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ISSN 2414-3146

N-{(*Z*)-3-Oxo-3-[(*E*)-(pyridin-2-ylmethyl)diazenyl]-1-(thiophen-2-yl)prop-1-en-2-yl}benzamide

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Received 28 July 2016
Accepted 8 August 2016

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

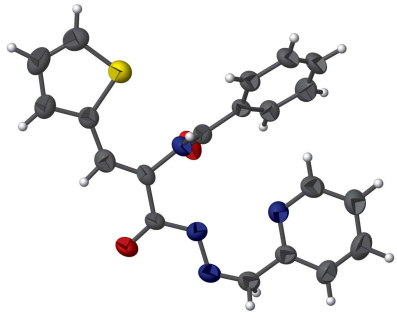
Keywords: crystal structure; diazo; benzamide; hydrogen bonding; C—H$\cdots\pi$ interactions.

CCDC reference: 1498199

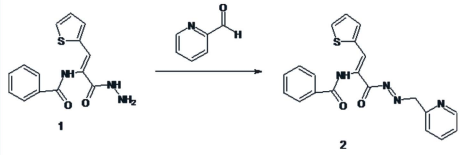
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{20}H_{16}N_4O_2S$, the thiophene ring subtends dihedral angles of 58.6 (3) and 9.8 (3)° with the benzamide and pyridine rings, respectively, whereas these two rings are inclined to one another by 59.3 (3)°. There is an intramolecular C—H$\cdots\pi$ interaction present involving the pyridine and benzamide rings. In the crystal, molecules are linked by N—H$\cdots$O hydrogen bonds, forming chains along the [010] direction. The chains are linked by C—H$\cdots$S hydrogen bonds and C—H$\cdots\pi$ interactions, forming sheets parallel to the *ab* plane.

3D view



Chemical scheme



Structure description

Azo compounds have a (–N=N–) linkage, and are highly coloured compounds. They are used as dyes and pigments for colouring fibers, optical storage devices, photo-electronic applications, printing systems, textile dyes *etc* (Wang *et al.*, 2000). The title compound is initially a hydrazone formed by the reaction of the precursor hydrazide **1** with pyridine 2-aldehyde (see Scheme). However, it rearranges to a diazo derivative by a 1,3 proton shift. Herein, we report on the crystal structure of compound **2**, containing a diazo (–N=N–) linkage.

In the title compound, Fig. 1, the thiophene ring forms a dihedral angle 9.8 (3)° with the pyridine ring. The benzamide ring is inclined to the thiophene and pyridine rings by 58.6 (3) and 59.3 (3)°, respectively. The molecule has an *E* conformation about the N1=N2 bond, and a *Z* conformation about the C5=C6 bond. There is an intramolecular C—H$\cdots\pi$ interaction present involving the pyridine and benzamide rings (Fig. 1 and Table 1).

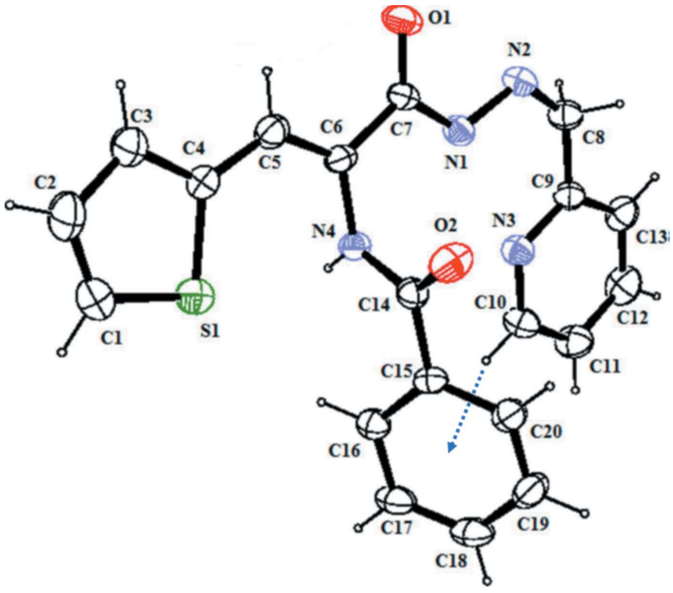


Figure 1
A view of the molecular structure of the title compound **2**, showing the atom labelling. Displacement ellipsoids are drawn at the 40% probability level. The intramolecular C—H···π interaction is shown as a blue dashed arrow (see Table 1).

