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6-(2-Methylphenyl)-3-(3,4,5-trimethoxyphenyl)-1,2,4-triazolo[3,4-*b*][1,3,4]thiadiazole

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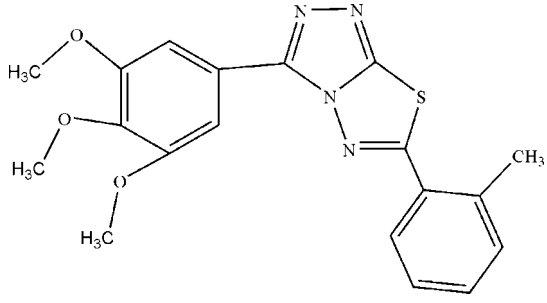
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.108; data-to-parameter ratio = 16.1.

In the molecule of the title compound, $C_{19}H_{18}N_4O_3S$, the planar central heterocylic ring system is oriented with respect to the trimethoxyphenyl and 2-methylphenyl rings at dihedral angles of 4.43 (3) and 4.32 (3)°, respectively. The dihedral angle between the two benzene rings is 7.65 (4)°. In the crystal structure, intermolecular C—H···N hydrogen bonds link the molecules into centrosymmetric $R_2^2(18)$ dimers. These dimers are connected *via* a C—H···π contact between the 2-methylphenyl and trimethoxyphenyl rings, and a π–π contact between the thiadiazole and trimethoxyphenyl rings [interplanar distance 3.51 Å, dihedral angles 4.17(4)°]. An intramolecular C—H···N hydrogen bond is also present.

Related literature

For general background, see: Karabasanagouda *et al.* (2007); Mathew *et al.* (2007). For ring motif details, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{19}H_{18}N_4O_3S$
M_r = 382.43
Monoclinic, $P2_1/c$
a = 7.5108 (15) Å
b = 15.950 (3) Å
c = 14.096 (3) Å
β = 91.88 (3)°
V = 1687.7 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 113 (2) K
0.24 × 0.20 × 0.16 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.923, T_{max} = 0.965
11990 measured reflections
3984 independent reflections
3408 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.108
S = 1.07
3984 reflections
248 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···N4	0.95	2.45	3.127 (3)	128
C7—H7C···N2^{i}	0.98	2.62	3.524 (3)	154
C19—H19B···CgA^{ii}	0.98	2.90	3.808 (3)	155

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+2, -y, -z$. *CgA* is the centroid of the trimethoxyphenyl ring.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2487).

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supporting information

Acta Cryst. (2008). E**64**, o1481 [doi:10.1107/S160053680802062X]

6-(2-Methylphenyl)-3-(3,4,5-trimethoxyphenyl)-1,2,4-triazolo[3,4-*b*][1,3,4]thiadiazole

Haitang Du, Haijun Du, Ying An and Shengnan Li

S1. Comment

1,2,4-Triazole and 1,3,4-thiadiazole represent one of the most biologically active classes of compounds, possessing a wide spectrum of activities. Various substituted 1,2,4-triazolo[3,4-b]-1,3,4-thiadiazoles are associated with diverse pharmacological activities such as antimicrobial (Karabasanagouda *et al.*, 2007) and anti-inflammatory activity (Mathew *et al.*, 2007). We report herein the crystal structure of the title compound.

In the molecule of the title compound (Fig. 1) the bond lengths and angles are within normal ranges. Rings A (C1-C6), B (N1-N3/C10/C11), C (S1/N3/N4/C11/C12) and D (C13-C18) are, of course, planar, and the dihedral angles between them are A/B = 4.63 (4)°, A/C = 4.08 (3)°, A/D = 7.65 (4)°, B/C = 0.94 (3)°, B/D = 4.59 (4)° and C/D = 4.25 (4)°. So, rings B and C are nearly coplanar. The coplanar ring system is oriented with respect to rings A and D at dihedral angles of 4.43 (3)° and 4.32 (3)°, respectively. The intra- molecular C-H···N hydrogen bond (Table 1) results in the formation of a planar six-membered ring E (N3/N4/C1/C2/C10/H2), in which it is oriented with respect to the other rings at dihedral angles of A/E = 3.24 (4)°, B/E = 1.39 (3)°, C/E = 1.03 (3)° and D/E = 5.25 (4)°. So, rings A, B, C and E are also nearly coplanar.

