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Ethyl 8-amino-2-(*o*-tolyloxy)-4-oxo-3-phenyl-3,4-dihydrothieno[2′,3′:2,3]-thieno[4,5-*d*]pyrimidine-6-carboxylate

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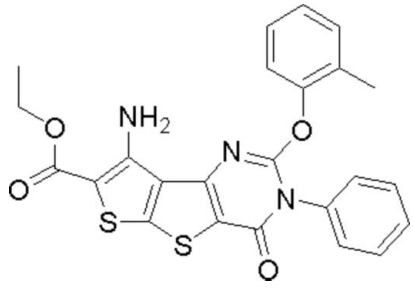
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.007 Å; R factor = 0.067; wR factor = 0.179; data-to-parameter ratio = 13.3.

In the title compound, $C_{24}H_{19}N_3O_4S_2$, the fused thieno-thienopyrimidine ring system is essentially planar, and makes a dihedral angle of 85.61 (2) and 72.02 (2)° with the phenyl and *o*-tolyloxy rings, respectively. The molecular structure is stabilized by intramolecular N—H···N and N—H···O hydrogen bonds. The crystal packing is stabilized mainly by intermolecular π–π interactions between adjacent thienothienopyrimidine ring systems; the centroid–centroid distances between the central and outer thiophene rings and between adjacent outer thiophene rings are 3.841 (4) and 3.696 (4) Å, respectively.

Related literature

Many derivatives of pyrimidinone have been prepared, and their biological and pharmaceutical activities have been studied by Modica *et al.* (2004) and Panico *et al.* (2001). For related literature, see: Janiak (2000); Ding *et al.* (2004); Liu *et al.* (2006).



Experimental

Crystal data

$C_{24}H_{19}N_3O_4S_2$
M_r = 477.54
Triclinic, $P\overline{1}$
a = 7.0996 (6) Å
b = 10.444 (9) Å
c = 16.9985 (13) Å
α = 104.447 (1)°
β = 97.120 (1)°
γ = 106.041 (1)°
V = 1147.5 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 292 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.924, T_{max} = 0.974
9743 measured reflections
3980 independent reflections
2644 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.179
S = 1.04
3980 reflections
300 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O5	0.86	2.22	2.799 (4)	124
N3—H3B···N2	0.86	2.56	3.158 (4)	128

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2198).

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supplementary materials

Acta Cryst. (2007). E**63**, o3664 [**doi:10.1107/S1600536807036781**]

Ethyl 8-amino-2-(*o*-tolyloxy)-4-oxo-3-phenyl-3,4-dihydrothieno[2',3':2,3]thieno[4,5-*d*]pyrimidine-6-carboxylate

M.-G. Liu, Z. Ma, T. Xie and Z.-Z. Yang

Comment

The derivatives of thienopyrimidine are of great importance because of their remarked biological properties (Panico *et al.*, 2001; Ding *et al.*, 2004; Modica *et al.*, 2004). We have recently focused on the synthesis of fused heterocyclic systems containing a fused pyrimidinone ring moiety using aza-Wittig reaction (Liu *et al.*, 2006). The title compound, (I), may be used as a new precursor for obtaining bioactive molecules and its structure is reported here (Fig. 1). The bond lengths and angles are unexceptional. The thienothienopyrimidinone ring system is essentially planar, with maximum deviations 0.034 (1) and 0.021 (3) Å for S1 and C20, respectively; the C1—C6 phenyl ring is twisted with respect to it, with a dihedral angle of 85.61 (2)°. Intramolecular N—H···O and N—H···N hydrogen bonds interactions are present which stabilize the molecular structure (Table 1). There are also intermolecular π-π interactions (Janiak, 2000; Fig. 2). In the thienothiophene system (ring A: S1/C18/C19/C20/C21 and B: S2/C10/C9/C19/C18), the interplanar perpendicular distances between them A/A^{i} and A/B^{i} [symmetry code (i): 2 − *x*, 2 − *y*, 2 − *z*] are 3.490 (3) and 3.471 (3) Å, respectively, and the center-to-center distances are 3.696 (4) and 3.841 (4) Å.