In the crystal, molecules are linked by N—H···O hydrogen bonds forming chains along the *b*-axis direction (Fig. 2 and Table 1). The chains are linked by C—H···S hydrogen bonds and C—H···π interactions, forming sheets parallel to the *ab* plane (Fig. 2 and Table 1).

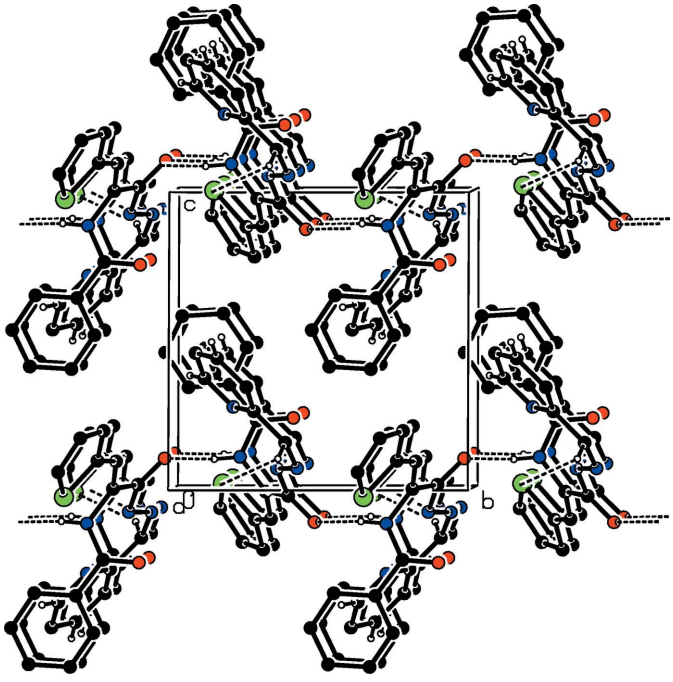


Figure 2
The crystal packing of the title compound **2**, viewed along the *a* axis. The N—H···O and C—H···S hydrogen bonds are shown as dashed lines (see Table 1). For clarity, only the H atoms involved in the various intra- and intermolecular interactions have been included.

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

*Cg*2 and *Cg*3 are the centroids of rings N3/C9–C13 and C15–C20, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···O1^{i}	0.86	2.18	2.931 (6)	145
C8—H8*B*···S1^{ii}	0.97	2.68	3.492 (5)	141
C10—H10···*Cg*3	0.93	2.89	3.627 (6)	137
C12—H12···*Cg*2^{ii}	0.93	2.92	3.648 (6)	136

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{16}N_4O_2S$
M_r	376.43
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	293
a, *b*, *c* (Å)	9.3289 (10), 9.9031 (10), 9.8984 (12)
β (°)	97.221 (11)
V (Å^3)	907.21 (17)
Z	2
Radiation type	Mo *K*α
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}	0.749, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3602, 2547, 1807
R_{int}	0.057
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.054, 0.137, 0.98
No. of reflections	2547
No. of parameters	244
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.27

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

Synthesis and crystallization

A mixture of [3-hydrazinyl-3-oxo-1-(thiophen-2-yl)prop-1-en-2-yl]benzamide **1** (2.87 g, 0.01 mol), and pyridine-2-carbaldehyde (1.07 g, 0.01 mol) in 20 ml ethanol were stirred for 3–4 h. The solid obtained was filtered, washed with cold water, dried and recrystallized from ethanol. Single crystals of **2** were grown from a methanol–1,4-dioxane (1:1) mixture by slow evaporation (m.p. 507–508 K).

