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1′-Phenyl-6′-thiacycloheptane-1-spiro-2′-perhydropyrrolizine-3′-spiro-3″-indoline-2,2″-dione

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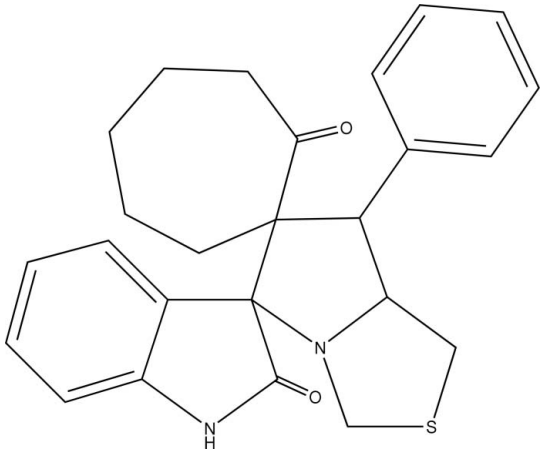
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.063; wR factor = 0.158; data-to-parameter ratio = 17.3.

The thiazolidine ring and the pyrrolidine ring in the title compound, $C_{25}H_{26}N_2O_2S$, both adopt an envelope conformation. The seven-membered ring has a twist-chair conformation. The crystal packing is stabilized by intermolecular N—H···O hydrogen bonds.

Related literature

For related literature, see: Amal Raj *et al.* (2003); Cremer & Pople (1975); Kumar *et al.* (2006); Nardelli (1983); Si *et al.* (2005).



Experimental

Crystal data

$C_{25}H_{26}N_2O_2S$
M_r = 418.54
Triclinic, $P\overline{1}$
a = 8.9846 (10) Å
b = 10.3564 (11) Å
c = 12.8124 (14) Å
α = 80.147 (2)°
β = 71.012 (2)°
γ = 67.497 (2)°
V = 1040.0 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 293 (2) K
0.26 × 0.25 × 0.23 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
11582 measured reflections
4697 independent reflections
3880 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.157
S = 1.08
4697 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1^{i}	0.86	2.04	2.859 (2)	160

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2666).

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1′-Phenyl-6′-thiacycloheptane-1-spiro-2′-perhydropyrrolizine-3′-spiro-3′′-indoline-2,2′′-dione

S. Sundaramoorthy, D. Gayathri, D. Velmurugan, M. Poornachandran and K. Ravikumar

S1. Comment

It has been reported that pyrrolidine derivatives reduce Coxsackievirus B3 replication through inhibition of the Ubiquitin-Proteasome pathway (Si *et al.*, 2005). They are found to have antimicrobial and antifungal activity against various pathogens except Bacillus subtilis (Amal Raj *et al.*, 2003). As the derivatives of pyrrolidine and oxindole are of pharmacological importance, we have undertaken the X-ray crystal structure determination of the title compound.

The bond lengths and bond angles of the title compound are comparable with a similar structure (Kumar *et al.*, 2006). The sum of the bond angles around N1 atom [341.8 (5)°] indicates sp^3 hybridization. The dihedral angle between the phenyl ring and the six membered in the oxindole moiety is 40.5 (1)°.

The thiazolidine ring adopts an envelope conformation with S1 atom deviating by 0.764 (1) Å. The pyrrolidine ring (N1/C1—C4) adopts an envelope conformation with C2 atom deviating by -0.655 (2) Å. The puckering parameters (Cremer & Pople, 1975) and the smallest displacement asymmetry parameters (Nardelli, 1983) for the pyrrolidine ring, five membered ring (N2/C7/C1/C13/C8) in the oxindole moiety and the thiazolidine ring are q_2 = 0.424 (2), 0.068 (2), 0.443 (2) Å, φ = 80.4 (3), 264.7 (18), 355.5 (3)° and $\Delta_s(C_2)$ = 7.7 (2), $\Delta_2(N_2)$ = 0.9 (3), $\Delta_s(S_1)$ = 5.9 (2).

