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3-[2-(5-Oxo-4,4-diphenyl-2-sulfanylideneimidazolidin-1-yl)ethyl]-1,3-oxazolidin-2-one

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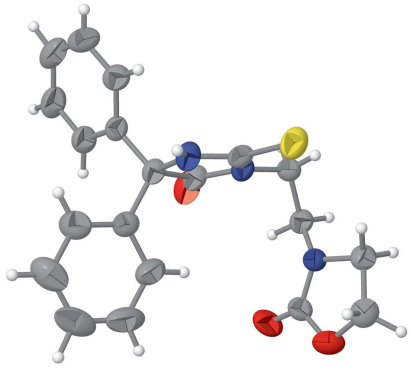
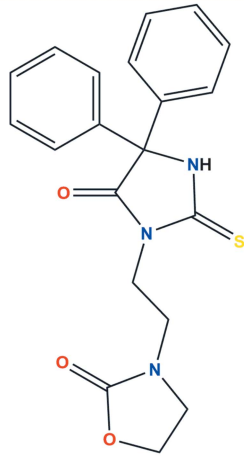
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{20}H_{19}N_3O_3S$, the conformation of the oxazolidine ring is characterized as twisted on the C—C bond. In the crystal, zigzag chains parallel to [101] are formed by N—H···O hydrogen bonds and are connected by C—H···O and C—H···π(ring) interactions.

3D view



Chemical scheme



Structure description

The imidazolidine-2,4-dione ring system is a core structure in various synthetic pharmaceutical agents, displaying a broad spectrum of biological activities, such as anticonvulsant (Weichet, 1974) antiarrhythmic (Havera *et al.*, 1976), fungicidal (Thenmozhiyal *et al.*, 2004), anticarcinogen (Lamothe *et al.*, 2002), antiviral (El-Barbary *et al.*, 1994) and anti-HIV (Khodair *et al.*, 1997). As a continuation of our research into hydantoin derivatives (Ramli *et al.*, 2017; Akrad *et al.*, 2017), the title compound, 3-[2-(5-oxo-4,4-diphenyl-2-sulfanylideneimidazolidin-1-yl)ethyl]-1,3-oxazolidin-2-one (Fig. 1), was prepared and its crystal structure is reported here. The pendant oxazolidine ring has a conformation described as twisted on the C19—C20 bond, with puckering parameters $Q(2)$ = 0.199 (2) Å and $\varphi(2)$ = 118.1 (5)°. The dihedral angle between the N1/C1/N2/C2/C3 and C4–C9 rings is 68.43 (8)°, while that between the former ring and the C10–C15 ring is 77.94 (9)°.

In the crystal, N2—H2···O3^{i} hydrogen bonds form zigzag chains parallel to the [101] direction. These are associated into a three-dimensional network by a combination of C17—H17*B*···O1^{ii} hydrogen bonds and C19—H19*A*···*Cg*1^{iii} (*Cg*1 is the centroid of the C4–C9 ring) interactions (Figs. 2 and 3, and Table 1).

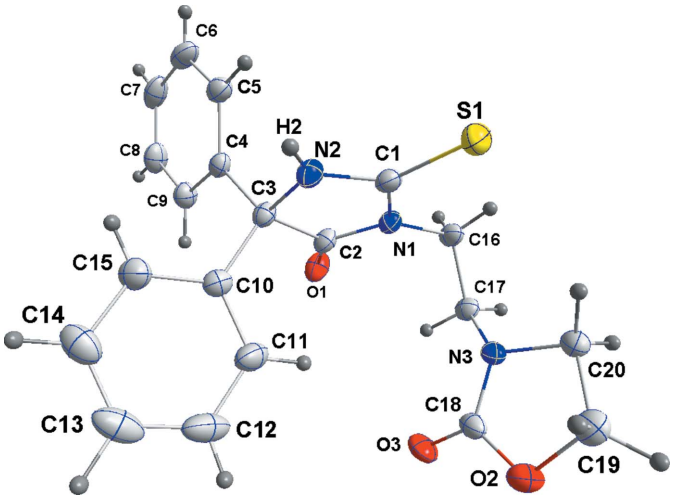


Figure 1
The title molecule, with the atom-labelling scheme and 25% probability displacement ellipsoids.