In the crystal structure, intermolecular weak C-H···N hydrogen bonds (Table 1) link the molecules to form a $\mathbf{R^2_2(18)}$ ring motif (Fig. 2) (Bernstein *et al.*, 1995), in which they may be effective in the stabilization of the structure. The C—H···π contact (Table 1) between the 2-methylphenyl and trimethoxyphenyl rings and a π—π contact between the thiadiazole and trimethoxyphenyl rings CgC···CgA^{i} [symmetry code: (i) 1 - x, 1 - y, 1 - z] further stabilize the structure, with centroid-centroid distance of 3.506 (1) Å.

S2. Experimental

For the preparation of the title compound, 4-amino-5-(3,4,5-trimethoxyphenyl) -4H-1,2,4-triazole-3-thiol (0.01 M) and 2-methylbenzoic acid (0.01 M) were dissolved in dry phosphorous oxychloride (10 ml). The resulted solution was further heated under reflux for 7 h. The reaction mixture was cooled to room temperature and the mixture was gradually poured onto crushed ice with stirring. Finally, powdered potassium carbonate and the required amount of solid potassium hydroxide were added until the pH of the mixture was raised to 8, to remove the excess of phosphorous oxychloride. The mixture was allowed to stand overnight and the solid was separated. It was filtered, washed with cold water, and then dried. Crystals suitable for X-ray analysis were obtained by the recrystallization of the solid residue from a mixture of N,N-dimethyl- formamide/ethanol (1:1) by slow evaporation at room temperature.

S3. Refinement

H atoms were positioned geometrically, with C-H = 0.95 and 0.98 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms with $U_{iso}(H) = xU_{eq}(C)$, where x = 1.5 for methyl H and x = 1.2 for aromatic H

atoms.

