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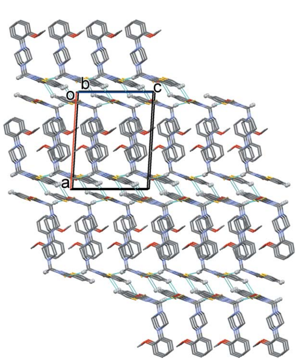

Crystal structure of 3-{[4-(2-methoxyphenyl)-piperazin-1-yl]methyl}-5-(thiophen-2-yl)-1,3,4-oxa-diazole-2(3*H*)-thione

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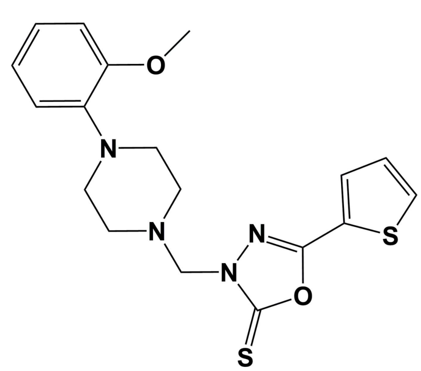
The title compound, $C_{18}H_{20}N_4O_2S_2$, is a new 1,3,4-oxadiazole and a key pharmacophore of several biologically active agents. It is composed of a methyl(thiophen-2-yl)-1,3,4-oxadiazole-2(3*H*)-thione moiety linked to a 2-methoxyphenyl unit *via* a piperazine ring that has a chair conformation. The thiophene ring mean plane lies almost in the plane of the oxadiazole ring, with a dihedral angle of 4.35 (9)°. The 2-methoxyphenyl ring is almost normal to the oxadiazole ring, with a dihedral angle of 84.17 (10)°. In the crystal, molecules are linked by weak C—H⋯S hydrogen bonds and C—H⋯π interactions, forming layers parallel to the *bc* plane. The layers are linked *via* weak C—H⋯O hydrogen bonds and slipped parallel π–π interactions [intercentroid distance = 3.6729 (10) Å], forming a three-dimensional structure. The thiophene ring has an approximate 180° rotational disorder about the bridging C—C bond.

1. Chemical context

1,3,4-Oxadiazole derivatives are structural motifs of particular value in material sciences (Zhang *et al.*, 2011) and agro-chemistry (Shi *et al.*, 2001; Milinkevich *et al.*, 2009; Li *et al.*, 2014). In addition, they occupy a unique situation in the field of medicinal chemistry as pharmacophores possessing diverse pharmacological activities including antibacterial (Ogata *et al.*, 1971; Rane *et al.*, 2012; Al-Omar, 2010), anticancer (Pinna *et al.*, 2009; Gamal El-Din *et al.*, 2015; Zhang *et al.*, 2014; Du *et al.*, 2013), antiviral (Summa *et al.*, 2008; Wu *et al.*, 2015; El-Emam *et al.*, 2004), antihypertensive (Vardan *et al.*, 1983; Schlecker & Thieme, 1988), anti-inflammatory (Bansal *et al.*, 2014; Kadi *et al.*, 2007) and anti-oxidant (Ma *et al.*, 2013) activities. In continuation to our previous studies on 1,3,4-oxadiazoles (El-Emam *et al.*, 2012), we report herein on the synthesis and crystal structure of the title compound.