The crystal packing is stabilized by intermolecular N—H···O hydrogen bonds generating a centrosymmetric dimeric ring motif [$R_2^2(8)$].

S2. Experimental

A mixture of isatin (0.147 g, 1 mmol), thiaproline, (0.135 g, 1 mmol) and benzylidenecycloheptanone (1 mmol) in methanol (20 ml) was refluxed until the disappearance of the starting materials. The reaction mixture was then concentrated *in vacuo* and extracted with water (50 ml) and dichloromethane (50 ml). The organic layer was washed with brine solution, dried with anhydrous sodium sulfate and concentrated *in vacuo*. The residue was purified by column chromatography with hexane-ethylacetate (8:2) mixture to get title compound. The pure compound was recrystallized from ethanol.

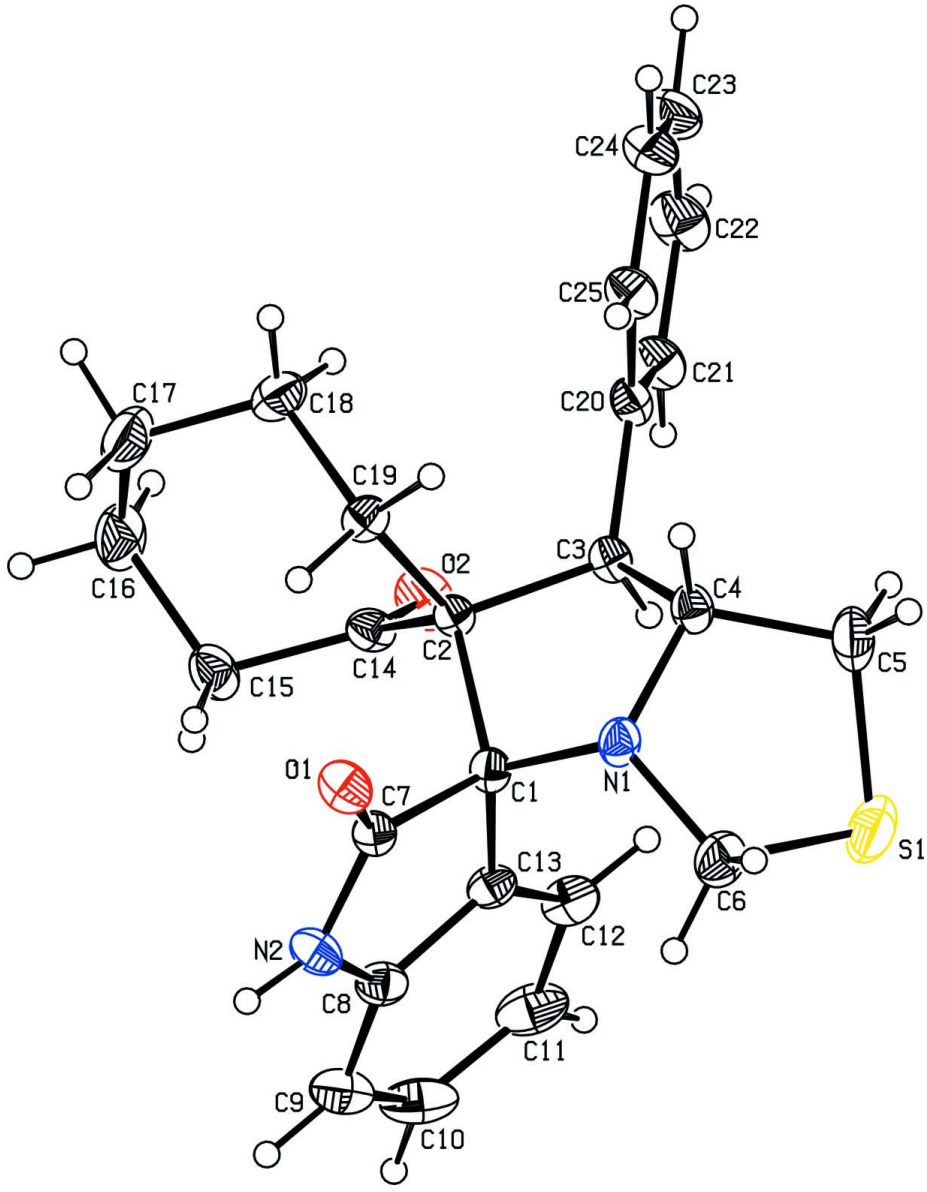

Figure 1

The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids.

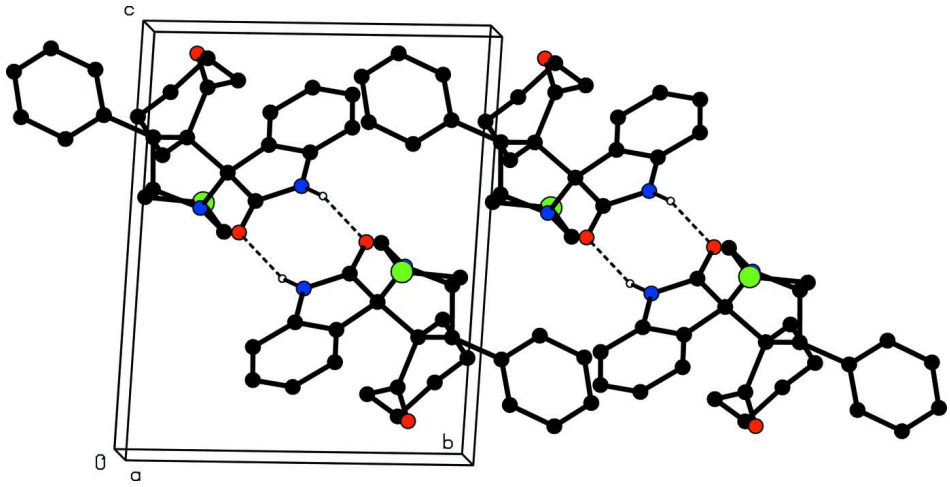

Figure 2

The packing of the title compound, viewed down the *a* axis, H atoms not involved in hydrogen bonding have been omitted.

1′-Phenyl-6′-thiacycloheptane-1-spiro-2′-perhydropyrrolizine-3′-spiro-3′′- indoline-2,2′′-dione

