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Synthesis and crystal structure of 5-{(*E*)-[(1*H*-indol-3-ylformamido)imino]methyl}-2-methoxyphenyl propane-1-sulfonate

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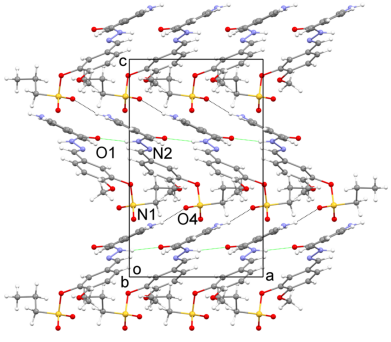
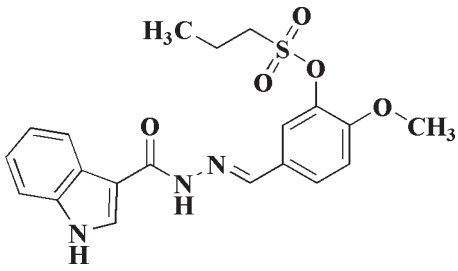
In the title molecule, $C_{20}H_{21}N_3O_5S$, the methylideneformohydrazide and methoxybenzene groups are almost coplanar, with the indolyl group being rotated farther from the plane. The molecules in the crystal structure form chains parallel to the *a*-axis direction through N—H···O hydrogen-bonding interactions. Neighbouring chains are linked by N—H···O contacts to form a three-dimensional network.

1. Chemical context

Indole-based compounds are important structural motifs found in numerous natural products and serve as key scaffolds in many clinical drugs, including anticancer agents, antiviral drugs, and non-steroidal anti-inflammatory agents (de Sa Alves *et al.*, 2009; Suzen, 2017). They also have various applications in biomedical research (Varun *et al.*, 2020; Facen *et al.*, 2024). As a result of their unique ability to mimic peptide structures and interact with enzymes, indole-based scaffolds are crucial in drug discovery (Kaushik *et al.*, 2013; Ubeid *et al.*, 2012; Citarella *et al.*, 2023). Recent advancements in drug discovery have driven the development of synthetic strategies to incorporate bioactive indole moieties into new molecules. Similarly to indole-based compounds, sulfonate derivatives have recently shown a wide range of pharmacological effects, such as antimicrobial, anticancer, and antiviral activities (Mohamed-Ezzat & Elgemeie, 2024*a*,*b*; Mohamed-Ezzat *et al.*, 2022, 2023*a*, 2024*a*,*b*). Conjugates that containing both sulfonate and indole moieties have demonstrated significant potency as inhibitors of various biological targets, such as carbonic anhydrase, tubulins, phosphatidylinositol 5-phosphate 4-kinase (PI5P4K), MET tyrosine kinase (Pingaew *et al.*, 2021), butyrylcholinesterase (BChE) (Omar *et al.*, 2023), and HIV protease inhibitors (Batool *et al.*, 2024). In line with our research on developing synthetic approaches for bioactive heterocycles (Mohamed-Ezzat & Srour, 2024; Mohamed-Ezzat *et al.*, 2023*b*,*c*), we have designed and synthesized a novel compound featuring a hydrazone scaffold. Recognizing the broad potency of hydrazine-based derivatives (Elgemeie & Mohamed, 2014; Mohamed-Ezzat & Elgemeie, 2023; Mohamed-Ezzat *et al.*, 2023*c*,*d*; Ragab *et al.*, 2024), the newly synthesized compound incorporates a conjugation of two bioactive moieties, indole and sulfonate, linked through a hydrazine linker (Fig. 1).





