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2-(3,4-Dimethyl-5,5-dioxo-2*H*,4*H*-pyrazolo[4,3-*c*][1,2]benzothiazin-2-yl)-1-(4-methoxyphenyl)ethanone

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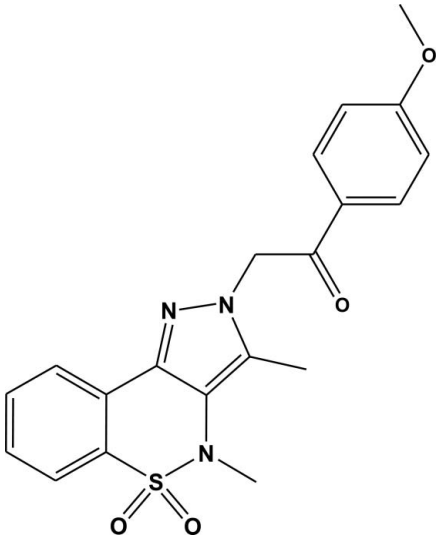
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.063; wR factor = 0.132; data-to-parameter ratio = 16.5.

In the title molecule, $C_{20}H_{19}N_3O_4S$, the heterocyclic thiazine ring adopts a half-chair conformation with the S and N atoms displaced by 0.492 (6) and 0.199 (6) Å, respectively, on opposite sides from the mean plane formed by the remaining ring atoms. The ethanone group lies at an angle of 9.4 (2)° with respect to the benzene ring, which lies almost perpendicular to the pyrazole ring, with a dihedral between the two planes of 78.07 (9)°. In the crystal, molecules are linked by weak C—H···O hydrogen bonds.

Related literature

For the biological activity of pyrazoles, see: Farag *et al.* (2008); Ciciani *et al.* (2008); Cunico *et al.* (2006); Ahmad *et al.* (2010). For a related structure, see: Siddiqui *et al.* (2008).



Experimental

Crystal data

$C_{20}H_{19}N_3O_4S$
M_r = 397.44
Monoclinic, $P2_1/n$
a = 13.862 (5) Å
b = 8.079 (2) Å
c = 17.748 (7) Å
β = 108.372 (18)°
V = 1886.3 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 173 K
0.14 × 0.09 × 0.07 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
T_{min} = 0.972, T_{max} = 0.986
7270 measured reflections
4221 independent reflections
3206 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.132
S = 1.15
4221 reflections
256 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O1^{i}	0.95	2.34	3.216 (3)	154
C4—H4···O4^{ii}	0.95	2.53	3.435 (4)	159
C9—H9*A*···O3^{iii}	0.98	2.54	3.335 (4)	138
C11—H11*C*···O2^{iv}	0.98	2.56	3.498 (4)	161
C12—H12*B*···O2^{iv}	0.99	2.33	3.309 (4)	170

Symmetry codes: (i) $x, y-1, z$; (ii) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x+1, -y+1, -z$.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* (Otwinowski & Minor, 1997); 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, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2223).

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supporting information

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2-(3,4-Dimethyl-5,5-dioxo-2*H*,4*H*-pyrazolo[4,3-*c*][1,2]benzothiazin-2-yl)-1-(4-methoxyphenyl)ethanone

Sana Aslam, Hamid Latif Siddiqui, Matloob Ahmad, Tanvir Hussain and Masood Parvez

S1. Comment

Both benzothiazines and pyrazoles are known as versatile biologically active heterocyclic nuclei. Pyrazoles are found to be cytotoxic agents (Ciciani *et al.*, 2008), anti–tumor (Farag *et al.*, 2008), anti–malarial (Cunico *et al.*, 2006), *etc*. In continuation to our research interests in biologically active molecules (Ahmad *et al.*, 2010), we have fused both of these heterocycles and herein report the synthesis and crystal structure of the title compound.

The bond distances and angles in the title compound (Fig. 1) agree very well with the corresponding bond distances and angles reported in closely related compounds (Siddiqui *et al.*, 2008). The heterocyclic thiazine ring adopts a half chair conformation with the atoms S1 and N1 displaced by 0.492 (5) and 0.199 (5) Å, respectively, on the opposite sides from the mean plane formed by the remaining ring atoms. The ethanone group O3/C12/C13/C14 is oriented at 9.4 (2)° with the benzene ring (C14–C19) which forms a dihedral angle 78.07 (9)° with the pyrazolyl ring (N2/N3/C7/C8/C10). The crystal packing (Fig. 2) is stabilized by weak intermolecular C—H···O hydrogen bonds (see, Table 1).