Crystal data

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$M_r = 418.54$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.9846$ (10) Å
$b = 10.3564$ (11) Å
$c = 12.8124$ (14) Å
$\alpha = 80.147$ (2)°
$\beta = 71.012$ (2)°
$\gamma = 67.497$ (2)°
$V = 1040.0$ (2) Å^3
$Z = 2$
$F(000) = 444$
$D_x = 1.337$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2358 reflections
$\theta = 1.7$–25.0°
$\mu = 0.18$ mm^{-1}
$T = 293$ K
Block, colorless
0.26 × 0.25 × 0.23 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
11582 measured reflections
4697 independent reflections
3880 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 28.0°$, $\theta_{min} = 1.7°$
$h = -11 \rightarrow 11$
$k = -13 \rightarrow 13$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.157$
$S = 1.08$
4697 reflections
271 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
$w = 1/[\sigma^2(F_o^2) + (0.0833P)^2 + 0.2981P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ 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}
C1	0.2327 (2)	0.71980 (19)	0.35784 (14)	0.0267 (4)
C2	0.1643 (2)	0.84561 (18)	0.27522 (14)	0.0245 (4)
C3	0.2629 (2)	0.93969 (19)	0.27834 (14)	0.0275 (4)
H3	0.3807	0.8916	0.2386	0.033*
C4	0.2543 (2)	0.9308 (2)	0.39991 (15)	0.0309 (4)
H4	0.1503	1.0022	0.4386	0.037*
C5	0.4043 (3)	0.9465 (3)	0.4219 (2)	0.0486 (6)
H5A	0.3675	0.9961	0.4887	0.058*
H5B	0.4568	0.9989	0.3607	0.058*
C6	0.3716 (3)	0.7143 (3)	0.4993 (2)	0.0477 (6)
H6A	0.4063	0.6146	0.4918	0.057*
H6B	0.3256	0.7325	0.5773	0.057*
C7	0.1116 (2)	0.63856 (19)	0.41978 (14)	0.0283 (4)
C8	0.3423 (3)	0.4830 (2)	0.31052 (16)	0.0340 (4)
C9	0.4440 (3)	0.3632 (2)	0.25409 (19)	0.0474 (6)
H9	0.4118	0.2855	0.2648	0.057*
C10	0.5958 (3)	0.3639 (3)	0.1810 (2)	0.0552 (7)
H10	0.6665	0.2857	0.1404	0.066*
C11	0.6440 (3)	0.4783 (3)	0.1674 (2)	0.0521 (6)
H11	0.7482	0.4750	0.1193	0.063*
C12	0.5404 (3)	0.5984 (2)	0.22390 (18)	0.0410 (5)
H12	0.5741	0.6752	0.2141	0.049*
C13	0.3852 (2)	0.6016 (2)	0.29553 (15)	0.0311 (4)
C14	0.2143 (3)	0.79473 (19)	0.15917 (15)	0.0312 (4)
C15	0.1212 (3)	0.7116 (2)	0.13959 (18)	0.0435 (5)
H15A	0.0694	0.6711	0.2093	0.052*
H15B	0.1990	0.6360	0.0920	0.052*
C16	−0.0142 (4)	0.8082 (3)	0.0852 (2)	0.0584 (7)
H16A	0.0370	0.8584	0.0216	0.070*
H16B	−0.0576	0.7514	0.0588	0.070*
C17	−0.1593 (3)	0.9132 (3)	0.1619 (2)	0.0600 (7)
H17A	−0.2234	0.8631	0.2172	0.072*
H17B	−0.2326	0.9763	0.1193	0.072*
C18	−0.1110 (3)	1.0007 (2)	0.22123 (19)	0.0433 (5)
H18A	−0.2113	1.0777	0.2538	0.052*

