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3-Ethyl-9-phenyl-2-tosyl-2,3,3a,4,9,9a-hexahydro-1*H*-pyrrolo[3,4-*b*]quinoline

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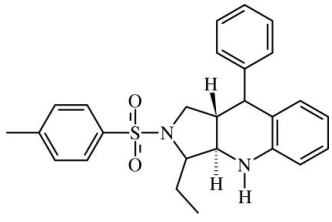
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.001 Å; R factor = 0.043; wR factor = 0.122; data-to-parameter ratio = 41.0.

In the molecule of the title compound, $C_{26}H_{28}N_2O_2S$, the pyrrolidine ring adopts an envelope conformation and the tetrahydropyridine ring is in a half-chair conformation; these two rings are *trans*-fused. The dihedral angle between the pyridine- and sulfonyl-bound benzene rings is 36.15 (5)°. In the crystalline state, the molecules are linked into a two-dimensional network parallel to the *ab* plane by C—H···O and C—H···π interactions.

Related literature

For the orientations of phenyl and ethyl substituents with respect to the fused ring system in the related 7-chloro- and 7-bromo-derivatives, see: Sudha *et al.* (2007, 2008). For biological activities of pyrrolo[3,4-*b*]quinoline derivatives, see: Anzini *et al.* (1990, 1992); Crenshaw *et al.* (1976); Fujita *et al.* (1996); Xiao *et al.* (2006). For related literature, see: Duax *et al.* (1976); Cremer & Pople (1975).



Experimental

Crystal data

$C_{26}H_{28}N_2O_2S$
M_r = 432.56
Triclinic, $P\overline{1}$
a = 9.3990 (1) Å
b = 10.9077 (2) Å
c = 12.5654 (3) Å
α = 64.3190 (8)°
β = 72.5291 (8)°
γ = 76.3803 (8)°
V = 1099.07 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.17 mm^{-1}
T = 100.0 (1) K
0.48 × 0.37 × 0.17 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.878, T_{max} = 0.971
49024 measured reflections
11697 independent reflections
9445 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.122
S = 1.03
11697 reflections
285 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C4–C9, C12–C17 and C19–C24 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O1^{i}	0.93	2.40	3.3215 (13)	171
C23—H23···O2^{ii}	0.93	2.53	3.2821 (13)	138
C2—H2···*Cg*1	0.98	2.94	3.8269 (9)	151
C7—H7···*Cg*3^{i}	0.93	2.95	3.7883 (12)	151
C10—H10···*Cg*2^{iii}	0.98	2.83	3.8072 (9)	178

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Version 5.1; Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2188).

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supporting information

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3-Ethyl-9-phenyl-2-tosyl-2,3,3a,4,9,9a-hexahydro-1*H*-pyrrolo[3,4-*b*]quinoline

D. Sudha, K. Chinnakali, M. Jayagobi, R. Raghunathan and Hoong-Kun Fun

S1. Comment

Pyrrolo[3,4-*b*]quinoline derivatives exhibit cytotoxic (Xiao *et al.*, 2006) and antibacterial (Fujita *et al.*, 1996) activities. The derivatives are also found to have interferon inducing activities (Crenshaw *et al.*, 1976) and ability to bind benzodiazepine receptors (Anzini *et al.*, 1990, 1992). We report here the crystal structure of the title compound, a pyrrolo[3,4-*b*]quinoline derivative (Fig. 1).

Bond lengths and angles are comparable with those in the 7-chloro- and 7-bromo- derivatives (Sudha *et al.*, 2007*a*,b). The pyrrolidine ring adopts an envelope conformation, with the local mirror plane passing through C2 and the midpoint of the bond N1—C11. The relevant asymmetry parameters (Duax *et al.*, 1976) are ΔC_s[C2] = 1.90 (7)° and the puckering parameters q_2 and φ_2 (Cremer & Pople, 1975) are 0.444 (1) Å and 74.6 (1)°. The tetrahydropyridine ring adopts a half-chair conformation, with the local twofold rotation axis passing through the midpoints of bonds C4—C9 and C2—C10. The asymmetry parameter ΔC_2[C4—c9] is 5.0 (1)°, and the puckering parameters Q, θ and φ are 0.505 (1) Å, 133.2 (1)° and 81.6 (1)°.