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

*Cg*1 is the centroid of the C4–C9 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O3^{i}	0.82 (2)	2.03 (2)	2.8214 (16)	161.9 (18)
C17—H17*B*···O1^{ii}	0.949 (17)	2.606 (17)	3.4068 (16)	142.3 (13)
C20—H20*A*···S1	1.01 (2)	2.95 (2)	3.8441 (16)	147.5 (16)
C19—H19*A*···*Cg*1^{iii}	1.01 (2)	2.58 (2)	3.563 (2)	163 (2)

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

Synthesis and crystallization

To a solution of 5,5-diphenyl-2-thioxoimidazolidin-4-one (1 g, 3.43 mmol), potassium carbonate (0.51 g, 3.73 mmol) and a catalytic amount of tetra-*n*-butylammonium bromide in dimethylformamide (DMF, 40 ml) was added bis(2-chloroethyl)amine hydrochloride (1.1 g, 6.87 mmol). The mixture was heated for 48 h. After completion of the reaction (as monitored by thin-layer chromatography), the inorganic material salt was filtered off and the solvent was removed under reduced pressure. The solid product was purified by recrys-

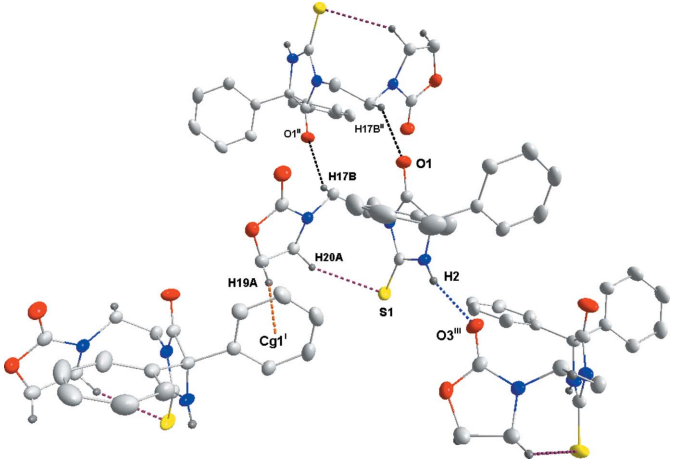


Figure 2
Detail of the N—H···O (blue dotted lines), C—H···O (black dotted lines) and C—H···S (purple dotted lines) hydrogen bonds, and the C—H···π(ring) (orange dotted line) interaction [symmetry codes: (i) $-1+x, y, z$; (ii) $1-x, 1-y, 1-z$; (iii) $\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$; *Cg*1 is the centroid of the C4–C9 ring].