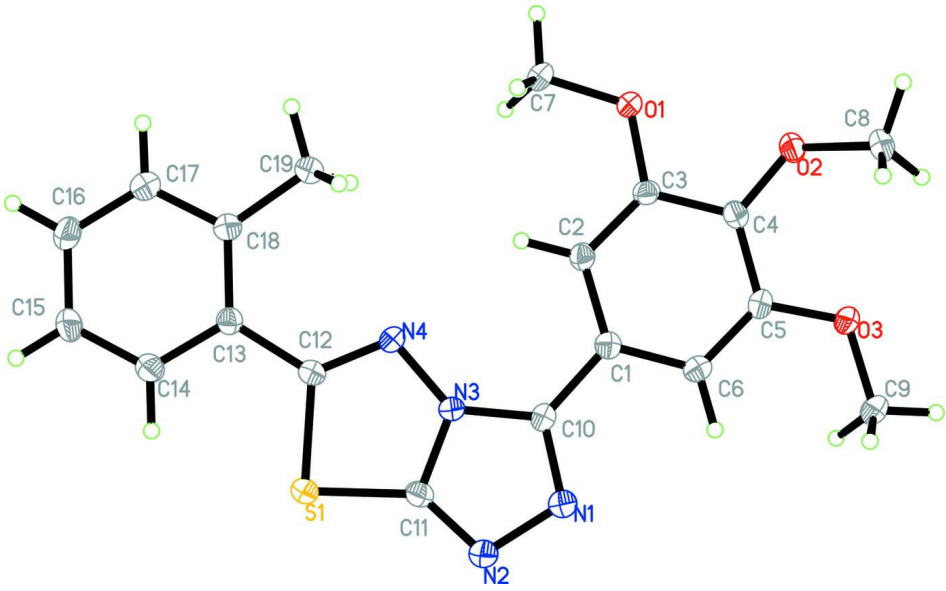

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

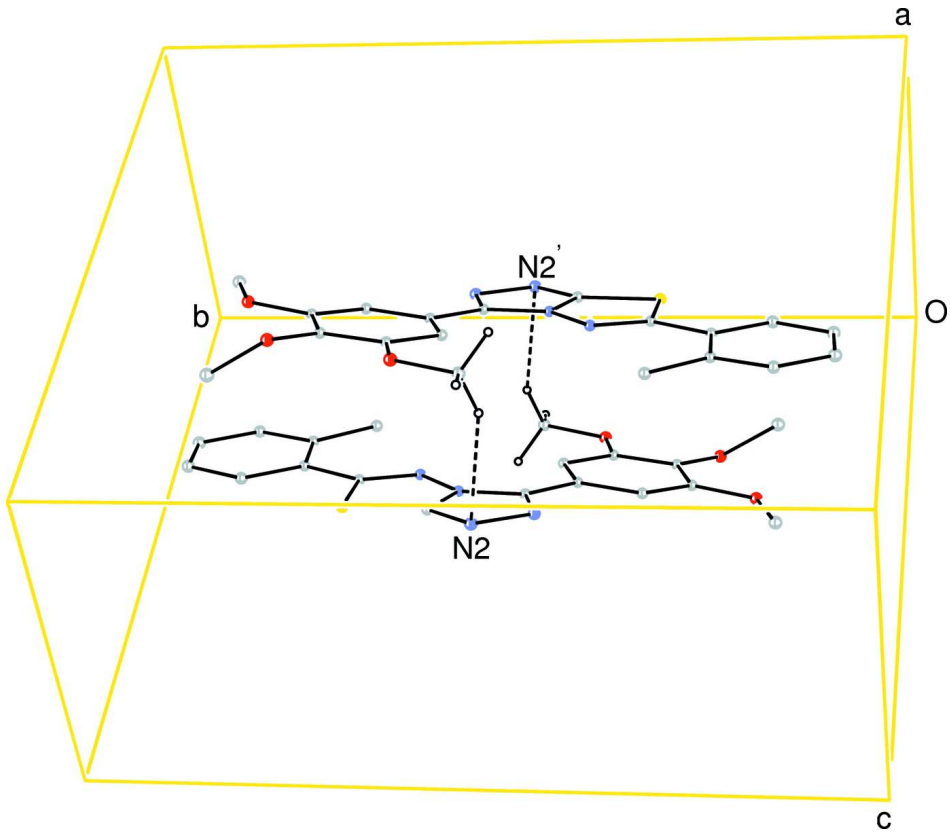

Figure 2

A partial packing diagram of the title compound [symmetry code: (′) -x, -y, -z]. Hydrogen bonds are shown as dashed lines.

6-(2-Methylphenyl)-3-(3,4,5-trimethoxyphenyl)-1,2,4- triazolo[3,4-*b*][1,3,4]thiadiazole

Crystal data

$C_{19}H_{18}N_4O_3S$
$M_r = 382.43$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.5108\ (15)$ Å
$b = 15.950\ (3)$ Å
$c = 14.096\ (3)$ Å
$\beta = 91.88\ (3)°$
$V = 1687.7\ (6)$ Å^3
$Z = 4$

$F(000) = 800$
$D_x = 1.505$ Mg m^{-3}
Melting point: 435 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4684 reflections
$\theta = 1.9–27.9°$
$\mu = 0.22$ mm^{-1}
$T = 113$ K
Prism, colorless
0.24 × 0.20 × 0.16 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Radiation source: rotating anode
Confocal monochromator
Detector resolution: 7.31 pixels mm^{-1}
ω and φ scans

Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min} = 0.923$, $T_{max} = 0.965$
11990 measured reflections
3984 independent reflections
3408 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$