Experimental

To a solution of diethyl 3-triphenylphosphoranylideneamino- 4-aminothieno[2,3-*b*]thiophene-2,5-dicarboxylate (3 mmol) in anhydrous dichloromethane (15 ml) was added phenyl isocyanate (3 mmol) under dry nitrogen at room temperature. The reaction mixture was left unstirred for 8 h at 273–278 K, then the solvent was removed under reduced pressure, which was used directly without further purification. To the reaction mixture was added anhydrous acetonitrile (15 ml) with 2-methyl-phenol (3 mmol) and anhydrous K_2CO_3 (1 mmol). The mixture was stirred for 6 h at 313–323 K, the solution concentrated under reduced pressure. The title compound was recrystallized from ethanol/dichloromethane (1:2 *v*/*v*) at room temperature, yielding single crystals suitable for X-ray diffraction.

Refinement

H atoms were located in a difference map and treated as riding, with C—H = 0.93–0.97 and N—H = 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(C, N) or 1.5U_{eq}(methyl C).

Figures

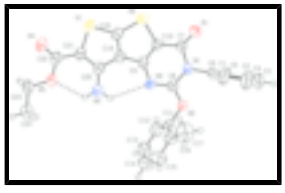


Fig. 1. The molecular structure of the title compound, with atom labels and 50% probability displacement ellipsoids for non-H atoms. The intramolecular N—H···N/O hydrogen bonds are indicated by dashed lines.

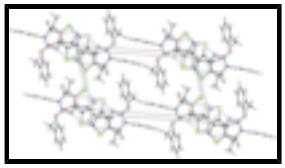


Fig. 2. A packing view of the title compound along the *a* axis, showing the hydrogen bonds as dashed lines.

Ethyl 8-amino-2-(*o*-tolyloxy)-4-oxo-3-phenyl-3,4-dihydro- thieno[2',3':2,3]thieno[4,5-*d*]pyrimidine-6-carboxylate

Crystal data

$C_{24}H_{19}N_3O_4S_2$	$Z = 2$
$M_r = 477.54$	$F_{000} = 496$
Triclinic, $P\overline{1}$	$D_x = 1.382$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.0996$ (6) Å	Cell parameters from 2292 reflections
$b = 10.444$ (9) Å	$\theta = 2.1$–22.0°
$c = 16.9985$ (13) Å	$\mu = 0.27$ mm^{-1}
$\alpha = 104.447$ (1)°	$T = 292$ (2) K
$\beta = 97.120$ (1)°	Plate, colorless
$\gamma = 106.041$ (1)°	0.30 × 0.20 × 0.10 mm
$V = 1147.5$ (10) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3980 independent reflections
Radiation source: fine-focus sealed tube	2644 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.058$
$T = 298$(2) K	$\theta_{max} = 25.0^\circ$
φ and ω scans	$\theta_{min} = 2.1^\circ$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -8 \rightarrow 8$
$T_{min} = 0.924$, $T_{max} = 0.974$	$k = -12 \rightarrow 12$
9743 measured reflections	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.067$	H-atom parameters constrained
$wR(F^2) = 0.179$	$w = 1/[\sigma^2(F_o^2) + (0.0925P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
3980 reflections	$\Delta\rho_{max} = 0.27$ e Å^{-3}