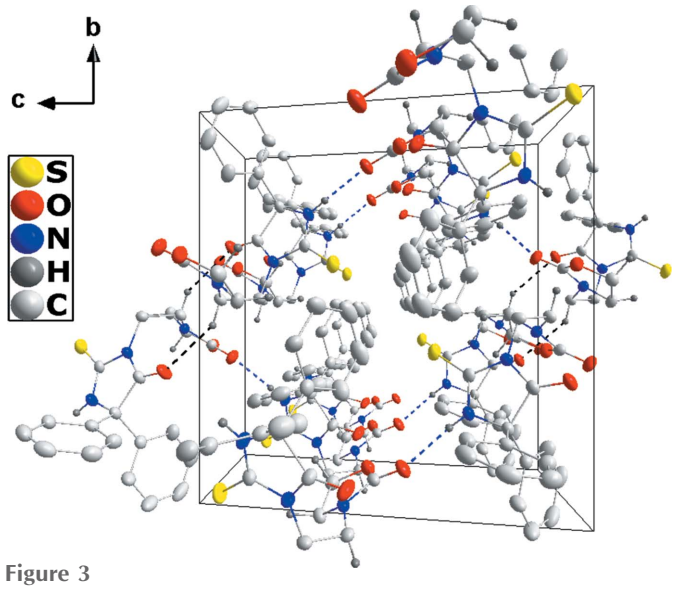


Figure 3
Packing viewed along the *a* axis, with N—H···O and C—H···O hydrogen bonds shown, respectively, as blue and black dotted lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{19}N_3O_3S$
M_r	381.44
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, *b*, *c* (Å)	9.1211 (6), 14.6521 (9), 14.2448 (9)
β (°)	104.037 (1)
V (Å^3)	1846.9 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.20
Crystal size (mm)	0.45 × 0.37 × 0.21
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.85, 0.96
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	34714, 4785, 3727
R_{int}	0.034
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.676
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.046, 0.136, 1.07
No. of reflections	4785
No. of parameters	320
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.20

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

tallization from ethanol solution to afford colourless block-like crystals of the title compound (yield 47%).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x171041 [https://doi.org/10.1107/S2414314617010410]

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Crystal data

$C_{20}H_{19}N_3O_3S$
M_r = 381.44
Monoclinic, $P2_1/n$
a = 9.1211 (6) Å
b = 14.6521 (9) Å
c = 14.2448 (9) Å
β = 104.037 (1)°
V = 1846.9 (2) Å^3
Z = 4
$F(000)$ = 800
D_x = 1.372 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9929 reflections
θ = 2.4–28.3°
μ = 0.20 mm^{-1}
T = 296 K
Thick plate, colourless
0.45 × 0.37 × 0.21 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 (*SADABS*; Bruker, 2016)
T_{min} = 0.85, T_{max} = 0.96
34714 measured reflections
4785 independent reflections
3727 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 28.7°, θ_{min} = 2.0°
h = −12→12
k = −19→19
l = −18→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.136
S = 1.07
4785 reflections
320 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0813P)^2 + 0.1546P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Special details

