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7′-Nitro-6′-phenyl-1′,6′,7′,7a′-tetrahydro-spiro-[indeno[1,2-*b*]quinoxaline-11,5′-pyrrolo[1,2-*c*]-[1,3]thiazole]

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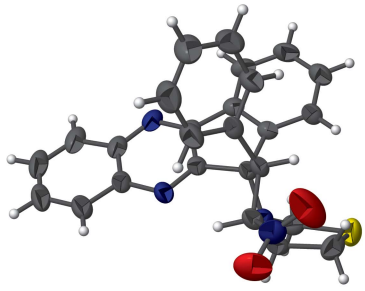
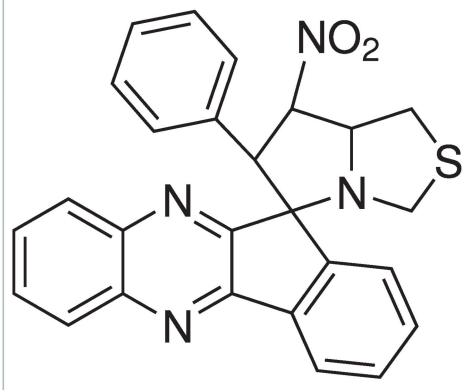
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{26}H_{20}N_4O_2S$, the thiazole and pyrrolidine rings adopt envelope conformations with the respective flap atoms being the N atom and the nitro-bearing C atom. The phenyl and indenoquinoxaline planes are oriented at an angle of 66.72 (1)° to each other. The molecular structure features two intramolecular interactions, *viz*. C—H···N and C—H···O. In the crystal, the molecules are connected through C—H···N and C—H···O interactions, forming ring motifs [two $R_2^1(7)$, $R_2^2(14)$, $R_2^2(22)$ and $R_2^2(16)$]. These ring motifs are connected through a $C(9)$ motif chain.

3D view



Chemical scheme



Structure description

Quinoxaline compounds and their derivatives possess many pharmaceutical applications, including as anticancer, antiviral and antibacterial agents (Seitz *et al.*, 2002; He *et al.*, 2003). Recently, new compounds have been investigated because of their biological and pharmaceutical applications (Zeb *et al.*, 2014; Arun *et al.*, 2014). Naturally occurring spiropyrrolidine derivatives are characterized by highly pronounced biological properties and are potential antileukemic, anticonvulsant, antiviral and anti-inflammatory agents (Anuradha *et al.*, 2014; Jiang *et al.*, 2006; Shao *et al.*, 2004). In addition, thiazole and its derivatives exhibit herbicidal, fungicidal, antitumour, anticancer, antiviral, antibacterial, antifungal and anti-inflammatory activities (He *et al.*, 2003; Campeau *et al.*, 2008; Muralikrishna *et al.*, 2013, Shruthy *et al.*, 2014). In view of the above, the title compound, containing spiropyrrolidine and thiazole groups, was synthesized and crystallized.

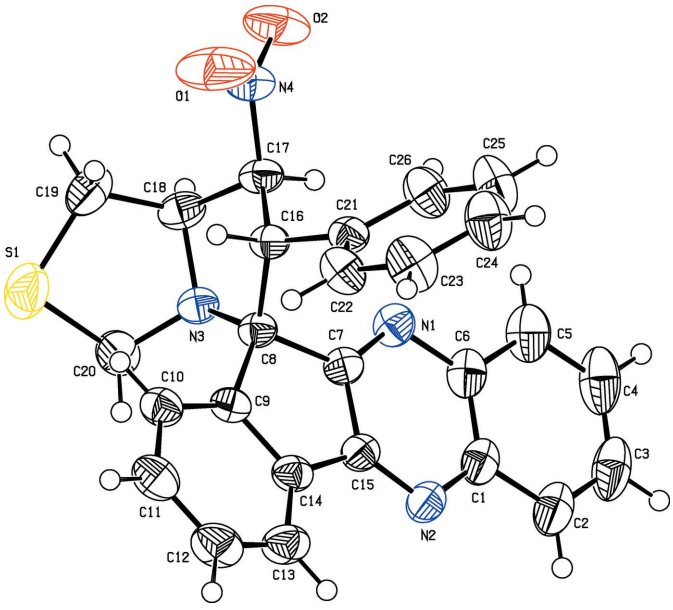


Figure 1
Perspective view of the title compound with the atom-numbering scheme and 50% probability displacement ellipsoids.