The tosyl group is attached to the pyrrolidine ring in a biaxial position. The sum of the bond angles around atoms N1 (342.6°) and N2 (347.2°) indicates sp^3 hybridization. The pyrrolidine and tetrahydropyridine rings show *trans*-fusion. The C19–C24 phenyl ring is equatorially attached to the tetrahydropyridine ring, and it forms dihedral angles of 74.80 (5) and 36.15 (5)°, respectively, with the C4–C9 and C12–C17 benzene rings.

An intramolecular C—H···π interaction involving the sulfonyl-bound phenyl ring (C12–C17, centroid *Cg*1) is observed. In the solid state, the molecules exist as centrosymmetrically C—H···π hydrogen-bonded dimers involving the C10—H10 group of the molecule at (*x*, *y*, *z*) and the C4–C9 benzene ring (centroid *Cg*2) of the molecule at (2 - *x*, -*y*, 1 - *z*). The dimers are linked into a chain along the *a* axis through C8—H8···O1^{i} hydrogen bonds, and C7—H7···π interaction involving the C19–C24 phenyl ring (centroid *Cg*3) of the molecule at (1 + *x*, *y*, *z*). The chains are cross-linked *via* C23—H23···O2^{ii} hydrogen bonds (Table 1), forming a two-dimensional network parallel to the *ab* plane (Fig. 2).

S2. Experimental

$InCl_3$ (20 mol%) was added to a mixture of 2-(*N*-cinnamyl-*N*-tosylamino)butanal (1 mmol) and arylamine (1 mmol) in acetonitrile (20 ml). The reaction mixture was stirred at room temperature for 30 min. On completion of the reaction, as indicated by TLC, the mixture was quenched with water and extracted with ethyl acetate. The organic layer was washed with brine and dried over Na_2SO_4. The solvent was evaporated *in vacuo* and the crude product was chromatographed using a hexane–ethyl acetate (8.5:1.5 *v*/*v*) mixture to obtain the title compound. The compound was recrystallized from ethyl acetate solution by slow evaporation.

S3. Refinement

The N-bound H atom was located from a difference map and refined freely. The remaining H atoms were positioned geometrically (C—H = 0.93–0.98 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl}). A rotating group model was used for the methyl groups attached to aromatic rings.