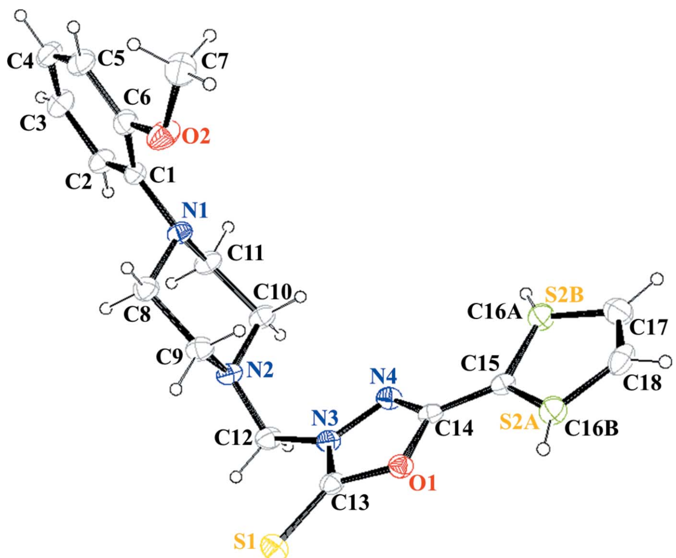


Figure 1
The molecular structure of the title compound, showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level. The thiophene ring has an approximate 180° rotational disorder about the bridging C—C bond.

2. Structural commentary

The title compound, Fig. 1, is composed of a methyl(thiophen-2-yl)-1,3,4-oxadiazole-2(3*H*)-thione moiety linked to a 2-methoxyphenyl unit *via* a bridging piperazine ring. The molecule is V-shaped with the mean plane of the piperazine ring, that has a chair conformation, making dihedral angles of 51.2 (1) and 77.8 (1)° with the 2-methoxyphenyl ring and the oxadiazole ring, respectively. The thiophene ring mean plane lies almost in the plane of the oxadiazole ring, with a dihedral angle of 4.35 (9)°. The thiophene ring has an approximate 180° rotational disorder about the bridging C14—C15 bond.

3. Supramolecular features

In the crystal, molecules are linked by weak C—H$\cdots$S hydrogen bonds and C—H$\cdots\pi$ interactions, forming layers in the *bc* plane (Table 1 and Fig. 2). The layers are linked *via* C—H$\cdots$O hydrogen bonds and slipped parallel π–π interactions [$Cg3\cdots Cg1^{i}$ = 3.6729 (10) Å, inter-planar distance = 3.4757 (7) Å, slippage = 0.967 Å; *Cg*1 and *Cg*3 are the centroids of the S2*A*/C15/C16*A*/C17/C18 and O1/ N3/N4/C13/C14 rings, respectively; symmetry code (i): $-x + 2, -y + 1, -z + 2$], forming a three-dimensional structure (Table 1 and Fig. 2).

4. Database survey

A search of the Cambridge Structural Database (Version 5.37, last update November 2015; Groom & Allen, 2014) for the 3-methyl-5-(thiophen-2-yl)-1,3,4-oxadiazole-2(3*H*)-thione moiety of the title compound gave three hits. Two of these compounds also contain a substituted piperazine ring, namely

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

*Cg*1 is the centroid of the S2*A*/C15/C16*A*/C17/C18 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C12—H12$A\cdots$S1^{i}	0.97	2.95	3.860 (2)	157
C17—H17$\cdots$O1^{ii}	0.93	2.69	3.475 (2)	143
C5—H5$\cdots Cg1^{iii}$	0.93	2.95	3.660 (2)	135

Symmetry codes: (i) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (ii) $-x + 2, y + \frac{1}{2}, -z + \frac{5}{2}$; (iii) $-x + 1, -y + 1, -z + 2$.

3-[(4-phenylpiperazin-1-yl)methyl]-5-(2-thienyl)-1,3,4-oxadiazole-2(3*H*)-thione (IDOBUA; El-Emam *et al.*, 2013) and 3-[(4-benzylpiperazin-1-yl)methyl]-5-(thiophen-2-yl)-2,3-dihydro-1,3,4-oxadiazole-2-thione (VUBYUO; Al-Omary *et al.*, 2015). In both of these molecules, the conformation is very similar to that of the title compound.