The title compound (Fig. 1) crystallizes with one molecule in the asymmetric unit. The thiazole ring exhibits an envelope conformation with the flap atom N3 deviating by 0.4598 (12) Å from the plane through the remaining ring atoms. The pyrroline ring also adopts an envelope conformation; the flap atom C17 deviates by 0.6678 (16) Å from the plane through the remaining ring atoms. The phenyl and indenoquinoxaline ring systems subtend an angle of 66.72 (1)°. The molecular conformation is stabilized by intramolecular C—H···N and C—H···O interactions (Table 1), each of which forms an *S*(6) motif.

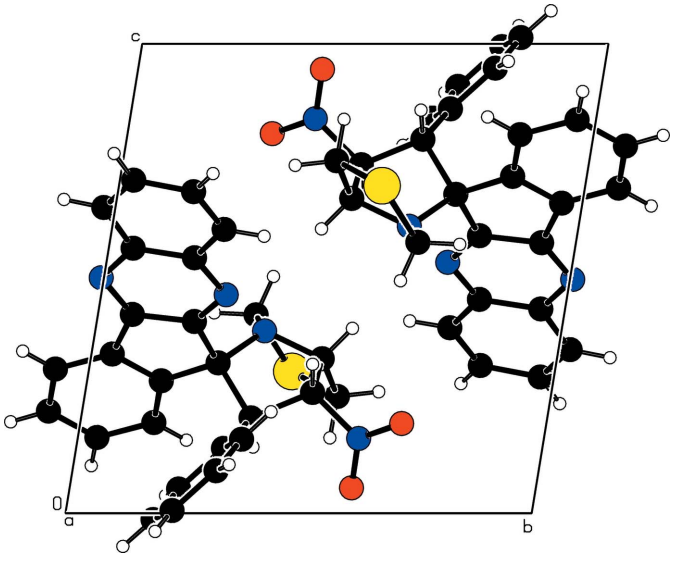


Figure 2
Packing diagram of the title compound viewed down the *a* axis. Hydrogen bonds (Table 1) are shown as dashed lines. **H bonds not shown**

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17···N1	0.98	2.56	3.208 (2)	123
C19—H19*B*···O1	0.97	2.54	3.182 (3)	124
C16—H16···O1^{i}	0.98	2.66	3.629 (2)	169
C10—H10···O1^{i}	0.93	2.62	3.355 (2)	136
C19—H19*B*···O1^{i}	0.97	2.98	3.832 (3)	148
C20—H20*A*···N2^{ii}	0.97	2.64	3.592 (2)	166
C4—H4···O2^{iii}	0.93	2.74	3.669 (3)	173
C13—H13···O2^{iv}	0.93	2.69	3.214 (2)	116
C18—H18···N3^{v}	0.98	2.76	3.7077 (19)	162

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

In the crystal (Fig. 2), the molecules are connected through C16—H16···O1^{i}, C10—H10···O1^{i}, C20—H20*A*···N2^{ii}, C4—H4···O2^{iii} and C18—H18···N3^{v} interactions, leading to $R_2^1(7)$, $R_2^1(7)$, $R_2^2(14)$, $R_2^2(22)$ and $R_2^2(6)$ ring motifs, respectively (Fig. 3; see Table 1 for symmetry codes). C13—H13···O2^{iv} interactions connect these hydrogen-bonded rings, leading to a *C*(9) chain motif along the *b*-axis direction (Fig. 4).

Synthesis and crystallization

20 ml of methanol was added to equimolar amounts of benzene-1,2-diamine, 1*H*-indene-1,2,3-trione and thiazolidine-4-carboxylic acid and refluxed in a water bath for 15 min. Then, an equimolar amount of substituted *trans*-*β*-nitrostyrenes was added to the reaction mixture and continued to

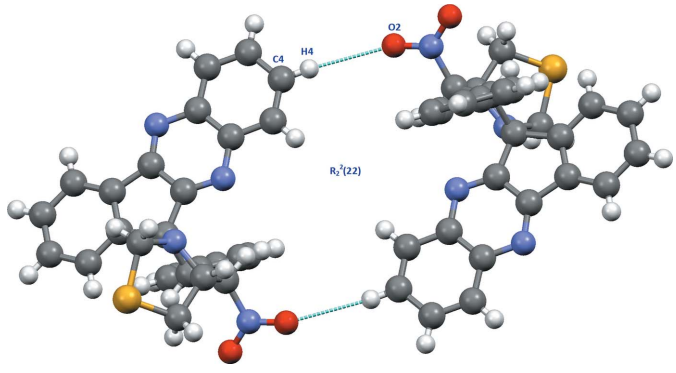


Figure 3
Centrosymmetric $R_2^2(22)$ ring motif formed through C—H···O interactions. Hydrogen bonds are shown as dashed lines.