2. Structural commentary

The asymmetric unit consists of one molecule of 5-((*E*)-(1*H*-indole-3-carboylimino)methyl)-2-methoxyphenyl propane-1-sulfonate (Fig. 2). The molecule comprises three planar fragments, namely indolyl (IND; C1–C8, N1), methylideneformohydrazide (MFH, C9, C10, N2, N3, O1), and methoxybenzene (MEB, C11–C17, O2) groups. In addition, the molecule has a propanesulfonate group (C18–C20, S1, O3–O5) with a nearly *trans* S1—C18—C19—C20 torsion angle [168.2 (4)°]. In the molecule, the methylideneformohydrazide and methoxybenzene groups are almost coplanar with a MFH/MEB twist angle of 13.67 (17)°. A similar conformation is also observed in the structure of (*E*)-2-methoxy-*N*′-[4-methoxy-3-(4-methylphenylsulfonyloxy) benzylidene] benzohydrazide ethanol solvate hemihydrate(Chen & Yu, 2006) where the twist angle is 7°. In the molecule of the title compound, the indolyl group is rotated farther from the plane defined by MFH and MEB with a IND/MFH twist angle of 25.93 (14)°. The geometry is similar to that of *N*′-(2-hydroxybenzylidene) indole-3-formylhydrazine (Li *et al.*, 2024), which has a corresponding twist angle of 18.1°.

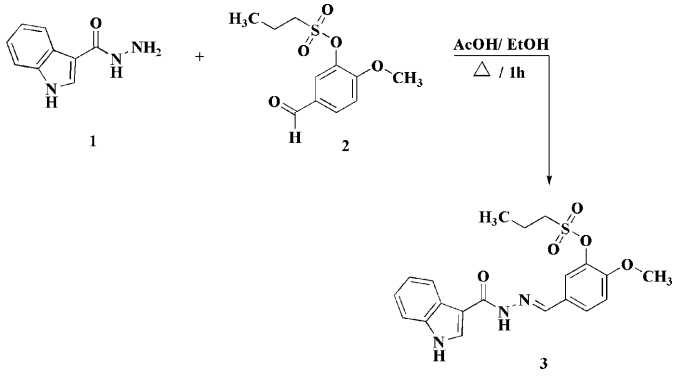


Figure 1
Synthesis of the novel title compound (**3**), which incorporates two bioactive moieties, indole and sulfonate, linked through a hydrazine linker.

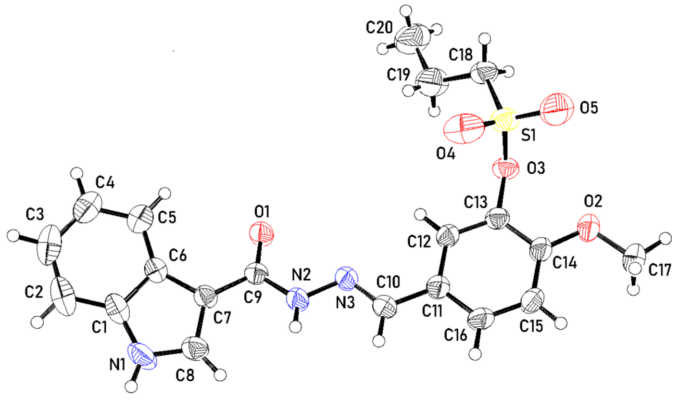


Figure 2
The molecular structure of the title compound showing 50% probability displacement ellipsoids.

3. Supramolecular features

In the crystal, the molecules are linked by N—H···O hydrogen-bonding interactions involving the N—H and carbonyls of methylideneformohydrazide groups of adjacent