300 parameters	$\Delta\rho_{min} = -0.32$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	0.9189 (7)	1.1256 (5)	0.6229 (3)	0.0784 (14)
H1	1.0236	1.1054	0.6504	0.094*
C2	0.9250 (9)	1.1479 (6)	0.5454 (3)	0.1021 (19)
H2	1.0353	1.1441	0.5217	0.122*
C3	0.7701 (11)	1.1754 (5)	0.5041 (3)	0.0965 (19)
H3	0.7751	1.1906	0.4527	0.116*
C4	0.6068 (10)	1.1805 (5)	0.5392 (3)	0.0949 (18)
H4	0.5012	1.1990	0.5110	0.114*
C5	0.5974 (8)	1.1584 (4)	0.6161 (3)	0.0774 (14)
H5	0.4855	1.1602	0.6390	0.093*
C6	0.7567 (6)	1.1337 (4)	0.6580 (2)	0.0543 (10)
C7	0.8496 (5)	1.2306 (4)	0.8098 (2)	0.0451 (9)
C8	0.6680 (5)	0.9832 (3)	0.7488 (2)	0.0447 (9)
C9	0.7561 (5)	1.0601 (3)	0.88721 (19)	0.0388 (8)
C10	0.8443 (5)	1.1936 (4)	0.8855 (2)	0.0456 (9)
C11	0.5062 (6)	0.7475 (4)	0.6740 (2)	0.0509 (10)
C12	0.3264 (7)	0.7053 (5)	0.6964 (3)	0.0694 (12)
H12	0.2603	0.7684	0.7157	0.083*
C13	0.2456 (8)	0.5640 (6)	0.6891 (3)	0.0939 (17)
H13	0.1256	0.5314	0.7055	0.113*
C14	0.3440 (12)	0.4740 (5)	0.6578 (4)	0.111 (2)
H14	0.2881	0.3792	0.6508	0.133*
C15	0.5262 (10)	0.5225 (5)	0.6362 (4)	0.1013 (18)
H15	0.5923	0.4595	0.6164	0.122*
C16	0.6118 (7)	0.6600 (4)	0.6431 (3)	0.0647 (11)
C17	0.8087 (8)	0.7118 (6)	0.6181 (4)	0.113 (2)
H17A	0.9056	0.7778	0.6655	0.170*
H17B	0.7907	0.7561	0.5758	0.170*
H17C	0.8553	0.6345	0.5969	0.170*
C18	0.8776 (5)	1.1747 (4)	1.0281 (2)	0.0447 (9)