Experimental. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5° in ω, colllected at φ = 0.00, 90.00 and 180.00° and 2 sets of 800 frames, each of width 0.45° in φ, collected at ω = –30.00 and 210.00°. The scan time was 25 sec/frame.

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	0.45439 (5)	0.10546 (3)	0.87115 (3)	0.06097 (15)
O1	0.63811 (14)	0.15767 (8)	0.57384 (8)	0.0606 (3)
O2	−0.00162 (13)	0.11450 (8)	0.54050 (8)	0.0589 (3)
O3	0.16876 (15)	0.13993 (9)	0.45325 (8)	0.0675 (3)
N1	0.54332 (13)	0.11617 (7)	0.70320 (8)	0.0415 (2)
N2	0.59571 (14)	0.23714 (8)	0.79636 (8)	0.0447 (3)
H2	0.597 (2)	0.2712 (13)	0.8418 (14)	0.060 (5)*
N3	0.22929 (13)	0.05952 (7)	0.59525 (8)	0.0414 (2)
C1	0.53205 (14)	0.15481 (9)	0.79080 (9)	0.0418 (3)
C2	0.61106 (15)	0.17427 (9)	0.65130 (10)	0.0434 (3)
C3	0.64881 (14)	0.26288 (9)	0.71114 (9)	0.0393 (3)
C4	0.81901 (15)	0.27814 (8)	0.73146 (9)	0.0406 (3)
C5	0.91493 (17)	0.26267 (10)	0.82159 (11)	0.0498 (3)
H5	0.872 (2)	0.2470 (12)	0.8716 (13)	0.056 (5)*
C6	1.0705 (2)	0.27260 (12)	0.83439 (15)	0.0630 (4)
H6	1.124 (3)	0.2629 (14)	0.8880 (16)	0.071 (6)*
C7	1.1302 (2)	0.29717 (12)	0.75892 (16)	0.0667 (5)
H7	1.240 (3)	0.2999 (15)	0.7689 (15)	0.082 (6)*
C8	1.0357 (2)	0.31437 (12)	0.66945 (15)	0.0629 (4)
H8	1.079 (3)	0.3304 (16)	0.6178 (17)	0.088 (7)*
C9	0.88057 (18)	0.30484 (10)	0.65535 (12)	0.0523 (3)
H9	0.817 (2)	0.3165 (13)	0.5906 (15)	0.066 (5)*
C10	0.55634 (15)	0.34371 (10)	0.66023 (10)	0.0435 (3)
C11	0.41904 (19)	0.33094 (15)	0.59418 (13)	0.0652 (5)
H11	0.381 (3)	0.2707 (17)	0.5755 (17)	0.091 (7)*
C12	0.3337 (2)	0.4056 (2)	0.55374 (17)	0.0836 (7)
H12	0.245 (4)	0.4032 (18)	0.515 (2)	0.123 (10)*
C13	0.3834 (3)	0.49273 (18)	0.57794 (15)	0.0789 (6)
H13	0.318 (3)	0.544 (2)	0.550 (2)	0.114 (9)*
C14	0.5185 (3)	0.50596 (14)	0.64244 (15)	0.0750 (6)
H14	0.556 (3)	0.566 (2)	0.655 (2)	0.118 (9)*
C15	0.6050 (2)	0.43190 (11)	0.68405 (13)	0.0600 (4)
H15	0.696 (3)	0.4400 (16)	0.7277 (16)	0.083 (6)*