S2. Experimental

Equimolar quantities of 3,4–dimethyl–2,4–dihydropyrazolo[4,3–*c*][1,2] benzothiazine 5,5–dioxide (1.0 g, 4.01 mmol) and *p*–methoxyphenacyl bromide (0.92 g, 4.01 mmol) were dissolved in acetonitrile (20 ml) followed by the addition of equimolar K_2CO_3 (0.55 g, 4.01 mmol). The mixture was subjected to reflux for 7 h. The completion of reaction was monitored with the help of TLC. The precipitates of the title compound formed were collected and washed with methanol. The crystals suitable for X–ray crystallographic analysis were grown from a solution of $CHCl_3$:MeOH in 1:1 ratio.

S3. Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95, 0.98 and 0.99 Å, for aryl, methyl and methylene H–atoms, respectively. The U_{iso}(H) were allowed at 1.5U_{eq}(C methyl) or 1.2U_{eq}(C non–methyl).

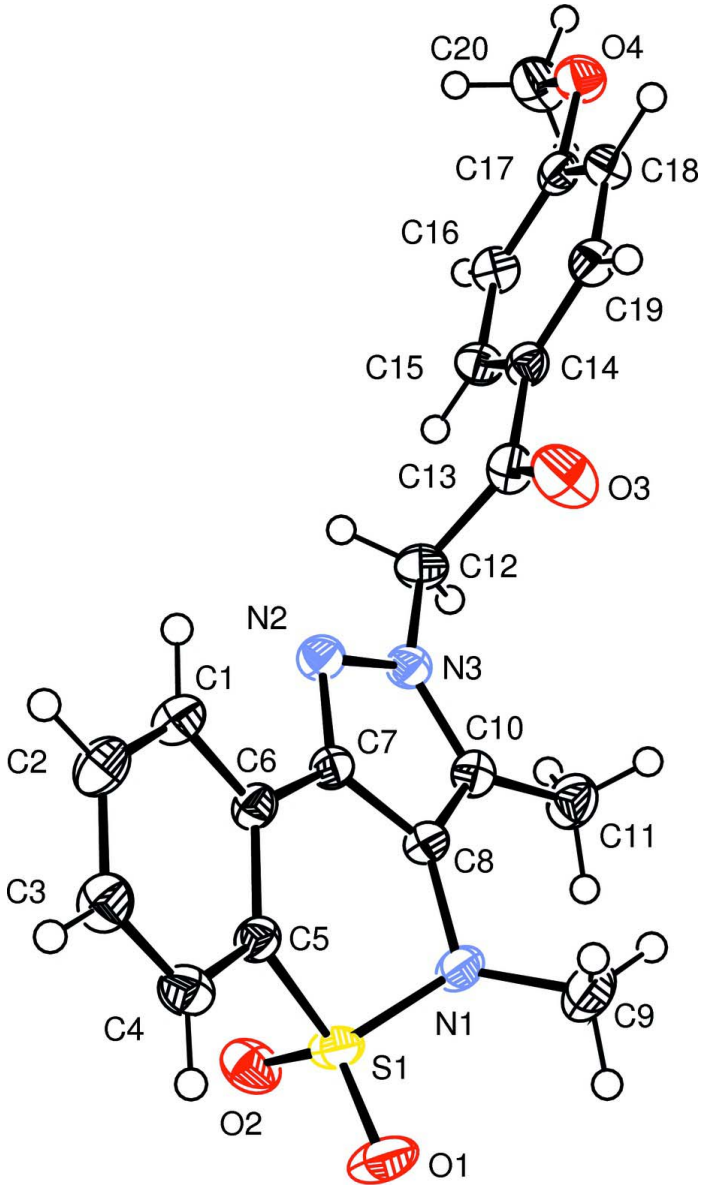

Figure 1

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are presented as small spheres of arbitrary radius.