C19	0.7735 (5)	1.0482 (3)	0.9699 (2)	0.0406 (8)
C20	0.7077 (5)	0.9386 (4)	1.0068 (2)	0.0435 (8)
C21	0.7692 (5)	0.9872 (4)	1.0933 (2)	0.0472 (9)
C22	0.7380 (6)	0.9123 (4)	1.1549 (2)	0.0517 (9)
C23	0.6039 (7)	0.6880 (4)	1.1759 (2)	0.0606 (11)
H23A	0.7302	0.6987	1.2104	0.073*
H23B	0.5168	0.7154	1.2118	0.073*
C24	0.5102 (9)	0.5422 (5)	1.1241 (3)	0.1020 (18)
H24A	0.3903	0.5341	1.0875	0.153*
H24B	0.4775	0.4834	1.1591	0.153*
H24C	0.6018	0.5140	1.0920	0.153*
N1	0.7524 (4)	1.1129 (3)	0.74015 (16)	0.0473 (7)
O1	0.9230 (4)	1.3454 (3)	0.80035 (16)	0.0630 (8)
N2	0.6637 (4)	0.9504 (3)	0.81807 (16)	0.0436 (7)
O2	0.5882 (4)	0.8878 (2)	0.67519 (14)	0.0580 (7)
N3	0.6009 (5)	0.8069 (3)	0.96004 (18)	0.0546 (8)
H3A	0.5636	0.7426	0.9835	0.066*
H3B	0.5702	0.7873	0.9069	0.066*
O4	0.7953 (5)	0.9629 (3)	1.22886 (16)	0.0710 (8)
O5	0.6378 (4)	0.7756 (3)	1.11951 (15)	0.0570 (7)
S1	0.90384 (15)	1.16428 (10)	1.12772 (6)	0.0569 (3)
S2	0.95315 (15)	1.30932 (10)	0.98436 (6)	0.0562 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.065 (3)	0.109 (4)	0.055 (3)	0.007 (3)	0.010 (2)	0.040 (3)
C2	0.090 (4)	0.135 (5)	0.067 (3)	−0.001 (4)	0.017 (3)	0.047 (3)
C3	0.136 (5)	0.088 (4)	0.052 (3)	0.007 (4)	0.004 (3)	0.038 (3)
C4	0.149 (6)	0.094 (4)	0.053 (3)	0.064 (4)	−0.010 (3)	0.027 (3)
C5	0.110 (4)	0.080 (3)	0.052 (3)	0.055 (3)	0.003 (3)	0.017 (2)
C6	0.075 (3)	0.042 (2)	0.042 (2)	0.0100 (19)	0.002 (2)	0.0180 (17)
C7	0.045 (2)	0.044 (2)	0.045 (2)	0.0117 (17)	0.0040 (16)	0.0163 (17)
C8	0.050 (2)	0.041 (2)	0.041 (2)	0.0144 (17)	0.0051 (16)	0.0103 (16)
C9	0.0333 (18)	0.049 (2)	0.0382 (18)	0.0165 (16)	0.0072 (15)	0.0161 (16)
C10	0.041 (2)	0.046 (2)	0.044 (2)	0.0119 (17)	0.0012 (16)	0.0091 (16)
C11	0.068 (3)	0.043 (2)	0.0343 (18)	0.0112 (19)	0.0013 (18)	0.0106 (16)
C12	0.066 (3)	0.079 (3)	0.060 (3)	0.014 (2)	0.014 (2)	0.023 (2)
C13	0.092 (4)	0.093 (4)	0.077 (3)	−0.013 (3)	0.011 (3)	0.040 (3)
C14	0.166 (7)	0.046 (3)	0.085 (4)	−0.007 (4)	−0.010 (4)	0.021 (3)
C15	0.139 (5)	0.058 (3)	0.104 (4)	0.031 (3)	0.026 (4)	0.019 (3)
C16	0.080 (3)	0.054 (3)	0.059 (3)	0.022 (2)	0.012 (2)	0.015 (2)
C17	0.096 (4)	0.137 (5)	0.128 (5)	0.056 (4)	0.049 (4)	0.042 (4)
C18	0.0339 (19)	0.056 (2)	0.0433 (19)	0.0166 (17)	0.0061 (15)	0.0109 (17)
C19	0.0374 (19)	0.048 (2)	0.0426 (19)	0.0195 (16)	0.0077 (16)	0.0186 (17)
C20	0.039 (2)	0.058 (2)	0.0403 (19)	0.0239 (18)	0.0071 (16)	0.0159 (17)
C21	0.043 (2)	0.058 (2)	0.044 (2)	0.0188 (18)	0.0059 (16)	0.0187 (17)
C22	0.053 (2)	0.067 (3)	0.044 (2)	0.029 (2)	0.0108 (18)	0.0201 (19)

C23	0.070 (3)	0.071 (3)	0.054 (2)	0.029 (2)	0.018 (2)	0.033 (2)
C24	0.146 (5)	0.076 (3)	0.070 (3)	0.011 (3)	0.010 (3)	0.030 (3)
N1	0.0583 (19)	0.0426 (17)	0.0393 (16)	0.0133 (15)	0.0054 (14)	0.0149 (13)
O1	0.0733 (19)	0.0456 (15)	0.0613 (17)	0.0070 (14)	0.0033 (14)	0.0189 (13)
N2	0.0517 (18)	0.0399 (16)	0.0371 (16)	0.0140 (14)	0.0038 (13)	0.0110 (13)
O2	0.086 (2)	0.0418 (14)	0.0378 (14)	0.0111 (13)	0.0043 (13)	0.0125 (11)
N3	0.066 (2)	0.0498 (18)	0.0440 (17)	0.0142 (16)	0.0050 (15)	0.0153 (14)
O4	0.092 (2)	0.0792 (19)	0.0401 (15)	0.0242 (16)	0.0034 (14)	0.0224 (14)
O5	0.0678 (18)	0.0602 (17)	0.0447 (14)	0.0181 (14)	0.0101 (13)	0.0222 (13)
S1	0.0593 (7)	0.0654 (7)	0.0403 (5)	0.0167 (5)	0.0036 (4)	0.0125 (5)
S2	0.0615 (7)	0.0490 (6)	0.0480 (6)	0.0095 (5)	0.0016 (5)	0.0109 (4)

Geometric parameters (Å, °)