C16	0.49753 (17)	0.02326 (9)	0.67036 (11)	0.0463 (3)
H16A	0.586 (2)	−0.0054 (12)	0.6560 (13)	0.059 (5)*
H16B	0.4752 (18)	−0.0049 (11)	0.7244 (12)	0.043 (4)*
C17	0.36826 (16)	0.02046 (9)	0.58082 (10)	0.0439 (3)
H17A	0.3944 (17)	0.0557 (11)	0.5276 (11)	0.045 (4)*
H17B	0.3498 (19)	−0.0416 (12)	0.5627 (12)	0.049 (4)*
C18	0.13715 (17)	0.10721 (9)	0.52403 (10)	0.0458 (3)
C19	−0.0003 (2)	0.07352 (12)	0.63277 (12)	0.0556 (4)
H19A	0.003 (2)	0.1271 (15)	0.6781 (15)	0.080 (6)*
H19B	−0.098 (2)	0.0367 (13)	0.6248 (13)	0.063 (5)*
C20	0.14379 (17)	0.01694 (11)	0.65766 (11)	0.0494 (3)
H20A	0.198 (3)	0.0250 (14)	0.7283 (16)	0.078 (6)*
H20B	0.1247 (19)	−0.0493 (12)	0.6376 (12)	0.053 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0601 (3)	0.0785 (3)	0.0440 (2)	−0.02252 (19)	0.01207 (18)	0.00519 (17)
O1	0.0711 (7)	0.0666 (7)	0.0509 (6)	−0.0187 (5)	0.0277 (5)	−0.0241 (5)
O2	0.0521 (6)	0.0678 (7)	0.0522 (6)	0.0130 (5)	0.0041 (5)	0.0052 (5)
O3	0.0776 (8)	0.0713 (7)	0.0518 (6)	0.0059 (6)	0.0125 (6)	0.0246 (5)
N1	0.0420 (6)	0.0413 (5)	0.0390 (6)	−0.0072 (4)	0.0054 (4)	−0.0053 (4)
N2	0.0511 (7)	0.0499 (6)	0.0348 (6)	−0.0119 (5)	0.0138 (5)	−0.0093 (5)
N3	0.0423 (6)	0.0431 (6)	0.0363 (5)	−0.0022 (4)	0.0045 (4)	0.0027 (4)
C1	0.0352 (6)	0.0503 (7)	0.0361 (6)	−0.0043 (5)	0.0016 (5)	−0.0014 (5)
C2	0.0415 (7)	0.0475 (7)	0.0410 (7)	−0.0077 (5)	0.0098 (5)	−0.0100 (5)
C3	0.0415 (7)	0.0429 (6)	0.0342 (6)	−0.0068 (5)	0.0106 (5)	−0.0069 (5)
C4	0.0408 (7)	0.0351 (6)	0.0455 (7)	−0.0033 (5)	0.0100 (5)	−0.0064 (5)
C5	0.0504 (8)	0.0471 (7)	0.0480 (8)	−0.0012 (6)	0.0045 (6)	−0.0073 (6)
C6	0.0499 (9)	0.0580 (9)	0.0697 (11)	0.0060 (7)	−0.0075 (8)	−0.0144 (8)
C7	0.0422 (8)	0.0567 (9)	0.1011 (15)	−0.0057 (7)	0.0173 (9)	−0.0207 (9)
C8	0.0525 (9)	0.0592 (9)	0.0836 (13)	−0.0075 (7)	0.0291 (9)	−0.0047 (8)
C9	0.0494 (8)	0.0529 (8)	0.0568 (9)	−0.0033 (6)	0.0171 (7)	0.0011 (6)
C10	0.0404 (7)	0.0533 (7)	0.0385 (6)	0.0005 (5)	0.0128 (5)	−0.0020 (5)
C11	0.0432 (8)	0.0866 (13)	0.0617 (10)	−0.0084 (8)	0.0047 (7)	0.0113 (9)
C12	0.0456 (10)	0.131 (2)	0.0721 (13)	0.0138 (11)	0.0098 (9)	0.0341 (12)
C13	0.0784 (13)	0.0989 (16)	0.0692 (12)	0.0434 (12)	0.0373 (11)	0.0306 (11)
C14	0.1022 (16)	0.0598 (11)	0.0675 (11)	0.0271 (10)	0.0293 (11)	0.0034 (8)
C15	0.0664 (10)	0.0513 (8)	0.0577 (9)	0.0088 (7)	0.0062 (8)	−0.0104 (7)
C16	0.0460 (8)	0.0371 (6)	0.0502 (8)	−0.0001 (5)	0.0010 (6)	−0.0022 (5)
C17	0.0453 (7)	0.0411 (7)	0.0428 (7)	−0.0034 (5)	0.0060 (6)	−0.0072 (5)
C18	0.0524 (8)	0.0398 (6)	0.0406 (7)	−0.0001 (5)	0.0024 (6)	0.0020 (5)
C19	0.0539 (9)	0.0592 (9)	0.0546 (9)	−0.0008 (7)	0.0152 (7)	−0.0053 (7)
C20	0.0475 (8)	0.0569 (8)	0.0416 (7)	−0.0054 (6)	0.0067 (6)	0.0063 (6)