Refinement

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

Acknowledgements

RK acknowledges the Indian Council of Medical Research, New Delhi, for financial support [research project No. BIC/12 (14)/2012] and the Department of Science and Technology Research (project No. EMR/2014/000467). KNS gratefully acknowledges the Department of Chemistry, Shri Madhwa Vadiraja Institute of Technology, Bantakal (VTU Belgam), for providing research facilities.

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full crystallographic data

IUCrData (2016). **1**, x161276 [doi:10.1107/S2414314616012761]

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Crystal data

$C_{20}H_{16}N_4O_2S$
M_r = 376.43
Monoclinic, $P2_1$
Hall symbol: P 2yb
a = 9.3289 (10) Å
b = 9.9031 (10) Å
c = 9.8984 (12) Å
β = 97.221 (11)°
V = 907.21 (17) Å^3
Z = 2
$F(000)$ = 392
D_x = 1.378 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 985 reflections
θ = 4.4–26.3°
μ = 0.20 mm^{-1}
T = 293 K
Rectangular, brown
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} = 0.749, T_{max} = 1.000
3602 measured reflections
2547 independent reflections
1807 reflections with $I > 2\sigma(I)$
R_{int} = 0.057
θ_{max} = 26.0°, θ_{min} = 3.5°
h = −9→11
k = −6→12
l = −11→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.137
S = 0.98
2547 reflections
244 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Special details

Experimental. CrysAlis Pro (Oxford Diffraction, 2010)

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	0.53359 (14)	0.16714 (15)	1.01498 (14)	0.0554 (4)
N1	1.0902 (4)	0.3655 (4)	1.0744 (4)	0.0444 (10)
N4	0.8437 (4)	0.2341 (4)	1.1093 (4)	0.0397 (9)
H4	0.8568	0.1485	1.1021	0.048*
O2	0.7951 (5)	0.4099 (3)	1.2397 (4)	0.0637 (11)
O1	0.9821 (4)	0.4880 (4)	0.8927 (4)	0.0664 (11)
N2	1.2188 (5)	0.4370 (4)	1.0774 (4)	0.0493 (11)
N3	1.2102 (4)	0.2226 (4)	1.2834 (4)	0.0473 (11)
C9	1.3313 (5)	0.2957 (5)	1.2705 (5)	0.0446 (12)
C8	1.3214 (5)	0.4001 (5)	1.1653 (5)	0.0484 (13)
H8A	1.3509	0.4822	1.2145	0.058*
H8B	1.3993	0.3788	1.1125	0.058*
C4	0.5869 (5)	0.2766 (5)	0.8944 (5)	0.0470 (12)
C15	0.8350 (5)	0.1983 (5)	1.3518 (5)	0.0401 (11)
C14	0.8217 (5)	0.2889 (5)	1.2308 (5)	0.0425 (12)
C7	0.9768 (5)	0.3999 (5)	0.9807 (5)	0.0421 (12)
C16	0.8130 (5)	0.0601 (5)	1.3426 (5)	0.0464 (12)
H16	0.7867	0.0198	1.2583	0.056*
C5	0.7281 (6)	0.3345 (5)	0.8987 (5)	0.0499 (13)
H5	0.7413	0.3901	0.8256	0.060*
C6	0.8447 (5)	0.3205 (5)	0.9930 (5)	0.0408 (11)
C20	0.8724 (5)	0.2558 (6)	1.4772 (5)	0.0500 (13)
H20	0.8837	0.3489	1.4842	0.060*
C11	1.3428 (6)	0.1005 (6)	1.4664 (6)	0.0637 (16)
H11	1.3449	0.0342	1.5332	0.076*
C13	1.4587 (6)	0.2743 (6)	1.3537 (6)	0.0564 (14)
H13	1.5398	0.3260	1.3436	0.068*
C17	0.8305 (6)	−0.0174 (6)	1.4596 (6)	0.0602 (15)
H17	0.8129	−0.1098	1.4541	0.072*
C1	0.3663 (6)	0.1528 (6)	0.9289 (6)	0.0634 (16)
H1	0.2947	0.0985	0.9578	0.076*
C3	0.4727 (6)	0.3004 (6)	0.7921 (6)	0.0612 (15)
H3	0.4781	0.3572	0.7180	0.073*
C10	1.2185 (6)	0.1270 (5)	1.3791 (6)	0.0559 (15)