θ_{max} = 27.9°, θ_{min} = 1.9°
h = −9→9
k = −20→20
l = −17→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.108
S = 1.07
3984 reflections
248 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
$w = 1/[\sigma^2(F_o^2) + (0.0664P)^2 + 0.1888P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-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 $F^2 > 2\text{sigma}(F^2)$ 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}
S1	0.45611 (5)	0.68554 (2)	0.69693 (2)	0.02005 (12)
O1	0.04396 (14)	0.40664 (6)	0.30838 (7)	0.0227 (2)
O2	0.03955 (14)	0.24866 (6)	0.34593 (7)	0.0223 (2)
O3	0.17803 (14)	0.18588 (6)	0.51532 (7)	0.0209 (2)
N1	0.43365 (17)	0.44321 (7)	0.69492 (9)	0.0208 (3)
N2	0.48819 (18)	0.51377 (8)	0.74703 (9)	0.0226 (3)
N3	0.36258 (15)	0.55345 (7)	0.61030 (8)	0.0156 (2)
N4	0.31020 (15)	0.61420 (7)	0.54614 (8)	0.0164 (2)
C1	0.27851 (18)	0.41101 (8)	0.54193 (10)	0.0162 (3)
C2	0.20134 (19)	0.44117 (8)	0.45750 (10)	0.0176 (3)
H2	0.2018	0.4995	0.4439	0.021*
C3	0.12374 (18)	0.38475 (9)	0.39346 (10)	0.0173 (3)
C4	0.12199 (18)	0.29857 (8)	0.41238 (10)	0.0170 (3)
C5	0.19617 (18)	0.26966 (8)	0.49906 (10)	0.0169 (3)
C6	0.27654 (18)	0.32539 (8)	0.56254 (10)	0.0174 (3)
H6	0.3303	0.3053	0.6201	0.021*
C7	0.0480 (2)	0.49299 (9)	0.28278 (11)	0.0232 (3)
H7A	−0.0099	0.5263	0.3314	0.035*
H7B	−0.0152	0.5009	0.2215	0.035*
H7C	0.1720	0.5112	0.2778	0.035*
C8	0.1222 (2)	0.17048 (9)	0.32363 (12)	0.0276 (4)
H8A	0.2513	0.1750	0.3349	0.041*
H8B	0.0968	0.1568	0.2568	0.041*

