IUCrData

ISSN 2414-3146

5-Methoxy-2-{[(4-methoxy-3,5-dimethylpyridin-2-yl)methyl)]sulfinyl}-1-(prop-2-yn-1-yl)-1*H*-benzimidazole

Youness El Bakri,[a]* Youssef Ramli,[b] Abdallah Harmaoui,[a] Mohamed Elhafi,[a] El Mokhtar Essassi[a] and Joel T. Mague[c]

[a]Laboratoire de Chimie Organique Hétérocyclique, URAC 21, Pôle de Compétence Pharmacochimie, Av. Ibn Battouta, BP 1014, Faculté des Sciences, Université Mohammed V, Rabat, Morocco, [b]Medicinal Chemistry Laboratory, Faculty of Medicine and Pharmacy, Mohammed V University in Rabat, 10170 Rabat, Morocco, and [c]Department of Chemistry, Tulane University, New Orleans, LA 70118, USA. *Correspondence e-mail: youness.chimie14@gmail.com

Received 22 October 2016
Accepted 22 October 2016

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

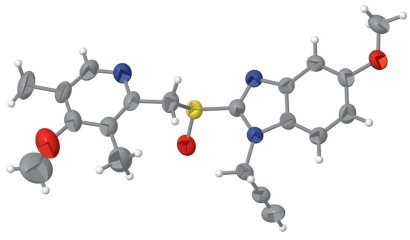
Keywords: crystal structure; omeprazole; benzimidazole; C—H···O hydrogen bonding; offset π–π stacking.

CCDC reference: 1511140

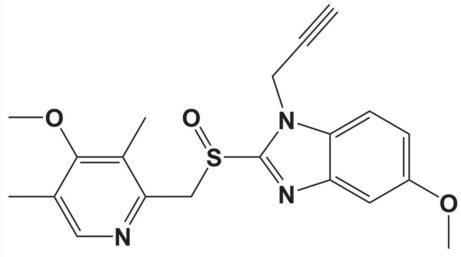
Structural data: full structural data are available from iucrdata.iucr.org

In the title omeprazole derivative, $C_{20}H_{21}N_3O_3S$, the benzimidazole ring is inclined to the pyridine ring by 21.21 (8)°. In the crystal, neighbouring molecules are linked by C—H···O hydrogen bonds, forming chains along the *a*-axis direction. Within the chains, there are offset π–π interactions [intercentroid distance = 3.880 (2) Å] involving neighbouring benzimidazole rings. There are no other significant intermolecular interactions present.

3D view



Chemical scheme

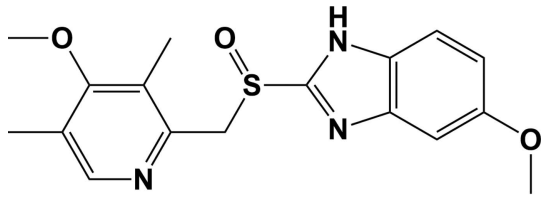


Structure description

Omeprazoles (Fig. 1) are a class of Proton Pump Inhibitors (PPIs) that inhibit the pump by irreversibly binding to cysteines in the pump. The irreversibility of the covalent bond results in inhibition of acid secretion until more enzymes are synthesized, *viz.* inhibition of enzymes H+, K+ ATPase (Hydrogen–Potassium Adenosine Triphosphates) at the secretory surface of the gastric parietal cells. This effect leads to inhibition of both basal and stimulated acid secretion, irrespective of the stimulus, for more than 24 h (Sachs *et al.*, 1976; Dibona *et al.*, 1979; Fellenius *et al.*, 1981).

In the title compound (Fig. 2), the benzimidazole moiety (N1/N2/C1–C6/C8) is planar (r.m.s. deviation = 0.008 Å) and it is inclined to the substituted pyridine ring (N1/C10–C14) by 21.21 (18)°.

In the crystal, neighbouring molecules are linked by C—H···O hydrogen bonds, forming chains along the *a*-axis direction (Table 1 and Figs. 3 and 4). Within the chains, there are offset π–π interactions present involving neighbouring benzimidazole rings



Omeprazole

Figure 1
The structure of omeprazole.