C1—C6	1.374 (6)	C13—H13	0.9300
C1—C2	1.398 (6)	C14—C15	1.382 (8)
C1—H1	0.9300	C14—H14	0.9300
C2—C3	1.366 (8)	C15—C16	1.364 (6)
C2—H2	0.9300	C15—H15	0.9300
C3—C4	1.375 (7)	C16—C17	1.508 (6)
C3—H3	0.9300	C17—H17A	0.9600
C4—C5	1.390 (6)	C17—H17B	0.9600
C4—H4	0.9300	C17—H17C	0.9600
C5—C6	1.381 (6)	C18—C19	1.378 (5)
C5—H5	0.9300	C18—S1	1.715 (3)
C6—N1	1.468 (4)	C18—S2	1.738 (4)
C7—O1	1.227 (4)	C19—C20	1.434 (5)
C7—N1	1.411 (4)	C20—N3	1.352 (5)
C7—C10	1.436 (5)	C20—C21	1.400 (5)
C8—N2	1.307 (4)	C21—C22	1.458 (5)
C8—O2	1.330 (4)	C21—S1	1.738 (4)
C8—N1	1.375 (4)	C22—O4	1.204 (4)
C9—N2	1.359 (4)	C22—O5	1.345 (4)
C9—C10	1.371 (5)	C23—C24	1.470 (6)
C9—C19	1.434 (4)	C23—O5	1.480 (4)
C10—S2	1.740 (3)	C23—H23A	0.9700
C11—C12	1.364 (5)	C23—H23B	0.9700
C11—C16	1.382 (6)	C24—H24A	0.9600
C11—O2	1.414 (4)	C24—H24B	0.9600
C12—C13	1.395 (7)	C24—H24C	0.9600
C12—H12	0.9300	N3—H3A	0.8600
C13—C14	1.364 (8)	N3—H3B	0.8600
C6—C1—C2	119.3 (5)	C15—C16—C17	121.7 (5)
C6—C1—H1	120.3	C11—C16—C17	122.6 (4)
C2—C1—H1	120.3	C16—C17—H17A	109.5
C3—C2—C1	120.5 (5)	C16—C17—H17B	109.5
C3—C2—H2	119.7	H17A—C17—H17B	109.5
C1—C2—H2	119.7	C16—C17—H17C	109.5
C2—C3—C4	119.6 (5)	H17A—C17—H17C	109.5