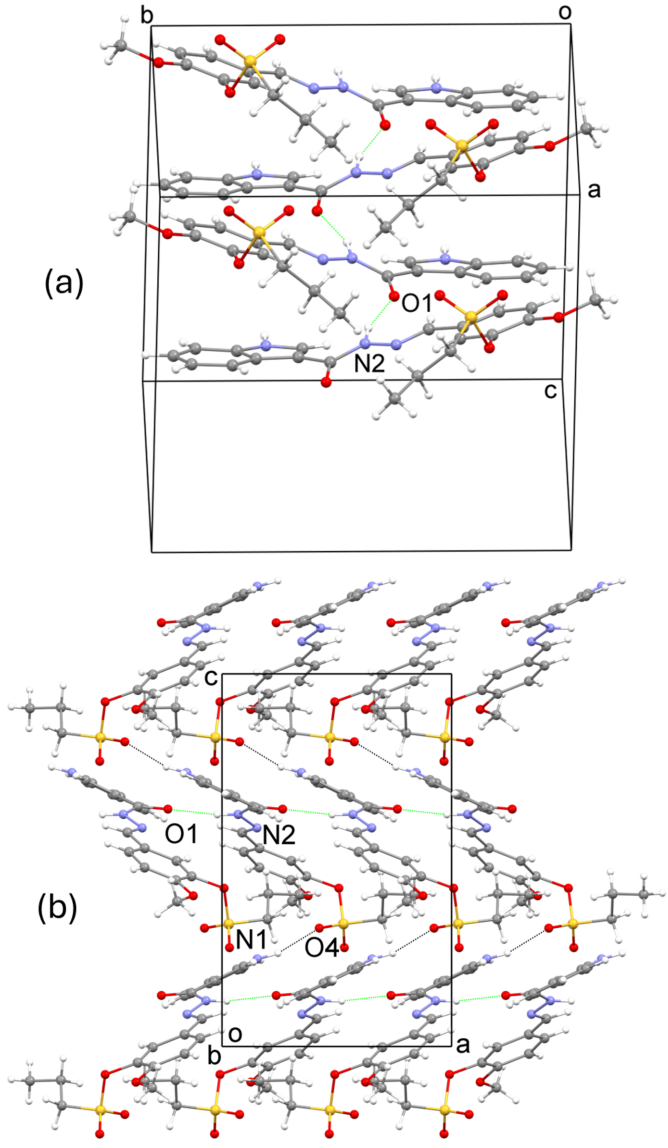


Figure 3
(*a*) A segment of the crystal structure showing molecules linked through N—H···O hydrogen bonds (green dotted lines). (*b*) The crystal structure viewed down the *b* axis with C—H···O interactions shown as black dotted lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···O1^{i}	0.93	2.51	3.325 (4)	146
C18—H18A···O1^{ii}	0.97	2.52	3.467 (5)	164
N2—H2A···O1^{i}	0.86 (1)	2.22 (2)	3.048 (4)	163 (4)
N1—H1···O4^{iii}	0.86 (1)	2.07 (3)	2.870 (5)	156 (5)

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

molecules. Thus, N2—H2A···O1 interactions link molecules related by glide symmetry to form chains parallel to the a axis (Fig. 3*a*, Table 1). The chains are linked through N1—H1···O4 interactions involving the N—H group of the indolyl fragment and an oxygen atom of the sulfonate group to form a three-dimensional network (Fig. 3*b*, Table 1). O1 is also an acceptor to longer intermolecular C—H···O interactions, namely C10—H10···O1 and C18—H18A···O1 (Table 1).

4. Database survey

A search of the CSD (version 5.46, November 2024; Groom *et al.*, 2016) for uncoordinated fragments of linked indolyl and methylideneformohydrazide groups revealed *N*′-[(2-hydroxyphenyl)methylidene]-1*H*-indole-3-carbohydrazide monohydrate (YODCIH; Chen & Yu, 2006), which has a similar twist angle to the title compound. The closest hit containing the sulfonate, methoxybenzene and methylideneformohydrazide groups was (*E*)-2-methoxy-*N*′-(4-methoxy-3-(4-methylbenzenesulfonyloxy)benzylidene)benzohydrazide ethanol solvate hemihydrate (HESRIH; Li *et al.*, 2024) in which the two planar fragments also have a twist angle (8.5°) comparable to the title compound.