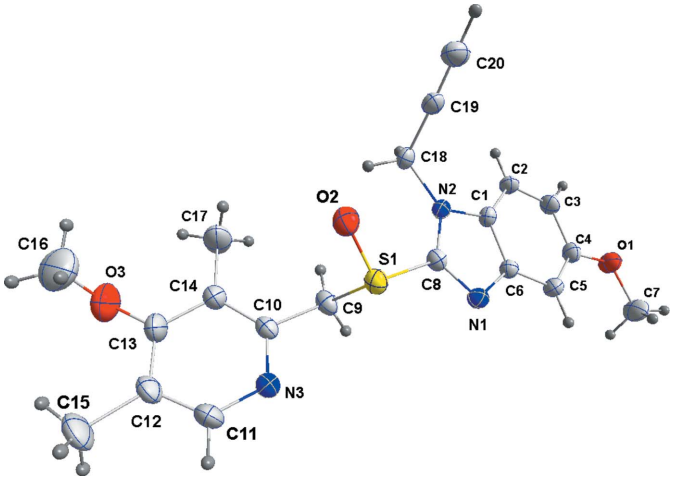


Figure 2
The molecular structure of the title compound, showing the atom labelling and 25% probability displacement ellipsoids.

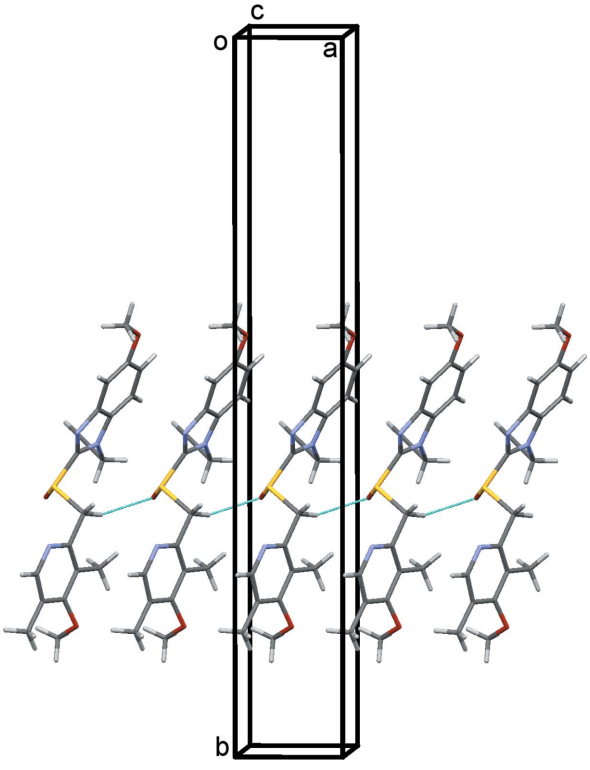


Figure 3
A partial view along the *c* axis of the crystal packing of the title compound, with the C—H···O hydrogen bonds (Table 1) shown as dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9*A*···O2^{i}	0.97	2.56	3.441 (5)	152

Symmetry code: (i) $x+1, y, z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{21}N_3O_3S$
M_r	383.46
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, *b*, *c* (Å)	4.5974 (3), 30.675 (2), 13.8090 (9)
β (°)	91.961 (1)
V (Å^3)	1946.3 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.19
Crystal size (mm)	0.32 × 0.12 × 0.06
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (TWINABS; Sheldrick, 2009)
T_{min}, T_{max}	0.82, 0.99
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	35690, 4617, 3504
R_{int}	0.039
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.659
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.083, 0.226, 1.10
No. of reflections	4617
No. of parameters	247
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.85, −0.37

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012), *Mercury* (Macrae *et al.*, 2008) and *SHELXTL* (Sheldrick, 2008).

[$Cg1\cdots Cg3(x-1, y, z)$ = 3.880 (2) Å; $Cg1$ and $Cg3$ are the centroids of rings N1/N2/C1/C6/C8 and C1–C6, interplanar distance = 3.620 (1) Å, slippage = 1.408 Å]. There are no other significant intermolecular interactions present.