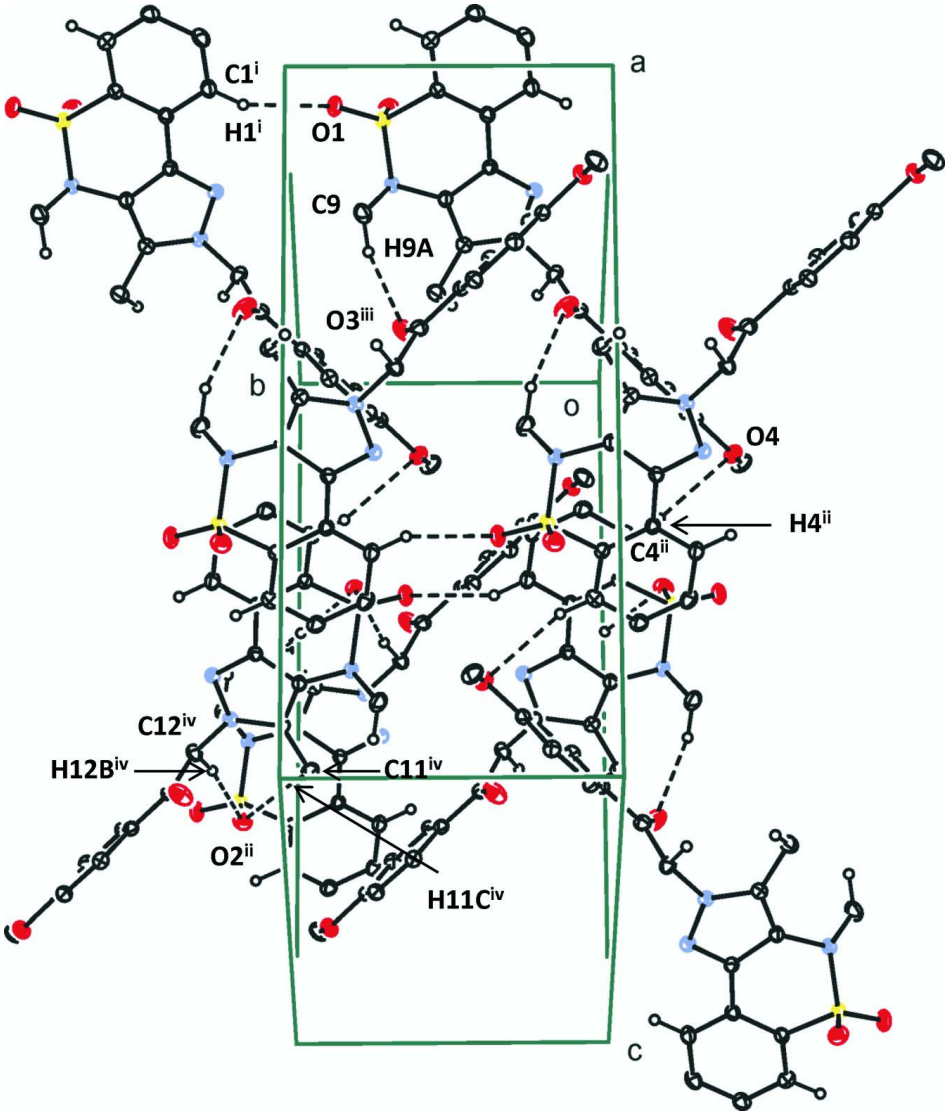

Figure 2

A view of the C—-H···O hydrogen bonds (dotted lines) in the crystal structure of the title compound. H atoms non-participating in hydrogen- bonding were omitted for clarity. [Symmetry codes: (i) *x*, *y* + 1, *z*; (ii) - *x* + 1/2, *y* + 1/2, - *z* + 1/2; (iii) - *x* + 3/2, *y* + 1/2, - *z* + 1/2; (iv) *x* - 1/2, *y* - 1/2, *z* + 1/2.]

