-0.0083 (6)	0.0069 (6)	-0.0038 (6)
C13	0.0205 (8)	0.0216 (9)	0.0131 (8)	0.0010 (6)	0.0060 (6)	-0.0011 (6)
C2	0.0171 (8)	0.0183 (8)	0.0175 (8)	0.0003 (6)	0.0028 (6)	0.0004 (6)
C4	0.0191 (8)	0.0222 (9)	0.0170 (8)	0.0003 (7)	0.0032 (7)	0.0008 (7)
C10	0.0178 (8)	0.0213 (9)	0.0184 (8)	0.0015 (6)	0.0025 (7)	0.0006 (7)
C3	0.0174 (8)	0.0184 (8)	0.0168 (8)	0.0013 (6)	0.0032 (6)	0.0017 (6)
C14	0.0222 (9)	0.0273 (10)	0.0309 (10)	-0.0057 (7)	-0.0011 (8)	-0.0059 (8)
C1	0.0181 (8)	0.0200 (8)	0.0185 (8)	0.0023 (6)	0.0013 (7)	0.0006 (7)
C6	0.0235 (8)	0.0226 (9)	0.0188 (8)	0.0000 (7)	0.0022 (7)	0.0008 (7)
C5	0.0267 (9)	0.0222 (9)	0.0188 (9)	-0.0013 (7)	0.0041 (7)	0.0005 (7)
C11	0.0380 (10)	0.0256 (9)	0.0154 (8)	0.0023 (8)	0.0080 (8)	-0.0038 (7)
C8	0.0314 (10)	0.0375 (11)	0.0174 (9)	0.0075 (8)	0.0076 (8)	0.0002 (8)
C7	0.0365 (10)	0.0259 (10)	0.0198 (9)	-0.0008 (8)	0.0061 (8)	-0.0038 (7)
C9	0.0266 (10)	0.0429 (12)	0.0278 (10)	-0.0014 (8)	0.0115 (8)	0.0052 (9)
C15	0.0236 (9)	0.0391 (11)	0.0303 (10)	0.0003 (8)	-0.0043 (8)	-0.0037 (9)
C12	0.0578 (14)	0.0241 (10)	0.0235 (10)	-0.0043 (10)	0.0078 (9)	-0.0049 (8)

Geometric parameters (Å, °)

S1—C1	1.7242 (18)	C14—C15	1.495 (3)
S1—C4	1.7633 (18)	C14—H14A	0.99
O3—C10	1.334 (2)	C14—H14B	0.99
O3—C11	1.4573 (19)	C6—C7	1.357 (2)