Synthesis and crystallization

To a solution of 5-methoxy-2-[(4-methoxy-3,5-dimethylpyridin-2-yl)methylsulfinyl]-1*H*-benzimidazole (0.5 g, 1.45 mmol) in *N*,*N*-dimethylformamide (15 ml) was added potassium

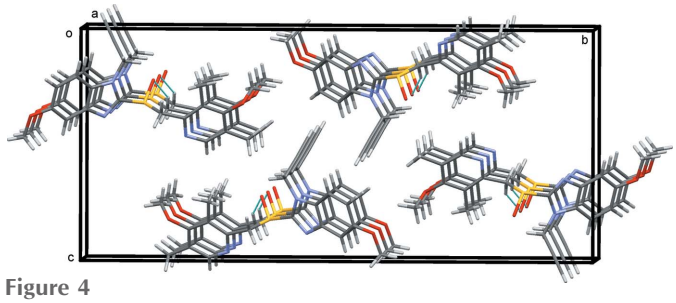


Figure 4
A view along the *a* axis of the crystal packing of the title compound, with the C—H···O hydrogen bonds (Table 1) shown as dashed lines.

carbonate (0.2 g, 1.21 mmol), propargyl bromide (0.1 ml, 1.21 mmol) and a catalytic amount of tetra-*n*-butylammonium bromide. The reaction mixture was stirred for 12 h. The solution was then concentrated to dryness under reduced pressure and the residue extracted with dichloromethane. The precipitate formed by cooling was filtered and crystallized from ethanol to give colourless rod-like crystals of the title compound (yield 76%).

Refinement

Crystal and refinement data are presented in Table 2. Trial refinements with both single- and two-component data files indicated the former to provide a better refinement.

Acknowledgements

JTM thanks Tulane University for support of the Tulane Crystallography Laboratory.

References

Brandenburg, K. & Putz, H. (2012). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2016). *APEX3*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dibona, D. R., Ito, S., Berglindh, T. & Sachs, G. (1979). *Proc. Natl Acad. Sci.* **76**, 6689–6693.
Fellenius, E., Berglindh, T. & Sachs, G. (1981). *Nature*, **290**, 156–161.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Sachs, G., Chang, H. H., Rabon, E., Schackman, R., Lewin, M. & Saccomani, G. (1976). *J. Biol. Chem.* **251**, 7690–7698.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2009). *TWINABS*. University of Göttingen, Göttingen, Germany.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

IUCrData (2016). **1**, x161695 [https://doi.org/10.1107/S2414314616016953]

5-Methoxy-2-{[(4-methoxy-3,5-dimethylpyridin-2-yl)methyl)]sulfinyl}-1-(prop-2-yn-1-yl)-1*H*-benzimidazole

Youness El Bakri, Youssef Ramli, Abdallah Harmaoui, Mohamed Elhafi, El Mokhtar Essassi and Joel T. Mague

5-Methoxy-2-{[(4-methoxy-3,5-dimethylpyridin-2-yl)methyl)]sulfinyl}-1-(prop-2-yn-1-yl)-1*H*-benzimidazole

Crystal data

$C_{20}H_{21}N_3O_3S$
M_r = 383.46
Monoclinic, $P2_1/c$
a = 4.5974 (3) Å
b = 30.675 (2) Å
c = 13.8090 (9) Å
β = 91.961 (1)°
V = 1946.3 (2) Å^3
Z = 4
$F(000)$ = 808
D_x = 1.309 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6538 reflections
θ = 2.5–25.3°
μ = 0.19 mm^{-1}
T = 296 K
Rod, colourless
0.32 × 0.12 × 0.06 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (TWINABS; Sheldrick, 2009)
T_{min} = 0.82, T_{max} = 0.99
35690 measured reflections
4617 independent reflections
3504 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 28.0°, θ_{min} = 1.3°
h = −6→6
k = −40→40
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.083
$wR(F^2)$ = 0.226
S = 1.10
4617 reflections
247 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
$w = 1/[\sigma^2(F_o^2) + (0.0777P)^2 + 2.7928P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.85 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Special details

Experimental. The diffraction data were collected in three sets of 363 frames (0.5° width in ω) at φ = 0, 120 and 240°. A scan time of 70 sec/frame was used. Analysis of 1608 reflections having I/σ(I) > 12 and chosen from the full data set with *CELL_NOW* (Sheldrick, 2008) showed the crystal to belong to the monoclinic system and to consist of two components, the minor one likely a parasite on the main crystal. The raw data were processed using the multi-component version of *SAINT* under control of the two-component orientation file generated by *CELL_NOW*.