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V = 1886.3 (11) Å^3
Z = 4
$F(000)$ = 832
D_x = 1.399 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7270 reflections
θ = 1.0–27.5°
μ = 0.20 mm^{-1}
T = 173 K
Block, colorless
0.14 × 0.09 × 0.07 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
T_{min} = 0.972, T_{max} = 0.986
7270 measured reflections
4221 independent reflections
3206 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 27.5°, θ_{min} = 2.8°
h = −17→17
k = −9→10
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.132
S = 1.15
4221 reflections
256 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0125P)^2 + 3.1849P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
S1	0.74841 (6)	0.70621 (8)	−0.04740 (5)	0.02818 (18)
O1	0.80588 (18)	0.8557 (2)	−0.03966 (15)	0.0421 (6)
O2	0.65575 (16)	0.6908 (3)	−0.11268 (13)	0.0364 (5)
O3	0.69947 (17)	0.1379 (3)	0.20986 (14)	0.0450 (6)
O4	0.42507 (16)	−0.3992 (2)	0.30314 (12)	0.0328 (5)
N1	0.71869 (18)	0.6790 (3)	0.03472 (15)	0.0278 (5)
N2	0.68248 (17)	0.2335 (3)	0.02702 (14)	0.0249 (5)
N3	0.61920 (17)	0.2872 (3)	0.06695 (14)	0.0247 (5)
C1	0.8567 (2)	0.2439 (3)	−0.04096 (18)	0.0285 (6)
H1	0.8446	0.1375	−0.0230	0.034*
C2	0.9282 (2)	0.2633 (4)	−0.08003 (19)	0.0318 (7)
H2	0.9630	0.1689	−0.0903	0.038*
C3	0.9497 (2)	0.4180 (4)	−0.10439 (18)	0.0305 (7)
H3	0.9994	0.4292	−0.1306	0.037*
C4	0.8986 (2)	0.5564 (4)	−0.09057 (17)	0.0290 (6)
H4	0.9138	0.6633	−0.1061	0.035*

C5	0.8247 (2)	0.5358 (3)	−0.05350 (16)	0.0225 (6)
C6	0.8025 (2)	0.3805 (3)	−0.02802 (16)	0.0226 (6)
C7	0.7262 (2)	0.3726 (3)	0.01260 (16)	0.0222 (5)
C8	0.6893 (2)	0.5120 (3)	0.04242 (16)	0.0238 (6)
C9	0.7789 (3)	0.7683 (4)	0.1072 (2)	0.0394 (8)
H9A	0.7481	0.7517	0.1493	0.059*
H9B	0.7799	0.8867	0.0956	0.059*
H9C	0.8486	0.7255	0.1248	0.059*
C10	0.6204 (2)	0.4540 (3)	0.07777 (17)	0.0248 (6)
C11	0.5603 (2)	0.5422 (4)	0.12170 (19)	0.0353 (7)
H11A	0.5545	0.6594	0.1068	0.053*
H11B	0.5947	0.5319	0.1789	0.053*
H11C	0.4923	0.4932	0.1083	0.053*
C12	0.5584 (2)	0.1665 (4)	0.09241 (18)	0.0287 (6)
H12A	0.5394	0.0759	0.0529	0.034*
H12B	0.4949	0.2199	0.0943	0.034*
C13	0.6139 (2)	0.0936 (4)	0.17351 (17)	0.0266 (6)
C14	0.5596 (2)	−0.0342 (3)	0.20525 (16)	0.0235 (6)
C15	0.4571 (2)	−0.0723 (3)	0.16869 (17)	0.0259 (6)
H15	0.4197	−0.0147	0.1220	0.031*
C16	0.4092 (2)	−0.1932 (3)	0.19962 (17)	0.0260 (6)
H16	0.3393	−0.2170	0.1747	0.031*
C17	0.4642 (2)	−0.2790 (3)	0.26725 (16)	0.0248 (6)
C18	0.5671 (2)	−0.2441 (3)	0.30382 (17)	0.0276 (6)
H18	0.6048	−0.3039	0.3498	0.033*
C19	0.6139 (2)	−0.1229 (3)	0.27307 (17)	0.0257 (6)
H19	0.6838	−0.0993	0.2982	0.031*
C20	0.3188 (2)	−0.4360 (4)	0.2697 (2)	0.0394 (8)
H20A	0.2989	−0.5161	0.3035	0.059*
H20B	0.3057	−0.4829	0.2164	0.059*
H20C	0.2792	−0.3342	0.2662	0.059*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0339 (4)	0.0189 (3)	0.0368 (4)	0.0020 (3)	0.0185 (3)	0.0031 (3)
O1	0.0553 (15)	0.0190 (10)	0.0655 (17)	−0.0036 (10)	0.0381 (13)	0.0001 (10)
O2	0.0346 (12)	0.0403 (12)	0.0350 (12)	0.0117 (10)	0.0121 (10)	0.0103 (10)
O3	0.0344 (13)	0.0554 (15)	0.0397 (13)	−0.0191 (11)	0.0039 (10)	0.0091 (11)
O4	0.0365 (12)	0.0297 (11)	0.0334 (12)	−0.0089 (9)	0.0127 (10)	0.0030 (9)
N1	0.0366 (14)	0.0194 (11)	0.0333 (14)	−0.0045 (10)	0.0192 (11)	−0.0043 (10)
N2	0.0261 (12)	0.0233 (11)	0.0282 (13)	−0.0023 (9)	0.0128 (10)	0.0000 (9)
N3	0.0280 (12)	0.0231 (11)	0.0255 (12)	−0.0010 (9)	0.0120 (10)	0.0012 (9)
C1	0.0302 (15)	0.0218 (14)	0.0339 (16)	−0.0019 (11)	0.0106 (13)	−0.0032 (12)
C2	0.0284 (15)	0.0289 (15)	0.0399 (17)	0.0046 (12)	0.0133 (13)	−0.0059 (13)
C3	0.0276 (15)	0.0327 (15)	0.0354 (17)	−0.0001 (12)	0.0157 (13)	−0.0026 (13)
C4	0.0284 (15)	0.0294 (15)	0.0293 (15)	−0.0024 (12)	0.0092 (13)	0.0034 (12)
C5	0.0238 (14)	0.0204 (13)	0.0243 (14)	0.0013 (10)	0.0088 (11)	−0.0010 (10)