H18B	−0.0339	1.0406	0.1669	0.052*
C19	−0.0288 (2)	0.9197 (2)	0.31231 (15)	0.0307 (4)
H19A	−0.0793	0.8497	0.3474	0.037*
H19B	−0.0561	0.9844	0.3679	0.037*
C20	0.2132 (2)	1.0876 (2)	0.22729 (15)	0.0300 (4)
C21	0.3124 (3)	1.1172 (2)	0.12397 (17)	0.0393 (5)
H21	0.4070	1.0459	0.0876	0.047*
C22	0.2726 (3)	1.2504 (3)	0.07487 (19)	0.0503 (6)
H22	0.3406	1.2681	0.0060	0.060*
C23	0.1336 (4)	1.3570 (2)	0.1268 (2)	0.0512 (6)
H23	0.1051	1.4461	0.0924	0.061*
C24	0.0365 (3)	1.3313 (2)	0.2302 (2)	0.0477 (6)
H24	−0.0565	1.4039	0.2665	0.057*
C25	0.0765 (3)	1.1980 (2)	0.28063 (18)	0.0385 (5)
H25	0.0110	1.1822	0.3511	0.046*
N1	0.2471 (2)	0.79135 (17)	0.44146 (12)	0.0312 (4)
N2	0.1822 (2)	0.50686 (17)	0.38528 (14)	0.0365 (4)
H2	0.1347	0.4451	0.4066	0.044*
O1	−0.02147 (18)	0.68469 (15)	0.49036 (11)	0.0377 (3)
O2	0.3167 (2)	0.82744 (17)	0.08308 (11)	0.0449 (4)
S1	0.55069 (8)	0.77332 (8)	0.43717 (6)	0.0609 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0286 (9)	0.0307 (9)	0.0235 (8)	−0.0144 (8)	−0.0074 (7)	0.0014 (7)
C2	0.0295 (9)	0.0258 (9)	0.0194 (8)	−0.0125 (7)	−0.0066 (7)	0.0012 (7)
C3	0.0301 (9)	0.0301 (9)	0.0234 (9)	−0.0143 (8)	−0.0045 (7)	−0.0014 (7)
C4	0.0358 (10)	0.0354 (10)	0.0264 (9)	−0.0176 (8)	−0.0091 (8)	−0.0014 (8)
C5	0.0577 (15)	0.0605 (15)	0.0485 (13)	−0.0368 (12)	−0.0255 (11)	0.0027 (11)
C6	0.0591 (15)	0.0524 (14)	0.0437 (12)	−0.0251 (12)	−0.0296 (11)	0.0099 (10)
C7	0.0345 (10)	0.0316 (10)	0.0220 (8)	−0.0166 (8)	−0.0096 (7)	0.0051 (7)
C8	0.0395 (11)	0.0309 (10)	0.0289 (9)	−0.0104 (9)	−0.0115 (8)	0.0039 (8)
C9	0.0591 (15)	0.0308 (11)	0.0446 (12)	−0.0088 (10)	−0.0154 (11)	0.0015 (9)
C10	0.0559 (15)	0.0376 (12)	0.0446 (13)	0.0071 (11)	−0.0077 (11)	−0.0015 (10)
C11	0.0362 (12)	0.0530 (15)	0.0435 (13)	−0.0005 (11)	−0.0028 (10)	0.0044 (11)
C12	0.0337 (11)	0.0433 (12)	0.0383 (11)	−0.0108 (9)	−0.0075 (9)	0.0052 (9)
C13	0.0316 (10)	0.0327 (10)	0.0259 (9)	−0.0092 (8)	−0.0100 (8)	0.0043 (7)
C14	0.0404 (11)	0.0272 (9)	0.0255 (9)	−0.0110 (8)	−0.0103 (8)	0.0001 (7)
C15	0.0661 (15)	0.0409 (12)	0.0357 (11)	−0.0268 (11)	−0.0212 (10)	−0.0010 (9)
C16	0.0824 (19)	0.0688 (17)	0.0485 (14)	−0.0382 (15)	−0.0401 (14)	0.0050 (12)
C17	0.0601 (16)	0.0745 (18)	0.0625 (16)	−0.0296 (14)	−0.0409 (14)	0.0135 (14)
C18	0.0408 (12)	0.0444 (12)	0.0435 (12)	−0.0107 (10)	−0.0202 (10)	0.0068 (10)
C19	0.0298 (10)	0.0352 (10)	0.0259 (9)	−0.0123 (8)	−0.0075 (8)	0.0028 (8)
C20	0.0372 (10)	0.0313 (10)	0.0273 (9)	−0.0189 (8)	−0.0090 (8)	0.0001 (7)
C21	0.0471 (12)	0.0397 (11)	0.0316 (10)	−0.0215 (10)	−0.0057 (9)	0.0000 (9)
C22	0.0710 (17)	0.0501 (14)	0.0367 (12)	−0.0360 (13)	−0.0131 (11)	0.0110 (10)
C23	0.0764 (17)	0.0352 (12)	0.0554 (14)	−0.0290 (12)	−0.0331 (13)	0.0147 (10)