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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 1.00 Å). All were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms. Trial refinements with both single- and two-component data files indicated the former to provide a better refinement.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.28987 (19)	0.62771 (3)	0.18681 (7)	0.0520 (3)
O1	1.0846 (7)	0.41553 (9)	0.1427 (2)	0.0689 (8)
O2	0.2040 (6)	0.64395 (9)	0.2825 (2)	0.0639 (7)
O3	0.4997 (10)	0.82164 (13)	0.1892 (4)	0.1150 (14)
N1	0.5178 (7)	0.55192 (10)	0.1319 (2)	0.0503 (7)
N2	0.6805 (6)	0.56988 (9)	0.28267 (19)	0.0440 (6)
N3	0.2691 (10)	0.70843 (12)	0.0456 (3)	0.0814 (12)
C1	0.8087 (7)	0.53035 (10)	0.2602 (2)	0.0429 (7)
C2	1.0008 (8)	0.50354 (12)	0.3125 (3)	0.0509 (8)
H2	1.0697	0.5108	0.3745	0.061*
C3	1.0830 (8)	0.46594 (12)	0.2678 (3)	0.0553 (9)
H3	1.2108	0.4471	0.3005	0.066*
C4	0.9807 (8)	0.45486 (11)	0.1741 (3)	0.0506 (8)
C5	0.7951 (8)	0.48130 (11)	0.1215 (3)	0.0503 (8)
H5	0.7302	0.4741	0.0590	0.060*
C6	0.7077 (7)	0.51995 (10)	0.1669 (2)	0.0430 (7)
C7	0.9808 (13)	0.40132 (16)	0.0497 (3)	0.0821 (14)
H7A	1.0581	0.4198	0.0007	0.123*
H7B	0.7721	0.4027	0.0463	0.123*
H7C	1.0423	0.3718	0.0392	0.123*
C8	0.5114 (7)	0.58028 (11)	0.2024 (2)	0.0457 (7)
C9	0.5748 (8)	0.66390 (12)	0.1477 (3)	0.0566 (9)
H9A	0.7239	0.6669	0.1987	0.068*
H9B	0.6641	0.6520	0.0908	0.068*
C10	0.4424 (8)	0.70796 (12)	0.1243 (3)	0.0521 (8)
C11	0.1534 (12)	0.74665 (16)	0.0195 (3)	0.0826 (14)
H11	0.0277	0.7468	−0.0347	0.099*
C12	0.2018 (11)	0.78517 (14)	0.0647 (3)	0.0683 (11)