5. Synthesis and crystallization

To a solution of 5-(thiophen-2-yl)-1,3,4-oxadiazole-2-thiol (920 mg, 5 mmol), in ethanol (15 ml), 1-(2-methoxyphenyl)-piperazine (960 mg, 5 mmol) and 37% formaldehyde solution (1.0 ml) were added and the mixture was stirred at room temperature for 3 h and then allowed to stand overnight at

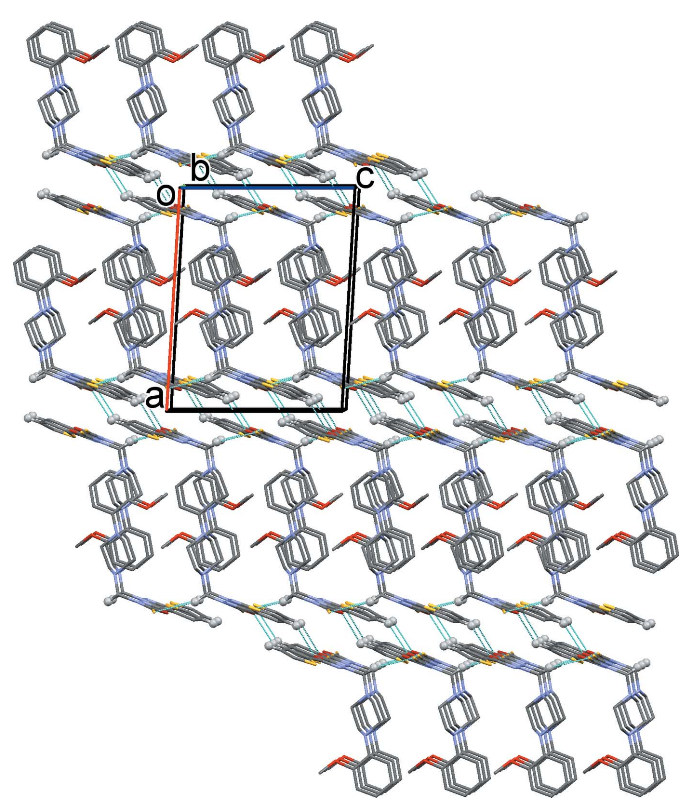


Figure 2
Crystal packing of the title compound, viewed along the *b* axis, showing the C—H$\cdots$S and C—H$\cdots$O hydrogen bonds (Table 1) as dashed lines. Only H atoms involved in intermolecular interactions have been included.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{20}N_4O_2S_2$
M_r	388.5
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, *b*, *c* (Å)	15.2925 (2), 10.0745 (1), 11.9726 (1)
β (°)	93.413 (1)
V (Å^3)	1841.28 (3)
Z	4
Radiation type	Cu *Kα*
μ (mm^{-1})	2.80
Crystal size (mm)	0.70 × 0.51 × 0.41
Data collection	
Diffractometer	Agilent Xcalibur Ruby Gemini
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.225, 0.315
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13494, 3545, 3401
R_{int}	0.026
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.612
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.045, 0.113, 1.04
No. of reflections	3494
No. of parameters	230
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.95, −0.65

Computer programs: *CrysAlis CCD* and *CrysAlis RED* (Oxford Diffraction, 2006), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008) and *publCIF* (Westrip, 2010).