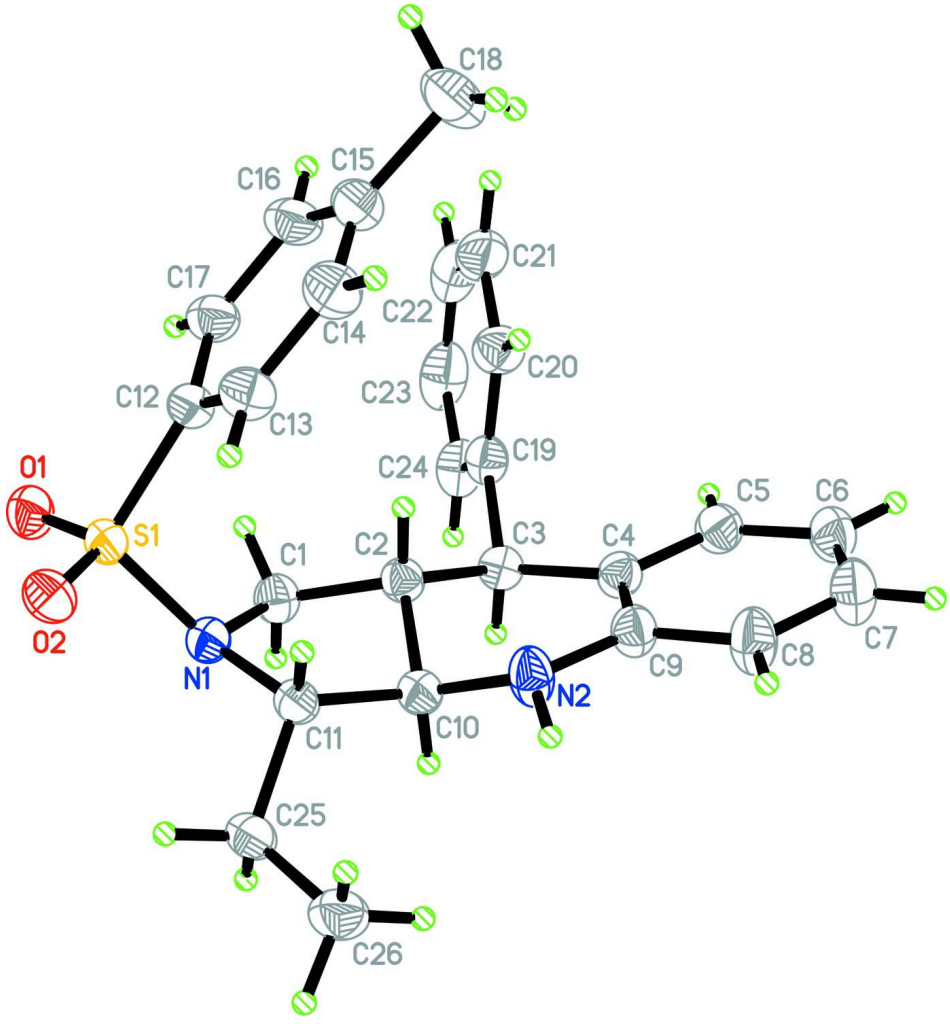

Figure 1

The molecular structure of the title compound, showing the atomic numbering. Displacement ellipsoids are drawn at the 80% probability level.

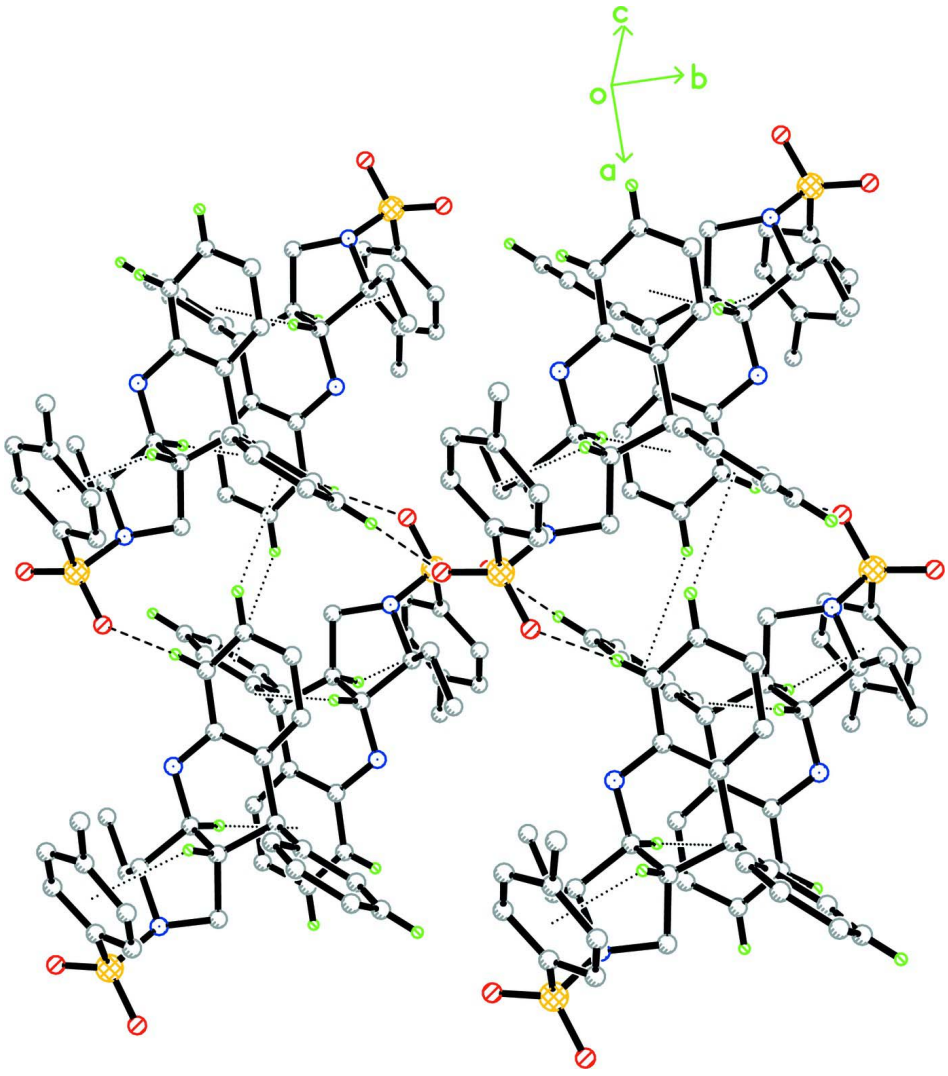

Figure 2

Part of the two-dimensional network in the title compound. Dashed and dotted lines indicate C—H···O and C—H···π interactions, respectively. For the sake of clarity, H atoms not involved in the interactions have been omitted.