C13	0.3896 (13)	0.78359 (14)	0.1456 (4)	0.0778 (13)
C14	0.5068 (10)	0.74393 (13)	0.1791 (3)	0.0622 (10)
C15	0.0700 (16)	0.82688 (18)	0.0263 (5)	0.109 (2)
H15A	0.1288	0.8506	0.0678	0.164*
H15B	0.1355	0.8321	−0.0379	0.164*
H15C	−0.1383	0.8245	0.0246	0.164*
C16	0.319 (2)	0.8389 (3)	0.2528 (7)	0.176 (4)
H16A	0.3030	0.8697	0.2419	0.265*
H16B	0.3940	0.8337	0.3175	0.265*
H16C	0.1305	0.8257	0.2446	0.265*
C17	0.7023 (16)	0.7420 (2)	0.2694 (5)	0.111 (2)
H17A	0.7778	0.7706	0.2835	0.166*
H17B	0.8606	0.7224	0.2591	0.166*
H17C	0.5925	0.7320	0.3229	0.166*
C18	0.7213 (8)	0.59296 (11)	0.3743 (2)	0.0496 (8)
H18A	0.6533	0.6227	0.3662	0.060*
H18B	0.9274	0.5940	0.3916	0.060*
C19	0.5667 (8)	0.57253 (12)	0.4531 (3)	0.0513 (8)
C20	0.4465 (11)	0.55728 (16)	0.5172 (3)	0.0753 (13)
H20	0.3500	0.5450	0.5687	0.090*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0460 (5)	0.0502 (5)	0.0595 (5)	0.0078 (4)	−0.0018 (4)	0.0003 (4)
O1	0.088 (2)	0.0551 (16)	0.0633 (17)	0.0187 (14)	−0.0071 (15)	−0.0094 (13)
O2	0.0613 (16)	0.0595 (16)	0.0722 (18)	0.0094 (13)	0.0213 (14)	−0.0005 (13)
O3	0.120 (3)	0.079 (3)	0.146 (4)	0.000 (2)	0.010 (3)	−0.014 (3)
N1	0.0529 (16)	0.0496 (16)	0.0480 (16)	0.0043 (13)	−0.0043 (13)	0.0003 (13)
N2	0.0474 (15)	0.0406 (14)	0.0437 (14)	−0.0018 (11)	−0.0016 (12)	−0.0024 (11)
N3	0.116 (3)	0.059 (2)	0.068 (2)	0.019 (2)	−0.025 (2)	−0.0048 (18)
C1	0.0421 (16)	0.0386 (16)	0.0480 (17)	−0.0029 (13)	0.0011 (13)	−0.0025 (13)
C2	0.056 (2)	0.0500 (19)	0.0454 (18)	0.0000 (15)	−0.0103 (15)	0.0005 (15)
C3	0.056 (2)	0.0497 (19)	0.059 (2)	0.0065 (16)	−0.0081 (17)	0.0052 (17)
C4	0.054 (2)	0.0419 (17)	0.056 (2)	0.0033 (15)	0.0037 (16)	−0.0010 (15)
C5	0.059 (2)	0.0494 (19)	0.0428 (18)	−0.0024 (16)	−0.0006 (15)	−0.0043 (15)
C6	0.0439 (17)	0.0418 (16)	0.0432 (17)	−0.0022 (13)	−0.0009 (13)	0.0015 (13)
C7	0.117 (4)	0.067 (3)	0.063 (3)	0.016 (3)	0.008 (3)	−0.018 (2)
C8	0.0440 (17)	0.0443 (17)	0.0487 (18)	0.0003 (13)	0.0014 (14)	0.0026 (14)
C9	0.051 (2)	0.054 (2)	0.065 (2)	0.0122 (16)	0.0132 (17)	0.0119 (18)
C10	0.0516 (19)	0.0509 (19)	0.054 (2)	0.0090 (15)	0.0078 (16)	0.0132 (16)
C11	0.110 (4)	0.071 (3)	0.065 (3)	0.016 (3)	−0.027 (3)	0.013 (2)
C12	0.083 (3)	0.056 (2)	0.066 (3)	0.014 (2)	0.008 (2)	0.021 (2)
C13	0.107 (4)	0.047 (2)	0.078 (3)	0.007 (2)	−0.003 (3)	−0.001 (2)
C14	0.074 (3)	0.053 (2)	0.059 (2)	0.0034 (19)	−0.0019 (19)	0.0034 (18)
C15	0.139 (5)	0.074 (3)	0.116 (5)	0.034 (3)	0.003 (4)	0.039 (3)
C16	0.181 (9)	0.200 (10)	0.151 (8)	0.091 (8)	0.044 (7)	−0.020 (7)
C17	0.141 (6)	0.088 (4)	0.100 (4)	0.012 (4)	−0.055 (4)	−0.009 (3)

C18	0.057 (2)	0.0431 (17)	0.0486 (19)	−0.0085 (15)	−0.0021 (15)	−0.0081 (14)
C19	0.056 (2)	0.052 (2)	0.0453 (19)	−0.0034 (16)	−0.0049 (16)	−0.0048 (15)
C20	0.089 (3)	0.085 (3)	0.052 (2)	−0.020 (3)	0.001 (2)	−0.001 (2)