C6	0.0228 (13)	0.0207 (13)	0.0242 (14)	−0.0026 (10)	0.0073 (11)	−0.0028 (10)
C7	0.0245 (14)	0.0203 (13)	0.0221 (13)	−0.0030 (10)	0.0078 (11)	−0.0008 (10)
C8	0.0269 (14)	0.0193 (13)	0.0247 (14)	−0.0009 (11)	0.0075 (12)	−0.0006 (10)
C9	0.047 (2)	0.0304 (16)	0.0435 (19)	−0.0080 (14)	0.0187 (16)	−0.0124 (14)
C10	0.0248 (14)	0.0254 (13)	0.0240 (14)	0.0004 (11)	0.0075 (12)	−0.0017 (11)
C11	0.0389 (18)	0.0334 (16)	0.0387 (18)	−0.0004 (13)	0.0197 (15)	−0.0057 (14)
C12	0.0277 (15)	0.0262 (14)	0.0339 (16)	−0.0051 (12)	0.0122 (13)	0.0029 (12)
C13	0.0248 (15)	0.0292 (14)	0.0273 (15)	−0.0037 (12)	0.0105 (12)	−0.0029 (12)
C14	0.0250 (14)	0.0225 (13)	0.0256 (14)	−0.0008 (11)	0.0116 (12)	−0.0019 (11)
C15	0.0245 (14)	0.0261 (14)	0.0278 (15)	0.0006 (11)	0.0094 (12)	0.0039 (11)
C16	0.0199 (13)	0.0287 (14)	0.0302 (15)	−0.0011 (11)	0.0092 (11)	0.0001 (12)
C17	0.0297 (15)	0.0207 (13)	0.0269 (14)	−0.0039 (11)	0.0131 (12)	−0.0039 (11)
C18	0.0307 (15)	0.0268 (14)	0.0245 (14)	0.0027 (12)	0.0074 (12)	0.0027 (11)
C19	0.0217 (14)	0.0264 (14)	0.0271 (14)	0.0003 (11)	0.0051 (12)	−0.0018 (11)
C20	0.0378 (18)	0.0431 (19)	0.0376 (18)	−0.0157 (15)	0.0124 (15)	0.0034 (15)

Geometric parameters (Å, º)