O5—C13	1.3272 (19)	C6—C5	1.420 (2)
O5—C14	1.451 (2)	C5—H5	0.95
O1—C9	1.364 (2)	C11—C12	1.494 (3)
O1—C6	1.370 (2)	C11—H11A	0.99
O4—C13	1.206 (2)	C11—H11B	0.99
O2—C10	1.224 (2)	C8—C9	1.340 (3)
N2—C5	1.289 (2)	C8—C7	1.416 (3)
N2—C4	1.382 (2)	C8—H8	0.95
N1—C1	1.349 (2)	C7—H7	0.95
N1—H1A	0.88	C9—H9	0.95
N1—H1B	0.88	C15—H15A	0.98
C13—C3	1.493 (2)	C15—H15B	0.98
C2—C1	1.385 (2)	C15—H15C	0.98
C2—C3	1.437 (2)	C12—H12A	0.98
C2—C10	1.452 (2)	C12—H12B	0.98
C4—C3	1.360 (2)	C12—H12C	0.98
C1—S1—C4	91.65 (8)	C7—C6—C5	129.21 (18)
C10—O3—C11	115.96 (13)	O1—C6—C5	120.86 (16)
C13—O5—C14	116.42 (14)	N2—C5—C6	125.07 (17)
C9—O1—C6	105.92 (15)	N2—C5—H5	117.5
C5—N2—C4	118.38 (15)	C6—C5—H5	117.5
C1—N1—H1A	120	O3—C11—C12	106.90 (15)
C1—N1—H1B	120	O3—C11—H11A	110.3
H1A—N1—H1B	120	C12—C11—H11A	110.3
O4—C13—O5	124.46 (16)	O3—C11—H11B	110.3
O4—C13—C3	124.88 (16)	C12—C11—H11B	110.3
O5—C13—C3	110.65 (14)	H11A—C11—H11B	108.6
C1—C2—C3	111.96 (15)	C9—C8—C7	106.42 (17)
C1—C2—C10	120.84 (15)	C9—C8—H8	126.8
C3—C2—C10	127.08 (15)	C7—C8—H8	126.8
C3—C4—N2	126.11 (16)	C6—C7—C8	106.60 (17)
C3—C4—S1	110.77 (13)	C6—C7—H7	126.7
N2—C4—S1	123.06 (13)	C8—C7—H7	126.7
O2—C10—O3	122.79 (16)	C8—C9—O1	111.14 (17)
O2—C10—C2	123.91 (16)	C8—C9—H9	124.4
O3—C10—C2	113.27 (14)	O1—C9—H9	124.4
C4—C3—C2	113.65 (15)	C14—C15—H15A	109.5
C4—C3—C13	121.43 (15)	C14—C15—H15B	109.5
C2—C3—C13	124.67 (15)	H15A—C15—H15B	109.5
O5—C14—C15	107.41 (15)	C14—C15—H15C	109.5
O5—C14—H14A	110.2	H15A—C15—H15C	109.5
C15—C14—H14A	110.2	H15B—C15—H15C	109.5
O5—C14—H14B	110.2	C11—C12—H12A	109.5
C15—C14—H14B	110.2	C11—C12—H12B	109.5
H14A—C14—H14B	108.5	H12A—C12—H12B	109.5
N1—C1—C2	128.96 (16)	C11—C12—H12C	109.5
N1—C1—S1	118.97 (13)	H12A—C12—H12C	109.5

C2—C1—S1	111.94 (13)	H12B—C12—H12C	109.5
C7—C6—O1	109.92 (16)		
C14—O5—C13—O4	3.5 (2)	O5—C13—C3—C4	-101.12 (18)
C14—O5—C13—C3	-177.89 (14)	O4—C13—C3—C2	-108.6 (2)
C5—N2—C4—C3	179.86 (17)	O5—C13—C3—C2	72.8 (2)
C5—N2—C4—S1	2.9 (2)	C13—O5—C14—C15	-167.31 (15)
C1—S1—C4—C3	-1.07 (14)	C3—C2—C1—N1	-177.66 (17)
C1—S1—C4—N2	176.35 (15)	C10—C2—C1—N1	-1.3 (3)
C11—O3—C10—O2	-5.4 (2)	C3—C2—C1—S1	-1.82 (18)
C11—O3—C10—C2	172.78 (14)	C10—C2—C1—S1	174.49 (12)
C1—C2—C10—O2	9.1 (3)	C4—S1—C1—N1	177.96 (14)
C3—C2—C10—O2	-175.17 (17)	C4—S1—C1—C2	1.66 (13)
C1—C2—C10—O3	-169.01 (15)	C9—O1—C6—C7	0.0 (2)
C3—C2—C10—O3	6.7 (2)	C9—O1—C6—C5	179.52 (17)
N2—C4—C3—C2	-177.09 (15)	C4—N2—C5—C6	178.96 (16)
S1—C4—C3—C2	0.22 (19)	C7—C6—C5—N2	179.79 (19)
N2—C4—C3—C13	-2.6 (3)	O1—C6—C5—N2	0.3 (3)
S1—C4—C3—C13	174.76 (12)	C10—O3—C11—C12	175.14 (15)
C1—C2—C3—C4	1.0 (2)	O1—C6—C7—C8	-0.1 (2)
C10—C2—C3—C4	-175.00 (16)	C5—C6—C7—C8	-179.58 (18)
C1—C2—C3—C13	-173.30 (15)	C9—C8—C7—C6	0.2 (2)
C10—C2—C3—C13	10.7 (3)	C7—C8—C9—O1	-0.2 (2)
O4—C13—C3—C4	77.5 (2)	C6—O1—C9—C8	0.1 (2)

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—H1A \cdots O2 ⁱ	0.88	2.20	2.889 (2)	135
N1—H1B \cdots O4 ⁱⁱ	0.88	2.50	3.059 (3)	122

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