room temperature. The precipitated crude product was filtered, washed with cold ethanol, dried, and crystallized from ethanol to yield the title compound as pale-yellow prismatic crystals(yield 1.67 g, 86%; m.p. 419–421 K). Single crystals suitable for X-ray analysis were obtained by slow evaporation of a $CHCl_3$:EtOH solution (1:1; 15 ml) at room temperature. ^{1}H NMR ($CDCl_3$, 500.13 MHz): δ 3.10 (*s*, 8H, piperazine-H), 3.85 (*s*, 3H, OCH_3), 5.15 (*s*, 2H, CH2), 6.85–6.87 (*m*, 1H, Ar-H), 6.92–6.95 (*m*, 2H, Ar-H), 7.01–7.03 (*m*, 1H, Ar-H), 7.18 (*t*, 1H, thiophene-H, *J* = 4.5 Hz), 7.59 (d, 1H, thiophene-H, *J* = 4.5 Hz), 7.75 (*d*, 1H, thiophene-H, *J* = 4.5 Hz). ^{13}C NMR ($CDCl_3$, 125.76 MHz): δ 50.43, 50.64 (piperazine-C), 55.33 (OCH_3), 70.44 (CH2), 111.05, 118.28, 120.94, 123.17, 123.68, 128.32, 130.74, 130.95, 141.09, 152.23 (Ar & thiophene-C), 155.42 (C=N), 177.74 (C=S).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C-bound H atoms were positioned geometrically and treated as riding atoms: C—H 0.95–0.97 Å with $U_{iso}(H) = 1.5U_{eq}$(C-methyl) and $1.2U_{eq}$(C) for other H atoms. The thienyl ring is disordered over two positions and in the final refinement cycles, the occupancy of atoms *S2A* and C16*A*, and S2*B* and C16*B*, were each fixed at 0.5.

Acknowledgements

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Acta Cryst. (2016). E**72**, 269-272 [doi:10.1107/S2056989016000992]

Crystal structure of 3-{[4-(2-methoxyphenyl)piperazin-1-yl]methyl}-5-(thiophen-2-yl)-1,3,4-oxadiazole-2(3*H*)-thione

Monirah A. Al-Alshaikh, Hatem A. Abuelizz, Ali A. El-Emam, Mohammed S. M. Abdelbaky and Santiago Garcia-Granda

Computing details

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis CCD* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED* (Oxford Diffraction, 2006); 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) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *publCIF* (Westrip, 2010).

3-{[4-(2-Methoxyphenyl)piperazin-1-yl]methyl}-5-(thiophen-2-yl)-1,3,4-oxadiazole-2(3*H*)-thione

Crystal data

$C_{18}H_{20}N_4O_2S_2$
M_r = 388.5
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 15.2925 (2) Å
b = 10.0745 (1) Å
c = 11.9726 (1) Å
β = 93.413 (1)°
V = 1841.28 (3) Å^3
Z = 4
$F(000)$ = 816
D_x = 1.401 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 11296 reflections
θ = 3.7–70.5°
μ = 2.80 mm^{-1}
T = 100 K
Prism, colourless
0.70 × 0.51 × 0.41 mm

Data collection

Agilent Xcalibur Ruby Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 10.2673 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min} = 0.225, T_{max} = 0.315
13494 measured reflections
3545 independent reflections
3401 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 70.7°, θ_{min} = 5.3°
h = −18→17
k = −8→12
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.113
S = 1.04
3494 reflections
230 parameters
0 restraints
0 constraints