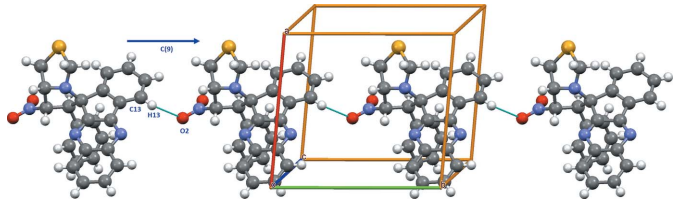


Figure 4
Chain *C*(9) motif, formed through a C—H···O interaction, extending along the *b*-axis direction. Hydrogen bonds are shown as dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{26}H_{20}N_4O_2S$
M_r	452.52
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	9.6591 (9), 10.5962 (11), 10.8001 (9)
α, β, γ (°)	80.389 (13), 85.626 (15), 85.030 (14)
V (Å^3)	1083.62 (18)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.18
Crystal size (mm)	0.22 × 0.18 × 0.16
Data collection	
Diffractometer	Bruker *SMART APEX* CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 2014
T_{min}, T_{max}	0.692, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	36403, 3811, 3556
R_{int}	0.020
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.594
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.105, 1.05
No. of reflections	3811
No. of parameters	299
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.26, −0.45

Computer programs: *SMART* and *SAINT* (Bruker, 2001), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *PLATON* (Spek, 2009).

reflux until completion of the reaction after 5 h, as monitored by TLC. The precipitated solid was filtered and washed with methanol to obtain the title compound in good yields (92–96%). Colourless block-shaped crystals were obtained by recrystallization from chloroform solution by slow evaporation.

Refinement

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

Acknowledgements

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References

Anuradha, T., Naga Siva Rao, J., Seshadri, P. R. & Raghunathan, R. (2014). *Acta Cryst.* E**70**, o38–o39.

Arun, Y., Saranraj, K., Balachandran, C. & Perumal, P. T. (2014). *Eur. J. Med. Chem.* **74**, 50–64.

Bruker (2001). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.

Campeau, L. C., Bertrand-Laperle, M., Leclerc, J. P., Villemure, E., Gorelsky, S. & Fagnou, K. (2008). *J. Am. Chem. Soc.* **130**, 3276–3277.

He, W., Myers, M. R., Hanney, B., Spada, A. P., Bilder, G., Galzcinski, H., Amin, D., Needle, S., Page, K., Jayyosi, Z. & Perrone, M. H. (2003). *Bioorg. Med. Chem. Lett.* **13**, 3097–3100.

Jiang, H., Zhao, J., Han, X. & Zhu, S. (2006). *Tetrahedron*, **62**, 11008–11011.

Muralikrishna, S., Raveendrareddy, P., Ravindranath, L. K., Harikrishna, S. & Jagadeeswara, R. P. (2013). *Pharma Chem.* **5**, 87–93.

Seitz, L. E., Suling, W. J. & Reynolds, R. C. (2002). *J. Med. Chem.* **45**, 5604–5606.

Shao, L., Jin, Z., Liu, J.-B., Zhou, X., Zhang, Q., Hu, Y. & Fang, J.-X. (2004). *Acta Cryst.* E**60**, o2517–o2519.

Sheldrick, G. M. (2014). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Shruthy, V. S. & Shakkeela, Y. (2014). *Int. J. Pharm. Pharm. Sci.* **6**, 271–275.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

Zeb, A., Hameed, A., Khan, L., Khan, I., Dalvandi, K., Choudhary, M. I. & Basha, F. (2014). *Med. Chem.* **10**, 724–729.

full crystallographic data

IUCrData (2017). **2**, x171305 [https://doi.org/10.1107/S2414314617013050]