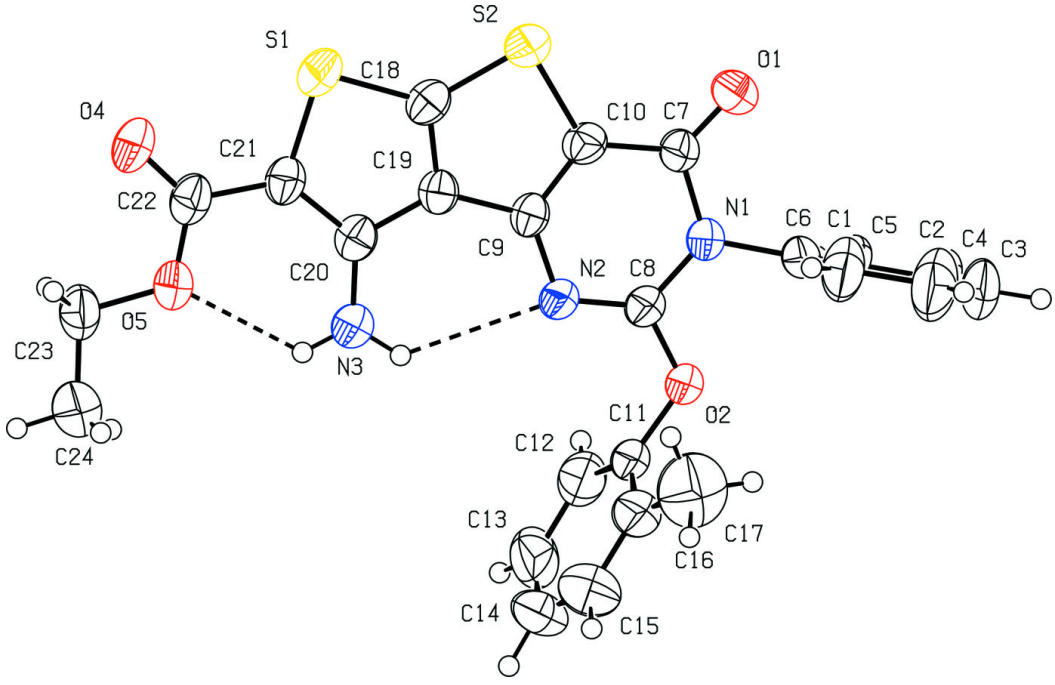
C2—C3—H3	120.2	H17B—C17—H17C	109.5
C4—C3—H3	120.2	C19—C18—S1	112.8 (3)
C3—C4—C5	120.9 (5)	C19—C18—S2	113.0 (3)
C3—C4—H4	119.6	S1—C18—S2	134.2 (2)
C5—C4—H4	119.6	C18—C19—C9	111.4 (3)
C6—C5—C4	119.0 (5)	C18—C19—C20	112.5 (3)
C6—C5—H5	120.5	C9—C19—C20	136.0 (3)
C4—C5—H5	120.5	N3—C20—C21	127.0 (3)
C1—C6—C5	120.6 (4)	N3—C20—C19	121.6 (3)
C1—C6—N1	119.3 (4)	C21—C20—C19	111.4 (3)
C5—C6—N1	120.1 (4)	C20—C21—C22	129.9 (3)
O1—C7—N1	120.2 (3)	C20—C21—S1	111.7 (3)
O1—C7—C10	128.9 (3)	C22—C21—S1	118.4 (3)
N1—C7—C10	110.9 (3)	O4—C22—O5	122.4 (3)
N2—C8—O2	121.7 (3)	O4—C22—C21	125.6 (4)
N2—C8—N1	127.2 (3)	O5—C22—C21	112.0 (3)
O2—C8—N1	111.1 (3)	C24—C23—O5	107.6 (3)
N2—C9—C10	123.7 (3)	C24—C23—H23A	110.2
N2—C9—C19	123.5 (3)	O5—C23—H23A	110.2
C10—C9—C19	112.7 (3)	C24—C23—H23B	110.2
C9—C10—C7	122.9 (3)	O5—C23—H23B	110.2
C9—C10—S2	112.4 (3)	H23A—C23—H23B	108.5
C7—C10—S2	124.6 (3)	C23—C24—H24A	109.5
C12—C11—C16	124.7 (4)	C23—C24—H24B	109.5
C12—C11—O2	119.7 (4)	H24A—C24—H24B	109.5
C16—C11—O2	115.4 (3)	C23—C24—H24C	109.5
C11—C12—C13	117.5 (5)	H24A—C24—H24C	109.5
C11—C12—H12	121.2	H24B—C24—H24C	109.5
C13—C12—H12	121.2	C8—N1—C7	121.5 (3)
C14—C13—C12	119.4 (5)	C8—N1—C6	121.5 (3)
C14—C13—H13	120.3	C7—N1—C6	116.9 (3)
C12—C13—H13	120.3	C8—N2—C9	113.8 (3)
C13—C14—C15	120.6 (5)	C8—O2—C11	117.6 (3)
C13—C14—H14	119.7	C20—N3—H3A	120.0
C15—C14—H14	119.7	C20—N3—H3B	120.0
C16—C15—C14	121.9 (5)	H3A—N3—H3B	120.0
C16—C15—H15	119.1	C22—O5—C23	116.8 (3)
C14—C15—H15	119.1	C18—S1—C21	91.53 (17)
C15—C16—C11	115.7 (4)	C18—S2—C10	90.37 (17)
C6—C1—C2—C3	−1.0 (8)	N3—C20—C21—C22	0.5 (6)
C1—C2—C3—C4	−0.3 (8)	C19—C20—C21—C22	−179.1 (3)
C2—C3—C4—C5	0.2 (8)	N3—C20—C21—S1	180.0 (3)
C3—C4—C5—C6	1.2 (7)	C19—C20—C21—S1	0.3 (4)
C2—C1—C6—C5	2.4 (7)	C20—C21—C22—O4	−179.4 (4)
C2—C1—C6—N1	−178.8 (4)	S1—C21—C22—O4	1.2 (5)
C4—C5—C6—C1	−2.5 (6)	C20—C21—C22—O5	1.5 (5)
C4—C5—C6—N1	178.7 (4)	S1—C21—C22—O5	−177.9 (2)
N2—C9—C10—C7	−0.7 (5)	N2—C8—N1—C7	0.3 (6)
C19—C9—C10—C7	178.7 (3)	O2—C8—N1—C7	−178.9 (3)