5. Synthesis and crystallization

For synthesis of (*E*)-5-{[2-(1*H*-indole-3-carbonyl)hydrazono]methyl}-2-methoxyphenyl propane-1-sulfonate (**3**), a mixture of 10 mmol of 1*H*-indole-3-carbohydrazide (**1**) and 10 mmol of 5-formyl-2-methoxyphenyl propane-1-sulfonate (**2**) in 20 ml of acetic acid/ethanol (1:2) was refluxed for 1 h. The mixture was filtered, and then the solid obtained was dried and recrystallized from ethanol. Yield: 91%; m.p. 485–486 K; Color: buff crystals; ^{1}H-NMR (500 MHz, DMSO-d_6) δ (ppm): 1.01 (*t*, 3H, J = 7.4 Hz, $CH_2CH_2CH_3$), 1.86 (*m*, 2H, $CH_2CH_2CH_3$), 3.46 (*t*, 2H, J = 7.6 Hz, $CH_2CH_2CH_3$), 3.86 (*s*, 3H, OCH_3), 7.13–7.19 (*m*, 2H, Ar-H), 7.22 (*d*, 1H, J = 8.6 Hz, Ar-H), 7.46 (*d*, 1H, J = 7.8 Hz, Ar-H), 7.59–7.64 (*m*, 2H, Ar-H), 8.21 (*br. s*, 3H, CH═N + Ar-H), 11.42 (*s*, 1H, NH), 11.76 (*s*, 1H, NH); ^{13}C-NMR (126 MHz, DMSO-d_6) δ (ppm): 12.38, 17.01, 51.45, 111.98, 120.80, 122.27, 122.65, 128.32, 133.86, 149.45; Analysis % for $C_{20}H_{21}N_3O_5S$ (415.46). Calculated: C, 57.82; H, 5.10; N, 10.11. Found: C, 57.78; H, 5.18; N, 9.96.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms were located in difference-Fourier maps. C-bound atoms were thereafter refined with restrained geometry using a riding model with displacement parameters constrained to either 1.2 or 1.5 times the equivalent isotropic displacement parameter of the parent C atom.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{21}N_3O_5S$
M_r	415.46
Crystal system, space group	Orthorhombic, $Pca2_1$
Temperature (K)	296
a, b, c (Å)	9.2969 (5), 14.0662 (7), 15.1168 (7)
V (Å^3)	1976.85 (17)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.20
Crystal size (mm)	0.34 × 0.14 × 0.09
Data collection	
Diffractometer	SuperNova, Dual, Cu at home/near, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2022)
T_{min}, T_{max}	0.618, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16123, 4696, 3791
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.698
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.111, 1.05
No. of reflections	4696
No. of parameters	272
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.23
Absolute structure	Flack x determined using 1389 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.05 (3)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020) and *ORTEP-3 for Windows* (Farrugia, 2012).

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Computing details

5-{(*E*)-[(1*H*-Indol-3-ylformamido)imino]methyl}-2-methoxyphenyl propane-1-sulfonate

Crystal data

$C_{20}H_{21}N_3O_5S$
M_r = 415.46
Orthorhombic, $Pca2_1$
a = 9.2969 (5) Å
b = 14.0662 (7) Å
c = 15.1168 (7) Å
V = 1976.85 (17) Å^3
Z = 4
$F(000)$ = 872
D_x = 1.396 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7123 reflections
θ = 3.9–28.6°
μ = 0.20 mm^{-1}
T = 296 K
Block, colourless
0.34 × 0.14 × 0.09 mm

Data collection

SuperNova, Dual, Cu at home/near, Atlas diffractometer
Detector resolution: 10.5082 pixels mm^{-1}
ω scans
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2022)
T_{min} = 0.618, T_{max} = 1.000
16123 measured reflections
4696 independent reflections
3791 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 29.7°, θ_{min} = 3.6°
h = −12→11
k = −18→19
l = −21→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.111
S = 1.05
4696 reflections
272 parameters
3 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0461P)^2 + 0.6044P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Absolute structure: Flack x determined using 1389 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.05 (3)

