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(4*Z*)-1-[(*E*)-(4-Methoxybenzylidene)amino]-2-phenyl-4-[(thiophen-2-yl)methylidene]-1*H*-imidazol-5(4*H*)-one

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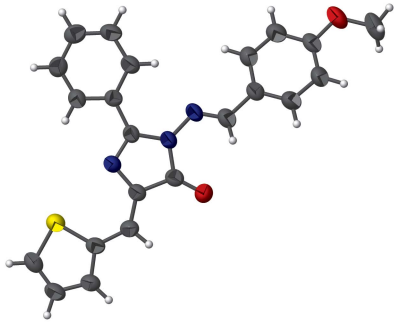
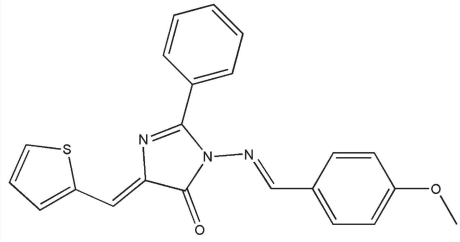
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{22}H_{17}N_3O_2S$, the imidazole ring forms dihedral angles of 9.2 (2), 10.9 (2) and 12.5 (2)° with the thiophene, phenyl and methoxy-substituted benzene rings, respectively. There are two intramolecular C—H···N hydrogen bonds forming *S*(5) and *S*(6) rings and one intramolecular C—H···O hydrogen bond forming an *S*(6) ring.

3D view



Chemical scheme



Structure description

Compounds containing the imidazolone as well as the imine moiety exhibit pharmaceutical activities such as antimicrobial (Suthakaran *et al.*, 2008; Patel *et al.*, 2006), antioxidant (Suhasini *et al.*, 2014), anticonvulsant (Mohamed *et al.*, 2012), anthelmintic (Patel *et al.*, 2010) antibacterial (Solankee *et al.*, 2011) analgesic (Sridhar & Ramesh, 2001), anti-inflammatory (Viveka *et al.*, 2015) and antitumor (Hodnett & Dunn, 1970). Apart from their biological activity, Schiff bases have assumed importance as ligands in coordination chemistry (Özkar *et al.* 2004, Pouralimardan *et al.*, 2007; Patti *et al.*, 2009). Structural information on the title compound is useful in developing the coordination properties of Schiff bases and to investigate new ligands.

The molecular structure of the title compound is shown in Fig. 1. The bond lengths and angles have normal values and all aromatic rings are essentially planar. The imidazole ring forms dihedral angles of 9.2 (2), 10.9 (2) and 12.5 (2)° with the thiophene (S1/C1–C4), phenyl (C9–C14) and methoxy-substituted benzene (C16–C21) rings, respectively. The methoxy group is essentially planar with the benzene ring to which it is attached, with

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···N1	0.93	2.46	2.792 (4)	101
C14—H14···N3	0.93	2.32	2.942 (4)	124
C15—H15···O1	0.93	2.21	2.867 (3)	127

a C22—O2—C19—C18 torsion angle of −0.8 (4)°. There are two intramolecular C—H···N hydrogen bonds (Table 1), forming $S(5)$ and $S(6)$ rings, and one intramolecular C—H···O hydrogen bond forming an $S(6)$ ring (Fig. 1).

Synthesis and crystallization

A mixture of 3-hydrazinyl-3-oxo-1-(thiophen-2-yl)prop-1-en-2-yl]benzamide (0.01 mol) in 2-propanol (30 ml) with 4-methoxybenzaldehyde (0.01 mol) in presence of one to two drops of sulfuric acid were heated under reflux for 8 h. The reaction mixture was cooled to ambient temperature and poured on cold water. The solid mass obtained was collected by filtration and washed with cold water. It was crystallized at ambient temperature in the presence of air from a mixture of methanol and *N*,*N*-dimethylformamide(1:1 *v*/*v*) (m.p. 421 K).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{17}N_3O_2S$
M_r	387.45
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	20.6796 (18), 5.4004 (4), 17.2537 (16)
β (°)	104.299 (9)
V (Å^3)	1867.2 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.20
Crystal size (mm)	0.30 × 0.20 × 0.20
Data collection	
Diffractometer	Oxford Diffraction Xcalibur Sapphire3
Absorption correction	Multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
T_{min}, T_{max}	0.769, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7300, 3663, 2215
R_{int}	0.028
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.136, 1.05
No. of reflections	3663
No. of parameters	255
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.23