Geometric parameters (Å, º)

S1—C1	1.6516 (14)	C8—C9	1.387 (2)
O1—C2	1.2122 (17)	C8—H8	0.95 (2)
O2—C18	1.346 (2)	C9—H9	0.98 (2)
O2—C19	1.442 (2)	C10—C15	1.382 (2)
O3—C18	1.2127 (18)	C10—C11	1.385 (2)
N1—C2	1.3693 (17)	C11—C12	1.385 (3)
N1—C1	1.3965 (17)	C11—H11	0.96 (2)
N1—C16	1.4669 (16)	C12—C13	1.370 (4)
N2—C1	1.3328 (18)	C12—H12	0.86 (3)
N2—C3	1.4614 (16)	C13—C14	1.361 (4)
N2—H2	0.82 (2)	C13—H13	0.98 (3)
N3—C18	1.3454 (17)	C14—C15	1.387 (3)
N3—C17	1.4502 (18)	C14—H14	0.95 (3)
N3—C20	1.4575 (18)	C15—H15	0.92 (2)
C2—C3	1.5454 (17)	C16—C17	1.5130 (19)
C3—C4	1.5251 (18)	C16—H16A	0.98 (2)
C3—C10	1.5308 (19)	C16—H16B	0.939 (16)
C4—C5	1.386 (2)	C17—H17A	0.994 (16)
C4—C9	1.393 (2)	C17—H17B	0.949 (17)
C5—C6	1.394 (2)	C19—C20	1.521 (2)
C5—H5	0.923 (18)	C19—H19A	1.01 (2)
C6—C7	1.366 (3)	C19—H19B	1.02 (2)
C6—H6	0.81 (2)	C20—H20A	1.01 (2)
C7—C8	1.378 (3)	C20—H20B	1.015 (18)
C7—H7	0.98 (2)		
C18—O2—C19	108.98 (12)	C10—C11—C12	120.0 (2)
C2—N1—C1	111.79 (10)	C10—C11—H11	121.3 (14)
C2—N1—C16	122.39 (11)	C12—C11—H11	118.6 (14)
C1—N1—C16	125.74 (11)	C13—C12—C11	120.9 (2)
C1—N2—C3	114.30 (11)	C13—C12—H12	113.6 (19)
C1—N2—H2	121.5 (13)	C11—C12—H12	125.4 (19)
C3—N2—H2	123.9 (13)	C14—C13—C12	119.50 (19)
C18—N3—C17	120.38 (12)	C14—C13—H13	121.6 (17)
C18—N3—C20	110.70 (12)	C12—C13—H13	118.8 (17)
C17—N3—C20	122.20 (11)	C13—C14—C15	120.3 (2)
N2—C1—N1	107.13 (11)	C13—C14—H14	119.5 (19)
N2—C1—S1	127.51 (10)	C15—C14—H14	120.1 (19)
N1—C1—S1	125.35 (10)	C10—C15—C14	120.76 (19)
O1—C2—N1	125.79 (12)	C10—C15—H15	118.2 (14)
O1—C2—C3	127.12 (12)	C14—C15—H15	121.1 (15)
N1—C2—C3	107.08 (10)	N1—C16—C17	113.42 (11)
N2—C3—C4	114.04 (11)	N1—C16—H16A	106.2 (11)
N2—C3—C10	109.73 (10)	C17—C16—H16A	109.1 (11)
C4—C3—C10	113.27 (10)	N1—C16—H16B	104.3 (9)
N2—C3—C2	99.62 (10)	C17—C16—H16B	113.6 (10)

C4—C3—C2	107.95 (10)	H16A—C16—H16B	109.9 (14)
C10—C3—C2	111.42 (11)	N3—C17—C16	113.52 (11)
C5—C4—C9	118.95 (14)	N3—C17—H17A	106.5 (9)
C5—C4—C3	122.46 (12)	C16—C17—H17A	110.3 (9)
C9—C4—C3	118.53 (12)	N3—C17—H17B	108.3 (10)
C4—C5—C6	119.87 (16)	C16—C17—H17B	107.8 (10)
C4—C5—H5	117.6 (12)	H17A—C17—H17B	110.5 (13)
C6—C5—H5	122.5 (12)	O3—C18—N3	126.96 (15)
C7—C6—C5	120.80 (17)	O3—C18—O2	122.46 (13)
C7—C6—H6	121.6 (15)	N3—C18—O2	110.58 (12)
C5—C6—H6	117.6 (15)	O2—C19—C20	104.79 (12)
C6—C7—C8	119.81 (16)	O2—C19—H19A	104.5 (12)
C6—C7—H7	119.1 (13)	C20—C19—H19A	112.8 (12)
C8—C7—H7	121.1 (13)	O2—C19—H19B	107.7 (11)
C7—C8—C9	120.19 (17)	C20—C19—H19B	114.6 (11)
C7—C8—H8	118.5 (15)	H19A—C19—H19B	111.5 (16)
C9—C8—H8	121.2 (15)	N3—C20—C19	100.62 (12)
C8—C9—C4	120.35 (16)	N3—C20—H20A	110.7 (13)
C8—C9—H9	118.0 (12)	C19—C20—H20A	110.5 (12)
C4—C9—H9	121.6 (12)	N3—C20—H20B	108.6 (10)
C15—C10—C11	118.48 (15)	C19—C20—H20B	112.1 (10)
C15—C10—C3	120.01 (13)	H20A—C20—H20B	113.5 (15)
C11—C10—C3	121.40 (14)		