Special details

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.0659 (4)	0.2094 (3)	0.7066 (3)	0.0495 (9)
C2	−0.0849 (6)	0.1109 (3)	0.7088 (3)	0.0697 (13)
H2	−0.168430	0.084058	0.731600	0.084*
C3	0.0230 (6)	0.0556 (3)	0.6765 (3)	0.0715 (13)
H3	0.013852	−0.010235	0.678105	0.086*
C4	0.1460 (5)	0.0956 (3)	0.6413 (3)	0.0624 (11)
H4	0.218451	0.055961	0.620438	0.075*
C5	0.1645 (4)	0.1927 (2)	0.6362 (3)	0.0488 (8)
H5	0.246976	0.218411	0.610950	0.059*
C6	0.0574 (4)	0.2512 (2)	0.6696 (2)	0.0361 (7)
C7	0.0362 (3)	0.3530 (2)	0.6756 (2)	0.0377 (7)
C8	−0.0946 (4)	0.3660 (3)	0.7149 (3)	0.0496 (8)
H8	−0.136701	0.424788	0.726252	0.059*
C9	0.1332 (3)	0.4263 (2)	0.6439 (2)	0.0361 (6)
C10	0.0879 (4)	0.6607 (2)	0.5743 (3)	0.0450 (8)
H10	−0.007127	0.668033	0.592203	0.054*
C11	0.1630 (4)	0.7397 (2)	0.5322 (2)	0.0415 (7)
C12	0.3017 (3)	0.7294 (2)	0.4981 (2)	0.0378 (7)
H12	0.349555	0.671639	0.503558	0.045*
C13	0.3671 (3)	0.8037 (2)	0.4567 (2)	0.0377 (7)
C14	0.2995 (4)	0.8918 (2)	0.4465 (2)	0.0420 (7)
C15	0.1624 (4)	0.9023 (2)	0.4804 (3)	0.0488 (9)
H15	0.114956	0.960221	0.475005	0.059*
C16	0.0953 (4)	0.8267 (2)	0.5223 (3)	0.0502 (9)
H16	0.002673	0.834642	0.544236	0.060*
C17	0.3050 (5)	1.0491 (2)	0.3895 (3)	0.0609 (11)
H17A	0.219977	1.038851	0.354718	0.091*
H17B	0.368862	1.091027	0.358372	0.091*
H17C	0.278991	1.077006	0.445144	0.091*
C18	0.6978 (4)	0.6949 (3)	0.3417 (3)	0.0489 (9)
H18A	0.728048	0.668857	0.285233	0.059*
H18B	0.766370	0.743790	0.358143	0.059*
C19	0.7020 (5)	0.6173 (4)	0.4099 (3)	0.0769 (14)
H19A	0.691877	0.645464	0.468136	0.092*
H19B	0.620706	0.575250	0.400642	0.092*
C20	0.8367 (6)	0.5601 (4)	0.4077 (4)	0.0939 (18)
H20A	0.841089	0.524917	0.353344	0.141*
H20B	0.837658	0.516757	0.456748	0.141*
H20C	0.918286	0.601747	0.411564	0.141*