Computer programs: *CrysAlis PRO* (Oxford Diffraction, 2010), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

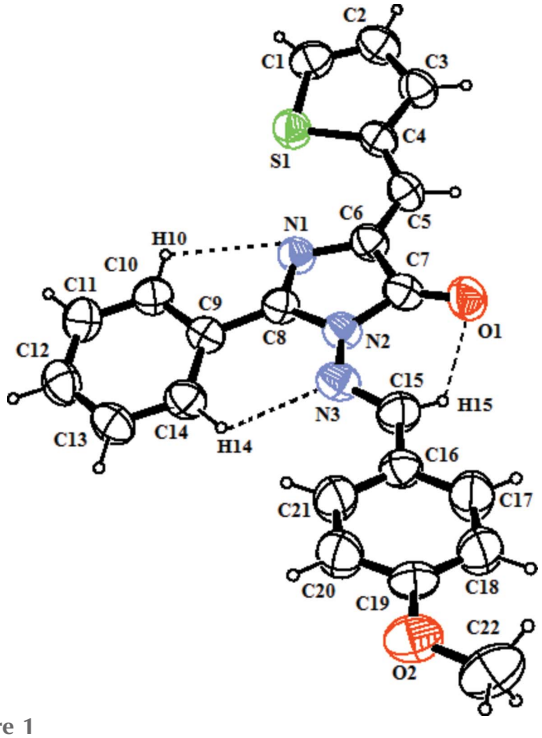


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 40% probability level. H atoms are shown as small spheres of arbitrary radii. Dashed lines indicate weak intramolecular hydrogen bonds.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x160566 [doi:10.1107/S2414314616005666]

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Crystal data

$C_{22}H_{17}N_3O_2S$
M_r = 387.45
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 20.6796 (18) Å
b = 5.4004 (4) Å
c = 17.2537 (16) Å
β = 104.299 (9)°
V = 1867.2 (3) Å^3
Z = 4
$F(000)$ = 808
D_x = 1.378 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1894 reflections
θ = 4.2–27.1°
μ = 0.20 mm^{-1}
T = 293 K
Rectangular, white
0.30 × 0.20 × 0.20 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 16.1049 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
T_{min} = 0.769, T_{max} = 1.000
7300 measured reflections
3663 independent reflections
2215 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 26.0°, θ_{min} = 3.9°
h = −21→25
k = −6→4
l = −21→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.136
S = 1.05
3663 reflections
255 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
$w = 1/[\sigma^2(F_o^2) + (0.0436P)^2 + 0.2269P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Special details

Experimental. Absorption correction: CrysAlisPro, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.44505 (4)	0.95712 (13)	0.26907 (4)	0.0566 (3)
N1	0.33090 (10)	0.8287 (4)	0.12524 (13)	0.0476 (6)
C9	0.28224 (12)	1.0201 (5)	−0.00327 (15)	0.0435 (6)
N2	0.23366 (10)	0.6575 (4)	0.05940 (13)	0.0469 (5)
O1	0.22389 (9)	0.3399 (4)	0.14907 (11)	0.0633 (6)
C7	0.25357 (14)	0.5141 (5)	0.12958 (16)	0.0498 (7)
C8	0.28221 (12)	0.8389 (5)	0.06065 (15)	0.0444 (6)
N3	0.17324 (11)	0.6492 (4)	0.00114 (13)	0.0518 (6)
C10	0.33009 (13)	1.2060 (5)	0.01438 (17)	0.0508 (7)
H10	0.3591	1.2132	0.0650	0.061*
C5	0.35065 (13)	0.5749 (5)	0.24616 (16)	0.0499 (7)
H5	0.3359	0.4344	0.2678	0.060*
C14	0.23988 (13)	1.0125 (5)	−0.07990 (17)	0.0539 (7)
H14	0.2079	0.8885	−0.0930	0.065*
O2	−0.11004 (10)	0.3630 (4)	−0.22410 (13)	0.0745 (6)
C4	0.40723 (13)	0.6972 (5)	0.29599 (15)	0.0473 (7)
C1	0.50041 (14)	0.9677 (6)	0.36046 (17)	0.0613 (8)
H1	0.5338	1.0866	0.3749	0.074*
C13	0.24499 (15)	1.1877 (5)	−0.13666 (17)	0.0595 (8)
H13	0.2164	1.1812	−0.1875	0.071*
C12	0.29240 (15)	1.3713 (5)	−0.11775 (18)	0.0600 (8)
H12	0.2957	1.4896	−0.1558	0.072*
C2	0.49050 (14)	0.7853 (6)	0.40935 (18)	0.0618 (8)
H2	0.5161	0.7651	0.4614	0.074*
C6	0.31598 (13)	0.6373 (5)	0.17177 (16)	0.0479 (7)
C16	0.07441 (14)	0.4331 (5)	−0.06258 (16)	0.0527 (7)
C15	0.13843 (14)	0.4562 (5)	−0.00441 (17)	0.0601 (8)
H15	0.1540	0.3241	0.0297	0.072*
C19	−0.04988 (14)	0.3744 (5)	−0.16912 (17)	0.0543 (7)
C21	0.05040 (15)	0.6050 (5)	−0.12224 (18)	0.0634 (8)
H21	0.0762	0.7426	−0.1268	0.076*
C3	0.43762 (14)	0.6291 (5)	0.37355 (16)	0.0555 (7)
H3	0.4243	0.4939	0.3992	0.067*