H8C	0.0751	0.1262	0.3639	0.041*
C9	0.2468 (2)	0.15402 (9)	0.60340 (11)	0.0247 (3)
H9A	0.3756	0.1639	0.6083	0.037*
H9B	0.2232	0.0937	0.6069	0.037*
H9C	0.1890	0.1826	0.6557	0.037*
C10	0.35879 (18)	0.46709 (8)	0.61313 (10)	0.0164 (3)
C11	0.44294 (18)	0.57788 (9)	0.69380 (10)	0.0182 (3)
C12	0.35200 (18)	0.68710 (8)	0.58207 (9)	0.0159 (3)
C13	0.32100 (18)	0.76838 (8)	0.53561 (10)	0.0167 (3)
C14	0.3639 (2)	0.84107 (9)	0.58780 (11)	0.0212 (3)
H14	0.4101	0.8357	0.6510	0.025*
C15	0.3405 (2)	0.92022 (9)	0.54955 (11)	0.0240 (3)
H15	0.3724	0.9686	0.5855	0.029*
C16	0.2700 (2)	0.92787 (9)	0.45800 (11)	0.0245 (3)
H16	0.2521	0.9819	0.4309	0.029*
C17	0.22563 (19)	0.85687 (9)	0.40588 (11)	0.0210 (3)
H17	0.1762	0.8634	0.3434	0.025*
C18	0.25090 (18)	0.77609 (9)	0.44191 (10)	0.0174 (3)
C19	0.2042 (2)	0.70232 (9)	0.37935 (10)	0.0206 (3)
H19A	0.1633	0.7224	0.3166	0.031*
H19B	0.1093	0.6697	0.4079	0.031*
H19C	0.3096	0.6669	0.3727	0.031*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0259 (2)	0.01750 (18)	0.01647 (19)	−0.00076 (13)	−0.00384 (14)	−0.00149 (12)
O1	0.0347 (6)	0.0148 (5)	0.0181 (5)	0.0021 (4)	−0.0071 (4)	0.0011 (4)
O2	0.0258 (6)	0.0165 (5)	0.0242 (6)	0.0014 (4)	−0.0056 (4)	−0.0036 (4)
O3	0.0278 (6)	0.0142 (5)	0.0203 (5)	−0.0019 (4)	−0.0035 (4)	0.0032 (4)
N1	0.0244 (7)	0.0189 (6)	0.0190 (6)	0.0012 (5)	−0.0023 (5)	−0.0002 (5)
N2	0.0287 (7)	0.0196 (6)	0.0193 (6)	0.0012 (5)	−0.0038 (5)	−0.0006 (5)
N3	0.0173 (6)	0.0158 (5)	0.0136 (5)	0.0000 (4)	−0.0010 (4)	0.0005 (4)
N4	0.0182 (6)	0.0149 (5)	0.0160 (6)	0.0005 (4)	−0.0002 (4)	0.0024 (4)
C1	0.0154 (6)	0.0170 (6)	0.0164 (7)	0.0007 (5)	0.0026 (5)	−0.0006 (5)
C2	0.0202 (7)	0.0150 (6)	0.0177 (7)	0.0015 (5)	0.0012 (5)	−0.0004 (5)
C3	0.0200 (7)	0.0179 (7)	0.0140 (6)	0.0031 (5)	0.0005 (5)	0.0003 (5)
C4	0.0171 (7)	0.0155 (6)	0.0184 (7)	−0.0001 (5)	0.0003 (5)	−0.0022 (5)
C5	0.0167 (7)	0.0142 (6)	0.0199 (7)	0.0010 (5)	0.0034 (5)	0.0014 (5)
C6	0.0168 (7)	0.0190 (7)	0.0165 (7)	0.0019 (5)	0.0005 (5)	0.0020 (5)
C7	0.0316 (8)	0.0161 (7)	0.0217 (7)	0.0028 (6)	−0.0042 (6)	0.0037 (5)
C8	0.0387 (9)	0.0170 (7)	0.0265 (8)	0.0034 (6)	−0.0065 (7)	−0.0061 (6)
C9	0.0335 (9)	0.0177 (7)	0.0227 (8)	−0.0002 (6)	−0.0037 (6)	0.0058 (6)
C10	0.0169 (7)	0.0146 (6)	0.0177 (7)	0.0008 (5)	0.0016 (5)	0.0014 (5)
C11	0.0196 (7)	0.0196 (6)	0.0154 (7)	−0.0006 (5)	−0.0010 (5)	−0.0013 (5)
C12	0.0147 (6)	0.0180 (7)	0.0149 (7)	−0.0003 (5)	0.0002 (5)	−0.0013 (5)
C13	0.0161 (7)	0.0163 (6)	0.0176 (7)	0.0005 (5)	0.0006 (5)	0.0000 (5)
C14	0.0233 (7)	0.0198 (7)	0.0204 (7)	0.0001 (6)	−0.0018 (6)	−0.0023 (6)

C15	0.0287 (8)	0.0161 (6)	0.0271 (8)	−0.0007 (6)	−0.0012 (6)	−0.0030 (6)
C16	0.0297 (8)	0.0168 (7)	0.0270 (8)	0.0013 (6)	0.0005 (6)	0.0025 (6)
C17	0.0218 (7)	0.0216 (7)	0.0198 (7)	0.0011 (6)	0.0004 (5)	0.0019 (5)
C18	0.0163 (7)	0.0190 (7)	0.0169 (7)	0.0004 (5)	0.0015 (5)	0.0003 (5)
C19	0.0245 (8)	0.0200 (7)	0.0172 (7)	−0.0012 (6)	−0.0015 (5)	−0.0009 (5)

Geometric parameters (Å, º)