N1	−0.1539 (3)	0.2809 (3)	0.7350 (3)	0.0614 (9)
N2	0.0700 (3)	0.5101 (2)	0.6228 (2)	0.0435 (6)
N3	0.1519 (3)	0.58184 (19)	0.58674 (19)	0.0414 (6)
O1	0.2641 (2)	0.41354 (16)	0.63705 (17)	0.0462 (6)
O2	0.3750 (3)	0.96064 (16)	0.40450 (19)	0.0560 (7)
O3	0.5089 (2)	0.79283 (17)	0.42481 (16)	0.0423 (5)
O4	0.4236 (3)	0.6744 (2)	0.3176 (2)	0.0725 (9)
O5	0.5327 (4)	0.8204 (3)	0.2653 (2)	0.0937 (12)
S1	0.52915 (9)	0.74697 (7)	0.32886 (7)	0.0473 (2)
H2A	−0.0209 (16)	0.520 (3)	0.622 (3)	0.051 (11)*
H1	−0.243 (2)	0.280 (4)	0.750 (4)	0.097 (17)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0429 (19)	0.053 (2)	0.053 (2)	−0.0118 (17)	−0.0035 (16)	0.0162 (18)
C2	0.075 (3)	0.064 (3)	0.071 (3)	−0.028 (2)	−0.010 (2)	0.024 (2)
C3	0.100 (4)	0.040 (2)	0.074 (3)	−0.011 (2)	−0.020 (3)	0.010 (2)
C4	0.083 (3)	0.046 (2)	0.059 (2)	0.008 (2)	−0.006 (2)	−0.0061 (19)
C5	0.053 (2)	0.0437 (19)	0.050 (2)	0.0015 (16)	−0.0070 (17)	−0.0011 (16)
C6	0.0348 (16)	0.0397 (16)	0.0338 (15)	−0.0036 (13)	−0.0045 (12)	0.0050 (13)
C7	0.0310 (16)	0.0406 (16)	0.0413 (16)	0.0016 (13)	0.0001 (13)	0.0060 (14)
C8	0.0355 (18)	0.053 (2)	0.060 (2)	0.0052 (15)	0.0062 (15)	0.0079 (19)
C9	0.0322 (16)	0.0389 (16)	0.0372 (15)	0.0004 (13)	0.0009 (12)	−0.0007 (13)
C10	0.0342 (17)	0.0419 (17)	0.059 (2)	−0.0021 (14)	0.0086 (15)	0.0023 (16)
C11	0.0370 (18)	0.0369 (16)	0.0507 (19)	0.0002 (13)	0.0036 (14)	0.0003 (14)
C12	0.0362 (16)	0.0354 (15)	0.0418 (16)	0.0050 (12)	−0.0009 (14)	0.0015 (14)
C13	0.0324 (16)	0.0380 (16)	0.0425 (17)	0.0008 (12)	0.0019 (13)	−0.0037 (13)
C14	0.0404 (18)	0.0317 (15)	0.054 (2)	−0.0017 (13)	0.0034 (15)	−0.0004 (15)
C15	0.043 (2)	0.0325 (16)	0.071 (2)	0.0056 (14)	0.0048 (17)	0.0010 (16)
C16	0.0350 (18)	0.0430 (18)	0.072 (3)	0.0066 (15)	0.0111 (17)	−0.0013 (17)
C17	0.070 (3)	0.0339 (18)	0.079 (3)	0.0034 (17)	0.013 (2)	0.009 (2)
C18	0.0393 (18)	0.053 (2)	0.054 (2)	0.0074 (15)	0.0061 (15)	−0.0021 (17)
C19	0.079 (3)	0.089 (3)	0.063 (3)	0.033 (3)	0.008 (2)	0.021 (2)
C20	0.107 (4)	0.097 (4)	0.078 (3)	0.053 (3)	0.010 (3)	0.018 (3)
N1	0.0344 (18)	0.071 (2)	0.079 (2)	−0.0050 (16)	0.0147 (16)	0.0224 (19)
N2	0.0314 (14)	0.0394 (14)	0.0596 (17)	0.0005 (12)	0.0067 (13)	0.0095 (14)
N3	0.0343 (14)	0.0379 (14)	0.0521 (16)	−0.0026 (12)	0.0046 (12)	0.0034 (12)
O1	0.0297 (12)	0.0447 (12)	0.0642 (15)	−0.0001 (10)	0.0019 (11)	0.0073 (12)
O2	0.0526 (15)	0.0357 (12)	0.0796 (19)	0.0012 (10)	0.0126 (13)	0.0106 (13)
O3	0.0312 (11)	0.0469 (13)	0.0488 (13)	0.0007 (10)	0.0042 (9)	−0.0045 (11)
O4	0.0489 (16)	0.093 (2)	0.076 (2)	−0.0002 (15)	−0.0067 (15)	−0.0299 (18)
O5	0.126 (3)	0.092 (2)	0.064 (2)	0.052 (2)	0.020 (2)	0.0295 (19)
S1	0.0443 (4)	0.0555 (5)	0.0420 (4)	0.0126 (4)	0.0015 (4)	0.0018 (4)

Geometric parameters (Å, º)

C1—N1	1.365 (5)	C13—O3	1.412 (4)
C1—C2	1.398 (6)	C14—O2	1.354 (4)
C1—C6	1.405 (5)	C14—C15	1.382 (5)
C2—C3	1.360 (7)	C15—C16	1.386 (5)
C2—H2	0.9300	C15—H15	0.9300
C3—C4	1.381 (7)	C16—H16	0.9300
C3—H3	0.9300	C17—O2	1.422 (4)
C4—C5	1.378 (5)	C17—H17A	0.9600
C4—H4	0.9300	C17—H17B	0.9600
C5—C6	1.387 (5)	C17—H17C	0.9600
C5—H5	0.9300	C18—C19	1.503 (6)
C6—C7	1.447 (5)	C18—S1	1.742 (3)
C7—C8	1.367 (5)	C18—H18A	0.9700
C7—C9	1.451 (4)	C18—H18B	0.9700
C8—N1	1.354 (5)	C19—C20	1.488 (6)
C8—H8	0.9300	C19—H19A	0.9700
C9—O1	1.235 (4)	C19—H19B	0.9700
C9—N2	1.355 (4)	C20—H20A	0.9600
C10—N3	1.273 (4)	C20—H20B	0.9600
C10—C11	1.458 (5)	C20—H20C	0.9600
C10—H10	0.9300	N1—H1	0.858 (14)
C11—C16	1.385 (5)	N2—N3	1.376 (4)
C11—C12	1.397 (5)	N2—H2A	0.856 (13)
C12—C13	1.361 (5)	O3—S1	1.599 (3)
C12—H12	0.9300	O4—S1	1.426 (3)
C13—C14	1.398 (4)	O5—S1	1.411 (3)