Geometric parameters (Å, º)

S1—O2	1.478 (3)	C7—H7C	0.9600
S1—C8	1.785 (3)	C9—C10	1.513 (5)
S1—C9	1.813 (4)	C9—H9A	0.9700
O1—C4	1.374 (4)	C9—H9B	0.9700
O1—C7	1.423 (5)	C10—C14	1.365 (6)
O3—C16	1.338 (8)	C11—C12	1.351 (6)
O3—C13	1.400 (6)	C11—H11	0.9300
N1—C8	1.307 (4)	C12—C13	1.390 (7)
N1—C6	1.389 (4)	C12—C15	1.504 (6)
N2—C8	1.370 (4)	C13—C14	1.402 (6)
N2—C1	1.388 (4)	C14—C17	1.514 (6)
N2—C18	1.456 (4)	C15—H15A	0.9600
N3—C10	1.325 (5)	C15—H15B	0.9600
N3—C11	1.332 (5)	C15—H15C	0.9600
C1—C2	1.391 (5)	C16—H16A	0.9600
C1—C6	1.392 (5)	C16—H16B	0.9600
C2—C3	1.368 (5)	C16—H16C	0.9600
C2—H2	0.9300	C17—H17A	0.9600
C3—C4	1.402 (5)	C17—H17B	0.9600
C3—H3	0.9300	C17—H17C	0.9600
C4—C5	1.368 (5)	C18—C19	1.461 (5)
C5—C6	1.407 (5)	C18—H18A	0.9700
C5—H5	0.9300	C18—H18B	0.9700
C7—H7A	0.9600	C19—C20	1.158 (6)
C7—H7B	0.9600	C20—H20	0.9300
O2—S1—C8	109.63 (17)	H9A—C9—H9B	108.3
O2—S1—C9	106.11 (18)	N3—C10—C14	124.0 (3)
C8—S1—C9	96.88 (16)	N3—C10—C9	114.3 (4)
C4—O1—C7	116.4 (3)	C14—C10—C9	121.7 (4)
C16—O3—C13	112.9 (7)	N3—C11—C12	126.0 (4)
C8—N1—C6	103.9 (3)	N3—C11—H11	117.0
C8—N2—C1	104.8 (3)	C12—C11—H11	117.0
C8—N2—C18	130.0 (3)	C11—C12—C13	115.4 (4)
C1—N2—C18	125.1 (3)	C11—C12—C15	121.6 (5)
C10—N3—C11	117.0 (4)	C13—C12—C15	123.0 (5)
N2—C1—C2	131.9 (3)	C12—C13—O3	121.5 (4)
N2—C1—C6	106.0 (3)	C12—C13—C14	121.1 (4)
C2—C1—C6	122.1 (3)	O3—C13—C14	116.9 (5)
C3—C2—C1	116.4 (3)	C10—C14—C13	116.5 (4)
C3—C2—H2	121.8	C10—C14—C17	122.5 (4)
C1—C2—H2	121.8	C13—C14—C17	121.0 (4)