S1—C11	1.7205 (15)	C7—H7A	0.9800
S1—C12	1.7749 (15)	C7—H7B	0.9800
O1—C3	1.3682 (17)	C7—H7C	0.9800
O1—C7	1.4244 (16)	C8—H8A	0.9800
O2—C4	1.3625 (16)	C8—H8B	0.9800
O2—C8	1.4325 (17)	C8—H8C	0.9800
O3—C5	1.3633 (16)	C9—H9A	0.9800
O3—C9	1.4229 (17)	C9—H9B	0.9800
N1—C10	1.3221 (18)	C9—H9C	0.9800
N1—N2	1.3978 (17)	C12—C13	1.4677 (19)
N2—C11	1.3067 (18)	C13—C14	1.4048 (19)
N3—C11	1.3619 (18)	C13—C18	1.411 (2)
N3—N4	1.3742 (16)	C14—C15	1.382 (2)
N3—C10	1.3783 (17)	C14—H14	0.9500
N4—C12	1.3026 (17)	C15—C16	1.384 (2)
C1—C2	1.392 (2)	C15—H15	0.9500
C1—C6	1.3964 (19)	C16—C17	1.385 (2)
C1—C10	1.4600 (19)	C16—H16	0.9500
C2—C3	1.3893 (19)	C17—C18	1.3956 (19)
C2—H2	0.9500	C17—H17	0.9500
C3—C4	1.4003 (19)	C18—C19	1.5050 (19)
C4—C5	1.404 (2)	C19—H19A	0.9800
C5—C6	1.3855 (19)	C19—H19B	0.9800
C6—H6	0.9500	C19—H19C	0.9800
C11—S1—C12	88.13 (6)	O3—C9—H9A	109.5
C3—O1—C7	117.15 (11)	O3—C9—H9B	109.5
C4—O2—C8	117.97 (11)	H9A—C9—H9B	109.5
C5—O3—C9	117.47 (11)	O3—C9—H9C	109.5
C10—N1—N2	109.59 (11)	H9A—C9—H9C	109.5
C11—N2—N1	105.19 (12)	H9B—C9—H9C	109.5
C11—N3—N4	118.44 (11)	N1—C10—N3	107.73 (12)
C11—N3—C10	105.66 (11)	N1—C10—C1	125.26 (12)
N4—N3—C10	135.89 (12)	N3—C10—C1	126.93 (12)
C12—N4—N3	108.26 (11)	N2—C11—N3	111.83 (13)
C2—C1—C6	120.59 (13)	N2—C11—S1	138.82 (11)
C2—C1—C10	121.79 (12)	N3—C11—S1	109.35 (10)
C6—C1—C10	117.59 (12)	N4—C12—C13	125.61 (13)
C3—C2—C1	119.05 (13)	N4—C12—S1	115.82 (10)
C3—C2—H2	120.5	C13—C12—S1	118.57 (10)

C1—C2—H2	120.5	C14—C13—C18	119.37 (13)
O1—C3—C2	124.52 (12)	C14—C13—C12	117.71 (13)
O1—C3—C4	114.26 (12)	C18—C13—C12	122.93 (12)
C2—C3—C4	121.23 (13)	C15—C14—C13	121.71 (14)
O2—C4—C3	116.72 (12)	C15—C14—H14	119.1
O2—C4—C5	124.38 (12)	C13—C14—H14	119.1
C3—C4—C5	118.83 (12)	C14—C15—C16	118.96 (14)
O3—C5—C6	124.34 (13)	C14—C15—H15	120.5
O3—C5—C4	115.42 (12)	C16—C15—H15	120.5
C6—C5—C4	120.22 (12)	C15—C16—C17	120.04 (14)
C5—C6—C1	120.03 (13)	C15—C16—H16	120.0
C5—C6—H6	120.0	C17—C16—H16	120.0
C1—C6—H6	120.0	C16—C17—C18	122.30 (14)
O1—C7—H7A	109.5	C16—C17—H17	118.8
O1—C7—H7B	109.5	C18—C17—H17	118.8
H7A—C7—H7B	109.5	C17—C18—C13	117.60 (13)
O1—C7—H7C	109.5	C17—C18—C19	118.83 (13)
H7A—C7—H7C	109.5	C13—C18—C19	123.57 (12)
H7B—C7—H7C	109.5	C18—C19—H19A	109.5
O2—C8—H8A	109.5	C18—C19—H19B	109.5
O2—C8—H8B	109.5	H19A—C19—H19B	109.5
H8A—C8—H8B	109.5	C18—C19—H19C	109.5
O2—C8—H8C	109.5	H19A—C19—H19C	109.5
H8A—C8—H8C	109.5	H19B—C19—H19C	109.5
H8B—C8—H8C	109.5		