3-Ethyl-9-phenyl-2-tosyl-2,3,3a,4,9,9a-hexahydro-1*H*- pyrrolo[3,4-*b*]quinoline

Crystal data

$C_{26}H_{28}N_2O_2S$
$M_r = 432.56$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.3990\ (1)$ Å
$b = 10.9077\ (2)$ Å
$c = 12.5654\ (3)$ Å
$\alpha = 64.3190\ (8)°$
$\beta = 72.5291\ (8)°$
$\gamma = 76.3803\ (8)°$
$V = 1099.07\ (4)$ Å^3
$Z = 2$
$F(000) = 460$
$D_x = 1.307$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7071 reflections
$\theta = 2.2–37.7°$
$\mu = 0.17$ mm^{-1}
$T = 100$ K
Block, colourless
0.48 × 0.37 × 0.17 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.33 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.878, T_{max} = 0.971
49024 measured reflections
11697 independent reflections
9445 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 37.8°, θ_{min} = 1.9°
h = −15→16
k = −18→18
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.122
S = 1.03
11697 reflections
285 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0632P)^2 + 0.2032P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Special details

Experimental. The low-temparture data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
S1	0.49683 (2)	0.424122 (19)	0.278537 (17)	0.01327 (5)
O1	0.35740 (7)	0.37308 (7)	0.30453 (6)	0.01740 (11)
O2	0.49608 (8)	0.55466 (6)	0.28077 (6)	0.01737 (11)
N1	0.59007 (8)	0.30981 (7)	0.37860 (6)	0.01346 (11)
N2	0.99769 (8)	0.23374 (7)	0.33005 (7)	0.01746 (13)
H1N2	1.0420 (18)	0.2777 (15)	0.3524 (14)	0.034 (4)*
C1	0.61499 (9)	0.16668 (8)	0.38536 (7)	0.01513 (13)
H1A	0.5572	0.1571	0.3377	0.018*
H1B	0.5887	0.1016	0.4685	0.018*
C2	0.78261 (9)	0.14729 (7)	0.33219 (7)	0.01321 (12)
H2	0.8007	0.2038	0.2451	0.016*
C3	0.86315 (9)	0.00361 (8)	0.34922 (7)	0.01390 (12)
H3	0.8397	−0.0548	0.4359	0.017*
C4	1.03201 (9)	0.01342 (8)	0.30922 (7)	0.01426 (12)