C2—C3—C4	122.1 (3)	C12—C15—H15A	109.5
C2—C3—H3	118.9	C12—C15—H15B	109.5
C4—C3—H3	118.9	H15A—C15—H15B	109.5
C5—C4—O1	124.7 (3)	C12—C15—H15C	109.5
C5—C4—C3	122.0 (3)	H15A—C15—H15C	109.5
O1—C4—C3	113.3 (3)	H15B—C15—H15C	109.5
C4—C5—C6	116.4 (3)	O3—C16—H16A	109.5
C4—C5—H5	121.8	O3—C16—H16B	109.5
C6—C5—H5	121.8	H16A—C16—H16B	109.5
N1—C6—C1	110.3 (3)	O3—C16—H16C	109.5
N1—C6—C5	128.7 (3)	H16A—C16—H16C	109.5
C1—C6—C5	121.0 (3)	H16B—C16—H16C	109.5
O1—C7—H7A	109.5	C14—C17—H17A	109.5
O1—C7—H7B	109.5	C14—C17—H17B	109.5
H7A—C7—H7B	109.5	H17A—C17—H17B	109.5
O1—C7—H7C	109.5	C14—C17—H17C	109.5
H7A—C7—H7C	109.5	H17A—C17—H17C	109.5
H7B—C7—H7C	109.5	H17B—C17—H17C	109.5
N1—C8—N2	114.9 (3)	N2—C18—C19	112.8 (3)
N1—C8—S1	118.7 (3)	N2—C18—H18A	109.0
N2—C8—S1	126.4 (3)	C19—C18—H18A	109.0
C10—C9—S1	108.8 (3)	N2—C18—H18B	109.0
C10—C9—H9A	109.9	C19—C18—H18B	109.0
S1—C9—H9A	109.9	H18A—C18—H18B	107.8
C10—C9—H9B	109.9	C20—C19—C18	178.1 (4)
S1—C9—H9B	109.9	C19—C20—H20	180.0

C8—N2—C1—C2	−179.8 (4)	C9—S1—C8—N1	−96.1 (3)
C18—N2—C1—C2	−1.1 (6)	O2—S1—C8—N2	−25.8 (4)
C8—N2—C1—C6	0.4 (3)	C9—S1—C8—N2	84.0 (3)
C18—N2—C1—C6	179.1 (3)	O2—S1—C9—C10	−69.6 (3)
N2—C1—C2—C3	179.4 (4)	C8—S1—C9—C10	177.6 (3)
C6—C1—C2—C3	−0.8 (5)	C11—N3—C10—C14	0.1 (7)
C1—C2—C3—C4	0.2 (6)	C11—N3—C10—C9	−178.0 (4)
C7—O1—C4—C5	−2.2 (6)	S1—C9—C10—N3	−69.5 (4)
C7—O1—C4—C3	177.6 (4)	S1—C9—C10—C14	112.3 (4)
C2—C3—C4—C5	0.8 (6)	C10—N3—C11—C12	1.6 (9)
C2—C3—C4—O1	−179.0 (4)	N3—C11—C12—C13	−0.3 (9)
O1—C4—C5—C6	178.7 (3)	N3—C11—C12—C15	177.1 (6)
C3—C4—C5—C6	−1.1 (5)	C11—C12—C13—O3	168.6 (5)
C8—N1—C6—C1	0.6 (4)	C15—C12—C13—O3	−8.8 (8)
C8—N1—C6—C5	179.6 (3)	C11—C12—C13—C14	−2.8 (8)
N2—C1—C6—N1	−0.6 (4)	C15—C12—C13—C14	179.8 (5)
C2—C1—C6—N1	179.5 (3)	C16—O3—C13—C12	84.8 (8)
N2—C1—C6—C5	−179.7 (3)	C16—O3—C13—C14	−103.5 (7)
C2—C1—C6—C5	0.5 (5)	N3—C10—C14—C13	−3.0 (7)
C4—C5—C6—N1	−178.4 (3)	C9—C10—C14—C13	175.0 (4)
C4—C5—C6—C1	0.5 (5)	N3—C10—C14—C17	179.1 (5)

C6—N1—C8—N2	−0.4 (4)	C9—C10—C14—C17	−3.0 (7)
C6—N1—C8—S1	179.7 (2)	C12—C13—C14—C10	4.3 (7)
C1—N2—C8—N1	0.0 (4)	O3—C13—C14—C10	−167.4 (4)
C18—N2—C8—N1	−178.6 (3)	C12—C13—C14—C17	−177.7 (5)
C1—N2—C8—S1	179.9 (2)	O3—C13—C14—C17	10.6 (8)
C18—N2—C8—S1	1.3 (5)	C8—N2—C18—C19	104.5 (4)
O2—S1—C8—N1	154.0 (3)	C1—N2—C18—C19	−73.8 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9*A*···O2^{i}	0.97	2.56	3.441 (5)	152

Symmetry code: (i) *x*+1, *y*, *z*.