C11	0.33506 (14)	1.3800 (5)	−0.04245 (18)	0.0580 (8)
H11	0.3673	1.5035	−0.0299	0.070*
C17	0.03512 (17)	0.2308 (6)	−0.0599 (2)	0.0823 (11)
H17	0.0507	0.1090	−0.0217	0.099*
C18	−0.02719 (16)	0.2015 (6)	−0.1122 (2)	0.0762 (10)
H18	−0.0532	0.0639	−0.1081	0.091*
C20	−0.01077 (15)	0.5760 (6)	−0.17477 (19)	0.0674 (9)
H20	−0.0259	0.6935	−0.2145	0.081*
C22	−0.15119 (16)	0.1525 (6)	−0.2217 (2)	0.0901 (12)
H22A	−0.1300	0.0068	−0.2357	0.135*
H22B	−0.1937	0.1750	−0.2590	0.135*
H22C	−0.1576	0.1342	−0.1687	0.135*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0543 (5)	0.0598 (5)	0.0512 (5)	−0.0039 (4)	0.0044 (4)	0.0050 (3)
N1	0.0426 (13)	0.0533 (13)	0.0432 (13)	−0.0023 (10)	0.0038 (11)	0.0027 (10)
C9	0.0389 (15)	0.0493 (15)	0.0421 (15)	0.0057 (12)	0.0096 (12)	0.0014 (12)
N2	0.0385 (12)	0.0565 (13)	0.0431 (13)	−0.0050 (11)	0.0051 (10)	−0.0003 (10)
O1	0.0606 (13)	0.0725 (13)	0.0539 (13)	−0.0183 (11)	0.0089 (11)	0.0084 (10)
C7	0.0466 (16)	0.0599 (18)	0.0420 (16)	−0.0003 (14)	0.0092 (13)	−0.0004 (13)
C8	0.0377 (14)	0.0510 (16)	0.0440 (16)	−0.0024 (13)	0.0090 (13)	−0.0023 (12)
N3	0.0378 (13)	0.0688 (15)	0.0450 (13)	−0.0054 (12)	0.0032 (11)	−0.0018 (11)
C10	0.0443 (16)	0.0549 (17)	0.0515 (17)	−0.0014 (13)	0.0089 (14)	−0.0028 (13)
C5	0.0461 (16)	0.0572 (16)	0.0457 (16)	0.0024 (13)	0.0103 (13)	0.0079 (13)
C14	0.0468 (16)	0.0619 (18)	0.0491 (17)	−0.0001 (14)	0.0042 (14)	0.0011 (14)
O2	0.0502 (13)	0.0910 (15)	0.0701 (15)	−0.0045 (12)	−0.0083 (11)	−0.0081 (12)
C4	0.0437 (15)	0.0558 (16)	0.0413 (15)	0.0073 (13)	0.0087 (13)	0.0036 (12)
C1	0.0500 (18)	0.0685 (19)	0.0581 (19)	−0.0053 (15)	−0.0002 (15)	−0.0074 (16)
C13	0.0559 (19)	0.070 (2)	0.0478 (17)	0.0097 (16)	0.0038 (15)	0.0091 (15)
C12	0.063 (2)	0.0571 (18)	0.063 (2)	0.0128 (16)	0.0204 (17)	0.0121 (15)
C2	0.0523 (18)	0.079 (2)	0.0469 (17)	0.0021 (16)	−0.0008 (15)	0.0030 (16)
C6	0.0422 (15)	0.0557 (16)	0.0431 (15)	−0.0012 (13)	0.0055 (13)	0.0026 (13)
C16	0.0495 (17)	0.0588 (17)	0.0459 (16)	−0.0063 (15)	0.0045 (14)	−0.0035 (14)
C15	0.0549 (18)	0.0609 (18)	0.0566 (19)	−0.0094 (16)	−0.0008 (15)	−0.0005 (15)
C19	0.0455 (16)	0.0651 (19)	0.0477 (17)	−0.0018 (15)	0.0029 (14)	−0.0114 (15)
C21	0.0567 (19)	0.0653 (19)	0.063 (2)	−0.0126 (16)	0.0040 (16)	0.0053 (16)
C3	0.0524 (17)	0.0639 (18)	0.0459 (17)	0.0007 (15)	0.0039 (14)	0.0076 (14)
C11	0.0522 (17)	0.0547 (17)	0.067 (2)	0.0003 (14)	0.0147 (16)	0.0052 (16)
C17	0.082 (2)	0.080 (2)	0.066 (2)	−0.027 (2)	−0.0183 (19)	0.0186 (18)
C18	0.071 (2)	0.080 (2)	0.064 (2)	−0.0310 (19)	−0.0078 (18)	0.0067 (18)
C20	0.063 (2)	0.069 (2)	0.061 (2)	−0.0026 (17)	−0.0006 (17)	0.0091 (16)
C22	0.054 (2)	0.098 (3)	0.105 (3)	−0.015 (2)	−0.005 (2)	−0.022 (2)