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Crystal data

$C_{26}H_{20}N_4O_2S$
M_r = 452.52
Triclinic, $P\overline{1}$
a = 9.6591 (9) Å
b = 10.5962 (11) Å
c = 10.8001 (9) Å
α = 80.389 (13)°
β = 85.626 (15)°
γ = 85.030 (14)°
V = 1083.62 (18) Å^3
Z = 2
$F(000)$ = 472
D_x = 1.387 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71072 Å
Cell parameters from 2626 reflections
θ = 2.3–25.1°
μ = 0.18 mm^{-1}
T = 293 K
Block, colourless
0.22 × 0.18 × 0.16 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2014
T_{min} = 0.692, T_{max} = 0.746
36403 measured reflections
3811 independent reflections
3556 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 25.0°, θ_{min} = 2.8°
h = −11→11
k = −12→12
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.105
S = 1.05
3811 reflections
299 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2 + 0.4417P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}
Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.025 (3)

Special details

Experimental. The following wavelength and cell were deduced by SADABS from the direction cosines etc. They are given here for emergency use only: CELL 0.71072 9.659 10.596 10.800 80.389 85.626 85.030

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. All H atoms were constrained and refined in the riding atom approximation with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2 U_{eq}(parent carbon atom).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.16821 (16)	0.94782 (16)	0.43525 (14)	0.0419 (4)
C2	0.08043 (18)	1.0250 (2)	0.34855 (16)	0.0552 (5)
H2	0.0870	1.1133	0.3314	0.066*
C3	−0.01329 (19)	0.9704 (2)	0.29033 (16)	0.0628 (6)
H3	−0.0703	1.0218	0.2335	0.075*
C4	−0.02495 (19)	0.8380 (2)	0.31488 (17)	0.0640 (6)
H4	−0.0917	0.8027	0.2763	0.077*
C5	0.06089 (19)	0.7593 (2)	0.39528 (16)	0.0555 (5)
H5	0.0534	0.6711	0.4098	0.067*
C6	0.16019 (16)	0.81288 (17)	0.45565 (14)	0.0423 (4)
C7	0.33029 (15)	0.79076 (14)	0.59133 (13)	0.0338 (3)
C8	0.44071 (15)	0.72538 (13)	0.67951 (13)	0.0320 (3)
C9	0.49965 (15)	0.84094 (13)	0.71767 (13)	0.0334 (3)
C10	0.59533 (16)	0.84225 (15)	0.80668 (14)	0.0398 (3)
H10	0.6413	0.7664	0.8443	0.048*
C11	0.62108 (18)	0.95912 (17)	0.83850 (17)	0.0494 (4)
H11	0.6845	0.9614	0.8986	0.059*
C12	0.5539 (2)	1.07226 (17)	0.78235 (18)	0.0543 (5)
H12	0.5727	1.1496	0.8052	0.065*
C13	0.45922 (18)	1.07213 (15)	0.69270 (17)	0.0479 (4)
H13	0.4146	1.1485	0.6546	0.057*
C14	0.43210 (15)	0.95551 (14)	0.66074 (13)	0.0358 (3)
C15	0.33201 (15)	0.92623 (14)	0.57640 (13)	0.0349 (3)
C16	0.38043 (15)	0.63542 (13)	0.79674 (12)	0.0323 (3)
H16	0.4513	0.6211	0.8589	0.039*
C17	0.38082 (17)	0.51239 (13)	0.74259 (14)	0.0376 (3)
H17	0.3080	0.5222	0.6825	0.045*
C18	0.52387 (17)	0.50359 (14)	0.67073 (14)	0.0406 (4)
H18	0.5213	0.4494	0.6059	0.049*
C19	0.6508 (2)	0.45782 (18)	0.75106 (18)	0.0568 (5)
H19A	0.6837	0.3707	0.7412	0.068*
H19B	0.6246	0.4593	0.8394	0.068*
C20	0.67779 (17)	0.66080 (16)	0.57722 (17)	0.0471 (4)
H20A	0.6906	0.7513	0.5729	0.057*
H20B	0.7051	0.6370	0.4954	0.057*