C24	0.0562 (14)	0.0318 (11)	0.0581 (14)	−0.0125 (10)	−0.0222 (12)	−0.0057 (10)
C25	0.0442 (12)	0.0363 (11)	0.0350 (10)	−0.0169 (9)	−0.0070 (9)	−0.0037 (9)
N1	0.0371 (9)	0.0375 (9)	0.0259 (8)	−0.0184 (7)	−0.0141 (7)	0.0032 (7)
N2	0.0430 (10)	0.0299 (8)	0.0372 (9)	−0.0191 (7)	−0.0074 (8)	0.0041 (7)
O1	0.0382 (8)	0.0393 (8)	0.0332 (7)	−0.0206 (6)	−0.0002 (6)	0.0013 (6)
O2	0.0558 (10)	0.0530 (9)	0.0247 (7)	−0.0257 (8)	0.0002 (7)	−0.0059 (6)
S1	0.0454 (4)	0.0753 (5)	0.0743 (5)	−0.0243 (3)	−0.0318 (3)	0.0007 (4)

Geometric parameters (Å, º)

C1—N1	1.466 (2)	C12—C13	1.389 (3)
C1—C13	1.534 (3)	C12—H12	0.9300
C1—C7	1.560 (2)	C14—O2	1.206 (2)
C1—C2	1.592 (2)	C14—C15	1.505 (3)
C2—C14	1.531 (2)	C15—C16	1.532 (3)
C2—C19	1.547 (3)	C15—H15A	0.9700
C2—C3	1.560 (2)	C15—H15B	0.9700
C3—C20	1.516 (3)	C16—C17	1.514 (4)
C3—C4	1.523 (2)	C16—H16A	0.9700
C3—H3	0.9800	C16—H16B	0.9700
C4—N1	1.469 (2)	C17—C18	1.530 (3)
C4—C5	1.535 (3)	C17—H17A	0.9700
C4—H4	0.9800	C17—H17B	0.9700
C5—S1	1.796 (3)	C18—C19	1.537 (3)
C5—H5A	0.9700	C18—H18A	0.9700
C5—H5B	0.9700	C18—H18B	0.9700
C6—N1	1.445 (3)	C19—H19A	0.9700
C6—S1	1.830 (2)	C19—H19B	0.9700
C6—H6A	0.9700	C20—C25	1.389 (3)
C6—H6B	0.9700	C20—C21	1.394 (3)
C7—O1	1.217 (2)	C21—C22	1.378 (3)
C7—N2	1.349 (2)	C21—H21	0.9300
C8—C9	1.381 (3)	C22—C23	1.370 (4)
C8—C13	1.388 (3)	C22—H22	0.9300
C8—N2	1.400 (3)	C23—C24	1.375 (4)
C9—C10	1.382 (3)	C23—H23	0.9300
C9—H9	0.9300	C24—C25	1.385 (3)
C10—C11	1.377 (4)	C24—H24	0.9300
C10—H10	0.9300	C25—H25	0.9300
C11—C12	1.386 (3)	N2—H2	0.8600
C11—H11	0.9300		

N1—C1—C13	120.41 (15)	O2—C14—C2	121.75 (17)
N1—C1—C7	106.89 (14)	C15—C14—C2	118.00 (17)
C13—C1—C7	100.64 (14)	C14—C15—C16	109.25 (18)
N1—C1—C2	102.68 (14)	C14—C15—H15A	109.8
C13—C1—C2	111.37 (14)	C16—C15—H15A	109.8
C7—C1—C2	115.44 (14)	C14—C15—H15B	109.8