C5	1.13274 (10)	−0.08705 (8)	0.27522 (8)	0.01671 (13)
H5	1.0951	−0.1589	0.2757	0.020*
C6	1.28696 (10)	−0.08326 (9)	0.24074 (8)	0.01913 (15)
H6	1.3514	−0.1511	0.2179	0.023*
C7	1.34377 (11)	0.02374 (9)	0.24084 (9)	0.02159 (16)
H7	1.4469	0.0269	0.2193	0.026*
C8	1.24635 (10)	0.12555 (9)	0.27314 (9)	0.02058 (15)
H8	1.2851	0.1966	0.2730	0.025*
C9	1.09059 (9)	0.12303 (8)	0.30597 (7)	0.01567 (13)
C10	0.84289 (9)	0.21313 (8)	0.39204 (7)	0.01400 (12)
H10	0.8370	0.1535	0.4778	0.017*
C11	0.73416 (9)	0.34598 (8)	0.38053 (7)	0.01333 (12)
H11	0.7704	0.4197	0.3031	0.016*
C12	0.60265 (9)	0.42650 (8)	0.13594 (7)	0.01398 (12)
C13	0.71831 (10)	0.50922 (8)	0.07365 (7)	0.01698 (14)
H13	0.7306	0.5714	0.1016	0.020*
C14	0.81489 (11)	0.49778 (9)	−0.03058 (8)	0.01997 (15)
H14	0.8916	0.5533	−0.0727	0.024*
C15	0.79834 (11)	0.40407 (9)	−0.07292 (7)	0.01950 (15)
C16	0.67845 (11)	0.32643 (9)	−0.01229 (7)	0.01902 (15)
H16	0.6639	0.2667	−0.0420	0.023*
C17	0.58026 (10)	0.33691 (8)	0.09193 (7)	0.01663 (13)
H17	0.5006	0.2847	0.1318	0.020*
C18	0.90773 (13)	0.38731 (12)	−0.18222 (9)	0.0290 (2)
H18A	0.9524	0.2936	−0.1608	0.044*
H18B	0.9849	0.4455	−0.2104	0.044*
H18C	0.8558	0.4122	−0.2452	0.044*
C19	0.81012 (9)	−0.05736 (8)	0.28198 (7)	0.01477 (13)
C20	0.83943 (11)	−0.00052 (9)	0.15531 (8)	0.01856 (14)
H20	0.8949	0.0734	0.1120	0.022*
C21	0.78685 (12)	−0.05303 (10)	0.09319 (9)	0.02300 (17)
H21	0.8071	−0.0142	0.0089	0.028*
C22	0.70390 (12)	−0.16372 (10)	0.15726 (11)	0.02572 (19)
H22	0.6683	−0.1987	0.1159	0.031*
C23	0.67453 (11)	−0.22161 (9)	0.28268 (11)	0.02484 (18)
H23	0.6191	−0.2956	0.3256	0.030*
C24	0.72808 (10)	−0.16905 (8)	0.34479 (9)	0.01953 (15)
H24	0.7088	−0.2090	0.4290	0.023*
C25	0.70648 (10)	0.39338 (8)	0.48343 (7)	0.01598 (13)
H25A	0.6292	0.4716	0.4719	0.019*
H25B	0.6690	0.3204	0.5594	0.019*
C26	0.84606 (11)	0.43310 (10)	0.49243 (8)	0.01998 (15)
H26A	0.8211	0.4619	0.5587	0.030*
H26B	0.8826	0.5069	0.4183	0.030*
H26C	0.9224	0.3556	0.5059	0.030*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01224 (8)	0.01495 (8)	0.01383 (8)	−0.00040 (6)	−0.00266 (6)	−0.00755 (6)
O1	0.0120 (3)	0.0218 (3)	0.0199 (3)	−0.0020 (2)	−0.0028 (2)	−0.0102 (2)
O2	0.0197 (3)	0.0158 (2)	0.0195 (3)	0.0003 (2)	−0.0050 (2)	−0.0105 (2)
N1	0.0123 (3)	0.0147 (2)	0.0142 (2)	−0.0013 (2)	−0.0032 (2)	−0.0064 (2)
N2	0.0121 (3)	0.0180 (3)	0.0266 (3)	−0.0015 (2)	−0.0028 (3)	−0.0138 (3)
C1	0.0138 (3)	0.0146 (3)	0.0168 (3)	−0.0023 (2)	−0.0026 (3)	−0.0063 (2)
C2	0.0128 (3)	0.0135 (3)	0.0138 (3)	−0.0018 (2)	−0.0026 (2)	−0.0060 (2)
C3	0.0142 (3)	0.0133 (3)	0.0140 (3)	−0.0022 (2)	−0.0030 (2)	−0.0050 (2)
C4	0.0141 (3)	0.0138 (3)	0.0154 (3)	−0.0009 (2)	−0.0041 (2)	−0.0061 (2)
C5	0.0172 (3)	0.0152 (3)	0.0190 (3)	0.0005 (3)	−0.0054 (3)	−0.0083 (2)
C6	0.0166 (4)	0.0190 (3)	0.0225 (4)	0.0021 (3)	−0.0046 (3)	−0.0108 (3)
C7	0.0139 (4)	0.0220 (3)	0.0297 (4)	0.0003 (3)	−0.0032 (3)	−0.0133 (3)
C8	0.0131 (3)	0.0207 (3)	0.0304 (4)	−0.0021 (3)	−0.0032 (3)	−0.0133 (3)
C9	0.0136 (3)	0.0157 (3)	0.0193 (3)	−0.0006 (2)	−0.0036 (3)	−0.0089 (2)
C10	0.0132 (3)	0.0153 (3)	0.0147 (3)	−0.0010 (2)	−0.0032 (2)	−0.0073 (2)
C11	0.0124 (3)	0.0155 (3)	0.0132 (3)	−0.0018 (2)	−0.0021 (2)	−0.0071 (2)
C12	0.0147 (3)	0.0147 (3)	0.0128 (3)	0.0001 (2)	−0.0035 (2)	−0.0064 (2)
C13	0.0179 (4)	0.0175 (3)	0.0155 (3)	−0.0033 (3)	−0.0027 (3)	−0.0066 (2)
C14	0.0184 (4)	0.0224 (3)	0.0160 (3)	−0.0037 (3)	−0.0012 (3)	−0.0058 (3)
C15	0.0201 (4)	0.0206 (3)	0.0146 (3)	0.0033 (3)	−0.0035 (3)	−0.0073 (3)
C16	0.0248 (4)	0.0182 (3)	0.0152 (3)	0.0000 (3)	−0.0048 (3)	−0.0087 (3)
C17	0.0190 (4)	0.0172 (3)	0.0154 (3)	−0.0020 (3)	−0.0046 (3)	−0.0077 (2)
C18	0.0290 (5)	0.0336 (5)	0.0188 (4)	0.0037 (4)	0.0008 (4)	−0.0130 (3)
C19	0.0138 (3)	0.0130 (3)	0.0187 (3)	−0.0014 (2)	−0.0038 (3)	−0.0073 (2)
C20	0.0202 (4)	0.0185 (3)	0.0195 (3)	−0.0021 (3)	−0.0059 (3)	−0.0090 (3)
C21	0.0232 (4)	0.0267 (4)	0.0266 (4)	0.0031 (3)	−0.0108 (3)	−0.0169 (3)
C22	0.0211 (4)	0.0255 (4)	0.0431 (5)	0.0049 (3)	−0.0149 (4)	−0.0237 (4)
C23	0.0187 (4)	0.0187 (3)	0.0428 (5)	−0.0015 (3)	−0.0103 (4)	−0.0153 (4)
C24	0.0167 (4)	0.0151 (3)	0.0266 (4)	−0.0026 (3)	−0.0046 (3)	−0.0078 (3)
C25	0.0151 (3)	0.0199 (3)	0.0153 (3)	−0.0019 (3)	−0.0019 (3)	−0.0101 (3)
C26	0.0190 (4)	0.0267 (4)	0.0198 (3)	−0.0047 (3)	−0.0036 (3)	−0.0136 (3)