H10	1.1365	0.0757	1.3875	0.067*
C19	0.8932 (5)	0.1783 (7)	1.5915 (5)	0.0640 (16)
H19	0.9211	0.2184	1.6757	0.077*
C18	0.8731 (6)	0.0402 (6)	1.5827 (6)	0.0633 (16)
H18	0.8887	−0.0130	1.6605	0.076*
C12	1.4648 (6)	0.1767 (8)	1.4506 (6)	0.0671 (16)
H12	1.5508	0.1608	1.5067	0.081*
C2	0.3467 (6)	0.2271 (7)	0.8149 (7)	0.0764 (19)
H2	0.2602	0.2304	0.7570	0.092*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0574 (8)	0.0551 (8)	0.0545 (8)	−0.0009 (7)	0.0105 (7)	0.0024 (7)
N1	0.040 (2)	0.045 (2)	0.048 (3)	−0.004 (2)	0.0056 (19)	0.003 (2)
N4	0.049 (2)	0.035 (2)	0.036 (2)	0.0003 (18)	0.0091 (19)	0.0022 (18)
O2	0.102 (3)	0.0386 (19)	0.051 (2)	0.020 (2)	0.012 (2)	0.0004 (19)
O1	0.063 (2)	0.068 (3)	0.066 (3)	−0.020 (2)	0.002 (2)	0.028 (2)
N2	0.048 (3)	0.046 (3)	0.055 (3)	−0.005 (2)	0.012 (2)	0.008 (2)
N3	0.045 (2)	0.046 (2)	0.050 (3)	0.003 (2)	0.004 (2)	0.006 (2)
C9	0.043 (3)	0.049 (3)	0.043 (3)	−0.003 (2)	0.012 (2)	0.000 (3)
C8	0.044 (3)	0.053 (3)	0.050 (3)	0.002 (2)	0.014 (3)	0.005 (3)
C4	0.051 (3)	0.050 (3)	0.040 (3)	−0.004 (3)	0.003 (2)	−0.001 (2)
C15	0.037 (2)	0.046 (3)	0.040 (3)	0.003 (2)	0.011 (2)	0.009 (2)
C14	0.044 (3)	0.039 (3)	0.044 (3)	−0.001 (2)	0.002 (2)	0.004 (2)
C7	0.043 (3)	0.042 (3)	0.042 (3)	−0.007 (2)	0.008 (2)	0.007 (2)
C16	0.047 (3)	0.044 (3)	0.048 (3)	0.001 (2)	0.007 (2)	0.006 (3)
C5	0.060 (3)	0.050 (3)	0.039 (3)	0.000 (3)	0.006 (3)	−0.002 (3)
C6	0.050 (3)	0.041 (3)	0.032 (2)	0.002 (2)	0.007 (2)	0.005 (2)
C20	0.052 (3)	0.056 (3)	0.043 (3)	0.000 (3)	0.006 (2)	0.002 (3)
C11	0.060 (4)	0.068 (4)	0.061 (4)	0.008 (3)	0.002 (3)	0.016 (3)
C13	0.043 (3)	0.073 (4)	0.052 (3)	0.004 (3)	0.000 (3)	0.000 (3)
C17	0.057 (3)	0.062 (4)	0.062 (4)	−0.005 (3)	0.011 (3)	0.026 (3)
C1	0.058 (3)	0.060 (4)	0.072 (4)	−0.009 (3)	0.007 (3)	−0.005 (4)
C3	0.055 (3)	0.066 (4)	0.059 (4)	−0.005 (3)	−0.006 (3)	0.006 (3)
C10	0.057 (3)	0.048 (3)	0.064 (4)	−0.001 (3)	0.011 (3)	0.010 (3)
C19	0.063 (3)	0.094 (5)	0.036 (3)	−0.005 (4)	0.008 (3)	−0.006 (3)
C18	0.063 (4)	0.069 (4)	0.059 (4)	0.001 (3)	0.011 (3)	0.031 (3)
C12	0.047 (3)	0.086 (4)	0.066 (4)	0.014 (4)	−0.006 (3)	0.001 (4)
C2	0.059 (4)	0.090 (5)	0.074 (4)	−0.007 (4)	−0.015 (3)	−0.001 (4)