C14—C2—C19	108.15 (15)	C16—C15—H15B	109.8
C14—C2—C3	111.12 (14)	H15A—C15—H15B	108.3
C19—C2—C3	113.41 (15)	C17—C16—C15	113.6 (2)
C14—C2—C1	110.81 (14)	C17—C16—H16A	108.8
C19—C2—C1	113.62 (14)	C15—C16—H16A	108.8
C3—C2—C1	99.60 (13)	C17—C16—H16B	108.8
C20—C3—C4	114.20 (15)	C15—C16—H16B	108.8
C20—C3—C2	118.60 (15)	H16A—C16—H16B	107.7
C4—C3—C2	103.40 (14)	C16—C17—C18	115.7 (2)
C20—C3—H3	106.6	C16—C17—H17A	108.4
C4—C3—H3	106.6	C18—C17—H17A	108.4
C2—C3—H3	106.6	C16—C17—H17B	108.4
N1—C4—C3	104.86 (14)	C18—C17—H17B	108.4
N1—C4—C5	109.38 (17)	H17A—C17—H17B	107.4
C3—C4—C5	114.85 (16)	C17—C18—C19	114.69 (19)
N1—C4—H4	109.2	C17—C18—H18A	108.6
C3—C4—H4	109.2	C19—C18—H18A	108.6
C5—C4—H4	109.2	C17—C18—H18B	108.6
C4—C5—S1	107.24 (15)	C19—C18—H18B	108.6
C4—C5—H5A	110.3	H18A—C18—H18B	107.6
S1—C5—H5A	110.3	C18—C19—C2	116.35 (16)
C4—C5—H5B	110.3	C18—C19—H19A	108.2
S1—C5—H5B	110.3	C2—C19—H19A	108.2
H5A—C5—H5B	108.5	C18—C19—H19B	108.2
N1—C6—S1	107.08 (15)	C2—C19—H19B	108.2
N1—C6—H6A	110.3	H19A—C19—H19B	107.4
S1—C6—H6A	110.3	C25—C20—C21	117.67 (18)
N1—C6—H6B	110.3	C25—C20—C3	123.12 (17)
S1—C6—H6B	110.3	C21—C20—C3	119.15 (18)
H6A—C6—H6B	108.6	C22—C21—C20	121.1 (2)
O1—C7—N2	125.70 (17)	C22—C21—H21	119.5
O1—C7—C1	125.71 (17)	C20—C21—H21	119.5
N2—C7—C1	108.54 (16)	C23—C22—C21	120.4 (2)
C9—C8—C13	123.1 (2)	C23—C22—H22	119.8
C9—C8—N2	126.65 (19)	C21—C22—H22	119.8
C13—C8—N2	110.23 (17)	C22—C23—C24	119.5 (2)
C8—C9—C10	117.0 (2)	C22—C23—H23	120.2
C8—C9—H9	121.5	C24—C23—H23	120.2
C10—C9—H9	121.5	C23—C24—C25	120.4 (2)
C11—C10—C9	121.1 (2)	C23—C24—H24	119.8
C11—C10—H10	119.5	C25—C24—H24	119.8
C9—C10—H10	119.5	C24—C25—C20	120.8 (2)
C10—C11—C12	121.4 (2)	C24—C25—H25	119.6
C10—C11—H11	119.3	C20—C25—H25	119.6
C12—C11—H11	119.3	C6—N1—C1	117.96 (17)
C11—C12—C13	118.6 (2)	C6—N1—C4	112.11 (16)
C11—C12—H12	120.7	C1—N1—C4	111.66 (14)
C13—C12—H12	120.7	C7—N2—C8	111.73 (16)

C8—C13—C12	118.80 (19)	C7—N2—H2	124.1
C8—C13—C1	108.37 (16)	C8—N2—H2	124.1
C12—C13—C1	132.51 (18)	C5—S1—C6	88.36 (11)
O2—C14—C15	120.06 (18)		