Geometric parameters (Å, º)

S1—O2	1.4346 (6)	C12—C17	1.3930 (11)
S1—O1	1.4363 (7)	C12—C13	1.3955 (12)
S1—N1	1.6406 (7)	C13—C14	1.3890 (12)
S1—C12	1.7613 (8)	C13—H13	0.93
N1—C1	1.4913 (10)	C14—C15	1.3957 (13)
N1—C11	1.5068 (10)	C14—H14	0.93
N2—C9	1.4049 (10)	C15—C16	1.3936 (14)
N2—C10	1.4478 (11)	C15—C18	1.5026 (13)
N2—H1N2	0.874 (15)	C16—C17	1.3907 (12)
C1—C2	1.5188 (11)	C16—H16	0.93
C1—H1A	0.97	C17—H17	0.93

C1—H1B	0.97	C18—H18A	0.96
C2—C10	1.5225 (11)	C18—H18B	0.96
C2—C3	1.5241 (10)	C18—H18C	0.96
C2—H2	0.98	C19—C24	1.3947 (11)
C3—C19	1.5167 (11)	C19—C20	1.3984 (12)
C3—C4	1.5289 (12)	C20—C21	1.3906 (12)
C3—H3	0.98	C20—H20	0.93
C4—C5	1.3979 (11)	C21—C22	1.3921 (15)
C4—C9	1.4100 (11)	C21—H21	0.93
C5—C6	1.3879 (13)	C22—C23	1.3846 (16)
C5—H5	0.93	C22—H22	0.93
C6—C7	1.3937 (13)	C23—C24	1.3967 (13)
C6—H6	0.93	C23—H23	0.93
C7—C8	1.3874 (12)	C24—H24	0.93
C7—H7	0.93	C25—C26	1.5234 (12)
C8—C9	1.4003 (12)	C25—H25A	0.97
C8—H8	0.93	C25—H25B	0.97
C10—C11	1.5410 (11)	C26—H26A	0.96
C10—H10	0.98	C26—H26B	0.96
C11—C25	1.5235 (10)	C26—H26C	0.96
C11—H11	0.98		