S1—O1	1.429 (2)	C8—C10	1.380 (4)
S1—O2	1.439 (2)	C9—H9A	0.9800
S1—N1	1.650 (3)	C9—H9B	0.9800
S1—C5	1.760 (3)	C9—H9C	0.9800
O3—C13	1.212 (3)	C10—C11	1.489 (4)
O4—C17	1.365 (3)	C11—H11A	0.9800
O4—C20	1.435 (4)	C11—H11B	0.9800
N1—C8	1.428 (3)	C11—H11C	0.9800
N1—C9	1.482 (4)	C12—C13	1.521 (4)
N2—C7	1.340 (3)	C12—H12A	0.9900
N2—N3	1.361 (3)	C12—H12B	0.9900
N3—C10	1.360 (3)	C13—C14	1.489 (4)
N3—C12	1.451 (3)	C14—C15	1.397 (4)
C1—C2	1.386 (4)	C14—C19	1.399 (4)
C1—C6	1.394 (4)	C15—C16	1.387 (4)
C1—H1	0.9500	C15—H15	0.9500
C2—C3	1.385 (4)	C16—C17	1.388 (4)
C2—H2	0.9500	C16—H16	0.9500
C3—C4	1.386 (4)	C17—C18	1.397 (4)
C3—H3	0.9500	C18—C19	1.378 (4)
C4—C5	1.391 (4)	C18—H18	0.9500
C4—H4	0.9500	C19—H19	0.9500
C5—C6	1.400 (4)	C20—H20A	0.9800
C6—C7	1.457 (4)	C20—H20B	0.9800
C7—C8	1.407 (4)	C20—H20C	0.9800
O1—S1—O2	118.68 (14)	H9B—C9—H9C	109.5
O1—S1—N1	108.34 (13)	N3—C10—C8	104.5 (2)
O2—S1—N1	106.97 (13)	N3—C10—C11	124.4 (3)
O1—S1—C5	109.83 (13)	C8—C10—C11	131.1 (3)

O2—S1—C5	106.49 (13)	C10—C11—H11A	109.5
N1—S1—C5	105.80 (13)	C10—C11—H11B	109.5
C17—O4—C20	117.5 (2)	H11A—C11—H11B	109.5
C8—N1—C9	118.4 (2)	C10—C11—H11C	109.5
C8—N1—S1	111.63 (18)	H11A—C11—H11C	109.5
C9—N1—S1	118.2 (2)	H11B—C11—H11C	109.5
C7—N2—N3	103.7 (2)	N3—C12—C13	112.6 (2)
C10—N3—N2	114.1 (2)	N3—C12—H12A	109.1
C10—N3—C12	127.2 (2)	C13—C12—H12A	109.1
N2—N3—C12	118.7 (2)	N3—C12—H12B	109.1
C2—C1—C6	120.0 (3)	C13—C12—H12B	109.1
C2—C1—H1	120.0	H12A—C12—H12B	107.8
C6—C1—H1	120.0	O3—C13—C14	122.0 (3)
C3—C2—C1	121.1 (3)	O3—C13—C12	120.5 (3)
C3—C2—H2	119.5	C14—C13—C12	117.5 (2)
C1—C2—H2	119.5	C15—C14—C19	118.6 (2)
C2—C3—C4	120.1 (3)	C15—C14—C13	122.6 (2)
C2—C3—H3	120.0	C19—C14—C13	118.8 (2)
C4—C3—H3	120.0	C16—C15—C14	121.0 (3)
C3—C4—C5	118.7 (3)	C16—C15—H15	119.5
C3—C4—H4	120.7	C14—C15—H15	119.5
C5—C4—H4	120.7	C15—C16—C17	119.5 (3)
C4—C5—C6	122.0 (3)	C15—C16—H16	120.2
C4—C5—S1	118.8 (2)	C17—C16—H16	120.2
C6—C5—S1	118.9 (2)	O4—C17—C16	124.6 (3)
C1—C6—C5	118.1 (2)	O4—C17—C18	115.2 (2)
C1—C6—C7	124.0 (2)	C16—C17—C18	120.2 (3)
C5—C6—C7	117.8 (2)	C19—C18—C17	119.9 (3)
N2—C7—C8	111.0 (2)	C19—C18—H18	120.1
N2—C7—C6	125.0 (2)	C17—C18—H18	120.1
C8—C7—C6	123.9 (2)	C18—C19—C14	120.8 (3)
C10—C8—C7	106.6 (2)	C18—C19—H19	119.6
C10—C8—N1	128.6 (2)	C14—C19—H19	119.6
C7—C8—N1	124.8 (2)	O4—C20—H20A	109.5
N1—C9—H9A	109.5	O4—C20—H20B	109.5
N1—C9—H9B	109.5	H20A—C20—H20B	109.5
H9A—C9—H9B	109.5	O4—C20—H20C	109.5
N1—C9—H9C	109.5	H20A—C20—H20C	109.5
H9A—C9—H9C	109.5	H20B—C20—H20C	109.5