N1—C1—C2—C14	154.06 (15)	C3—C2—C14—O2	−0.4 (3)
C13—C1—C2—C14	23.9 (2)	C1—C2—C14—O2	−110.2 (2)
C7—C1—C2—C14	−90.04 (18)	C19—C2—C14—C15	−50.3 (2)
N1—C1—C2—C19	−83.94 (17)	C3—C2—C14—C15	−175.42 (17)
C13—C1—C2—C19	145.89 (16)	C1—C2—C14—C15	74.8 (2)
C7—C1—C2—C19	32.0 (2)	O2—C14—C15—C16	−75.9 (3)
N1—C1—C2—C3	36.98 (16)	C2—C14—C15—C16	99.2 (2)
C13—C1—C2—C3	−93.19 (16)	C14—C15—C16—C17	−70.3 (3)
C7—C1—C2—C3	152.88 (15)	C15—C16—C17—C18	52.0 (3)
C14—C2—C3—C20	74.5 (2)	C16—C17—C18—C19	−71.4 (3)
C19—C2—C3—C20	−47.6 (2)	C17—C18—C19—C2	87.6 (2)
C1—C2—C3—C20	−168.64 (15)	C14—C2—C19—C18	−34.2 (2)
C14—C2—C3—C4	−157.92 (15)	C3—C2—C19—C18	89.6 (2)
C19—C2—C3—C4	80.01 (17)	C1—C2—C19—C18	−157.62 (16)
C1—C2—C3—C4	−41.06 (17)	C4—C3—C20—C25	−42.5 (3)
C20—C3—C4—N1	160.57 (15)	C2—C3—C20—C25	79.8 (2)
C2—C3—C4—N1	30.29 (18)	C4—C3—C20—C21	134.67 (19)
C20—C3—C4—C5	−79.4 (2)	C2—C3—C20—C21	−103.0 (2)
C2—C3—C4—C5	150.37 (17)	C25—C20—C21—C22	−2.2 (3)
N1—C4—C5—S1	22.4 (2)	C3—C20—C21—C22	−179.53 (19)
C3—C4—C5—S1	−95.20 (18)	C20—C21—C22—C23	−0.2 (4)
N1—C1—C7—O1	45.1 (2)	C21—C22—C23—C24	2.1 (4)
C13—C1—C7—O1	171.63 (18)	C22—C23—C24—C25	−1.5 (4)
C2—C1—C7—O1	−68.4 (2)	C23—C24—C25—C20	−1.0 (3)
N1—C1—C7—N2	−132.43 (16)	C21—C20—C25—C24	2.8 (3)
C13—C1—C7—N2	−5.90 (18)	C3—C20—C25—C24	−179.97 (19)
C2—C1—C7—N2	114.09 (17)	S1—C6—N1—C1	101.84 (17)
C13—C8—C9—C10	0.9 (3)	S1—C6—N1—C4	−30.0 (2)
N2—C8—C9—C10	177.8 (2)	C13—C1—N1—C6	−27.7 (2)
C8—C9—C10—C11	1.4 (4)	C7—C1—N1—C6	86.0 (2)
C9—C10—C11—C12	−1.9 (4)	C2—C1—N1—C6	−152.11 (16)
C10—C11—C12—C13	0.1 (4)	C13—C1—N1—C4	104.30 (18)
C9—C8—C13—C12	−2.7 (3)	C7—C1—N1—C4	−142.00 (16)
N2—C8—C13—C12	179.99 (17)	C2—C1—N1—C4	−20.10 (19)
C9—C8—C13—C1	171.59 (19)	C3—C4—N1—C6	128.85 (18)
N2—C8—C13—C1	−5.7 (2)	C5—C4—N1—C6	5.2 (2)
C11—C12—C13—C8	2.1 (3)	C3—C4—N1—C1	−6.0 (2)
C11—C12—C13—C1	−170.5 (2)	C5—C4—N1—C1	−129.71 (17)
N1—C1—C13—C8	123.82 (18)	O1—C7—N2—C8	−174.57 (18)
C7—C1—C13—C8	6.88 (19)	C1—C7—N2—C8	3.0 (2)
C2—C1—C13—C8	−116.00 (16)	C9—C8—N2—C7	−175.5 (2)
N1—C1—C13—C12	−63.0 (3)	C13—C8—N2—C7	1.8 (2)
C7—C1—C13—C12	−179.9 (2)	C4—C5—S1—C6	−33.23 (16)

C2—C1—C13—C12	57.2 (3)	N1—C6—S1—C5	36.70 (17)
C19—C2—C14—O2	124.6 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.86	2.04	2.859 (2)	160

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