C10—N1—N2—C11	0.13 (16)	C2—C1—C10—N1	179.68 (13)
C11—N3—N4—C12	−0.04 (16)	C6—C1—C10—N1	1.6 (2)
C10—N3—N4—C12	−178.51 (15)	C2—C1—C10—N3	3.3 (2)
C6—C1—C2—C3	−0.6 (2)	C6—C1—C10—N3	−174.73 (13)
C10—C1—C2—C3	−178.64 (13)	N1—N2—C11—N3	−0.07 (16)
C7—O1—C3—C2	2.7 (2)	N1—N2—C11—S1	−179.34 (13)
C7—O1—C3—C4	−177.29 (12)	N4—N3—C11—N2	−178.90 (12)
C1—C2—C3—O1	−179.99 (13)	C10—N3—C11—N2	−0.01 (16)
C1—C2—C3—C4	0.0 (2)	N4—N3—C11—S1	0.58 (15)
C8—O2—C4—C3	138.95 (14)	C10—N3—C11—S1	179.48 (9)
C8—O2—C4—C5	−44.2 (2)	C12—S1—C11—N2	178.60 (18)
O1—C3—C4—O2	−1.28 (18)	C12—S1—C11—N3	−0.68 (10)
C2—C3—C4—O2	178.74 (12)	N3—N4—C12—C13	179.15 (12)
O1—C3—C4—C5	−178.28 (12)	N3—N4—C12—S1	−0.53 (14)
C2—C3—C4—C5	1.7 (2)	C11—S1—C12—N4	0.74 (11)
C9—O3—C5—C6	−0.1 (2)	C11—S1—C12—C13	−178.97 (11)
C9—O3—C5—C4	−178.32 (12)	N4—C12—C13—C14	175.74 (13)
O2—C4—C5—O3	−1.3 (2)	S1—C12—C13—C14	−4.59 (17)
C3—C4—C5—O3	175.43 (12)	N4—C12—C13—C18	−4.3 (2)
O2—C4—C5—C6	−179.60 (13)	S1—C12—C13—C18	175.39 (11)
C3—C4—C5—C6	−2.9 (2)	C18—C13—C14—C15	−0.5 (2)
O3—C5—C6—C1	−175.88 (13)	C12—C13—C14—C15	179.46 (13)

C4—C5—C6—C1	2.2 (2)	C13—C14—C15—C16	1.2 (2)
C2—C1—C6—C5	−0.5 (2)	C14—C15—C16—C17	−0.6 (2)
C10—C1—C6—C5	177.61 (12)	C15—C16—C17—C18	−0.7 (2)
N2—N1—C10—N3	−0.13 (15)	C16—C17—C18—C13	1.3 (2)
N2—N1—C10—C1	−177.07 (12)	C16—C17—C18—C19	−178.14 (14)
C11—N3—C10—N1	0.09 (15)	C14—C13—C18—C17	−0.7 (2)
N4—N3—C10—N1	178.69 (14)	C12—C13—C18—C17	179.32 (13)
C11—N3—C10—C1	176.96 (13)	C14—C13—C18—C19	178.70 (13)
N4—N3—C10—C1	−4.4 (3)	C12—C13—C18—C19	−1.3 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···N4	0.95	2.45	3.127 (3)	128
C7—H7*C*···N2^{i}	0.98	2.62	3.524 (3)	154
C19—H19*B*···CgA^{ii}	0.98	2.90	3.808 (3)	155

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