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
$w = 1/[\sigma^2(F_o^2) + (0.0574P)^2 + 2.048P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.95$ e Å^{-3}
$\Delta\rho_{min} = -0.65$ 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 $F^2 > \sigma(F^2)$ 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}	Occ. (<1)
S1	0.89998 (3)	0.09896 (5)	0.99378 (4)	0.02414 (15)	
S2A	0.87403 (4)	0.74266 (6)	1.04820 (5)	0.02497 (16)	0.7913 (14)
C16A	0.94021 (8)	0.57554 (13)	1.21094 (10)	0.02497 (16)	0.7913 (14)
H16A	0.9598	0.501	1.2508	0.03*	0.7913 (14)
S2B	0.94021 (8)	0.57554 (13)	1.21094 (10)	0.02497 (16)	0.2087 (14)
C16B	0.87403 (4)	0.74266 (6)	1.04820 (5)	0.02497 (16)	0.2087 (14)
H16B	0.8502	0.779	0.9817	0.03*	0.2087 (14)
O1	0.90631 (8)	0.35048 (13)	1.06190 (11)	0.0189 (3)	
O2	0.43793 (9)	0.38449 (17)	0.90935 (12)	0.0312 (4)	
N3	0.85646 (10)	0.33316 (16)	0.89001 (13)	0.0192 (3)	
N1	0.55319 (10)	0.37224 (16)	0.74811 (13)	0.0198 (3)	
N4	0.85770 (10)	0.46847 (16)	0.91387 (13)	0.0204 (3)	
N2	0.73225 (10)	0.29806 (17)	0.75238 (13)	0.0210 (3)	
C1	0.46191 (12)	0.37565 (18)	0.71654 (16)	0.0202 (4)	
C15	0.90176 (11)	0.58606 (19)	1.08927 (15)	0.0183 (4)	
C14	0.88737 (11)	0.47285 (19)	1.01696 (15)	0.0180 (4)	
C13	0.88567 (12)	0.26006 (19)	0.97769 (15)	0.0187 (4)	
C6	0.40227 (13)	0.3813 (2)	0.80197 (17)	0.0229 (4)	
C9	0.67626 (13)	0.2461 (2)	0.83683 (17)	0.0237 (4)	
H9A	0.6806	0.3025	0.9026	0.028*	
H9B	0.6955	0.1577	0.8589	0.028*	
C11	0.61058 (12)	0.4202 (2)	0.66366 (16)	0.0231 (4)	
H11A	0.5908	0.5066	0.6368	0.028*	
H11B	0.6088	0.3596	0.6007	0.028*	
C4	0.28120 (13)	0.3853 (2)	0.66375 (19)	0.0278 (5)	
H4	0.2211	0.3875	0.6463	0.033*	
C3	0.33874 (14)	0.3826 (2)	0.57913 (18)	0.0284 (5)	
H3	0.3177	0.3844	0.5046	0.034*	
C2	0.42871 (13)	0.3770 (2)	0.60627 (17)	0.0249 (4)	
H2	0.4672	0.3741	0.5491	0.03*	