Geometric parameters (Å, º)

S1—C1	1.687 (5)	C16—H16	0.9300
S1—C4	1.731 (5)	C5—C6	1.349 (7)
N1—C7	1.359 (7)	C5—H5	0.9300
N1—N2	1.389 (5)	C20—C19	1.361 (7)
N4—C14	1.359 (6)	C20—H20	0.9300

N4—C6	1.436 (6)	C11—C10	1.382 (7)
N4—H4	0.8600	C11—C12	1.390 (8)
O2—C14	1.229 (5)	C11—H11	0.9300
O1—C7	1.238 (6)	C13—C12	1.358 (8)
N2—C8	1.264 (6)	C13—H13	0.9300
N3—C10	1.335 (6)	C17—C18	1.358 (8)
N3—C9	1.362 (6)	C17—H17	0.9300
C9—C13	1.374 (6)	C1—C2	1.341 (8)
C9—C8	1.462 (6)	C1—H1	0.9300
C8—H8A	0.9700	C3—C2	1.423 (8)
C8—H8B	0.9700	C3—H3	0.9300
C4—C3	1.395 (7)	C10—H10	0.9300
C4—C5	1.432 (7)	C19—C18	1.382 (9)
C15—C20	1.370 (6)	C19—H19	0.9300
C15—C16	1.385 (7)	C18—H18	0.9300
C15—C14	1.490 (6)	C12—H12	0.9300
C7—C6	1.479 (7)	C2—H2	0.9300
C16—C17	1.382 (7)		

C1—S1—C4	91.9 (3)	C5—C6—C7	119.8 (5)
C7—N1—N2	118.9 (4)	N4—C6—C7	118.2 (4)
C14—N4—C6	119.2 (4)	C19—C20—C15	120.8 (5)
C14—N4—H4	120.4	C19—C20—H20	119.6
C6—N4—H4	120.4	C15—C20—H20	119.6
C8—N2—N1	116.4 (4)	C10—C11—C12	117.4 (5)
C10—N3—C9	118.0 (4)	C10—C11—H11	121.3
N3—C9—C13	121.8 (5)	C12—C11—H11	121.3
N3—C9—C8	117.6 (4)	C12—C13—C9	119.3 (5)
C13—C9—C8	120.6 (5)	C12—C13—H13	120.4
N2—C8—C9	132.0 (5)	C9—C13—H13	120.4
N2—C8—H8A	104.2	C18—C17—C16	120.6 (5)
C9—C8—H8A	104.2	C18—C17—H17	119.7
N2—C8—H8B	104.2	C16—C17—H17	119.7
C9—C8—H8B	104.2	C2—C1—S1	113.5 (5)
H8A—C8—H8B	105.5	C2—C1—H1	123.3
C3—C4—C5	124.7 (5)	S1—C1—H1	123.3
C3—C4—S1	110.3 (4)	C4—C3—C2	111.7 (6)
C5—C4—S1	125.0 (4)	C4—C3—H3	124.2
C20—C15—C16	119.3 (5)	C2—C3—H3	124.2
C20—C15—C14	117.6 (4)	N3—C10—C11	123.2 (5)
C16—C15—C14	123.1 (4)	N3—C10—H10	118.4
O2—C14—N4	120.5 (4)	C11—C10—H10	118.4
O2—C14—C15	121.8 (5)	C20—C19—C18	120.1 (5)
N4—C14—C15	117.7 (4)	C20—C19—H19	120.0
O1—C7—N1	124.0 (4)	C18—C19—H19	120.0
O1—C7—C6	122.6 (5)	C17—C18—C19	119.6 (5)
N1—C7—C6	113.3 (4)	C17—C18—H18	120.2
C17—C16—C15	119.5 (5)	C19—C18—H18	120.2