N1—C1—C2	130.3 (4)	C16—C15—H15	119.9
N1—C1—C6	107.9 (3)	C11—C16—C15	121.6 (3)
C2—C1—C6	121.8 (4)	C11—C16—H16	119.2
C3—C2—C1	117.8 (4)	C15—C16—H16	119.2
C3—C2—H2	121.1	O2—C17—H17A	109.5
C1—C2—H2	121.1	O2—C17—H17B	109.5
C2—C3—C4	121.0 (4)	H17A—C17—H17B	109.5
C2—C3—H3	119.5	O2—C17—H17C	109.5
C4—C3—H3	119.5	H17A—C17—H17C	109.5
C5—C4—C3	121.9 (4)	H17B—C17—H17C	109.5
C5—C4—H4	119.0	C19—C18—S1	113.9 (3)
C3—C4—H4	119.0	C19—C18—H18A	108.8
C4—C5—C6	118.6 (4)	S1—C18—H18A	108.8
C4—C5—H5	120.7	C19—C18—H18B	108.8
C6—C5—H5	120.7	S1—C18—H18B	108.8
C5—C6—C1	118.8 (3)	H18A—C18—H18B	107.7
C5—C6—C7	135.0 (3)	C20—C19—C18	113.5 (4)
C1—C6—C7	106.1 (3)	C20—C19—H19A	108.9
C8—C7—C6	106.3 (3)	C18—C19—H19A	108.9

C8—C7—C9	126.9 (3)	C20—C19—H19B	108.9
C6—C7—C9	126.7 (3)	C18—C19—H19B	108.9
N1—C8—C7	109.9 (3)	H19A—C19—H19B	107.7
N1—C8—H8	125.0	C19—C20—H20A	109.5
C7—C8—H8	125.0	C19—C20—H20B	109.5
O1—C9—N2	122.3 (3)	H20A—C20—H20B	109.5
O1—C9—C7	122.4 (3)	C19—C20—H20C	109.5
N2—C9—C7	115.3 (3)	H20A—C20—H20C	109.5
N3—C10—C11	120.3 (3)	H20B—C20—H20C	109.5
N3—C10—H10	119.8	C8—N1—C1	109.7 (3)
C11—C10—H10	119.8	C8—N1—H1	117 (4)
C16—C11—C12	118.1 (3)	C1—N1—H1	131 (4)
C16—C11—C10	120.3 (3)	C9—N2—N3	119.5 (3)
C12—C11—C10	121.6 (3)	C9—N2—H2A	124 (3)
C13—C12—C11	120.2 (3)	N3—N2—H2A	115 (3)
C13—C12—H12	119.9	C10—N3—N2	116.1 (3)
C11—C12—H12	119.9	C14—O2—C17	117.6 (3)
C12—C13—C14	122.1 (3)	C13—O3—S1	117.6 (2)
C12—C13—O3	119.4 (3)	O5—S1—O4	117.3 (3)
C14—C13—O3	118.6 (3)	O5—S1—O3	108.98 (19)
O2—C14—C15	125.1 (3)	O4—S1—O3	108.43 (17)
O2—C14—C13	116.9 (3)	O5—S1—C18	111.2 (2)
C15—C14—C13	117.9 (3)	O4—S1—C18	109.37 (19)
C14—C15—C16	120.2 (3)	O3—S1—C18	100.09 (16)
C14—C15—H15	119.9		
C20—C19—C18—S1	168.2 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···O1^{i}	0.93	2.51	3.325 (4)	146
C18—H18*A*···O1^{ii}	0.97	2.52	3.467 (5)	164
N2—H2*A*···O1^{i}	0.86 (1)	2.22 (2)	3.048 (4)	163 (4)
N1—H1···O4^{iii}	0.86 (1)	2.07 (3)	2.870 (5)	156 (5)

Symmetry codes: (i) $x-1/2, -y+1, z$; (ii) $-x+1, -y+1, z-1/2$; (iii) $-x, -y+1, z+1/2$.