C10	0.70379 (12)	0.4304 (2)	0.71497 (16)	0.0228 (4)
H10A	0.7424	0.4638	0.66	0.027*
H10B	0.7058	0.4912	0.7779	0.027*
C8	0.58162 (13)	0.2411 (2)	0.78978 (18)	0.0240 (4)
H8A	0.5763	0.177	0.7292	0.029*
H8B	0.5441	0.2125	0.8478	0.029*
C5	0.31283 (13)	0.3849 (2)	0.77469 (18)	0.0275 (5)
H5	0.2738	0.3869	0.8313	0.033*
C12	0.82390 (12)	0.2821 (2)	0.77866 (15)	0.0224 (4)
H12A	0.8555	0.3268	0.7217	0.027*
H12B	0.8379	0.1883	0.7749	0.027*
C17	0.93757 (13)	0.7167 (2)	1.24746 (17)	0.0268 (4)
H17	0.9571	0.7421	1.3193	0.032*
C7	0.38537 (15)	0.4430 (3)	0.99152 (19)	0.0342 (5)
H7A	0.4167	0.4403	1.0634	0.051*
H7B	0.3316	0.3943	0.9947	0.051*
H7C	0.3726	0.5335	0.9715	0.051*
C18	0.90558 (13)	0.8060 (2)	1.1716 (2)	0.0297 (5)
H18	0.9016	0.8961	1.1874	0.036*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0282 (3)	0.0197 (3)	0.0246 (3)	0.00178 (18)	0.00181 (19)	0.00051 (18)
S2A	0.0229 (3)	0.0257 (3)	0.0265 (3)	−0.0011 (2)	0.0022 (2)	−0.0008 (2)
C16A	0.0229 (3)	0.0257 (3)	0.0265 (3)	−0.0011 (2)	0.0022 (2)	−0.0008 (2)
S2B	0.0229 (3)	0.0257 (3)	0.0265 (3)	−0.0011 (2)	0.0022 (2)	−0.0008 (2)
C16B	0.0229 (3)	0.0257 (3)	0.0265 (3)	−0.0011 (2)	0.0022 (2)	−0.0008 (2)
O1	0.0189 (6)	0.0199 (6)	0.0177 (6)	0.0015 (5)	0.0001 (5)	0.0003 (5)
O2	0.0213 (7)	0.0510 (10)	0.0218 (7)	−0.0010 (6)	0.0057 (6)	−0.0044 (6)
N3	0.0175 (7)	0.0216 (8)	0.0184 (8)	0.0028 (6)	0.0006 (6)	−0.0007 (6)
N1	0.0161 (8)	0.0234 (8)	0.0201 (8)	0.0005 (6)	0.0037 (6)	0.0027 (6)
N4	0.0196 (8)	0.0219 (8)	0.0197 (8)	0.0030 (6)	0.0022 (6)	0.0002 (6)
N2	0.0170 (8)	0.0260 (8)	0.0201 (8)	0.0035 (6)	0.0011 (6)	0.0002 (7)
C1	0.0175 (9)	0.0190 (9)	0.0244 (10)	−0.0012 (7)	0.0030 (7)	0.0003 (7)
C15	0.0141 (8)	0.0219 (9)	0.0191 (9)	0.0009 (7)	0.0019 (7)	0.0014 (7)
C14	0.0128 (8)	0.0209 (9)	0.0204 (9)	0.0022 (7)	0.0029 (7)	0.0023 (7)
C13	0.0143 (8)	0.0241 (10)	0.0182 (9)	0.0006 (7)	0.0031 (7)	−0.0016 (7)
C6	0.0216 (10)	0.0233 (10)	0.0239 (10)	−0.0022 (8)	0.0034 (8)	0.0000 (8)
C9	0.0218 (10)	0.0248 (10)	0.0245 (10)	0.0031 (8)	0.0021 (8)	0.0047 (8)
C11	0.0177 (9)	0.0309 (11)	0.0211 (9)	0.0008 (8)	0.0031 (7)	0.0060 (8)
C4	0.0163 (9)	0.0309 (11)	0.0360 (11)	−0.0025 (8)	0.0000 (8)	0.0014 (9)
C3	0.0228 (10)	0.0351 (12)	0.0267 (10)	−0.0024 (8)	−0.0019 (8)	0.0032 (9)
C2	0.0197 (9)	0.0309 (11)	0.0246 (10)	−0.0008 (8)	0.0042 (8)	0.0010 (8)
C10	0.0177 (9)	0.0284 (10)	0.0224 (9)	−0.0002 (8)	0.0024 (7)	0.0055 (8)
C8	0.0203 (9)	0.0228 (10)	0.0290 (10)	−0.0003 (7)	0.0030 (8)	0.0035 (8)
C5	0.0197 (10)	0.0331 (11)	0.0307 (11)	−0.0032 (8)	0.0087 (8)	−0.0001 (9)
C12	0.0204 (9)	0.0295 (10)	0.0174 (9)	0.0047 (8)	0.0017 (7)	−0.0042 (8)

C17	0.0173 (9)	0.0420 (12)	0.0211 (9)	−0.0069 (8)	0.0027 (7)	−0.0057 (9)
C7	0.0326 (11)	0.0442 (13)	0.0272 (11)	−0.0067 (10)	0.0117 (9)	−0.0083 (10)
C18	0.0240 (10)	0.0230 (10)	0.0432 (12)	−0.0017 (8)	0.0102 (9)	−0.0017 (9)

Geometric parameters (Å, º)