O2—S1—O1	119.99 (4)	N1—C11—H11	109.5
O2—S1—N1	106.92 (4)	C25—C11—H11	109.5
O1—S1—N1	106.32 (4)	C10—C11—H11	109.5
O2—S1—C12	107.98 (4)	C17—C12—C13	120.56 (7)
O1—S1—C12	108.51 (4)	C17—C12—S1	120.00 (6)
N1—S1—C12	106.36 (4)	C13—C12—S1	119.15 (6)
C1—N1—C11	109.19 (6)	C14—C13—C12	119.34 (8)
C1—N1—S1	116.25 (5)	C14—C13—H13	120.3
C11—N1—S1	117.17 (5)	C12—C13—H13	120.3
C9—N2—C10	116.54 (7)	C13—C14—C15	120.86 (8)
C9—N2—H1N2	113.8 (10)	C13—C14—H14	119.6
C10—N2—H1N2	116.9 (10)	C15—C14—H14	119.6
N1—C1—C2	102.47 (6)	C16—C15—C14	118.90 (8)
N1—C1—H1A	111.3	C16—C15—C18	120.51 (9)
C2—C1—H1A	111.3	C14—C15—C18	120.59 (9)
N1—C1—H1B	111.3	C17—C16—C15	120.98 (8)
C2—C1—H1B	111.3	C17—C16—H16	119.5
H1A—C1—H1B	109.2	C15—C16—H16	119.5
C1—C2—C10	101.01 (6)	C16—C17—C12	119.25 (8)
C1—C2—C3	119.66 (6)	C16—C17—H17	120.4
C10—C2—C3	111.59 (6)	C12—C17—H17	120.4
C1—C2—H2	108.0	C15—C18—H18A	109.5
C10—C2—H2	108.0	C15—C18—H18B	109.5
C3—C2—H2	108.0	H18A—C18—H18B	109.5
C19—C3—C2	111.25 (6)	C15—C18—H18C	109.5
C19—C3—C4	113.39 (6)	H18A—C18—H18C	109.5

C2—C3—C4	107.44 (6)	H18B—C18—H18C	109.5
C19—C3—H3	108.2	C24—C19—C20	118.46 (8)
C2—C3—H3	108.2	C24—C19—C3	120.93 (7)
C4—C3—H3	108.2	C20—C19—C3	120.59 (7)
C5—C4—C9	118.20 (8)	C21—C20—C19	120.91 (8)
C5—C4—C3	120.56 (7)	C21—C20—H20	119.5
C9—C4—C3	121.24 (7)	C19—C20—H20	119.5
C6—C5—C4	122.28 (8)	C20—C21—C22	119.93 (9)
C6—C5—H5	118.9	C20—C21—H21	120.0
C4—C5—H5	118.9	C22—C21—H21	120.0
C5—C6—C7	118.98 (8)	C23—C22—C21	119.88 (8)
C5—C6—H6	120.5	C23—C22—H22	120.1
C7—C6—H6	120.5	C21—C22—H22	120.1
C8—C7—C6	119.98 (9)	C22—C23—C24	120.05 (9)
C8—C7—H7	120.0	C22—C23—H23	120.0
C6—C7—H7	120.0	C24—C23—H23	120.0
C7—C8—C9	121.06 (8)	C19—C24—C23	120.76 (9)
C7—C8—H8	119.5	C19—C24—H24	119.6
C9—C8—H8	119.5	C23—C24—H24	119.6
C8—C9—N2	118.22 (7)	C26—C25—C11	113.64 (7)
C8—C9—C4	119.46 (7)	C26—C25—H25A	108.8
N2—C9—C4	122.27 (8)	C11—C25—H25A	108.8
N2—C10—C2	108.59 (6)	C26—C25—H25B	108.8
N2—C10—C11	114.73 (6)	C11—C25—H25B	108.8
C2—C10—C11	103.44 (6)	H25A—C25—H25B	107.7
N2—C10—H10	109.9	C25—C26—H26A	109.5
C2—C10—H10	109.9	C25—C26—H26B	109.5
C11—C10—H10	109.9	H26A—C26—H26B	109.5
N1—C11—C25	109.71 (6)	C25—C26—H26C	109.5
N1—C11—C10	103.05 (6)	H26A—C26—H26C	109.5
C25—C11—C10	115.45 (6)	H26B—C26—H26C	109.5