C17—C16—H16	120.2	C13—C12—C11	120.2 (5)
C15—C16—H16	120.2	C13—C12—H12	119.9
C6—C5—C4	129.7 (5)	C11—C12—H12	119.9
C6—C5—H5	115.2	C1—C2—C3	112.7 (5)
C4—C5—H5	115.2	C1—C2—H2	123.7
C5—C6—N4	122.0 (5)	C3—C2—H2	123.7
C7—N1—N2—C8	−179.2 (5)	C14—N4—C6—C7	78.7 (5)
C10—N3—C9—C13	−0.8 (7)	O1—C7—C6—C5	6.0 (8)
C10—N3—C9—C8	179.9 (4)	N1—C7—C6—C5	−173.6 (4)
N1—N2—C8—C9	−1.9 (8)	O1—C7—C6—N4	−171.7 (5)
N3—C9—C8—N2	−1.5 (8)	N1—C7—C6—N4	8.7 (6)
C13—C9—C8—N2	179.2 (5)	C16—C15—C20—C19	2.4 (8)
C1—S1—C4—C3	0.9 (4)	C14—C15—C20—C19	−176.8 (5)
C1—S1—C4—C5	−179.0 (5)	N3—C9—C13—C12	0.6 (8)
C6—N4—C14—O2	4.0 (7)	C8—C9—C13—C12	179.9 (5)
C6—N4—C14—C15	−174.4 (4)	C15—C16—C17—C18	−2.0 (8)
C20—C15—C14—O2	−24.7 (7)	C4—S1—C1—C2	−0.8 (5)
C16—C15—C14—O2	156.1 (5)	C5—C4—C3—C2	179.1 (5)
C20—C15—C14—N4	153.6 (4)	S1—C4—C3—C2	−0.8 (6)
C16—C15—C14—N4	−25.6 (7)	C9—N3—C10—C11	1.0 (7)
N2—N1—C7—O1	3.3 (8)	C12—C11—C10—N3	−1.1 (9)
N2—N1—C7—C6	−177.1 (4)	C15—C20—C19—C18	−1.7 (9)
C20—C15—C16—C17	−0.6 (7)	C16—C17—C18—C19	2.7 (9)
C14—C15—C16—C17	178.6 (5)	C20—C19—C18—C17	−0.9 (9)
C3—C4—C5—C6	178.8 (5)	C9—C13—C12—C11	−0.7 (9)
S1—C4—C5—C6	−1.3 (8)	C10—C11—C12—C13	0.9 (9)
C4—C5—C6—N4	2.4 (8)	S1—C1—C2—C3	0.5 (7)
C4—C5—C6—C7	−175.1 (5)	C4—C3—C2—C1	0.2 (8)
C14—N4—C6—C5	−98.9 (5)		

Hydrogen-bond geometry (Å, º)

Cg2 and Cg3 are the centroids of rings N3/C9–C13 and C15–C20, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···O1^{i}	0.86	2.18	2.931 (6)	145
C8—H8*B*···S1^{ii}	0.97	2.68	3.492 (5)	141
C10—H10···*Cg*3	0.93	2.89	3.627 (6)	137
C12—H12···*Cg*2^{ii}	0.93	2.92	3.648 (6)	136

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