S1—C13	1.647 (2)	C9—H9A	0.97
S2A—C18	1.655 (2)	C9—H9B	0.97
S2A—C15	1.6988 (19)	C11—C10	1.522 (3)
C16A—C17	1.489 (3)	C11—H11A	0.97
C16A—C15	1.542 (2)	C11—H11B	0.97
C16A—H16A	0.93	C4—C3	1.381 (3)
O1—C14	1.369 (2)	C4—C5	1.386 (3)
O1—C13	1.381 (2)	C4—H4	0.93
O2—C6	1.367 (3)	C3—C2	1.396 (3)
O2—C7	1.434 (3)	C3—H3	0.93
N3—C13	1.337 (2)	C2—H2	0.93
N3—N4	1.393 (2)	C10—H10A	0.97
N3—C12	1.487 (2)	C10—H10B	0.97
N1—C1	1.425 (2)	C8—H8A	0.97
N1—C11	1.460 (2)	C8—H8B	0.97
N1—C8	1.469 (2)	C5—H5	0.93
N4—C14	1.290 (2)	C12—H12A	0.97
N2—C12	1.427 (2)	C12—H12B	0.97
N2—C9	1.460 (2)	C17—C18	1.349 (3)
N2—C10	1.464 (3)	C17—H17	0.93
C1—C2	1.386 (3)	C7—H7A	0.96
C1—C6	1.412 (3)	C7—H7B	0.96
C15—C14	1.441 (3)	C7—H7C	0.96
C6—C5	1.388 (3)	C18—H18	0.93
C9—C8	1.522 (3)		
C18—S2A—C15	92.58 (10)	C3—C4—C5	120.10 (19)
C17—C16A—C15	101.32 (13)	C3—C4—H4	120
C17—C16A—H16A	129.3	C5—C4—H4	120
C15—C16A—H16A	129.3	C4—C3—C2	119.49 (19)
C14—O1—C13	105.85 (14)	C4—C3—H3	120.3
C6—O2—C7	116.52 (17)	C2—C3—H3	120.3
C13—N3—N4	112.23 (15)	C1—C2—C3	121.48 (19)
C13—N3—C12	126.27 (17)	C1—C2—H2	119.3
N4—N3—C12	121.49 (15)	C3—C2—H2	119.3
C1—N1—C11	115.34 (15)	N2—C10—C11	108.46 (16)
C1—N1—C8	112.16 (15)	N2—C10—H10A	110
C11—N1—C8	110.80 (15)	C11—C10—H10A	110
C14—N4—N3	103.26 (15)	N2—C10—H10B	110
C12—N2—C9	114.55 (15)	C11—C10—H10B	110
C12—N2—C10	116.12 (16)	H10A—C10—H10B	108.4
C9—N2—C10	111.25 (15)	N1—C8—C9	110.57 (16)

C2—C1—C6	118.29 (18)	N1—C8—H8A	109.5
C2—C1—N1	123.40 (17)	C9—C8—H8A	109.5
C6—C1—N1	118.28 (17)	N1—C8—H8B	109.5
C14—C15—C16A	123.32 (15)	C9—C8—H8B	109.5
C14—C15—S2A	122.32 (14)	H8A—C8—H8B	108.1
C16A—C15—S2A	114.33 (12)	C4—C5—C6	120.56 (19)
N4—C14—O1	113.53 (16)	C4—C5—H5	119.7
N4—C14—C15	129.37 (18)	C6—C5—H5	119.7
O1—C14—C15	117.09 (16)	N2—C12—N3	115.51 (15)
N3—C13—O1	105.12 (16)	N2—C12—H12A	108.4
N3—C13—S1	132.09 (15)	N3—C12—H12A	108.4
O1—C13—S1	122.77 (14)	N2—C12—H12B	108.4
O2—C6—C5	123.60 (18)	N3—C12—H12B	108.4
O2—C6—C1	116.35 (17)	H12A—C12—H12B	107.5
C5—C6—C1	120.05 (19)	C18—C17—C16A	117.01 (18)
N2—C9—C8	109.84 (16)	C18—C17—H17	121.5
N2—C9—H9A	109.7	C16A—C17—H17	121.5
C8—C9—H9A	109.7	O2—C7—H7A	109.5
N2—C9—H9B	109.7	O2—C7—H7B	109.5
C8—C9—H9B	109.7	H7A—C7—H7B	109.5
H9A—C9—H9B	108.2	O2—C7—H7C	109.5
N1—C11—C10	109.26 (15)	H7A—C7—H7C	109.5
N1—C11—H11A	109.8	H7B—C7—H7C	109.5
C10—C11—H11A	109.8	C17—C18—S2A	114.76 (17)
N1—C11—H11B	109.8	C17—C18—H18	122.6
C10—C11—H11B	109.8	S2A—C18—H18	122.6
H11A—C11—H11B	108.3		