O2—S1—N1—C1	−175.61 (6)	S1—N1—C11—C25	100.35 (7)
O1—S1—N1—C1	55.08 (6)	C1—N1—C11—C10	−1.35 (7)
C12—S1—N1—C1	−60.43 (6)	S1—N1—C11—C10	−136.16 (5)
O2—S1—N1—C11	−43.94 (6)	N2—C10—C11—N1	146.21 (6)
O1—S1—N1—C11	−173.24 (5)	C2—C10—C11—N1	28.11 (7)
C12—S1—N1—C11	71.25 (6)	N2—C10—C11—C25	−94.20 (8)
C11—N1—C1—C2	−25.88 (8)	C2—C10—C11—C25	147.70 (7)
S1—N1—C1—C2	109.40 (6)	O2—S1—C12—C17	−157.41 (7)
N1—C1—C2—C10	42.60 (7)	O1—S1—C12—C17	−25.90 (8)
N1—C1—C2—C3	165.43 (6)	N1—S1—C12—C17	88.13 (7)
C1—C2—C3—C19	66.47 (9)	O2—S1—C12—C13	28.75 (8)
C10—C2—C3—C19	−176.03 (6)	O1—S1—C12—C13	160.27 (7)
C1—C2—C3—C4	−168.88 (7)	N1—S1—C12—C13	−85.71 (7)
C10—C2—C3—C4	−51.38 (8)	C17—C12—C13—C14	−2.42 (13)
C19—C3—C4—C5	−34.90 (10)	S1—C12—C13—C14	171.38 (7)
C2—C3—C4—C5	−158.25 (7)	C12—C13—C14—C15	−0.53 (13)

C19—C3—C4—C9	145.35 (7)	C13—C14—C15—C16	3.15 (13)
C2—C3—C4—C9	22.00 (10)	C13—C14—C15—C18	−176.99 (9)
C9—C4—C5—C6	1.08 (12)	C14—C15—C16—C17	−2.88 (13)
C3—C4—C5—C6	−178.67 (7)	C18—C15—C16—C17	177.26 (8)
C4—C5—C6—C7	0.52 (13)	C15—C16—C17—C12	0.00 (13)
C5—C6—C7—C8	−1.07 (14)	C13—C12—C17—C16	2.68 (12)
C6—C7—C8—C9	0.01 (15)	S1—C12—C17—C16	−171.07 (6)
C7—C8—C9—N2	−175.93 (9)	C2—C3—C19—C24	−112.37 (8)
C7—C8—C9—C4	1.62 (14)	C4—C3—C19—C24	126.40 (8)
C10—N2—C9—C8	−165.08 (8)	C2—C3—C19—C20	66.09 (10)
C10—N2—C9—C4	17.45 (12)	C4—C3—C19—C20	−55.15 (10)
C5—C4—C9—C8	−2.12 (12)	C24—C19—C20—C21	0.65 (13)
C3—C4—C9—C8	177.63 (8)	C3—C19—C20—C21	−177.84 (8)
C5—C4—C9—N2	175.32 (8)	C19—C20—C21—C22	−0.05 (14)
C3—C4—C9—N2	−4.93 (12)	C20—C21—C22—C23	−0.27 (14)
C9—N2—C10—C2	−45.97 (9)	C21—C22—C23—C24	−0.02 (14)
C9—N2—C10—C11	−161.12 (7)	C20—C19—C24—C23	−0.94 (13)
C1—C2—C10—N2	−166.38 (6)	C3—C19—C24—C23	177.54 (8)
C3—C2—C10—N2	65.36 (8)	C22—C23—C24—C19	0.64 (14)
C1—C2—C10—C11	−44.09 (7)	N1—C11—C25—C26	−179.71 (7)
C3—C2—C10—C11	−172.34 (6)	C10—C11—C25—C26	64.43 (9)
C1—N1—C11—C25	−124.83 (7)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O1^{i}	0.93	2.40	3.3215 (13)	171
C23—H23···O2^{ii}	0.93	2.53	3.2821 (13)	138
C2—H2···*Cg*1	0.98	2.94	3.8269 (9)	151
C7—H7···*Cg*3^{i}	0.93	2.95	3.7883 (12)	151
C10—H10···*Cg*2^{iii}	0.98	2.83	3.8072 (9)	178

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