O1—S1—N1—C8	−162.2 (2)	C6—C7—C8—N1	2.2 (4)
O2—S1—N1—C8	68.8 (2)	C9—N1—C8—C10	69.1 (4)
C5—S1—N1—C8	−44.4 (2)	S1—N1—C8—C10	−148.3 (3)
O1—S1—N1—C9	−19.6 (3)	C9—N1—C8—C7	−112.1 (3)
O2—S1—N1—C9	−148.6 (2)	S1—N1—C8—C7	30.4 (4)
C5—S1—N1—C9	98.2 (2)	N2—N3—C10—C8	−0.1 (3)
C7—N2—N3—C10	0.6 (3)	C12—N3—C10—C8	−179.5 (3)
C7—N2—N3—C12	180.0 (2)	N2—N3—C10—C11	−178.1 (3)

C6—C1—C2—C3	2.2 (5)	C12—N3—C10—C11	2.5 (5)
C1—C2—C3—C4	−0.7 (5)	C7—C8—C10—N3	−0.4 (3)
C2—C3—C4—C5	−1.3 (4)	N1—C8—C10—N3	178.5 (3)
C3—C4—C5—C6	1.7 (4)	C7—C8—C10—C11	177.4 (3)
C3—C4—C5—S1	−171.8 (2)	N1—C8—C10—C11	−3.7 (5)
O1—S1—C5—C4	−33.1 (3)	C10—N3—C12—C13	−92.9 (3)
O2—S1—C5—C4	96.6 (2)	N2—N3—C12—C13	87.7 (3)
N1—S1—C5—C4	−149.8 (2)	N3—C12—C13—O3	0.4 (4)
O1—S1—C5—C6	153.1 (2)	N3—C12—C13—C14	−179.0 (2)
O2—S1—C5—C6	−77.2 (2)	O3—C13—C14—C15	172.2 (3)
N1—S1—C5—C6	36.4 (3)	C12—C13—C14—C15	−8.5 (4)
C2—C1—C6—C5	−1.8 (4)	O3—C13—C14—C19	−9.7 (4)
C2—C1—C6—C7	−179.8 (3)	C12—C13—C14—C19	169.6 (3)
C4—C5—C6—C1	−0.2 (4)	C19—C14—C15—C16	1.3 (4)
S1—C5—C6—C1	173.3 (2)	C13—C14—C15—C16	179.4 (3)
C4—C5—C6—C7	178.0 (3)	C14—C15—C16—C17	−0.9 (4)
S1—C5—C6—C7	−8.5 (3)	C20—O4—C17—C16	−1.8 (4)
N3—N2—C7—C8	−0.8 (3)	C20—O4—C17—C18	177.9 (3)
N3—N2—C7—C6	178.8 (2)	C15—C16—C17—O4	179.5 (3)
C1—C6—C7—N2	−15.4 (4)	C15—C16—C17—C18	−0.1 (4)
C5—C6—C7—N2	166.6 (3)	O4—C17—C18—C19	−179.0 (2)
C1—C6—C7—C8	164.2 (3)	C16—C17—C18—C19	0.7 (4)
C5—C6—C7—C8	−13.9 (4)	C17—C18—C19—C14	−0.2 (4)
N2—C7—C8—C10	0.8 (3)	C15—C14—C19—C18	−0.7 (4)
C6—C7—C8—C10	−178.8 (3)	C13—C14—C19—C18	−179.0 (3)
N2—C7—C8—N1	−178.2 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O1^{i}	0.95	2.34	3.216 (3)	154
C4—H4···O4^{ii}	0.95	2.53	3.435 (4)	159
C9—H9*A*···O3^{iii}	0.98	2.54	3.335 (4)	138
C11—H11*C*···O2^{iv}	0.98	2.56	3.498 (4)	161
C12—H12*B*···O2^{iv}	0.99	2.33	3.309 (4)	170

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) *x*+1/2, −*y*+1/2, *z*−1/2; (iii) −*x*+3/2, *y*+1/2, −*z*+1/2; (iv) −*x*+1, −*y*+1, −*z*.