C13—N3—N4—C14	−0.5 (2)	N1—C1—C6—O2	0.7 (3)
C12—N3—N4—C14	178.38 (15)	C2—C1—C6—C5	1.5 (3)
C11—N1—C1—C2	22.5 (3)	N1—C1—C6—C5	179.97 (18)
C8—N1—C1—C2	−105.7 (2)	C12—N2—C9—C8	−167.82 (16)
C11—N1—C1—C6	−155.90 (18)	C10—N2—C9—C8	58.0 (2)
C8—N1—C1—C6	76.0 (2)	C1—N1—C11—C10	171.49 (16)
C17—C16A—C15—C14	−177.76 (16)	C8—N1—C11—C10	−59.7 (2)
C17—C16A—C15—S2A	0.16 (15)	C5—C4—C3—C2	1.1 (3)
C18—S2A—C15—C14	177.79 (16)	C6—C1—C2—C3	−0.5 (3)
C18—S2A—C15—C16A	−0.16 (13)	N1—C1—C2—C3	−178.91 (19)
N3—N4—C14—O1	0.53 (19)	C4—C3—C2—C1	−0.8 (3)
N3—N4—C14—C15	−178.64 (17)	C12—N2—C10—C11	165.92 (15)
C13—O1—C14—N4	−0.4 (2)	C9—N2—C10—C11	−60.7 (2)
C13—O1—C14—C15	178.90 (15)	N1—C11—C10—N2	60.7 (2)
C16A—C15—C14—N4	−178.37 (16)	C1—N1—C8—C9	−172.53 (16)
S2A—C15—C14—N4	3.9 (3)	C11—N1—C8—C9	57.0 (2)
C16A—C15—C14—O1	2.5 (2)	N2—C9—C8—N1	−55.2 (2)
S2A—C15—C14—O1	−175.28 (13)	C3—C4—C5—C6	−0.2 (3)
N4—N3—C13—O1	0.29 (19)	O2—C6—C5—C4	178.1 (2)
C12—N3—C13—O1	−178.53 (15)	C1—C6—C5—C4	−1.2 (3)

N4—N3—C13—S1	−178.25 (15)	C9—N2—C12—N3	−52.8 (2)
C12—N3—C13—S1	2.9 (3)	C10—N2—C12—N3	79.1 (2)
C14—O1—C13—N3	0.03 (18)	C13—N3—C12—N2	110.8 (2)
C14—O1—C13—S1	178.74 (13)	N4—N3—C12—N2	−67.9 (2)
C7—O2—C6—C5	−24.0 (3)	C15—C16A—C17—C18	−0.1 (2)
C7—O2—C6—C1	155.31 (19)	C16A—C17—C18—S2A	0.0 (2)
C2—C1—C6—O2	−177.78 (18)	C15—S2A—C18—C17	0.11 (17)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the S2*A*/C15/C16*A*/C17/C18 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12*A*···S1^{i}	0.97	2.95	3.860 (2)	157
C17—H17···O1^{ii}	0.93	2.69	3.475 (2)	143
C5—H5···*Cg*1^{iii}	0.93	2.95	3.660 (2)	135

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (ii) −*x*+2, *y*+1/2, −*z*+5/2; (iii) −*x*+1, −*y*+1, −*z*+2.