C3—N2—C1—N1	2.78 (16)	C5—C4—C9—C8	1.0 (2)
C3—N2—C1—S1	−177.54 (10)	C3—C4—C9—C8	−176.30 (13)
C2—N1—C1—N2	−1.37 (15)	N2—C3—C10—C15	91.40 (15)
C16—N1—C1—N2	175.39 (12)	C4—C3—C10—C15	−37.31 (17)
C2—N1—C1—S1	178.93 (10)	C2—C3—C10—C15	−159.25 (13)
C16—N1—C1—S1	−4.31 (19)	N2—C3—C10—C11	−84.74 (16)
C1—N1—C2—O1	178.35 (15)	C4—C3—C10—C11	146.55 (14)
C16—N1—C2—O1	1.5 (2)	C2—C3—C10—C11	24.61 (18)
C1—N1—C2—C3	−0.42 (15)	C15—C10—C11—C12	−0.1 (3)
C16—N1—C2—C3	−177.31 (11)	C3—C10—C11—C12	176.09 (16)
C1—N2—C3—C4	−117.55 (12)	C10—C11—C12—C13	0.2 (3)
C1—N2—C3—C10	114.16 (13)	C11—C12—C13—C14	0.1 (3)
C1—N2—C3—C2	−2.86 (15)	C12—C13—C14—C15	−0.5 (3)
O1—C2—C3—N2	−176.91 (15)	C11—C10—C15—C14	−0.3 (3)
N1—C2—C3—N2	1.84 (13)	C3—C10—C15—C14	−176.51 (16)
O1—C2—C3—C4	−57.62 (19)	C13—C14—C15—C10	0.6 (3)
N1—C2—C3—C4	121.13 (12)	C2—N1—C16—C17	−68.04 (18)
O1—C2—C3—C10	67.35 (18)	C1—N1—C16—C17	115.52 (15)
N1—C2—C3—C10	−113.91 (12)	C18—N3—C17—C16	143.55 (13)
N2—C3—C4—C5	4.19 (18)	C20—N3—C17—C16	−67.86 (16)
C10—C3—C4—C5	130.65 (13)	N1—C16—C17—N3	−63.23 (17)
C2—C3—C4—C5	−105.49 (14)	C17—N3—C18—O3	−17.3 (2)
N2—C3—C4—C9	−178.64 (12)	C20—N3—C18—O3	−169.18 (15)
C10—C3—C4—C9	−52.18 (16)	C17—N3—C18—O2	162.26 (12)

C2—C3—C4—C9	71.68 (15)	C20—N3—C18—O2	10.39 (16)
C9—C4—C5—C6	−1.0 (2)	C19—O2—C18—O3	−176.59 (14)
C3—C4—C5—C6	176.19 (13)	C19—O2—C18—N3	3.82 (16)
C4—C5—C6—C7	−0.2 (2)	C18—O2—C19—C20	−15.49 (16)
C5—C6—C7—C8	1.4 (3)	C18—N3—C20—C19	−18.81 (15)
C6—C7—C8—C9	−1.4 (3)	C17—N3—C20—C19	−170.09 (12)
C7—C8—C9—C4	0.2 (2)	O2—C19—C20—N3	19.90 (15)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O3^{i}	0.82 (2)	2.03 (2)	2.8214 (16)	161.9 (18)
C17—H17*B*···O1^{ii}	0.949 (17)	2.606 (17)	3.4068 (16)	142.3 (13)
C20—H20*A*···S1	1.01 (2)	2.95 (2)	3.8441 (16)	147.5 (16)
C19—H19*A*···*Cg*1^{iii}	1.01 (2)	2.58 (2)	3.563 (2)	163 (2)

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