N2—C9—C10—S2	−179.0 (3)	N2—C8—N1—C6	176.4 (4)
C19—C9—C10—S2	0.4 (4)	O2—C8—N1—C6	−2.8 (5)
O1—C7—C10—C9	179.8 (4)	O1—C7—N1—C8	−179.7 (3)
N1—C7—C10—C9	0.4 (5)	C10—C7—N1—C8	−0.2 (5)
O1—C7—C10—S2	−2.1 (6)	O1—C7—N1—C6	4.1 (5)
N1—C7—C10—S2	178.5 (3)	C10—C7—N1—C6	−176.4 (3)
C16—C11—C12—C13	1.4 (6)	C1—C6—N1—C8	−91.1 (5)
O2—C11—C12—C13	176.0 (4)	C5—C6—N1—C8	87.7 (4)
C11—C12—C13—C14	−2.2 (7)	C1—C6—N1—C7	85.1 (4)
C12—C13—C14—C15	2.5 (8)	C5—C6—N1—C7	−96.1 (4)
C13—C14—C15—C16	−1.8 (9)	O2—C8—N2—C9	178.6 (3)
C14—C15—C16—C11	0.8 (8)	N1—C8—N2—C9	−0.5 (5)
C14—C15—C16—C17	−178.8 (5)	C10—C9—N2—C8	0.7 (5)
C12—C11—C16—C15	−0.7 (6)	C19—C9—N2—C8	−178.7 (3)
O2—C11—C16—C15	−175.5 (4)	N2—C8—O2—C11	−3.0 (5)
C12—C11—C16—C17	179.0 (4)	N1—C8—O2—C11	176.3 (3)
O2—C11—C16—C17	4.2 (6)	C12—C11—O2—C8	74.9 (4)
S1—C18—C19—C9	−179.3 (2)	C16—C11—O2—C8	−110.0 (4)
S2—C18—C19—C9	0.7 (4)	O4—C22—O5—C23	−1.3 (5)
S1—C18—C19—C20	1.4 (4)	C21—C22—O5—C23	177.8 (3)
S2—C18—C19—C20	−178.6 (2)	C24—C23—O5—C22	−174.7 (4)
N2—C9—C19—C18	178.7 (3)	C19—C18—S1—C21	−1.0 (3)
C10—C9—C19—C18	−0.7 (4)	S2—C18—S1—C21	178.9 (3)
N2—C9—C19—C20	−2.3 (6)	C20—C21—S1—C18	0.4 (3)
C10—C9—C19—C20	178.3 (4)	C22—C21—S1—C18	179.9 (3)
C18—C19—C20—N3	179.2 (3)	C19—C18—S2—C10	−0.4 (3)
C9—C19—C20—N3	0.3 (6)	S1—C18—S2—C10	179.6 (3)
C18—C19—C20—C21	−1.1 (4)	C9—C10—S2—C18	0.0 (3)
C9—C19—C20—C21	179.9 (4)	C7—C10—S2—C18	−178.3 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3A···O5	0.86	2.22	2.799 (4)	124
N3—H3B···N2	0.86	2.56	3.158 (4)	128

Fig. 1


S2
S1
C18
O1
O4
C10
C7
C21
C19
C22
N1
C6
C1
C5
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C4
C3
C9
N2
C8
C20
O5
N3
C23
C11
O2
C12
C24
C13
C17
C16
C14
C15

Fig. 2