C21	0.24702 (15)	0.68381 (14)	0.86165 (13)	0.0355 (3)
C22	0.25499 (18)	0.76582 (17)	0.94828 (15)	0.0470 (4)
H22	0.3413	0.7915	0.9626	0.056*
C23	0.1374 (2)	0.8099 (2)	1.01342 (18)	0.0599 (5)
H23	0.1449	0.8652	1.0706	0.072*
C24	0.0088 (2)	0.7723 (2)	0.99425 (18)	0.0625 (5)
H24	−0.0705	0.8015	1.0387	0.075*
C25	−0.00121 (19)	0.6919 (2)	0.90945 (19)	0.0651 (5)
H25	−0.0878	0.6661	0.8965	0.078*
C26	0.11658 (18)	0.64828 (19)	0.84232 (17)	0.0527 (4)
H26	0.1079	0.5947	0.7838	0.063*
N1	0.24762 (14)	0.73187 (13)	0.53455 (11)	0.0404 (3)
N2	0.25567 (13)	1.00594 (13)	0.49817 (12)	0.0415 (3)
N3	0.53473 (13)	0.63686 (11)	0.61145 (11)	0.0351 (3)
N4	0.35731 (15)	0.39744 (12)	0.84065 (14)	0.0482 (4)
O1	0.3921 (2)	0.39548 (16)	0.94584 (14)	0.0938 (6)
O2	0.30317 (17)	0.31038 (13)	0.80879 (15)	0.0753 (4)
S1	0.78439 (6)	0.56426 (5)	0.69783 (6)	0.0733 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0359 (8)	0.0552 (10)	0.0292 (7)	0.0073 (7)	0.0049 (6)	0.0002 (6)
C2	0.0432 (9)	0.0741 (12)	0.0388 (9)	0.0140 (8)	0.0033 (7)	0.0059 (8)
C3	0.0438 (10)	0.1011 (17)	0.0359 (9)	0.0196 (10)	−0.0031 (7)	−0.0015 (9)
C4	0.0438 (10)	0.1116 (19)	0.0388 (9)	0.0078 (10)	−0.0100 (8)	−0.0222 (10)
C5	0.0506 (10)	0.0767 (13)	0.0427 (9)	0.0018 (9)	−0.0103 (8)	−0.0202 (9)
C6	0.0389 (8)	0.0593 (10)	0.0279 (7)	0.0031 (7)	−0.0023 (6)	−0.0084 (7)
C7	0.0385 (7)	0.0358 (7)	0.0264 (7)	−0.0030 (6)	−0.0008 (6)	−0.0037 (5)
C8	0.0375 (7)	0.0304 (7)	0.0286 (7)	−0.0048 (6)	−0.0048 (6)	−0.0035 (5)
C9	0.0377 (7)	0.0319 (7)	0.0310 (7)	−0.0075 (6)	0.0023 (6)	−0.0055 (5)
C10	0.0427 (8)	0.0399 (8)	0.0384 (8)	−0.0099 (6)	−0.0038 (6)	−0.0065 (6)
C11	0.0500 (9)	0.0531 (10)	0.0501 (9)	−0.0162 (8)	−0.0034 (8)	−0.0167 (8)
C12	0.0612 (11)	0.0420 (9)	0.0655 (11)	−0.0135 (8)	0.0012 (9)	−0.0235 (8)
C13	0.0551 (10)	0.0323 (8)	0.0560 (10)	−0.0024 (7)	0.0041 (8)	−0.0105 (7)
C14	0.0380 (8)	0.0336 (7)	0.0348 (7)	−0.0047 (6)	0.0060 (6)	−0.0053 (6)
C15	0.0353 (7)	0.0356 (7)	0.0307 (7)	0.0000 (6)	0.0058 (6)	−0.0014 (6)
C16	0.0395 (8)	0.0304 (7)	0.0280 (7)	−0.0077 (6)	−0.0079 (6)	−0.0024 (5)
C17	0.0503 (9)	0.0299 (7)	0.0337 (7)	−0.0089 (6)	−0.0094 (6)	−0.0023 (6)
C18	0.0570 (9)	0.0307 (7)	0.0352 (8)	−0.0033 (6)	−0.0050 (7)	−0.0079 (6)
C19	0.0604 (11)	0.0520 (10)	0.0522 (10)	0.0139 (8)	−0.0065 (8)	0.0007 (8)
C20	0.0444 (9)	0.0466 (9)	0.0524 (10)	−0.0049 (7)	0.0017 (7)	−0.0149 (7)
C21	0.0406 (8)	0.0374 (8)	0.0277 (7)	−0.0075 (6)	−0.0048 (6)	0.0005 (6)
C22	0.0452 (9)	0.0590 (10)	0.0401 (8)	−0.0128 (8)	0.0002 (7)	−0.0147 (7)
C23	0.0583 (11)	0.0767 (13)	0.0494 (10)	−0.0087 (9)	0.0063 (8)	−0.0262 (9)
C24	0.0484 (10)	0.0895 (15)	0.0493 (10)	−0.0025 (10)	0.0067 (8)	−0.0161 (10)
C25	0.0402 (10)	0.0965 (16)	0.0622 (12)	−0.0155 (10)	−0.0042 (8)	−0.0172 (11)
C26	0.0475 (9)	0.0670 (11)	0.0486 (9)	−0.0140 (8)	−0.0060 (8)	−0.0178 (8)