Geometric parameters (Å, º)

S1—C1	1.705 (3)	C1—H1	0.9300
S1—C4	1.725 (3)	C13—C12	1.376 (4)
N1—C8	1.306 (3)	C13—H13	0.9300
N1—C6	1.389 (3)	C12—C11	1.379 (4)
C9—C10	1.390 (3)	C12—H12	0.9300
C9—C14	1.395 (3)	C2—C3	1.398 (4)
C9—C8	1.475 (3)	C2—H2	0.9300
N2—N3	1.398 (3)	C16—C17	1.369 (4)
N2—C8	1.399 (3)	C16—C21	1.384 (4)
N2—C7	1.410 (3)	C16—C15	1.456 (4)
O1—C7	1.215 (3)	C15—H15	0.9300
C7—C6	1.475 (3)	C19—C18	1.353 (4)
N3—C15	1.257 (3)	C19—C20	1.374 (4)
C10—C11	1.380 (4)	C21—C20	1.371 (4)
C10—H10	0.9300	C21—H21	0.9300
C5—C6	1.349 (3)	C3—H3	0.9300
C5—C4	1.431 (3)	C11—H11	0.9300
C5—H5	0.9300	C17—C18	1.388 (4)
C14—C13	1.384 (4)	C17—H17	0.9300
C14—H14	0.9300	C18—H18	0.9300
O2—C19	1.367 (3)	C20—H20	0.9300
O2—C22	1.426 (3)	C22—H22A	0.9600
C4—C3	1.380 (3)	C22—H22B	0.9600
C1—C2	1.345 (4)	C22—H22C	0.9600
C1—S1—C4	91.37 (14)	C1—C2—H2	123.6
C8—N1—C6	106.9 (2)	C3—C2—H2	123.6
C10—C9—C14	118.4 (2)	C5—C6—N1	126.4 (2)
C10—C9—C8	116.6 (2)	C5—C6—C7	123.5 (3)
C14—C9—C8	125.0 (2)	N1—C6—C7	110.0 (2)
N3—N2—C8	123.0 (2)	C17—C16—C21	117.0 (3)
N3—N2—C7	128.3 (2)	C17—C16—C15	119.4 (3)
C8—N2—C7	108.4 (2)	C21—C16—C15	123.6 (3)
O1—C7—N2	127.0 (3)	N3—C15—C16	122.0 (3)
O1—C7—C6	130.8 (3)	N3—C15—H15	119.0
N2—C7—C6	102.1 (2)	C16—C15—H15	119.0
N1—C8—N2	112.5 (2)	C18—C19—O2	124.4 (3)
N1—C8—C9	121.6 (2)	C18—C19—C20	119.6 (3)
N2—C8—C9	125.9 (2)	O2—C19—C20	115.9 (3)
C15—N3—N2	118.3 (2)	C20—C21—C16	121.2 (3)
C11—C10—C9	120.7 (3)	C20—C21—H21	119.4
C11—C10—H10	119.7	C16—C21—H21	119.4
C9—C10—H10	119.7	C4—C3—C2	112.7 (3)
C6—C5—C4	128.3 (3)	C4—C3—H3	123.6
C6—C5—H5	115.8	C2—C3—H3	123.6
C4—C5—H5	115.8	C12—C11—C10	120.2 (3)