N1	0.0444 (7)	0.0442 (7)	0.0337 (6)	−0.0024 (6)	−0.0087 (5)	−0.0070 (5)
N2	0.0389 (7)	0.0421 (7)	0.0379 (7)	0.0051 (5)	0.0045 (5)	0.0022 (5)
N3	0.0417 (7)	0.0315 (6)	0.0324 (6)	−0.0036 (5)	−0.0022 (5)	−0.0053 (5)
N4	0.0587 (9)	0.0323 (7)	0.0525 (9)	−0.0099 (6)	0.0005 (7)	−0.0023 (6)
O1	0.1585 (18)	0.0699 (10)	0.0520 (9)	−0.0439 (11)	−0.0338 (10)	0.0234 (7)
O2	0.0975 (11)	0.0412 (7)	0.0912 (11)	−0.0303 (7)	0.0084 (9)	−0.0158 (7)
S1	0.0592 (3)	0.0578 (3)	0.1089 (5)	0.0028 (2)	−0.0391 (3)	−0.0195 (3)

Geometric parameters (Å, º)

C1—N2	1.368 (2)	C16—C21	1.511 (2)
C1—C2	1.418 (2)	C16—C17	1.5150 (19)
C1—C6	1.418 (2)	C16—H16	0.9800
C2—C3	1.360 (3)	C17—N4	1.4957 (19)
C2—H2	0.9300	C17—C18	1.536 (2)
C3—C4	1.396 (3)	C17—H17	0.9800
C3—H3	0.9300	C18—N3	1.4590 (19)
C4—C5	1.373 (3)	C18—C19	1.552 (2)
C4—H4	0.9300	C18—H18	0.9800
C5—C6	1.407 (2)	C19—S1	1.786 (2)
C5—H5	0.9300	C19—H19A	0.9700
C6—N1	1.384 (2)	C19—H19B	0.9700
C7—N1	1.3007 (19)	C20—N3	1.436 (2)
C7—C15	1.419 (2)	C20—S1	1.8387 (18)
C7—C8	1.5268 (19)	C20—H20A	0.9700
C8—N3	1.4918 (18)	C20—H20B	0.9700
C8—C9	1.5227 (19)	C21—C26	1.386 (2)
C8—C16	1.5592 (19)	C21—C22	1.389 (2)
C9—C10	1.386 (2)	C22—C23	1.378 (3)
C9—C14	1.397 (2)	C22—H22	0.9300
C10—C11	1.386 (2)	C23—C24	1.377 (3)
C10—H10	0.9300	C23—H23	0.9300
C11—C12	1.381 (3)	C24—C25	1.365 (3)
C11—H11	0.9300	C24—H24	0.9300
C12—C13	1.382 (3)	C25—C26	1.389 (3)
C12—H12	0.9300	C25—H25	0.9300
C13—C14	1.388 (2)	C26—H26	0.9300
C13—H13	0.9300	N4—O1	1.205 (2)
C14—C15	1.463 (2)	N4—O2	1.2082 (19)
C15—N2	1.3114 (19)		
N2—C1—C2	119.06 (16)	C8—C16—H16	106.9
N2—C1—C6	122.22 (14)	N4—C17—C16	113.18 (12)
C2—C1—C6	118.71 (16)	N4—C17—C18	113.06 (13)
C3—C2—C1	120.3 (2)	C16—C17—C18	103.43 (12)
C3—C2—H2	119.9	N4—C17—H17	109.0
C1—C2—H2	119.9	C16—C17—H17	109.0
C2—C3—C4	120.77 (17)	C18—C17—H17	109.0

C2—C3—H3	119.6	N3—C18—C17	101.11 (12)
C4—C3—H3	119.6	N3—C18—C19	109.68 (13)
C5—C4—C3	120.84 (19)	C17—C18—C19	116.57 (13)
C5—C4—H4	119.6	N3—C18—H18	109.7
C3—C4—H4	119.6	C17—C18—H18	109.7
C4—C5—C6	119.7 (2)	C19—C18—H18	109.7
C4—C5—H5	120.2	C18—C19—S1	107.71 (12)
C6—C5—H5	120.2	C18—C19—H19A	110.2
N1—C6—C5	118.86 (16)	S1—C19—H19A	110.2
N1—C6—C1	121.49 (14)	C18—C19—H19B	110.2
C5—C6—C1	119.66 (15)	S1—C19—H19B	110.2
N1—C7—C15	123.98 (14)	H19A—C19—H19B	108.5
N1—C7—C8	125.36 (13)	N3—C20—S1	107.83 (11)
C15—C7—C8	110.64 (12)	N3—C20—H20A	110.1
N3—C8—C9	119.03 (12)	S1—C20—H20A	110.1
N3—C8—C7	108.41 (11)	N3—C20—H20B	110.1
C9—C8—C7	101.22 (11)	S1—C20—H20B	110.1
N3—C8—C16	103.78 (11)	H20A—C20—H20B	108.5
C9—C8—C16	111.13 (11)	C26—C21—C22	117.76 (15)
C7—C8—C16	113.64 (11)	C26—C21—C16	123.68 (14)
C10—C9—C14	120.35 (13)	C22—C21—C16	118.53 (13)
C10—C9—C8	128.25 (13)	C23—C22—C21	121.20 (16)
C14—C9—C8	111.01 (12)	C23—C22—H22	119.4
C9—C10—C11	118.57 (15)	C21—C22—H22	119.4
C9—C10—H10	120.7	C24—C23—C22	120.28 (18)
C11—C10—H10	120.7	C24—C23—H23	119.9
C12—C11—C10	121.00 (16)	C22—C23—H23	119.9
C12—C11—H11	119.5	C25—C24—C23	119.41 (18)
C10—C11—H11	119.5	C25—C24—H24	120.3
C11—C12—C13	120.90 (15)	C23—C24—H24	120.3
C11—C12—H12	119.6	C24—C25—C26	120.68 (17)
C13—C12—H12	119.6	C24—C25—H25	119.7
C12—C13—C14	118.54 (16)	C26—C25—H25	119.7
C12—C13—H13	120.7	C21—C26—C25	120.65 (17)
C14—C13—H13	120.7	C21—C26—H26	119.7
C13—C14—C9	120.63 (15)	C25—C26—H26	119.7
C13—C14—C15	130.20 (14)	C7—N1—C6	114.26 (13)
C9—C14—C15	109.07 (13)	C15—N2—C1	114.29 (14)
N2—C15—C7	123.56 (14)	C20—N3—C18	110.29 (12)
N2—C15—C14	128.65 (14)	C20—N3—C8	121.53 (12)
C7—C15—C14	107.79 (12)	C18—N3—C8	110.98 (11)
C21—C16—C17	118.23 (12)	O1—N4—O2	123.38 (15)
C21—C16—C8	117.04 (12)	O1—N4—C17	119.57 (13)
C17—C16—C8	99.98 (11)	O2—N4—C17	117.05 (15)
C21—C16—H16	106.9	C19—S1—C20	92.82 (8)
C17—C16—H16	106.9		

N2—C1—C2—C3	−176.11 (15)	C21—C16—C17—N4	−64.47 (17)