C13—C14—C9	120.7 (3)	C12—C11—H11	119.9
C13—C14—H14	119.6	C10—C11—H11	119.9
C9—C14—H14	119.6	C16—C17—C18	122.2 (3)
C19—O2—C22	117.6 (2)	C16—C17—H17	118.9
C3—C4—C5	124.6 (3)	C18—C17—H17	118.9
C3—C4—S1	110.5 (2)	C19—C18—C17	119.6 (3)
C5—C4—S1	124.9 (2)	C19—C18—H18	120.2
C2—C1—S1	112.6 (2)	C17—C18—H18	120.2
C2—C1—H1	123.7	C21—C20—C19	120.4 (3)
S1—C1—H1	123.7	C21—C20—H20	119.8
C12—C13—C14	119.9 (3)	C19—C20—H20	119.8
C12—C13—H13	120.0	O2—C22—H22A	109.5
C14—C13—H13	120.0	O2—C22—H22B	109.5
C13—C12—C11	120.0 (3)	H22A—C22—H22B	109.5
C13—C12—H12	120.0	O2—C22—H22C	109.5
C11—C12—H12	120.0	H22A—C22—H22C	109.5
C1—C2—C3	112.9 (3)	H22B—C22—H22C	109.5

N3—N2—C7—O1	7.1 (4)	C4—C5—C6—N1	4.4 (5)
C8—N2—C7—O1	−180.0 (3)	C4—C5—C6—C7	−172.6 (2)
N3—N2—C7—C6	−170.7 (2)	C8—N1—C6—C5	−174.8 (3)
C8—N2—C7—C6	2.3 (3)	C8—N1—C6—C7	2.5 (3)
C6—N1—C8—N2	−1.0 (3)	O1—C7—C6—C5	−3.1 (5)
C6—N1—C8—C9	−179.0 (2)	N2—C7—C6—C5	174.5 (2)
N3—N2—C8—N1	172.4 (2)	O1—C7—C6—N1	179.5 (3)
C7—N2—C8—N1	−1.0 (3)	N2—C7—C6—N1	−2.9 (3)
N3—N2—C8—C9	−9.6 (4)	N2—N3—C15—C16	179.1 (2)
C7—N2—C8—C9	177.0 (2)	C17—C16—C15—N3	−172.5 (3)
C10—C9—C8—N1	−10.9 (4)	C21—C16—C15—N3	8.1 (5)
C14—C9—C8—N1	166.7 (2)	C22—O2—C19—C18	−0.8 (4)
C10—C9—C8—N2	171.4 (2)	C22—O2—C19—C20	178.1 (3)
C14—C9—C8—N2	−11.1 (4)	C17—C16—C21—C20	1.6 (5)
C8—N2—N3—C15	166.7 (2)	C15—C16—C21—C20	−179.0 (3)
C7—N2—N3—C15	−21.3 (4)	C5—C4—C3—C2	−178.0 (2)
C14—C9—C10—C11	0.6 (4)	S1—C4—C3—C2	−0.3 (3)
C8—C9—C10—C11	178.3 (2)	C1—C2—C3—C4	−0.1 (4)
C10—C9—C14—C13	−0.7 (4)	C13—C12—C11—C10	−0.5 (4)
C8—C9—C14—C13	−178.2 (2)	C9—C10—C11—C12	0.0 (4)
C6—C5—C4—C3	176.1 (3)	C21—C16—C17—C18	−2.4 (5)
C6—C5—C4—S1	−1.3 (4)	C15—C16—C17—C18	178.1 (3)
C1—S1—C4—C3	0.5 (2)	O2—C19—C18—C17	179.3 (3)
C1—S1—C4—C5	178.2 (2)	C20—C19—C18—C17	0.4 (5)
C4—S1—C1—C2	−0.6 (2)	C16—C17—C18—C19	1.5 (6)
C9—C14—C13—C12	0.2 (4)	C16—C21—C20—C19	0.2 (5)
C14—C13—C12—C11	0.4 (4)	C18—C19—C20—C21	−1.2 (5)
S1—C1—C2—C3	0.5 (3)	O2—C19—C20—C21	179.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···N1	0.93	2.46	2.792 (4)	101
C14—H14···N3	0.93	2.32	2.942 (4)	124
C15—H15···O1	0.93	2.21	2.867 (3)	127