C6—C1—C2—C3	2.6 (2)	C8—C16—C17—N4	167.34 (12)
C1—C2—C3—C4	0.1 (3)	C21—C16—C17—C18	172.83 (12)
C2—C3—C4—C5	−2.1 (3)	C8—C16—C17—C18	44.63 (13)
C3—C4—C5—C6	1.2 (3)	N4—C17—C18—N3	−164.28 (12)
C4—C5—C6—N1	−178.79 (15)	C16—C17—C18—N3	−41.50 (13)
C4—C5—C6—C1	1.6 (2)	N4—C17—C18—C19	−45.48 (18)
N2—C1—C6—N1	−4.4 (2)	C16—C17—C18—C19	77.31 (15)
C2—C1—C6—N1	176.92 (13)	N3—C18—C19—S1	−19.19 (16)
N2—C1—C6—C5	175.24 (14)	C17—C18—C19—S1	−133.25 (12)
C2—C1—C6—C5	−3.5 (2)	C17—C16—C21—C26	−20.8 (2)
N1—C7—C8—N3	55.24 (18)	C8—C16—C21—C26	98.89 (17)
C15—C7—C8—N3	−123.18 (12)	C17—C16—C21—C22	157.41 (14)
N1—C7—C8—C9	−178.78 (13)	C8—C16—C21—C22	−82.94 (17)
C15—C7—C8—C9	2.80 (14)	C26—C21—C22—C23	0.4 (3)
N1—C7—C8—C16	−59.58 (18)	C16—C21—C22—C23	−177.91 (16)
C15—C7—C8—C16	122.01 (13)	C21—C22—C23—C24	0.5 (3)
N3—C8—C9—C10	−68.10 (19)	C22—C23—C24—C25	−0.5 (3)
C7—C8—C9—C10	173.32 (14)	C23—C24—C25—C26	−0.2 (3)
C16—C8—C9—C10	52.33 (19)	C22—C21—C26—C25	−1.1 (3)
N3—C8—C9—C14	119.07 (13)	C16—C21—C26—C25	177.07 (17)
C7—C8—C9—C14	0.50 (15)	C24—C25—C26—C21	1.1 (3)
C16—C8—C9—C14	−120.50 (13)	C15—C7—N1—C6	0.6 (2)
C14—C9—C10—C11	0.6 (2)	C8—C7—N1—C6	−177.62 (13)
C8—C9—C10—C11	−171.59 (14)	C5—C6—N1—C7	−176.33 (14)
C9—C10—C11—C12	−0.5 (2)	C1—C6—N1—C7	3.3 (2)
C10—C11—C12—C13	−0.1 (3)	C7—C15—N2—C1	2.9 (2)
C11—C12—C13—C14	0.4 (3)	C14—C15—N2—C1	−177.84 (13)
C12—C13—C14—C9	−0.3 (2)	C2—C1—N2—C15	179.77 (13)
C12—C13—C14—C15	175.64 (15)	C6—C1—N2—C15	1.1 (2)
C10—C9—C14—C13	−0.3 (2)	S1—C20—N3—C18	−35.00 (14)
C8—C9—C14—C13	173.21 (13)	S1—C20—N3—C8	97.43 (13)
C10—C9—C14—C15	−176.97 (13)	C17—C18—N3—C20	159.14 (12)
C8—C9—C14—C15	−3.50 (16)	C19—C18—N3—C20	35.48 (17)
N1—C7—C15—N2	−4.0 (2)	C17—C18—N3—C8	21.51 (14)
C8—C7—C15—N2	174.44 (12)	C19—C18—N3—C8	−102.16 (14)
N1—C7—C15—C14	176.59 (13)	C9—C8—N3—C20	−2.32 (19)
C8—C7—C15—C14	−4.97 (15)	C7—C8—N3—C20	112.47 (14)
C13—C14—C15—N2	9.6 (3)	C16—C8—N3—C20	−126.41 (14)
C9—C14—C15—N2	−174.13 (14)	C9—C8—N3—C18	129.83 (13)
C13—C14—C15—C7	−171.05 (15)	C7—C8—N3—C18	−115.38 (13)
C9—C14—C15—C7	5.25 (16)	C16—C8—N3—C18	5.73 (14)
N3—C8—C16—C21	−159.76 (11)	C16—C17—N4—O1	−28.0 (2)
C9—C8—C16—C21	71.16 (15)	C18—C17—N4—O1	89.1 (2)
C7—C8—C16—C21	−42.22 (16)	C16—C17—N4—O2	151.84 (15)
N3—C8—C16—C17	−30.78 (13)	C18—C17—N4—O2	−90.97 (18)
C9—C8—C16—C17	−159.87 (12)	C18—C19—S1—C20	−0.35 (13)
C7—C8—C16—C17	86.75 (13)	N3—C20—S1—C19	19.92 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17···N1	0.98	2.56	3.208 (2)	123
C19—H19*B*···O1	0.97	2.54	3.182 (3)	124
C16—H16···O1^{i}	0.98	2.66	3.629 (2)	169
C10—H10···O1^{i}	0.93	2.62	3.355 (2)	136
C19—H19*B*···O1^{i}	0.97	2.98	3.832 (3)	148
C20—H20*A*···N2^{ii}	0.97	2.64	3.592 (2)	166
C4—H4···O2^{iii}	0.93	2.74	3.669 (3)	173
C13—H13···O2^{iv}	0.93	2.69	3.214 (2)	116
C18—H18···N3^{v}	0.98	2.76	3.7077 (19)	162

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